

Supporting Information

Mass spectrometric Imaging of Organic and Metallic Metabolites by Plasmon-Induced Interfacial Charge-Transfer Transition (PICTT) on Au Sputtered ITO Slides

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1. Supplementary notes

1.1. Notes S1. Reagents and apparatus

Chloroform was purchased from Chron Chemical Co. Ltd. (Chengdu, China). Methanol and ether were purchased from Fisher Scientific (NJ, USA). 9-aminoacridine (9-AA), iohexol and paraformaldehyde were purchased from Aladdin Industrial Corporation (Shanghai, China). ESI-L low concentration tuning mix was purchased from Agilent Technologies Inc. (CA, USA). All standard free fatty acids (including C4:0, C6:0, C8:0, C10:0, C12:0, C14:0, C16:0, C18:0, C20:0, C22:0, C18:1C9, C18:T9, C18:1C6, C16:1C9, C16:1T9, C20:1C11, C20:1T11, C18:2C9,12, C20:4C5, 8, 11, 14) and various lipids such as 18:1 (Δ 9-cis) PC, 18:1 (Δ 9-cis) PE, 18:1 (Δ 9-cis) PG, 18:1 (Δ 6-cis) PC, 18:1 (Δ 6-cis) PC, C16:0/C18:1 Δ 9-cis PC, C18:1 (Δ 9-cis) TG and C18:2 Δ 9-cis, Δ 12-cis TG were purchased from Nu-ChekPrep Inc (MN, USA). Stock solutions of various free fatty acids and lipids were prepared at a concentration of 0.01 mol·L⁻¹ in solutions containing dichloromethane and methanol (3:1, v/v). Iohexol was dissolved in a solution of water containing 70% ethanol at a concentration of 0.05 mol/L. The stock solutions of 9-AA was prepared at a concentration of 0.01 mol·L⁻¹ in a solution containing 80% methanol. IntellislideTM ITO glass slides were purchased from Bruker Daltonics (Billerica, USA). Leica

CM1860 freezing microtome and tissue embedding media were purchased from Leica (Wetzlar, Germany).

1.2. Notes S2. Preparation of tissue slices for mass spectrometric imaging.

4T1 tumor-bearing BALB/c adult female nude mice weighting 15~17g were purchased from Nanjing Cavans Biotechnology Co. Ltd. (Nanjing, China). Those mice were etherized before the brain was taken out. It was washed with several cycles of 0.9% NaCl solution in order to clean blood contamination. Then brain was freshly frozen and stored at -80 °C. For the preparation of tissue slices, the mouse brain was placed in the cryochamber of a Leica CM1860 microtome (Wetzlar, Germany) at -20°C for half hour. And then the frozen tissues were fixed with the embedding media, respectively. These tissues were sectioned serially at 20 µm thickness and directly blotted on the surface of the ITO glass slide sputtered with Au nanoparticles.

1.3. Notes S3. Calibration of the mass spectrometer.

All mass spectrometric analysis was conducted on a Bruker Daltonics timsTOF Flex MALDI 2The mass spectrometer. It was calibrated before experiments every day in the morning with the Agilent ESI-L low concentration tuning mix (CA, USA). The mass accuracy is usually about 0.5 ppm. Fig. S1 is a representative calibration result.

1.4. Notes S4. Homogenization of brain tissues.

4T1 tumor-bearing BALB/c adult female nude mice and control mice weighting 15~17g were etherized before the brain was taken out. It was washed with several cycles of 0.9% NaCl solution in order to clean blood contamination. The homogenates of whole brains of a 4T1 mouse or a control mouse were mixed with 9-AA solution for mass spectrometric analysis.

1.5. Notes S5. Spraying of auxiliary matrix materials on tissue slices.

In order to localize double bond, metal ions or compare with regular deprotonation

ionization, surfaces of tissue slices that were blotted on the thin film of Au nanoparticles sputtered on ITO glass slides have been coated with auxiliary matrix materials including iohexol and 9-aminoacridine (9-AA). Stock solutions of these materials were sprayed on tissue slices with a HTX TM-SprayerTM (NC, USA). Major parameters including nozzle height, temperature, flow rate, nitrogen gas pressure, flow rate and dry time were set as 40 mm, 60 °C, 0.125 mL·min⁻¹, 10 psi, 3 L·min⁻¹ and 2 s, respectively.

1.6. Notes S6. Comparedoxome v 1.0

```
import base64

from tkinter import filedialog

import os

import pandas as pd

from PIL import Image, ImageTk

from openpyxl import load_workbook

from openpyxl.styles import Alignment

import tkinter as tk

from pandas.core.window import Window

from Picture.image import *

inmzfilename1=""

inmzfilename2=""

inmzfilename3=""

def run():

    # Set error tolerance range

    tolerance = 0.0030

    # Load data and forward-fill to handle merged cells

    normal_df = pd.read_excel(inmzfilename1)

    cancer_df = pd.read_excel(inmzfilename2)
```

```
# Forward-fill the 'm/z' column (first column) and the second column
normal_df.iloc[:, [0, 1]] = normal_df.iloc[:, [0, 1]].fillna(method='ffill')
cancer_df.iloc[:, [0, 1]] = cancer_df.iloc[:, [0, 1]].fillna(method='ffill')
```

```
# Ensure m/z data is of float type
normal_mz = normal_df.iloc[:, 0].astype(float)
cancer_mz = cancer_df.iloc[:, 0].astype(float)
```

```
# Get column names with prefixes to avoid duplicates
normal_cols = [f"Inputfile1_{col}" for col in normal_df.columns]
cancer_cols = [f"Inputfile2_{col}" for col in cancer_df.columns]
```

```
# Rename columns to avoid conflicts
normal_df.columns = normal_cols
cancer_df.columns = cancer_cols
```

```
# Initialize result lists and matched indices
matched_rows = []
remaining_normal = []
matched_cancer_indices = set()
```

```
# Find matched items
for i, mz_normal in normal_mz.items():
    found_match = False
    for j, mz_cancer in cancer_mz.items():
        if abs(mz_normal - mz_cancer) <= tolerance and j not in
```

```

matched_cancer_indices:
    combined_row = pd.concat([normal_df.iloc[i], cancer_df.iloc[j]],
axis=0)

    matched_rows.append(combined_row)
    matched_cancer_indices.add(j)
    found_match = True
    break

if not found_match:
    remaining_normal.append(normal_df.iloc[i])

# Find remaining cancer items
remaining_cancer = [cancer_df.iloc[j] for j in range(len(cancer_mz)) if j not in
matched_cancer_indices]

# Create DataFrame for matched results
if matched_rows:
    matched_df = pd.DataFrame(matched_rows)

else:
    matched_df = pd.DataFrame(columns=normal_cols + cancer_cols)

# Write results to files
with pd.ExcelWriter(inmzfilename3, engine='openpyxl',mode='w') as writer:
    matched_df.to_excel(writer, index=False, sheet_name='Common')

with pd.ExcelWriter(inmzfilename3, engine='openpyxl',mode='a') as writer:
    pd.DataFrame(remaining_normal).to_excel(writer, index=False,
sheet_name='Inputfile1 only', header=normal_cols)

```

```

with pd.ExcelWriter(inmzfilename3, engine='openpyxl', mode='a') as writer:
    pd.DataFrame(remaining_cancer).to_excel(writer, index=False,
sheet_name='Inputfile2 only', header=cancer_cols)
tk.messagebox.showinfo(title="", message='Completed successfully')
def getuploadfilename1():
    infile1=filedialog.askopenfilename(filetypes=((('Excel files','*.xlsx'),))
    inpath_text1.set(infile1)
    global inmzfilename1
    inmzfilename1=infile1
def getuploadfilename2():
    infile2=filedialog.askopenfilename(filetypes=((('Excel files','*.xlsx'),))
    inpath_text2.set(infile2)
    global inmzfilename2
    inmzfilename2=infile2
def getuploadfilename3():
    infile3=filedialog.askopenfilename(filetypes=((('Excel files','*.xlsx'),))
    inpath_text3.set(infile3)
    global inmzfilename3
    inmzfilename3=infile3

def decode_base64(base64_string):
    decoded_bytes = base64.b64decode(base64_string)
    return decoded_bytes

def save_image(decoded_bytes, file_path):
    with open(file_path, 'wb') as image_file:
        image_file.write(decoded_bytes)

```

```

mw=tk.Tk()
mw.title('Comparedoxome')
mw.geometry('590x300')

decode_bytes=decode_base64(compare_png)
file_path='backimg.png'
save_image(decode_bytes,file_path)

with Image.open(file_path) as img:
    img=img.resize((590,300))
backg=ImageTk.PhotoImage(img)
backglable=tk.Label(mw,image=backg)
backglable.pack()
os.remove('backimg.png')

Text_input1=tk.Label(mw,text='Input file 1',font=('Times New Roman',10))
Text_input1.place(x=20,y=110)
Text_input2=tk.Label(mw,text='Input file 2',font=('Times New Roman',10))
Text_input2.place(x=20,y=160)
Text_input3=tk.Label(mw,text='Output file',font=('Times New Roman',10))
Text_input3.place(x=20,y=210)

uploadbutton1=tk.Button(mw,text='Select
file',command=getuploadfilename1,width=10,height=1,font=('Times New
Roman',10))
uploadbutton1.pack()
uploadbutton1.place(x=475,y=107)
uploadbutton2=tk.Button(mw,text='Select

```

```

file',command=getuploadfilename2,width=10,height=1,font=('Times New
Roman',10))
uploadbutton2.pack()
uploadbutton2.place(x=475,y=157)
uploadbutton3=tk.Button(mw,text='Save
to',command=getuploadfilename3,width=10,height=1,font=('Times New Roman',10))
uploadbutton3.pack()
uploadbutton3.place(x=475,y=207)
outbutton=tk.Button(mw,text='Run',command=run,width=10,height=1,font=('Times
New Roman',10))
outbutton.pack()
outbutton.place(x=245,y=260)

```

```

inpath_text1=tk.StringVar()
entry_inpath1=tk.Entry(mw,textvariable=inpath_text1,width=50,state='readonly')
entry_inpath1.place(x=100,y=110)
inpath_text2=tk.StringVar()
entry_inpath2=tk.Entry(mw,textvariable=inpath_text2,width=50,state='readonly')
entry_inpath2.place(x=100,y=160)
inpath_text3=tk.StringVar()
entry_inpath3=tk.Entry(mw,textvariable=inpath_text3,width=50,state='readonly')
entry_inpath3.place(x=100,y=210)

mw.mainloop().

```

1. 7. Notes S7. Computational method

The electronic structures of molecules were investigated with DFT. Generalized gradient approximation (GGA) was used as a quantum mechanistic modeling method

for exchange-correlation potential in the form of Perdew-Burke-Ernzerhof (PBE) function. A Gaussian software (Wallingford, CT, USA) was used to calculate ground state electronic energies. All structures were optimized with B3LYP/6-31G+ (d) basis set. And ground state electronic energies were calculated at the B3LYP/6-31G++(d) level. Charge distribution of molecules was evaluated with Natural Bond Orbital (NBO) calculation. All the calculations were performed using the Cambridge Serial Total Energy Package (CASTEP).

2. Supplementary Figures

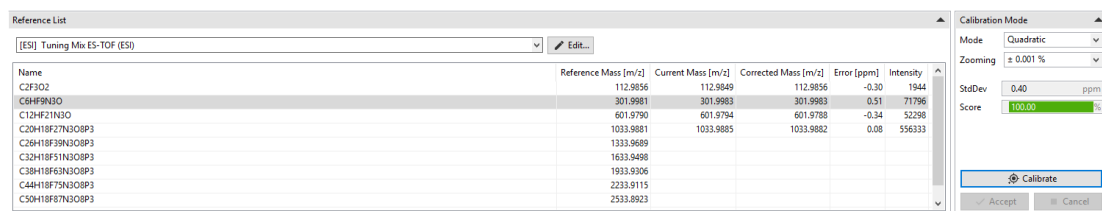


Fig. S1. A representative calibration result of the mass spectrometer.

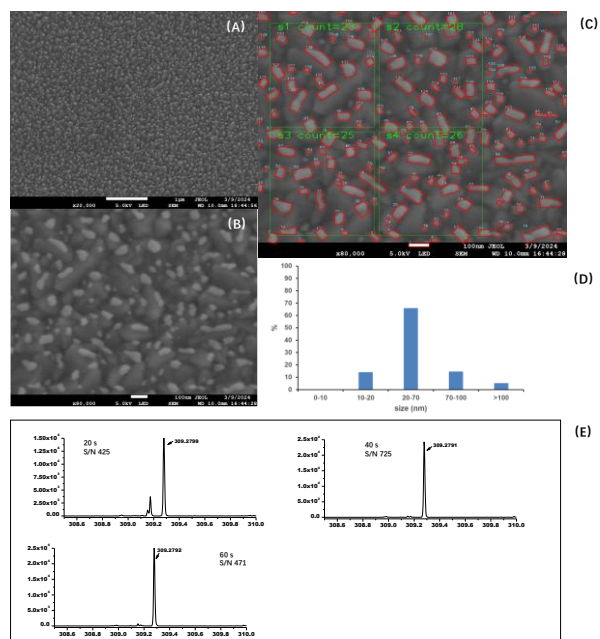


Fig. S2. Characterization of Au sputtered ITO glass slide under 10 mA current , 40 s deposition time, 0.08 mbar pressure and 4 cm distance.. (A) SEM x 20, 000. (B) SEM x 80, 000. (C) Uniformity of Au film analyzed with Opencv-python code. Averaged density is 25.5 $\uparrow$ /250000nm² in the four labeled regions and the coefficient of variation is about 8%. (D) Size distribution. About 95% particle sizes are between 10 nm and 100 nm. Only 5% particles are more than 100 nm. (E) Detection of C20:1 on Au sputtered ITO slides with different deposition time with different S/N ratios.

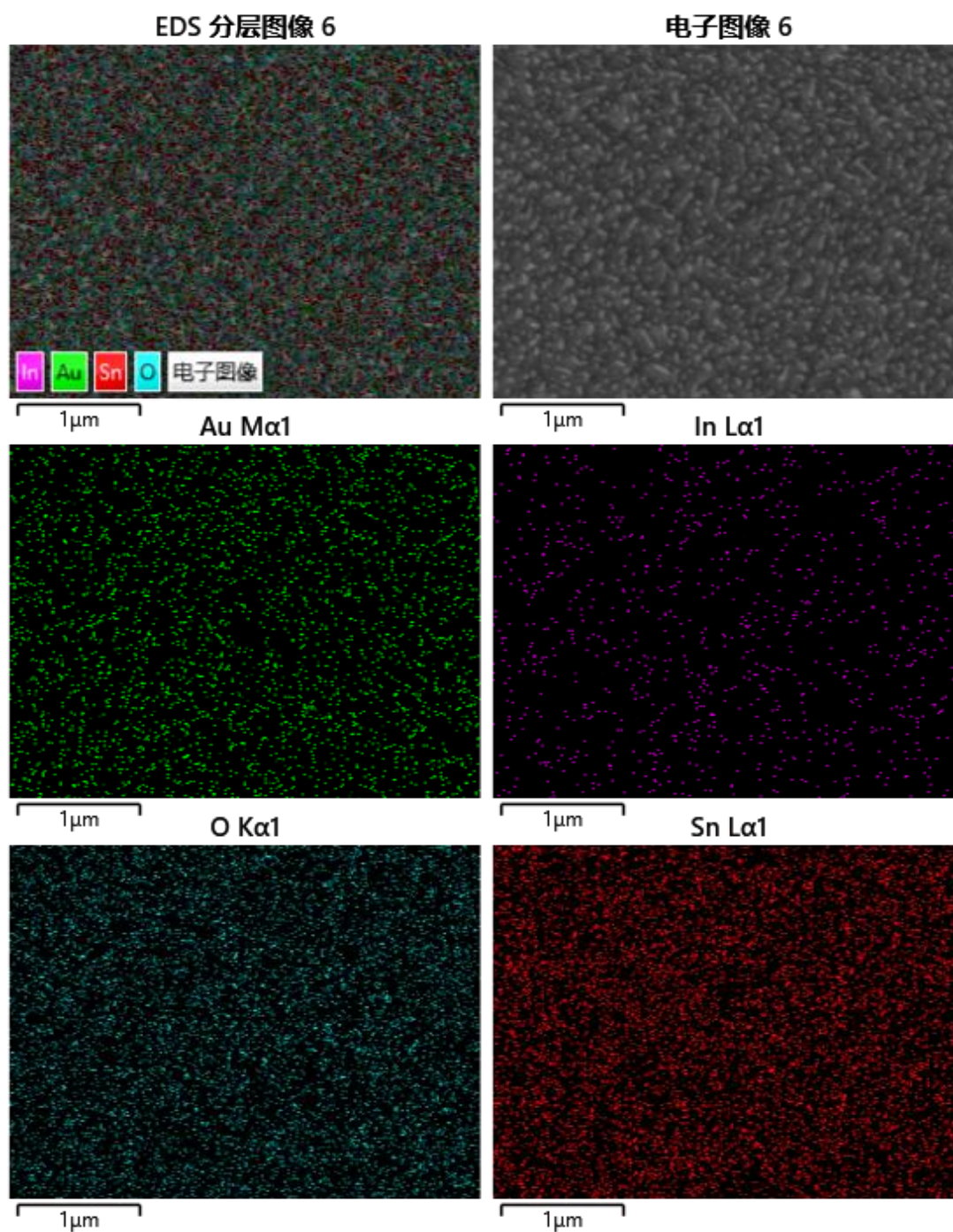


Fig. S3. EDS characterization of Au sputtered ITO glass slide.

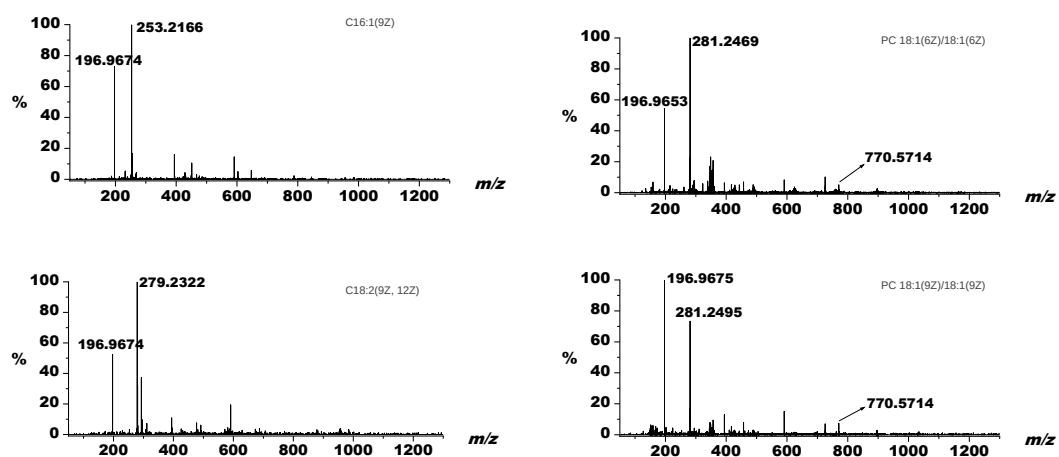


Fig. S4. MS spectra of free fatty acids and phospholipids spotted on Au sputtered ITO glass slides with 9-AA as auxiliary matrix.

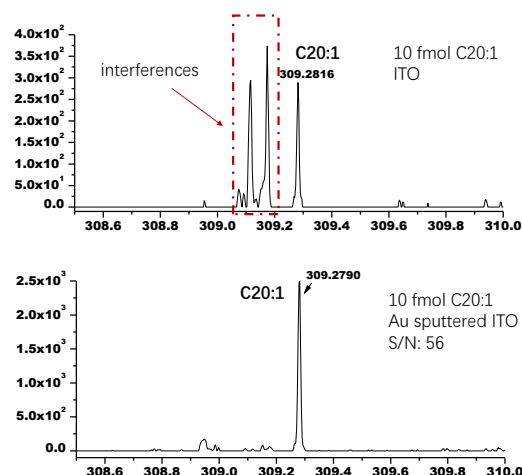


Fig. S5. MS spectra of C20:1 spotted on Au sputtered ITO glass slides or non-sputtered ITO with 9-AA as auxiliary matrix. The absolute intensity of C20:1 generated with PICTT MS is about 8 times more than that of general MALDI MS. It is shown the detection limit of PICTT MS can be down to 10 fmol and signal-to-noise ratio (S/N) is about 56.

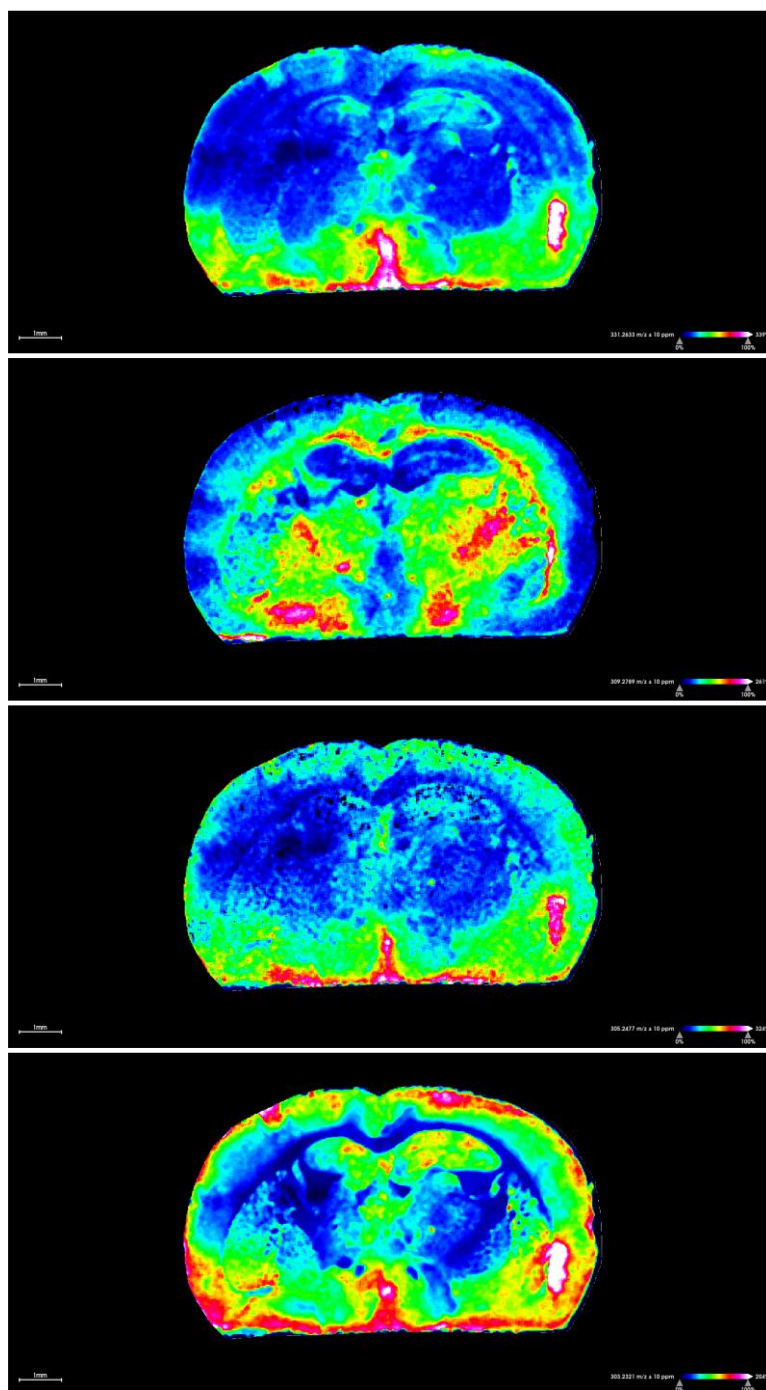


Fig. S6. Mass spectrometric imaging of fatty acids of 4T1 tumor-bearing BALB/c nude mouse brain slice on Au sputtered ITO glass slide with auxiliary matrix 9-AA.

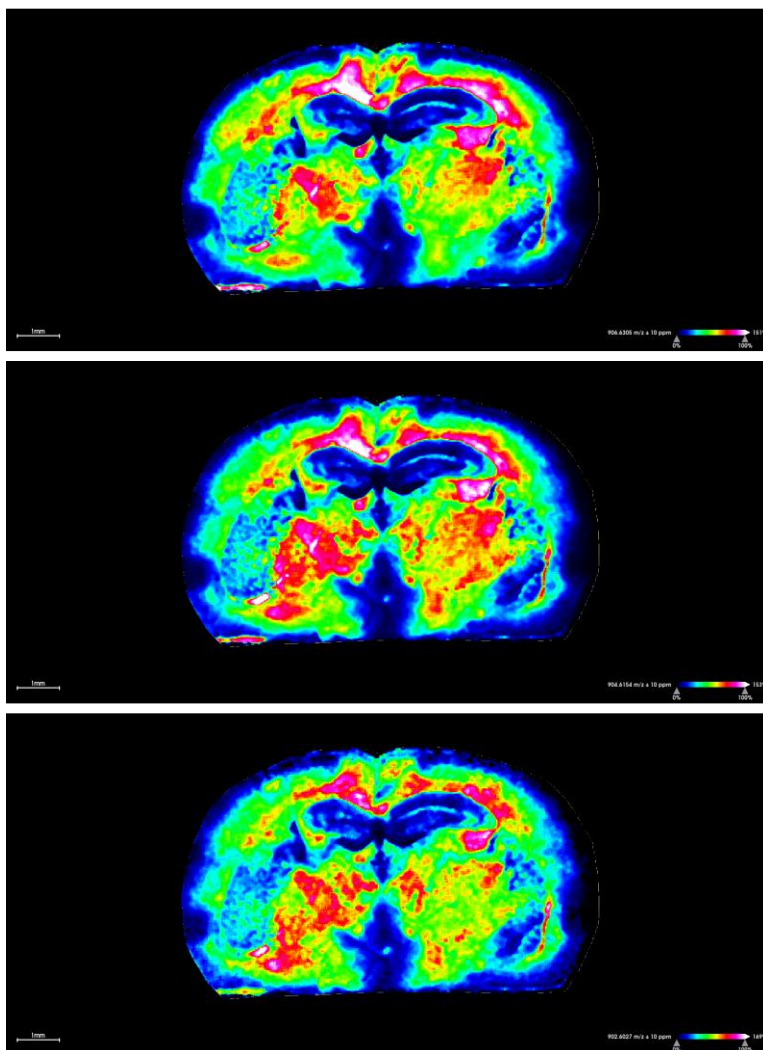


Fig. S7. Mass spectrometric imaging of three PCs at m/z 902, 904 and 906 of 4T1 tumor-bearing BALB/c nude mouse brain slice on Au sputtered ITO slide with 9-AA auxiliary matrix.

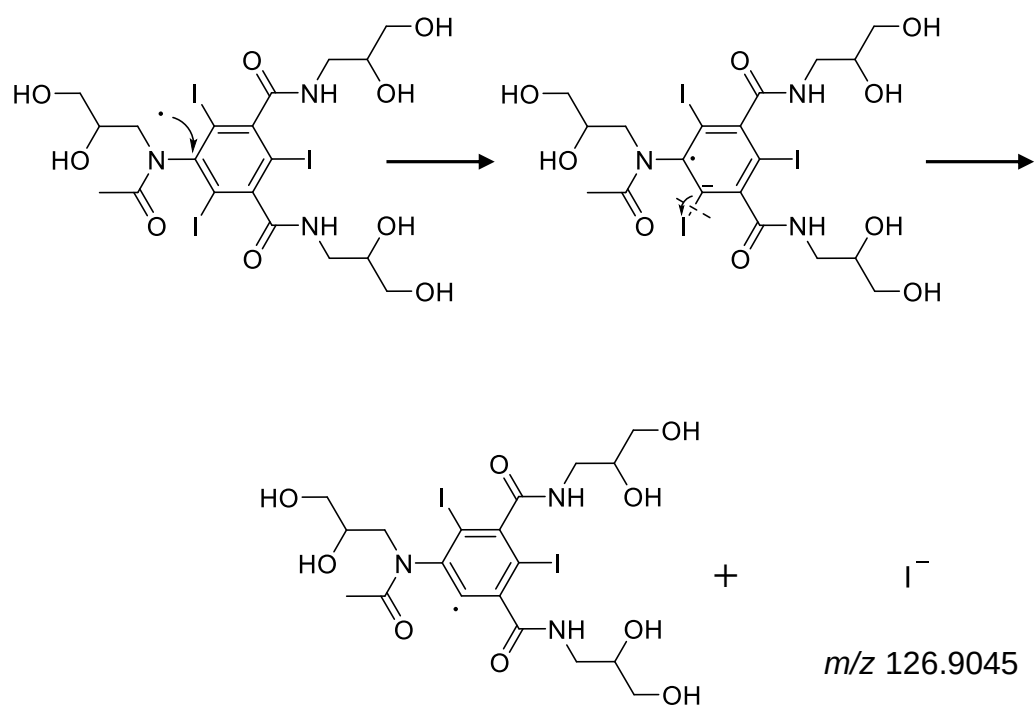


Fig. S8. Electron transfer produced iodide from iothalamate upon laser irradiation at 355 nm.

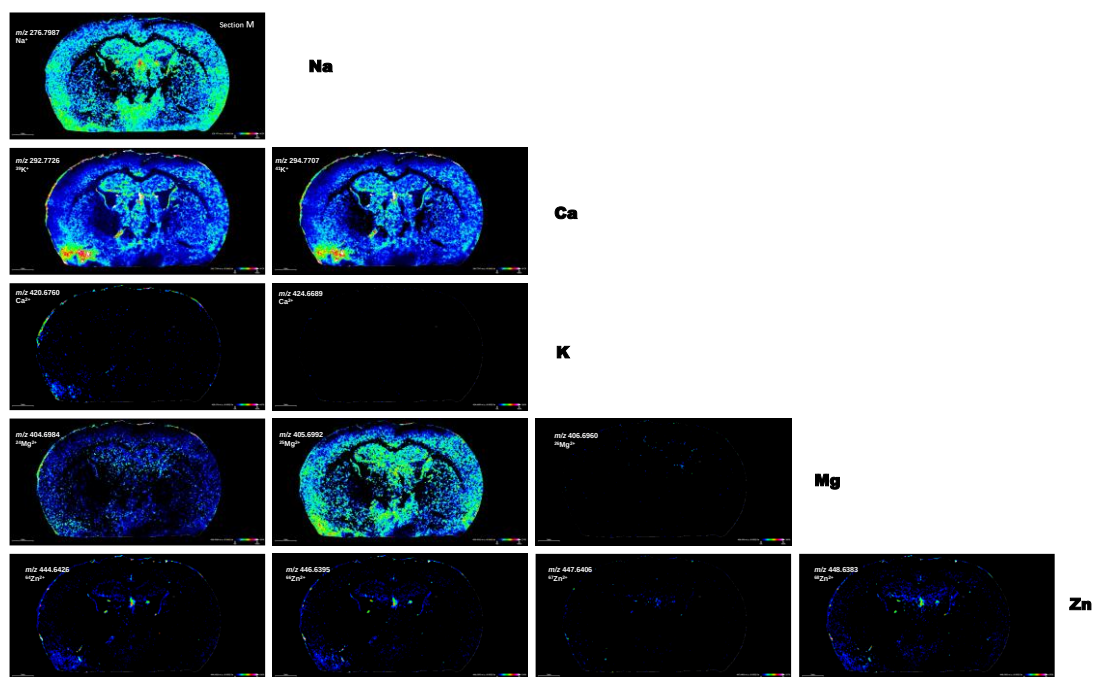


Fig. S9. Mass spectrometric imaging of redox inert metal ions and isotope of a section M of a control BALB/c nude mouse brain.

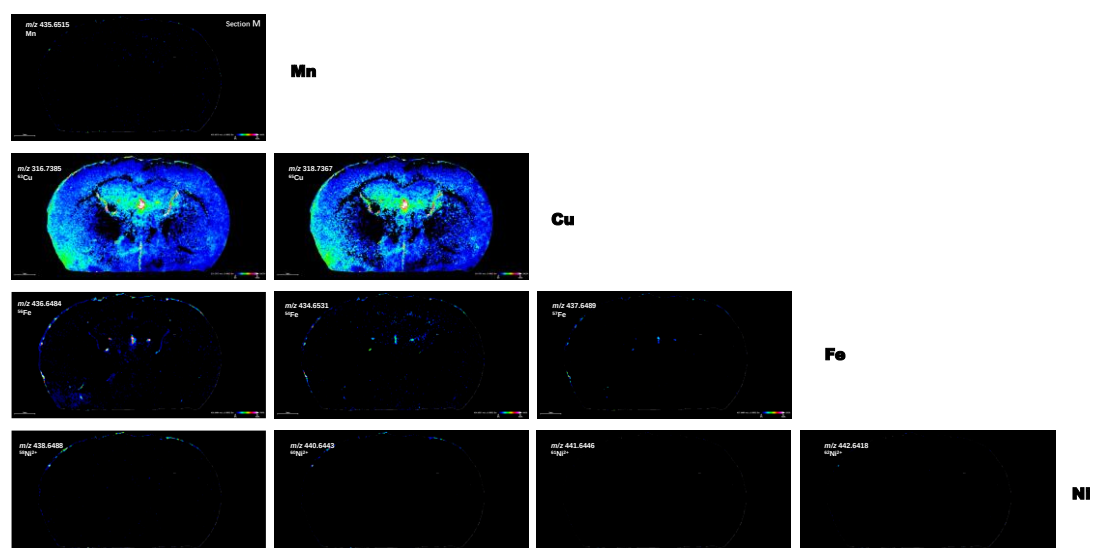


Fig. S10. Mass spectrometric imaging of redox active metal ions and isotopes of a section M of a control BALB/c nude mouse brain.

3. Supplementary Tables

3.1. Table S1. Detected metabolites in the brain of a 4T1 breast tumor-bearing mouse by electron transfer ionization (the ions that were only detected in 4T1 mouse brain were indicated with red color).

N o.	mz	Monisotopic _Mass	Error (Da)	Mode	IUPAC_name	Name	Accession Number	Chemical_Form ula	KE GG
1	124.00 63	125.0146638	0.0005 638	Proton ation	b'2-aminoethane-1-sulfonic acid'	b'Taurine'	HMDB00 00251	C2H7NO3S	C00 245
		125.0146643	0.0005 643	Proton ation	b'(2-aminoethylidene)dihydroxy-lambda6-sulfanone'	b'3h-Taurine'	HMDB02 46277	C2H7NO3S	
		125.0146643	0.0005 643	Proton ation	b'1-hydroxyethane-1-sulfonamide'	b'Sulfonamidoethanol'	HMDB02 58596	C2H7NO3S	
2	126.00 22	127.0091845	0.0008 155	Proton ation	b'1-(1,3-thiazol-2-yl)ethan-1-one'	b'2-Acetylthiazole'	HMDB00 32964	C5H5NOS	
		127.009185	0.0008 15	Proton ation	b'4-thia-1-azabicyclo[3.2.0]hept-2-en-7-one'	b'Penem'	HMDB02 56222	C5H5NOS	
		127.009185	0.0008 15	Proton ation	b'1-hydroxy-1,2-dihydropyridine-2-thione'	b'pyrithione'	HMDB02 56986	C5H5NOS	
		127.0091845	0.0008 155	Proton ation	b'(2E)-but-2-enecarbonyl isothiocyanate'	b'Crotonyl isothiocyanate'	HMDB03 02364	C5H5NOS	
3	126.90 41	127.9122935	0.0003 935	Proton ation	b'hydrogen iodide'	b'I(-)'	HMDB00 59634	HI	C05 590
		126.9044684	0.0003 684	Redox	b'iodide'	b'Iodide'	HMDB00 12238	I	C00 708
4	127.05 02	128.0585775	0.0005 775	Proton ation	b'(5S)-5-methyl-1,3-diazinane-2,4-dione'	b'Dihydrothymine'	HMDB00 00079	C5H8N2O2	C00 906
		128.0585775	0.0005 775	Proton ation	b'2-oxopyrrolidine-1-carboxamide'	b'Squamolone'	HMDB00 29874	C5H8N2O2	
		128.0585775	0.0005	Proton	b'3-methylpiperazine-2,5-dione'	b'L-Cyclo(alanylglycyl)'	HMDB00	C5H8N2O2	

5	128.03		775	ation			31547		
		128.0585775	0.0005 775	Proton ation	b'(3S)-3-aminopiperidine-2,6-dione'	b'Pyroglutamine'	HMDB00 62558	C5H8N2O2	
		128.0585775	0.0005 775	Proton ation	b'3-aminopiperidine-2,6-dione'	b'3-Aminopiperidine-2,6-dione'	HMDB02 42134	C5H8N2O2	
		128.0585775	0.0005 775	Proton ation	b'5-methyl-1,3-diazinane-2,4-dione'	b'5,6-dihydrothymine'	HMDB03 04210	C5H8N2O2	C00 906
	45	129.0425931	0.0002 931	Proton ation	b'(2S)-5-oxopyrrolidine-2-carboxylic acid'	b'Pyroglutamic acid'	HMDB00 00267	C5H7NO3	C01 879
		129.0425931	0.0002 931	Proton ation	b'4-hydroxy-3,4-dihydro-2H-pyrrole-2-carboxylic acid'	b'Pyrroline hydroxycarboxylic acid'	HMDB00 01369	C5H7NO3	C04 281
		129.0425931	0.0002 931	Proton ation	b'2-(prop-2-enamido)acetic acid'	b'N-Acryloylglycine'	HMDB00 01843	C5H7NO3	
		129.0425931	0.0002 931	Proton ation	b'3-hydroxy-3,4-dihydro-2H-pyrrole-5-carboxylic acid'	b'1-Pyrroline-4-hydroxy-2-carboxylate'	HMDB00 02234	C5H7NO3	C04 282
		129.0425931	0.0002 931	Proton ation	b'4-hydroxy-5,5-dimethyl-2,5-dihydro-1,3-oxazol-2-one'	b'dimethadione'	HMDB00 61093	C5H7NO3	
		129.0425931	0.0002 931	Proton ation	b'(2S,4R)-4-hydroxy-3,4-dihydro-2H-pyrrole-2-carboxylic acid'	b'(3R,5S)-1-pyrroline-3-hydroxy-5-carboxylic Acid'	HMDB00 62585	C5H7NO3	C04 281
		129.0425931	0.0002 931	Proton ation	b'3-hydroxy-1-methylpyrrolidine-2,5-dione'	b'3-Hydroxy-1-methylpyrrolidine-2,5-dione'	HMDB02 45148	C5H7NO3	
		129.0425931	0.0002 931	Proton ation	b'4-oxopyrrolidine-2-carboxylic acid'	b'4-Oxo-L-proline'	HMDB02 46561	C5H7NO3	
		129.0425931	0.0002 931	Proton ation	b'1-methyl-1H-pyrrole-2,3,5-triol'	b'1-Methylpyrrole-2,3,5-triol'	HMDB02 55336	C5H7NO3	
		129.0425931	0.0002	Proton	b'2-oxopyrrolidine-1-carboxylic acid'	b'pyrrolidone carboxylic acid'	HMDB02	C5H7NO3	

6	130.0501		931	ation			57001		
		129.0425931	0.0002 931	Proton ation	b'6-oxa-1-azabicyclo[3.1.0]hexane-2-carboxylic acid'	b'(2S)-6-Oxa-1-azabicyclo[3.1.0]hexane-2-carboxylic acid'	HMDB02 60147	C5H7NO3	
		128.0334254	0.0010 746	Redox	b'6-amino-1,3,5-triazine-2,4-diol'	b'Ammelide'	HMDB02 48340	C3H4N4O2	C08 734
		128.0353166	0.0008 166	Redox	b'4-oxopyrrolidine-2-carboxylate'	b'4-Oxoproline'	HMDB03 04793	C5H6NO3	
	130.0501	131.0582432	0.0003 432	Proton ation	b'(2S,4R)-4-hydroxypyrrolidine-2-carboxylic acid'	b'4-Hydroxyproline'	HMDB00 00725	C5H9NO3	C011 57
		131.0582432	0.0003 432	Proton ation	b'(2S)-2-acetamidopropanoic acid'	b'N-Acetyl-L-alanine'	HMDB00 00766	C5H9NO3	
		131.0582432	0.0003 432	Proton ation	b'2-propanamidoacetic acid'	b'Propionylglycine'	HMDB00 00783	C5H9NO3	
		131.0582432	0.0003 432	Proton ation	b'5-amino-4-oxopentanoic acid'	b'5-Aminolevulinic acid'	HMDB00 01149	C5H9NO3	C00 430
		131.0582432	0.0003 432	Proton ation	b'(2S)-2-amino-5-oxopentanoic acid'	b'L-Glutamic gamma-semialdehyde'	HMDB00 02104	C5H9NO3	C011 65
		131.0582432	0.0003 432	Proton ation	b'(2R,3S)-3-hydroxypyrrolidine-2-carboxylic acid'	b'3-Hydroxy-L-proline'	HMDB00 02113	C5H9NO3	C04 397
		131.0582432	0.0003 432	Proton ation	b'5-amino-2-oxopentanoic acid'	b'5-Amino-2-oxopentanoic acid'	HMDB00 06272	C5H9NO3	C011 10
		131.0582432	0.0003 432	Proton ation	b'(2S,3S)-3-hydroxypyrrolidine-2-carboxylic acid'	b'Trans-3-hydroxy-L-proline'	HMDB00 59659	C5H9NO3	C05 147
		131.0582432	0.0003 432	Proton ation		b'cis-4-Hydroxy-D-proline'	HMDB00 60460	C5H9NO3	C03 440

		131.0582432	0.0003 432	Proton ation	b'3-acetamidopropanoic acid'	b'N-Acetyl-beta-alanine'	HMDB00 61880	C5H9NO3	C01 073
		131.0582432	0.0003 432	Proton ation	b'(2S,4S)-4-hydroxypyrrolidine-2-carboxylic acid'	b'cis-4-Hydroxyproline'	HMDB02 40251	C5H9NO3	C01 015
		131.0582432	0.0003 432	Proton ation	b'1-hydroxypyrrolidine-2-carboxylic acid'	b'N-Hydroxy-L-proline'	HMDB02 43901	C5H9NO3	
		131.0582432	0.0003 432	Proton ation	b'1-hydroxypyrrolidine-3-carboxylic acid'	b'1-Hydroxypyrrolidine-3-carboxylic acid'	HMDB02 43902	C5H9NO3	
		131.0582432	0.0003 432	Proton ation	b'2-amino-4-oxopentanoic acid'	b'2-Amino-4-oxopentanoic acid'	HMDB02 44991	C5H9NO3	
		131.0582432	0.0003 432	Proton ation	b'3-hydroxypyrrolidine-2-carboxylic acid'	b'3-Hydroxyproline'	HMDB02 45903	C5H9NO3	
		131.0582432	0.0003 432	Proton ation	b'4-amino-5-oxopentanoic acid'	b'4-Amino-5-oxo-pentanoic acid'	HMDB02 46349	C5H9NO3	
		131.0582432	0.0003 432	Proton ation	b'4-carbamoylbutanoic acid'	b'Glutamic acid'	HMDB02 46746	C5H9NO3	
		131.0582432	0.0003 432	Proton ation	b'5-hydroxypyrrolidine-2-carboxylic acid'	b'5-Hydroxyproline'	HMDB02 46811	C5H9NO3	
		131.0582432	0.0003 432	Proton ation	b'2-acetamidopropanoic acid'	b'N-Acetyl-DL-alanine'	HMDB02 55053	C5H9NO3	
		130.0530982	0.0029 982	Redox	b'1,5-naphthyridine'	b'1,5-Naphthyridine'	HMDB02 44238	C8H6N2	
		130.0530982	0.0029 982	Redox	b'1,8-naphthyridine'	b'1,8-Naphthyridine'	HMDB02 44251	C8H6N2	
		130.0530982	0.0029 982	Redox	b'cinoline'	b'Cinoline'	HMDB02 50265	C8H6N2	

		130.0530982	0.0029 982	Redox	b'phthalazine'	b'Phthalazine'	HMDB02 56500	C8H6N2	
		130.0530982	0.0029 982	Redox	b'quinazoline'	b'QUINAZOLINE'	HMDB02 57035	C8H6N2	
		130.0530982	0.0029 982	Redox	b'quinoxaline'	b'QUINOXALINE'	HMDB02 57053	C8H6N2	C18 575
7	132.02 94	133.0375077	0.0003 077	Proton ation	b'(2S)-2-aminobutanedioic acid'	b'L-Aspartic acid'	HMDB00 00191	C4H7NO4	C00 049
		133.0375077	0.0003 077	Proton ation	b'(2R)-2-aminobutanedioic acid'	b'D-Aspartic acid'	HMDB00 06483	C4H7NO4	C00 402
		133.0375077	0.0003 077	Proton ation	b'2-[(carboxymethyl)amino]acetic acid'	b'Iminodiacetic acid'	HMDB00 11753	C4H7NO4	C19 911
		132.0323628	0.0029 628	Redox	b'3H-indazol-3-one'	b'3H-Indazol-3-one'	HMDB02 46268	C7H4N2O	
8	133.01 33	134.0215233	0.0004 233	Proton ation	b'(2S)-2-hydroxybutanedioic acid'	b'Malic acid'	HMDB00 00156	C4H6O5	C00 149
		134.0215233	0.0004 233	Proton ation	b'(2R)-2-hydroxybutanedioic acid'	b'D-Malic acid'	HMDB00 31518	C4H6O5	C00 497
		134.0215233	0.0004 233	Proton ation	b'dimethyl dicarbonate'	b'Velcorin'	HMDB00 32872	C4H6O5	
		134.0223917	0.0012 917	Proton ation	b'3,3-dimethyl-1,2-dithiolane'	b'3,3-Dimethyl-1,2-dithiolane'	HMDB00 38974	C5H10S2	
		134.0223917	0.0012 917	Proton ation	b'2-methylthiolane-2-thiol'	b'Tetrahydro-2-methyl-2-thiophenethiol'	HMDB00 39789	C5H10S2	
		134.0223917	0.0012 917	Proton ation	b'2-methylthiolane-3-thiol'	b'Tetrahydro-2-methyl-3-thiophenethiol'	HMDB00 39790	C5H10S2	

9		134.0190214	0.0020 786	Proton ation	b'1-benzothiophene'	b'Benzothiophene'	HMDB02 49003	C8H6S	
		134.0215233	0.0004 233	Proton ation	b'2-(carboxymethoxy)acetic acid'	b'Diglycolic acid'	HMDB02 51283	C4H6O5	
		134.0228607	0.0017 607	Proton ation	b'3H-pyrazolo[4,3-d]pyrimidin-3-one'	b'Pyrazolopyrimidinone'	HMDB02 56955	C5H2N4O	
		134.0215233	0.0004 233	Proton ation	b'2-(carboxyoxo)propanoic acid'	b'2-Carboxyoxopropanoic acid'	HMDB02 57720	C4H6O5	
		134.0223927	0.0012 927	Proton ation	b'cyclopentane-1,2-dithiol'	b'1,2-Dimercaptocyclopentane'	HMDB03 02171	C5H10S2	
	134.04 65	135.0544952	0.0001 952	Proton ation	b'7H-purin-6-amine'	b'Adenine'	HMDB00 00034	C5H5N5	C00 147
		135.0531578	0.0011 422	Proton ation	b'2-amino-3,4-dihydroxybutanoic acid'	b'(+)-threo-2-Amino-3,4- dihydroxybutanoic acid'	HMDB00 29389	C4H9NO4	
		135.0558379	0.0015 379	Proton ation	b'4-(hydroxymethyl)benzene-1-diazonium'	b'4- (Hydroxymethyl)benzenediazonium(1+)'	HMDB00 32593	C7H7N2O	
		135.0544952	0.0001 952	Proton ation	b'1H-pyrazolo[3,4-d]pyrimidin-4-amine'	b'1H-Pyrazolo[3,4-d]pyrimidin-4- amine'	HMDB02 44899	C5H5N5	
		135.0544952	0.0001 952	Proton ation	b'2,3-dihydro-1H-purin-2-imine'	b'2-Aminopurine'	HMDB02 45025	C5H5N5	
		135.0544952	0.0001 952	Proton ation	b'9H-purin-9-amine'	b'9h-Purin-9-amine'	HMDB02 47703	C5H5N5	
		134.0480128	0.0015 128	Redox	b'1H-indazol-3-ol'	b'1H-Indazol-3-ol'	HMDB02 44883	C7H6N2O	
		134.0480128	0.0015	Redox	b'N-iminobenzamide'	b'Benzoyl hydrazone'	HMDB02	C7H6N2O	

			128				49039		
1 0	135.03	136.0385108	0.0007 108	Proton ation	b'7H-purin-6-ol'	b'Hypoxanthine'	HMDB00 00157	C5H4N4O	C00 262
		136.0371734	0.0006 266	Proton ation	b'(2R,3R)-2,3,4-trihydroxybutanoic acid'	b'Erythronic acid'	HMDB00 00613	C4H8O5	
		136.0371734	0.0006 266	Proton ation	b'(2R,3S)-2,3,4-trihydroxybutanoic acid'	b'Thronic acid'	HMDB00 00943	C4H8O5	C01 620
		136.0385108	0.0007 108	Proton ation	b'1H,2H,4H-pyrazolo[3,4-d]pyrimidin-4-one'	b'Allopurinol'	HMDB00 14581	C5H4N4O	
		136.0380418	0.0002 418	Proton ation	b'pentane-1-dithioperoxol'	b'1-Pentanesulfenothioic acid'	HMDB00 31160	C5H12S2	
		136.0380418	0.0002 418	Proton ation	b'1-(ethylsulfanyl)propane'	b'Ethyl propyl disulfide'	HMDB00 33053	C5H12S2	
		136.0380418	0.0002 418	Proton ation	b'2-(ethylsulfanyl)propane'	b'Ethyl isopropyl disulfide'	HMDB00 33054	C5H12S2	
		136.0385108	0.0007 108	Proton ation	b'7H-purin-2-ol'	b'2-Hydroxypurine'	HMDB02 45165	C5H4N4O	
		136.0371734	0.0006 266	Proton ation	b'2,3,4-trihydroxybutanoic acid'	b'2,3,4-Trihydroxybutanoic acid'	HMDB02 45425	C4H8O5	C01 620
		136.0385108	0.0007 108	Proton ation	b'9H-purin-9-ol'	b'9H-Purine-9-ol'	HMDB02 47704	C5H4N4O	
		136.0398534	0.0020 534	Proton ation	b'4-aminobenzoate'	b'4-aminobenzoate'	HMDB03 04171	C7H6NO2	
		135.0320284	0.0020 284	Redox		b'2-Benzoxazolol'	HMDB00 32931	C7H5NO2	
		135.0320284	0.0020	Redox	b'2,3-dihydro-1,2-benzoxazol-3-one'	b'Benzo[d]isoxazol-3-ol'	HMDB02	C7H5NO2	

			284				49006		
11	136.00	137.0146643	0.0004 643	Proton ation	b'2-amino-3-sulfinylpropanoic acid'	b'S-oxocysteine'	HMDB02 57422	C3H7NO3S	
	64	137.0146643	0.0004 643	Proton ation	b'2-amino-3-hydroxypropane(thioperoxoic) OS-acid'	b'serine thiol'	HMDB02 58249	C3H7NO3S	
1	136.99	138.0081952	0.0005 952	Proton ation	b'[(2R,3S)-3-methyloxiran-2-yl]phosphonic acid'	b'Fosfomycin'	HMDB00 14966	C3H7O4P	C06 454
2	98	138.0081957	0.0005 957	Proton ation	b'(3-methyloxiran-2-yl)phosphonic acid'	b'(2S,3R)-3-Methyloxiran-2-ylphosphonic acid'	HMDB02 42559	C3H7O4P	
1 3	140.01 08	141.0190943	0.0004 943	Proton ation	b'(2-aminoethoxy)phosphonic acid'	b'O-Phosphoethanolamine'	HMDB00 00224	C2H8NO4P	C00 346
		141.0190947	0.0004 947	Proton ation	b'(1-aminoethoxy)phosphonic acid'	b'Aminoethanol phosphate'	HMDB02 48314	C2H8NO4P	
		140.0109586	0.0001 586	Redox	b'2-[(2E)-5-oxo-2,5-dihydrofuran-2-ylidene]acetic acid'	b'cis-4-Carboxymethylenebut-2-en-4-olide'	HMDB00 60459	C6H4O4	C04 431
		140.0109586	0.0001 586	Redox	b'2-(5-oxo-2,5-dihydrofuran-2-ylidene)acetic acid'	b'trans-4-Carboxymethylenebut-2-en-4-olide'	HMDB00 60518	C6H4O4	
1 4	145.06 06	146.0691422	0.0007 422	Proton ation	b'(2S)-2-amino-4-carbamoylbutanoic acid'	b'L-Glutamine'	HMDB00 00641	C5H10N2O3	C00 064
		146.0691422	0.0007 422	Proton ation	b'(2S)-3-(carbamoylamino)-2-methylpropanoic acid'	b'Ureidoisobutyric acid'	HMDB00 02031	C5H10N2O3	C05 100
		146.0691422	0.0007 422	Proton ation	b'(2R)-2-amino-4-carbamoylbutanoic acid'	b'D-Glutamine'	HMDB00 03423	C5H10N2O3	C00 819
		146.0691422	0.0007 422	Proton ation	b'2-[(2S)-2-aminopropanamido]acetic acid'	b'Alanylglycine'	HMDB00 06899	C5H10N2O3	
		146.0691422	0.0007	Proton	b'5,6-dihydroxy-1,3-diazepan-2-one'	b'Cyclic Urea'	HMDB02	C5H10N2O3	

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		146.0691422	0.0007 422	Proton ation	b'2-(2-aminoacetamido)propanoic acid'	b'Glycyl-D-Alanine'	HMDB02 52875	C5H10N2O3	
		146.0691422	0.0007 422	Proton ation	b'2-(2-amino-N-methylacetamido)acetic acid'	b'Glycylsarcosine'	HMDB02 52887	C5H10N2O3	
		146.0691422	0.0007 422	Proton ation	b'2-[[[(2R)-2-amino-1-hydroxypropylidene]amino}acetic acid'	b'D-Alanyl glycine'	HMDB03 02832	C5H10N2O3	
		146.0691422	0.0007 422	Proton ation	b'3-(carbamoylamino)-2-methylpropanoic acid'	b'3-ureido-isobutyrate'	HMDB03 04156	C5H10N2O3	C05 100
1 5	146.04 49	147.0531578	0.0004 578	Proton ation	b'(2S)-2-aminopentanedioic acid'	b'L-Glutamic acid'	HMDB00 00148	C5H9NO4	C00 025
		147.0531578	0.0004 578	Proton ation	b'(2R)-2-(methylamino)butanedioic acid'	b'N-Methyl-D-aspartic acid'	HMDB00 02393	C5H9NO4	C12 269
		147.0531578	0.0004 578	Proton ation	b'(2S)-2-acetamido-3-hydroxypropanoic acid'	b'N-Acetylserine'	HMDB00 02931	C5H9NO4	
		147.0531578	0.0004 578	Proton ation	b'(2S)-3-(acetyloxy)-2-aminopropanoic acid'	b'O-Acetylserine'	HMDB00 03011	C5H9NO4	C00 979
		147.0531578	0.0004 578	Proton ation	b'(2R)-2-aminopentanedioic acid'	b'D-Glutamic acid'	HMDB00 03339	C5H9NO4	C00 217
		147.0531578	0.0004 578	Proton ation	b'(2S,4R)-2-amino-4-hydroxy-5-oxopentanoic acid'	b'L-4-Hydroxyglutamate semialdehyde'	HMDB00 06556	C5H9NO4	C05 938
		147.0531578	0.0004 578	Proton ation	b'3-[(carboxymethyl)amino]propanoic acid'	b'3-(Carboxymethylamino)propanoic acid'	HMDB00 33550	C5H9NO4	
		147.0531578	0.0004 578	Proton ation	b'2-aminopentanedioic acid'	b'DL-Glutamate'	HMDB00 60475	C5H9NO4	C00 302
		147.0531578	0.0004	Proton	b'2-[(2S)-2-hydroxypropanamido]acetic acid'	b'N-lactoyl-Glycine'	HMDB00	C5H9NO4	

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		147.0531578	0.0004 578	Proton ation	b'2-amino-5-hydroxy-4-oxopentanoic acid'	b'5-Hydroxy-4-oxo-L-norvaline'	HMDB02 46802	C5H9NO4	
		147.0531578	0.0004 578	Proton ation	b'2-aminopropanoyl ethaneperoxoate'	b'Alanine acetate'	HMDB02 48101	C5H9NO4	
		147.0531578	0.0004 578	Proton ation	b'2-(methylamino)butanedioic acid'	b'N-Methyl-DL-aspartic acid'	HMDB02 55174	C5H9NO4	
1 6	150.02 16	151.0303138	0.0009 138	Proton ation	b'2-amino-3-methanesulfinylpropanoic acid'	b'(S)C(S)S-S-Methylcysteine sulfoxide'	HMDB00 29432	C4H9NO3S	
		151.026943	0.0024 57	Proton ation	b'3-nitrobenzaldehyde'	b'3-Nitrobenzaldehyde'	HMDB02 45945	C7H5NO3	
		151.026943	0.0024 57	Proton ation	b'4-nitrobenzaldehyde'	b'4-Nitrobenzaldehyde'	HMDB02 46531	C7H5NO3	
1 7	150.04	151.0494098	0.0016 098	Proton ation	b'2-amino-6,7-dihydro-3H-purin-6-one'	b'Guanine'	HMDB00 00132	C5H5N5O	C00 242
		151.0494098	0.0016 098	Proton ation	b'6-amino-7H-purin-2-ol'	b'2-Hydroxyadenine'	HMDB00 00403	C5H5N5O	
		151.0494098	0.0016 098	Proton ation	b'6-amino-7H-purin-8-ol'	b'8-Hydroxyadenine'	HMDB00 00542	C5H5N5O	
		151.0455705	0.0022 295	Proton ation	b'4-methylbenzene-1-carbothioamide'	b'4-Methylbenzenecarbothioamide'	HMDB02 45645	C8H9NS	
		151.0494098	0.0016 098	Proton ation	b'2-amino-8,9-dihydro-7H-purin-8-one'	b'8-Oxo-7,8-dihydrodeoxyguanine'	HMDB02 47457	C5H5N5O	
		151.0489418	0.0011 418	Proton ation	b'2-amino-4-(methylsulfonyl)butane-1-thiol'	b'(S)-2-Amino-4-methylsulfonyl- butane-1-thiol'	HMDB02 49989	C5H13NS2	
		151.0455705	0.0022	Proton	b'N-phenylethanethioamide'	b'Thiacetanilide'	HMDB02	C8H9NS	

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		150.0429274	0.0029 274	Redox	b'5-(prop-1-yn-1-yl)-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'5-Propynyluracil'	HMDB02 46840	C7H6N2O2	
1 8	151.02 48	152.0334254	0.0008 254	Proton ation	b'2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Xanthine'	HMDB00 00292	C5H4N4O2	C00 385
		152.0334254	0.0008 254	Proton ation	b'1H,2H,4H,5H,6H-pyrazolo[3,4-d]pyrimidine-4,6-dione'	b'Oxypurinol'	HMDB00 00786	C5H4N4O2	C07 599
		152.0334254	0.0008 254	Proton ation	b'6,7,8,9-tetrahydro-3H-purine-6,8-dione'	b'6,8-Dihydroxypurine'	HMDB00 01182	C5H4N4O2	
1 9	152.00 13	153.0095784	0.0004 784	Proton ation	b'(2R)-2-amino-3-[(R)-sulfinio]propanoic acid'	b'3-Sulfinioalanine'	HMDB00 00996	C3H7NO4S	C00 606
		153.0095789	0.0004 789	Proton ation	b'2-amino-3-sulfinopropanoic acid'	b'Cysteine sulfinic acid'	HMDB02 50705	C3H7NO4S	
		152.0027164	0.0014 164	Redox	b'1,2,3-benzodioxaphosphinine'	b'Benzodioxaphosphorin'	HMDB02 49013	C7H5O2P	
2 0	152.99 49	154.0031103	0.0004 103	Proton ation	b'2-phosphonopropanoic acid'	b'2-Phosphonopropionic acid'	HMDB02 45296	C3H7O5P	
2 1	153.99 72	155.0074709	0.0024 709	Proton ation	b'1-amino-3-sulfanylpropane-1-sulfinic acid'	b'(1R)-1-Amino-3-sulfanylpropane-1-sulfinic acid'	HMDB02 42354	C3H9NO2S2	
		155.0040996	0.0009 004	Proton ation	b'2-sulfanylidene-1,2-dihydropyridine-3-carboxylic acid'	b'2-Mercaptopicotinic acid'	HMDB02 45193	C6H5NO2S	
		155.0040996	0.0009 004	Proton ation	b'3-sulfanylpuridine-2-carboxylic acid'	b'3-Mercaptopicolinic acid'	HMDB02 45916	C6H5NO2S	
		155.0040996	0.0009 004	Proton ation	b'4-nitrobenzene-1-thiol'	b'4-Nitrothiophenol'	HMDB02 46550	C6H5NO2S	
		153.9944624	0.0027	Redox	b'1-methyl-3-propyltrisulfane'	b'Methyl propyl trisulfide'	HMDB00	C4H10S3	

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		153.9944624	0.0027 376	Redox	b'(methylsulfanyl)((methylsulfanyl)methyl)sulfanyl)methane'	b'2,4,6-Trithiaheptane'	HMDB00 32547	C4H10S3	
		153.9944624	0.0027 376	Redox	b'([(methylsulfanyl)methyl]disulfanyl)ethane'	b'Ethyl (methylthio)methyl disulfide'	HMDB00 33047	C4H10S3	
		153.9944624	0.0027 376	Redox	b'diethyltrisulfane'	b'Diethyl trisulfide'	HMDB00 39524	C4H10S3	
		153.9944624	0.0027 376	Redox	b'1-[(1-sulfanylethyl)sulfanyl]ethane-1-thiol'	b"1,1'-Thiobisethanethiol"	HMDB00 40239	C4H10S3	
		153.9952203	0.0019 797	Redox	b'3,3-bis(chloromethyl)oxetane'	b'3,3-Bis(chloromethyl)oxetane'	HMDB02 45991	C5H8Cl2O	
2	154.04	155.0582432	0.0005	Proton	b'3-amino-4-methoxybenzene-1,2-diol'	b'methoxycatecholamine'	HMDB02 54544	C7H9NO3	
2	99		432	ation					
2	154.06	155.0694765	0.0005 765	Proton ation	b'(2S)-2-amino-3-(1H-imidazol-5-yl)propanoic acid'	b'L-Histidine'	HMDB00 00177	C6H9N3O2	C00 135
		155.0694765	0.0005 765	Proton ation	b'2-amino-3-(1H-pyrazol-1-yl)propanoic acid'	b'L-2-Amino-3-(1-pyrazolyl)propanoic acid'	HMDB00 34267	C6H9N3O2	
		155.0694765	0.0005 765	Proton ation	b'2-amino-3-(1H-imidazol-5-yl)propanoic acid'	b'D-Histidine'	HMDB02 50763	C6H9N3O2	C00 768
3	11	155.0713678	0.0024 678	Proton ation	b'2-methyl-4-oxo-5-propyl-4,5-dihydrofuran-3-olate'	b'4-hydroxy-5-methyl-2-propyl-3(2H)-furanone'	HMDB03 04179	C8H11O3	
		154.0629942	0.0018 942	Redox	b'4-(2-hydroxyethyl)benzene-1,2-diol'	b'Hydroxytyrosol'	HMDB00 05784	C8H10O3	
		154.0629942	0.0018 942	Redox	b'3-(hydroxymethyl)-5-methoxyphenol'	b'Sylvopinol'	HMDB00 30570	C8H10O3	
		154.0629942	0.0018	Redox	b'4-(hydroxymethyl)-2-methoxyphenol'	b'4-Hydroxy-3-	HMDB00	C8H10O3	C06

2	156.02		942			methoxybenzenemethanol'	32012		317
		154.0629942	0.0018 942	Redox	b'2,6-dimethoxyphenol'	b'2,6-Dimethoxyphenol'	HMDB00 34158	C8H10O3	C10 787
		154.0629942	0.0018 942	Redox	b'propyl furan-2-carboxylate'	b'Propyl 2-furoate'	HMDB00 37724	C8H10O3	
		154.0629942	0.0018 942	Redox	b'furan-2-ylmethyl propanoate'	b'2-Furanylmethyl propanoate'	HMDB00 37728	C8H10O3	
		154.0629942	0.0018 942	Redox	b'3,5-dimethoxyphenol'	b'3,5-Dimethoxyphenol'	HMDB00 59966	C8H10O3	
		154.0629942	0.0018 942	Redox	b'6-ethyl-3-hydroxy-2-methyl-4H-pyran-4-one'	b'6-Ethyl-3-hydroxy-2-methyl-4-pyrone'	HMDB02 47055	C8H10O3	
		154.0629942	0.0018 942	Redox	b'octahydro-2-benzofuran-1,3-dione'	b'Hexahydrophthalic anhydride'	HMDB02 53140	C8H10O3	
		154.0629942	0.0018 942	Redox	b'3a-hydroxy-2,3,3a,6,7,7a-hexahydro-1-benzofuran-6-one'	b'Halleridone'	HMDB03 02803	C8H10O3	
		154.0629942	0.0018 942	Redox	b'4-acetyl-2,5-dimethyl-2,3-dihydrofuran-3-one'	b'4-Acetyl-2,5-dimethyl-3(2H)-furanone'	HMDB03 03185	C8H10O3	
2	156.02	157.0375077	0.0003 077	Proton ation	b'(2Z,4E)-5-amino-2,4-dienedioic acid'	b'2-Aminomuconic acid'	HMDB00 01241	C6H7NO4	C02 220
		157.0375077	0.0003 077	Proton ation	b'2,5-dioxopyrrolidin-1-yl acetate'	b'Succinimidyl acetate'	HMDB02 44630	C6H7NO4	
		157.0375077	0.0003 077	Proton ation	b'1,2-dimethyl-3,4-dioxazetidine-2-carboxylic acid'	b'(2S)-1,2-Dimethyl-3,4-dioxazetidine-2-carboxylic acid'	HMDB02 57875	C6H7NO4	
		156.02834	0.0010 6	Redox	b'4,6-dioxo-1,4,5,6-tetrahydro-1,3,5-triazine-2-carboxamide'	b'Allantoxanamide'	HMDB02 47204	C4H4N4O3	
2	158.92	158.92535	0.0008	Redox	b'terbium'	b'Terbium'	HMDB03	Tb	

5	45		5				03932		
2	160.84		0.0008						
6	07	160.8415003	003	Redox	b'iron(3+) ion trichloride'	b'Iron(III) chloride'	HMDB03 03404	Cl3Fe	
2	163.01	164.0255633	0.0024 633	Proton ation	b'2-amino-4-(nitrososulfinyl)butanoic acid'	b'S-Nitrosomocysteine'	HMDB02 57418	C4H8N2O3S	
7	53	163.0125553	0.0027 447	Redox	b'1-isothiocyanato-3-methanesulfinylpropane'	b'3-Methylsulfinylpropyl isothiocyanate'	HMDB00 06095	C5H9NOS2	
2	164.03	165.0459644	0.0007 644	Proton ation	b'(2S)-2-amino-4-methanesulfinylbutanoic acid'	b'Methionine sulfoxide'	HMDB00 02005	C5H11NO3S	C02 989
8	74	165.0425931	0.0026 069	Proton ation	b'7-hydroxy-6-methyl-1H,3H-furo[3,4-c]pyridin-1-one'	b'4-Pyridoxolactone'	HMDB00 03454	C8H7NO3	C00 971
		165.0425931	0.0026 069	Proton ation	b'2-formamidobenzoic acid'	b'Formylanthranilic acid'	HMDB00 04089	C8H7NO3	C05 653
		165.0425931	0.0026 069	Proton ation	b'7-hydroxy-6-methyl-1H,3H-furo[3,4-c]pyridin-3-one'	b'5-Pyridoxolactone'	HMDB00 04291	C8H7NO3	C06 052
		165.0425931	0.0026 069	Proton ation	b'3-hydroxy-3,5,6,7-tetrahydro-2H-indole-5,6-dione'	b'Noradrenochrome'	HMDB00 13030	C8H7NO3	
		165.0425931	0.0026 069	Proton ation	b'6-methoxy-2,3-dihydro-1,3-benzoxazol-2-one'	b'6-Methoxy-2(3H)-benzoxazolone'	HMDB00 36582	C8H7NO3	
		165.0459639	0.0007 639	Proton ation	b'2-amino-3-(ethanesulfinyl)propanoic acid'	b'Ethiin'	HMDB00 37057	C5H11NO3S	
		165.0425931	0.0026 069	Proton ation	b'2-hydroxy-3,4-dihydro-2H-1,4-benzoxazin-3-one'	b'(R)-2-Hydroxy-2H-1,4-benzoxazin- 3(4H)-one'	HMDB00 38318	C8H7NO3	C15 769
		165.0459644	0.0007 644	Proton ation	b'2-amino-2-hydroxy-4-(methylsulfinyl)butanoic acid'	b'2-Hydroxy-L-methionine'	HMDB02 46915	C5H11NO3S	
		165.0459639	0.0007	Proton	b'2-amino-4-methanesulfinylbutanoic acid'	b'D-Methionine (S)-S-oxide'	HMDB02	C5H11NO3S	

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		165.0425931	0.0026 069	Proton ation	b'1-(4-nitrophenyl)ethan-1-one'	b"4'-Nitroacetophenone"	HMDB02 56052	C8H7NO3	C02 803
		165.0425931	0.0026 069	Proton ation	b'2-(C-hydroxycarbonimidoyl)benzoic acid'	b'Phthalamic acid'	HMDB02 56499	C8H7NO3	
		164.038591	0.0011 91	Redox	b'3-fluoro-1,2-dihydro-1,8-naphthyridin-2-one'	b'Fluoronaphthyridone'	HMDB02 52387	C8H5FN2O	
2	164.04	164.0473441	0.0023 559	Redox	b'2-oxo-3-phenylpropanoic acid'	b'Phenylpyruvic acid'	HMDB00 00205	C9H8O3	C00 166
9	97	164.0473441	0.0023 559	Redox	b'(2E)-3-(3-hydroxyphenyl)prop-2-enoic acid'	b'm-Coumaric acid'	HMDB00 01713	C9H8O3	C12 621
		164.0473441	0.0023 559	Redox	b'(2E)-3-(4-hydroxyphenyl)prop-2-enoic acid'	b'4-Hydroxycinnamic acid'	HMDB00 02035	C9H8O3	C00 811
		164.0473441	0.0023 559	Redox	b'(2E)-3-(2-hydroxyphenyl)prop-2-enoic acid'	b'2-Hydroxycinnamic acid'	HMDB00 02641	C9H8O3	C01 772
		164.0473441	0.0023 559	Redox	b'(2Z)-2-hydroxy-3-phenylprop-2-enoic acid'	b'Enol-phenylpyruvate'	HMDB00 12225	C9H8O3	C02 763
		164.0473441	0.0023 559	Redox	b'(2Z)-3-(4-hydroxyphenyl)prop-2-enoic acid'	b'cis-p-Coumaric acid'	HMDB00 30677	C9H8O3	C06 738
		164.0473441	0.0023 559	Redox	b'(2Z)-3-(2-hydroxyphenyl)prop-2-enoic acid'	b'Coumarinic acid'	HMDB00 41592	C9H8O3	C05 838
		164.0473441	0.0023 559	Redox	b'methyl 2-oxo-2-phenylacetate'	b'Methyl Phenylglyoxalate'	HMDB00 62605	C9H8O3	
		164.0473441	0.0023 559	Redox	b'methyl 4-formylbenzoate'	b'METHYL 4-FORMYLBENZOATE'	HMDB02 54568	C9H8O3	
3	165.04	166.0504181	0.0017	Proton	b'(3,6-dihydroxy-2,3-dihydro-1H-indol-5-yl)oxidanyl'	b'Noradrenochrome o-semiquinone'	HMDB00	C8H8NO3	

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3	166.01	167.0218577	0.0027 423	Proton ation	b'pyridine-2,3-dicarboxylic acid'	b'Quinolinic acid'	HMDB00 00232	C7H5NO4	C03 722
		167.0252285	0.0006 285	Proton ation	b'2-amino-4-sulfinoethanoic acid'	b'Homocysteinesulfonic acid'	HMDB00 06462	C4H9NO4S	
		167.0265659	0.0019 659	Proton ation	b'2-amino-6,7-dihydro-3H-purine-6-thione'	b'Thioguanine'	HMDB00 14496	C5H5N5S	C07 648
		167.0218577	0.0027 423	Proton ation	b'pyridine-2,6-dicarboxylic acid'	b'2,6-Pyridinedicarboxylic acid'	HMDB00 33161	C7H5NO4	
		167.0252289	0.0006 289	Proton ation	b'2-acetamidoethane-1-sulfonic acid'	b'N-Acetyltaurine'	HMDB02 40253	C4H9NO4S	
		167.0218576	0.0027 424	Proton ation	b'2-nitrobenzoic acid'	b'2-Nitrobenzoic acid'	HMDB02 45255	C7H5NO4	C16 234
		167.0218576	0.0027 424	Proton ation	b'3-hydroxy-2-nitrobenzaldehyde'	b'3-Hydroxy-2-nitrobenzaldehyde'	HMDB02 45884	C7H5NO4	
		167.0218577	0.0027 423	Proton ation	b'4-nitrobenzoic acid'	b'4-Nitrobenzoic acid'	HMDB02 46532	C7H5NO4	C18 625
		167.0218576	0.0027 424	Proton ation	b'pyridine-3,5-dicarboxylic acid'	b'Pyridine-3,5-dicarboxylic acid'	HMDB02 56966	C7H5NO4	
		167.0229548	0.0016 452	Proton ation	b'(2S)-2,3-dihydropyridine-2,6-dicarboxylate'	b'(S)-2,3-dihydrodipicolinate'	HMDB03 03995	C7H5NO4	
3	166.06	167.0734993	0.0006 993	Proton ation	b'9H-carbazole'	b'Carbazole'	HMDB02 49614	C12H9N	C08 060
		167.0713678	0.0014 322	Proton ation	b'5-butylidene-2-methyl-4-oxo-4,5-dihydrofuran-3-olate'	b'(2E)-2-butylidene-4-hydroxy-5-methyl-3(2H)-furanone'	HMDB03 03965	C9H11O3	
		167.0713678	0.0014	Proton	b'6-(2-methylpropyl)-2-oxo-2H-pyran-4-olate'	b'6-isobutyl-4-hydroxy-2-pyrone'	HMDB03	C9H11O3	

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166.0629942	0.0020 058	Redox	b'3-(3-hydroxyphenyl)propanoic acid'	b'3-(3-Hydroxyphenyl)propanoic acid'	HMDB00 00375	C9H10O3	C114 57	
166.0629942	0.0020 058	Redox	b'(2S)-2-hydroxy-3-phenylpropanoic acid'	b'D-Phenyllactic acid'	HMDB00 00563	C9H10O3	C05 607	
166.0629942	0.0020 058	Redox	b'(2R)-2-hydroxy-3-phenylpropanoic acid'	b'L-3-Phenyllactic acid'	HMDB00 00748	C9H10O3	C05 607	
166.0629942	0.0020 058	Redox		b'Phenyllactic acid'	HMDB00 00779	C9H10O3	C01 479	
166.0629942	0.0020 058	Redox	b'2-(4-methoxyphenyl)acetic acid'	b'4-Methoxyphenylacetic acid'	HMDB00 02072	C9H10O3		
166.0629942	0.0020 058	Redox	b'3-(4-hydroxyphenyl)propanoic acid'	b'Desaminotyrosine'	HMDB00 02199	C9H10O3	C01 744	
166.0629942	0.0020 058	Redox	b'3-phenoxypropanoic acid'	b'3-Phenoxypionic acid'	HMDB00 02229	C9H10O3		
166.0629942	0.0020 058	Redox	b'2-(4-hydroxy-3-methoxyphenyl)acetaldehyde'	b'Homovanillin'	HMDB00 05175	C9H10O3	C05 581	
166.0629942	0.0020 058	Redox	b'3-ethoxy-4-hydroxybenzaldehyde'	b'Ethyl vanillin'	HMDB00 29665	C9H10O3		
166.0629942	0.0020 058	Redox	b'ethyl 2-hydroxybenzoate'	b'Ethyl salicylate'	HMDB00 29817	C9H10O3		
166.0629942	0.0020 058	Redox	b'1-(3,4-dihydroxyphenyl)propan-2-one'	b'3,4-Dihydroxyphenylacetone'	HMDB00 31132	C9H10O3		
166.0629942	0.0020 058	Redox	b'2-methoxyphenyl acetate'	b'Guaicyl acetate'	HMDB00 32030	C9H10O3		
166.0629942	0.0020	Redox	b'3,4-dimethoxybenzaldehyde'	b'3,4-Dimethoxybenzaldehyde'	HMDB00	C9H10O3	C02	

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166.0629942	0.0020 058	Redox	b'ethyl 4-hydroxybenzoate'	b'Ethylparaben'	HMDB00 32573	C9H10O3			
166.0629942	0.0020 058	Redox	b'methyl 2-methoxybenzoate'	b'Methyl 2-methoxybenzoate'	HMDB00 32605	C9H10O3			
166.0629942	0.0020 058	Redox	b'methyl 4-methoxybenzoate'	b'Methyl 4-methoxybenzoate'	HMDB00 32639	C9H10O3			
166.0629942	0.0020 058	Redox	b'3-(2-hydroxyphenyl)propanoic acid'	b'3-(2-Hydroxyphenyl)propanoic acid'	HMDB00 33752	C9H10O3		C011 98	
166.0629942	0.0020 058	Redox	b'1-(furan-3-yl)pentane-1,4-dione'	b'Ipomeanine'	HMDB00 34243	C9H10O3			
166.0629942	0.0020 058	Redox	b'(4-methoxyphenyl)methyl formate'	b'4-Methoxybenzyl formate'	HMDB00 34993	C9H10O3			
166.0629942	0.0020 058	Redox	b'3-hydroxy-1-(4-hydroxyphenyl)propan-1-one'	b'3-Hydroxy-1-(4-hydroxyphenyl)-1-propanone'	HMDB00 40645	C9H10O3			
166.0629942	0.0020 058	Redox	b'ethyl (2Z)-3-(furan-2-yl)prop-2-enoate'	b'Ethyl 2-furanacrylate'	HMDB00 41611	C9H10O3			
166.0629942	0.0020 058	Redox	b'2-(4-hydroxyphenyl)propanoic acid'	b'4-Hydroxyphenyl-2-propionic acid'	HMDB00 41683	C9H10O3		C03 080	
166.0629942	0.0020 058	Redox	b'2-(3-methoxyphenyl)acetic acid'	b'3-Methoxyphenylacetic acid'	HMDB00 59969	C9H10O3			
166.0629942	0.0020 058	Redox	b'3,5-dimethoxybenzaldehyde'	b'3,5-Dimethoxybenzaldehyde'	HMDB00 62348	C9H10O3			
166.0629942	0.0020 058	Redox	b'3-hydroxy-2-phenylpropanoic acid'	b'Tropate'	HMDB00 62590	C9H10O3		C01 456	
166.0629942	0.0020	Redox	b'(3R)-3-hydroxy-3-phenylpropanoic acid'	b'3-Hydroxy-3-phenylpropanoic acid'	HMDB01	C9H10O3			

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		166.0629942	0.0020 058	Redox	b'4-methyl-1,3,3a,4,5,7a-hexahydro-2-benzofuran-1,3-dione'	b'3-Methyltetrahydrophthalic anhydride'	HMDB02 45936	C9H10O3		
		166.0629942	0.0020 058	Redox	b'1-(4-hydroxy-3-methoxyphenyl)ethan-1-one'	b'Acetovanillone'	HMDB02 47918	C9H10O3	C113 80	
		166.0663655	0.0013 655	Redox	b'hexane-1-sulfonic acid'	b'Hexanesulfonic acid'	HMDB02 53146	C6H14O3S		
		166.0629942	0.0020 058	Redox	b'3a-methyl-1,3,3a,4,7,7a-hexahydro-2-benzofuran-1,3-dione'	b'1,2,3,6-Tetrahydromethylphthalic anhydride'	HMDB02 54937	C9H10O3		
		166.0629942	0.0020 058	Redox	b'1-(2-hydroxy-4-methoxyphenyl)ethan-1-one'	b'Paconol'	HMDB02 56081	C9H10O3	C10 712	
		166.0629942	0.0020 058	Redox	b'octahydro-1H-indene-1,2,3-trione'	b'3a,4,5,6,7,7a-Hexahydroindene-1,2,3- trione'	HMDB02 60012	C9H10O3		
		166.0629942	0.0020 058	Redox	b'2-methoxy-2-phenylacetic acid'	b'Methoxyphenylacetic acid'	HMDB03 01734	C9H10O3		
3	166.97 38	167.9823744	0.0007 744	Proton ation	b'2-(phosphonoxy)prop-2-enoic acid'	b'Phosphoenolpyruvic acid'	HMDB00 00263	C3H5O6P	C00 074	
		167.983472	0.0018 72	Proton ation	b'2-hydroxy-3-(phosphonatoxy)propanal'	b'L-glyceraldehyde 3-phosphate'	HMDB03 04402	C3H5O6P		
3 4	167.05 98	168.0687483	0.0011 483	Proton ation	b'9H-pyrido[3,4-b]indole'	b'beta-Carboline'	HMDB00 12897	C11H8N2	C20 157	
		168.0687483	0.0011 483	Proton ation	b'6H-pyrrolo[2,3-f]quinoline'	b'1H-Pyrrolo[2,3-f]quinoline'	HMDB02 44904	C11H8N2		
		168.0687483	0.0011 483	Proton ation	b'5H-pyrido[4,3-b]indole'	b'5H-Pyrido[4,3-b]indole'	HMDB02 47024	C11H8N2		
		168.0687483	0.0011	Proton	b'7H-pyrrolo[2,3-h]quinoline'	b'Pyrroloquinoline'	HMDB02	C11H8N2		

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		167.0582432	0.0015 568	Redox	b'3-hydroxy-5-(hydroxymethyl)-2-methylpyridine-4-carbaldehyde'	b'Pyridoxal'	HMDB00 01545	C8H9NO3	C00 250
		167.0582432	0.0015 568	Redox	b'5-hydroxy-4-(hydroxymethyl)-6-methylpyridine-3-carbaldehyde'	b'Isopyridoxal'	HMDB00 04290	C8H9NO3	C06 051
		167.0582432	0.0015 568	Redox	b'5-hydroxy-2,3,3a,4,5,7a-hexahydro-1H-isoindole-1,3-dione'	b'3alpha,4,5,7alpha-Tetrahydro-5-hydroxy-1H-isoindole-1,3(2H)-dione'	HMDB00 34887	C8H9NO3	
		167.0582432	0.0015 568	Redox	b'4-hydroxy-2,3,3a,4,7,7a-hexahydro-1H-isoindole-1,3-dione'	b'3alpha,4,7,7alpha-Tetrahydro-4-hydroxy-1H-isoindole-1,3(2H)-dione'	HMDB00 34889	C8H9NO3	
		167.0582432	0.0015 568	Redox	b'2-amino-3-methoxybenzoic acid'	b'3-Methoxyanthranilate'	HMDB00 60374	C8H9NO3	C05 831
		167.0582432	0.0015 568	Redox	b'2-hydroxy-N-(2-hydroxyphenyl)acetamide'	b'2-Hydroxy-N-(2-hydroxyphenyl)acetamide'	HMDB02 40370	C8H9NO3	
		167.0582432	0.0015 568	Redox	b'2-amino-2-(4-hydroxyphenyl)acetic acid'	b'4-Hydroxyphenylglycine'	HMDB02 44973	C8H9NO3	
		167.0582432	0.0015 568	Redox	b'2-[(4-hydroxyphenyl)amino]acetic acid'	b'N-(4-Hydroxyphenyl)glycine'	HMDB02 55011	C8H9NO3	
3 5	168.02 65	169.0351024	0.0008 024	Proton ation	b'sodium 2-amino-4-carboxybutanoate'	b'Monosodium glutamate'	HMDB03 03331	C5H8NNaO4	
		168.02834	0.0018 4	Redox	b'2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'	b'Uric acid'	HMDB00 00289	C5H4N4O3	C00 366
		168.0245007	0.0019 993	Redox	b'2-(phenylsulfanyl)acetic acid'	b'(Phenylthio)acetic acid'	HMDB02 43657	C8H8O2S	
3 6	168.04 2	169.0503944	0.0005 944	Proton ation	b'[2-(dimethylamino)ethoxy]phosphonic acid'	b'Phosphodimethylethanolamine'	HMDB00 60244	C4H12NO4P	C13 482
		169.0527638	0.0029	Proton	b'1-isocyanatonaphthalene'	b'1-Naphthyl isocyanate'	HMDB02	C11H7NO	

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168.0422587	0.0002 587	Redox	b'2-(2,5-dihydroxyphenyl)acetic acid'	b'Homogentisic acid'	HMDB00 00130	C8H8O4	C00 544	
168.0422587	0.0002 587	Redox	b'4-hydroxy-3-methoxybenzoic acid'	b'Vanillic acid'	HMDB00 00484	C8H8O4	C06 672	
168.0422587	0.0002 587	Redox	b'2-hydroxy-2-(3-hydroxyphenyl)acetic acid'	b'3-Hydroxymandelic acid'	HMDB00 00750	C8H8O4		
168.0422587	0.0002 587	Redox	b'2-hydroxy-2-(4-hydroxyphenyl)acetic acid'	b'p-Hydroxymandelic acid'	HMDB00 00822	C8H8O4	C115 27	
168.0422587	0.0002 587	Redox	b'2-(3,4-dihydroxyphenyl)acetic acid'	b'3,4-Dihydroxybenzeneacetic acid'	HMDB00 01336	C8H8O4	C011 61	
168.0422587	0.0002 587	Redox	b'2-hydroxy-5-methoxybenzoic acid'	b'5-Methoxysalicylic acid'	HMDB00 01868	C8H8O4		
168.0422587	0.0002 587	Redox	b'2-(3,4-dihydroxyphenyl)-2-hydroxyacetaldehyde'	b'3,4-Dihydroxymandelaldehyde'	HMDB00 06242	C8H8O4	C05 577	
168.0422587	0.0002 587	Redox	b'1-(2,4,6-trihydroxyphenyl)ethan-1-one'	b"2",4',6'-Trihydroxyacetophenone"	HMDB00 29644	C8H8O4		
168.0422587	0.0002 587	Redox	b'2,6-dimethoxycyclohexa-2,5-diene-1,4-dione'	b'2,6-Dimethoxy-1,4-benzoquinone'	HMDB00 29673	C8H8O4	C10 331	
168.0422587	0.0002 587	Redox	b'3-acetyl-4-hydroxy-6-methyl-2H-pyran-2-one'	b'3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one'	HMDB00 33129	C8H8O4		
168.0422587	0.0002 587	Redox	b'2,5-dimethoxycyclohexa-2,5-diene-1,4-dione'	b'Thermophilin'	HMDB00 34335	C8H8O4	C01 692	
168.0422587	0.0002 587	Redox	b'2-hydroxy-3-methoxybenzoic acid'	b'3-Methoxysalicylic acid'	HMDB00 59713	C8H8O4		
168.0422587	0.0002	Redox	b'3-hydroxy-4-methoxybenzoic acid'	b'Isovanillic acid'	HMDB00	C8H8O4		

			587					60003		
		168.0422587	0.0002 587	Redox	b'2-(3,5-dihydroxyphenyl)acetic acid'	b'3, 5-Dihydroxyphenylacetic acid'	HMDB00 94709	C8H8O4		
		168.0422587	0.0002 587	Redox	b'2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)acetic acid'	b'Quinolacetic acid'	HMDB02 40257	C8H8O4		
		168.0422587	0.0002 587	Redox	b'4,10-dioxatricyclo[5.2.1.0 ^{2,6}]{2,6}]decane-3,5-dione'	b'4,7-Epoxyisobenzofuran-1,3-dione, hexahydro-, (3aR,4S,7R,7aS)-rel.'	HMDB02 45751	C8H8O4		
		168.0422587	0.0002 587	Redox	b'3-acetyl-6-methyl-3,4-dihydro-2H-pyran-2,4-dione'	b'Dehydroacetic acid'	HMDB02 50943	C8H8O4		
		168.0422587	0.0002 587	Redox	b'1-(2,4-dihydroxyphenyl)-2-hydroxyethan-1-one'	b'1-(2,4-Dihydroxyphenyl)-2- hydroxyethanone'	HMDB02 57566	C8H8O4		
		168.0434016	0.0014 016	Redox	b'3-fluoro-5-(hydroxymethyl)oxolane-2,3,4-triol'	b'(3R,4R,5R)-3-Fluoro-5- (hydroxymethyl)oxolane-2,3,4-triol'	HMDB02 57780	C5H9FO5		
		168.0422587	0.0002 587	Redox	b'3,4-dihydroxyphenyl acetate'	b'(3,4-Dihydroxyphenyl) acetate'	HMDB02 58013	C8H8O4		
		168.0422587	0.0002 587	Redox	b'2,2-dihydroxy-2-phenylacetic acid'	b'2,2-Dihydroxy-2-phenylacetic acid'	HMDB02 58145	C8H8O4		
		168.0422587	0.0002 587	Redox	b'3,5-dihydroxy-4-methoxybenzaldehyde'	b'3,5-Dihydroxy-4- methoxybenzaldehyde'	HMDB03 01768	C8H8O4		
3 7	171.00 52	172.0136745	0.0006 745	Proton ation	b'[(2R)-2,3-dihydroxypropoxy]phosphonic acid'	b'Glycerol 3-phosphate'	HMDB00 00126	C3H9O6P	C00 093	
		172.0136745	0.0006 745	Proton ation	b'[(1,3-dihydroxypropan-2-yl)oxy]phosphonic acid'	b'beta-Glycerophosphoric acid'	HMDB00 02520	C3H9O6P	C02 979	
		172.0136745	0.0006 745	Proton ation	b'(2,3-dihydroxypropoxy)phosphonic acid'	b'Glycerophosphoric acid'	HMDB02 52849	C3H9O6P	C03 189	
		171.0023845	0.0028	Redox	b'(1R)-1-amino-3-sulfanylpropane-1-sulfonic acid'	b'L-Homocysteine sulfonic acid'	HMDB00	C3H9NO3S2		

			155				02238		
3 8	174.03 98	175.0480724	0.0004 724	Proton ation	b'(2S)-2-acetamidobutanedioic acid'	b'N-Acetyl-L-aspartic acid'	HMDB00 00812	C6H9NO5	C01 042
		175.0480724	0.0004 724	Proton ation	b'(2S)-2-formamidopentanedioic acid'	b'N-Formyl-L-glutamic acid'	HMDB00 03470	C6H9NO5	C01 045
		175.0489408	0.0013 408	Proton ation	b'1-isothiocyanato-5-(methylsulfanyl)pentane'	b'Berteroin'	HMDB00 31577	C7H13NS2	
		175.0480724	0.0004 724	Proton ation	b'2-(2-carboxyacetylamido)propanoic acid'	b'D-N-(Carboxyacetyl)alanine'	HMDB00 39163	C6H9NO5	
		175.0480724	0.0004 724	Proton ation	b'2-amino-3-oxohexanedioic acid'	b'2-Amino-3-oxoadipate'	HMDB00 60273	C6H9NO5	C05 520
		175.0480724	0.0004 724	Proton ation	b'2-aminopropanoyl 2-oxopropaneperoxoate'	b'Alanine pyruvate'	HMDB02 48106	C6H9NO5	
		175.0480724	0.0004 724	Proton ation	b'methyl [(2-methoxy-2-oxoethyl)carbamoyl]formate'	b'Dimethylalanyl glycine'	HMDB02 51540	C6H9NO5	
		175.04557	0.0020 3	Proton ation	b'2-methyl-1,4-dihydroquinoline-4-thione'	b'2-Methylquinoline'	HMDB03 02391	C10H9NS	
3 9	175.04 3	176.0507149	8.51E- 05	Proton ation	b'1-(methylsulfanyl)-1-oxopropan-2-yl propanoate'	b'Methylthio 2-(propanoyloxy)propanoate'	HMDB00 40003	C7H12O3S	
		175.043439	0.0004 39	Redox	b'6-(methylsulfanyl)-2-oxohexanoate'	b'2-oxo-6-methylthiohexanoate'	HMDB03 04083	C7H11O3S	
4 0	176.93 49	177.9432255	0.0005 255	Proton ation	b'(phosphonoxy)phosphonic acid'	b'Pyrophosphate'	HMDB00 00250	H4O7P2	C00 013
4 1	178.01 66	179.0252285	0.0008 285	Proton ation	b'2-amino-3-[(carboxymethyl)sulfanyl]propanoic acid'	b'S-Carboxymethyl-L-cysteine'	HMDB00 29415	C5H9NO4S	
		179.0250249	0.0006	Proton	b'2-[2-(3-chlorophenyl)diazene-1-yl]acetonitrile'	b'2-[(3-	HMDB02	C8H6ClN3	

			249	ation		Chlorophenyl]diazenyl]acetonitrile'	55365		
		178.0185425	0.0019 425	Redox	b'4-chloronaphthalen-1-ol'	b'4-Chloro-1-naphthol'	HMDB02 47127	C10H7ClO	
		178.0145198	0.0020 802	Redox	b'2-amino-2-(3-chloro-4,5-dihydro-1,2-oxazol-5-yl)acetic acid'	b'Acivicin'	HMDB02 47942	CSH7CIN2O3	
4 2	179.05 48	180.0633881	0.0007 881	Proton ation	b'(2R,3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Glucose'	HMDB00 00122	C6H12O6	C00 221
		180.0633881	0.0007 881	Proton ation	b'(2S,3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Galactose'	HMDB00 00143	C6H12O6	C00 984
		180.0633881	0.0007 881	Proton ation	b'(2S,3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Mannose'	HMDB00 00169	C6H12O6	C00 936
		180.0633881	0.0007 881	Proton ation	b'(1R,2R,3r,4S,5S,6s)-cyclohexane-1,2,3,4,5,6-hexol'	b'myo-Inositol'	HMDB00 00211	C6H12O6	C00 137
		180.0633881	0.0007 881	Proton ation	b'(2S,4S,5R)-2,4,5,6-tetrahydroxyhexanoic acid'	b'3-Deoxyarabinohexonic acid'	HMDB00 00346	C6H12O6	
		180.0633881	0.0007 881	Proton ation	b'(2R,3S,4S,5R)-2,5-bis(hydroxymethyl)oxolane-2,3,4-triol'	b'D-Fructose'	HMDB00 00660	C6H12O6	C02 336
		180.0633881	0.0007 881	Proton ation	b'(3S,4S,5R,6S)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'Allose'	HMDB00 01151	C6H12O6	C01 487
		180.0633881	0.0007 881	Proton ation	b'(2R,3S,4R,5S)-2-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'L-Sorbose'	HMDB00 01266	C6H12O6	C08 356
		180.0647255	0.0021 255	Proton ation		b'Paraxanthine'	HMDB00 01860	C7H8N4O2	C13 747
		180.0647255	0.0021 255	Proton ation	b'1,3-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Theophylline'	HMDB00 01889	C7H8N4O2	C07 130
		180.0647255	0.0021	Proton	b'3,7-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Theobromine'	HMDB00	C7H8N4O2	C07

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180.0633881	0.0007 881	Proton ation	b'(2S,3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'alpha-D-Glucose'	HMDB00 03345	C6H12O6	C00 267	
180.0633881	0.0007 881	Proton ation	b'(2R,3S,4S,5R)-2-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Tagatose'	HMDB00 03418	C6H12O6	C00 795	
180.0633881	0.0007 881	Proton ation	b'(2R,3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'beta-D-Galactose'	HMDB00 03449	C6H12O6	C00 962	
180.0633881	0.0007 881	Proton ation	b'(1r,2r,3r,4r,5r,6r)-cyclohexane-1,2,3,4,5,6-hexol'	b'scyllo-Inositol'	HMDB00 06088	C6H12O6	C06 153	
180.0633881	0.0007 881	Proton ation	b'(3S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'L-Gulose'	HMDB00 12326	C6H12O6	C15 923	
180.0633881	0.0007 881	Proton ation	b'2,5-bis(hydroxymethyl)-1,4-dioxane-2,5-diol'	b'Dihydroxyacetone (dimer)'	HMDB00 32222	C6H12O6		
180.0633881	0.0007 881	Proton ation	b'(2R,3S,4R,5S,6S)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'L-Galactose'	HMDB00 33704	C6H12O6	C01 825	
180.0633881	0.0007 881	Proton ation	b'(1R,2R,3R,4R,5S,6S)-cyclohexane-1,2,3,4,5,6-hexol'	b'Levoinositol'	HMDB00 34220	C6H12O6		
180.0633881	0.0007 881	Proton ation	b'(1R,2S,3S,4R,5S,6r)-cyclohexane-1,2,3,4,5,6-hexol'	b'muco-Inositol'	HMDB00 62138	C6H12O6	C06 152	
180.0633881	0.0007 881	Proton ation	b'(2S,3S,4R,5R)-2,3,4,5,6-pentahydroxyhexanal'	b'Glycoprotein-phospho-D-mannose'	HMDB00 62473	C6H12O6		
180.0633881	0.0007 881	Proton ation	b'(1R,2S,3r,4R,5S,6s)-cyclohexane-1,2,3,4,5,6-hexol'	b'epi-Inositol'	HMDB02 40207	C6H12O6		
180.0633881	0.0007 881	Proton ation	b'(1R,2R,3S,4S,5S,6s)-cyclohexane-1,2,3,4,5,6-hexol'	b'neo-Inositol'	HMDB02 40208	C6H12O6		
180.0633881	0.0007	Proton	b'(1R,2R,3S,4S,5S,6S)-cyclohexane-1,2,3,4,5,6-hexol'	b'D-chiro-Inositol'	HMDB02	C6H12O6	C19	

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		180.0633881	0.0007 881	Proton ation	b'(1R,2R,3S,4S,5s,6s)-cyclohexane-1,2,3,4,5,6-hexol'	b'cis-Inositol'	HMDB02 40210	C6H12O6	
		180.0633881	0.0007 881	Proton ation	b'(1R,2R,3S,4R,5S,6S)-cyclohexane-1,2,3,4,5,6-hexol'	b'allo-Inositol'	HMDB02 40211	C6H12O6	
		180.0633881	0.0007 881	Proton ation	b'2,3,4,5,6-pentahydroxyhexanal'	b'(2R,3R,4R,5R)-2,3,4,5,6-Pentahydroxyhexanal'	HMDB02 42534	C6H12O6	
		180.0633881	0.0007 881	Proton ation	b'1,2,4,5,6-pentahydroxyhexan-3-one'	b'(2R,4S,5S)-1,2,4,5,6-Pentahydroxyhexan-3-one'	HMDB02 42761	C6H12O6	C01 383
		180.0633881	0.0007 881	Proton ation	b'1,3,4,5,6-pentahydroxyhexan-2-one'	b'(3R,4R,5R)-1,3,4,5,6-Pentahydroxyhexan-2-one'	HMDB02 46950	C6H12O6	C01 452
		180.0633881	0.0007 881	Proton ation	b'5-(1,2-dihydroxyethyl)oxolane-2,3,4-triol'	b'alpha-D-Galactofuranose'	HMDB02 48203	C6H12O6	
		180.0633881	0.0007 881	Proton ation	b'2,5-bis(hydroxymethyl)oxolane-2,3,4-triol'	b'D-Fructofuranose'	HMDB02 50747	C6H12O6	
		180.0633881	0.0007 881	Proton ation	b'6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Gulose'	HMDB02 50761	C6H12O6	C00 738
		180.0633881	0.0007 881	Proton ation	b'2-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Psicose'	HMDB02 50793	C6H12O6	
		180.0647255	0.0021 255	Proton ation	b'1-[(1H-imidazol-1-yl)amino]pyrrolidine-2,5-dione'	b'Succinylaminoimidazole'	HMDB02 58546	C7H8N4O2	
		180.0633881	0.0007 881	Proton ation	b'(3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'Glucose'	HMDB03 04632	C6H12O6	C00 031
		180.0633881	0.0007 881	Proton ation	b'(2S,3R,4S,5R)-5-[(1R)-1,2-dihydroxyethyl]oxolane-2,3,4-triol'	b'alpha-D-Allofuranose'	HMDB03 04814	C6H12O6	
4	180.04	181.0503944	0.0007	Proton	b'2-amino-4-[hydroxy(methyl)phosphoryl]butanoic acid'	b'Glufosinate'	HMDB02	C5H12NO4P	C05

3	18		944	ation			52799		042
		181.0506324	0.0010 324	Proton ation	b'4-[(2R)-2-carboxy-2-hydroxyethyl]benzen-1-olate'	b'(R+)-3-(4-hydroxyphenyl)lactate'	HMDB03 03993	C9H9O4	
		180.0422587	0.0004 587	Redox	b'3-(4-hydroxyphenyl)-2-oxopropanoic acid'	b'4-Hydroxyphenylpyruvic acid'	HMDB00 00707	C9H8O4	C011 79
		180.0422587	0.0004 587	Redox	b'2-(acetyloxy)benzoic acid'	b'Aspirin'	HMDB00 01879	C9H8O4	C01 405
		180.0422587	0.0004 587	Redox	b'(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid'	b'Caffeic acid'	HMDB00 01964	C9H8O4	C01 481
		180.0422587	0.0004 587	Redox	b'2-(methoxycarbonyl)benzoic acid'	b'Monomethyl phthalate'	HMDB00 02130	C9H8O4	
		180.0422587	0.0004 587	Redox	b'(2Z)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid'	b'cis-Caffeic acid'	HMDB00 03501	C9H8O4	C01 481
		180.0422587	0.0004 587	Redox	b'(2Z)-2-hydroxy-3-(4-hydroxyphenyl)prop-2-enoic acid'	b'2-Hydroxy-3-(4-hydroxyphenyl)propenoic acid'	HMDB00 06915	C9H8O4	C05 350
		180.0422587	0.0004 587	Redox	b'3-(3-hydroxyphenyl)-2-oxopropanoic acid'	b'3-Hydroxyphenylpyruvic acid'	HMDB00 11663	C9H8O4	
		180.0422587	0.0004 587	Redox	b'3-(2,3-dihydroxyphenyl)prop-2-enoic acid'	b'(E)-3-(2,3-Dihydroxyphenyl)-2-propenoic acid'	HMDB00 32057	C9H8O4	C12 623
		180.0422587	0.0004 587	Redox	b'(2E)-3-(3,5-dihydroxyphenyl)prop-2-enoic acid'	b'3,5-Dihydroxycinnamic acid'	HMDB00 32131	C9H8O4	
4	180.06	181.0738932	0.0005 068	Proton ation	b'(2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid'	b'L-Tyrosine'	HMDB00 00158	C9H11NO3	C00 082
		181.0738932	0.0005 068	Proton ation	b'4-hydroxy-4-(pyridin-3-yl)butanoic acid'	b'4-Hydroxy-4-(3-pyridyl)-butanoic acid'	HMDB00 01119	C9H11NO3	C19 579
		181.0738932	0.0005	Proton	b'(2S)-2-amino-3-hydroxy-3-phenylpropanoic acid'	b'L-Threo-3-Phenylserine'	HMDB00	C9H11NO3	

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		181.0738932	0.0005 068	Proton ation	b'3-amino-3-(4-hydroxyphenyl)propanoic acid'	b'Beta-Tyrosine'	HMDB00 03831	C9H11NO3	C04 368
		181.0738932	0.0005 068	Proton ation	b'2-amino-3-(2-hydroxyphenyl)propanoic acid'	b'o-Tyrosine'	HMDB00 06050	C9H11NO3	
		181.0738932	0.0005 068	Proton ation	b'(2S)-2-amino-3-(3-hydroxyphenyl)propanoic acid'	b'Meta-Tyrosine'	HMDB00 59720	C9H11NO3	
		181.0738932	0.0005 068	Proton ation	b'1,2,3,4-tetrahydroisoquinoline-4,6,7-triol'	b'4,6,7-Trihydroxy-1,2,3,4-tetrahydroisoquinoline'	HMDB00 60280	C9H11NO3	
		181.0738932	0.0005 068	Proton ation	b'2-amino-3-hydroxy-3-phenylpropanoic acid'	b'2-Amino-3-hydroxy-3-phenylpropanoic acid'	HMDB02 44981	C9H11NO3	
		181.0738932	0.0005 068	Proton ation	b'2-amino-3-(4-hydroxyphenyl)propanoic acid'	b'D-Tyrosine'	HMDB02 50803	C9H11NO3	C01 536
		180.0660682	0.0005 318	Redox	b'(3,6-dihydroxy-1-methyl-2,3-dihydro-1H-indol-5-yl)oxidanyl'	b'Adrenochrome o-semiquinone'	HMDB00 12883	C9H10NO3	
		180.0687483	0.0021 483	Redox	b'1,10-phenanthroline'	b'1,10-Phenanthroline'	HMDB02 44053	C12H8N2	C00 604
		180.0687483	0.0021 483	Redox	b'1,7-phenanthroline'	b'1,7-Phenanthroline'	HMDB02 44247	C12H8N2	
		180.0687483	0.0021 483	Redox	b'benzo[c]cinnoline'	b'Benzo[c]cinnoline'	HMDB02 49005	C12H8N2	
		180.0687483	0.0021 483	Redox	b'phenazine'	b'Phenazine'	HMDB02 56395	C12H8N2	
4 5	181.96 5	182.9711102	0.0016 898	Proton ation	b'3-hydroxy-2-(phosphonatoxy)propanoate'	b'2-phospho-D-glycerate'	HMDB03 04085	C3H4O7P	
4	182.01	183.0201431	0.0005	Proton	b'(2S)-2-amino-4-sulfobutanoic acid'	b'L-Homocysteic acid'	HMDB00	C4H9NO5S	C16

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		183.0214805	0.0018 805	Proton ation	b'2-imino-6-sulfanyl-3,9-dihydro-2H-purin-8-ol'	b'8-Hydroxythioguanine'	HMDB00 60804	C5H5N5OS	
		183.0201436	0.0005 436	Proton ation	b'2-amino-4-sulfobutanoic acid'	b'DL-Homocysteic acid'	HMDB02 51520	C4H9NO5S	
		182.0109759	0.0008 241	Redox	b'[(carbamoylamino)sulfonyl]urea'	b"N,N"-Sulfonylbisurea"	HMDB02 55277	C2H6N4O4S	
4 7	182.04	183.0531578	0.0007 578	Proton ation	b'3-hydroxy-5-(hydroxymethyl)-2-methylpyridine-4-carboxylic acid'	b'4-Pyridoxic acid'	HMDB00 00017	C8H9NO4	C00 847
		183.0531578	0.0007 578	Proton ation	b'2-amino-2-(3,5-dihydroxyphenyl)acetic acid'	b'3,5-Dihydroxyphenylglycine'	HMDB02 43702	C8H9NO4	
		183.0531578	0.0007 578	Proton ation	b'2-[(3,5-dihydroxyphenyl)amino]acetic acid'	b'2-[(3,5-Dihydroxyphenyl)amino]acetic acid'	HMDB02 44908	C8H9NO4	
		183.0544952	0.0020 952	Proton ation	b'3,4,5,13,14-pentaaazatricyclo[7.5.0.0 ⁰]{2,6}]tetradeca-1(14),2,4,6,8,10,12-heptaene'	b'triazolobenzodiazepine'	HMDB02 59157	C9H5N5	
	46	182.0439901	0.0006 099	Redox	b'3-methyl-2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'	b'3-Methyluric acid'	HMDB00 01970	C6H6N4O3	
		182.0439901	0.0006 099	Redox	b'9-methyl-2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'	b'9-Methyluric acid'	HMDB00 01973	C6H6N4O3	
		182.0439901	0.0006 099	Redox	b'1-methyl-2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'	b'1-Methyluric acid'	HMDB00 03099	C6H6N4O3	C16 359
		182.0439901	0.0006 099	Redox	b'7-methyl-7H-purine-2,6,8-triol'	b'7-Methyluric acid'	HMDB00 11107	C6H6N4O3	C16 355
4 8	184.00 06	185.0089235	0.0005 235	Proton ation	b'(2S)-2-amino-3-(phosphonoxy)propanoic acid'	b'Phosphoserine'	HMDB00 00272	C3H8NO6P	C01 005
		185.0089235	0.0005	Proton	b'2-amino-3-(phosphonoxy)propanoic acid'	b'DL-O-Phosphoserine'	HMDB00	C3H8NO6P	C01

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		185.0089235	0.0005 235	Proton ation	b'(2R)-2-amino-3-(phosphonoxy)propanoic acid'	b'3-phospho-L-serine'	HMDB03 04154	C3H8NO6P	C02 532
		184.0007879	0.0001 879	Redox	b'4-oxo-4H-pyran-2,6-dicarboxylic acid'	b'Chelidonic acid'	HMDB02 49899	C7H4O6	C08 476
4 9	184.98 44	185.9929391	0.0007 391	Proton ation	b'3-hydroxy-2-(phosphonoxy)propanoic acid'	b'2-Phosphoglyceric acid'	HMDB00 00362	C3H7O7P	
		185.9929391	0.0007 391	Proton ation	b'2-hydroxy-3-(phosphonoxy)propanoic acid'	b'3-Phosphoglyceric acid'	HMDB00 00807	C3H7O7P	C00 597
		185.9929391	0.0007 391	Proton ation	b'(2R)-3-hydroxy-2-(phosphonoxy)propanoic acid'	b'2-Phospho-D-glyceric acid'	HMDB00 03391	C3H7O7P	C00 631
		185.9944531	0.0022 531	Proton ation	b'8-chloro-2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'8-Chloroxanthine'	HMDB00 06039	C5H3ClN4O2	
		185.9929391	0.0007 391	Proton ation	b'(2R)-2-hydroxy-3-(phosphonoxy)propanoic acid'	b'D-Glycerate 3-phosphate'	HMDB00 60180	C3H7O7P	C00 197
		185.9938075	0.0016 075	Proton ation	b'O,O-diethyl sulfanylphosphonothioate'	b'Diethyldithiophosphate'	HMDB00 61736	C4H11O2PS2	
		185.9904192	0.0017 808	Proton ation	b'hexafluorobenzene'	b'Hexafluorobenzene'	HMDB02 53133	C6F6	
5 0	185.96 19	186.9704025	0.0007 025	Proton ation	b'5,7-dichloropyrazolo[1,5-a]pyrimidine'	b'5,7-Dichloropyrazolo[1,5-a]pyrimidine'	HMDB02 46869	C6H3Cl2N3	
5 1	189.04 48	189.0425931	0.0022 069	Redox		b'Kynurenic acid'	HMDB00 00715	C10H7NO3	C01 717
		189.0425931	0.0022 069	Redox	b'5-nitro-1aH,7aH-naphtho[1,2-b]oxirene'	b'1-Nitronaphthalene-5,6-oxide'	HMDB00 60331	C10H7NO3	C14 800
		189.0425931	0.0022	Redox	b'7-nitro-1aH,7bH-naphtho[1,2-b]oxirene'	b'1-Nitronaphthalene-7,8-oxide'	HMDB00	C10H7NO3	C14

5	191.01		069					60332		802
		189.0425931	0.0022 069	Redox	b'2-(1H-indol-3-yl)-2-oxoacetic acid'	b'3-Indoleglyoxylic acid'	HMDB02 42143	C10H7NO3		
		189.0425931	0.0022 069	Redox	b'2-oxo-1,2-dihydroquinoline-3-carboxylic acid'	b'2-Hydroxyquinoline-3-carboxylic acid'	HMDB02 45167	C10H7NO3		
		189.0425931	0.0022 069	Redox	b'4-oxo-1,4-dihydroquinoline-3-carboxylic acid'	b'4-Oxo-1,4-dihydroquinoline-3-carboxylic acid'	HMDB02 46559	C10H7NO3		
		189.0425931	0.0022 069	Redox	b'2-cyano-3-(4-hydroxyphenyl)prop-2-enoic acid'	b'alpha-Cyano-4-hydroxycinnamate'	HMDB02 48196	C10H7NO3		
	87	192.0270026	0.0005 026	Proton ation	b'2-hydroxypropane-1,2,3-tricarboxylic acid'	b'Citric acid'	HMDB00 00094	C6H8O7	C00 158	
		192.0270026	0.0005 026	Proton ation	b'1-hydroxypropane-1,2,3-tricarboxylic acid'	b'Isocitric acid'	HMDB00 00193	C6H8O7	C00 311	
		192.0270026	0.0005 026	Proton ation	b'(1R,2S)-1-hydroxypropane-1,2,3-tricarboxylic acid'	b'D-threo-Isocitric acid'	HMDB00 01874	C6H8O7	C00 451	
		192.0270026	0.0005 026	Proton ation	b'(4R,5S)-4,5,6-trihydroxy-2,3-dioxohexanoic acid'	b'Diketogulonic acid'	HMDB00 05971	C6H8O7	C04 575	
		192.0270026	0.0005 026	Proton ation	b'(5S)-4,5,6-trihydroxy-2,3-dioxohexanoic acid'	b'2,3-Diketo-L-gulonate'	HMDB00 06511	C6H8O7	C04 575	
		192.0270026	0.0005 026	Proton ation	b'(1R,2R)-1-hydroxypropane-1,2,3-tricarboxylic acid'	b'(1R,2R)-Isocitric acid'	HMDB00 33717	C6H8O7	C04 617	
		192.0245002	0.0019 998	Proton ation	b'(5E)-5-[(5-methylthiophen-2-yl)methylidene]-2,5-dihydrofuran-2-one'	b'(Z)-5-[(5-Methyl-2-thienyl)methylene]-2(5H)-furanone'	HMDB00 33845	C10H8O2S		
		192.0270026	0.0005 026	Proton ation	b'(2S)-2-[(2S,3R,4R)-3,4-dihydroxy-5-oxoxolan-2-yl]-2-hydroxyacetic acid'	b'D-Glucaro-1,4-lactone'	HMDB00 41862	C6H8O7		
		192.0270026	0.0005	Proton	b'4,5,6-trihydroxy-2,3-dioxohexanoic acid'	b'2,3-diketogulonate'	HMDB00	C6H8O7		

			026	ation			62803		
		192.0270026	0.0005 026	Proton ation	b'3,3,3a,6-tetrahydroxy-hexahydrofuro[3,2-b]furan-2-one'	b'dehydroascorbate (bicyclic form)'	HMDB03 04326	C6H8O7	
		191.0194129	0.0007 129	Redox	b'2-(trifluoromethyl)pyridine-4-carboxylic acid'	b'2-(Trifluoromethyl)isonicotinic acid'	HMDB02 44959	C7H4F3NO2	
		191.0197261	0.0010 261	Redox	b'4,5,6-trihydroxy-2,3-dioxohexanoate'	b'2,3-dioxo-L-gulonate'	HMDB03 04040	C6H7O7	
		191.0197261	0.0010 261	Redox	b'3,4-dihydroxy-5-(hydroxymethyl)-2-oxooxolane-3-carboxylate'	b'2-carboxy-L-xylonolactone'	HMDB03 04063	C6H7O7	
5 3	191.06 03	192.0687483	0.0006 483	Proton ation	b'2H-benzof[flisoindole-1-carbonitrile'	b'2H-Benzo[F]isoindole-1-carbonitrile'	HMDB02 45761	C13H8N2	
		191.0582432	0.0020 568	Redox	b'2-(5-hydroxy-1H-indol-3-yl)acetic acid'	b'5-Hydroxyindoleacetic acid'	HMDB00 00763	C10H9NO3	C05 635
		191.061614	0.0013 14	Redox	b'(2S)-2-acetamido-4-(methylsulfonyl)butanoic acid'	b'N-Acetyl-L-methionine'	HMDB00 11745	C7H13NO3S	C02 712
		191.0582432	0.0020 568	Redox	b'2-(2-hydroxy-3H-indol-3-yl)acetic acid'	b'xi-2,3-Dihydro-2-oxo-1H-indole-3-acetic acid'	HMDB00 35514	C10H9NO3	
		191.0582432	0.0020 568	Redox	b'4-hydroxy-5-phenyl-5,6-dihydro-2H-1,3-oxazin-2-one'	b'5-Phenyl-1,3-oxazinane-2,4-dione'	HMDB00 60400	C10H9NO3	C16 596
		191.0582432	0.0020 568	Redox		b'5-Methoxyindole-2-carboxylic acid'	HMDB02 46823	C10H9NO3	
		191.0616145	0.0013 145	Redox	b'ethyl 2-acetamido-3-sulfanylpropanoate'	b'L-Cysteine, N-acetyl-, ethyl ester'	HMDB02 47004	C7H13NO3S	
		191.0616145	0.0013 145	Redox	b'2-acetamido-3-methyl-3-sulfanylbutanoic acid'	b'N-Acetyl-dl-penicillamine'	HMDB02 55055	C7H13NO3S	
		191.0616145	0.0013	Redox	b'2-(2-methylpropanamido)-3-sulfanylpropanoic acid'	b'N-Isobutyryl-L-cysteine'	HMDB02	C7H13NO3S	

5 4	192.06 36		145				55162		
		191.0582432	0.0020 568	Redox	b'2H,5H,6H,7H,8H-[1,3]dioxolo[4,5-g]isoquinolin-5-one'	b'Noroxyhydrastinine'	HMDB02 55749	C10H9NO3	
		191.0582432	0.0020 568	Redox	b'2-(3-hydroxy-1H-indol-2-yl)acetic acid'	b'2-(3-Hydroxy-1H-indol-2-yl)acetic acid'	HMDB02 57584	C10H9NO3	
		191.0582432	0.0020 568	Redox	b'2-(5-hydroxy-1H-indol-2-yl)acetic acid'	b'2-(5-Hydroxy-1H-indol-2-yl)acetic acid'	HMDB02 57587	C10H9NO3	
		191.0582432	0.0020 568	Redox	b'1H-indol-3-yl 2-hydroxyacetate'	b'1H-Indol-3-yl 2-hydroxyacetate'	HMDB02 57908	C10H9NO3	
	192.06 36	193.0738932	0.0024 932	Proton ation	b'2-(2-phenylacetamido)acetic acid'	b'Phenylacetyl glycine'	HMDB00 00821	C10H11NO3	C05 598
		193.0738932	0.0024 932	Proton ation	b'methyl 2-(phenylformamido)acetate'	b'Methyl hippurate'	HMDB00 00859	C10H11NO3	
		193.0738932	0.0024 932	Proton ation	b'2-[(2-methylphenyl)formamido]acetic acid'	b'2-Methylhippuric acid'	HMDB00 11723	C10H11NO3	C01 586
		193.0738932	0.0024 932	Proton ation	b'2-[(3-methylphenyl)formamido]acetic acid'	b'm-Methylhippuric acid'	HMDB00 13245	C10H11NO3	
		193.0738932	0.0024 932	Proton ation	b'2-[(4-methylphenyl)formamido]acetic acid'	b'p-Methylhippuric acid'	HMDB00 13292	C10H11NO3	
		193.0738932	0.0024 932	Proton ation	b'methyl 2-acetamidobenzoate'	b'Methyl n-acetylanthranilate'	HMDB00 32388	C10H11NO3	C06 332
		193.0738932	0.0024 932	Proton ation	b'3-(phenylformamido)propanoic acid'	b'Betamipron'	HMDB00 34250	C10H11NO3	
		193.0738932	0.0024 932	Proton ation	b'3-(C-hydroxycarbonimidoyloxy)-2-phenylpropanal'	b'3-Carbamoyl-2-phenylpropionaldehyde'	HMDB00 60366	C10H11NO3	C16 587
		193.0738932	0.0024	Proton	b'5-phenyl-5,6-dihydro-4H-1,3-oxazine-2,4-diol'	b'4-Hydroxy-5-phenyltetrahydro-1,3-	HMDB00	C10H11NO3	C16

			932	ation		oxazin-2-one'	60389		595
		193.0738932	0.0024 932	Proton ation	b'3-(phenyl-C-hydroxycarbonimidoyl)propanoic acid'	b'4-Anilino-4-oxobutanoic acid'	HMDB00 60758	C10H11NO3	
		193.0738932	0.0024 932	Proton ation	b'(2S)-2-formamido-3-phenylpropanoic acid'	b'N-Formylphenylalanine'	HMDB02 40317	C10H11NO3	
		193.0738932	0.0024 932	Proton ation	b'2-[4-[(1-hydroxyethylidene)amino]phenyl]acetic acid'	b'Actarit'	HMDB02 47976	C10H11NO3	
		193.0738932	0.0024 932	Proton ation	b'2-(phenylformamido)propanoic acid'	b'n-benzoyl-d-alanine'	HMDB02 55085	C10H11NO3	
		193.0738932	0.0024 932	Proton ation	b'2-formamido-3-phenylpropanoic acid'	b'N-Formyl-dl-phenylalanine'	HMDB02 55143	C10H11NO3	
		192.0633881	0.0002 119	Redox		b'Quinic acid'	HMDB00 03072	C7H12O6	C00 296
		192.0608857	0.0027 143	Redox	b'(2E)-2-[(methylsulfanyl)methyl]-3-phenylprop-2-enal'	b'2-(Methylthiomethyl)-3-phenyl-2-propenal'	HMDB00 37166	C11H12OS	
		192.0642575	0.0006 575	Redox	b'6,8-disulfanyloctanal'	b'6,8-Bis(sulfanyl)octanal'	HMDB02 58126	C8H16OS2	
		192.0633881	0.0002 119	Redox	b'(2R,3R)-2,3-dihydroxy-4-oxo-4-(propan-2-yloxy)butanoic acid'	b'Isopropyl tartaric acid'	HMDB03 02348	C7H12O6	
5 5	193.07 56	194.0843983	0.0009 983	Proton ation	b'acridin-1-amine'	b'1-Aminoacridine'	HMDB02 43819	C13H10N2	
		194.0843983	0.0009 983	Proton ation	b'2-phenylimidazo[1,2-a]pyridine'	b'2-Phenylimidazo[1,2-a]pyridine'	HMDB02 45292	C13H10N2	
		194.0843983	0.0009 983	Proton ation	b'acridin-9-amine'	b'9-Aminoacridine'	HMDB02 47578	C13H10N2	
		194.0843983	0.0009	Proton	b'2-cyclopropylpyrrolo[2,3-g]indole'	b'Cyclopropylpyrroloindole'	HMDB02	C13H10N2	

			983	ation			50679		
		194.0843983	0.0009 983	Proton ation	b'8,9-diazatricyclo[9.4.0.0°{2,7}]pentadeca-1(15),2,4,6,9,11,13-heptaene'	b'Dibenzodiazepine'	HMDB02 51163	C13H10N2	
		193.077264	0.0016 64	Redox	b'(2R)-2-amino-3-(butane-1-sulfinyl)propanoic acid'	b'S-Butylcysteine sulfoxide'	HMDB03 02178	C7H15NO3S	
5 6	193.09 24	194.0976656	0.0025 344	Proton ation	b'octane-1-sulfonic acid'	b'1-Octanesulfonic acid'	HMDB02 43978	C8H18O3S	
		193.0950226	0.0026 226	Redox	b'2,6-bis(hydroxymethyl)piperidine-3,4,5-triol'	b'(2r,3r,5s,6r)-2,6-Bis(hydroxymethyl)piperidine-3,4,5-triol'	HMDB02 42543	C7H15NO5	
		193.0950226	0.0026 226	Redox	b'3,4,5,6-tetrahydroxy-2-(methylamino)hexanal'	b'N-Methylglucosamine'	HMDB02 55188	C7H15NO5	
5 7	194.05 98	195.0684139	0.0008 139	Proton ation	b'9H-carbazole-3-carbaldehyde'	b'9H-Carbazole-3-carboxaldehyde'	HMDB00 29743	C13H9NO	
		195.0684139	0.0008 139	Proton ation	b'2-oxa-9-azatricyclo[9.4.0.0°\xc2\xb3,\xc2\xb3,\xc2\xb3]pentadeca-1(15),3,5,7,9,11,13-heptaene'	b'Dibenz[b,f][1,4]oxazepine'	HMDB02 45702	C13H9NO	
		195.0684139	0.0008 139	Proton ation	b'9,10-dihydroacridin-9-one'	b'Acridone'	HMDB02 46984	C13H9NO	C20 142
		195.0684139	0.0008 139	Proton ation	b'phenanthridin-6-ol'	b'6(5H)-Phenanthridinone'	HMDB02 47116	C13H9NO	
		195.0695567	0.0019 567	Proton ation	b'10-fluoro-2,8-dioxa-5-azatricyclo[7.4.0.0°{3,7}]trideca-1(9),10,12-triene'	b'Fluparoxan'	HMDB02 52395	C10H10FNO2	
		195.0684139	0.0008 139	Proton ation	b'phenanthridin-1-ol'	b'Phenanthridinol'	HMDB02 56393	C13H9NO	
		194.0579088	0.0018 912	Redox	b'(2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid'	b'Ferulic acid'	HMDB00 00954	C10H10O4	C01 494

		194.0579088	0.0018 912	Redox	b'(2E)-3-(3-hydroxy-4-methoxyphenyl)prop-2-enoic acid'	b'Isoferulic acid'	HMDB00 00955	C10H10O4	C10 470
		194.0579088	0.0018 912	Redox	b'2-(ethoxycarbonyl)benzoic acid'	b'Monoethyl phthalate'	HMDB00 02120	C10H10O4	
		194.0579088	0.0018 912	Redox	b'4-formyl-2-methoxyphenyl acetate'	b'Vanillin acetate'	HMDB00 29663	C10H10O4	
		194.0579088	0.0018 912	Redox	b'4,8-dihydroxy-3-methyl-3,4-dihydro-1H-2-benzopyran-1-one'	b'(-)-trans-3,4-Dihydro-4,8-dihydroxy-3-methyl-1H-2-benzopyran-1-one'	HMDB00 30765	C10H10O4	
		194.0579088	0.0018 912	Redox	b'2H-1,3-benzodioxol-5-ylmethyl acetate'	b'Piperonyl acetate'	HMDB00 32614	C10H10O4	
		194.0579088	0.0018 912	Redox	b'6,7-dimethoxy-1,3-dihydro-2-benzofuran-1-one'	b'Meconine'	HMDB00 32652	C10H10O4	
		194.0579088	0.0018 912	Redox	b'(2E)-3-(2-hydroxy-3-methoxyphenyl)prop-2-enoic acid'	b'3-(2-Hydroxy-3-methoxyphenyl)-2-propenoic acid'	HMDB00 37644	C10H10O4	
		194.0579088	0.0018 912	Redox	b'(3-{4-[3-(hydroxymethyl)oxiran-2-yl]buta-1,3-diyn-1-yl}oxiran-2-yl)methanol'	b'Repandiol'	HMDB00 39606	C10H10O4	
		194.0579088	0.0018 912	Redox	b'3-(benzyloxy)-3-oxopropanoic acid'	b'mono-Benzyl malonate'	HMDB00 59721	C10H10O4	
		194.0579088	0.0018 912	Redox	b'methyl (2E)-3-(2,5-dihydroxyphenyl)prop-2-enoate'	b'2,5-Dihydroxycinnamic acid methyl ester'	HMDB00 61686	C10H10O4	
		194.0579088	0.0018 912	Redox	b'(2Z)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid'	b'cis-Ferulic acid'	HMDB02 40705	C10H10O4	
		194.0579088	0.0018 912	Redox	b'methyl 3-(3,4-dihydroxyphenyl)prop-2-enoate'	b'Methyl 3,4-dihydroxycinnamate'	HMDB02 46032	C10H10O4	
		194.0579088	0.0018 912	Redox	b'1,2-dimethyl benzene-1,2-dicarboxylate'	b'Dimethyl phthalate'	HMDB02 51388	C10H10O4	C112 33

5 8	194.07	194.0579088	0.0018 912	Redox	b'3-(3-hydroxy-4-methoxyphenyl)prop-2-enoic acid'	b'cis-Isoferulic acid'	HMDB02 59693	C10H10O4	
		194.0579088	0.0018 912	Redox	b'6,8-dihydroxy-3-methyl-3,4-dihydro-1H-2-benzopyran-1-one'	b'(R)-3,4-Dihydro-6,8-dihydroxy-3-methyl-1H-2-benzopyran-1-one'	HMDB03 03675	C10H10O4	
		194.0579088	0.0018 912	Redox	b'3-(3,4-dihydroxy-5-methoxyphenyl)prop-2-enal'	b'5-hydroxy-coniferaldehyde'	HMDB03 04215	C10H10O4	
	92	195.0895433	0.0025 433	Proton ation	b'(2S)-2-amino-3-(4-hydroxyphenyl)-2-methylpropanoic acid'	b'Metyrosine'	HMDB00 14903	C10H13NO3	C07 921
		195.0895433	0.0025 433	Proton ation	b'methyl (2S)-2-amino-3-(4-hydroxyphenyl)propanoate'	b'Tyrosine methylester'	HMDB00 29217	C10H13NO3	C03 404
		195.0895433	0.0025 433	Proton ation	b'N-[2-(3,4-dihydroxyphenyl)ethyl]ethanimidic acid'	b'N-Acetyldopamine'	HMDB00 41943	C10H13NO3	
		195.0895433	0.0025 433	Proton ation	b'2-methyl-1,2,3,4-tetrahydroisoquinoline-4,6,7-triol'	b'N-methyl-4,6,7-trihydroxy-1,2,3,4-tetrahydroisoquinoline'	HMDB00 60065	C10H13NO3	
		195.0895433	0.0025 433	Proton ation	b'3-(C-hydroxycarbonimidoyloxy)-2-phenylpropan-1-ol'	b'2-Phenyl-1,3-propanediol monocarbamate'	HMDB00 60351	C10H13NO3	C16 586
		195.0895433	0.0025 433	Proton ation	b'2-amino-3-(4-hydroxyphenyl)-2-methylpropanoic acid'	b'Racemetirosine'	HMDB02 47174	C10H13NO3	
		195.0895433	0.0025 433	Proton ation	b'2-amino-3-(3-hydroxyphenyl)-2-methylpropanoic acid'	b'alpha-Methyl-m-tyrosine'	HMDB02 48232	C10H13NO3	C118 20
		195.0895433	0.0025 433	Proton ation	b'3-amino-2-hydroxy-4-phenylbutanoic acid'	b'3-Amino-2-hydroxy-4-phenylbutanoic acid'	HMDB02 56443	C10H13NO3	
		195.0895433	0.0025 433	Proton ation	b'5-(2-aminopropyl)-2-hydroxybenzoic acid'	b'5-[(2R)-2-Aminopropyl]-2-hydroxybenzoic acid'	HMDB02 57825	C10H13NO3	
		195.0895433	0.0025 433	Proton ation	b'2-(2-aminopropyl)-5-hydroxybenzoic acid'	b'2-[(2R)-2-Aminopropyl]-5-hydroxybenzoic acid'	HMDB02 57865	C10H13NO3	

		194.0803756	0.0011 756	Redox	b'1,3,7-trimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Caffeine'	HMDB00 01847	C8H10N4O2	C07 481
		194.0803756	0.0011 756	Redox	b'3-propyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Enprofylline'	HMDB00 14962	C8H10N4O2	
		194.0790382	0.0001 618	Redox	b'(1R,2R,3R,4R,5S,6R)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'D-4-O-Methyl-myo-inositol'	HMDB00 29915	C7H14O6	C06 353
		194.0790382	0.0001 618	Redox	b'(2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-methoxyoxane-3,4,5-triol'	b'Methyl beta-D-glucopyranoside'	HMDB00 29965	C7H14O6	
		194.0790382	0.0001 618	Redox	b'(1R,2R,3S,4S,5R,6S)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'(-)-Bornesitol'	HMDB00 31437	C7H14O6	C03 659
		194.0790382	0.0001 618	Redox	b'(1R,2S,3r,4R,5S,6r)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'Sequoyitol'	HMDB00 31449	C7H14O6	C03 365
		194.0790382	0.0001 618	Redox	b'(1r,2R,3S,4s,5R,6S)-1-methylcyclohexane-1,2,3,4,5,6-hexol'	b'Mytilitol'	HMDB00 33816	C7H14O6	
		194.0790382	0.0001 618	Redox	b'(1R,2S,3R,4S,5S,6S)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'D-Pinitol'	HMDB00 34219	C7H14O6	C03 844
		194.0790382	0.0001 618	Redox	b'(1R,2S,3S,4S,5R,6R)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'L-Quebrachitol'	HMDB00 34221	C7H14O6	C08 257
		194.0799066	0.0007 066	Redox	b'3-[(3-sulfanylbutan-2-yl)sulfanyl]butan-2-ol'	b'3-[(2-Mercapto-1-methylpropyl)thio]- 2-butanol'	HMDB00 37295	C8H18OS2	
		194.0790382	0.0001 618	Redox	b'(1S,2R,3R,4R,5S,6S)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'1D-5-O-Methyl-chiro-inositol'	HMDB00 62564	C7H14O6	
		194.0790382	0.0001 618	Redox	b'3,4,5,6,7-pentahydroxyheptan-2-one'	b'1-Deoxy-D-manno-heptulose'	HMDB02 43861	C7H14O6	
		194.0790382	0.0001 618	Redox	b'2,4,5,6-tetrahydroxy-3-methoxyhexanal'	b'3-O-Methyl-d-glucose'	HMDB02 45931	C7H14O6	

5	195.06	194.0790382	0.0001 618	Redox	b'1,4,5,6-tetrahydroxy-3-methoxyhexan-2-one'	b'3-O-Methyl-D-fructose'	HMDB02 45957	C7H14O6	
		194.0790382	0.0001 618	Redox	b'6-(hydroxymethyl)-4-methoxyoxane-2,3,5-triol'	b'3-O-Methyl-D-glucopyranose'	HMDB02 45958	C7H14O6	
		194.0790382	0.0001 618	Redox	b'2-(hydroxymethyl)-6-methoxyoxane-3,4,5-triol'	b'Methyl alpha-D-galactopyranoside'	HMDB02 46173	C7H14O6	
		194.0790382	0.0001 618	Redox	b'1,2,3,5,6-pentahydroxyheptan-4-one'	b'(2R,3R,5S)-1,2,3,5,6-Pentahydroxyheptan-4-one'	HMDB02 55312	C7H14O6	
		194.0790382	0.0001 618	Redox	b'(1R,2S,4S,5S)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'D-ononitol'	HMDB03 04321	C7H14O6	
	33	196.0735589	0.0024 589	Proton ation	b'2-(3,4-dimethoxyphenyl)acetic acid'	b'Homoveratric acid'	HMDB00 00434	C10H12O4	
		196.0735589	0.0024 589	Proton ation	b'1-(2-hydroxy-4,6-dimethoxyphenyl)ethan-1-one'	b'Xanthoxylin'	HMDB00 29645	C10H12O4	C10 726
		196.0735589	0.0024 589	Proton ation	b'2,4,5-trimethoxybenzaldehyde'	b'2,4,5-Trimethoxybenzaldehyde'	HMDB00 29648	C10H12O4	
		196.0735589	0.0024 589	Proton ation	b'3-(2H-1,3-benzodioxol-5-yl)propane-1,2-diol'	b'(+)-3-(3,4-Methylenedioxyphenyl)-1,2-propanediol'	HMDB00 30571	C10H12O4	
		196.0735589	0.0024 589	Proton ation	b'2-methyl-4-oxo-4H-pyran-3-yl 2-methylpropanoate'	b'Maltol isobutyrate'	HMDB00 32365	C10H12O4	
		196.0735589	0.0024 589	Proton ation	b'5-(furan-3-yl)-2-methyl-5-oxopentanoic acid'	b'(S)-Batatic acid'	HMDB00 35721	C10H12O4	
		196.0735589	0.0024 589	Proton ation	b'1-(2,4,5-trihydroxyphenyl)butan-1-one'	b'1-(2,4,5-Trihydroxyphenyl)-1-butanone'	HMDB00 37177	C10H12O4	
		196.0735589	0.0024 589	Proton ation	b'2-hydroxy-3-(4-methoxyphenyl)propanoic acid'	b'2-Hydroxy-3-(4-methoxyphenyl)propanoic acid'	HMDB00 39427	C10H12O4	

196.0735589	0.0024 589	Proton ation	b'2-(4-methoxyphenoxy)propanoic acid'	b'(S)-2-(4-Methoxyphenoxy)propanoic acid'	HMDB00 40256	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'3-butanoyl-4-hydroxy-6-methyl-2H-pyran-2-one'	b'4-Hydroxy-6-methyl-3-(1-oxobutyl)-2H-pyran-2-one'	HMDB00 40637	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'5-[(1E)-3-hydroxyprop-1-en-1-yl]-3-methoxybenzene-1,2-diol'	b'5-Hydroxyconiferyl alcohol'	HMDB00 60398	C10H12O4	C12 205
196.0735589	0.0024 589	Proton ation	b'2-hydroxy-3-(3-hydroxyphenyl)-2-methylpropanoic acid'	b'3-(3-Hydroxyphenyl)-2-methylactic acid'	HMDB00 60733	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'3-(3,4-dihydroxyphenyl)-2-methylpropanoic acid'	b'3-(3,4-Dihydroxyphenyl)-2-methylpropionic acid'	HMDB00 60735	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'3-(4-hydroxy-3-methoxyphenyl)propanoic acid'	b'Dihydroferulic acid'	HMDB00 62121	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'3-(3-hydroxy-4-methoxyphenyl)propanoic acid'	b'3-(3-hydroxy-4-methoxyphenyl)propanoic acid'	HMDB01 31138	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'2,6-dimethyl-4,10-dioxatricyclo[5.2.1.0'xc2'xb2,\xc2'x81'xb6]decane-3,5-dione'	b'Cantharidin'	HMDB02 49592	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'2-(3,4-dihydroxyphenyl)ethyl acetate'	b'Hydroxytyrosol Acetate'	HMDB02 53298	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'3-(5-methoxy-4-oxocyclohex-2-en-1-yl)prop-2-enoic acid'	b'3-(5-Methoxy-4-oxocyclohex-2-en-1-yl)prop-2-enoic acid'	HMDB02 55409	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'4,4,4-trihydroxy-1-phenylbutan-1-one'	b'trihydroxybutyrophenone'	HMDB02 59219	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'ethyl 4-hydroxy-3-methoxybenzoate'	b'4-hydroxy-3-methoxybenzoic acid ethyl ester'	HMDB03 03913	C10H12O4	
196.0735589	0.0024 589	Proton ation	b'2-methyl-1-(2,4,6-trihydroxyphenyl)propan-1-one'	b'phlorisobutyrophenone'	HMDB03 04461	C10H12O4	C07 351

60	195.0823	196.0921858	0.0020858	Protonation	b'1-(thiophen-2-yl)heptan-1-one'	b'1-(2-Thienyl)-1-heptanone'	HMDB0040241	C11H16OS	
		196.088815	0.001285	Protonation	b'(2R,3S)-2,3-diphenyloxirane'	b'Cis-stilbene oxide'	HMDB0059631	C14H12O	C16014
		196.088815	0.001285	Protonation	b'1,2-diphenylethan-1-one'	b'Deoxybenzoin'	HMDB0244095	C14H12O	
		196.088815	0.001285	Protonation	b'4-(2-phenylethenyl)phenol'	b'4-Hydroxystilbene'	HMDB0246467	C14H12O	
		196.088815	0.001285	Protonation	b'2-(2-phenylethenyl)phenol'	b'hydroxystilbene'	HMDB0253294	C14H12O	
		196.088815	0.001285	Protonation	b'2,3-diphenyloxirane'	b'Stilbene oxide'	HMDB0258501	C14H12O	
		195.0814772	0.0008228	Redox	b'8-chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine'	b'8-Chloro-1-methyl-2,3,4,5-tetrahydro-1H-benzo[d]azepine'	HMDB0247137	C11H14ClN	
		195.0814772	0.0008228	Redox	b'6-chloro-3-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine'	b'benalfocin'	HMDB0248942	C11H14ClN	C10970
61	195.9906	196.9955004	0.0028996	Protonation	b'(2S)-2-amino-4-(methylsclanyl)butanoic acid'	b'Selenomethionine'	HMDB0003966	C5H11NO2Se	C05335
62	196.0219	197.0324223	0.0027223	Protonation	b'5-hydroxy-6-methylpyridine-3,4-dicarboxylic acid'	b'3-Hydroxy-2-methylpyridine-4,5-dicarboxylate'	HMDB0006955	C8H7NO5	C04604
		197.0324223	0.0027223	Protonation	b'2-(4-hydroxy-3-nitrophenyl)acetic acid'	b'4-hydroxy-3-nitrophenylacetate'	HMDB0062403	C8H7NO5	
		197.0324223	0.0027223	Protonation	b'4-hydroxy-3-nitrophenyl acetate'	b'4-Hydroxy-3-nitrophenyl acetate'	HMDB0246444	C8H7NO5	
63	196.0366	197.0436557	0.0007443	Protonation	b'2-methyl-3,5-dinitroaniline'	b'2-Amino-4,6-dinitrotoluene'	HMDB0245219	C7H7N3O4	C16395

		197.0436557	0.0007 443	Proton ation	b'4-methyl-3,5-dinitroaniline'	b'4-Amino-2,6-dinitrotoluene'	HMDB02 46344	C7H7N3O4	C16 394
		197.0453095	0.0009 095	Proton ation	b'2-amino-5-phosphonopentanoic acid'	b'2-Amino-5-phosphonopentanoic acid'	HMDB02 47376	C5H12NO5P	C13 734
		197.045547	0.0011 47	Proton ation	b'2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetate'	b'vanillyl mandelate'	HMDB03 04531	C9H9O5	
		196.0371734	0.0005 734	Redox	b'7-methoxy-2H-1,3-benzodioxole-5-carboxylic acid'	b'3-Methoxy-4,5-methylenedioxybenzoic acid'	HMDB00 30800	C9H8O5	
		196.0371734	0.0005 734	Redox	b'3-(4-hydroxyphenoxy)-3-oxopropanoic acid'	b'4-Hydroxy-benzenepropanedioate'	HMDB00 59809	C9H8O5	
		196.034488	0.0021 12	Redox	b'2-amino-8-nitro-6,7-dihydro-1H-purin-6-one'	b'8-Nitroguanine'	HMDB02 47453	C5H4N6O3	
6 4	196.96 56	196.9665516	0.0009 516	Redox	b'gold(1+) ion'	b'Gold'	HMDB00 04138	Au	
6 5	196.98 23	197.9929391	0.0028 391	Proton ation	b'[3-(formyloxy)-2-oxopropoxy]phosphonic acid'	b'Dihydroxyacetone Phosphate Acyl Ester'	HMDB00 11750	C4H7O7P	C03 372
		197.99055	0.0004 5	Proton ation	b'1-iodopentane'	b'1-Iodopentane'	HMDB02 43909	C5H11I	
6 6	197.02 12	198.0295012	0.0005 012	Proton ation	b'3-chloro-6-(hydroxymethyl)oxane-2,4,5-triol'	b'2-Chloro-DG'	HMDB02 45057	C6H11ClO5	
		198.0276713	0.0013 287	Proton ation	b'2-methyl-4,6-dinitrophenol'	b'4,6-Dinitro-O-cresol'	HMDB02 45221	C7H6N2O5	C18 653
		198.0276713	0.0013 287	Proton ation	b'1-methoxy-2,4-dinitrobenzene'	b'2,4-Dinitroanisole'	HMDB02 45458	C7H6N2O5	
		197.0201569	0.0010 431	Redox	b'2-[(E)-[amino(phosphonoamino)methylidene]amino]acetic acid'	b'Phosphoguanidinooacetate'	HMDB00 03705	C3H8N3O5P	C03 166

6 7	198.98 14	199.9872256	0.0019 744	Proton ation	b'octafluorocyclobutane'	b'Octafluorocyclobutane'	HMDB00 31292	C4F8	
		199.9872253	0.0019 747	Proton ation	b'1,1,3,3,3-pentafluoro-2-(trifluoromethyl)prop-1-ene'	b'Perfluoroisobutylene'	HMDB02 56325	C4F8	
		198.9784686	0.0029 314	Redox	b'4-chloro-7-nitro-2,1,3-benzoxadiazole'	b'4-Chloro-7-nitrobenzofurazan'	HMDB02 46389	C6H2ClN3O3	
6 8	207.04 35	208.051776	0.0004 776	Proton ation	b'2-[(2-amino-1-hydroxy-3-sulfanylpropylidene)amino]-3-hydroxypropanoic acid'	b'Cysteinyl-Serine'	HMDB00 28784	C6H12N2O4S	
		208.051778	0.0004 78	Proton ation	b'(2R)-2-[(2S)-2-amino-3-hydroxypropanamido]-3-sulfanylpropanoic acid'	b'Serylcyserine'	HMDB00 29036	C6H12N2O4S	
		208.051778	0.0004 78	Proton ation	b'(2R)-2-amino-3-[(2R)-2-amino-2-carboxyethyl]sulfanyl]propanoic acid'	b'Lanthionine'	HMDB02 40656	C6H12N2O4S	
		208.0524295	0.0011 295	Proton ation	b'1,2-dihydroanthracene-1,2-dione'	b'1,2-Anthraquinone'	HMDB02 44055	C14H8O2	
		208.0524295	0.0011 295	Proton ation	b'9,10-dihydroanthracene-9,10-dione'	b'Anthraquinone'	HMDB02 48468	C14H8O2	C16 207
		208.051778	0.0004 78	Proton ation	b'2-amino-3-[(2-amino-2-carboxyethyl)sulfanyl]propanoic acid'	b'DL-Lanthionine'	HMDB02 51521	C6H12N2O4S	
		208.0524295	0.0011 295	Proton ation	b'9,10-dihydrophenanthrene-9,10-dione'	b'9,10-Phenanthrenequinone'	HMDB02 56391	C14H8O2	C03 243
6 9	208.02 72	209.0335195	0.0014 805	Proton ation	b'4-(2-oxoethylidene)-1,2,3,4-tetrahydropyridine-2,6-dicarboxylate'	b'betalamate'	HMDB03 04273	C9H7NO5	
7 0	208.06 26	209.0688078	0.0015 922	Proton ation	b'2-[2-(4-hydroxyphenyl)acetamido]acetic acid'	b'Hydroxyphenylacetyl glycine'	HMDB00 00735	C10H11NO4	C05 596
		209.0688078	0.0015 922	Proton ation	b'3-(C-hydroxycarbonimidoyloxy)-2-phenylpropanoic acid'	b'3-Carbamoyl-2-phenylpropionic acid'	HMDB00 60367	C10H11NO4	C16 591

		209.0688078	0.0015 922	Proton ation	b'4-(1-amino-1-carboxyethyl)benzoic acid'	b'alpha-Methyl-4-carboxyphenylglycine'	HMDB02 43703	C10H11NO4	
		209.0688078	0.0015 922	Proton ation	b'4-nitrophenyl butanoate'	b'4-Nitrophenyl butyrate'	HMDB02 46539	C10H11NO4	
		209.0688078	0.0015 922	Proton ation	b'4-[amino(carboxy)methyl]-3-methylbenzoic acid'	b'4-[(S)-Amino(carboxy)methyl]-3-methylbenzoic acid'	HMDB02 54239	C10H11NO4	
		209.0721787	0.0017 787	Proton ation	b'3-(morpholin-4-yl)propane-1-sulfonic acid'	b'3[N-Morpholino]propane sulfonic acid'	HMDB02 54880	C7H15NO4S	
		208.0596401	0.0029 599	Redox	b'1- {[5-aminofuran-2-yl)methylidene]amino}-4-hydroxy-2,5-dihydro-1H-imidazol-2-one'	b'Aminofurantoin'	HMDB00 60589	C8H8N4O3	
7 1	209.07 05	210.079313	0.0010 13	Proton ation	b'1-methoxyphenazine'	b'1-Methoxyphenazine'	HMDB02 43918	C13H10N2O	
		210.079313	0.0010 13	Proton ation	b'2-amino-9,10-dihydroacridin-9-one'	b'2-Aminoacridone'	HMDB02 45005	C13H10N2O	C12 143
		210.079313	0.0010 13	Proton ation	b'5-methyl-1,5-dihydrophenazin-1-one'	b'Pyocyanin'	HMDB02 56934	C13H10N2O	
		210.079313	0.0010 13	Proton ation	b'2-aminoacridin-1-ol'	b'C1=CC=CC2=CC3=C(O)C(N)=CC=C3N=C21'	HMDB02 58097	C13H10N2O	
7 2	210.07 33	211.079587	0.0015 13	Proton ation	b'ethyl {[2-(dimethylamino)ethyl]sulfanyl}(methyl)phosphinate'	b'Medemo'	HMDB02 54401	C7H18NO2PS	
		210.0752902	0.0019 902	Redox	b'1,3,7-trimethyl-2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'	b'1,3,7-Trimethyluric acid'	HMDB00 02123	C8H10N4O3	C16 361
		210.0739528	0.0006 528	Redox	b'(2R,3S,4R,5S,6R)-2,6-bis(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'Sedoheptulose'	HMDB00 03219	C7H14O7	C08 355
		210.0739528	0.0006 528	Redox	b'(2R,3S,4R,5S,6S)-2,6-bis(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'L-galacto-2-Heptulose'	HMDB00 29901	C7H14O7	

		210.0739528	0.0006 528	Redox	b'(2S,3S,4S,5S,6R)-2,6-bis(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-manno-2-Heptulose'	HMDB00 29935	C7H14O7	C08 236
		210.0739528	0.0006 528	Redox	b'6-(1,2-dihydroxyethyl)oxane-2,3,4,5-tetrol'	b'D-altro-D-manno-Heptose'	HMDB00 29952	C7H14O7	C06 397
		210.0752902	0.0019 902	Redox	b'1,3,9-trimethyl-2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'	b'1,3,9-Trimethyluric acid'	HMDB00 36431	C8H10N4O3	
		210.0752902	0.0019 902	Redox	b'1-(hydroxymethyl)-3,7-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Caffeinol'	HMDB02 49533	C8H10N4O3	
		210.0739528	0.0006 528	Redox	b'2,3,4,5,6,7-hexahydroxyheptanal'	b'd-Glycero-d-galacto-heptose'	HMDB02 53107	C7H14O7	
		210.0739528	0.0006 528	Redox	b'1,3,4,5,6,7-hexahydroxyheptan-2-one'	b'MANNOHEPTULOSE'	HMDB02 54327	C7H14O7	
		210.0739528	0.0006 528	Redox	b'1,2,3,5,6,7-hexahydroxyheptan-4-one'	b'(3R,5R,6R)-1,2,3,5,6,7-Hexahydroxyheptan-4-one'	HMDB02 55327	C7H14O7	
		210.0739528	0.0006 528	Redox	b'(2R,4R,5R,6R)-1,2,4,5,6,7-hexahydroxyheptan-3-one'	b'Crocose'	HMDB03 02576	C7H14O7	C19 612
7 3	211.00 02	212.0069359	0.0010 641	Proton ation	b'3,5-dinitrobenzoic acid'	b'3,5-Dinitrobenzoic acid'	HMDB02 46067	C7H4N2O6	
7 4	212.02 18	213.0307083	0.0011 083	Proton ation	b'2-amino-1-[(2-hydroxypropanoyl)oxy]ethane-1-sulfonic acid'	b'Taurine lactate'	HMDB02 58739	C5H11NO6S	
7 5	212.03 13	213.0402236	0.0011 236	Proton ation	b'[2-(2-hydroxypropanamido)ethoxy]phosphonic acid'	b'N-Lactoyl ethanolamine phosphate'	HMDB00 32357	C5H12NO6P	
		213.0385703	0.0005 297	Proton ation	b'N-(2-methyl-3,5-dinitrophenyl)hydroxylamine'	b'2-hydroxylamino-4,6-dinitrotoluene'	HMDB03 04072	C7H7N3O5	C16 393
		213.0385703	0.0005 297	Proton ation	b'N-(4-methyl-3,5-dinitrophenyl)hydroxylamine'	b'4-hydroxylamino-2,6-dinitrotoluene'	HMDB03 04181	C7H7N3O5	C16 392

		212.0295861	0.0017 139	Redox	b'9H-thioxanthen-9-one'	b'Thioxanthen-9-one'	HMDB02 59037	C13H8OS	
7 6	214.04 72	215.0558737	0.0008 737	Proton ation	b'(2-aminoethoxy)(2,3-dihydroxypropoxy)phosphinic acid'	b'Glycerylphosphorylethanolamine'	HMDB00 00114	C5H14NO6P	C01 233
		215.0558737	0.0008 737	Proton ation	b'(2-aminoethoxy)((2S)-2,3-dihydroxypropoxy)phosphinic acid'	b'sn-glycero-3-Phosphoethanolamine'	HMDB00 59660	C5H14NO6P	
		214.0490754	0.0018 754	Redox	b'1H,2H,3H,4H-benzo[g]pteridine-2,4-dione'	b'Alloxazine'	HMDB02 48162	C10H6N4O2	
7 7	215.05 13	216.056863	0.0022 37	Proton ation	b'3-[(3aS,4S,6aR)-2-oxo-hexahydro-1H-thieno[3,4-d]imidazolidin-4-yl]propanoic acid'	b'Bisnorbiotin'	HMDB00 04821	C8H12N2O3S	C20 384
		216.056863	0.0022 37	Proton ation	b'(2S,5R,6R)-6-amino-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid'	b'6-Aminopenicillanic acid'	HMDB00 60618	C8H12N2O3S	C02 954
		216.0568634	0.0022 366	Proton ation	b'3-[(2-cyanoethyl)sulfanyl]-2-acetamidopropanoic acid'	b'N-Acetyl-S-(2-cyanoethyl)-L-cysteine'	HMDB02 55060	C8H12N2O3S	
7 8	218.07 06	218.0731649	0.0025 649	Redox	b'pyren-1-ol'	b'1-Hydroxypyrene'	HMDB00 13139	C16H10O	C14 519
		218.072513	0.0019 13	Redox	b'1-(2-amino-3-sulfanylpropanoyl)pyrrolidine-2-carboxylic acid'	b'Cysteinyl-Proline'	HMDB00 28783	C8H14N2O3S	
		218.072513	0.0019 13	Redox	b'2-[(pyrrolidin-2-yl)formamido]-3-sulfanylpropanoic acid'	b'Prolyl-Cysteine'	HMDB00 29014	C8H14N2O3S	
		218.0691422	0.0014 578	Redox	b'2-[[cyano(phenyl)methyl]carbamoyl]acetic acid'	b'(S)-3-[(Cyanophenylmethyl)amino]-3-oxopropanoic acid'	HMDB00 34911	C11H10N2O3	
7 9	221.90 49	221.9071148	0.0022 148	Redox	b'disodium hydrogen (hydrogen phosphonatoxy)phosphonate'	b'Disodium pyrophosphate'	HMDB03 03490	H2Na2O7P2	
8 0	222.05 31	223.0609591	5.91E- 05	Proton ation	b'(2E)-3-[(dimethoxyphosphoryl)oxy]-N-methylbut-2-enamide'	b'(E)-Monocrotophos'	HMDB00 31805	C7H14NO5P	C18 663

		223.0609596	5.96E-05	Protonation	b'3-[(dimethoxyphosphoryl)oxy]-N-methylbut-2-enamide'	b'Alphate'	HMDB02 45618	C7H14NO5P	
		223.0609596	5.96E-05	Protonation	b'4-(phosphonomethyl)piperidine-2-carboxylic acid'	b'4-(Phosphonomethyl)piperidine-2-carboxylic acid'	HMDB02 46313	C7H14NO5P	
		223.0633285	0.0024285	Protonation	b'9-nitrophenanthrene'	b'9-Nitrophenanthrene'	HMDB02 47604	C14H9NO2	
		223.0633285	0.0024285	Protonation	b'9-azatricyclo[9.4.0.0^{2,7}]pentadeca-1(15),2,4,6,11,13-hexaene-8,10-dione'	b'Benzo[d][2]benzazepine-5,7-dione'	HMDB02 51445	C14H9NO2	
		223.0633285	0.0024285	Protonation	b'2-phenyl-2,3-dihydro-1H-isoindole-1,3-dione'	b'N-Phenylphthalimide'	HMDB02 55231	C14H9NO2	
		222.0528234	0.0002766	Redox	b'7-hydroxy-6,8-dimethoxy-2H-chromen-2-one'	b'Isofraxidin'	HMDB02 53642	C11H10O5	C17 480
		222.0519679	0.0011321	Redox	b"2-:[N-(2-chloroethyl)-N'-oxohydrazinecarbonyl]amino}propanamide"	b'N-Chloroethylnitrosourea sarcosinamide'	HMDB02 55103	C6H11ClN4O3	
		222.0519679	0.0011321	Redox	b"2-:[N-(2-chloroethyl)-N'-oxohydrazinecarbonyl](methyl)amino}acetamide"	b'Sarcnu'	HMDB02 57494	C6H11ClN4O3	
		222.0528234	0.0002766	Redox	b'acetyl 2-(acetyloxy)benzoate'	b'Acetyl 2-acetyloxybenzoate'	HMDB02 57655	C11H10O5	
		222.0528234	0.0002766	Redox	b'2-:[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy}acetic acid'	b'p-Coumaroyl glycolic acid'	HMDB03 01727	C11H10O5	
		222.0528234	0.0002766	Redox	b'2-(3-carboxypropanoyl)benzoic acid'	b'2-succinylbenzoate'	HMDB03 04087	C11H10O5	C02 730
8	223.00	224.0078052	0.0004948	Protonation	b"4-amino-[2,3'-bithiophene]-5-carboxamide"	b'3-Amino-5-(3-thiophenyl)-2-thiophenecarboxamide'	HMDB02 57535	C9H8N2OS2	
1	05	223	0.0005	Redox	b'francium'	b'FR'	HMDB03 03046	Fr	

8	2	224.06	73	225.0766096	0.0015 096	Proton ation	b'2-amino-7-phosphonoheptanoic acid'	b'(+)-2-Amino-7-phosphonoheptanoic acid'	HMDB02 42241	C7H16NO5P	
				225.0749558	0.0001 442	Proton ation	b'4-(hydroxymethyl)-10-imino-3,7-dioxo-1,9-diazatricyclo[6.4.0.0']{2,6}dodeca-8,11-dien-5-ol'	b''2,2'-Anhydrocytidine"	HMDB02 43629	C9H11N3O4	
				225.077947	0.0028 47	Proton ation	b'9-[2-(phosphanylmethoxy)ethyl]-9H-purin-6-amine'	b'9-[2-(Phosphanylmethoxy)ethyl]purin-6-amine'	HMDB02 47656	C8H12N5OP	
				224.0684735	0.0011 735	Redox	b'methyl 2-oxo-4-[(2Z)-1-oxobut-2-en-2-yl]-3,4-dihydro-2H-pyran-5-carboxylate'	b'Elenolide'	HMDB00 30018	C11H12O5	C09 506
				224.0684735	0.0011 735	Redox	b'(2E)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoic acid'	b'Sinapic acid'	HMDB00 32616	C11H12O5	C00 482
				224.0684735	0.0011 735	Redox	b'(2Z)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoic acid'	b'cis-Sinapic acid'	HMDB00 34069	C11H12O5	
				224.0684735	0.0011 735	Redox	b'5-[(3,4,5-trihydroxyphenyl)methyl]oxolan-2-one'	b''5-(3',4',5'-Trihydroxyphenyl)-gamma-valerolactone"	HMDB00 41691	C11H12O5	
				224.0684735	0.0011 735	Redox	b'2-oxo-2-(3,4,5-trimethoxyphenyl)acetaldehyde'	b'2-Oxo-2-(3,4,5-trimethoxyphenyl)acetaldehyde'	HMDB02 45283	C11H12O5	
8	3	225.09	81	226.1065903	0.0006 903	Proton ation	b'(2S)-2-(3-aminopropanamido)-3-(1H-imidazol-5-yl)propanoic acid'	b'Carnosine'	HMDB00 00033	C9H14N4O3	C00 386
				226.1065903	0.0006 903	Proton ation	b'(2S)-2-[(2S)-2-aminopropanamido]-3-(1H-imidazol-4-yl)propanoic acid'	b'Alanylhistidine'	HMDB00 28689	C9H14N4O3	
				226.1065903	0.0006 903	Proton ation	b'(2S)-2-[(2S)-2-amino-3-(1H-imidazol-5-yl)propanamido]propanoic acid'	b'Histidylalanine'	HMDB00 28878	C9H14N4O3	
				226.1065903	0.0006 903	Proton ation	b'4-[2-(5-nitro-1H-imidazol-1-yl)ethyl]morpholine'	b'Nimorazole'	HMDB02 55612	C9H14N4O3	
				226.1065903	0.0006	Proton	b'2-[(3-amino-1-hydroxypropylidene)amino]-3-(1H-imidazol-5-yl)propanoic acid'	b'beta-Alanyl-L-histidine'	HMDB02	C9H14N4O3	

			903	ation			56117		
		226.1065903	0.0006 903	Proton ation	b'2-[(2-amino-1-hydroxypropylidene)amino]-3-(1H-imidazol-5-yl)propanoic acid'	b'Alanyl-Histidine'	HMDB03 04775	C9H14N4O3	
		226.1065903	0.0006 903	Proton ation	b'2-[(2-amino-1-hydroxy-3-(1H-imidazol-5-yl)propylidene)amino]propanoic acid'	b'Histidinyl-Alanine'	HMDB03 04819	C9H14N4O3	
		225.100108	0.0020 08	Redox	b'4-(2-amino-3,3-dihydroxypropyl)phenyl acetate'	b'Hydroxy Tyrosol -Acetate'	HMDB02 53254	C11H15NO4	
8 4	227.91 18	227.9130813	0.0012 813	Redox	b'tetrahydroxyiodous acid'	b'Orthoperiodic acid'	HMDB00 34831	H5IO6	
8 5	228.95 52	229.9649828	0.0019 828	Proton ation	b'6,7-dichloro-3-nitroso-1H-indol-2-ol'	b'(Z)-6,7-Dichloro-3-(hydroxyimino)indolin-2-one'	HMDB02 55775	C8H4Cl2N2O2	
8 6	229.01 07	230.0191538	0.0006 538	Proton ation	b'{{{(2R,3R)-2,3,5-trihydroxy-4-oxopentyl}oxy}phosphonic acid'	b'D-Ribulose 5-phosphate'	HMDB00 00618	C5H11O8P	C00 199
		230.0191538	0.0006 538	Proton ation	b'{{{(2R,3S)-2,3,5-trihydroxy-4-oxopentyl}oxy}phosphonic acid'	b'Xylulose 5-phosphate'	HMDB00 00868	C5H11O8P	C00 231
		230.0191538	0.0006 538	Proton ation	b'{{{(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl}oxy}phosphonic acid'	b'Ribose 1-phosphate'	HMDB00 01489	C5H11O8P	C00 620
		230.0191538	0.0006 538	Proton ation	b'{{{(2R,3S,4R,5S)-3,4,5-trihydroxyoxolan-2-yl}methoxy}phosphonic acid'	b'D-Ribose 5-phosphate'	HMDB00 01548	C5H11O8P	C03 736
		230.0191543	0.0006 543	Proton ation	b'{{{(3S,4R)-3,4,5-trihydroxy-2-oxopentyl}oxy}phosphonic acid'	b'D-Xylulose 1-phosphate'	HMDB00 06534	C5H11O8P	
		230.0191538	0.0006 538	Proton ation	b'{{{(2R,3R,4S)-2,3,4-trihydroxy-5-oxopentyl}oxy}phosphonic acid'	b'D-Arabinose 5-phosphate'	HMDB00 11734	C5H11O8P	C011 12
		230.0191538	0.0006 538	Proton ation	b'{{{(2R,3R,4S,5S)-3,4,5-trihydroxyoxan-2-yl}oxy}phosphonic acid'	b'beta-L-Arabinose 1-phosphate'	HMDB00 12195	C5H11O8P	C03 906
		230.0190785	0.0005	Proton	b'7-hydroxy-4-(trifluoromethyl)-2H-chromen-2-one'	b'7-Hydroxy-4-	HMDB02	C10H5F3O3	

			785	ation		(trifluoromethyl)coumarin'	47257		
		230.0191543	0.0006 543	Proton ation	b'[[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]oxy]phosphonic acid'	b'D-Ribose 1-phosphate'	HMDB02 50796	C5H11O8P	
		230.0200237	0.0015 237	Proton ation	b'dimethyl {[2-(ethylsulfanyl)ethyl]sulfanyl}phosphonate'	b'Demeton-S-methyl'	HMDB02 50995	C6H15O3PS2	C18 655
		230.0191543	0.0006 543	Proton ation	b'[(3,4,5-trihydroxy-1-oxopentan-2-yl)oxy]phosphonic acid'	b'Phosphoribose'	HMDB02 56491	C5H11O8P	
		230.0191543	0.0006 543	Proton ation	b'[(2,3,4-trihydroxy-5-oxopentyl)oxy]phosphonic acid'	b'ribose-5-phosphate'	HMDB02 57215	C5H11O8P	
		230.0191538	0.0006 538	Proton ation	b'[(3,4,5-trihydroxy-2-oxopentyl)oxy]phosphonic acid'	b'[(3R)-3,4,5-Trihydroxy-2-oxopentyl] dihydrogen phosphate'	HMDB02 60227	C5H11O8P	
		230.0167119	0.0017 881	Proton ation	b'disodium 7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylate'	b'Pancrelipase'	HMDB03 04827	C8H8Na2O5	C18 724
		229.0117407	0.0010 407	Redox	b'1-(2,2,2-trifluoroacetyl)pyrrolidine-2-carbonyl chloride'	b'N-Trifluoroacetylprolyl chloride'	HMDB02 46206	C7H7ClF3NO2	
8	230.00	230.0109759	0.0018 759	Redox	b'4-hydroxy-1-(5-nitro-1,3-thiazol-2-yl)imidazolidin-2-one'	b'2-Imidazolidinone, 4-hydroxy-1-(5- nitro-2-thiazolyl)-'	HMDB02 46460	C6H6N4O4S	
7	91	230.0076046	0.0014 954	Redox	b'7-nitro-2,3-dioxo-2,3-dihydroquinoxaline-6-carbonitrile'	b'7-Nitro-2,3-Dioxo-2,3- Dihydroquinoxaline-6-Carbonitrile'	HMDB02 50068	C9H2N4O4	
8	233.93	233.9290379	0.0025 621	Redox	b'dipotassium oxoboranyl [(oxoboranyl boronato)oxy]boronate'	b'Potassium tetraborate'	HMDB03 03558	B4K2O7	
8	238.89	239.8989912	0.0009 912	Proton ation	b'trihydroxy-1,3,5,2'\xcce'\xbbb'\xc2'\xb81'\xb5,4'\xcce'\xbbb'\xc2'\xb81'\xb5,6'\xcce'\xbbb'\xc2'\xb81'\xb5- trioxatriphosphinane-2,4,6-trione'	b'Trimetaphosphoric acid'	HMDB00 59921	H3O9P3	C02 466
9	238.96	239.9737284	0.0023 284	Proton ation	b'5-(4-methoxyphenyl)-3H-1,2-dithiole-3-thione'	b'Anethole trithione'	HMDB02 48420	C10H8OS3	
9	238.97	238.9748609	0.0007	Redox	b'[[hydroxy(pyridin-2-yl)phosphoryl]oxy]phosphonic acid'	b'Diphosphopyridine'	HMDB02	C5H7NO6P2	

1	56		391				51464		
9	239.11	240.1222404	0.0002 404	Proton ation	b'(2S)-2-(3-aminopropanamido)-3-(1-methyl-1H-imidazol-5-yl)propanoic acid'	b'Anserine'	HMDB00 00194	C10H16N4O3	C01 262
		240.1222404	0.0002 404	Proton ation	b'(2S)-2-(4-aminobutanamido)-3-(1H-imidazol-4-yl)propanoic acid'	b'Homocarnosine'	HMDB00 00745	C10H16N4O3	C00 884
		240.1222404	0.0002 404	Proton ation	b'(2S)-2-(3-aminopropanamido)-3-(1-methyl-1H-imidazol-4-yl)propanoic acid'	b'Balenine'	HMDB00 05769	C10H16N4O3	
		240.1222404	0.0002 404	Proton ation	b'1-(2,3-dimethylaziridin-1-yl)-3-(2-nitro-1H-imidazol-1-yl)propan-2-ol'	b'alpha-((2,3-Dimethyl-1-aziridinyl)methyl)-2-nitro-1H-imidazole-1-ethanol'	HMDB02 43785	C10H16N4O3	
		240.120903	0.0010 97	Proton ation	b'3-[3-(2,3-dihydroxypropoxy)-2-hydroxypropoxy]propane-1,2-diol'	b'Triglycerol'	HMDB02 59216	C9H20O7	
2	42	239.115758	0.0015 58	Redox	b'ethyl 2-amino-3-(3,4-dihydroxyphenyl)-2-methylpropanoate'	b'Methylidopate'	HMDB02 54628	C12H17NO4	
9	239.97	240.9812326	0.0022 326	Proton ation	b'2-oxo-2H-chromen-7-yl sulfate'	b'Umbelliferone sulfate'	HMDB02 40565	C9H5O6S	
3	12								
9	240.04	241.0586371	0.0010 371	Proton ation	b'2,4-dihydroxy-6,7-dimethoxy-3,4-dihydro-2H-1,4-benzoxazin-3-one'	b'2,4-Dihydroxy-6,7-dimethoxy-2H-1,4-benzoxazin-3(4H)-one'	HMDB00 37548	C10H11NO6	
		241.0586371	0.0010 371	Proton ation	b'2,4-dihydroxy-7,8-dimethoxy-3,4-dihydro-2H-1,4-benzoxazin-3-one'	b'2,4-Dihydroxy-7,8-dimethoxy-2H-1,4-benzoxazin-3(4H)-one'	HMDB00 37549	C10H11NO6	
		241.0561352	0.0014 648	Proton ation	b'1-(10H-phenothiazin-2-yl)ethan-1-one'	b'1-(10H-Phenothiazin-2-yl)ethanone'	HMDB02 44969	C14H11NOS	
		241.0561352	0.0014 648	Proton ation	b'N-phenyl-N-(prop-2-yn-1-yl)thiophene-2-carboxamide'	b'Morin-5'-sulfonic acid"	HMDB02 54884	C14H11NOS	
9	241.01	242.0191538	0.0012 538	Proton ation	b'(3aR,4R,5S,6S,7R,7aS)-2,4,5,6,7-pentahydroxy-hexahydro-2H-1,3,2'-xcccxbbx2'x81'xb5-benzodioxaphosphol-2-one'	b'Inositol cyclic phosphate'	HMDB00 01125	C6H11O8P	C04 299
5	01								

		242.0191543	0.0012 543	Proton ation	b'6-(hydroxymethyl)-2-phosphooxane-2,3,4,5-tetrol'	b'Phosphohexose'	HMDB02 56479	C6H11O8P	
		242.0191543	0.0012 543	Proton ation	b'2,6,7,8-tetrahydroxy-1,3,2lambda5-dioxaphosphanone-2,5-dione'	b'(6S,7R)-2,6,7,8-Tetrahydroxy-2-oxo-1,3,2lambda5-dioxaphosphanone-5-one'	HMDB02 60167	C6H11O8P	
		242.0202515	0.0023 515	Proton ation	b'3,4,5-trihydroxy-6-methylloxan-2-yl phosphate'	b'beta-L-fucose 1-phosphate'	HMDB03 04542	C6H11O8P	
		241.0078638	0.0022 362	Redox	b'3-[[{(2R)-2-amino-2-carboxyethyl]disulfanyl}-2-hydroxypropanoic acid'	b'3-Mercaptolactate-cysteine disulfide'	HMDB00 06512	C6H11NO5S2	
9 6	242.03 29	242.0319012	0.0009 988	Redox	b'3-(2-chloroethyl)-4-oxo-3H,4H-imidazo[4,3-d][1,2,3,5]tetrazine-8-carboxamide'	b'Mitozolomide'	HMDB02 54765	C7H7ClN6O2	
9 7	242.07 89	243.0855205	0.0011 795	Proton ation	b'4-amino-1-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one'	b'Cytidine'	HMDB00 00089	C9H13N3O5	C00 475
		243.0855205	0.0011 795	Proton ation	b'4-amino-1-[(2R,3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one'	b'Cytarabine'	HMDB00 15122	C9H13N3O5	C02 961
		243.0855205	0.0011 795	Proton ation	b'(2S)-2-amino-4-[[{(1S)-1-carboxy-2-cyanoethyl]-C-hydroxycarbonimidoyl]butanoic acid'	b'gamma-Glutamyl-beta-cyanoalanine'	HMDB00 60478	C9H13N3O5	C05 711
		243.0855205	0.0011 795	Proton ation	b'4-amino-1-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one'	b'Arabinofuranosylcytosine'	HMDB02 48553	C9H13N3O5	
		243.0855205	0.0011 795	Proton ation	b'4-amino-5-hydroxy-1-[4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one'	b'4-Amino-5-hydroxy-1-[(2R,5R)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidin-2-one'	HMDB02 58026	C9H13N3O5	
		242.0790382	0.0001 382	Redox	b'2'-[3-hydroxy-1H,3H,4H,5H,6H-cyclopenta[c]furan-4-yl]-3-methoxy-3-oxopropanoic acid'	b'Genipinic acid'	HMDB00 38126	C11H14O6	
		242.0790382	0.0001 382	Redox	b'2-[3-formyl-5-(methoxycarbonyl)-2-methyl-3,4-dihydro-2H-pyran-4-yl]acetic acid'	b'Elenaic acid'	HMDB00 39136	C11H14O6	
		242.0803756	0.0014	Redox	b'7,8-dimethyl-1H,2H,3H,4H-benzo[g]pteridine-2,4-dione'	b'Lumichrome'	HMDB02	C12H10N4O2	C01

			756				54199		727
9 8	243.08 14	244.0881631	0.0010 369	Proton ation	b'5-[(3aS,4S,6aR)-2-oxo-hexahydro-1H-thieno[3,4-d]imidazol-4-yl]pentanoic acid'	b'Biotin'	HMDB00 00030	C10H16N2O3S	C00 120
		244.0899579	0.0007 579	Proton ation	b''2-[2-fluoro-[1,1'-biphenyl]-4-yl]propanoic acid''	b'Flurbiprofen'	HMDB00 14850	C15H13FO2	
		244.088815	0.0003 85	Proton ation	b'tetraphen-3-ol'	b'3-Hydroxybenz[a]anthracene'	HMDB02 46692	C18H12O	
		244.0881636	0.0010 364	Proton ation	b'N-{3-[1-hydroxy-2-(methylanino)ethyl]phenyl}methanesulfonamide'	b'Amidephrine'	HMDB02 48297	C10H16N2O3S	
		244.0881631	0.0010 369	Proton ation	b'5-[2-hydroxy-1H,3aH,4H,6H,6aH-thieno[3,4-d]imidazol-6-yl]pentanoic acid'	b'Bioepiderm'	HMDB02 49220	C10H16N2O3S	
		243.0830181	0.0016 181	Redox	b'2-propyl-4H,5H-[1,3]thiazolo[4,5-c]quinolin-4-imine'	b'2-Propylthiazolo[4,5-c]quinolin-4-amine'	HMDB02 45307	C13H13N3S	
9 9	243.88 55	243.8860163	0.0005 163	Redox	b'[dichloro(phosphono)methyl]phosphonic acid'	b'Clodronate'	HMDB00 14858	CH4Cl2O6P2	
1 0 0	245.04 12	246.0504544	0.0014 544	Proton ation	b'[(2R)-2,3-dihydroxypropoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'Glycerophosphoglycerol'	HMDB02 40316	C6H15O8P	
		245.0436557	0.0024 557	Redox	b'7-methoxy-2-oxo-2H-chromene-3-carbonyl azide'	b'7-Methoxycoumarin-3-carbonyl azide'	HMDB02 47270	C11H7N3O4	
		245.0412109	1.09E- 05	Redox	b'N-[4-(trifluoromethoxy)phenyl]carbamoyl cyanide'	b'1-Cyano-N-[4-(trifluoromethoxy)phenyl]formohydrazide'	HMDB02 58057	C9H6F3N3O2	
1 0 1	245.95 81	246.9632125	0.0026 875	Proton ation	b'2-chloro-1,3,5-trinitrobenzene'	b'Picryl chloride'	HMDB02 56541	C6H2ClN3O6	
		246.9650522	0.0008 478	Proton ation	b'2-hydroxypropane-1,2,3-tricarboxylic acid manganese'	b'Manganese citrate'	HMDB03 03646	C6H8MnO7	

1 0 2	245.98 27	245.9834232	0.0007 232	Redox	b'5-sulfobenzene-1,3-dicarboxylic acid'	b'5-Sulfo-1,3-benzenedicarboxylic acid'	HMDB00 32822	C8H6O7S	
1 0 3	247.97 71	247.9788138	0.0017 138	Redox	b'2,5-bis(thiophen-2-yl)thiophene'	b''2,2':5',2''-Terthiophene''	HMDB02 45378	C12H8S3	C08 460
1 0 4	248.93 74	249.9461916 249.94624	0.0009 916 0.0010 4	Proton ation Proton ation	b'[(methanesulfonylmethyl)disulfanyl]methanesulfonylmethane'	b'Bis(methylsulfonylmethyl) disulfide'	HMDB00 41188	C4H10O4S4	
					b'dioxotungstendiol'	b'Tungstic acid'	HMDB02 59326	H2O4W	
1 0 5	248.97 16	249.9799642 249.9815051 249.9783383 249.9783383	0.0005 642 0.0021 051 0.0010 617 0.0010 617	Proton ation Proton ation Proton ation Proton ation	b'3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoic acid'	b'3,5-Dichloro-4-hydroxy-2-methoxy-6-methylbenzoic acid'	HMDB00 33822	C9H8Cl2O4	
					b'2-amino-4-chloro-5-sulfamoylbenzoic acid'	b'4-Chloro-5-sulfamoylanthranilic acid'	HMDB00 60761	C7H7ClN2O4S	
					b'3,5-dihydroxy-4-(sulfooxy)benzoic acid'	b'3,5-dihydroxy-4-(sulfooxy)benzoic acid'	HMDB01 26639	C7H6O8S	
					b'3,4-dihydroxy-5-(sulfooxy)benzoic acid'	b'Gallic acid 3-sulfate'	HMDB02 40519	C7H6O8S	
1 0 6	253.04 85	254.0579088 254.0572569 254.0579088 254.0579088	0.0016 088 0.0009 569 0.0016 088 0.0016 088	Proton ation Proton ation Proton ation Proton ation	b'7-hydroxy-3-(4-hydroxyphenyl)-4H-chromen-4-one'	b'Daidzein'	HMDB00 03312	C15H10O4	C10 208
					b'(2S)-2-amino-4-[(2-sulfoethyl)carbamoyl]butanoic acid'	b'5-L-Glutamyl-taurine'	HMDB00 04195	C7H14N2O6S	C05 844
					b'1,8-dihydroxy-3-methyl-9,10-dihydroanthracene-9,10-dione'	b'Chrysophanol'	HMDB00 30670	C15H10O4	C10 315
					b'5,7-dihydroxy-3-phenyl-4H-chromen-4-one'	b'5,7-Dihydroxyisoflavone'	HMDB00 30699	C15H10O4	C02 168

		254.2245802	0.0011 802	Proton ation	b'5-dodecylloxolan-2-one'	b'5-Dodecylidihydro-2(3H)-furanone'	HMDB00 31145	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'16-methyl-1-oxacyclohexadecan-2-one'	b'15-Hexadecanolide'	HMDB00 31711	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'(5E)-hexadec-5-enoic acid'	b'(Z)-5-Hexadecenoic acid'	HMDB00 32638	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'(3Z)-hexadec-3-enoic acid'	b'(E)-3-Hexadecenoic acid'	HMDB00 33791	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'(13Z)-hexadec-13-enoic acid'	b'(Z)-13-Hexadecenoic acid'	HMDB00 35877	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'(11E)-hexadec-11-enoic acid'	b'(E)-11-Hexadecenoic acid'	HMDB00 37647	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'3,7-dimethyloct-6-en-1-yl hexanoate'	b'Citronellyl hexanoate'	HMDB00 38958	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'(6E)-14-methylpentadec-6-enoic acid'	b'(Z)-14-Methyl-6-pentadecenoic acid'	HMDB00 41422	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'hexadec-15-enoic acid'	b'15-Hexadecenoic acid'	HMDB02 44666	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'hexadec-9-enoic acid'	b'9-Hexadecenoic acid, (9Z)-'	HMDB02 47596	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'dodecyl 2-methylprop-2-enoate'	b'Dodecyl methacrylate'	HMDB02 51570	C16H30O2	
		254.2245802	0.0011 802	Proton ation	b'hexadec-6-enoic acid'	b'Sapienic acid'	HMDB02 57483	C16H30O2	
1 0	254.92 42	254.9256761	0.0014 761	Redox	b'2-[(3,5,6-trichloropyridin-2-yl)oxy]acetic acid'	b'TRICLOPYR'	HMDB02 59186	C7H4Cl3NO3	C110 32

8									
109	255.0313	256.0371734	0.0019266	Protonation	b'1,2,4-trihydroxy-9,10-dihydroanthracene-9,10-dione'	b'PURPURIN'	HMDB0256928	C14H8O5	C10395
110	255.2316	256.2402303	0.0008303	Protonation	b'hexadecanoic acid'	b'Palmitic acid'	HMDB0000220	C16H32O2	C00249
		256.2402303	0.0008303	Protonation	b'4,8,12-trimethyltridecanoic acid'	b'Trimethyltridecanoic acid'	HMDB0002396	C16H32O2	
		256.2402303	0.0008303	Protonation	b'14-methylpentadecanoic acid'	b'Isopalmitic acid'	HMDB0031068	C16H32O2	
		256.2402303	0.0008303	Protonation	b'butyl dodecanoate'	b'Butyl dodecanoate'	HMDB0032065	C16H32O2	
		256.2402303	0.0008303	Protonation	b'dodecyl butanoate'	b'Dodecyl butyrate'	HMDB0032249	C16H32O2	
		256.2402303	0.0008303	Protonation	b'hexyl decanoate'	b'Hexyl decanoate'	HMDB0032324	C16H32O2	
		256.2402303	0.0008303	Protonation	b'octyl octanoate'	b'Octyl octanoate'	HMDB0033166	C16H32O2	
		256.2402303	0.0008303	Protonation	b'ethyl tetradecanoate'	b'Ethyl tetradecanoate'	HMDB0034153	C16H32O2	
		256.2402303	0.0008303	Protonation	b'dodecyl 2-methylpropanoate'	b'Dodecyl 2-methylpropanoate'	HMDB0036210	C16H32O2	
		256.2402303	0.0008303	Protonation	b'methyl pentadecanoate'	b'Methyl pentadecanoate'	HMDB0254606	C16H32O2	
		256.2402303	0.0008303	Protonation	b'tetradecyl acetate'	b'Tetradecyl acetate'	HMDB0258885	C16H32O2	

11	256.05	257.0688078	0.0024 078	Proton ation	b'1,3,5-trihydroxy-10-methyl-9,10-dihydroacridin-9-one'	b'1,3,5-Trihydroxy-10-methylacridone'	HMDB00 41468	C14H11NO4	
		257.0688078	0.0024 078	Proton ation	b'1-(3,7-dihydroxy-10H-phenoxazin-10-yl)ethan-1-one'	b'10-Acetyl-3,7-dihydroxyphenoxazine'	HMDB02 44436	C14H11NO4	
		257.0641125	0.0022 875	Proton ation	b'N,N-diethyl{[(4-chlorophenyl)methyl]sulfanyl}formamide'	b'Thiobencarb'	HMDB02 48966	C12H16ClNOS	C14 428
		256.0583027	0.0002 973	Redox	b'2,3-dihydroxy-2-[(4-hydroxyphenyl)methyl]butanedioic acid'	b'(2R,3S)-Piscidic acid'	HMDB00 30809	C11H12O7	
11	256.90	257.9095559	0.0006 559	Proton ation	b' {[hydroxy(phosphonooxy)phosphoryl]oxy}phosphonic acid'	b'Triphosphate'	HMDB00 03379	H5O10P3	C02 174
		257.9075832	0.0013 168	Proton ation	b'1,3,5-trichloro-2-methanesulfonylbenzene'	b'1,3,5-Trichloro-(2-methylsulfonyl)benzene'	HMDB00 37120	C7H5Cl3O2S	
11	256.99	256.9945372	0.0009 628	Redox	b'O,O-dimethyl {[2-(N-methylformamido)-2-oxoethyl]sulfanyl}phosphonothioate'	b'Formothion'	HMDB02 52447	C6H12NO4PS2	C18 988
11	258.03	259.0457029	0.0013 029	Proton ation	b' {[(2S,3R,4R,5S,6R)-3-amino-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phosphonic acid'	b'Glucosamine-1P'	HMDB00 01109	C6H14NO8P	
		259.0457029	0.0013 029	Proton ation	b' {[(2R,3S,4R,5R,6S)-5-amino-3,4,6-trihydroxyoxan-2-yl]methoxy}phosphonic acid'	b'Glucosamine 6-phosphate'	HMDB00 01254	C6H14NO8P	C00 352
		259.0457029	0.0013 029	Proton ation	b' {[(2R,3S,4S)-4-amino-3,5-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]methoxy}phosphonic acid'	b'Aminofructose 6-phosphate'	HMDB00 60436	C6H14NO8P	C12 214
		259.0457034	0.0013 034	Proton ation	b' [(5-amino-2,3,4-trihydroxy-6-oxohexyl)oxy]phosphonic acid'	b'D-Glucosamine-6-phosphate'	HMDB02 50754	C6H14NO8P	
		259.0457034	0.0013 034	Proton ation	b'2-amino-3- {[(2,3-dihydroxypropoxy)(hydroxy)phosphoryl]oxy}propanoic acid'	b'Glycerophosphoserine'	HMDB02 52850	C6H14NO8P	
		258.0375673	0.0009 673	Redox	b'6-(acetyloxy)-2,5-dioxo-hexahydrofuro[3,2-b]furan-3-yl acetate'	b'Glucaron'	HMDB02 47896	C10H10O8	

11	259.01	260.0219757	0.0029	Proton	b'3-fluoro-5-{2-[2-(fluoromethyl)-1,3-thiazol-4-yl]ethynyl} benzonitrile'	b'Benzonitrile, 3-fluoro-5-(2-(2-(fluoromethyl)-4-thiazolyl)ethynyl)-'	HMDB02 58401	C13H6F2N2S	
5	12		757	ation					
11	259.02	260.0297185	0.0010	Proton	b'{{{(2R,3R,4S)-2,3,4,6-tetrahydroxy-5-oxohexyl}oxy} phosphonic acid'}	b'Fructose 6-phosphate'	HMDB00 00124	C6H13O9P	C00 085
		260.029719	0.0010	Proton	b'{{{(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl}oxy} phosphonic acid'}	b'myo-Inositol 1-phosphate'	HMDB00 00213	C6H13O9P	C011 77
		260.0297185	0.0010	Proton	b'{{{(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl}oxy} phosphonic acid'}	b'Galactose 1-phosphate'	HMDB00 00645	C6H13O9P	C00 446
		260.0297185	0.0010	Proton	b'{{{(2S,3S,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl}oxy} phosphonic acid'}	b'Dolichyl phosphate D-mannose'	HMDB00 00994	C6H13O9P	C03 862
		260.0297185	0.0010	Proton	b'{{{(2R,3S,4S,5R)-2,3,4-trihydroxy-5-(hydroxymethyl)oxolan-2-yl}methoxy} phosphonic acid'}	b'Fructose 1-phosphate'	HMDB00 01076	C6H13O9P	C01 094
		260.0297185	0.0010	Proton	b'{{{(2R,3S,4S,5S,6R)-3,4,5,6-tetrahydroxyoxan-2-yl}methoxy} phosphonic acid'}	b'Mannose 6-phosphate'	HMDB00 01078	C6H13O9P	C00 275
		260.0297185	0.0010	Proton	b'{{{(1S,2R,3S,4S,5S,6S)-2,3,4,5,6-pentahydroxycyclohexyl}oxy} phosphonic acid'}	b'D-myo-Inositol 4-phosphate'	HMDB00 01313	C6H13O9P	C03 546
		260.0297185	0.0010	Proton	b'{{{(2R,3S,4S,5R)-3,4,5,6-tetrahydroxyoxan-2-yl}methoxy} phosphonic acid'}	b'Glucose 6-phosphate'	HMDB00 01401	C6H13O9P	C00 092
		260.0297185	0.0010	Proton	b'{{{(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl}oxy} phosphonic acid'}	b'Glucose 1-phosphate'	HMDB00 01586	C6H13O9P	C00 103
		260.0297185	0.0010	Proton	b'{{{(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl}oxy} phosphonic acid'}	b'myo-Inositol 6-phosphate'	HMDB00 02985	C6H13O9P	
		260.0297185	0.0010	Proton	b'{{{(2R,3S,4S,5R,6R)-3,4,5,6-tetrahydroxyoxan-2-yl}methoxy} phosphonic acid'}	b'beta-D-Glucose 6-phosphate'	HMDB00 03498	C6H13O9P	C011 72
		260.0297185	0.0010	Proton	b'{{{(2R,3S,4S,5R)-3,4,5-trihydroxy-5-(hydroxymethyl)oxolan-2-yl}methoxy} phosphonic acid'}	b'Beta-D-Fructose 6-phosphate'	HMDB00 03971	C6H13O9P	C05 345

		260.0297185	0.0010 185	Proton ation	b'[{(3S,4S,5R)-3,4,5,6-tetrahydroxy-2-oxohexyl}oxy]phosphonic acid'	b'D-Tagatose 1-phosphate'	HMDB00 06328	C6H13O9P	
		260.0297185	0.0010 185	Proton ation	b'[{(2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl}oxy]phosphonic acid'	b'D-Mannose 1-phosphate'	HMDB00 06330	C6H13O9P	C00 636
		260.0297185	0.0010 185	Proton ation	b'[{(3S,4R,5S)-3,4,5,6-tetrahydroxy-2-oxohexyl}oxy]phosphonic acid'	b'Sorbose 1-phosphate'	HMDB00 06797	C6H13O9P	C02 888
		260.0297185	0.0010 185	Proton ation	b'[{(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl}oxy]phosphonic acid'	b'Beta-D-Fructose 2-phosphate'	HMDB00 06800	C6H13O9P	C03 267
		260.0297185	0.0010 185	Proton ation	b'[{(1R,2S,3R,4R,5S,6S)-2,3,4,5,6-pentahydroxycyclohexyl}oxy]phosphonic acid'	b'D-myo-Inositol 3-phosphate'	HMDB00 06814	C6H13O9P	C04 006
		260.0297185	0.0010 185	Proton ation	b'[{(2R,3R,4S)-3,4,5-trihydroxy-5-(hydroxymethyl)oxolan-2-yl}methoxy]phosphonic acid'	b'D-Tagatose 6-phosphate'	HMDB00 06873	C6H13O9P	C01 097
		260.0297185	0.0010 185	Proton ation	b'[{(3S,4R,5R)-3,4,5,6-tetrahydroxy-2-oxohexyl}oxy]phosphonic acid'	b'D-fructose 1-phosphate'	HMDB00 60467	C6H13O9P	
		260.029719	0.0010 19	Proton ation	b'[(2,3,4,5,6-pentahydroxycyclohexyl)oxy]phosphonic acid'	b'(2,3,4,5,6-Pentahydroxycyclohexyl) dihydrogen phosphate'	HMDB02 42486	C6H13O9P	
		260.029719	0.0010 19	Proton ation	b'[(2,3,4,5-tetrahydroxy-6-oxohexyl)oxy]phosphonic acid'	b'(2R,3R,4S,5R)-2,3,4,5-Tetrahydroxy- 6-oxohexyl dihydrogen phosphate'	HMDB02 42558	C6H13O9P	
		260.0297185	0.0010 185	Proton ation	b'[(3,4,5,6-tetrahydroxy-2-oxohexyl)oxy]phosphonic acid'	b'(3S,4R)-Ketose 1-phosphate'	HMDB02 43608	C6H13O9P	
		260.029719	0.0010 19	Proton ation	b'[(2,3,4,5-tetrahydroxyoxan-2-yl)methoxy]phosphonic acid'	b'beta-D-Fructopyranose 1-phosphate'	HMDB02 43977	C6H13O9P	
		260.0297185	0.0010 185	Proton ation	b'[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]phosphonic acid'	b'[(2R,3R,4S,5S)-3,4,5,6- Tetrahydroxyoxan-2-yl]methyl dihydrogen phosphate'	HMDB02 46205	C6H13O9P	C02 965
		260.029719	0.0010	Proton	b'[(3,4,5,6-tetrahydroxy-1-oxohexan-2-yl)oxy]phosphonic acid'	b'D-Glucose 2-phosphate'	HMDB02	C6H13O9P	

			19	ation			47860		
		260.0297185	0.0010 185	Proton ation	b' {[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy} phosphonic acid'	b'beta-D-Glucose 1-phosphate'	HMDB02 49121	C6H13O9P	C01 002
		260.029719	0.0010 19	Proton ation	b'[(1,4,5,6-tetrahydroxy-2-oxohexan-3-yl)oxy] phosphonic acid'	b'Fructose 3-phosphate'	HMDB02 52488	C6H13O9P	
		260.029719	0.0010 19	Proton ation	b' {[3,4,5-trihydroxy-5-(hydroxymethyl)oxolan-2-yl]methoxy} phosphonic acid'	b'Fructose-6-Phosphate (closed form)'	HMDB02 57695	C6H13O9P	
		260.0297185	0.0010 185	Proton ation	b' {[(2R,3S,4S,5S)-3,4,5,6-tetrahydroxyoxan-2-yl]methoxy} phosphonic acid'	b'D-mannose 6-phosphate'	HMDB03 04312	C6H13O9P	C00 275
11	260.02	261.0307083	0.0010 917	Proton ation	b'(4-acetamido-3-methoxyphenyl)oxidanesulfonic acid'	b'2-Methoxyacetaminophen sulfate'	HMDB00 62550	C9H11NO6S	
7	4	261.0307078	0.0010 922	Proton ation	b'(2S)-2-amino-3-[4-(sulfooxy)phenyl]propanoic acid'	b'O-Sulfotyrosine'	HMDB01 55722	C9H11NO6S	
		260.0248197	0.0008 197	Redox	b'2-[bis(2-chloroethyl)amino]-1,3,2lambda5-oxazaphosphinan-2-one'	b'Cyclophosphamide'	HMDB00 14672	C7H15Cl2N2O2 P	C07 888
		260.0248197	0.0008 197	Redox	b'3-(2-chloroethyl)-2-[(2-chloroethyl)amino]-1,3,2lambda5-oxazaphosphinan-2-one'	b'Ifosfamide'	HMDB00 15312	C7H15Cl2N2O2 P	C07 047
		260.0248201	0.0008 201	Redox	b'2-[bis(2-chloroethyl)amino]-1,3,2-oxazaphosphinan-4-ol'	b'2-(Bis(2-chloroethyl)amino)-4-hydroxytetrahydro-2H-1,3,2-oxazaphosphorine'	HMDB02 46558	C7H15Cl2N2O2 P	
11	261.93	262.9411083	0.0010 083	Proton ation	b'(4-hydroxy-3-nitrophenyl)arsonic acid'	b'Roxarsone'	HMDB00 33205	C6H6AsNO6	
8	23								
11	263.97	263.9718274	0.0009 274	Redox	b'[(2-hydroxy-6-sulfanyl-9H-purin-9-yl)oxy] phosphonic acid'	b'Thioxanthine monophosphate'	HMDB00 60876	C5H5N4O5PS	
9	09								
1	264.95	265.9592695	0.0007 695	Proton ation	b' {[(2R)-2-hydroxy-3-(phosphonoxy)propanoyl]oxy} phosphonic acid'	b'Glyceric acid 1,3-biphosphate'	HMDB00 01270	C3H8O10P2	C00 236
2	07								

0		265.9592695	0.0007 695	Proton ation	b'(2R)-2,3-bis(phosphonoxy)propanoic acid'	b'2,3-Diphosphoglyceric acid'	HMDB00 01294	C3H8O10P2	C011 59
		265.9592705	0.0007 705	Proton ation	b'3-hydroxy-2- {[hydroxy(phosphonoxy)phosphoryl]oxy} propanoic acid'	b'3-Hydroxy-2- [hydroxy(phosphonoxy)phosphoryl]oxypropanoic acid'	HMDB02 58120	C3H8O10P2	
1 2 1	267.07 21	268.0807695	0.0008 695	Proton ation	b'9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-3H-purin-6-one'	b'Inosine'	HMDB00 00195	C10H12N4O5	C00 294
		268.0794321	0.0004 679	Proton ation	b'(4S,5R,6R,7R,8S)-4,5,6,7,8,9-hexahydroxy-2-oxononanoic acid'	b'3-Deoxy-D-glycero-D-galacto-2- nonulosonic acid'	HMDB00 00425	C9H16O9	
		268.0807695	0.0008 695	Proton ation	b'1-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1H,4H,7H-pyrazolo[3,4-d]pyrimidin-4-one'	b'Allopurinol riboside'	HMDB00 00481	C10H12N4O5	
		268.0807695	0.0008 695	Proton ation	b'9-[(3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-3H-purin-6-one'	b'Arabinosylhypoxanthine'	HMDB00 03040	C10H12N4O5	
		268.0807695	0.0008 695	Proton ation	b'2-(6-hydroxy-9H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol'	b'Ara-HX'	HMDB02 47301	C10H12N4O5	
		268.0807695	0.0008 695	Proton ation	b'3-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1H,6H,7H-pyrazolo[4,3-d]pyrimidin-7-one'	b'Formycin b'	HMDB02 52449	C10H12N4O5	
		268.0794321	0.0004 679	Proton ation	b'3,4,5,6-tetrahydroxy-6-(hydroxymethyl)oxan-2-yl 2-hydroxypropanoate'	b'Fructose lactate'	HMDB02 52491	C9H16O9	
		268.0794321	0.0004 679	Proton ation	b'2,3,4,5-tetrahydroxy-6-(hydroxymethyl)oxan-2-yl 2-hydroxypropanoate'	b'galactose lactate'	HMDB02 52580	C9H16O9	
1 2 2	267.26 78	268.2766158	0.0010 158	Proton ation	b'octadecanal'	b'Stearaldehyde'	HMDB00 02384	C18H36O	C01 838
		268.2766158	0.0010 158	Proton ation	b'(9Z)-octadec-9-en-1-ol'	b'Oleil alcohol'	HMDB00 29632	C18H36O	
		268.2766158	0.0010	Proton	b'2-octyl-3-pentyloxane'	b'(2R,3S)-2-Octyl-3-pentyloxane'	HMDB02	C18H36O	

			158	ation			42702		
		268.2766158	0.0010 158	Proton ation	b'octadec-9-en-1-ol'	b'9-Octadecen-1-ol, (9Z)-'	HMDB02 47606	C18H36O	
		268.2766158	0.0010 158	Proton ation	b'6,10,14-trimethylpentadecan-2-one'	b'6,10,14-Trimethylpentadecan-2-one'	HMDB03 03073	C18H36O	
1 2 3	272.00 52	273.0129492	5.08E- 05	Proton ation	b'2-[2-(thiophene-2-carbonylsulfanyl)propanamido]acetic acid'	b'Stepronin'	HMDB00 15492	C10H11NO4S2	
1 2 4	272.08 68	272.0896029	0.0028 029	Redox	b'(2R,3S,4S,5R,6S)-2-(hydroxymethyl)-6-(4-hydroxyphenoxy)oxane-3,4,5-triol'	b'Arbutin'	HMDB00 29943	C12H16O7	C06 186
1 2 5	272.99 92	274.0089831 274.0040842 274.0040842	0.0019 831 0.0029 158 0.0029 158	Proton ation Proton ation Proton ation	b'(2S,3S,4S,5R,6R)-3,4,5-trihydroxy-6-(phosphonoxy)oxane-2-carboxylic acid'	b'D-Glucuronic acid 1-phosphate'	HMDB00 03976	C6H11O10P	C05 385
					b'2-[bis(2-chloroethyl)amino]-1,3,2'x'ce'x'bb'xe2'x81'xb5-oxazaphosphinane-2,4-dione'	b'4-Ketocyclophosphamide'	HMDB00 60686	C7H13Cl2N2O3 P	C07 644
					b'3-(2-chloroethyl)-2-[(2-chloroethyl)amino]-1,3,2'x'ce'x'bb'xe2'x81'xb5-oxazaphosphinane-2,4-dione'	b'4-Ketofosfamide'	HMDB00 60690	C7H13Cl2N2O3 P	C16 554
1 2 6	273.03 26	274.0396719	0.0007 281	Proton ation	b'methyl 2-chloro-9-hydroxy-9H-fluorene-9-carboxylate'	b'Chlorfluorenol-methyl'	HMDB02 50098	C15H11ClO3	
1 2 7	279.23 15	280.2402303 280.2402303 280.2402303	0.0009 303 0.0009 303 0.0009 303	Proton ation Proton ation Proton ation	b'(9Z,12Z)-octadeca-9,12-dienoic acid'	b'Linoleic acid'	HMDB00 00673	C18H32O2	C01 595
					b'(9Z,11E)-octadeca-9,11-dienoic acid'	b'Bovinic acid'	HMDB00 03797	C18H32O2	C04 056
					b'(9E,11E)-octadeca-9,11-dienoic acid'	b'(9E,11E)-Octadecadienoic acid'	HMDB00 05047	C18H32O2	

		280.2402303	0.0009 303	Proton ation	b'(10E,12Z)-octadeca-10,12-dienoic acid'	b'(10E,12Z)-Octadecadienoic acid'	HMDB00 05048	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'(9E,12E)-octadeca-9,12-dienoic acid'	b'Linoelaidic acid'	HMDB00 06270	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'(9E,15E)-octadeca-9,15-dienoic acid'	b'Mangiferic acid'	HMDB00 29800	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'3,7-dimethylocta-1,6-dien-3-yl octanoate'	b'Linalyl caprylate'	HMDB00 30430	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'ethyl (2E,4Z)-hexadeca-2,4-dienoate'	b'Ethyl 2E,4Z-hexadecadienoate'	HMDB00 31051	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'octadec-5-ynoic acid'	b'5-Octadecynoic acid'	HMDB00 31097	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'(10Z,12Z)-octadeca-10,12-dienoic acid'	b'Dihomolinoleic acid'	HMDB00 61864	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'(6Z,9Z)-octadeca-6,9-dienoic acid'	b'6Z,9Z-octadecadienoic acid'	HMDB00 62238	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'(2E,4E)-octadeca-2,4-dienoic acid'	b'Octadecadienoate'	HMDB00 62784	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'octadeca-10,12-dienoic acid'	b'Octadeca-10,12-dienoic acid'	HMDB02 44277	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'octadec-17-ynoic acid'	b'17-Octadecynoic acid'	HMDB02 44776	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'octadec-7-ynoic acid'	b'7-Octadecynoic acid'	HMDB02 47278	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'octadeca-8,12-dienoic acid'	b'8,12-Octadecadienoic acid'	HMDB02 47466	C18H32O2	

		280.2402303	0.0009 303	Proton ation	b'octadeca-9,11-dienoic acid'	b'Octadeca-9,11-dienoic acid'	HMDB02 47620	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'octadeca-9,12-dienoic acid'	b'9Z,12E-Octadecadienoic acid'	HMDB02 47706	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'octadeca-2,4-dienoic acid'	b'Octadeca-2,4-dienoic acid'	HMDB02 55894	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'7-(2-octylcycloprop-1-en-1-yl)heptanoic acid'	b'Malvalic acid'	HMDB03 02286	C18H32O2	C08 321
		280.2402303	0.0009 303	Proton ation	b'octadeca-2,9-dienoic acid'	b'Octadeca-2,9-dienoic acid'	HMDB03 02650	C18H32O2	
		280.2402303	0.0009 303	Proton ation	b'(11E,15Z)-octadeca-11,15-dienoic acid'	b'trans-11,cis-15-Octadecadienoic acid'	HMDB03 04773	C18H32O2	
1 2 8	280.02	280.0170463	0.0029 537	Redox	b'dimethyl {[[(5-methoxy-4-oxo-4H-pyran-2-yl)methyl]sulfanyl}phosphonate'	b'Endothion'	HMDB02 51802	C9H13O6PS	C18 982
1 2 9	281.24 71	282.2558803	0.0009 803	Proton ation	b'(9Z)-octadec-9-enoic acid'	b'Oleic acid'	HMDB00 00207	C18H34O2	C00 712
		282.2558803	0.0009 803	Proton ation	b'(9E)-octadec-9-enoic acid'	b'Elaidic acid'	HMDB00 00573	C18H34O2	C01 712
		282.2558803	0.0009 803	Proton ation	b'octadec-6-enoic acid'	b'Petroselinic acid'	HMDB00 02080	C18H34O2	
		282.2558803	0.0009 803	Proton ation	b'(11E)-octadec-11-enoic acid'	b'Vaccenic acid'	HMDB00 03231	C18H34O2	C08 367
		282.2558803	0.0009 803	Proton ation	b'(13Z)-octadec-13-enoic acid'	b'(Z)-13-Octadecenoic acid'	HMDB00 41480	C18H34O2	
		282.2558803	0.0009	Proton	b'ethyl (9E)-hexadec-9-enoate'	b'Ethyl 9-hexadecenoate'	HMDB00	C18H34O2	

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282.2558803	0.0009 803	Proton ation	b'(7Z)-octadec-7-enoic acid'	b'7Z-octadecenoic acid'	HMDB00 62242	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'octadec-9-enoic acid'	b'Octadec-9-enoic Acid'	HMDB00 62703	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'(11Z)-octadec-11-enoic acid'	b'cis-Vaccenic acid'	HMDB02 40219	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'octadec-11-enoic acid'	b'11-Aoctadecenoic acid'	HMDB02 44344	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'octadec-2-enoic acid'	b'Octadecenoic acid'	HMDB02 45277	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'octadec-5-enoic acid'	b'Octadec-5-enoic acid'	HMDB02 46833	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'(7E)-octadec-7-enoic acid'	b'7-Octadecenoic acid'	HMDB03 02159	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'(10E)-octadec-10-enoic acid'	b'trans-10-Octadecenoic acid'	HMDB03 02289	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'(6E)-octadec-6-enoic acid'	b'6-Octadecenoic acid'	HMDB03 03337	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'(12Z)-octadec-12-enoic acid'	b'cis-12-Octadecenoic acid'	HMDB03 04764	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'octadec-15-enoic acid'	b'cis-15-Octadecenoic acid'	HMDB03 04765	C18H34O2			
282.2558803	0.0009 803	Proton ation	b'(12E)-octadec-12-enoic acid'	b'trans-12-Octadecenoic acid'	HMDB03 04766	C18H34O2			
282.2558803	0.0009	Proton	b'(14E)-octadec-14-enoic acid'	b'trans-14-Octadecenoic acid'	HMDB03	C18H34O2			

			803	ation			04767		
		282.2558803	0.0009 803	Proton ation	b'(15E)-octadec-15-enoic acid'	b'trans-15-Octadecenoic acid'	HMDB03 04768	C18H34O2	
		282.2558803	0.0009 803	Proton ation	b'(16E)-octadec-16-enoic acid'	b'trans-16-Octadecenoic acid'	HMDB03 04769	C18H34O2	
		282.2558803	0.0009 803	Proton ation	b'(4E)-octadec-4-enoic acid'	b'trans-4-Octadecenoic acid'	HMDB03 04770	C18H34O2	
		282.2558803	0.0009 803	Proton ation	b'(8E)-octadec-8-enoic acid'	b'trans-8-Elaidic acid'	HMDB03 04817	C18H34O2	
		281.2480553	0.0009 553	Redox	b'(6Z)-octadec-6-enoate'	b'petroselinic acid'	HMDB03 04458	C18H33O2	
1 3 0	282.03 71	282.0375673	0.0004 673	Redox	b'3-hydroxy-2-[3-hydroxy-6-(hydroxymethyl)-4-oxo-4H-pyran-2-yl]-6-(hydroxymethyl)-4H-pyran-4-one'	b'Bikojic acid'	HMDB00 34034	C12H10O8	
		282.0375673	0.0004 673	Redox	b'2-[[[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy]propanedioic acid'	b'2-O-Caffeoyltartronic acid'	HMDB00 40869	C12H10O8	
		282.0344139	0.0026 861	Redox	b'2-amino-3-[(2-carboxy-2-acetamidoethyl)disulfanyl]propanoic acid'	b'3-[[[(2R)-2-Acetamido-2-carboxyethyl]disulfanyl]-2-aminopropanoic acid'	HMDB02 47775	C8H14N2O5S2	
1 3 1	282.08 29	283.0916686	0.0009 686	Proton ation	b'2-amino-9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-1H-purin-6-one'	b'Guanosine'	HMDB00 00133	C10H13N5O5	C00 387
		283.0916686	0.0009 686	Proton ation	b'2-amino-8-hydroxy-9-[(2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-1H-purin-6-one'	b'8-Hydroxy-deoxyguanosine'	HMDB00 03333	C10H13N5O5	
		283.0916686	0.0009 686	Proton ation	b'2-(6-hydroxy-2-imino-3,9-dihydro-2H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol'	b'9-beta-D-Arabinofuranosylguanine'	HMDB02 46240	C10H13N5O5	
		283.0916685	0.0009 685	Proton ation	b'2-amino-9-[4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,7,8,9-tetrahydro-1H-purine-6,8-dione'	b'8-Hydroxy-2-desoxyguanosine'	HMDB02 47436	C10H13N5O5	

		283.0916685	0.0009 685	Proton ation	b'2-amino-9-[2,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-1H-purin-6-one'	b'hydroxydeoxyguanosine'	HMDB02 53263	C10H13N5O5	
		283.0916685	0.0009 685	Proton ation	b'1-[4-(azidoxy)-5-(hydroxymethyl)oxolan-2-yl]-5-methyl-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'1-[(2R,5R)-4-Azidoxy-5-(hydroxymethyl)oxolan-2-yl]-5-methylpyrimidine-2,4-dione'	HMDB02 57735	C10H13N5O5	
		283.0916685	0.0009 685	Proton ation	b'2-amino-9-[5-(hydroperoxymethyl)-4-hydroxyoxolan-2-yl]-6,9-dihydro-1H-purin-6-one'	b'2-Amino-9-[(2R,4S,5R)-5-(hydroperoxymethyl)-4-hydroxyoxolan-2-yl]-1H-purin-6-one'	HMDB02 57980	C10H13N5O5	
		282.0851862	0.0022 862	Redox	b'2-(butan-2-yl)-4,6-dinitrophenyl acetate'	b'Dinoseb acetate'	HMDB00 32560	C12H14N2O6	C19 119
		282.0804558	0.0024 442	Redox	b'2-(4-fluorophenyl)-5-(1-isocyanatoethyl)-1,3-benzoxazole'	b'Flunoxaprogen isocyanate'	HMDB02 52342	C16H11FN2O2	
		282.0851862	0.0022 862	Redox	b'4-acetamidophenyl 4-(nitrooxy)butanoate'	b'Nitroparacetamol'	HMDB02 55491	C12H14N2O6	
		282.0851862	0.0022 862	Redox	b'1-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-5-(prop-1-yn-1-yl)-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'Netivudine'	HMDB02 55549	C12H14N2O6	
1 3 2	283.00 26	283.0010747	0.0015 253	Redox	b'[1-hydroxy-1-phosphono-2-(pyridin-3-yl)ethyl]phosphonic acid'	b'Risedronate'	HMDB00 15022	C7H11NO7P2	C08 233
1 3 3	283.26 24	284.2715304	0.0013 304	Proton ation	b'octadecanoic acid'	b'Stearic acid'	HMDB00 00827	C18H36O2	C01 530
		284.2715304	0.0013 304	Proton ation	b'ethyl hexadecanoate'	b'Ethyl hexadecanoate'	HMDB00 29811	C18H36O2	
		284.2715304	0.0013 304	Proton ation	b'16-methylheptadecanoic acid'	b'16-Methylheptadecanoic acid'	HMDB00 31066	C18H36O2	C20 356
		284.2715304	0.0013	Proton	b'hexyl dodecanoate'	b'Hexyl dodecanoate'	HMDB00	C18H36O2	

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		284.2715304	0.0013 304	Proton ation	b'3-hydroxyoctadecan-2-one'	b'2-Octadecanone, 3-hydroxy-'	HMDB02 45276	C18H36O2	
		284.2688451	0.0013 549	Proton ation	b'3,6,10,13,16,19-hexaazabicyclo[6.6.6]icosane'	b'Sar chelate'	HMDB02 57487	C14H32N6	
1 3 4	285.07 18	286.082581 285.0722705	0.0029 81 0.0004 705	Proton ation Redox	b'4-amino-1-[5-azido-3-fluoro-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one'	b'Azvudine'	HMDB02 48824	C9H11FN6O4	
					b'2-amino-1H,1'H,6H,6'H-[9,9'-bipurine]-6,6'-dione"	b'2-Amino-9-(6-oxo-1H-purin-9-yl)- 1H-purin-6-one'	HMDB02 57944	C10H7N9O2	
1 3 5	286.07 42	287.0793725 287.0793725 287.0793725	0.0026 275 0.0026 275 0.0026 275	Proton ation Proton ation Proton ation	b'1,3,5-trihydroxy-4-methoxy-10-methyl-9,10-dihydroacridin-9-one'	b'Citrusinine II'	HMDB00 30373	C15H13NO5	
					b'1,3,6-trihydroxy-5-methoxy-10-methyl-9,10-dihydroacridin-9-one'	b'Grandisine III'	HMDB00 40683	C15H13NO5	
					b'2-methoxy-4-(4-methylbenzoyl)-6-nitrophenol'	b'3-O-Methyltolcapone'	HMDB02 44556	C15H13NO5	
1 3 6	286.97 6	287.980838	0.0029 62	Proton ation	b'dodecafluoropentane'	b'Dodecafluoropentane'	HMDB02 51565	C5F12	
1 3 7	290.08 71	291.0967539 291.0954165 291.0967539 291.0967539	0.0018 539 0.0005 165 0.0018 539 0.0018 539	Proton ation Proton ation Proton ation Proton ation	b'2-(hydroxymethyl)-5-{3H-imidazo[2,1-f]purin-3-yl}oxolane-3,4-diol'	b'1,N6-Ethenoadenosine'	HMDB02 44260	C12H13N5O4	
					b'3-acetamido-4-hydroxy-2-(1,2,3-trihydroxypropyl)-3,4-dihydro-2H-pyran-6-carboxylic acid'	b'2-Deoxy-2,3-dehydro-n-acetyl- neuraminic acid'	HMDB02 45680	C11H17NO8	
					b'methyl N-[2-oxo-5-(1,2,3,6-tetrahydropyridin-1-yl)-2H-[1,2,4]oxadiazolo[2,3-a]pyrimidin-7-yl]carbamate'	b'Carprazidil'	HMDB02 49688	C12H13N5O4	
					b'1-(6-amino-9H-purin-9-yl)-3-(hydroxymethyl)-2-oxabicyclo[3.2.0]hept-6-ene-4,5-diol'	b'Ethenoadenosine'	HMDB02 52011	C12H13N5O4	

1 3 8	291.08 96	292.0946882	0.0027 118	Proton ation	b'4-hydroxy-7-(hydroxymethyl)-2-(2-hydroxypropan-2-yl)-2H,3H,5H-furo[3,2-g]chromen-5-one'	b'(S)-Angelica'	HMDB00 30120	C15H16O6	
		292.0946882	0.0027 118	Proton ation	b'13,14-dihydroxy-8-methoxy-12,12-dimethyl-3,11-dioxatricyclo[8.4.0.0'xc2'xb2,\xc2'x81'xb7]tetradeca-1(10),2(7),5,8-tetraen-4-one'	b'trans-Grandmarin'	HMDB00 39030	C15H16O6	
		292.0946882	0.0027 118	Proton ation	b'(1R,5S,8S,13R,14R)-1-hydroxy-13-methyl-14-(prop-1-en-2-yl)-4,7,10-trioxapentacyclo[6.4.1.1'^{9,12}.0^{3,5}.0^{5,13}]tetradecane-6,11-dione'	b'Picrotoxinin'	HMDB02 40274	C15H16O6	
		292.0978555	0.0004 555	Proton ation	b'6-chloro-12-methyl-2-oxa-12,15-diazatetracyclo[7.5.3.0'xc2'xb9,\xc2'xb9'xc2'xb8'xc2'xb3,\xc2'xb8'xc2'xb8]heptadeca-3,5,7-trien-16-one'	b'(+)-(4Ar*,10R*,10aS*)-8-Chloro-1,2,3,4,10,10a-hexahydro-2-methyl-4a,10-(iminoethano)-4aH-(1)benzopyrano(3,2-c)pyridin-12-one'	HMDB02 42234	C15H17CIN2O2	
		291.0895433	5.67E- 05	Redox	b'2-[(1Z,3E)-4-(4-hydroxyphenyl)buta-1,3-dien-1-yl]-4H-3,1-benzoxazin-4-one'	b'Avenalumin III'	HMDB00 38956	C18H13NO3	
1 3 9	293.04 13	294.0496691	0.0005 691	Proton ation	b'(3E)-3-([bis(methylsulfanyl)methylidene]amino)methylidene)-1-methoxy-2,3-dihydro-1H-indol-2-one'	b'Wasalexin A'	HMDB00 34765	C13H14N2O2S2	
		294.0496691	0.0005 691	Proton ation	b'(3Z)-3-([bis(methylsulfanyl)methylidene]amino)methylidene)-1-methoxy-2,3-dihydro-1H-indol-2-one'	b'Wasalexin B'	HMDB00 34768	C13H14N2O2S2	
		294.0496691	0.0005 691	Proton ation	b'N-[bis(methylsulfanyl)methylidene]-1-methoxy-1H-indole-3-carboxamide'	b'Methoxybrassenin B'	HMDB00 38636	C13H14N2O2S2	
		293.0421561	0.0008 561	Redox	b'([2-(diethylamino)-6-methylpyrimidin-4-yl]oxy)(sulfanyl)sulfanylidene phosphinous acid'	b'Pirimiphos'	HMDB02 56599	C9H16N3O2PS2	
1 4 0	297.01 75	297.0145755	0.0029 245	Redox	b'2-chloro-5-[(2-chlorophenyl)methyl]-4H,5H,6H,7H-thieno[3,2-c]pyridine'	b'2-Chloroticlopidine'	HMDB00 13922	C14H13Cl2NS	
1 4 1	299.05 23	299.0518514	0.0004 486	Redox	b'([amino]{2-[(2-hydroxypropanoyl)peroxy]-2-oxoethyl}(methyl)amino)methylidene]amino]phosphonic acid'	b'Phosphocreatine lactate'	HMDB02 56473	C7H14N3O8P	

1 4 2	300.03 86	301.0467518	0.0003 518	Proton ation	b'[(2R,3R,4R,5R,6R)-5-acetamido-4,6-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxidanesulfonic acid'	b'N-Acetyl galactosamine 4-sulphate'	HMDB00 00781	C8H15NO9S	C16 265
		301.0467518	0.0003 518	Proton ation	b'([(2R,3S,4R,5R,6R)-5-acetamido-3,4,6-trihydroxyoxan-2-yl]methoxy)sulfonic acid'	b'N-Acetyl glucosamine 6-sulfate'	HMDB00 00814	C8H15NO9S	C04 132
		301.0467518	0.0003 518	Proton ation	b'([(2R,3R,4R,5R)-5-acetamido-2,3,4-trihydroxy-6-oxohexyl]oxy)sulfonic acid'	b'N-Acetyl galactosamine 6-sulfate'	HMDB00 00841	C8H15NO9S	
		301.0467522	0.0003 522	Proton ation	b'N-{2,4,5-trihydroxy-6-[(sulfooxy)methyl]oxan-3-yl}ethanimidic acid'	b'2-(Acetyl amino)-2-Deoxy-6-O-Sulfo- alpha-D-Glucopyranose'	HMDB02 44937	C8H15NO9S	
		300.038236 64	0.0003	Redox	b'2-amino-3-oxo-3H-phenoxazine-1,9-dicarboxylic acid'	b'Cinnavalinate'	HMDB00 04078	C14H8N2O6	C05 640
1 4 3	300.04 68	301.0562676	0.0016 676	Proton ation	b'([(2R,3S,4R,5R)-5-acetamido-3,4,6-trihydroxyoxan-2-yl]methoxy)phosphonic acid'	b'N-Acetyl-D-Glucosamine 6- Phosphate'	HMDB00 01062	C8H16NO9P	C00 357
		301.0562676	0.0016 676	Proton ation	b'([(2R,3S,4R,5S,6S)-5-acetamido-3,4,6-trihydroxyoxan-2-yl]methoxy)phosphonic acid'	b'N-Acetyl-D-mannosamine 6- phosphate'	HMDB00 01121	C8H16NO9P	C04 257
		301.0562676	0.0016 676	Proton ation	b'([(3R,4R,5S,6R)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)phosphonic acid'	b'N-Acetyl-glucosamine 1-phosphate'	HMDB00 01367	C8H16NO9P	C04 256
		301.0562676	0.0016 676	Proton ation	b'([(2R,3S,4R,5R,6S)-5-acetamido-3,4,6-trihydroxyoxan-2-yl]methoxy)phosphonic acid'	b'N-Acetyl glucosamine 6-phosphate'	HMDB00 02817	C8H16NO9P	
		301.0562676	0.0016 676	Proton ation	b'([(3R,4R,5R,6R)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)phosphonic acid'	b'N-Acetyl-D-galactosamine 1- phosphate'	HMDB00 06480	C8H16NO9P	
		301.0562676	0.0016 676	Proton ation	b'N-[(2R,3R,4R,5R,6R)-4,5-dihydroxy-6-(hydroxymethyl)-2-(phosphonoxy)oxan-3-yl]ethanimidic acid'	b'N-acetyl-alpha-D-galactosamine 1- phosphate'	HMDB00 59626	C8H16NO9P	C18 060
		301.0562681	0.0016 681	Proton ation	b'([(2R,3S,4R,5S,6R)-5-acetamido-3,4,6-trihydroxyoxan-2-yl]methoxy)phosphonic acid'	b'N-Acetylmannosamine-6P'	HMDB00 62500	C8H16NO9P	
		301.0562681	0.0016 681	Proton ation	b'[(5-acetamido-3,4,6-trihydroxyoxan-2-yl)methoxy]phosphonic acid'	b'(5-Acetamido-3,4,6-trihydroxyoxan- 2-yl)methyl dihydrogen phosphate'	HMDB02 52741	C8H16NO9P	

		301.0521119	0.0024 881	Proton ation	b'methyl N-[6-(thiophene-2-carbonyl)-1H-1,3-benzodiazol-2-yl]carbamate'	b'Nocodazole'	HMDB02 55688	C14H11N3O3S	C13 719
		300.048132	0.0013 32	Redox	b'2-{2-[(5-formylfuran-2-yl)methoxy]-2-oxoethyl}-2-hydroxybutanedioic acid'	b'Mumefural'	HMDB00 35179	C12H12O9	
1	301.06	301.0636342	0.0001 342	Redox	b'4-{4-[bis(2-chloroethyl)amino]phenyl}but-3-enoic acid'	b'3,4-Dehydrochlorambucil'	HMDB02 46018	C14H17Cl2NO2	
4	35	301.0636342	0.0001 342	Redox	b'N-(2,3-dichloro-4-hydroxyphenyl)-1-methylcyclohexane-1-carboxamide'	b'Fenhexamid'	HMDB02 52201	C14H17Cl2NO2	C18 593
1	302.05	302.0473614	0.0029 386	Redox	b'5-{[(4-hydroxyphenyl)methylidene]amino}-3-methyl-4H,5H,6H,7H-[1,2]thiazolo[5,4-d]pyrimidine-4,6-dione'	b'5-((p-Hydroxybenzylidene)amino)-3-methylisothiazolo[5,4-d]pyrimidine-4,6(5H,7H)-dione'	HMDB02 53558	C13H10N4O3S	
4	03	302.0512007	0.0009 007	Redox	b''1H,1'H,2H,2'H,3H,3'H,6H,6'H-[9,9'-bipurine]-2,2',6,6'-tetrone"	b'9-(2,6-Dioxo-3H-purin-9-yl)-3H-purine-2,6-dione'	HMDB02 57773	C10H6N8O4	
1	303.08	304.0906655	0.0015 655	Proton ation	b'(2S)-2-[(2S)-3-carboxy-2-acetamidopropanamido]pentanedioic acid'	b'N-Acetylasparylglutamic acid'	HMDB00 01067	C11H16N2O8	C12 270
4	13	304.0866221	0.0024 779	Proton ation	b''2-({4'-chloro-[1,1'-biphenyl]-4-yl} methoxy)-2-methylpropanoic acid"	b'Cloubazart'	HMDB02 50334	C17H17ClO3	
6		304.0911006	0.0020 006	Proton ation	b''4-{2',4'-difluoro-[1,1'-biphenyl]-4-yl}-2-methyl-4-oxobutanoic acid"	b'Floubufen'	HMDB02 52307	C17H14F2O3	
		304.0866221	0.0024 779	Proton ation	b'methyl 2-({4'-chloro-[1,1'-biphenyl]-4-yl}oxy)-2-methylpropanoate"	b'Methyl clofenapate'	HMDB02 54582	C17H17ClO3	
		304.0906655	0.0015 655	Proton ation	b'2-(3-carboxy-2-acetamidopropanamido)pentanedioic acid'	b'N-Acetyl-L-aspartylglutamic acid'	HMDB02 55414	C11H16N2O8	C12 270
		304.0898173	0.0007 173	Proton ation	b'4-(methylsulfanyl)phenyl dipropyl phosphate'	b'Propaphos'	HMDB02 56818	C13H21O4PS	C19 013
		303.0792843	0.0020	Redox	b'4-{4-[bis(2-chloroethyl)amino]phenyl}butanoic acid'	b'Chlorambucil'	HMDB00	C14H19Cl2NO2	C06

			157				14436		900
1 4 7	303.23 21	304.2402303	0.0003 303	Proton ation	b'(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid'	b'Arachidonic acid'	HMDB00 01043	C20H32O2	C00 219
		304.2402303	0.0003 303	Proton ation	b'(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoic acid'	b'Cis-8,11,14,17-Eicosatetraenoic acid'	HMDB00 02177	C20H32O2	
		304.2402303	0.0003 303	Proton ation	b'(1S,2S,3S,7S,10R,11S,14S,15S)-14-hydroxy-2,3,15-trimethyltetracyclo[8.7.0.0\xc2\xba2,\xc2\xba1\xb7.0\xc2\xba9\xc2\xba9,\xc2\xba9\xc2\xba1\xb5]heptadecan-5-one'	b'Mesterolone'	HMDB00 06036	C20H32O2	D04 947
		304.2402303	0.0003 303	Proton ation	b'(1S,2S,4R,7S,10R,11S,14S,15S)-14-hydroxy-2,4,15-trimethyltetracyclo[8.7.0.0\xc2\xba2,\xc2\xba1\xb7.0\xc2\xba9\xc2\xba9,\xc2\xba9\xc2\xba1\xb5]heptadecan-5-one'	b'Drostanolone'	HMDB00 14996	C20H32O2	C14 605
		304.2402303	0.0003 303	Proton ation	b'5-(hydroxymethyl)-5,9,14-trimethyltetracyclo[11.2.1.0\xc2\xba9,\xc2\xba9\xc2\xba1\xb0.0\xc2\xba1\xb4,\xc2\xba1\xb9]hexadec-14-en-2-ol'	b'Sideridiol'	HMDB00 36702	C20H32O2	
		304.2402303	0.0003 303	Proton ation	b'14-(hydroxymethyl)-5,9-dimethyltetracyclo[11.2.1.0\xc2\xba9,\xc2\xba9\xc2\xba1\xb0.0\xc2\xba1\xb4,\xc2\xba1\xb9]hexadecane-5-carbaldehyde'	b'ent-17-Hydroxy-16beta-kauran-19-al'	HMDB00 36721	C20H32O2	
		304.2402303	0.0003 303	Proton ation	b'7-ethenyl-1,1,4a,7-tetramethyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrene-2,6-diol'	b'Yucalexin P21'	HMDB00 36754	C20H32O2	
		304.2402303	0.0003 303	Proton ation	b'(2Z)-5-(5,5,8a-trimethyl-2-methylidene-decahydronaphthalen-1-yl)-3-methylpent-2-enoic acid'	b'Copalic acid'	HMDB00 36829	C20H32O2	
		304.2402303	0.0003 303	Proton ation	b'1,4a-dimethyl-5-(3-methyl-5-oxopentyl)-6-methylidene-decahydronaphthalene-1-carbaldehyde'	b'Junicedral'	HMDB00 36830	C20H32O2	
		304.2402303	0.0003 303	Proton ation	b'(2Z)-5-(2,5,5,8a-tetramethyl-1,4,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)-3-methylpent-2-enoic acid'	b'7,13-Eperudien-15-oic acid'	HMDB00 37824	C20H32O2	
		304.2402303	0.0003 303	Proton ation	b'6-(hydroxymethyl)-2,6,12-trimethyltetracyclo[11.2.1.0\xc2\xba9,\xc2\xba9\xc2\xba1\xb0.0\xc2\xba2,\xc2\xba1\xb7]hexadec-11-en-4-ol'	b'Oryzalexin S'	HMDB00 39687	C20H32O2	
		304.2402303	0.0003 303	Proton ation	b'(2R,4aR,4bS,7S,10aR)-7-ethenyl-1,1,4a,7-tetramethyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrene-2,4b-diol'	b'Oryzalexin E'	HMDB00 39702	C20H32O2	
		304.2402303	0.0003	Proton	b'3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenoic acid'	b'2,6,10,14-Hexadecatetraenoic acid,	HMDB02	C20H32O2	

			973				03943		617
1 4 9	305.01 66	306.0253019	0.0009 019	Proton ation	b'1-[(3aR,4R,6R,6aR)-2-hydroxy-6-(hydroxymethyl)-2-oxo-tetrahydro-2H-2'xco'xb'x2'x81'xb5-furo[3,4-d][1,3,2]dioxaphosphol-4-yl]-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'Uridine 2',3'-cyclic phosphate"	HMDB00 11640	C9H11N2O8P	C02 355
1 5 0	305.24 69	306.2558803	0.0011 803	Proton ation	b'(8Z,11Z,14Z)-icosa-8,11,14-trienoic acid'	b'Dihomo-gamma-linolenic acid'	HMDB00 02925	C20H34O2	C03 242
		306.2558803	0.0011 803	Proton ation	b'(5Z,8Z,11Z)-icosa-5,8,11-trienoic acid'	b'5,8,11-Eicosatrienoic acid'	HMDB00 10378	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'(5Z,11E,14E)-icosa-5,11,14-trienoic acid'	b'Sciadonic acid'	HMDB00 31058	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'5-[5-(hydroxymethyl)-1,2,4a-trimethyl-1,2,3,4,4a,7,8,8a-octahydronaphthalen-1-yl]-3-methylpent-1-en-3-ol'	b'Sagittariol'	HMDB00 36835	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'(11Z,14Z,17Z)-icosa-11,14,17-trienoic acid'	b'Dihomo-alpha-linolenic acid'	HMDB00 60039	C20H34O2	C16 522
		306.2558803	0.0011 803	Proton ation		b'11-Eicosatrienoic acid'	HMDB02 44353	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'icosa-11,14,17-trienoic acid'	b'Eicosa-11,14,17-trienoic acid'	HMDB02 44373	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'icosa-5,8,11-trienoic acid'	b'Eicosa-5,8,11-trienoic acid'	HMDB02 45590	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'icosa-5,11,14-trienoic acid'	b'5,11,14-Eicosatrienoic acid'	HMDB02 46847	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'icosa-8,11,14-trienoic acid'	b'Dihomo-linolenic acid'	HMDB02 47333	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'icosa-2,4,6-trienoic acid'	b'Icosa-2,4,6-trienoic acid'	HMDB02 51723	C20H34O2	

1 5 1	306.07 53	306.2558803	0.0011 803	Proton ation	b'ethyl octadeca-9,12,15-trienoate'	b'Ethyl octadeca-9,12,15-trienoate'	HMDB02 52049	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'ethyl (9Z,12Z,15Z)-octadeca-9,12,15-trienoate'	b'Ethyl alpha-linolenate'	HMDB03 02158	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'(1S,4S,5R,9S,10R,13R,14R)-5-(hydroxymethyl)-5,9,14-trimethyltetraacyclo[11.2.1.0'xc2'xb9,\xc2'xb9'\xc2'xb0.0'xc2'xb4,\xc2'xb8'\xc2'xb9]hexadecan-14-ol'	b'ent-16b-Kauran-16,19-diol'	HMDB03 02662	C20H34O2	
		306.2558803	0.0011 803	Proton ation	b'ethyl (9E,12E,15E)-octadeca-9,12,15-trienoate'	b'Ethyl linolenate'	HMDB03 02813	C20H34O2	
		306.253475	0.0012 25	Proton ation	b'sodium octadecanoate'	b'Sodium octadecanoate'	HMDB03 03349	C18H35NaO2	
		305.2486039	0.0017 039	Redox	b'icosa-8,11,14-trienoate'	b'di-homo-gamma-linolenate'	HMDB03 04332	C20H33O2	
	306.07 53	307.083806	0.0007 06	Proton ation	b'(2S)-2-amino-4-([(1R)-1-[(carboxymethyl)carbamoyl]-2-sulfanylethyl]carbamoyl)butanoic acid'	b'Glutathione'	HMDB00 00125	C10H17N3O6S	C00 051
		307.0844579	0.0013 579	Proton ation	b'2-acetyl-5-hydroxy-11-methyl-6H,11H-furo[2,3-c]acridin-6-one'	b'Hallacridone'	HMDB00 29826	C18H13NO4	
		307.0844579	0.0013 579	Proton ation	b'15-hydroxy-16-methoxy-10-methyl-10-azatetracyclo[7.7.1.0'xc2'xb2,\xc2'xb8'\xc2'xb7.0'xc2'xb9'\xc2'xb3,\xc2'xb9'\xc2'xb8'\xc2'xb7]heptadeca-1(17),2,4,6,8,13,15-heptaene-11,12-dione'	b'Aristolodione'	HMDB00 33247	C18H13NO4	
		307.0838065	0.0007 065	Proton ation	b'2-amino-4-([1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-sulfanylethyl]-C-hydroxycarbonimidoyl)butanoic acid'	b'Glutathione(1-)'	HMDB00 62697	C10H17N3O6S	
		307.0844579	0.0013 579	Proton ation	b'methyl 2-[(3,4-dioxo-3,4-dihydronaphthalen-1-yl)amino]benzoate'	b'Methyl 2-[(3,4-dihydro-3,4-dioxo-1-naphthalenyl)amino]benzoate'	HMDB02 44408	C18H13NO4	
		306.0739528	0.0013 472	Redox	b'(2R,3R)-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol'	b'(-)-Epigallocatechin'	HMDB00 38361	C15H14O7	C12 136
		306.0739528	0.0013 472	Redox	b'(2R,3S)-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol'	b'(+) -Gallocatechin'	HMDB00 38365	C15H14O7	C12 127

		306.0739528	0.0013 472	Redox	b'(2S,3R)-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol'	b'4-Gallocatechol'	HMDB03 02404	C15H14O7	
		306.0739528	0.0013 472	Redox	b'2-(3,4-dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,4,5,7-tetrol'	b'Leucocyanidin'	HMDB03 03660	C15H14O7	
1 5 2	307.26 21	308.2715304	0.0016 304	Proton ation	b'(11Z,14Z)-icosa-11,14-dienoic acid'	b'Eicosadienoic acid'	HMDB00 05060	C20H36O2	C16 525
		308.2715304	0.0016 304	Proton ation	b'1-(3-hydroxy-3-methylpent-4-en-1-yl)-2,5,5,8a-tetramethyl-decahydronaphthalen-2-ol'	b'Sclareol'	HMDB00 36827	C20H36O2	C09 183
		308.2715304	0.0016 304	Proton ation	b'(8Z,11Z)-icosa-8,11-dienoic acid'	b'8Z,11Z-eicosadienoic acid'	HMDB00 62432	C20H36O2	
		308.2715304	0.0016 304	Proton ation	b'icosa-11,14-dienoic acid'	b'11,14-Eicosadienoic acid'	HMDB02 44372	C20H36O2	
		308.2715304	0.0016 304	Proton ation	b'icosa-2,4-dienoic acid'	b'Eicosadienic acid'	HMDB02 51719	C20H36O2	
		308.2715304	0.0016 304	Proton ation	b'ethyl octadeca-9,12-dienoate'	b'Ethyl linoleate'	HMDB02 52048	C20H36O2	
		308.2715304	0.0016 304	Proton ation	b'methyl 8-(2-octylcycloprop-1-en-1-yl)octanoate'	b'Methyl sterculate'	HMDB02 54613	C20H36O2	
		308.2715304	0.0016 304	Proton ation	b'icosa-2,6-dienoic acid'	b'Icosa-2,6-dienoic acid'	HMDB02 60426	C20H36O2	
		308.2715304	0.0016 304	Proton ation	b'ethyl (9E,12Z)-octadeca-9,12-dienoate'	b'Ethyl (Z,Z)-9,12-octadecadienoate'	HMDB03 03389	C20H36O2	
1 5 3	308.09 74	309.1059812	0.0007 812	Proton ation	b'(2S,4S,5R,6R)-5-acetamido-2,4-dihydroxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]oxane-2-carboxylic acid'	b'N-Acetylneuraminic acid'	HMDB00 00230	C11H19NO9	C19 910
		309.1059812	0.0007 812	Proton ation	b'(2R,4S,5R,6R)-5-acetamido-2,4-dihydroxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]oxane-2-carboxylic acid'	b'N-Acetyl-a-neuraminic acid'	HMDB00 00773	C11H19NO9	C19 909

		309.1059812	0.0007 812	Proton ation	b'5-acetamido-2,4-dihydroxy-6-(1,2,3-trihydroxypropyl)oxane-2-carboxylic acid'	b'3h-Sialic acid'	HMDB02 46275	C11H19NO9	
		309.1059812	0.0007 812	Proton ation	b'4-amino-5-oxo-5-[(2,3,4,5-tetrahydroxy-6-oxohexyl)oxy]pentanoic acid'	b'Glucose-6-glutamate'	HMDB02 52776	C11H19NO9	
		309.1059812	0.0007 812	Proton ation	b'6-[3-(acetyloxy)-1,2-dihydroxypropyl]-5-amino-2,4-dihydroxyoxane-2-carboxylic acid'	b'9-O-Acetylneuraminic acid'	HMDB02 55839	C11H19NO9	
		309.1059812	0.0007 812	Proton ation	b'5-acetamido-4,6,7,8,9-pentahydroxy-2-oxononanoic acid'	b'Aceneuramic acid'	HMDB02 59583	C11H19NO9	
1 5 4	308.97 83	309.9854843	0.0006 157	Proton ation	b' {[(2R,3R,4S,5R)-3,4-dihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl]oxy} phosphonic acid'	b'Ribose 1,5-bisphosphate'	HMDB00 11688	C5H12O11P2	C011 51
		309.9854852	0.0006 148	Proton ation	b' {[3,4-dihydroxy-2-oxo-5-(phosphonoxy)pentyl]oxy} phosphonic acid'	b'D-Ribulose 1,5-bisphosphate'	HMDB02 44230	C5H12O11P2	
		309.9854852	0.0006 148	Proton ation	b' ({hydroxy[(3,4,5-trihydroxy-2-oxopentyl)oxy]phosphoryl}oxy) phosphonic acid'	b'Phosphono [(3S,4S)-3,4,5-trihydroxy-2-oxopentyl] hydrogen phosphate'	HMDB02 60366	C5H12O11P2	
		309.9854843	0.0006 157	Proton ation	b' {[(3R,4R)-3,4-dihydroxy-2-oxo-5-(phosphonoxy)pentyl]oxy} phosphonic acid'	b'D-ribulose-1,5-bisphosphate'	HMDB03 04322	C5H12O11P2	C011 82
1 5 5	309.27 89	310.2871805	0.0004 805	Proton ation	b'(11Z)-icos-11-enoic acid'	b'11Z-Eicosenoic acid'	HMDB00 02231	C20H38O2	C16 526
		310.2871805	0.0004 805	Proton ation	b'ethyl (9E)-octadec-9-enoate'	b'Ethyl oleate'	HMDB00 34451	C20H38O2	C03 425
		310.2871805	0.0004 805	Proton ation	b'(13Z)-icos-13-enoic acid'	b'Paullinic acid'	HMDB00 35159	C20H38O2	
		310.2871805	0.0004 805	Proton ation	b'icosane-6,8-dione'	b'6,8-Icosanedione'	HMDB00 35572	C20H38O2	
		310.2871805	0.0004 805	Proton ation	b'icosane-5,7-dione'	b'5,7-Icosanedione'	HMDB00 35573	C20H38O2	

		310.2871805	0.0004 805	Proton ation	b'icosane-4,6-dione'	b'4,6-Icosanedione'	HMDB00 35574	C20H38O2	
		310.2871805	0.0004 805	Proton ation	b'(9E)-octadec-9-en-1-yl acetate'	b'Oleoyl acetate'	HMDB00 37127	C20H38O2	
		310.2871805	0.0004 805	Proton ation	b'(9Z)-icos-9-enoic acid'	b'9Z-Eicosenoic acid'	HMDB00 62436	C20H38O2	
		310.2871805	0.0004 805	Proton ation	b'icos-2-enoic acid'	b'Icos-2-enoic acid'	HMDB02 47671	C20H38O2	
		310.2871805	0.0004 805	Proton ation	b'ethyl octadec-9-enoate'	b'Ethyl octadec-9-enoate'	HMDB02 52058	C20H38O2	
1 5 6	309.87 1	309.87154	0.0005 4	Redox	b'1,4-diiodobutane'	b'1,4-Diiodobutane'	HMDB02 44214	C4H8I2	
1 5 7	312.06 88	312.0665554 312.0699267	0.0022 446 0.0011 267	Redox Redox	b'2-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]acetic acid'	b'Lonazolac'	HMDB02 54157	C17H13ClN2O2	
					b'N-(4-aminobutyl)-5-chloronaphthalene-2-sulfonamide'	b'N-(4-Aminobutyl)-5-chloronaphthalene-2-sulfonamide'	HMDB02 59886	C14H17ClN2O2 S	
1 5 8	316.07 39	316.0729074 316.0729074	0.0009 926 0.0009 926	Redox Redox	b'(2R)-2-amino-3-({6-[(2S)-2-amino-2-carboxyethyl]-2,3-dihydroxyphenyl}sulfanyl)propanoic acid'	b'2-S-cysteinyl-DOPA'	HMDB00 62734	C12H16N2O6S	
					b'2-amino-3-([5-(2-amino-2-carboxyethyl)-2,3-dihydroxyphenyl]sulfanyl)propanoic acid'	b'5-S-Cysteinyl-Dopa'	HMDB02 44850	C12H16N2O6S	
1 5 9	319.04 3	320.0532174 320.0532173 320.0532174	0.0024 174 0.0024 173 0.0024	Proton ation Proton ation Proton	b'3,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-4-one'	b'trans-3,3',4',5,5',7'-Hexahydroxyflavanone"	HMDB00 30835	C15H12O8	
					b'4,5,7-trihydroxy-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3-one'	b'(2S)-4,5,7-Trihydroxy-2-(3,4,5-trihydroxyphenyl)-4H-chromen-3-one'	HMDB02 55326	C15H12O8	
					b'ethyl 7,8,9-trihydroxy-3,5-dioxo-1H,2H,3H,5H-cyclopenta[c]isochromene-1-carboxylate'	b'Ethyl brevifolincarboxylate'	HMDB03	C15H12O8	

			174	ation			03706		
1 6 0	322.04 25	323.051851	0.0015 51	Proton ation	b'{{{(2R,3S,4R,5R)-5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl}methoxy}phosphonic acid'	b'Cytidine monophosphate'	HMDB00 00095	C9H14N3O8P	C00 055
		323.051851	0.0015 51	Proton ation	b'{{{(3R,4R,5R)-2-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-4-hydroxy-5-(hydroxymethyl)oxolan-3-yl}oxy}phosphonic acid'	b"Cytidine 2'-phosphate"	HMDB00 11692	C9H14N3O8P	C03 104
		323.051851	0.0015 51	Proton ation	b'{{{(2R,3S,4R,5R)-5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl}oxy}phosphonic acid'	b"Cytidine 3'-monophosphate"	HMDB02 40312	C9H14N3O8P	C05 822
		323.051851	0.0015 51	Proton ation	b'{{{3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl}methoxy}phosphonic acid'	b"Cytosine arabinose-5'-phosphate"	HMDB02 43501	C9H14N3O8P	
		323.0479841	0.0023 159	Proton ation	b'1-chloro-4-[1-(4-chlorophenyl)-2-nitrobutyl]benzene'	b'BULAN'	HMDB02 49435	C16H15Cl2NO2	
		323.0495256	0.0007 744	Proton ation	b'4-{2-[4-(dimethylamino)phenyl]diazen-1-yl}benzene-1-sulfonyl chloride'	b'Dabsyl chloride'	HMDB02 50819	C14H14ClN3O2 S	
		323.0495251	0.0007 749	Proton ation	b'2-{(4-chloro-6-[(2,3-dimethylphenyl)amino]pyrimidin-2-yl)sulfonyl}acetic acid'	b'Pirininix acid'	HMDB02 56601	C14H14ClN3O2 S	C15 617
1 6 1	323.02 7	324.0358665	0.0010 665	Proton ation	b'{{{(2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl}methoxy}phosphonic acid'	b"Uridine 5'-monophosphate"	HMDB00 00288	C9H13N2O9P	C00 105
		324.0358665	0.0010 665	Proton ation	b'{{{(2R,3S,4R,5S)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)-3,4-dihydroxyoxolan-2-yl}methoxy}phosphonic acid'	b"Pseudouridine 5'-phosphate"	HMDB00 01271	C9H13N2O9P	C011 68
		324.0358665	0.0010 665	Proton ation	b'{{{(2R,3R,4R,5R)-2-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-4-hydroxy-5-(hydroxymethyl)oxolan-3-yl}oxy}phosphonic acid'	b"Uridine 2'-phosphate"	HMDB00 11641	C9H13N2O9P	C03 031
		324.0358665	0.0010 665	Proton ation	b'{{{(2R,3S,4R,5R)-4-hydroxy-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)-2-(hydroxymethyl)oxolan-3-yl}oxy}phosphonic acid'	b"Uridine 3'-monophosphate"	HMDB00 60282	C9H13N2O9P	C01 368
		324.0335412	0.0012 588	Proton ation	b'1-(4-chlorophenyl)-3-(4-methylbenzenesulfonyl)urea'	b'1-(4-Chlorophenyl)-3-((4-methylphenyl)sulfonyl)urea'	HMDB02 46250	C14H13ClN2O3 S	
		324.035867	0.0010	Proton	b'{{{5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl}methoxy}phosphonic acid'	b'[(2S,3R,4R,5R)-5-(2,4-	HMDB02	C9H13N2O9P	

			67	ation		Dioxypyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl dihydrogen phosphate'	47871		
		324.0319997	0.0028 003	Proton ation	b'4-chlorophenyl 2-(4-chlorophenoxy)-2-methylpropanoate'	b'Dulofibrate'	HMDB02 51637	C16H14Cl2O3	
1 6 2	324.03	325.0401358	0.0023 358	Proton ation	b'[(2,5-dichlorophenyl)amino](hexyloxy)phosphinic acid'	b'Hexyl 2,5-dichlorophenylphosphoramidate'	HMDB02 53167	C12H18Cl2NO3 P	
		324.0272191	0.0027 809	Redox	b'(2S,4S)-4-(ethylamino)-2-methyl-1,1-dioxo-2H,3H,4H-1'x'ce'x'bb'x'e2'x'81'x'b6'-thieno[2,3-b]thiopyran-6-sulfonamide'	b'Dorzolamide'	HMDB00 15007	C10H16N2O4S3	C06 969
1 6 3	325.02 95	326.0394993	0.0021 993	Proton ation	b'2-{2-oxo-1-[2-(thiophen-2-yl)acetamido]ethyl}-5,6-dihydro-2H-1,3-thiazine-4-carboxylic acid'	b'(2R)-2-{(1R)-2-Oxo-1-[(2-thienylacetyl)amino]ethyl}-5,6-dihydro-2H-1,3-thiazine-4-carboxylic acid'	HMDB02 42604	C13H14N2O4S2	
		326.0394983	0.0021 983	Proton ation	b'7-hydroxy-11-(hydroxymethyl)-15-methyl-12,13-dithia-9,15-diazatetracyclo[9.2.2.0'x'c2'x'b9.0'x'e2'x'81'x'b9.0'x'e2'x'b3'x'e2'x'81'x'b8]pentadeca-3,5-diene-10,14-dione'	b'Gliotoxin'	HMDB02 52746	C13H14N2O4S2	
		325.0303306	0.0008 306	Redox	b'2-amino-7-(1,2-dihydroxyethyl)-6-(methylsulfonyl)-1H,4H-thieno[3,2-g]pteridin-4-one'	b'Urothion'	HMDB00 02377	C11H11N5O3S2	
		325.0272487	0.0022 513	Redox	b'2-{2-[(2,6-dichloro-4-methoxyphenyl)amino]phenyl}acetic acid'	b'2-{(2,6-Dichloro-4-methoxyphenyl)amino}phenylacetic acid'	HMDB02 50053	C15H13Cl2NO3	
		325.0287901	0.0007 099	Redox	b'2-[6-(5-chloro-2-methoxyphenyl)-4-oxo-2-sulfonylidene-1,2,3,4-tetrahydropyrimidin-1-yl]acetamide'	b'2-(6-(5-Chloro-2-methoxyphenyl)-4-oxo-2-thioxo-3,4-dihydropyrimidin-1(2H)-yl)acetamide'	HMDB02 56364	C13H12ClN3O3 S	
1 6 4	325.06 37	326.070796	0.0007 04	Proton ation	b'triphenyl phosphate'	b'TRIPHENYL PHOSPHATE'	HMDB02 59262	C18H15O4P	C14 235

1 6 5	327.23 17	328.2402303	0.0007 303	Proton ation	b'(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoic acid'	b'Docosahexaenoic acid'	HMDB00 02183	C22H32O2	C06 429
		328.2402303	0.0007 303	Proton ation	b'5-methyl-4-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-yl]benzene-1,3-diol'	b'Neogrifolin'	HMDB00 30053	C22H32O2	
		328.2402303	0.0007 303	Proton ation	b'5-methyl-2-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-yl]benzene-1,3-diol'	b'Grifolin'	HMDB00 30446	C22H32O2	
		328.2402303	0.0007 303	Proton ation	b'(2E,4E,6Z,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-yl acetate'	b'Retinol acetate'	HMDB00 35185	C22H32O2	
		328.2402303	0.0007 303	Proton ation	b'2-methyl-5-[(8Z,11E)-pentadeca-8,11,14-trien-1-yl]benzene-1,3-diol'	b'(Z,Z)-2-Methyl-5-(8,11,14-pentadecatrienyl)-1,3-benzenediol'	HMDB00 38908	C22H32O2	
		328.2402303	0.0007 303	Proton ation	b'docosa-2,4,6,8,10,12-hexaenoic acid'	b'Docosahexaenoic acid(DHA)'	HMDB02 44316	C22H32O2	
		328.2402303	0.0007 303	Proton ation	b'3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-yl acetate'	b'9-cis Retinol Acetate'	HMDB02 47587	C22H32O2	
		328.2402303	0.0007 303	Proton ation	b'docosa-4,7,10,13,16,19-hexaenoic acid'	b'(4E,7E,10Z,13E,16E,19E)-Docosa-4,7,10,13,16,19-hexaenoic acid'	HMDB02 51558	C22H32O2	
		328.2402303	0.0007 303	Proton ation	b'14-methoxy-15-methyl-5-propoxytetraacyclo[8.7.0.0^(2,7).0^(11,15)]heptadeca-2(7),3,5-triene'	b'Promestrienum'	HMDB02 56803	C22H32O2	
1 6 6	328.04 34	329.0525197	0.0013 197	Proton ation	b'(4aR,6R,7R,7aS)-6-(6-amino-9H-purin-9-yl)-2,7-dihydroxy-hexahydro-2lambda5-furo[3,2-d][1,3,2]dioxaphosphinin-2-one'	b'Cyclic AMP'	HMDB00 00058	C10H12N5O6P	C00 575
		329.0525197	0.0013 197	Proton ation	b'4-(6-amino-9H-purin-9-yl)-2-hydroxy-6-(hydroxymethyl)-tetrahydro-2H-2'xcelxbbxe2\x81\x85-furo[3,4-d][1,3,2]dioxaphosphol-2-one'	b"Adenosine 2',3'-cyclic phosphate"	HMDB00 11616	C10H12N5O6P	C08 355
		329.0511071	9.29E- 05	Proton ation	b'2-[2-nitro-4-(trifluoromethyl)benzoyl]cyclohexane-1,3-dione'	b'Nitisinone'	HMDB00 14492	C14H10F3NO5	
		329.0520506	0.0008 506	Proton ation	b'ethyl N-(2-[[diethoxy(sulfanylidene)-\xcelxbbxe2\x81\x85-phosphanyl]sulfonyl]acetyl)-N-methylcarbamate'	b'Mecarbam'	HMDB00 31800	C10H20NO5PS2	C18 661

1	328.23		0.0008							
6	54	328.2362075	075	Redox	b'4-carbamoyl-2-dodecanamidobutanoic acid'	b'N-Lauroyl Glutamine'	HMDB02 42031	C17H32N2O4		
7										
1	331.26	332.2715304	0.0012 304	Proton ation	b'(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoic acid'	b'Adrenic acid'	HMDB00 02226	C22H36O2	C16	527
6	25	332.2715304	0.0012 304	Proton ation	b'1-hydroxy-1-phenylhexadecan-3-one'	b'1-Hydroxy-1-phenyl-3-hexadecanone'	HMDB00 35676	C22H36O2		
8		332.2715304	0.0012 304	Proton ation	b'3-hydroxy-1-phenylhexadecan-1-one'	b'3-Hydroxy-1-phenyl-1-hexadecanone'	HMDB00 35677	C22H36O2		
		332.2715304	0.0012 304	Proton ation	b'2-methyl-5-[(8Z)-pentadec-8-en-1-yl]benzene-1,3-diol'	b'2-Methyl-5-(8-pentadecenyl)-1,3-benzenediol'	HMDB00 38910	C22H36O2		
		332.2715304	0.0012 304	Proton ation	b'ethyl (5Z,8Z,14Z)-icosa-5,8,11,14-tetraenoate'	b'Ethyl Arachidonate'	HMDB00 62725	C22H36O2		
		332.2715304	0.0012 304	Proton ation	b'docosa-2,4,6,8-tetraenoic acid'	b'Docosa-2,4,6,8-tetraenoic acid'	HMDB02 51563	C22H36O2		
		332.2715304	0.0012 304	Proton ation		b'Ganaxolone'	HMDB02 52627	C22H36O2		
		332.2715304	0.0012 304	Proton ation	b'ethyl icosa-6,9,12,15-tetraenoate'	b'Ethyl icosa-6,9,12,15-tetraenoate'	HMDB02 60406	C22H36O2		
1	332.01	333.0237849	0.0026 151	Proton ation	b'6-[(2-chloro-4-fluorophenyl)sulfamoyl]cyclohex-1-ene-1-carboxylic acid'	b'(6R)-6-[(2-Chloro-4-fluorophenyl)sulfamoyl]cyclohexene-1-carboxylic acid'	HMDB02 58104	C13H13ClFNO4 S		
6	86	333.0260651	0.0003 349	Proton ation	b'1-{3,4-dihydroxy-5-[(phosphonatoxy)methyl]oxolan-2-yl}-1'x'ce'xb'x'ce2'x81'xb5'-pyridin-1-ylum-3-carboxylate'	b'beta-nicotinate D-ribonucleotide'	HMDB03 04543	C11H12NO9P		
9										
1	333.05	334.066498	0.0008 98	Proton ation	b'[(2R)-2,3-dihydroxypropoxy]([[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy])phosphinic acid'	b'Glycerophosphoinositol'	HMDB00 11649	C9H19O11P	C01	225
7	78									

0		333.0548009	0.0029 991	Redox	b'1-[(E)-[(4-chlorophenyl)methylidene]amino]-3-[(Z)-[(4-chlorophenyl)methylidene]amino]guanidine'	b'Robenidine'	HMDB00 31785	C15H13Cl2N5	
1 7 1	334.06 18	335.0704031	0.0008 031	Proton ation	b'3-[(4-aminophenyl)sulfanyl]-3-imino-2-[2-(trifluoromethyl)phenyl]propanenitrile'	b'MEK1-2-inhibitor'	HMDB02 48914	C16H12F3N3S	
		335.0724492	0.0028 492	Proton ation	b'methyl 2-[N-(3-chloro-4-fluorophenyl)-1-phenylformamido]propanoate'	b'Flamprop-methyl'	HMDB02 52289	C17H15ClFNO3	
		335.0704031	0.0008 031	Proton ation	b'3-amino-3-[(4-aminophenyl)sulfanyl]-2-[2-(trifluoromethyl)phenyl]prop-2-enenitrile'	b'(Z)-3-Amino-3-(4-aminophenylthio)- 2-(2-(trifluoromethyl)phenyl)acrylonitrile'	HMDB02 58336	C16H12F3N3S	
		335.0724492	0.0028 492	Proton ation	b'4-[[[(4-chlorophenyl)(5-fluoro-2-hydroxyphenyl)methylidene]amino]butanoic acid'	b'Progabide acid'	HMDB02 59499	C17H15ClFNO3	
		334.0623427	0.0005 427	Redox	b'2-(4-benzamidobenzenesulfonamido)acetic acid'	b'2-[(4-Benzamidophenyl)sulfonylamino]acetic acid'	HMDB02 49991	C15H14N2O5S	
1 7 2	338.84 69	339.854981	0.0002 81	Proton ation	b'1,7,8,9,10,10-hexachloro-4-oxatricyclo[5.2.1.0 ^{2,5}]\xc2\x81\x81\dec-8-ene'	b'Endosulfan-ether'	HMDB02 46167	C9H6Cl6O	
1 7 3	338.98 67	339.9960489	0.0015 489	Proton ation	b'[[[(1R,2R,3R,4R,5R,6S)-2,3,5,6-tetrahydroxy-4-(phosphonooxy)cyclohexyl]oxy]phosphonic acid'	b'D-myo-Inositol 1,4-bisphosphate'	HMDB00 00968	C6H14O12P2	C01 220
		339.9960489	0.0015 489	Proton ation	b'[[[(2R,3S,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)-5-(phosphonooxy)oxolan-2-yl]methoxy]phosphonic acid'	b'D-Fructose 2,6-bisphosphate'	HMDB00 01047	C6H14O12P2	C00 665
		339.9960489	0.0015 489	Proton ation	b'[[[(2R,3S,4S,5R)-3,4,5-trihydroxy-5-[(phosphonooxy)methyl]oxolan-2-yl]methoxy]phosphonic acid'	b'Fructose 1,6-bisphosphate'	HMDB00 01058	C6H14O12P2	C05 378
		339.9960489	0.0015 489	Proton ation	b'[[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[(phosphonooxy)methyl]oxan-2-yl]oxy]phosphonic acid'	b'alpha-D-Glucose 1,6-bisphosphate'	HMDB00 03514	C6H14O12P2	C01 231
		339.9960489	0.0015	Proton	b'[[[(1S,2R,3s,4S,5R,6s)-2,3,4,6-tetrahydroxy-5-(phosphonooxy)cyclohexyl]oxy]phosphonic acid'	b'D-myo-Inositol 1,3-bisphosphate'	HMDB00	C6H14O12P2	C04

			489	ation			06234		062
		339.9960489	0.0015 489	Proton ation	b'{{{(1S,2S,3S,4S,5R,6S)-2,3,4,5-tetrahydroxy-6-(phosphonoxy)cyclohexyl}oxy}phosphonic acid'	b'D-myo-Inositol 3,4-bisphosphate'	HMDB00 06235	C6H14O12P2	C04 063
		339.9960489	0.0015 489	Proton ation	b'{{{(2R,3R,4S)-3,4,5-trihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl}methoxy}phosphonic acid'	b'D-Tagatose 1,6-bisphosphate'	HMDB00 06872	C6H14O12P2	C03 785
		339.9960489	0.0015 489	Proton ation	b'{{{(2R,3S,4S,5S,6S)-3,4,5-trihydroxy-6-(phosphonoxy)oxan-2-yl}methoxy}phosphonic acid'	b'D-Mannose 1,6-bisphosphate'	HMDB00 60269	C6H14O12P2	
		339.9960499	0.0015 499	Proton ation	b'{{{3,4,5-trihydroxy-2-oxo-6-(phosphonoxy)hexyl}oxy}phosphonic acid'	b'1,6-Di-O-phosphono-D-fructose'	HMDB02 44239	C6H14O12P2	
		339.9960499	0.0015 499	Proton ation	b'({2,3,4-trihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl}methoxy)phosphonic acid'	b'Fructose-1,6-diphosphate'	HMDB02 44240	C6H14O12P2	
		339.9960499	0.0015 499	Proton ation	b'{{4,5,6-trihydroxy-2-oxo-1-(phosphonoxy)hexan-3-yl}oxy}phosphonic acid'	b'Di-phosphofructose'	HMDB02 51116	C6H14O12P2	
		339.9960499	0.0015 499	Proton ation	b'({hydroxy[(3,4,5,6-tetrahydroxy-1-oxohexan-2-yl)oxy]phosphoryl}oxy)phosphonic acid'	b'Diphosphoglucose'	HMDB02 51461	C6H14O12P2	
		339.9960499	0.0015 499	Proton ation	b'{{2,4,5-trihydroxy-3-oxo-6-(phosphonoxy)hexyl}oxy}phosphonic acid'	b'[(2R,3R)-2,3,5-Trihydroxy-4-oxo-6-phosphonoxyhexyl] dihydrogen phosphate'	HMDB02 60218	C6H14O12P2	
1	341.03	342.0439018	0.0008 982	Proton ation	b'12-chloro-9-(2-chlorophenyl)-3-methyl-2,4,5,8-tetraazatricyclo[8.4.0.0'xc2'xb2,\xc2'x81'xb6]tetradeca-1(10),3,5,8,11,13-hexaene'	b'Triazolam'	HMDB00 15034	C17H12Cl2N4	
7	7	342.0456463	0.0008 463	Proton ation	b'methyl N-{{2-([[(methoxycarbonyl)amino]methanethioyl)amino]phenyl}carbamothioyl} carbamate'	b'Thiophanate-methyl'	HMDB02 59025	C12H14N4O4S2	C14 432
4		341.0391649	0.0021 649	Redox	b'2-([5-(2-benzenesulfonamidoethyl)thiophen-2-yl]oxy)acetic acid'	b'Linotroban'	HMDB02 54105	C14H15NO5S2	
1	344.03	345.0474343	0.0011 343	Proton ation	b'9-[(4aR,6R,7R,7aS)-2,7-dihydroxy-2-oxo-hexahydro-2'xc2'xb2'x81'xb5-furo[3,2-d][1,3,2]dioxaphosphinin-6-yl]-2-amino-6,9-dihydro-1H-purin-6-one'	b'Cyclic GMP'	HMDB00 01314	C10H12N5O7P	C00 942

5		345.0474343	0.0011 343	Proton ation	b'9-[(3aR,4R,6R,6aR)-2-hydroxy-6-(hydroxymethyl)-2-oxo-tetrahydro-2H-2'xccc'x81'xb5-furo[3,4-d][1,3,2]dioxaphosphol-4-yl]-2-amino-6,9-dihydro-3H-purin-6-one'	b"Guanosine 2',3'-cyclic phosphate"	HMDB00 11629	C10H12N5O7P	
		345.0474347	0.0011 347	Proton ation	b'2-amino-6-(2,5-dihydroxy-2-oxo-1,3,2lambda5-dioxaphosphinane-4-carbonyl)-4,6,7,8-tetrahydropteridin-4-one'	b'Molybdopterin precursor Z'	HMDB00 11683	C10H12N5O7P	
		344.0379612	0.0005 388	Redox	b'2-hydroxy-2-[3-hydroxy-5-oxo-4-(3,4,5-trihydroxybenzoyloxy)oxolan-2-yl]acetic acid'	b'2-O-Galloyl-1,4-galactarolactone'	HMDB00 37199	C13H12O11	
		344.0379612	0.0005 388	Redox	b'2-hydroxy-2-[4-hydroxy-5-oxo-3-(3,4,5-trihydroxybenzoyloxy)oxolan-2-yl]acetic acid'	b'3-O-Galloyl-1,4-galactarolactone'	HMDB00 37201	C13H12O11	
		344.0379612	0.0005 388	Redox	b'2-(3,4-dihydroxy-5-oxooxolan-2-yl)-2-(3,4,5-trihydroxybenzoyloxy)acetic acid'	b'5-O-Galloyl-1,4-galactarolactone'	HMDB00 37202	C13H12O11	
1 7 6	346.05 35	347.0630843	0.0017 843	Proton ation	b'([(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)phosphonic acid'	b'Adenosine monophosphate'	HMDB00 00045	C10H14N5O7P	C00 020
		347.0630843	0.0017 843	Proton ation	b'([(2R,3S,5R)-5-(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)-3-hydroxyoxolan-2-yl]methoxy)phosphonic acid'	b"2'-Deoxyguanosine 5'- monophosphate"	HMDB00 01044	C10H14N5O7P	C00 362
		347.0630843	0.0017 843	Proton ation	b'([(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]oxy)phosphonic acid'	b"3'-AMP"	HMDB00 03540	C10H14N5O7P	C01 367
		347.0630843	0.0017 843	Proton ation	b'([(3R,4R,5R)-2-(6-amino-9H-purin-9-yl)-4-hydroxy-5-(hydroxymethyl)oxolan-3-yl]oxy)phosphonic acid'	b"Adenosine 2'-phosphate"	HMDB00 11617	C10H14N5O7P	C00 946
		347.0630843	0.0017 843	Proton ation	b'([(2R,3S,5R)-5-(6-amino-2-hydroxy-9H-purin-9-yl)-3-hydroxyoxolan-2-yl]methoxy)phosphonic acid'	b'2-hydroxy-dAMP'	HMDB00 59594	C10H14N5O7P	C19 970
		347.0630843	0.0017 843	Proton ation	b'[{5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy}phosphonic acid'	b'Vidarabine phosphate'	HMDB02 45755	C10H14N5O7P	
		347.0630848	0.0017 848	Proton ation	b'9-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6-imino-6,9-dihydro-3H-purin-3-yl}phosphonic acid'	b'3-Phosphoadenosine'	HMDB02 45974	C10H14N5O7P	
		347.0630848	0.0017 848	Proton ation	b'[{3-azido-5-(5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)oxolan-2-yl]methoxy}phosphonic acid'	b'Zidovudine monophosphate'	HMDB02 48821	C10H14N5O7P	

		347.0630848	0.0017 848	Proton ation	b' {[5-(6-amino-9H-purin-9-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]oxy} phosphonic acid'	b'[(2R,5R)-5-(6-Aminopurin-9-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl] dihydrogen phosphate'	HMDB02 58140	C10H14N5O7P	
		346.0536113	0.0001 113	Redox	b'6-(4-carboxy-2,6-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'6-(4-carboxy-2,6-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	HMDB01 26636	C13H14O11	
		346.0536113	0.0001 113	Redox	b'6-(5-carboxy-2,3-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'6-(5-carboxy-2,3-dihydroxyphenoxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	HMDB01 26637	C13H14O11	
1 7 7	347.03 86	348.0470999	0.0006 999	Proton ation	b' {[(2R,3S,4R,5R)-3,4-dihydroxy-5-(6-oxo-6,9-dihydro-1H-purin-9-yl)oxolan-2-yl]methoxy} phosphonic acid'	b'Inosinic acid'	HMDB00 00175	C10H13N4O8P	C00 130
		348.0470999	0.0006 999	Proton ation	b' {[(2R,3R,4R,5R)-4-hydroxy-5-(hydroxymethyl)-2-(6-oxo-6,9-dihydro-3H-purin-9-yl)oxolan-3-yl]oxy} phosphonic acid'	b"Inosine 2'-phosphate"	HMDB00 11681	C10H13N4O8P	
		348.0457625	0.0006 375	Proton ation	b'(2R)-3-hydroxy-2- {[(2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-[(phosphonoxy)methyl]oxan-2-yl]oxy} propanoic acid'	b'2-O-(6-Phospho- α -mannosyl)-D-glycerate'	HMDB00 12152	C9H17O12P	C16 699
		348.045763	0.0006 37	Proton ation	b' ({3,4,5,6-tetrahydroxy-6-[(2-hydroxypropanoyl)oxy]oxan-2-yl} methoxy) phosphonic acid'	b'Glucose-6-phosphate lactate'	HMDB02 52789	C9H17O12P	
		348.0470999	0.0006 999	Proton ation	b' {[3,4-dihydroxy-5-(6-hydroxy-9H-purin-9-yl)oxolan-2-yl]methoxy} phosphonic acid'	b'[(2R,5R)-3,4-Dihydroxy-5-(6-oxo-1H-purin-9-yl)oxolan-2-yl]methyl dihydrogen phosphate'	HMDB02 57686	C10H13N4O8P	
1 7 8	347.05 68	347.0575912	0.0007 912	Redox	b'4-hydroxy-N-(5-hydroxypyridin-2-yl)-2-methyl-1,1-dioxo-2H-1H-cyclobutene-2,2-benzothiazine-3-carboxamide'	b"5'-Hydroxypiroxicam"	HMDB00 14096	C15H13N3O5S	
1 7 9	348.04 04	348.0432331	0.0028 331	Redox	b'13-chloro-2-(2-chlorophenyl)-3-oxa-6,9-diazatricyclo[8.4.0.0'xc2'xb2,\xc2'x81'xb6]tetradeca-1(10),11,13-trien-8-one'	b'Cloxazolam, (R)-'	HMDB02 59410	C17H14Cl2N2O 2	

180	352.9481	353.9578531	0.0019531	Protonation	b'3-bromo-1-[4-(3-bromopropanoyl)piperazin-1-yl]propan-1-one'	b'Pipobroman'	HMDB0014381	C10H16Br2N2O2	C07362
181	353.0028	354.0083924	0.0022076	Protonation	b'11-hydroxy-8,13,16-trioxa-1,5,7,14-tetraazatetracyclo[9.4.3.0 ^{3,7} .0 ^{4,14}]octadec-3-ene-2,6,9,12,15,17-hexone'	b'uric acid citrate'	HMDB0259718	C11H6N4O10	
1882	354.0598	355.0694197	0.0018197	Protonation	b'2-[(2-amino-1-hydroxy-3-[(4-methanesulfinylbutyl)thio(carbonoimidyl)sulfonyl]propylidene)amino]acetic acid'	b'Sulforaphane-cysteine-glycine'	HMDB0240559	C11H21N3O4S3	
182	98	354.0586967	0.0011033	Redox	b'2-hydroxy-1-[[[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy]propane-1,2,3-tricarboxylic acid'	b'2-O-p-Coumaroylhydroxycitric acid'	HMDB0040570	C15H14O10	
183	361.0435	362.0485259	0.0027741	Protonation	b'2,3,4-trihydroxy-5-(3,4,5-trihydroxybenzoyloxy)hexanedioic acid'	b'2-O-Galloylgalactaric acid'	HMDB0036932	C13H14O12	
183	35	362.0489965	0.0023035	Protonation	b'1-[2-hydroxy-5-(trifluoromethyl)phenyl]-5-(trifluoromethyl)-2,3-dihydro-1H-1,3-benzodiazol-2-one'	b'1-(2-Hydroxy-5-(trifluoromethyl)phenyl)-5-(trifluoromethyl)-1H-benzo[d]imidazol-2(3H)-one'	HMDB0255771	C15H8F6N2O2	C13833
184	362.0024	362.0031981	0.0007981	Redox	b'tris(4-chlorophenyl)methanol'	b'Tris(4-chlorophenyl)methanol'	HMDB0259279	C19H13Cl3O	
185	362.0486	363.057999	0.001599	Protonation	b'[[[(2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy]phosphonic acid'	b'Guanosine monophosphate'	HMDB0001397	C10H14N5O8P	C00144
185	86	363.057999	0.001599	Protonation	b'[[[(3S)-5-(2-amino-6,8-dioxo-6,7,8,9-tetrahydro-3H-purin-9-yl)-3-hydroxyoxolan-2-yl]methoxy]phosphonic acid'	b'8-Oxo-dGMP'	HMDB0011670	C10H14N5O8P	
185	99	363.057999	0.001599	Protonation	b'(4aR,5aR,11aR,12aS)-2,10,12,12-tetrahydroxy-8-imino-4,4a,5a,6,7,8,11,11a,12,12a-decahydro-2H-1,3,5-trioxa-6,7,9,11-tetraaza-2lambda5-phosphatetracen-2-one'	b'Cyclic pyranopterin monophosphate'	HMDB0059639	C10H14N5O8P	C18239
185	99	363.057999	0.0015	Protonation	b'[[[(2R,3R,4R,5R)-2-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-4-hydroxy-5-(hydroxymethyl)oxolan-3-yl]oxy]phosphonic acid'	b'Guanosine 2'-monophosphate"	HMDB02	C10H14N5O8P	

			99	ation			40586		
		363.057999	0.0015 99	Proton ation	b'[{(2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]oxy} phosphonic acid'	b'Guanosine 3'-monophosphate"	HMDB02 40587	C10H14N5O8P	C06 193
		363.057999	0.0015 99	Proton ation	b'[{3,4-dihydroxy-5-(6-hydroxy-2-imino-3,9-dihydro-2H-purin-9-yl)oxolan-2-yl]methoxy} phosphonic acid'	b'[(2R,5R)-5-(2-Amino-6-oxo-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl dihydrogen phosphate'	HMDB02 57693	C10H14N5O8P	
1 8 6	363.05 19	364.0583027	0.0013 973	Proton ation	b"3',4',5',6'-tetrahydroxy-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'Gallicin'	HMDB02 52597	C20H12O7	
1 8 7	368.99 7	370.0073427	0.0025 427	Proton ation	b'2-chloro-5-(2H-1,2,3,4-tetrazol-5-yl)-4-[(thiophen-2-ylmethyl)amino]benzene-1-sulfonamide'	b'Azosemid'	HMDB00 41831	C12H11ClN6O2 S2	
		370.0066136	0.0018 136	Proton ation	b'[{(3S,4R,5R,6R)-3,4,5,6-tetrahydroxy-2-oxo-7-(phosphonoxy)heptyl]oxy} phosphonic acid'	b'Sedoheptulose 1,7-bisphosphate'	HMDB00 60274	C7H16O13P2	C00 447
1 8 8	369.02	370.027583	0.0002 17	Proton ation	b'3-(2,4-dichlorophenyl)-4-(1-methyl-1H-indol-3-yl)-2,5-dihydro-1H-pyrrole-2,5-dione'	b'3-(2,4-Dichlorophenyl)-4-(1-methyl-1H-indol-3-yl)-1H-pyrrole-2,5-dione'	HMDB02 45731	C19H12Cl2N2O 2	
		369.0170779	0.0029 221	Redox	b'2-[(2-{(2,6-dichloro-4-hydroxyphenyl)amino}phenyl)acetyl]oxy]acetic acid'	b"4'-Hydroxy Aceclofenac"	HMDB02 46629	C16H13Cl2NO5	
1 8 9	377.01 82	378.028931	0.0029 31	Proton ation	b'1,1,1,2,2,3,3,4,4,5,5,6,6-tridecafluoro-6-(propan-2-yloxy)hexane'	b'Casoxin D'	HMDB03 03768	C9H7F13O	
1 9 0	380.01 31	380.011933	0.0011 67	Redox	b'4,11-dichloro-5,7,12,14-tetrahydro-5,12-diazapentacene-7,14-dione'	b'4,11-Dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione'	HMDB00 37810	C20H10Cl2N2O 2	
1 9 1	381.10 82	382.1181401	0.0021 401	Proton ation	b"(3-{3'-methoxy Spiro[adamantane-2,2'-[1,4]dioxetane]-3'-yl}phenoxy)phosphonic acid"	b'Amppd'	HMDB02 48363	C18H23O7P	
		382.1182557	0.0022	Proton	b'potassium (5R,9S,11R,12S)-12-hydroxy-5,11-dimethyl-6-methylidene-16-oxo-15-	b'Potassium gibberellate'	HMDB03	C20H23KO5	

			557	ation	oxapentacyclo[9.3.2.1\ce2\81\85,\ce2\81\88.0\ce2\89\ce2\81\80.0\ce2\82,\ce2\81\88]heptadec-13-ene-9-carboxylate'		03277		
1	382.09	383.1077125	0.0024	Proton	b'(2S)-2-((9-((2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl)-9H-purin-6-yl)amino)butanedioic acid'	b'Succinyladenosine'	HMDB0000912	C14H17N5O8	
9		383.1077125	0.0024	Proton	b'2-((9-((3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl)-9H-purin-6-yl)amino)butanedioic acid'	b'N6-Succinyl Adenosine'	HMDB0255303	C14H17N5O8	
2	75		125	ation					
1	384.98	385.9894834	0.0010	Proton	b'1-(3,4-dichlorophenyl)-3-(2,3-dihydro-1-benzofuran-5-sulfonyl)urea'	b"N-(5-(2,3-Dihydrobenzofuryl)sulfonyl)-N'-(3,4-dichlorophenyl)urea"	HMDB0254244	C15H12Cl2N2O4S	
9			166	ation					
3	27								
1	385.14	386.1486548	0.0025	Proton	b'2-methanesulfinyl-10-[2-(1-methylpiperidin-2-yl)ethyl]-10H-phenothiazine'	b'Mesoridazine'	HMDB0015068	C21H26N2OS2	C07
9			452	ation					143
4	34	386.1486558	0.0025	Proton	b'10-[2-(1-methylpiperidin-2-yl)ethyl]-2-(methylsulfonyl)-10H-5lambda4-phenothiazin-5-one'	b'Thioridazine 5-Sulfoxide'	HMDB0243502	C21H26N2OS2	
1	386.03	387.0406215	0.0015	Proton	b'2-amino-4-((1-((carboxymethyl)(sulfo)amino)-1-oxo-3-sulfanylpropan-2-yl)carbamoyl)butanoic acid'	b'2-Amino-5-[[1-(carboxymethyl)(sulfo)amino]-1-oxo-3-sulfanylpropan-2-yl]amino]-5-oxopentanoic acid'	HMDB0257661	C10H17N3O9S2	
9			215	ation					
5	13								
1	386.98	387.9922734	0.0024	Proton	b'(3-hydroxy-5-((E)-2-[4-(sulfooxy)phenyl]ethenyl)phenyl)oxidanefulfonic acid'	b'trans-Resveratrol 3,4'-disulfate"	HMDB0041780	C14H12O9S2	
9			266	ation					
6	69	387.9922734	0.0024	Proton	b'(3-((E)-2-(4-hydroxyphenyl)ethenyl)-5-(sulfooxy)phenyl)oxidanefulfonic acid'	b'trans-Resveratrol 3,5'-disulfate'	HMDB0041781	C14H12O9S2	
1	388.02	389.0357936	0.0003	Proton	b'3',6'-dihydroxy-4-isothiocyanato-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'3',6'-Dihydroxy-6-isothiocyanatospiro[isobenzofuran-1(3H),9'-[9H]xanthene]-3-one"	HMDB0246164	C21H11NO5S	
9			064	ation					
7		389.0357932	0.0003	Proton	b'3',6'-dihydroxy-5-isothiocyanato-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'Fluorescein-5-isothiocyanate'	HMDB0246165	C21H11NO5S	
1	83	389.0357936	0.0003	Proton	b'3',6'-dihydroxy-8'-isothiocyanato-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'Fluoresceine isothiocyanate'	HMDB02	C21H11NO5S	

			064	ation			52364		
1	391.22	392.2327754	0.0017	Proton	b'(2-hydroxy-2-oxo-1,3,2\xce\xbb\xce2\x81\x85-dioxaphospholan-4-yl)methyl hexadecanoate'	b'CPA(16:0/0:0)'	HMDB00	C19H37O6P	
9			754	ation			07003		
8	32	391.2259772	0.0027	Redox	b'N-[4-(1-benzoylpiperidin-4-yl)butyl]-3-(pyridin-3-yl)prop-2-enamide'	b'Daporinad'	HMDB02	C24H29N3O2	
			772				47176		
1	392.22		0.0017						
9		392.2252489	0.0017	Redox	b'(diphenylmethyl)({2-[(diphenylmethyl)amino]ethyl})amine'	b"N,N'-Dibenzhydriethane-1,2-diamine"	HMDB02	C28H28N2	
9	7		511				54810		
2	393.23		0.0013	Proton					
0		394.2484255	0.0013	ation	b'[(2R)-3-[(1Z)-hexadec-1-en-1-yloxy]-2-hydroxypropoxy]phosphonic acid'	b'LysoPA(P-16:0/0:0)'	HMDB00	C19H39O6P	C15
0	93		255				11154		646
2	401.24	401.2426899	0.0017	Redox	b'8-{4-[1-oxo-4-(pyrimidin-2-yl)-1\xce\xbb\xce2\x81\x85-piperazin-1-yl]butyl}-8-azaspiro[4.5]decane-7,9-dione'	b'Buspirone N-oxide'	HMDB00	C21H31N5O3	
			101				61107		
		401.2426899	0.0017	Redox	b'2-hydroxy-8-{4-[4-(pyrimidin-2-yl)piperazin-1-yl]butyl}-8-azaspiro[4.5]decane-7,9-dione'	b"3'-Hydroxybuspirone"	HMDB00	C21H31N5O3	
			101				61108		
		401.2426899	0.0017	Redox	b'8-{4-[4-(5-hydroxypyrimidin-2-yl)piperazin-1-yl]butyl}-8-azaspiro[4.5]decane-7,9-dione'	b'5-Hydroxybuspirone'	HMDB00	C21H31N5O3	
1	44		101				61109		
		401.2426899	0.0017	Redox	b'6-hydroxy-8-{4-[4-(pyrimidin-2-yl)piperazin-1-yl]butyl}-8-azaspiro[4.5]decane-7,9-dione'	b"6'-Hydroxybuspirone"	HMDB00	C21H31N5O3	
			101				61110		
		401.2426899	0.0017	Redox	b'6-({3-[4-(2-methoxyphenyl)piperazin-1-yl]propyl} amino)-1,3,5-trimethyl-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'5-Methylurapidil'	HMDB02	C21H31N5O3	
			101				46828		
2	402.00	403.0181814	0.0018	Proton	b'[({(2R,3S,4R,5R)-5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy}(hydroxy)phosphoryl]oxy]phosphonic acid'	b'CDP'	HMDB00	C9H15N3O11P2	C00
0			814	ation			01546		112
2	85	403.0181823	0.0018	Proton	b'[({(5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy}(hydroxy)phosphoryl]oxy]phosphonic acid'	b'[(2S,3R,4R,5R)-5-(4-Amino-2-oxopyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl	HMDB02	C9H15N3O11P2	
			823	ation			57860		

						phosphono hydrogen phosphate'			
		402.0061789	0.0023 211	Redox	b'2-(2,7-dichloro-3,6-dihydroxy-9H-xanthen-9-yl)benzoic acid'	b'2,7-Dichlorofluorescin'	HMDB02 50892	C20H12Cl2O5	
		402.0061789	0.0023 211	Redox	b'1',2'-dichloro-3',6'-dihydroxy-1',2'-dihydro-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'dichlorodihydrofluorescein'	HMDB02 51190	C20H12Cl2O5	
		402.0061789	0.0023 211	Redox	b'2-(1,2-dichloro-3,6-dihydroxy-9H-xanthen-9-yl)benzoic acid'	b'Dichlorofluorescin'	HMDB02 51194	C20H12Cl2O5	
		402.0061789	0.0023 211	Redox	b'3a,4-dichloro-3',6'-dihydroxy-3a,4-dihydro-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'7,7a-Dichloro-3',6'- dihydroxyspiro[7H-2-benzofuran-3,9'- xanthene]-1-one"	HMDB02 57577	C20H12Cl2O5	
2 0 3	402.24 78	402.2478348	3.48E- 05	Redox	b'(5E)-2,10-diamino-5-{{(5-amino-5-carboxypentyl)amino)methyl}undec-5-enedioic acid'	b'Merodesmosine'	HMDB00 30407	C18H34N4O6	
2 0 4	402.99 26	404.0021969	0.0017 969	Proton ation	b'({{(2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy}(hydroxy)phosphoryl)oxy]phosphonic acid'	b'Uridine 5'-diphosphate"	HMDB00 00295	C9H14N2O12P2	C00 015
2 0 5	403.26 07	404.2675076	0.0009 924	Proton ation	b'N-[1-(2,3-dihydro-1,4-benzodioxin-6-yl)-1-hydroxy-3-(pyrrolidin-1-yl)propan-2-yl]octanamide'	b'Eliglustat'	HMDB02 51746	C23H36N2O4	
2 0 6	408.01 06	408.0085921	0.0020 079	Redox	b'6-hydroxy-5-[(E)-2-(4-sulfofenyl)diazene-1-yl]naphthalene-2-sulfonic acid'	b'6-Hydroxy-5-[(4-sulfofenyl)azo]-2- naphthalenesulfonic acid'	HMDB00 34022	C16H12N2O7S2	
2 0 7	409.01 25	410.0178024	0.0024 976	Proton ation	b'1-[4-(4-chlorophenyl)-2-[(2,6-dichlorophenyl)sulfanyl]butyl]-1H-imidazole'	b'Butoconazole'	HMDB00 14777	C19H17Cl3N2S	C08 065
2	409.23	410.2433401	0.0010	Proton	b'[2-(hexadecanoyloxy)-3-hydroxypropoxy]phosphonic acid'	b'LysoPA(0:0/16:0)	HMDB00	C19H39O7P	

1	45		756	ation			07004		
3									
2	421.26	422.2797256	0.0022 256	Proton ation	b'[3-(octadecyloxy)-2-oxopropoxy]phosphonic acid'	b'DHAP(O-18:0)'	HMDB00 11142	C21H43O6P	
1 4		422.2780723	0.0005 723	Proton ation	b'7-{3-[(2-heptanamidoacetamido)methyl]-7-oxabicyclo[2.2.1]heptan-2-yl}hept-5-enoic acid'	b'3-(((Oxoheptyl)amino)acetyl)amino)methyl-7-oxobicyclo[2.2.1]hept-2-yl-5-heptenoic acid'	HMDB02 58446	C23H38N2O5	
2 1 5	422.03 08	422.0283709	0.0024 291	Redox	b'4-[2-(2-dichloroacetamido)-3-hydroxy-3-(4-nitrophenyl)propoxy]-4-oxobutanoic acid'	b'Chloramphenicol succinate'	HMDB02 50088	C15H16Cl2N2O 8	
2 1 6	426.01 98	427.0294147	0.0018 147	Proton ation	b'([(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonoxy)oxolan-2-yl]methoxy)phosphonic acid'	b'Adenosine 3',5'-diphosphate"	HMDB00 00061	C10H15N5O10P 2	C00 054
		427.0294147	0.0018 147	Proton ation	b'([(2R,3S,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3-hydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryloxy]phosphonic acid'	b'dGDP"	HMDB00 00960	C10H15N5O10P 2	C00 361
		427.0294147	0.0018 147	Proton ation	b'([(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryloxy]phosphonic acid'	b'ADP"	HMDB00 01341	C10H15N5O10P 2	C00 008
		427.0294147	0.0018 147	Proton ation	b'([(5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryloxy]phosphonic acid'	b'[(2S,3R,4R,5R)-5-(6-Aminopurin-9-yl)-3,4-dihydroxyoxolan-2-yl]methylphosphono hydrogen phosphate'	HMDB02 47869	C10H15N5O10P 2	
		427.0294157	0.0018 157	Proton ation	b'([(3-azido-5-(5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryloxy]phosphonic acid'	b'Zidovudine diphosphate'	HMDB02 48820	C10H15N5O10P 2	
2 1 7	427.02 21	427.0198989	0.0022 011	Redox	b'([(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryloxy]sulfonic acid'	b'Adenosine phosphosulfate'	HMDB00 01003	C10H14N5O10P S	C00 224
2	428.02	429.0336711	0.0012	Proton	b'2,2,4,4-tetrafluoro-6-(2-phenylethynyl)-6-[4-(prop-1-en-2-yl)phenyl]-1,3,5,2lambda5,4lambda5,6lambda5-triazatriphosphinine'	b'Geminal'	HMDB02	C17H14F4N3P3	

18	46		711	ation			52673		
219	429.0563	430.0654659	0.0013659	Protonation	b'(2-aminoethyl)(({(2R,3S,4R,5R)-3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl)methoxy}(hydroxy)phosphoryl)oxy]phosphinic acid'	b'CMP-2-aminoethylphosphonate'	HMDB0060067	C11H20N4O10P2	C05673
		430.0635466	0.0005534	Protonation	b'calcium bis(2,3,4,5,6-pentahydroxyhexanoate)'	b'Calcium gluconate'	HMDB0302138	C12H22CaO14	
220	435.2501	436.2589907	0.0010907	Protonation	b'{3-hydroxy-2-[(9Z)-octadec-9-enoyloxy]propoxy}phosphonic acid'	b'LysoPA(0:0/18:1(9Z))'	HMDB0007851	C21H41O7P	
		436.2589907	0.0010907	Protonation	b'{2-hydroxy-3-[(9Z)-octadec-9-enoyloxy]propoxy}phosphonic acid'	b'LysoPA(18:1(9Z)/0:0)'	HMDB0007855	C21H41O7P	
		436.2589902	0.0010902	Protonation	b'[3-(octadecanoyloxy)-2-oxopropoxy]phosphonic acid'	b'DHAP(18:0)'	HMDB0011133	C21H41O7P	C03805
		436.2589902	0.0010902	Protonation	b'[2-hydroxy-3-(octadec-9-enoyloxy)propoxy]phosphonic acid'	b'(2-Hydroxy-3-phosphonoxypropyl)octadec-9-enoate'	HMDB0242470	C21H41O7P	
221	436.2817	437.2906247	0.0011247	Protonation	b'(2-aminoethoxy)((2R)-3-[(1Z)-hexadec-1-en-1-yloxy]-2-hydroxypropoxy]phosphinic acid'	b'LysoPE(P-16:0/0:0)'	HMDB0011152	C21H44NO6P	
		436.282489	0.000789	Redox	b'(3R,5R)-7-[(1S,2S,6R,8S,8aR)-8-[(2,2-dimethylbutanoyl)oxy]-2,6-dimethyl-1,2,6,7,8,8a-hexahydronaphthalen-1-yl]-3,5-dihydroxyheptanoic acid'	b'simvastatin hydroxy acid'	HMDB0061047	C25H40O6	
		436.282489	0.000789	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienoate'	b'DG(2:0/20:3(5Z,8Z,11Z)-O(14R,15S)/0:0)'	HMDB0296847	C25H40O6	
		436.282489	0.000789	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienoate'	b'DG(20:3(5Z,8Z,11Z)-O(14R,15S)/2:0/0:0)'	HMDB0296848	C25H40O6	
		436.282489	0.000789	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienoate'	b'DG(2:0/0:0/20:3(5Z,8Z,11Z)-O(14R,15S))'	HMDB0296849	C25H40O6	
		436.282489	0.000789	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienoate'	b'DG(20:3(5Z,8Z,11Z)-O(14R,15S)/0:0/2:0)'	HMDB0296850	C25H40O6	

		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoate'	b'DG(2:0/20:3(5Z,8Z,14Z)- O(11S,12R)/0:0)'	HMDB02 96851	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoate'	b'DG(20:3(5Z,8Z,14Z)- O(11S,12R)/2:0/0:0)'	HMDB02 96852	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoate'	b'DG(2:0/0:0/20:3(5Z,8Z,14Z)- O(11S,12R))'	HMDB02 96853	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoate'	b'DG(20:3(5Z,8Z,14Z)- O(11S,12R)/0:0/2:0)'	HMDB02 96854	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoate'	b'DG(2:0/20:3(5Z,11Z,14Z)- O(8,9)/0:0)'	HMDB02 96855	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoate'	b'DG(20:3(5Z,11Z,14Z)- O(8,9)/2:0/0:0)'	HMDB02 96856	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoate'	b'DG(2:0/0:0/20:3(5Z,11Z,14Z)- O(8,9))'	HMDB02 96857	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoate'	b'DG(20:3(5Z,11Z,14Z)- O(8,9)/0:0/2:0)'	HMDB02 96858	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl 4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoate'	b'DG(2:0/20:3(8Z,11Z,14Z)- O(5,6)/0:0)'	HMDB02 96859	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl 4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoate'	b'DG(20:3(8Z,11Z,14Z)- O(5,6)/2:0/0:0)'	HMDB02 96860	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl 4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoate'	b'DG(2:0/0:0/20:3(8Z,11Z,14Z)- O(5,6))'	HMDB02 96861	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl 4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoate'	b'DG(20:3(8Z,11Z,14Z)- O(5,6)/0:0/2:0)'	HMDB02 96862	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z)-20-hydroxyicos-5,8,11,14-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,11Z,14Z)- OH(20)/0:0)'	HMDB02 96863	C25H40O6	

		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(20)/2:0/0:0)'	HMDB02 96864	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,14Z)- OH(20))'	HMDB02 96865	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(20)/0:0/2:0)'	HMDB02 96866	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5R,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoate'	b'DG(2:0/20:4(6E,8Z,11Z,14Z)- OH(5S)/0:0)'	HMDB02 96867	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)- OH(5S)/2:0/0:0)'	HMDB02 96868	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(6E,8Z,11Z,14Z)- OH(5S))'	HMDB02 96869	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)- OH(5S)/0:0/2:0)'	HMDB02 96870	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z,19S)-19-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,11Z,14Z)- OH(19S)/0:0)'	HMDB02 96871	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(19S)/2:0/0:0)'	HMDB02 96872	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,14Z)- OH(19S))'	HMDB02 96873	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(19S)/0:0/2:0)'	HMDB02 96874	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z,18R)-18-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,11Z,14Z)- OH(18R)/0:0)'	HMDB02 96875	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z,18S)-18-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(18R)/2:0/0:0)'	HMDB02 96876	C25H40O6	

		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,18S)-18-hydroxyicosanoate	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,14Z)-OH(18R))'	HMDB02 96877	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,18S)-18-hydroxyicosanoate	b'DG(20:4(5Z,8Z,11Z,14Z)-OH(18R)/0:0/2:0)'	HMDB02 96878	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z)-17-hydroxyicosanoate	b'DG(2:0/20:4(5Z,8Z,11Z,14Z)-OH(17)/0:0)'	HMDB02 96879	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z)-17-hydroxyicosanoate	b'DG(20:4(5Z,8Z,11Z,14Z)-OH(17)/2:0/0:0)'	HMDB02 96880	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z)-17-hydroxyicosanoate	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,14Z)-OH(17))'	HMDB02 96881	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z)-17-hydroxyicosanoate	b'DG(20:4(5Z,8Z,11Z,14Z)-OH(17)/0:0/2:0)'	HMDB02 96882	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z,16R)-16-hydroxyicosanoate	b'DG(2:0/20:4(5Z,8Z,11Z,14Z)-OH(16R)/0:0)'	HMDB02 96883	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z,16S)-16-hydroxyicosanoate	b'DG(20:4(5Z,8Z,11Z,14Z)-OH(16R)/2:0/0:0)'	HMDB02 96884	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,16S)-16-hydroxyicosanoate	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,14Z)-OH(16R))'	HMDB02 96885	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,16S)-16-hydroxyicosanoate	b'DG(20:4(5Z,8Z,11Z,14Z)-OH(16R)/0:0/2:0)'	HMDB02 96886	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,13E,15S)-15-hydroxyicosanoate	b'DG(2:0/20:4(5Z,8Z,11Z,13E)-OH(15S)/0:0)'	HMDB02 96887	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,13E,15R)-15-hydroxyicosanoate	b'DG(20:4(5Z,8Z,11Z,13E)-OH(15S)/2:0/0:0)'	HMDB02 96888	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E,15R)-15-hydroxyicosanoate	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,13E)-OH(15S))'	HMDB02 96889	C25H40O6	

		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E,15R)-15-hydroxyicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)- OH(15S)0:0/2:0)'	HMDB02 96890	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,10E,12S,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,10E,14Z)- OH(12S)0:0)'	HMDB02 96891	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoate'	b'DG(20:4(5Z,8Z,10E,14Z)- OH(12S)2:0/0:0)'	HMDB02 96892	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,8Z,10E,14Z)- OH(12S))'	HMDB02 96893	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoate'	b'DG(20:4(5Z,8Z,10E,14Z)- OH(12S)0:0/2:0)'	HMDB02 96894	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5E,8Z,11R,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoate'	b'DG(2:0/20:4(5E,8Z,12Z,14Z)- OH(11R)0:0)'	HMDB02 96895	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5E,8Z,11S,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoate'	b'DG(20:4(5E,8Z,12Z,14Z)- OH(11R)2:0/0:0)'	HMDB02 96896	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5E,8Z,11S,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoate'	b'DG(2:0/0:0/20:4(5E,8Z,12Z,14Z)- OH(11R))'	HMDB02 96897	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5E,8Z,11S,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoate'	b'DG(20:4(5E,8Z,12Z,14Z)- OH(11R)0:0/2:0)'	HMDB02 96898	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoate'	b'DG(2:0/20:4(5Z,7E,11Z,14Z)- OH(9)0:0)'	HMDB02 96899	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoate'	b'DG(20:4(5Z,7E,11Z,14Z)- OH(9)2:0/0:0)'	HMDB02 96900	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,7E,11Z,14Z)- OH(9))'	HMDB02 96901	C25H40O6	
		436.282489	0.0007 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoate'	b'DG(20:4(5Z,7E,11Z,14Z)- OH(9)0:0/2:0)'	HMDB02 96902	C25H40O6	

2	437.26	438.2746402	0.0012 402	Proton ation	b'[3-hydroxy-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'LysoPA(0:0/18:0)	HMDB00 07850	C21H43O7P	
2	56	438.2746407	0.0012 407	Proton ation	b'[2-hydroxy-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'LysoPA(18:0/0:0)	HMDB00 07854	C21H43O7P	
2	442.01	443.0243294	0.0007 294	Proton ation	b'[({(2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy}(hydroxy)phosphoryl]oxy]phosphonic acid'	b'Guanosine diphosphate'	HMDB00 01201	C10H15N5O11P 2	C00 035
2	58	443.0243294	0.0007 294	Proton ation	b'[({(2R,3S,5R)-5-(6,8-dihydroxy-2-imino-3,9-dihydro-2H-purin-9-yl)-3-hydroxyoxolan-2-yl)methoxy}(hydroxy)phosphoryl]oxy]phosphonic acid'	b'8-oxo-dGDP"	HMDB00 59648	C10H15N5O11P 2	C20 176
3		443.0243303	0.0007 303	Proton ation	b'[({(5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy}(hydroxy)phosphoryl]oxy]phosphonic acid'	b'Guanosine diphos-phate'	HMDB02 52974	C10H15N5O11P 2	
		443.0243303	0.0007 303	Proton ation	b'[(5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-4-hydroxy-2-[(phosphonoxy)methyl]oxolan-3-yl]oxy]phosphonic acid'	b"Guanosine-3',5'-Diphosphate"	HMDB02 52975	C10H15N5O11P 2	
2	445.05	446.0603805	0.0018 805	Proton ation	b'(2-aminoethoxy)[({(2R,3S,4R,5R)-3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl)methoxy}(hydroxy)phosphoryl]oxy]phosphinic acid'	b'CDP-ethanolamine'	HMDB00 01564	C11H20N4O11P 2	C00 570
4	07	446.0572574	0.0012 426	Proton ation	b'2-(6-hydroxy-3-oxo-3H-xanthen-9-yl)-5-(5-oxo-2-sulfanylideneimidazolidin-1-yl)benzoic acid'	b'Fluorescein thiohydantoin'	HMDB02 52361	C23H14N2O6S	
2	446.30	446.3032245	0.0024 245	Redox	b"5,7,9,13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[10.8.0.0'xc2'xb2,\xc2'x81'xb9.0'xc2'x81'xb4,\xc2'x81'xb8.0'xc2'xb9'xc2'xb3,\xc2'xb9'xc2'x81'xb8]icosan]-18'-ene-4,14',16'-triol"	b'Cepagenin'	HMDB00 30913	C27H42O5	
2	08	446.3032245	0.0024 245	Redox	b"16',19'-dihydroxy-5,7',9',13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[10.8.0.0'xc2'xb2,\xc2'x81'xb9.0'xc2'x81'xb4,\xc2'x81'xb8.0'xc2'xb9'xc2'xb3,\xc2'xb9'xc2'x81'xb8]icosane]-10'-one"	b'12-Ketoporrigenin'	HMDB00 31079	C27H42O5	
2		446.3032245	0.0024 245	Redox	b"16',19'-dihydroxy-5,7',9',13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[10.8.0.0'xc2'xb2,\xc2'x81'xb9.0'xc2'x81'xb4,\xc2'x81'xb8.0'xc2'xb9'xc2'xb3,\xc2'xb9'xc2'x81'xb8]icosane]-15'-one"	b'Neoporrigenin B'	HMDB00 32680	C27H42O5	
5		446.3032245	0.0024 245	Redox	b"16',18'-dihydroxy-5,7',9',13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[10.7.0.0'xc2'xb2,\xc2'x81'xb9.0'xc2'x81'xb4,\xc2'x81'xb8.0'xc2'xb9'xc2'xb3,\xc2'xb9'xc2'x81'xb8]nonadecane]-19'-carbaldehyde"	b'Leontogenin'	HMDB00 33583	C27H42O5	
		446.3032245	0.0024 245	Redox	b"5,5-bis(hydroxymethyl)-7',9',13'-trimethyl-5'-oxaspiro[oxolane-2,6'-pentacyclo[10.8.0.0'xc2'xb2,\xc2'x81'xb9.0'xc2'x81'xb4,\xc2'x81'xb8.0'xc2'xb9'xc2'xb3,\xc2'xb9'xc2'x81'xb8]icosan]-18'-en-16'-ol"	b'Taccagenin'	HMDB00 34189	C27H42O5	

		446.3032245	0.0024 245	Redox	b'5-(hydroxymethyl)-7,9,13'-trimethyl-5'-oxaspiro[oxane-2,6'- pentaacyclo[10.8.0.0'xc2'xb2,\xc2'xb1'xb9.0'xc2'xb1'xb4,\xc2'xb1'xb8.0'xc2'xb9'xc2'xb3,\xc2'xb9'xc2'xb1'xb8]icosan]-18'-ene-5,16'-diol"	b'Spirotaecagenin'	HMDB00 34424	C27H42O5	
		446.3032245	0.0024 245	Redox	b'(4R,6R)-6-[(1R,3aS,4E,7aR)-4-{2-[(1E,3S,5R)-3,5-dihydroxy-2-methylidenecyclohexylidene]ethylidene}-7a-methyl-octahydro-1H-inden-1-yl]-2,4-dihydroxy-2-methylheptan-3-one'	b'24-Oxo-1alpha,23,25-trihydroxyvitamin D3'	HMDB00 60129	C27H42O5	
2 2 6	447.05 57	448.0610216	0.0024 784	Proton ation	b'([(E)-[2-(1H-indol-3-yl)-1-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]sulfonyl}ethylidene]amino]oxy)sulfonic acid'	b'Glucobrassicin'	HMDB00 30243	C16H20N2O9S2	
		448.064176	0.0006 76	Proton ation	b'7,13,14-trihydroxy-6-[(3,4,5-trihydroxy-6-methyloxan-2-yl)oxy]-2,9-dioxatetracyclo[6.6.2.0'xc2'xb1'xb4,\xc2'xb9'xc2'xb1'xb6.0'xc2'xb9'xc2'xb9,\xc2'xb9'xc2'xb1'xb5]hexadeca-1(15),4(16),5,7,11,13-hexaene-3,10-dione'	b'Ellagic acid 2-rhamnoside'	HMDB03 03358	C20H16O12	
2 2 7	452.27 62	453.2855393	0.0015 393	Proton ation	b'(2-aminoethoxy)[(2R)-2-(hexadecanoyloxy)-3-hydroxypropoxy]phosphinic acid'	b'LysoPE(0:0/16:0)'	HMDB00 11473	C21H44NO7P	
		453.2855393	0.0015 393	Proton ation	b'(2-aminoethoxy)[(2R)-3-(hexadecanoyloxy)-2-hydroxypropoxy]phosphinic acid'	b'LysoPE(16:0/0:0)'	HMDB00 11503	C21H44NO7P	
		453.2855393	0.0015 393	Proton ation	b'(2-aminoethoxy)[3-(hexadecanoyloxy)-2-hydroxypropoxy]phosphinic acid'	b'[3-[2-Aminoethoxy(hydroxy)phosphoryl]oxy-2-hydroxypropyl] hexadecanoate'	HMDB02 56030	C21H44NO7P	
		452.2774036	0.0012 036	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxyicosanoic acid'	b'DG(2:0/20:4(6Z,8E,10E,14Z)-2OH(5S,12R)/0:0)'	HMDB02 96927	C25H40O7	
		452.2774036	0.0012 036	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosanoic acid'	b'DG(20:4(6Z,8E,10E,14Z)-2OH(5S,12R)/2:0/0:0)'	HMDB02 96928	C25H40O7	
		452.2774036	0.0012 036	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosanoic acid'	b'DG(2:0/0:0/20:4(6Z,8E,10E,14Z)-2OH(5S,12R))'	HMDB02 96929	C25H40O7	
		452.2774036	0.0012 036	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosanoic acid'	b'DG(20:4(6Z,8E,10E,14Z)-2OH(5S,12R)/0:0/2:0)'	HMDB02 96930	C25H40O7	
		452.2774036	0.0012 036	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosanoic acid'	b'DG(2:0/20:4(6E,8Z,11Z,13E)-2OH(5S,15S)/0:0)'	HMDB02 96999	C25H40O7	
		452.2774036	0.0012	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosanoic acid'	b'DG(20:4(6E,8Z,11Z,13E)-	HMDB02	C25H40O7	

			036			2OH(5S,15S)/2:0/0:0)'	97000		
		452.2774036	0.0012 036	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoate'	b'DG(2:0/0:0/20:4(6E,8Z,11Z,13E)- 2OH(5S,15S))'	HMDB02 97001	C25H40O7	
		452.2774036	0.0012 036	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoate'	b'DG(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/0:0/2:0)'	HMDB02 97002	C25H40O7	
		452.2774036	0.0012 036	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoate'	b'DG(2:0/20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/0:0)'	HMDB02 97003	C25H40O7	
		452.2774036	0.0012 036	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoate'	b'DG(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/2:0/0:0)'	HMDB02 97004	C25H40O7	
		452.2774036	0.0012 036	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoate'	b'DG(2:0/0:0/20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R))'	HMDB02 97005	C25H40O7	
		452.2774036	0.0012 036	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoate'	b'DG(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/0:0/2:0)'	HMDB02 97006	C25H40O7	
2	462.06	463.074043	0.0012 43	Proton ation	b'(2S)-2-({9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl]-9H-purin-6-yl}amino)butanedioic acid'	b'Adenylsuccinic acid'	HMDB00 00536	C14H18N5O11P	C03 794
2	5	463.0740434	0.0012 434	Proton ation	b'2-[(9-{3,4-dihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl]-9H-purin-6-yl}amino)butanedioic acid'	b'Adenylsuccinic acid'	HMDB02 48010	C14H18N5O11P	
2	462.29	463.3062752	0.0023 752	Proton ation	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'LysoPE(P-18:1(9Z)/0:0)'	HMDB02 40599	C23H46NO6P	
9	61	462.2981391	0.0020 391	Redox	b'4-{5,9,12-trihydroxy-2,6,6,11,15-pentamethyl-17-oxotetracyclo[8.7.0.0'xc2'xb2'xc2'x81'xb7.0'xc2'xb9'xc2'xb9'xc2'xb9'xc2'xb9'xc2'x81'xb5]heptadec-1(10)-en-14-yl}pentanoic acid'	b'Lucidenic acid M'	HMDB00 35973	C27H42O6	C10 029
2	463.06	464.0724331	0.0029 669	Proton ation	b'2-(hydroxymethyl)-6-({7-methanesulfinyl-1-[(sulfonatoxy)imino]heptyl)sulfanyl}oxane-3,4,5-triol'	b'6-methylsulfinylhexyl glucosinolate'	HMDB03 04231	C14H26NO10S3	
2	463.27 95	464.2902908	0.0029 908	Proton ation	b'[(2R)-2-hydroxy-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphonic acid'	b'1-(11Z-eicosenoyl)-glycero-3- phosphate'	HMDB00 62305	C23H45O7P	

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2	463.30	463.3005987	0.0010 013	Redox	b'2-[(4,6-diamino-3-[(3-amino-6-(1-aminoethyl)oxan-2-yl)oxy]-2-hydroxycyclohexyl)oxy]-5-methyl-4-(methylamino)oxane-3,5-diol'	b'Gentamicin C2'	HMDB02 52691	C20H41N5O7	
3	16	463.3005987	0.0010 013	Redox	b'2-[(4,6-diamino-3-[(3-amino-6-(methylamino)methyl)oxan-2-yl]oxy)-2-hydroxycyclohexyl]oxy]-5-methyl-4-(methylamino)oxane-3,5-diol'	b'Micronomicin'	HMDB02 54707	C20H41N5O7	
2	463.97	464.9851805	8.05E- 05	Proton ation	b'[[hydroxy([hydroxy([2-[(6-hydroxy-2-imino-3,9-dihydro-2H-purin-9-yl)methoxy]ethoxy)]phosphoryl]oxy)]phosphoryl]oxy]phosphonic acid'	b'Acyclovir triphosphate'	HMDB02 47992	C8H14N5O12P3	
3	73	463.9786995	0.0013 995	Redox	b'[[hydroxy([hydroxy([5-(5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-2,5-dihydrofuran-2-yl]methoxy)]phosphoryl]oxy)]phosphoryl]oxy]phosphonic acid'	b'Stavudine triphosphate'	HMDB02 58490	C10H15N2O13P 3	
2	464.31	465.3219253	0.0015 253	Proton ation	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(1Z)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'LysoPE(P-18:0:0:0)'	HMDB02 40598	C23H48NO6P	
3	26	464.3137891	0.0011 891	Redox	b'14-(3,6-dihydroxy-6-methylheptan-2-yl)-4,5,11-trihydroxy-2,15-dimethyltetraacyclo[8.7.0.0'xc2'xb2,\xc2'xb7.0'xc2'xb9'xc2'xb9,\xc2'xb9'xc2'xb5]heptadec-9-en-8-one'	b'Ecdysone'	HMDB02 51684	C27H44O6	
4		464.3137891	0.0011 891	Redox	b'14-(2,3-dihydroxy-6-methylheptan-2-yl)-4,5,11-trihydroxy-2,15-dimethyltetraacyclo[8.7.0.0'xc2'xb2,\xc2'xb7.0'xc2'xb9'xc2'xb9,\xc2'xb9'xc2'xb5]heptadec-9-en-8-one'	b'Ponasterone A'	HMDB02 56697	C27H44O6	
2	465.17	466.1813952	0.0022 952	Proton ation	b'3,3-bis[4-hydroxy-2-methyl-5-(propan-2-yl)phenyl]-3H-2,1lambda6-benzoxathiole-1,1-dione'	b'Thymol blue'	HMDB02 59055	C27H30O5S	
3	13								
5									
2	471.06	472.0765801	0.0004 801	Proton ation	b'(2-[[[([5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methyl]phosphonato)oxy]phosphinato]oxy)ethyl]dimethylazaniumyl'	b'CDP-N-dimethylethanolamine'	HMDB03 04286	C13H22N4O11P 2	
3	83	471.0689409	0.0006 409	Redox	b'5-chloro-2-methoxy-N-[2-(4-methoxy-3-[(methylcarbamothioyl)amino]sulfonyl)phenyl]ethyl]benzamide'	b'Clamikalant'	HMDB02 50313	C19H22ClN3O5 S2	
6									
2	478.29	479.3011893	0.0017 893	Proton ation	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(0:0/18:1(11Z))'	HMDB00 11475	C23H46NO7P	
3	16	479.3011893	0.0017 893	Proton ation	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(0:0/18:1(9Z))'	HMDB00 11476	C23H46NO7P	
7									

		479.3011893	0.0017 893	Proton ation	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(18:1(11Z)/0:0)'	HMDB00 11505	C23H46NO7P	
		479.3011893	0.0017 893	Proton ation	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(18:1(9Z)/0:0)'	HMDB00 11506	C23H46NO7P	
		478.2930537	0.0014 537	Redox	b'9-ethoxy-3a,5a-dimethyl-1-(propan-2-yl)-6-[(3,4,5-trihydroxyoxan-2-yl)oxy]-2H,3H,3aH,4H,5H,5aH,6H,9H,10H,10aH-cyclohepta[e]indene-8-carbaldehyde'	b'Erinacine D'	HMDB00 31896	C27H42O7	
		478.2930537	0.0014 537	Redox	b'3-{1-hydroxy-2-[2-hydroxy-2-(hydroxymethyl)-4b,8,8,10a-tetramethyl-tetradecahydrophenanthren-1-yl]ethyl}-5-oxo-2,5-dihydrofuran-2-yl acetate'	b'25-Acetylvulgaroside'	HMDB00 41365	C27H42O7	
		478.2903683	0.0012 317	Redox	b'6-amino-2-[2-(2-amino-3-methylbutanamido)-4-methylpentanamido]-N-(4-nitrophenyl)hexanamide'	b'Valyl-leucyl-lysine 4-nitroanilide'	HMDB02 50805	C23H38N6O5	
		478.2903683	0.0012 317	Redox	b'6-amino-2-[2-(2-amino-3-methylbutanamido)-3-methylpentanamido]-N-(4-nitrophenyl)hexanamide'	b'H-D-Val-Leu-Lys-pNA'	HMDB02 57385	C23H38N6O5	
2 3 8	480.30 71	481.3168394	0.0019 394	Proton ation	b'(2-([(2R)-2-hydroxy-3-(pentadecanoyloxy)propyl phosphono]oxy)ethyl)trimethylazanium'	b'LysoPC(15:0/0:0)'	HMDB00 10381	C23H48NO7P	C04 230
		481.3168394	0.0019 394	Proton ation	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'LysoPE(0:0/18:0)'	HMDB00 11129	C23H48NO7P	
		481.3168394	0.0019 394	Proton ation	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'LysoPE(18:0/0:0)'	HMDB00 11130	C23H48NO7P	
		481.3151861	0.0002 861	Proton ation	b'N-{1-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-2-oxo-1,2-dihydropyrimidin-4-yl}hexadecanamide'	b'Palmitoyl Ara-C'	HMDB02 56087	C25H43N3O6	
		480.3087038	0.0016 038	Redox	b'(1R,2R,4S,5R,7R,11S,14S,15R)-4,5,11-trihydroxy-2,15-dimethyl-14-[(2R,3R)-2,3,6-trihydroxy-6-methylheptan-2-yl]tetracyclo[8.7.0.0.0^{2,7}.0^{11,15}]heptadec-9-en-8-one'	b'Crustecdysone'	HMDB00 30180	C27H44O7	
		480.3087038	0.0016 038	Redox	b'4,5,11-trihydroxy-2,15-dimethyl-14-(2,3,6-trihydroxy-6-methylheptan-2-yl)tetracyclo[8.7.0.0.0^{2,7}.0^{11,15}]heptadec-9-en-8-one'	b'Ecysterone'	HMDB02 42587	C27H44O7	
2 3	481.23 37	482.2433406	0.0018 406	Proton ation	b'[(2R)-3-[(4Z,7Z,10Z,13Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-hydroxypropoxy]phosphonic acid'	b'1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-glycero-3-phosphate'	HMDB00 62307	C25H39O7P	

9		482.2433406	0.0018 406	Proton ation	b'[3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-hydroxypropoxy]phosphonic acid'	b'LysoPA(22:6(4Z,7Z,10Z,13Z,16Z,19Z)0:0)'	HMDB01 14755	C25H39O7P	
		481.2365419	0.0028 419	Redox	b'1-[4-[2-hydroxy-3-(quinolin-5-yloxy)propyl]piperazin-1-yl]-2,2-diphenylethan-1-one'	b'Dofequidar'	HMDB02 51575	C30H31N3O3	
2 4 0	481.97 78	482.9845118	0.0010 882	Proton ation	b'(((2R,3S,4R,5R)-5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)phosphonic acid'	b'Cytidine triphosphate'	HMDB00 00082	C9H16N3O14P3	C00 063
		482.9845118	0.0010 882	Proton ation	b'(((3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)phosphonic acid'	b'Arabinofuranosylcytosine triphosphate'	HMDB02 48548	C9H16N3O14P3	
2 4 1	482.95 84	483.9685274	0.0023 274	Proton ation	b'(((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)phosphonic acid'	b'Uridine triphosphate'	HMDB00 00285	C9H15N2O15P3	C00 075
		483.9685288	0.0023 288	Proton ation	b'(((5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)phosphonic acid'	b'([(2S,5S)-5-(2,4-Dioxopyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy-hydroxyphosphoryl] phosphono hydrogen phosphate'	HMDB02 58116	C9H15N2O15P3	
2 4 2	483.00 43	484.0116582	0.0004 418	Proton ation	b"6'-(acetyloxy)-2',7'-dichloro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-3'-yl acetate"	b'Diacetyldichlorofluorescein'	HMDB02 45587	C24H14Cl2O7	
		484.0116582	0.0004 418	Proton ation	b"3'-(acetyloxy)-4',5'-dichloro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-6'-yl acetate"	b'Dichlorofluorescein diacetate'	HMDB02 51193	C24H14Cl2O7	
		484.0116582	0.0004 418	Proton ation	b"3'-(acetyloxy)-4,5-dichloro-3-oxo-3H-spiro[2-benzofuran-1,9'-xanthene]-6'-yl acetate"	b"(6'-Acetyloxy-4,5-dichloro-3-oxospiro[2-benzofuran-1,9'-xanthene]-3'-yl) acetate"	HMDB02 57840	C24H14Cl2O7	
		484.0116582	0.0004 418	Proton ation	b"6,7-diacetyl-4,5-dichloro-3',6'-dihydroxy-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b"4,5-Diacetyl-6,7-dichloro-3',6'-dihydroxyspiro[2-benzofuran-3,9'-xanthene]-1-one"	HMDB02 58000	C24H14Cl2O7	
2 4	484.02 45	485.0325692	0.0002 692	Proton ation	b'6-{6-amino-8-[(4-chlorophenyl)sulfanyl]-9H-purin-9-yl}-2-hydroxy-7-methoxy-hexahydro-2lambda5-furo[3,2-d][1,3,2]dioxaphosphinin-2-one'	b"8-Pcpt-2'-O-Me-cAMP"	HMDB02 47461	C17H17ClN5O6 PS	

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2	488.31	488.3137891	0.0012	Redox	b'2-methyl-3-methylidene-6-{5,6,9-trihydroxy-2,6,15-trimethyl-17-oxotetracyclo[8.7.0.0\xc2\x82,\xc2\x81\x87.0\xc2\x89\xc2\x89,\xc2\x89\xc2\x81\x85]heptadec-1(10)-en-14-yl}heptanoic acid'	b'Antcin K'	HMDB02 49891	C29H44O6	
4	25		891						
4									
2	492.98	493.9991602	0.0017	Proton	b'[(4-{[(2,3-dihydroxypropoxy)(hydroxy)phosphoryl]oxy}-2,3,5-trihydroxy-6-(phosphonoxy)cyclohexyl)oxy]phosphonic acid'	b'Phosphatidylinositol 4,5-diphosphate'	HMDB02 52943	C9H21O17P3	
4	96		602	ation					
5									
2	493.16	493.1631194	0.0027	Redox	b'6-{2-[2-amino-3-(methylcarbamoyl)propanamido]-2-(4-hydroxyphenyl)acetamido}-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid'	b'6-[[2-[[2-Amino-4-(methylamino)-4-oxobutanoyl]amino]-2-(4-hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid'	HMDB02 48670	C21H27N5O7S	
4	59		806						
6		493.1671422	0.0012	Redox	b'N-{6-[3-tert-butyl-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-2-methoxyphenyl]naphthalen-2-yl}methanesulfonamide'	b'Dasabuvir'	HMDB02 50872	C26H27N3O5S	
		493.1631194	0.0027	Redox	b'6-(((3-carbamoyl-2-(methylamino)propanoyl)carbamoyl)(4-hydroxyphenyl)methyl)amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid'	b'L-Aspoxicillin trihydrate'	HMDB02 53876	C21H27N5O7S	
2	495.04	496.0590608	0.0015	Proton	b'N-{1-[bis(4-chlorophenyl)methyl]azetidin-3-yl}-N-(3,5-difluorophenyl)methanesulfonamide'	b'Drinabant'	HMDB02 51620	C23H20Cl2F2N2 O2S	
4	97		608	ation					
7									
2	501.95	502.9641976	0.0013	Proton	b'4-(3-sulfanylidene-3H-1,2-dithiol-5-yl)phenyl 2-{2-[(2,6-dichlorophenyl)amino]phenyl}acetate'	b'S-Diclofenac'	HMDB02 47974	C23H15Cl2NO2 S3	
4	5		976	ation					
8									
2	503.97	504.9800965	0.0015	Proton	b'(((2-[1-(6-amino-9H-purin-9-yl)-2-oxoethoxy]-3-oxopropoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b''2',3'-Dialdehyde ATP''	HMDB02 55984	C10H14N5O13P 3	
4	07		965	ation					
9									

250	504.3072	505.3168394	0.0018394	Protonation	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'LysoPE(0:0/20:2(11Z,14Z))'	HMDB0011483	C25H48NO7P	
		505.3168394	0.0018394	Protonation	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'LysoPE(20:2(11Z,14Z)/0:0)'	HMDB0011513	C25H48NO7P	
		505.3168399	0.0018399	Protonation	b'(2-{[3-(heptadeca-9,12-dienyloxy)-2-hydroxypropyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(17:2(9Z,12Z)/0:0)'	HMDB0256157	C25H48NO7P	
		504.3087038	0.0015038	Redox	b'4-{5-[(4,5-dihydroxy-6-methyloxan-2-yl)oxy]-11-hydroxy-2,15-dimethyltetraacyclo[8.7.0.0'xc2'xb2,\xc2'x81'xb7.0'xc2'xb9'xc2'xb9,\xc2'xb9'xc2'x81'xb5]heptadecan-14-yl}-2,5-dihydrofuran-2-one'	b'Desglucocorolide'	HMDB0033709	C29H44O7	
251	505.9868	506.9957452	0.0011452	Protonation	b'(((((((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy) (hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl}oxy)phosphonic acid'	b'Adenosine triphosphate'	HMDB0000538	C10H16N5O13P3	C00002
		506.9957452	0.0011452	Protonation	b'(((((((2R,3S,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3-hydroxyoxolan-2-yl)methoxy) (hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl}oxy)phosphonic acid'	b'dGTP'	HMDB0001440	C10H16N5O13P3	C00286
		506.9957452	0.0011452	Protonation	b'(((((((2R,3S,5R)-5-(6-amino-2-hydroxy-9H-purin-9-yl)-3-hydroxyoxolan-2-yl)methoxy) (hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl}oxy)phosphonic acid'	b'2-hydroxy-dATP'	HMDB0059593	C10H16N5O13P3	C19969
		506.9957452	0.0011452	Protonation	b'(((([5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy) (hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl}oxy)phosphonic acid'	b'[(2R,5R)-5-(6-Aminopurin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy-hydroxyphosphoryl] phosphono hydrogen phosphate'	HMDB0257997	C10H16N5O13P3	
252	506.2867	506.2879683	0.0012683	Redox	b'6-(1-hydroxy-1-{7,8,11-trihydroxy-2,15-dimethyl-3-oxotetracyclo[8.7.0.0'xc2'xb2,\xc2'x81'xb7.0'xc2'xb9'xc2'xb9,\xc2'xb9'xc2'x81'xb5]heptadecan-14-yl}ethyl)-3-(hydroxymethyl)-4-methyl-5,6-dihydro-2H-pyran-2-one'	b'(5alpha,6beta,14alpha,20R,22R)-5,6,14,20,27-Pentahydroxy-1-oxowith-24-enolide'	HMDB0033198	C28H42O8	
253	506.3221	507.3324895	0.0025895	Protonation	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(0:0/20:1(11Z))'	HMDB0011482	C25H50NO7P	
		507.3324895	0.0025895	Protonation	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(20:1(11Z)/0:0)'	HMDB0011512	C25H50NO7P	
254	506.98	506.9862293	0.0021	Redox	b'(((((((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonoxy)oxolan-2-yl)methoxy) (hydroxy)phosphoryl)oxy)sulfonic acid'	b'Phosphoadenosine phosphosulfate'	HMDB00	C10H15N5O13P	C00

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260	521.9806	522.9906598	0.0022598	Protonation	b'(((2R,3S,4R,5R)-5-(2-amino-6-oxo-6,7,8,9-tetrahydro-3H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)phosphonic acid'	b'Guanosine triphosphate'	HMDB0001273	C10H16N5O14P3	C00044
		522.9906598	0.0022598	Protonation	b'(((2S,3R,4R,5R)-5-(2-amino-6-oxo-6,7,8,9-tetrahydro-3H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)phosphonic acid'	b'8-Oxo-dGTP'	HMDB0011615	C10H16N5O14P3	
		522.9906612	0.0022612	Protonation	b'(((5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)phosphonic acid'	b'(((2S,3R,4R,5R)-5-(2-Amino-6-oxo-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy-hydroxyphosphoryl)phosphono hydrogen phosphate'	HMDB0047873	C10H16N5O14P3	
261	522.2809	523.2910191	0.0023191	Protonation	b'2-amino-3-(hydroxy[2-hydroxy-3-(octadec-9-enoyloxy)propoxy]phosphoryl)oxy)propanoic acid'	b'1-Oleoylglycerophosphoserine'	HMDB0061694	C24H46NO9P	
		523.2910186	0.0023186	Protonation	b'(2S)-2-amino-3-(hydroxy[(2R)-2-hydroxy-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl)oxy)propanoic acid'	b'LysoPS(18:1(9Z)/0:0)'	HMDB0040603	C24H46NO9P	
		522.2828829	0.0019829	Redox	b'15-[1-(4,5-dihydroxy-4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-5,6-dihydroxy-2,16-dimethyl-8-oxapentacyclo[9.7.0.0'xc2'xb2,\xc2'xb7,\xc2'xb7,\xc2'xb7,\xc2'xb9,\xc2'xb2,\xc2'xb2,\xc2'xb9,\xc2'xb6]octadecan-3-one'	b'Physangulide'	HMDB0037381	C28H42O9	
262	524.2772	525.2855393	0.0005393	Protonation	b'(2-aminoethoxy)[(2R)-2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-hydroxypropoxy]phosphinic acid'	b'LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB0011496	C27H44NO7P	
		525.2855393	0.0005393	Protonation	b'(2-aminoethoxy)[(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-hydroxypropoxy]phosphinic acid'	b'LysoPE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/0:0)'	HMDB0011526	C27H44NO7P	
		524.2765481	0.0006519	Redox	b'methyl N-[2-[(3-chlorophenyl)(1-[(2-(methylamino)-3-(oxan-3-yl)propyl]carbamoylethyl)methoxyethyl]carbamate'	b'Methyl 2-((R)-(3-chlorophenyl)((R)-1-((S)-2-(methylamino)-3-((R)-tetrahydro-2H-pyran-3-yl)propyl)carbamoylethyl)methoxyethyl]carbamate'	HMDB0047675	C26H41ClN4O5	
266	524.2968	525.3066691	0.0020691	Protonation	b'2-amino-3-(hydroxy[2-hydroxy-3-(octadecanoyloxy)propoxy]phosphoryl)oxy)propanoic acid'	b'1-Stearoylglycerophosphoserine'	HMDB0061698	C24H48NO9P	

3		525.3066687	0.0020 687	Proton ation	b'(2S)-2-amino-3-(hydroxy((2R)-2-hydroxy-3-(octadecanoyloxy)propoxy)phosphoryl oxy)propanoic acid'	b'LysoPS(18:0/0:0)	HMDB02 40606	C24H48NO9P	
2 6 4	525.30 05	526.3056245	0.0026 755	Proton ation	b'1-(butan-2-yl)-N-[(4,6-dimethyl-2-oxo-1,2-dihydropyridin-3-yl)methyl]-3-methyl-6-[6-(piperazin-1-yl)pyridin-3-yl]-1H-indole-4-carboxamide'	b'(S)-1-(Sec-Butyl)-N-[(4,6-dimethyl-2-oxo-1,2-dihydropyridin-3-yl)methyl]-3-methyl-6-(6-(piperazin-1-yl)pyridin-3-yl)-1H-indole-4-carboxamide'	HMDB02 52950	C31H38N6O2	
2 6 5	535.03 54	536.0444557	0.0012 557	Proton ation	b'(((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl oxy)((2R,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl)oxy)phosphinic acid'	b'UDP-D-Xylose'	HMDB00 01018	C14H22N2O16P 2	C00 190
		536.0444557	0.0012 557	Proton ation	b'(((2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl)oxy)(hydroxy)phosphoryl oxy)((2R,3S,4R,5R)-3,4-dihydroxy-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-2-yl)methoxy)phosphinic acid'	b'UDP-D-apiose'	HMDB00 12301	C14H22N2O16P 2	C01 623
		536.0444557	0.0012 557	Proton ation	b'(((2R,3S,4R,5R)-3,4-dihydroxy-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-2-yl)methoxy)((hydroxy)((2R,3R,4S,5S)-3,4,5-trihydroxyoxan-2-yl)oxy)phosphoryl oxy)phosphinic acid'	b'UDP-L-arabinose'	HMDB00 12303	C14H22N2O16P 2	C00 935
2 6 6	537.19 2	538.1991533	0.0006 467	Proton ation	b'3,8,22,27,29-pentamethyl-11,15,19-trioxaoctacyclo[14.14.1.0]xc2xb2,xc2xb9xc2xb1xb4.0xc2xb1xb4,xc2xb9xc2xb2.0xc2xb5,xc2xb9xc2xb1xb0.0xc2xb9xc2xb1xb8,xc2xb2xc2xb1xb6.0xc2xb2xc2xb1xb0,xc2xb2xc2xb1xb5.0xc2xb2xc2xb1xb7,xc2xb3xc2xb9]hentriaconta-2,4(12),5,7,9,13,18(26),20,22,24,29-undecaene-6,16,17,24-tetrol'	b'Asticlorin A'	HMDB00 30133	C33H30O7	
2 6 7	540.05 2	541.0611098	0.0013 098	Proton ation	b'3,4,8,10,14,15-hexahydroxy-24-imino-7,9,11,25,26-pentaosa-1,17,19,22-tetraaza-8lambda5,10lambda5-diphosphapentacyclo[18.3.1.1^(2,5).1^(13,16).0^(17,21)]hexacosa-18,20,22-triene-8,10-dione'	b'Cyclic ADP-ribose'	HMDB02 49529	C15H21N5O13P 2	
		541.0614413	0.0016 413	Proton ation	b'3-[2-(2-chloro-4-[[3-(2,6-dichlorophenyl)-5-(propan-2-yl)-1,2-oxazol-4-yl]methoxy]phenyl)ethenyl]benzoic acid'	b'3-[2-[2-Chloro-4-[[3-(2,6-dichlorophenyl)-5-propan-2-yl-4-isoxazolyl]methoxy]phenyl]ethenyl]benzoic acid'	HMDB02 49972	C28H22Cl3NO4	
2 6 8	540.28 29	541.2920674	0.0013 674	Proton ation	b'(((2S,4R,5S,6S)-6-((2S,3R,4E)-2-amino-3-hydroxyoctadec-4-en-1-yl)oxy)-3,4,5-trihydroxyoxan-2-yl)methoxy)sulfonic acid'	b'Psychosine sulfate'	HMDB00 13046	C24H47NO10S	
		541.2920679	0.0013 679	Proton ation	b'2-[(2-amino-3-hydroxyoctadec-4-en-1-yl)oxy]-3,5-dihydroxy-6-(hydroxymethyl)oxan-4-yl]oxidanefulfonic acid'	b'Lysosulfatide'	HMDB02 54273	C24H47NO10S	
2	558.06	559.0716735	0.0016	Proton	b'[[5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy]((hydroxy((3,4,5-trihydroxyoxolan-2-yl)methoxy)phosphoryl oxy)phosphinic acid'	b'Adenosine diphosphate ribose'	HMDB00	C15H23N5O14P	C00

6	22		735	ation			01178	2	301
9		559.0716735	0.0016 735	Proton ation	b'[[[(2R,3S,4R,5R)-5-{1-[(2R,3R,4S,5R)-3,4-dihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl]-6-imino-6,9-dihydro-1H-purin-9-yl}-3,4-dihydroxyoxolan-2-yl]methoxy} phosphonic acid'	b'Phosphoribosyl-AMP'	HMDB00 12276	C15H23N5O14P 2	C02 741
		559.0716744	0.0016 744	Proton ation	b'[[5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy}{(hydroxy[(2,3,4-trihydroxy-5-oxopentyl)oxy]phosphoryl)oxy}phosphinic acid'	b'ADP Ribose'	HMDB02 48024	C15H23N5O14P 2	
		559.0716735	0.0016 735	Proton ation	b'[[[(2R,3S,4R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy}{(hydroxy[(2R,3S,4R,5R)-3,4,5-trihydroxyoxolan-2-yl]methoxy)}phosphoryl]oxy}phosphinic acid'	b'Adenosine diphosphate-D-ribose'	HMDB03 03049	C15H23N5O14P 2	
2 7 0	563.03 14	564.0404684	0.0012 684	Proton ation	b'[5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl {3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl phosphonato}oxy}phosphonate'	b'UDP-alpha-D-galactose'	HMDB03 04527	C15H22N2O17P 2	
2 7 1	563.06 38	564.07171	0.0001 1	Proton ation	b'2-[[[(1-carboxy-5-[[[(4-iodophenyl)carbamoyl]amino]pentyl)carbamoyl]amino]pentanedioic acid'	b'L-Glutamic acid, N-((((1S)-1-carboxy-5-[[[(4-iodophenyl)amino]carbonyl]amino]pentyl)amino]carbonyl)-'	HMDB02 50018	C19H25N4O8	
2 7 2	565.04 5	566.0550204	0.0022 204	Proton ation	b'[([(2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)[[(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy} phosphinic acid'	b'Uridine diphosphate glucose'	HMDB00 00286	C15H24N2O17P 2	C00 029
		566.0550204	0.0022 204	Proton ation	b'[([(2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)[[(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy} phosphinic acid'	b'Uridine diphosphategalactose'	HMDB00 00302	C15H24N2O17P 2	C00 052
		566.0550204	0.0022 204	Proton ation	b'[([(3,4-dihydroxy-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)[[(3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy} phosphinic acid'	b"Glucose-uridine-C1,5'-diphosphate"	HMDB02 59387	C15H24N2O17P 2	
2 7 3	565.13 54	566.1424263	0.0007 737	Proton ation	b'2-[[[3,5-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl]oxy]-4,5-dihydroxy-6-methylxan-3-yl 2-methoxybenzoate'	b'Gladioside C2'	HMDB00 36254	C29H26O12	
		566.1424263	0.0007 737	Proton ation	b'2-[[[3,5-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl]oxy]-3,5-dihydroxy-6-methylxan-4-yl 2-methoxybenzoate'	b'Gladioside C1'	HMDB00 36255	C29H26O12	
2 7	568.27 64	569.2849486	0.0007 486	Proton ation	b'2-[2-(2-[2-amino-3-(4-hydroxyphenyl)propanamido]propanamido}acetamido)-3-phenylpropanamido]-4-methylpentanoic acid'	b'Leuphasyl'	HMDB02 47171	C29H39N5O7	

4									
2	571.28	572.2961635	0.0020 635	Proton ation	b'[(2R)-3-(hexadecanoyloxy)-2-hydroxypropoxy](((1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl)oxy)]phosphonic acid'	b'LysoPI(16:0/0:0)'	HMDB00 61695	C25H49O12P	
7	63	571.2866799	0.0003 799	Redox	b'(2S)-2-(((2S)-1-((2S)-2-[(2S)-2-amino-5-carbamimidamidopentanamido]-3-(1H-imidazol-4-yl)propanoyl)pyrrolidin-2-yl)]formamido)-3-(4-hydroxyphenyl)propanoic acid'	b'Kinetensin 4-7'	HMDB00 12986	C26H37N9O6	
2	573.01	574.0264698	0.0016 698	Proton ation	b'6-([2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-4-oxo-3-(sulfooxy)-4H-chromen-8-yl]oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'Gossypetin 8-glucuronide 3-sulfate'	HMDB00 37752	C21H18O17S	
7	7	574.02284	0.0019 6	Proton ation	b'N-([5-(2-chloro-6-((3-iodophenyl)methyl)amino)-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl](hydroxy)methyl)-N-methylformamide'	b'N-([[(2S,3S,4R,5R)-5-[2-Chloro-6-((3-iodophenyl)methylamino)purin-9-yl]-3,4-dihydroxyoxolan-2-yl]-hydroxymethyl]-N-methylformamide'	HMDB02 57746	C19H20ClN6O5	
2	579.02	580.0342849	0.0015 849	Proton ation	b'(2S,3S,4S,5R,6R)-6-((((((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'Uridine diphosphate glucuronic acid'	HMDB00 00935	C15H22N2O18P 2	C00 167
7	49	580.0342849	0.0015 849	Proton ation	b'(2S,3R,4S,5R,6R)-6-((((((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'UDP-D-galacturonic acid'	HMDB00 12302	C15H22N2O18P 2	C00 617
7	7	580.0342849	0.0015 849	Proton ation	b'(2R,3S,4S,5R,6R)-6-((((((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'UDP-L-iduronate'	HMDB00 12304	C15H22N2O18P 2	C02 330
2	579.02	580.0342859	0.0015 859	Proton ation	b'6-((((([5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'(2R,3R,4R,5S,6R)-6-([[(2S,3R,4R,5R)-5-(2,4-Dioxypyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy-hydroxyphosphoryl]oxy-hydroxyphosphoryl]oxy-3,4,5-trihydroxyoxane-2-carboxylic acid'	HMDB02 60120	C15H22N2O18P 2	
7	7	580.0342859	0.0015 859	Proton ation	b'([5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-4-hydroxy-3-((3,4,5,6-tetrahydroxy-2-oxohexanoyl)oxy)oxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'[(2R,3S,4R,5R)-5-(2,4-Dioxypyrimidin-1-yl)-4-hydroxy-2-	HMDB02 60220	C15H22N2O18P 2	

						[[hydroxy(phosphonooxy)phosphoryl]oxymethyl]oxolan-3-yl] (3S,4R,5S)-3,4,5,6-tetrahydroxy-2-oxohexanoate'			
2	581.17	582.1889826	0.0012 826	Proton ation	b'2-[6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-5-[(E)-2-(2,4-dihydroxyphenyl)ethenyl]benzene-1,3-diol'	b'Kuwanon Y'	HMDB00 33296	C34H30O9	
7	99	582.1849598	0.0027 402	Proton ation		b'Glucuronidated Sn-38'	HMDB02 52796	C29H30N2O11	
2	585.95 2	586.9620756	0.0022 756	Proton ation	b'(((((((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl]oxy) phosphonic acid'	b'Adenosine tetraphosphate'	HMDB00 01364	C10H17N5O16P 4	C03 483
2 8 0	588.07 26	589.0822382	0.0018 382	Proton ation	b'(((((((2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(((((3S,4R,5S,6S)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy))phosphonic acid'	b'GDP-L-fucose'	HMDB00 01095	C16H25N5O15P 2	C00 325
		589.0822382	0.0018 382	Proton ation	b'(((((((2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(((((2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy))phosphonic acid'	b'GDP-D-Rhamnose'	HMDB00 01499	C16H25N5O15P 2	C03 117
		589.0822382	0.0018 382	Proton ation	b'(((((((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(((((2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy))phosphonic acid'	b'ADP-Mannose'	HMDB00 06369	C16H25N5O15P 2	C06 192
		589.0822382	0.0018 382	Proton ation	b'(((((((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(((((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy))phosphonic acid'	b'ADP-glucose'	HMDB00 06557	C16H25N5O15P 2	C00 498
		589.0822382	0.0018 382	Proton ation	b'(((((((3,4-dihydroxy-5-(6-hydroxy-2-imino-3,9-dihydro-2H-purin-9-yl)oxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(((((3,4,5-trihydroxy-6-methyloxan-2-yl]oxy))phosphonic acid'	b'GDP-fucose'	HMDB02 52660	C16H25N5O15P 2	
2	599.31	600.3274637	0.0028 637	Proton ation	b'[(2R)-3-hydroxy-2-(octadecanoyloxy)propoxy](((((1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy))phosphonic acid'	b'LysoPI(0:0/18:0)'	HMDB00 61704	C27H53O12P	
8	68	600.3274637	0.0028 637	Proton ation	b'[(2R)-2-hydroxy-3-(octadecanoyloxy)propoxy](((((1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy))phosphonic acid'	b'LysoPI(18:0/0:0)'	HMDB02 40261	C27H53O12P	
2	603.00 19	604.0125343	0.0028 343	Proton ation	b'4,5,6,12,19,20,21,27-octahydroxy-10,14,25,29-tetraoxaocetacyclo[14.14.2.0]xc2'xb2,\xc2'xb9'xc2'xb9.0'xc2'xb3,\xc2'xb8'xb8.0'xc2'xb9'xc2'xb3,\xc2'xb3'xc2'xb9.0'xc2'xb9'xc2'xb8'xb7,\xc2'xb2'xc2'xb8'xb6.0'xc2'xb9'xc2'xb8	b'Gallagic acid'	HMDB00 29275	C28H12O16	

2					\xb8,\xc2\xb2\xc2\xb3.0\xc2\xb2\xc2\x81\xb8,\xc2\xb3\xc2\xb2\xb2]dotriaconta-1(31),2(11),3(8),4,6,12,16(32),18(23),19,21,27-undecaene-9,15,24,30-tetrone'				
2	604.06 71	605.0771528	0.0022 528	Proton ation	b'[([(2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy[([(2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)]phosphinic acid'	b'Guanosine diphosphate mannose'	HMDB00 01163	C16H25N5O16P 2	C00 096
3		605.0771528	0.0022 528	Proton ation	b'[([(2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy[([(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)]phosphinic acid'	b'GDP-glucose'	HMDB00 03351	C16H25N5O16P 2	C00 394
2 8 4	605.06 92	605.0670175	0.0021 825	Redox	b'[5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl [(3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl phosphonato]oxy]phosphonate'	b'UDP-N-acetyl-alpha-D-glucosamine'	HMDB03 04526	C17H25N3O17P 2	
2 8 5	606.07 14	607.0815695	0.0023 695	Proton ation	b'[([(2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy[([(2R,3R,4S,5S,6R)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)]phosphinic acid'	b'Uridine diphosphate-N-acetylglucosamine'	HMDB00 00290	C17H27N3O17P 2	C00 043
		607.0815695	0.0023 695	Proton ation	b'[([(5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy[([(3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)]phosphinic acid'	b'Uridine diphosphate-N-acetylgalactosamine'	HMDB00 00304	C17H27N3O17P 2	
		607.0815695	0.0023 695	Proton ation	b'[([(2S,3R,4S,5S)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy[([(3R,4S,5R,6S)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)]phosphinic acid'	b'UDP-N-acetyl-D-mannosamine'	HMDB00 13112	C17H27N3O17P 2	C011 70
		607.0815695	0.0023 695	Proton ation	b'[([(2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy[([(2R,3R,4R,5R,6R)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)]phosphinic acid'	b'UDP-N-acetyl-alpha-D-galactosamine'	HMDB00 60522	C17H27N3O17P 2	
2 8 6	611.14 26	612.1519619	0.0015 619	Proton ation	b'(2S)-2-amino-4-[((1R)-2-[((2R)-2-[(4S)-4-amino-4-carboxybutanamido]-2-[(carboxymethyl)carbamoyl]ethyl]disulfanyl)-1-[(carboxymethyl)carbamoyl]ethyl]carbamoyl]butanoic acid'	b'Oxidized glutathione'	HMDB00 03337	C20H32N6O12S 2	C00 127
		611.1400806	0.0025 194	Redox	b'3-[((2S,3R,4S,5R,6R)-3,5-dihydroxy-6-(hydroxymethyl)-4-[((2E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy)oxan-2-yl]oxy)-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-1'\xc2\xbb'\xc2\x81'\xb4-chromen-1-ylum'	b'Delphinidin 3-(3"-p-coumaroylglucoside)"	HMDB00 30099	C30H27O14	
		611.1400806	0.0025 194	Redox	b'5,7-dihydroxy-3-[(3,4,5-trihydroxy-6-[((2E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy)methyl]oxan-2-yl]oxy)-2-(3,4,5-trihydroxyphenyl)-1'\xc2\xbb'\xc2\x81'\xb4-chromen-1-ylum'	b'Delphinidin 3-(6-p-coumaroylglactoside)'	HMDB00 37089	C30H27O14	
2 8 7	619.28 64	620.2961635	0.0019 635	Proton ation	b'[(2R)-2-hydroxy-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy)[[((1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy)]phosphinic acid'	b'LysoPI(20:4(5Z,8Z,11Z,14Z)/0:0)'	HMDB00 61690	C29H49O12P	
		620.296164	0.0019 64	Proton ation	b'[2-hydroxy-3-(icosa-5,8,11,14-tetraenoyloxy)propoxy)[[(2,3,4,5,6-pentahydroxycyclohexyl]oxy)]phosphinic acid'	b'PI(20:4(5Z,8Z,11Z,14Z)/0:0)'	HMDB02 56523	C29H49O12P	

		620.2918249	0.0023 751	Proton ation	b'2-[2-[5-({amino({methylcarbamoyl}amino)methylidene}amino)-2-(2-acetamidopropanamido)-N-methylpentanamido]-3-phenylpropanamido]butanedioic acid'	b'Tetrapeptide'	HMDB02 58927	C27H40N8O9	
2 8 8	619.33 75	619.3369842	0.0005 158	Redox	b'2-(2-[2-[(azepane-1-carbonyl)amino]-4-methylpentanamido]-3-(1-methyl-1H-indol-3-yl)propanamido)-3-(4-hydroxyphenyl)propanoic acid'	b'N-(Hexahydro-1-azepinyl)carbonyl- leucyl(1-methyl)-tryptophyl- tryptophan'	HMDB02 56177	C34H45N5O6	
2 8 9	620.01 76	621.0274392	0.0020 392	Proton ation	b' [{ (2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy } [{ ((5R)-2,6-dihydroxy-2-oxo-tetrahydro-2H-2'xccc'x'bb'xe2'x81'xb5-furo[2,3-d][1,3,2]dioxaphosphol-5-yl]methoxy } (hydroxy)phosphoryl]oxy]phosphinic acid'	b'ADP-ribose 1"-2" cyclic phosphate'	HMDB00 11671	C15H22N5O16P 3	
2 9 0	644.49 87	644.5015899	0.0028 899	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(17:0/20:4(6E,8Z,11Z,14Z)+=O(5))0:0)'	HMDB02 95699	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)+=O(5)/17: 0/0:0)'	HMDB02 95700	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(17:0/0:0/20:4(6E,8Z,11Z,14Z)+= O(5))'	HMDB02 95701	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)+=O(5)/0:0/ 17:0)'	HMDB02 95702	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(17:0/20:4(5Z,8Z,11Z,13E)+=O(1 5)/0:0)'	HMDB02 95703	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15)/17 :0/0:0)'	HMDB02 95704	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(17:0/0:0/20:4(5Z,8Z,11Z,13E)+= O(15))'	HMDB02 95705	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15)/0: 0/17:0)'	HMDB02 95706	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(17:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/0:0)'	HMDB02 95727	C40H68O6	

		644.5015899	0.0028 899	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicos-5,8,11,14,16-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/17:0/0:0)'	HMDB02 95728	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicos-5,8,11,14,16-pentaenoate'	b'DG(17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 95729	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicos-5,8,11,14,16-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/0:0/17:0)'	HMDB02 95730	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicos-5,8,11,13,17-pentaenoate'	b'DG(17:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/0:0)'	HMDB02 95731	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicos-5,8,11,13,17-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/17:0/0:0)'	HMDB02 95732	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicos-5,8,11,13,17-pentaenoate'	b'DG(17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	HMDB02 95733	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicos-5,8,11,13,17-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/0:0/17:0)'	HMDB02 95734	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicos-5,8,10,14,17-pentaenoate'	b'DG(17:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/0:0)'	HMDB02 95735	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicos-5,8,10,14,17-pentaenoate'	b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/17:0/0:0)'	HMDB02 95736	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicos-5,8,10,14,17-pentaenoate'	b'DG(17:0/0:0/20:5(5Z,8Z,10E,14Z,17Z)-OH(12))'	HMDB02 95737	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicos-5,8,10,14,17-pentaenoate'	b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/0:0/17:0)'	HMDB02 95738	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicos-6,8,11,14,17-pentaenoate'	b'DG(17:0/20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/0:0)'	HMDB02 95739	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicos-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/17:0/0:0)'	HMDB02 95740	C40H68O6	

		644.5015899	0.0028 899	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(17:0/0:0/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 95741	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/0:0/17:0))'	HMDB02 95742	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(a-17:0/20:4(6E,8Z,11Z,14Z)+=O(5)/0:0))'	HMDB02 97779	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)+=O(5)/a-17:0/0:0))'	HMDB02 97780	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(a-17:0/0:0/20:4(6E,8Z,11Z,14Z)+=O(5))'	HMDB02 97781	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(a-17:0/20:4(5Z,8Z,11Z,13E)+=O(15)/0:0))'	HMDB02 97782	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15)/a-17:0/0:0))'	HMDB02 97783	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(a-17:0/0:0/20:4(5Z,8Z,11Z,13E)+=O(15))'	HMDB02 97784	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15)/0:0/a-17:0))'	HMDB02 97785	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(a-17:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/0:0))'	HMDB02 97806	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/a-17:0/0:0))'	HMDB02 97807	C40H68O6	
		644.5015899	0.0028	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(a-	HMDB02	C40H68O6	

		899				17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R))'	97808		
644.5015899	0.0028 899	Redox		b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/0:0/a-17:0)'	HMDB02 97809		C40H68O6	
644.5015899	0.0028 899	Redox		b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(a- 17:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/0:0)'	HMDB02 97810		C40H68O6	
644.5015899	0.0028 899	Redox		b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/a-17:0/0:0)'	HMDB02 97811		C40H68O6	
644.5015899	0.0028 899	Redox		b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(a- 17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18))'	HMDB02 97812		C40H68O6	
644.5015899	0.0028 899	Redox		b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/0:0/a-17:0)'	HMDB02 97813		C40H68O6	
644.5015899	0.0028 899	Redox		b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(a- 17:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/0:0)'	HMDB02 97814		C40H68O6	
644.5015899	0.0028 899	Redox		b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/a-17:0/0:0)'	HMDB02 97815		C40H68O6	
644.5015899	0.0028 899	Redox		b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(a- 17:0/0:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12))'	HMDB02 97816		C40H68O6	
644.5015899	0.0028 899	Redox		b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/0:0/a-17:0)'	HMDB02 97817		C40H68O6	
644.5015899	0.0028 899	Redox		b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(a- 17:0/20:5(6E,8Z,11Z,14Z,17Z)-	HMDB02 97818		C40H68O6	

					OH(5)/0:0)			
644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/a-17:0/0:0)	HMDB02 97819	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(a- 17:0/0:0/20:5(6E,8Z,11Z,14Z,17Z)- OH(5))'	HMDB02 97820	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/0:0/a-17:0)	HMDB02 97821	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(i- 17:0/20:4(6E,8Z,11Z,14Z)+=O(5)/0:0)	HMDB02 99440	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)+=O(5)/i- 17:0/0:0)	HMDB02 99441	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(i- 17:0/0:0/20:4(6E,8Z,11Z,14Z)+=O(5))'	HMDB02 99442	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)+=O(5)/0:0/ i-17:0)	HMDB02 99443	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(i- 17:0/20:4(5Z,8Z,11Z,13E)+=O(15)/0:0 y	HMDB02 99444	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15)/i- 17:0/0:0)	HMDB02 99445	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(i- 17:0/0:0/20:4(5Z,8Z,11Z,13E)+=O(15) y	HMDB02 99446	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15)/0: 0/i-17:0)	HMDB02 99447	C40H68O6		

		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(i-17:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/0:0)'	HMDB02 99468	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/i-17:0/0:0)'	HMDB02 99469	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(i- 17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R))'	HMDB02 99470	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/0:0/i-17:0)'	HMDB02 99471	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(i-17:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/0:0)'	HMDB02 99472	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/i-17:0/0:0)'	HMDB02 99473	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(i- 17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18))'	HMDB02 99474	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/0:0/i-17:0)'	HMDB02 99475	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(i-17:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/0:0)'	HMDB02 99476	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/i-17:0/0:0)'	HMDB02 99477	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(i- 17:0/0:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12))'	HMDB02 99478	C40H68O6	
		644.5015899	0.0028	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(20:5(5Z,8Z,10E,14Z,17Z)-	HMDB02	C40H68O6	

2 9 1	647.46		899			OH(12)/0:0/i-17:0)	99479		
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(i-17:0/20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/0:0)	HMDB02 99480	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/i-17:0/0:0)	HMDB02 99481	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(i-17:0/0:0/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 99482	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/0:0/i-17:0)	HMDB02 99483	C40H68O6	
	37	648.4730062	0.0015 062	Proton ation	b'[(2R)-2,3-bis(hexadecanoyloxy)propoxy]phosphonic acid'	b'PA(16:0/16:0)	HMDB00 00674	C35H69O8P	C00 416
		648.4730062	0.0015 062	Proton ation	b'[(2R)-3-(decanoyloxy)-2-(docosanoyloxy)propoxy]phosphonic acid'	b'PA(10:0/22:0)	HMDB01 14777	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-3-(octadecanoyloxy)-2-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/14:0)	HMDB01 14873	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-2-(dodecanoyloxy)-3-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:0/12:0)	HMDB01 15059	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-2-(decanoyloxy)-3-(docosanoyloxy)propoxy]phosphonic acid'	b'PA(22:0/10:0)	HMDB01 15237	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-3-(decanoyloxy)-2-[(20-methylhenicosanoyl)oxy]propoxy]phosphonic acid'	b'PA(10:0/i-22:0)	HMDB01 15621	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-3-(icosanoyloxy)-2-[(10-methylundecanoyl)oxy]propoxy]phosphonic acid'	b'PA(20:0/i-12:0)	HMDB01 15634	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-2-[(22-methyltricosanoyl)oxy]-3-(octanoyloxy)propoxy]phosphonic acid'	b'PA(8:0/i-24:0)	HMDB01 15696	C35H69O8P	

		648.4730062	0.0015 062	Proton ation	b'[(2R)-3-[(10-methyldodecanoyl)oxy]-2-[(17-methyloctadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(a-13:0/i-19:0)	HMDB01 15710	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-2-[(18-methylnonadecanoyl)oxy]-3-[(10-methylundecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-12:0/i-20:0)	HMDB01 15789	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-3-[(11-methyldodecanoyl)oxy]-2-[(17-methyloctadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-13:0/i-19:0)	HMDB01 15806	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-2-(dodecanoyloxy)-3-[(18-methylnonadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-20:0/12:0)	HMDB01 15831	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-3-[(18-methylnonadecanoyl)oxy]-2-[(10-methylundecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-20:0/i-12:0)	HMDB01 15848	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-2-(decanoyloxy)-3-[(20-methylhenicosanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-22:0/10:0)	HMDB01 15890	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[(2R)-3-[(22-methyltricosanoyl)oxy]-2-(octanoyloxy)propoxy]phosphonic acid'	b'PA(i-24:0/8:0)	HMDB01 15932	C35H69O8P	
		648.4730062	0.0015 062	Proton ation	b'[2,3-bis(hexadecanoyloxy)propoxy]phosphonic acid'	b'2,3-Bis(palmitoyloxy)propyl dihydrogen phosphate'	HMDB02 44852	C35H69O8P	
2 9 2	652.07 87	653.0883871	0.0018 871	Proton ation	b'({3-([5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy}(hydroxy)phosphoryl)oxy)-4-hydroxy-5-(6-oxo-6,9-dihydro-1H-purin-9-yl)oxolan-2-yl]methoxy}phosphonic acid'	b"Cytidyl-yl-(5'-3')-5'-inosinic acid homopolymer"	HMDB02 56667	C19H25N7O15P 2	
2 9 3	670.51 44	670.51724	0.0028 4	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(17:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/0:0)	HMDB02 95759	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/17:0/0:0)	HMDB02 95760	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(17:0/0:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 95761	C42H70O6	
		670.51724	0.0028	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-	HMDB02	C42H70O6	

			4			OH(4)/0:0/17:0)	95762		
670.51724	0.0028 4	Redox		b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(17:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/0:0)	HMDB02 95763	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/17:0/0:0)	HMDB02 95764	C42H70O6		
670.51724	0.0028 4	Redox		b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(17:0/0:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 95765	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/0:0/17:0)	HMDB02 95766	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(17:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0)	HMDB02 95767	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/17:0/0:0)	HMDB02 95768	C42H70O6		
670.51724	0.0028 4	Redox		b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(17:0/0:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 95769	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0/17:0)	HMDB02 95770	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(17:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/0:0)	HMDB02 95771	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/17:0/0:0)	HMDB02 95772	C42H70O6		
670.51724	0.0028 4	Redox		b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(17:0/0:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 95773	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/0:0/17:0)	HMDB02 95774	C42H70O6		
670.51724	0.0028	Redox		b'(2S)-3-hydroxy-2-[[[4Z,7Z,10Z,13Z]15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl]pentadeca-4,7,10,13-tetraenyl}oxy]propyl heptadecanoate'	b'DG(17:0/22:5(4Z,7Z,10Z,13Z,19Z)-	HMDB02	C42H70O6		

		4				O(16,17)0:0)'	95779		
670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-{{{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}propan-2-yl heptadecanoate'		b'DG(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)17:0/0:0)'	HMDB02 95780	C42H70O6		
670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-{{{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}propyl heptadecanoate'		b'DG(17:0/0:0/22:5(4Z,7Z,10Z,13Z,19Z)- Z)-O(16,17))'	HMDB02 95781	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-{{{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}propyl heptadecanoate'		b'DG(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)0:0/17:0)'	HMDB02 95782	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'		b'DG(a- 17:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)0:0)'	HMDB02 97838	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'		b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)a-17:0/0:0)'	HMDB02 97839	C42H70O6		
670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'		b'DG(a- 17:0/0:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)- -OH(4))'	HMDB02 97840	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'		b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)0:0/a-17:0)'	HMDB02 97841	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'		b'DG(a- 17:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)0:0)'	HMDB02 97842	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'		b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)a-17:0/0:0)'	HMDB02 97843	C42H70O6		
670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'		b'DG(a- 17:0/0:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)- -OH(7))'	HMDB02 97844	C42H70O6		
670.51724	0.0028	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'		b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-	HMDB02	C42H70O6		

		4				OH(7)/0:0/a-17:0)	97845		
670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'		b'DG(a-17:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0)	HMDB02 97846	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'		b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/a-17:0/0:0)	HMDB02 97847	C42H70O6		
670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'		b'DG(a-17:0/0:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 97848	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'		b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0/a-17:0)	HMDB02 97849	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'		b'DG(a-17:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/0:0)	HMDB02 97850	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'		b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/a-17:0/0:0)	HMDB02 97851	C42H70O6		
670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'		b'DG(a-17:0/0:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 97852	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'		b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/0:0/a-17:0)	HMDB02 97853	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-([(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy)propyl 14-methylhexadecanoate'		b'DG(a-17:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/0:0)	HMDB02 97858	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-([(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy)propan-2-yl 14-methylhexadecanoate'		b'DG(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/a-17:0/0:0)	HMDB02 97859	C42H70O6		

		670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-{{[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy}propyl 14-methylhexadecanoate'	b'DG(a- 17:0/0:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))'	HMDB02 97860	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-{{[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy}propyl 14-methylhexadecanoate'	b'DG(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/0:0/a-17:0)'	HMDB02 97861	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(i- 17:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)/0:0)'	HMDB02 99500	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)/i-17:0/0:0)'	HMDB02 99501	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(i- 17:0/0:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)- -OH(4))'	HMDB02 99502	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)/0:0/i-17:0)'	HMDB02 99503	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(i- 17:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/0:0)'	HMDB02 99504	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/i-17:0/0:0)'	HMDB02 99505	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(i- 17:0/0:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)- -OH(7))'	HMDB02 99506	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/0:0/i-17:0)'	HMDB02 99507	C42H70O6	
		670.51724	0.0028	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(i-	HMDB02	C42H70O6	

		4				17:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/0:0)	99508		
670.51724	0.0028 4	Redox		b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/i-17:0/0:0)	HMDB02 99509		C42H70O6	
670.51724	0.0028 4	Redox		b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(i- 17:0/0:0/22:6(4Z,7Z,10Z,12E,16Z,19Z) -OH(14))'	HMDB02 99510		C42H70O6	
670.51724	0.0028 4	Redox		b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/0:0/i-17:0)	HMDB02 99511		C42H70O6	
670.51724	0.0028 4	Redox		b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(i- 17:0/22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/0:0)	HMDB02 99512		C42H70O6	
670.51724	0.0028 4	Redox		b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/i-17:0/0:0)	HMDB02 99513		C42H70O6	
670.51724	0.0028 4	Redox		b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(i- 17:0/0:0/22:6(4Z,7Z,10Z,13E,15E,19Z) -OH(17))'	HMDB02 99514		C42H70O6	
670.51724	0.0028 4	Redox		b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/0:0/i-17:0)	HMDB02 99515		C42H70O6	
670.51724	0.0028 4	Redox		b'(2S)-3-hydroxy-2-([(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}]pentadeca-4,7,10,13-tetraenyl)oxy]propyl 15-methylhexadecanoate'	b'DG(i-17:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/0:0)	HMDB02 99520		C42H70O6	
670.51724	0.0028 4	Redox		b'(2S)-1-hydroxy-3-([(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}]pentadeca-4,7,10,13-tetraenyl)oxy]propan-2-yl 15-methylhexadecanoate'	b'DG(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/i-17:0/0:0)	HMDB02 99521		C42H70O6	
670.51724	0.0028 4	Redox		b'(2R)-2-hydroxy-3-([(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}]pentadeca-4,7,10,13-tetraenyl)oxy]propyl 15-methylhexadecanoate'	b'DG(i- 17:0/0:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))'	HMDB02 99522		C42H70O6	

		670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-([(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy)propyl 15-methylhexadecanoate'	b'DG(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)0:0/i-17:0)'	HMDB02 99523	C42H70O6	
2 9 4	673.47 79	674.4886562	0.0029 562	Proton ation	b'[(2R)-3-(hexadecanoyloxy)-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(16:0/18:1(11Z))'	HMDB00 07858	C37H71O8P	C00 416
		674.4886562	0.0029 562	Proton ation	b'[(2R)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(16:0/18:1(9Z))'	HMDB00 07859	C37H71O8P	C00 416
		674.4886558	0.0029 558	Proton ation	b'[2-(hexadecanoyloxy)-3-[(9E)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'9-Octadecenoic acid 1-[[[(1-oxohexadecyl)oxy]methyl]-2-(phosphonoxy)ethyl ester'	HMDB00 31130	C37H71O8P	
		674.4886558	0.0029 558	Proton ation	b'[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/16:1(9Z))'	HMDB01 14877	C37H71O8P	
		674.4886562	0.0029 562	Proton ation	b'[(2R)-2-(hexadecanoyloxy)-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/16:0)'	HMDB01 14899	C37H71O8P	
		674.4886562	0.0029 562	Proton ation	b'[(2R)-2-(hexadecanoyloxy)-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/16:0)'	HMDB01 14924	C37H71O8P	
		674.4886562	0.0029 562	Proton ation	b'[(2R)-3-(icosanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(20:0/14:1(9Z))'	HMDB01 15062	C37H71O8P	
		674.4886562	0.0029 562	Proton ation	b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(20:1(11Z)/14:0)'	HMDB01 15091	C37H71O8P	
2 9 5	678.09 35	679.1026988	0.0013 988	Proton ation	b'2-([2-([([5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)(hydroxy)phosphoryl]oxy)-3-acetamido-5-hydroxy-6-(hydroxymethyl)oxan-4-yl]oxy]propanoic acid'	b'UDP-N-acetyluraminate'	HMDB00 11720	C20H31N3O19P 2	
2 9 6	685.51 32	685.5128829	0.0003 171	Redox	b'2-hydroxy-N-[(4Z,8Z)-3-hydroxy-1-([3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)octadeca-4,8-dien-2-yl]tetradecanamide'	b'AS 1-1'	HMDB00 32794	C38H71NO9	
2	699.49	700.5043058	0.0022	Proton	b'[(2R)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/18:2(9Z,12Z))'	HMDB00	C39H73O8P	C00

9	7	43		058	ation			07861		416
			700.5043063	0.0022 063	Proton ation	b'[(2R)-2,3-bis[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/18:1(11Z))'	HMDB00 07862	C39H73O8P	C00 416
			700.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/18:1(9Z))'	HMDB00 07863	C39H73O8P	
			700.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/18:1(11Z))'	HMDB00 07864	C39H73O8P	
			700.5043063	0.0022 063	Proton ation	b'[(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/18:1(9Z))'	HMDB00 07865	C39H73O8P	
			700.5043058	0.0022 058	Proton ation	b'[2,3-bis(octadec-9-enoyloxy)propoxy]phosphonic acid'	b'9-Octadecenoic acid 1- [(phosphonoxy)methyl]-1,2-ethanediyl ester'	HMDB00 31129	C39H73O8P	
			700.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(14:1(9Z)/22:1(13Z))'	HMDB01 14804	C39H73O8P	
			700.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:2(9Z,12Z)/18:0)'	HMDB01 14951	C39H73O8P	
			700.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/16:1(9Z))'	HMDB01 15095	C39H73O8P	
			700.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(22:1(13Z)/14:1(9Z))'	HMDB01 15271	C39H73O8P	
			700.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(22:2(13Z,16Z)/14:0)'	HMDB01 15296	C39H73O8P	
			700.5043063	0.0022 063	Proton ation	b'[(2R)-3-(hexadecanoyloxy)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphonic acid'	b'PA(16:0/20:2(11Z,14Z))'	HMDB01 15510	C39H73O8P	
			700.5043063	0.0022 063	Proton ation	b'[(2R)-2-(hexadecanoyloxy)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphonic acid'	b'PA(20:2(11Z,14Z)/16:0)'	HMDB01 15535	C39H73O8P	

		700.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(13Z,16Z)-docosa-13,16-dienyloxy]-3-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(14:0/22:2(13Z,16Z))'	HMDB01 16699	C39H73O8P	
2 9 8	700.49 88	701.5091349	0.0025 349	Proton ation	b'2-(dimethylamino)-N-(1-([3-methoxy-1-(2-{1-methoxy-2-methyl-2-[(2-phenylethyl)carbamoyl]ethyl}pyrrolidin-1-yl)-5-methyl-1-oxoheptan-4-yl](methyl)carbamoyl)-2-methylpropyl)-3-methylbutanamide'	b'Soblidotin'	HMDB02 58356	C39H67N5O6	
2 9 9	700.52 51	700.5278047	0.0027 047	Redox	b'(2S)-1-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate'	b'DG(11D3/11D3/0:0)'	HMDB01 16369	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-2-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropyl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate'	b'DG(11D3/9D5/0:0)'	HMDB01 16376	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-2-([9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropyl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'	b'DG(11D5/9D3/0:0)'	HMDB01 16384	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-hydroxy-3-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate'	b'DG(11M3/11M5/0:0)'	HMDB01 16390	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-hydroxy-3-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propan-2-yl 11-(3-methyl-5-propylfuran-2-yl)undecanoate'	b'DG(11M5/11M3/0:0)'	HMDB01 16398	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-3-hydroxy-2-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propyl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate'	b'DG(11M5/9M5/0:0)'	HMDB01 16404	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-([9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'	b'DG(9D3/11D5/0:0)'	HMDB01 16423	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate'	b'DG(9D5/11D3/0:0)'	HMDB01 16431	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropan-2-yl 9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoate'	b'DG(9D5/9D5/0:0)'	HMDB01 16438	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-hydroxy-3-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate'	b'DG(9M5/11M5/0:0)'	HMDB01 16443	C43H72O7	
		700.5278047	0.0027	Redox	b'(2S)-1-hydroxy-3-(octadecanoyloxy)propan-2-yl (5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(18:0/22:6(5Z,8E,10Z,13Z,15E,19	HMDB02	C43H72O7	

		047				Z)-2OH(7S, 17S)/0:0)	95951		
700.5278047	0.0027 047	Redox	b'(2S)-3-hydroxy-2-(octadecanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'		b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S)/18:0/0:0)	HMDB02 95952	C43H72O7		
700.5278047	0.0027 047	Redox	b'(2R)-2-hydroxy-3-(octadecanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'		b'DG(18:0/0:0/22:6(5Z,8E,10Z,13Z,15 E,19Z)-2OH(7S, 17S))'	HMDB02 95953	C43H72O7		
700.5278047	0.0027 047	Redox	b'(2S)-2-hydroxy-3-(octadecanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'		b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S)/0:0/18:0)	HMDB02 95954	C43H72O7		
700.5278047	0.0027 047	Redox	b'(2S)-1-hydroxy-3-(octadecanoyloxy)propan-2-yl (4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'		b'DG(18:0/22:6(4Z,7Z,11E,13Z,15E,19 Z)-2OH(10S,17)/0:0)	HMDB02 95983	C43H72O7		
700.5278047	0.0027 047	Redox	b'(2S)-3-hydroxy-2-(octadecanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'		b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/18:0/0:0)	HMDB02 95984	C43H72O7		
700.5278047	0.0027 047	Redox	b'(2R)-2-hydroxy-3-(octadecanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'		b'DG(18:0/0:0/22:6(4Z,7Z,11E,13Z,15 E,19Z)-2OH(10S,17))'	HMDB02 95985	C43H72O7		
700.5278047	0.0027 047	Redox	b'(2S)-2-hydroxy-3-(octadecanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'		b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/0:0/18:0)	HMDB02 95986	C43H72O7		
700.5278047	0.0027 047	Redox	b'(2S)-1-hydroxy-3-[(16-methylheptadecanoyl)oxy]propan-2-yl (5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'		b'DG(i- 18:0/22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S)/0:0)	HMDB02 99692	C43H72O7		
700.5278047	0.0027 047	Redox	b'(2S)-3-hydroxy-2-[(16-methylheptadecanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'		b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S)/i-18:0/0:0)	HMDB02 99693	C43H72O7		
700.5278047	0.0027 047	Redox	b'(2R)-2-hydroxy-3-[(16-methylheptadecanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'		b'DG(i- 18:0/0:0/22:6(5Z,8E,10Z,13Z,15E,19Z) -2OH(7S, 17S))'	HMDB02 99694	C43H72O7		
700.5278047	0.0027 047	Redox	b'(2S)-2-hydroxy-3-[(16-methylheptadecanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'		b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S)/0:0/i-18:0)	HMDB02 99695	C43H72O7		
700.5278047	0.0027	Redox	b'(2S)-1-hydroxy-3-[(16-methylheptadecanoyl)oxy]propan-2-yl (4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'		b'DG(i-	HMDB02	C43H72O7		

			047			18:0/22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/0:0)	99723		
		700.5278047	0.0027 047	Redox	b'(2S)-3-hydroxy-2-[(16-methylheptadecanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/i-18:0/0:0)	HMDB02 99724	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2R)-2-hydroxy-3-[(16-methylheptadecanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(i- 18:0/0:0/22:6(4Z,7Z,11E,13Z,15E,19Z) -2OH(10S,17))'	HMDB02 99725	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-2-hydroxy-3-[(16-methylheptadecanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/0:0/i-18:0)	HMDB02 99726	C43H72O7	
3 0 0	701.51	702.5199564	0.0021 564	Proton ation	b'[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(14:0/22:1(13Z))'	HMDB01 14789	C39H75O8P	
		702.5199564	0.0021 564	Proton ation	b'[(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:1(11Z)/18:0)	HMDB01 14901	C39H75O8P	
		702.5199564	0.0021 564	Proton ation	b'[(2R)-3-{(9Z)-octadec-9-enoyloxy}-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:1(9Z)/18:0)	HMDB01 14926	C39H75O8P	
		702.5199564	0.0021 564	Proton ation	b'[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:0/16:1(9Z))'	HMDB01 15065	C39H75O8P	
		702.5199564	0.0021 564	Proton ation	b'[(2R)-2-(hexadecanoyloxy)-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/16:0)	HMDB01 15094	C39H75O8P	
		702.5199564	0.0021 564	Proton ation	b'[(2R)-3-(docosanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(22:0/14:1(9Z))'	HMDB01 15241	C39H75O8P	
		702.5199564	0.0021 564	Proton ation	b'[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(22:1(13Z)/14:0)	HMDB01 15270	C39H75O8P	
3 0 1	703.51 75	704.5227193	0.0025 807	Proton ation	b'(2S)-1-hydroxy-3-(nonadecanoyloxy)propan-2-yl (5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(19:0/20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15)/0:0)	HMDB02 96163	C42H72O8	
		704.5227193	0.0025	Proton	b'(2S)-3-hydroxy-2-(nonadecanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:5(7Z,9Z,11E,13E,17Z)-	HMDB02	C42H72O8	

		807	ation			3OH(5,6,15)/19:0/0:0)	96164		
704.5227193	0.0025 807	Proton ation	b'(2R)-2-hydroxy-3-(nonadecanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(19:0/0:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 96165	C42H72O8		
704.5227193	0.0025 807	Proton ation	b'(2S)-2-hydroxy-3-(nonadecanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/0:0/19:0)	HMDB02 96166	C42H72O8		
704.5227193	0.0025 807	Proton ation	b'(2S)-1-hydroxy-3-[(17-methyloctadecanoyl)oxy]propan-2-yl (5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(i-19:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/0:0)	HMDB02 99903	C42H72O8		
704.5227193	0.0025 807	Proton ation	b'(2S)-3-hydroxy-2-[(17-methyloctadecanoyl)oxy]propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/i-19:0/0:0)	HMDB02 99904	C42H72O8		
704.5227193	0.0025 807	Proton ation	b'(2R)-2-hydroxy-3-[(17-methyloctadecanoyl)oxy]propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(i-19:0/0:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 99905	C42H72O8		
704.5227193	0.0025 807	Proton ation	b'(2S)-2-hydroxy-3-[(17-methyloctadecanoyl)oxy]propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/0:0/i-19:0)	HMDB02 99906	C42H72O8		
703.5152049	0.0022 951	Redox	b'(2-){[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-(tetradecanoyloxy)propyl phosphonato]oxy}ethyl)trimethylazanium'		b'PC(14:0/16:1(9Z))'	HMDB00 07870	C38H74NO8P		
703.5152049	0.0022 951	Redox	b'(2-){[(2R)-2-(hexadecanoyloxy)-3-[(9Z)-tetradec-9-enoyloxy]propyl phosphonato]oxy}ethyl)trimethylazanium'		b'PC(14:1(9Z)/16:0)	HMDB00 07902	C38H74NO8P		
703.5152049	0.0022 951	Redox	b'(2-){[(2R)-3-(hexadecanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propyl phosphonato]oxy}ethyl)trimethylazanium'		b'PC(16:0/14:1(9Z))'	HMDB00 07966	C38H74NO8P	C00 157	
703.5152049	0.0022 951	Redox	b'(2-){[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-(tetradecanoyloxy)propyl phosphonato]oxy}ethyl)trimethylazanium'		b'PC(16:1(9Z)/14:0)	HMDB00 07998	C38H74NO8P		
703.5152049	0.0022 951	Redox	b'(2-aminoethoxy)[(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-(pentadecanoyloxy)propoxy]phosphinic acid'		b'PE(15:0/18:1(11Z))'	HMDB00 08893	C38H74NO8P		
703.5152053	0.0022 947	Redox	b'(2-aminoethoxy)[(2R)-2-[(9Z)-octadec-9-enoyloxy]-3-(pentadecanoyloxy)propoxy]phosphinic acid'		b'PE(15:0/18:1(9Z))'	HMDB00 08894	C38H74NO8P		

		703.5152049	0.0022 951	Redox	b'(2-aminoethoxy){(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-(pentadecanoyloxy)propoxy}phosphinic acid'	b'PE(18:1(11Z)/15:0)'	HMDB00 09021	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'(2-aminoethoxy){(2R)-3-[(9Z)-octadec-9-enoyloxy]-2-(pentadecanoyloxy)propoxy}phosphinic acid'	b'PE(18:1(9Z)/15:0)'	HMDB00 09054	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'[2-[(9Z)-hexadec-9-enoyloxy]-3-(hexadecanoyloxy)propoxy]{2-(methylamino)ethoxy}phosphinic acid'	b'PE-NMe(16:0/16:1(9Z))'	HMDB01 12949	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy]{2-[(9Z)-octadec-9-enoyloxy]-3-(tetradecanoyloxy)propoxy}phosphinic acid'	b'PE-NMe(14:0/18:1(9Z))'	HMDB01 12950	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy]{2-[(11Z)-octadec-11-enoyloxy]-3-(tetradecanoyloxy)propoxy}phosphinic acid'	b'PE-NMe(14:0/18:1(11Z))'	HMDB01 12951	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy][2-(octadecanoyloxy)-3-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE-NMe(14:1(9Z)/18:0)'	HMDB01 12952	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'[3-[(9Z)-hexadec-9-enoyloxy]-2-(hexadecanoyloxy)propoxy]{2-(methylamino)ethoxy}phosphinic acid'	b'PE-NMe(16:1(9Z)/16:0)'	HMDB01 13064	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy][3-(octadecanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE-NMe(18:0/14:1(9Z))'	HMDB01 13085	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy]{3-[(11Z)-octadec-11-enoyloxy]-2-(tetradecanoyloxy)propoxy}phosphinic acid'	b'PE-NMe(18:1(11Z)/14:0)'	HMDB01 13110	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy]{3-[(9Z)-octadec-9-enoyloxy]-2-(tetradecanoyloxy)propoxy}phosphinic acid'	b'PE-NMe(18:1(9Z)/14:0)'	HMDB01 13137	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'[2-(dimethylamino)ethoxy]{2-[(9Z)-hexadec-9-enoyloxy]-3-(pentadecanoyloxy)propoxy}phosphinic acid'	b'PE-NMe2(15:0/16:1(9Z))'	HMDB01 13846	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'[2-(dimethylamino)ethoxy]{3-[(9Z)-hexadec-9-enoyloxy]-2-(pentadecanoyloxy)propoxy}phosphinic acid'	b'PE-NMe2(16:1(9Z)/15:0)'	HMDB01 13964	C38H74NO8P	
		703.5152053	0.0022 947	Redox	b'(2-[(2R)-3-(dodecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl phosphono]oxy)ethyl)trimethylazanium'	b'10E-heptadecenoic acid'	HMDB03 04753	C38H74NO8P	

3 0 2	716.52 11	717.5308549	0.0019 549	Proton ation	b'(2-[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-(pentadecanoyloxy)propyl phosphonato]oxy)ethyl)trimethylazanium'	b'PC(15:0/16:1(9Z))'	HMDB00 07936	C39H76NO8P	C00 157
		717.5308549	0.0019 549	Proton ation	b'(2-[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-(pentadecanoyloxy)propyl phosphonato]oxy)ethyl)trimethylazanium'	b'PC(16:1(9Z)/15:0)'	HMDB00 08000	C39H76NO8P	
		717.5308549	0.0019 549	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-(tetradecanoyloxy)propoxy]phosphinic acid'	b'PE(14:0/20:1(11Z))'	HMDB00 08834	C39H76NO8P	
		717.5308549	0.0019 549	Proton ation	b'(2-aminoethoxy)[(2R)-2-(icosanoyloxy)-3-(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(14:1(9Z)/20:0)'	HMDB00 08866	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'(2-aminoethoxy)[(2R)-3-(hexadecanoyloxy)-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(16:0/18:1(11Z))'	HMDB00 08926	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'(2-aminoethoxy)[(2R)-3-(hexadecanoyloxy)-2-(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(16:0/18:1(9Z))'	HMDB00 08927	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(16:1(9Z)/18:0)'	HMDB00 08958	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/16:1(9Z))'	HMDB00 08990	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'(2-aminoethoxy)[(2R)-2-(hexadecanoyloxy)-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(11Z)/16:0)'	HMDB00 09022	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'(2-aminoethoxy)[(2R)-2-(hexadecanoyloxy)-3-(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)/16:0)'	HMDB00 09055	C39H76NO8P	
		717.5308549	0.0019 549	Proton ation	b'(2-aminoethoxy)[(2R)-3-(icosanoyloxy)-2-(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(20:0/14:1(9Z))'	HMDB00 09218	C39H76NO8P	
		717.5308549	0.0019 549	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-(tetradecanoyloxy)propoxy]phosphinic acid'	b'PE(20:1(11Z)/14:0)'	HMDB00 09250	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(methylamino)ethoxy]({2-[(9Z)-octadec-9-enoyloxy]-3-(pentadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe(15:0/18:1(9Z))'	HMDB01 12953	C39H76NO8P	

		717.5308554	0.0019 554	Proton ation	b'[2-(methylamino)ethoxy]({2-[(11Z)-octadec-11-enoyloxy]-3-(pentadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe(15:0/18:1(11Z))'	HMDB01 12954	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(methylamino)ethoxy]({3-[(11Z)-octadec-11-enoyloxy]-2-(pentadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe(18:1(11Z)/15:0)'	HMDB01 13112	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(methylamino)ethoxy]({3-[(9Z)-octadec-9-enoyloxy]-2-(pentadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe(18:1(9Z)/15:0)'	HMDB01 13139	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(9Z)-hexadec-9-enoyloxy]-3-(hexadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(16:0/16:1(9Z))'	HMDB01 13850	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(9Z)-octadec-9-enoyloxy]-3-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(14:0/18:1(9Z))'	HMDB01 13851	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(11Z)-octadec-11-enoyloxy]-3-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(14:0/18:1(11Z))'	HMDB01 13852	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(dimethylamino)ethoxy][2-(octadecanoyloxy)-3-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE-NMe2(14:1(9Z)/18:0)'	HMDB01 13853	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(9Z)-hexadec-9-enoyloxy]-2-(hexadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(16:1(9Z)/16:0)'	HMDB01 13965	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(dimethylamino)ethoxy][3-(octadecanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE-NMe2(18:0/14:1(9Z))'	HMDB01 13986	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(11Z)-octadec-11-enoyloxy]-2-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(18:1(11Z)/14:0)'	HMDB01 14011	C39H76NO8P	
		717.5308554	0.0019 554	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(9Z)-octadec-9-enoyloxy]-2-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(18:1(9Z)/14:0)'	HMDB01 14038	C39H76NO8P	
3	718.53	718.5383693	0.0028 693	Redox	b'(2S)-1-hydroxy-3-(icosanoyloxy)propan-2-yl (5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicoso-7,9,11,13,17-pentaenoate'	b'DG(20:0/20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15)/0:0)'	HMDB02 96371	C43H74O8	
0	55	718.5383693	0.0028 693	Redox	b'(2S)-3-hydroxy-2-(icosanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicoso-7,9,11,13,17-pentaenoate'	b'DG(20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15)/20:0/0:0)'	HMDB02 96372	C43H74O8	

3 0 4	723.49	718.5383693	0.0028 693	Redox	b'(2R)-2-hydroxy-3-(icosanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:0/0:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 96373	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2S)-2-hydroxy-3-(icosanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/0:0/20:0)'	HMDB02 96374	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2S)-1-hydroxy-3-[(18-methylnonadecanoyloxy)propan-2-yl (5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(i-20:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/0:0)'	HMDB03 00110	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2S)-3-hydroxy-2-[(18-methylnonadecanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/i-20:0/0:0)'	HMDB03 00111	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2R)-2-hydroxy-3-[(18-methylnonadecanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(i-20:0/0:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB03 00112	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2S)-2-hydroxy-3-[(18-methylnonadecanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/0:0/i-20:0)'	HMDB03 00113	C43H74O8	
	43	724.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-(hexadecanoyloxy)propoxy]phosphonic acid'	b'PA(16:0/22:4(7Z,10Z,13Z,16Z))'	HMDB01 14846	C41H73O8P	
		724.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/20:4(5Z,8Z,11Z,14Z))'	HMDB01 14884	C41H73O8P	
		724.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/20:4(8Z,11Z,14Z,17Z))'	HMDB01 14885	C41H73O8P	
		724.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/20:3(5Z,8Z,11Z))'	HMDB01 14908	C41H73O8P	
		724.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/20:3(5Z,8Z,11Z))'	HMDB01 14933	C41H73O8P	
		724.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphonic acid'	b'PA(18:3(6Z,9Z,12Z)/20:1(11Z))'	HMDB01 14986	C41H73O8P	
		724.5043063	0.0022	Proton	b'[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphonic acid'	b'PA(18:3(9Z,12Z,15Z)/20:1(11Z))'	HMDB01	C41H73O8P	

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724.5043063	0.0022 063	Proton ation	b'[(2R)-2-(icosanoyloxy)-3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphonic acid'	b'PA(18:4(6Z,9Z,12Z,15Z)/20:0)'	HMDB01 15039	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-3-(icosanoyloxy)-2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphonic acid'	b'PA(20:0/18:4(6Z,9Z,12Z,15Z))'	HMDB01 15073	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/18:3(6Z,9Z,12Z))'	HMDB01 15100	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/18:3(9Z,12Z,15Z))'	HMDB01 15101	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(20:3(5Z,8Z,11Z)/18:1(11Z))'	HMDB01 15124	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(20:3(5Z,8Z,11Z)/18:1(9Z))'	HMDB01 15125	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(20:4(5Z,8Z,11Z,14Z)/18:0)'	HMDB01 15149	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(20:4(8Z,11Z,14Z,17Z)/18:0)'	HMDB01 15176	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(hexadecanoyloxy)propoxy]phosphonic acid'	b'PA(22:4(7Z,10Z,13Z,16Z)/16:0)'	HMDB01 15326	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'	b'PA(20:2(11Z,14Z)/18:2(9Z,12Z))'	HMDB01 15493	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/20:3(8Z,11Z,14Z))'	HMDB01 15517	C41H73O8P		
724.5043063	0.0022 063	Proton ation	b'[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/20:3(8Z,11Z,14Z))'	HMDB01 15519	C41H73O8P		
724.5043063	0.0022	Proton	b'[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'	b'PA(18:2(9Z,12Z)/20:2(11Z,14Z))'	HMDB01	C41H73O8P		

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		724.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(20:3(8Z,11Z,14Z)/18:1(11Z))'	HMDB01 15567	C41H73O8P	
		724.5043063	0.0022 063	Proton ation	b'[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(20:3(8Z,11Z,14Z)/18:1(9Z))'	HMDB01 15568	C41H73O8P	
	727.52 63	728.5356064	0.0015 064	Proton ation	b'[(2R)-2-[(15Z)-tetracos-15-enoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(14:1(9Z)/24:1(15Z))'	HMDB01 14811	C41H77O8P	
		728.5356064	0.0015 064	Proton ation	b'[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-(hexadecanoyloxy)propoxy]phosphonic acid'	b'PA(16:0/22:2(13Z,16Z))'	HMDB01 14845	C41H77O8P	
		728.5356064	0.0015 064	Proton ation	b'[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(9Z)-hexadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(16:1(9Z)/22:1(13Z))'	HMDB01 14865	C41H77O8P	
		728.5356064	0.0015 064	Proton ation	b'[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/20:1(11Z))'	HMDB01 14907	C41H77O8P	
		728.5356064	0.0015 064	Proton ation	b'[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/20:1(11Z))'	HMDB01 14932	C41H77O8P	
		728.5356064	0.0015 064	Proton ation	b'[(2R)-2-(icosanoyloxy)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'	b'PA(18:2(9Z,12Z)/20:0)'	HMDB01 14958	C41H77O8P	
		728.5356064	0.0015 064	Proton ation	b'[(2R)-3-(icosanoyloxy)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'	b'PA(20:0/18:2(9Z,12Z))'	HMDB01 15070	C41H77O8P	
		728.5356064	0.0015 064	Proton ation	b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/18:1(11Z))'	HMDB01 15097	C41H77O8P	
		728.5356064	0.0015 064	Proton ation	b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/18:1(9Z))'	HMDB01 15098	C41H77O8P	
		728.5356064	0.0015 064	Proton ation	b'[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(9Z)-hexadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(22:1(13Z)/16:1(9Z))'	HMDB01 15274	C41H77O8P	
		728.5356064	0.0015	Proton	b'[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-(hexadecanoyloxy)propoxy]phosphonic acid'	b'PA(22:2(13Z,16Z)/16:0)'	HMDB01	C41H77O8P	

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		728.5356064	0.0015 064	Proton ation	b'[(2R)-3-[(15Z)-tetracos-15-enoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(24:1{(15Z)/14:1(9Z)})'	HMDB01 15456	C41H77O8P	
		728.5356064	0.0015 064	Proton ation	b'[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/20:2{(11Z,14Z)})'	HMDB01 15514	C41H77O8P	
	728.52 55	728.5356064	0.0015 064	Proton ation	b'[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(20:2{(11Z,14Z)/18:0})'	HMDB01 15537	C41H77O8P	
		729.5308549	0.0024 451	Proton ation	b'trimethyl(2-[[{(2R)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-3-(tetradecanoyloxy)propyl phosphono]oxy}ethyl]azanium'	b'PC(14:0/18:2(9Z,12Z))'	HMDB00 07874	C40H76NO8P	
		729.5308549	0.0024 451	Proton ation	b'trimethyl(2-[[{(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propyl phosphono]oxy}ethyl]azanium'	b'PC(14:1(9Z)/18:1(11Z))'	HMDB00 07905	C40H76NO8P	
		729.5308549	0.0024 451	Proton ation	b'trimethyl(2-[[{(2R)-2-[(9Z)-octadec-9-enoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propyl phosphono]oxy}ethyl]azanium'	b'PC(14:1(9Z)/18:1(9Z))'	HMDB00 07906	C40H76NO8P	
		729.5308549	0.0024 451	Proton ation	b'(2-[[{(2R)-2,3-bis[(9Z)-hexadec-9-enoyloxy]propyl phosphono]oxy}ethyl]trimethylazanium'	b'PC(16:1(9Z)/16:1(9Z))'	HMDB00 08002	C40H76NO8P	C00 157
		729.5308549	0.0024 451	Proton ation	b'trimethyl(2-[[{(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propyl phosphono]oxy}ethyl]azanium'	b'PC(18:1{(11Z)/14:1(9Z)})'	HMDB00 08065	C40H76NO8P	C00 157
		729.5308549	0.0024 451	Proton ation	b'trimethyl(2-[[{(2R)-3-[(9Z)-octadec-9-enoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propyl phosphono]oxy}ethyl]azanium'	b'PC(18:1(9Z)/14:1(9Z))'	HMDB00 08098	C40H76NO8P	
		729.5308549	0.0024 451	Proton ation	b'trimethyl(2-[[{(2R)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-2-(tetradecanoyloxy)propyl phosphono]oxy}ethyl]azanium'	b'PC(18:2(9Z,12Z)/14:0))'	HMDB00 08130	C40H76NO8P	
		729.5308549	0.0024 451	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-(pentadecanoyloxy)propoxy]phosphinic acid'	b'PE(15:0/20:2{(11Z,14Z)})'	HMDB00 08901	C40H76NO8P	
		729.5308549	0.0024 451	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-(pentadecanoyloxy)propoxy]phosphinic acid'	b'PE(20:2{(11Z,14Z)/15:0})'	HMDB00 09285	C40H76NO8P	
		729.5308554	0.0024	Proton	b'[2-[(11Z)-icos-11-enoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(14:1(9Z)/20:1(11Z))'	HMDB01	C40H76NO8P	

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		729.5308554	0.0024 446	Proton ation	b'3-[(9Z)-hexadec-9-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(16:1(9Z)/18:1(9Z))'	HMDB01 12956	C40H76NO8P	
		729.5308554	0.0024 446	Proton ation	b'3-[(9Z)-hexadec-9-enoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(16:1(9Z)/18:1(11Z))'	HMDB01 12957	C40H76NO8P	
		729.5308554	0.0024 446	Proton ation	b'2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-(tetradecanoyloxy)propoxy[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(14:0/20:2(11Z,14Z))'	HMDB01 12984	C40H76NO8P	
		729.5308554	0.0024 446	Proton ation	b'3-(hexadecanoyloxy)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(16:0/18:2(9Z,12Z))'	HMDB01 13042	C40H76NO8P	
		729.5308554	0.0024 446	Proton ation	b'2-[(9Z)-hexadec-9-enoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(18:1(11Z)/16:1(9Z))'	HMDB01 13114	C40H76NO8P	
		729.5308554	0.0024 446	Proton ation	b'2-[(9Z)-hexadec-9-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(18:1(9Z)/16:1(9Z))'	HMDB01 13141	C40H76NO8P	
		729.5308554	0.0024 446	Proton ation	b'2-(hexadecanoyloxy)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(18:2(9Z,12Z)/16:0)'	HMDB01 13167	C40H76NO8P	
		729.5308554	0.0024 446	Proton ation	b'3-[(11Z)-icos-11-enoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(20:1(11Z)/14:1(9Z))'	HMDB01 13309	C40H76NO8P	
		729.5308554	0.0024 446	Proton ation	b'3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-(tetradecanoyloxy)propoxy[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(20:2(11Z,14Z)/14:0)'	HMDB01 13337	C40H76NO8P	
		729.5308554	0.0024 446	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-3-(pentadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(15:0/18:2(9Z,12Z))'	HMDB01 13920	C40H76NO8P	
		729.5308554	0.0024 446	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-2-(pentadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(18:2(9Z,12Z)/15:0)'	HMDB01 14067	C40H76NO8P	
3	728.55	729.5672404	0.0011 404	Proton ation	b'trimethyl[2-({2-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]-3-(pentadecanoyloxy)propyl phosphonato}oxy)ethyl]azanium'	b'PC(15:0/P-18:1(11Z))'	HMDB00 07963	C41H80NO7P	
0	83	729.5672404	0.0011	Proton	b'trimethyl[2-({2-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]-3-(pentadecanoyloxy)propyl phosphonato}oxy)ethyl]azanium'	b'PC(15:0/P-18:1(9Z))'	HMDB00	C41H80NO7P	C00

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729.5672404	0.0011 404	Proton ation	b'(2-aminoethoxy)((2R)-2-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'		b'PE(18:0/P-18:1(11Z))'	HMDB00 09017	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'(2-aminoethoxy)((2R)-2-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'		b'PE(18:0/P-18:1(9Z))'	HMDB00 09018	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'(2-aminoethoxy)((2R)-2-[(1Z)-octadec-1-en-1-yloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'		b'PE(18:1(11Z)/P-18:0)'	HMDB00 09049	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'(2-aminoethoxy)((2R)-2-[(1Z)-octadec-1-en-1-yloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'		b'PE(18:1(9Z)/P-18:0)'	HMDB00 09082	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'(2-aminoethoxy)((2R)-2-[(1Z)-hexadec-1-en-1-yloxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'		b'PE(20:1(11Z)/P-16:0)'	HMDB00 09279	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'trimethyl(2-([(2R)-3-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]-2-(pentadecanoyloxy)propyl phosphonato]oxy)ethyl)azanium'		b'PC(P-18:1(11Z)/15:0)'	HMDB00 11271	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'trimethyl[2-({3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]-2-(pentadecanoyloxy)propyl phosphonato} oxy)ethyl]azanium'		b'PC(P-18:1(9Z)/15:0)'	HMDB00 11304	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'(2-aminoethoxy)((2R)-3-[(1Z)-hexadec-1-en-1-yloxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'		b'PE(P-16:0/20:1(11Z))'	HMDB00 11348	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'(2-aminoethoxy)((2R)-3-[(1Z)-octadec-1-en-1-yloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'		b'PE(P-18:0/18:1(11Z))'	HMDB00 11374	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'(2-aminoethoxy)((2R)-3-[(1Z)-octadec-1-en-1-yloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'		b'PE(P-18:0/18:1(9Z))'	HMDB00 11375	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'(2-aminoethoxy)((2R)-3-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'		b'PE(P-18:1(11Z)/18:0)'	HMDB00 11406	C41H80NO7P	
729.5672404	0.0011 404	Proton ation	b'(2-aminoethoxy)((2R)-3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'		b'PE(P-18:1(9Z)/18:0)'	HMDB00 11439	C41H80NO7P	
728.5591048	0.0008	Redox	b'(2S)-1-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'		b'DG(11D3/11D5/0:0)'	HMDB01	C45H76O7	

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728.5591048	0.0008 048	Redox	b'(2S)-1-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate'		b'DG(11D5/11D3/0:0)'	HMDB01 16378	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-2-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropyl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'		b'DG(11D5/9D5/0:0)'	HMDB01 16385	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-1-hydroxy-3-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate'		b'DG(11M3/13M5/0:0)'	HMDB01 16392	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-1-hydroxy-3-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate'		b'DG(11M5/11M5/0:0)'	HMDB01 16399	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-2-([9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate'		b'DG(13D5/9D3/0:0)'	HMDB01 16411	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-3-hydroxy-2-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate'		b'DG(13M5/11M3/0:0)'	HMDB01 16416	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-3-hydroxy-2-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate'		b'DG(13M5/9M5/0:0)'	HMDB01 16421	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-1-([9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate'		b'DG(9D3/13D5/0:0)'	HMDB01 16426	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-1-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'		b'DG(9D5/11D5/0:0)'	HMDB01 16432	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-1-hydroxy-3-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate'		b'DG(9M5/13M5/0:0)'	HMDB01 16445	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-1-hydroxy-3-(icosanoyloxy)propan-2-yl (5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'		b'DG(20:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/0:0)'	HMDB02 96367	C45H76O7		
728.5591048	0.0008 048	Redox	b'(2S)-3-hydroxy-2-(icosanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'		b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/20:0/0:0)'	HMDB02 96368	C45H76O7		
728.5591048	0.0008	Redox	b'(2R)-2-hydroxy-3-(icosanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'		b'DG(20:0/0:0/22:6(5Z,8E,10Z,13Z,15	HMDB02	C45H76O7		

			048			E,19Z)-2OH(7S, 17S))'	96369		
728.5591048	0.0008 048	Redox		b'(2S)-2-hydroxy-3-(icosanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S))0:0/20:0)'	HMDB02 96370	C45H76O7		
728.5591048	0.0008 048	Redox		b'(2S)-1-hydroxy-3-(icosanoyloxy)propan-2-yl (4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(20:0/22:6(4Z,7Z,11E,13Z,15E,19Z)- Z)-2OH(10S,17)/0:0)'	HMDB02 96399	C45H76O7		
728.5591048	0.0008 048	Redox		b'(2S)-3-hydroxy-2-(icosanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/20:0/0:0)'	HMDB02 96400	C45H76O7		
728.5591048	0.0008 048	Redox		b'(2R)-2-hydroxy-3-(icosanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(20:0/0:0/22:6(4Z,7Z,11E,13Z,15E,19Z)- E,19Z)-2OH(10S,17))'	HMDB02 96401	C45H76O7		
728.5591048	0.0008 048	Redox		b'(2S)-2-hydroxy-3-(icosanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/0:0/20:0)'	HMDB02 96402	C45H76O7		
728.5591048	0.0008 048	Redox		b'(2S)-1-hydroxy-3-[(18-methylnonadecanoyl)oxy]propan-2-yl (5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(i- 20:0/22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S))0:0)'	HMDB03 00106	C45H76O7		
728.5591048	0.0008 048	Redox		b'(2S)-3-hydroxy-2-[(18-methylnonadecanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S))i-20:0/0:0)'	HMDB03 00107	C45H76O7		
728.5591048	0.0008 048	Redox		b'(2R)-2-hydroxy-3-[(18-methylnonadecanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(i- 20:0/0:0/22:6(5Z,8E,10Z,13Z,15E,19Z)- -2OH(7S, 17S))'	HMDB03 00108	C45H76O7		
728.5591048	0.0008 048	Redox		b'(2S)-2-hydroxy-3-[(18-methylnonadecanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S))0:0/i-20:0)'	HMDB03 00109	C45H76O7		
728.5591048	0.0008 048	Redox		b'(2S)-1-hydroxy-3-[(18-methylnonadecanoyl)oxy]propan-2-yl (4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(i- 20:0/22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/0:0)'	HMDB03 00138	C45H76O7		
728.5591048	0.0008 048	Redox		b'(2S)-3-hydroxy-2-[(18-methylnonadecanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/i-20:0/0:0)'	HMDB03 00139	C45H76O7		

		728.5591048	0.0008 048	Redox	b'(2R)-2-hydroxy-3-[(18-methylnonadecanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(i- 20:0/0:0/22:6(4Z,7Z,11E,13Z,15E,19Z)- -2OH(10S,17))'	HMDB03 00140	C45H76O7	
		728.5591048	0.0008 048	Redox	b'(2S)-2-hydroxy-3-[(18-methylnonadecanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/0:0/i-20:0)'	HMDB03 00141	C45H76O7	
3 0 8	742.53 7	743.546505	0.0017 05	Proton ation	b'trimethyl(2-([(2R)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-3-(pentadecanoyloxy)propyl phosphonato]oxy)ethyl)azanium'	b'PC(15:0/18:2(9Z,12Z))'	HMDB00 07940	C41H78NO8P	C00 157
		743.546505	0.0017 05	Proton ation	b'trimethyl(2-([(2R)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-3-(pentadecanoyloxy)propyl phosphonato]oxy)ethyl)azanium'	b'PC(18:2(9Z,12Z)/15:0)'	HMDB00 08132	C41H78NO8P	
		743.546505	0.0017 05	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-(tetradecanoyloxy)propoxy]phosphinic acid'	b'PE(14:0/22:2(13Z,16Z))'	HMDB00 08843	C41H78NO8P	C00 350
		743.546505	0.0017 05	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docosa-13-enoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(14:1(9Z)/22:1(13Z))'	HMDB00 08875	C41H78NO8P	
		743.546505	0.0017 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-(hexadecanoyloxy)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphinic acid'	b'PE(16:0/20:2(11Z,14Z))'	HMDB00 08934	C41H78NO8P	
		743.546505	0.0017 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(16:1(9Z)/20:1(11Z))'	HMDB00 08966	C41H78NO8P	
		743.546505	0.0017 05	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/18:2(9Z,12Z))'	HMDB00 08994	C41H78NO8P	
		743.5465055	0.0017 055	Proton ation	b'(2-aminoethoxy)[(2R)-2,3-bis[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(11Z)/18:1(11Z))'	HMDB00 09025	C41H78NO8P	
		743.546505	0.0017 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(11Z)/18:1(9Z))'	HMDB00 09026	C41H78NO8P	
		743.546505	0.0017 05	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)/18:1(11Z))'	HMDB00 09058	C41H78NO8P	
		743.5465055	0.0017	Proton	b'(2-aminoethoxy)[(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)/18:1(9Z))'	HMDB00	C41H78NO8P	

		055	ation			09059		
743.546505	0.0017 05	Proton ation		b'(2-aminoethoxy)[(2R)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:2(9Z,12Z)/18:0)'	HMDB00 09090	C41H78NO8P	
743.546505	0.0017 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/16:1(9Z))'	HMDB00 09254	C41H78NO8P	
743.546505	0.0017 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-(hexadecanoyloxy)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/16:0)'	HMDB00 09286	C41H78NO8P	
743.546505	0.0017 05	Proton ation		b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/14:1(9Z))'	HMDB00 09515	C41H78NO8P	
743.546505	0.0017 05	Proton ation		b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-(tetradecanoyloxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/14:0)'	HMDB00 09547	C41H78NO8P	
743.5465055	0.0017 055	Proton ation		b'[2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-(pentadecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(15:0/20:2(11Z,14Z))'	HMDB01 13025	C41H78NO8P	
743.5465055	0.0017 055	Proton ation		b'[3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-(pentadecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(20:2(11Z,14Z)/15:0)'	HMDB01 13339	C41H78NO8P	
743.5465055	0.0017 055	Proton ation		b'[2-(dimethylamino)ethoxy]({2-[(11Z)-icos-11-enoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propoxy})phosphinic acid'	b'PE-NMe2(14:1(9Z)/20:1(11Z))'	HMDB01 13856	C41H78NO8P	
743.5465055	0.0017 055	Proton ation		b'[2-(dimethylamino)ethoxy]({3-[(9Z)-hexadec-9-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy})phosphinic acid'	b'PE-NMe2(16:1(9Z)/18:1(9Z))'	HMDB01 13857	C41H78NO8P	
743.5465055	0.0017 055	Proton ation		b'[2-(dimethylamino)ethoxy]({3-[(9Z)-hexadec-9-enoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy})phosphinic acid'	b'PE-NMe2(16:1(9Z)/18:1(11Z))'	HMDB01 13858	C41H78NO8P	
743.5465055	0.0017 055	Proton ation		b'[2-(dimethylamino)ethoxy]({2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(14:0/20:2(11Z,14Z))'	HMDB01 13884	C41H78NO8P	
743.5465055	0.0017 055	Proton ation		b'[2-(dimethylamino)ethoxy][3-(hexadecanoyloxy)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PE-NMe2(16:0/18:2(9Z,12Z))'	HMDB01 13943	C41H78NO8P	
743.5465055	0.0017	Proton		b'[2-(dimethylamino)ethoxy]({2-[(9Z)-hexadec-9-enoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy})phosphinic acid'	b'PE-NMe2(18:1(11Z)/16:1(9Z))'	HMDB01	C41H78NO8P	

			055	ation			14015		
		743.5465055	0.0017 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(9Z)-hexadec-9-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy})phosphinic acid'	b'PE-NMe2(18:1(9Z)/16:1(9Z))'	HMDB01 14042	C41H78NO8P	
		743.5465055	0.0017 055	Proton ation	b'[2-(dimethylamino)ethoxy][2-(hexadecanoyloxy)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PE-NMe2(18:2(9Z,12Z)/16:0)'	HMDB01 14068	C41H78NO8P	
		743.5465055	0.0017 055	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(11Z)-icos-11-enoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy})phosphinic acid'	b'PE-NMe2(20:1(11Z)/14:1(9Z))'	HMDB01 14211	C41H78NO8P	
		743.5465055	0.0017 055	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(20:2(11Z,14Z)/14:0)'	HMDB01 14239	C41H78NO8P	
		743.5465055	0.0017 055	Proton ation	b'(2-aminoethoxy)[2,3-bis(octadec-9-enoyloxy)propoxy]phosphinic acid'	b'1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine'	HMDB02 44088	C41H78NO8P	
		743.5465055	0.0017 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyloxy)-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:0/18:1(12Z)-O(9S,10R))'	HMDB02 85330	C41H78NO8P	
		743.5465055	0.0017 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyloxy)-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(18:1(12Z)-O(9S,10R)/P-18:0)'	HMDB02 85331	C41H78NO8P	
		743.5465055	0.0017 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(1E)-octadec-1-en-1-yloxy]-2-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(P-18:0/18:1(9Z)-O(12,13))'	HMDB02 85332	C41H78NO8P	
		743.5465055	0.0017 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(1E)-octadec-1-en-1-yloxy]-3-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)-O(12,13)/P-18:0)'	HMDB02 85333	C41H78NO8P	
3 0 9	746.50 71	746.5097851	0.0026 851	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-(hexadecanoyloxy)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(16:0/18:2(9Z,12Z))'	HMDB00 10575	C40H75O10P	
		746.5097851	0.0026 851	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-(9Z)-hexadec-9-enoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(16:1(9Z)/18:1(11Z))'	HMDB00 10588	C40H75O10P	
		746.5097851	0.0026 851	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-(9Z)-hexadec-9-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(16:1(9Z)/18:1(9Z))'	HMDB00 10589	C40H75O10P	
		746.5097851	0.0026	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(9Z)-hexadec-9-enoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(11Z)/16:1(9Z))'	HMDB00	C40H75O10P	

		063	ation			5Z))'	15307		
748.5043063	0.0015 063	Proton ation	b'[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'		b'PA(22:4(7Z,10Z,13Z,16Z)/18:2(9Z,12Z))'	HMDB01 15331	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'		b'PA(22:5(4Z,7Z,10Z,13Z,16Z)/18:1(11Z))'	HMDB01 15355	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'		b'PA(22:5(4Z,7Z,10Z,13Z,16Z)/18:1(9Z))'	HMDB01 15356	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'		b'PA(22:5(7Z,10Z,13Z,16Z,19Z)/18:1(11Z))'	HMDB01 15381	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'		b'PA(22:5(7Z,10Z,13Z,16Z,19Z)/18:1(9Z))'	HMDB01 15382	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'		b'PA(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0))'	HMDB01 15406	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphonic acid'		b'PA(20:3(5Z,8Z,11Z)/20:3(8Z,11Z,14Z))'	HMDB01 15494	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphonic acid'		b'PA(20:3(8Z,11Z,14Z)/20:3(5Z,8Z,11Z))'	HMDB01 15496	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-2,3-bis[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphonic acid'		b'PA(20:3(8Z,11Z,14Z)/20:3(8Z,11Z,14Z))'	HMDB01 15497	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]phosphonic acid'		b'PA(20:4(5Z,8Z,11Z,14Z)/20:2(11Z,14Z))'	HMDB01 15498	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]phosphonic acid'		b'PA(20:4(8Z,11Z,14Z,17Z)/20:2(11Z,14Z))'	HMDB01 15500	C43H73O8P		
748.5043063	0.0015 063	Proton ation	b'[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]phosphonic acid'		b'PA(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z))'	HMDB01 15548	C43H73O8P		
748.5043063	0.0015	Proton	b'[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]phosphonic acid'		b'PA(20:2(11Z,14Z)/20:4(8Z,11Z,14Z,17Z))'	HMDB01	C43H73O8P		

			063	ation		17Z))'	15549		
3 11	747.51 56	748.5254352	0.0020 352	Proton ation		b'PG(16:0/18:1(11Z))'	HMDB00 10573	C40H77O10P	
		748.5254352	0.0020 352	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(16:0/18:1(9Z))'	HMDB00 10574	C40H77O10P	
		748.5254352	0.0020 352	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(16:1(9Z)/18:0)'	HMDB00 10587	C40H77O10P	
		748.5254352	0.0020 352	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(18:0/16:1(9Z))'	HMDB00 10601	C40H77O10P	
		748.5254352	0.0020 352	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(11Z)/16:0)'	HMDB00 10615	C40H77O10P	
		748.5254352	0.0020 352	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)/16:0)'	HMDB00 10630	C40H77O10P	
		748.5254357	0.0020 357	Proton ation	b'(2,3-dihydroxypropoxy)[3-(hexadecanoyloxy)-2-(octadec-9-enoyloxy)propoxy]phosphinic acid'	b'1-Palmitoyl-2-oleoylglycero-3-phosphoglycerol'	HMDB02 44000	C40H77O10P	
		748.5254357	0.0020 357	Proton ation	b'[(2R)-2-[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-3-(nonadecanoyloxy)propoxy]phosphonic acid'	b'PA(19:0/18:1(12Z)-2OH(9,10))'	HMDB02 64462	C40H77O10P	
		748.5254357	0.0020 357	Proton ation	b'[(2R)-3-[(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-2-(nonadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:1(12Z)-2OH(9,10)/19:0)'	HMDB02 64463	C40H77O10P	
		748.5254357	0.0020 357	Proton ation	b'[(2R)-2-[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-3-[(17-methyloctadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-19:0/18:1(12Z)-2OH(9,10))'	HMDB02 68092	C40H77O10P	
		748.5254357	0.0020 357	Proton ation	b'[(2R)-3-[(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-2-[(17-methyloctadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(18:1(12Z)-2OH(9,10)/i-19:0)'	HMDB02 68093	C40H77O10P	
3 1	749.49 91	750.5070692	0.0001 692	Proton ation	b'28- {[(2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoyl]oxy} hexacosyl (2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate'	b'1,26-Hexacosanediol diferulate'	HMDB00 30751	C46H70O8	
2		750.5070692	0.0001	Proton	b'28- {[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy} octacosyl (2E)-3-(3,4-dihydroxyphenyl)prop-2-enoate'	b'1,28-Dicaffeoyloctacosanediol'	HMDB00	C46H70O8	

		692	ation				38064		
749.4995548	0.0004 548	Redox	b'(2-{{(2R)-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propyl phosphonato}oxy}ethyl)trimethylazanium'		b'PC(14:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))' Z))'		HMDB00 07918	C42H72NO8P	
749.4995548	0.0004 548	Redox	b'(2-{{(2R)-3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propyl phosphonato}oxy}ethyl)trimethylazanium'		b'PC(20:5(5Z,8Z,11Z,14Z,17Z)/14:1(9Z))' Z))'		HMDB00 08493	C42H72NO8P	
749.4995548	0.0004 548	Redox	b'(2-aminoethoxy)[(2R)-2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-(pentadecanoyloxy)propoxy]phosphinic acid'		b'PE(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))' Z))'		HMDB00 08913	C42H72NO8P	
749.4995548	0.0004 548	Redox	b'(2-aminoethoxy)[(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(pentadecanoyloxy)propoxy]phosphinic acid'		b'PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/15:0)' :0)'		HMDB00 09681	C42H72NO8P	
749.4995553	0.0004 553	Redox	b'[2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-(tetradecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'		b'PE- NMe(14:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))' Z))'		HMDB01 12996	C42H72NO8P	
749.4995553	0.0004 553	Redox	b'[2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'		b'PE- NMe(14:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))' Z))'		HMDB01 13013	C42H72NO8P	
749.4995553	0.0004 553	Redox	b'[2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'		b'PE- NMe(14:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))' 9Z))'		HMDB01 13014	C42H72NO8P	
749.4995553	0.0004 553	Redox	b'[3-[(9Z)-hexadec-9-enoyloxy]-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'		b'PE- NMe(16:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))' Z))'		HMDB01 13074	C42H72NO8P	
749.4995553	0.0004 553	Redox	b'[2-(methylamino)ethoxy]({2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy})phosphinic acid'		b'PE- NMe(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))' Z))'		HMDB01 13175	C42H72NO8P	
749.4995553	0.0004 553	Redox	b'[2,3-bis[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'		b'PE- NMe(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))' Z))'		HMDB01 13201	C42H72NO8P	

						)Y'			
		749.4995553	0.0004 553	Redox	b'[2-(methylamino)ethoxy]({3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))'	HMDB01 13202	C42H72NO8P	
		749.4995553	0.0004 553	Redox	b'[2-(methylamino)ethoxy]({2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe(18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))'	HMDB01 13230	C42H72NO8P	
		749.4995553	0.0004 553	Redox	b'[2,3-bis[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE- NMe(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))'	HMDB01 13231	C42H72NO8P	
		749.4995553	0.0004 553	Redox	b'[2-(methylamino)ethoxy]({3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy})phosphinic acid'	b'PE- NMe(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))'	HMDB01 13258	C42H72NO8P	
		749.4995553	0.0004 553	Redox	b'[2-[(9Z)-hexadec-9-enoyloxy]-3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE- NMe(20:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))'	HMDB01 13483	C42H72NO8P	
		749.4995553	0.0004 553	Redox	b'[3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE- NMe(22:5(4Z,7Z,10Z,13Z,16Z)/14:1(9Z))'	HMDB01 13621	C42H72NO8P	
		749.4995553	0.0004 553	Redox	b'[3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE- NMe(22:5(7Z,10Z,13Z,16Z,19Z)/14:1(9Z))'	HMDB01 13647	C42H72NO8P	
		749.4995553	0.0004 553	Redox	b'[3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(tetradecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE- NMe(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/14:0))'	HMDB01 13673	C42H72NO8P	
3	750.54	751.5515904	0.0021	Proton	b'(2-aminoethoxy)((2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-[(1Z)-octadec-1-en-1-yloxy]propoxy)phosphinic acid'	b'PE(P-18:0/20:4(5Z,8Z,11Z,14Z))'	HMDB00	C43H78NO7P	C00

1	16		904	ation			05779		350
3		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)/P-18:1(11Z))'	HMDB00 09347	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)/P-18:1(9Z))'	HMDB00 09348	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)/P-18:1(11Z))'	HMDB00 09380	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)/P-18:1(9Z))'	HMDB00 09381	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-[(1Z)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)/P-18:0)'	HMDB00 09412	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-[(1Z)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(20:4(8Z,11Z,14Z,17Z)/P-18:0)'	HMDB00 09445	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-[(1Z)-hexadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(22:4(7Z,10Z,13Z,16Z)/P-16:0)'	HMDB00 09609	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-[(1Z)-hexadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-16:0/22:4(7Z,10Z,13Z,16Z))'	HMDB00 11358	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-3-[(1Z)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:0/20:4(8Z,11Z,14Z,17Z))'	HMDB00 11386	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:1(11Z)/20:3(5Z,8Z,11Z))'	HMDB00 11416	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:1(11Z)/20:3(8Z,11Z,14Z))'	HMDB00 11417	C43H78NO7P	
		751.5515904	0.0021 904	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:1(9Z)/20:3(5Z,8Z,11Z))'	HMDB00 11449	C43H78NO7P	
		750.5410853	0.0005	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-(hexadecanoyloxy)-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(16:0/18:0)'	HMDB00	C40H79O10P	

3	1	4		147				10572		
			750.5410853	0.0005 147	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PG(18:0/16:0)'	HMDB00 10600	C40H79O10P	
			750.5410857	0.0005 143	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(10-methyldodecanoyl)oxy]-2-[(18-methylicosanoyl)oxy]propoxy]phosphonic acid'	b'PG(a-13:0/a-21:0)'	HMDB01 16640	C40H79O10P	
			750.5410857	0.0005 143	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(10-methyldodecanoyl)oxy]-2-[(19-methylicosanoyl)oxy]propoxy]phosphonic acid'	b'PG(a-13:0/i-21:0)'	HMDB01 16651	C40H79O10P	
			750.5410857	0.0005 143	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(20-methylhenicosanoyl)oxy]-3-[(10-methylundecanoyl)oxy]propoxy]phosphonic acid'	b'PG(i-12:0/i-22:0)'	HMDB01 16670	C40H79O10P	
			750.5410857	0.0005 143	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(11-methyldodecanoyl)oxy]-2-[(18-methylicosanoyl)oxy]propoxy]phosphonic acid'	b'PG(i-13:0/a-21:0)'	HMDB01 16676	C40H79O10P	
			750.5410857	0.0005 143	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(11-methyldodecanoyl)oxy]-2-[(19-methylicosanoyl)oxy]propoxy]phosphonic acid'	b'PG(i-13:0/i-21:0)'	HMDB01 16687	C40H79O10P	
3	1	4	752.5356064	0.0023 064	Proton ation	b'[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/22:4(7Z,10Z,13Z,16Z))'	HMDB01 14890	C43H77O8P	
			752.5356064	0.0023 064	Proton ation	b'[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'	b'PA(18:2(9Z,12Z)/22:2(13Z,16Z))'	HMDB01 14966	C43H77O8P	
			752.5356064	0.0023 064	Proton ation	b'[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphonic acid'	b'PA(18:3(6Z,9Z,12Z)/22:1(13Z))'	HMDB01 14992	C43H77O8P	
			752.5356064	0.0023 064	Proton ation	b'[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphonic acid'	b'PA(18:3(9Z,12Z,15Z)/22:1(13Z))'	HMDB01 15019	C43H77O8P	
			752.5356064	0.0023 064	Proton ation	b'[(2R)-2-(docosanoyloxy)-3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphonic acid'	b'PA(18:4(6Z,9Z,12Z,15Z)/22:0)'	HMDB01 15045	C43H77O8P	
			752.5356064	0.0023 064	Proton ation	b'[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:0/20:4(5Z,8Z,11Z,14Z))'	HMDB01 15078	C43H77O8P	
			752.5356064	0.0023	Proton	b'[(2R)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-3-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:0/20:4(8Z,11Z,14Z,17Z))'	HMDB01	C43H77O8P	

			064	ation			15079		
		752.5356064	0.0023 064	Proton ation	b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/20:3(5Z,8Z,11Z))'	HMDB01 15105	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:3(5Z,8Z,11Z)/20:1(11Z))'	HMDB01 15131	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:4(5Z,8Z,11Z,14Z)/20:0)'	HMDB01 15156	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:4(8Z,11Z,14Z,17Z)/20:0)'	HMDB01 15183	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-3-(docosanoyloxy)-2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphonic acid'	b'PA(22:0/18:4(6Z,9Z,12Z,15Z))'	HMDB01 15251	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphonic acid'	b'PA(22:1(13Z)/18:3(6Z,9Z,12Z))'	HMDB01 15279	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphonic acid'	b'PA(22:1(13Z)/18:3(9Z,12Z,15Z))'	HMDB01 15280	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'	b'PA(22:2(13Z,16Z)/18:2(9Z,12Z))'	HMDB01 15304	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(22:4(7Z,10Z,13Z,16Z)/18:0)'	HMDB01 15328	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/20:3(8Z,11Z,14Z))'	HMDB01 15531	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-2,3-bis[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphonic acid'	b'PA(20:2(11Z,14Z)/20:2(11Z,14Z))'	HMDB01 15545	C43H77O8P	
		752.5356064	0.0023 064	Proton ation	b'[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:3(8Z,11Z,14Z)/20:1(11Z))'	HMDB01 15573	C43H77O8P	
3	754.57	755.5828905	0.0016	Proton	b'(2-aminoethoxy)((2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/P-18:1(11Z))'	HMDB00	C43H82NO7P	

1	34		905	ation			09281		
5		755.5828905	0.0016 905	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/P-18:1(9Z))'	HMDB00 09282	C43H82NO7P	
		755.5828905	0.0016 905	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(1Z)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/P-18:0)'	HMDB00 09313	C43H82NO7P	
		755.5828905	0.0016 905	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[(1Z)-hexadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/P-16:0)'	HMDB00 09576	C43H82NO7P	
		755.5828905	0.0016 905	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[(1Z)-hexadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-16:0/22:2(13Z,16Z))'	HMDB00 11357	C43H82NO7P	
		755.5828905	0.0016 905	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(1Z)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:0/20:2(11Z,14Z))'	HMDB00 11382	C43H82NO7P	
		755.5828905	0.0016 905	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:1(11Z)/20:1(11Z))'	HMDB00 11414	C43H82NO7P	
		755.5828905	0.0016 905	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:1(9Z)/20:1(11Z))'	HMDB00 11447	C43H82NO7P	
3	755.07	756.0819344	0.0006 344	Proton ation	b' {[[(2S,3R,4S,5S)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy}([(((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy]phosphinic acid'	b'Diadenosine triphosphate'	HMDB00 01155	C20H27N10O16 P3	C06 197
1		756.0810078	0.0002 922	Proton ation	b'3,4,5,12,13,21,25,26,27-nonahydroxy-8,18-dioxo-9,14,17,23,30-pentaohexacyclo[17.12.0.0.0xc2xb2,\xc2xb81xb7.0xc2xb9xc2xb81xb0,\xc2xb9xc2xb81xb5.0xc2xb2xc2xb2,\xc2xb3xc2xb9.0xc2xb2xc2xb81xb4,\xc2xb2xc2xb81xb9]hentriaconta-1(19),2,4,6,20,22(31),24(29),25,27-nonaen-11-yl 3,4,5-trihydroxybenzoate'	b'Syzyginin B'	HMDB00 30237	C33H24O21	
6	35	756.0819358	0.0006 358	Proton ation	b'bis([5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]phosphinic acid'	b'AP3A-lyophilized'	HMDB02 47779	C20H27N10O16 P3	
		756.0819358	0.0006 358	Proton ation	b'([([1,2-bis[5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]ethoxy)(hydroxy)phosphoryl)oxy](hydroxy)phosphoryl)oxy]phosphonic acid'	b'Ppapa'	HMDB02 56716	C20H27N10O16 P3	
3	756.58	757.5985406	0.0017 406	Proton ation	b'(2-aminoethoxy)[(2R)-3-(icosanoyloxy)-2-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:0/P-18:1(11Z))'	HMDB00 09248	C43H84NO7P	
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7	757.5985406	0.0017 406	Proton ation	b'(2-aminoethoxy)[(2R)-3-(icosanoyloxy)-2-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:0/P-18:1(9Z))'	HMDB00 09249	C43H84NO7P	
	757.5985406	0.0017 406	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(1Z)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/P-18:0)'	HMDB00 09280	C43H84NO7P	
	757.5985406	0.0017 406	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(1Z)-hexadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/P-16:0)'	HMDB00 09543	C43H84NO7P	
	757.5985406	0.0017 406	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(1Z)-hexadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-16:0/22:1(13Z))'	HMDB00 11356	C43H84NO7P	
	757.5985406	0.0017 406	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(1Z)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:0/20:1(11Z))'	HMDB00 11381	C43H84NO7P	
	757.5985406	0.0017 406	Proton ation	b'(2-aminoethoxy)[(2R)-2-(icosanoyloxy)-3-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:1(11Z)/20:0)'	HMDB00 11413	C43H84NO7P	
	757.5985406	0.0017 406	Proton ation	b'(2-aminoethoxy)[(2R)-2-(icosanoyloxy)-3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:1(9Z)/20:0)'	HMDB00 11446	C43H84NO7P	
	756.5904049	0.0014 049	Redox	b'(2S)-1-[[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy]-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate'	b'DG(11D3/13D5/0:0)'	HMDB01 16373	C47H80O7	
	756.5904049	0.0014 049	Redox	b'(2S)-1-[[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy]-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'	b'DG(11D5/11D5/0:0)'	HMDB01 16379	C47H80O7	
	756.5904049	0.0014 049	Redox	b'(2S)-1-hydroxy-3-[[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy]propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate'	b'DG(11M5/13M5/0:0)'	HMDB01 16401	C47H80O7	
	756.5904049	0.0014 049	Redox	b'(2S)-2-[[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy]-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate'	b'DG(13D5/11D3/0:0)'	HMDB01 16405	C47H80O7	
	756.5904049	0.0014 049	Redox	b'(2S)-2-[[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy]-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate'	b'DG(13D5/9D5/0:0)'	HMDB01 16412	C47H80O7	
	756.5904049	0.0014 049	Redox	b'(2S)-3-hydroxy-2-[[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy]propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate'	b'DG(13M5/11M5/0:0)'	HMDB01 16417	C47H80O7	

		756.5904049	0.0014 049	Redox	b'(2S)-1-[(9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl)oxy]-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate'	b'DG(9D5/13D5/0:0)'	HMDB01 16435	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-1-(docosanoyloxy)-3-hydroxypropan-2-yl (5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/0:0)'	HMDB02 96783	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-2-(docosanoyloxy)-3-hydroxypropyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/22:0/0:0)'	HMDB02 96784	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2R)-3-(docosanoyloxy)-2-hydroxypropyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:0/0:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S))'	HMDB02 96785	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-3-(docosanoyloxy)-2-hydroxypropyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/0:0/22:0)'	HMDB02 96786	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-1-(docosanoyloxy)-3-hydroxypropan-2-yl (4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/0:0)'	HMDB02 96815	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-2-(docosanoyloxy)-3-hydroxypropyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/22:0/0:0)'	HMDB02 96816	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2R)-3-(docosanoyloxy)-2-hydroxypropyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:0/0:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17))'	HMDB02 96817	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-3-(docosanoyloxy)-2-hydroxypropyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/0:0/22:0)'	HMDB02 96818	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-1-hydroxy-3-[(20-methylhenicosanoyl)oxy]propan-2-yl (5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(i-22:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/0:0)'	HMDB03 00522	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-3-hydroxy-2-[(20-methylhenicosanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/i-22:0/0:0)'	HMDB03 00523	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2R)-2-hydroxy-3-[(20-methylhenicosanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(i-22:0/0:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S))'	HMDB03 00524	C47H80O7	

		756.5904049	0.0014 049	Redox	b'(2S)-2-hydroxy-3-[(20-methylhenicosanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S,17S)/0:0/i-22:0)'	HMDB03 00525	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-1-hydroxy-3-[(20-methylhenicosanoyl)oxy]propan-2-yl (4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(i- 22:0/22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/0:0)'	HMDB03 00554	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-3-hydroxy-2-[(20-methylhenicosanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/i-22:0/0:0)'	HMDB03 00555	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2R)-2-hydroxy-3-[(20-methylhenicosanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(i- 22:0/0:0/22:6(4Z,7Z,11E,13Z,15E,19Z) -2OH(10S,17))'	HMDB03 00556	C47H80O7	
		756.5904049	0.0014 049	Redox	b'(2S)-2-hydroxy-3-[(20-methylhenicosanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/0:0/i-22:0)'	HMDB03 00557	C47H80O7	
3 1 8	757.58 83	758.59379	0.0023 1	Proton ation	b'(2-:{{(2S,3R)-3-hydroxy-2-(8-:[3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanamido)nonadecyl phosphono}oxy)ethyl}trimethylazanium'	b'SM(d19:0/18:1(12Z)-O(9S,10R))'	HMDB02 90636	C42H83N2O7P	
		758.59379	0.0023 1	Proton ation	b'(2-:{{(2S,3R)-3-hydroxy-2-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enamido]nonadecyl phosphono}oxy)ethyl}trimethylazanium'	b'SM(d19:0/18:1(9Z)-O(12,13))'	HMDB02 90637	C42H83N2O7P	
3 1 9	762.50 58	763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-(hexadecanoyloxy)propoxy]phosphinic acid'	b'PE(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19 Z))'	HMDB00 08946	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-(9Z)-hexadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(16:1(9Z)/22:5(4Z,7Z,10Z,13Z,16 Z))'	HMDB00 08977	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-(9Z)-hexadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(16:1(9Z)/22:5(7Z,10Z,13Z,16Z,1 9Z))'	HMDB00 08978	C43H74NO8P	C00 350
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(11Z)/20:5(5Z,8Z,11Z,14Z,1 7Z))'	HMDB00 09038	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17 Z))'	HMDB00 09071	C43H74NO8P	

		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PE(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))'	HMDB00 09102	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PE(18:2(9Z,12Z)/20:4(8Z,11Z,14Z,17Z))'	HMDB00 09103	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphinic acid'	b'PE(18:3(6Z,9Z,12Z)/20:3(5Z,8Z,11Z))'	HMDB00 09133	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphinic acid'	b'PE(18:3(6Z,9Z,12Z)/20:3(8Z,11Z,14Z))'	HMDB00 09134	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphinic acid'	b'PE(18:3(9Z,12Z,15Z)/20:3(5Z,8Z,11Z))'	HMDB00 09166	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphinic acid'	b'PE(18:3(9Z,12Z,15Z)/20:3(8Z,11Z,14Z))'	HMDB00 09167	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphinic acid'	b'PE(18:4(6Z,9Z,12Z,15Z)/20:2(11Z,14Z))'	HMDB00 09198	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))'	HMDB00 09294	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))'	HMDB00 09325	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))'	HMDB00 09326	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))'	HMDB00 09358	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))'	HMDB00 09359	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))'	HMDB00 09390	C43H74NO8P	

		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PE(20:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))'	HMDB00 09423	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))'	HMDB00 09454	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))'	HMDB00 09455	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(9Z)-hexadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,16Z)/16:1(9Z))'	HMDB00 09617	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(9Z)-hexadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(22:5(7Z,10Z,13Z,16Z,19Z)/16:1(9Z))'	HMDB00 09650	C43H74NO8P	
		763.5152049	0.0016 049	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(hexadecanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:0)	HMDB00 09682	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'[2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-(pentadecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB01 13036	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'[3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(pentadecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/15:0)	HMDB01 13675	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'[2-(dimethylamino)ethoxy]([2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-(tetradecanoyloxy)propoxy])phosphinic acid'	b'PE-NMe2(14:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB01 13896	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'[2-(dimethylamino)ethoxy]([2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propoxy])phosphinic acid'	b'PE-NMe2(14:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB01 13913	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'[2-(dimethylamino)ethoxy]([2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propoxy])phosphinic acid'	b'PE-NMe2(14:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB01 13914	C43H74NO8P	

						19Z))'			
763.5152053	0.0016 053	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(9Z)-hexadec-9-enoyloxy]-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]propoxy})phosphinic acid'		b'PE- NMc2(16:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))'	HMDB01 13975	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy})phosphinic acid'		b'PE- NMc2(18:2(9Z,12Z)/18:4(6Z,9Z,12Z,15Z))'	HMDB01 14076	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b' {2,3-bis[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy}[2-(dimethylamino)ethoxy]phosphinic acid'		b'PE- NMc2(18:3(6Z,9Z,12Z)/18:3(6Z,9Z,12Z))'	HMDB01 14103	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'		b'PE- NMc2(18:3(6Z,9Z,12Z)/18:3(9Z,12Z,15Z))'	HMDB01 14104	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'		b'PE- NMc2(18:3(9Z,12Z,15Z)/18:3(6Z,9Z,12Z))'	HMDB01 14132	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b' {2,3-bis[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy}[2-(dimethylamino)ethoxy]phosphinic acid'		b'PE- NMc2(18:3(9Z,12Z,15Z)/18:3(9Z,12Z,15Z))'	HMDB01 14133	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy})phosphinic acid'		b'PE- NMc2(18:4(6Z,9Z,12Z,15Z)/18:2(9Z,12Z))'	HMDB01 14160	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(9Z)-hexadec-9-enoyloxy]-3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]propoxy})phosphinic acid'		b'PE- NMc2(20:5(5Z,8Z,11Z,14Z,17Z)/16:1(9Z))'	HMDB01 14385	C43H74NO8P		
763.5152053	0.0016	Proton	b'[2-(dimethylamino)ethoxy]({3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy})phosphinic acid'		b'PE-	HMDB01	C43H74NO8P		

			053	ation		NMe2(22:5(4Z,7Z,10Z,13Z,16Z)/14:1(9Z))'	14524		
763.5152053	0.0016053	Protonation			b'[2-(dimethylamino)ethoxy]({3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy})phosphinic acid'	b'PE-NMe2(22:5(7Z,10Z,13Z,16Z,19Z)/14:1(9Z))'	HMDB0114550	C43H74NO8P	
763.5152053	0.0016053	Protonation			b'[2-(dimethylamino)ethoxy]({3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/14:0)'	HMDB0114576	C43H74NO8P	
763.5152053	0.0016053	Protonation			b'(2-aminoethoxy)((2R)-3-[(1E)-hexadec-1-en-1-yloxy]-2-[[{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(P-16:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB0285246	C43H74NO8P	
763.5152053	0.0016053	Protonation			b'(2-aminoethoxy)((2R)-2-[(1E)-hexadec-1-en-1-yloxy]-3-[[{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/P-16:0)'	HMDB0285247	C43H74NO8P	
763.5152053	0.0016053	Protonation			b'(2-aminoethoxy)((2R)-3-[(1E)-hexadec-1-en-1-yloxy]-2-[[{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(P-16:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB0285248	C43H74NO8P	
763.5152053	0.0016053	Protonation			b'(2-aminoethoxy)((2R)-2-[(1E)-hexadec-1-en-1-yloxy]-3-[[{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/P-16:0)'	HMDB0285249	C43H74NO8P	
763.5152053	0.0016053	Protonation			b'(2-aminoethoxy)((2R)-3-[(1E)-hexadec-1-en-1-yloxy]-2-[[{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(P-16:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB0285250	C43H74NO8P	
763.5152053	0.0016053	Protonation			b'(2-aminoethoxy)((2R)-2-[(1E)-hexadec-1-en-1-yloxy]-3-[[{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/P-16:0)'	HMDB0285251	C43H74NO8P	
763.5152053	0.0016053	Protonation			b'(2-aminoethoxy)((2R)-3-[(1E)-hexadec-1-en-1-yloxy]-2-[[{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(P-16:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB0285252	C43H74NO8P	

		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(1E)-hexadec-1-en-1-yloxy]-3-[[{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/P-16:0)'	HMDB02 85253	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(1E)-hexadec-1-en-1-yloxy]-2-[[{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(P-16:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))'	HMDB02 85256	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(1E)-hexadec-1-en-1-yloxy]-3-[[{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/P-16:0)'	HMDB02 85257	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]-2-[[{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(P- 18:1(11Z)/20:4(6E,8Z,11Z,14Z)+=O(5))'	HMDB02 85424	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]-3-[[{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)+=O(5)P- 18:1(11Z))'	HMDB02 85425	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]-2-[[{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(P- 18:1(11Z)/20:4(5Z,8Z,11Z,13E)+=O(1 5))'	HMDB02 85426	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation		b'PE(20:4(5Z,8Z,11Z,13E)+=O(15)P- 18:1(11Z))'	HMDB02 85427	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoyl]oxy}-3-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P- 18:1(11Z)/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R))'	HMDB02 85438	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoyl]oxy}-2-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/P-18:1(11Z))'	HMDB02 85439	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoyl]oxy}-3-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P- 18:1(11Z)/20:5(5Z,8Z,11Z,14Z,16E)- OH(18))'	HMDB02 85440	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoyl]oxy}-2-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/P-18:1(11Z))'	HMDB02 85441	C43H74NO8P	

		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}-3-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P- 18:1(11Z)/20:5(5Z,8Z,10E,14Z,17Z)- OH(12))'	HMDB02 85442	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}-2-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/P-18:1(11Z))'	HMDB02 85443	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}-3-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P- 18:1(11Z)/20:5(6E,8Z,11Z,14Z,17Z)- OH(5))'	HMDB02 85444	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}-2-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/P-18:1(11Z))'	HMDB02 85445	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation		b'PE(P- 18:1(9Z)/20:4(6E,8Z,11Z,14Z)+=O(5))'	HMDB02 85525	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]-3-{{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl}oxy}propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)+=O(5)P- 18:1(9Z))'	HMDB02 85526	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation		b'PE(P- 18:1(9Z)/20:4(5Z,8Z,11Z,13E)+=O(15) y'	HMDB02 85527	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation		b'PE(20:4(5Z,8Z,11Z,13E)+=O(15)P- 18:1(9Z))'	HMDB02 85528	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenyl}oxy}-3-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P- 18:1(9Z)/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R))'	HMDB02 85538	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl}oxy}-2-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/P-18:1(9Z))'	HMDB02 85539	C43H74NO8P	
		763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl}oxy}-3-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P- 18:1(9Z)/20:5(5Z,8Z,11Z,14Z,16E)-	HMDB02 85540	C43H74NO8P	

						OH(18))'			
763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{5Z,8Z,11Z,13E,17Z}-16-hydroxyicosa-5,8,11,13,17-pentaenoyl}oxy}-2-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'		b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18))P-18:1(9Z))'	HMDB02 85541	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{5Z,8Z,10E,14Z,17Z}-12-hydroxyicosa-5,8,10,14,17-pentaenoyl}oxy}-3-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'		b'PE(P- 18:1(9Z)/20:5(5Z,8Z,10E,14Z,17Z)- OH(12))'	HMDB02 85542	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{5Z,8Z,10E,14Z,17Z}-12-hydroxyicosa-5,8,10,14,17-pentaenoyl}oxy}-2-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'		b'PE(20:5(5Z,8Z,10E,14Z,17Z)- OH(12))P-18:1(9Z))'	HMDB02 85543	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{6E,8Z,11Z,14Z,17Z}-5-hydroxyicosa-6,8,11,14,17-pentaenoyl}oxy}-3-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'		b'PE(P- 18:1(9Z)/20:5(6E,8Z,11Z,14Z,17Z)- OH(5))'	HMDB02 85544	C43H74NO8P		
763.5152053	0.0016 053	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{6E,8Z,11Z,14Z,17Z}-5-hydroxyicosa-6,8,11,14,17-pentaenoyl}oxy}-2-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'		b'PE(20:5(6E,8Z,11Z,14Z,17Z)- OH(5))P-18:1(9Z))'	HMDB02 85545	C43H74NO8P		
762.5047002	0.0010 998	Redox	b'[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-(heptadecanoyloxy)propoxy]phosphonic acid'		b'PA(17:0/PGF1alpha)'	HMDB02 63569	C40H75O11P		
762.5047002	0.0010 998	Redox	b'[(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-(heptadecanoyloxy)propoxy]phosphonic acid'		b'PA(PGF1alpha/17:0)'	HMDB02 63570	C40H75O11P		
762.5047002	0.0010 998	Redox	b'[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[(14-methylhexadecanoyl)oxy]propoxy]phosphonic acid'		b'PA(a-17:0/PGF1alpha)'	HMDB02 67099	C40H75O11P		
762.5047002	0.0010 998	Redox	b'[(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(14-methylhexadecanoyl)oxy]propoxy]phosphonic acid'		b'PA(PGF1alpha/a-17:0)'	HMDB02 67100	C40H75O11P		
762.5047002	0.0010 998	Redox	b'[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[(15-methylhexadecanoyl)oxy]propoxy]phosphonic acid'		b'PA(i-17:0/PGF1alpha)'	HMDB02 67926	C40H75O11P		
762.5047002	0.0010 998	Redox	b'[(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(15-methylhexadecanoyl)oxy]propoxy]phosphonic acid'		b'PA(PGF1alpha/i-17:0)'	HMDB02 67927	C40H75O11P		
762.5047002	0.0010	Redox	b'[(2S)-2,3-dihydroxypropoxy][[(2R)-3-(hexadecanoyloxy)-2-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl]octanoyl)oxy]propoxy]phosphinic acid'		b'PG(16:0/18:1(12Z)-O(9S,10R))'	HMDB02	C40H75O11P		

			998					68611		
		762.5047002	0.0010 998	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphinic acid'	b'PG(18:1(12Z)-O(9S,10R)/16:0)'	HMDB02 68612	C40H75O11P		
		762.5047002	0.0010 998	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-2-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphinic acid'	b'PG(16:0/18:1(9Z)-O(12,13))'	HMDB02 68613	C40H75O11P		
		762.5047002	0.0010 998	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)-O(12,13)/16:0)'	HMDB02 68614	C40H75O11P		
		762.5047002	0.0010 998	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(14-methylpentadecanoyl)oxy]-2-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphinic acid'	b'PG(i-16:0/18:1(12Z)-O(9S,10R))'	HMDB02 71520	C40H75O11P		
		762.5047002	0.0010 998	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(14-methylpentadecanoyl)oxy]-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphinic acid'	b'PG(18:1(12Z)-O(9S,10R)/i-16:0)'	HMDB02 71521	C40H75O11P		
		762.5047002	0.0010 998	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(14-methylpentadecanoyl)oxy]-2-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphinic acid'	b'PG(i-16:0/18:1(9Z)-O(12,13))'	HMDB02 71522	C40H75O11P		
		762.5047002	0.0010 998	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(14-methylpentadecanoyl)oxy]-3-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)-O(12,13)/i-16:0)'	HMDB02 71523	C40H75O11P		
3 2 0	766.53 67	767.546505	0.0020 05	Proton ation	b'(2-[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-(pentadecanoyloxy)propyl phosphonato]oxy)ethyl)trimethylazanium'	b'PC(15:0/20:4(5Z,8Z,11Z,14Z))'	HMDB00 07949	C43H78NO8P		
		767.546505	0.0020 05	Proton ation		b'PC(15:0/20:4(8Z,11Z,14Z,17Z))'	HMDB00 07950	C43H78NO8P		
		767.546505	0.0020 05	Proton ation	b'(2-[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-(pentadecanoyloxy)propyl phosphonato]oxy)ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)/15:0)'	HMDB00 08428	C43H78NO8P	C00 157	
		767.546505	0.0020 05	Proton ation	b'(2-[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-(pentadecanoyloxy)propyl phosphonato]oxy)ethyl)trimethylazanium'	b'PC(20:4(8Z,11Z,14Z,17Z)/15:0)'	HMDB00 08461	C43H78NO8P		
		767.546505	0.0020 05	Proton ation	b'(2-aminoethoxy)((2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-(hexadecanoyloxy)propoxy]phosphinic acid'	b'PE(16:0/22:4(7Z,10Z,13Z,16Z))'	HMDB00 08943	C43H78NO8P		
		767.546505	0.0020	Proton	b'(2-aminoethoxy)((2R)-2-[(10Z,13Z,16Z)-docosa-10,13,16-trienoyloxy]-3-(9Z)-hexadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(16:1(9Z)/20:3(8Z,11Z,14Z))'	HMDB00	C43H78NO8P		

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767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/20:4(5Z,8Z,11Z,14Z))'	HMDB00 09003		C43H78NO8P	
767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14,17-tetraenoxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/20:4(8Z,11Z,14Z,17Z))'	HMDB00 09004		C43H78NO8P	
767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(11Z)/20:3(5Z,8Z,11Z))'	HMDB00 09034		C43H78NO8P	
767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(11Z)/20:3(8Z,11Z,14Z))'	HMDB00 09035		C43H78NO8P	
767.546505	0.0020 05	Proton ation			b'PE(18:1(9Z)/20:3(5Z,8Z,11Z))'	HMDB00 09067		C43H78NO8P	
767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)/20:3(8Z,11Z,14Z))'	HMDB00 09068		C43H78NO8P	
767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PE(18:2(9Z,12Z)/20:2(11Z,14Z))'	HMDB00 09099		C43H78NO8P	
767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphinic acid'	b'PE(18:3(6Z,9Z,12Z)/20:1(11Z))'	HMDB00 09131		C43H78NO8P	
767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphinic acid'	b'PE(18:3(9Z,12Z,15Z)/20:1(11Z))'	HMDB00 09164		C43H78NO8P	
767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-2-(icosanoyloxy)-3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoxy]propoxy]phosphinic acid'	b'PE(18:4(6Z,9Z,12Z,15Z)/20:0)'	HMDB00 09196		C43H78NO8P	
767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-3-(icosanoyloxy)-2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoxy]propoxy]phosphinic acid'	b'PE(20:0/18:4(6Z,9Z,12Z,15Z))'	HMDB00 09228		C43H78NO8P	
767.546505	0.0020 05	Proton ation		b'(2-aminoethoxy)[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/18:3(6Z,9Z,12Z))'	HMDB00 09259		C43H78NO8P	
767.546505	0.0020	Proton		b'(2-aminoethoxy)[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/18:3(9Z,12Z,15Z))'	HMDB00		C43H78NO8P	

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767.546505	0.0020 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/18:2(9Z,12Z))'	HMDB00 09291	C43H78NO8P		
767.546505	0.0020 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)/18:1(11Z))'	HMDB00 09322	C43H78NO8P		
767.546505	0.0020 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)/18:1(9Z))'	HMDB00 09323	C43H78NO8P		
767.546505	0.0020 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)/18:1(11Z))'	HMDB00 09355	C43H78NO8P		
767.546505	0.0020 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)/18:1(9Z))'	HMDB00 09356	C43H78NO8P		
767.546505	0.0020 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)/18:0)'	HMDB00 09387	C43H78NO8P		
767.546505	0.0020 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(20:4(8Z,11Z,14Z,17Z)/18:0)'	HMDB00 09420	C43H78NO8P		
767.546505	0.0020 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(hexadecanoyloxy)propoxy]phosphinic acid'	b'PE(22:4(7Z,10Z,13Z,16Z)/16:0)'	HMDB00 09583	C43H78NO8P		
767.5465055	0.0020 055	Proton ation	b'[2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-(pentadecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE- NMe(15:0/22:4(7Z,10Z,13Z,16Z))'	HMDB01 13034	C43H78NO8P		
767.5465055	0.0020 055	Proton ation	b'[3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(pentadecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE- NMe(22:4(7Z,10Z,13Z,16Z)/15:0)'	HMDB01 13594	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'PE- NMe2(14:0/22:4(7Z,10Z,13Z,16Z))'	HMDB01 13893	C43H78NO8P		
767.5465055	0.0020 055	Proton ation	b'[2-(dimethylamino)ethoxy][3-(hexadecanoyloxy)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]phosphinic acid'	b'PE- NMe2(16:0/20:4(5Z,8Z,11Z,14Z))'	HMDB01 13951	C43H78NO8P		
767.5465055	0.0020	Proton	b'[2-(dimethylamino)ethoxy][(3-[(9Z)-hexadec-9-enoyloxy]-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy)]phosphinic acid'	b'PE-	HMDB01	C43H78NO8P		

		055	ation			NMe2(16:1(9Z)/20:3(5Z,8Z,11Z))'	13971		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]({3-[(9Z)-hexadec-9-enoyloxy]-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(16:1(9Z)/20:3(8Z,11Z,14Z))'	HMDB01 13972	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]({2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]-3-(octadecanoyloxy)propoxy})phosphinic acid'	b'PE- NMe2(18:0/18:4(6Z,9Z,12Z,15Z))'	HMDB01 13993	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]({3-[(11Z)-octadec-11-enoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:1(11Z)/18:3(6Z,9Z,12Z))'	HMDB01 14018	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]({3-[(11Z)-octadec-11-enoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:1(11Z)/18:3(9Z,12Z,15Z))'	HMDB01 14019	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]({3-[(9Z)-octadec-9-enoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:1(9Z)/18:3(6Z,9Z,12Z))'	HMDB01 14045	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]({3-[(9Z)-octadec-9-enoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:1(9Z)/18:3(9Z,12Z,15Z))'	HMDB01 14046	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'[2,3-bis[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE- NMe2(18:2(9Z,12Z)/18:2(9Z,12Z))'	HMDB01 14073	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]({2-[(11Z)-octadec-11-enoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:3(6Z,9Z,12Z)/18:1(11Z))'	HMDB01 14100	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]({2-[(9Z)-octadec-9-enoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:3(6Z,9Z,12Z)/18:1(9Z))'	HMDB01 14101	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]({2-[(11Z)-octadec-11-enoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:3(9Z,12Z,15Z)/18:1(11Z))'	HMDB01 14129	C43H78NO8P		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]({2-[(9Z)-octadec-9-enoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:3(9Z,12Z,15Z)/18:1(9Z))'	HMDB01 14130	C43H78NO8P		
767.5465055	0.0020 055	Proton ation			b'PE- NMe2(18:4(6Z,9Z,12Z,15Z)/18:0))'	HMDB01 14157	C43H78NO8P		
767.5465055	0.0020	Proton		b'[2-(dimethylamino)ethoxy]({2-[(9Z)-hexadec-9-enoyloxy]-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy})phosphinic acid'	b'PE-	HMDB01	C43H78NO8P		

		055	ation			NMe2(20:3(5Z,8Z,11Z)/16:1(9Z))'	14272		
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]([2-[(9Z)-hexadec-9-enoyloxy]-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy])phosphinic acid'	b'PE- NMe2(20:3(8Z,11Z,14Z)/16:1(9Z))'	HMDB01 14300		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy][2-(hexadecanoyloxy)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]phosphinic acid'	b'PE- NMe2(20:4(5Z,8Z,11Z,14Z)/16:0)'	HMDB01 14327		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy][2-(hexadecanoyloxy)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]phosphinic acid'	b'PE- NMe2(20:4(8Z,11Z,14Z,17Z)/16:0)'	HMDB01 14355		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy]([3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(tetradecanoyloxy)propoxy])phosphinic acid'	b'PE- NMe2(22:4(7Z,10Z,13Z,16Z)/14:0)'	HMDB01 14495		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'[2-(dimethylamino)ethoxy][3-(hexadecanoyloxy)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]phosphinic acid'	b'PE- NMe2(16:0/20:4(8Z,11Z,14Z,17Z))'	HMDB01 16711		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'(2-aminoethoxy)((2R)-3-[(1E)-octadec-1-en-1-yloxy]-2-[(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienoyloxy]propoxy]phosphinic acid'	b'PE(P-18:0/20:3(5Z,8Z,11Z)- O(14R,15S))'	HMDB02 85270		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'(2-aminoethoxy)((2R)-2-[(1E)-octadec-1-en-1-yloxy]-3-[(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)-O(14R,15S)/P- 18:0)'	HMDB02 85271		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'(2-aminoethoxy)((2R)-2-[(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyloxy]-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:0/20:3(5Z,8Z,14Z)- O(11S,12R))'	HMDB02 85272		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'(2-aminoethoxy)((2R)-3-[(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyloxy]-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,14Z)-O(11S,12R)/P- 18:0)'	HMDB02 85273		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'(2-aminoethoxy)((2R)-3-[(1E)-octadec-1-en-1-yloxy]-2-[(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyloxy]propoxy]phosphinic acid'	b'PE(P-18:0/20:3(5Z,11Z,14Z)-O(8,9))'	HMDB02 85274		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'(2-aminoethoxy)((2R)-2-[(1E)-octadec-1-en-1-yloxy]-3-[(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,11Z,14Z)-O(8,9)/P-18:0)'	HMDB02 85275		C43H78NO8P	
767.5465055	0.0020 055	Proton ation		b'(2-aminoethoxy)((2R)-3-[(1E)-octadec-1-en-1-yloxy]-2-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyloxy]propoxy]phosphinic acid'	b'PE(P-18:0/20:3(8Z,11Z,14Z)-O(5,6))'	HMDB02 85276		C43H78NO8P	
767.5465055	0.0020	Proton			b'PE(20:3(8Z,11Z,14Z)-O(5,6)/P-18:0)'	HMDB02		C43H78NO8P	

		055	ation				85277		
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(P-18:0/20:4(5Z,8Z,11Z,14Z)-OH(20))'	HMDB02 85278		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(20:4(5Z,8Z,11Z,14Z)-OH(20))/P-18:0)'	HMDB02 85279		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5R,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(P-18:0/20:4(6E,8Z,11Z,14Z)-OH(5S))'	HMDB02 85280		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(20:4(6E,8Z,11Z,14Z)-OH(5S))/P-18:0)'	HMDB02 85281		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,8Z,11Z,14Z,19S)-19-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(P-18:0/20:4(5Z,8Z,11Z,14Z)-OH(19S))'	HMDB02 85282		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(20:4(5Z,8Z,11Z,14Z)-OH(19S))/P-18:0)'	HMDB02 85283		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,8Z,11Z,14Z,18R)-18-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(P-18:0/20:4(5Z,8Z,11Z,14Z)-OH(18R))'	HMDB02 85284		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,8Z,11Z,14Z,18S)-18-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(20:4(5Z,8Z,11Z,14Z)-OH(18R))/P-18:0)'	HMDB02 85285		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(P-18:0/20:4(5Z,8Z,11Z,14Z)-OH(17))'	HMDB02 85286		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(20:4(5Z,8Z,11Z,14Z)-OH(17))/P-18:0)'	HMDB02 85287		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,8Z,11Z,14Z,16R)-16-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(P-18:0/20:4(5Z,8Z,11Z,14Z)-OH(16R))'	HMDB02 85288		C43H78NO8P	
767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,8Z,11Z,14Z,16S)-16-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(20:4(5Z,8Z,11Z,14Z)-OH(16R))/P-18:0)'	HMDB02 85289		C43H78NO8P	
767.5465055	0.0020	Proton	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,8Z,11Z,13E,15S)-15-hydroxyicosa-5,8,11,13-tetraenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy}phosphinic acid'		b'PE(P-18:0/20:4(5Z,8Z,11Z,13E)-	HMDB02		C43H78NO8P	

			055	ation		OH(15S))'	85290		
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,11Z,13E,15R)-15-hydroxyicoso-5,8,11,13-tetraenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)-OH(15S))P-18:0)'	HMDB02 85291	C43H78NO8P	
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,10E,12S,14Z)-12-hydroxyicoso-5,8,10,14-tetraenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:0/20:4(5Z,8Z,10E,14Z)-OH(12S))'	HMDB02 85292	C43H78NO8P	
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,10E,12R,14Z)-12-hydroxyicoso-5,8,10,14-tetraenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,10E,14Z)-OH(12S))P-18:0)'	HMDB02 85293	C43H78NO8P	
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-2-{{(5E,8Z,11R,12Z,14Z)-11-hydroxyicoso-5,8,12,14-tetraenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:0/20:4(5E,8Z,12Z,14Z)-OH(11R))'	HMDB02 85294	C43H78NO8P	
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-3-{{(5E,8Z,11S,12Z,14Z)-11-hydroxyicoso-5,8,12,14-tetraenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(20:4(5E,8Z,12Z,14Z)-OH(11R))P-18:0)'	HMDB02 85295	C43H78NO8P	
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-2-{{(5E,7Z,11Z,14Z)-9-hydroxyicoso-5,7,11,14-tetraenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:0/20:4(5Z,7E,11Z,14Z)-OH(9))'	HMDB02 85296	C43H78NO8P	
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-3-{{(5E,7Z,11Z,14Z)-9-hydroxyicoso-5,7,11,14-tetraenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,7E,11Z,14Z)-OH(9))P-18:0)'	HMDB02 85297	C43H78NO8P	
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-2-{{(6E,8E,11E)-5-hydroxyicoso-6,8,11-trienoyl}oxy}-3-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:1(11Z)/20:3(6,8,11)-OH(5))'	HMDB02 85473	C43H78NO8P	
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-3-{{(6E,8E,11E)-5-hydroxyicoso-6,8,11-trienoyl}oxy}-2-[(1E,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:3(6,8,11)-OH(5))P-18:1(11Z))'	HMDB02 85474	C43H78NO8P	
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-2-{{(6E,8E,11E)-5-hydroxyicoso-6,8,11-trienoyl}oxy}-3-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:1(9Z)/20:3(6,8,11)-OH(5))'	HMDB02 85576	C43H78NO8P	
		767.5465055	0.0020 055	Proton ation	b'(2-aminoethoxy)((2R)-3-{{(6E,8E,11E)-5-hydroxyicoso-6,8,11-trienoyl}oxy}-2-[(1E,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'PE(20:3(6,8,11)-OH(5))P-18:1(9Z))'	HMDB02 85577	C43H78NO8P	
3	772.58	773.5934552	0.0021	Proton	b'(2-{{(2R)-2-[(11Z)-icos-11-enoyloxy]-3-(pentadecanoyloxy)propyl phosphonato}oxy}ethyl)trimethylazanium'	b'PC(15:0/20:1(11Z))'	HMDB00 07945	C43H84NO8P	
2	35	773.5934552	552	ation					
1		773.5934552	0.0021	Proton	b'(2-{{(2R)-3-[(11Z)-icos-11-enoyloxy]-2-(pentadecanoyloxy)propyl phosphonato}oxy}ethyl)trimethylazanium'	b'PC(20:1(11Z)/15:0)'	HMDB00	C43H84NO8P	

		552	ation			08297		
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(15Z)-tetracos-15-enoyloxy]-3-(tetradecanoyloxy)propoxy]phosphinic acid'		b'PE(14:0/24:1(15Z))'	HMDB00 08849	C43H84NO8P	C00 350
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-2-(tetracosanoyloxy)-3-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'		b'PE(14:1(9Z)/24:0)'	HMDB00 08881	C43H84NO8P	
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-(hexadecanoyloxy)propoxy]phosphinic acid'		b'PE(16:0/22:1(13Z))'	HMDB00 08941	C43H84NO8P	
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-[(9Z)-hexadec-9-enoyloxy]propoxy]phosphinic acid'		b'PE(16:1(9Z)/22:0)'	HMDB00 08973	C43H84NO8P	
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'		b'PE(18:0/20:1(11Z))'	HMDB00 08999	C43H84NO8P	
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-2-(icosanoyloxy)-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'		b'PE(18:1(11Z)/20:0)'	HMDB00 09031	C43H84NO8P	
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-2-(icosanoyloxy)-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'		b'PE(18:1(9Z)/20:0)'	HMDB00 09064	C43H84NO8P	
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-3-(icosanoyloxy)-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'		b'PE(20:0/18:1(11Z))'	HMDB00 09223	C43H84NO8P	
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-3-(icosanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'		b'PE(20:0/18:1(9Z))'	HMDB00 09224	C43H84NO8P	
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'		b'PE(20:1(11Z)/18:0)'	HMDB00 09255	C43H84NO8P	
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-[(9Z)-hexadec-9-enoyloxy]propoxy]phosphinic acid'		b'PE(22:0/16:1(9Z))'	HMDB00 09485	C43H84NO8P	
773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-(hexadecanoyloxy)propoxy]phosphinic acid'		b'PE(22:1(13Z)/16:0)'	HMDB00 09517	C43H84NO8P	
773.5934552	0.0021	Proton	b'(2-aminoethoxy)[(2R)-3-(tetracosanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'		b'PE(24:0/14:1(9Z))'	HMDB00	C43H84NO8P	

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773.5934552	0.0021 552	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(15Z)-tetracos-15-enoyloxy]-2-(tetradecanoyloxy)propoxy]phosphinic acid'	b'PE(24:1(15Z)/14:0)'	HMDB00 09745	C43H84NO8P		
773.5934557	0.0021 557	Proton ation	b'[2-[(13Z)-docos-13-enoyloxy]-3-(pentadecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMc(15:0/22:1(13Z))'	HMDB01 13032	C43H84NO8P		
773.5934557	0.0021 557	Proton ation	b'[3-[(13Z)-docos-13-enoyloxy]-2-(pentadecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMc(22:1(13Z)/15:0)'	HMDB01 13537	C43H84NO8P		
773.5934557	0.0021 557	Proton ation	b'[2-(dimethylamino)ethoxy][(2-[(9Z)-octadec-9-enoyloxy]-3-(octadecanoyloxy)propoxy)]phosphinic acid'	b'PE-NMc2(18:0/18:1(9Z))'	HMDB01 13871	C43H84NO8P		
773.5934557	0.0021 557	Proton ation	b'[2-(dimethylamino)ethoxy][(2-[(11Z)-octadec-11-enoyloxy]-3-(octadecanoyloxy)propoxy)]phosphinic acid'	b'PE-NMc2(18:0/18:1(11Z))'	HMDB01 13872	C43H84NO8P		
773.5934557	0.0021 557	Proton ation	b'[2-(dimethylamino)ethoxy][2-(docosanoyloxy)-3-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE-NMc2(14:1(9Z)/22:0)'	HMDB01 13873	C43H84NO8P		
773.5934557	0.0021 557	Proton ation	b'[2-(dimethylamino)ethoxy][3-(hexadecanoyloxy)-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE-NMc2(16:0/20:1(11Z))'	HMDB01 13874	C43H84NO8P		
773.5934557	0.0021 557	Proton ation	b'[2-(dimethylamino)ethoxy][(3-[(9Z)-hexadec-9-enoyloxy]-2-(icosanoyloxy)propoxy)]phosphinic acid'	b'PE-NMc2(16:1(9Z)/20:0)'	HMDB01 13875	C43H84NO8P		
773.5934557	0.0021 557	Proton ation	b'[2-(dimethylamino)ethoxy][(2-[(13Z)-docos-13-enoyloxy]-3-(tetradecanoyloxy)propoxy)]phosphinic acid'	b'PE-NMc2(14:0/22:1(13Z))'	HMDB01 13891	C43H84NO8P		
773.5934557	0.0021 557	Proton ation	b'[2-(dimethylamino)ethoxy][(3-[(11Z)-octadec-11-enoyloxy]-2-(octadecanoyloxy)propoxy)]phosphinic acid'	b'PE-NMc2(18:1(11Z)/18:0)'	HMDB01 14016	C43H84NO8P		
773.5934557	0.0021 557	Proton ation		b'PE-NMc2(18:1(9Z)/18:0)'	HMDB01 14043	C43H84NO8P		
773.5934557	0.0021 557	Proton ation	b'[2-(dimethylamino)ethoxy][(2-[(9Z)-hexadec-9-enoyloxy]-3-(icosanoyloxy)propoxy)]phosphinic acid'	b'PE-NMc2(20:0/16:1(9Z))'	HMDB01 14185	C43H84NO8P		
773.5934557	0.0021	Proton	b'[2-(dimethylamino)ethoxy][2-(hexadecanoyloxy)-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE-NMc2(20:1(11Z)/16:0)'	HMDB01	C43H84NO8P		

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		773.5934557	0.0021 557	Proton ation	b'[2-(dimethylamino)ethoxy][(3-(docosanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE-NMc2(22:0/14:1(9Z))'	HMDB01 14411	C43H84NO8P	
		773.5934557	0.0021 557	Proton ation	b'[2-(dimethylamino)ethoxy]((13-(13Z)-docos-13-enoyloxy)-2-(tetradecanoyloxy)propoxy)]phosphinic acid'	b'PE-NMc2(22:1(13Z)/14:0)'	HMDB01 14437	C43H84NO8P	
		773.5934557	0.0021 557	Proton ation	b'(2-[(2-(heptadecanoyloxy)-3-(octadec-9-enoyloxy)propyl phosphono]oxy)ethyl]trimethylazanium'	b'PC(18:1(9Z)/17:0)'	HMDB02 56160	C43H84NO8P	
3 2 2	773.94 25	774.9483145	0.0019 855	Proton ation	b'[dichloro({((2R,3S,4R,5R)-3,4-dihydroxy-5-(6-[(2-(methylsulfonyl)ethyl]amino)-2-[(3,3,3-trifluoropropyl)sulfonyl]-9H-purin-9-yl)oxolan-2-yl)methoxy}(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)methyl]phosphonic acid'	b'Cangrelor'	HMDB02 40386	C17H25Cl2F3N5 O12P3S2	
3 2 3	774.54 06	774.5410853	0.0004 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(18:0/18:2(9Z,12Z))'	HMDB00 10605	C42H79O10P	
		774.5410857	0.0004 857	Redox	b'[(2R)-2,3-bis[(11Z)-octadec-11-enoyloxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(18:1(11Z)/18:1(11Z))'	HMDB00 10618	C42H79O10P	
		774.5410853	0.0004 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(11Z)/18:1(9Z))'	HMDB00 10619	C42H79O10P	
		774.5410853	0.0004 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)/18:1(11Z))'	HMDB00 10633	C42H79O10P	
		774.5410857	0.0004 857	Redox	b'[(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(18:1(9Z)/18:1(9Z))'	HMDB00 10634	C42H79O10P	
		774.5410853	0.0004 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(18:2(9Z,12Z)/18:0)'	HMDB00 10647	C42H79O10P	
		774.5410857	0.0004 857	Redox	b'[2,3-bis(octadec-9-enoyloxy)propoxy](2,3-dihydroxypropoxy)phosphinic acid'	b'1,2-Dioleoyl-sn-glycero-3-phosphoglycerol'	HMDB02 44089	C42H79O10P	
3 2	781.47 65	782.4816423	0.0026 577	Proton ation	b'2-[(14-(3,4-dihydroxy-6-methylhept-5-en-2-yl)-1,6,6,11,15-pentamethyltetracyclo[8.7.0.0\xc2\x82.\xc2\x81\x87.0\xc2\x82.\xc2\x89\xc2\x89.\xc2\x89\xc2\x81\x85]heptadec-7-en-5-yl)oxy]-6-([3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)methyl]oxane-3,4,5-triol'	b'Momordicoside D'	HMDB00 35011	C42H70O13	

4		782.4816423	0.0026 577	Proton ation	b'2-([1,2,6,6,10,17-hexamethyl-15-(2-methylprop-1-en-1-yl)-7-([3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)-14-oxapentacyclo[11.7.1.0'xc2'xb2,'xc2'xb9'xc2'xb9.0'xc2'xb5,'xc2'xb9'xc2'xb8,'xc2'xb2'xb9]henicosan-17-yl]oxy)-6-(hydroxymethyl)oxane-3,4,5-triol'	b'Ginsenoside La'	HMDB00 39647	C42H70O13	
3 2 5	784.14 59	784.1486935	0.0027 935	Redox	b'5,7-dihydroxy-2-([3,4,5-trihydroxy-2-[2,3,4-trihydroxy-6-(3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-2-yl)phenyl]phenyl]-3-([3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)-4H-chromen-4-one'	b'Degalloyltheaflavin'	HMDB00 40548	C36H32O20	
3 2 6	785.15 42	785.1571345 785.1571354	0.0029 345 0.0029 354	Redox Redox	b'([(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)([(2R,3S,4S)-5-(7,8-dimethyl-2,4-dioxo-2H,3H,4H,10H-benzo[g]pteridin-10-yl)-2,3,4-trihydroxypentyl]oxy)(hydroxy)phosphoryl]oxy]phosphinic acid'	b'FAD'	HMDB00 01248	C27H33N9O15P 2	C00 016
					b'([5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)([(5-(7,8-dimethyl-2,4-dioxo-2H,3H,4H,10H-benzo[g]pteridin-10-yl)-2,3,4-trihydroxypentyl]oxy)(hydroxy)phosphoryl]oxy]phosphinic acid'	b'Flavinat'	HMDB02 52293	C27H33N9O15P 2	
3 2 7	790.53 71	791.546505 791.546505 791.546505 791.546505 791.546505 791.546505 791.546505	0.0016 05 0.0016 05 0.0016 05 0.0016 05 0.0016 05 0.0016 05	Proton ation Proton ation Proton ation Proton ation Proton ation	b'(2-([(2R)-2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-(pentadecanoyloxy)propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(15:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB00 07958	C45H78NO8P	C00 157
					b'(2-([(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(pentadecanoyloxy)propyl phosphonato]oxy)ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/15:0)'	HMDB00 08724	C45H78NO8P	
					b'(2-aminoethoxy)((2R)-2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB00 09012	C45H78NO8P	
					b'(2-aminoethoxy)((2R)-2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB00 09043	C45H78NO8P	
					b'(2-aminoethoxy)((2R)-2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(11Z)/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB00 09044	C45H78NO8P	
					b'(2-aminoethoxy)((2R)-2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB00 09076	C45H78NO8P	
					b'(2-aminoethoxy)((2R)-2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB00 09077	C45H78NO8P	
					b'(2-aminoethoxy)((2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PE(18:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z))'	HMDB00 09108	C45H78NO8P	

		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphinic acid'	b'PE(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))'	HMDB00 09206	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:5(5Z,8Z,11Z,14Z,17Z))'	HMDB00 09269	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z))'	HMDB00 09300	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(8Z,11Z,14Z,17Z))'	HMDB00 09301	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-2,3-bis[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)/20:3(5Z,8Z,11Z))'	HMDB00 09331	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)/20:3(8Z,11Z,14Z))'	HMDB00 09332	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)/20:3(5Z,8Z,11Z))'	HMDB00 09364	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-2,3-bis[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)/20:3(8Z,11Z,14Z))'	HMDB00 09365	C45H78NO8P	C00 350
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)/20:2(11Z,14Z))'	HMDB00 09396	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]phosphinic acid'	b'PE(20:4(8Z,11Z,14Z,17Z)/20:2(11Z,14Z))'	HMDB00 09429	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,17Z)/20:1(11Z))'	HMDB00 09461	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))'	HMDB00 09558	C45H78NO8P	C00 350
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)((2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PE(22:4(7Z,10Z,13Z,16Z)/18:2(9Z,12Z))'	HMDB00 09588	C45H78NO8P	

		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,16Z)/18:1(1Z))'	HMDB00 09619	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,16Z)/18:1(9Z))'	HMDB00 09620	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(22:5(7Z,10Z,13Z,16Z,19Z)/18:1(11Z))'	HMDB00 09652	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(22:5(7Z,10Z,13Z,16Z,19Z)/18:1(9Z))'	HMDB00 09653	C45H78NO8P	
		791.546505	0.0016 05	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	HMDB00 09684	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-(hexadecanoyloxy)propoxy})phosphinic acid'	b'PE- NMe2(16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB01 13959	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-[(9Z)-hexadec-9-enoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(16:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB01 13980	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-[(9Z)-hexadec-9-enoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(16:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB01 13981	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:1(11Z)/20:5(5Z,8Z,11Z,14Z,17Z))'	HMDB01 14028	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))'	HMDB01 14055	C45H78NO8P	
		791.5465055	0.0016	Proton	b'[2-(dimethylamino)ethoxy]({2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy})phosphinic acid'	b'PE-	HMDB01	C45H78NO8P	

			055	ation		NMe2(18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))'	14082		
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:2(9Z,12Z)/20:4(8Z,11Z,14Z,17Z))'	HMDB01 14083	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:3(6Z,9Z,12Z)/20:3(5Z,8Z,11Z))'	HMDB01 14109	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:3(6Z,9Z,12Z)/20:3(8Z,11Z,14Z))'	HMDB01 14110	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:3(9Z,12Z,15Z)/20:3(5Z,8Z,11Z))'	HMDB01 14138	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:3(9Z,12Z,15Z)/20:3(8Z,11Z,14Z))'	HMDB01 14139	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(18:4(6Z,9Z,12Z,15Z)/20:2(11Z,14Z))'	HMDB01 14166	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(20:2(11Z,14Z)/18:4(6Z,9Z,12Z,15Z))'	HMDB01 14250	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(20:3(5Z,8Z,11Z)/18:3(6Z,9Z,12Z))'	HMDB01 14277	C45H78NO8P	

		791.5465055	0.0016 055	Proton ation	b[2-(dimethylamino)ethoxy]({3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(20:3(5Z,8Z,11Z)/18:3(9Z,12Z,15Z))'	HMDB01 14278	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b[2-(dimethylamino)ethoxy]({3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(20:3(8Z,11Z,14Z)/18:3(6Z,9Z,12Z))'	HMDB01 14305	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b[2-(dimethylamino)ethoxy]({3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(20:3(8Z,11Z,14Z)/18:3(9Z,12Z,15Z))'	HMDB01 14306	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b[2-(dimethylamino)ethoxy]({3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(20:4(5Z,8Z,11Z,14Z)/18:2(9Z,12Z))'	HMDB01 14332	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b[2-(dimethylamino)ethoxy]({3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(20:4(8Z,11Z,14Z,17Z)/18:2(9Z,12Z))'	HMDB01 14360	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b[2-(dimethylamino)ethoxy]({3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(11Z))'	HMDB01 14387	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b[2-(dimethylamino)ethoxy]({3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(20:5(5Z,8Z,11Z,14Z,17Z)/18:1(9Z))'	HMDB01 14388	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b[2-(dimethylamino)ethoxy]({3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(9Z)-hexadec-9-enoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(22:5(4Z,7Z,10Z,13Z,16Z)/16:1(9Z))'	HMDB01 14526	C45H78NO8P	
		791.5465055	0.0016 055	Proton ation	b[2-(dimethylamino)ethoxy]({3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(9Z)-hexadec-9-enoyloxy]propoxy})phosphinic acid'	b'PE- NMe2(22:5(7Z,10Z,13Z,16Z,19Z)/16:1(9Z))'	HMDB01 14553	C45H78NO8P	

						(9Z))'			
791.5465055	0.0016 055	Proton ation	b'[2-(dimethylamino)ethoxy]({3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(hexadecanoyloxy)propoxy})phosphinic acid'		b'PE- NMe2(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/ 16:0))'	HMDB01 14579	C45H78NO8P		
791.5465055	0.0016 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{5Z,7Z,10Z,13Z,16Z,19Z}-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'		b'PE(P- 18:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4))'	HMDB02 85350	C45H78NO8P		
791.5465055	0.0016 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{5Z,7Z,10Z,13Z,16Z,19Z}-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'		b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)/P-18:0))'	HMDB02 85351	C45H78NO8P		
791.5465055	0.0016 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{4Z,8Z,10Z,13Z,16Z,19Z}-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'		b'PE(P- 18:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7))'	HMDB02 85352	C45H78NO8P		
791.5465055	0.0016 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{4Z,8Z,10Z,13Z,16Z,19Z}-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'		b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/P-18:0))'	HMDB02 85353	C45H78NO8P		
791.5465055	0.0016 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{4Z,7Z,10Z,12E,16Z,19Z}-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'		b'PE(P- 18:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14))'	HMDB02 85354	C45H78NO8P		
791.5465055	0.0016 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{4Z,7Z,10Z,12E,16Z,19Z}-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'		b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/P-18:0))'	HMDB02 85355	C45H78NO8P		
791.5465055	0.0016 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{4Z,7Z,10Z,13E,15E,19Z}-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'		b'PE(P- 18:0/22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17))'	HMDB02 85356	C45H78NO8P		
791.5465055	0.0016 055	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{4Z,7Z,10Z,13E,15E,19Z}-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'		b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/P-18:0))'	HMDB02 85357	C45H78NO8P		
791.5465055	0.0016 055	Proton ation			b'PE(P-18:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))'	HMDB02 85360	C45H78NO8P		

		791.5465055	0.0016 055	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(1E)-octadec-1-en-1-yloxy]-3-[[4Z,7Z,10Z,13Z]-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)P-18:0)'	HMDB02 85361	C45H78NO8P	
		790.5360004	0.0010 996	Redox	b'[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-(nonadecanoyloxy)propoxy]phosphonic acid'	b'PA(19:0/PGF1alpha)'	HMDB02 64504	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-(nonadecanoyloxy)propoxy]phosphonic acid'	b'PA(PGF1alpha/19:0)'	HMDB02 64505	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[(17-methyloctadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-19:0/PGF1alpha)'	HMDB02 68134	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(17-methyloctadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(PGF1alpha/i-19:0)'	HMDB02 68135	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PG(18:0/18:1(12Z)-O(9S,10R))'	HMDB02 68819	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PG(18:1(12Z)-O(9S,10R)/18:0)'	HMDB02 68820	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-(octadecanoyloxy)-2-[[9Z]-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphonic acid'	b'PG(18:0/18:1(9Z)-O(12,13))'	HMDB02 68821	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(octadecanoyloxy)-3-[[9Z]-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphonic acid'	b'PG(18:1(9Z)-O(12,13)/18:0)'	HMDB02 68822	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(16-methylheptadecanoyl)oxy]-2-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphonic acid'	b'PG(i-18:0/18:1(12Z)-O(9S,10R))'	HMDB02 71728	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(16-methylheptadecanoyl)oxy]-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphonic acid'	b'PG(18:1(12Z)-O(9S,10R)/i-18:0)'	HMDB02 71729	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(16-methylheptadecanoyl)oxy]-2-[[9Z]-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphonic acid'	b'PG(i-18:0/18:1(9Z)-O(12,13))'	HMDB02 71730	C42H79O11P	
		790.5360004	0.0010 996	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(16-methylheptadecanoyl)oxy]-3-[[9Z]-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphonic acid'	b'PG(18:1(9Z)-O(12,13)/i-18:0)'	HMDB02 71731	C42H79O11P	

3 2 8	792.54 56	793.5526397	0.0007 603	Proton ation	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-(((2S)-1-hydroxy-3-(nonadecanoyloxy)propan-2-yl)oxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(19:0/LTE4/0:0)'	HMDB02 96091	C45H79NO8S	
		793.5526397	0.0007 603	Proton ation	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-((2S)-3-hydroxy-2-(nonadecanoyloxy)propoxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(LTE4/19:0/0:0)'	HMDB02 96092	C45H79NO8S	
		793.5526397	0.0007 603	Proton ation	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-((2R)-2-hydroxy-3-(nonadecanoyloxy)propoxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(19:0/0:0/LTE4)'	HMDB02 96093	C45H79NO8S	
		793.5526397	0.0007 603	Proton ation	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-((2S)-2-hydroxy-3-(nonadecanoyloxy)propoxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(LTE4/0:0/19:0)'	HMDB02 96094	C45H79NO8S	
		793.5526397	0.0007 603	Proton ation	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-(((2S)-1-hydroxy-3-((17-methyloctadecanoyl)oxy)propan-2-yl)oxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(i-19:0/LTE4/0:0)'	HMDB02 99831	C45H79NO8S	
		793.5526397	0.0007 603	Proton ation	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-((2S)-3-hydroxy-2-((17-methyloctadecanoyl)oxy)propoxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(LTE4/i-19:0/0:0)'	HMDB02 99832	C45H79NO8S	
		793.5526397	0.0007 603	Proton ation	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-((2R)-2-hydroxy-3-((17-methyloctadecanoyl)oxy)propoxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(i-19:0/0:0/LTE4)'	HMDB02 99833	C45H79NO8S	
		793.5526397	0.0007 603	Proton ation	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-((2S)-2-hydroxy-3-((17-methyloctadecanoyl)oxy)propoxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(LTE4/0:0/i-19:0)'	HMDB02 99834	C45H79NO8S	
3 2 9	795.51 11	794.5213987	0.0024 987	Proton ation	b'(6-[2,3-bis(hexadecanoyloxy)propoxy]-3,4,5-trihydroxyoxan-2-yl) methanesulfonic acid'	b'1,2-Di-O-palmitoyl-3-O-(6-sulfoquinovopyranosyl)glycerol'	HMDB00 41202	C41H78O12S	
		794.521019	0.0021 19	Proton ation	b(2-(((2S,3R,4E,14Z)-3-hydroxy-2-((5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenamido]octadeca-4,14-dien-1-yl phosphono]oxy)ethyl)trimethylazanium'	b'SM(d18:2(4E,14Z)/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 90591	C43H75N2O9P	
		793.5105139	0.0005 861	Redox	b'(2S)-2-amino-3-(((2R)-2-(((9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl)oxy)-3-(hexadecanoyloxy)propoxy)(hydroxy)phosphoryl)oxy)propanoic acid'	b'PS(16:0/18:1(12Z)-2OH(9,10))'	HMDB02 81164	C40H76NO12P	
		793.5105139	0.0005 861	Redox	b'(2S)-2-amino-3-(((2R)-3-(((9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl)oxy)-2-(hexadecanoyloxy)propoxy)(hydroxy)phosphoryl)oxy)propanoic acid'	b'PS(18:1(12Z)-2OH(9,10)/16:0)'	HMDB02 81165	C40H76NO12P	
3 3	795.52 72	796.5366691	0.0016 691	Proton ation	b(2-(((2S,3R,4E)-3-hydroxy-2-((5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenamido]octadec-4-en-1-yl phosphono]oxy)ethyl)trimethylazanium'	b'SM(d18:1/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 90539	C43H77N2O9P	

0		796.5366691	0.0016 691	Proton ation	b'(2-([(2S,3R,4E,14Z)-3-hydroxy-2-[(5Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]hept-5-enamido]octadeca-4,14-dien-1-yl phosphono)oxy)ethyl)trimethylazanium'	b'SM(d18:2(4E,14Z)/PGE2)'	HMDB02 90568	C43H77N2O9P	
		796.5366691	0.0016 691	Proton ation	b'(2-([(2S,3R,4E,14Z)-3-hydroxy-2-[(5Z)-7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]hept-5-enamido]octadeca-4,14-dien-1-yl phosphono)oxy)ethyl)trimethylazanium'	b'SM(d18:2(4E,14Z)/PGD2)'	HMDB02 90569	C43H77N2O9P	
		796.5366691	0.0016 691	Proton ation	b'(2-([(2S,3R,4E,14Z)-3-hydroxy-2-[(5S,6S,7E,9E,11Z,13E,15S)-5,6,15-trihydroxyicos-7,9,11,13-tetraenamido]octadeca-4,14-dien-1-yl phosphono)oxy)ethyl)trimethylazanium'	b'SM(d18:2(4E,14Z)/20:4(7E,9E,11Z,13E)-3OH(5S,6R,15S))'	HMDB02 90576	C43H77N2O9P	
3 3 1	806.54 33	807.5530331	0.0019 331	Proton ation	b'[(2R,5S,6R)-3,5-dihydroxy-2-([(2S,3R,4E)-3-hydroxy-2-octadecanamido]octadec-4-en-1-yl)oxy]-6-(hydroxymethyl)oxan-4-yl]oxidanesulfonic acid'	b'3-O-Sulfogalactosylceramide (d18:1/18:0)'	HMDB00 12314	C42H81NO11S	C06 125
		806.541832	0.0014 68	Redox	b'N-{1,6-dicyclohexyl-3,4-dihydroxy-5-[3-methyl-2-({methyl[(pyridin-2-yl)methyl]carbamoyl} amino)butanamido]hexan-2-yl}-3-methyl-2-({methyl[(pyridin-2-yl)methyl]carbamoyl} amino)butanamide'	b'Inhibitor CC'	HMDB02 60354	C44H70N8O6	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-(henicosanoyloxy)-2-([(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl]oxy)propoxy]phosphonic acid'	b'PA(21:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 65523	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-(henicosanoyloxy)-3-([(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl]oxy)propoxy]phosphonic acid'	b'PA(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/21:0)'	HMDB02 65524	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-(henicosanoyloxy)-2-([(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl]oxy)propoxy]phosphonic acid'	b'PA(21:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 65525	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-(henicosanoyloxy)-3-([(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl]oxy)propoxy]phosphonic acid'	b'PA(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/21:0)'	HMDB02 65526	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-(henicosanoyloxy)-2-([(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy)propoxy]phosphonic acid'	b'PA(21:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 65527	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-(henicosanoyloxy)-3-([(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy)propoxy]phosphonic acid'	b'PA(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/21:0)'	HMDB02 65528	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-(henicosanoyloxy)-3-([(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy)propoxy]phosphonic acid'	b'PA(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/21:0)'	HMDB02 65529	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-(henicosanoyloxy)-2-([(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl} pentadeca-4,7,10,13-tetraenoyl]oxy)propoxy]phosphonic acid'	b'PA(21:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 65532	C46H79O9P	

		806.5461711	0.0028 711	Redox	b'[(2R)-2-(hencosanoyloxy)-3-[[4Z,7Z,10Z,13Z]-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propoxy]phosphonic acid'	b'PA(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/21:0)'	HMDB02 65533	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-[[[5Z,7Z,10Z,13Z,16Z,19Z]-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy]-3-[(18-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(a- 21:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4))'	HMDB02 67183	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-[[[5Z,7Z,10Z,13Z,16Z,19Z]-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy]-2-[(18-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)/a-21:0)'	HMDB02 67184	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-[[[4Z,8Z,10Z,13Z,16Z,19Z]-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy]-3-[(18-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(a- 21:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7))'	HMDB02 67185	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-[[[4Z,8Z,10Z,13Z,16Z,19Z]-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy]-2-[(18-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/a-21:0)'	HMDB02 67186	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-[[[4Z,7Z,10Z,12E,16Z,19Z]-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl]oxy]-3-[(18-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(a- 21:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14))'	HMDB02 67187	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-[[[4Z,7Z,10Z,12E,16Z,19Z]-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl]oxy]-2-[(18-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/a-21:0)'	HMDB02 67188	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-[[[4Z,7Z,10Z,13E,15E,19Z]-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl]oxy]-3-[(18-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(a- 21:0/22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17))'	HMDB02 67189	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-[[[4Z,7Z,10Z,13E,15E,19Z]-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl]oxy]-2-[(18-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/a-21:0)'	HMDB02 67190	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-[(18-methylcosanoyl)oxy]-2-[[[4Z,7Z,10Z,13Z]-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propoxy]phosphonic acid'	b'PA(a-21:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))'	HMDB02 67193	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-[(18-methylcosanoyl)oxy]-3-[[[4Z,7Z,10Z,13Z]-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propoxy]phosphonic acid'	b'PA(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/a-21:0)'	HMDB02 67194	C46H79O9P	

		806.5461711	0.0028 711	Redox	b'[(2R)-2-{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}-3-[(19-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(i- 21:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4))'	HMDB02 68322	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}-2-[(19-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4))i-21:0)	HMDB02 68323	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}-3-[(19-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(i- 21:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7))'	HMDB02 68324	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}-2-[(19-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7))i-21:0)	HMDB02 68325	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy}-3-[(19-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(i- 21:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14))'	HMDB02 68326	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy}-2-[(19-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14))i-21:0)	HMDB02 68327	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy}-3-[(19-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(i- 21:0/22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17))'	HMDB02 68328	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy}-2-[(19-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17))i-21:0)	HMDB02 68329	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-3-[(19-methylcosanoyl)oxy]-2-{{(4Z,7Z,10Z,13Z)-15-[3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl]pentadeca-4,7,10,13-tetraenoyl}oxy]propoxy]phosphonic acid'	b'PA(i-21:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))'	HMDB02 68332	C46H79O9P	
		806.5461711	0.0028 711	Redox	b'[(2R)-2-[(19-methylcosanoyl)oxy]-3-{{(4Z,7Z,10Z,13Z)-15-[3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl]pentadeca-4,7,10,13-tetraenoyl}oxy]propoxy]phosphonic acid'	b'PA(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))i-21:0)	HMDB02 68333	C46H79O9P	
3 3	808.55	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-(icosanoyloxy)-2-{{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl}oxy]propoxy]phosphonic acid'	b'PE(20:0/20:4(6E,8Z,11Z,14Z))+O(5) y'	HMDB02 61864	C45H80NO9P	

2	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-(icosanoyloxy)-3-{{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl}oxy}propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z))+O(5)/20:0 y'	HMDB02 61865	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-(icosanoyloxy)-2-{{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl}oxy}propoxy]phosphinic acid'	b'PE(20:0/20:4(5Z,8Z,11Z,13E))+O(1 5))'	HMDB02 61866	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-(icosanoyloxy)-3-{{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl}oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E))+O(15)/20: 0y'	HMDB02 61867	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenyl}oxy}-3-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R))'	HMDB02 61878	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl}oxy}-2-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/20:0y'	HMDB02 61879	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl}oxy}-3-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18))'	HMDB02 61880	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl}oxy}-2-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/20:0y'	HMDB02 61881	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}-3-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12))'	HMDB02 61882	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}-2-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/20:0y'	HMDB02 61883	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}-3-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:0/20:5(6E,8Z,11Z,14Z,17Z)- OH(5))'	HMDB02 61884	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}-2-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/20:0y'	HMDB02 61885	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(11Z)-icos-11-enoyloxy}-2-{{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl}oxy}propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:3(5Z,8Z,11Z)- O(14R,15S))'	HMDB02 61918	C45H80NO9P	
	809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(11Z)-icos-11-enoyloxy}-3-{{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl}oxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)- O(14R,15S)/20:1(11Z))'	HMDB02 61919	C45H80NO9P	

		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[[[(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyl]oxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:3(5Z,8Z,14Z)- O(11S,12R))'	HMDB02 61920	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[[[(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyl]oxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,14Z)- O(11S,12R)/20:1(11Z))'	HMDB02 61921	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[[[(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl]oxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:3(5Z,11Z,14Z)- O(8,9))'	HMDB02 61922	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[[[(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl]oxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,11Z,14Z)- O(8,9)/20:1(11Z))'	HMDB02 61923	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl]oxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:3(8Z,11Z,14Z)- O(5,6))'	HMDB02 61924	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl]oxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)- O(5,6)/20:1(11Z))'	HMDB02 61925	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[[[(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(5Z,8Z,11Z,14Z)- OH(20))'	HMDB02 61926	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[[[(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(20)/20:1(11Z))'	HMDB02 61927	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[[[(5R,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(6E,8Z,11Z,14Z)- OH(5S))'	HMDB02 61928	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[[[(5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)- OH(5S)/20:1(11Z))'	HMDB02 61929	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[[[(5Z,8Z,11Z,14Z,19S)-19-hydroxyicosa-5,8,11,14-tetraenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(5Z,8Z,11Z,14Z)- OH(19S))'	HMDB02 61930	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[[[(5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(19S)/20:1(11Z))'	HMDB02 61931	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[[[(5Z,8Z,11Z,14Z,18R)-18-hydroxyicosa-5,8,11,14-tetraenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(5Z,8Z,11Z,14Z)- OH(18R))'	HMDB02 61932	C45H80NO9P	

		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,8Z,11Z,14Z,18S)-18-hydroxyicos-5,8,11,14-tetraenyl}oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(18R)/20:1(11Z))'	HMDB02 61933	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,8Z,11Z,14Z)-17-hydroxyicos-5,8,11,14-tetraenyl}oxy}-3-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:1(11Z)/20:4(5Z,8Z,11Z,14Z)- OH(17))'	HMDB02 61934	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,8Z,11Z,14Z)-17-hydroxyicos-5,8,11,14-tetraenyl}oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(17)/20:1(11Z))'	HMDB02 61935	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,8Z,11Z,14Z,16R)-16-hydroxyicos-5,8,11,14-tetraenyl}oxy}-3-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:1(11Z)/20:4(5Z,8Z,11Z,14Z)- OH(16R))'	HMDB02 61936	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,8Z,11Z,14Z,16S)-16-hydroxyicos-5,8,11,14-tetraenyl}oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(16R)/20:1(11Z))'	HMDB02 61937	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,8Z,11Z,13E,15S)-15-hydroxyicos-5,8,11,13-tetraenyl}oxy}-3-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:1(11Z)/20:4(5Z,8Z,11Z,13E)- OH(15S))'	HMDB02 61938	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,8Z,11Z,13E,15R)-15-hydroxyicos-5,8,11,13-tetraenyl}oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)- OH(15S)/20:1(11Z))'	HMDB02 61939	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,8Z,10E,12S,14Z)-12-hydroxyicos-5,8,10,14-tetraenyl}oxy}-3-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:1(11Z)/20:4(5Z,8Z,10E,14Z)- OH(12S))'	HMDB02 61940	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,8Z,10E,12R,14Z)-12-hydroxyicos-5,8,10,14-tetraenyl}oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:4(5Z,8Z,10E,14Z)- OH(12S)/20:1(11Z))'	HMDB02 61941	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5E,8Z,11R,12Z,14Z)-11-hydroxyicos-5,8,12,14-tetraenyl}oxy}-3-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:1(11Z)/20:4(5E,8Z,12Z,14Z)- OH(11R))'	HMDB02 61942	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5E,8Z,11S,12Z,14Z)-11-hydroxyicos-5,8,12,14-tetraenyl}oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:4(5E,8Z,12Z,14Z)- OH(11R)/20:1(11Z))'	HMDB02 61943	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{{(5E,7Z,11Z,14Z)-9-hydroxyicos-5,7,11,14-tetraenyl}oxy}-3-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:1(11Z)/20:4(5Z,7E,11Z,14Z)- OH(9))'	HMDB02 61944	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{{(5E,7Z,11Z,14Z)-9-hydroxyicos-5,7,11,14-tetraenyl}oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy}phosphinic acid'	b'PE(20:4(5Z,7E,11Z,14Z)- OH(9)/20:1(11Z))'	HMDB02 61945	C45H80NO9P	

		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl}oxy}-3-[(11Z,14Z)-icosa-11,14-dienoyl}oxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:3(6,8,11)-OH(5))'	HMDB02 62124	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl}oxy}-2-[(11Z,14Z)-icosa-11,14-dienoyl}oxy]propoxy]phosphinic acid'	b'PE(20:3(6,8,11)-OH(5)/20:2(11Z,14Z))'	HMDB02 62125	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyl}oxy]-2-{{(10E,12Z)-9-oxooctadeca-10,12-dienoyl}oxy]propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/18:2(10E,12Z)+=O(9))'	HMDB02 83972	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyl}oxy]-3-{{(10E,12Z)-9-oxooctadeca-10,12-dienoyl}oxy]propoxy]phosphinic acid'	b'PE(18:2(10E,12Z)+=O(9)/22:2(13Z,16Z))'	HMDB02 83973	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyl}oxy]-2-{{(9Z,11E)-13-oxooctadeca-9,11-dienoyl}oxy]propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/18:2(9Z,11E)+=O(13))'	HMDB02 83974	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyl}oxy]-3-{{(9Z,11E)-13-oxooctadeca-9,11-dienoyl}oxy]propoxy]phosphinic acid'	b'PE(18:2(9Z,11E)+=O(13)/22:2(13Z,16Z))'	HMDB02 83975	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyl}oxy]-2-{{(10E,12E,15E)-9-hydroxyoctadeca-10,12,15-trienoyl}oxy]propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/18:3(10,12,15)-OH(9))'	HMDB02 84010	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyl}oxy]-3-{{(10E,12E,15E)-9-hydroxyoctadeca-10,12,15-trienoyl}oxy]propoxy]phosphinic acid'	b'PE(18:3(10,12,15)-OH(9)/22:2(13Z,16Z))'	HMDB02 84011	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyl}oxy]-2-{{(9E,11E,15E)-13-hydroxyoctadeca-9,11,15-trienoyl}oxy]propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/18:3(9,11,15)-OH(13))'	HMDB02 84012	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyl}oxy]-3-{{(9E,11E,15E)-13-hydroxyoctadeca-9,11,15-trienoyl}oxy]propoxy]phosphinic acid'	b'PE(18:3(9,11,15)-OH(13)/22:2(13Z,16Z))'	HMDB02 84013	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-{{(2R)-3-(heptadecanoyl}oxy)-2-{{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy)ethyl)trimethylazanium'	b'PC(17:0/20:4(6E,8Z,11Z,14Z)+=O(5))'	HMDB02 86149	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-{{(2R)-2-(heptadecanoyl}oxy)-3-{{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy)ethyl)trimethylazanium'	b'PC(20:4(6E,8Z,11Z,14Z)+=O(5)/17:0))'	HMDB02 86150	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2-{{(2R)-3-(heptadecanoyl}oxy)-2-{{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl}oxy}propyl phosphono}oxy)ethyl)trimethylazanium'	b'PC(17:0/20:4(5Z,8Z,11Z,13E)+=O(15))'	HMDB02 86151	C45H80NO9P	

		809.5570702	0.0007 298	Proton ation	b'(2- -{[(2R)-2-(heptadecanoyloxy)-3- -{[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,13E)+=O(15)/17:0)	HMDB02 86152	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2- -{[(2R)-3-(heptadecanoyloxy)-2- -{[(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(17:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 86163	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2- -{[(2R)-2-(heptadecanoyloxy)-3- -{[(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/17:0)	HMDB02 86164	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2- -{[(2R)-3-(heptadecanoyloxy)-2- -{[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(17:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	HMDB02 86165	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2- -{[(2R)-2-(heptadecanoyloxy)-3- -{[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:5(5Z,8Z,11Z,14Z,16E)-OH(18)/17:0)	HMDB02 86166	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2- -{[(2R)-3-(heptadecanoyloxy)-2- -{[(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(17:0/20:5(5Z,8Z,10E,14Z,17Z)-OH(12))'	HMDB02 86167	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2- -{[(2R)-2-(heptadecanoyloxy)-3- -{[(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:5(5Z,8Z,10E,14Z,17Z)-OH(12)/17:0)	HMDB02 86168	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2- -{[(2R)-3-(heptadecanoyloxy)-2- -{[(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(17:0/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 86169	C45H80NO9P	
		809.5570702	0.0007 298	Proton ation	b'(2- -{[(2R)-2-(heptadecanoyloxy)-3- -{[(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/17:0)	HMDB02 86170	C45H80NO9P	
3 3 3	820.52 35	820.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(11Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB00 10629	C46H77O10P	
		820.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB00 10644	C46H77O10P	
		820.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(18:2(9Z,12Z)/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB00 10657	C46H77O10P	
		820.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(18:2(9Z,12Z)/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB00 10658	C46H77O10P	

		820.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphinic acid'	b'PG(18:3(6Z,9Z,12Z)/22:4(7Z,10Z,13Z,16Z))'	HMDB00 10671	C46H77O10P	
		820.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphinic acid'	b'PG(18:3(9Z,12Z,15Z)/22:4(7Z,10Z,13Z,16Z))'	HMDB00 10686	C46H77O10P	
		820.5254357	0.0019 357	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy]phosphinic acid'	b'PG(20:4(5Z,8Z,11Z,14Z)/20:3(5Z,8Z,11Z))'	HMDB01 16587	C46H77O10P	
		820.5254357	0.0019 357	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphinic acid'	b'PG(20:4(5Z,8Z,11Z,14Z)/20:3(8Z,11Z,14Z))'	HMDB01 16588	C46H77O10P	
		820.5254357	0.0019 357	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(8Z,11Z,14Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]phosphinic acid'	b'PG(20:4(8Z,11Z,14Z,17Z)/20:3(5Z,8Z,11Z,14Z))'	HMDB01 16594	C46H77O10P	
		820.5254357	0.0019 357	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphinic acid'	b'PG(20:4(8Z,11Z,14Z,17Z)/20:3(8Z,11Z,14Z))'	HMDB01 16595	C46H77O10P	
		820.5254357	0.0019 357	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(22:5(4Z,7Z,10Z,13Z,16Z)/18:2(9Z,12Z))'	HMDB01 16598	C46H77O10P	
		820.5254357	0.0019 357	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(22:5(7Z,10Z,13Z,16Z,19Z)/18:2(9Z,12Z))'	HMDB01 16599	C46H77O10P	
		820.5254357	0.0019 357	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(11Z))'	HMDB01 16632	C46H77O10P	
		820.5254357	0.0019 357	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:1(9Z))'	HMDB01 16633	C46H77O10P	
3	821.54 36	821.541814	0.0017 86	Redox	b'(2S)-2-amino-3-({[(2R)-2-[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-3-(octadecanoyloxy)propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(18:0/18:1(12Z)-2OH(9,10))'	HMDB02 81372	C42H80NO12P	
4		821.541814	0.0017 86	Redox	b'(2S)-2-amino-3-({[(2R)-3-[(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-2-(octadecanoyloxy)propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(18:1(12Z)-2OH(9,10)/18:0)'	HMDB02 81373	C42H80NO12P	
3 3	822.53 83	822.5410853	0.0027 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB00 10614	C46H79O10P	

5	822.5410853	0.0027 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB00 10627	C46H79O10P	
	822.5410853	0.0027 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(11Z)/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB00 10628	C46H79O10P	
	822.5410853	0.0027 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB00 10642	C46H79O10P	
	822.5410853	0.0027 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB00 10643	C46H79O10P	
	822.5410853	0.0027 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(18:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z))'	HMDB00 10656	C46H79O10P	
	822.5410857	0.0027 857	Redox	b'[(2R)-2,3-bis[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(20:3(5Z,8Z,11Z)/20:3(5Z,8Z,11Z))'	HMDB01 16579	C46H79O10P	
	822.5410857	0.0027 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphinic acid'	b'PG(20:3(5Z,8Z,11Z)/20:3(8Z,11Z,14Z))'	HMDB01 16580	C46H79O10P	
	822.5410857	0.0027 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphinic acid'	b'PG(20:3(8Z,11Z,14Z)/20:3(5Z,8Z,11Z))'	HMDB01 16582	C46H79O10P	
	822.5410857	0.0027 857	Redox	b'[(2R)-2,3-bis[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(20:3(8Z,11Z,14Z)/20:3(8Z,11Z,14Z))'	HMDB01 16583	C46H79O10P	
	822.5410857	0.0027 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]phosphinic acid'	b'PG(20:4(5Z,8Z,11Z,14Z)/20:2(11Z,14Z))'	HMDB01 16586	C46H79O10P	
	822.5410857	0.0027 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]phosphinic acid'	b'PG(20:4(8Z,11Z,14Z,17Z)/20:2(11Z,14Z))'	HMDB01 16593	C46H79O10P	
	822.5410857	0.0027 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(22:5(4Z,7Z,10Z,13Z,16Z)/18:1(11Z))'	HMDB01 16616	C46H79O10P	
	822.5410857	0.0027 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(22:5(4Z,7Z,10Z,13Z,16Z)/18:1(9Z))'	HMDB01 16617	C46H79O10P	

		822.5410857	0.0027 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PG(22:5(7Z,10Z,13Z,16Z,19Z)/18:1(11Z))'	HMDB01 16624	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PG(22:5(7Z,10Z,13Z,16Z,19Z)/18:1(9Z))'	HMDB01 16625	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0)	HMDB01 16630	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-2-3-[(5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyloxy]-3-(henicosanoyloxy)propoxy]phosphonic acid'	b'PA(21:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S))'	HMDB02 65515	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-2-3-[(5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyloxy]-2-(henicosanoyloxy)propoxy]phosphonic acid'	b'PA(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/21:0)	HMDB02 65516	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-2-3-[(4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyloxy]-3-(henicosanoyloxy)propoxy]phosphonic acid'	b'PA(21:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17))'	HMDB02 65530	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-2-3-[(4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyloxy]-2-(henicosanoyloxy)propoxy]phosphonic acid'	b'PA(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/21:0)	HMDB02 65531	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-2-3-[(5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyloxy]-3-[(18-methylcosanoyloxy)propoxy]phosphonic acid'	b'PA(a-21:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S))'	HMDB02 67175	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-2-3-[(5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyloxy]-2-[(18-methylcosanoyloxy)propoxy]phosphonic acid'	b'PA(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/a-21:0)	HMDB02 67176	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-2-3-[(4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyloxy]-3-[(18-methylcosanoyloxy)propoxy]phosphonic acid'	b'PA(a-21:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17))'	HMDB02 67191	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-2-3-[(4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyloxy]-2-[(18-methylcosanoyloxy)propoxy]phosphonic acid'	b'PA(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/a-21:0)	HMDB02 67192	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-2-3-[(5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyloxy]-3-[(19-methylcosanoyloxy)propoxy]phosphonic acid'	b'PA(i-21:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-	HMDB02 68314	C46H79O10P	

						2OH(7S, 17S))'			
		822.5410857	0.0027 857	Redox	b'[(2R)-3-{{(5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-2-[(19-methylicosanoyl)oxy]propoxy]phosphonic acid'	b'PA(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S))i-21:0)'	HMDB02 68315	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-2-{{(4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl}oxy}-3-[(19-methylicosanoyl)oxy]propoxy]phosphonic acid'	b'PA(i- 21:0/22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17))'	HMDB02 68330	C46H79O10P	
		822.5410857	0.0027 857	Redox	b'[(2R)-3-{{(4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl}oxy}-2-[(19-methylicosanoyl)oxy]propoxy]phosphonic acid'	b'PA(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17))i-21:0)'	HMDB02 68331	C46H79O10P	
3 3 6	823.54 86	824.5567353	0.0003 353	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyl]oxy]-3-(octadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(18:0/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB00 10612	C46H81O10P	
		824.5567353	0.0003 353	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyl]oxy]-3-(octadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(18:0/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB00 10613	C46H81O10P	
		824.5567353	0.0003 353	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyl]oxy]-3-[(11Z)-octadec-11-enoyl]oxy]propoxy]phosphinic acid'	b'PG(18:1(11Z)/22:4(7Z,10Z,13Z,16Z) y'	HMDB00 10626	C46H81O10P	
		824.5567353	0.0003 353	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyl]oxy]-3-[(9Z)-octadec-9-enoyl]oxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)/22:4(7Z,10Z,13Z,16Z))'	HMDB00 10641	C46H81O10P	
		824.5567358	0.0003 358	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(11Z)-icos-11-enoyl]oxy]-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyl]oxy]propoxy]phosphinic acid'	b'PG(20:4(5Z,8Z,11Z,14Z)/20:1(11Z))'	HMDB01 16585	C46H81O10P	
		824.5567358	0.0003 358	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(11Z)-icos-11-enoyl]oxy]-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyl]oxy]propoxy]phosphinic acid'	b'PG(20:4(8Z,11Z,14Z,17Z)/20:1(11Z) y'	HMDB01 16592	C46H81O10P	
		824.5567358	0.0003 358	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyl]oxy]-2-(octadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(22:5(4Z,7Z,10Z,13Z,16Z)/18:0)'	HMDB01 16614	C46H81O10P	
		824.5567358	0.0003 358	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyl]oxy]-2-(octadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(22:5(7Z,10Z,13Z,16Z,19Z)/18:0)'	HMDB01 16622	C46H81O10P	
3 3	825.55 02	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)((2R)-2-{{(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl}oxy}-3-(icosanoyl)oxy]propoxy]phosphinic acid'	b'PE(20:0/PGJ2)'	HMDB02 61850	C45H80NO10P	

7	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-3-[[[(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy]-2-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(PGJ2/20:0)'	HMDB02 61851	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-2-[[[(5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(6Z,8E,10E,14Z)- 2OH(5S,12R))'	HMDB02 61958	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-3-[[[(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6Z,8E,10E,14Z)- 2OH(5S,12R)/20:1(11Z))'	HMDB02 61959	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-2-[[[(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(6E,8Z,11Z,13E)- 2OH(5S,15S))'	HMDB02 61994	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-3-[[[(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/20:1(11Z))'	HMDB02 61995	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-2-[[[(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R))'	HMDB02 61996	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-3-[[[(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/20:1(11Z))'	HMDB02 61997	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-2-[[[(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl]oxy]-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:3(8Z,11Z,14Z)- 2OH(5,6))'	HMDB02 62068	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-3-[[[(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl]oxy]-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)- 2OH(5,6)/20:2(11Z,14Z))'	HMDB02 62069	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-2-[[[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]propoxy]phosphinic acid'	b'PE(22:4(7Z,10Z,13Z,16Z)/18:1(12Z)- 2OH(9,10))'	HMDB02 84080	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-3-[[[(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]propoxy]phosphinic acid'	b'PE(18:1(12Z)- 2OH(9,10)/22:4(7Z,10Z,13Z,16Z))'	HMDB02 84081	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-3-[[[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy]-2-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphinic acid'	b'PE(DiMe(11,5)/18:1(12Z)- O(9S,10R))'	HMDB02 84810	C45H80NO10P	
	825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-2-[[[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy]-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphinic acid'	b'PE(18:1(12Z)- O(9S,10R)/DiMe(11,5))'	HMDB02 84811	C45H80NO10P	

3 3 8		825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-3-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-2-{{(9Z)-11-(3-pentoxiran-2-yl)undec-9-enoyl}oxy}propoxy]phosphinic acid'	b'PE(DiMe(11,5)/18:1(9Z)-O(12,13))'	HMDB02 84812	C45H80NO10P	
		825.5519848	0.0017 848	Redox	b'(2-aminoethoxy)[(2R)-2-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-3-{{(9Z)-11-(3-pentoxiran-2-yl)undec-9-enoyl}oxy}propoxy]phosphinic acid'	b'PE(18:1(9Z)-O(12,13)/DiMe(11,5))'	HMDB02 84813	C45H80NO10P	
		825.5519848	0.0017 848	Redox	b'(2-{{(2R)-3-(heptadecanoyloxy)-2-{{(5Z)-7-{{(1S,5R)-3-hydroxyoct-1-en-1-yl}}-4-oxocyclopent-2-en-1-yl}hept-5-enoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(17:0/PGJ2)'	HMDB02 86135	C45H80NO10P	
		825.5519848	0.0017 848	Redox	b'(2-{{(2R)-2-(heptadecanoyloxy)-3-{{(5Z)-7-{{(1S,5R)-3-hydroxyoct-1-en-1-yl}}-4-oxocyclopent-2-en-1-yl}hept-5-enoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(PGJ2/17:0)'	HMDB02 86136	C45H80NO10P	
	832.55 14	833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}-3-{{(11Z)-icos-11-enoyloxy}propoxy]phosphinic acid'	b'PE(20:1(11Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 61998	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}-2-{{(11Z)-icos-11-enoyloxy}propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/20:1(11Z))'	HMDB02 61999	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}-3-{{(11Z)-icos-11-enoyloxy}propoxy]phosphinic acid'	b'PE(20:1(11Z)/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 62000	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}-2-{{(11Z)-icos-11-enoyloxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/20:1(11Z))'	HMDB02 62001	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy}-3-{{(11Z)-icos-11-enoyloxy}propoxy]phosphinic acid'	b'PE(20:1(11Z)/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 62002	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy}-2-{{(11Z)-icos-11-enoyloxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/20:1(11Z))'	HMDB02 62003	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy}-3-{{(11Z)-icos-11-enoyloxy}propoxy]phosphinic acid'	b'PE(20:1(11Z)/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 62004	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy}-2-{{(11Z)-icos-11-enoyloxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/20:1(11Z))'	HMDB02 62005	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(11Z)-icos-11-enoyloxy}-2-{{(4Z,7Z,10Z,13Z)-15-{{3-{{(2Z)-pent-2-en-1-yl}oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl}oxy}propoxy]phosphinic acid'	b'PE(20:1(11Z)/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 62008	C47H80NO9P	

		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-2-((11Z)-icos-11-enyloxy)-3-(((4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl)oxy)propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)20:1(11Z))'	HMDB02 62009	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienyloxy)-2-(((6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(6E,8Z,11Z,1 4Z)+=O(5))'	HMDB02 83968	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienyloxy)-3-(((6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl)oxy)propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)+=O(5)/22:2 (13Z,16Z))'	HMDB02 83969	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienyloxy)-2-(((5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(5Z,8Z,11Z,1 3E)+=O(15))'	HMDB02 83970	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienyloxy)-3-(((5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl)oxy)propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)+=O(15)/22: 2(13Z,16Z))'	HMDB02 83971	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienyloxy)-2-(((5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:5(5Z,8Z,11Z,1 4Z,16E)-OH(18R))'	HMDB02 83982	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienyloxy)-3-(((5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl)oxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/22:2(13Z,16Z))'	HMDB02 83983	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienyloxy)-2-(((5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:5(5Z,8Z,11Z,1 4Z,16E)-OH(18))'	HMDB02 83984	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienyloxy)-3-(((5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl)oxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/22:2(13Z,16Z))'	HMDB02 83985	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienyloxy)-2-(((5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:5(5Z,8Z,10E,1 4Z,17Z)-OH(12))'	HMDB02 83986	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienyloxy)-3-(((5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl)oxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/22:2(13Z,16Z))'	HMDB02 83987	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienyloxy)-2-(((6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:5(6E,8Z,11Z,1 4Z,17Z)-OH(5))'	HMDB02 83988	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienyloxy)-3-(((6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl)oxy)propoxy]phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/22:2(13Z,16Z))'	HMDB02 83989	C47H80NO9P	

3 3 9		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-[[[(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl]oxy]propoxy]phosphinic acid'	b'PE(22:4(7Z,10Z,13Z,16Z)/20:3(6,8,11)-OH(5))'	HMDB02 84124	C47H80NO9P	
		833.5570702	0.0021 298	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-[[[(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl]oxy]propoxy]phosphinic acid'	b'PE(20:3(6,8,11)-OH(5)/22:4(7Z,10Z,13Z,16Z))'	HMDB02 84125	C47H80NO9P	
	834.52 69	835.5363342	0.0016 342	Proton ation	b'(2S)-2-amino-3-([[(2R)-2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-(octadecanoyloxy)propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(18:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB00 10167	C46H78NO10P	C02 737
		835.5363342	0.0016 342	Proton ation	b'(2S)-2-amino-3-([[(2R)-2,3-bis[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(20:3(8Z,11Z,14Z)/20:3(8Z,11Z,14Z))'	HMDB00 12426	C46H78NO10P	
		835.5363342	0.0016 342	Proton ation	b'(2S)-2-amino-3-([[(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-(octadecanoyloxy)propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/18:0))'	HMDB00 12444	C46H78NO10P	
		835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-([[(2R)-2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(18:1(11Z)/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB01 12404	C46H78NO10P	
		835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-([[(2R)-2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(18:1(11Z)/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB01 12405	C46H78NO10P	
		835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-([[(2R)-2-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(18:1(9Z)/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB01 12421	C46H78NO10P	
		835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-([[(2R)-2-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(18:1(9Z)/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB01 12422	C46H78NO10P	
		835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-([[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(18:2(9Z,12Z)/22:4(7Z,10Z,13Z,16Z))'	HMDB01 12438	C46H78NO10P	
		835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-([[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(18:4(6Z,9Z,12Z,15Z)/22:2(13Z,16Z))'	HMDB01 12505	C46H78NO10P	
		835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-([hydroxy[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]propoxy]phosphoryl]oxy)propanoic acid'	b'PS(20:1(11Z)/20:5(5Z,8Z,11Z,14Z,17Z))'	HMDB01 12557	C46H78NO10P	
		835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-([hydroxy[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]phosphoryl]oxy)propanoic acid'	b'PS(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14Z))'	HMDB01 12583	C46H78NO10P	

835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({hydroxy[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(8Z,11Z,14Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:2(11Z,14Z)/20:4(8Z,11Z,14Z,17Z))'	HMDB01 12584	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({[(2R)-2,3-bis[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:3(5Z,8Z,11Z)/20:3(5Z,8Z,11Z))'	HMDB01 12608	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({hydroxy[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:3(5Z,8Z,11Z)/20:3(8Z,11Z,14Z))'	HMDB01 12609	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({hydroxy[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:3(8Z,11Z,14Z)/20:3(5Z,8Z,11Z))'	HMDB01 12628	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({hydroxy[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:4(5Z,8Z,11Z,14Z)/20:2(11Z,14Z))'	HMDB01 12642	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({hydroxy[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(8Z,11Z,14Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:4(8Z,11Z,14Z,17Z)/20:2(11Z,14Z))'	HMDB01 12667	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({hydroxy[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:5(5Z,8Z,11Z,14Z,17Z)/20:1(11Z))'	HMDB01 12691	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:2(13Z,16Z)/18:4(6Z,9Z,12Z,15Z))'	HMDB01 12772	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:4(7Z,10Z,13Z,16Z)/18:2(9Z,12Z))'	HMDB01 12796	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({[(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:5(4Z,7Z,10Z,13Z,16Z)/18:1(11Z))'	HMDB01 12820	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({[(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:5(4Z,7Z,10Z,13Z,16Z)/18:1(9Z))'	HMDB01 12821	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({[(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:5(7Z,10Z,13Z,16Z,19Z)/18:1(11Z))'	HMDB01 12845	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2S)-2-amino-3-({[(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:5(7Z,10Z,13Z,16Z,19Z)/18:1(9Z))'	HMDB01 12846	C46H78NO10P	

835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[(5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl]oxy}-3-[(9Z)-hexadec-9-enoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(16:1(9Z)/22:6(5Z,8E,10Z,13Z,15 E,19Z)-2OH(7S, 17S))'	HMDB02 86067	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{[(5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl]oxy}-2-[(9Z)-hexadec-9-enoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S)/16:1(9Z))'	HMDB02 86068	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[(4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl]oxy}-3-[(9Z)-hexadec-9-enoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(16:1(9Z)/22:6(4Z,7Z,11E,13Z,15 E,19Z)-2OH(10S,17))'	HMDB02 86083	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{[(4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl]oxy}-2-[(9Z)-hexadec-9-enoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/16:1(9Z))'	HMDB02 86084	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(18:2(9Z,12Z)PGJ2)'	HMDB02 86550	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{[(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(PGJ2/18:2(9Z,12Z))'	HMDB02 86551	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[(5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxydocosa-6,8,10,14-tetraenoyl]oxy}-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(18:3(6Z,9Z,12Z)/20:4(6Z,8E,10E, 14Z)-2OH(5S,12R))'	HMDB02 86658	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{[(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxydocosa-6,8,10,14-tetraenoyl]oxy}-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(6Z,8E,10E,14Z)- 2OH(5S,12R)/18:3(6Z,9Z,12Z))'	HMDB02 86659	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[(5S,6E,8Z,11Z,13E,15S)-5,15-dihydroxydocosa-6,8,11,13-tetraenoyl]oxy}-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(18:3(6Z,9Z,12Z)/20:4(6E,8Z,11Z, 13E)-2OH(5S,15S))'	HMDB02 86694	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{[(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxydocosa-6,8,11,13-tetraenoyl]oxy}-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/18:3(6Z,9Z,12Z))'	HMDB02 86695	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxydocosa-8,11,14,17-tetraenoyl]oxy}-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(18:3(6Z,9Z,12Z)/20:4(8Z,11Z,14 Z,17Z)-2OH(5S,6R))'	HMDB02 86696	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{[(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxydocosa-8,11,14,17-tetraenoyl]oxy}-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/18:3(6Z,9Z,12Z))'	HMDB02 86697	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[(5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxydocosa-6,8,10,14-tetraenoyl]oxy}-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(18:3(9Z,12Z,15Z)/20:4(6Z,8E,10 E,14Z)-2OH(5S,12R))'	HMDB02 86762	C46H78NO10P	

835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl]oxy}-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(6Z,8E,10E,14Z)- 2OH(5S,12R)/18:3(9Z,12Z,15Z))'	HMDB02 86763	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy}-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(18:3(9Z,12Z,15Z)/20:4(6E,8Z,11 Z,13E)-2OH(5S,15S))'	HMDB02 86798	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy}-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/18:3(9Z,12Z,15Z))'	HMDB02 86799	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy}-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(18:3(9Z,12Z,15Z)/20:4(8Z,11Z,1 4Z,17Z)-2OH(5S,6R))'	HMDB02 86800	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy}-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/18:3(9Z,12Z,15Z))'	HMDB02 86801	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl]oxy}-3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(18:4(6Z,9Z,12Z,15Z)/20:3(8Z,11 Z,14Z)-2OH(5,6))'	HMDB02 86872	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl]oxy}-2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:3(8Z,11Z,14Z)- 2OH(5,6)/18:4(6Z,9Z,12Z,15Z))'	HMDB02 86873	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-2- -{[(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienoyl]oxy}propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:3(5Z,8Z,11Z)- O(14R,15S))'	HMDB02 89213	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3- -{[(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienoyl]oxy}propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:3(5Z,8Z,11Z)- O(14R,15S)/DiMe(9,3))'	HMDB02 89214	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-2- -{[(5Z,8Z)-10- -{3-(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyl]oxy}propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:3(5Z,8Z,14Z)- O(11S,12R))'	HMDB02 89215	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3- -{[(5Z,8Z)-10- -{3-(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyl]oxy}propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:3(5Z,8Z,14Z)- O(11S,12R)/DiMe(9,3))'	HMDB02 89216	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-3- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-2- -{[(5Z)-7- -{3-(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl]oxy}propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:3(5Z,11Z,14Z)- O(8,9))'	HMDB02 89217	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-3- -{[(5Z)-7- -{3-(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl]oxy}propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:3(5Z,11Z,14Z)- O(8,9)/DiMe(9,3))'	HMDB02 89218	C46H78NO10P	

835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-2-{{4-{{3-{{(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl}oxiran-2-yl}butanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:3(8Z,11Z,14Z)- O(5,6))'	HMDB02 89219	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-{{4-{{3-{{(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl}oxiran-2-yl}butanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:3(8Z,11Z,14Z)- O(5,6)/DiMe(9,3))'	HMDB02 89220	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-2-:{{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:4(5Z,8Z,11Z,14Z)- OH(20))'	HMDB02 89221	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-2-:{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-:{{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)- OH(20)/DiMe(9,3))'	HMDB02 89222	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-2-:{{(5R,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:4(6E,8Z,11Z,14Z)- OH(5S))'	HMDB02 89223	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-:{{(5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:4(6E,8Z,11Z,14Z)- OH(5S)/DiMe(9,3))'	HMDB02 89224	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-2-:{{(5Z,8Z,11Z,14Z,19S)-19-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:4(5Z,8Z,11Z,14Z)- OH(19S))'	HMDB02 89225	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-:{{(5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)- OH(19S)/DiMe(9,3))'	HMDB02 89226	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-2-:{{(5Z,8Z,11Z,14Z,18R)-18-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:4(5Z,8Z,11Z,14Z)- OH(18R))'	HMDB02 89227	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-:{{(5Z,8Z,11Z,14Z,18S)-18-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)- OH(18R)/DiMe(9,3))'	HMDB02 89228	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-2-:{{(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:4(5Z,8Z,11Z,14Z)- OH(17))'	HMDB02 89229	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-:{{(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)- OH(17)/DiMe(9,3))'	HMDB02 89230	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2-:{{(2R)-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-2-:{{(5Z,8Z,11Z,14Z,16R)-16-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:4(5Z,8Z,11Z,14Z)- OH(16R))'	HMDB02 89231	C46H78NO10P	

835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -3- -{[(5Z,8Z,11Z,14Z,16S)-16-hydroxyicos-5,8,11,14-tetraenoyl]oxy} propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)- OH(16R)/DiMe(9,3))'	HMDB02 89232	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -2- -{[(5Z,8Z,11Z,13E,15S)-15-hydroxyicos-5,8,11,13-tetraenoyl]oxy} propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:4(5Z,8Z,11Z,13E)- OH(15S))'	HMDB02 89233	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -3- -{[(5Z,8Z,11Z,13E,15R)-15-hydroxyicos-5,8,11,13-tetraenoyl]oxy} propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,13E)- OH(15S)/DiMe(9,3))'	HMDB02 89234	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -2- -{[(5Z,8Z,10E,12S,14Z)-12-hydroxyicos-5,8,10,14-tetraenoyl]oxy} propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:4(5Z,8Z,10E,14Z)- OH(12S))'	HMDB02 89235	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -3- -{[(5Z,8Z,10E,12R,14Z)-12-hydroxyicos-5,8,10,14-tetraenoyl]oxy} propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,10E,14Z)- OH(12S)/DiMe(9,3))'	HMDB02 89236	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -2- -{[(5Z,8Z,11R,12Z,14Z)-11-hydroxyicos-5,8,12,14-tetraenoyl]oxy} propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:4(5E,8Z,12Z,14Z)- OH(11R))'	HMDB02 89237	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -3- -{[(5E,8Z,11S,12Z,14Z)-11-hydroxyicos-5,8,12,14-tetraenoyl]oxy} propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(5E,8Z,12Z,14Z)- OH(11R)/DiMe(9,3))'	HMDB02 89238	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -2- -{[(5E,7Z,11Z,14Z)-9-hydroxyicos-5,7,11,14-tetraenoyl]oxy} propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(DiMe(9,3)/20:4(5Z,7E,11Z,14Z)- OH(9))'	HMDB02 89239	C46H78NO10P	
835.5363347	0.0016 347	Proton ation	b'(2- -{[(2R)-2- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy} -3- -{[(5E,7Z,11Z,14Z)-9-hydroxyicos-5,7,11,14-tetraenoyl]oxy} propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(5Z,7E,11Z,14Z)- OH(9)/DiMe(9,3))'	HMDB02 89240	C46H78NO10P	
834.5258296	0.0010 704	Redox	b'[(2R)-3-(hexadecanoyloxy)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]([[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy])phosphinic acid'	b'PI(16:0/18:2(9Z,12Z))'	HMDB00 09784	C43H79O13P	
834.5258291	0.0010 709	Redox	b'[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]([[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy])phosphinic acid'	b'PI(16:1(9Z)/18:1(11Z))'	HMDB00 09800	C43H79O13P	
834.5258291	0.0010 709	Redox	b'[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]([[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy])phosphinic acid'	b'PI(16:1(9Z)/18:1(9Z))'	HMDB00 09801	C43H79O13P	C00 626
834.5258291	0.0010 709	Redox	b'[(2R)-3-[(9Z,12Z)-hexadeca-9,12-dienoyloxy]-2-(octadecanoyloxy)propoxy]([[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy])phosphinic acid'	b'PI(16:2(9Z,12Z)/18:0)	HMDB00 09803	C43H79O13P	

		834.5258291	0.0010 709	Redox	b'[(2R)-2-[(9Z,12Z)-hexadeca-9,12-dienyloxy]-3-(octadecanoyloxy)propoxy]({[(1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:0/16:2(9Z,12Z))'	HMDB00 09807	C43H79O13P	
		834.5258291	0.0010 709	Redox	b'[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]({[(1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(11Z)/16:1(9Z))'	HMDB00 09823	C43H79O13P	
		834.5258291	0.0010 709	Redox	b'[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]({[(1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(9Z)/16:1(9Z))'	HMDB00 09835	C43H79O13P	
		834.5258291	0.0010 709	Redox	b'[(2R)-2-(hexadecanoyloxy)-3-[(9Z,12Z)-octadeca-9,12-dienyloxy]propoxy]({[(1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:2(9Z,12Z)/16:0)'	HMDB00 09846	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2R)-2-[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl]oxy]-3-[(14-methylhexadecanoyl)oxy]propoxy]((2S)-2,3-dihydroxypropoxy)phosphinic acid'	b'PG(a-17:0/PGF2alpha)'	HMDB02 70768	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2R)-3-[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl]oxy]-2-[(14-methylhexadecanoyl)oxy]propoxy]((2S)-2,3-dihydroxypropoxy)phosphinic acid'	b'PG(PGF2alpha/a-17:0)'	HMDB02 70769	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-2-[(7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl)oxy)-3-[(14-methylhexadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(a-17:0/PGE1)'	HMDB02 70829	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-3-[(7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl)oxy)-2-[(14-methylhexadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(PGE1/a-17:0)'	HMDB02 70830	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-2-[(7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl)oxy)-3-[(14-methylhexadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(a-17:0/PGD1)'	HMDB02 70831	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-3-[(7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl)oxy)-2-[(14-methylhexadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(PGD1/a-17:0)'	HMDB02 70832	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2R)-2-[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl]oxy]-3-[(15-methylhexadecanoyl)oxy]propoxy]((2S)-2,3-dihydroxypropoxy)phosphinic acid'	b'PG(i-17:0/PGF2alpha)'	HMDB02 71598	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2R)-3-[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl]oxy]-2-[(15-methylhexadecanoyl)oxy]propoxy]((2S)-2,3-dihydroxypropoxy)phosphinic acid'	b'PG(PGF2alpha/i-17:0)'	HMDB02 71599	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-2-[(7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl)oxy)-3-[(15-methylhexadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(i-17:0/PGE1)'	HMDB02 71660	C43H79O13P	

3 4 0	836.58	834.5258296	0.0010 704	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-({7-[(1R,2R,3R)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-2-[(1S-methylhexadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(PGE1/i-17:0)	HMDB02 71661	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-3-[(1S-methylhexadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(i-17:0/PGD1)	HMDB02 71662	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-2-[(1S-methylhexadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(PGD1/i-17:0)	HMDB02 71663	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2R)-2-({[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy)-3-[(17-methyloctadecanoyl)oxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(i-19:0/5-iso PGF2VI)	HMDB02 71820	C43H79O13P	
		834.5258296	0.0010 704	Redox	b'[(2R)-3-({[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy)-2-[(17-methyloctadecanoyl)oxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(5-iso PGF2VI/i-19:0)	HMDB02 71821	C43H79O13P	
	24	837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-({[(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:0/20:4(6E,8Z,11Z,14Z)+=O(5))	HMDB02 83760	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-({[(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)+=O(5)/22:0)	HMDB02 83761	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-({[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:0/20:4(5Z,8Z,11Z,13E)+=O(1 5))'	HMDB02 83762	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-({[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)+=O(15)/22: 0)	HMDB02 83763	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-({[(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenyl]oxy}propoxy]phosphinic acid'	b'PE(22:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R))'	HMDB02 83774	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-({[(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl]oxy}propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/22:0)	HMDB02 83775	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-({[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl]oxy}propoxy]phosphinic acid'	b'PE(22:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18))'	HMDB02 83776	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-({[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl]oxy}propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/22:0)	HMDB02 83777	C47H84NO9P	

837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12))'	HMDB02 83778	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/22:0)	HMDB02 83779	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/20:5(6E,8Z,11Z,14Z,17Z)- OH(5))'	HMDB02 83780	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/22:0)	HMDB02 83781	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-{{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl}oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:3(5Z,8Z,11Z)- O(14R,15S))'	HMDB02 83814	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-{{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl}oxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)- O(14R,15S)/22:1(13Z))'	HMDB02 83815	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-{{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienyl}oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:3(5Z,8Z,14Z)- O(11S,12R))'	HMDB02 83816	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-{{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienyl}oxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,14Z)- O(11S,12R)/22:1(13Z))'	HMDB02 83817	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-{{(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl}oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:3(5Z,11Z,14Z)- O(8,9))'	HMDB02 83818	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-{{(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl}oxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,11Z,14Z)- O(8,9)/22:1(13Z))'	HMDB02 83819	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl]oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:3(8Z,11Z,14Z)- O(5,6))'	HMDB02 83820	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl]oxy}propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)- O(5,6)/22:1(13Z))'	HMDB02 83821	C47H84NO9P	
837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-{{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenyl}oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)- OH(20))'	HMDB02 83822	C47H84NO9P	

		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[5Z,8Z,11Z,14Z]-20-hydroxyicosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(20)/22:1(13Z))'	HMDB02 83823	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[5R,6E,8Z,11Z,14Z]-5-hydroxyicosa-6,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(6E,8Z,11Z,14Z)- OH(5S))'	HMDB02 83824	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[5S,6E,8Z,11Z,14Z]-5-hydroxyicosa-6,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)- OH(5S)/22:1(13Z))'	HMDB02 83825	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[5Z,8Z,11Z,14Z,19S]-19-hydroxyicosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)- OH(19S))'	HMDB02 83826	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[5Z,8Z,11Z,14Z,19R]-19-hydroxyicosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(19S)/22:1(13Z))'	HMDB02 83827	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[5Z,8Z,11Z,14Z,18R]-18-hydroxyicosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)- OH(18R))'	HMDB02 83828	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[5Z,8Z,11Z,14Z,18S]-18-hydroxyicosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(18R)/22:1(13Z))'	HMDB02 83829	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[5Z,8Z,11Z,14Z]-17-hydroxyicosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)- OH(17))'	HMDB02 83830	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[5Z,8Z,11Z,14Z]-17-hydroxyicosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(17)/22:1(13Z))'	HMDB02 83831	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[5Z,8Z,11Z,14Z,16R]-16-hydroxyicosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)- OH(16R))'	HMDB02 83832	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[5Z,8Z,11Z,14Z,16S]-16-hydroxyicosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(16R)/22:1(13Z))'	HMDB02 83833	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[5Z,8Z,11Z,13E,15S]-15-hydroxyicosa-5,8,11,13-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,13E)- OH(15S))'	HMDB02 83834	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[5Z,8Z,11Z,13E,15R]-15-hydroxyicosa-5,8,11,13-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)- OH(15S)/22:1(13Z))'	HMDB02 83835	C47H84NO9P	

		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[[(5Z,8Z,10E,12S,14Z)-12-hydroxyicosa-5,8,10,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,10E,14Z)-OH(12S))'	HMDB02 83836	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[[(5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,10E,14Z)-OH(12S)/22:1(13Z))'	HMDB02 83837	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[[(5E,8Z,11R,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5E,8Z,12Z,14Z)-OH(11R))'	HMDB02 83838	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[[(5E,8Z,11S,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5E,8Z,12Z,14Z)-OH(11R)/22:1(13Z))'	HMDB02 83839	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[[(5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,7E,11Z,14Z)-OH(9))'	HMDB02 83840	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[[(5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,7E,11Z,14Z)-OH(9)/22:1(13Z))'	HMDB02 83841	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[[(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:3(6,8,11)-OH(5))'	HMDB02 84020	C47H84NO9P	
		837.5883703	0.0018 297	Proton ation	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[[(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienyl]oxy}propoxy]phosphinic acid'	b'PE(20:3(6,8,11)-OH(5)/22:2(13Z,16Z))'	HMDB02 84021	C47H84NO9P	
3 4 1	847.55 86	847.5574641	0.0011 359	Redox	b'(2S)-2-amino-3-({[(2R)-2-({[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-3-[(11Z)-icos-11-enoyloxy]propoxy](hydroxy)phosphoryl]oxy}propanoic acid'	b'PS(20:1(11Z)/18:1(12Z)-2OH(9,10))'	HMDB02 82203	C44H82NO12P	
		847.5574641	0.0011 359	Redox	b'(2S)-2-amino-3-({[(2R)-3-({[(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy](hydroxy)phosphoryl]oxy}propanoic acid'	b'PS(18:1(12Z)-2OH(9,10)/20:1(11Z))'	HMDB02 82204	C44H82NO12P	
		847.5574641	0.0011 359	Redox	b'(2-({[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]-6-oxoheptanoyl]oxy}-3-(hexadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(16:0/6 keto-PGF1alpha)'	HMDB02 85923	C44H82NO12P	
		847.5574641	0.0011 359	Redox	b'(2-({[(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]-6-oxoheptanoyl]oxy}-2-(hexadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(6 keto-PGF1alpha/16:0)'	HMDB02 85924	C44H82NO12P	
		847.5574641	0.0011 359	Redox	b'(2-({[(2R)-2-({[(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl]oxy}-3-(hexadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(16:0/TXB2)'	HMDB02 85933	C44H82NO12P	

		847.5574641	0.0011 359	Redox	b'(2- -{(2R)-3- -{(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl}oxy}-2-(hexadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(TXB2/16:0)'	HMDB02 85934	C44H82NO12P	
3	849.57 4	849.5731141	0.0008 859	Redox	b'(2S)-2-amino-3- -{(2R)-2- -{(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-3- -{icosanoyloxy}propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:0/18:1(12Z)-2OH(9,10))'	HMDB02 82099	C44H84NO12P	
2		849.5731141	0.0008 859	Redox	b'(2S)-2-amino-3- -{(2R)-3- -{(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-2- -{icosanoyloxy}propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(18:1(12Z)-2OH(9,10)/20:0)'	HMDB02 82100	C44H84NO12P	
3	851.57 92	852.5880359	0.0010 359	Proton ation	b'[(2R)-2- -{(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}-3- -{(2-methyltetracosanoyl)oxy}propoxy]phosphonic acid'	b'PA(a-25:0/PGJ2)'	HMDB02 67243	C48H85O10P	
4		852.5880359	0.0010 359	Proton ation	b'[(2R)-3- -{(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}-2- -{(2-methyltetracosanoyl)oxy}propoxy]phosphonic acid'	b'PA(PGJ2/a-25:0)'	HMDB02 67244	C48H85O10P	
3 4 4	853.58 27	853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)[(2R)-3- -{docosanoyloxy}-3- -{(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}propoxy]phosphinic acid'	b'PE(22:0/PGJ2)'	HMDB02 83746	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)[(2R)-2- -{docosanoyloxy}-3- -{(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}propoxy]phosphinic acid'	b'PE(PGJ2/22:0)'	HMDB02 83747	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)[(2R)-2- -{(5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl]oxy}-3- -{(13Z)-docos-13-enoyloxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(6Z,8E,10E,14Z)- 2OH(5S,12R))'	HMDB02 83854	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)[(2R)-3- -{(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl]oxy}-2- -{(13Z)-docos-13-enoyloxy}propoxy]phosphinic acid'	b'PE(20:4(6Z,8E,10E,14Z)- 2OH(5S,12R)/22:1(13Z))'	HMDB02 83855	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)[(2R)-2- -{(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy}-3- -{(13Z)-docos-13-enoyloxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(6E,8Z,11Z,13E)- 2OH(5S,15S))'	HMDB02 83890	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)[(2R)-3- -{(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy}-2- -{(13Z)-docos-13-enoyloxy}propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/22:1(13Z))'	HMDB02 83891	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)[(2R)-2- -{(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy}-3- -{(13Z)-docos-13-enoyloxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R))'	HMDB02 83892	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)[(2R)-3- -{(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy}-2- -{(13Z)-docos-13-enoyloxy}propoxy]phosphinic acid'	b'PE(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/22:1(13Z))'	HMDB02 83893	C47H84NO10P	

		853.5832849	0.0005 849	Redox		b'PE(22:2(13Z,16Z)/20:3(8Z,11Z,14Z)-2OH(5,6))'	HMDB02 83964	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)((2R)-3-{{(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl}oxy}-2-{{(13Z,16Z)-docosa-13,16-dienoyl}oxy}propoxy]phosphonic acid'	b'PE(20:3(8Z,11Z,14Z)-2OH(5,6)/22:2(13Z,16Z))'	HMDB02 83965	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)((2R)-3-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{(8-{3-{{(2Z)-oct-2-en-1-yl}oxiran-2-yl}octanoyl}oxy}propoxy]phosphonic acid'	b'PE(DiMe(13,5)'18:1(12Z)-O(9S,10R))'	HMDB02 84914	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)((2R)-2-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-{{(8-{3-{{(2Z)-oct-2-en-1-yl}oxiran-2-yl}octanoyl}oxy}propoxy]phosphonic acid'	b'PE(18:1(12Z)-O(9S,10R)/DiMe(13,5))'	HMDB02 84915	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)((2R)-3-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl}oxy}propoxy]phosphonic acid'	b'PE(DiMe(13,5)'18:1(9Z)-O(12,13))'	HMDB02 84916	C47H84NO10P	
		853.5832849	0.0005 849	Redox	b'(2-aminoethoxy)((2R)-2-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-{{(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl}oxy}propoxy]phosphonic acid'	b'PE(18:1(9Z)-O(12,13)/DiMe(13,5))'	HMDB02 84917	C47H84NO10P	
3 4 5	854.60 13	854.603686	0.0023 86	Redox	b'[(2R)-2-{{(5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl}oxy}-3-{{(22-methyltetracosanoyl}oxy}propoxy]phosphonic acid'	b'PA(a-25:0/20:4(6Z,8E,10E,14Z)-2OH(5S,12R))'	HMDB02 67247	C48H87O10P	
		854.603686	0.0023 86	Redox	b'[(2R)-3-{{(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl}oxy}-2-{{(22-methyltetracosanoyl}oxy}propoxy]phosphonic acid'	b'PA(20:4(6Z,8E,10E,14Z)-2OH(5S,12R)/a-25:0)'	HMDB02 67248	C48H87O10P	
		854.603686	0.0023 86	Redox	b'[(2R)-2-{{(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl}oxy}-3-{{(22-methyltetracosanoyl}oxy}propoxy]phosphonic acid'	b'PA(a-25:0/20:4(6E,8Z,11Z,13E)-2OH(5S,15S))'	HMDB02 67283	C48H87O10P	
		854.603686	0.0023 86	Redox	b'[(2R)-3-{{(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl}oxy}-2-{{(22-methyltetracosanoyl}oxy}propoxy]phosphonic acid'	b'PA(20:4(6E,8Z,11Z,13E)-2OH(5S,15S)/a-25:0)'	HMDB02 67284	C48H87O10P	
		854.603686	0.0023 86	Redox	b'[(2R)-2-{{(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl}oxy}-3-{{(22-methyltetracosanoyl}oxy}propoxy]phosphonic acid'	b'PA(a-25:0/20:4(8Z,11Z,14Z,17Z)-2OH(5S,6R))'	HMDB02 67285	C48H87O10P	
		854.603686	0.0023 86	Redox	b'[(2R)-3-{{(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl}oxy}-2-{{(22-methyltetracosanoyl}oxy}propoxy]phosphonic acid'	b'PA(20:4(8Z,11Z,14Z,17Z)-2OH(5S,6R)/a-25:0)'	HMDB02 67286	C48H87O10P	
3 4	856.53 7	857.541814	0.0029 86	Proton ation	b'(2-aminoethoxy)((2R)-2-(7-{{(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]-6-oxoheptanoyl}oxy)-3-{{(11Z,14Z)-icosa-11,14-dienoyl}oxy}propoxy]phosphonic acid'	b'PE(20:2(11Z,14Z)/6 keto-PGF1alpha)'	HMDB02 62054	C45H80NO12P	

6		857.541814	0.0029 86	Proton ation	b'(2-aminoethoxy)[(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]-6-oxoheptanoyl}oxy)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphinic acid'	b'PE(6 keto-PGF1alpha/20:2(11Z,14Z))'	HMDB02 62055	C45H80NO12P	
		857.541814	0.0029 86	Proton ation	b'(2-aminoethoxy)[(2R)-2-({[(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl}oxy)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/TXB2)'	HMDB02 62064	C45H80NO12P	
		857.541814	0.0029 86	Proton ation	b'(2-aminoethoxy)[(2R)-3-({[(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl}oxy)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphinic acid'	b'PE(TXB2/20:2(11Z,14Z))'	HMDB02 62065	C45H80NO12P	
		857.541814	0.0029 86	Proton ation	b'(2-aminoethoxy)[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy]propoxy]phosphinic acid'	b'PE(DiMe(11,3)/PGF1alpha)'	HMDB02 84746	C45H80NO12P	
		857.541814	0.0029 86	Proton ation		b'PE(PGF1alpha/DiMe(11,3))'	HMDB02 84747	C45H80NO12P	
		857.541814	0.0029 86	Proton ation	b'(2-aminoethoxy)[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy]propoxy]phosphinic acid'	b'PE(DiMe(9,5)/PGF1alpha)'	HMDB02 85162	C45H80NO12P	
		857.541814	0.0029 86	Proton ation	b'(2-aminoethoxy)[(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy]propoxy]phosphinic acid'	b'PE(PGF1alpha/DiMe(9,5))'	HMDB02 85163	C45H80NO12P	
3 4 7	857.51 61	858.5258296	0.0019 296	Proton ation	b'[(2R)-3-(hexadecanoyloxy)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]({[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(16:0/20:4(5Z,8Z,11Z,14Z))'	HMDB00 09789	C45H79O13P	
		858.5258291	0.0019 291	Proton ation	b'[(2R)-3-(hexadecanoyloxy)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(16:0/20:4(8Z,11Z,14Z,17Z))'	HMDB00 09790	C45H79O13P	
		858.5258291	0.0019 291	Proton ation	b'[(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(11Z)/18:3(6Z,9Z,12Z))'	HMDB00 09827	C45H79O13P	
		858.5258291	0.0019 291	Proton ation	b'[(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(11Z)/18:3(9Z,12Z,15Z))'	HMDB00 09828	C45H79O13P	
		858.5258291	0.0019 291	Proton ation	b'[(2R)-3-[(9Z)-octadec-9-enoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(9Z)/18:3(6Z,9Z,12Z))'	HMDB00 09839	C45H79O13P	
		858.5258291	0.0019 291	Proton ation	b'[(2R)-3-[(9Z)-octadec-9-enoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(9Z)/18:3(9Z,12Z,15Z))'	HMDB00 09840	C45H79O13P	

		858.5258296	0.0019 296	Proton ation	b'[(2R)-2,3-bis[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]({[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:2(9Z,12Z)/18:2(9Z,12Z))'	HMDB00 09850	C45H79O13P	
		858.5258291	0.0019 291	Proton ation	b'[(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:3(6Z,9Z,12Z)/18:1(11Z))'	HMDB00 09859	C45H79O13P	
		858.5258291	0.0019 291	Proton ation	b'[(2R)-2-[(9Z)-octadec-9-enoyloxy]-3-[(9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:3(6Z,9Z,12Z)/18:1(9Z))'	HMDB00 09860	C45H79O13P	
		858.5258291	0.0019 291	Proton ation	b'[(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:3(9Z,12Z,15Z)/18:1(11Z))'	HMDB00 09863	C45H79O13P	
		858.5258291	0.0019 291	Proton ation	b'[(2R)-2-[(9Z)-octadec-9-enoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:3(9Z,12Z,15Z)/18:1(9Z))'	HMDB00 09864	C45H79O13P	
		858.5258291	0.0019 291	Proton ation	b'[(2R)-2-(hexadecanoyloxy)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(20:4(5Z,8Z,11Z,14Z)/16:0)	HMDB00 09893	C45H79O13P	C00 626
		858.5258291	0.0019 291	Proton ation	b'[(2R)-2-(hexadecanoyloxy)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(20:4(8Z,11Z,14Z,17Z)/16:0)	HMDB00 09899	C45H79O13P	
		858.5258296	0.0019 296	Proton ation	b'[3-(hexadecanoyloxy)-2-(icosa-5,8,11,14-tetraenoyloxy)propoxy]((2,3,4,5,6-pentahydroxycyclohexyl)oxy)phosphinic acid'	b'Phosphatidylinositol(36:4)'	HMDB02 56468	C45H79O13P	
		858.5258296	0.0019 296	Proton ation	b'[(2S)-2,3-dihydroxypropoxy]((2R)-3-[(17-methyloctadecanoyl)oxy]-2-({[(5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl]oxy}propoxy)phosphinic acid'	b'PG(i-19:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 71846	C45H79O13P	
		858.5258296	0.0019 296	Proton ation	b'[(2S)-2,3-dihydroxypropoxy]((2R)-2-[(17-methyloctadecanoyl)oxy]-3-({[(5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl]oxy}propoxy)phosphinic acid'	b'PG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/i-19:0)	HMDB02 71847	C45H79O13P	
3 4 8	858.51 79	858.5193049	0.0014 049	Redox	b'(5S,6R,7E,9E,11Z,14Z)-6-({[(2R)-2-amino-3-({[(2R)-1-({[(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-3-(hexadec-1-en-1-yloxy)propan-2-yl]oxy}-3-oxopropyl)sulfanyl}-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'PE(P-16:0/LTE4)'	HMDB02 85204	C44H79N2O10P S	
		858.5193049	0.0014 049	Redox	b'(5S,6R,7E,9E,11Z,14Z)-6-({[(2R)-2-amino-3-({[(2R)-3-({[(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(hexadec-1-en-1-yloxy)propoxy]-3-oxopropyl)sulfanyl}-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'PE(LTE4/P-16:0)	HMDB02 85205	C44H79N2O10P S	
3 4	858.56 94	858.5692281	0.0001 719	Redox	b'({[(3,7,11,15,19,23,27,31,35,39-decamethyltetraconta-2,6,10,14,18,22,26,30,34,38-decaen-1-yl)oxy](hydroxy)phosphoryl]oxy})phosphonic acid'	b'all-trans-Decaprenyl diphosphate'	HMDB00 59616	C50H84O7P2	C17 432

[illegible]

5	55		334	ation		(d18:1/22:0)'	12316		125
1									
3	863.55		0.0023		b'8-[3-methoxy-4,8-dimethyl-9-(2-methyl-1,3-oxazol-4-yl)nona-4,6,8-trien-2-yl]-11,16-dimethyl-6,19-dioxo-4,7,12,18-tetraoxatetracyclo[15.3.1.0 ³ {3,5}.0 ⁶ {11,13}]benicos-14-en-				
5	71	863.5547477	523	Redox	10-yl hexadecanoate'	b'Palmitoyl rhizoxin'	HMDB02 56089	C51H77NO10	
2									
3	863.60	864.6161783	0.0016 783	Proton ation	b'bis(3-methylbut-2-en-1-yl) {[hexakis(3-methylbut-2-en-1-yl)bis[(3-methylbut-2-en-1-yl)oxy]phosphoroso]oxy}phosphonate'	b'All trans decaprenyl diphosphate'	HMDB00 06288	C50H90O7P2	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{{(4Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 83790	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{{(4Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/22:0)'	HMDB02 83791	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 83792	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/22:0)'	HMDB02 83793	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 83794	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/22:0)'	HMDB02 83795	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 83796	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/22:0)'	HMDB02 83797	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{{(4Z,7Z,10Z,13Z,15-3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 83800	C49H86NO9P	
		863.6040204	0.0026	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{{(4Z,7Z,10Z,13Z,15-3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl}oxy}propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)-	HMDB02	C49H86NO9P	

			796				O(16,17)/22:0)	83801		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-{{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(6E,8Z,11Z,14Z)+ =O(5))'	HMDB02 84592	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-{{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)+=O(5)/24:1 (15Z))'	HMDB02 84593	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,13E)+ =O(15))'	HMDB02 84594	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)+=O(15)/24:1 1(15Z))'	HMDB02 84595	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:5(5Z,8Z,11Z,14Z,1 6E)-OH(18R))'	HMDB02 84606	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/24:1(15Z))'	HMDB02 84607	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:5(5Z,8Z,11Z,14Z,1 6E)-OH(18))'	HMDB02 84608	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/24:1(15Z))'	HMDB02 84609	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:5(5Z,8Z,10E,14Z,1 7Z)-OH(12))'	HMDB02 84610	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/24:1(15Z))'	HMDB02 84611	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:5(6E,8Z,11Z,14Z,1 7Z)-OH(5))'	HMDB02 84612	C49H86NO9P		
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/24:1(15Z))'	HMDB02 84613	C49H86NO9P		
		863.6040204	0.0026	Redox	b'trimethyl(2-{{(2R)-3-{{(10E,12Z)-9-oxooctadeca-10,12-dienyl}oxy}-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienyloxy]propyl phosphono}oxy)ethyl)azanium'	b'PC(18:2(10E,12Z)+=O(9)/22:3(10Z,1	HMDB02	C49H86NO9P		

			796			3Z,16Z))'	88125		
		863.6040204	0.0026 796	Redox	b'trimethyl(2-{{(2R)-2-{{(9Z,11E)-13-oxooctadeca-9,11-dienoyl}oxy}-3-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)azanum'	b'PC(22:3(10Z,13Z,16Z)/18:2(9Z,11E) +=O(13))'	HMDB02 88126	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'trimethyl(2-{{(2R)-3-{{(9Z,11E)-13-oxooctadeca-9,11-dienoyl}oxy}-2-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)azanum'	b'PC(18:2(9Z,11E)+=O(13)/22:3(10Z,1 3Z,16Z))'	HMDB02 88127	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-{{(2R)-2-{{(10E,12E,15E)-9-hydroxyoctadeca-10,12,15-trienoyl}oxy}-3-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanum'	b'PC(22:3(10Z,13Z,16Z)/18:3(10,12,15)-OH(9))'	HMDB02 88162	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-{{(2R)-3-{{(10E,12E,15E)-9-hydroxyoctadeca-10,12,15-trienoyl}oxy}-2-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanum'	b'PC(18:3(10,12,15)- OH(9)/22:3(10Z,13Z,16Z))'	HMDB02 88163	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-{{(2R)-2-{{(9E,11E,15E)-13-hydroxyoctadeca-9,11,15-trienoyl}oxy}-3-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanum'	b'PC(22:3(10Z,13Z,16Z)/18:3(9,11,15) -OH(13))'	HMDB02 88164	C49H86NO9P	
		863.6040204	0.0026 796	Redox	b'(2-{{(2R)-3-{{(9E,11E,15E)-13-hydroxyoctadeca-9,11,15-trienoyl}oxy}-2-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanum'	b'PC(18:3(9,11,15)- OH(13)/22:3(10Z,13Z,16Z))'	HMDB02 88165	C49H86NO9P	
3 5 4	864.57 02	864.5727793	0.0025 793	Redox	b'[(2R)-2-{{(9Z)-octadec-9-enoyloxy}-3-(octadecanoyloxy)propoxy}][{(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl}oxy]phosphinic acid'	b'PI(18:0/18:1(9Z))'	HMDB02 40667	C45H85O13P	
		864.5727798	0.0025 798	Redox	b'[(2R)-2-{{7-{{(1R,2R,3R,5S)-3,5-dihydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}cyclopentyl}heptanoyl}oxy}-3-{{(17-methyloctadecanoyl}oxy)propoxy}}[(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(i-19:0/PGF1a)alpha)'	HMDB02 71872	C45H85O13P	
		864.5727798	0.0025 798	Redox	b'[(2R)-3-{{7-{{(1R,2R,3R,5S)-3,5-dihydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}cyclopentyl}heptanoyl}oxy}-2-{{(17-methyloctadecanoyl}oxy)propoxy}}[(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(PGF1a)alpha/i-19:0)'	HMDB02 71873	C45H85O13P	
3 5 5	864.61 12	865.6196704	0.0006 704	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:4(6E,8Z,11Z,14Z)+=O(5))'	HMDB02 84488	C49H88NO9P	
		865.6196704	0.0006 704	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)+=O(5)/24:0)'	HMDB02 84489	C49H88NO9P	
		865.6196704	0.0006 704	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:4(5Z,8Z,11Z,13E)+=O(1 5))'	HMDB02 84490	C49H88NO9P	
		865.6196704	0.0006	Proton	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)+=O(15)/24:	HMDB02	C49H88NO9P	

			704	ation		0)	84491		
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 84502	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/24:0)'	HMDB02 84503	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	HMDB02 84504	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)-OH(18)/24:0)'	HMDB02 84505	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:5(5Z,8Z,10E,14Z,17Z)-OH(12))'	HMDB02 84506	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)-OH(12)/24:0)'	HMDB02 84507	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 84508	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/24:0)'	HMDB02 84509	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:3(5Z,8Z,11Z)-O(14R,15S))'	HMDB02 84542	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)-O(14R,15S)/24:1(15Z))'	HMDB02 84543	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:3(5Z,8Z,14Z)-O(11S,12R))'	HMDB02 84544	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,14Z)-O(11S,12R)/24:1(15Z))'	HMDB02 84545	C49H88NO9P	
865.6196704	0.0006	Proton			b'(2-aminoethoxy)((2R)-3-{{(15Z)-tetracos-15-enoyloxy}-2-{{(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl}oxy}propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:3(5Z,11Z,14Z)-	HMDB02	C49H88NO9P	

			704	ation		O(8,9))'	84546		
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-2-[(15Z)-tetracos-15-enoyloxy]-3-[[{(5Z)-7-[3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl]oxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,11Z,14Z)- O(8,9)/24:1(15Z))'	HMDB02 84547	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-2-[(15Z)-tetracos-15-enoyloxy]-2-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl)oxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:3(8Z,11Z,14Z)- O(5,6))'	HMDB02 84548	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-2-[(15Z)-tetracos-15-enoyloxy]-3-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl)oxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)- O(5,6)/24:1(15Z))'	HMDB02 84549	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenyl]oxy]-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,14Z)- OH(20))'	HMDB02 84550	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenyl]oxy]-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(20)/24:1(15Z))'	HMDB02 84551	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-2-[[{(5R,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenyl]oxy]-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(6E,8Z,11Z,14Z)- OH(5S))'	HMDB02 84552	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-3-[[{(5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenyl]oxy]-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)- OH(5S)/24:1(15Z))'	HMDB02 84553	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,14Z,19S)-19-hydroxyicosa-5,8,11,14-tetraenyl]oxy]-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,14Z)- OH(19S))'	HMDB02 84554	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenyl]oxy]-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(19S)/24:1(15Z))'	HMDB02 84555	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,14Z,18R)-18-hydroxyicosa-5,8,11,14-tetraenyl]oxy]-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,14Z)- OH(18R))'	HMDB02 84556	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,11Z,14Z,18S)-18-hydroxyicosa-5,8,11,14-tetraenyl]oxy]-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(18R)/24:1(15Z))'	HMDB02 84557	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenyl]oxy]-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,14Z)- OH(17))'	HMDB02 84558	C49H88NO9P	
865.6196704	0.0006	Proton			b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenyl]oxy]-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)-	HMDB02	C49H88NO9P	

			704	ation		OH(17)/24:1(15Z))'	84559		
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(5Z,8Z,11Z,14Z,16R)-16-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,14Z)-OH(16R))'	HMDB02 84560	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,11Z,14Z,16S)-16-hydroxyicosa-5,8,11,14-tetraenoyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)-OH(16R)/24:1(15Z))'	HMDB02 84561	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(5Z,8Z,11Z,13E,15S)-15-hydroxyicosa-5,8,11,13-tetraenoyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,13E)-OH(15S))'	HMDB02 84562	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,11Z,13E,15R)-15-hydroxyicosa-5,8,11,13-tetraenoyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)-OH(15S)/24:1(15Z))'	HMDB02 84563	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(5Z,8Z,10E,12S,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,10E,14Z)-OH(12S))'	HMDB02 84564	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(20:4(5Z,8Z,10E,14Z)-OH(12S)/24:1(15Z))'	HMDB02 84565	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(5E,8Z,11R,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(24:1(15Z)/20:4(5E,8Z,12Z,14Z)-OH(11R))'	HMDB02 84566	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(5E,8Z,11S,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(20:4(5E,8Z,12Z,14Z)-OH(11R)/24:1(15Z))'	HMDB02 84567	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-2-{{(5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,7E,11Z,14Z)-OH(9))'	HMDB02 84568	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'(2-aminoethoxy)((2R)-3-{{(5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(20:4(5Z,7E,11Z,14Z)-OH(9)/24:1(15Z))'	HMDB02 84569	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'trimethyl(2-{{(2R)-2-{{(8-{{3-{{(2Z)-oct-2-en-1-yl}oxiran-2-yl}octanoyl}oxy}-3-{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/18:1(12Z)-O(9S,10R))'	HMDB02 88130	C49H88NO9P	
865.6196704	0.0006	Proton	704	ation	b'trimethyl(2-{{(2R)-3-{{(8-{{3-{{(2Z)-oct-2-en-1-yl}oxiran-2-yl}octanoyl}oxy}-2-{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)azanium'	b'PC(18:1(12Z)-O(9S,10R)/22:3(10Z,13Z,16Z))'	HMDB02 88131	C49H88NO9P	
865.6196704	0.0006	Proton		ation	b'trimethyl(2-{{(2R)-2-{{(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl}oxy}-3-{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/18:1(9Z)-	HMDB02	C49H88NO9P	

			704	ation		O(12,13))'	88132		
		865.6196704	0.0006 704	Proton ation	b'trimethyl(2-{{(2R)-3-{{(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl}oxy}-2-{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)azanium'	b'PC(18:1(9Z)- O(12,13)22:3(10Z,13Z,16Z))'	HMDB02 88133	C49H88NO9P	
		864.6091653	0.0020 347	Redox	b'[(2R)-2-{{(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl}oxy}-3-{{(20-methylhenicosanoyl)oxy}propoxy}[(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(i-22:0/18:1(12Z)-2OH(9,10))'	HMDB02 72141	C46H89O12P	
		864.6091653	0.0020 347	Redox	b'[(2R)-3-{{(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl}oxy}-2-{{(20-methylhenicosanoyl)oxy}propoxy}[(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(18:1(12Z)-2OH(9,10)/i-22:0)'	HMDB02 72142	C46H89O12P	
3	877.60	877.6044143	0.0013 857	Redox	b'(2S)-2-amino-3-({(2R)-2-{{(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl}oxy}-3-(docosanoyloxy)propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:0/18:1(12Z)-2OH(9,10))'	HMDB02 82930	C46H88NO12P	
5	58	877.6044143	0.0013 857	Redox	b'(2S)-2-amino-3-({(2R)-3-{{(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl}oxy}-2-(docosanoyloxy)propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(18:1(12Z)-2OH(9,10)/22:0)'	HMDB02 82931	C46H88NO12P	
		881.614585	0.0011 15	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5Z)-7-{{(1S,5R)-5-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-4-oxocyclopent-2-en-1-yl}hept-5-enoyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/PGJ2)'	HMDB02 84474	C49H88NO10P	
		881.614585	0.0011 15	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(5Z)-7-{{(1S,5R)-5-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-4-oxocyclopent-2-en-1-yl}hept-5-enoyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(PGJ2/24:0)'	HMDB02 84475	C49H88NO10P	
		881.614585	0.0011 15	Proton ation		b'PE(24:1(15Z)/20:4(6Z,8E,10E,14Z)- 2OH(5S,12R))'	HMDB02 84582	C49H88NO10P	
		881.614585	0.0011 15	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicos-6,8,10,14-tetraenoyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy]phosphinic acid'	b'PE(20:4(6Z,8E,10E,14Z)- 2OH(5S,12R)/24:1(15Z))'	HMDB02 84583	C49H88NO10P	
		881.614585	0.0011 15	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicos-6,8,11,13-tetraenoyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(6E,8Z,11Z,13E)- 2OH(5S,15S))'	HMDB02 84618	C49H88NO10P	
		881.614585	0.0011 15	Proton ation	b'(2-aminoethoxy)[(2R)-3-{{(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicos-6,8,11,13-tetraenoyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/24:1(15Z))'	HMDB02 84619	C49H88NO10P	
		881.614585	0.0011 15	Proton ation	b'(2-aminoethoxy)[(2R)-2-{{(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicos-8,11,14,17-tetraenoyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R))'	HMDB02 84620	C49H88NO10P	
		881.614585	0.0011	Proton	b'(2-aminoethoxy)[(2R)-3-{{(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicos-8,11,14,17-tetraenoyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy]phosphinic acid'	b'PE(20:4(8Z,11Z,14Z,17Z)-	HMDB02	C49H88NO10P	

			15	ation		2OH(5S,6R)/24:1(15Z))'	84621		
		880.6067595	0.0011 405	Redox	b'(3-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-2-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(11,3)/MonoMe(11,5))'	HMDB00 61396	C49H87NO10P	
		880.6067595	0.0011 405	Redox	b'(3-{[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-2-{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(11,5)/MonoMe(11,3))'	HMDB00 61404	C49H87NO10P	
		880.6067595	0.0011 405	Redox	b'(3-{[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-2-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(11,5)/MonoMe(9,5))'	HMDB00 61407	C49H87NO10P	
		880.6067595	0.0011 405	Redox	b'(3-{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-2-{[13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(9,3)/MonoMe(13,5))'	HMDB00 61424	C49H87NO10P	
		880.6067595	0.0011 405	Redox	b'(3-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-2-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(9,5)/MonoMe(11,5))'	HMDB00 61432	C49H87NO10P	
		880.6067595	0.0011 405	Redox	b'(2-{[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,3)/DiMe(11,5))'	HMDB00 61436	C49H87NO10P	
		880.6067595	0.0011 405	Redox	b'(2-{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-3-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,5)/DiMe(11,3))'	HMDB00 61444	C49H87NO10P	
		880.6067595	0.0011 405	Redox	b'(2-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,5)/DiMe(9,5))'	HMDB00 61448	C49H87NO10P	
		880.6067595	0.0011 405	Redox	b'(2-{[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-3-{[13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(13,5)/DiMe(9,3))'	HMDB00 61456	C49H87NO10P	
		880.6067595	0.0011 405	Redox	b'(2-{[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-3-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(9,5)/DiMe(11,5))'	HMDB00 61463	C49H87NO10P	
3	883.52 97	884.534955	0.0025 45	Proton ation	b'(5S,6R,7E,9E,11Z,14Z)-6-{{{(2R)-2-amino-3-{{{(2R)-1-{{{(2-aminoethoxy)(hydroxy)phosphoryl}oxy}-3-{{(11Z)-octadeca-1,11-dien-1-yloxy}propan-2-yl}oxy}-3-oxopropyl}sulfanyl}-5-hydroxyicos-7,9,11,14-tetraenoic acid'	b'PE(P-18:1(11Z)/LTE4))'	HMDB02 85412	C46H81N2O10P S	
5		884.534955	0.0025 45	Proton ation	b'(5S,6R,7E,9E,11Z,14Z)-6-{{{(2R)-2-amino-3-{{{(2R)-3-{{{(2-aminoethoxy)(hydroxy)phosphoryl}oxy}-2-{{(11Z)-octadeca-1,11-dien-1-yloxy}propoxy}-3-oxopropyl}sulfanyl}-5-hydroxyicos-7,9,11,14-tetraenoic acid'	b'PE(LTE4/P-18:1(11Z))'	HMDB02 85413	C46H81N2O10P S	
8		884.534955	0.0025	Proton	b'(5S,6R,7E,9E,11Z,14Z)-6-{{{(2R)-2-amino-3-{{{(2R)-1-{{{(2-aminoethoxy)(hydroxy)phosphoryl}oxy}-3-{{(9Z)-octadeca-1,9-dien-1-yloxy}propan-2-yl}oxy}-3-oxopropyl}sulfanyl}-5-	b'PE(P-18:1(9Z)/LTE4))'	HMDB02	C46H81N2O10P	

			45	ation	hydroxyicosa-7,9,11,14-tetraenoic acid'		85513	S	
		884.534955	0.0025	Proton	b'(5S,6R,7E,9E,11Z,14Z)-6-{{(2R)-2-amino-3-[(2R)-3-{{(2-aminoethoxy)(hydroxy)phosphoryl}oxy}-2-[(9Z)-octadeca-1,9-dien-1-yloxy]propoxy}-3-oxopropyl)sulfanyl}-5-	b'PE(LTE4/P-18:1(9Z))'	HMDB02	C46H81N2O10P	
			45	ation	hydroxyicosa-7,9,11,14-tetraenoic acid'		85514	S	
3 5 9	884.53 09	885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({hydroxy[(2R)-3-(icosanoyloxy)-2-{{(5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl}oxy}propoxy]phosphoryl}oxy)propanoic	b'PS(20:0/20:5(7Z,9Z,11E,13E,17Z)-	HMDB02	C46H80NO13P	
			714	ation	acid'	3OH(5,6,15))'	82115		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({hydroxy[(2R)-2-(icosanoyloxy)-3-{{(5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl}oxy}propoxy]phosphoryl}oxy)propanoic	b'PS(20:5(7Z,9Z,11E,13E,17Z)-	HMDB02	C46H80NO13P	
			714	ation	acid'	3OH(5,6,15)/20:0)'	82116		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({hydroxy[(2R)-2-{{(5Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]hept-5-enoyl}oxy}-3-[(11Z)-icos-11-	b'PS(20:1(11Z)/PGE2)'	HMDB02	C46H80NO13P	
			714	ation	enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'		82173		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({hydroxy[(2R)-3-{{(5Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]hept-5-enoyl}oxy}-2-[(11Z)-icos-11-	b'PS(PGE2/20:1(11Z))'	HMDB02	C46H80NO13P	
			714	ation	enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'		82174		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({hydroxy[(2R)-2-{{(5Z)-7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]hept-5-enoyl}oxy}-3-[(11Z)-icos-11-	b'PS(20:1(11Z)/PGD2)'	HMDB02	C46H80NO13P	
			714	ation	enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'		82175		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({hydroxy[(2R)-3-{{(5Z)-7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]hept-5-enoyl}oxy}-2-[(11Z)-icos-11-	b'PS(PGD2/20:1(11Z))'	HMDB02	C46H80NO13P	
			714	ation	enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'		82176		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({hydroxy[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-{{(5S,6S,7E,9E,11Z,13E,15S)-5,6,15-trihydroxyicosa-7,9,11,13-tetraenoyl}oxy}propoxy]phosphoryl}oxy)propanoic	b'PS(20:1(11Z)/20:4(7E,9E,11Z,13E)-	HMDB02	C46H80NO13P	
			714	ation	acid'	3OH(5S,6R,15S))'	82189		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({hydroxy[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-{{(5R,6R,7E,9E,11Z,13E,15R)-5,6,15-trihydroxyicosa-7,9,11,13-tetraenoyl}oxy}propoxy]phosphoryl}oxy)propanoic	b'PS(20:4(7E,9E,11Z,13E)-	HMDB02	C46H80NO13P	
			714	ation	acid'	3OH(5S,6R,15S)/20:1(11Z))'	82190		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({{(2R)-2-{{(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl}oxy}-3-[(11Z,14Z)-icosa-11,14-	b'PS(20:2(11Z,14Z)/PGF2alpha)'	HMDB02	C46H80NO13P	
			714	ation	dienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'		82283		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({{(2R)-3-{{(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl}oxy}-2-[(11Z,14Z)-icosa-11,14-	b'PS(PGF2alpha/20:2(11Z,14Z))'	HMDB02	C46H80NO13P	
			714	ation	dienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'		82284		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({hydroxy[(2R)-2-[(7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-3-[(11Z,14Z)-icosa-11,14-	b'PS(20:2(11Z,14Z)/PGE1)'	HMDB02	C46H80NO13P	
			714	ation	dienoyloxy]propoxy]phosphoryl}oxy)propanoic acid'		82345		
		885.5367286	0.0019	Proton	b'(2S)-2-amino-3-({hydroxy[(2R)-3-({7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-2-[(11Z,14Z)-icosa-11,14-	b'PS(PGE1/20:2(11Z,14Z))'	HMDB02	C46H80NO13P	

			714	ation	dienoyloxy]propoxy]phosphoryl]oxy]propanoic acid'		82346		
	885.5367286	0.0019	714	Proton ation	b'(2S)-2-amino-3-({hydroxy{(2R)-2-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-3-[(11Z,14Z)-icosa-11,14- dienoyloxy]propoxy]phosphoryl]oxy]propanoic acid'	b'PS(20:2(11Z,14Z)/PGD1)'	HMDB02 82347	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2S)-2-amino-3-({hydroxy{(2R)-3-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-2-[(11Z,14Z)-icosa-11,14- dienoyloxy]propoxy]phosphoryl]oxy]propanoic acid'	b'PS(PGD1/20:2(11Z,14Z))'	HMDB02 82348	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2S)-2-amino-3-({[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[(5Z,8Z,11Z)-icosa-5,8,11- trienoyloxy]propoxy](hydroxy)phosphoryl]oxy]propanoic acid'	b'PS(20:3(5Z,8Z,11Z)/PGF1alpha)'	HMDB02 82453	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2S)-2-amino-3-({[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(5Z,8Z,11Z)-icosa-5,8,11- trienoyloxy]propoxy](hydroxy)phosphoryl]oxy]propanoic acid'	b'PS(PGF1alpha/20:3(5Z,8Z,11Z))'	HMDB02 82454	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2S)-2-amino-3-({[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[(8Z,11Z,14Z)-icosa-8,11,14- trienoyloxy]propoxy](hydroxy)phosphoryl]oxy]propanoic acid'	b'PS(20:3(8Z,11Z,14Z)/PGF1alpha)'	HMDB02 82557	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2S)-2-amino-3-({[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(8Z,11Z,14Z)-icosa-8,11,14- trienoyloxy]propoxy](hydroxy)phosphoryl]oxy]propanoic acid'	b'PS(PGF1alpha/20:3(8Z,11Z,14Z))'	HMDB02 82558	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2S)-2-amino-3-({[(2R)-2-([(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl]oxy)-3-[(13Z,16Z)-docosa-13,16- dienoyloxy]propoxy](hydroxy)phosphoryl]oxy]propanoic acid'	b'PS(22:2(13Z,16Z)/5-iso PGF2VI)'	HMDB02 83128	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2S)-2-amino-3-({[(2R)-3-([(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl]oxy)-2-[(13Z,16Z)-docosa-13,16- dienoyloxy]propoxy](hydroxy)phosphoryl]oxy]propanoic acid'	b'PS(5-iso PGF2VI/22:2(13Z,16Z))'	HMDB02 83129	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2-([(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]-6-oxoheptanoyl}oxy)-3-[(9-(3,4-dimethyl-5-propylfuran-2- yl)nonanoyl]oxy]propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(DiMe(9,3)/6 keto-PGF1alpha)'	HMDB02 89245	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2-([(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]-6-oxoheptanoyl}oxy)-2-[(9-(3,4-dimethyl-5-propylfuran-2- yl)nonanoyl]oxy]propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(6 keto-PGF1alpha/DiMe(9,3))'	HMDB02 89246	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2-([(2R)-2-([(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl]oxy)-3-[(9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy]propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(DiMe(9,3)/TXB2)'	HMDB02 89255	C46H80NO13P	
	885.5367286	0.0019	714	Proton ation	b'(2-([(2R)-3-([(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl]oxy)-2-[(9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy]propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(TXB2/DiMe(9,3))'	HMDB02 89256	C46H80NO13P	
3	885.54	886.5571293	0.0028	Proton	b'[(2R)-2-[(10Z,13Z,16Z,19Z)-docosa-10,13,16,19-tetraenoyloxy]-3-(hexadecanoyloxy)propoxy]([[(1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy])phosphinic acid'	b'PI(16:0/22:4(10Z,13Z,16Z,19Z))'	HMDB00	C47H83O13P	

6 0	65		293	ation			09793		
		886.5571293	0.0028 293	Proton ation	b'[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-(hexadecanoyloxy)propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(16:0/22:4(7Z,10Z,13Z,16Z))'	HMDB00 09794	C47H83O13P	
		886.5571297	0.0028 297	Proton ation	b'[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-(octadecanoyloxy)propoxy]({[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:0/20:4(5Z,8Z,11Z,14Z))'	HMDB00 09815	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-3-(octadecanoyloxy)propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:0/20:4(8Z,11Z,14Z,17Z))'	HMDB00 09816	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(11Z)/20:3(5Z,8Z,11Z))'	HMDB00 09830	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(11Z)/20:3(8Z,11Z,14Z))'	HMDB00 09831	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(9Z)/20:3(5Z,8Z,11Z))'	HMDB00 09842	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(9Z)/20:3(8Z,11Z,14Z))'	HMDB00 09843	C47H83O13P	C00 626
		886.5571293	0.0028 293	Proton ation	b'[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:2(9Z,12Z)/20:2(11Z,14Z))'	HMDB00 09853	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(20:2(11Z,14Z)/18:2(9Z,12Z))'	HMDB00 09877	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(20:3(5Z,8Z,11Z)/18:1(11Z))'	HMDB00 09881	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(20:3(5Z,8Z,11Z)/18:1(9Z))'	HMDB00 09882	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(20:3(8Z,11Z,14Z)/18:1(11Z))'	HMDB00 09888	C47H83O13P	C00 626
		886.5571293	0.0028	Proton	b'[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(20:3(8Z,11Z,14Z)/18:1(9Z))'	HMDB00	C47H83O13P	

			293	ation			09889		
		886.5571293	0.0028 293	Proton ation	b'[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-(octadecanoyloxy)propoxy](((1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl)oxy))phosphinic acid'	b'PI(20:4(5Z,8Z,11Z,14Z)/18:0)	HMDB00 09894	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-(octadecanoyloxy)propoxy](((1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl)oxy))phosphinic acid'	b'PI(20:4(8Z,11Z,14Z,17Z)/18:0)	HMDB00 09900	C47H83O13P	C00 626
		886.5571293	0.0028 293	Proton ation	b'[(2R)-3-[(10Z,13Z,16Z,19Z)-docosa-10,13,16,19-tetraenoyloxy]-2-(hexadecanoyloxy)propoxy](((1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl)oxy))phosphinic acid'	b'PI(22:4(10Z,13Z,16Z,19Z)/16:0)	HMDB00 09912	C47H83O13P	
		886.5571293	0.0028 293	Proton ation	b'[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(hexadecanoyloxy)propoxy](((1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl)oxy))phosphinic acid'	b'PI(22:4(7Z,10Z,13Z,16Z)/16:0)	HMDB00 09914	C47H83O13P	
		886.5571297	0.0028 297	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(18-methylcosanoyloxy)-2-[[[5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenyl]oxy]propoxy]phosphinic acid'	b'PG(a-21:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 70911	C47H83O13P	
		886.5571297	0.0028 297	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(18-methylcosanoyloxy)-3-[[[5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenyl]oxy]propoxy]phosphinic acid'	b'PG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/a-21:0)	HMDB02 70912	C47H83O13P	
		886.5571297	0.0028 297	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(19-methylcosanoyloxy)-2-[[[5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenyl]oxy]propoxy]phosphinic acid'	b'PG(i-21:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 72053	C47H83O13P	
		886.5571297	0.0028 297	Proton ation	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(19-methylcosanoyloxy)-3-[[[5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenyl]oxy]propoxy]phosphinic acid'	b'PG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/i-21:0)	HMDB02 72054	C47H83O13P	
3 6 1	886.54 99	886.5506051	0.0007 051	Redox	b'(5S,6R,7E,9E,11Z,14Z)-6-[[[(2R)-2-amino-3-[[[(2R)-1-[[[(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-3-(octadec-1-en-1-yloxy)propan-2-yl]oxy]-3-oxopropyl]sulfanyl}-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'PE(P-18:0/LTE4)	HMDB02 85308	C46H83N2O10P S	
		886.5506051	0.0007 051	Redox	b'(5S,6R,7E,9E,11Z,14Z)-6-[[[(2R)-2-amino-3-[(2R)-3-[[[(2-aminoethoxy)(hydroxy)phosphoryl]oxy]-2-(octadec-1-en-1-yloxy)propoxy]-3-oxopropyl]sulfanyl}-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'PE(LTE4/P-18:0)	HMDB02 85309	C46H83N2O10P S	
3 6 2	887.55 45	887.5523787	0.0021 213	Redox	b'(2S)-2-amino-3-[(hydroxy[(2R)-2-[[[(5Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]hept-5-enoyl]oxy]-3-(icosanoyloxy)propoxy]phosphoryl]oxy)propanoic acid'	b'PS(20:0/PGE2)	HMDB02 82069	C46H82NO13P	
		887.5523787	0.0021 213	Redox	b'(2S)-2-amino-3-[(hydroxy[(2R)-3-[[[(5Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]hept-5-enoyl]oxy]-2-(icosanoyloxy)propoxy]phosphoryl]oxy)propanoic acid'	b'PS(PGE2/20:0)	HMDB02 82070	C46H82NO13P	
		887.5523787	0.0021	Redox	b'(2S)-2-amino-3-[(hydroxy[(2R)-2-[[[(5Z)-7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]hept-5-enoyl]oxy]-3-(icosanoyloxy)propoxy]phosphoryl]oxy)propanoic acid'	b'PS(20:0/PGD2)	HMDB02	C46H82NO13P	

			213		(icosanoyloxy)propoxy]phosphoryl}oxy)propanoic acid'		82071		
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({hydroxy[(2R)-3-{{(5Z)-7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]hept-5-enoyl}oxy]-2- (icosanoyloxy)propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGD2/20:0)'	HMDB02 82072	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({hydroxy[(2R)-3-(icosanoyloxy)-2-{{(5S,6S,7E,9E,11Z,13E,15S)-5,6,15-trihydroxyicosa-7,9,11,13-tetraenoyl}oxy}propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:0/20:4(7E,9E,11Z,13E)- 3OH(5S,6R,15S))'	HMDB02 82085	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({hydroxy[(2R)-2-(icosanoyloxy)-3-{{(5R,6R,7E,9E,11Z,13E,15R)-5,6,15-trihydroxyicosa-7,9,11,13-tetraenoyl}oxy}propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:4(7E,9E,11Z,13E)- 3OH(5S,6R,15S)/20:0)'	HMDB02 82086	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({{(2R)-2-{{(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl}oxy}-3-[(11Z)-icos-11- enoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:1(11Z)/PGF2alpha)'	HMDB02 82179	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({{(2R)-3-{{(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl}oxy}-2-[(11Z)-icos-11- enoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(PGF2alpha/20:1(11Z))'	HMDB02 82180	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-2-[(11Z)-icos-11- enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:1(11Z)/PGE1)'	HMDB02 82241	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({hydroxy[(2R)-3-({7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-2-[(11Z)-icos-11- enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGE1/20:1(11Z))'	HMDB02 82242	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-3-[(11Z)-icos-11- enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:1(11Z)/PGD1)'	HMDB02 82243	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({hydroxy[(2R)-3-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-2-[(11Z)-icos-11- enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGD1/20:1(11Z))'	HMDB02 82244	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({{(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[(11Z,14Z)-icosa-11,14- dienoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:2(11Z,14Z)/PGF1alpha)'	HMDB02 82349	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({{(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(11Z,14Z)-icosa-11,14- dienoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(PGF1alpha/20:2(11Z,14Z))'	HMDB02 82350	C46H82NO13P	
887.5523787	0.0021	Redox	213		b'(2S)-2-amino-3-({{(2R)-2-{{(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy}-3-[(13Z)-docos-13- enoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:1(13Z)/5-iso PGF2VI)'	HMDB02 83024	C46H82NO13P	
887.5523787	0.0021	Redox			b'(2S)-2-amino-3-({{(2R)-3-{{(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy}-2-[(13Z)-docos-13- enoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(5-iso PGF2VI/22:1(13Z))'	HMDB02	C46H82NO13P	

			213		enoyloxy]propoxy](hydroxy)phosphoryl}oxy]propanoic acid'		83025		
3 6 3	889.56 71	889.5680288	0.0009 288	Redox	b'(2S)-2-amino-3-({[(2R)-2-({[(5E)-7-({(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl}oxy)-3-(icosanoyloxy)propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:0/PGF2alpha)'	HMDB02 82075	C46H84NO13P	
		889.5680288	0.0009 288	Redox	b'(2S)-2-amino-3-({[(2R)-3-({[(5E)-7-({(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl}oxy)-2-(icosanoyloxy)propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(PGF2alpha/20:0)'	HMDB02 82076	C46H84NO13P	
		889.5680288	0.0009 288	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-({(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-3-(icosanoyloxy)propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:0/PGE1)'	HMDB02 82137	C46H84NO13P	
		889.5680288	0.0009 288	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-3-({7-({(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-2-(icosanoyloxy)propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGE1/20:0)'	HMDB02 82138	C46H84NO13P	
		889.5680288	0.0009 288	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-({(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-3-(icosanoyloxy)propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:0/PGD1)'	HMDB02 82139	C46H84NO13P	
		889.5680288	0.0009 288	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-3-({7-({(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-2-(icosanoyloxy)propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGD1/20:0)'	HMDB02 82140	C46H84NO13P	
		889.5680288	0.0009 288	Redox	b'(2S)-2-amino-3-({[(2R)-2-({7-({(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-({(11Z)-icos-11-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:1(11Z)/PGF1alpha)'	HMDB02 82245	C46H84NO13P	
		889.5680288	0.0009 288	Redox	b'(2S)-2-amino-3-({[(2R)-3-({7-({(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-({(11Z)-icos-11-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(PGF1alpha/20:1(11Z))'	HMDB02 82246	C46H84NO13P	
		889.5680288	0.0009 288	Redox	b'(2S)-2-amino-3-({[(2R)-2-({[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy)-3-(docosanoyloxy)propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:0/5-iso PGF2VI)'	HMDB02 82920	C46H84NO13P	
		889.5680288	0.0009 288	Redox	b'(2S)-2-amino-3-({[(2R)-3-({[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy)-2-(docosanoyloxy)propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(5-iso PGF2VI/22:0)'	HMDB02 82921	C46H84NO13P	
3 6 4	891.63 78	891.6353205	0.0024 795	Redox	b'(2-aminoethoxy)[(2R)-2-({[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy)-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 84518	C51H90NO9P	
		891.6353205	0.0024 795	Redox	b'(2-aminoethoxy)[(2R)-3-({[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy)-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/24:0)'	HMDB02 84519	C51H90NO9P	
		891.6353205	0.0024	Redox	b'(2-aminoethoxy)[(2R)-2-({[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy)-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02	C51H90NO9P	

			795			Z)-OH(7))'	84520		
		891.6353205	0.0024 795	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,12,16,19-hexaenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/24:0))'	HMDB02 84521	C51H90NO9P	
		891.6353205	0.0024 795	Redox	b'(2-aminoethoxy)[(2R)-2-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/22:6(4Z,7Z,10Z,12E,16Z,19 Z)-OH(14))'	HMDB02 84522	C51H90NO9P	
		891.6353205	0.0024 795	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/24:0))'	HMDB02 84523	C51H90NO9P	
		891.6353205	0.0024 795	Redox	b'(2-aminoethoxy)[(2R)-2-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/22:6(4Z,7Z,10Z,13E,15E,19 Z)-OH(17))'	HMDB02 84524	C51H90NO9P	
		891.6353205	0.0024 795	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/24:0))'	HMDB02 84525	C51H90NO9P	
		891.6353205	0.0024 795	Redox	b'(2-aminoethoxy)[(2R)-2-{{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))'	HMDB02 84528	C51H90NO9P	
		891.6353205	0.0024 795	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/24:0))'	HMDB02 84529	C51H90NO9P	
		891.6353205	0.0024 795	Redox	b'(2-{{(2R)-2-{{(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienyl}oxy}-3-[(10Z,13Z,16Z)-tricoso-10,13,16-trienyloxy]propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:3(6,8,11)- OH(5))'	HMDB02 88172	C51H90NO9P	
		891.6353205	0.0024 795	Redox	b'(2-{{(2R)-3-{{(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienyl}oxy}-2-[(10Z,13Z,16Z)-tricoso-10,13,16-trienyloxy]propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:3(6,8,11)- OH(5)/22:3(10Z,13Z,16Z))'	HMDB02 88173	C51H90NO9P	
3 6 5	895.62 78	895.6302351	0.0024 351	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-3-{{(5Z,8Z,11Z)-icosa-5,8,11-trienyloxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphoryl}oxy}propanoic acid'	b'PS(20:3(5Z,8Z,11Z)/24:1(15Z))'	HMDB01 12620	C50H90NO10P	
		895.6302351	0.0024 351	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-3-{{(8Z,11Z,14Z)-icosa-8,11,14-trienyloxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphoryl}oxy}propanoic acid'	b'PS(20:3(8Z,11Z,14Z)/24:1(15Z))'	HMDB01 12635	C50H90NO10P	
		895.6302351	0.0024 351	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-3-{{(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenyloxy}-2-(tetracosanoyloxy)propoxy]phosphoryl}oxy}propanoic acid'	b'PS(20:4(5Z,8Z,11Z,14Z)/24:0))'	HMDB01 12652	C50H90NO10P	
		895.6302351	0.0024	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-3-{{(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenyloxy}-2-(tetracosanoyloxy)propoxy]phosphoryl}oxy}propanoic acid'	b'PS(20:4(8Z,11Z,14Z,17Z)/24:0))'	HMDB01	C50H90NO10P	

			351				12678		
895.6302351	0.0024 351	Redox	b'(2S)-2-amino-3-({(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-(docosanoyloxy)propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'		b'PS(22:0/22:4(7Z,10Z,13Z,16Z))'		HMDB01 12730	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2S)-2-amino-3-({(2R)-2,3-bis[(13Z,16Z)-docosa-13,16-dienoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'		b'PS(22:2(13Z,16Z)/22:2(13Z,16Z))'		HMDB01 12781	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2S)-2-amino-3-({(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(docosanoyloxy)propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'		b'PS(22:4(7Z,10Z,13Z,16Z)/22:0)'		HMDB01 12807	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-(tetracosanoyloxy)propoxy}phosphoryl}oxy)propanoic acid'		b'PS(24:0/20:4(5Z,8Z,11Z,14Z))'		HMDB01 12898	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-3-(tetracosanoyloxy)propoxy}phosphoryl}oxy)propanoic acid'		b'PS(24:0/20:4(8Z,11Z,14Z,17Z))'		HMDB01 12899	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(15Z)-tetracos-15-enoyloxy]propoxy}phosphoryl}oxy)propanoic acid'		b'PS(24:1(15Z)/20:3(5Z,8Z,11Z))'		HMDB01 12924	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(15Z)-tetracos-15-enoyloxy]propoxy}phosphoryl}oxy)propanoic acid'		b'PS(24:1(15Z)/20:3(8Z,11Z,14Z))'		HMDB01 12925	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2-({(2R)-3-(docosanoyloxy)-2-({(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl}oxy}propyl phosphono}oxy)ethyl)trimethylazanium'		b'PC(22:0/PJ2)'		HMDB02 87795	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2-({(2R)-2-(docosanoyloxy)-3-({(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl}oxy}propyl phosphono}oxy)ethyl)trimethylazanium'		b'PC(PJ2/22:0)'		HMDB02 87796	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2-({(2R)-2-({(5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl}oxy)-3-[(13Z)-docos-13-enoyloxy]propyl phosphono}oxy)ethyl)trimethylazanium'		b'PC(22:1(13Z)/20:4(6Z,8E,10E,14Z)-2OH(5S,12R))'		HMDB02 87903	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2-({(2R)-3-({(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl}oxy)-2-[(13Z)-docos-13-enoyloxy]propyl phosphono}oxy)ethyl)trimethylazanium'		b'PC(20:4(6Z,8E,10E,14Z)-2OH(5S,12R)/22:1(13Z))'		HMDB02 87904	C50H90NO10P	
895.6302351	0.0024 351	Redox	b'(2-({(2R)-2-({(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl}oxy)-3-[(13Z)-docos-13-enoyloxy]propyl phosphono}oxy)ethyl)trimethylazanium'		b'PC(22:1(13Z)/20:4(6E,8Z,11Z,13E)-2OH(5S,15S))'		HMDB02 87939	C50H90NO10P	
895.6302351	0.0024	Redox	b'(2-({(2R)-3-({(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl}oxy)-2-[(13Z)-docos-13-enoyloxy]propyl phosphono}oxy)ethyl)trimethylazanium'		b'PC(20:4(6E,8Z,11Z,13E)-		HMDB02	C50H90NO10P	

			351			2OH(5S,15S)/22:1(13Z))'	87940		
		895.6302351	0.0024 351	Redox	b'(2-:{{(2R)-2-:{{(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxydocosa-8,11,14,17-tetraenyl}oxy}-3-:{{(13Z)-docos-13-enoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:1(13Z)/20:4(8Z,11Z,14Z,17Z)- -2OH(5S,6R))'	HMDB02 87941	C50H90NO10P	
		895.6302351	0.0024 351	Redox	b'(2-:{{(2R)-3-:{{(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxydocosa-8,11,14,17-tetraenyl}oxy}-2-:{{(13Z)-docos-13-enoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/22:1(13Z))'	HMDB02 87942	C50H90NO10P	
		895.6302351	0.0024 351	Redox	b'(2-:{{(2R)-2-:{{(8Z,11Z,14Z)-5,6-dihydroxydocosa-8,11,14-trienyl}oxy}-3-:{{(13Z,16Z)-docosa-13,16-dienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:2(13Z,16Z)/20:3(8Z,11Z,14Z)- -2OH(5,6))'	HMDB02 88013	C50H90NO10P	
		895.6302351	0.0024 351	Redox	b'(2-:{{(2R)-3-:{{(8Z,11Z,14Z)-5,6-dihydroxydocosa-8,11,14-trienyl}oxy}-2-:{{(13Z,16Z)-docosa-13,16-dienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:3(8Z,11Z,14Z)- 2OH(5,6)/22:2(13Z,16Z))'	HMDB02 88014	C50H90NO10P	
		895.6302351	0.0024 351	Redox	b'(2-:{{(2R)-3-:{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-:{{8-:{{3-:{{(2Z)-oct-2-en-1-yl}oxiran-2-yl}octanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(13,5)/18:1(12Z)- O(9S,10R))'	HMDB02 89169	C50H90NO10P	
		895.6302351	0.0024 351	Redox	b'(2-:{{(2R)-2-:{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-:{{8-:{{3-:{{(2Z)-oct-2-en-1-yl}oxiran-2-yl}octanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(18:1(12Z)- O(9S,10R)/DiMe(13,5))'	HMDB02 89170	C50H90NO10P	
		895.6302351	0.0024 351	Redox	b'(2-:{{(2R)-3-:{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-:{{(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(13,5)/18:1(9Z)-O(12,13))'	HMDB02 89171	C50H90NO10P	
		895.6302351	0.0024 351	Redox	b'(2-:{{(2R)-2-:{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-:{{(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(18:1(9Z)-O(12,13)/DiMe(13,5))'	HMDB02 89172	C50H90NO10P	
3 6 6	903.60 06	903.598935	0.0016 65	Redox	b'(2-:{{(2R)-2-:{{(5Z)-7-:{{(1S,5R)-5-:{{(1E,3S)-3-hydroxyoct-1-en-1-yl}4-oxocyclopent-2-en-1-yl}hept-5-enoyl}oxy}-3-:{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/PGJ2)'	HMDB02 88107	C51H86NO10P	
		903.598935	0.0016 65	Redox	b'(2-:{{(2R)-3-:{{(5Z)-7-:{{(1S,5R)-5-:{{(1E,3S)-3-hydroxyoct-1-en-1-yl}4-oxocyclopent-2-en-1-yl}hept-5-enoyl}oxy}-2-:{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(PGJ2/22:3(10Z,13Z,16Z))'	HMDB02 88108	C51H86NO10P	
3 6 7	903.63 67	903.6353205	0.0013 795	Redox	b'(2-:{{(2R)-3-:{{(13Z)-docos-13-enoyloxy}-2-:{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:1(13Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 87943	C52H90NO9P	
		903.6353205	0.0013 795	Redox	b'(2-:{{(2R)-2-:{{(13Z)-docos-13-enoyloxy}-3-:{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)/22:1(13Z))'	HMDB02 87944	C52H90NO9P	
		903.6353205	0.0013	Redox	b'(2-:{{(2R)-3-:{{(13Z)-docos-13-enoyloxy}-2-:{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:1(13Z)/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02	C52H90NO9P	

3 6 8	907.63 28		795			6Z,19Z)-OH(7))'	87945		
		903.6353205	0.0013 795	Redox	b'(2-){[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-}{[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/22:1(13Z))'	HMDB02 87946	C52H90NO9P	
		903.6353205	0.0013 795	Redox	b'(2-){[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-}{[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:1(13Z)/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/22:1(13Z))'	HMDB02 87947	C52H90NO9P	
		903.6353205	0.0013 795	Redox	b'(2-){[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-}{[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/22:1(13Z))'	HMDB02 87948	C52H90NO9P	
		903.6353205	0.0013 795	Redox	b'(2-){[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-}{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:1(13Z)/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/22:1(13Z))'	HMDB02 87949	C52H90NO9P	
		903.6353205	0.0013 795	Redox	b'(2-){[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-}{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/22:1(13Z))'	HMDB02 87950	C52H90NO9P	
		903.6353205	0.0013 795	Redox	b'(2-){[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-}{[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:1(13Z)/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 87953	C52H90NO9P	
		903.6353205	0.0013 795	Redox	b'(2-){[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-}{[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/22:1(13Z))'	HMDB02 87954	C52H90NO9P	
	907.63 28	908.6380596	0.0025 404	Proton ation	b'(3-){[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-2-{[13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy}propoxy}[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(11,3)/MonoMe(13,5))'	HMDB00 61397	C51H91NO10P	
		908.6380596	0.0025 404	Proton ation	b'(3-){[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-2-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propoxy}[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(11,5)/MonoMe(11,5))'	HMDB00 61405	C51H91NO10P	
		908.6380596	0.0025 404	Proton ation	b'(3-){[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy}-2-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propoxy}[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(13,5)/MonoMe(11,3))'	HMDB00 61413	C51H91NO10P	
		908.6380596	0.0025 404	Proton ation	b'(3-){[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy}-2-{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propoxy}[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(13,5)/MonoMe(9,5))'	HMDB00 61416	C51H91NO10P	
		908.6380596	0.0025 404	Proton ation	b'(3-){[9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy}-2-{[13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy}propoxy}[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(9,5)/MonoMe(13,5))'	HMDB00 61433	C51H91NO10P	
		908.6380596	0.0025	Proton	b'(2-){[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy}-3-{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propoxy}[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,3)/DiMe(13,5))'	HMDB00	C51H91NO10P	

		404	ation				61437		
908.6380596	0.0025 404	Proton ation	b'(2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,5)/DiMe(11,5))'	HMDB00 61445	C51H91NO10P			
908.6380596	0.0025 404	Proton ation	b'(2-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(13,5)/DiMe(11,3))'	HMDB00 61453	C51H91NO10P			
908.6380596	0.0025 404	Proton ation	b'(2-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(13,5)/DiMe(9,5))'	HMDB00 61457	C51H91NO10P			
908.6380596	0.0025 404	Proton ation	b'(2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(9,5)/DiMe(13,5))'	HMDB00 61464	C51H91NO10P			
907.6302346	0.0025 654	Redox	b'(2-aminoethoxy)((2R)-2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)phosphinic acid'	b'PE(DiMe(11,5)/DiMe(13,5))'	HMDB00 61482	C51H90NO10P			
907.6302346	0.0025 654	Redox	b'(2-aminoethoxy)((2R)-3-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)phosphinic acid'	b'PE(DiMe(13,5)/DiMe(11,5))'	HMDB00 61490	C51H90NO10P			
907.6302346	0.0025 654	Redox	b'(2-aminoethoxy)((2R)-2,3-bis([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)phosphinic acid'	b'PE(MonoMe(13,5)/MonoMe(13,5))'	HMDB00 61541	C51H90NO10P			
907.6302351	0.0025 649	Redox	b'((2R)-3-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-2-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11D5/13M5)'	HMDB01 13770	C51H90NO10P			
907.6302351	0.0025 649	Redox	b'((2R)-2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11M5/13D5)'	HMDB01 13787	C51H90NO10P			
907.6302351	0.0025 649	Redox	b'((2R)-3-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(13D5/11M5)'	HMDB01 13795	C51H90NO10P			
907.6302351	0.0025 649	Redox	b'((2R)-2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(13M5/11D5)'	HMDB01 13802	C51H90NO10P			
907.6302351	0.0025 649	Redox	b'((2R)-2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMe2(11D3/13D5)'	HMDB01 14664	C51H90NO10P			
907.6302351	0.0025	Redox	b'((2R)-2,3-bis([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMe2(11D5/11D5)'	HMDB01	C51H90NO10P			

			649				14670		
		907.6302351	0.0025 649	Redox	b'[2-(dimethylamino)ethoxy][(2R)-2-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy]phosphinic acid'	b'PE-NMc2(11M5/13M5)'	HMDB01 14692	C51H90NO10P	
		907.6302351	0.0025 649	Redox	b'[(2R)-3-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(13D5/11D3)'	HMDB01 14696	C51H90NO10P	
		907.6302351	0.0025 649	Redox	b'[(2R)-2-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(13D5/9D5)'	HMDB01 14703	C51H90NO10P	
		907.6302351	0.0025 649	Redox	b'[2-(dimethylamino)ethoxy][(2R)-3-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy]phosphinic acid'	b'PE-NMc2(13M5/11M5)'	HMDB01 14708	C51H90NO10P	
		907.6302351	0.0025 649	Redox	b'[(2R)-3-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-2-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(9D5/13D5)'	HMDB01 14727	C51H90NO10P	
		907.6302351	0.0025 649	Redox	b'(2-aminoethoxy)[(2R)-2-{{{{(5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-3-(tetracosanoyloxy)propoxy}phosphinic acid'	b'PE(24:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S,17S))'	HMDB02 84510	C51H90NO10P	
		907.6302351	0.0025 649	Redox	b'(2-aminoethoxy)[(2R)-3-{{{{(5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-2-(tetracosanoyloxy)propoxy}phosphinic acid'	b'PE(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S,17S)/24:0)'	HMDB02 84511	C51H90NO10P	
		907.6302351	0.0025 649	Redox	b'(2-aminoethoxy)[(2R)-2-{{{{(4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl}oxy}-3-(tetracosanoyloxy)propoxy}phosphinic acid'	b'PE(24:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17S))'	HMDB02 84526	C51H90NO10P	
		907.6302351	0.0025 649	Redox	b'(2-aminoethoxy)[(2R)-3-{{{{(4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl}oxy}-2-(tetracosanoyloxy)propoxy}phosphinic acid'	b'PE(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17S)/24:0)'	HMDB02 84527	C51H90NO10P	
		907.6302351	0.0025 649	Redox	b'(2-{{(2R)-2-{{{{(8Z,11Z,14Z)-5,6-dihydroxydocosa-8,11,14-trienoyl}oxy}-3-{{(10Z,13Z,16Z)-tricosanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'}	b'PC(22:3(10Z,13Z,16Z)/20:3(8Z,11Z,14Z)-2OH(5,6))'	HMDB02 88117	C51H90NO10P	
		907.6302351	0.0025 649	Redox	b'(2-{{(2R)-3-{{{{(8Z,11Z,14Z)-5,6-dihydroxydocosa-8,11,14-trienoyl}oxy}-2-{{(10Z,13Z,16Z)-tricosanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'}	b'PC(20:3(8Z,11Z,14Z)-2OH(5,6)/22:3(10Z,13Z,16Z))'	HMDB02 88118	C51H90NO10P	
3	931.51	932.5262235	0.0013	Proton	b'[(2R)-3-(octadecanoyloxy)-2-{{{{(5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxydocosa-7,9,11,13,17-pentaenoyl}oxy}propoxy}({{1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl}oxy)]phosphinic acid'	b'PI(18:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 76410	C47H81O16P	
6	98	932.5262235	0.0013	Proton	b'[(2R)-2-(octadecanoyloxy)-3-{{{{(5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxydocosa-7,9,11,13,17-pentaenoyl}oxy}propoxy}({{1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl}oxy)]phosphinic acid'	b'PI(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02	C47H81O16P	

			765	ation	pentahydroxycyclohexyl]oxy))phosphinic acid'	3OH(5,6,15)/18:0)	76411		
932.5262235	0.0013	Proton	765	ation	b'[(1R,6R,12Z,15R,18R,19S,20R,21R,22R,23S,24R)-3,18,20,21,22,23,24-heptahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8,16-trioxo-2,4,7-trioxa-3lambda5-phosphabicyclo[13.6.3]tetracos-12-en-6-yl)methyl (11Z)-octadec-11-enoate'	b'PI(18:1(11Z)/PGE2)'	HMDB02 76468	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'(1R,6R,13Z,16R,19R,20S,21R,22R,23R,24S,25R)-3,19,21,22,23,24,25-heptahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9,17-trioxo-2,4,8-trioxa-3lambda5-phosphabicyclo[14.6.3]pentacos-13-en-6-yl (11Z)-octadec-11-enoate'	b'PI(PGE2/18:1(11Z))'	HMDB02 76469	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'[(1R,6R,12Z,15S,16S,19R,20R,21R,22R,23S,24R)-3,16,20,21,22,23,24-heptahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8,18-trioxo-2,4,7-trioxa-3lambda5-phosphabicyclo[13.6.3]tetracos-12-en-6-yl)methyl (11Z)-octadec-11-enoate'	b'PI(18:1(11Z)/PGD2)'	HMDB02 76470	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'(1R,6R,13Z,16S,17S,20R,21R,22R,23R,24S,25R)-3,17,21,22,23,24,25-heptahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9,19-trioxo-2,4,8-trioxa-3lambda5-phosphabicyclo[14.6.3]pentacos-13-en-6-yl (11Z)-octadec-11-enoate'	b'PI(PGD2/18:1(11Z))'	HMDB02 76471	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'[(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-[[[(5S,6S,7E,9E,11Z,13E,15S)-5,6,15-trihydroxycosa-7,9,11,13-tetraenyl]oxy]propoxy]([[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy))phosphinic acid'	b'PI(18:1(11Z)/20:4(7E,9E,11Z,13E)-3OH(5S,6R,15S))'	HMDB02 76484	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'[(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-[[[(5R,6R,7E,9E,11Z,13E,15R)-5,6,15-trihydroxycosa-7,9,11,13-tetraenyl]oxy]propoxy]([[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy))phosphinic acid'	b'PI(20:4(7E,9E,11Z,13E)-3OH(5S,6R,15S)/18:1(11Z))'	HMDB02 76485	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'[(1R,6R,12Z,15R,18R,19S,20R,21R,22R,23S,24R)-3,18,20,21,22,23,24-heptahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8,16-trioxo-2,4,7-trioxa-3lambda5-phosphabicyclo[13.6.3]tetracos-12-en-6-yl)methyl (9Z)-octadec-9-enoate'	b'PI(18:1(9Z)/PGE2)'	HMDB02 76572	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'(1R,6R,13Z,16R,19R,20S,21R,22R,23R,24S,25R)-3,19,21,22,23,24,25-heptahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9,17-trioxo-2,4,8-trioxa-3lambda5-phosphabicyclo[14.6.3]pentacos-13-en-6-yl (9Z)-octadec-9-enoate'	b'PI(PGE2/18:1(9Z))'	HMDB02 76573	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'[(1R,6R,12Z,15S,16S,19R,20R,21R,22R,23S,24R)-3,16,20,21,22,23,24-heptahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8,18-trioxo-2,4,7-trioxa-3lambda5-phosphabicyclo[13.6.3]tetracos-12-en-6-yl)methyl (9Z)-octadec-9-enoate'	b'PI(18:1(9Z)/PGD2)'	HMDB02 76574	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'(1R,6R,13Z,16S,17S,20R,21R,22R,23R,24S,25R)-3,17,21,22,23,24,25-heptahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9,19-trioxo-2,4,8-trioxa-3lambda5-phosphabicyclo[14.6.3]pentacos-13-en-6-yl (9Z)-octadec-9-enoate'	b'PI(PGD2/18:1(9Z))'	HMDB02 76575	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'[(2R)-3-[(9Z)-octadec-9-enoyloxy]-2-[[[(5S,6S,7E,9E,11Z,13E,15S)-5,6,15-trihydroxycosa-7,9,11,13-tetraenyl]oxy]propoxy]([[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy))phosphinic acid'	b'PI(18:1(9Z)/20:4(7E,9E,11Z,13E)-3OH(5S,6R,15S))'	HMDB02 76588	C47H81O16P	
932.5262235	0.0013	Proton	765	ation	b'[(2R)-2-[(9Z)-octadec-9-enoyloxy]-3-[[[(5R,6R,7E,9E,11Z,13E,15R)-5,6,15-trihydroxycosa-7,9,11,13-tetraenyl]oxy]propoxy]([[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy))phosphinic acid'	b'PI(20:4(7E,9E,11Z,13E)-3OH(5S,6R,15S)/18:1(9Z))'	HMDB02 76589	C47H81O16P	
932.5262235	0.0013	Proton			b'[(1R,6R,12E,15S,16S,18R,19S,20R,21R,22R,23S,24R)-3,16,18,20,21,22,23,24-octahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8-dioxo-2,4,7-trioxa-3lambda5-	b'PI(18:2(9Z,12Z)/PGF2alpha)'	HMDB02	C47H81O16P	

			765	ation	phosphabicyclo[13.6.3]tetracos-12-en-6-yl)methyl (9Z,12Z)-octadeca-9,12-dienoate'		76682		
		932.5262235	0.0013	Proton	b'[(1R,6R,13E,16S,17S,19R,20S,21R,22R,23R,24S,25R)-3,17,19,21,22,23,24,25-octahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9-dioxo-2,4,8-trioxa-3lambda5-	b'PI(PGF2alpha/18:2(9Z,12Z))'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[14.6.3]pentacos-en-6-yl (9Z,12Z)-octadeca-9,12-dienoate'		76683		
		932.5262235	0.0013	Proton	b'[(1R,6R,15R,18R,19S,20R,21R,22R,23S,24R)-3,18,20,21,22,23,24,25-heptahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8,16-trioxo-2,4,7-trioxa-3lambda5-	b'PI(18:2(9Z,12Z)/PGE1)'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[13.6.3]tetracosan-6-yl)methyl (9Z,12Z)-octadeca-9,12-dienoate'		76743		
		932.5262235	0.0013	Proton	b'[(1R,6R,16R,19R,20S,21R,22R,23R,24S,25R)-3,19,21,22,23,24,25-heptahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9,17-trioxo-2,4,8-trioxa-3lambda5-	b'PI(PGE1/18:2(9Z,12Z))'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[14.6.3]pentacosan-6-yl (9Z,12Z)-octadeca-9,12-dienoate'		76744		
		932.5262235	0.0013	Proton	b'[(1R,6R,15S,16S,19R,20R,21R,22R,23S,24R)-3,16,20,21,22,23,24,25-heptahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8,18-trioxo-2,4,7-trioxa-3lambda5-	b'PI(18:2(9Z,12Z)/PGD1)'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[13.6.3]tetracosan-6-yl)methyl (9Z,12Z)-octadeca-9,12-dienoate'		76745		
		932.5262235	0.0013	Proton	b'[(1R,6R,16S,17S,20R,21R,22R,23R,24S,25R)-3,17,21,22,23,24,25-heptahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9,19-trioxo-2,4,8-trioxa-3lambda5-	b'PI(PGD1/18:2(9Z,12Z))'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[14.6.3]pentacosan-6-yl (9Z,12Z)-octadeca-9,12-dienoate'		76746		
		932.5262235	0.0013	Proton	b'[(1R,6R,15S,16S,18R,19S,20R,21R,22R,23S,24R)-3,16,18,20,21,22,23,24-octahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8-dioxo-2,4,7-trioxa-3lambda5-	b'PI(18:3(6Z,9Z,12Z)/PGF1alpha)'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[13.6.3]tetracosan-6-yl)methyl (6Z,9Z,12Z)-octadeca-6,9,12-trienoate'		76851		
3 7 0	949.52 79	932.5262235	0.0013	Proton	b'[(1R,6R,16S,17S,19R,20S,21R,22R,23R,24S,25R)-3,17,19,21,22,23,24,25-octahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9-dioxo-2,4,8-trioxa-3lambda5-	b'PI(PGF1alpha/18:3(6Z,9Z,12Z))'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[14.6.3]pentacosan-6-yl (6Z,9Z,12Z)-octadeca-6,9,12-trienoate'		76852		
		932.5262235	0.0013	Proton	b'[(1R,6R,15S,16S,18R,19S,20R,21R,22R,23S,24R)-3,16,18,20,21,22,23,24-octahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8-dioxo-2,4,7-trioxa-3lambda5-	b'PI(18:3(9Z,12Z,15Z)/PGF1alpha)'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[13.6.3]tetracosan-6-yl)methyl (9Z,12Z,15Z)-octadeca-9,12,15-trienoate'		76955		
		932.5262235	0.0013	Proton	b'[(1R,6R,16S,17S,19R,20S,21R,22R,23R,24S,25R)-3,17,19,21,22,23,24,25-octahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9-dioxo-2,4,8-trioxa-3lambda5-	b'PI(PGF1alpha/18:3(9Z,12Z,15Z))'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[14.6.3]pentacosan-6-yl (9Z,12Z,15Z)-octadeca-9,12,15-trienoate'		76956		
		932.5262235	0.0013	Proton	b'[(1R,6R,10Z,13R,14S,16R,17S,18R,19R,20R,21S,22R)-3,14,16,18,19,20,21,22-octahydroxy-17-[(1E,3R)-3-hydroxyoct-1-en-1-yl]-3,8-dioxo-2,4,7-trioxa-3lambda5-	b'PI(20:2(11Z,14Z)/5-iso PGF2VI)'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[11.6.3]docos-10-en-6-yl)methyl (11Z,14Z)-icosa-11,14-dienoate'		77215		
		932.5262235	0.0013	Proton	b'[(1R,6R,11Z,14R,15S,17R,18S,19R,20R,21R,22S,23R)-3,15,17,19,20,21,22,23-octahydroxy-18-[(1E,3R)-3-hydroxyoct-1-en-1-yl]-3,9-dioxo-2,4,8-trioxa-3lambda5-	b'PI(5-iso PGF2VI/20:2(11Z,14Z))'	HMDB02	C47H81O16P	
			765	ation	phosphabicyclo[12.6.3]tricos-11-en-6-yl (11Z,14Z)-icosa-11,14-dienoate'		77216		
		950.5367882	0.0010	Proton	b'[(1R,6R,15S,16S,18R,19S,20R,21R,22R,23S,24R)-3,16,18,20,21,22,23,24-octahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8,13-trioxo-2,4,7-trioxa-3lambda5-	b'PI(18:1(11Z)/6 keto-PGF1alpha)'	HMDB02	C47H83O17P	
			882	ation	phosphabicyclo[13.6.3]tetracosan-6-yl)methyl (11Z)-octadec-11-enoate'		76472		
		950.5367882	0.0010	Proton	b'[(1R,6R,16S,17S,19R,20S,21R,22R,23R,24S,25R)-3,17,19,21,22,23,24,25-octahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9,14-trioxo-2,4,8-trioxa-3lambda5-	b'PI(6 keto-PGF1alpha/18:1(11Z))'	HMDB02	C47H83O17P	

3	965.51		882	ation	phosphabicyclo[14.6.3]pentacosan-6-yl (11Z)-octadec-11-enoate'		76473		
		950.5367882	0.0010 882	Proton ation	b'[(1S,6R,12Z,15S,16S,20R,21S,22R,23R,24S,25R)-3,16,18,21,22,23,24,25-octahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8-dioxo-2,4,7,19-tetraoxa-3lambda5-phosphabicyclo[13.7.3]pentacos-12-en-6-yl]methyl (11Z)-octadec-11-enoate'	b'PI(18:1(11Z)/TXB2)'	HMDB02 76482	C47H83O17P	
		950.5367882	0.0010 882	Proton ation	b'(1S,6R,13Z,16S,17S,21R,22S,23R,24R,25S,26R)-3,17,19,22,23,24,25,26-octahydroxy-21-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9-dioxo-2,4,8,20-tetraoxa-3lambda5-phosphabicyclo[14.7.3]hexacos-13-en-6-yl (11Z)-octadec-11-enoate'	b'PI(TXB2/18:1(11Z))'	HMDB02 76483	C47H83O17P	
		950.5367882	0.0010 882	Proton ation	b'[(1R,6R,15S,16S,18R,19S,20R,21R,22R,23S,24R)-3,16,18,20,21,22,23,24-octahydroxy-19-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8,13-trioxo-2,4,7-trioxa-3lambda5-phosphabicyclo[13.6.3]tetracosan-6-yl]methyl (9Z)-octadec-9-enoate'	b'PI(18:1(9Z)/6 keto-PGF1alpha)'	HMDB02 76576	C47H83O17P	
		950.5367882	0.0010 882	Proton ation	b'(1R,6R,16S,17S,19R,20S,21R,22R,23R,24S,25R)-3,17,19,21,22,23,24,25-octahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9,14-trioxo-2,4,8-trioxa-3lambda5-phosphabicyclo[14.6.3]pentacosan-6-yl (9Z)-octadec-9-enoate'	b'PI(6 keto-PGF1alpha/18:1(9Z))'	HMDB02 76577	C47H83O17P	
		950.5367882	0.0010 882	Proton ation	b'[(1S,6R,12Z,15S,16S,20R,21S,22R,23R,24S,25R)-3,16,18,21,22,23,24,25-octahydroxy-20-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,8-dioxo-2,4,7,19-tetraoxa-3lambda5-phosphabicyclo[13.7.3]pentacos-12-en-6-yl]methyl (9Z)-octadec-9-enoate'	b'PI(18:1(9Z)/TXB2)'	HMDB02 76586	C47H83O17P	
		950.5367882	0.0010 882	Proton ation	b'(1S,6R,13Z,16S,17S,21R,22S,23R,24R,25S,26R)-3,17,19,22,23,24,25,26-octahydroxy-21-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3,9-dioxo-2,4,8,20-tetraoxa-3lambda5-phosphabicyclo[14.7.3]hexacos-13-en-6-yl (9Z)-octadec-9-enoate'	b'PI(TXB2/18:1(9Z))'	HMDB02 76587	C47H83O17P	
7 1	965.51	966.5234597	4.03E-05	Proton ation	b'[{(1R,3S)-3-({(2R)-2-[(10Z,13Z,16Z,19Z)-docosa-10,13,16,19-tetraenoyloxy]-3-(hexadecanoyloxy)propoxy}(hydroxy)phosphoryl}oxy)-2,4,5,6-tetrahydroxycyclohexyl}oxy] phosphonic acid'	b'PIP(16:0/22:4(10Z,13Z,16Z,19Z))'	HMDB00 09922	C47H84O16P2	
		966.5234597	4.03E-05	Proton ation	b'[{(1R,3S)-3-({(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-(hexadecanoyloxy)propoxy}(hydroxy)phosphoryl}oxy)-2,4,5,6-tetrahydroxycyclohexyl}oxy] phosphonic acid'	b'PIP(16:0/22:4(7Z,10Z,13Z,16Z))'	HMDB00 09936	C47H84O16P2	
		966.5234597	4.03E-05	Proton ation	b'[{(1R,5S)-2,3,4,6-tetrahydroxy-5-({hydroxy[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-(octadecanoyloxy)propoxy}phosphoryl}oxy)cyclohexyl}oxy] phosphonic acid'	b'PIP(18:0/20:4(5Z,8Z,11Z,14Z))'	HMDB00 09956	C47H84O16P2	
		966.5234597	4.03E-05	Proton ation	b'[{(1R,5S)-2,3,4,6-tetrahydroxy-5-({hydroxy[(2R)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-3-(octadecanoyloxy)propoxy}phosphoryl}oxy)cyclohexyl}oxy] phosphonic acid'	b'PIP(18:0/20:4(8Z,11Z,14Z,17Z))'	HMDB00 09957	C47H84O16P2	
		966.5234597	4.03E-05	Proton ation	b'[{(1R,5S)-2,3,4,6-tetrahydroxy-5-({hydroxy[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy}phosphoryl}oxy)cyclohexyl}oxy] phosphonic acid'	b'PIP(18:1(11Z)/20:3(5Z,8Z,11Z))'	HMDB00 09965	C47H84O16P2	C00 626
		966.5234597	4.03E-05	Proton ation	b'[{(1R,5S)-2,3,4,6-tetrahydroxy-5-({hydroxy[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy}phosphoryl}oxy)cyclohexyl}oxy] phosphonic acid'	b'PIP(18:1(11Z)/20:3(8Z,11Z,14Z))'	HMDB00 09966	C47H84O16P2	C00 626
		966.5234597	4.03E-05	Proton	b'[{(1R,5S)-2,3,4,6-tetrahydroxy-5-({hydroxy[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy}phosphoryl}oxy)cyclohexyl}oxy] phosphonic acid'	b'PIP(18:1(9Z)/20:3(5Z,8Z,11Z))'	HMDB00	C47H84O16P2	

			05	ation	acid'		09978		
966.5234597	4.03E-05	Proton		ation	b'{{{1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl}oxy)cyclohexyl}oxy}phosphonic acid'	b'PIP(18:1(9Z)/20:3(8Z,11Z,14Z))'	HMDB0009979	C47H84O16P2	
966.5234597	4.03E-05	Proton		ation	b'{{{1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphoryl}oxy)cyclohexyl}oxy}phosphonic acid'	b'PIP(18:2(9Z,12Z)/20:2(11Z,14Z))'	HMDB0009990	C47H84O16P2	C00626
966.5234597	4.03E-05	Proton		ation	b'{{{1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphoryl}oxy)cyclohexyl}oxy}phosphonic acid'	b'PIP(20:2(11Z,14Z)/18:2(9Z,12Z))'	HMDB0010004	C47H84O16P2	C00626
966.5234597	4.03E-05	Proton		ation	b'{{{1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphoryl}oxy)cyclohexyl}oxy}phosphonic acid'	b'PIP(20:3(5Z,8Z,11Z)/18:1(11Z))'	HMDB0010007	C47H84O16P2	C00626
966.5234597	4.03E-05	Proton		ation	b'{{{1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(8Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl}oxy)cyclohexyl}oxy}phosphonic acid'	b'PIP(20:3(8Z,8Z,11Z)/18:1(9Z))'	HMDB0010008	C47H84O16P2	C00626
966.5234597	4.03E-05	Proton		ation	b'{{{1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphoryl}oxy)cyclohexyl}oxy}phosphonic acid'	b'PIP(20:3(8Z,11Z,14Z)/18:1(11Z))'	HMDB0010012	C47H84O16P2	C00626
966.5234597	4.03E-05	Proton		ation	b'{{{1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl}oxy)cyclohexyl}oxy}phosphonic acid'	b'PIP(20:3(8Z,11Z,14Z)/18:1(9Z))'	HMDB0010013	C47H84O16P2	C00626
966.5234597	4.03E-05	Proton		ation	b'{{{1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphoryl}oxy)cyclohexyl}oxy}phosphonic acid'	b'PIP(20:4(5Z,8Z,11Z,14Z)/18:0)'	HMDB0010016	C47H84O16P2	C00626
966.5234597	4.03E-05	Proton		ation	b'{{{1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphoryl}oxy)cyclohexyl}oxy}phosphonic acid'	b'PIP(20:4(8Z,11Z,14Z,17Z)/18:0)'	HMDB0010020	C47H84O16P2	C00626
966.5234597	4.03E-05	Proton		ation	b'{{{1R,3S)-3-[(2R)-3-[(10Z,13Z,16Z,19Z)-docosa-10,13,16,19-tetraenoyloxy]-2-(hexadecanoyloxy)propoxy](hydroxy)phosphoryl}oxy)-2,4,5,6-tetrahydroxycyclohexyl}oxy}phosphonic acid'	b'PIP(22:4(10Z,13Z,16Z,19Z)/16:0)'	HMDB0010027	C47H84O16P2	
966.5234597	4.03E-05	Proton		ation	b'{{{1R,3S)-3-[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(hexadecanoyloxy)propoxy](hydroxy)phosphoryl}oxy)-2,4,5,6-tetrahydroxycyclohexyl}oxy}phosphonic acid'	b'PIP(22:4(7Z,10Z,13Z,16Z)/16:0)'	HMDB0010028	C47H84O16P2	C00626
966.5234606	3.94E-05	Proton		ation	b'[(2S)-2-hydroxy-3-(hydroxy[(2R)-3-[(18-methylcosanoyl)oxy]-2-[(5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxycosa-7,9,11,13,17-pentaenoyl]oxy]propoxy]phosphoryl}oxy)propoxy]phosphonic acid'	b'PGP(a-21:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB0074647	C47H84O16P2	

		966.5234606	3.94E-05	Protonation	b'[(2S)-2-hydroxy-3-({hydroxy[(2R)-2-[(18-methylicosanoyl)oxy]-3-{{(5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl}oxy}propoxy]phosphoryl}oxy)propoxy]phosphonic acid'	b'PGP(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/a-21:0)'	HMDB02 74648	C47H84O16P2	
		966.5234606	3.94E-05	Protonation	b'[(2S)-2-hydroxy-3-({hydroxy[(2R)-3-[(19-methylicosanoyl)oxy]-2-{{(5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl}oxy}propoxy]phosphoryl}oxy)propoxy]phosphonic acid'	b'PGP(i-21:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 75788	C47H84O16P2	
		966.5234606	3.94E-05	Protonation	b'[(2S)-2-hydroxy-3-({hydroxy[(2R)-2-[(19-methylicosanoyl)oxy]-3-{{(5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl}oxy}propoxy]phosphoryl}oxy)propoxy]phosphonic acid'	b'PGP(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/i-21:0)'	HMDB02 75789	C47H84O16P2	
372	1037.6251	1038.634335	0.001435	Protonation	b'(2-{{[(2R)-2-{{[(2R)-2-amino-3-{{(4S,5R,6E,8E,10Z,13Z)-1-carboxy-4-hydroxynonadeca-6,8,10,13-tetraen-5-yl}sulfanyl}propanoyl}oxy}-3-{{[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propyl phosphono]oxy}ethyl}trimethylazanium'	b'PC(DiMe(13,5)/LTE4)'	HMDB02 89147	C55H95N2O12P S	
		1038.634335	0.001435	Protonation	b'(2-{{[(2R)-3-{{[(2R)-2-amino-3-{{(4S,5R,6E,8E,10Z,13Z)-1-carboxy-4-hydroxynonadeca-6,8,10,13-tetraen-5-yl}sulfanyl}propanoyl}oxy}-2-{{[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propyl phosphono]oxy}ethyl}trimethylazanium'	b'PC(LTE4/DiMe(13,5))'	HMDB02 89148	C55H95N2O12P S	

3.2. Table S2. Detected metabolites in the brain of a control mouse by electron transfer ionization.

Table S2. Detected metabolites in the brain of a control mouse by electron transfer ionization.									
N o.	m/z	Monoisotopic _Mass	Error(Da)	Mode	IUPAC_Name	Name	Accession Number	Chemical_F ormula	KE GG
1	124.00 63	125.0146638	0.0005 638	Protona tion	b'2-aminoethane-1-sulfonic acid'	b'Taurine'	HMDB00 00251	C2H7NO3S	C002 45
		125.0146643	0.0005 643	Protona tion	b'(2-aminoethylidene)dihydroxy-lambda6-sulfanone'	b'3h-Taurine'	HMDB02 46277	C2H7NO3S	
		125.0146643	0.0005 643	Protona tion	b'1-hydroxyethane-1-sulfonamide'	b'Sulfonamidoethanol'	HMDB02 58596	C2H7NO3S	
2	126.00 19	127.0091845	0.0005 155	Protona tion	b'1-(1,3-thiazol-2-yl)ethan-1-one'	b'2-Acetylthiazole'	HMDB00 32964	C5H5NOS	
		127.009185	0.0005 15	Protona tion	b'4-thia-1-azabicyclo[3.2.0]hept-2-en-7-one'	b'Penem'	HMDB02 56222	C5H5NOS	
		127.009185	0.0005 15	Protona tion	b'1-hydroxy-1,2-dihydropyridine-2-thione'	b'pyrithione'	HMDB02 56986	C5H5NOS	
		127.0091845	0.0005 155	Protona tion	b'(2E)-but-2-enecarbonyl isothiocyanate'	b'Crotonyl isothiocyanate'	HMDB03 02364	C5H5NOS	
3	126.90 38	127.9122935	0.0006 935	Protona tion	b'hydrogen iodide'	b'I(-)'	HMDB00 59634	HI	C055 90
		126.9044684	0.0006 684	Redox	b'iodide'	b'Iodide'	HMDB00 12238	I	C007 08
4	127.04 98	128.0585775	0.0009 775	Protona tion	b'(5S)-5-methyl-1,3-diazinane-2,4-dione'	b'Dihydrothymine'	HMDB00 00079	C5H8N2O2	C009 06
		128.0585775	0.0009 775	Protona tion	b'2-oxopyrrolidine-1-carboxamide'	b'Squamolone'	HMDB00 29874	C5H8N2O2	
		128.0585775	0.0009	Protona	b'3-methylpiperazine-2,5-dione'	b'L-Cyclo(alanylglycyl)'	HMDB00	C5H8N2O2	

			775	tion				31547		
		128.0585775	0.0009 775	Protona tion	b'(3S)-3-aminopiperidine-2,6-dione'	b'Pyroglutamine'	HMDB00 62558	C5H8N2O2		
		128.0585775	0.0009 775	Protona tion	b'3-aminopiperidine-2,6-dione'	b'3-Aminopiperidine-2,6-dione'	HMDB02 42134	C5H8N2O2		
		128.0585775	0.0009 775	Protona tion	b'5-methyl-1,3-diazinane-2,4-dione'	b'5,6-dihydrothymine'	HMDB03 04210	C5H8N2O2	C009 06	
5	128.03 45	129.0425931	0.0002 931	Protona tion	b'(2S)-5-oxopyrrolidine-2-carboxylic acid'	b'Pyroglutamic acid'	HMDB00 00267	C5H7NO3	C018 79	
		129.0425931	0.0002 931	Protona tion	b'4-hydroxy-3,4-dihydro-2H-pyrrole-2-carboxylic acid'	b'Pyrroline hydroxycarboxylic acid'	HMDB00 01369	C5H7NO3	C042 81	
		129.0425931	0.0002 931	Protona tion	b'2-(prop-2-enamido)acetic acid'	b'N-Acryloylglycine'	HMDB00 01843	C5H7NO3		
		129.0425931	0.0002 931	Protona tion	b'3-hydroxy-3,4-dihydro-2H-pyrrole-5-carboxylic acid'	b'1-Pyrroline-4-hydroxy-2-carboxylate'	HMDB00 02234	C5H7NO3	C042 82	
		129.0425931	0.0002 931	Protona tion	b'4-hydroxy-5,5-dimethyl-2,5-dihydro-1,3-oxazol-2-one'	b'dimethadione'	HMDB00 61093	C5H7NO3		
		129.0425931	0.0002 931	Protona tion	b'(2S,4R)-4-hydroxy-3,4-dihydro-2H-pyrrole-2-carboxylic acid'	b'(3R,5S)-1-pyrroline-3-hydroxy-5-carboxylic Acid'	HMDB00 62585	C5H7NO3	C042 81	
		129.0425931	0.0002 931	Protona tion	b'3-hydroxy-1-methylpyrrolidine-2,5-dione'	b'3-Hydroxy-1-methylpyrrolidine-2,5-dione'	HMDB02 45148	C5H7NO3		
		129.0425931	0.0002 931	Protona tion	b'4-oxopyrrolidine-2-carboxylic acid'	b'4-Oxo-L-proline'	HMDB02 46561	C5H7NO3		
		129.0425931	0.0002 931	Protona tion	b'1-methyl-1H-pyrrole-2,3,5-triol'	b'1-Methylpyrrole-2,3,5-triol'	HMDB02 55336	C5H7NO3		
		129.0425931	0.0002	Protona	b'2-oxopyrrolidine-1-carboxylic acid'	b'pyrrolidone carboxylic acid'	HMDB02	C5H7NO3		

6	130.0494		931	tion				57001		
		129.0425931	0.0002 931	Protontion	b'6-oxa-1-azabicyclo[3.1.0]hexane-2-carboxylic acid'	b'(2S)-6-Oxa-1-azabicyclo[3.1.0]hexane-2-carboxylic acid'	HMDB02 60147	C5H7NO3		
		128.0334254	0.0010 746	Redox	b'6-amino-1,3,5-triazine-2,4-diol'	b'Ammelide'	HMDB02 48340	C3H4N4O2	C087	34
		128.0353166	0.0008 166	Redox	b'4-oxopyrrolidine-2-carboxylate'	b'4-Oxoproline'	HMDB03 04793	C5H6NO3		
	130.0494	131.0582432	0.0010 432	Protontion	b'(2S,4R)-4-hydroxypyrrolidine-2-carboxylic acid'	b'4-Hydroxyproline'	HMDB00 00725	C5H9NO3	C011	57
		131.0582432	0.0010 432	Protontion	b'(2S)-2-acetamidopropanoic acid'	b'N-Acetyl-L-alanine'	HMDB00 00766	C5H9NO3		
		131.0582432	0.0010 432	Protontion	b'2-propanamidoacetic acid'	b'Propionylglycine'	HMDB00 00783	C5H9NO3		
		131.0582432	0.0010 432	Protontion	b'5-amino-4-oxopentanoic acid'	b'5-Aminolevulinic acid'	HMDB00 01149	C5H9NO3	C004	30
		131.0582432	0.0010 432	Protontion	b'(2S)-2-amino-5-oxopentanoic acid'	b'L-Glutamic gamma-semialdehyde'	HMDB00 02104	C5H9NO3	C011	65
		131.0582432	0.0010 432	Protontion	b'(2R,3S)-3-hydroxypyrrolidine-2-carboxylic acid'	b'3-Hydroxy-L-proline'	HMDB00 02113	C5H9NO3	C043	97
		131.0582432	0.0010 432	Protontion	b'5-amino-2-oxopentanoic acid'	b'5-Amino-2-oxopentanoic acid'	HMDB00 06272	C5H9NO3	C011	10
		131.0582432	0.0010 432	Protontion	b'(2S,3S)-3-hydroxypyrrolidine-2-carboxylic acid'	b'Trans-3-hydroxy-L-proline'	HMDB00 59659	C5H9NO3	C051	47
		131.0582432	0.0010 432	Protontion		b'cis-4-Hydroxy-D-proline'	HMDB00 60460	C5H9NO3	C034	40

		131.0582432	0.0010 432	Protone tion	b'3-acetamidopropanoic acid'	b'N-Acetyl-beta-alanine'	HMDB00 61880	C5H9NO3	C010 73
		131.0582432	0.0010 432	Protone tion	b'(2S,4S)-4-hydroxypyrrolidine-2-carboxylic acid'	b'cis-4-Hydroxyproline'	HMDB02 40251	C5H9NO3	C010 15
		131.0582432	0.0010 432	Protone tion	b'1-hydroxypyrrolidine-2-carboxylic acid'	b'N-Hydroxy-L-proline'	HMDB02 43901	C5H9NO3	
		131.0582432	0.0010 432	Protone tion	b'1-hydroxypyrrolidine-3-carboxylic acid'	b'1-Hydroxypyrrolidine-3-carboxylic acid'	HMDB02 43902	C5H9NO3	
		131.0582432	0.0010 432	Protone tion	b'2-amino-4-oxopentanoic acid'	b'2-Amino-4-oxopentanoic acid'	HMDB02 44991	C5H9NO3	
		131.0582432	0.0010 432	Protone tion	b'3-hydroxypyrrolidine-2-carboxylic acid'	b'3-Hydroxyproline'	HMDB02 45903	C5H9NO3	
		131.0582432	0.0010 432	Protone tion	b'4-amino-5-oxopentanoic acid'	b'4-Amino-5-oxo-pentanoic acid'	HMDB02 46349	C5H9NO3	
		131.0582432	0.0010 432	Protone tion	b'4-carbamoylbutanoic acid'	b'Glutamic acid'	HMDB02 46746	C5H9NO3	
		131.0582432	0.0010 432	Protone tion	b'5-hydroxypyrrolidine-2-carboxylic acid'	b'5-Hydroxyproline'	HMDB02 46811	C5H9NO3	
		131.0582432	0.0010 432	Protone tion	b'2-acetamidopropanoic acid'	b'N-Acetyl-DL-alanine'	HMDB02 55053	C5H9NO3	
7	131.02 29	132.0335056	0.0028 056	Protone tion	b'5-fluoro-1,3-diazinane-2,4-dione'	b'5,6-Dihydro-5-fluorouracil'	HMDB00 60402	C4H5FN2O2	C166 30
		132.0323628	0.0016 628	Protone tion	b'3H-indazol-3-one'	b'3H-Indazol-3-one'	HMDB02 46268	C7H4N2O	
		132.0335056	0.0028 056	Protone tion	b'1-fluoro-1,3-diazinane-2,4-dione'	b'Fluorodihydrouracil'	HMDB02 52374	C4H5FN2O2	

		131.0218577	0.0010 423	Redox	b'2-iminobutanedioic acid'	b'Iminoaspartic acid'	HMDB00 01131	C4H5NO4	C058 40
		131.0218577	0.0010 423	Redox	b'3-(C-hydroxycarbonimidoyl)-2-oxopropanoic acid'	b'2-Oxosuccinamate'	HMDB00 60350	C4H5NO4	C023 62
8	132.02 94	133.0375077	0.0003 077	Protona tion	b'(2S)-2-aminobutanedioic acid'	b'L-Aspartic acid'	HMDB00 00191	C4H7NO4	C000 49
		133.0375077	0.0003 077	Protona tion	b'(2R)-2-aminobutanedioic acid'	b'D-Aspartic acid'	HMDB00 06483	C4H7NO4	C004 02
		133.0375077	0.0003 077	Protona tion	b'2-[(carboxymethyl)amino]acetic acid'	b'Iminodiacetic acid'	HMDB00 11753	C4H7NO4	C199 11
9	133.01 33	134.0215233	0.0004 233	Protona tion	b'(2S)-2-hydroxybutanedioic acid'	b'Malic acid'	HMDB00 00156	C4H6O5	C001 49
		134.0215233	0.0004 233	Protona tion	b'(2R)-2-hydroxybutanedioic acid'	b'D-Malic acid'	HMDB00 31518	C4H6O5	C004 97
		134.0215233	0.0004 233	Protona tion	b'dimethyl dicarbonate'	b'Velcorin'	HMDB00 32872	C4H6O5	
		134.0223917	0.0012 917	Protona tion	b'3,3-dimethyl-1,2-dithiolane'	b'3,3-Dimethyl-1,2-dithiolane'	HMDB00 38974	C5H10S2	
		134.0223917	0.0012 917	Protona tion	b'2-methylthiolane-2-thiol'	b'Tetrahydro-2-methyl-2-thiophenethiol'	HMDB00 39789	C5H10S2	
		134.0223917	0.0012 917	Protona tion	b'2-methylthiolane-3-thiol'	b'Tetrahydro-2-methyl-3-thiophenethiol'	HMDB00 39790	C5H10S2	
		134.0190214	0.0020 786	Protona tion	b'1-benzothiophene'	b'Benzoithiophene'	HMDB02 49003	C8H6S	
		134.0215233	0.0004 233	Protona tion	b'2-(carboxymethoxy)acetic acid'	b'Diglycolic acid'	HMDB02 51283	C4H6O5	

		134.0228607	0.0017 607	Protone tion	b'3H-pyrazolo[4,3-d]pyrimidin-3-one'	b'Pyrazolopyrimidinone'	HMDB02 56955	C5H2N4O	
		134.0215233	0.0004 233	Protone tion	b'2-(carboxyoxo)propanoic acid'	b'2-Carboxyoxopropanoic acid'	HMDB02 57720	C4H6O5	
		134.0223927	0.0012 927	Protone tion	b'cyclopentane-1,2-dithiol'	b'1,2-Dimercaptocyclopentane'	HMDB03 02171	C5H10S2	
10	134.02 17	135.0320284	0.0025 284	Protone tion		b'2-Benzoxazolol'	HMDB00 32931	C7H5NO2	
		135.0320284	0.0025 284	Protone tion	b'2,3-dihydro-1,2-benzoxazol-3-one'	b'Benzo[d]isoxazol-3-ol'	HMDB02 49006	C7H5NO2	
11	134.04 59	135.0544952	0.0007 952	Protone tion	b'7H-purin-6-amine'	b'Adenine'	HMDB00 00034	C5H5N5	C001 47
		135.0531578	0.0005 422	Protone tion	b'2-amino-3,4-dihydroxybutanoic acid'	b'(+)-threo-2-Amino-3,4-dihydroxybutanoic acid'	HMDB00 29389	C4H9NO4	
		135.0558379	0.0021 379	Protone tion	b'4-(hydroxymethyl)benzene-1-diazonium'	b'4-(Hydroxymethyl)benzenediazonium(1+)	HMDB00 32593	C7H7N2O	
		135.0544952	0.0007 952	Protone tion	b'1H-pyrazolo[3,4-d]pyrimidin-4-amine'	b'1H-Pyrazolo[3,4-d]pyrimidin-4-amine'	HMDB02 44899	C5H5N5	
		135.0544952	0.0007 952	Protone tion	b'2,3-dihydro-1H-purin-2-imine'	b'2-Aminopurine'	HMDB02 45025	C5H5N5	
		135.0544952	0.0007 952	Protone tion	b'9H-purin-9-amine'	b'9h-Purin-9-amine'	HMDB02 47703	C5H5N5	
		134.0480128	0.0021 128	Redox	b'1H-indazol-3-ol'	b'1H-Indazol-3-ol'	HMDB02 44883	C7H6N2O	
		134.0480128	0.0021	Redox	b'N-iminobenzamide'	b'Benzoyl hydrazone'	HMDB02	C7H6N2O	

			128				49039		
12	135.03	136.0385108	0.0007 108	Protone tion	b'7H-purin-6-ol'	b'Hypoxanthine'	HMDB00 00157	C5H4N4O	C002 62
		136.0371734	0.0006 266	Protone tion	b'(2R,3R)-2,3,4-trihydroxybutanoic acid'	b'Erythronic acid'	HMDB00 00613	C4H8O5	
		136.0371734	0.0006 266	Protone tion	b'(2R,3S)-2,3,4-trihydroxybutanoic acid'	b'Threonine acid'	HMDB00 00943	C4H8O5	C016 20
		136.0385108	0.0007 108	Protone tion	b'1H,2H,4H-pyrazolo[3,4-d]pyrimidin-4-one'	b'Allopurinol'	HMDB00 14581	C5H4N4O	
		136.0380418	0.0002 418	Protone tion	b'pentane-1-dithioperoxol'	b'1-Pentanesulfenothioic acid'	HMDB00 31160	C5H12S2	
		136.0380418	0.0002 418	Protone tion	b'1-(ethylidisulfanyl)propane'	b'Ethyl propyl disulfide'	HMDB00 33053	C5H12S2	
		136.0380418	0.0002 418	Protone tion	b'2-(ethylidisulfanyl)propane'	b'Ethyl isopropyl disulfide'	HMDB00 33054	C5H12S2	
		136.0385108	0.0007 108	Protone tion	b'7H-purin-2-ol'	b'2-Hydroxypurine'	HMDB02 45165	C5H4N4O	
		136.0371734	0.0006 266	Protone tion	b'2,3,4-trihydroxybutanoic acid'	b'2,3,4-Trihydroxybutanoic acid'	HMDB02 45425	C4H8O5	C016 20
		136.0385108	0.0007 108	Protone tion	b'9H-purin-9-ol'	b'9H-Purine-9-ol'	HMDB02 47704	C5H4N4O	
		136.0398534	0.0020 534	Protone tion	b'4-aminobenzoate'	b'4-aminobenzoate'	HMDB03 04171	C7H6NO2	
13	136.00 61	137.0146643	0.0007 643	Protone tion	b'2-amino-3-sulfinylpropanoic acid'	b'S-oxocysteine'	HMDB02 57422	C3H7NO3S	
		137.0146643	0.0007	Protone	b'2-amino-3-hydroxypropane(thioperoxoic) OS-acid'	b'serine thiol'	HMDB02	C3H7NO3S	

			643	tion			58249		
14	136.99	138.0081952	0.0008 952	Protona tion	b'[(2R,3S)-3-methyloxiran-2-yl]phosphonic acid'	b'Fosfomicin'	HMDB00 14966	C3H7O4P	C064 54
	95	138.0081957	0.0008 957	Protona tion	b'(3-methyloxiran-2-yl)phosphonic acid'	b'(2S,3R)-3-Methyloxiran-2-ylphosphonic acid'	HMDB02 42559	C3H7O4P	
15	138.97	139.9874598	0.0004 598	Protona tion	b'(acetyloxy)phosphonic acid'	b'Acetylphosphate'	HMDB00 01494	C2H5O5P	C002 27
	92	139.9874598	0.0004 598	Protona tion	b'2-phosphonoacetic acid'	b'Phosphonoacetate'	HMDB00 04110	C2H5O5P	C056 82
16	140.01	141.0190943	0.0008 943	Protona tion	b'(2-aminoethoxy)phosphonic acid'	b'O-Phosphoethanolamine'	HMDB00 00224	C2H8NO4P	C003 46
		141.0190947	0.0008 947	Protona tion	b'(1-aminoethoxy)phosphonic acid'	b'Aminoethanol phosphate'	HMDB02 48314	C2H8NO4P	
		140.0109586	0.0005 586	Redox	b'2-[(2E)-5-oxo-2,5-dihydrofuran-2-ylidene]acetic acid'	b'cis-4-Carboxymethylenebut-2-en-4-olide'	HMDB00 60459	C6H4O4	C044 31
		140.0109586	0.0005 586	Redox	b'2-(5-oxo-2,5-dihydrofuran-2-ylidene)acetic acid'	b'trans-4-Carboxymethylenebut-2-en-4-olide'	HMDB00 60518	C6H4O4	
17	144.03	145.0375077	0.0002 923	Protona tion	b'4-carbamoyl-2-oxobutanoic acid'	b'2-Keto-glutaramic acid'	HMDB00 01552	C5H7NO4	C009 40
18	145.06	146.0691422	0.0007 422	Protona tion	b'(2S)-2-amino-4-carbamoylbutanoic acid'	b'L-Glutamine'	HMDB00 00641	C5H10N2O3	C000 64
		146.0691422	0.0007 422	Protona tion	b'(2S)-3-(carbamoylamino)-2-methylpropanoic acid'	b'Ureidoisobutyric acid'	HMDB00 02031	C5H10N2O3	C051 00
		146.0691422	0.0007 422	Protona tion	b'(2R)-2-amino-4-carbamoylbutanoic acid'	b'D-Glutamine'	HMDB00 03423	C5H10N2O3	C008 19
		146.0691422	0.0007	Protona	b'2-[(2S)-2-aminopropanamido]acetic acid'	b'Alanylglycine'	HMDB00	C5H10N2O3	

19	146.04		422	tion			06899		
		146.0691422	0.0007 422	Protone tion	b'5,6-dihydroxy-1,3-diazepan-2-one'	b'Cyclic Urea'	HMDB02 50626	C5H10N2O3	
		146.0691422	0.0007 422	Protone tion	b'2-(2-aminoacetamido)propanoic acid'	b'Glycyl-D-Alanine'	HMDB02 52875	C5H10N2O3	
		146.0691422	0.0007 422	Protone tion	b'2-(2-amino-N-methylacetamido)acetic acid'	b'Glycylsarcosine'	HMDB02 52887	C5H10N2O3	
		146.0691422	0.0007 422	Protone tion	b'2-[(2R)-2-amino-1-hydroxypropylidene]amino]acetic acid'	b'D-Alanyl glycine'	HMDB03 02832	C5H10N2O3	
		146.0691422	0.0007 422	Protone tion	b'3-(carbamoylamino)-2-methylpropanoic acid'	b'3-urcido-isobutyrate'	HMDB03 04156	C5H10N2O3	C051 00
	146.04 46	147.0531578	0.0007 578	Protone tion	b'(2S)-2-aminopentanedioic acid'	b'L-Glutamic acid'	HMDB00 00148	C5H9NO4	C000 25
		147.0531578	0.0007 578	Protone tion	b'(2R)-2-(methylamino)butanedioic acid'	b'N-Methyl-D-aspartic acid'	HMDB00 02393	C5H9NO4	C122 69
		147.0531578	0.0007 578	Protone tion	b'(2S)-2-acetamido-3-hydroxypropanoic acid'	b'N-Acetylserine'	HMDB00 02931	C5H9NO4	
		147.0531578	0.0007 578	Protone tion	b'(2S)-3-(acetyloxy)-2-aminopropanoic acid'	b'O-Acetylserine'	HMDB00 03011	C5H9NO4	C009 79
		147.0531578	0.0007 578	Protone tion	b'(2R)-2-aminopentanedioic acid'	b'D-Glutamic acid'	HMDB00 03339	C5H9NO4	C002 17
		147.0531578	0.0007 578	Protone tion	b'(2S,4R)-2-amino-4-hydroxy-5-oxopentanoic acid'	b'L-4-Hydroxyglutamate semialdehyde'	HMDB00 06556	C5H9NO4	C059 38
		147.0531578	0.0007 578	Protone tion	b'3-[(carboxymethyl)amino]propanoic acid'	b'3-(Carboxymethylamino)propanoic acid'	HMDB00 33550	C5H9NO4	
		147.0531578	0.0007	Protone	b'2-aminopentanedioic acid'	b'DL-Glutamate'	HMDB00	C5H9NO4	C003

			578	tion			60475		02
		147.0531578	0.0007 578	Protona tion	b'2-[(2S)-2-hydroxypropanamido]acetic acid'	b'N-lactoyl-Glycine'	HMDB00 62183	C5H9NO4	
		147.0531578	0.0007 578	Protona tion	b'2-amino-5-hydroxy-4-oxopentanoic acid'	b'5-Hydroxy-4-oxo-L-norvaline'	HMDB02 46802	C5H9NO4	
		147.0531578	0.0007 578	Protona tion	b'2-aminopropanoyl ethaneperoxoate'	b'Alanine acetate'	HMDB02 48101	C5H9NO4	
		147.0531578	0.0007 578	Protona tion	b'2-(methylamino)butanedioic acid'	b'N-Methyl-DL-aspartic acid'	HMDB02 55174	C5H9NO4	
20	150.02 16	151.0303138	0.0009 138	Protona tion	b'2-amino-3-methanesulfinylpropanoic acid'	b'(S)C(S)S-S-Methylcysteine sulfoxide'	HMDB00 29432	C4H9NO3S	
		151.026943	0.0024 57	Protona tion	b'3-nitrobenzaldehyde'	b'3-Nitrobenzaldehyde'	HMDB02 45945	C7H5NO3	
		151.026943	0.0024 57	Protona tion	b'4-nitrobenzaldehyde'	b'4-Nitrobenzaldehyde'	HMDB02 46531	C7H5NO3	
21	150.04 07	151.0494098	0.0009 098	Protona tion	b'2-amino-6,7-dihydro-3H-purin-6-one'	b'Guanine'	HMDB00 00132	C5H5N5O	C002 42
		151.0494098	0.0009 098	Protona tion	b'6-amino-7H-purin-2-ol'	b'2-Hydroxyadenine'	HMDB00 00403	C5H5N5O	
		151.0494098	0.0009 098	Protona tion	b'6-amino-7H-purin-8-ol'	b'8-Hydroxyadenine'	HMDB00 00542	C5H5N5O	
		151.0455705	0.0029 295	Protona tion	b'4-methylbenzene-1-carbothioamide'	b'4-Methylbenzenecarbothioamide'	HMDB02 45645	C8H9NS	
		151.0494098	0.0009 098	Protona tion	b'2-amino-8,9-dihydro-7H-purin-8-one'	b'8-Oxo-7,8-dihydrodeoxyguanine'	HMDB02 47457	C5H5N5O	
		151.0489418	0.0004	Protona	b'2-amino-4-(methylsulfonyl)butane-1-thiol'	b'(S)-2-Amino-4-methylsulfonyl-	HMDB02	C5H13NS2	

			418	tion		butane-1-thiol'	49989		
		151.0455705	0.0029 295	Protona tion	b'N-phenylethanethioamide'	b'Thioacetanilide'	HMDB02 58998	C8H9NS	
		150.0429274	0.0022 274	Redox	b'5-(prop-1-yn-1-yl)-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'5-Propynyluracil'	HMDB02 46840	C7H6N2O2	
22	151.02 48	152.0334254	0.0008 254	Protona tion	b'2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Xanthine'	HMDB00 00292	C5H4N4O2	C003 85
		152.0334254	0.0008 254	Protona tion	b'1H,2H,4H,5H,6H-pyrazolo[3,4-d]pyrimidine-4,6-dione'	b'Oxypurinol'	HMDB00 00786	C5H4N4O2	C075 99
		152.0334254	0.0008 254	Protona tion	b'6,7,8,9-tetrahydro-3H-purine-6,8-dione'	b'6,8-Dihydroxypurine'	HMDB00 01182	C5H4N4O2	
23	152.00 13	153.0095784	0.0004 784	Protona tion	b'(2R)-2-amino-3-[(R)-sulfinio]propanoic acid'	b'3-Sulfinioalanine'	HMDB00 00996	C3H7NO4S	C006 06
		153.0095789	0.0004 789	Protona tion	b'2-amino-3-sulfinopropanoic acid'	b'Cysteine sulfinic acid'	HMDB02 50705	C3H7NO4S	
		152.0027164	0.0014 164	Redox	b'1,2,3-benzodioxaphosphinine'	b'Benzodioxaphosphorin'	HMDB02 49013	C7H5O2P	
24	152.99 45	154.0031103	0.0008 103	Protona tion	b'2-phosphonopropanoic acid'	b'2-Phosphonopropionic acid'	HMDB02 45296	C3H7O5P	
		152.9918199	0.0026 801	Redox	b'(2S)-2-amino-3-disulfanypropanoic acid'	b'Thiocysteine'	HMDB00 03585	C3H7NO2S2	C019 62
		152.9918208	0.0026 792	Redox	b'2-amino-3-sulfanylpropane(thioperoxoic) OS-acid'	b'Cysteine thiol'	HMDB02 50706	C3H7NO2S2	
		152.9918208	0.0026 792	Redox	b'3-sulfanyl-2-(sulfanylamino)propanoic acid'	b'Sulfhydryl cysteine'	HMDB02 58584	C3H7NO2S2	
25	153.06	154.0742276	0.0011	Protona	b'(8aS)-octahydropyrrolo[1,2-a]piperazine-1,4-dione'	b'(S)-Hexahydropyrrolo[1,2-a]pyrazine-	HMDB02	C7H10N2O2	

53		276	tion			1,4-dione'	42137		
	154.0742276	0.0011 276	Protona tion	b'6-propyl-1,2,3,4-tetrahydropyrimidine-2,4-dione'		b'6-n-Propyluracil'	HMDB02 47095	C7H10N2O2	
	154.0742276	0.0011 276	Protona tion	b'octahydropyrrolo[1,2-a]piperazine-1,4-dione'		b'Hexahydropyrrolo[1,2-a]piperazine-1,4-dione'	HMDB02 53141	C7H10N2O2	
	154.0742276	0.0011 276	Protona tion	b'hepta-2,5-dienediamide'		b'Methylene bisacrylamide'	HMDB02 54632	C7H10N2O2	
	154.0742276	0.0011 276	Protona tion	b'N- {[(1-hydroxyprop-2-en-1-ylidene)amino]methyl}prop-2-enimidic acid'		b''N,N'- METHYLENEBISACRYLAMIDE''	HMDB02 55276	C7H10N2O2	
	153.0650599	0.0002 401	Redox	b'N-(4,6-diaminopyrimidin-5-yl)formamide'		b'FAPy-adenine'	HMDB00 04816	C5H7N5O	C065 02
26	153.99 76	155.0074709	0.0020 709	Protona tion	b'1-amino-3-sulfanylpropane-1-sulfonic acid'	b'(1R)-1-Amino-3-sulfanylpropane-1-sulfonic acid'	HMDB02 42354	C3H9NO2S2	
		155.0040996	0.0013 004	Protona tion	b'2-sulfanylidene-1,2-dihydropyridine-3-carboxylic acid'	b'2-Mercaptionicotinic acid'	HMDB02 45193	C6H5NO2S	
		155.0040996	0.0013 004	Protona tion	b'3-sulfanylpyridine-2-carboxylic acid'	b'3-Mercaptopicolinic acid'	HMDB02 45916	C6H5NO2S	
		155.0040996	0.0013 004	Protona tion	b'4-nitrobenzene-1-thiol'	b'4-Nitrothiophenol'	HMDB02 46550	C6H5NO2S	
		153.9952203	0.0023 797	Redox	b'3,3-bis(chloromethyl)oxetane'	b'3,3-Bis(chloromethyl)oxetane'	HMDB02 45991	C5H8Cl2O	
27	154.04 99	155.0582432	0.0005 432	Protona tion	b'3-amino-4-methoxybenzene-1,2-diol'	b'methoxycatecholamine'	HMDB02 54544	C7H9NO3	
28	154.06 07	155.0694765	0.0009 765	Protona tion	b'(2S)-2-amino-3-(1H-imidazol-5-yl)propanoic acid'	b'L-Histidine'	HMDB00 00177	C6H9N3O2	C001 35
		155.0694765	0.0009	Protona	b'2-amino-3-(1H-pyrazol-1-yl)propanoic acid'	b'L-2-Amino-3-(1-pyrazolyl)propanoic	HMDB00	C6H9N3O2	

		765	tion			acid'	34267		
155.0694765	0.0009	Protona		b'2-amino-3-(1H-imidazol-5-yl)propanoic acid'	b'D-Histidine'	HMDB02	C6H9N3O2	C007	
	765	tion				50763		68	
155.0713678	0.0028	Protona		b'2-methyl-4-oxo-5-propyl-4,5-dihydrofuran-3-olate'	b'4-hydroxy-5-methyl-2-propyl-3(2H)-furanone'	HMDB03	C8H11O3		
	678	tion				04179			
154.0629942	0.0022	Redox		b'4-(2-hydroxyethyl)benzene-1,2-diol'	b'Hydroxytyrosol'	HMDB00	C8H10O3		
	942					05784			
154.0629942	0.0022	Redox		b'3-(hydroxymethyl)-5-methoxyphenol'	b'Sylvopinol'	HMDB00	C8H10O3		
	942					30570			
154.0629942	0.0022	Redox		b'4-(hydroxymethyl)-2-methoxyphenol'	b'4-Hydroxy-3-methoxybenzenemethanol'	HMDB00	C8H10O3	C063	
	942					32012		17	
154.0629942	0.0022	Redox		b'2,6-dimethoxyphenol'	b'2,6-Dimethoxyphenol'	HMDB00	C8H10O3	C107	
	942					34158		87	
154.0629942	0.0022	Redox		b'propyl furan-2-carboxylate'	b'Propyl 2-furoate'	HMDB00	C8H10O3		
	942					37724			
154.0629942	0.0022	Redox		b'furan-2-ylmethyl propanoate'	b'2-Furanylmethyl propanoate'	HMDB00	C8H10O3		
	942					37728			
154.0629942	0.0022	Redox		b'3,5-dimethoxyphenol'	b'3,5-Dimethoxyphenol'	HMDB00	C8H10O3		
	942					59966			
154.0629942	0.0022	Redox		b'6-ethyl-3-hydroxy-2-methyl-4H-pyran-4-one'	b'6-Ethyl-3-hydroxy-2-methyl-4-pyrone'	HMDB02	C8H10O3		
	942					47055			
154.0629942	0.0022	Redox		b'octahydro-2-benzofuran-1,3-dione'	b'Hexahydrophthalic anhydride'	HMDB02	C8H10O3		
	942					53140			
154.0629942	0.0022	Redox		b'3a-hydroxy-2,3,3a,6,7,7a-hexahydro-1-benzofuran-6-one'	b'Halleridone'	HMDB03	C8H10O3		
	942					02803			
154.0629942	0.0022	Redox		b'4-acetyl-2,5-dimethyl-2,3-dihydrofuran-3-one'	b'4-Acetyl-2,5-dimethyl-3(2H)-	HMDB03	C8H10O3		

			942			furanone'	03185		
29	155.08 17	156.0898776	0.0003 776	Protone tion	b'2-ethyl-1-[(C-hydroxycarbonimidoyl)imino]but-2-en-1-ol'	b'(2-Ethylcrotonoyl)urea'	HMDB02 42468	C7H12N2O2	
30	156.02 9	157.0375077	0.0007 077	Protone tion	b'(2Z,4E)-5-aminohexa-2,4-dienedioic acid'	b'2-Aminomuconic acid'	HMDB00 01241	C6H7NO4	C022 20
		157.0375077	0.0007 077	Protone tion	b'2,5-dioxopyrrolidin-1-yl acetate'	b'Succinimidyl acetate'	HMDB02 44630	C6H7NO4	
		157.0375077	0.0007 077	Protone tion	b'1,2-dimethyl-3,4-dioxazetidine-2-carboxylic acid'	b'(2S)-1,2-Dimethyl-3,4-dioxazetidine-2-carboxylic acid'	HMDB02 57875	C6H7NO4	
		156.02834	0.0006 6	Redox	b'4,6-dioxo-1,4,5,6-tetrahydro-1,3,5-triazine-2-carboxamide'	b'Allantoxanamide'	HMDB02 47204	C4H4N4O3	
31	158.92 37	158.92535	0.0016 5	Redox	b'terbium'	b'Terbium'	HMDB03 03932	Tb	
32	159.02 82	160.0371734	0.0011 734	Protone tion	b'2-oxohexanedioic acid'	b'Oxoadipic acid'	HMDB00 00225	C6H8O5	C003 22
		160.0371734	0.0011 734	Protone tion	b'3-oxohexanedioic acid'	b'3-Oxoadipic acid'	HMDB00 00398	C6H8O5	C008 46
		160.0346709	0.0013 291	Protone tion	b'naphthalene-2-thiol'	b'2-Naphthalenethiol'	HMDB00 29689	C10H8S	
		160.0371734	0.0011 734	Protone tion	b'2-methyl-4-oxopentanedioic acid'	b'2-Methyl-4-oxopentanedioic acid'	HMDB00 39447	C6H8O5	
		160.0346714	0.0013 286	Protone tion	b'1-benzothiepine'	b'1-Benzothiepin'	HMDB02 43832	C10H8S	
		160.0371734	0.0011 734	Protone tion	b'2-[(2-oxopropanoyl)oxy]propanoic acid'	b'2-(2-Oxopropanoyloxy)propanoic acid'	HMDB02 58108	C6H8O5	
		160.0382705	0.0022	Protone	b'2-hydroxy-2,3-dimethylbutanedioate'	b'(2R,3S)-2,3-dimethylmalate'	HMDB03	C6H8O5	

			705	tion			03969		
33	160.06 13	161.0688078	0.0002 922	Protone tion	b'(2S)-2-aminohexanedioic acid'	b'Aminoadipic acid'	HMDB00 00510	C6H11NO4	C009 56
		161.0688078	0.0002 922	Protone tion	b'4-(acetyloxy)-2-aminobutanoic acid'	b'Acetylhomoserine'	HMDB00 29423	C6H11NO4	
		161.0688078	0.0002 922	Protone tion	b'2-[(1-carboxyethyl)amino]propanoic acid'	b'('xc2'xb1)-2,2'-Iminobispropanoic acid''	HMDB00 33747	C6H11NO4	C032 10
		161.0688078	0.0002 922	Protone tion	b'(2S)-2-amino-5-methoxy-5-oxopentanoic acid'	b'Glutamic acid gamma-methyl ester'	HMDB00 61715	C6H11NO4	
		161.0688078	0.0002 922	Protone tion	b'(2S,3R)-2-acetamido-3-hydroxybutanoic acid'	b'N-Acetylthreonine'	HMDB00 62557	C6H11NO4	
		161.0688078	0.0002 922	Protone tion	b'(2S)-2-(methylamino)pentanedioic acid'	b'N-methyl-L-glutamic Acid'	HMDB00 62660	C6H11NO4	C010 46
		161.0688078	0.0002 922	Protone tion	b'2-[(1,4-dihydroxybutylidene)amino]acetic acid'	b'hydroxybutyrylglycine'	HMDB00 94716	C6H11NO4	
		161.0688078	0.0002 922	Protone tion	b'3-aminohexanedioic acid'	b'3-Aminoadipic acid'	HMDB02 45812	C6H11NO4	
		161.0688078	0.0002 922	Protone tion	b'2-carboxy-2-(trimethylazaniumyl)acetate'	b'Carboxybetaine'	HMDB02 49655	C6H11NO4	
		161.0688078	0.0002 922	Protone tion	b'2-aminohexanedioic acid'	b'2-Aminoadipic acid'	HMDB03 02754	C6H11NO4	C009 56
		160.0636629	0.0023 629	Redox	b'1H-indole-2-carboxamide'	b'1H-Indole-2-carboxamide'	HMDB02 44889	C9H8N2O	
		160.0636629	0.0023 629	Redox	b'1H-indole-5-carboxamide'	b'1H-Indole-5-carboxamide'	HMDB02 44894	C9H8N2O	
		160.0636629	0.0023	Redox	b'2-methylquinazolin-4-ol'	b'2-Methyl-4(3H)-quinazolinone'	HMDB02	C9H8N2O	

			629				45238		
		160.0636629	0.0023 629	Redox	b'1H-1,4-benzodiazepin-3-ol'	b'3-Hydroxy-1,4-benzodiazepine'	HMDB02 45882	C9H8N2O	
		160.0636629	0.0023 629	Redox	b'N-(quinolin-4-yl)hydroxylamine'	b'4-Quinolinamine, N-hydroxy-	HMDB02 46579	C9H8N2O	
		160.0636629	0.0023 629	Redox	b'5-amino-1,2-dihydroisoquinolin-1-one'	b'5-Aminoisoquinolin-1(2H)-one'	HMDB02 46750	C9H8N2O	
34	160.84 11	160.8415003	0.0004 003	Redox	b'iron(3+) ion trichloride'	b'Iron(III) chloride'	HMDB03 03404	Cl3Fe	
35	163.01 49	164.0255633	0.0028 633	Protone tion	b'2-amino-4-(nitrososulfanyl)butanoic acid'	b'S-Nitrosohomocysteine'	HMDB02 57418	C4H8N2O3S	
		163.0125553	0.0023 447	Redox	b'1-isothiocyanato-3-methanesulfinylpropane'	b'3-Methylsulfinylpropyl isothiocyanate'	HMDB00 06095	C5H9NOS2	
36	164.03 7	165.0459644	0.0011 644	Protone tion	b'(2S)-2-amino-4-methanesulfinylbutanoic acid'	b'Methionine sulfoxide'	HMDB00 02005	C5H11NO3S	C029 89
		165.0425931	0.0022 069	Protone tion	b'7-hydroxy-6-methyl-1H,3H-furo[3,4-c]pyridin-1-one'	b'4-Pyridoxolactone'	HMDB00 03454	C8H7NO3	C009 71
		165.0425931	0.0022 069	Protone tion	b'2-formamidobenzoic acid'	b'Formylanthranilic acid'	HMDB00 04089	C8H7NO3	C056 53
		165.0425931	0.0022 069	Protone tion	b'7-hydroxy-6-methyl-1H,3H-furo[3,4-c]pyridin-3-one'	b'5-Pyridoxolactone'	HMDB00 04291	C8H7NO3	C060 52
		165.0425931	0.0022 069	Protone tion	b'3-hydroxy-3,5,6,7-tetrahydro-2H-indole-5,6-dione'	b'Noradrenochrome'	HMDB00 13030	C8H7NO3	
		165.0425931	0.0022 069	Protone tion	b'6-methoxy-2,3-dihydro-1,3-benzoxazol-2-one'	b'6-Methoxy-2(3H)-benzoxazolone'	HMDB00 36582	C8H7NO3	
		165.0459639	0.0011	Protone	b'2-amino-3-(ethanesulfinyl)propanoic acid'	b'Ethiin'	HMDB00	C5H11NO3S	

37	164.04 93		639	tion			37057		
		165.0425931	0.0022 069	Protona tion	b'2-hydroxy-3,4-dihydro-2H-1,4-benzoxazin-3-one'	b'(R)-2-Hydroxy-2H-1,4-benzoxazin-3(4H)-one'	HMDB00 38318	C8H7NO3	C157 69
		165.0459644	0.0011 644	Protona tion	b'2-amino-2-hydroxy-4-(methylsulfonyl)butanoic acid'	b'2-Hydroxy-L-methionine'	HMDB02 46915	C5H11NO3S	
		165.0459639	0.0011 639	Protona tion	b'2-amino-4-methanesulfinylbutanoic acid'	b'D-Methionine (S)-S-oxide'	HMDB02 50776	C5H11NO3S	
		165.0425931	0.0022 069	Protona tion	b'1-(4-nitrophenyl)ethan-1-one'	b"4'-Nitroacetophenone"	HMDB02 56052	C8H7NO3	C028 03
		165.0425931	0.0022 069	Protona tion	b'2-(C-hydroxycarbonimidoyl)benzoic acid'	b'Phthamic acid'	HMDB02 56499	C8H7NO3	
		164.038591	0.0015 91	Redox	b'3-fluoro-1,2-dihydro-1,8-naphthyridin-2-one'	b'Fluoronaphthyridone'	HMDB02 52387	C8H5FN2O	
	164.04 93	164.0473441	0.0019 559	Redox	b'2-oxo-3-phenylpropanoic acid'	b'Phenylpyruvic acid'	HMDB00 00205	C9H8O3	C001 66
		164.0473441	0.0019 559	Redox	b'(2E)-3-(3-hydroxyphenyl)prop-2-enoic acid'	b'm-Coumaric acid'	HMDB00 01713	C9H8O3	C126 21
		164.0473441	0.0019 559	Redox	b'(2E)-3-(4-hydroxyphenyl)prop-2-enoic acid'	b'4-Hydroxycinnamic acid'	HMDB00 02035	C9H8O3	C008 11
		164.0473441	0.0019 559	Redox	b'(2E)-3-(2-hydroxyphenyl)prop-2-enoic acid'	b'2-Hydroxycinnamic acid'	HMDB00 02641	C9H8O3	C017 72
		164.0473441	0.0019 559	Redox	b'(2Z)-2-hydroxy-3-phenylprop-2-enoic acid'	b'Enol-phenylpyruvate'	HMDB00 12225	C9H8O3	C027 63
		164.0473441	0.0019 559	Redox	b'(2Z)-3-(4-hydroxyphenyl)prop-2-enoic acid'	b'cis-p-Coumaric acid'	HMDB00 30677	C9H8O3	C067 38
		164.0473441	0.0019	Redox	b'(2Z)-3-(2-hydroxyphenyl)prop-2-enoic acid'	b'Coumarinic acid'	HMDB00	C9H8O3	C058

			559					41592		38
		164.0473441	0.0019 559	Redox	b'methyl 2-oxo-2-phenylacetate'		b'Methyl Phenylglyoxalate'	HMDB00 62605	C9H8O3	
		164.0473441	0.0019 559	Redox	b'methyl 4-formylbenzoate'		b'METHYL 4-FORMYLBENZOATE'	HMDB02 54568	C9H8O3	
38	165.04 39	166.0490755	0.0026 245	Protona tion	b'3-methyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'		b'3-Methylxanthine'	HMDB00 01886	C6H6N4O2	C163 57
		166.0490755	0.0026 245	Protona tion	b'7-methyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'		b'7-Methylxanthine'	HMDB00 01991	C6H6N4O2	C163 53
		166.0490755	0.0026 245	Protona tion	b'2-hydroxy-1-methyl-6,9-dihydro-1H-purin-6-one'		b'1-Methylxanthine'	HMDB00 10738	C6H6N4O2	C163 58
		166.0504181	0.0012 819	Protona tion	b'(3,6-dihydroxy-2,3-dihydro-1H-indol-5-yl)oxidanil'		b'Noradrenochrome o-semiquinone'	HMDB00 13029	C8H8NO3	
		166.0490755	0.0026 245	Protona tion	b'9-methyl-2,3,6,9-tetrahydro-1H-purine-2,6-dione'		b'9-Methylxanthine'	HMDB00 59716	C6H6N4O2	
39	166.01 68	167.0218577	0.0027 423	Protona tion	b'pyridine-2,3-dicarboxylic acid'		b'Quinolinic acid'	HMDB00 00232	C7H5NO4	C037 22
		167.0252285	0.0006 285	Protona tion	b'2-amino-4-sulfinobutanoic acid'		b'Homocysteinesulfinic acid'	HMDB00 06462	C4H9NO4S	
		167.0265659	0.0019 659	Protona tion	b'2-amino-6,7-dihydro-3H-purine-6-thione'		b'Thioguanine'	HMDB00 14496	C5H5N5S	C076 48
		167.0218577	0.0027 423	Protona tion	b'pyridine-2,6-dicarboxylic acid'		b'2,6-Pyridinedicarboxylic acid'	HMDB00 33161	C7H5NO4	
		167.0252289	0.0006 289	Protona tion	b'2-acetamidoethane-1-sulfonic acid'		b'N-Acetyltaurine'	HMDB02 40253	C4H9NO4S	
		167.0218576	0.0027	Protona	b'2-nitrobenzoic acid'		b'2-Nitrobenzoic acid'	HMDB02	C7H5NO4	C162

40			424	tion			45255		34
		167.0218576	0.0027 424	Protona tion	b'3-hydroxy-2-nitrobenzaldehyde'	b'3-Hydroxy-2-nitrobenzaldehyde'	HMDB02 45884	C7H5NO4	
		167.0218577	0.0027 423	Protona tion	b'4-nitrobenzoic acid'	b'4-Nitrobenzoic acid'	HMDB02 46532	C7H5NO4	C186 25
		167.0218576	0.0027 424	Protona tion	b'pyridine-3,5-dicarboxylic acid'	b'Pyridine-3,5-dicarboxylic acid'	HMDB02 56966	C7H5NO4	
		167.0229548	0.0016 452	Protona tion	b'(2S)-2,3-dihydropyridine-2,6-dicarboxylate'	b'(S)-2,3-dihydrodipicolinate'	HMDB03 03995	C7H5NO4	
	166.06 5	167.0734993	0.0006 993	Protona tion	b'9H-carbazole'	b'Carbazole'	HMDB02 49614	C12H9N	C080 60
		167.0713678	0.0014 322	Protona tion	b'5-butylidene-2-methyl-4-oxo-4,5-dihydrofuran-3-olate'	b'(2E)-2-butylidene-4-hydroxy-5-methyl-3(2H)-furanone'	HMDB03 03965	C9H11O3	
		167.0713678	0.0014 322	Protona tion	b'6-(2-methylpropyl)-2-oxo-2H-pyran-4-olate'	b'6-isobutyl-4-hydroxy-2-pyrone'	HMDB03 04229	C9H11O3	
		166.0629942	0.0020 058	Redox	b'3-(3-hydroxyphenyl)propanoic acid'	b'3-(3-Hydroxyphenyl)propanoic acid'	HMDB00 00375	C9H10O3	C114 57
		166.0629942	0.0020 058	Redox	b'(2S)-2-hydroxy-3-phenylpropanoic acid'	b'D-Phenyllactic acid'	HMDB00 00563	C9H10O3	C056 07
		166.0629942	0.0020 058	Redox	b'(2R)-2-hydroxy-3-phenylpropanoic acid'	b'L-3-Phenyllactic acid'	HMDB00 00748	C9H10O3	C056 07
		166.0629942	0.0020 058	Redox		b'Phenyllactic acid'	HMDB00 00779	C9H10O3	C014 79
		166.0629942	0.0020 058	Redox	b'2-(4-methoxyphenyl)acetic acid'	b'4-Methoxyphenylacetic acid'	HMDB00 02072	C9H10O3	
		166.0629942	0.0020	Redox	b'3-(4-hydroxyphenyl)propanoic acid'	b'Desaminotyrosine'	HMDB00	C9H10O3	C017

		058					02199		44
166.0629942	0.0020 058	Redox		b'3-phenoxypropanoic acid'		b'3-Phenoxypropionic acid'	HMDB00 02229	C9H10O3	
166.0629942	0.0020 058	Redox		b'2-(4-hydroxy-3-methoxyphenyl)acetaldehyde'		b'Homovanillin'	HMDB00 05175	C9H10O3	C055 81
166.0629942	0.0020 058	Redox		b'3-ethoxy-4-hydroxybenzaldehyde'		b'Ethyl vanillin'	HMDB00 29665	C9H10O3	
166.0629942	0.0020 058	Redox		b'ethyl 2-hydroxybenzoate'		b'Ethyl salicylate'	HMDB00 29817	C9H10O3	
166.0629942	0.0020 058	Redox		b'1-(3,4-dihydroxyphenyl)propan-2-one'		b'3,4-Dihydroxyphenylacetone'	HMDB00 31132	C9H10O3	
166.0629942	0.0020 058	Redox		b'2-methoxyphenyl acetate'		b'Guaicyl acetate'	HMDB00 32030	C9H10O3	
166.0629942	0.0020 058	Redox		b'3,4-dimethoxybenzaldehyde'		b'3,4-Dimethoxybenzaldehyde'	HMDB00 32138	C9H10O3	C022 01
166.0629942	0.0020 058	Redox		b'ethyl 4-hydroxybenzoate'		b'Ethylparaben'	HMDB00 32573	C9H10O3	
166.0629942	0.0020 058	Redox		b'methyl 2-methoxybenzoate'		b'Methyl 2-methoxybenzoate'	HMDB00 32605	C9H10O3	
166.0629942	0.0020 058	Redox		b'methyl 4-methoxybenzoate'		b'Methyl 4-methoxybenzoate'	HMDB00 32639	C9H10O3	
166.0629942	0.0020 058	Redox		b'3-(2-hydroxyphenyl)propanoic acid'		b'3-(2-Hydroxyphenyl)propanoic acid'	HMDB00 33752	C9H10O3	C011 98
166.0629942	0.0020 058	Redox		b'1-(furan-3-yl)pentane-1,4-dione'		b'Ipomeanine'	HMDB00 34243	C9H10O3	
166.0629942	0.0020	Redox		b'(4-methoxyphenyl)methyl formate'		b'4-Methoxybenzyl formate'	HMDB00	C9H10O3	

			058					34993		
166.0629942	0.0020 058	Redox		b'3-hydroxy-1-(4-hydroxyphenyl)propan-1-one'		b'3-Hydroxy-1-(4-hydroxyphenyl)-1-propanone'		HMDB00 40645	C9H10O3	
166.0629942	0.0020 058	Redox		b'ethyl (2Z)-3-(furan-2-yl)prop-2-enoate'		b'Ethyl 2-furanacrylate'		HMDB00 41611	C9H10O3	
166.0629942	0.0020 058	Redox		b'2-(4-hydroxyphenyl)propanoic acid'		b'4-Hydroxyphenyl-2-propionic acid'		HMDB00 41683	C9H10O3	C030 80
166.0629942	0.0020 058	Redox		b'2-(3-methoxyphenyl)acetic acid'		b'3-Methoxyphenylacetic acid'		HMDB00 59969	C9H10O3	
166.0629942	0.0020 058	Redox		b'3,5-dimethoxybenzaldehyde'		b'3,5-Dimethoxybenzaldehyde'		HMDB00 62348	C9H10O3	
166.0629942	0.0020 058	Redox		b'3-hydroxy-2-phenylpropanoic acid'		b'Tropate'		HMDB00 62590	C9H10O3	C014 56
166.0629942	0.0020 058	Redox		b'(3R)-3-hydroxy-3-phenylpropanoic acid'		b'3-Hydroxy-3-phenylpropanoic acid'		HMDB01 24925	C9H10O3	
166.0629942	0.0020 058	Redox		b'4-methyl-1,3,3a,4,5,7a-hexahydro-2-benzofuran-1,3-dione'		b'3-Methyltetrahydrophthalic anhydride'		HMDB02 45936	C9H10O3	
166.0629942	0.0020 058	Redox		b'1-(4-hydroxy-3-methoxyphenyl)ethan-1-one'		b'Acetovanillone'		HMDB02 47918	C9H10O3	C113 80
166.0663655	0.0013 655	Redox		b'hexane-1-sulfonic acid'		b'Hexanesulfonic acid'		HMDB02 53146	C6H14O3S	
166.0629942	0.0020 058	Redox		b'3a-methyl-1,3,3a,4,7,7a-hexahydro-2-benzofuran-1,3-dione'		b'1,2,3,6-Tetrahydromethylphthalic anhydride'		HMDB02 54937	C9H10O3	
166.0629942	0.0020 058	Redox		b'1-(2-hydroxy-4-methoxyphenyl)ethan-1-one'		b'Paeonol'		HMDB02 56081	C9H10O3	C107 12
166.0629942	0.0020	Redox		b'octahydro-1H-indene-1,2,3-trione'		b'3a,4,5,6,7,7a-Hexahydroindene-1,2,3-		HMDB02	C9H10O3	

			058			trione'	60012		
		166.0629942	0.0020 058	Redox	b'2-methoxy-2-phenylacetic acid'	b'Methoxyphenylacetic acid'	HMDB03 01734	C9H10O3	
41	166.97 34	167.9823744	0.0011 744	Protona tion	b'2-(phosphonoxy)prop-2-enoic acid'	b'Phosphoenolpyruvic acid'	HMDB00 00263	C3H5O6P	C000 74
		167.983472	0.0022 72	Protona tion	b'2-hydroxy-3-(phosphonatoxy)propanal'	b'L-glyceraldehyde 3-phosphate'	HMDB03 04402	C3H5O6P	
		168.0687483	0.0011 483	Protona tion	b'9H-pyrido[3,4-b]indole'	b'beta-Carboline'	HMDB00 12897	C11H8N2	C201 57
		168.0687483	0.0011 483	Protona tion	b'6H-pyrrolo[2,3-f]quinoline'	b'1H-Pyrrolo[2,3-f]quinoline'	HMDB02 44904	C11H8N2	
		168.0687483	0.0011 483	Protona tion	b'5H-pyrido[4,3-b]indole'	b'5H-Pyrido[4,3-b]indole'	HMDB02 47024	C11H8N2	
		168.0687483	0.0011 483	Protona tion	b'7H-pyrrolo[2,3-h]quinoline'	b'Pyrroloquinoline'	HMDB02 57007	C11H8N2	
42	167.05 98	167.0582432	0.0015 568	Redox	b'3-hydroxy-5-(hydroxymethyl)-2-methylpyridine-4-carbaldehyde'	b'Pyridoxal'	HMDB00 01545	C8H9NO3	C002 50
		167.0582432	0.0015 568	Redox	b'5-hydroxy-4-(hydroxymethyl)-6-methylpyridine-3-carbaldehyde'	b'Isopyridoxal'	HMDB00 04290	C8H9NO3	C060 51
		167.0582432	0.0015 568	Redox	b'5-hydroxy-2,3,3a,4,5,7a-hexahydro-1H-isoindole-1,3-dione'	b'3alpha,4,5,7alpha-Tetrahydro-5-hydroxy-1H-isoindole-1,3(2H)-dione'	HMDB00 34887	C8H9NO3	
		167.0582432	0.0015 568	Redox	b'4-hydroxy-2,3,3a,4,7,7a-hexahydro-1H-isoindole-1,3-dione'	b'3alpha,4,7,7alpha-Tetrahydro-4-hydroxy-1H-isoindole-1,3(2H)-dione'	HMDB00 34889	C8H9NO3	
		167.0582432	0.0015 568	Redox	b'2-amino-3-methoxybenzoic acid'	b'3-Methoxyanthranilate'	HMDB00 60374	C8H9NO3	C058 31
		167.0582432	0.0015	Redox	b'2-hydroxy-N-(2-hydroxyphenyl)acetamide'	b'2-Hydroxy-N-(2-	HMDB02	C8H9NO3	

			568			hydroxyphenyl)acetamide'	40370		
		167.0582432	0.0015 568	Redox	b'2-amino-2-(4-hydroxyphenyl)acetic acid'	b'4-Hydroxyphenylglycine'	HMDB02 44973	C8H9NO3	
		167.0582432	0.0015 568	Redox	b'2-[(4-hydroxyphenyl)amino]acetic acid'	b'N-(4-Hydroxyphenyl)glycine'	HMDB02 55011	C8H9NO3	
43	167.08 15	168.0898776	0.0005 776	Protone tion	b'4-(aminomethyl)-5-(hydroxymethyl)-2-methylpyridin-3-ol'	b'Pyridoxamine'	HMDB00 01431	C8H12N2O2	C005 34
		168.0898776	0.0005 776	Protone tion	b'1,6-diisocyanatohexane'	b'Hexamethylene diisocyanate'	HMDB02 44241	C8H12N2O2	
		168.0898776	0.0005 776	Protone tion	b'4,5-dimethoxybenzene-1,2-diamine'	b'4,5-Dimethoxybenzene-1,2-diamine'	HMDB02 46610	C8H12N2O2	
		168.0898776	0.0005 776	Protone tion	b'1-(2-hydroxyethyl)-4,6-dimethyl-1,2-dihydropyrimidin-2-one'	b'xymedon'	HMDB02 59943	C8H12N2O2	
		168.0898776	0.0005 776	Protone tion	b'3-methyl-octahydropyrrolol[1,2-a]piperazine-1,4-dione'	b'L,L-Cyclo(propylalanyl)'	HMDB03 03321	C8H12N2O2	
		167.0807099	0.0007 901	Redox	b'2-amino-1,2,3,4,6,7-hexahydropteridin-4-one'	b'2-Amino-2,3,6,7-tetrahydro-1H- pteridin-4-one'	HMDB02 55369	C6H9N5O	
		167.0807099	0.0007 901	Redox	b'2-amino-3,4,5,6,7,8-hexahydropteridin-4-one'	b'tetrahydropterin'	HMDB02 58903	C6H9N5O	
44	168.02 65	169.0351024	0.0008 024	Protone tion	b'sodium 2-amino-4-carboxybutanoate'	b'Monosodium glutamate'	HMDB03 03331	C5H8NNaO4	
		168.02834	0.0018 4	Redox	b'2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'	b'Uric acid'	HMDB00 00289	C5H4N4O3	C003 66
		168.0245007	0.0019 993	Redox	b'2-(phenylsulfonyl)acetic acid'	b'(Phenylthio)acetic acid'	HMDB02 43657	C8H8O2S	
45	168.04	169.0503944	0.0009	Protone	b'[2-(dimethylamino)ethoxy]phosphonic acid'	b'Phosphodimethylethanolamine'	HMDB00	C4H12NO4P	C134

16		944	tion				60244		82
	168.0422587	0.0006 587	Redox	b'2-(2,5-dihydroxyphenyl)acetic acid'	b'Homogentisic acid'	HMDB00 00130	C8H8O4	C005 44	
	168.0422587	0.0006 587	Redox	b'4-hydroxy-3-methoxybenzoic acid'	b'Vanillic acid'	HMDB00 00484	C8H8O4	C066 72	
	168.0422587	0.0006 587	Redox	b'2-hydroxy-2-(3-hydroxyphenyl)acetic acid'	b'3-Hydroxymandelic acid'	HMDB00 00750	C8H8O4		
	168.0422587	0.0006 587	Redox	b'2-hydroxy-2-(4-hydroxyphenyl)acetic acid'	b'p-Hydroxymandelic acid'	HMDB00 00822	C8H8O4	C115 27	
	168.0422587	0.0006 587	Redox	b'2-(3,4-dihydroxyphenyl)acetic acid'	b'3,4-Dihydroxybenzeneacetic acid'	HMDB00 01336	C8H8O4	C011 61	
	168.0422587	0.0006 587	Redox	b'2-hydroxy-5-methoxybenzoic acid'	b'5-Methoxysalicylic acid'	HMDB00 01868	C8H8O4		
	168.0422587	0.0006 587	Redox	b'2-(3,4-dihydroxyphenyl)-2-hydroxyacetaldehyde'	b'3,4-Dihydroxymandelaldehyde'	HMDB00 06242	C8H8O4	C055 77	
	168.0422587	0.0006 587	Redox	b'1-(2,4,6-trihydroxyphenyl)ethan-1-one'	b"2',4',6'-Trihydroxyacetophenone"	HMDB00 29644	C8H8O4		
	168.0422587	0.0006 587	Redox	b'2,6-dimethoxycyclohexa-2,5-diene-1,4-dione'	b'2,6-Dimethoxy-1,4-benzoquinone'	HMDB00 29673	C8H8O4	C103 31	
	168.0422587	0.0006 587	Redox	b'3-acetyl-4-hydroxy-6-methyl-2H-pyran-2-one'	b'3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one'	HMDB00 33129	C8H8O4		
	168.0422587	0.0006 587	Redox	b'2,5-dimethoxycyclohexa-2,5-diene-1,4-dione'	b'Thermophilin'	HMDB00 34335	C8H8O4	C016 92	
	168.0422587	0.0006 587	Redox	b'2-hydroxy-3-methoxybenzoic acid'	b'3-Methoxysalicylic acid'	HMDB00 59713	C8H8O4		
	168.0422587	0.0006	Redox	b'3-hydroxy-4-methoxybenzoic acid'	b'Isovanillic acid'	HMDB00	C8H8O4		

			587					60003		
		168.0422587	0.0006 587	Redox	b'2-(3,5-dihydroxyphenyl)acetic acid'	b'3, 5-Dihydroxyphenylacetic acid'	HMDB00 94709	C8H8O4		
		168.0422587	0.0006 587	Redox	b'2-(1-hydroxy-4-oxocyclohexa-2,5-dien-1-yl)acetic acid'	b'Quinolacetic acid'	HMDB02 40257	C8H8O4		
		168.0422587	0.0006 587	Redox	b'4,10-dioxatricyclo[5.2.1.0^{2,6}]decane-3,5-dione'	b'4,7-Epoxyisobenzofuran-1,3-dione, hexahydro-, (3aR,4S,7R,7aS)-rel-'	HMDB02 45751	C8H8O4		
		168.0422587	0.0006 587	Redox	b'3-acetyl-6-methyl-3,4-dihydro-2H-pyran-2,4-dione'	b'Dehydroacetic acid'	HMDB02 50943	C8H8O4		
		168.0422587	0.0006 587	Redox	b'1-(2,4-dihydroxyphenyl)-2-hydroxyethan-1-one'	b'1-(2,4-Dihydroxyphenyl)-2- hydroxyethanone'	HMDB02 57566	C8H8O4		
		168.0434016	0.0018 016	Redox	b'3-fluoro-5-(hydroxymethyl)oxolane-2,3,4-triol'	b'(3R,4R,5R)-3-Fluoro-5- (hydroxymethyl)oxolane-2,3,4-triol'	HMDB02 57780	C5H9FO5		
		168.0422587	0.0006 587	Redox	b'3,4-dihydroxyphenyl acetate'	b'(3,4-Dihydroxyphenyl) acetate'	HMDB02 58013	C8H8O4		
		168.0422587	0.0006 587	Redox	b'2,2-dihydroxy-2-phenylacetic acid'	b'2,2-Dihydroxy-2-phenylacetic acid'	HMDB02 58145	C8H8O4		
		168.0422587	0.0006 587	Redox	b'3,5-dihydroxy-4-methoxybenzaldehyde'	b'3,5-Dihydroxy-4- methoxybenzaldehyde'	HMDB03 01768	C8H8O4		
46	170.09 24	170.0942943	0.0018 943	Redox	b'1-(furan-3-yl)pentane-1,4-diol'	b'1,4-Isopentadiol'	HMDB00 30471	C9H14O3		
		170.0942943	0.0018 943	Redox	b'(3Z)-hex-3-en-1-yl 2-oxopropanoate'	b'cis-3-Hexenyl pyruvate'	HMDB00 38276	C9H14O3		
		170.091609	0.0007 91	Redox	b' {N-[(1-oxopropan-2-ylidene)amino]carbamimidamido}methanimidamide'	b'Methylglyoxal-bis-guanyldiazone'	HMDB02 58082	C5H10N6O		
47	171.00	172.0136745	0.0006	Protona	b'[(2R)-2,3-dihydroxypropoxy]phosphonic acid'	b'Glycerol 3-phosphate'	HMDB00	C3H9O6P	C000	

48	52		745	tion			00126		93
		172.0136745	0.0006 745	Protona tion	b'[(1,3-dihydroxypropan-2-yl)oxy]phosphonic acid'	b'beta-Glycerophosphoric acid'	HMDB00 02520	C3H9O6P	C029 79
		172.0136745	0.0006 745	Protona tion	b'(2,3-dihydroxypropoxy)phosphonic acid'	b'Glycerophosphoric acid'	HMDB02 52849	C3H9O6P	C031 89
		171.0023845	0.0028 155	Redox	b'(1R)-1-amino-3-sulfanylpropane-1-sulfonic acid'	b'L-Homocysteine sulfonic acid'	HMDB00 02238	C3H9NO3S2	
	173.00 82	174.0164379	0.0004 379	Protona tion	b'(1Z)-prop-1-ene-1,2,3-tricarboxylic acid'	b'cis-Aconitic acid'	HMDB00 00072	C6H6O6	C004 17
		174.0164379	0.0004 379	Protona tion	b'(1E)-prop-1-ene-1,2,3-tricarboxylic acid'	b'trans-Aconitic acid'	HMDB00 00958	C6H6O6	C023 41
		174.0164379	0.0004 379	Protona tion	b'(5R)-5-[(1S)-1,2-dihydroxyethyl]oxolane-2,3,4-trione'	b'Dehydroascorbic acid'	HMDB00 01264	C6H6O6	C054 22
		174.0173063	0.0013 063	Protona tion	b'2,5-dimethyl-3-(methylsulfonyl)furan'	b'2,5-Dimethyl-3-(methylthio)furan'	HMDB00 40200	C7H10OS2	
		174.0164379	0.0004 379	Protona tion	b'5-(1,2-dihydroxyethyl)-4-hydroxy-2,3-dihydrofuran-2,3-dione'	b'Dehydroascorbide(1-)'	HMDB00 62706	C6H6O6	
		174.0164379	0.0004 379	Protona tion	b'prop-1-ene-1,2,3-tricarboxylic acid'	b'Aconitic acid'	HMDB02 47961	C6H6O6	
		174.0150788	0.0009 212	Protona tion	b'4-methylbenzene-1-sulfonyl fluoride'	b'p-TOLUENESULFONYL FLUORIDE'	HMDB02 56057	C7H7FO2S	
		174.0150788	0.0009 212	Protona tion	b'phenylmethanesulfonyl fluoride'	b'Phenylmethylsulfonyl fluoride'	HMDB02 56652	C7H7FO2S	C067 47
49	174.03	175.0480724	0.0008 724	Protona tion	b'(2S)-2-acetamidobutanedioic acid'	b'N-Acetyl-L-aspartic acid'	HMDB00 00812	C6H9NO5	C010 42
	94	175.0480724	0.0008	Protona	b'(2S)-2-formamidopentanedioic acid'	b'N-Formyl-L-glutamic acid'	HMDB00	C6H9NO5	C010

			724	tion			03470		45
		175.0489408	0.0017 408	Protona tion	b'1-isothiocyanato-5-(methylsulfanyl)pentane'	b'Berteroin'	HMDB00 31577	C7H13NS2	
		175.0480724	0.0008 724	Protona tion	b'2-(2-carboxyacetamido)propanoic acid'	b'D-N-(Carboxyacetyl)alanine'	HMDB00 39163	C6H9NO5	
		175.0480724	0.0008 724	Protona tion	b'2-amino-3-oxohexanedioic acid'	b'2-Amino-3-oxoadipate'	HMDB00 60273	C6H9NO5	C055 20
		175.0480724	0.0008 724	Protona tion	b'2-aminopropanoyl 2-oxopropaneperoxoate'	b'Alanine pyruvate'	HMDB02 48106	C6H9NO5	
		175.0480724	0.0008 724	Protona tion	b'methyl [(2-methoxy-2-oxoethyl)carbamoyl]formate'	b'Dimethyloxalylglycine'	HMDB02 51540	C6H9NO5	
		175.04557	0.0016 3	Protona tion	b'2-methyl-1,4-dihydroquinoline-4-thione'	b'2-Methylquinoline'	HMDB03 02391	C10H9NS	
50	175.04 3	176.0507149	8.51E- 05	Protona tion	b'1-(methylsulfanyl)-1-oxopropan-2-yl propanoate'	b'Methylthio 2- (propanoyloxy)propanoate'	HMDB00 40003	C7H12O3S	
		175.043439	0.0004 39	Redox	b'6-(methylsulfanyl)-2-oxohexanoate'	b'2-oxo-6-methylthiohexanoate'	HMDB03 04083	C7H11O3S	
51	176.93 4	177.9432255	0.0014 255	Protona tion	b'(phosphonoxy)phosphonic acid'	b'Pyrophosphate'	HMDB00 00250	H4O7P2	C000 13
52	178.01 66	179.0252285	0.0008 285	Protona tion	b'2-amino-3-[(carboxymethyl)sulfanyl]propanoic acid'	b'S-Carboxymethyl-L-cysteine'	HMDB00 29415	C5H9NO4S	
		179.0250249	0.0006 249	Protona tion	b'2-[2-(3-chlorophenyl)diazene-1-yl]acetonitrile'	b'2-[(3- Chlorophenyl)diazene]acetonitrile'	HMDB02 55365	C8H6ClN3	
		178.0185425	0.0019 425	Redox	b'4-chloronaphthalen-1-ol'	b'4-Chloro-1-naphthol'	HMDB02 47127	C10H7ClO	
		178.0145198	0.0020	Redox	b'2-amino-2-(3-chloro-4,5-dihydro-1,2-oxazol-5-yl)acetic acid'	b'Acivicin'	HMDB02	C5H7ClN2O	

			802				47942	3	
53	178.02 59	178.0266087	0.0007 087	Redox	b'6,7-dihydroxy-2H-chromen-2-one'	b'Aesculetin'	HMDB00 30819	C9H6O4	C092 63
		178.0266087	0.0007 087	Redox	b'5,7-dihydroxy-4H-chromen-4-one'	b'5,7-Dihydroxy-4H-1-benzopyran-4-one'	HMDB00 32950	C9H6O4	C090 01
		178.0266087	0.0007 087	Redox	b'4,7-dihydroxy-2H-chromen-2-one'	b'4,7-Dihydroxy-2H-1-benzopyran-2-one'	HMDB00 32951	C9H6O4	
		178.0266087	0.0007 087	Redox	b'2,2-dihydroxy-2,3-dihydro-1H-indene-1,3-dione'	b'Ninhydrin'	HMDB02 55614	C9H6O4	
54	178.05 17	179.0582432	0.0012 568	Protone tion	b'2-(phenylformamido)acetic acid'	b'Hippuric acid'	HMDB00 00714	C9H9NO3	C015 86
		179.0582432	0.0012 568	Protone tion	b'4-oxo-4-(pyridin-3-yl)butanoic acid'	b'3-Succinoylpyridine'	HMDB00 00992	C9H9NO3	C195 69
		179.0582432	0.0012 568	Protone tion	b'(3R)-3-hydroxy-1-methyl-2,3,5,6-tetrahydro-1H-indole-5,6-dione'	b'Adrenochrome'	HMDB00 12884	C9H9NO3	
		179.061614	0.0021 14	Protone tion	b'2-amino-3-(propane-1-sulfinyl)propanoic acid'	b'(R)C(R)S-S-Propylcysteine sulfoxide'	HMDB00 29442	C6H13NO3S	
		179.061614	0.0021 14	Protone tion	b'N-cyclohexylsulfamic acid'	b'Cyclamic acid'	HMDB00 31340	C6H13NO3S	C028 24
		179.0582432	0.0012 568	Protone tion	b'methyl 2-formamidobenzoate'	b'Methyl n-formylanthranilate'	HMDB00 32398	C9H9NO3	
		179.0582432	0.0012 568	Protone tion	b'1-methoxy-4-[(E)-2-nitroethenyl]benzene'	b'1-(4-Methoxyphenyl)-2-nitroethylene'	HMDB00 32595	C9H9NO3	
		179.0582432	0.0012 568	Protone tion	b'3-(3,4-dihydroxyphenyl)prop-2-enamide'	b'2-Propenamide, 3-(3,4-dihydroxyphenyl)-'	HMDB02 45300	C9H9NO3	
		179.0582432	0.0012	Protone	b'4-acetamidobenzoic acid'	b'4-Acetamidobenzoic acid'	HMDB02	C9H9NO3	

55	178.0638		568	tion			46328		
		179.0582432	0.0012568	Protonation	b'5,6-dihydroxy-1-methyl-2,3-dihydro-1H-indol-3-one'	b'Adrenolutin'	HMDB0248030	C9H9NO3	
		179.0582432	0.0012568	Protonation	b'N-[2-(2,5-dihydroxyphenyl)ethenyl]formamide'	b'Erbstatin'	HMDB0251902	C9H9NO3	
		179.0616145	0.0021145	Protonation	b'2-amino-3-[(3-hydroxypropyl)sulfonyl]propanoic acid'	b'Fudosteine'	HMDB0252511	C6H13NO3S	
		179.0582432	0.0012568	Protonation	b'N-(2-hydroxybenzoyl)ethanimidic acid'	b'N-Acetyl-2-hydroxybenzamide'	HMDB0255046	C9H9NO3	
		179.0582432	0.0012568	Protonation	b'1-methyl-1H-indole-3,5,6-triol'	b'1-Methyl-1H-indole-3,5,6-triol'	HMDB0257859	C9H9NO3	
		179.061614	0.002114	Protonation	b'(2R)-2-amino-3-(propane-1-sulfinyl)propanoic acid'	b'S-Propylcysteine sulphoxide'	HMDB0302213	C6H13NO3S	
		178.0490755	0.0026245	Redox	b'3-(1H-1,2,3,4-tetrazol-5-yloxy)phenol'	b'Melizame'	HMDB0029684	C7H6N4O2	
		179.0694765	0.0021235	Protonation	b'N-(pyridine-4-carbonyl)ethanehydrazonic acid'	b'Acetylisoniazid'	HMDB0041821	C8H9N3O2	C07585
		179.0694765	0.0021235	Protonation	b'2-acetylpyridine-4-carbohydrazide'	b'2-Acetylisonicotinohydrazide'	HMDB0244968	C8H9N3O2	
		179.0694765	0.0021235	Protonation	b'4-carbamimidamidobenzoic acid'	b'4-Guanidinobenzoic acid'	HMDB0246433	C8H9N3O2	
55	178.0638	179.0734993	0.0018993	Protonation	b'acridine'	b'Acridine'	HMDB0247968	C13H9N	C20141
		179.0734993	0.0018993	Protonation	b'benzo[f]quinoline'	b'Benzo[f]quinoline'	HMDB0249008	C13H9N	
		179.0734993	0.0018	Protonation	b'phenanthridine'	b'Phenanthridine'	HMDB02	C13H9N	

			993	tion			56392		
178.0629942	0.0008 058	Redox		b'(2E)-3-(4-methoxyphenyl)prop-2-enoic acid'	b'4-Methoxycinnamic acid'	HMDB00 02040	C10H10O3		
178.0629942	0.0008 058	Redox		b'3-(4-methylphenyl)oxirane-2-carboxylic acid'	b'3-(4-Methylphenyl)oxiranecarboxylic acid'	HMDB00 30903	C10H10O3		
178.0629942	0.0008 058	Redox		b'(8Z)-10-hydroxydec-8-en-4,6-diynoic acid'	b'(Z)-10-Hydroxy-8-decene-4,6-diynoic acid'	HMDB00 31055	C10H10O3		
178.0629942	0.0008 058	Redox		b'2-[(furan-2-ylmethoxy)methyl]furan'	b'Di-alpha-furfuryl ether'	HMDB00 33248	C10H10O3		
178.0629942	0.0008 058	Redox		b'4,8-dihydroxy-1,2,3,4-tetrahydronaphthalen-1-one'	b'(S)-Isosclerone'	HMDB00 38712	C10H10O3		
178.0629942	0.0008 058	Redox		b'(2E)-10-hydroxydec-2-en-4,6-diynoic acid'	b'(E)-10-Hydroxy-2-decene-4,6-diynoic acid'	HMDB00 38965	C10H10O3		
178.0629942	0.0008 058	Redox		b'(2E)-3-(4-hydroxy-2-methoxyphenyl)prop-2-enal'	b'3-(4-Hydroxy-2-methoxyphenyl)-2-propenal'	HMDB00 39471	C10H10O3		
178.0629942	0.0008 058	Redox		b'1aH,6H,7H,7aH-naphtho[1,2-b]oxirene-6,7-diol'	b'1,2-Dihydroxy-3,4-epoxy-1,2,3,4-tetrahydronaphthalene'	HMDB00 62273	C10H10O3	C147 84	
178.0629942	0.0008 058	Redox		b'ethyl 2-oxo-2-phenylacetate'	b'Ethyl Phenylglyoxylate'	HMDB00 62729	C10H10O3		
178.0629942	0.0008 058	Redox		b'(2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enal'	b'Coniferaldehyde'	HMDB01 41782	C10H10O3	C026 66	
178.0629942	0.0008 058	Redox		b'3-(4-methoxyphenyl)prop-2-enoic acid'	b'(Z)-p-Methoxycinnamic acid'	HMDB02 46971	C10H10O3		
178.0629942	0.0008 058	Redox		b'(3R)-8-hydroxy-3-methyl-3,4-dihydro-1H-2-benzopyran-1-one'	b'Mellein'	HMDB03 01747	C10H10O3		
178.0629942	0.0008	Redox		b'methyl 3-(4-hydroxyphenyl)prop-2-enoate'	b'Methyl p-coumarate'	HMDB03	C10H10O3		

			058				02074		
		178.0629942	0.0008 058	Redox	b'(2E)-3-(2-methoxyphenyl)prop-2-enoic acid'	b'trans-2-Methoxycinnamic acid'	HMDB03 02514	C10H10O3	
56	179.05 48	180.0633881	0.0007 881	Protona tion	b'(2R,3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Glucose'	HMDB00 00122	C6H12O6	C002 21
		180.0633881	0.0007 881	Protona tion	b'(2S,3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Galactose'	HMDB00 00143	C6H12O6	C009 84
		180.0633881	0.0007 881	Protona tion	b'(2S,3S,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Mannose'	HMDB00 00169	C6H12O6	C009 36
		180.0633881	0.0007 881	Protona tion	b'(1R,2R,3r,4S,5S,6s)-cyclohexane-1,2,3,4,5,6-hexol'	b'myo-Inositol'	HMDB00 00211	C6H12O6	C001 37
		180.0633881	0.0007 881	Protona tion	b'(2S,4S,5R)-2,4,5,6-tetrahydroxyhexanoic acid'	b'3-Deoxyarabinohexonic acid'	HMDB00 00346	C6H12O6	
		180.0633881	0.0007 881	Protona tion	b'(2R,3S,4S,5R)-2,5-bis(hydroxymethyl)oxolane-2,3,4-triol'	b'D-Fructose'	HMDB00 00660	C6H12O6	C023 36
		180.0633881	0.0007 881	Protona tion	b'(3S,4S,5R,6S)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'Allose'	HMDB00 01151	C6H12O6	C014 87
		180.0633881	0.0007 881	Protona tion	b'(2R,3S,4R,5S)-2-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'L-Sorbose'	HMDB00 01266	C6H12O6	C083 56
		180.0647255	0.0021 255	Protona tion		b'Paraxanthine'	HMDB00 01860	C7H8N4O2	C137 47
		180.0647255	0.0021 255	Protona tion	b'1,3-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Theophylline'	HMDB00 01889	C7H8N4O2	C071 30
		180.0647255	0.0021 255	Protona tion	b'3,7-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Theobromine'	HMDB00 02825	C7H8N4O2	C074 80
		180.0633881	0.0007	Protona	b'(2S,3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'alpha-D-Glucose'	HMDB00	C6H12O6	C002

		881	tion				03345		67
180.0633881	0.0007 881	Protone tion	b'(2R,3S,4S,5R)-2-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Tagatose'	HMDB00 03418	C6H12O6	C007 95		
180.0633881	0.0007 881	Protone tion	b'(2R,3R,4S,5R,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'beta-D-Galactose'	HMDB00 03449	C6H12O6	C009 62		
180.0633881	0.0007 881	Protone tion	b'(1r,2r,3r,4r,5r,6r)-cyclohexane-1,2,3,4,5,6-hexol'	b'scylo-Inositol'	HMDB00 06088	C6H12O6	C061 53		
180.0633881	0.0007 881	Protone tion	b'(3S,4S,5S,6S)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'L-Gulose'	HMDB00 12326	C6H12O6	C159 23		
180.0633881	0.0007 881	Protone tion	b'2,5-bis(hydroxymethyl)-1,4-dioxane-2,5-diol'	b'Dihydroxyacetone (dimer)'	HMDB00 32222	C6H12O6			
180.0633881	0.0007 881	Protone tion	b'(2R,3S,4R,5S,6S)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'L-Galactose'	HMDB00 33704	C6H12O6	C018 25		
180.0633881	0.0007 881	Protone tion	b'(1R,2R,3R,4R,5S,6S)-cyclohexane-1,2,3,4,5,6-hexol'	b'Levoinositol'	HMDB00 34220	C6H12O6			
180.0633881	0.0007 881	Protone tion	b'(1R,2S,3S,4R,5S,6r)-cyclohexane-1,2,3,4,5,6-hexol'	b'muco-Inositol'	HMDB00 62138	C6H12O6	C061 52		
180.0633881	0.0007 881	Protone tion	b'(2S,3S,4R,5R)-2,3,4,5,6-pentahydroxyhexanal'	b'Glycoprotein-phospho-D-mannose'	HMDB00 62473	C6H12O6			
180.0633881	0.0007 881	Protone tion	b'(1R,2S,3r,4R,5S,6s)-cyclohexane-1,2,3,4,5,6-hexol'	b'epi-Inositol'	HMDB02 40207	C6H12O6			
180.0633881	0.0007 881	Protone tion	b'(1R,2R,3S,4S,5S,6s)-cyclohexane-1,2,3,4,5,6-hexol'	b'neo-Inositol'	HMDB02 40208	C6H12O6			
180.0633881	0.0007 881	Protone tion	b'(1R,2R,3S,4S,5S,6S)-cyclohexane-1,2,3,4,5,6-hexol'	b'D-chiro-Inositol'	HMDB02 40209	C6H12O6	C198 91		
180.0633881	0.0007	Protone	b'(1R,2R,3S,4S,5s,6s)-cyclohexane-1,2,3,4,5,6-hexol'	b'cis-Inositol'	HMDB02	C6H12O6			

			881	tion			40210		
		180.0633881	0.0007 881	Protona tion	b'(1R,2R,3S,4R,5S,6S)-cyclohexane-1,2,3,4,5,6-hexol'	b'allo-Inositol'	HMDB02 40211	C6H12O6	
		180.0633881	0.0007 881	Protona tion	b'2,3,4,5,6-pentahydroxyhexanal'	b'(2R,3R,4R,5R)-2,3,4,5,6-Pentahydroxyhexanal'	HMDB02 42534	C6H12O6	
		180.0633881	0.0007 881	Protona tion	b'1,2,4,5,6-pentahydroxyhexan-3-one'	b'(2R,4S,5S)-1,2,4,5,6-Pentahydroxyhexan-3-one'	HMDB02 42761	C6H12O6	C013 83
		180.0633881	0.0007 881	Protona tion	b'1,3,4,5,6-pentahydroxyhexan-2-one'	b'(3R,4R,5R)-1,3,4,5,6-Pentahydroxyhexan-2-one'	HMDB02 46950	C6H12O6	C014 52
		180.0633881	0.0007 881	Protona tion	b'5-(1,2-dihydroxyethyl)oxolane-2,3,4-triol'	b'alpha-D-Galactofuranose'	HMDB02 48203	C6H12O6	
		180.0633881	0.0007 881	Protona tion	b'2,5-bis(hydroxymethyl)oxolane-2,3,4-triol'	b'D-Fructofuranose'	HMDB02 50747	C6H12O6	
		180.0633881	0.0007 881	Protona tion	b'6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Gulose'	HMDB02 50761	C6H12O6	C007 38
		180.0633881	0.0007 881	Protona tion	b'2-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-Psicose'	HMDB02 50793	C6H12O6	
		180.0647255	0.0021 255	Protona tion	b'1-[(1H-imidazol-1-yl)amino]pyrrolidine-2,5-dione'	b'Succinylaminoimidazole'	HMDB02 58546	C7H8N4O2	
		180.0633881	0.0007 881	Protona tion	b'(3R,4S,5S,6R)-6-(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'Glucose'	HMDB03 04632	C6H12O6	C000 31
		180.0633881	0.0007 881	Protona tion	b'(2S,3R,4S,5R)-5-[(1R)-1,2-dihydroxyethyl]oxolane-2,3,4-triol'	b'alpha-D-Allofuranose'	HMDB03 04814	C6H12O6	
57	180.04 18	181.0503944	0.0007 944	Protona tion	b'2-amino-4-[hydroxy(methyl)phosphoryl]butanoic acid'	b'Glufosinate'	HMDB02 52799	C5H12NO4P	C050 42
		181.0506324	0.0010	Protona	b'4-[(2R)-2-carboxy-2-hydroxyethyl]benzen-1-olate'	b'(R+)-3-(4-hydroxyphenyl)lactate'	HMDB03	C9H9O4	

58	180.06 7		324	tion			03993		
		180.0422587	0.0004 587	Redox	b'3-(4-hydroxyphenyl)-2-oxopropanoic acid'	b'4-Hydroxyphenylpyruvic acid'	HMDB00 00707	C9H8O4	C011 79
		180.0422587	0.0004 587	Redox	b'2-(acetyloxy)benzoic acid'	b'Aspirin'	HMDB00 01879	C9H8O4	C014 05
		180.0422587	0.0004 587	Redox	b'(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid'	b'Caffeic acid'	HMDB00 01964	C9H8O4	C014 81
		180.0422587	0.0004 587	Redox	b'2-(methoxycarbonyl)benzoic acid'	b'Monomethyl phthalate'	HMDB00 02130	C9H8O4	
		180.0422587	0.0004 587	Redox	b'(2Z)-3-(3,4-dihydroxyphenyl)prop-2-enoic acid'	b'cis-Caffeic acid'	HMDB00 03501	C9H8O4	C014 81
		180.0422587	0.0004 587	Redox	b'(2Z)-2-hydroxy-3-(4-hydroxyphenyl)prop-2-enoic acid'	b'2-Hydroxy-3-(4-hydroxyphenyl)propenoic acid'	HMDB00 06915	C9H8O4	C053 50
		180.0422587	0.0004 587	Redox	b'3-(3-hydroxyphenyl)-2-oxopropanoic acid'	b'3-Hydroxyphenylpyruvic acid'	HMDB00 11663	C9H8O4	
		180.0422587	0.0004 587	Redox	b'3-(2,3-dihydroxyphenyl)prop-2-enoic acid'	b'(E)-3-(2,3-Dihydroxyphenyl)-2-propenoic acid'	HMDB00 32057	C9H8O4	C126 23
		180.0422587	0.0004 587	Redox	b'(2E)-3-(3,5-dihydroxyphenyl)prop-2-enoic acid'	b'3,5-Dihydroxycinnamic acid'	HMDB00 32131	C9H8O4	
		181.0738932	0.0009 068	Protontion	b'(2S)-2-amino-3-(4-hydroxyphenyl)propanoic acid'	b'L-Tyrosine'	HMDB00 00158	C9H11NO3	C000 82
		181.0738932	0.0009 068	Protontion	b'4-hydroxy-4-(pyridin-3-yl)butanoic acid'	b'4-Hydroxy-4-(3-pyridyl)-butanoic acid'	HMDB00 01119	C9H11NO3	C195 79
		181.0738932	0.0009 068	Protontion	b'(2S)-2-amino-3-hydroxy-3-phenylpropanoic acid'	b'L-Threo-3-Phenylserine'	HMDB00 02184	C9H11NO3	
		181.0738932	0.0009	Protontion	b'3-amino-3-(4-hydroxyphenyl)propanoic acid'	b'Beta-Tyrosine'	HMDB00	C9H11NO3	C043

			068	tion			03831		68
		181.0738932	0.0009 068	Protona tion	b'2-amino-3-(2-hydroxyphenyl)propanoic acid'	b'o-Tyrosine'	HMDB00 06050	C9H11NO3	
		181.0738932	0.0009 068	Protona tion	b'(2S)-2-amino-3-(3-hydroxyphenyl)propanoic acid'	b'Meta-Tyrosine'	HMDB00 59720	C9H11NO3	
		181.0738932	0.0009 068	Protona tion	b'1,2,3,4-tetrahydroisoquinoline-4,6,7-triol'	b'4,6,7-Trihydroxy-1,2,3,4-tetrahydroisoquinoline'	HMDB00 60280	C9H11NO3	
		181.0738932	0.0009 068	Protona tion	b'2-amino-3-hydroxy-3-phenylpropanoic acid'	b'2-Amino-3-hydroxy-3-phenylpropanoic acid'	HMDB02 44981	C9H11NO3	
		181.0738932	0.0009 068	Protona tion	b'2-amino-3-(4-hydroxyphenyl)propanoic acid'	b'D-Tyrosine'	HMDB02 50803	C9H11NO3	C015 36
		180.0660682	0.0009 318	Redox	b'(3,6-dihydroxy-1-methyl-2,3-dihydro-1H-indol-5-yl)oxidanyl'	b'Adrenochrome o-semiquinone'	HMDB00 12883	C9H10NO3	
		180.0687483	0.0017 483	Redox	b'1,10-phenanthroline'	b'1,10-Phenanthroline'	HMDB02 44053	C12H8N2	C006 04
		180.0687483	0.0017 483	Redox	b'1,7-phenanthroline'	b'1,7-Phenanthroline'	HMDB02 44247	C12H8N2	
		180.0687483	0.0017 483	Redox	b'benzo[c]cinnoline'	b'Benzo[c]cinnoline'	HMDB02 49005	C12H8N2	
		180.0687483	0.0017 483	Redox	b'phenazine'	b'Phenazine'	HMDB02 56395	C12H8N2	
59	181.96 4	182.9711102	0.0006 898	Protona tion	b'3-hydroxy-2-(phosphonatoxy)propanoate'	b'2-phospho-D-glycerate'	HMDB03 04085	C3H4O7P	
		181.9616394	0.0023 606	Redox	b'4,5-dihydroxy-2,6,7-trioxo-11lambda5-phosphabicyclo[2.2.1]heptane-1,3-dione'	b'Glyceraldehyde phosphate'	HMDB02 52837	C3H3O7P	
60	182.01	183.0201431	0.0009	Protona	b'(2S)-2-amino-4-sulfobutanoic acid'	b'L-Homocysteic acid'	HMDB00	C4H9NO5S	C165

	14		431	tion				02205		11
		183.0214805	0.0022 805	Protona tion	b'2-imino-6-sulfanyl-3,9-dihydro-2H-purin-8-ol'	b'8-Hydroxythioguanine'	HMDB00 60804	C5H5N5OS		
		183.0201436	0.0009 436	Protona tion	b'2-amino-4-sulfobutanoic acid'	b'DL-Homocysteic acid'	HMDB02 51520	C4H9NO5S		
		182.0109759	0.0004 241	Redox	b'[(carbamoylamino)sulfonyl]urea'	b"N,N".Sulfonylbisurea"	HMDB02 55277	C2H6N4O4S		
61	182.02 14	183.0296594	0.0004 594	Protona tion	b'2-amino-4-phosphonobutanoic acid'	b'2-Amino-4-phosphonobutyric acid'	HMDB02 44992	C4H10NO5P		
		183.0280057	0.0011 943	Protona tion	b'N,N-dinitroaniline'	b'N-Nitro-N-phenylnitramide'	HMDB02 48976	C6H5N3O4		
		183.0296589	0.0004 589	Protona tion	b'[3-(N-hydroxyformamido)propyl]phosphonic acid'	b'Fosmidomycin'	HMDB02 52468	C4H10NO5P		
		182.0215233	0.0001 233	Redox	b'2-hydroxybenzene-1,4-dicarboxylic acid'	b'2-Hydroxyterephthalic acid'	HMDB02 45171	C8H6O5		
62	182.04 46	183.0531578	0.0007 578	Protona tion	b'3-hydroxy-5-(hydroxymethyl)-2-methylpyridine-4-carboxylic acid'	b'4-Pyridoxic acid'	HMDB00 00017	C8H9NO4	C008 47	
		183.0531578	0.0007 578	Protona tion	b'2-amino-2-(3,5-dihydroxyphenyl)acetic acid'	b'3,5-Dihydroxyphenylglycine'	HMDB02 43702	C8H9NO4		
		183.0531578	0.0007 578	Protona tion	b'2-[(3,5-dihydroxyphenyl)amino]acetic acid'	b'2-[(3,5-Dihydroxyphenyl)amino]acetic acid'	HMDB02 44908	C8H9NO4		
		183.0544952	0.0020 952	Protona tion	b'3,4,5,13,14-pentaazatricyclo[7.5.0.0^{2,6}]tetradeca-1(14),2,4,6,8,10,12-heptaene'	b'triazolobenzodiazepine'	HMDB02 59157	C9H5N5		
		182.0439901	0.0006 099	Redox	b'3-methyl-2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'	b'3-Methyluric acid'	HMDB00 01970	C6H6N4O3		
		182.0439901	0.0006	Redox	b'9-methyl-2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'	b'9-Methyluric acid'	HMDB00	C6H6N4O3		

			099					01973		
		182.0439901	0.0006 099	Redox	b'1-methyl-2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'	b'1-Methyluric acid'	HMDB00 03099	C6H6N4O3	C163 59	
		182.0439901	0.0006 099	Redox	b'7-methyl-7H-purine-2,6,8-triol'	b'7-Methyluric acid'	HMDB00 11107	C6H6N4O3	C163 55	
63	184.00 02	185.0089235	0.0009 235	Protone tion	b'(2S)-2-amino-3-(phosphonoxy)propanoic acid'	b'Phosphoserine'	HMDB00 00272	C3H8NO6P	C010 05	
		185.0089235	0.0009 235	Protone tion	b'2-amino-3-(phosphonoxy)propanoic acid'	b'DL-O-Phosphoserine'	HMDB00 01721	C3H8NO6P	C010 05	
		185.0089235	0.0009 235	Protone tion	b'(2R)-2-amino-3-(phosphonoxy)propanoic acid'	b'3-phospho-L-serine'	HMDB03 04154	C3H8NO6P	C025 32	
		184.0007879	0.0005 879	Redox	b'4-oxo-4H-pyran-2,6-dicarboxylic acid'	b'Chelidonic acid'	HMDB02 49899	C7H4O6	C084 76	
64	184.10 74	184.1099444	0.0025 444	Redox	b'2-methyl-5-(1-oxopropan-2-yl)cyclopentane-1-carboxylic acid'	b'('1'R)-Nepetalic acid''	HMDB00 36117	C10H16O3		
		184.1099444	0.0025 444	Redox	b'4-(2-hydroxypropan-2-yl)cyclohex-1-ene-1-carboxylic acid'	b'(S)-Oleuropeic acid'	HMDB00 36998	C10H16O3		
		184.1099444	0.0025 444	Redox	b'5-(1,2-dihydroxypropan-2-yl)-2-methylcyclohex-2-en-1-one'	b'(4S,8R)-8,9-Dihydroxy-p-menth-1(6)- en-2-one'	HMDB00 39052	C10H16O3		
		184.1099444	0.0025 444	Redox	b'1-acetylcyclohexyl acetate'	b'1-Acetylcyclohexyl acetate'	HMDB00 39710	C10H16O3		
		184.1099444	0.0025 444	Redox	b'(8E)-10-oxodec-8-enoic acid'	b'(E)-10-Oxo-8-decenoic acid'	HMDB00 40883	C10H16O3		
		184.1099444	0.0025 444	Redox	b'1-methyl-4-(prop-1-en-2-yl)-7,8,9-trioxabicyclo[4.2.1]nonane'	b'r-limonene'	HMDB02 57077	C10H16O3		
		184.1099444	0.0025	Redox	b'2-(2,2,3-trimethyl-4-oxocyclopentyl)acetic acid'	b'alpha-Campholonic acid'	HMDB03	C10H16O3		

68	191.05		026	tion			01874		51
		192.0270026	0.0009 026	Protona tion	b'(4R,5S)-4,5,6-trihydroxy-2,3-dioxohexanoic acid'	b'Diketogulonic acid'	HMDB00 05971	C6H8O7	C045 75
		192.0270026	0.0009 026	Protona tion	b'(5S)-4,5,6-trihydroxy-2,3-dioxohexanoic acid'	b'2,3-Diketo-L-gulonate'	HMDB00 06511	C6H8O7	C045 75
		192.0270026	0.0009 026	Protona tion	b'(1R,2R)-1-hydroxypropane-1,2,3-tricarboxylic acid'	b'(1R,2R)-Isocitric acid'	HMDB00 33717	C6H8O7	C046 17
		192.0245002	0.0015 998	Protona tion	b'(5E)-5-[(5-methylthiophen-2-yl)methylidene]-2,5-dihydrofuran-2-one'	b'(Z)-5-[(5-Methyl-2-thienyl)methylene]-2(5H)-furanone'	HMDB00 33845	C10H8O2S	
		192.0270026	0.0009 026	Protona tion	b'(2S)-2-[(2S,3R,4R)-3,4-dihydroxy-5-oxoxolan-2-yl]-2-hydroxyacetic acid'	b'D-Glucaro-1,4-lactone'	HMDB00 41862	C6H8O7	
		192.0270026	0.0009 026	Protona tion	b'4,5,6-trihydroxy-2,3-dioxohexanoic acid'	b'2,3-diketogulonate'	HMDB00 62803	C6H8O7	
		192.0270026	0.0009 026	Protona tion	b'3,3,3a,6-tetrahydroxy-hexahydrofuro[3,2-b]furan-2-one'	b'dehydroascorbate (bicyclic form)'	HMDB03 04326	C6H8O7	
		191.0194129	0.0011 129	Redox	b'2-(trifluoromethyl)pyridine-4-carboxylic acid'	b'2-(Trifluoromethyl)isonicotinic acid'	HMDB02 44959	C7H4F3NO2	
		191.0197261	0.0014 261	Redox	b'4,5,6-trihydroxy-2,3-dioxohexanoate'	b'2,3-dioxo-L-gulonate'	HMDB03 04040	C6H7O7	
		191.0197261	0.0014 261	Redox	b'3,4-dihydroxy-5-(hydroxymethyl)-2-oxoxolane-3-carboxylate'	b'2-carboxy-L-xylonolactone'	HMDB03 04063	C6H7O7	
68	191.05 98	192.0687483	0.0011 483	Protona tion	b'2H-benzo[f]isoindole-1-carbonitrile'	b'2H-Benzo[F]isoindole-1-carbonitrile'	HMDB02 45761	C13H8N2	
		191.0582432	0.0015 568	Redox	b'2-(5-hydroxy-1H-indol-3-yl)acetic acid'	b'5-Hydroxyindoleacetic acid'	HMDB00 00763	C10H9NO3	C056 35
		191.061614	0.0018	Redox	b'(2S)-2-acetamido-4-(methylsulfonyl)butanoic acid'	b'N-Acetyl-L-methionine'	HMDB00	C7H13NO3S	C027

69	192.06		14					11745		12
		191.0582432	0.0015 568	Redox	b'2-(2-hydroxy-3H-indol-3-yl)acetic acid'	b'xi-2,3-Dihydro-2-oxo-1H-indole-3-acetic acid'	HMDB00 35514	C10H9NO3		
		191.0582432	0.0015 568	Redox	b'4-hydroxy-5-phenyl-5,6-dihydro-2H-1,3-oxazin-2-one'	b'5-Phenyl-1,3-oxazinane-2,4-dione'	HMDB00 60400	C10H9NO3	C165 96	
		191.0582432	0.0015 568	Redox		b'5-Methoxyindole-2-carboxylic acid'	HMDB02 46823	C10H9NO3		
		191.0616145	0.0018 145	Redox	b'ethyl 2-acetamido-3-sulfanylpropanoate'	b'L-Cysteine, N-acetyl-, ethyl ester'	HMDB02 47004	C7H13NO3S		
		191.0616145	0.0018 145	Redox	b'2-acetamido-3-methyl-3-sulfanylbutoanoic acid'	b'N-Acetyl-dl-penicillamine'	HMDB02 55055	C7H13NO3S		
		191.0616145	0.0018 145	Redox	b'2-(2-methylpropanamido)-3-sulfanylpropanoic acid'	b'N-Isobutyryl-L-cysteine'	HMDB02 55162	C7H13NO3S		
		191.0582432	0.0015 568	Redox	b'2H,5H,6H,7H,8H-[1,3]dioxolo[4,5-g]isoquinolin-5-one'	b'Noroxyhydrastinine'	HMDB02 55749	C10H9NO3		
		191.0582432	0.0015 568	Redox	b'2-(3-hydroxy-1H-indol-2-yl)acetic acid'	b'2-(3-Hydroxy-1H-indol-2-yl)acetic acid'	HMDB02 57584	C10H9NO3		
		191.0582432	0.0015 568	Redox	b'2-(5-hydroxy-1H-indol-2-yl)acetic acid'	b'2-(5-Hydroxy-1H-indol-2-yl)acetic acid'	HMDB02 57587	C10H9NO3		
		191.0582432	0.0015 568	Redox	b'1H-indol-3-yl 2-hydroxyacetate'	b'1H-Indol-3-yl 2-hydroxyacetate'	HMDB02 57908	C10H9NO3		
		193.0738932	0.0024 932	Protonation	b'2-(2-phenylacetamido)acetic acid'	b'Phenylacetylglutamine'	HMDB00 00821	C10H11NO3	C055 98	
		193.0738932	0.0024 932	Protonation	b'methyl 2-(phenylformamido)acetate'	b'Methyl hippurate'	HMDB00 00859	C10H11NO3		
		193.0738932	0.0024	Protonation	b'2-[(2-methylphenyl)formamido]acetic acid'	b'2-Methylhippuric acid'	HMDB00	C10H11NO3	C015	

		932	tion				11723		86
193.0738932	0.0024 932	Protona tion		b'2-[(3-methylphenyl)formamido]acetic acid'	b'm-Methylhippuric acid'	HMDB00 13245	C10H11NO3		
193.0738932	0.0024 932	Protona tion		b'2-[(4-methylphenyl)formamido]acetic acid'	b'p-Methylhippuric acid'	HMDB00 13292	C10H11NO3		
193.0738932	0.0024 932	Protona tion		b'methyl 2-acetamidobenzoate'	b'Methyl n-acetylanthranilate'	HMDB00 32388	C10H11NO3	C063 32	
193.0738932	0.0024 932	Protona tion		b'3-(phenylformamido)propanoic acid'	b'Betamipron'	HMDB00 34250	C10H11NO3		
193.0738932	0.0024 932	Protona tion		b'3-(C-hydroxycarbonimidoyloxy)-2-phenylpropanal'	b'3-Carbamoyl-2-phenylpropionaldehyde'	HMDB00 60366	C10H11NO3	C165 87	
193.0738932	0.0024 932	Protona tion		b'5-phenyl-5,6-dihydro-4H-1,3-oxazine-2,4-diol'	b'4-Hydroxy-5-phenyltetrahydro-1,3-oxazin-2-one'	HMDB00 60389	C10H11NO3	C165 95	
193.0738932	0.0024 932	Protona tion		b'3-(phenyl-C-hydroxycarbonimidoyl)propanoic acid'	b'4-Anilino-4-oxobutanoic acid'	HMDB00 60758	C10H11NO3		
193.0738932	0.0024 932	Protona tion		b'(2S)-2-formamido-3-phenylpropanoic acid'	b'N-Formylphenylalanine'	HMDB02 40317	C10H11NO3		
193.0738932	0.0024 932	Protona tion		b'2-{4-[(1-hydroxyethylidene)amino]phenyl}acetic acid'	b'Actarit'	HMDB02 47976	C10H11NO3		
193.0738932	0.0024 932	Protona tion		b'2-(phenylformamido)propanoic acid'	b'n-benzoyl-d-alanine'	HMDB02 55085	C10H11NO3		
193.0738932	0.0024 932	Protona tion		b'2-formamido-3-phenylpropanoic acid'	b'N-Formyl-dl-phenylalanine'	HMDB02 55143	C10H11NO3		
192.0633881	0.0002 119	Redox			b'Quinic acid'	HMDB00 03072	C7H12O6	C002 96	
192.0608857	0.0027	Redox		b'(2E)-2-[(methylsulfonyl)methyl]-3-phenylprop-2-enal'	b'2-(Methylthiomethyl)-3-phenyl-2-	HMDB00	C11H12OS		

			143			propenal'	37166		
		192.0642575	0.0006 575	Redox	b'6,8-disulfanyloctanal'	b'6,8-Bis(sulfanyl)octanal'	HMDB02 58126	C8H16OS2	
		192.0633881	0.0002 119	Redox	b'(2R,3R)-2,3-dihydroxy-4-oxo-4-(propan-2-yloxy)butanoic acid'	b'Isopropyl tartaric acid'	HMDB03 02348	C7H12O6	
70	193.07 56	194.0843983	0.0009 983	Protona tion	b'acridin-1-amine'	b'1-Aminoacridine'	HMDB02 43819	C13H10N2	
		194.0843983	0.0009 983	Protona tion	b'2-phenylimidazo[1,2-a]pyridine'	b'2-Phenylimidazo[1,2-a]pyridine'	HMDB02 45292	C13H10N2	
		194.0843983	0.0009 983	Protona tion	b'acridin-9-amine'	b'9-Aminoacridine'	HMDB02 47578	C13H10N2	
		194.0843983	0.0009 983	Protona tion	b'2-cyclopropylpyrrolo[2,3-g]indole'	b'Cyclopropylpyrroloindole'	HMDB02 50679	C13H10N2	
		194.0843983	0.0009 983	Protona tion	b'8,9-diazatricyclo[9.4.0.0^{2,7}]pentadeca-1(15),2,4,6,9,11,13-heptaene'	b'Dibenzodiazepine'	HMDB02 51163	C13H10N2	
		193.077264	0.0016 64	Redox	b'(2R)-2-amino-3-(butane-1-sulfinyl)propanoic acid'	b'S-Butylcysteine sulfoxide'	HMDB03 02178	C7H15NO3S	
71	193.09 24	194.0976656	0.0025 344	Protona tion	b'octane-1-sulfonic acid'	b'1-Octanesulfonic acid'	HMDB02 43978	C8H18O3S	
		193.0950226	0.0026 226	Redox	b'2,6-bis(hydroxymethyl)piperidine-3,4,5-triol'	b'(2r,3r,5s,6r)-2,6-Bis(hydroxymethyl)piperidine-3,4,5-triol'	HMDB02 42543	C7H15NO5	
		193.0950226	0.0026 226	Redox	b'3,4,5,6-tetrahydroxy-2-(methyldamino)hexanal'	b'N-Methylglucosamine'	HMDB02 55188	C7H15NO5	
72	193.15 86	194.1670653	0.0006 653	Protona tion	b'(5Z)-6,10-dimethylundeca-5,9-dien-2-one'	b'Geranylacetone'	HMDB00 31846	C13H22O	C132 97

		194.1670653	0.0006 653	Protona tion	b'(6E)-8-methyl-5-(propan-2-yl)nona-6,8-dien-2-one'	b'(+/-)-[R-(E)]-5-Isopropyl-8-methylnona-6,8-dien-2-one'	HMDB00 32355	C13H22O	
		194.1670653	0.0006 653	Protona tion	b'4-(2,6,6-trimethylcyclohex-1-en-1-yl)butan-2-one'	b'4-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-2-butanone'	HMDB00 32913	C13H22O	C035 27
		194.1670653	0.0006 653	Protona tion	b'6-(propan-2-yl)-decahydronaphthalen-2-one'	b'Octahydro-6-isopropyl-2(1H)-naphthalenone'	HMDB00 36026	C13H22O	
		194.1670653	0.0006 653	Protona tion	b'4-(2,6,6-trimethylcyclohexa-1,3-dien-1-yl)butan-2-ol'	b'7,8-Dehydro-3,4-dihydro-beta-ionol'	HMDB00 36184	C13H22O	
		194.1670653	0.0006 653	Protona tion	b'(3E)-4-(2,6,6-trimethylcyclohex-1-en-1-yl)but-3-en-2-ol'	b'beta-Ionol'	HMDB00 36820	C13H22O	
		194.1670653	0.0006 653	Protona tion	b'2,6,10,10-tetramethyl-1-oxaspiro[4.5]dec-6-ene'	b'Theaspirane'	HMDB00 36823	C13H22O	
		194.1670653	0.0006 653	Protona tion	b'4-[(1R)-2,6,6-trimethylcyclohex-2-en-1-yl]butan-2-one'	b'Dihydro-alpha-ionone'	HMDB00 38026	C13H22O	
		194.1670653	0.0006 653	Protona tion	b'2-(2-methylpropyl)-5-(propan-2-yl)cyclohex-2-en-1-one'	b'5-Isopropyl-2-(2-methylpropyl)-2-cyclohexen-1-one'	HMDB00 38216	C13H22O	
		194.1670653	0.0006 653	Protona tion	b'(3E)-4-(2,6,6-trimethylcyclohex-2-en-1-yl)but-3-en-2-ol'	b'4,7-Megastigmadien-9-ol'	HMDB00 38731	C13H22O	
		194.1670653	0.0006 653	Protona tion	b'2-[(2E)-oct-2-en-1-yl]cyclopentan-1-one'	b'(E)-2-(2-Octenyl)cyclopentanone'	HMDB00 38897	C13H22O	
73	194.02 1	195.0296594	0.0008 594	Protona tion	b'2-amino-5-phosphonopent-3-enoic acid'	b'(E)-2-Amino-5-phosphonopent-3-enoic acid'	HMDB02 44997	C5H10NO5P	
		195.0298969	0.0010 969	Protona tion	b'3-(3,4-dihydroxyphenyl)-2-oxopropanoate'	b'3,4-dihydroxyphenylpyruvate'	HMDB03 04103	C9H7O5	

		194.0183699	0.0026 301	Redox	b'pyrrolidin-1-yl N,N-disulfanylcabamate'	b'Pyrrolidin-1-yl N,N-bis(sulfanyl)carbamate'	HMDB02 57676	C5H10N2O2 S2	
74	194.05 98	195.0684139	0.0008 139	Protontion	b'9H-carbazole-3-carbaldehyde'	b'9H-Carbazole-3-carboxaldehyde'	HMDB00 29743	C13H9NO	
		195.0684139	0.0008 139	Protontion	b'2-oxa-9-azatricyclo[9.4.0.0'xc2'xb3,xc2'xb8]pentadeca-1(15),3,5,7,9,11,13-heptaene'	b'Dibenz[b,f][1,4]oxazepine'	HMDB02 45702	C13H9NO	
		195.0684139	0.0008 139	Protontion	b'9,10-dihydroacridin-9-one'	b'Acridone'	HMDB02 46984	C13H9NO	C201 42
		195.0684139	0.0008 139	Protontion	b'phenanthridin-6-ol'	b'6(SH)-Phenanthridinone'	HMDB02 47116	C13H9NO	
		195.0695567	0.0019 567	Protontion	b'10-fluoro-2,8-dioxo-5-azatricyclo[7.4.0.0' {3,7}]trideca-1(9),10,12-triene'	b'Fluparoxan'	HMDB02 52395	C10H10FNO 2	
		195.0684139	0.0008 139	Protontion	b'phenanthridin-1-ol'	b'Phenanthridinol'	HMDB02 56393	C13H9NO	
		194.0579088	0.0018 912	Redox	b'(2E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid'	b'Ferulic acid'	HMDB00 00954	C10H10O4	C014 94
		194.0579088	0.0018 912	Redox	b'(2E)-3-(3-hydroxy-4-methoxyphenyl)prop-2-enoic acid'	b'Isoferulic acid'	HMDB00 00955	C10H10O4	C104 70
		194.0579088	0.0018 912	Redox	b'2-(ethoxycarbonyl)benzoic acid'	b'Monoethyl phthalate'	HMDB00 02120	C10H10O4	
		194.0579088	0.0018 912	Redox	b'4-formyl-2-methoxyphenyl acetate'	b'Vanillin acetate'	HMDB00 29663	C10H10O4	
		194.0579088	0.0018 912	Redox	b'4,8-dihydroxy-3-methyl-3,4-dihydro-1H-2-benzopyran-1-one'	b'(-)-trans-3,4-Dihydro-4,8-dihydroxy-3-methyl-1H-2-benzopyran-1-one'	HMDB00 30765	C10H10O4	
		194.0579088	0.0018 912	Redox	b'2H-1,3-benzodioxol-5-ylmethyl acetate'	b'Piperonyl acetate'	HMDB00 32614	C10H10O4	

		194.0579088	0.0018 912	Redox	b'6,7-dimethoxy-1,3-dihydro-2-benzofuran-1-one'	b'Meconine'	HMDB00 32652	C10H10O4	
		194.0579088	0.0018 912	Redox	b'(2E)-3-(2-hydroxy-3-methoxyphenyl)prop-2-enoic acid'	b'3-(2-Hydroxy-3-methoxyphenyl)-2-propenoic acid'	HMDB00 37644	C10H10O4	
		194.0579088	0.0018 912	Redox	b'(3-{4-[3-(hydroxymethyl)oxiran-2-yl]buta-1,3-diyn-1-yl} oxiran-2-yl)methanol'	b'Repandiol'	HMDB00 39606	C10H10O4	
		194.0579088	0.0018 912	Redox	b'3-(benzyloxy)-3-oxopropanoic acid'	b'mono-Benzyl malonate'	HMDB00 59721	C10H10O4	
		194.0579088	0.0018 912	Redox	b'methyl (2E)-3-(2,5-dihydroxyphenyl)prop-2-enoate'	b'2,5-Dihydroxycinnamic acid methyl ester'	HMDB00 61686	C10H10O4	
		194.0579088	0.0018 912	Redox	b'(2Z)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid'	b'cis-Ferulic acid'	HMDB02 40705	C10H10O4	
		194.0579088	0.0018 912	Redox	b'methyl 3-(3,4-dihydroxyphenyl)prop-2-enoate'	b'Methyl 3,4-dihydroxycinnamate'	HMDB02 46032	C10H10O4	
		194.0579088	0.0018 912	Redox	b'1,2-dimethyl benzene-1,2-dicarboxylate'	b'Dimethyl phthalate'	HMDB02 51388	C10H10O4	C112 33
		194.0579088	0.0018 912	Redox	b'3-(3-hydroxy-4-methoxyphenyl)prop-2-enoic acid'	b'cis-Isoferulic acid'	HMDB02 59693	C10H10O4	
		194.0579088	0.0018 912	Redox	b'6,8-dihydroxy-3-methyl-3,4-dihydro-1H-2-benzopyran-1-one'	b'(R)-3,4-Dihydro-6,8-dihydroxy-3-methyl-1H-2-benzopyran-1-one'	HMDB03 03675	C10H10O4	
		194.0579088	0.0018 912	Redox	b'3-(3,4-dihydroxy-5-methoxyphenyl)prop-2-enal'	b'5-hydroxy-coniferaldehyde'	HMDB03 04215	C10H10O4	
75	194.07 88	195.0895433	0.0029 433	Protontion	b'(2S)-2-amino-3-(4-hydroxyphenyl)-2-methylpropanoic acid'	b'Metyrosine'	HMDB00 14903	C10H13NO3	C079 21
		195.0895433	0.0029 433	Protontion	b'methyl (2S)-2-amino-3-(4-hydroxyphenyl)propanoate'	b'Tyrosine methylester'	HMDB00 29217	C10H13NO3	C034 04

		195.0895433	0.0029 433	Protona tion	b'N-[2-(3,4-dihydroxyphenyl)ethyl]ethanimidic acid'	b'N-Acetyldopamine'	HMDB00 41943	C10H13NO3	
		195.0895433	0.0029 433	Protona tion	b'2-methyl-1,2,3,4-tetrahydroisoquinoline-4,6,7-triol'	b'N-methyl-4,6,7-trihydroxy-1,2,3,4-tetrahydroisoquinoline'	HMDB00 60065	C10H13NO3	
		195.0895433	0.0029 433	Protona tion	b'3-(C-hydroxycarbonimidoyloxy)-2-phenylpropan-1-ol'	b'2-Phenyl-1,3-propanediol monocarbamate'	HMDB00 60351	C10H13NO3	C165 86
		195.0895433	0.0029 433	Protona tion	b'2-amino-3-(4-hydroxyphenyl)-2-methylpropanoic acid'	b'Racemetirosine'	HMDB02 47174	C10H13NO3	
		195.0895433	0.0029 433	Protona tion	b'2-amino-3-(3-hydroxyphenyl)-2-methylpropanoic acid'	b'alpha-Methyl-m-tyrosine'	HMDB02 48232	C10H13NO3	C118 20
		195.0895433	0.0029 433	Protona tion	b'3-amino-2-hydroxy-4-phenylbutanoic acid'	b'3-Amino-2-hydroxy-4-phenylbutanoic acid'	HMDB02 56443	C10H13NO3	
		195.0895433	0.0029 433	Protona tion	b'5-(2-aminopropyl)-2-hydroxybenzoic acid'	b'5-[(2R)-2-Aminopropyl]-2-hydroxybenzoic acid'	HMDB02 57825	C10H13NO3	
		195.0895433	0.0029 433	Protona tion	b'2-(2-aminopropyl)-5-hydroxybenzoic acid'	b'2-[(2R)-2-Aminopropyl]-5-hydroxybenzoic acid'	HMDB02 57865	C10H13NO3	
		194.0803756	0.0015 756	Redox	b'1,3,7-trimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Caffeine'	HMDB00 01847	C8H10N4O2	C074 81
		194.0803756	0.0015 756	Redox	b'3-propyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'	b'Enprofylline'	HMDB00 14962	C8H10N4O2	
		194.0790382	0.0002 382	Redox	b'(1R,2R,3R,4R,5S,6R)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'D-4-O-Methyl-myo-inositol'	HMDB00 29915	C7H14O6	C063 53
		194.0790382	0.0002 382	Redox	b'(2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-methoxyoxane-3,4,5-triol'	b'Methyl beta-D-glucopyranoside'	HMDB00 29965	C7H14O6	
		194.0790382	0.0002 382	Redox	b'(1R,2R,3S,4S,5R,6S)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'(-)-Bornesitol'	HMDB00 31437	C7H14O6	C036 59

		194.0790382	0.0002 382	Redox	b'(1R,2S,3r,4R,5S,6r)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'Sequoyitol'	HMDB00 31449	C7H14O6	C033 65
		194.0790382	0.0002 382	Redox	b'(1r,2R,3S,4s,5R,6S)-1-methylcyclohexane-1,2,3,4,5,6-hexol'	b'Mytilitol'	HMDB00 33816	C7H14O6	
		194.0790382	0.0002 382	Redox	b'(1R,2S,3R,4S,5S,6S)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'D-Pinitol'	HMDB00 34219	C7H14O6	C038 44
		194.0790382	0.0002 382	Redox	b'(1R,2S,3S,4S,5R,6R)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'L-Quebrachitol'	HMDB00 34221	C7H14O6	C082 57
		194.0799066	0.0011 066	Redox	b'3-[(3-sulfanylbutan-2-yl)sulfanyl]butan-2-ol'	b'3-[(2-Mercapto-1-methylpropyl)thio]- 2-butanol'	HMDB00 37295	C8H18OS2	
		194.0790382	0.0002 382	Redox	b'(1S,2R,3R,4R,5S,6S)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'1D-5-O-Methyl-chiro-inositol'	HMDB00 62564	C7H14O6	
		194.0790382	0.0002 382	Redox	b'3,4,5,6,7-pentahydroxyheptan-2-one'	b'1-Deoxy-D-manno-heptulose'	HMDB02 43861	C7H14O6	
		194.0790382	0.0002 382	Redox	b'2,4,5,6-tetrahydroxy-3-methoxyhexanal'	b'3-O-Methyl-d-glucose'	HMDB02 45931	C7H14O6	
		194.0790382	0.0002 382	Redox	b'1,4,5,6-tetrahydroxy-3-methoxyhexan-2-one'	b'3-O-Methyl-D-fructose'	HMDB02 45957	C7H14O6	
		194.0790382	0.0002 382	Redox	b'6-(hydroxymethyl)-4-methoxyoxane-2,3,5-triol'	b'3-O-Methyl-D-glucopyranose'	HMDB02 45958	C7H14O6	
		194.0790382	0.0002 382	Redox	b'2-(hydroxymethyl)-6-methoxyoxane-3,4,5-triol'	b'Methyl alpha-D-galactopyranoside'	HMDB02 46173	C7H14O6	
		194.0790382	0.0002 382	Redox	b'1,2,3,5,6-pentahydroxyheptan-4-one'	b'(2R,3R,5S)-1,2,3,5,6- Pentahydroxyheptan-4-one'	HMDB02 55312	C7H14O6	
		194.0790382	0.0002 382	Redox	b'(1R,2S,4S,5S)-6-methoxycyclohexane-1,2,3,4,5-pentol'	b'D-ononitol'	HMDB03 04321	C7H14O6	

76	195.06 28	196.0735589	0.0029 589	Protone	b'2-(3,4-dimethoxyphenyl)acetic acid'	b'Homoveratric acid'	HMDB00 00434	C10H12O4	
		196.0735589	0.0029 589	Protone	b'1-(2-hydroxy-4,6-dimethoxyphenyl)ethan-1-one'	b'Xanthoxylin'	HMDB00 29645	C10H12O4	C107 26
		196.0735589	0.0029 589	Protone	b'2,4,5-trimethoxybenzaldehyde'	b'2,4,5-Trimethoxybenzaldehyde'	HMDB00 29648	C10H12O4	
		196.0735589	0.0029 589	Protone	b'3-(2H-1,3-benzodioxol-5-yl)propane-1,2-diol'	b'(+)-3-(3,4-Methylenedioxyphenyl)- 1,2-propanediol'	HMDB00 30571	C10H12O4	
		196.0735589	0.0029 589	Protone	b'2-methyl-4-oxo-4H-pyran-3-yl 2-methylpropanoate'	b'Maltol isobutyrate'	HMDB00 32365	C10H12O4	
		196.0735589	0.0029 589	Protone	b'5-(furan-3-yl)-2-methyl-5-oxopentanoic acid'	b'(S)-Batatic acid'	HMDB00 35721	C10H12O4	
		196.0735589	0.0029 589	Protone	b'1-(2,4,5-trihydroxyphenyl)butan-1-one'	b'1-(2,4,5-Trihydroxyphenyl)-1- butanone'	HMDB00 37177	C10H12O4	
		196.0735589	0.0029 589	Protone	b'2-hydroxy-3-(4-methoxyphenyl)propanoic acid'	b'2-Hydroxy-3-(4- methoxyphenyl)propanoic acid'	HMDB00 39427	C10H12O4	
		196.0735589	0.0029 589	Protone	b'2-(4-methoxyphenoxy)propanoic acid'	b'(S)-2-(4-Methoxyphenoxy)propanoic acid'	HMDB00 40256	C10H12O4	
		196.0735589	0.0029 589	Protone	b'3-butanoyl-4-hydroxy-6-methyl-2H-pyran-2-one'	b'4-Hydroxy-6-methyl-3-(1-oxobutyl)- 2H-pyran-2-one'	HMDB00 40637	C10H12O4	
		196.0735589	0.0029 589	Protone	b'5-[(1E)-3-hydroxyprop-1-en-1-yl]-3-methoxybenzene-1,2-diol'	b'5-Hydroxyconiferyl alcohol'	HMDB00 60398	C10H12O4	C122 05
		196.0735589	0.0029 589	Protone	b'2-hydroxy-3-(3-hydroxyphenyl)-2-methylpropanoic acid'	b'3-(3-Hydroxyphenyl)-2-methylactic acid'	HMDB00 60733	C10H12O4	
		196.0735589	0.0029 589	Protone	b'3-(3,4-dihydroxyphenyl)-2-methylpropanoic acid'	b'3-(3,4-Dihydroxyphenyl)-2- methylpropionic acid'	HMDB00 60735	C10H12O4	

77	195.08 18	196.0735589	0.0029 589	Protone tion	b'3-(4-hydroxy-3-methoxyphenyl)propanoic acid'	b'Dihydroferulic acid'	HMDB00 62121	C10H12O4	
		196.0735589	0.0029 589	Protone tion	b'3-(3-hydroxy-4-methoxyphenyl)propanoic acid'	b'3-(3-hydroxy-4-methoxyphenyl)propanoic acid'	HMDB01 31138	C10H12O4	
		196.0735589	0.0029 589	Protone tion	b'2,6-dimethyl-4,10-dioxatricyclo[5.2.1.0]xc2'xb2,\xe2\x81\xb6]decane-3,5-dione'	b'Cantharidin'	HMDB02 49592	C10H12O4	
		196.0735589	0.0029 589	Protone tion	b'2-(3,4-dihydroxyphenyl)ethyl acetate'	b'Hydroxytyrosol Acetate'	HMDB02 53298	C10H12O4	
		196.0735589	0.0029 589	Protone tion	b'3-(5-methoxy-4-oxocyclohex-2-en-1-yl)prop-2-enoic acid'	b'3-(5-Methoxy-4-oxocyclohex-2-en-1-yl)prop-2-enoic acid'	HMDB02 55409	C10H12O4	
		196.0735589	0.0029 589	Protone tion	b'4,4,4-trihydroxy-1-phenylbutan-1-one'	b'trihydroxybutyrophene'	HMDB02 59219	C10H12O4	
		196.0735589	0.0029 589	Protone tion	b'ethyl 4-hydroxy-3-methoxybenzoate'	b'4-hydroxy-3-methoxybenzoic acid ethyl ester'	HMDB03 03913	C10H12O4	
		196.0735589	0.0029 589	Protone tion	b'2-methyl-1-(2,4,6-trihydroxyphenyl)propan-1-one'	b'phlorisobutyrophene'	HMDB03 04461	C10H12O4	C073 51
	195.08 18	196.0921858	0.0025 858	Protone tion	b'1-(thiophen-2-yl)heptan-1-one'	b'1-(2-Thienyl)-1-heptanone'	HMDB00 40241	C11H16OS	
		196.088815	0.0007 85	Protone tion	b'(2R,3S)-2,3-diphenyloxirane'	b'Cis-stilbene oxide'	HMDB00 59631	C14H12O	C160 14
		196.088815	0.0007 85	Protone tion	b'1,2-diphenylethan-1-one'	b'Deoxybenzoin'	HMDB02 44095	C14H12O	
		196.088815	0.0007 85	Protone tion	b'4-(2-phenylethenyl)phenol'	b'4-Hydroxystilbene'	HMDB02 46467	C14H12O	
		196.088815	0.0007 85	Protone tion	b'2-(2-phenylethenyl)phenol'	b'hydroxystilbene'	HMDB02 53294	C14H12O	

		196.088815	0.0007 85	Protona tion	b'2,3-diphenyloxirane'	b'Stilbene oxide'	HMDB02 58501	C14H12O	
		195.0814772	0.0003 228	Redox	b'8-chloro-1-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine'	b'8-Chloro-1-methyl-2,3,4,5-tetrahydro-1H-benzof[d]azepine'	HMDB02 47137	C11H14CIN	
		195.0814772	0.0003 228	Redox	b'6-chloro-3-methyl-2,3,4,5-tetrahydro-1H-3-benzazepine'	b'benalfocin'	HMDB02 48942	C11H14CIN	C109 70
78	195.99 06	196.9955004	0.0028 996	Protona tion	b'(2S)-2-amino-4-(methylelanil)butanoic acid'	b'Selenomethionine'	HMDB00 03966	C5H11NO2S e	C053 35
79	196.03 66	197.0436557	0.0007 443	Protona tion	b'2-methyl-3,5-dinitroaniline'	b'2-Amino-4,6-dinitrotoluene'	HMDB02 45219	C7H7N3O4	C163 95
		197.0436557	0.0007 443	Protona tion	b'4-methyl-3,5-dinitroaniline'	b'4-Amino-2,6-dinitrotoluene'	HMDB02 46344	C7H7N3O4	C163 94
		197.0453095	0.0009 095	Protona tion	b'2-amino-5-phosphonopentanoic acid'	b'2-Amino-5-phosphonopentanoic acid'	HMDB02 47376	C5H12NO5P	C137 34
		197.045547	0.0011 47	Protona tion	b'2-hydroxy-2-(4-hydroxy-3-methoxyphenyl)acetate'	b'vanillyl mandelate'	HMDB03 04531	C9H9O5	
		196.0371734	0.0005 734	Redox	b'7-methoxy-2H-1,3-benzodioxole-5-carboxylic acid'	b'3-Methoxy-4,5-methylenedioxybenzoic acid'	HMDB00 30800	C9H8O5	
		196.0371734	0.0005 734	Redox	b'3-(4-hydroxyphenoxy)-3-oxopropanoic acid'	b'4-Hydroxy-benzenepropanedioate'	HMDB00 59809	C9H8O5	
		196.034488	0.0021 12	Redox	b'2-amino-8-nitro-6,7-dihydro-1H-purin-6-one'	b'8-Nitroguanine'	HMDB02 47453	C5H4N6O3	
80	196.96 56	196.9665516	0.0009 516	Redox	b'gold(1+) ion'	b'Gold'	HMDB00 04138	Au	
81	196.98 18	197.99055	0.0009 5	Protona tion	b'1-iodopentane'	b'1-Iodopentane'	HMDB02 43909	C5H11I	

82	197.0203	198.0295012	0.0014012	Protonation	b'3-chloro-6-(hydroxymethyl)oxane-2,4,5-triol'	b'2-Chloro-DG'	HMDB0245057	C6H11ClO5	
		198.0276713	0.0004287	Protonation	b'2-methyl-4,6-dinitrophenol'	b'4,6-Dinitro-O-cresol'	HMDB0245221	C7H6N2O5	C18653
		198.0276713	0.0004287	Protonation	b'1-methoxy-2,4-dinitrobenzene'	b'2,4-Dinitroanisole'	HMDB0245458	C7H6N2O5	
		197.0201569	0.0001431	Redox	b'2-[(E)-[amino(phosphonoamino)methylidene]amino]acetic acid'	b'Phosphoguanidinoacetate'	HMDB0003705	C3H8N3O5P	C03166
83	198.9809	199.9872256	0.0014744	Protonation	b'octafluorocyclobutane'	b'Octafluorocyclobutane'	HMDB0031292	C4F8	
		199.9872253	0.0014747	Protonation	b'1,1,3,3,3-pentafluoro-2-(trifluoromethyl)prop-1-ene'	b'Perfluoroisobutylene'	HMDB0256325	C4F8	
		198.9784686	0.0024314	Redox	b'4-chloro-7-nitro-2,1,3-benzoxadiazole'	b'4-Chloro-7-nitrobenzofurazan'	HMDB0246389	C6H2ClN3O3	
84	204.0676	205.0738932	0.0015068	Protonation	b'(2S)-2-hydroxy-3-(1H-indol-3-yl)propanoic acid'	b'Indolelactic acid'	HMDB0000671	C11H11NO3	C02043
		205.0738932	0.0015068	Protonation	b'2-(5-methoxy-1H-indol-3-yl)acetic acid'	b'5-Methoxyindoleacetate'	HMDB0004096	C11H11NO3	C05660
		205.0738932	0.0015068	Protonation	b'2-[(2E)-3-phenylprop-2-enamido]acetic acid'	b'Cinnamoylglycine'	HMDB0011621	C11H11NO3	
		205.0738932	0.0015068	Protonation	b'4,8-dimethoxy-1,2-dihydroquinolin-2-one'	b'Edulitine'	HMDB0030179	C11H11NO3	
		205.0738932	0.0015068	Protonation	b'methyl 1-methoxy-1H-indole-3-carboxylate'	b'Methyl 1-methoxy-1H-indole-3-carboxylate'	HMDB0032755	C11H11NO3	
		205.0738932	0.0015068	Protonation	b'3-hydroxy-3-(1H-indol-3-yl)propanoic acid'	b'3-Indolehydracrylic acid'	HMDB0059765	C11H11NO3	

		205.0772645	0.0018 645	Protona tion	b'(2S)-2-[(1-hydroxypropylidene)amino]-4-(methylsulfonyl)butanoic acid'	b'N-Propionylmethionine'	HMDB00 94704	C8H15NO3S	
		205.0738932	0.0015 068	Protona tion	b'5-ethyl-5-phenyl-1,3-oxazolidine-2,4-dione'	b'5-Ethyl-5-phenyl-1,3-oxazolidine-2,4-dione'	HMDB02 46785	C11H11NO3	
		205.0738932	0.0015 068	Protona tion	b'methyl 2-(2-hydroxy-3H-indol-3-yl)acetate'	b'Methyl oxindole-3-acetate'	HMDB03 03691	C11H11NO3	
		204.0687483	0.0011 483	Redox	b'2,8-diazatetracyclo[7.6.1.0]x81xb5,\xc2\xb9xc2\x81xb6.0xc2\xb9xc2\x81xb0,\xc2\xb9xc2\x81xb5]hexadeca-1,3,5(16),6,8,10,12,14-octaene'	b'Eupolauridine'	HMDB00 30182	C14H8N2	
85	206.04 75	207.0531578	0.0021 422	Protona tion	b'4-(2-aminophenyl)-2,4-dioxobutanoic acid'	b'4-(2-Aminophenyl)-2,4-dioxobutanoic acid'	HMDB00 00978	C10H9NO4	C012 52
		207.0565286	0.0012 286	Protona tion	b'2-amino-3-[(2-carboxy-2-methylethyl)sulfonyl]propanoic acid'	b'(2R,2'S)-Isobutene"	HMDB00 30411	C7H13NO4S	
		207.0565286	0.0012 286	Protona tion	b'2-methyl-2-(prop-2-enamido)propane-1-sulfonic acid'	b'2-Methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid'	HMDB00 31200	C7H13NO4S	
		207.0531578	0.0021 422	Protona tion	b'5-nitro-1,2-dihydronaphthalene-1,2-diol'	b'1-Nitro-5,6-dihydroxy-dihydronaphthalene'	HMDB00 60328	C10H9NO4	C148 01
		207.056325	0.0010 25	Protona tion	b'1-(4-chlorophenyl)-3-methyl-1H-pyrazol-5-amine'	b'chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 3'	HMDB00 62463	C10H10ClN	3
		207.0565291	0.0012 291	Protona tion	b'(2S)-2-acetamido-4-methanesulfonylbutanoic acid'	b'N-Acetyl methionine sulfoxide'	HMDB02 40343	C7H13NO4S	
		207.0531578	0.0021 422	Protona tion	b'6-hydroxy-5-methoxy-1H-indole-2-carboxylic acid'	b'6-Hydroxy-5-methoxy-1H-indole-2-carboxylic acid'	HMDB02 45714	C10H9NO4	
		207.0531578	0.0021 422	Protona tion	b'5-hydroxy-6-methoxy-1H-indole-2-carboxylic acid'	b'5-Hydroxy-6-methoxy-1H-indole-2-carboxylic acid'	HMDB02 46803	C10H9NO4	
86	207.04	208.0517776	0.0014	Protona	b'2-[(2-amino-1-hydroxy-3-sulfonylpropylidene)amino]-3-hydroxypropanoic acid'	b'Cysteinyl-Serine'	HMDB00	C6H12N2O4	

25		776	tion				28784	S	
	208.051778	0.0014 78	Protone tion	b'(2R)-2-[(2S)-2-amino-3-hydroxypropanamido]-3-sulfanylpropanoic acid'	b'Serylcycteine'	HMDB00 29036	C6H12N2O4 S		
	208.051778	0.0014 78	Protone tion	b'(2R)-2-amino-3-[(2R)-2-amino-2-carboxyethyl]sulfanyl]propanoic acid'	b'Lanthionine'	HMDB02 40656	C6H12N2O4 S		
	208.0524295	0.0021 295	Protone tion	b'1,2-dihydroanthracene-1,2-dione'	b'1,2-Anthraquinone'	HMDB02 44055	C14H8O2		
	208.0524295	0.0021 295	Protone tion	b'9,10-dihydroanthracene-9,10-dione'	b'Anthraquinone'	HMDB02 48468	C14H8O2	C162 07	
	208.051778	0.0014 78	Protone tion	b'2-amino-3-[(2-amino-2-carboxyethyl)sulfanyl]propanoic acid'	b'DL-Lanthionine'	HMDB02 51521	C6H12N2O4 S		
	208.0524295	0.0021 295	Protone tion	b'9,10-dihydrophenanthrene-9,10-dione'	b'9,10-Phenanthrenequinone'	HMDB02 56391	C14H8O2	C032 43	
87	207.05 44	208.0596401 599	0.0025 599	Protone tion	b'1-([(5-aminofuran-2-yl)methylidene]amino)-4-hydroxy-2,5-dihydro-1H-imidazol-2-one'	b'Aminofurantoine'	HMDB00 60589	C8H8N4O3	
88	208.02 67	209.0335195 805	0.0009 805	Protone tion	b'4-(2-oxoethylidene)-1,2,3,4-tetrahydropyridine-2,6-dicarboxylate'	b'betalamate'	HMDB03 04273	C9H7NO5	
89	208.06 26	209.0688078	0.0015 922	Protone tion	b'2-[2-(4-hydroxyphenyl)acetamido]acetic acid'	b'Hydroxyphenylacetyl glycine'	HMDB00 00735	C10H11NO4	C055 96
		209.0688078	0.0015 922	Protone tion	b'3-(C-hydroxycarbonimidoyloxy)-2-phenylpropanoic acid'	b'3-Carbamoyl-2-phenylpropionic acid'	HMDB00 60367	C10H11NO4	C165 91
		209.0688078	0.0015 922	Protone tion	b'4-(1-amino-1-carboxyethyl)benzoic acid'	b'alpha-Methyl-4-carboxyphenylglycine'	HMDB02 43703	C10H11NO4	
		209.0688078	0.0015 922	Protone tion	b'4-nitrophenyl butanoate'	b'4-Nitrophenyl butyrate'	HMDB02 46539	C10H11NO4	
		209.0688078	0.0015	Protone	b'4-[amino(carboxy)methyl]-3-methylbenzoic acid'	b'4-[(S)-Amino(carboxy)methyl]-3-	HMDB02	C10H11NO4	

			922	tion		methylbenzoic acid'	54239		
		209.0721787	0.0017 787	Protona tion	b'3-(morpholin-4-yl)propane-1-sulfonic acid'	b'3[N-Morpholino]propane sulfonic acid'	HMDB02 54880	C7H15NO4S	
90	208.07 25	209.0800412	0.0002 588	Protona tion	b'N-(3-amino-4-methyl-5-nitrophenyl)ethanimidic acid'	b'4-Acetamido-2-amino-6-nitrotoluene'	HMDB00 60384	C9H11N3O3	C164 20
		209.0800412	0.0002 588	Protona tion	b'2-amino-N-(4-nitrophenyl)propanamide'	b'L-Alanine-4-nitroanilide'	HMDB02 44748	C9H11N3O3	
		209.0800412	0.0002 588	Protona tion	b'4-amino-1-[5-(hydroxymethyl)-2,5-dihydrofuran-2-yl]-1,2-dihydropyrimidin-2-one'	b"2',3'-Didehydro-2',3'-dideoxycytidine"	HMDB02 45545	C9H11N3O3	
		209.0818711	0.0015 711	Protona tion	b'2-[(3-chloro-2-hydroxypropyl)amino]-3-methylbutanoic acid'	b'n-(3-Chloro-2-hydroxypropyl)valine'	HMDB02 55000	C8H16ClNO 3	
		209.0819325	0.0016 325	Protona tion	b'6-(4-methyl-2-oxopentyl)-2-oxo-2H-pyran-4-olate'	b'6-(4-methyl-2-oxopentyl)-4-hydroxy-2-pyrone'	HMDB03 04223	C11H13O4	
		208.0735589	0.0010 589	Redox	b'(2S)-2-benzylbutanedioic acid'	b'(R)-2-Benzylsuccinate'	HMDB00 12127	C11H12O4	C098 16
		208.0735589	0.0010 589	Redox	b'(5R)-5-[(3,4-dihydroxyphenyl)methyl]oxolan-2-one'	b"5-(3',4'-Dihydroxyphenyl)-gamma-valerolactone"	HMDB00 29185	C11H12O4	
		208.0735589	0.0010 589	Redox	b'(2E)-3-(3,4-dimethoxyphenyl)prop-2-enoic acid'	b'3-(3,4-Dimethoxyphenyl)-2-propenoic acid'	HMDB00 34315	C11H12O4	
		208.0735589	0.0010 589	Redox	b'8-methoxy-11-methyl-4,6,10-trioxatricyclo[7.3.0.0]xc2'xb3,\xc2'x81'xb7]dodeca-1,3(7),8-triene'	b'Furapiole'	HMDB00 36055	C11H12O4	
		208.0735589	0.0010 589	Redox	b'1-(4-methoxy-2H-1,3-benzodioxol-5-yl)propan-1-one'	b'1-(2-Methoxy-3,4-methylenedioxyphenyl)-1-propanone'	HMDB00 37308	C11H12O4	
		208.0735589	0.0010 589	Redox	b'8-hydroxy-6-methoxy-3-methyl-3,4-dihydro-1H-2-benzopyran-1-one'	b'6-Methoxymellein'	HMDB00 38510	C11H12O4	C023 81
		208.0735589	0.0010	Redox	b'(2Z)-3-(7-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-en-1-ol'	b'3-(3-Methoxy-4,5-	HMDB00	C11H12O4	

91	209.07		589				methylenedioxyphenyl)-2-propen-1-ol'	40892		
		208.0735589	0.0010 589	Redox	b'1-(7-methoxy-2H-1,3-benzodioxol-5-yl)prop-2-en-1-ol'		b'Anthriscinol'	HMDB00 41461	C11H12O4	
		208.0735589	0.0010 589	Redox	b'5-[(3,5-dihydroxyphenyl)methyl]oxolan-2-one'		b'5-(3',5'-Dihydroxyphenyl)-gamma-valerolactone"	HMDB00 41692	C11H12O4	
		208.0735589	0.0010 589	Redox	b'5-[(3,4-dihydroxyphenyl)methyl]oxolan-2-one'		b'5-(3',4'-Dihydroxyphenyl)-\xc3-valerolactone"	HMDB02 40472	C11H12O4	
		208.0735589	0.0010 589	Redox	b'2-(2-phenylethyl)propanedioic acid'		b'Propanedioic acid, (2-phenylethyl)-'	HMDB02 46216	C11H12O4	
		208.0735589	0.0010 589	Redox	b'3,4-dihydroxy-3-phenyloxan-2-one'		b'Dihydroxyphenyl-valerolactone'	HMDB02 51346	C11H12O4	
		208.0735589	0.0010 589	Redox	b'3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enal'		b'Sinapaldehyde'	HMDB02 58301	C11H12O4	
		208.0735589	0.0010 589	Redox	b'ethyl (2E)-3-(3,4-dihydroxyphenyl)prop-2-enoate'		b'Caffeic acid ethyl ester'	HMDB03 01712	C11H12O4	
		208.0735589	0.0010 589	Redox	b'methyl 3-(4-hydroxy-3-methoxyphenyl)prop-2-enoate'		b'Methyl ferulate'	HMDB03 02072	C11H12O4	
	209.07	210.0752902	0.0025 098	Protonation	b'1,3,7-trimethyl-2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'		b'1,3,7-Trimethyluric acid'	HMDB00 02123	C8H10N4O3	C163 61
		210.0752902	0.0025 098	Protonation	b'1,3,9-trimethyl-2,3,6,7,8,9-hexahydro-1H-purine-2,6,8-trione'		b'1,3,9-Trimethyluric acid'	HMDB00 36431	C8H10N4O3	
		210.079313	0.0015 13	Protonation	b'1-methoxyphenazine'		b'1-Methoxyphenazine'	HMDB02 43918	C13H10N2O	
		210.079313	0.0015 13	Protonation	b'2-amino-9,10-dihydroacridin-9-one'		b'2-Aminoacridone'	HMDB02 45005	C13H10N2O	C121 43
		210.0752902	0.0025	Protonation	b'1-(hydroxymethyl)-3,7-dimethyl-2,3,6,7-tetrahydro-1H-purine-2,6-dione'		b'Caffeinol'	HMDB02	C8H10N4O3	

			098	tion			49533		
		210.079313	0.0015 13	Protone tion	b'5-methyl-1,5-dihydrophenazin-1-one'	b'Pyocyanin'	HMDB02 56934	C13H10N2O	
		210.079313	0.0015 13	Protone tion	b'2-aminoacridin-1-ol'	b'C1=CC=CC2=CC3=C(O)C(N)=CC=C3N=C21'	HMDB02 58097	C13H10N2O	
92	210.05 28	211.0633285	0.0027 285	Protone tion	b'2-hydroxy-9H-carbazole-3-carbaldehyde'	b'Mukonal'	HMDB00 30216	C13H9NO2	
		211.0633285	0.0027 285	Protone tion	b'2-nitro-9H-fluorene'	b'2-Nitrofluorene'	HMDB02 45257	C13H9NO2	C109 23
		211.062473	0.0018 73	Protone tion	b"N"-(4-chlorophenyl)-N-(diaminomethylidene)guanidine"	b'4-Chlorophenylbiguanide'	HMDB02 46402	C8H10ClN5	
		211.0609591	0.0003 591	Protone tion	b'propan-2-yl N-(dimethoxyphosphoryl)carbamate'	b'Avenin'	HMDB02 48738	C6H14NO5P	
		211.062473	0.0018 73	Protone tion	b"N"-(3-chlorophenyl)-N-(diaminomethylidene)guanidine"	b'm-Chlorophenylbiguanide'	HMDB02 54274	C8H10ClN5	C136 46
		211.0593058	0.0012 942	Protone tion	b'2-[(pyridin-3-yl)formamido]ethyl nitrate'	b'Nicorandil'	HMDB02 55584	C8H9N3O4	C132 80
		210.0528234	2.34E- 05	Redox	b'3-(4-hydroxy-3-methoxyphenyl)-2-oxopropanoic acid'	b'Vanilpyruvic acid'	HMDB00 11714	C10H10O5	
		210.0528234	2.34E- 05	Redox	b'(2E)-3-(3,4-dihydroxy-5-methoxyphenyl)prop-2-enoic acid'	b'5-Hydroxyferulic acid'	HMDB00 35484	C10H10O5	C056 19
93	210.07 33	211.079587	0.0015 13	Protone tion	b'ethyl {[2-(dimethylamino)ethyl]sulfanyl}(methyl)phosphinate'	b'Medemo'	HMDB02 54401	C7H18NO2P S	
		210.0739528	0.0006 528	Redox	b'(2R,3S,4R,5S,6R)-2,6-bis(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'Sedoheptulose'	HMDB00 03219	C7H14O7	C083 55
		210.0739528	0.0006	Redox	b'(2R,3S,4R,5S,6S)-2,6-bis(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'L-galacto-2-Heptulose'	HMDB00	C7H14O7	

			528					29901		
		210.0739528	0.0006 528	Redox	b'(2S,3S,4S,5S,6R)-2,6-bis(hydroxymethyl)oxane-2,3,4,5-tetrol'	b'D-manno-2-Heptulose'	HMDB00 29935	C7H14O7	C082 36	
		210.0739528	0.0006 528	Redox	b'6-(1,2-dihydroxyethyl)oxane-2,3,4,5-tetrol'	b'D-altro-D-manno-Heptose'	HMDB00 29952	C7H14O7	C063 97	
		210.0739528	0.0006 528	Redox	b'2,3,4,5,6,7-hexahydroxyheptanal'	b'd-Glycero-d-galacto-heptose'	HMDB02 53107	C7H14O7		
		210.0739528	0.0006 528	Redox	b'1,3,4,5,6,7-hexahydroxyheptan-2-one'	b'MANNOHEPTULOSE'	HMDB02 54327	C7H14O7		
		210.0739528	0.0006 528	Redox	b'1,2,3,5,6,7-hexahydroxyheptan-4-one'	b'(3R,5R,6R)-1,2,3,5,6,7-Hexahydroxyheptan-4-one'	HMDB02 55327	C7H14O7		
		210.0739528	0.0006 528	Redox	b'(2R,4R,5R,6R)-1,2,4,5,6,7-hexahydroxyheptan-3-one'	b'Crocose'	HMDB03 02576	C7H14O7	C196 12	
94	210.99 97	212.0069359	0.0005 641	Protone tion	b'3,5-dinitrobenzoic acid'	b'3,5-Dinitrobenzoic acid'	HMDB02 46067	C7H4N2O6		
95	211.99 53	213.0038381	0.0007 381	Protone tion	b'(2S)-2-amino-4-oxo-4-(phosphonoxy)butanoic acid'	b'L-Aspartyl-4-phosphate'	HMDB00 12250	C4H8NO7P	C030 82	
		213.0021848	0.0009 152	Protone tion	b'1,3,5-trinitrobenzene'	b'1,3,5-Trinitrobenzene'	HMDB02 44187	C6H3N3O6		
		211.9955403	0.0002 403	Redox	b'(((amino-lambda4-sulfanylidene)methyl)amino)(methyl)phosphoryl)((aminomethylidene)-lambda4-sulfanyl)amine'	b'Antipyrine'	HMDB02 48492	C3H9N4OPS 2		
96	212.02 18	213.0307083	0.0011 083	Protone tion	b'2-amino-1-[(2-hydroxypropanoyl)oxy]ethane-1-sulfonic acid'	b'Taurine lactate'	HMDB02 58739	C5H11NO6S		
97	212.03 13	213.0402236	0.0011 236	Protone tion	b'[2-(2-hydroxypropanamido)ethoxy]phosphonic acid'	b'N-Lactoyl ethanolamine phosphate'	HMDB00 32357	C5H12NO6P		
		213.0385703	0.0005	Protone	b'N-(2-methyl-3,5-dinitrophenyl)hydroxylamine'	b'2-hydroxylamino-4,6-dinitrotoluene'	HMDB03	C7H7N3O5	C163	

			297	tion				04072		93
		213.0385703	0.0005 297	Protona tion	b'N-(4-methyl-3,5-dinitrophenyl)hydroxylamine'	b'4-hydroxylamino-2,6-dinitrotoluene'	HMDB03 04181	C7H7N3O5	C163 92	
		212.0295861	0.0017 139	Redox	b'9H-thioxanthen-9-one'	b'Thioxanthen-9-one'	HMDB02 59037	C13H8OS		
98	214.04 72	215.0558737	0.0008 737	Protona tion	b'(2-aminoethoxy)(2,3-dihydroxypropoxy)phosphinic acid'	b'Glycerylphosphorylethanolamine'	HMDB00 00114	C5H14NO6P	C012 33	
		215.0558737	0.0008 737	Protona tion	b'(2-aminoethoxy)[(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'sn-glycero-3-Phosphoethanolamine'	HMDB00 59660	C5H14NO6P		
		214.0490754	0.0018 754	Redox	b'1H,2H,3H,4H-benzo[g]pteridine-2,4-dione'	b'Alloxazine'	HMDB02 48162	C10H6N4O2		
99	215.05 02	216.056863	0.0011 37	Protona tion	b'3-[(3aS,4S,6aR)-2-oxo-hexahydro-1H-thieno[3,4-d]imidazolidin-4-yl]propanoic acid'	b'Bisnorbiotin'	HMDB00 04821	C8H12N2O3 S	C203 84	
		216.056863	0.0011 37	Protona tion	b'(2S,5R,6R)-6-amino-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid'	b'6-Aminopenicillanic acid'	HMDB00 60618	C8H12N2O3 S	C029 54	
		216.0568634	0.0011 366	Protona tion	b'3-[(2-cyanoethyl)sulfanyl]-2-acetamidopropanoic acid'	b'N-Acetyl-S-(2-cyanoethyl)-L-cysteine'	HMDB02 55060	C8H12N2O3 S		
100	217.07 58	218.0843983	0.0007 983	Protona tion	b'9-(diazomethyl)anthracene'	b'9-Anthryldiazomethane'	HMDB02 47582	C15H10N2		
		217.077264	0.0014 64	Redox	b'(2S)-1-[(2S)-2-methyl-3-sulfanylpropanoyl]pyrrolidine-2-carboxylic acid'	b'Captopril'	HMDB00 15328	C9H15NO3S		
		217.0738932	0.0019 068	Redox	b'2-(quinolin-8-yloxy)propanoic acid'	b'2-(Quinolin-8-yloxy)propanoic acid'	HMDB02 44957	C12H11NO3		
		217.0772645	0.0014 645	Redox	b'1-(2-methyl-3-sulfanylpropanoyl)pyrrolidine-2-carboxylic acid'	b'1-(D-3-Mercapto-2-methyl-1-oxopropyl)-L-proline'	HMDB02 47169	C9H15NO3S		
		217.0738932	0.0019	Redox	b'4-(ethoxymethylidene)-2-phenyl-4,5-dihydro-1,3-oxazol-5-one'	b'4-Ethoxymethylene-2-phenyl-2-	HMDB02	C12H11NO3		

			068			oxazolin-5-one'	52118		
		217.0772645	0.0014 645	Redox	b'N-[4-(hydroxymethyl)-3-oxo-1-sulfanythex-4-en-2-yl]acetamide'	b'N-[(2R)-4-(Hydroxymethyl)-3-oxo-1-sulfanythex-4-en-2-yl]acetamide'	HMDB02 60423	C9H15NO3S	
10 1	218.07 06	218.0731649	0.0025 649	Redox	b'pyren-1-ol'	b'1-Hydroxypyrene'	HMDB00 13139	C16H10O	C145 19
		218.072513	0.0019 13	Redox	b'1-(2-amino-3-sulfanylpropanoyl)pyrrolidine-2-carboxylic acid'	b'Cysteinyl-Proline'	HMDB00 28783	C8H14N2O3 S	
		218.072513	0.0019 13	Redox	b'2-[(pyrrolidin-2-yl)formamido]-3-sulfanylpropanoic acid'	b'Prolyl-Cysteine'	HMDB00 29014	C8H14N2O3 S	
		218.0691422	0.0014 578	Redox	b'2-[[cyano(phenyl)methyl]carbonyl]acetic acid'	b'(S)-3-[(Cyanophenylmethyl)amino]-3-oxopropanoic acid'	HMDB00 34911	C11H10N2O 3	
10 2	222.05 2	223.0609591	0.0011 591	Protontion	b'(2E)-3-[(dimethoxyphosphoryl)oxy]-N-methylbut-2-enamide'	b'(E)-Monocrotophos'	HMDB00 31805	C7H14NO5P	C186 63
		223.0609596	0.0011 596	Protontion	b'3-[(dimethoxyphosphoryl)oxy]-N-methylbut-2-enamide'	b'Alphate'	HMDB02 45618	C7H14NO5P	
		223.0609596	0.0011 596	Protontion	b'4-(phosphonomethyl)piperidine-2-carboxylic acid'	b'4-(Phosphonomethyl)piperidine-2-carboxylic acid'	HMDB02 46313	C7H14NO5P	
		222.0528234	0.0008 234	Redox	b'7-hydroxy-6,8-dimethoxy-2H-chromen-2-one'	b'Isoraxidin'	HMDB02 53642	C11H10O5	C174 80
		222.0519679	3.21E-05	Redox	b'2-[[N-(2-chloroethyl)-N'-oxohydrazinecarbonyl]amino]propanamide"	b'N-Chlorothynitrosourea sarcosinamide'	HMDB02 55103	C6H11CIN4 O3	
		222.0519679	3.21E-05	Redox	b'2-[[N-(2-chloroethyl)-N'-oxohydrazinecarbonyl](methyl)amino]acetamide"	b'Sarcnu'	HMDB02 57494	C6H11CIN4 O3	
		222.0528234	0.0008 234	Redox	b'acetyl 2-(acetyloxy)benzoate'	b'Acetyl 2-acetyloxybenzoate'	HMDB02 57655	C11H10O5	
		222.0528234	0.0008	Redox	b'2-[[{(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy]acetic acid'	b'p-Coumaroyl glycolic acid'	HMDB03	C11H10O5	

			234				01727		
		222.0528234	0.0008 234	Redox	b'2-(3-carboxypropanoyl)benzoic acid'	b'2-succinylbenzoate'	HMDB03 04087	C11H10O5	C027 30
10	222.99	224.0078052	0.0006 052	Protone tion	b'4-amino-[2,3'-bithiophene]-5-carboxamide"	b'3-Amino-5-(3-thiophenyl)-2- thiophenecarboxamide'	HMDB02 57535	C9H8N2OS2	
3	94	223	0.0006	Redox	b'francium'	b'FR'	HMDB03 03046	Fr	
10	224.06	225.0766096	0.0015 096	Protone tion	b'2-amino-7-phosphonoheptanoic acid'	b'(+)-2-Amino-7-phosphonoheptanoic acid'	HMDB02 42241	C7H16NO5P	
		225.0749558	0.0001 442	Protone tion	b'4-(hydroxymethyl)-10-imino-3,7-dioxo-1,9-diazatricyclo[6.4.0.0 ² {2,6}]dodeca-8,11-dien-5-ol'	b'2,2'-Anhydrocytidine"	HMDB02 43629	C9H11N3O4	
		225.077947	0.0028 47	Protone tion	b'9-[2-(phosphanylmethoxy)ethyl]-9H-purin-6-amine'	b'9-[2- (Phosphanylmethoxy)ethyl]purin-6- amine'	HMDB02 47656	C8H12N5OP	
		224.0684735	0.0011 735	Redox	b'methyl 2-oxo-4-[(2Z)-1-oxobut-2-en-2-yl]-3,4-dihydro-2H-pyran-5-carboxylate'	b'Elenolide'	HMDB00 30018	C11H12O5	C095 06
		224.0684735	0.0011 735	Redox	b'(2E)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoic acid'	b'Sinapic acid'	HMDB00 32616	C11H12O5	C004 82
		224.0684735	0.0011 735	Redox	b'(2Z)-3-(4-hydroxy-3,5-dimethoxyphenyl)prop-2-enoic acid'	b'cis-Sinapic acid'	HMDB00 34069	C11H12O5	
		224.0684735	0.0011 735	Redox	b'5-[(3,4,5-trihydroxyphenyl)methyl]oxolan-2-one'	b'5-(3',4',5'-Trihydroxyphenyl)-gamma- valerolactone"	HMDB00 41691	C11H12O5	
		224.0684735	0.0011 735	Redox	b'2-oxo-2-(3,4,5-trimethoxyphenyl)acetaldehyde'	b'2-Oxo-2-(3,4,5- trimethoxyphenyl)acetaldehyde'	HMDB02 45283	C11H12O5	
10	225.09	226.1065903	0.0011 903	Protone tion	b'(2S)-2-(3-aminopropanamido)-3-(1H-imidazol-5-yl)propanoic acid'	b'Carnosine'	HMDB00 00033	C9H14N4O3	C003 86
5	76								

		226.1065903	0.0011 903	Protone tion	b'(2S)-2-[(2S)-2-aminopropanamido]-3-(1H-imidazol-4-yl)propanoic acid'	b'Alanylhistidine'	HMDB00 28689	C9H14N4O3	
		226.1065903	0.0011 903	Protone tion	b'(2S)-2-[(2S)-2-amino-3-(1H-imidazol-5-yl)propanamido]propanoic acid'	b'Histidylalanine'	HMDB00 28878	C9H14N4O3	
		226.1027505	0.0026 495	Protone tion	b'3-[(2-methylfuran-3-yl)sulfanyl]heptan-4-one'	b'3-[(2-Methyl-3-furanyl)thio]-4-heptanone'	HMDB00 37158	C12H18O2S	
		226.1065903	0.0011 903	Protone tion	b'4-[2-(5-nitro-1H-imidazol-1-yl)ethyl]morpholine'	b'Nimorazole'	HMDB02 55612	C9H14N4O3	
		226.1065903	0.0011 903	Protone tion	b'2-[(3-amino-1-hydroxypropylidene)amino]-3-(1H-imidazol-5-yl)propanoic acid'	b'beta-Alanyl-L-histidine'	HMDB02 56117	C9H14N4O3	
		226.1065903	0.0011 903	Protone tion	b'2-[(2-amino-1-hydroxypropylidene)amino]-3-(1H-imidazol-5-yl)propanoic acid'	b'Alanyl-Histidine'	HMDB03 04775	C9H14N4O3	
		226.1065903	0.0011 903	Protone tion	b'2-[(2-amino-1-hydroxy-3-(1H-imidazol-5-yl)propylidene)amino]propanoic acid'	b'HistidinyL-Alanine'	HMDB03 04819	C9H14N4O3	
		225.100108	0.0025 08	Redox	b'4-(2-amino-3,3-dihydroxypropyl)phenyl acetate'	b'Hydroxy Tyrosol -Acetate'	HMDB02 53254	C11H15NO4	
		226.0477381	0.0005 381	Redox	b'(3R,4R)-3-[(1-carboxyeth-1-en-1-yl)oxy]-4-hydroxycyclohexa-1,5-diene-1-carboxylic acid'	b'Chorismate'	HMDB00 12199	C10H10O6	C002 51
		226.0477381	0.0005 381	Redox	b'(1s,4s)-1-(2-carboxy-2-oxoethyl)-4-hydroxycyclohexa-2,5-diene-1-carboxylic acid'	b'Prephenate'	HMDB00 12283	C10H10O6	C002 54
		226.0477381	0.0005 381	Redox	b'3,4-dimethoxybenzene-1,2-dicarboxylic acid'	b'3,4-Dimethoxy-1,2-benzenedicarboxylic acid'	HMDB00 33842	C10H10O6	
10 6	226.04 72	226.0477381	0.0005 381	Redox	b'4,5-dimethoxybenzene-1,2-dicarboxylic acid'	b'4,5-Dimethoxy-1,2-benzenedicarboxylic acid'	HMDB00 33893	C10H10O6	
		226.0477381	0.0005 381	Redox	b'(5S,6S)-5-[(1-carboxyeth-1-en-1-yl)oxy]-6-hydroxycyclohexa-1,3-diene-1-carboxylic acid'	b'isochorismate'	HMDB03 04395	C10H10O6	C008 85

10	227.91	227.9130813	0.0017	Redox	b'tetrahydroxyiodous acid'	b'Orthoperiodic acid'	HMDB00	H5IO6	
7	13	813				34831			
10	228.95	229.9649828	0.0019	Protone	b'6,7-dichloro-3-nitroso-1H-indol-2-ol'	b'(Z)-6,7-Dichloro-3-(hydroxyimino)indolin-2-one'	HMDB02	C8H4Cl2N2	
8	52	828		tion		55775	O2		
10	229.01	230.0191538	0.0011	Protone	b'[{(2R,3R)-2,3,5-trihydroxy-4-oxopentyl}oxy]phosphonic acid'	b'D-Ribulose 5-phosphate'	HMDB00	C5H11O8P	C001
		538		tion		00618			99
		230.0191538	0.0011	Protone	b'[{(2R,3S)-2,3,5-trihydroxy-4-oxopentyl}oxy]phosphonic acid'	b'Xylulose 5-phosphate'	HMDB00	C5H11O8P	C002
		538		tion		00868			31
		230.0191538	0.0011	Protone	b'[{(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl}oxy]phosphonic acid'	b'Ribose 1-phosphate'	HMDB00	C5H11O8P	C006
		538		tion		01489			20
		230.0191538	0.0011	Protone	b'[{(2R,3S,4R,5S)-3,4,5-trihydroxyoxolan-2-yl}methoxy]phosphonic acid'	b'D-Ribose 5-phosphate'	HMDB00	C5H11O8P	C037
		538		tion		01548			36
		230.0191543	0.0011	Protone	b'[{(3S,4R)-3,4,5-trihydroxy-2-oxopentyl}oxy]phosphonic acid'	b'D-Xylulose 1-phosphate'	HMDB00	C5H11O8P	
		543		tion		06534			
9	02	230.0191538	0.0011	Protone	b'[{(2R,3R,4S)-2,3,4-trihydroxy-5-oxopentyl}oxy]phosphonic acid'	b'D-Arabinose 5-phosphate'	HMDB00	C5H11O8P	C011
		538		tion		11734			12
		230.0191538	0.0011	Protone	b'[{(2R,3R,4S,5S)-3,4,5-trihydroxyoxan-2-yl}oxy]phosphonic acid'	b'beta-L-Arabinose 1-phosphate'	HMDB00	C5H11O8P	C039
		538		tion		12195			06
		230.0190785	0.0010	Protone	b'7-hydroxy-4-(trifluoromethyl)-2H-chromen-2-one'	b'7-Hydroxy-4-(trifluoromethyl)coumarin'	HMDB02	C10H5F3O3	
		785		tion		47257			
		230.0191543	0.0011	Protone	b'[{3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl}oxy]phosphonic acid'	b'D-Ribose 1-phosphate'	HMDB02	C5H11O8P	
		543		tion		50796			
		230.0200237	0.0020	Protone	b'dimethyl {[2-(ethylsulfanyl)ethyl]sulfanyl}phosphonate'	b'Demeton-S-methyl'	HMDB02	C6H15O3PS	C186
		237		tion		50995	2		55
		230.0191543	0.0011	Protone	b'[(3,4,5-trihydroxy-1-oxopentan-2-yl)oxy]phosphonic acid'	b'Phosphoribose'	HMDB02	C5H11O8P	
		543		tion		56491			

		230.0191543	0.0011 543	Protona tion	b'[(2,3,4-trihydroxy-5-oxopentyl)oxy]phosphonic acid'	b'ribose-5-phosphate'	HMDB02 57215	C5H11O8P	
		230.0191538	0.0011 538	Protona tion	b'[(3,4,5-trihydroxy-2-oxopentyl)oxy]phosphonic acid'	b'[(3R)-3,4,5-Trihydroxy-2-oxopentyl] dihydrogen phosphate'	HMDB02 60227	C5H11O8P	
		230.0167119	0.0012 881	Protona tion	b'disodium 7-oxabicyclo[2.2.1]heptane-2,3-dicarboxylate'	b'Pancrelipase'	HMDB03 04827	C8H8Na2O5	C187 24
		229.0117407	0.0015 407	Redox	b'1-(2,2,2-trifluoroacetyl)pyrrolidine-2-carbonyl chloride'	b'N-Trifluoroacetylprolyl chloride'	HMDB02 46206	C7H7ClF3N O2	
11 0	230.00 85	231.0136189	0.0026 811	Protona tion	b'benzenesulfonamidothiourea'	b'Benzenesulfonamidothiourea'	HMDB02 44954	C7H9N3O2S 2	
		230.0109759	0.0024 759	Redox	b'4-hydroxy-1-(5-nitro-1,3-thiazol-2-yl)imidazolidin-2-one'	b'2-Imidazolidinone, 4-hydroxy-1-(5- nitro-2-thiazolyl)-'	HMDB02 46460	C6H6N4O4S	
		230.0076046	0.0008 954	Redox	b'7-nitro-2,3-dioxo-2,3-dihydroquinoxaline-6-carbonitrile'	b'7-Nitro-2,3-Dioxo-2,3- Dihydroquinoxaline-6-Carbonitrile'	HMDB02 50068	C9H2N4O4	
11 1	233.93 1	233.9290379	0.0019 621	Redox	b'dipotassium oxoboranyl [(oxoboranyl boronato)oxy]boronate'	b'Potassium tetraborate'	HMDB03 03558	B4K2O7	
11 2	237.96 8	238.9748609	0.0009 391	Protona tion	b'[{hydroxy(pyridin-2-yl)phosphoryl]oxy}phosphonic acid'	b'Diphosphopyridine'	HMDB02 51464	C5H7NO6P2	
		237.9693103	0.0013 103	Redox	b'[{(1,3-benzothiazol-2-ylsulfanyl)methyl}sulfanyl]carbonitrile'	b'2- (Thiocyanomethylthio)benzothiazole'	HMDB02 45617	C9H6N2S3	
11 3	237.99 18	237.9935945	0.0017 945	Redox	b'3,4-dioxo-3,4-dihydronaphthalene-1-sulfonic acid'	b'1-Naphthalenesulfonic acid, 3,4- dihydro-3,4-dioxo-'	HMDB02 45592	C10H6O5S	
11 4	238.04 78	239.0582432	0.0026 432	Protona tion	b'4-methyl-1H,2H,5H,10H-benzo[g]quinoline-2,5,10-trione'	b'Marcanine A'	HMDB00 33757	C14H9NO3	
		238.0477381	6.19E- 05	Redox	b'2-(benzoyloxy)butanedioic acid'	b'Benzoilmalic acid'	HMDB00 39494	C11H10O6	

			58						
11	239.23	240.2453156	0.0019 156	Protone tion	b'hexadecanal'	b'Palmitaldehyde'	HMDB00 01551	C16H32O	C005 17
9	56	240.2453156	0.0019 156	Protone tion	b'hexadecan-2-one'	b'2-Hexadecanone'	HMDB00 31052	C16H32O	
12 0	239.97 06	240.9812326	0.0028 326	Protone tion	b'2-oxo-2H-chromen-7-yl sulfate'	b'Umbelliferone sulfate'	HMDB02 40565	C9H5O6S	
12 1	240.04 98	241.0586371	0.0010 371	Protone tion	b'2,4-dihydroxy-6,7-dimethoxy-3,4-dihydro-2H-1,4-benzoxazin-3-one'	b'2,4-Dihydroxy-6,7-dimethoxy-2H-1,4-benzoxazin-3(4H)-one'	HMDB00 37548	C10H11NO6	
		241.0586371	0.0010 371	Protone tion	b'2,4-dihydroxy-7,8-dimethoxy-3,4-dihydro-2H-1,4-benzoxazin-3-one'	b'2,4-Dihydroxy-7,8-dimethoxy-2H-1,4-benzoxazin-3(4H)-one'	HMDB00 37549	C10H11NO6	
		241.0561352	0.0014 648	Protone tion	b'1-(10H-phenothiazin-2-yl)ethan-1-one'	b'1-(10H-Phenothiazin-2-yl)ethanone'	HMDB02 44969	C14H11NOS	
		241.0561352	0.0014 648	Protone tion	b'N-phenyl-N-(prop-2-yn-1-yl)thiophene-2-carboxamide'	b'Morin-5'-sulfonic acid"	HMDB02 54884	C14H11NOS	
12 2	240.06 24	241.0730377	0.0028 377	Protone tion	b'4-chloro-N-(4,5-dihydro-1H-imidazol-2-yl)-6-methoxy-2-methylpyrimidin-5-amine'	b'Moxonidine'	HMDB00 41938	C9H12CIN5 O	C074 51
		241.0728616	0.0026 616	Protone tion	b'2-amino-9-[2-(phosphanylmethoxy)ethyl]-6,9-dihydro-1H-purin-6-one'	b'2-Amino-9-[2-(phosphanylmethoxy)ethyl]-1H-purin-6-one'	HMDB02 57768	C8H12NSO2 P	
		240.0633881	0.0009 881	Redox	b'(1R,6R)-2-(3-carboxypropanoyl)-6-hydroxycyclohexa-2,4-diene-1-carboxylic acid'	b'(1R,6R)-6-hydroxy-2-succinylcyclohexa-2,4-diene-1-carboxylate'	HMDB03 03951	C11H12O6	C058 17
12 3	241.01 01	242.0191538	0.0012 538	Protone tion	b'(3aR,4R,5S,6S,7R,7aS)-2,4,5,6,7-pentahydroxy-hexahydro-2H-1,3,2\xce\xbb\xce2\x81\xbb5-benzodioxaphosphol-2-one'	b'Inositol cyclic phosphate'	HMDB00 01125	C6H11O8P	C042 99
		242.0191543	0.0012	Protone	b'6-(hydroxymethyl)-2-phosphooxane-2,3,4,5-tetrol'	b'Phosphohexose'	HMDB02	C6H11O8P	

			543	tion			56479		
		242.0191543	0.0012 543	Protona tion	b'2,6,7,8-tetrahydroxy-1,3,2lambda5-dioxaphosponane-2,5-dione'	b'(6S,7R)-2,6,7,8-Tetrahydroxy-2-oxo-1,3,2lambda5-dioxaphosponan-5-one'	HMDB02 60167	C6H11O8P	
		242.0202515	0.0023 515	Protona tion	b'3,4,5-trihydroxy-6-methyloxan-2-yl phosphate'	b'beta-L-fucose 1-phosphate'	HMDB03 04542	C6H11O8P	
		241.0078638	0.0022 362	Redox	b'3- {[(2R)-2-amino-2-carboxyethyl]disulfanyl} -2-hydroxypropanoic acid'	b'3-Mercaptolactate-cysteine disulfide'	HMDB00 06512	C6H11NO5S 2	
12 4	242.03 23	242.0319012	0.0003 988	Redox	b'3-(2-chloroethyl)-4-oxo-3H,4H-imidazo[4,3-d][1,2,3,5]tetrazine-8-carboxamide'	b'Mitozolomide'	HMDB02 54765	C7H7ClN6O 2	
12 5	242.07 83	243.0855205	0.0005 795	Protona tion	b'4-amino-1-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one'	b'Cytidine'	HMDB00 00089	C9H13N3O5	C004 75
		243.0855205	0.0005 795	Protona tion	b'4-amino-1-[(2R,3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one'	b'Cytarabine'	HMDB00 15122	C9H13N3O5	C029 61
		243.0855205	0.0005 795	Protona tion	b'(2S)-2-amino-4- {[(1S)-1-carboxy-2-cyanoethyl]-C-hydroxycarbonimidoyl} butanoic acid'	b'gamma-Glutamyl-beta-cyanoalanine'	HMDB00 60478	C9H13N3O5	C057 11
		243.0855205	0.0005 795	Protona tion	b'4-amino-1-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one'	b'Arabinofuranosylcytosine'	HMDB02 48553	C9H13N3O5	
		243.0855205	0.0005 795	Protona tion	b'4-amino-5-hydroxy-1-[4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,2-dihydropyrimidin-2-one'	b'4-Amino-5-hydroxy-1-[(2R,5R)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]pyrimidin-2-one'	HMDB02 58026	C9H13N3O5	
		242.0790382	0.0007 382	Redox	b'2-{3-hydroxy-1H,3H,4H,5H,6H-cyclopenta[c]furan-4-yl}-3-methoxy-3-oxopropanoic acid'	b'Genipinic acid'	HMDB00 38126	C11H14O6	
		242.0790382	0.0007 382	Redox	b'2-[3-formyl-5-(methoxycarbonyl)-2-methyl-3,4-dihydro-2H-pyran-4-yl]acetic acid'	b'Elenaic acid'	HMDB00 39136	C11H14O6	
		242.0803756	0.0020 756	Redox	b'7,8-dimethyl-1H,2H,3H,4H-benzo[g]pteridine-2,4-dione'	b'Lumichrome'	HMDB02 54199	C12H10N4O 2	C017 27

12	243.08 6	244.0881631	0.0004 369	Protone tion	b'5-[(3aS,4S,6aR)-2-oxo-hexahydro-1H-thienof[3,4-d]imidazol-4-yl]pentanoic acid'	b'Biotin'	HMDB00 00030	C10H16N2O 3S	C001 20
		244.0899579	0.0013 579	Protone tion	b''2-{2-fluoro-[1,1'-biphenyl]-4-yl}propanoic acid''	b'Flurbiprofen'	HMDB00 14850	C15H13FO2	
		244.0859351	0.0026 649	Protone tion	b'1-[4-fluoro-5-(hydroxymethyl)oxolan-2-yl]-5-methyl-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b''3'-DEOXY-3'- FLUOROTHYMIDINE''	HMDB02 46092	C10H13FN2 O4	
		244.088815	0.0002 15	Protone tion	b'tetraphen-3-ol'	b'3-Hydroxybenz[a]anthracene'	HMDB02 46692	C18H12O	
		244.0881636	0.0004 364	Protone tion	b'N-{3-[1-hydroxy-2-(methylamino)ethyl]phenyl}methanesulfonamide'	b'Amidephrine'	HMDB02 48297	C10H16N2O 3S	
		244.0881631	0.0004 369	Protone tion	b'5-{2-hydroxy-1H,3aH,4H,6H,6aH-thieno[3,4-d]imidazol-6-yl}pentanoic acid'	b'Bioepiderm'	HMDB02 49220	C10H16N2O 3S	
		243.0830181	0.0022 181	Redox	b'2-propyl-4H,5H-[1,3]thiazolo[4,5-c]quinolin-4-imine'	b'2-Propylthiazolo[4,5-c]quinolin-4- amine'	HMDB02 45307	C13H13N3S	
12	243.88 7	243.8860163	0.0005 163	Redox	b'[dichloro(phosphono)methyl]phosphonic acid'	b'Clodronate'	HMDB00 14858	CH4Cl2O6P 2	
12	245.04 8	246.0504544	0.0014 544	Protone tion	b'[(2R)-2,3-dihydroxypropoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'Glycerophosphoglycerol'	HMDB02 40316	C6H15O8P	
		245.0436557	0.0024 557	Redox	b'7-methoxy-2-oxo-2H-chromene-3-carbonyl azide'	b'7-Methoxycoumarin-3-carbonyl azide'	HMDB02 47270	C11H7N3O4	
		245.0412109	1.09E- 05	Redox	b'N-[4-(trifluoromethoxy)phenyl]carbamoyl cyanide'	b'1-Cyano-N-[4- (trifluoromethoxy)phenyl]formohydrazide'	HMDB02 58057	C9H6F3N3O 2	
12	245.95 9	246.9632125	0.0026 875	Protone tion	b'2-chloro-1,3,5-trinitrobenzene'	b'Picryl chloride'	HMDB02 56541	C6H2ClN3O 6	
		246.9650522	0.0008	Protone	b'2-hydroxypropane-1,2,3-tricarboxylic acid manganese'	b'Manganese citrate'	HMDB03	C6H8MnO7	

			478	tion			03646		
13	245.98	245.9834232	0.0007	Redox	b'5-sulfobenzene-1,3-dicarboxylic acid'	b'5-Sulfo-1,3-benzenedicarboxylic acid'	HMDB00	C8H6O7S	
0	27		232				32822		
13	246.96	247.9739217	0.0012	Protone	b'2,4-dinitrobenzene-1-sulfonic acid'	b'2,4-Dinitrobenzenesulfonic acid'	HMDB02	C6H4N2O7S	
1	74	247.9739217	0.0012	Protone	b'2,3-dinitrobenzene-1-sulfonic acid'	b'Dinitrobenzene sulfonic acid'	HMDB02	C6H4N2O7S	
			783	tion			51418		
13	247.97	247.9788138	0.0023	Redox	b'2,5-bis(thiophen-2-yl)thiophene'	b"2,2':5',2"-Terthiophene"	HMDB02	C12H8S3	C084
2	65		138				45378		60
13	248.93	249.9461916	0.0016	Protone	b'[(methanesulfonylmethyl)disulfanyl]methanesulfonylmethane'	b'Bis(methylsulfonylmethyl) disulfide'	HMDB00	C4H10O4S4	
3	67	249.94624	0.0017	Protone	b'dioxotungstendiol'	b'Tungstic acid'	HMDB02	H2O4W	
			916	tion			41188		
			4	tion			59326		
13	248.97	249.9799642	0.0011	Protone	b'3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoic acid'	b'3,5-Dichloro-4-hydroxy-2-methoxy-6-methylbenzoic acid'	HMDB00	C9H8Cl2O4	
4	1	249.9815051	0.0027	Protone	b'2-amino-4-chloro-5-sulfamoylbenzoic acid'	b'4-Chloro-5-sulfamoylanthranilic acid'	HMDB00	C7H7ClN2O	
			051	tion			60761	4S	
		249.9783383	0.0004	Protone	b'3,5-dihydroxy-4-(sulfooxy)benzoic acid'	b'3,5-dihydroxy-4-(sulfooxy)benzoic acid'	HMDB01	C7H6O8S	
			617	tion			26639		
		249.9783383	0.0004	Protone	b'3,4-dihydroxy-5-(sulfooxy)benzoic acid'	b'Gallic acid 3-sulfate'	HMDB02	C7H6O8S	
			617	tion			40519		
13	253.04	254.0579088	0.0016	Protone	b'7-hydroxy-3-(4-hydroxyphenyl)-4H-chromen-4-one'	b'Daidzein'	HMDB00	C15H10O4	C102
5	85	254.0572569	0.0009	Protone	b'(2S)-2-amino-4-[(2-sulfoethyl)carbamoyl]butanoic acid'	b'5-L-Glutamyl-L-tyrosine'	HMDB00	C7H14N2O6	C058
			569	tion			04195	S	44
		254.0579088	0.0016	Protone	b'1,8-dihydroxy-3-methyl-9,10-dihydroanthracene-9,10-dione'	b'Chrysophanol'	HMDB00	C15H10O4	C103

13	7			494	tion		nonanone'	37141		
			254.1340506	0.0020 494	Protona tion	b'2,6-dimethyl-3-[(2-methylfuran-3-yl)sulfanyl]heptan-4-one'	b'2,6-Dimethyl-3-[(2-methyl-3-furanyl)thio]-4-heptanone'	HMDB00 37154	C14H22O2S	
			254.1378905	0.0017 905	Protona tion	b'2-amino-5-[(5-hydroxy-4,6-dimethylpyrimidin-2-yl)amino]pentanoic acid'	b'(S)-Argpyrimidine'	HMDB00 37180	C11H18N4O 3	
			254.1378905	0.0017 905	Protona tion	b'1-(2-nitro-1H-imidazol-1-yl)-3-(piperidin-1-yl)propan-2-ol'	b'Pimonidazole'	HMDB02 56554	C11H18N4O 3	
	56	253.21	254.2245802	0.0011 802	Protona tion	b'(7Z)-hexadec-7-enoic acid'	b'Hypogeic acid'	HMDB00 02186	C16H30O2	
			254.2245802	0.0011 802	Protona tion	b'(9Z)-hexadec-9-enoic acid'	b'Palmitoleic acid'	HMDB00 03229	C16H30O2	C083 62
			254.2245802	0.0011 802	Protona tion	b'(2E)-hexadec-2-enoic acid'	b'Trans-Hexa-dec-2-enoic acid'	HMDB00 10735	C16H30O2	
			254.2245802	0.0011 802	Protona tion	b'(9E)-hexadec-9-enoic acid'	b'Palmitelaidic acid'	HMDB00 12328	C16H30O2	
			254.2245802	0.0011 802	Protona tion	b'(6E)-hexadec-6-enoic acid'	b'(E)-6-Hexadecenoic acid'	HMDB00 31053	C16H30O2	
			254.2245802	0.0011 802	Protona tion	b'5-dodecyloxolan-2-one'	b'5-Dodecyldihydro-2(3H)-furanone'	HMDB00 31145	C16H30O2	
			254.2245802	0.0011 802	Protona tion	b'16-methyl-1-oxacyclohexadecan-2-one'	b'15-Hexadecanolide'	HMDB00 31711	C16H30O2	
			254.2245802	0.0011 802	Protona tion	b'(5E)-hexadec-5-enoic acid'	b'(Z)-5-Hexadecenoic acid'	HMDB00 32638	C16H30O2	
			254.2245802	0.0011 802	Protona tion	b'(3Z)-hexadec-3-enoic acid'	b'(E)-3-Hexadecenoic acid'	HMDB00 33791	C16H30O2	
			254.2245802	0.0011	Protona	b'(13Z)-hexadec-13-enoic acid'	b'(Z)-13-Hexadecenoic acid'	HMDB00	C16H30O2	

			802	tion			35877		
		254.2245802	0.0011 802	Protona tion	b'(11E)-hexadec-11-enoic acid'	b'(E)-11-Hexadecenoic acid'	HMDB00 37647	C16H30O2	
		254.2245802	0.0011 802	Protona tion	b'3,7-dimethyloct-6-en-1-yl hexanoate'	b'Citronellyl hexanoate'	HMDB00 38958	C16H30O2	
		254.2245802	0.0011 802	Protona tion	b'(6E)-14-methylpentadec-6-enoic acid'	b'(Z)-14-Methyl-6-pentadecenoic acid'	HMDB00 41422	C16H30O2	
		254.2245802	0.0011 802	Protona tion	b'hexadec-15-enoic acid'	b'15-Hexadecenoic acid'	HMDB02 44666	C16H30O2	
		254.2245802	0.0011 802	Protona tion	b'hexadec-9-enoic acid'	b'9-Hexadecenoic acid, (9Z)-'	HMDB02 47596	C16H30O2	
		254.2245802	0.0011 802	Protona tion	b'dodecyl 2-methylprop-2-enoate'	b'Dodecyl methacrylate'	HMDB02 51570	C16H30O2	
		254.2245802	0.0011 802	Protona tion	b'hexadec-6-enoic acid'	b'Sapenic acid'	HMDB02 57483	C16H30O2	
13 8	254.92 36	254.9256761	0.0020 761	Redox	b'2-[(3,5,6-trichloropyridin-2-yl)oxy]acetic acid'	b'TRICLOPYR'	HMDB02 59186	C7H4Cl3NO 3	C110 32
13 9	255.03 07	256.0371734	0.0013 266	Protona tion	b'1,2,4-trihydroxy-9,10-dihydroanthracene-9,10-dione'	b'PURPURIN'	HMDB02 56928	C14H8O5	C103 95
14 0	255.23 16	256.2402303	0.0008 303	Protona tion	b'hexadecanoic acid'	b'Palmitic acid'	HMDB00 00220	C16H32O2	C002 49
		256.2402303	0.0008 303	Protona tion	b'4,8,12-trimethyltridecanoic acid'	b'Trimethyltridecanoic acid'	HMDB00 02396	C16H32O2	
		256.2402303	0.0008 303	Protona tion	b'14-methylpentadecanoic acid'	b'Isopalmitic acid'	HMDB00 31068	C16H32O2	
		256.2402303	0.0008	Protona	b'butyl dodecanoate'	b'Butyl dodecanoate'	HMDB00	C16H32O2	

			303	tion			32065		
		256.2402303	0.0008 303	Protona tion	b'dodecyl butanoate'	b'Dodecyl butyrate'	HMDB00 32249	C16H32O2	
		256.2402303	0.0008 303	Protona tion	b'hexyl decanoate'	b'Hexyl decanoate'	HMDB00 32324	C16H32O2	
		256.2402303	0.0008 303	Protona tion	b'octyl octanoate'	b'Octyl octanoate'	HMDB00 33166	C16H32O2	
		256.2402303	0.0008 303	Protona tion	b'ethyl tetradecanoate'	b'Ethyl tetradecanoate'	HMDB00 34153	C16H32O2	
		256.2402303	0.0008 303	Protona tion	b'dodecyl 2-methylpropanoate'	b'Dodecyl 2-methylpropanoate'	HMDB00 36210	C16H32O2	
		256.2402303	0.0008 303	Protona tion	b'methyl pentadecanoate'	b'Methyl pentadecanoate'	HMDB02 54606	C16H32O2	
		256.2402303	0.0008 303	Protona tion	b'tetradecyl acetate'	b'Tetradecyl acetate'	HMDB02 58885	C16H32O2	
14	256.05	257.0641125	0.0015 875	Protona tion	b'N,N-diethyl {[4-chlorophenyl)methyl]sulfonyl}formamide'	b'Thiobencarb'	HMDB02 48966	C12H16ClN OS	C144 28
1	79	256.0583027	0.0004 027	Redox	b'2,3-dihydroxy-2-[(4-hydroxyphenyl)methyl]butanedioic acid'	b'(2R,3S)-Piscidic acid'	HMDB00 30809	C11H12O7	
14	256.89	257.9095559	0.0019 559	Protona tion	b'[[hydroxy(phosphonooxy)phosphoryl]oxy]phosphonic acid'	b'Triphosphate'	HMDB00 03379	H5O10P3	C021 74
2	98	257.9075832	1.68E- 05	Protona tion	b'1,3,5-trichloro-2-methanesulfonylbenzene'	b'1,3,5-Trichloro-(2-methylsulfonyl)benzene'	HMDB00 37120	C7H5Cl3O2 S	
14	256.99	256.9945372	0.0009 628	Redox	b'O,O-dimethyl {[2-(N-methylformamido)-2-oxoethyl]sulfonyl}phosphonothioate'	b'Formothion'	HMDB02 52447	C6H12NO4P S2	C189 88
3	55								
14	257.23	258.2433043	0.0010	Protona	b'[2-(decanoyloxy)ethyl]trimethylazanium'	b'Decanoylcholine'	HMDB00	C15H32NO2	

4	66		957	tion			13228		
		257.2354792	0.0011 208	Redox	b'2-[dodecyl(methyl)amino]acetic acid'	b'N-Dodecylsarcosinate'	HMDB02 55129	C15H31NO2	
14 5	258.03 72	259.0457029	0.0007 029	Protone tion	b'([(2S,3R,4R,5S,6R)-3-amino-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)phosphonic acid'	b'Glucosamine-1P'	HMDB00 01109	C6H14NO8P	
		259.0457029	0.0007 029	Protone tion	b'([(2R,3S,4R,5R,6S)-5-amino-3,4,6-trihydroxyoxan-2-yl]methoxy)phosphonic acid'	b'Glucosamine 6-phosphate'	HMDB00 01254	C6H14NO8P	C003 52
		259.0457029	0.0007 029	Protone tion	b'([(2R,3S,4S)-4-amino-3,5-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]methoxy)phosphonic acid'	b'Aminofructose 6-phosphate'	HMDB00 60436	C6H14NO8P	C122 14
		259.0457034	0.0007 034	Protone tion	b'[(5-amino-2,3,4-trihydroxy-6-oxohexyl)oxy]phosphonic acid'	b'D-Glucosamine-6-phosphate'	HMDB02 50754	C6H14NO8P	
		259.0457034	0.0007 034	Protone tion	b'2-amino-3-([(2,3-dihydroxypropoxy)(hydroxy)phosphoryl]oxy)propanoic acid'	b'Glycerophosphoserine'	HMDB02 52850	C6H14NO8P	
		258.0375673	0.0003 673	Redox	b'6-(acetyloxy)-2,5-dioxo-hexahydrofuro[3,2-b]furan-3-yl acetate'	b'Glucaron'	HMDB02 47896	C10H10O8	
14 6	259.01 12	260.0219757	0.0029 757	Protone tion	b'3-fluoro-5-[2-[2-(fluoromethyl)-1,3-thiazol-4-yl]ethynyl]benzonitrile'	b'Benzonitrile, 3-fluoro-5-(2-(2-(fluoromethyl)-4-thiazolyl)ethynyl)-'	HMDB02 58401	C13H6F2N2 S	
14 7	259.02 09	260.0297185	0.0010 185	Protone tion	b'([(2R,3R,4S)-2,3,4,6-tetrahydroxy-5-oxohexyl]oxy)phosphonic acid'	b'Fructose 6-phosphate'	HMDB00 00124	C6H13O9P	C000 85
		260.029719	0.0010 19	Protone tion	b'([(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy)phosphonic acid'	b'myo-Inositol 1-phosphate'	HMDB00 00213	C6H13O9P	C011 77
		260.0297185	0.0010 185	Protone tion	b'([(2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)phosphonic acid'	b'Galactose 1-phosphate'	HMDB00 00645	C6H13O9P	C004 46
		260.0297185	0.0010 185	Protone tion	b'([(2S,3S,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)phosphonic acid'	b'Dolichyl phosphate D-mannose'	HMDB00 00994	C6H13O9P	C038 62
		260.0297185	0.0010	Protone	b'([(2R,3S,4S,5R)-2,3,4-trihydroxy-5-(hydroxymethyl)oxolan-2-yl]methoxy)phosphonic acid'	b'Fructose 1-phosphate'	HMDB00	C6H13O9P	C010

		185	tion				01076		94
260.0297185	0.0010 185	Protone tion	b'([(2R,3S,4S,5S,6R)-3,4,5,6-tetrahydroxyoxan-2-yl]methoxy)phosphonic acid'	b'Mannose 6-phosphate'	HMDB00 01078	C6H13O9P	C002 75		
260.0297185	0.0010 185	Protone tion	b'([(1S,2R,3S,4S,5S,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy)phosphonic acid'	b'D-myo-Inositol 4-phosphate'	HMDB00 01313	C6H13O9P	C035 46		
260.0297185	0.0010 185	Protone tion	b'([(2R,3S,4S,5R)-3,4,5,6-tetrahydroxyoxan-2-yl]methoxy)phosphonic acid'	b'Glucose 6-phosphate'	HMDB00 01401	C6H13O9P	C000 92		
260.0297185	0.0010 185	Protone tion	b'([(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)phosphonic acid'	b'Glucose 1-phosphate'	HMDB00 01586	C6H13O9P	C001 03		
260.0297185	0.0010 185	Protone tion	b'([(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy)phosphonic acid'	b'myo-Inositol 6-phosphate'	HMDB00 02985	C6H13O9P			
260.0297185	0.0010 185	Protone tion	b'([(2R,3S,4S,5R,6R)-3,4,5,6-tetrahydroxyoxan-2-yl]methoxy)phosphonic acid'	b'beta-D-Glucose 6-phosphate'	HMDB00 03498	C6H13O9P	C011 72		
260.0297185	0.0010 185	Protone tion	b'([(2R,3S,4S,5R)-3,4,5-trihydroxy-5-(hydroxymethyl)oxolan-2-yl]methoxy)phosphonic acid'	b'Beta-D-Fructose 6-phosphate'	HMDB00 03971	C6H13O9P	C053 45		
260.0297185	0.0010 185	Protone tion	b'([(3S,4S,5R)-3,4,5,6-tetrahydroxy-2-oxohexyl]oxy)phosphonic acid'	b'D-Tagatose 1-phosphate'	HMDB00 06328	C6H13O9P			
260.0297185	0.0010 185	Protone tion	b'([(2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy)phosphonic acid'	b'D-Mannose 1-phosphate'	HMDB00 06330	C6H13O9P	C006 36		
260.0297185	0.0010 185	Protone tion	b'([(3S,4R,5S)-3,4,5,6-tetrahydroxy-2-oxohexyl]oxy)phosphonic acid'	b'Sorbose 1-phosphate'	HMDB00 06797	C6H13O9P	C028 88		
260.0297185	0.0010 185	Protone tion	b'([(2S,3S,4S,5R)-3,4-dihydroxy-2,5-bis(hydroxymethyl)oxolan-2-yl]oxy)phosphonic acid'	b'Beta-D-Fructose 2-phosphate'	HMDB00 06800	C6H13O9P	C032 67		
260.0297185	0.0010 185	Protone tion	b'([(1R,2S,3R,4R,5S,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy)phosphonic acid'	b'D-myo-Inositol 3-phosphate'	HMDB00 06814	C6H13O9P	C040 06		
260.0297185	0.0010	Protone	b'([(2R,3R,4S)-3,4,5-trihydroxy-5-(hydroxymethyl)oxolan-2-yl]methoxy)phosphonic acid'	b'D-Tagatose 6-phosphate'	HMDB00	C6H13O9P	C010		

			185	tion			06873		97
		260.0297185	0.0010 185	Protona tion	b'[(3S,4R,5R)-3,4,5,6-tetrahydroxy-2-oxohexyl]oxy}phosphonic acid'	b'D-fructose 1-phosphate'	HMDB00 60467	C6H13O9P	
		260.029719	0.0010 19	Protona tion	b'[(2,3,4,5,6-pentahydroxycyclohexyl)oxy]phosphonic acid'	b'(2,3,4,5,6-Pentahydroxycyclohexyl) dihydrogen phosphate'	HMDB02 42486	C6H13O9P	
		260.029719	0.0010 19	Protona tion	b'[(2,3,4,5-tetrahydroxy-6-oxohexyl)oxy]phosphonic acid'	b'(2R,3R,4S,5R)-2,3,4,5-Tetrahydroxy- 6-oxohexyl dihydrogen phosphate'	HMDB02 42558	C6H13O9P	
		260.0297185	0.0010 185	Protona tion	b'[(3,4,5,6-tetrahydroxy-2-oxohexyl)oxy]phosphonic acid'	b'(3S,4R)-Ketose 1-phosphate'	HMDB02 43608	C6H13O9P	
		260.029719	0.0010 19	Protona tion	b'[(2,3,4,5-tetrahydroxyoxan-2-yl)methoxy]phosphonic acid'	b'beta-D-Fructopyranose 1-phosphate'	HMDB02 43977	C6H13O9P	
		260.0297185	0.0010 185	Protona tion	b'[(3,4,5,6-tetrahydroxyoxan-2-yl)methoxy]phosphonic acid'	b'[(2R,3R,4S,5S)-3,4,5,6- Tetrahydroxyoxan-2-yl]methyl dihydrogen phosphate'	HMDB02 46205	C6H13O9P	C029 65
		260.029719	0.0010 19	Protona tion	b'[(3,4,5,6-tetrahydroxy-1-oxohexan-2-yl)oxy]phosphonic acid'	b'D-Glucose 2-phosphate'	HMDB02 47860	C6H13O9P	
		260.0297185	0.0010 185	Protona tion	b'[{3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy}phosphonic acid'	b'beta-D-Glucose 1-phosphate'	HMDB02 49121	C6H13O9P	C010 02
		260.029719	0.0010 19	Protona tion	b'[(1,4,5,6-tetrahydroxy-2-oxohexan-3-yl)oxy]phosphonic acid'	b'Fructose 3-phosphate'	HMDB02 52488	C6H13O9P	
		260.029719	0.0010 19	Protona tion	b'[{3,4,5-trihydroxy-5-(hydroxymethyl)oxolan-2-yl]methoxy}phosphonic acid'	b'Fructose-6-Phosphate (closed form)'	HMDB02 57695	C6H13O9P	
		260.0297185	0.0010 185	Protona tion	b'[{(2R,3S,4S,5S)-3,4,5,6-tetrahydroxyoxan-2-yl]methoxy}phosphonic acid'	b'D-mannose 6-phosphate'	HMDB03 04312	C6H13O9P	C002 75
14 8	259.03 97	260.0466927	0.0008 073	Protona tion	b'3-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6-imino-3,6-dihydro-2H-1,3-thiazin-2-one'	b'3-Thiacytidine'	HMDB02 45986	C9H12N2O5 S	

		260.0466927	0.0008 073	Protone tion	b'1-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-4-sulfanylidene-1,2,3,4-tetrahydropyrimidin-2-one'	b'4-Thiouridine'	HMDB02 46588	C9H12N2O5 S	
		260.0466927	0.0008 073	Protone tion	b'2-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1,3-thiazole-4-carboxamide'	b'TIAZOFURIN'	HMDB02 59072	C9H12N2O5 S	
14 9	259.93 17	260.941805	0.0023 05	Protone tion	b'3-(3,5-dichlorophenyl)-4-hydroxy-2,3-dihydro-1,3-thiazol-2-one'	b'3-(3,5-Dichlorophenyl)-4-hydroxy- 1,3-thiazol-2-one'	HMDB02 55405	C9H5Cl2NO 2S	
15 0	260.02 27	261.0307083	0.0002 083	Protone tion	b'(4-acetamido-3-methoxyphenyl)oxidanesulfonic acid'	b'2-Methoxyacetaminophen sulfate'	HMDB00 62550	C9H11NO6S	
		261.0307078	0.0002 078	Protone tion	b'(2S)-2-amino-3-[4-(sulfooxy)phenyl]propanoic acid'	b'O-Sulfofytrosine'	HMDB01 55722	C9H11NO6S	
		260.0248197	0.0021 197	Redox	b'2-[bis(2-chloroethyl)amino]-1,3,2lambda5-oxazaphosphinan-2-one'	b'Cyclophosphamide'	HMDB00 14672	C7H15Cl2N 2O2P	C078 88
		260.0248197	0.0021 197	Redox	b'3-(2-chloroethyl)-2-[(2-chloroethyl)amino]-1,3,2lambda5-oxazaphosphinan-2-one'	b'Ifosfamide'	HMDB00 15312	C7H15Cl2N 2O2P	C070 47
		260.0248201	0.0021 201	Redox	b'2-[bis(2-chloroethyl)amino]-1,3,2-oxazaphosphinan-4-ol'	b'2-(Bis(2-chloroethyl)amino)-4- hydroxytetrahydro-2H-1,3,2- oxazaphosphorine'	HMDB02 46558	C7H15Cl2N 2O2P	
15 1	261.93 17	262.9411083	0.0016 083	Protone tion	b'(4-hydroxy-3-nitrophenyl)arsonic acid'	b'Roxarsone'	HMDB00 33205	C6H6AsNO6	
15 2	262.98 61	263.9939879	8.79E- 05	Protone tion	b'(3,4,5-trihydroxy-2-methylbenzoyloxy)sulfonic acid'	b'Methylgallic acid-O-sulphate'	HMDB00 60005	C8H8O8S	
		263.9939884	8.84E- 05	Protone tion	b'3-hydroxy-4-methoxy-5-(sulfooxy)benzoic acid'	b'4-Methylgallic acid 3-sulfate'	HMDB02 40463	C8H8O8S	
15 3	263.97 09	263.9718274	0.0009 274	Redox	b'[(2-hydroxy-6-sulfanyl-9H-purin-9-yl)oxy]phosphonic acid'	b'Thioxanthine monophosphate'	HMDB00 60876	C5H5N4O5P S	
15	264.95	265.9592695	0.0014	Protone	b'[{(2R)-2-hydroxy-3-(phosphonoxy)propanoyl}oxy]phosphonic acid'	b'Glyceric acid 1,3-biphosphate'	HMDB00	C3H8O10P2	C002

4			695	tion				01270		36
		265.9592695	0.0014 695	Protona tion	b'(2R)-2,3-bis(phosphonoxy)propanoic acid'	b'2,3-Diphosphoglyceric acid'	HMDB00 01294	C3H8O10P2	C011 59	
		265.9592705	0.0014 705	Protona tion	b'3-hydroxy-2-([hydroxy(phosphonoxy)phosphoryl]oxy)propanoic acid'	b'3-Hydroxy-2- [hydroxy(phosphonoxy)phosphoryl]oxypropanoic acid'	HMDB02 58120	C3H8O10P2		
15 5	265.25 22	266.2609657	0.0009 657	Protona tion	b'(9E)-octadec-9-enal'	b'9-Octadecenal'	HMDB00 30965	C18H34O		
		266.2609657	0.0009 657	Protona tion	b'2-tetradecylcyclobutan-1-one'	b'2-Tetradecylcyclobutanone'	HMDB00 37517	C18H34O		
		266.2609657	0.0009 657	Protona tion	b'octadec-9-enal'	b'Octadec-9-enal'	HMDB02 50283	C18H34O		
15 6	266.08 71	267.0967539	0.0018 539	Protona tion	b'(2R,3R,4S,5R)-2-(6-amino-9H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol'	b'Adenosine'	HMDB00 00050	C10H13N5O 4	C002 12	
		267.0967539	0.0018 539	Protona tion	b'2-amino-9-[(2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-1H-purin-6-one'	b'Deoxyguanosine'	HMDB00 00085	C10H13N5O 4	C003 30	
		267.0954165	0.0005 165	Protona tion	b'(2S,4S,5R,6R)-5-amino-2,4-dihydroxy-6-[(1R,2R)-1,2,3-trihydroxypropyl]oxane-2-carboxylic acid'	b'Neuraminic acid'	HMDB00 00830	C9H17NO8	C064 69	
		267.0967539	0.0018 539	Protona tion	b'(2R,3S,4S,5R)-2-(6-amino-9H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol'	b'Vidarabine'	HMDB00 14340	C10H13N5O 4	C071 95	
		267.0967539	0.0018 539	Protona tion	b'1-[(2R,4S,5S)-4-azido-5-(hydroxymethyl)oxolan-2-yl]-5-methyl-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'Zidovudine'	HMDB00 14638	C10H13N5O 4	C072 10	
		267.0954165	0.0005 165	Protona tion	b'(2S)-3-hydroxy-2-([(3S,4S,5R)-2,3,4-trihydroxy-5-(hydroxymethyl)oxolan-2-yl]methyl)amino)propanoic acid'	b'N-(1-Deoxy-1-fructosyl)serine'	HMDB00 37842	C9H17NO8		
		267.0967539	0.0018 539	Protona tion	b'1-[4-azido-5-(hydroxymethyl)oxolan-2-yl]-5-methyl-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'3'-Azido-3'-deoxythymidine, 98%"	HMDB02 46088	C10H13N5O 4		

15	267.07	267.0967539	0.0018 539	Protone	b'6-amino-9-[4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-8,9-dihydro-7H-purin-8-one'	b"8-Oxo-2'-deoxyadenosine"	HMDB02 47147	C10H13N5O 4	
		267.0967539	0.0018 539	Protone	b'2-(6-amino-9H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol'	b'9-Arabinofuranosyladenine'	HMDB02 47583	C10H13N5O 4	
		267.0967539	0.0018 539	Protone	b'2-{7-amino-2H-pyrazolo[4,3-d]pyrimidin-3-yl}-5-(hydroxymethyl)oxolane-3,4-diol'	b'Formycin A'	HMDB02 52448	C10H13N5O 4	
		267.0954165	0.0005 165	Protone	b'2-(hydroxymethyl)-6-(3-nitropropoxy)oxane-3,4,5-triol'	b'Miserotoxin'	HMDB02 54754	C9H17NO8	
		267.0929146	0.0019 854	Protone	b'3-(2-benzyl-3-sulfanylpropanamido)propanoic acid'	b'3-[(2-Benzyl-3-sulfanylpropanoyl)amino]propanoic acid'	HMDB02 58443	C13H17NO3 S	
	267.07 14	268.0807695	0.0015 695	Protone	b'9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-3H-purin-6-one'	b'Inosine'	HMDB00 00195	C10H12N4O 5	C002 94
		268.0794321	0.0002 321	Protone	b'(4S,5R,6R,7R,8S)-4,5,6,7,8,9-hexahydroxy-2-oxononanoic acid'	b'3-Deoxy-D-glycero-D-galacto-2-nonulosonic acid'	HMDB00 00425	C9H16O9	
		268.0807695	0.0015 695	Protone	b'1-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1H,4H,7H-pyrazolo[3,4-d]pyrimidin-4-one'	b'Allopurinol riboside'	HMDB00 00481	C10H12N4O 5	
		268.0807695	0.0015 695	Protone	b'9-[(3S,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-3H-purin-6-one'	b'Arabinosylhypoxanthine'	HMDB00 03040	C10H12N4O 5	
		268.0807695	0.0015 695	Protone	b'2-(6-hydroxy-9H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol'	b'Ara-HX'	HMDB02 47301	C10H12N4O 5	
		268.0807695	0.0015 695	Protone	b'3-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-1H,6H,7H-pyrazolo[4,3-d]pyrimidin-7-one'	b'Formycin b'	HMDB02 52449	C10H12N4O 5	
		268.0794321	0.0002 321	Protone	b'3,4,5,6-tetrahydroxy-6-(hydroxymethyl)oxan-2-yl 2-hydroxypropanoate'	b'Fructose lactate'	HMDB02 52491	C9H16O9	
		268.0794321	0.0002	Protone	b'2,3,4,5-tetrahydroxy-6-(hydroxymethyl)oxan-2-yl 2-hydroxypropanoate'	b'galactose lactate'	HMDB02	C9H16O9	

			321	tion			52580		
158	267.2672	268.2766158	0.0016158	Protonation	b'octadecanal'	b'Stearaldehyde'	HMDB0002384	C18H36O	C01838
		268.2766158	0.0016158	Protonation	b'(9Z)-octadec-9-en-1-ol'	b'Oleyl alcohol'	HMDB0029632	C18H36O	
		268.2766158	0.0016158	Protonation	b'2-octyl-3-pentyloxane'	b'(2R,3S)-2-Octyl-3-pentyloxane'	HMDB0242702	C18H36O	
		268.2766158	0.0016158	Protonation	b'octadec-9-en-1-ol'	b'9-Octadecen-1-ol, (9Z)-'	HMDB0247606	C18H36O	
		268.2766158	0.0016158	Protonation	b'6,10,14-trimethylpentadecan-2-one'	b'6,10,14-Trimethylpentadecan-2-one'	HMDB0303073	C18H36O	
159	268.0735	268.0729069	0.0005931	Redox	b'2-amino-4-(3-amino-3-carboxypropanesulfonyl)butanoic acid'	b'Homolanthionine'	HMDB0002034	C8H16N2O6S	
		268.0735589	5.89E-05	Redox	b'7-hydroxy-3-(4-methoxyphenyl)-4H-chromen-4-one'	b'Formononetin'	HMDB0005808	C16H12O4	C00858
		268.0711894	0.0023106	Redox	b'[3-(hexanoyloxy)-2-oxopropoxy]phosphonic acid'	b'DHAP(6:0)'	HMDB0011679	C9H17O7P	
		268.0735589	5.89E-05	Redox	b'7-hydroxy-6-methoxy-2-phenyl-4H-chromen-4-one'	b'Triglucum'	HMDB0030720	C16H12O4	
		268.0735589	5.89E-05	Redox	b'8-hydroxy-1-methoxy-3-methyl-9,10-dihydroanthracene-9,10-dione'	b'8-Hydroxy-1-methoxy-3-methylantraquinone'	HMDB0033036	C16H12O4	
		268.0735589	5.89E-05	Redox	b'3-(4-hydroxyphenyl)-7-methoxy-4H-chromen-4-one'	b'Isoformononetin'	HMDB0033994	C16H12O4	C12125
		268.0735589	5.89E-05	Redox	b'1,3-dimethoxy-9,10-dihydroanthracene-9,10-dione'	b'1,3-Dimethoxyanthraquinone'	HMDB0036586	C16H12O4	
		268.0735589	5.89E-05	Redox	b'2-(8-methyl-9-oxo-9H-xanthen-4-yl)acetic acid'	b'8-Methylxanthen-9-one-4-acetic acid'	HMDB02	C16H12O4	

			05					44424		
		268.0735589	5.89E-05	Redox	b'4-{8-oxatricyclo[7.4.0.0'xc2'xb2,\xc2'x81'xb7]trideca-1(13),2,4,6,9,11-hexaen-4-yl}-4-oxobutanoic acid'	b'Furobufen'	HMDB0252542	C16H12O4		
		268.0735589	5.89E-05	Redox	b'6-hydroxy-7-methoxy-4-phenyl-2H-chromen-2-one'	b'Dalbergin'	HMDB0303925	C16H12O4	C10414	
		268.0735589	5.89E-05	Redox	b'14-methoxy-8,17-dioxatetracyclo[8.7.0.0'xc2'xb2,\xc2'x81'xb7.0'xc2'xb9'xc2'xb9,\xc2'xb9'xc2'xb9'xc2'xb9'xc2'xb9]heptadeca-2,4,6,9,11,13,15-heptaen-5-ol'	b'(-)-medicarpin'	HMDB0303947	C16H12O4		
160	268.0762	268.0735589	0.0026411	Redox	b'7-hydroxy-3-(4-methoxyphenyl)-4H-chromen-4-one'	b'Formononetin'	HMDB0005808	C16H12O4	C00858	
		268.0735589	0.0026411	Redox	b'7-hydroxy-6-methoxy-2-phenyl-4H-chromen-4-one'	b'Trigraecum'	HMDB0030720	C16H12O4		
		268.0735589	0.0026411	Redox	b'8-hydroxy-1-methoxy-3-methyl-9,10-dihydroanthracene-9,10-dione'	b'8-Hydroxy-1-methoxy-3-methylantraquinone'	HMDB0033036	C16H12O4		
		268.0735589	0.0026411	Redox	b'3-(4-hydroxyphenyl)-7-methoxy-4H-chromen-4-one'	b'Isoformononetin'	HMDB0033994	C16H12O4	C12125	
		268.0735589	0.0026411	Redox	b'1,3-dimethoxy-9,10-dihydroanthracene-9,10-dione'	b'1,3-Dimethoxyanthraquinone'	HMDB0036586	C16H12O4		
		268.0735589	0.0026411	Redox	b'2-(8-methyl-9-oxo-9H-xanthen-4-yl)acetic acid'	b'8-Methylxanthen-9-one-4-acetic acid'	HMDB0244424	C16H12O4		
		268.0735589	0.0026411	Redox	b'4-{8-oxatricyclo[7.4.0.0'xc2'xb2,\xc2'x81'xb7]trideca-1(13),2,4,6,9,11-hexaen-4-yl}-4-oxobutanoic acid'	b'Furobufen'	HMDB0252542	C16H12O4		
		268.0735589	0.0026411	Redox	b'6-hydroxy-7-methoxy-4-phenyl-2H-chromen-2-one'	b'Dalbergin'	HMDB0303925	C16H12O4	C10414	
		268.0735589	0.0026411	Redox	b'14-methoxy-8,17-dioxatetracyclo[8.7.0.0'xc2'xb2,\xc2'x81'xb7.0'xc2'xb9'xc2'xb9,\xc2'xb9'xc2'xb9'xc2'xb9'xc2'xb9]heptadeca-2,4,6,9,11,13,15-heptaen-5-ol'	b'(-)-medicarpin'	HMDB0303947	C16H12O4		
16	272.00	273.0129492	0.0006	Protona	b'2-[2-(thiophene-2-carbonylsulfanyl)propanamido]acetic acid'	b'Stepronin'	HMDB00	C10H11NO4		

1	45		492	tion			15492	S2	
16	272.08		0.0028	Redox					
2	68	272.0896029	029		b'(2R,3S,4S,5R,6S)-2-(hydroxymethyl)-6-(4-hydroxyphenoxy)oxane-3,4,5-triol'	b'Arbutin'	HMDB00 29943	C12H16O7	C061 86
16	272.99	274.0040842	0.0015 158	Protona tion	b'2-[bis(2-chloroethyl)amino]-1,3,2'xccc'xb'x81'xb5-oxazaphosphinane-2,4-dione'	b'4-Ketocyclophosphamide'	HMDB00 60686	C7H13Cl2N 2O3P	C076 44
3	78	274.0040842	0.0015 158	Protona tion	b'3-(2-chloroethyl)-2-[(2-chloroethyl)amino]-1,3,2'xccc'xb'x81'xb5-oxazaphosphinane-2,4-dione'	b'4-Ketoifosamide'	HMDB00 60690	C7H13Cl2N 2O3P	C165 54
		272.9959486	0.0018 514	Redox	b'1-[(2,4-dichlorophenyl)-C-hydroxycarbonimidoyl]cyclopropane-1-carboxylic acid'	b'Cyclanilide'	HMDB02 50621	C11H9Cl2N O3	
16	273.03		2.81E-	Protona					
4	19	274.0396719	05	tion	b'methyl 2-chloro-9-hydroxy-9H-fluorene-9-carboxylate'	b'Chlorflurenol-methyl'	HMDB02 50098	C15H11ClO3	
16	275.08		0.0012	Protona					
5	67	276.0957509	509	tion	b'(2S)-2-[(4S)-4-amino-4-carboxybutanamido]pentanedioic acid'	b'gamma-Glutamylglutamic acid'	HMDB00 11737	C10H16N2O 7	C052 82
		276.0957509	0.0012 509	Protona tion	b'(2S)-2-[(2S)-2-amino-4-carboxybutanamido]pentanedioic acid'	b'Glutamylglutamic acid'	HMDB00 28818	C10H16N2O 7	C014 25
		276.0957509	0.0012 509	Protona tion	b'4,5,6-trihydroxy-1-[(2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-5-methyl-1,2,5,6-tetrahydropyrimidin-2-one'	b'Thymidine glycol'	HMDB00 42036	C10H16N2O 7	
		276.0939004	0.0005 996	Protona tion	b'hexacyclo[12.8.0.0^{2,11}.0^{3,8}.0^{4,21}.0^{17,22}]docosa-1(14),2,4,6,8,10,12,15,17(22),18,20-undecaene'	b'Benzo[ghi]perylene'	HMDB02 49010	C22H12	C143 18
		276.0957509	0.0012 509	Protona tion	b'2-(4-amino-4-carboxybutanamido)pentanedioic acid'	b'D-gamma-Glutamyl-D-glutamic acid'	HMDB02 50751	C10H16N2O 7	
		276.0939004	0.0005 996	Protona tion	b'hexacyclo[16.3.1.0^{2,7}.0^{8,21}.0^{11,20}.0^{14,19}]docosa-1(22),2,4,6,8(21),9,11(20),12,14(19),15,17-undecaene'	b'Indeno[1,2,3-cd]pyrene'	HMDB02 53452	C22H12	C192 51
16	279.23		0.0016	Protona					
6	08	280.2402303	303	tion	b'(9Z,12Z)-octadeca-9,12-dienoic acid'	b'Linoleic acid'	HMDB00 00673	C18H32O2	C015 95
		280.2402303	0.0016	Protona	b'(9Z,11E)-octadeca-9,11-dienoic acid'	b'Bovinic acid'	HMDB00	C18H32O2	C040

		303	tion				03797		56
280.2402303	0.0016 303	Protona tion	b'(9E,11E)-octadeca-9,11-dienoic acid'	b'(9E,11E)-Octadecadienoic acid'	HMDB00 05047	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'(10E,12Z)-octadeca-10,12-dienoic acid'	b'(10E,12Z)-Octadecadienoic acid'	HMDB00 05048	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'(9E,12E)-octadeca-9,12-dienoic acid'	b'Linoelaidic acid'	HMDB00 06270	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'(9E,15E)-octadeca-9,15-dienoic acid'	b'Mangiferic acid'	HMDB00 29800	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'3,7-dimethylocta-1,6-dien-3-yl octanoate'	b'Linalyl caprylate'	HMDB00 30430	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'ethyl (2E,4Z)-hexadeca-2,4-dienoate'	b'Ethyl 2E,4Z-hexadecadienoate'	HMDB00 31051	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'octadec-5-ynoic acid'	b'5-Octadecynoic acid'	HMDB00 31097	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'(10Z,12Z)-octadeca-10,12-dienoic acid'	b'Dihomolinoleic acid'	HMDB00 61864	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'(6Z,9Z)-octadeca-6,9-dienoic acid'	b'6Z,9Z-octadecadienoic acid'	HMDB00 62238	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'(2E,4E)-octadeca-2,4-dienoic acid'	b'Octadecadienoate'	HMDB00 62784	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'octadeca-10,12-dienoic acid'	b'Octadeca-10,12-dienoic acid'	HMDB02 44277	C18H32O2			
280.2402303	0.0016 303	Protona tion	b'octadec-17-ynoic acid'	b'17-Octadecynoic acid'	HMDB02 44776	C18H32O2			
280.2402303	0.0016	Protona	b'octadec-7-ynoic acid'	b'7-Octadecynoic acid'	HMDB02	C18H32O2			

			303	tion			47278		
		280.2402303	0.0016 303	Protona tion	b'octadeca-8,12-dienoic acid'	b'8,12-Octadecadienoic acid'	HMDB02 47466	C18H32O2	
		280.2402303	0.0016 303	Protona tion	b'octadeca-9,11-dienoic acid'	b'Octadeca-9,11-dienoic acid'	HMDB02 47620	C18H32O2	
		280.2402303	0.0016 303	Protona tion	b'octadeca-9,12-dienoic acid'	b'9Z,12E-Octadecadienoic acid'	HMDB02 47706	C18H32O2	
		280.2402303	0.0016 303	Protona tion	b'octadeca-2,4-dienoic acid'	b'Octadeca-2,4-dienoic acid'	HMDB02 55894	C18H32O2	
		280.2402303	0.0016 303	Protona tion	b'7-(2-octylcycloprop-1-en-1-yl)heptanoic acid'	b'Malvalic acid'	HMDB03 02286	C18H32O2	C083 21
		280.2402303	0.0016 303	Protona tion	b'octadeca-2,9-dienoic acid'	b'Octadeca-2,9-dienoic acid'	HMDB03 02650	C18H32O2	
		280.2402303	0.0016 303	Protona tion	b'(11E,15Z)-octadeca-11,15-dienoic acid'	b'trans-11,cis-15-Octadecadienoic acid'	HMDB03 04773	C18H32O2	
16 7	280.01 93	280.0170463	0.0022 537	Redox	b'dimethyl (((5-methoxy-4-oxo-4H-pyran-2-yl)methyl)sulfanyl)phosphonate'	b'Endothion'	HMDB02 51802	C9H13O6PS	C189 82
16 8	281.24 64	282.2558803	0.0016 803	Protona tion	b'(9Z)-octadec-9-enoic acid'	b'Oleic acid'	HMDB00 00207	C18H34O2	C007 12
		282.2558803	0.0016 803	Protona tion	b'(9E)-octadec-9-enoic acid'	b'Elaidic acid'	HMDB00 00573	C18H34O2	C017 12
		282.2558803	0.0016 803	Protona tion	b'octadec-6-enoic acid'	b'Petroselinic acid'	HMDB00 02080	C18H34O2	
		282.2558803	0.0016 803	Protona tion	b'(11E)-octadec-11-enoic acid'	b'Vaccenic acid'	HMDB00 03231	C18H34O2	C083 67
		282.2558803	0.0016	Protona	b'(13Z)-octadec-13-enoic acid'	b'(Z)-13-Octadecenoic acid'	HMDB00	C18H34O2	

		803	tion				41480		
282.2558803	0.0016 803	Protone tion		b'ethyl (9E)-hexadec-9-enoate'	b'Ethyl 9-hexadecenoate'	HMDB00 59871	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'(7Z)-octadec-7-enoic acid'	b'7Z-octadecenoic acid'	HMDB00 62242	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'octadec-9-enoic acid'	b'Octadec-9-enoic Acid'	HMDB00 62703	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'(11Z)-octadec-11-enoic acid'	b'cis-Vaccenic acid'	HMDB02 40219	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'octadec-11-enoic acid'	b'11-Octadecenoic acid'	HMDB02 44344	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'octadec-2-enoic acid'	b'Octadecenoic acid'	HMDB02 45277	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'octadec-5-enoic acid'	b'Octadec-5-enoic acid'	HMDB02 46833	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'(7E)-octadec-7-enoic acid'	b'7-Octadecenoic acid'	HMDB03 02159	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'(10E)-octadec-10-enoic acid'	b'trans-10-Octadecenoic acid'	HMDB03 02289	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'(6E)-octadec-6-enoic acid'	b'6-Octadecenoic acid'	HMDB03 03337	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'(12Z)-octadec-12-enoic acid'	b'cis-12-Octadecenoic acid'	HMDB03 04764	C18H34O2		
282.2558803	0.0016 803	Protone tion		b'octadec-15-enoic acid'	b'cis-15-Octadecenoic acid'	HMDB03 04765	C18H34O2		
282.2558803	0.0016	Protone		b'(12E)-octadec-12-enoic acid'	b'trans-12-Octadecenoic acid'	HMDB03	C18H34O2		

			803	tion			04766		
		282.2558803	0.0016 803	Protona tion	b'(14E)-octadec-14-enoic acid'	b'trans-14-Octadecenoic acid'	HMDB03 04767	C18H34O2	
		282.2558803	0.0016 803	Protona tion	b'(15E)-octadec-15-enoic acid'	b'trans-15-Octadecenoic acid'	HMDB03 04768	C18H34O2	
		282.2558803	0.0016 803	Protona tion	b'(16E)-octadec-16-enoic acid'	b'trans-16-Octadecenoic acid'	HMDB03 04769	C18H34O2	
		282.2558803	0.0016 803	Protona tion	b'(4E)-octadec-4-enoic acid'	b'trans-4-Octadecenoic acid'	HMDB03 04770	C18H34O2	
		282.2558803	0.0016 803	Protona tion	b'(8E)-octadec-8-enoic acid'	b'trans-8-Elaidic acid'	HMDB03 04817	C18H34O2	
		281.2480553	0.0016 553	Redox	b'(6Z)-octadec-6-enoate'	b'petroselinic acid'	HMDB03 04458	C18H33O2	
16 9	282.03 64	282.0375673	0.0011 673	Redox	b'3-hydroxy-2-[3-hydroxy-6-(hydroxymethyl)-4-oxo-4H-pyran-2-yl]-6-(hydroxymethyl)-4H-pyran-4-one'	b'Bikojic acid'	HMDB00 34034	C12H10O8	
		282.0375673	0.0011 673	Redox	b'2-[[[(2E)-3-(3,4-dihydroxyphenyl)prop-2-enoyl]oxy]propanedioic acid'	b'2-O-Caffeoyltartronic acid'	HMDB00 40869	C12H10O8	
		282.0344139	0.0019 861	Redox	b'2-amino-3-[(2-carboxy-2-acetamidoethyl)disulfanyl]propanoic acid'	b'3-[[[(2R)-2-Acetamido-2-carboxyethyl]disulfanyl]-2-aminopropanoic acid'	HMDB02 47775	C8H14N2O5 S2	
17 0	282.08 29	283.0916686	0.0009 686	Protona tion	b'2-amino-9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-1H-purin-6-one'	b'Guanosine'	HMDB00 00133	C10H13N5O 5	C003 87
		283.0916686	0.0009 686	Protona tion	b'2-amino-8-hydroxy-9-[(2R,4S,5R)-4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-1H-purin-6-one'	b'8-Hydroxy-deoxyguanosine'	HMDB00 03333	C10H13N5O 5	
		283.0916686	0.0009 686	Protona tion	b'2-(6-hydroxy-2-imino-3,9-dihydro-2H-purin-9-yl)-5-(hydroxymethyl)oxolane-3,4-diol'	b'9-beta-d-Arabinofuranosylguanine'	HMDB02 46240	C10H13N5O 5	

		283.0916685	0.0009 685	Protone tion	b'2-amino-9-[4-hydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,7,8,9-tetrahydro-1H-purine-6,8-dione'	b'8-Hydroxy-2-desoxyguanosine'	HMDB02 47436	C10H13N5O 5	
		283.0916685	0.0009 685	Protone tion	b'2-amino-9-[2,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6,9-dihydro-1H-purin-6-one'	b'hydroxydeoxyguanosine'	HMDB02 53263	C10H13N5O 5	
		283.0916685	0.0009 685	Protone tion	b'1-[4-(azidoxy)-5-(hydroxymethyl)oxolan-2-yl]-5-methyl-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'1-[(2R,5R)-4-Azidoxy-5-(hydroxymethyl)oxolan-2-yl]-5-methylpyrimidine-2,4-dione'	HMDB02 57735	C10H13N5O 5	
		283.0916685	0.0009 685	Protone tion	b'2-amino-9-[5-(hydroperoxymethyl)-4-hydroxyoxolan-2-yl]-6,9-dihydro-1H-purin-6-one'	b'2-Amino-9-[(2R,4S,5R)-5-(hydroperoxymethyl)-4-hydroxyoxolan-2-yl]-1H-purin-6-one'	HMDB02 57980	C10H13N5O 5	
		282.0851862	0.0022 862	Redox	b'2-(butan-2-yl)-4,6-dinitrophenyl acetate'	b'Dinoseb acetate'	HMDB00 32560	C12H14N2O 6	C191 19
		282.0804558	0.0024 442	Redox	b'2-(4-fluorophenyl)-5-(1-isocyanatoethyl)-1,3-benzoxazole'	b'Flunoxaprofen isocyanate'	HMDB02 52342	C16H11FN2 O2	
		282.0851862	0.0022 862	Redox	b'4-acetamidophenyl 4-(nitrooxy)butanoate'	b'Nitroparacetamol'	HMDB02 55491	C12H14N2O 6	
		282.0851862	0.0022 862	Redox	b'1-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-5-(prop-1-yn-1-yl)-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'Netivudine'	HMDB02 55549	C12H14N2O 6	
17 1	283.00 12	283.0010747	0.0001 253	Redox	b'[1-hydroxy-1-phosphono-2-(pyridin-3-yl)ethyl]phosphonic acid'	b'Risedronate'	HMDB00 15022	C7H11NO7P 2	C082 33
17 2	283.26 24	284.2715304	0.0013 304	Protone tion	b'octadecanoic acid'	b'Stearic acid'	HMDB00 00827	C18H36O2 C18H36O2	C015 30
		284.2715304	0.0013 304	Protone tion	b'ethyl hexadecanoate'	b'Ethyl hexadecanoate'	HMDB00 29811	C18H36O2	
		284.2715304	0.0013 304	Protone tion	b'16-methylheptadecanoic acid'	b'16-Methylheptadecanoic acid'	HMDB00 31066	C18H36O2	C203 56

		284.2715304	0.0013 304	Protona tion	b'hexyl dodecanoate'	b'Hexyl dodecanoate'	HMDB00 61946	C18H36O2	
		284.2715304	0.0013 304	Protona tion	b'3-hydroxyoctadecan-2-one'	b'2-Octadecanone, 3-hydroxy-'	HMDB02 45276	C18H36O2	
		284.2688451	0.0013 549	Protona tion	b'3,6,10,13,16,19-hexaazabicyclo[6.6.6]icosane'	b'Sar chelate'	HMDB02 57487	C14H32N6	
17 3	285.07 11	285.0722705	0.0011 705	Redox	b"2-amino-1H,1'H,6H,6'H-[9,9'-bipurine]-6,6'-dione"	b'2-Amino-9-(6-oxo-1H-purin-9-yl)- 1H-purin-6-one'	HMDB02 57944	C10H7N9O2	
17 4	286.07 42	287.0793725	0.0026 275	Protona tion	b'1,3,5-trihydroxy-4-methoxy-10-methyl-9,10-dihydroacridin-9-one'	b'Citrusinine II'	HMDB00 30373	C15H13NO5	
		287.0793725	0.0026 275	Protona tion	b'1,3,6-trihydroxy-5-methoxy-10-methyl-9,10-dihydroacridin-9-one'	b'Grandisine III'	HMDB00 40683	C15H13NO5	
		287.0793725	0.0026 275	Protona tion	b'2-methoxy-4-(4-methylbenzoyl)-6-nitrophenol'	b'3-O-Methyltolcapone'	HMDB02 44556	C15H13NO5	
17 5	287.97 86	287.980838	0.0022 38	Redox	b'dodecafluoropentane'	b'Dodecafluoropentane'	HMDB02 51565	C5F12	
17 6	290.08 64	291.0967539	0.0025 539	Protona tion	b'2-(hydroxymethyl)-5-{3H-imidazo[2,1-f]purin-3-yl}oxolane-3,4-diol'	b'1,N6-Ethenoadenosine'	HMDB02 44260	C12H13N5O 4	
		291.0954165	0.0012 165	Protona tion	b'3-acetamido-4-hydroxy-2-(1,2,3-trihydroxypropyl)-3,4-dihydro-2H-pyran-6-carboxylic acid'	b'2-Deoxy-2,3-dehydro-n-acetyl- neuraminic acid'	HMDB02 45680	C11H17NO8	
		291.0967539	0.0025 539	Protona tion	b'methyl N-[2-oxo-5-(1,2,3,6-tetrahydropyridin-1-yl)-2H-[1,2,4]oxadiazolo[2,3-a]pyrimidin-7-yl]carbamate'	b'Carprazidil'	HMDB02 49688	C12H13N5O 4	
		291.0967539	0.0025 539	Protona tion	b'1-(6-amino-9H-purin-9-yl)-3-(hydroxymethyl)-2-oxabicyclo[3.2.0]hept-6-ene-4,5-diol'	b'Ethenoadenosine'	HMDB02 52011	C12H13N5O 4	
17 7	291.08 89	292.0946882	0.0020 118	Protona tion	b'4-hydroxy-7-(hydroxymethyl)-2-(2-hydroxypropan-2-yl)-2H,3H,5H-furo[3,2-g]chromen-5-one'	b'(S)-Angelica'	HMDB00 30120	C15H16O6	

		292.0946882	0.0020 118	Protone tion	b'13,14-dihydroxy-8-methoxy-12,12-dimethyl-3,11-dioxatricyclo[8.4.0.0]xc2'xb2,\xc2'x81'xb7]tetradeca-1(10),2(7),5,8-tetraen-4-one'	b'trans-Grandmarin'	HMDB00 39030	C15H16O6	
		292.0946882	0.0020 118	Protone tion	b'(1R,5S,8S,13R,14R)-1-hydroxy-13-methyl-14-(prop-1-en-2-yl)-4,7,10-trioxapentacyclo[6.4.1.1^9,12].0^3,5}.0^5{5,13}]tetradecane-6,11-dione'	b'Picrotoxinin'	HMDB02 40274	C15H16O6	
		292.0978555	0.0011 555	Protone tion	b'6-chloro-12-methyl-2-oxa-12,15-diazatetracyclo[7.5.3.0]xc2'xb9,\xc2'xb9'xc2'x81'xb0.0]xc2'xb3,\xc2'x81'xb8]heptadeca-3,5,7-trien-16-one'	b'(+)-(4Ar*,10R*,10aS*)-8-Chloro-1,2,3,4,10,10a-hexahydro-2-methyl-4a,10-(iminoethano)-4aH-(1)benzopyrano(3,2-c)pyridin-12-one'	HMDB02 42234	C15H17ClN 2O2	
		291.0895433	0.0006 433	Redox	b'2-[(1Z,3E)-4-(4-hydroxyphenyl)buta-1,3-dien-1-yl]-4H-3,1-benzoxazin-4-one'	b'Avenalumin III'	HMDB00 38956	C18H13NO3	
17 8	293.04 06	294.0496691	0.0012 691	Protone tion	b'(3E)-3-([bis(methylsulfanyl)methylidene]amino)methylidene)-1-methoxy-2,3-dihydro-1H-indol-2-one'	b'Wasalexin A'	HMDB00 34765	C13H14N2O 2S2	
		294.0496691	0.0012 691	Protone tion	b'(3Z)-3-([bis(methylsulfanyl)methylidene]amino)methylidene)-1-methoxy-2,3-dihydro-1H-indol-2-one'	b'Wasalexin B'	HMDB00 34768	C13H14N2O 2S2	
		294.0496691	0.0012 691	Protone tion	b'N-[bis(methylsulfanyl)methylidene]-1-methoxy-1H-indole-3-carboxamide'	b'Methoxybrassenin B'	HMDB00 38636	C13H14N2O 2S2	
		293.0421561	0.0015 561	Redox	b'[[2-(diethylamino)-6-methylpyrimidin-4-yl]oxy](sulfanyl)sulfanylidene phosphinous acid'	b'Pirimiphos'	HMDB02 56599	C9H16N3O2 PS2	
17 9	299.05 16	299.0518514	0.0002 514	Redox	b'[[amino(2-[(2-hydroxypropanoyl)peroxy]-2-oxoethyl)(methylamino)methylidene]amino]phosphonic acid'	b'Phosphocreatine lactate'	HMDB02 56473	C7H14N3O8 P	
18 0	300.03 71	301.0467518	0.0018 518	Protone tion	b'[(2R,3R,4R,5R,6R)-5-acetamido-4,6-dihydroxy-2-(hydroxymethyl)oxan-3-yl]oxidanesulfonic acid'	b'N-Acetylgalactosamine 4-sulphate'	HMDB00 00781	C8H15NO9S 65	C162
		301.0467518	0.0018 518	Protone tion	b'[[[(2R,3S,4R,5R,6R)-5-acetamido-3,4,6-trihydroxyoxan-2-yl]methoxy]sulfonic acid'	b'N-Acetylglucosamine 6-sulfate'	HMDB00 00814	C8H15NO9S 32	C041
		301.0467518	0.0018 518	Protone tion	b'[[[(2R,3R,4R,5R)-5-acetamido-2,3,4-trihydroxy-6-oxohexyl]oxy]sulfonic acid'	b'N-Acetylgalactosamine 6-sulfate'	HMDB00 00841	C8H15NO9S	

18	1	300.04	61	301.0467522	0.0018 522	Protone	b'N-{2,4,5-trihydroxy-6-[(sulfooxy)methyl]oxan-3-yl}ethanimidic acid'	b'2-(Acetyl amino)-2-Deoxy-6-O-Sulfo- alpha-D-Glucopyranose'	HMDB02 44937	C8H15NO9S	
				300.038236	0.0011 36	Redox	b'2-amino-3-oxo-3H-phenoxazine-1,9-dicarboxylic acid'	b'Cinnalinate'	HMDB00 04078	C14H8N2O6	C056 40
				301.0562676	0.0023 676	Protone	b'{{{(2R,3S,4R,5R)-5-acetamido-3,4,6-trihydroxyoxan-2-yl}methoxy}phosphonic acid'	b'N-Acetyl-D-Glucosamine 6- Phosphate'	HMDB00 01062	C8H16NO9P	C003 57
				301.0562676	0.0023 676	Protone	b'{{{(2R,3S,4R,5S,6S)-5-acetamido-3,4,6-trihydroxyoxan-2-yl}methoxy}phosphonic acid'	b'N-Acetyl-D-mannosamine 6- phosphate'	HMDB00 01121	C8H16NO9P	C042 57
				301.0562676	0.0023 676	Protone	b'{{{(3R,4R,5S,6R)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl}oxy}phosphonic acid'	b'N-Acetyl-glucosamine 1-phosphate'	HMDB00 01367	C8H16NO9P	C042 56
				301.0562676	0.0023 676	Protone	b'{{{(2R,3S,4R,5R,6S)-5-acetamido-3,4,6-trihydroxyoxan-2-yl}methoxy}phosphonic acid'	b'N-Acetylglucosamine 6-phosphate'	HMDB00 02817	C8H16NO9P	
				301.0562676	0.0023 676	Protone	b'{{{(3R,4R,5R,6R)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl}oxy}phosphonic acid'	b'N-Acetyl-D-galactosamine 1- phosphate'	HMDB00 06480	C8H16NO9P	
				301.0562676	0.0023 676	Protone	b'N-[(2R,3R,4R,5R,6R)-4,5-dihydroxy-6-(hydroxymethyl)-2-(phosphonoxy)oxan-3-yl]ethanimidic acid'	b'N-acetyl-alpha-D-galactosamine 1- phosphate'	HMDB00 59626	C8H16NO9P	C180 60
				301.0562681	0.0023 681	Protone	b'{{{(2R,3S,4R,5S,6R)-5-acetamido-3,4,6-trihydroxyoxan-2-yl}methoxy}phosphonic acid'	b'N-Acetylmannosamine-6P'	HMDB00 62500	C8H16NO9P	
				301.0562681	0.0023 681	Protone	b'[(5-acetamido-3,4,6-trihydroxyoxan-2-yl)methoxy]phosphonic acid'	b'(5-Acetamido-3,4,6-trihydroxyoxan-2- yl)methyl dihydrogen phosphate'	HMDB02 52741	C8H16NO9P	
18	1	300.04	61	301.0521119	0.0017 881	Protone	b'methyl N-[6-(thiophene-2-carbonyl)-1H-1,3-benzodiazol-2-yl]carbamate'	b'Nocodazole'	HMDB02 55688	C14H11N3O 3S	C137 19
				300.048132	0.0020 32	Redox	b'2-{2-[(5-formylfuran-2-yl)methoxy]-2-oxoethyl}-2-hydroxybutanedioic acid'	b'Mumefural'	HMDB00 35179	C12H12O9	
				300.0432331	0.0028 669	Redox	b'5-[bis(2-chloroethyl)amino]-1H-indole-2-carboxylic acid'	b'Indole-2-carboxylic acid, 5-(bis(2- chloroethyl)amino)-'	HMDB02 48682	C13H14Cl2 N2O2	

18	301.06	301.0636342	0.0001 342	Redox	b'4-{4-[bis(2-chloroethyl)amino]phenyl}but-3-enoic acid'	b'3,4-Dehydrochlorambucil'	HMDB02 46018	C14H17Cl2 NO2	
		301.0636342	0.0001 342	Redox	b'N-(2,3-dichloro-4-hydroxyphenyl)-1-methylcyclohexane-1-carboxamide'	b'Fenhexamid'	HMDB02 52201	C14H17Cl2 NO2	C185 93
18	302.05	302.0538861	0.0027 861	Redox	b'5-[(E)-2-(3-carboxy-4-hydroxyphenyl)diazene-1-yl]-2-hydroxybenzoic acid'	b'Olsalazine'	HMDB00 15380	C14H10N2O 6	C073 23
		302.0512007	0.0001 007	Redox	b"1H,1'H,2H,2'H,3H,3'H,6H,6'H-[9,9'-bipurine]-2,2',6,6'-tetrone"	b'9-(2,6-Dioxo-3H-purin-9-yl)-3H-purine-2,6-dione'	HMDB02 57773	C10H6N8O4	
18	303.08	304.0906655	0.0015 655	Protontion	b'(2S)-2-[(2S)-3-carboxy-2-acetamidopropanamido]pentanedioic acid'	b'N-Acetylaspartylglutamic acid'	HMDB00 01067	C11H16N2O 8	C122 70
		304.0866221	0.0024 779	Protontion	b"2-({4'-chloro-[1,1'-biphenyl]-4-yl} methoxy)-2-methylpropanoic acid"	b'Clobuzarit'	HMDB02 50334	C17H17ClO 3	
		304.0911006	0.0020 006	Protontion	b"4-{2,4'-difluoro-[1,1'-biphenyl]-4-yl}-2-methyl-4-oxobutanoic acid"	b'Flobufen'	HMDB02 52307	C17H14F2O 3	
		304.0866221	0.0024 779	Protontion	b"methyl 2-({4'-chloro-[1,1'-biphenyl]-4-yl} oxy)-2-methylpropanoate"	b'Methyl clofenapate'	HMDB02 54582	C17H17ClO 3	
		304.0906655	0.0015 655	Protontion	b'2-(3-carboxy-2-acetamidopropanamido)pentanedioic acid'	b'N-Acetyl-L-aspartylglutamic acid'	HMDB02 55414	C11H16N2O 8	C122 70
		304.0898173	0.0007 173	Protontion	b'4-(methylsulfanyl)phenyl dipropyl phosphate'	b'Propaphos'	HMDB02 56818	C13H21O4P S	C190 13
		303.0792843	0.0020 157	Redox	b'4-{4-[bis(2-chloroethyl)amino]phenyl} butanoic acid'	b'Chlorambucil'	HMDB00 14436	C14H19Cl2 NO2	C069 00
18	303.23	304.2402303	0.0010 303	Protontion	b'(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoic acid'	b'Arachidonic acid'	HMDB00 01043	C20H32O2	C002 19
		304.2402303	0.0010 303	Protontion	b'(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoic acid'	b'Cis-8,11,14,17-Eicosatetraenoic acid'	HMDB00 02177	C20H32O2	

		304.2402303	0.0010 303	Protona tion	b'(1S,2S,3S,7S,10R,11S,14S,15S)-14-hydroxy-2,3,15-trimethyltetracyclo[8.7.0.0'xc2'xb2,\xc2'x81'xb7.0'xc2'xb9'xc2'xb9,\xc2'xb9'xc2'xb5]heptadecan-5-one'	b'Mesterolone'	HMDB00 06036	C20H32O2	D04 947
		304.2402303	0.0010 303	Protona tion	b'(1S,2S,4R,7S,10R,11S,14S,15S)-14-hydroxy-2,4,15-trimethyltetracyclo[8.7.0.0'xc2'xb2,\xc2'x81'xb7.0'xc2'xb9'xc2'xb9,\xc2'xb9'xc2'xb5]heptadecan-5-one'	b'Drostanolone'	HMDB00 14996	C20H32O2	C146 05
		304.2402303	0.0010 303	Protona tion	b'5-(hydroxymethyl)-5,9,14-trimethyltetracyclo[11.2.1.0'xc2'xb9,\xc2'xb9'xc2'xb0.0'xc2'xb4,\xc2'xb9]hexadec-14-en-2-ol'	b'Sideridiol'	HMDB00 36702	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'14-(hydroxymethyl)-5,9-dimethyltetracyclo[11.2.1.0'xc2'xb9,\xc2'xb9'xc2'xb0.0'xc2'xb4,\xc2'xb9]hexadecan-5-carbaldehyde'	b'ent-17-Hydroxy-16beta-kauran-19-al'	HMDB00 36721	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'7-ethenyl-1,1,4a,7-tetramethyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrene-2,6-diol'	b'Yucalexin P21'	HMDB00 36754	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'(2Z)-5-(5,5,8a-trimethyl-2-methylidene-decahydronaphthalen-1-yl)-3-methylpent-2-enoic acid'	b'Copalic acid'	HMDB00 36829	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'1,4a-dimethyl-5-(3-methyl-5-oxopentyl)-6-methylidene-decahydronaphthalene-1-carbaldehyde'	b'Junicedral'	HMDB00 36830	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'(2Z)-5-(2,5,5,8a-tetramethyl-1,4,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)-3-methylpent-2-enoic acid'	b'7,13-Eperudien-15-oic acid'	HMDB00 37824	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'6-(hydroxymethyl)-2,6,12-trimethyltetracyclo[11.2.1.0'xc2'xb9,\xc2'xb9'xc2'xb0.0'xc2'xb2,\xc2'xb7]hexadec-11-en-4-ol'	b'Oryzalexin S'	HMDB00 39687	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'(2R,4aR,4bS,7S,10aR)-7-ethenyl-1,1,4a,7-tetramethyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrene-2,4b-diol'	b'Oryzalexin E'	HMDB00 39702	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraenoic acid'	b'2,6,10,14-Hexadecatetraenoic acid, 3,7,11,15-tetramethyl-, (Z,E,E)-'	HMDB02 45522	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'icosa-5,8,11,14-tetraenoic acid'	b'5,8,11,14-Icosatetraenoic Acid'	HMDB02 46871	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'icosa-2,4,6,8-tetraenoic acid'	b'Eicosatetraenoic acid'	HMDB02 51721	C20H32O2	

		304.2402303	0.0010 303	Protona tion		b'Mestaline'	HMDB02 54484	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'2,14,15-trimethyltetraacyclo[8.7.0.0 ⁺ {2,7}.0 ⁺ {11,15}]heptadec-7-ene-5,14-diol'	b'Methandriol'	HMDB02 54517	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'(2R,4aR,4bS,7S,10aS)-7-ethenyl-1,1,4a,7-tetramethyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthrene-2,9-diol'	b'Oryzalexin D'	HMDB03 02102	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'(2R,4aS,4bR,7S,10aS)-7-ethenyl-1-(hydroxymethyl)-1,4a,7-trimethyl-1,2,3,4,4a,4b,5,6,7,9,10,10a-dodecahydrophenanthren-2-ol'	b'Oryzalexin F'	HMDB03 02103	C20H32O2	
		304.2402303	0.0010 303	Protona tion	b'[(1R,4aR,4bR)-1,4a-dimethyl-7-(propan-2-yl)-1,2,3,4,4a,4b,5,6,10,10a-decahydrophenanthren-1-yl]methanediol'	b'abietadiene-diol'	HMDB03 04255	C20H32O2	
18 6	304.05 88	305.0688078	0.0022 078	Protona tion	b'11-methyl-3,5-dioxa-11-azapentacyclo[10.7.1.0 ⁺ xc2\xb2,\xc2\xb81\xb6.0\xc2\xb81\xb8,\xc2\xb2\xc2\xb81\xb0.0\xc2\xb9\xc2\xb81\xb4,\xc2\xb9\xc2\xb81\xb9]jicosa-1(20),2(6),7,12,14,16,18-heptaene-9,10-dione'	b'Cepharadione A'	HMDB00 34364	C18H11NO4	
		305.0688078	0.0022 078	Protona tion	b'16-methoxy-3,5-dioxa-11-azapentacyclo[10.7.1.0 ⁺ xc2\xb2,\xc2\xb81\xb6.0\xc2\xb81\xb8,\xc2\xb2\xc2\xb81\xb0.0\xc2\xb9\xc2\xb81\xb4,\xc2\xb9\xc2\xb81\xb9]jicosa-1(20),2(6),7,9,11,14(19),15,17-octaen-13-one'	b'Oxoxypine'	HMDB03 02035	C18H11NO4	
		304.0583027	0.0004 973	Redox	b'(2E)-3-(7-hydroxy-2H-chromen-3-yl)-4-oxohex-2-enedioic acid'	b'Pratenol B'	HMDB00 40631	C15H12O7	
		304.0583027	0.0004 973	Redox	b'2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one'	b'(2R)-2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-2,3-dihydrochromen-4-one'	HMDB02 42509	C15H12O7	
		304.0583027	0.0004 973	Redox	b'2-(3,4-dihydroxyphenyl)-4,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-3-one'	b'2-(3,4-Dihydroxy-phenyl)-3,5,7-trihydroxy-chroman-4-one'	HMDB02 43555	C15H12O7	
		304.0583027	0.0004 973	Redox	b'(2R,3R)-2-(3,4-dihydroxyphenyl)-3,5,7-trihydroxy-3,4-dihydro-2H-1-benzopyran-4-one'	b'(+)-taxifolin'	HMDB03 03943	C15H12O7	C016 17
18 7	305.01 58	306.0253019	0.0017 019	Protona tion	b'1-[(3aR,4R,6R,6aR)-2-hydroxy-6-(hydroxymethyl)-2-oxo-tetrahydro-2H-2\xc2\xb2\xc2\xb81\xb5-furo[3,4-d][1,3,2]dioxaphosphol-4-yl]-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b''Uridine 2',3'-cyclic phosphate"	HMDB00 11640	C9H11N2O8 P	C023 55
18 8	305.24 69	306.2558803	0.0011 803	Protona tion	b'(8Z,11Z,14Z)-icosa-8,11,14-trienoic acid'	b'Dihomo-gamma-linolenic acid'	HMDB00 02925	C20H34O2	C032 42

		306.2558803	0.0011 803	Protona tion	b'(5Z,8Z,11Z)-icosa-5,8,11-trienoic acid'	b'5,8,11-Eicosatrienoic acid'	HMDB00 10378	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'(5Z,11E,14E)-icosa-5,11,14-trienoic acid'	b'Sciadonic acid'	HMDB00 31058	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'5-[5-(hydroxymethyl)-1,2,4a-trimethyl-1,2,3,4,4a,7,8,8a-octahydronaphthalen-1-yl]-3-methylpent-1-en-3-ol'	b'Sagittario'	HMDB00 36835	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'(11Z,14Z,17Z)-icosa-11,14,17-trienoic acid'	b'Dihomo-alpha-linolenic acid'	HMDB00 60039	C20H34O2	C165 22
		306.2558803	0.0011 803	Protona tion		b'11-Eicosatrienoic acid'	HMDB02 44353	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'icosa-11,14,17-trienoic acid'	b'Eicosa-11,14,17-trienoic acid'	HMDB02 44373	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'icosa-5,8,11-trienoic acid'	b'Eicosa-5,8,11-trienoic acid'	HMDB02 45590	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'icosa-5,11,14-trienoic acid'	b'5,11,14-Eicosatrienoic acid'	HMDB02 46847	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'icosa-8,11,14-trienoic acid'	b'Dihomo--linolenic acid'	HMDB02 47333	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'icosa-2,4,6-trienoic acid'	b'Icosa-2,4,6-trienoic acid'	HMDB02 51723	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'ethyl octadeca-9,12,15-trienoate'	b'Ethyl octadeca-9,12,15-trienoate'	HMDB02 52049	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'ethyl (9Z,12Z,15Z)-octadeca-9,12,15-trienoate'	b'Ethyl alpha-linolenate'	HMDB03 02158	C20H34O2	
		306.2558803	0.0011 803	Protona tion	b'(1S,4S,5R,9S,10R,13R,14R)-5-(hydroxymethyl)-5,9,14-trimethyltricyclo[11.2.1.0\xc2\xb9,\xc2\xb9\x81\xb0.0\xc2\x81\xb4,\xc2\x81\xb9]hexadecan-14-ol'	b'ent-16b-Kauran-16,19-diol'	HMDB03 02662	C20H34O2	

		306.2558803	0.0011 803	Protone tion	b'ethyl (9E,12E,15E)-octadeca-9,12,15-trienoate'	b'Ethyl linolenate'	HMDB03 02813	C20H34O2	
		306.253475	0.0012 25	Protone tion	b'sodium octadecanoate'	b'Sodium octadecanoate'	HMDB03 03349	C18H35NaO 2	
		305.2486039	0.0017 039	Redox	b'icosa-8,11,14-trienoate'	b'di-homo-gamma-linolenate'	HMDB03 04332	C20H33O2	
18 9	306.07 45	307.083806	0.0015 06	Protone tion	b'(2S)-2-amino-4-{{(1R)-1-[(carboxymethyl)carbamoyl]-2-sulfanylethyl}carbamoyl}butanoic acid'	b'Glutathione'	HMDB00 00125	C10H17N3O 6S	C000 51
		307.0844579	0.0021 579	Protone tion	b'2-acetyl-5-hydroxy-11-methyl-6H,11H-furo[2,3-c]acridin-6-one'	b'Hallacridone'	HMDB00 29826	C18H13NO4	
		307.0844579	0.0021 579	Protone tion	b'15-hydroxy-16-methoxy-10-methyl-10-azatetracyclo[7.7.1.0'xc2'xb2,'xc2'xb7.0'xc2'xb9'xc2'xb3,'xc2'xb9'xc2'xb7]heptadeca-1(17),2,4,6,8,13,15-heptaene-11,12-dione'	b'Aristolodione'	HMDB00 33247	C18H13NO4	
		307.0838065	0.0015 065	Protone tion	b'2-amino-4-{{(1-[(carboxymethyl)-C-hydroxycarbonimidoyl]-2-sulfanylethyl)-C-hydroxycarbonimidoyl}butanoic acid'	b'Glutathionate(1-)'	HMDB00 62697	C10H17N3O 6S	
		307.0844579	0.0021 579	Protone tion	b'methyl 2-[(3,4-dioxo-3,4-dihydronaphthalen-1-yl)amino]benzoate'	b'Methyl 2-[(3,4-dihydro-3,4-dioxo-1-naphthalenyl)amino]benzoate'	HMDB02 44408	C18H13NO4	
		306.0739528	0.0005 472	Redox	b'(2R,3R)-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol'	b'(-)-Epigallocatechin'	HMDB00 38361	C15H14O7	C121 36
		306.0739528	0.0005 472	Redox	b'(2R,3S)-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol'	b'(+-)-Gallocatechin'	HMDB00 38365	C15H14O7	C121 27
		306.0739528	0.0005 472	Redox	b'(2S,3R)-2-(3,4,5-trihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,5,7-triol'	b'4-Gallocatechol'	HMDB03 02404	C15H14O7	
		306.0739528	0.0005 472	Redox	b'2-(3,4-dihydroxyphenyl)-3,4-dihydro-2H-1-benzopyran-3,4,5,7-tetrol'	b'Leucocyanidin'	HMDB03 03660	C15H14O7	
19 0	307.26 13	308.2715304	0.0024 304	Protone tion	b'(11Z,14Z)-icosa-11,14-dienoic acid'	b'Eicosadienoic acid'	HMDB00 05060	C20H36O2	C165 25

		308.2715304	0.0024 304	Protona tion	b'1-(3-hydroxy-3-methylpent-4-en-1-yl)-2,5,5,8a-tetramethyl-decahydronaphthalen-2-ol'	b'Sclareol'	HMDB00 36827	C20H36O2	C091 83
		308.2715304	0.0024 304	Protona tion	b'(8Z,11Z)-icosa-8,11-dienoic acid'	b'8Z,11Z-eicosadienoic acid'	HMDB00 62432	C20H36O2	
		308.2715304	0.0024 304	Protona tion	b'icosa-11,14-dienoic acid'	b'11,14-Eicosadienoic acid'	HMDB02 44372	C20H36O2	
		308.2715304	0.0024 304	Protona tion	b'icosa-2,4-dienoic acid'	b'Eicosadienic acid'	HMDB02 51719	C20H36O2	
		308.2715304	0.0024 304	Protona tion	b'ethyl octadeca-9,12-dienoate'	b'Ethyl linolate'	HMDB02 52048	C20H36O2	
		308.2715304	0.0024 304	Protona tion	b'methyl 8-(2-octylcycloprop-1-en-1-yl)octanoate'	b'Methyl sterculate'	HMDB02 54613	C20H36O2	
		308.2715304	0.0024 304	Protona tion	b'icosa-2,6-dienoic acid'	b'icosa-2,6-dienoic acid'	HMDB02 60426	C20H36O2	
		308.2715304	0.0024 304	Protona tion	b'ethyl (9E,12Z)-octadeca-9,12-dienoate'	b'Ethyl (Z,Z)-9,12-octadecadienoate'	HMDB03 03389	C20H36O2	
19 1	308.29 39	309.3031649	0.0014 649	Protona tion	b'1-(pyrrolidin-1-yl)hexadecan-1-one'	b'N-Hexadecanoylpyrrolidine'	HMDB00 32740	C20H39NO	
19 2	308.97 83	309.9854843	0.0006 157	Protona tion	b'{{{(2R,3R,4S,5R)-3,4-dihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl}oxy}phosphonic acid'	b'Ribose 1,5-bisphosphate'	HMDB00 11688	C5H12O11P 2	C011 51
		309.9854852	0.0006 148	Protona tion	b' {[3,4-dihydroxy-2-oxo-5-(phosphonoxy)pentyl]oxy}phosphonic acid'	b'D-Ribulose 1,5-bisphosphate'	HMDB02 44230	C5H12O11P 2	
		309.9854852	0.0006 148	Protona tion	b'([hydroxy[(3,4,5-trihydroxy-2-oxopentyl]oxy]phosphoryl]oxy)phosphonic acid'	b'Phosphono [(3S,4S)-3,4,5-trihydroxy-2-oxopentyl] hydrogen phosphate'	HMDB02 60366	C5H12O11P 2	
		309.9854843	0.0006 157	Protona tion	b'{{{(3R,4R)-3,4-dihydroxy-2-oxo-5-(phosphonoxy)pentyl}oxy}phosphonic acid'	b'D-ribulose-1,5-bisphosphate'	HMDB03 04322	C5H12O11P 2	C011 82

19	3	309.27	82	310.2871805	0.0011 805	Protone tion	b'(11Z)-icos-11-enoic acid'	b'11Z-Eicosenoic acid'	HMDB00 02231	C20H38O2	C165 26
				310.2871805	0.0011 805	Protone tion	b'ethyl (9E)-octadec-9-enoate'	b'Ethyl oleate'	HMDB00 34451	C20H38O2	C034 25
				310.2871805	0.0011 805	Protone tion	b'(13Z)-icos-13-enoic acid'	b'Pallinic acid'	HMDB00 35159	C20H38O2	
				310.2871805	0.0011 805	Protone tion	b'icosane-6,8-dione'	b'6,8-Icosanedione'	HMDB00 35572	C20H38O2	
				310.2871805	0.0011 805	Protone tion	b'icosane-5,7-dione'	b'5,7-Icosanedione'	HMDB00 35573	C20H38O2	
				310.2871805	0.0011 805	Protone tion	b'icosane-4,6-dione'	b'4,6-Icosanedione'	HMDB00 35574	C20H38O2	
				310.2871805	0.0011 805	Protone tion	b'(9E)-octadec-9-en-1-yl acetate'	b'Oleyl acetate'	HMDB00 37127	C20H38O2	
				310.2871805	0.0011 805	Protone tion	b'(9Z)-icos-9-enoic acid'	b'9Z-Eicosenoic acid'	HMDB00 62436	C20H38O2	
				310.2871805	0.0011 805	Protone tion	b'icos-2-enoic acid'	b'Icos-2-enoic acid'	HMDB02 47671	C20H38O2	
				310.2871805	0.0011 805	Protone tion	b'ethyl octadec-9-enoate'	b'Ethyl octadec-9-enoate'	HMDB02 52058	C20H38O2	
19	4	309.87 1		309.87154	0.0005 4	Redox	b'1,4-diiodobutane'	b'1,4-Diiodobutane'	HMDB02 44214	C4H8I2	
19	5	311.29 27		312.3028305	0.0023 305	Protone tion	b'(3R,7R,11R)-3,7,11,15-tetramethylhexadecanoic acid'	b'3D,7D,11D-Phytanic acid'	HMDB00 00417	C20H40O2	
				312.3028305	0.0023 305	Protone tion	b'(3S,7R,11R)-3,7,11,15-tetramethylhexadecanoic acid'	b'3L,7D,11D-Phytanic acid'	HMDB00 00553	C20H40O2	

		312.3028305	0.0023 305	Protona tion	b'3,7,11,15-tetramethylhexadecanoic acid'	b'Phytanic acid'	HMDB00 00801	C20H40O2	C016 07
		312.3028305	0.0023 305	Protona tion	b'icosanoic acid'	b'Arachidic acid'	HMDB00 02212	C20H40O2	C064 25
		312.3028305	0.0023 305	Protona tion	b'2,2,6,10,14-pentamethylpentadecanoic acid'	b'2,2,6,10,14-Pentamethylpentadecanoic acid'	HMDB00 31318	C20H40O2	
		312.3028305	0.0023 305	Protona tion	b'ethyl octadecanoate'	b'Ethyl stearate'	HMDB00 34156	C20H40O2	
		312.3028305	0.0023 305	Protona tion	b'5-hydroxyicosan-7-one'	b'5-Hydroxy-7-eicosanone'	HMDB00 35672	C20H40O2	
		312.3028305	0.0023 305	Protona tion	b'4-hydroxyicosan-6-one'	b'4-Hydroxy-6-eicosanone'	HMDB00 35673	C20H40O2	
		312.3028305	0.0023 305	Protona tion	b'(7R,11R)-3,7,11,15-tetramethylhexadecanoic acid'	b'3,7R,11R,15-tetramethyl-hexadecanoic acid'	HMDB00 62520	C20H40O2	
		312.3028305	0.0023 305	Protona tion	b'2-(octadec-9-en-1-yloxy)ethan-1-ol'	b'Emulphor'	HMDB02 51781	C20H40O2	
		312.3028305	0.0023 305	Protona tion	b'butyl hexadecanoate'	b'Butyl palmitate'	HMDB03 03179	C20H40O2	
19	312.06 8	312.0665554	0.0014 446	Redox	b'2-[3-(4-chlorophenyl)-1-phenyl-1H-pyrazol-4-yl]acetic acid'	b'Lonazolac'	HMDB02 54157	C17H13ClN 2O2	
		312.0699267	0.0019 267	Redox	b'N-(4-aminobutyl)-5-chloronaphthalene-2-sulfonamide'	b'N-(4-Aminobutyl)-5-chloronaphthalene-2-sulfonamide'	HMDB02 59886	C14H17ClN 2O2S	
19	316.07 39	316.0729074	0.0009 926	Redox	b'(2R)-2-amino-3-({6-[(2S)-2-amino-2-carboxyethyl]-2,3-dihydroxyphenyl}sulfanyl)propanoic acid'	b'2-S-cysteinyl-DOPA'	HMDB00 62734	C12H16N2O 6S	
		316.0729074	0.0009 926	Redox	b'2-amino-3-({5-(2-amino-2-carboxyethyl)-2,3-dihydroxyphenyl}sulfanyl)propanoic acid'	b'5-S-Cysteinyl-D-dopa'	HMDB02 44850	C12H16N2O 6S	

19	8	322.04 25	323.051851	0.0015 51	Protone	b'[(2R,3S,4R,5R)-5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy]phosphonic acid'	b'Cytidine monophosphate'	HMDB00 00095	C9H14N3O8 P	C000 55
			323.051851	0.0015 51	Protone	b'[(3R,4R,5R)-2-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-4-hydroxy-5-(hydroxymethyl)oxolan-3-yl]oxy]phosphonic acid'	b"Cytidine 2'-phosphate"	HMDB00 11692	C9H14N3O8 P	C031 04
			323.051851	0.0015 51	Protone	b'[(2R,3S,4R,5R)-5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]oxy]phosphonic acid'	b"Cytidine 3'-monophosphate"	HMDB02 40312	C9H14N3O8 P	C058 22
			323.051851	0.0015 51	Protone	b'[[3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy]phosphonic acid'	b"Cytosine arabinose-5'-phosphate"	HMDB02 43501	C9H14N3O8 P	
			323.0479841	0.0023 159	Protone	b'1-chloro-4-[1-(4-chlorophenyl)-2-nitrobutyl]benzene'	b'BULAN'	HMDB02 49435	C16H15Cl2 NO2	
			323.0495256	0.0007 744	Protone	b'4-{2-[4-(dimethylamino)phenyl]diazene-1-yl}benzene-1-sulfonyl chloride'	b'Dabsyl chloride'	HMDB02 50819	C14H14ClN 3O2S	
			323.0495251	0.0007 749	Protone	b'2-(4-chloro-6-[(2,3-dimethylphenyl)amino]pyrimidin-2-yl)sulfany]acetic acid'	b'Pirimixic acid'	HMDB02 56601	C14H14ClN 3O2S	C156 17
19	9	323.02 7	324.0358665	0.0010 665	Protone	b'[(2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy]phosphonic acid'	b"Uridine 5'-monophosphate"	HMDB00 00288	C9H13N2O9 P	C001 05
			324.0358665	0.0010 665	Protone	b'[(2R,3S,4R,5S)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl)-3,4-dihydroxyoxolan-2-yl]methoxy]phosphonic acid'	b"Pseudouridine 5'-phosphate"	HMDB00 01271	C9H13N2O9 P	C011 68
			324.0358665	0.0010 665	Protone	b'[(2R,3R,4R,5R)-2-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-4-hydroxy-5-(hydroxymethyl)oxolan-3-yl]oxy]phosphonic acid'	b"Uridine 2'-phosphate"	HMDB00 11641	C9H13N2O9 P	C030 31
			324.0358665	0.0010 665	Protone	b'[(2R,3S,4R,5R)-4-hydroxy-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)-2-(hydroxymethyl)oxolan-3-yl]oxy]phosphonic acid'	b"Uridine 3'-monophosphate"	HMDB00 60282	C9H13N2O9 P	C013 68
			324.0335412	0.0012 588	Protone	b'1-(4-chlorophenyl)-3-(4-methylbenzenesulfonyl)urea'	b'1-(4-Chlorophenyl)-3-(4-methylphenyl)sulfonyl]urea'	HMDB02 46250	C14H13ClN 2O3S	
			324.035867	0.0010 67	Protone	b'[(5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy]phosphonic acid'	b'[(2S,3R,4R,5R)-5-(2,4-Dioxypyrimidin-1-yl)-3,4-	HMDB02 47871	C9H13N2O9 P	

						dihydroxyoxolan-2-yl)methyl dihydrogen phosphate'			
		324.0319997	0.0028 003	Protona tion	b'4-chlorophenyl 2-(4-chlorophenoxy)-2-methylpropanoate'	b'Dulofibrate'	HMDB02 51637	C16H14Cl2 O3	
20 0	324.03	325.0401358	0.0023 358	Protona tion	b'[(2,5-dichlorophenyl)amino](hexyloxy)phosphinic acid'	b'Hexyl 2,5- dichlorophenylphosphoroamidate'	HMDB02 53167	C12H18Cl2 NO3P	
		324.0272191	0.0027 809	Redox	b'(2S,4S)-4-(ethylamino)-2-methyl-1,1-dioxo-2H,3H,4H-1'xccc'x'bb'x'c2'x'81'x'b6'-thieno[2,3-b]thiopyran-6-sulfonamide'	b'Dorzolamide'	HMDB00 15007	C10H16N2O 4S3	C069 69
20 1	325.02 95	326.0394993	0.0021 993	Protona tion	b'2-[2-oxo-1-[2-(thiophen-2-yl)acetamido]ethyl]-5,6-dihydro-2H-1,3-thiazine-4-carboxylic acid'	b'(2R)-2-[(1R)-2-Oxo-1-[(2- thienylacetyl)amino]ethyl]-5,6-dihydro- 2H-1,3-thiazine-4-carboxylic acid'	HMDB02 42604	C13H14N2O 4S2	
		326.0394983	0.0021 983	Protona tion	b'7-hydroxy-11-(hydroxymethyl)-15-methyl-12,13-dithia-9,15-diazatetracyclo[9.2.2.0'xc2'xb9,\xc2'x81'xb9.0'xc2'xb3,\xc2'x81'xb8]pentadeca-3,5-diene-10,14-dione'	b'Gliotoxin'	HMDB02 52746	C13H14N2O 4S2	
		325.0303306	0.0008 306	Redox	b'2-amino-7-(1,2-dihydroxyethyl)-6-(methylsulfanyl)-1H,4H-thieno[3,2-g]pteridin-4-one'	b'Urothion'	HMDB00 02377	C11H11N5O 3S2	
		325.0272487	0.0022 513	Redox	b'2-[2-[(2,6-dichloro-4-methoxyphenyl)amino]phenyl]acetic acid'	b'2-[(2,6-Dichloro-4- methoxyphenyl)amino]phenylacetic acid'	HMDB02 50053	C15H13Cl2 NO3	
		325.0287901	0.0007 099	Redox	b'2-[6-(5-chloro-2-methoxyphenyl)-4-oxo-2-sulfanylidene-1,2,3,4-tetrahydropyrimidin-1-yl]acetamide'	b'2-(6-(5-Chloro-2-methoxyphenyl)-4- oxo-2-thioxo-3,4-dihydropyrimidin- 1(2H)-yl)acetamide'	HMDB02 56364	C13H12ClN 3O3S	
20 2	325.06 28	326.070796	0.0001 96	Protona tion	b'triphenyl phosphate'	b'TRIPHENYL PHOSPHATE'	HMDB02 59262	C18H15O4P	C142 35
20 3	327.23 09	328.2402303	0.0015 303	Protona tion	b'(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoic acid'	b'Docosahexaenoic acid'	HMDB00 02183	C22H32O2	C064 29
		328.2402303	0.0015	Protona	b'5-methyl-4-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-yl]benzene-1,3-diol'	b'Neogrifolin'	HMDB00	C22H32O2	

20	328.04		303	tion			30053		
		328.2402303	0.0015 303	Protona tion	b'5-methyl-2-[(2E,6E)-3,7,11-trimethyldodeca-2,6,10-trien-1-yl]benzene-1,3-diol'	b'Grifolin'	HMDB00 30446	C22H32O2	
		328.2402303	0.0015 303	Protona tion	b'(2E,4E,6Z,8E)-3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-yl acetate'	b'Retinol acetate'	HMDB00 35185	C22H32O2	
		328.2402303	0.0015 303	Protona tion	b'2-methyl-5-[(8Z,11E)-pentadeca-8,11,14-trien-1-yl]benzene-1,3-diol'	b'(Z,Z)-2-Methyl-5-(8,11,14-pentadecatrienyl)-1,3-benzenediol'	HMDB00 38908	C22H32O2	
		328.2362075	0.0024 925	Protona tion	b'4-carbamoyl-2-dodecanamidobutanoic acid'	b'N-Lauroyl Glutamine'	HMDB02 42031	C17H32N2O 4	
		328.2402303	0.0015 303	Protona tion	b'docos-2,4,6,8,10,12-hexaenoic acid'	b'Docosahexaenoic acid(DHA)'	HMDB02 44316	C22H32O2	
		328.2402303	0.0015 303	Protona tion	b'3,7-dimethyl-9-(2,6,6-trimethylcyclohex-1-en-1-yl)nona-2,4,6,8-tetraen-1-yl acetate'	b'9-cis Retinol Acetate'	HMDB02 47587	C22H32O2	
		328.2402303	0.0015 303	Protona tion	b'docosa-4,7,10,13,16,19-hexaenoic acid'	b'(4E,7E,10Z,13E,16E,19E)-Docosa-4,7,10,13,16,19-hexaenoic acid'	HMDB02 51558	C22H32O2	
		328.2402303	0.0015 303	Protona tion	b'14-methoxy-15-methyl-5-propoxytetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadeca-2(7),3,5-triene'	b'Promestrienum'	HMDB02 56803	C22H32O2	
20	328.04	329.0525197	0.0021 197	Protona tion	b'(4aR,6R,7R,7aS)-6-(6-amino-9H-purin-9-yl)-2,7-dihydroxy-hexahydro-2lambda5-furo[3,2-d][1,3,2]dioxaphosphinin-2-one'	b'Cyclic AMP'	HMDB00 00058	C10H12N5O 6P	C005 75
		329.0525197	0.0021 197	Protona tion	b'4-(6-amino-9H-purin-9-yl)-2-hydroxy-6-(hydroxymethyl)-tetrahydro-2H-2'\xce'\xbb'\xe2'\xb5-furo[3,2-d][1,3,2]dioxaphosphol-2-one'	b'Adenosine 2',3'-cyclic phosphate"	HMDB00 11616	C10H12N5O 6P	C083 55
		329.0511071	0.0007 071	Protona tion	b'2-[2-nitro-4-(trifluoromethyl)benzoyl]cyclohexane-1,3-dione'	b'Nitisinone'	HMDB00 14492	C14H10F3N O5	
		329.0520506	0.0016 506	Protona tion	b'ethyl N-(2-[(diethoxy(sulfanylidene)-\xce'\xbb'\xe2'\xb5-phosphanyl]sulfanyl)acetyl)-N-methylcarbamate'	b'Mecarbam'	HMDB00 31800	C10H20NO5 PS2	C186 61
20	331.26	332.2715304	0.0021	Protona	b'(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoic acid'	b'Adrenic acid'	HMDB00	C22H36O2	C165

5	16		304	tion			02226		27
		332.2715304	0.0021 304	Protona tion	b'1-hydroxy-1-phenylhexadecan-3-one'	b'1-Hydroxy-1-phenyl-3-hexadecanone'	HMDB00 35676	C22H36O2	
		332.2715304	0.0021 304	Protona tion	b'3-hydroxy-1-phenylhexadecan-1-one'	b'3-Hydroxy-1-phenyl-1-hexadecanone'	HMDB00 35677	C22H36O2	
		332.2715304	0.0021 304	Protona tion	b'2-methyl-5-[(8Z)-pentadec-8-en-1-yl]benzene-1,3-diol'	b'2-Methyl-5-(8-pentadecenyl)-1,3-benzenediol'	HMDB00 38910	C22H36O2	
		332.2715304	0.0021 304	Protona tion	b'ethyl (5Z,8Z,14Z)-icosa-5,8,11,14-tetraenoate'	b'Ethyl Arachidonate'	HMDB00 62725	C22H36O2	
		332.2715304	0.0021 304	Protona tion	b'docosa-2,4,6,8-tetraenoic acid'	b'Docosa-2,4,6,8-tetraenoic acid'	HMDB02 51563	C22H36O2	
		332.2715304	0.0021 304	Protona tion		b'Ganaxolone'	HMDB02 52627	C22H36O2	
		332.2715304	0.0021 304	Protona tion	b'ethyl icosa-6,9,12,15-tetraenoate'	b'Ethyl icosa-6,9,12,15-tetraenoate'	HMDB02 60406	C22H36O2	
20 6	332.01 86	333.0237849	0.0026 151	Protona tion	b'6-[(2-chloro-4-fluorophenyl)sulfamoyl]cyclohex-1-ene-1-carboxylic acid'	b'(6R)-6-[(2-Chloro-4-fluorophenyl)sulfamoyl]cyclohexene-1-carboxylic acid'	HMDB02 58104	C13H13ClF NO4S	
		333.0260651	0.0003 349	Protona tion	b'1-{3,4-dihydroxy-5-[(phosphonatoxy)methyl]oxolan-2-yl}-1'xccc'xb'x81'xb5-pyridin-1-ylum-3-carboxylate'	b'beta-nicotinate D-ribonucleotide'	HMDB03 04543	C11H12NO9 P	
20 7	333.00 28	333.0000559	0.0027 441	Redox	b'2-[2-amino-3-(4-bromobenzoyl)phenyl]acetic acid'	b'Bromfenac'	HMDB00 15098	C15H12BrN O3	
20 8	333.05 69	334.066498	0.0017 98	Protona tion	b'[(2R)-2,3-dihydroxypropoxy]([[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy])phosphinic acid'	b'Glycerophosphoinositol'	HMDB00 11649	C9H19O11P	C012 25
		334.0623427	0.0023 573	Protona tion	b'2-(4-benzamidobenzenesulfonamido)acetic acid'	b'2-[(4-Benzamidophenyl)sulfonylamino]acetic	HMDB02 49991	C15H14N2O 5S	

						acid'			
		333.0548009	0.0020 991	Redox	b'1-[(E)-[(4-chlorophenyl)methylidene]amino]-3-[(Z)-[(4-chlorophenyl)methylidene]amino]guanidine'	b'Robenidine'	HMDB00 31785	C15H13Cl2 N5	
20 9	334.06 01	335.0704031	0.0025 031	Protone tion	b'3-[(4-aminophenyl)sulfanyl]-3-imino-2-[2-(trifluoromethyl)phenyl]propanenitrile'	b'MEK1-2-inhibitor'	HMDB02 48914	C16H12F3N 3S	
		335.0704031	0.0025 031	Protone tion	b'3-amino-3-[(4-aminophenyl)sulfanyl]-2-[2-(trifluoromethyl)phenyl]prop-2-enenitrile'	b'(Z)-3-Amino-3-(4-aminophenylthio)- 2-(2-(trifluoromethyl)phenyl)acrylonitrile'	HMDB02 58336	C16H12F3N 3S	
		334.0583565	0.0017 435	Redox	b'7-tert-butyl-6-chloro-2-(trifluoromethyl)-2H-chromene-3-carboxylic acid'	b'(2s)-7-Tert-Butyl-6-Chloro-2-(Trifluoromethyl)-2h-Chromene-3-Carboxylic Acid'	HMDB02 60149	C15H14ClF3 O3	
		334.0576996	0.0024 004	Redox	b'[5-(3-carbamoyl-1,4-dihydropyridin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl phosphate'	b'NMNH'	HMDB03 04437	C11H15N2O 8P	
21 0	337.30 95	338.3184806	0.0011 806	Protone tion	b'(13Z)-docos-13-enoic acid'	b'Erucic acid'	HMDB00 02068	C22H42O2	C083 16
		338.3184806	0.0011 806	Protone tion	b'(11Z)-docos-11-enoic acid'	b'Cetoleic acid'	HMDB00 02884	C22H42O2	
		338.3184806	0.0011 806	Protone tion	b'(11E)-docos-11-enoic acid'	b'Catelaidic acid'	HMDB00 31013	C22H42O2	
		338.3184806	0.0011 806	Protone tion	b'(2E)-3,7,11,15-tetramethylhexadec-2-en-1-yl acetate'	b'Phytyl acetate'	HMDB00 32470	C22H42O2	
		338.3184806	0.0011 806	Protone tion	b'docosane-7,9-dione'	b'7,9-Docosanedione'	HMDB00 35566	C22H42O2	
		338.3184806	0.0011 806	Protone tion	b'docosane-6,8-dione'	b'6,8-Docosanedione'	HMDB00 35567	C22H42O2	
		338.3184806	0.0011	Protone	b'docosane-5,7-dione'	b'5,7-Docosanedione'	HMDB00	C22H42O2	

			806	tion			35568		
		338.3184806	0.0011 806	Protona tion	b'docosane-4,6-dione'	b'4,6-Docosanedione'	HMDB00 35569	C22H42O2	
		338.3184806	0.0011 806	Protona tion	b'butyl (9Z)-octadec-9-enoate'	b'N-butyl Oleate'	HMDB00 62659	C22H42O2	
		338.3184806	0.0011 806	Protona tion	b'docos-13-enoic acid'	b'Brassicidic acid'	HMDB02 49369	C22H42O2	
		338.3184806	0.0011 806	Protona tion	b'docos-15-enoic acid'	b'15-Docosenoic acid'	HMDB03 02279	C22H42O2	
		338.3184806	0.0011 806	Protona tion	b'(2E)-docos-2-enoic acid'	b'Docosenic acid'	HMDB03 02285	C22H42O2	
		338.3184806	0.0011 806	Protona tion	b'docos-2-enoic acid'	b'Docosenoic acid'	HMDB03 02620	C22H42O2	
21 1	338.84 61	339.854981	0.0010 81	Protona tion	b'1,7,8,9,10,10-hexachloro-4-oxatricyclo[5.2.1.0\xc2\xb2,\xc2\xb81\b6]dec-8-ene'	b'Endosulfan-ether'	HMDB02 46167	C9H6Cl6O	
21 2	338.98 67	339.9960489	0.0015 489	Protona tion	b'{{{(1R,2R,3R,4R,5R,6S)-2,3,5,6-tetrahydroxy-4-(phosphonoxy)cyclohexyl}oxy}phosphonic acid'	b'D-myo-Inositol 1,4-bisphosphate'	HMDB00 00968	C6H14O12P 2	C012 20
		339.9960489	0.0015 489	Protona tion	b'{{{(2R,3S,4S,5S)-3,4-dihydroxy-5-(hydroxymethyl)-5-(phosphonoxy)oxolan-2-yl}methoxy}phosphonic acid'	b'D-Fructose 2,6-bisphosphate'	HMDB00 01047	C6H14O12P 2	C006 65
		339.9960489	0.0015 489	Protona tion	b'{{{(2R,3S,4S,5R)-3,4,5-trihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl}methoxy}phosphonic acid'	b'Fructose 1,6-bisphosphate'	HMDB00 01058	C6H14O12P 2	C053 78
		339.9960489	0.0015 489	Protona tion	b'{{{(2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-[(phosphonoxy)methyl]oxan-2-yl}oxy}phosphonic acid'	b'alpha-D-Glucose 1,6-bisphosphate'	HMDB00 03514	C6H14O12P 2	C012 31
		339.9960489	0.0015 489	Protona tion	b'{{{(1S,2R,3s,4S,5R,6s)-2,3,4,6-tetrahydroxy-5-(phosphonoxy)cyclohexyl}oxy}phosphonic acid'	b'D-myo-Inositol 1,3-bisphosphate'	HMDB00 06234	C6H14O12P 2	C040 62
		339.9960489	0.0015	Protona	b'{{{(1S,2S,3S,4S,5R,6S)-2,3,4,5-tetrahydroxy-6-(phosphonoxy)cyclohexyl}oxy}phosphonic acid'	b'D-myo-Inositol 3,4-bisphosphate'	HMDB00	C6H14O12P	C040

			489	tion			06235	2	63
		339.9960489	0.0015 489	Protona tion	b'{{{(2R,3R,4S)-3,4,5-trihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl]methoxy}phosphonic acid'}	b'D-Tagatose 1,6-bisphosphate'	HMDB00 06872	C6H14O12P 2	C037 85
		339.9960489	0.0015 489	Protona tion	b'{{{(2R,3S,4S,5S,6S)-3,4,5-trihydroxy-6-(phosphonoxy)oxan-2-yl]methoxy}phosphonic acid'}	b'D-Mannose 1,6-bisphosphate'	HMDB00 60269	C6H14O12P 2	
		339.9960499	0.0015 499	Protona tion	b'[[3,4,5-trihydroxy-2-oxo-6-(phosphonoxy)hexyl]oxy]phosphonic acid'	b'1,6-Di-O-phosphono-D-fructose'	HMDB02 44239	C6H14O12P 2	
		339.9960499	0.0015 499	Protona tion	b'((2,3,4-trihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl]methoxy)phosphonic acid'	b'Fructose-1,6-diphosphate'	HMDB02 44240	C6H14O12P 2	
		339.9960499	0.0015 499	Protona tion	b'[[4,5,6-trihydroxy-2-oxo-1-(phosphonoxy)hexan-3-yl]oxy]phosphonic acid'	b'Di-phosphofructose'	HMDB02 51116	C6H14O12P 2	
		339.9960499	0.0015 499	Protona tion	b'([hydroxy[(3,4,5,6-tetrahydroxy-1-oxohexan-2-yl)oxy]phosphoryl]oxy)phosphonic acid'	b'Diphosphoglucose'	HMDB02 51461	C6H14O12P 2	
		339.9960499	0.0015 499	Protona tion	b'[[2,4,5-trihydroxy-3-oxo-6-(phosphonoxy)hexyl]oxy]phosphonic acid'	b'[(2R,3R)-2,3,5-Trihydroxy-4-oxo-6-phosphonoxyhexyl] dihydrogen phosphate'	HMDB02 60218	C6H14O12P 2	
21	341.03	342.0439018	0.0008 982	Protona tion	b'12-chloro-9-(2-chlorophenyl)-3-methyl-2,4,5,8-tetraazatricyclo[8.4.0.0]x2'xb2,\xc2'x81'xb6]tetradeca-1(10),3,5,8,11,13-hexaene'	b'Triazolam'	HMDB00 15034	C17H12Cl2 N4	
3	7	342.0456463	0.0008 463	Protona tion	b'methyl N-[[2-([[(methoxycarbonyl)amino]methanethioyl)amino]phenyl]carbamothioyl]carbamate'	b'Thiophanate-methyl'	HMDB02 59025	C12H14N4O 4S2	C144 32
		341.0391649	0.0021 649	Redox	b'2-[[5-(2-benzenesulfonamidoethyl)thiophen-2-yl]oxy]acetic acid'	b'Linotroban'	HMDB02 54105	C14H15NO5 S2	
21	344.03	345.0474343	0.0020 343	Protona tion	b'9-[(4aR,6R,7R,7aS)-2,7-dihydroxy-2-oxo-hexahydro-2'xc2'xb2'x81'xb5-furo[3,2-d][1,3,2]dioxaphosphinin-6-yl]-2-amino-6,9-dihydro-1H-purin-6-one'	b'Cyclic GMP'	HMDB00 01314	C10H12N5O 7P	C009 42
4	76	345.0474343	0.0020 343	Protona tion	b'9-[(3aR,4R,6R,6aR)-2-hydroxy-6-(hydroxymethyl)-2-oxo-tetrahydro-2H-2'xc2'xb2'x81'xb5-furo[3,4-d][1,3,2]dioxaphosphol-4-yl]-2-amino-6,9-dihydro-3H-purin-6-one'	b'Guanosine 2',3'-cyclic phosphate"	HMDB00 11629	C10H12N5O 7P	

21	5	346.05	345.0474347	0.0020 347	Protone tion	b'2-amino-6-(2,5-dihydroxy-2-oxo-1,3,2lambda5-dioxaphosphinane-4-carbonyl)-4,6,7,8-tetrahydropteridin-4-one'	b'Molybdopterin precursor Z'	HMDB00 11683	C10H12N5O 7P	
			344.0379612	0.0003 612	Redox	b'2-hydroxy-2-[3-hydroxy-5-oxo-4-(3,4,5-trihydroxybenzoyloxy)oxolan-2-yl]acetic acid'	b'2-O-Galloyl-1,4-galactarolactone'	HMDB00 37199	C13H12O11	
			344.0379612	0.0003 612	Redox	b'2-hydroxy-2-[4-hydroxy-5-oxo-3-(3,4,5-trihydroxybenzoyloxy)oxolan-2-yl]acetic acid'	b'3-O-Galloyl-1,4-galactarolactone'	HMDB00 37201	C13H12O11	
			344.0379612	0.0003 612	Redox	b'2-(3,4-dihydroxy-5-oxoxolan-2-yl)-2-(3,4,5-trihydroxybenzoyloxy)acetic acid'	b'5-O-Galloyl-1,4-galactarolactone'	HMDB00 37202	C13H12O11	
	35	346.05	347.0630843	0.0017 843	Protone tion	b' {[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy} phosphonic acid'	b'Adenosine monophosphate'	HMDB00 00045	C10H14N5O 7P	C000 20
			347.0630843	0.0017 843	Protone tion	b' {[(2R,3S,5R)-5-(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)-3-hydroxyoxolan-2-yl]methoxy} phosphonic acid'	b"2'-Deoxyguanosine 5'- monophosphate"	HMDB00 01044	C10H14N5O 7P	C003 62
			347.0630843	0.0017 843	Protone tion	b' {[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]oxy} phosphonic acid'	b"3'-AMP"	HMDB00 03540	C10H14N5O 7P	C013 67
			347.0630843	0.0017 843	Protone tion	b' {[(3R,4R,5R)-2-(6-amino-9H-purin-9-yl)-4-hydroxy-5-(hydroxymethyl)oxolan-3-yl]oxy} phosphonic acid'	b"Adenosine 2'-phosphate"	HMDB00 11617	C10H14N5O 7P	C009 46
			347.0630843	0.0017 843	Protone tion	b' {[(2R,3S,5R)-5-(6-amino-2-hydroxy-9H-purin-9-yl)-3-hydroxyoxolan-2-yl]methoxy} phosphonic acid'	b'2-hydroxy-dAMP"	HMDB00 59594	C10H14N5O 7P	C199 70
			347.0630843	0.0017 843	Protone tion	b' {[(5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy} phosphonic acid'	b'Vidarabine phosphate'	HMDB02 45755	C10H14N5O 7P	
			347.0630848	0.0017 848	Protone tion	b' {9-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-6-imino-6,9-dihydro-3H-purin-3-yl} phosphonic acid'	b'3-Phosphoadenosine'	HMDB02 45974	C10H14N5O 7P	
			347.0630848	0.0017 848	Protone tion	b' {[3-azido-5-(5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)oxolan-2-yl]methoxy} phosphonic acid'	b'Zidovudine monophosphate'	HMDB02 48821	C10H14N5O 7P	
			347.0630848	0.0017 848	Protone tion	b' {[5-(6-amino-9H-purin-9-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]oxy} phosphonic acid'	b' [(2R,5R)-5-(6-Aminopurin-9-yl)-4- hydroxy-2-(hydroxymethyl)oxolan-3-yl]	HMDB02 58140	C10H14N5O 7P	

22	0	354.05	9	355.0694197	0.0026 197	Protone	b'2-[(2-amino-1-hydroxy-3-[(4-methanesulfinylbutyl)thio(carbonoimidyl)]sulfinyl)propylidene)amino]acetic acid'	b'Sulforaphane-cysteine-glycine'	HMDB02 40559	C11H21N3O 4S3	
				355.0645065	0.0022 935	Protone	b'propan-2-yl 2-chloro-5-(2-methyl-5,6-dihydro-1,4-oxathine-3-amido)benzoate'	b'1-Methyl ethyl 1-chloro-5- [[[(5,6dihydro-2-methyl-1,4-oxathin-3-yl)carbonyl]amino]benzoate'	HMDB02 59386	C16H18ClN O4S	
				355.0645069	0.0022 931	Protone	b'2-[1-[1-(2-chlorophenyl)-2-methoxy-2-oxoethyl]-4-sulfanylpiperidin-3-ylidene]acetic acid'	b'Clotidogrel active metabolite'	HMDB02 59496	C16H18ClN O4S	
				354.0586967	0.0003 033	Redox	b'2-hydroxy-1-[[[(2E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy]propane-1,2,3-tricarboxylic acid'	b'2-O-p-Coumaroylhydroxycitric acid'	HMDB00 40570	C15H14O10	
22	1	356.83	85	357.8444164	0.0018 836	Protone	b'1,2,4-trichloro-3-(2,3,6-trichlorophenyl)benzene'	b"2,2',3,3',6,6'-Hexachlorobiphenyl"	HMDB02 45362	C12H4Cl6	C143 69
				357.8444164	0.0018 836	Protone	b'1,2,5-trichloro-3-(2,4,5-trichlorophenyl)benzene'	b"2,2',3,4',5,5'-Hexachlorobiphenyl"	HMDB02 45366	C12H4Cl6	
				357.8444164	0.0018 836	Protone	b'1,2,4-trichloro-5-(2,4,5-trichlorophenyl)benzene'	b"2,2',4,4',5,5'-Hexachlorobiphenyl"	HMDB02 45372	C12H4Cl6	C142 01
				357.8444164	0.0018 836	Protone	b'1,3,5-trichloro-2-(2,4,6-trichlorophenyl)benzene'	b"2,2',4,4',6,6'-Hexachlorobiphenyl"	HMDB02 45374	C12H4Cl6	C142 02
				357.8444164	0.0018 836	Protone	b'1,2,3,4-tetrachloro-5-(3,4-dichlorophenyl)benzene'	b"2,3,3',4,4',5'-Hexachlorobiphenyl"	HMDB02 45418	C12H4Cl6	C181 20
				357.8444164	0.0018 836	Protone	b'1,2,3-trichloro-4-(3,4,5-trichlorophenyl)benzene'	b"2,3,3',4,4',5'-Hexachlorobiphenyl"	HMDB02 45420	C12H4Cl6	C181 21
				357.8444164	0.0018 836	Protone	b'1,2,4,5-tetrachloro-3-(3,4-dichlorophenyl)benzene'	b"2,3,3',4',5,6'-Hexachlorobiphenyl"	HMDB02 45421	C12H4Cl6	
				357.8444164	0.0018 836	Protone	b'1,2,4-trichloro-5-(3,4,5-trichlorophenyl)benzene'	b"2,3',4,4',5,5'-Hexachlorobiphenyl"	HMDB02 45441	C12H4Cl6	C181 22
				357.8444164	0.0018	Protone	b'1,2,3-trichloro-5-(3,4,5-trichlorophenyl)benzene'	b"3,3',4,4',5,5'-Hexachlorobiphenyl"	HMDB02	C12H4Cl6	C181

			836	tion			46011		15
		357.8444164	0.0018 836	Protona tion	b'1,2,3-trichloro-4-(2,4,5-trichlorophenyl)benzene'	b"2,2',3,4,4',5'-Hexachlorobiphenyl"	HMDB02 46191	C12H4Cl6	
		357.8444164	0.0018 836	Protona tion	b'1,2,4-trichloro-5-(2,3,6-trichlorophenyl)benzene'	b"2,2',3,4',5',6'-Hexachlorobiphenyl"	HMDB02 46230	C12H4Cl6	
		357.8444164	0.0018 836	Protona tion	b'1,2,3,4,5-pentachloro-6-(2-chlorophenyl)benzene'	b"2,2',3,4,5,6'-Hexachlorobiphenyl"	HMDB02 46652	C12H4Cl6	
		357.8444164	0.0018 836	Protona tion	b'1,2,4,5-tetrachloro-3-(2,5-dichlorophenyl)benzene'	b"2,2',3,5,5',6'-Hexachlorobiphenyl"	HMDB02 46909	C12H4Cl6	
		357.8444164	0.0018 836	Protona tion	b'1,2,3-trichloro-4-(2,3,4-trichlorophenyl)benzene'	b"2,2',3,3',4,4'-Hexachlorobiphenyl"	HMDB02 48611	C12H4Cl6	
22	361.04	362.0485259	0.0027 741	Protona tion	b'2,3,4-trihydroxy-5-(3,4,5-trihydroxybenzoyloxy)hexanedioic acid'	b'2-O-Galloylgalactaric acid'	HMDB00 36932	C13H14O12	
2	35	362.0489965	0.0023 035	Protona tion	b'1-[2-hydroxy-5-(trifluoromethyl)phenyl]-5-(trifluoromethyl)-2,3-dihydro-1H-1,3-benzodiazol-2-one'	b'1-(2-Hydroxy-5-(trifluoromethyl)phenyl)-5-(trifluoromethyl)-1H-benzodiazol-2-one'	HMDB02 55771	C15H8F6N2 O2	C138 33
22	362.00	362.0031981	0.0007 981	Redox	b'tris(4-chlorophenyl)methanol'	b'Tris(4-chlorophenyl)methanol'	HMDB02 59279	C19H13Cl3 O	
22	362.04	363.057999	0.0015 99	Protona tion	b'([(2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)phosphonic acid'	b'Guanosine monophosphate'	HMDB00 01397	C10H14N5O 8P	C001 44
		363.057999	0.0015 99	Protona tion	b'([(3S)-5-(2-amino-6,8-dioxo-6,7,8,9-tetrahydro-3H-purin-9-yl)-3-hydroxyoxolan-2-yl]methoxy)phosphonic acid'	b'8-Oxo-dGMP'	HMDB00 11670	C10H14N5O 8P	
		363.057999	0.0015 99	Protona tion	b'(4aR,5aR,11aR,12aS)-2,10,12,12-tetrahydroxy-8-imino-4,4a,5a,6,7,8,11,11a,12,12a-decahydro-2H-1,3,5-trioxo-6,7,9,11-tetraaza-2lambda5-phosphatetracen-2-one'	b'Cyclic pyranopterin monophosphate'	HMDB00 59639	C10H14N5O 8P	C182 39
		363.057999	0.0015	Protona	b'([(2R,3R,4R,5R)-2-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-4-hydroxy-5-(hydroxymethyl)oxolan-3-yl]oxy)phosphonic acid'	b"Guanosine 2'-monophosphate"	HMDB02	C10H14N5O	

			99	tion			40586	8P	
		363.057999	0.0015 99	Protona tion	b' {[(2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]oxy} phosphonic acid'	b"Guanosine 3'-monophosphate"	HMDB02 40587	C10H14N5O 8P	C061 93
		363.057999	0.0015 99	Protona tion	b' {[3,4-dihydroxy-5-(6-hydroxy-2-imino-3,9-dihydro-2H-purin-9-yl)oxolan-2-yl]methoxy} phosphonic acid'	b'[(2R,5R)-5-(2-Amino-6-oxo-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl dihydrogen phosphate'	HMDB02 57693	C10H14N5O 8P	
22 5	363.00 47	364.0132809	0.0007 809	Protona tion	b'3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctan-1-ol'	b'3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctan-1-ol'	HMDB02 60260	C8H5F13O	
22 6	363.05 1	364.0583027	0.0004 973	Protona tion	b"3',4',5',6'-tetrahydroxy-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'Gallein'	HMDB02 52597	C20H12O7	
22 7	369.01 91	370.027583 369.0170779	0.0006 83 0.0020 221	Protona tion Redox	b'3-(2,4-dichlorophenyl)-4-(1-methyl-1H-indol-3-yl)-2,5-dihydro-1H-pyrrole-2,5-dione' b'2-[(2-{2-[(2,6-dichloro-4-hydroxyphenyl)amino]phenyl}acetyl)oxy]acetic acid'	b'3-(2,4-Dichlorophenyl)-4-(1-methyl-1H-indol-3-yl)-1H-pyrrole-2,5-dione' b"4'-Hydroxy Aceclofenac"	HMDB02 45731 HMDB02 46629	C19H12Cl2 N2O2 C16H13Cl2 NO5	
22 8	380.01 31	380.011933	0.0011 67	Redox	b'4,11-dichloro-5,7,12,14-tetrahydro-5,12-diazapentacene-7,14-dione'	b'4,11-Dichloro-5,12-dihydroquino[2,3-b]acridine-7,14-dione'	HMDB00 37810	C20H10Cl2 N2O2	
22 9	381.10 82	382.1181401 382.1182557	0.0021 401 0.0022 557	Protona tion Protona tion	b"(3-{3'-methoxyspiro[adamantane-2,2'-(1,4)dioxetane]-3'-yl}phenoxy)phosphonic acid" b'potassium (5R,9S,11R,12S)-12-hydroxy-5,11-dimethyl-6-methylidene-16-oxo-15-oxapentacyclo[9.3.2.1'xe2\x81\x85,\xc2\x81\x8b8.0'xc2\x8b9,\xc2\x8b9'xc2\x81\x8b0.0'xc2\x8b2,\xc2\x81\x8b8]heptadec-13-ene-9-carboxylate'	b'Amppd' b'Potassium gibberellate'	HMDB02 48363 HMDB03 03277	C18H23O7P C20H23KO5	
23 0	382.09 85	383.1077125 383.1077125	0.0014 125 0.0014 125	Protona tion Protona tion	b'(2S)-2-({9-[(2R,3R,4S,5R)-3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-9H-purin-6-yl} amino)butanedioic acid' b'2-({9-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-9H-purin-6-yl} amino)butanedioic acid'	b'Succinyladenosine' b'N6-Succinyl Adenosine'	HMDB00 00912 HMDB02 55303	C14H17N5O 8 C14H17N5O 8	
23 1	384.98 17	385.9894834	1.66E- 05	Protona tion	b'1-(3,4-dichlorophenyl)-3-(2,3-dihydro-1-benzofuran-5-sulfonyl)urea'	b"N-(5-(2,3-Dihydrobenzofuryl)sulfonyl)-N'-(3,4-	HMDB02 54244	C15H12Cl2 N2O4S	

						dichlorophenyl)urea"			
23	385.14	386.1486548	0.0025 452	Protona tion	b'2-methanesulfinyl-10-[2-(1-methylpiperidin-2-yl)ethyl]-10H-phenothiazine'	b'Mesoridazine'	HMDB00 15068	C21H26N2O S2	C071 43
2	34	386.1486558	0.0025 442	Protona tion	b'10-[2-(1-methylpiperidin-2-yl)ethyl]-2-(methylsulfonyl)-10H-5lambda4-phenothiazin-5-one'	b'Thioridazine 5-Sulfoxide'	HMDB02 43502	C21H26N2O S2	
23	386.03	387.0406215	0.0025 215	Protona tion	b'2-amino-4-({1-[(carboxymethyl)(sulfo)amino]-1-oxo-3-sulfonylpropan-2-yl}carbonyl)butanoic acid'	b'2-Amino-5-[[1-[carboxymethyl(sulfo)amino]-1-oxo-3-sulfonylpropan-2-yl]amino]-5-oxopentanoic acid'	HMDB02 57661	C10H17N3O 9S2	
23	386.98	387.9922734	0.0014 266	Protona tion	b' {3-hydroxy-5-[(E)-2-[4-(sulfooxy)phenyl]ethenyl]phenyl} oxidanesulfonic acid'	b'trans-Resveratrol 3,4'-disulfate"	HMDB00 41780	C14H12O9S 2	
4	59	387.9922734	0.0014 266	Protona tion	b' {3-[(E)-2-(4-hydroxyphenyl)ethenyl]-5-(sulfooxy)phenyl} oxidanesulfonic acid'	b'trans-Resveratrol 3,5-disulfate'	HMDB00 41781	C14H12O9S 2	
23	388.02	389.0357936	0.0015 936	Protona tion	b"3',6'-dihydroxy-4-isothiocyanato-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b"3',6'-Dihydroxy-6-isothiocyanatospiro[isobenzofuran-1(3H),9'-[9H]xanthen]-3-one"	HMDB02 46164	C21H11NO5 S	
5	64	389.0357932	0.0015 932	Protona tion	b"3',6'-dihydroxy-5-isothiocyanato-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'Fluorescein-5-isothiocyanate'	HMDB02 46165	C21H11NO5 S	
		389.0357936	0.0015 936	Protona tion	b"3',6'-dihydroxy-8'-isothiocyanato-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'Fluoresceine isothiocyanate'	HMDB02 52364	C21H11NO5 S	
23	391.22	392.2327754	0.0017 754	Protona tion	b'(2-hydroxy-2-oxo-1,3,2'wce'x'bb'xe2'x81'xb5-dioxaphospholan-4-yl)methyl hexadecanoate'	b'CPA(16:0/0:0)'	HMDB00 07003	C19H37O6P	
6	32	391.2259772	0.0027 772	Redox	b'N-[4-(1-benzoylpiperidin-4-yl)butyl]-3-(pyridin-3-yl)prop-2-enamide'	b'Daporinad'	HMDB02 47176	C24H29N3O 2	
23	392.22	392.2252489	0.0007 511	Redox	b'(diphenylmethyl)({2-[(diphenylmethyl)amino]ethyl})amine'	b"N,N'-Dibenzhydylethane-1,2-diamine"	HMDB02 54810	C28H28N2	

23	393.23	394.2484255	0.0023	Protona	b'[(2R)-3-[(1Z)-hexadec-1-en-1-yloxy]-2-hydroxypropoxy]phosphonic acid'	b'LysoPA(P-16:0/0:0)'	HMDB00	C19H39O6P	C156
8	83		255	tion			11154		46
23	401.24	401.2426899	0.0007	Redox	b'8-{4-[1-oxo-4-(pyrimidin-2-yl)-1'xcel'xb'xe2'x81'xb5-piperazin-1-yl]butyl}-8-azaspiro[4.5]decane-7,9-dione'	b'Buspirone N-oxide'	HMDB00	C21H31N5O	
			101				61107	3	
		401.2426899	0.0007	Redox	b'2-hydroxy-8-{4-[4-(pyrimidin-2-yl)piperazin-1-yl]butyl}-8-azaspiro[4.5]decane-7,9-dione'	b'3'-Hydroxybuspirone"	HMDB00	C21H31N5O	
			101				61108	3	
		401.2426899	0.0007	Redox	b'8-{4-[4-(5-hydroxypyrimidin-2-yl)piperazin-1-yl]butyl}-8-azaspiro[4.5]decane-7,9-dione'	b'5-Hydroxybuspirone'	HMDB00	C21H31N5O	
9	34		101				61109	3	
		401.2426899	0.0007	Redox	b'6-hydroxy-8-{4-[4-(pyrimidin-2-yl)piperazin-1-yl]butyl}-8-azaspiro[4.5]decane-7,9-dione'	b'6'-Hydroxybuspirone"	HMDB00	C21H31N5O	
			101				61110	3	
		401.2426899	0.0007	Redox	b'6-{[3-{4-(2-methoxyphenyl)piperazin-1-yl]propyl}amino]-1,3,5-trimethyl-1,2,3,4-tetrahydropyrimidine-2,4-dione'	b'5-Methylurapidi'	HMDB02	C21H31N5O	
			101				46828	3	
24	402.00	403.0181814	0.0028	Protona	b'[(2R,3S,4R,5R)-5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy(hydroxy)phosphoryloxy]phosphonic acid'	b'CDP"	HMDB00	C9H15N3O1	C001
			814	tion			01546	1P2	12
		403.0181823	0.0028	Protona	b'[(5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy(hydroxy)phosphoryloxy]phosphonic acid'	b'[(2S,3R,4R,5R)-5-(4-Amino-2-oxopyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl phosphono hydrogen phosphate'	HMDB02	C9H15N3O1	
			823	tion			57860	1P2	
		402.0061789	0.0013	Redox	b'2-(2,7-dichloro-3,6-dihydroxy-9H-xanthen-9-yl)benzoic acid'	b'2,7-Dichlorofluorescin'	HMDB02	C20H12Cl2	
			211				50892	O5	
0	75	402.0061789	0.0013	Redox	b'1',2'-dichloro-3',6'-dihydroxy-1',2'-dihydro-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'dichlorodihydrofluorescein'	HMDB02	C20H12Cl2	
			211				51190	O5	
		402.0061789	0.0013	Redox	b'2-(1,2-dichloro-3,6-dihydroxy-9H-xanthen-9-yl)benzoic acid'	b'Dichlorofluorescin'	HMDB02	C20H12Cl2	
			211				51194	O5	
		402.0061789	0.0013	Redox	b'3a,4-dichloro-3',6'-dihydroxy-3a,4-dihydro-3H-spiro[2-benzofuran-1,9'-xanthene]-3-one"	b'7,7a-Dichloro-3',6'-dihydroxy Spiro[7H-2-benzofuran-3,9'-	HMDB02	C20H12Cl2	
			211				57577	O5	

8	67		887	tion			34590		
24	417.23	418.2484255	0.0020 255	Protone tion	b'(2-hydroxy-2-oxo-1,3,2\xce\xbb\xce2\x81\x85-dioxaphospholan-4-yl)methyl (11Z)-octadec-11-enoate'	b'CPA(18:1(11Z)/0:0)'	HMDB00 07005	C21H39O6P	
9	86	418.2484255	0.0020 255	Protone tion	b'(2-hydroxy-2-oxo-1,3,2\xce\xbb\xce2\x81\x85-dioxaphospholan-4-yl)methyl (9Z)-octadec-9-enoate'	b'CPA(18:1(9Z)/0:0)'	HMDB00 07006	C21H39O6P	
25 0	418.07 5	418.07534	0.0003 4	Redox	b'N-[(1-ethylpyrrolidin-2-yl)methyl]-5-iodo-2,3-dimethoxybenzamide'	b'Epidipride'	HMDB02 51845	C16H23IN2 O3	
25 1	418.27	418.2719243	0.0004 243	Redox	b'(1S,3R,7S,8S,8aR)-8-{2-[(2R,4R)-4-hydroxy-6-oxooxan-2-yl]ethyl}-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl 2,2-dimethylbutanoate'	b'Simvastatin'	HMDB00 05007	C25H38O5	
		418.2719243	0.0004 243	Redox	b'(2E)-4-[(2E,6E,10E,14E)-16-hydroxy-3,7,11,15-tetramethylhexadeca-2,6,10,14-tetraen-1-yl]oxy]-3-methyl-4-oxobut-2-enoic acid'	b'Cavipetin D'	HMDB00 30365	C25H38O5	
		418.2719243	0.0004 243	Redox	b'8-[2-(4-hydroxy-6-oxooxan-2-yl)ethyl]-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl 2,2-dimethylbutanoate'	b'(1R,3S,7R,8R,8As)-8-{2-[(2R,4S)-4-hydroxy-6-oxooxan-2-yl]ethyl}-3,7-dimethyl-1,2,3,7,8,8a-hexahydronaphthalen-1-yl 2,2-dimethylbutanoate'	HMDB02 57813	C25H38O5	
		418.2719243	0.0004 243	Redox	b'(2S)-2,3-dihydroxypropyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'MG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/0:0/0:0)'	HMDB02 60501	C25H38O5	
		418.2719243	0.0004 243	Redox	b'(2S)-2,3-dihydroxypropyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'MG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/0:0/0:0)'	HMDB02 60502	C25H38O5	
		418.2719243	0.0004 243	Redox	b'(2S)-2,3-dihydroxypropyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'MG(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0/0:0)'	HMDB02 60503	C25H38O5	
		418.2719243	0.0004 243	Redox	b'(2S)-2,3-dihydroxypropyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'MG(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/0:0/0:0)'	HMDB02 60504	C25H38O5	
		418.2719243	0.0004 243	Redox	b'(2S)-2,3-dihydroxypropyl (4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoate'	b'MG(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/0:0/0:0)'	HMDB02 60506	C25H38O5	

		418.2719243	0.0004 243	Redox	b'1,3-dihydroxypropan-2-yl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'MG(0:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/0:0)'	HMDB02 60553	C25H38O5	
		418.2719243	0.0004 243	Redox	b'1,3-dihydroxypropan-2-yl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'MG(0:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/0:0)'	HMDB02 60554	C25H38O5	
		418.2719243	0.0004 243	Redox	b'1,3-dihydroxypropan-2-yl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'MG(0:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0)'	HMDB02 60555	C25H38O5	
		418.2719243	0.0004 243	Redox	b'1,3-dihydroxypropan-2-yl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'MG(0:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/0:0)'	HMDB02 60556	C25H38O5	
		418.2719243	0.0004 243	Redox	b'1,3-dihydroxypropan-2-yl (4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoate'	b'MG(0:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/0:0)'	HMDB02 60558	C25H38O5	
25 2	419.25 45	420.2640756	0.0017 756	Protontion	b'(2-hydroxy-2-oxo-1,3,2'-dioxaphospholan-4-yl)methyl octadecanoate'	b'CPA(18:0/0:0)'	HMDB00 07004	C21H41O6P	
25 3	421.02 33	422.0283709	0.0027 291	Protontion	b'4-[2-(2,2-dichloroacetamido)-3-hydroxy-3-(4-nitrophenyl)propoxy]-4-oxobutanoic acid'	b'Chloramphenicol succinate'	HMDB02 50088	C15H16Cl2 N2O8	
25 4	421.26 76	422.2780723	0.0026 723	Protontion	b'7-{3-[(2-heptanamidoacetamido)methyl]-7-oxabicyclo[2.2.1]heptan-2-yl}hept-5-enoic acid'	b'3-(((Oxoheptylamino)acetyl)amino)methyl-7-oxobicyclo(2.2.1)hept-2-yl-5-heptenoic acid'	HMDB02 58446	C23H38N2O 5	
25 5	426.01 87	427.0294147	0.0029 147	Protontion	b'(((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonoxy)oxolan-2-yl)methoxy)phosphonic acid'	b'Adenosine 3',5'-diphosphate"	HMDB00 00061	C10H15N5O 10P2	C000 54
		427.0294147	0.0029 147	Protontion	b'(((2R,3S,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3-hydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'dGDP"	HMDB00 00960	C10H15N5O 10P2	C003 61
		427.0294147	0.0029 147	Protontion	b'(((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'ADP"	HMDB00 01341	C10H15N5O 10P2	C000 08
		427.0294147	0.0029 147	Protontion	b'(((5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'[(2S,3R,4R,5R)-5-(6-Aminopurin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl	HMDB02 47869	C10H15N5O 10P2	

						phosphono hydrogen phosphate'			
		427.0294157	0.0029 157	Protone tion	b'([3-azido-5-(5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'Zidovudine diphosphate'	HMDB02 48820	C10H15N5O 10P2	
25 6	427.00 71	428.0134303	0.0014 697	Protone tion	b'([[(2R,3S,4R)-3,4-dihydroxy-5-(6-oxo-6,9-dihydro-3H-purin-9-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'IDP'	HMDB00 03335	C10H14N4O 11P2	C001 04
25 7	427.02 1	427.0198989	0.0011 011	Redox	b'([[(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]sulfonic acid'	b'Adenosine phosphosulfate'	HMDB00 01003	C10H14N5O 10PS	C002 24
25 8	428.02 46	429.0336711	0.0012 711	Protone tion	b'2,2,4,4-tetrafluoro-6-(2-phenylethynyl)-6-[4-(prop-1-en-2-yl)phenyl]-1,3,5,2lambda5,4lambda5,6lambda5-triazatriphosphinine'	b'Geminal'	HMDB02 52673	C17H14F4N 3P3	
25 9	429.05 53	430.0610405	0.0020 595	Protone tion		b'Bicalutamide'	HMDB00 15260	C18H14F4N 2O4S	C081 60
		430.0654659	0.0023 659	Protone tion	b'(2-aminoethyl)([[(2R,3S,4R,5R)-3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]phosphinic acid'	b'CMP-2-aminoethylphosphonate'	HMDB00 60067	C11H20N4O 10P2	C056 73
		430.0635466	0.0004 466	Protone tion	b'calcium bis(2,3,4,5,6-pentahydroxyhexanoate)'	b'Calcium gluconate'	HMDB03 02138	C12H22CaO 14	
26 0	433.97 12	434.9766663	0.0023 337	Protone tion	b'([6-(4-chlorophenyl)imidazo[2,1-b][1,3]thiazol-5-yl]methylidene)[(3,4-dichlorophenyl)methoxy]amine'	b'6-(4-Chlorophenyl)imidazo[2,1-B][1,3]thiazole-5-carbaldehyde O-(3,4-dichlorobenzyl)oxime'	HMDB02 50300	C19H12Cl3 N3OS	
26 1	435.00 42	436.0100324	0.0019 676	Protone tion	b'2,6-dihydroxy-4-[4-hydroxy-7-(hydroxymethyl)-11-oxo-2,8-dioxatricyclo[7.3.1.0^{5,13}]trideca-1(12),3,5(13),6,9-pentaen-3-yl]phenyl]oxidanefulfonic acid'	b'2,6-dihydroxy-4-[4-hydroxy-7-(hydroxymethyl)-11-oxo-2,8-dioxatricyclo[7.3.1.0^{x81'xb5','xc2'xb9'xc2'xb3']trideca-1(12),3,5(13),6,9-pentaen-3-yl]phenoxy]dihydroxyoxo-\xce\xbb\x81'xb6-sulfanylium'	HMDB01 24760	C18H20I1 S	
26 2	435.24 9	436.2589907	0.0021 907	Protone tion	b'3-hydroxy-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'LysoPA(0/0/18:1(9Z))'	HMDB00 07851	C21H41O7P	

26	436.27	436.2589907	0.0021 907	Protona tion	b'[2-hydroxy-3-[(9Z)-octadec-9-enyloxy]propoxy]phosphonic acid'	b'LysoPA(18:1(9Z)/0:0)'	HMDB00 07855	C21H41O7P	
		436.2589902	0.0021 902	Protona tion	b'[3-(octadecanoyloxy)-2-oxopropoxy]phosphonic acid'	b'DHAP(18:0)'	HMDB00 11133	C21H41O7P	C038 05
		436.2589902	0.0021 902	Protona tion	b'[2-hydroxy-3-(octadec-9-enyloxy)propoxy]phosphonic acid'	b'(2-Hydroxy-3-phosphonoxypropyl) octadec-9-enoate'	HMDB02 42470	C21H41O7P	
	95	436.2784663	0.0010 337	Redox	b'6-({2,2-bis[bis(propan-2-yl)amino]acetyl oxy)-2,3,4,5-tetrahydroxyhexanoic acid'	b'Pangamic acid'	HMDB00 29949	C20H40N2O 8	
		436.282489	0.0029 89	Redox	b'(3R,5R)-7-[(1S,2S,6R,8S,8aR)-8-[(2,2-dimethylbutanoyl)oxy]-2,6-dimethyl-1,2,6,7,8,8a-hexahydronaphthalen-1-yl]-3,5-dihydroxyheptanoic acid'	b'simvastatin hydroxy acid'	HMDB00 61047	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z)-13-(3-pentyloxiran-2-yl)trideca-5,8,11-trienoate'	b'DG(2:0/20:3(5Z,8Z,11Z)- O(14R,15S)/0:0)'	HMDB02 96847	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z)-13-(3-pentyloxiran-2-yl)trideca-5,8,11-trienoate'	b'DG(20:3(5Z,8Z,11Z)- O(14R,15S)/2:0/0:0)'	HMDB02 96848	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z)-13-(3-pentyloxiran-2-yl)trideca-5,8,11-trienoate'	b'DG(2:0/0:0/20:3(5Z,8Z,11Z)- O(14R,15S))'	HMDB02 96849	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z)-13-(3-pentyloxiran-2-yl)trideca-5,8,11-trienoate'	b'DG(20:3(5Z,8Z,11Z)- O(14R,15S)/0:0/2:0)'	HMDB02 96850	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl} deca-5,8-dienoate'	b'DG(2:0/20:3(5Z,8Z,14Z)- O(11S,12R)/0:0)'	HMDB02 96851	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl} deca-5,8-dienoate'	b'DG(20:3(5Z,8Z,14Z)- O(11S,12R)/2:0/0:0)'	HMDB02 96852	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl} deca-5,8-dienoate'	b'DG(2:0/0:0/20:3(5Z,8Z,14Z)- O(11S,12R))'	HMDB02 96853	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl} deca-5,8-dienoate'	b'DG(20:3(5Z,8Z,14Z)- O(11S,12R)/0:0/2:0)'	HMDB02 96854	C25H40O6	

		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoate'	b'DG(2:0/20:3(5Z,11Z,14Z)- O(8,9)/0:0)'	HMDB02 96855	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoate'	b'DG(20:3(5Z,11Z,14Z)- O(8,9)/2:0/0:0)'	HMDB02 96856	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoate'	b'DG(2:0/0:0/20:3(5Z,11Z,14Z)- O(8,9))'	HMDB02 96857	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoate'	b'DG(20:3(5Z,11Z,14Z)- O(8,9)/0:0/2:0)'	HMDB02 96858	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl 4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoate'	b'DG(2:0/20:3(8Z,11Z,14Z)- O(5,6)/0:0)'	HMDB02 96859	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl 4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoate'	b'DG(20:3(8Z,11Z,14Z)- O(5,6)/2:0/0:0)'	HMDB02 96860	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl 4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoate'	b'DG(2:0/0:0/20:3(8Z,11Z,14Z)- O(5,6))'	HMDB02 96861	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl 4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoate'	b'DG(20:3(8Z,11Z,14Z)- O(5,6)/0:0/2:0)'	HMDB02 96862	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,11Z,14Z)- OH(20)/0:0)'	HMDB02 96863	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(20)/2:0/0:0)'	HMDB02 96864	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,14Z)- OH(20))'	HMDB02 96865	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(20)/0:0/2:0)'	HMDB02 96866	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5R,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoate'	b'DG(2:0/20:4(6E,8Z,11Z,14Z)- OH(5S)/0:0)'	HMDB02 96867	C25H40O6	

		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)- OH(5S)/2:0/0:0)'	HMDB02 96868	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(6E,8Z,11Z,14Z)- OH(5S))'	HMDB02 96869	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)- OH(5S)/0:0/2:0)'	HMDB02 96870	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z,19S)-19-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,11Z,14Z)- OH(19S)/0:0)'	HMDB02 96871	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(19S)/2:0/0:0)'	HMDB02 96872	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,14Z)- OH(19S))'	HMDB02 96873	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(19S)/0:0/2:0)'	HMDB02 96874	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z,18R)-18-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,11Z,14Z)- OH(18R)/0:0)'	HMDB02 96875	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z,18S)-18-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(18R)/2:0/0:0)'	HMDB02 96876	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,18S)-18-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,14Z)- OH(18R))'	HMDB02 96877	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,18S)-18-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(18R)/0:0/2:0)'	HMDB02 96878	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,11Z,14Z)- OH(17)/0:0)'	HMDB02 96879	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(17)/2:0/0:0)'	HMDB02 96880	C25H40O6	

		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,14Z)- OH(17))'	HMDB02 96881	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(17)/0:0/2:0)'	HMDB02 96882	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z,16R)-16-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,11Z,14Z)- OH(16R)/0:0)'	HMDB02 96883	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z,16S)-16-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(16R)/2:0/0:0)'	HMDB02 96884	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,16S)-16-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,14Z)- OH(16R))'	HMDB02 96885	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,16S)-16-hydroxyicosa-5,8,11,14-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,14Z)- OH(16R)/0:0/2:0)'	HMDB02 96886	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,13E,15S)-15-hydroxyicosa-5,8,11,13-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,11Z,13E)- OH(15S)/0:0)'	HMDB02 96887	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,11Z,13E,15R)-15-hydroxyicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)- OH(15S)/2:0/0:0)'	HMDB02 96888	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E,15R)-15-hydroxyicosa-5,8,11,13-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,8Z,11Z,13E)- OH(15S))'	HMDB02 96889	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E,15R)-15-hydroxyicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)- OH(15S)/0:0/2:0)'	HMDB02 96890	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,8Z,10E,12S,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoate'	b'DG(2:0/20:4(5Z,8Z,10E,14Z)- OH(12S)/0:0)'	HMDB02 96891	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoate'	b'DG(20:4(5Z,8Z,10E,14Z)- OH(12S)/2:0/0:0)'	HMDB02 96892	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,8Z,10E,14Z)- OH(12S))'	HMDB02 96893	C25H40O6	

		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoate'	b'DG(20:4(5Z,8Z,10E,14Z)- OH(12S)/0:0/2:0)'	HMDB02 96894	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5E,8Z,11R,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoate'	b'DG(2:0/20:4(5E,8Z,12Z,14Z)- OH(11R)/0:0)'	HMDB02 96895	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5E,8Z,11S,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoate'	b'DG(20:4(5E,8Z,12Z,14Z)- OH(11R)/2:0/0:0)'	HMDB02 96896	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5E,8Z,11S,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoate'	b'DG(2:0/0:0/20:4(5E,8Z,12Z,14Z)- OH(11R))'	HMDB02 96897	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5E,8Z,11S,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoate'	b'DG(20:4(5E,8Z,12Z,14Z)- OH(11R)/0:0/2:0)'	HMDB02 96898	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoate'	b'DG(2:0/20:4(5Z,7E,11Z,14Z)- OH(9)/0:0)'	HMDB02 96899	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoate'	b'DG(20:4(5Z,7E,11Z,14Z)- OH(9)/2:0/0:0)'	HMDB02 96900	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoate'	b'DG(2:0/0:0/20:4(5Z,7E,11Z,14Z)- OH(9))'	HMDB02 96901	C25H40O6	
		436.282489	0.0029 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoate'	b'DG(20:4(5Z,7E,11Z,14Z)- OH(9)/0:0/2:0)'	HMDB02 96902	C25H40O6	
26	437.26 45	438.2746402	0.0023 402	Protone tion	b'[3-hydroxy-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'LysoPA(0:0/18:0)'	HMDB00 07850	C21H43O7P	
		438.2746407	0.0023 407	Protone tion	b'[2-hydroxy-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'LysoPA(18:0/0:0)'	HMDB00 07854	C21H43O7P	
26	439.04 89	439.0507913	0.0018 913	Redox	b'[2-[(2-{4-[(2,4-dioxo-1,3-thiazolidin-5-yl)methyl]phenoxy}ethyl)amino]pyridin-3-yl]oxidanesulfonic acid'	b'N-Desmethyl-o-O-sulfate rosiglitazone'	HMDB00 60837	C17H17N3O 7S2	
		439.0507913	0.0018 913	Redox	b'[6-[(2-{4-[(2,4-dioxo-1,3-thiazolidin-5-yl)methyl]phenoxy}ethyl)amino]pyridin-3-yl]oxidanesulfonic acid'	b'N-Desmethyl-p-O-sulfate rosiglitazone'	HMDB00 60839	C17H17N3O 7S2	

26 6	439.22 23	440.2311221	0.0010 221	Protone tion	b'3-[2-(3-[4-(pentylcarbamoyl)-1,3-oxazol-2-yl]-7-oxabicyclo[2.2.1]heptan-2-yl)methyl]phenyl]propanoic acid'	b'3-[2-[[[(1S,2R,3S)-3-[4-(Pentylcarbamoyl)-1,3-oxazol-2-yl]-7-oxabicyclo[2.2.1]heptan-2-yl)methyl]phenyl]propanoic acid'	HMDB02 47885	C25H32N2O 5	
		440.2324595	0.0023 595	Protone tion	b'6-(1H-indol-4-yl)-4-(5-[[4-(propan-2-yl)piperazin-1-yl)methyl]-1,3-oxazol-2-yl]-1H-indazole'	b'Nemiralisib'	HMDB02 55509	C26H28N6O	
		439.220617	0.0016 83	Redox	b'(2S,3S,4S,5R,6S)-6-[4-[2-(dimethylamino)-1-(1-hydroxycyclohexyl)ethyl]phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'O-Desmethylvenlafaxine glucuronide'	HMDB00 61172	C22H33NO8	
		439.2219544	0.0003 456	Redox	b'3-(6-methoxypyridin-3-yl)-3-[2-oxo-3-[3-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)propyl]imidazolidin-1-yl]propanoic acid'	b'(S)-3-(6-Methoxypyridin-3-yl)-3-(2-oxo-3-(3-(5,6,7,8-tetrahydro-1,8-naphthyridin-2-yl)propyl)imidazolidin-1-yl)propanoic acid'	HMDB02 54780	C23H29N5O 4	
26 7	440.04 33	440.0418031	0.0014 969	Redox	b'5-[4-phenyl-5-(trifluoromethyl)thiophen-2-yl]-3-[3-(trifluoromethyl)phenyl]-1,2,4-oxadiazole'	b'5-[4-Phenyl-5-(trifluoromethyl)-2-thienyl]-3-[3-(trifluoromethyl)phenyl]-1,2,4-oxadiazole'	HMDB02 58264	C20H10F6N 2OS	
26 8	442.01 36	443.0243294	0.0029 294	Protone tion	b'([([2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'Guanosine diphosphate'	HMDB00 01201	C10H15N5O 11P2	C000 35
		443.0243294	0.0029 294	Protone tion	b'([([2R,3S,5R)-5-(6,8-dihydroxy-2-imino-3,9-dihydro-2H-purin-9-yl)-3-hydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'8-oxo-dGDP'	HMDB00 59648	C10H15N5O 11P2	C201 76
		443.0243303	0.0029 303	Protone tion	b'([5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'Guanosine diphosphate'	HMDB02 52974	C10H15N5O 11P2	
		443.0243303	0.0029 303	Protone tion	b'([5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-4-hydroxy-2-[(phosphonoxy)methyl]oxolan-3-yl]oxy]phosphonic acid'	b"Guanosine-3',5'-Diphosphate"	HMDB02 52975	C10H15N5O 11P2	
26 9	444.28 59	444.2875744	0.0016 744	Redox	b'(3R,5S)-5-[(2R)-2-[(1R,3aS,4E,7aR)-4-{2-[(1Z,3S,5R)-3,5-dihydroxy-2-methylidenecyclohexylidene]ethylidene}-7a-methyl-octahydro-1H-inden-1-yl]propyl]-3-hydroxy-3-methyloxolan-2-one'	b'1,25-Dihydroxyvitamin D3-26,23-lactone'	HMDB00 00969	C27H40O5	
		444.2875744	0.0016	Redox	b'14-acetyl-14-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.0.0^{2,7}.0^{11,15}]heptadec-6-en-3-yl hexanoate'	b'17-hydroxyprogesterone caproate'	HMDB02	C27H40O5	

			744					44774		
		444.2875744	0.0016 744	Redox	b'5-{2-{4-[2-(3,5-dihydroxy-2-methylidenecyclohexylidene)ethylidene]-7a-methyl-octahydro-1H-inden-1-yl}propyl}-3-hydroxy-3-methylloxan-2-one'	b'Calcitriol lactone'	HMDB02 49548	C27H40O5		
		444.2875744	0.0016 744	Redox	b'2-{2,13-dihydroxy-3a,6,10,14-tetramethyl-3-oxo-3H,3aH,4H,7H,8H,11H,12H,13H,16H,16aH-cyclopenta[15]annulen-1-yl}propyl acetate'	b'Proliferin'	HMDB02 52552	C27H40O5		
27	445.04	446.0603805	0.0029 805	Protone tion	b'(2-aminoethoxy){((2R,3S,4R,5R)-3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl)methoxy}(hydroxy)phosphoryloxy]phosphinic acid'	b'CDP-ethanolamine'	HMDB00 01564	C11H20N4O 11P2	C005 70	
0	96	446.0572574	0.0001 426	Protone tion	b'2-(6-hydroxy-3-oxo-3H-xanthen-9-yl)-5-(5-oxo-2-sulfanylideneimidazolidin-1-yl)benzoic acid'	b'Fluorescein thiohydantoin'	HMDB02 52361	C23H14N2O 6S		
27	446.30	446.3032245	0.0013 245	Redox	b'5,7,9,13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[10.8.0.0xc2xb2,\xc2\x81\xb9.0xc2\x81\xb4,\xc2\x81\xb8.0xc2\xb9xc2\xb3,\xc2\xb9xc2\x81\xb8]icosan]-18'-ene-4,14',16'-triol"	b'Cepagenin'	HMDB00 30913	C27H42O5		
		446.3032245	0.0013 245	Redox	b'16',19'-dihydroxy-5,7,9,13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[10.8.0.0xc2xb2,\xc2\x81\xb9.0xc2\x81\xb4,\xc2\x81\xb8.0xc2\xb9xc2\xb3,\xc2\xb9xc2\x81\xb8]icosane]-10'-one"	b'12-Ketoporrigenin'	HMDB00 31079	C27H42O5		
		446.3032245	0.0013 245	Redox	b'16',19'-dihydroxy-5,7,9,13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[10.8.0.0xc2xb2,\xc2\x81\xb9.0xc2\x81\xb4,\xc2\x81\xb8.0xc2\xb9xc2\xb3,\xc2\xb9xc2\x81\xb8]icosane]-15'-one"	b'Neoporrigenin B'	HMDB00 32680	C27H42O5		
1	19	446.3032245	0.0013 245	Redox	b'16',18'-dihydroxy-5,7,9,13'-tetramethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[10.7.0.0xc2xb2,\xc2\x81\xb9.0xc2\x81\xb4,\xc2\x81\xb8.0xc2\xb9xc2\xb3,\xc2\xb9xc2\x81\xb8]nonadecane]-19'-carbaldehyde"	b'Leontogenin'	HMDB00 33583	C27H42O5		
		446.3032245	0.0013 245	Redox	b'5,5-bis(hydroxymethyl)-7',9',13'-trimethyl-5'-oxaspiro[oxolane-2,6'-pentacyclo[10.8.0.0xc2xb2,\xc2\x81\xb9.0xc2\x81\xb4,\xc2\x81\xb8.0xc2\xb9xc2\xb3,\xc2\xb9xc2\x81\xb8]icosan]-18'-en-16'-ol"	b'Taccagenin'	HMDB00 34189	C27H42O5		
		446.3032245	0.0013 245	Redox	b'5-(hydroxymethyl)-7',9',13'-trimethyl-5'-oxaspiro[oxane-2,6'-pentacyclo[10.8.0.0xc2xb2,\xc2\x81\xb9.0xc2\x81\xb4,\xc2\x81\xb8.0xc2\xb9xc2\xb3,\xc2\xb9xc2\x81\xb8]icosan]-18'-ene-5,16'-diol"	b'Spirotaccagenin'	HMDB00 34424	C27H42O5		
		446.3032245	0.0013 245	Redox	b'(4R,6R)-6-[(1R,3aS,4E,7aR)-4-{2-[(1E,3S,5R)-3,5-dihydroxy-2-methylidenecyclohexylidene]ethylidene]-7a-methyl-octahydro-1H-inden-1-yl]-2,4-dihydroxy-2-methylheptan-3-one'	b'24-Oxo-1alpha,23,25-trihydroxyvitamin D3'	HMDB00 60129	C27H42O5		
27	447.05	448.0610216	0.0013 784	Protone tion	b'[(E)-[2-(1H-indol-3-yl)-1-{[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]sulfanyl}ethylidene]amino]oxy]sulfonic acid'	b'Glucobrassicin'	HMDB00 30243	C16H20N2O 9S2		
2	46	448.064176	0.0017	Protone	b'7,13,14-trihydroxy-6-[(3,4,5-trihydroxy-6-methylloxan-2-yl)oxy]-2,9-dioxatetracyclo[6.6.2.0xc2\x81\xb4,\xc2\xb9xc2\x81\xb6.0xc2\xb9xc2\xb9,\xc2\xb9xc2\x81\xb5]hexadeca-	b'Ellagic acid 2-rhamnoside'	HMDB03	C20H16O12		

			76	tion	1(15),4(16),5,7,11,13-hexaene-3,10-dione'		03358		
27 3	452.27 51	453.2855393	0.0026 393	Protone tion	b'(2-aminoethoxy)[(2R)-2-(hexadecanoyloxy)-3-hydroxypropoxy]phosphinic acid'	b'LysoPE(0:0/16:0)'	HMDB00 11473	C21H44NO7 P	
		453.2855393	0.0026 393	Protone tion	b'(2-aminoethoxy)[(2R)-3-(hexadecanoyloxy)-2-hydroxypropoxy]phosphinic acid'	b'LysoPE(16:0/0:0)'	HMDB00 11503	C21H44NO7 P	
		453.2855393	0.0026 393	Protone tion	b'(2-aminoethoxy)[3-(hexadecanoyloxy)-2-hydroxypropoxy]phosphinic acid'	b'[3-[2-Aminoethoxy(hydroxy)phosphoryl]oxy-2-hydroxypropyl] hexadecanoate'	HMDB02 56030	C21H44NO7 P	
		452.2774036	0.0023 036	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoate'	b'DG(2:0/20:4(6Z,8E,10E,14Z)-2OH(5S,12R)/0:0)'	HMDB02 96927	C25H40O7	
		452.2774036	0.0023 036	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoate'	b'DG(20:4(6Z,8E,10E,14Z)-2OH(5S,12R)/2:0/0:0)'	HMDB02 96928	C25H40O7	
		452.2774036	0.0023 036	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoate'	b'DG(2:0/0:0/20:4(6Z,8E,10E,14Z)-2OH(5S,12R))'	HMDB02 96929	C25H40O7	
		452.2774036	0.0023 036	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoate'	b'DG(20:4(6Z,8E,10E,14Z)-2OH(5S,12R)/0:0/2:0)'	HMDB02 96930	C25H40O7	
		452.2774036	0.0023 036	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoate'	b'DG(2:0/20:4(6E,8Z,11Z,13E)-2OH(5S,15S)/0:0)'	HMDB02 96999	C25H40O7	
		452.2774036	0.0023 036	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoate'	b'DG(20:4(6E,8Z,11Z,13E)-2OH(5S,15S)/2:0/0:0)'	HMDB02 97000	C25H40O7	
		452.2774036	0.0023 036	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoate'	b'DG(2:0/0:0/20:4(6E,8Z,11Z,13E)-2OH(5S,15S))'	HMDB02 97001	C25H40O7	
		452.2774036	0.0023 036	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoate'	b'DG(20:4(6E,8Z,11Z,13E)-2OH(5S,15S)/0:0/2:0)'	HMDB02 97002	C25H40O7	
		452.2774036	0.0023 036	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoate'	b'DG(2:0/20:4(8Z,11Z,14Z,17Z)-2OH(5S,6R)/0:0)'	HMDB02 97003	C25H40O7	

		452.2774036	0.0023 036	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxycosa-8,11,14,17-tetraenoate'	b'DG(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)2:0/0:0)'	HMDB02 97004	C25H40O7	
		452.2774036	0.0023 036	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxycosa-8,11,14,17-tetraenoate'	b'DG(2:0/0:0/20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R))'	HMDB02 97005	C25H40O7	
		452.2774036	0.0023 036	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxycosa-8,11,14,17-tetraenoate'	b'DG(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)0:0/2:0)'	HMDB02 97006	C25H40O7	
27 4	453.27 8	454.2831577	0.0026 423	Protona tion	b'2-(3,4-dimethoxyphenyl)-5-([2-(3,4-dimethoxyphenyl)ethyl](methyl)amino)-2-(propan-2-yl)pentanenitrile'	b'Verapamil'	HMDB00 01850	C27H38N2O 4	C071 88
27 5	460.28 03	461.2889714	0.0008 714	Protona tion	b'benzyl N-[3-methyl-1-((3-methyl-1-((1-oxopentan-2-yl)carbamoyl)butyl)carbamoyl)butyl]carbamate'	b'Z-Leu-Leu-Norvalinal'	HMDB02 44548	C25H39N3O 5	
		460.282489	0.0021 89	Redox	b"2-{5,7',9',13'-tetramethyl-16'-oxo-5',17'-dioxaspiro[oxane-2,6'- pentacyclo[10.7.0.0xc2xb2,\xc2\x81\xb9.0\xc2\x81\xb4,\xc2\x81\xb8.0\xc2\xb9\xc2\x81\xb4,\xc2\xb9\xc2\x81\xb8]nonadecane]-13'-yl}acetic acid"	b'2,3-Secoporigenin'	HMDB00 30909	C27H40O6	
		460.282489	0.0021 89	Redox	b'4-{5,9-dihydroxy-2,6,6,11,15-pentamethyl-12,17-dioxotetracyclo[8.7.0.0xc2xb2,\xc2\x81\xb7.0\xc2\xb9\xc2\xb9,\xc2\xb9\xc2\x81\xb5]heptadec-1(10)-en-14-yl}pentanoic acid'	b'Lucidenic acid N'	HMDB00 38352	C27H40O6	
		460.282489	0.0021 89	Redox	b'4-(2-hydroxy-5-oxo-2,5-dihydrofuran-3-yl)-1,11,15,15-tetramethyl-5-oxatetracyclo[8.8.0.0xc2xb2,\xc2\x81\xb7.0\xc2\xb9\xc2\xb9,\xc2\xb9\xc2\x81\xb6]octadecan-6-yl acetate'	b'Petrospongiolide m'	HMDB02 56357	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(2:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)0:0)'	HMDB02 97007	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)2:0/0:0)'	HMDB02 97008	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(2:0/0:0/22:6(5Z,7Z,10Z,13Z,16Z, 19Z)-OH(4))'	HMDB02 97009	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)0:0/2:0)'	HMDB02 97010	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(2:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)0:0)'	HMDB02 97011	C27H40O6	

		460.282489	0.0021 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/2:0/0:0)'	HMDB02 97012	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(2:0/0:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 97013	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/0:0/2:0)'	HMDB02 97014	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(2:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0)'	HMDB02 97015	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/2:0/0:0)'	HMDB02 97016	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(2:0/0:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 97017	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0/2:0)'	HMDB02 97018	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(2:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/0:0)'	HMDB02 97019	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/2:0/0:0)'	HMDB02 97020	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(2:0/0:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 97021	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/0:0/2:0)'	HMDB02 97022	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-1-(acetyloxy)-3-hydroxypropan-2-yl (4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoate'	b'DG(2:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/0:0)'	HMDB02 97027	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-2-(acetyloxy)-3-hydroxypropyl (4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoate'	b'DG(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/2:0/0:0)'	HMDB02 97028	C27H40O6	

		460.282489	0.0021 89	Redox	b'(2R)-3-(acetyloxy)-2-hydroxypropyl (4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoate'	b'DG(2:0/0:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 97029	C27H40O6	
		460.282489	0.0021 89	Redox	b'(2S)-3-(acetyloxy)-2-hydroxypropyl (4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoate'	b'DG(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/0:0/2:0)'	HMDB02 97030	C27H40O6	
27	462.06	463.074043	0.0023 43	Protona tion	b'(2S)-2-(9-{(2R,3R,4S,5R)-3,4-dihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl}-9H-purin-6-yl)amino)butanedioic acid'	b'Adenylsuccinic acid'	HMDB00 00536	C14H18N5O 11P	C037 94
6	39	463.0740434	0.0023 434	Protona tion	b'2-[(9-{3,4-dihydroxy-5-[(phosphonoxy)methyl]oxolan-2-yl}-9H-purin-6-yl)amino]butanedioic acid'	b'Adenylsuccinic acid'	HMDB02 48010	C14H18N5O 11P	
27	462.29	463.3062752	0.0023 752	Protona tion	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphinic acid'	b'LysoPE(P-18:1(9Z)/0:0)'	HMDB02 40599	C23H46NO6 P	
7	61	462.2981391	0.0020 391	Redox	b'4-{5,9,12-trihydroxy-2,6,6,11,15-pentamethyl-17-oxotetracyclo[8.7.0.0xc2xb2,\xc2\x81\xb7.0xc2xb9xc2xb9,\xc2xb9xc2\x81\xb5]heptadec-1(10)-en-14-yl}pentanoic acid'	b'Lucidenic acid M'	HMDB00 35973	C27H42O6	C100 29
27	463.06	464.0724331	0.0029 669	Protona tion	b'2-(hydroxymethyl)-6-{(7-methanesulfinyl-1-[(sulfonatoxy)imino]heptyl)sulfanyl}oxane-3,4,5-triol'	b'6-methylsulfinylhexyl glucosinolate'	HMDB03 04231	C14H26NO1 0S3	
27	463.30	463.3005987	0.0001 987	Redox	b'2-[(4,6-diamino-3-{[3-amino-6-(1-aminoethoxy)oxan-2-yl]oxy}-2-hydroxycyclohexyl)oxy]-5-methyl-4-(methyldiamino)oxane-3,5-diol'	b'Gentamicin C2'	HMDB02 52691	C20H41N5O 7	
9	04	463.3005987	0.0001 987	Redox	b'2-[(4,6-diamino-3-{[3-amino-6-(methyldiamino)methyl]oxan-2-yl}oxy)-2-hydroxycyclohexyl]oxy]-5-methyl-4-(methyldiamino)oxane-3,5-diol'	b'Micronomicin'	HMDB02 54707	C20H41N5O 7	
28	463.97	464.9851805	0.0012 805	Protona tion	b'[[hydroxy{[hydroxy{2-[(6-hydroxy-2-imino-3,9-dihydro-2H-purin-9-yl)methoxy]ethoxy}phosphoryl]oxy}phosphoryl]oxy]phosphonic acid'	b'Acyclovir triphosphate'	HMDB02 47992	C8H14N5O1 2P3	
0	61	463.9786995	0.0025 995	Redox	b'[[hydroxy{[hydroxy{[5-(5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-2,5-dihydrofuran-2-yl]methoxy}phosphoryl]oxy}phosphoryl]oxy]phosphonic acid'	b'Stavudine triphosphate'	HMDB02 58490	C10H15N2O 13P3	
28	464.31	465.3219253	0.0026 253	Protona tion	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(1Z)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'LysoPE(P-18:0/0:0)'	HMDB02 40598	C23H48NO6 P	
1	15	464.3137891	0.0022 891	Redox	b'14-(3,6-dihydroxy-6-methylheptan-2-yl)-4,5,11-trihydroxy-2,15-dimethyltetracyclo[8.7.0.0xc2xb2,\xc2\x81\xb7.0xc2xb9xc2xb9,\xc2xb9xc2\x81\xb5]heptadec-9-en-8-one'	b'Ecdysone'	HMDB02 51684	C27H44O6	

		464.3137891	0.0022 891	Redox	b'14-(2,3-dihydroxy-6-methylheptan-2-yl)-4,5,11-trihydroxy-2,15-dimethyltetracyclo[8.7.0.0 [^] {2,7}.0 [^] {11,15}]heptadec-9-en-8-one'	b'Ponasterone A'	HMDB02 56697	C27H44O6	
28 2	465.16 66	466.175831	0.0014 31	Protona tion	b'chloromethyl 14-[(ethoxycarbonyloxy]-17-hydroxy-2,15-dimethyl-5-oxotetracyclo[8.7.0.0 [^] {2,7}.0 [^] {11,15}]heptadeca-3,6-diene-14-carboxylate'	b'Loteprednol etabonate'	HMDB02 42700	C24H31ClO 7	
28 3	465.17 13	466.1813952	0.0022 952	Protona tion	b'3,3-bis[4-hydroxy-2-methyl-5-(propan-2-yl)phenyl]-3H-2,1lambda6-benzoxathiole-1,1-dione'	b'Thymol blue'	HMDB02 59055	C27H30O5S	
28 4	465.31 43	466.3195432	0.0025 568	Protona tion	b'3-(1H-indol-3-yl)-2-(octadeca-9,12-dienamido)propanoic acid'	b'N-Linoleoyl Tryptophan'	HMDB02 41986	C29H42N2O 3	
		466.321197	0.0009 03	Protona tion	b'[[2,15-dimethyl-14-(6-methylheptan-2-yl)tetracyclo[8.7.0.0 [^] {2,7}.0 [^] {11,15}]heptadec-7-en-5-yl]oxy]phosphonic acid'	b'Cholesterol phosphate'	HMDB02 50176	C27H47O4P	
28 5	471.06 83	472.0765801	0.0004 801	Protona tion	b'2-[[{[5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl phosphonato}oxy]phosphinato]oxy]ethyl]dimethylazaniumyl'	b'CDP-N-dimethylethanolamine'	HMDB03 04286	C13H22N4O 11P2	
		471.0689409	0.0006 409	Redox	b'5-chloro-2-methoxy-N-[2-(4-methoxy-3-[[[(methylcarbamothioyl)amino]sulfonyl]phenyl]ethyl]benzamide'	b'Clamikalant'	HMDB02 50313	C19H22ClN 3O5S2	
28 6	478.29 04	479.3011893	0.0029 893	Protona tion	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(0:0/18:1(11Z))'	HMDB00 11475	C23H46NO7 P	
		479.3011893	0.0029 893	Protona tion	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(0:0/18:1(9Z))'	HMDB00 11476	C23H46NO7 P	
		479.3011893	0.0029 893	Protona tion	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(18:1(11Z)/0:0)'	HMDB00 11505	C23H46NO7 P	
		479.3011893	0.0029 893	Protona tion	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(18:1(9Z)/0:0)'	HMDB00 11506	C23H46NO7 P	
		478.2930537	0.0026 537	Redox	b'9-ethoxy-3a,5a-dimethyl-1-(propan-2-yl)-6-[(3,4,5-trihydroxyoxan-2-yl)oxy]-2H,3H,3aH,4H,5H,5aH,6H,9H,10H,10aH-cyclohepta[c]indene-8-carbaldehyde'	b'Erinacine D'	HMDB00 31896	C27H42O7	
		478.2930537	0.0026 537	Redox	b'3-{1-hydroxy-2-[2-hydroxy-2-(hydroxymethyl)-4b,8,8,10a-tetramethyl-tetradecahydrophenanthren-1-yl]ethyl}-5-oxo-2,5-dihydrofuran-2-yl acetate'	b'25-Acetylvulgaroside'	HMDB00 41365	C27H42O7	

		478.2903683	3.17E-05	Redox	b'6-amino-2-[2-(2-amino-3-methylbutanamido)-4-methylpentanamido]-N-(4-nitrophenyl)hexanamide'	b'Valyl-leucyl-lysine 4-nitroanilide'	HMDB02 50805	C23H38N6O 5	
		478.2903683	3.17E-05	Redox	b'6-amino-2-[2-(2-amino-3-methylbutanamido)-3-methylpentanamido]-N-(4-nitrophenyl)hexanamide'	b'H-D-Val-Leu-Lys-pNA'	HMDB02 57385	C23H38N6O 5	
28	480.30	481.3151861	0.0014861	Protonation	b'N-{1-[3,4-dihydroxy-5-(hydroxymethyl)oxolan-2-yl]-2-oxo-1,2-dihydropyrimidin-4-yl}hexadecanamide'	b'Palmitoyl Ara-C'	HMDB02 56087	C25H43N3O 6	
7	59	480.3087038	0.0028038	Redox	b'(1R,2R,4S,5R,7R,11S,14S,15R)-4,5,11-trihydroxy-2,15-dimethyl-14-[(2R,3R)-2,3,6-trihydroxy-6-methylheptan-2-yl]tetracyclo[8.7.0.0 ² .0 ⁶]{11,15}heptadec-9-en-8-one'	b'Crustecdysone'	HMDB00 30180	C27H44O7	
		480.3087038	0.0028038	Redox	b'4,5,11-trihydroxy-2,15-dimethyl-14-(2,3,6-trihydroxy-6-methylheptan-2-yl)tetracyclo[8.7.0.0 ² .0 ⁶]{11,15}heptadec-9-en-8-one'	b'Ecdysterone'	HMDB02 42587	C27H44O7	
28	481.97	482.9845118	0.0001118	Protonation	b'([([([([2R,3S,4R,5R)-5-(4-amino-2-oxo-1,2-dihydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy}(hydroxy)phosphoryl)oxy](hydroxy)phosphoryl)oxy)phosphonic acid'	b'Cytidine triphosphate'	HMDB00 00082	C9H16N3O1 4P3	C000 63
8	66	482.9845118	0.0001118	Protonation	b'([([([([3,4-dihydroxy-5-(2-hydroxy-4-imino-1,4-dihydropyrimidin-1-yl)oxolan-2-yl)methoxy}(hydroxy)phosphoryl)oxy](hydroxy)phosphoryl)oxy)phosphonic acid'	b'Arabinofuranosylcytosine triphosphate'	HMDB02 48548	C9H16N3O1 4P3	
28	488.31	489.3162487	0.0028513	Protonation	b'2-[(4-amino-3-[[3-amino-6-(1-aminoethyl)-3,4-dihydro-2H-pyran-2-yl]oxy]-6-(ethylamino)-2-hydroxycyclohexyl]oxy]-5-methyl-4-(methylamino)oxane-3,5-diol'	b'Vertilmicin'	HMDB02 42753	C22H43N5O 7	
9	13	488.3137891	0.0024891	Redox	b'2-methyl-3-methylidene-6-{5,6,9-trihydroxy-2,6,15-trimethyl-17-oxotetracyclo[8.7.0.0 ² .xc2'xb2,xc2'xb81'xb7.0'xc2'xb9'xc2'xb9,xc2'xb9'xc2'xb81'xb5]heptadec-1(10)-en-14-yl}heptanoic acid'	b'Antcin K'	HMDB02 49891	C29H44O6	
29	492.98	493.9991602	0.0029602	Protonation	b'[(4-{([([2,3-dihydroxypropoxy)(hydroxy)phosphoryl]oxy)-2,3,5-trihydroxy-6-(phosphonoxy)cyclohexyl)oxy}phosphonic acid'	b'Phosphatidylinositol 4,5-diphosphate'	HMDB02 52943	C9H21O17P 3	
29	493.16	493.1631194	0.0014806	Redox	b'6-[2-[2-amino-3-(methylcarbamoyl)propanamido]-2-(4-hydroxyphenyl)acetamido]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid'	b'6-[2-[[2-Amino-4-(methylamino)-4-oxobutanoyl]amino]-2-(4-hydroxyphenyl)acetyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid'	HMDB02 48670	C21H27N5O 7S	

		493.1671422	0.0025 422	Redox	b'N-{6-[3-tert-butyl-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-2-methoxyphenyl]naphthalen-2-yl} methanesulfonamide'	b'Dasabuvir'	HMDB02 50872	C26H27N3O 5S	
		493.1631194	0.0014 806	Redox	b'6-[[[3-carbamoyl-2-(methylamino)propanoyl]carbamoyl](4-hydroxyphenyl)methyl]amino]-3,3-dimethyl-7-oxo-4-thia-1-azabicyclo[3.2.0]heptane-2-carboxylic acid'	b'L-Aspicillin trihydrate'	HMDB02 53876	C21H27N5O 7S	
29 2	500.27 51	501.2855393	0.0026 393	Protona tion	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoxyloxy]propoxy]phosphinic acid'	b'LysoPE(0:0/20:4(5Z,8Z,11Z,14Z))'	HMDB00 11487	C25H44NO7 P	
		501.2855393	0.0026 393	Protona tion	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoxyloxy]propoxy]phosphinic acid'	b'LysoPE(0:0/20:4(8Z,11Z,14Z,17Z))'	HMDB00 11488	C25H44NO7 P	
		501.2855393	0.0026 393	Protona tion	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoxyloxy]propoxy]phosphinic acid'	b'LysoPE(20:4(5Z,8Z,11Z,14Z)/0:0)'	HMDB00 11517	C25H44NO7 P	
		501.2855393	0.0026 393	Protona tion	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoxyloxy]propoxy]phosphinic acid'	b'LysoPE(20:4(8Z,11Z,14Z,17Z)/0:0)'	HMDB00 11518	C25H44NO7 P	
		501.2855398	0.0026 398	Protona tion	b'(2,3-dihydroxypropoxy)[2-(icosa-5,8,11,14-tetraenamido)ethoxy]phosphinic acid'	b'Glycerophospho-N-Arachidonoyl Ethanolamine'	HMDB02 52848	C25H44NO7 P	
29 3	504.07 52	505.0854017	0.0024 017	Protona tion	b'N-{3-[5-(2-aminopyrimidin-4-yl)-2-(propan-2-yl)-1,3-thiazol-4-yl]-2-fluorophenyl}-2,6-difluorobenzene-1-sulfonamide'	b'Desmethyl dabrafenib'	HMDB02 51052	C22H18F3N 5O2S2	
29 4	504.30 59	504.3087038	0.0028 038	Redox	b'4-{5-[(4,5-dihydroxy-6-methyloxan-2-yl)oxy]-11-hydroxy-2,15-dimethyltetracyclo[8.7.0.0'xc2'xb2,xc2'xb81'xb7.0'xc2'xb9'xc2'xb9,xc2'xb9'xc2'xb81'xb5]heptadecan-14-yl}-2,5-dihydrofuran-2-one'	b'Desglucocorolide'	HMDB00 33709	C29H44O7	
29 5	505.98 55	506.9957452	0.0024 452	Protona tion	b'([(((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'Adenosine triphosphate'	HMDB00 00538	C10H16N5O 13P3	C000 02
		506.9957452	0.0024 452	Protona tion	b'([(((2R,3S,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3-hydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'dGTP'	HMDB00 01440	C10H16N5O 13P3	C002 86
		506.9957452	0.0024 452	Protona tion	b'([(((2R,3S,5R)-5-(6-amino-2-hydroxy-9H-purin-9-yl)-3-hydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'2-hydroxy-dATP'	HMDB00 59593	C10H16N5O 13P3	C199 69
		506.9957452	0.0024 452	Protona tion	b'([(((5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy]phosphonic acid'	b'[(2R,5R)-5-(6-Aminopurin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy-	HMDB02 57997	C10H16N5O 13P3	

						hydroxyphosphoryl] phosphono hydrogen phosphate'			
29 6	506.28 54	506.2879683	0.0025 683	Redox	b'6-(1-hydroxy-1-{7,8,11-trihydroxy-2,15-dimethyl-3-oxotetracyclo[8.7.0.0\xc2\xb2,\xc2\x81\xb7.0\xc2\xb9\xc2\xb9,\xc2\xb9\xc2\x81\xb5]heptadecan-14-yl}ethyl)-3-(hydroxymethyl)-4-methyl-5,6-dihydro-2H-pyran-2-one'	b'(5alpha,6beta,14alpha,20R,22R)- 5,6,14,20,27-Pentahydroxy-1-oxowith- 24-enolide'	HMDB00 33198	C28H42O8	
29 7	506.32 21	507.3324895	0.0025 895	Protona tion	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(0:0/20:1(11Z))'	HMDB00 11482	C25H50NO7 P	
		507.3324895	0.0025 895	Protona tion	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'LysoPE(20:1(11Z)/0:0)'	HMDB00 11512	C25H50NO7 P	
29 8	506.98 71	506.9862293	0.0008 707	Redox	b'([(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonoxy)oxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]sulfonic acid'	b'Phosphoadenosine phosphosulfate'	HMDB00 01134	C10H15N5O 13P2S	C000 53
		506.9862307	0.0008 693	Redox	b'([(5-(6-amino-9H-purin-9-yl)-4-hydroxy-3-(phosphonoxy)oxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy]sulfonic acid' Sulfate(4-)-"	b"3'-phosphonato-5'-adenyl Sulfate(4-)-"	HMDB00 62646	C10H15N5O 13P2S	
		506.9862307	0.0008 693	Redox	b'([(5-(6-amino-9H-purin-9-yl)-4-hydroxy-2-[(phosphonoxy)methyl]oxolan-3-yl]oxy)(hydroxy)phosphoryl)oxy]sulfonic acid'	b'[(2R,3S,4R,5R)-5-(6-Aminopurin-9- yl)-4-hydroxy-2- (phosphonooxymethyl)oxolan-3-yl] sulfo hydrogen phosphate'	HMDB02 57827	C10H15N5O 13P2S	
29 9	508.33 75	509.3481395	0.0028 395	Protona tion	b'(2-aminoethoxy)[(2R)-3-hydroxy-2-(icosanoyloxy)propoxy]phosphinic acid'	b'LysoPE(0:0/20:0)'	HMDB00 11481	C25H52NO7 P	
		509.3481395	0.0028 395	Protona tion	b'(2-aminoethoxy)[(2R)-2-hydroxy-3-(icosanoyloxy)propoxy]phosphinic acid'	b'LysoPE(20:0/0:0)'	HMDB00 11511	C25H52NO7 P	
		509.3481395	0.0028 395	Protona tion	b'(2-[(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl phosphono]oxy]ethyl)trimethylazanium'	b'LysoPC(17:0/0:0)'	HMDB00 12108	C25H52NO7 P	C042 30
		508.3400039	0.0025 039	Redox	b'5,6,8,9-tetrahydroxy-14-{1-[6-hydroxy-4-(propan-2-yl)oxan-2-yl]ethyl}-2,15-dimethyltetracyclo[8.7.0.0\xc2\xb2,\xc2\x81\xb7.0\xc2\xb9\xc2\xb9,\xc2\xb9\xc2\x81\xb5]heptadecan- 12-one'	b'Contignasterol'	HMDB02 50439	C29H48O7	
30	515.03	516.0409558	0.0009	Protona	b'3-[2-(2,4-dinitrophenyl)ethenyl]-8-oxo-7-[2-(thiophen-2-yl)acetamido]-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylic acid'	b'Nitrocefin'	HMDB02	C21H16N4O	

0	41		442	tion			59569	8S2	
30	521.98	522.9906598	0.0022 598	Protone tion	b'(((((((2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)phosphonic acid'	b'Guanosine triphosphate'	HMDB00 01273	C10H16N5O 14P3	C000 44
		522.9906598	0.0022 598	Protone tion	b'(((((((3S)-5-(2-amino-6,8-dioxo-6,7,8,9-tetrahydro-3H-purin-9-yl)-3-hydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)phosphonic acid'	b'8-Oxo-dGTP'	HMDB00 11615	C10H16N5O 14P3	
		522.9906612	0.0022 612	Protone tion	b'(((((([5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)oxy)phosphonic acid'	b'((([2S,3R,4R,5R)-5-(2-Amino-6-oxo-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy-hydroxyphosphoryl]phosphono hydrogen phosphate'	HMDB02 47873	C10H16N5O 14P3	
30	522.28 09	523.2910191	0.0023 191	Protone tion	b'2-amino-3-({hydroxy[2-hydroxy-3-(octadec-9-enoyloxy)propoxy]phosphoryl}oxy)propanoic acid'	b'1-Oleoylglycerophosphoserine'	HMDB00 61694	C24H46NO9 P	
		523.2910186	0.0023 186	Protone tion	b'(2S)-2-amino-3-({hydroxy[(2R)-2-hydroxy-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'LysoPS(18:1(9Z)0:0)'	HMDB02 40603	C24H46NO9 P	
		522.2828829	0.0019 829	Redox	b'15-[1-(4,5-dihydroxy-4,5-dimethyl-6-oxooxan-2-yl)-1-hydroxyethyl]-5,6-dihydroxy-2,16-dimethyl-8-oxapentacyclo[9.7.0.0\xc2\xb2,\xc2\xb81\b7.0\xc2\xb81\b7,\xc2\xb81\b9.0\xc2\xb9\xc2\xb2,\xc2\xb9\xc2\xb6]octadecan-3-one'	b'Physangulide'	HMDB00 37381	C28H42O9	
30	524.27 59	525.2855393	0.0018 393	Protone tion	b'(2-aminoethoxy)((2R)-2-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-3-hydroxypropoxy]phosphinic acid'	b'LysoPE(0:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB00 11496	C27H44NO7 P	
		525.2855393	0.0018 393	Protone tion	b'(2-aminoethoxy)((2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-hydroxypropoxy]phosphinic acid'	b'LysoPE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)0:0)'	HMDB00 11526	C27H44NO7 P	
		524.2765481	0.0006 481	Redox	b'methyl N-{2-[(3-chlorophenyl)(1-{[2-(methylamino)-3-(oxan-3-yl)propyl]carbonyl}piperidin-3-yl)methoxy]ethyl} carbamate'	b'Methyl (2-((R)-(3-chlorophenyl)((R)-1-(((S)-2-(methylamino)-3-((R)-tetrahydro-2H-pyran-3-yl)propyl)carbonyl)piperidin-3-yl)methoxy)ethyl)carbamate'	HMDB02 47675	C26H41ClN 4O5	
30	525.30 4	526.3056245	0.0026 755	Protone tion	b'1-(butan-2-yl)-N-[(4,6-dimethyl-2-oxo-1,2-dihydropyridin-3-yl)methyl]-3-methyl-6-[6-(piperazin-1-yl)pyridin-3-yl]-1H-indole-4-carboxamide'	b'(S)-1-(Sec-Butyl)-N-((4,6-dimethyl-2-oxo-1,2-dihydropyridin-3-yl)methyl)-3-	HMDB02 52950	C31H38N6O 2	

						methyl-6-(6-(piperazin-1-yl)pyridin-3-yl)-1H-indole-4-carboxamide'				
305	535.0341	536.0444557	0.0025557	Protonation	b'(((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(((2R,3R,4S,5R)-3,4,5-trihydroxyoxan-2-yl)oxy))phosphinic acid'	b'UDP-D-Xylose'	HMDB00101018	C14H22N2O16P2	C00190	
		536.0444557	0.0025557	Protonation	b'(((2S,3R,4R)-3,4-dihydroxy-4-(hydroxymethyl)oxolan-2-yl)oxy)(hydroxy)phosphoryl)oxy)(((2R,3S,4R,5R)-3,4-dihydroxy-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-2-yl)methoxy))phosphinic acid'	b'UDP-D-apiose'	HMDB0012301	C14H22N2O16P2	C01623	
		536.0444557	0.0025557	Protonation	b'(((2R,3S,4R,5R)-3,4-dihydroxy-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-2-yl)methoxy)((hydroxy((2R,3R,4S,5S)-3,4,5-trihydroxyoxan-2-yl)oxy))phosphoryl)oxy))phosphinic acid'	b'UDP-L-arabinose'	HMDB0012303	C14H22N2O16P2	C00935	
306	537.1906	538.1991533	0.0007533	Protonation	b'3,8,22,27,29-pentamethyl-11,15,19-trioxaoctacyclo[14.14.1.0'xc2'xb2,\xc2'xb9'xc2'xb4.0'xc2'xb4,\xc2'xb9'xc2'xb2.0'xc2'xb5,\xc2'xb9'xc2'xb8,\xc2'xb2'xc2'xb6.0'xc2'xb2'\xc2'xb0,\xc2'xb2'xc2'xb1'\xc2'xb5.0'xc2'xb2'xc2'xb1'\xc2'xb7,\xc2'xb3'xc2'xb9]hentriaconta-2,4(12),5,7,9,13,18(26),20,22,24,29-undecaene-6,16,17,24-tetrol'	b'Asticlorin A'	HMDB0030133		C33H30O7	
307	540.0507	541.0611098	0.0026098	Protonation	b'3,4,8,10,14,15-hexahydroxy-24-imino-7,9,11,25,26-pentaosa-1,17,19,22-tetraaza-8lambda5,10lambda5-diphosphapentacyclo[18.3.1.1'^{2,5}.1'^{13,16}.0'^{17,21}]hexacos-18,20,22-triene-8,10-dione'	b'Cyclic ADP-ribose'	HMDB0249529		C15H21N5O13P2	
		541.0614413	0.0029413	Protonation	b'3-[2-(2-chloro-4-([3-(2,6-dichlorophenyl)-5-(propan-2-yl)-1,2-oxazol-4-yl]methoxy)phenyl)ethenyl]benzoic acid'	b'3-[2-[2-Chloro-4-([3-(2,6-dichlorophenyl)-5-propan-2-yl-4-isoxazolyl]methoxy)phenyl]ethenyl]benzoic acid'	HMDB0249972		C28H22Cl3NO4	
308	540.2829	541.2920674	0.0013674	Protonation	b'(((2S,4R,5S,6S)-6-(((2S,3R,4E)-2-amino-3-hydroxyoctadec-4-en-1-yl)oxy)-3,4,5-trihydroxyoxan-2-yl)methoxy)sulfonic acid'	b'Psychosine sulfate'	HMDB0013046		C24H47NO10S	
		541.2920679	0.0013679	Protonation	b'[2-((2-amino-3-hydroxyoctadec-4-en-1-yl)oxy)-3,5-dihydroxy-6-(hydroxymethyl)oxan-4-yl]oxidanesulfonic acid'	b'Lysosulfatide'	HMDB0254273		C24H47NO10S	
309	563.03	564.0404684	0.0026684	Protonation	b'[5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl {[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl phosphonato]oxy}phosphonate'	b'UDP-alpha-D-galactose'	HMDB0304527		C15H22N2O17P2	
310	563.0652	564.0757558	0.0027558	Protonation	b'[[hydroxy(((2R,3S,5R)-3-hydroxy-5-(5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)oxolan-2-yl)methoxy))phosphoryl]oxy)(((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy))phosphinic acid'	b'dTDP-D-glucose'	HMDB0001328		C16H26N2O16P2	C00842
		564.0757558	0.0027	Protonation	b'[[hydroxy(((2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl)oxy))phosphoryl]oxy)(((2R,3S,5R)-3-hydroxy-5-(5-methyl-2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-	b'dTDP-D-galactose'	HMDB00		C16H26N2O	C020

			558	tion	yl)oxolan-2-yl]methoxy})phosphinic acid'		06876	16P2	97
		564.0757568	0.0027 568	Protona tion	b' {[hydroxy({[3-hydroxy-5-(4-hydroxy-5-methyl-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy})phosphoryl]oxy} ({[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphinic acid'	b'DTDP- α -D-glucose(2-)'	HMDB00 62805	C16H26N2O 16P2	
		564.07171	0.0012 9	Protona tion	b'2- {[(1-carboxy-5- {[(4-iodophenyl)carbamoyl]amino} pentyl)carbamoyl]amino} pentanedioic acid'	b'L-Glutamic acid, N-((((1S)-1-carboxy-5-((((4-iodophenyl)amino)carbonyl)amino)pentyl)amino)carbonyl)-'	HMDB02 50018	C19H25IN4 O8	
31	565.04 5	566.0550204	0.0022 204	Protona tion	b'([(((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)([((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphinic acid'	b'Uridine diphosphate glucose'	HMDB00 00286	C15H24N2O 17P2	C000 29
		566.0550204	0.0022 204	Protona tion	b'([(((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)([((2R,3R,4S,5R,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphinic acid'	b'Uridine diphosphategalactose'	HMDB00 00302	C15H24N2O 17P2	C000 52
		566.0550204	0.0022 204	Protona tion	b'([(([3,4-dihydroxy-5-(4-hydroxy-2-oxo-1,2-dihydropyrimidin-1-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)([([3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphinic acid'	b"Glucose-uridine-C1,5'-diphosphate"	HMDB02 59387	C15H24N2O 17P2	
31	565.13	566.1424263	0.0006 263	Protona tion	b'2- {[3,5-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl]oxy}-4,5-dihydroxy-6-methylloxan-3-yl 2-methoxybenzoate'	b'Gladioside C2'	HMDB00 36254	C29H26O12	
2	4	566.1424263	0.0006 263	Protona tion	b'2- {[3,5-dihydroxy-2-(4-hydroxyphenyl)-4-oxo-4H-chromen-7-yl]oxy}-3,5-dihydroxy-6-methylloxan-4-yl 2-methoxybenzoate'	b'Gladioside C1'	HMDB00 36255	C29H26O12	
31	568.27 3	569.2849486	0.0021 486	Protona tion	b'2-[2-(2-[2-amino-3-(4-hydroxyphenyl)propanamido]propanamido)acetamido]-3-phenylpropanamido]-4-methylpentanoic acid'	b'Leuphasyl'	HMDB02 47171	C29H39N5O 7	
31	571.28	572.2961635	0.0020 635	Protona tion	b'[(2R)-3-(hexadecanoyloxy)-2-hydroxypropoxy]([((1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'LysoPI(16:0/0:0)'	HMDB00 61695	C25H49O12 P	
4	63	571.2866799	0.0003 799	Redox	b'(2S)-2- [((2S)-1- [((2S)-2- [(2S)-2-amino-5-carbamimidamidopentanamido]-3-(1H-imidazol-4-yl)propanoyl]pyrrolidin-2-yl]formamido)-3-(4-hydroxyphenyl)propanoic acid'	b'Kinetensin 4-7'	HMDB00 12986	C26H37N9O 6	
31	573.01 5	574.02284	0.0005 6	Protona tion	b'N- {[5-(2-chloro-6- {[(3-iodophenyl)methyl]amino}-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl](hydroxy)methyl}-N-methylformamide'	b'N- [((2S,3S,4R,5R)-5-[2-Chloro-6- [(3-iodophenyl)methylamino]purin-9-yl]-3,4-dihydroxyoxolan-2-yl]-	HMDB02 57746	C19H20ClIN 6O5	

						hydroxymethyl]-N-methylformamide'			
31	579.02	580.0342849	0.0015 849	Protone	b'(2S,3S,4S,5R,6R)-6-(((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryloxy)(hydroxy)phosphoryloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'Uridine diphosphate glucuronic acid'	HMDB00 00935	C15H22N2O 18P2	C001 67
		580.0342849	0.0015 849	Protone	b'(2S,3R,4S,5R,6R)-6-(((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryloxy)(hydroxy)phosphoryloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'UDP-D-galacturonic acid'	HMDB00 12302	C15H22N2O 18P2	C006 17
		580.0342849	0.0015 849	Protone	b'(2R,3S,4S,5R,6R)-6-(((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryloxy)(hydroxy)phosphoryloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'UDP-L-iduronate'	HMDB00 12304	C15H22N2O 18P2	C023 30
		580.0342859	0.0015 859	Protone	b'6-(((5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryloxy)(hydroxy)phosphoryloxy)-3,4,5-trihydroxyoxane-2-carboxylic acid'	b'(2R,3R,4R,5S,6R)-6-[[[(2S,3R,4R,5R)-5-(2,4-Dioxypyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxyhydroxyphosphoryloxyhydroxyphosphoryloxy]-3,4,5-trihydroxyoxane-2-carboxylic acid'	HMDB02 60120	C15H22N2O 18P2	
		580.0342859	0.0015 859	Protone	b'([5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-4-hydroxy-3-[(3,4,5,6-tetrahydroxy-2-oxohexanoyloxy)oxolan-2-yl)methoxy](hydroxy)phosphoryloxy]phosphonic acid'	b'[(2R,3S,4R,5R)-5-(2,4-Dioxypyrimidin-1-yl)-4-hydroxy-2-[[hydroxy(phosphonoxy)phosphoryloxy]oxymethyl]oxolan-3-yl] (3S,4R,5S)-3,4,5,6-tetrahydroxy-2-oxohexanoate'	HMDB02 60220	C15H22N2O 18P2	
31	581.17	582.1889826	0.0012 826	Protone	b'2-[6-(2,4-dihydroxybenzoyl)-5-(2,4-dihydroxyphenyl)-3-methylcyclohex-2-en-1-yl]-5-[(E)-(2,4-dihydroxyphenyl)ethenyl]benzene-1,3-diol'	b'Kuwanon Y'	HMDB00 33296	C34H30O9	
		582.1849598	0.0027 402	Protone		b'Glucuronidated Sn-38'	HMDB02 52796	C29H30N2O 11	
31	581.30	582.3125603	0.0001 397	Protone	b'2-([1-(2-([1-(2-amino-3-methylbutanoyl)pyrrolidin-2-yl]formamido)-3-carboxypropanoyl)pyrrolidin-2-yl]formamido)-5-[(diaminomethylidene)amino]pentanoic acid'	b'Val-Pro-Asp-Pro-Arg'	HMDB02 44421	C25H42N8O 8	
31	588.07	589.0822382	0.0018	Protone	b'([[(2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-1H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy](hydroxy)phosphoryloxy]([[(3S,4R,5S,6S)-3,4,5-trihydroxy-6-methyloxan-2-	b'GDP-L-fucose'	HMDB00	C16H25N5O	C003

9	26		382	tion	y]oxy})phosphinic acid'		01095	15P2	25
		589.0822382	0.0018 382	Protona tion	b'(((2R,3S,4R,5R)-5-(2-amino-6-oxo-6,9-dihydro-3H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(((2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-methyloxan-2-yl]oxy})phosphinic acid'	b'GDP-D-Rhamnose'	HMDB00 01499	C16H25N5O 15P2	C031 17
		589.0822382	0.0018 382	Protona tion	b'(((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(((2R,3S,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphinic acid'	b'ADP-Mannose'	HMDB00 06369	C16H25N5O 15P2	C061 92
		589.0822382	0.0018 382	Protona tion	b'(((2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(((2R,3R,4S,5S,6R)-3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphinic acid'	b'ADP-glucose'	HMDB00 06557	C16H25N5O 15P2	C004 98
		589.0822382	0.0018 382	Protona tion	b'([3,4-dihydroxy-5-(6-hydroxy-2-imino-3,9-dihydro-2H-purin-9-yl)oxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy]((3,4,5-trihydroxy-6-methyloxan-2-yl)oxy]phosphinic acid'	b'GDP-fucose'	HMDB02 52660	C16H25N5O 15P2	
32	599.31	600.3274637	0.0028 637	Protona tion	b'[(2R)-3-hydroxy-2-(octadecanoyloxy)propoxy]([1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'LysoPI(0:0/18:0)'	HMDB00 61704	C27H53O12 P	
		600.3274637	0.0028 637	Protona tion	b'[(2R)-2-hydroxy-3-(octadecanoyloxy)propoxy]([1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'LysoPI(18:0/0:0)'	HMDB02 40261	C27H53O12 P	
32	605.06	605.0670175	0.0006 825	Redox	b'[5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methyl [3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl phosphonato]oxy} phosphonate'	b'UDP-N-acetyl-alpha-D-glucosamine'	HMDB03 04526	C17H25N3O 17P2	
32	606.07	607.0815695	0.0023 695	Protona tion	b'(((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy)(((2R,3R,4R,5S,6R)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphinic acid'	b'Uridine diphosphate-N-acetylglucosamine'	HMDB00 00290	C17H27N3O 17P2	C000 43
		607.0815695	0.0023 695	Protona tion	b'([5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy]([3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphinic acid'	b'Uridine diphosphate-N-acetyl galactosamine'	HMDB00 00304	C17H27N3O 17P2	
		607.0815695	0.0023 695	Protona tion	b'([((2S,3R,4S,5S)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy]([3R,4S,5R,6S)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphinic acid'	b'UDP-N-acetyl-D-mannosamine'	HMDB00 13112	C17H27N3O 17P2	C011 70
		607.0815695	0.0023 695	Protona tion	b'([(((2R,3S,4R,5R)-5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl)methoxy)(hydroxy)phosphoryl)oxy]([2R,3R,4R,5R,6R)-3-acetamido-4,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy})phosphinic acid'	b'UDP-N-acetyl-alpha-D-galactosamine'	HMDB00 60522	C17H27N3O 17P2	
32	611.14	611.1400806	0.0010 194	Redox	b'3-(((2S,3R,4S,5R,6R)-3,5-dihydroxy-6-(hydroxymethyl)-4-(((2E)-3-(4-hydroxyphenyl)prop-2-enoyl)oxy) oxan-2-yl]oxy)-5,7-dihydroxy-2-(3,4,5-trihydroxyphenyl)-1'x'ce'x'bb'x'e2'x'81'x'b4'-chromen-1-ylum'	b'Delphinidin 3-(3"-p-coumaroylglucoside)"	HMDB00 30099	C30H27O14	
		611.1400806	0.0010	Redox	b'5,7-dihydroxy-3-([3,4,5-trihydroxy-6-(((2E)-3-(4-hydroxyphenyl)prop-2-enoyl]oxy) methyl)oxan-2-yl]oxy)-2-(3,4,5-trihydroxyphenyl)-1'x'ce'x'bb'x'e2'x'81'x'b4'-chromen-1-ylum'	b'Delphinidin 3-(6-p-	HMDB00	C30H27O14	

			194			coumaroylgalactoside'	37089		
		611.139532	0.0015 68	Redox	b'[3-(3,4-dihydroxyphenyl)-1-hydroxyprop-2-en-1-ylidene]([[(3S,6S)-6-{[2-(3,4-dihydroxyphenyl)-7-hydroxy-5-oxo-5H-chromen-3-yl]oxy}-3,4,5-trihydroxyoxan-2-yl]methyl])oxidanium'	b'Cyanidin 3-(caffeoylglucoside)'	HMDB03 03636	C30H27O14	
32 4	619.28 48	620.2918249	0.0007 751	Protone tion	b'2-[2-[5-({amino(methylcarbamoyl)amino)methylidene}amino)-2-(2-acetamidopropanamido)-N-methylpentanamido]-3-phenylpropanamido]butanedioic acid'	b'Tetrapeptide'	HMDB02 58927	C27H40N8O 9	
32 5	619.33 9	619.3369842	0.0020 158	Redox	b'2-(2-[2-[(azepane-1-carbonyl)amino]-4-methylpentanamido]-3-(1-methyl-1H-indol-3-yl)propanamido)-3-(4-hydroxyphenyl)propanoic acid'	b'N-((Hexahydro-1-azepinyl)carbonyl)- leucyl(1-methyl)-tryptophyl-tryptophan'	HMDB02 56177	C34H45N5O 6	
32 6	640.04 62	640.04416	0.0020 4	Redox	b'7-[(4,5-dihydroxy-3-iodo-6-methyloxan-2-yl)oxy]-6,9,11-trihydroxy-9-(2-hydroxyacetyl)-5,7,8,9,10,12-hexahydro-1,4-dione'	b'Annamycin'	HMDB02 48448	C26H25O11	
32 7	644.49 87	644.5015899	0.0028 899	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(17:0/20:4(6E,8Z,11Z,14Z)+=O(5) /0:0)'	HMDB02 95699	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)+=O(5)/17:0 /0:0)'	HMDB02 95700	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(17:0/0:0/20:4(6E,8Z,11Z,14Z)+= O(5))'	HMDB02 95701	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)+=O(5)/0:0/ 17:0)'	HMDB02 95702	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(17:0/20:4(5Z,8Z,11Z,13E)+=O(1 5)/0:0)'	HMDB02 95703	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15)/17: 0/0:0)'	HMDB02 95704	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(17:0/0:0/20:4(5Z,8Z,11Z,13E)+= O(15))'	HMDB02 95705	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15)/0:0/ /17:0)'	HMDB02 95706	C40H68O6	
		644.5015899	0.0028	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(17:0/20:5(5Z,8Z,11Z,14Z,16E)-	HMDB02	C40H68O6	

			899				OH(18R)/0:0)	95727		
644.5015899	0.0028 899	Redox		b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'		b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/17:0/0:0)	HMDB02 95728	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'		b'DG(17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 95729	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'		b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/0:0/17:0)	HMDB02 95730	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'		b'DG(17:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/0:0)	HMDB02 95731	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'		b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/17:0/0:0)	HMDB02 95732	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'		b'DG(17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	HMDB02 95733	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'		b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/0:0/17:0)	HMDB02 95734	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'		b'DG(17:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/0:0)	HMDB02 95735	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'		b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/17:0/0:0)	HMDB02 95736	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'		b'DG(17:0/0:0/20:5(5Z,8Z,10E,14Z,17Z)-OH(12))'	HMDB02 95737	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'		b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/0:0/17:0)	HMDB02 95738	C40H68O6		
644.5015899	0.0028 899	Redox		b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'		b'DG(17:0/20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/0:0)	HMDB02 95739	C40H68O6		
644.5015899	0.0028	Redox		b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'		b'DG(20:5(6E,8Z,11Z,14Z,17Z)-	HMDB02	C40H68O6		

			899				OH(5)/17:0/0:0)	95740		
644.5015899	0.0028 899	Redox		b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(17:0/0:0/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 95741	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/0:0/17:0)	HMDB02 95742	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(a-17:0/20:4(6E,8Z,11Z,14Z)+=O(5)/0:0)	HMDB02 97779	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)+=O(5)/a-17:0/0:0)	HMDB02 97780	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(a-17:0/0:0/20:4(6E,8Z,11Z,14Z)+=O(5))'	HMDB02 97781	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(a-17:0/20:4(5Z,8Z,11Z,13E)+=O(15)/0:0)	HMDB02 97782	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15)/a-17:0/0:0)	HMDB02 97783	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(a-17:0/0:0/20:4(5Z,8Z,11Z,13E)+=O(15))'	HMDB02 97784	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15)/0:0/a-17:0)	HMDB02 97785	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(a-17:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/0:0)	HMDB02 97806	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/a-17:0/0:0)	HMDB02 97807	C40H68O6			
644.5015899	0.0028 899	Redox		b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(a-17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 97808	C40H68O6			

		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)0:0/a-17:0)'	HMDB02 97809	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(a-17:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18)0:0)'	HMDB02 97810	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/a-17:0/0:0)'	HMDB02 97811	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(a- 17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18))'	HMDB02 97812	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)0:0/a-17:0)'	HMDB02 97813	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(a-17:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12)0:0)'	HMDB02 97814	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/a-17:0/0:0)'	HMDB02 97815	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(a- 17:0/0:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12))'	HMDB02 97816	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)0:0/a-17:0)'	HMDB02 97817	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(a-17:0/20:5(6E,8Z,11Z,14Z,17Z)- OH(5)0:0)'	HMDB02 97818	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/a-17:0/0:0)'	HMDB02 97819	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(a- 17:0/0:0/20:5(6E,8Z,11Z,14Z,17Z)-	HMDB02 97820	C40H68O6	

					OH(5))'			
644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)- OH(5))0:0/a-17:0)'	HMDB02 97821	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(i- 17:0/20:4(6E,8Z,11Z,14Z)+=O(5))0:0)'	HMDB02 99440	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)+=O(5))i- 17:0/0:0)'	HMDB02 99441	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(i- 17:0/0:0/20:4(6E,8Z,11Z,14Z)+=O(5))'	HMDB02 99442	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoate'	b'DG(20:4(6E,8Z,11Z,14Z)+=O(5))0:0/i -17:0)'	HMDB02 99443	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(i- 17:0/20:4(5Z,8Z,11Z,13E)+=O(15))0:0)'	HMDB02 99444	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15))i- 17:0/0:0)'	HMDB02 99445	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(i- 17:0/0:0/20:4(5Z,8Z,11Z,13E)+=O(15))'	HMDB02 99446	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoate'	b'DG(20:4(5Z,8Z,11Z,13E)+=O(15))0:0 /i-17:0)'	HMDB02 99447	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(i-17:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R))0:0)'	HMDB02 99468	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R))i-17:0/0:0)'	HMDB02 99469	C40H68O6		
644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(i- 17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R))'	HMDB02 99470	C40H68O6		

		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)0:0/i-17:0)'	HMDB02 99471	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(i-17:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18)0:0)'	HMDB02 99472	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)i-17:0/0:0)'	HMDB02 99473	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(i- 17:0/0:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18))'	HMDB02 99474	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoate'	b'DG(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)0:0/i-17:0)'	HMDB02 99475	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(i-17:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12)0:0)'	HMDB02 99476	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)i-17:0/0:0)'	HMDB02 99477	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(i- 17:0/0:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12))'	HMDB02 99478	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoate'	b'DG(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)0:0/i-17:0)'	HMDB02 99479	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(i-17:0/20:5(6E,8Z,11Z,14Z,17Z)- OH(5)0:0)'	HMDB02 99480	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)i-17:0/0:0)'	HMDB02 99481	C40H68O6	
		644.5015899	0.0028 899	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(i- 17:0/0:0/20:5(6E,8Z,11Z,14Z,17Z)- OH(5))'	HMDB02 99482	C40H68O6	

						OH(5)'			
		644.5015899	0.0028 899	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoate'	b'DG(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/0:0/i-17:0)	HMDB02 99483	C40H68O6	
32 8	647.36 82	647.3682843	8.43E- 05	Redox	b'(Z)-N-{1-[(8Z,11E,13E)-10-(butan-2-yl)-8,11-dihydroxy-16-methoxy-2-oxa-6,9,12-triazatricyclo[13.3.1.0 ^{xc2xb3} , ^{xe2xb81xb7}]nonadeca-1(18),8,11,13,15(19),16-hexaen-6-yl]-4-methyl-1-oxopentan-2-yl}-2-(methylamino)-3-phenylpropimide acid'	b'Nummularine A'	HMDB00 29336	C36H49N5O 6	C100 11
32 9	647.46 37	648.4730062	0.0015 062	Protone tion	b'[(2R)-2,3-bis(hexadecanoyloxy)propoxy]phosphonic acid'	b'PA(16:0/16:0)'	HMDB00 00674	C35H69O8P	C004 16
		648.4730062	0.0015 062	Protone tion	b'[(2R)-3-(decanoyloxy)-2-(docosanoyloxy)propoxy]phosphonic acid'	b'PA(10:0/22:0)'	HMDB01 14777	C35H69O8P	
		648.4730062	0.0015 062	Protone tion	b'[(2R)-3-(octadecanoyloxy)-2-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/14:0)'	HMDB01 14873	C35H69O8P	
		648.4730062	0.0015 062	Protone tion	b'[(2R)-2-(dodecanoyloxy)-3-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:0/12:0)'	HMDB01 15059	C35H69O8P	
		648.4730062	0.0015 062	Protone tion	b'[(2R)-2-(decanoyloxy)-3-(docosanoyloxy)propoxy]phosphonic acid'	b'PA(22:0/10:0)'	HMDB01 15237	C35H69O8P	
		648.4730062	0.0015 062	Protone tion	b'[(2R)-3-(decanoyloxy)-2-[(20-methylhenicosanoyl)oxy]propoxy]phosphonic acid'	b'PA(10:0/i-22:0)'	HMDB01 15621	C35H69O8P	
		648.4730062	0.0015 062	Protone tion	b'[(2R)-3-(icosanoyloxy)-2-[(10-methylundecanoyl)oxy]propoxy]phosphonic acid'	b'PA(20:0/i-12:0)'	HMDB01 15634	C35H69O8P	
		648.4730062	0.0015 062	Protone tion	b'[(2R)-2-[(22-methyltricosanoyl)oxy]-3-(octanoyloxy)propoxy]phosphonic acid'	b'PA(8:0/i-24:0)'	HMDB01 15696	C35H69O8P	
		648.4730062	0.0015 062	Protone tion	b'[(2R)-3-[(10-methyldodecanoyl)oxy]-2-[(17-methyloctadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(a-13:0/i-19:0)'	HMDB01 15710	C35H69O8P	
		648.4730062	0.0015 062	Protone tion	b'[(2R)-2-[(18-methylnonadecanoyl)oxy]-3-[(10-methylundecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-12:0/i-20:0)'	HMDB01 15789	C35H69O8P	
		648.4730062	0.0015	Protone	b'[(2R)-3-[(11-methyldodecanoyl)oxy]-2-[(17-methyloctadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-13:0/i-19:0)'	HMDB01	C35H69O8P	

			062	tion			15806		
		648.4730062	0.0015 062	Protona tion	b'[(2R)-2-(dodecanoyloxy)-3-[(18-methylnonadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-20:0/12:0)'	HMDB01 15831	C35H69O8P	
		648.4730062	0.0015 062	Protona tion	b'[(2R)-3-[(18-methylnonadecanoyl)oxy]-2-[(10-methylundecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-20:0/i-12:0)'	HMDB01 15848	C35H69O8P	
		648.4730062	0.0015 062	Protona tion	b'[(2R)-2-(decanoyloxy)-3-[(20-methylhenicosanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-22:0/10:0)'	HMDB01 15890	C35H69O8P	
		648.4730062	0.0015 062	Protona tion	b'[(2R)-3-[(22-methyltricosanoyl)oxy]-2-(octanoyloxy)propoxy]phosphonic acid'	b'PA(i-24:0/8:0)'	HMDB01 15932	C35H69O8P	
		648.4730062	0.0015 062	Protona tion	b'[2,3-bis(hexadecanoyloxy)propoxy]phosphonic acid'	b'2,3-Bis(palmitoyloxy)propyl dihydrogen phosphate'	HMDB02 44852	C35H69O8P	
33 0	648.37 41	648.3720919	0.0020 081	Redox	b'2- {[(6E,10E)-2-hydroxy-2,6,10,14-tetramethyl-14- {[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy} hexadeca-6,10,15-trien-3-yl]oxy}-6-(hydroxymethyl)oxane-3,4,5-triol'	b'Lyciumoside III'	HMDB00 39553	C32H56O13	
33 1	670.51 44	670.51724	0.0028 4	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(17:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/0:0)'	HMDB02 95759	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/17:0/0:0)'	HMDB02 95760	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(17:0/0:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 95761	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/0:0/17:0)'	HMDB02 95762	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(17:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-Z)-OH(7)/0:0)'	HMDB02 95763	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/17:0/0:0)'	HMDB02 95764	C42H70O6	
		670.51724	0.0028	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(17:0/0:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/17:0/0:0)'	HMDB02	C42H70O6	

			4				,19Z)-OH(7))'	95765		
670.51724	0.0028 4	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'		b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/0:0/17:0))'	HMDB02 95766	C42H70O6			
670.51724	0.0028 4	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'		b'DG(17:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0))'	HMDB02 95767	C42H70O6			
670.51724	0.0028 4	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'		b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/17:0/0:0))'	HMDB02 95768	C42H70O6			
670.51724	0.0028 4	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'		b'DG(17:0/0:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 95769	C42H70O6			
670.51724	0.0028 4	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'		b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0/17:0))'	HMDB02 95770	C42H70O6			
670.51724	0.0028 4	Redox	b'(2S)-1-(heptadecanoyloxy)-3-hydroxypropan-2-yl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'		b'DG(17:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/0:0))'	HMDB02 95771	C42H70O6			
670.51724	0.0028 4	Redox	b'(2S)-2-(heptadecanoyloxy)-3-hydroxypropyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'		b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/17:0/0:0))'	HMDB02 95772	C42H70O6			
670.51724	0.0028 4	Redox	b'(2R)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'		b'DG(17:0/0:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 95773	C42H70O6			
670.51724	0.0028 4	Redox	b'(2S)-3-(heptadecanoyloxy)-2-hydroxypropyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'		b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/0:0/17:0))'	HMDB02 95774	C42H70O6			
670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-{{{4Z,7Z,10Z,13Z}-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}propyl heptadecanoate'		b'DG(17:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/0:0))'	HMDB02 95779	C42H70O6			
670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-{{{4Z,7Z,10Z,13Z}-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}propan-2-yl heptadecanoate'		b'DG(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/17:0/0:0))'	HMDB02 95780	C42H70O6			
670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-{{{4Z,7Z,10Z,13Z}-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}propyl heptadecanoate'		b'DG(17:0/0:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 95781	C42H70O6			
670.51724	0.0028	Redox	b'(2S)-2-hydroxy-3-{{{4Z,7Z,10Z,13Z}-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}propyl heptadecanoate'		b'DG(22:5(4Z,7Z,10Z,13Z,19Z)-	HMDB02	C42H70O6			

			4				O(16,17)/0:0/17:0)	95782		
670.51724	0.0028 4	Redox		b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'		b'DG(a-17:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/0:0)	HMDB02 97838	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'		b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/a-17:0/0:0)	HMDB02 97839	C42H70O6		
670.51724	0.0028 4	Redox		b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'		b'DG(a-17:0/0:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 97840	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'		b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/0:0/a-17:0)	HMDB02 97841	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'		b'DG(a-17:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/0:0)	HMDB02 97842	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'		b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/a-17:0/0:0)	HMDB02 97843	C42H70O6		
670.51724	0.0028 4	Redox		b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'		b'DG(a-17:0/0:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 97844	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'		b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/0:0/a-17:0)	HMDB02 97845	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'		b'DG(a-17:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/0:0)	HMDB02 97846	C42H70O6		
670.51724	0.0028 4	Redox		b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'		b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/a-17:0/0:0)	HMDB02 97847	C42H70O6		

		670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(a- 17:0/0:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)- -OH(14))'	HMDB02 97848	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/0:0/a-17:0)'	HMDB02 97849	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(14-methylhexadecanoyl)oxy]propan-2-yl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(a- 17:0/22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/0:0)'	HMDB02 97850	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/a-17:0/0:0)'	HMDB02 97851	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(a- 17:0/0:0/22:6(4Z,7Z,10Z,13E,15E,19Z)- -OH(17))'	HMDB02 97852	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(14-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/0:0/a-17:0)'	HMDB02 97853	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[[4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propyl 14-methylhexadecanoate'	b'DG(a-17:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/0:0)'	HMDB02 97858	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[[4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propan-2-yl 14-methylhexadecanoate'	b'DG(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/a-17:0/0:0)'	HMDB02 97859	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[[4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propyl 14-methylhexadecanoate'	b'DG(a- 17:0/0:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))'	HMDB02 97860	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[[4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propyl 14-methylhexadecanoate'	b'DG(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/0:0/a-17:0)'	HMDB02 97861	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(i- 17:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-	HMDB02 99500	C42H70O6	

					OH(4)/0:0)			
670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)/i-17:0/0:0)	HMDB02 99501	C42H70O6		
670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(i- 17:0/0:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)- -OH(4))'	HMDB02 99502	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoate'	b'DG(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)/0:0/i-17:0)	HMDB02 99503	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(i- 17:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/0:0)	HMDB02 99504	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/i-17:0/0:0)	HMDB02 99505	C42H70O6		
670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(i- 17:0/0:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)- -OH(7))'	HMDB02 99506	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoate'	b'DG(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/0:0/i-17:0)	HMDB02 99507	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(i- 17:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/0:0)	HMDB02 99508	C42H70O6		
670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/i-17:0/0:0)	HMDB02 99509	C42H70O6		
670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(i- 17:0/0:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)- -OH(14))'	HMDB02 99510	C42H70O6		

		670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/0:0/i-17:0)'	HMDB02 99511	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[(15-methylhexadecanoyl)oxy]propan-2-yl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(i- 17:0/22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/0:0)'	HMDB02 99512	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/i-17:0/0:0)'	HMDB02 99513	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(i- 17:0/0:0/22:6(4Z,7Z,10Z,13E,15E,19Z)- -OH(17))'	HMDB02 99514	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[(15-methylhexadecanoyl)oxy]propyl (4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/0:0/i-17:0)'	HMDB02 99515	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-3-hydroxy-2-[[[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propyl 15-methylhexadecanoate'	b'DG(i-17:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/0:0)'	HMDB02 99520	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-1-hydroxy-3-[[[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propan-2-yl 15-methylhexadecanoate'	b'DG(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/i-17:0/0:0)'	HMDB02 99521	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2R)-2-hydroxy-3-[[[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propyl 15-methylhexadecanoate'	b'DG(i- 17:0/0:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))'	HMDB02 99522	C42H70O6	
		670.51724	0.0028 4	Redox	b'(2S)-2-hydroxy-3-[[[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy]propyl 15-methylhexadecanoate'	b'DG(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/0:0/i-17:0)'	HMDB02 99523	C42H70O6	
33	671.51 59	671.5158602	3.98E- 05	Redox	b'2-amino-3-[[2,3-bis(hexadecanoyloxy)propyl]sulfonyl]propanoic acid'	b'2,3-Dipalmitoyl-S-glycerylcysteine'	HMDB02 56098	C38H73NO6 S	
		671.5158602	3.98E- 05	Redox	b'3-[(2,3-dihydroxypropyl)sulfonyl]-2-(N-hexadecanoylhexadecanamido)propanoic acid'	b'Dipalmitoyl-s-glyceryl cysteine'	HMDB02 57984	C38H73NO6 S	
33	673.47	674.4886562	0.0029	Protone	b'[(2R)-3-(hexadecanoyloxy)-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(16:0/18:1(11Z))'	HMDB00	C37H71O8P	C004

3	79		562	tion			07858		16
		674.4886562	0.0029 562	Protone tion	b'[(2R)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(16:0/18:1(9Z))'	HMDB00 07859	C37H71O8P	C004 16
		674.4886558	0.0029 558	Protone tion	b'[2-(hexadecanoyloxy)-3-[(9E)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'9-Octadecenoic acid 1-[[1-oxohexadecyl]oxy]methyl]-2-(phosphonoxy)ethyl ester'	HMDB00 31130	C37H71O8P	
		674.4886558	0.0029 558	Protone tion	b'[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/16:1(9Z))'	HMDB01 14877	C37H71O8P	
		674.4886562	0.0029 562	Protone tion	b'[(2R)-2-(hexadecanoyloxy)-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/16:0)'	HMDB01 14899	C37H71O8P	
		674.4886562	0.0029 562	Protone tion	b'[(2R)-2-(hexadecanoyloxy)-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/16:0)'	HMDB01 14924	C37H71O8P	
		674.4886562	0.0029 562	Protone tion	b'[(2R)-3-(icosanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(20:0/14:1(9Z))'	HMDB01 15062	C37H71O8P	
		674.4886562	0.0029 562	Protone tion	b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(20:1(11Z)/14:0)'	HMDB01 15091	C37H71O8P	
33 4	674.48 05	675.4862742	0.0020 258	Protone tion	b'(3E)-1-(3,3-dimethyloxiran-2-yl)-3-methyl-5-[4-[2-(phenylformamido)ethyl]phenoxy]pent-3-en-2-yl octadecanoate'	b'Acidissiminin epoxide'	HMDB00 38620	C43H65NO5	
33 5	675.10 64	676.115604	0.0014 04	Protone tion	b'[{(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methoxy}[{(2R,3S,4R,5S)-5-(6-amino-9H-purin-9-yl)-4-hydroxy-2-(hydroxymethyl)oxolan-3-yl]oxy](hydroxy)phosphoryl]oxy]phosphonic acid'	b'Diadenosine diphosphate'	HMDB00 01312	C20H26N10 O13P2	
33 6	678.09 35	679.1026988	0.0013 988	Protone tion	b'2-[[2-([[(5-(2,4-dioxo-1,2,3,4-tetrahydropyrimidin-1-yl)-3,4-dihydroxyoxolan-2-yl]methoxy)(hydroxy)phosphoryl]oxy)(hydroxy)phosphoryl]oxy]-3-acetamido-5-hydroxy-6-(hydroxymethyl)oxan-4-yl]oxy]propanoic acid'	b'UDP-N-acetylmuramate'	HMDB00 11720	C20H31N3O 19P2	
33 7	685.51 49	685.5128829	0.0020 171	Redox	b'2-hydroxy-N-[(4Z,8Z)-3-hydroxy-1-[[3,4,5-trihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy]octadeca-4,8-dien-2-yl]tetradecanamide'	b'AS 1-1'	HMDB00 32794	C38H71NO9	
33 8	699.49 43	700.5043058	0.0022 058	Protone tion	b'[(2R)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/18:2(9Z,12Z))'	HMDB00 07861	C39H73O8P	C004 16

		700.5043063	0.0022 063	Protone tion	b'[(2R)-2,3-bis[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/18:1(11Z))'	HMDB00 07862	C39H73O8P	C004 16
		700.5043063	0.0022 063	Protone tion	b'[(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/18:1(9Z))'	HMDB00 07863	C39H73O8P	
		700.5043063	0.0022 063	Protone tion	b'[(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/18:1(11Z))'	HMDB00 07864	C39H73O8P	
		700.5043063	0.0022 063	Protone tion	b'[(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/18:1(9Z))'	HMDB00 07865	C39H73O8P	
		700.5043058	0.0022 058	Protone tion	b'[2,3-bis(octadec-9-enoyloxy)propoxy]phosphonic acid'	b'9-Octadecenoic acid 1- [(phosphonoxy)methyl]-1,2-ethanediyl ester'	HMDB00 31129	C39H73O8P	
		700.5043063	0.0022 063	Protone tion	b'[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(14:1(9Z)/22:1(13Z))'	HMDB01 14804	C39H73O8P	
		700.5043063	0.0022 063	Protone tion	b'[(2R)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:2(9Z,12Z)/18:0)	HMDB01 14951	C39H73O8P	
		700.5043063	0.0022 063	Protone tion	b'[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/16:1(9Z))'	HMDB01 15095	C39H73O8P	
		700.5043063	0.0022 063	Protone tion	b'[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(22:1(13Z)/14:1(9Z))'	HMDB01 15271	C39H73O8P	
		700.5043063	0.0022 063	Protone tion	b'[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(22:2(13Z,16Z)/14:0)	HMDB01 15296	C39H73O8P	
		700.5043063	0.0022 063	Protone tion	b'[(2R)-3-(hexadecanoyloxy)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphonic acid'	b'PA(16:0/20:2(11Z,14Z))'	HMDB01 15510	C39H73O8P	
		700.5043063	0.0022 063	Protone tion	b'[(2R)-2-(hexadecanoyloxy)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphonic acid'	b'PA(20:2(11Z,14Z)/16:0)	HMDB01 15535	C39H73O8P	
		700.5043063	0.0022	Protone	b'[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(14:0/22:2(13Z,16Z))'	HMDB01	C39H73O8P	

			063	tion			16699		
33 9	700.52 51	700.5278047	0.0027 047	Redox	b'(2S)-1-{{11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl}oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate'	b'DG(11D3/11D3/0:0)'	HMDB01 16369	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-2-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-hydroxypropyl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate'	b'DG(11D3/9D5/0:0)'	HMDB01 16376	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-hydroxypropyl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'	b'DG(11D5/9D3/0:0)'	HMDB01 16384	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-hydroxy-3-{{11-(3-methyl-5-propylfuran-2-yl)undecanoyl}oxy}propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate'	b'DG(11M3/11M5/0:0)'	HMDB01 16390	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-hydroxy-3-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propan-2-yl 11-(3-methyl-5-propylfuran-2-yl)undecanoate'	b'DG(11M5/11M3/0:0)'	HMDB01 16398	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-3-hydroxy-2-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}propyl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate'	b'DG(11M5/9M5/0:0)'	HMDB01 16404	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'	b'DG(9D3/11D5/0:0)'	HMDB01 16423	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate'	b'DG(9D5/11D3/0:0)'	HMDB01 16431	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-hydroxypropan-2-yl 9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoate'	b'DG(9D5/9D5/0:0)'	HMDB01 16438	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-hydroxy-3-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate'	b'DG(9M5/11M5/0:0)'	HMDB01 16443	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-1-hydroxy-3-(octadecanoyloxy)propan-2-yl (5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(18:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/0:0)'	HMDB02 95951	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-3-hydroxy-2-(octadecanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/18:0/0:0)'	HMDB02 95952	C43H72O7	
		700.5278047	0.0027	Redox	b'(2R)-2-hydroxy-3-(octadecanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(18:0/0:0/22:6(5Z,8E,10Z,13Z,15E	HMDB02	C43H72O7	

		700.5278047	0.0027 047	Redox	b'(2R)-2-hydroxy-3-[(16-methylheptadecanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(i- 18:0/0:0/22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17))'	HMDB02 99725	C43H72O7	
		700.5278047	0.0027 047	Redox	b'(2S)-2-hydroxy-3-[(16-methylheptadecanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/0:0/i-18:0)'	HMDB02 99726	C43H72O7	
34 0	701.51	702.5199564	0.0021 564	Protona tion	b'[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(14:0/22:1(13Z))'	HMDB01 14789	C39H75O8P	
		702.5199564	0.0021 564	Protona tion	b'[(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:1(11Z)/18:0)'	HMDB01 14901	C39H75O8P	
		702.5199564	0.0021 564	Protona tion	b'[(2R)-3-[(9Z)-octadec-9-enoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:1(9Z)/18:0)'	HMDB01 14926	C39H75O8P	
		702.5199564	0.0021 564	Protona tion	b'[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:0/16:1(9Z))'	HMDB01 15065	C39H75O8P	
		702.5199564	0.0021 564	Protona tion	b'[(2R)-2-(hexadecanoyloxy)-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/16:0)'	HMDB01 15094	C39H75O8P	
		702.5199564	0.0021 564	Protona tion	b'[(2R)-3-(docosanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(22:0/14:1(9Z))'	HMDB01 15241	C39H75O8P	
		702.5199564	0.0021 564	Protona tion	b'[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(22:1(13Z)/14:0)'	HMDB01 15270	C39H75O8P	
		701.5091349	0.0008 651	Redox	b'2-(dimethylamino)-N-(1-[[3-methoxy-1-(2-{1-methoxy-2-methyl-2-[(2-phenylethyl)carbamoyl]ethyl}pyrrolidin-1-yl)-5-methyl-1-oxoheptan-4-yl](methyl)carbamoyl]-2-methylpropyl)-3-methylbutanamide'	b'Sobidotin'	HMDB02 58356	C39H67N5O 6	
34 1	703.51 75	704.5227193	0.0025 807	Protona tion	b'(2S)-1-hydroxy-3-(nonadecanoyloxy)propan-2-yl (5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(19:0/20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15)/0:0)'	HMDB02 96163	C42H72O8	
		704.5227193	0.0025 807	Protona tion	b'(2S)-3-hydroxy-2-(nonadecanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15)/19:0/0:0)'	HMDB02 96164	C42H72O8	
		704.5227193	0.0025	Protona	b'(2R)-2-hydroxy-3-(nonadecanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(19:0/0:0/20:5(7Z,9Z,11E,13E,17Z)-	HMDB02	C42H72O8	

		807	tion			)·3OH(5,6,15))'	96165		
704.5227193	0.0025 807	Protona tion	b'(2S)-2-hydroxy-3-(nonadecanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15)0:0/19:0)'	HMDB02 96166	C42H72O8		
704.5227193	0.0025 807	Protona tion	b'(2S)-1-hydroxy-3-[(17-methyloctadecanoyl)oxy]propan-2-yl (5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(i-19:0/20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15)0:0)'	HMDB02 99903	C42H72O8		
704.5227193	0.0025 807	Protona tion	b'(2S)-3-hydroxy-2-[(17-methyloctadecanoyl)oxy]propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15)i-19:0/0:0)'	HMDB02 99904	C42H72O8		
704.5227193	0.0025 807	Protona tion	b'(2R)-2-hydroxy-3-[(17-methyloctadecanoyl)oxy]propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(i- 19:0/0:0/20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15))'	HMDB02 99905	C42H72O8		
704.5227193	0.0025 807	Protona tion	b'(2S)-2-hydroxy-3-[(17-methyloctadecanoyl)oxy]propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'		b'DG(20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15)0:0/i-19:0)'	HMDB02 99906	C42H72O8		
703.5152049	0.0022 951	Redox	b'(2- -{[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-(tetradecanoyloxy)propyl phosphonato]oxy}ethyl)trimethylazanium'		b'PC(14:0/16:1(9Z))'	HMDB00 07870	C38H74NO8 P		
703.5152049	0.0022 951	Redox	b'(2- -{[(2R)-2-(hexadecanoyloxy)-3-[(9Z)-tetradec-9-enoyloxy]propyl phosphonato]oxy}ethyl)trimethylazanium'		b'PC(14:1(9Z)/16:0)'	HMDB00 07902	C38H74NO8 P		
703.5152049	0.0022 951	Redox	b'(2- -{[(2R)-3-(hexadecanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propyl phosphonato]oxy}ethyl)trimethylazanium'		b'PC(16:0/14:1(9Z))'	HMDB00 07966	C38H74NO8 P	C001 57	
703.5152049	0.0022 951	Redox	b'(2- -{[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-(tetradecanoyloxy)propyl phosphonato]oxy}ethyl)trimethylazanium'		b'PC(16:1(9Z)/14:0)'	HMDB00 07998	C38H74NO8 P		
703.5152049	0.0022 951	Redox	b'(2-aminoethoxy)[(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-(pentadecanoyloxy)propoxy]phosphinic acid'		b'PE(15:0/18:1(11Z))'	HMDB00 08893	C38H74NO8 P		
703.5152053	0.0022 947	Redox	b'(2-aminoethoxy)[(2R)-2-[(9Z)-octadec-9-enoyloxy]-3-(pentadecanoyloxy)propoxy]phosphinic acid'		b'PE(15:0/18:1(9Z))'	HMDB00 08894	C38H74NO8 P		
703.5152049	0.0022 951	Redox	b'(2-aminoethoxy)[(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-(pentadecanoyloxy)propoxy]phosphinic acid'		b'PE(18:1(11Z)/15:0)'	HMDB00 09021	C38H74NO8 P		

		703.5152053	0.0022 947	Redox	b'(2-aminoethoxy)[(2R)-3-[(9Z)-octadec-9-enoyloxy]-2-(pentadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:1(9Z)/15:0)'	HMDB00 09054	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'[2-[(9Z)-hexadec-9-enoyloxy]-3-(hexadecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(16:0/16:1(9Z))'	HMDB01 12949	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy]({2-[(9Z)-octadec-9-enoyloxy]-3-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe(14:0/18:1(9Z))'	HMDB01 12950	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy]({2-[(11Z)-octadec-11-enoyloxy]-3-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe(14:0/18:1(11Z))'	HMDB01 12951	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy][2-(octadecanoyloxy)-3-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE-NMe(14:1(9Z)/18:0)'	HMDB01 12952	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'[3-[(9Z)-hexadec-9-enoyloxy]-2-(hexadecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(16:1(9Z)/16:0)'	HMDB01 13064	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy][3-(octadecanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphinic acid'	b'PE-NMe(18:0/14:1(9Z))'	HMDB01 13085	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy]({3-[(11Z)-octadec-11-enoyloxy]-2-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe(18:1(11Z)/14:0)'	HMDB01 13110	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'[2-(methylamino)ethoxy]({3-[(9Z)-octadec-9-enoyloxy]-2-(tetradecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe(18:1(9Z)/14:0)'	HMDB01 13137	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'[2-(dimethylamino)ethoxy]({2-[(9Z)-hexadec-9-enoyloxy]-3-(pentadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(15:0/16:1(9Z))'	HMDB01 13846	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'[2-(dimethylamino)ethoxy]({3-[(9Z)-hexadec-9-enoyloxy]-2-(pentadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(16:1(9Z)/15:0)'	HMDB01 13964	C38H74NO8 P	
		703.5152053	0.0022 947	Redox	b'(2-[(2R)-3-(dodecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl phosphono]oxy)ethyltrimethylazanium'	b'10E-heptadecenoic acid'	HMDB03 04753	C38H74NO8 P	
34 2	718.53 55	718.5383693	0.0028 693	Redox	b'(2S)-1-hydroxy-3-(icosanoyloxy)propan-2-yl (5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:0/20:5(7Z,9Z,11E,13E,17Z)- 3OH(5,6,15)/0:0)'	HMDB02 96371	C43H74O8	

34	723.49	718.5383693	0.0028 693	Redox	b'(2S)-3-hydroxy-2-(icosanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/20:0/0:0)'	HMDB02 96372	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2R)-2-hydroxy-3-(icosanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:0/0:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 96373	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2S)-2-hydroxy-3-(icosanoyloxy)propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/0:0/20:0)'	HMDB02 96374	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2S)-1-hydroxy-3-[(18-methylnonadecanoyl)oxy]propan-2-yl (5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(i-20:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/0:0)'	HMDB03 00110	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2S)-3-hydroxy-2-[(18-methylnonadecanoyl)oxy]propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/i-20:0/0:0)'	HMDB03 00111	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2R)-2-hydroxy-3-[(18-methylnonadecanoyl)oxy]propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(i-20:0/0:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB03 00112	C43H74O8	
		718.5383693	0.0028 693	Redox	b'(2S)-2-hydroxy-3-[(18-methylnonadecanoyl)oxy]propyl (5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoate'	b'DG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/0:0/i-20:0)'	HMDB03 00113	C43H74O8	
34	723.49	724.5043063	0.0022 063	Protontaion	b'[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-(hexadecanoyloxy)propoxy]phosphonic acid'	b'PA(16:0/22:4(7Z,10Z,13Z,16Z))'	HMDB01 14846	C41H73O8P	
		724.5043063	0.0022 063	Protontaion	b'[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/20:4(5Z,8Z,11Z,14Z))'	HMDB01 14884	C41H73O8P	
		724.5043063	0.0022 063	Protontaion	b'[(2R)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/20:4(8Z,11Z,14Z,17Z))'	HMDB01 14885	C41H73O8P	
		724.5043063	0.0022 063	Protontaion	b'[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/20:3(5Z,8Z,11Z))'	HMDB01 14908	C41H73O8P	
		724.5043063	0.0022 063	Protontaion	b'[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/20:3(5Z,8Z,11Z))'	HMDB01 14933	C41H73O8P	
		724.5043063	0.0022	Protontaion	b'[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphonic acid'	b'PA(18:3(6Z,9Z,12Z)/20:1(11Z))'	HMDB01	C41H73O8P	

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724.5043063	0.0022 063	Protona tion		b'[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphonic acid'	b'PA(18:3(9Z,12Z,15Z)/20:1(11Z))'	HMDB01 15013	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-2-(icosanoyloxy)-3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphonic acid'	b'PA(18:4(6Z,9Z,12Z,15Z)/20:0)'	HMDB01 15039	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-3-(icosanoyloxy)-2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphonic acid'	b'PA(20:0/18:4(6Z,9Z,12Z,15Z))'	HMDB01 15073	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/18:3(6Z,9Z,12Z))'	HMDB01 15100	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/18:3(9Z,12Z,15Z))'	HMDB01 15101	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(20:3(5Z,8Z,11Z)/18:1(11Z))'	HMDB01 15124	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(20:3(5Z,8Z,11Z)/18:1(9Z))'	HMDB01 15125	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(20:4(5Z,8Z,11Z,14Z)/18:0)'	HMDB01 15149	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(20:4(8Z,11Z,14Z,17Z)/18:0)'	HMDB01 15176	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(hexadecanoyloxy)propoxy]phosphonic acid'	b'PA(22:4(7Z,10Z,13Z,16Z)/16:0)'	HMDB01 15326	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'	b'PA(20:2(11Z,14Z)/18:2(9Z,12Z))'	HMDB01 15493	C41H73O8P		
724.5043063	0.0022 063	Protona tion		b'[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/20:3(8Z,11Z,14Z))'	HMDB01 15517	C41H73O8P		
724.5043063	0.0022	Protona		b'[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/20:3(8Z,11Z,14Z))'	HMDB01	C41H73O8P		

34	4	728.52	37		063	tion			15519		
				724.5043063	0.0022 063	Protona tion	b'[(2R)-2-[(11Z,14Z)-icosa-11,14-dienyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienyloxy]propoxy]phosphonic acid'	b'PA(18:2(9Z,12Z)/20:2(11Z,14Z))'	HMDB01 15520	C41H73O8P	
				724.5043063	0.0022 063	Protona tion	b'[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienyloxy]-2-[(11Z)-octadec-11-enyloxy]propoxy]phosphonic acid'	b'PA(20:3(8Z,11Z,14Z)/18:1(11Z))'	HMDB01 15567	C41H73O8P	
				724.5043063	0.0022 063	Protona tion	b'[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienyloxy]-2-[(9Z)-octadec-9-enyloxy]propoxy]phosphonic acid'	b'PA(20:3(8Z,11Z,14Z)/18:1(9Z))'	HMDB01 15568	C41H73O8P	
				729.5308549	0.0006 451	Protona tion	b'trimethyl(2-[[[(2R)-2-[(9Z,12Z)-octadeca-9,12-dienyloxy]-3-(tetradecanoyloxy)propyl phosphono]oxy]ethyl]azanium'	b'PC(14:0/18:2(9Z,12Z))'	HMDB00 07874	C40H76NO8 P	
				729.5308549	0.0006 451	Protona tion	b'trimethyl(2-[[[(2R)-2-[(11Z)-octadec-11-enyloxy]-3-[(9Z)-tetradec-9-enyloxy]propyl phosphono]oxy]ethyl]azanium'	b'PC(14:1(9Z)/18:1(11Z))'	HMDB00 07905	C40H76NO8 P	
				729.5308549	0.0006 451	Protona tion	b'trimethyl(2-[[[(2R)-2-[(9Z)-octadec-9-enyloxy]-3-[(9Z)-tetradec-9-enyloxy]propyl phosphono]oxy]ethyl]azanium'	b'PC(14:1(9Z)/18:1(9Z))'	HMDB00 07906	C40H76NO8 P	
				729.5308549	0.0006 451	Protona tion	b'(2-[[[(2R)-2,3-bis[(9Z)-hexadec-9-enyloxy]propyl phosphono]oxy]ethyl]trimethylazanium'	b'PC(16:1(9Z)/16:1(9Z))'	HMDB00 08002	C40H76NO8 P	C001 57
				729.5308549	0.0006 451	Protona tion	b'trimethyl(2-[[[(2R)-3-[(11Z)-octadec-11-enyloxy]-2-[(9Z)-tetradec-9-enyloxy]propyl phosphono]oxy]ethyl]azanium'	b'PC(18:1(11Z)/14:1(9Z))'	HMDB00 08065	C40H76NO8 P	C001 57
				729.5308549	0.0006 451	Protona tion	b'trimethyl(2-[[[(2R)-3-[(9Z)-octadec-9-enyloxy]-2-[(9Z)-tetradec-9-enyloxy]propyl phosphono]oxy]ethyl]azanium'	b'PC(18:1(9Z)/14:1(9Z))'	HMDB00 08098	C40H76NO8 P	
				729.5308549	0.0006 451	Protona tion	b'trimethyl(2-[[[(2R)-3-[(9Z,12Z)-octadeca-9,12-dienyloxy]-2-(tetradecanoyloxy)propyl phosphono]oxy]ethyl]azanium'	b'PC(18:2(9Z,12Z)/14:0)	HMDB00 08130	C40H76NO8 P	
				729.5308549	0.0006 451	Protona tion	b'(2-aminoethoxy)[(2R)-2-[(11Z,14Z)-icosa-11,14-dienyloxy]-3-(pentadecanoyloxy)propoxy]phosphinic acid'	b'PE(15:0/20:2(11Z,14Z))'	HMDB00 08901	C40H76NO8 P	
				729.5308549	0.0006 451	Protona tion	b'(2-aminoethoxy)[(2R)-3-[(11Z,14Z)-icosa-11,14-dienyloxy]-2-(pentadecanoyloxy)propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/15:0)	HMDB00 09285	C40H76NO8 P	
				729.5308554	0.0006	Protona	b'[2-[(11Z)-icos-11-enyloxy]-3-[(9Z)-tetradec-9-enyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(14:1(9Z)/20:1(11Z))'	HMDB01	C40H76NO8	

			446	tion			12955	P	
		729.5308554	0.0006 446	Protona tion	b'3-[(9Z)-hexadec-9-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy}[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(16:1(9Z)/18:1(9Z))'	HMDB01 12956	C40H76NO8 P	
		729.5308554	0.0006 446	Protona tion	b'3-[(9Z)-hexadec-9-enoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy}[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(16:1(9Z)/18:1(11Z))'	HMDB01 12957	C40H76NO8 P	
		729.5308554	0.0006 446	Protona tion	b'2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-(tetradecanoyloxy)propoxy}[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(14:0/20:2(11Z,14Z))'	HMDB01 12984	C40H76NO8 P	
		729.5308554	0.0006 446	Protona tion	b'[3-(hexadecanoyloxy)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(16:0/18:2(9Z,12Z))'	HMDB01 13042	C40H76NO8 P	
		729.5308554	0.0006 446	Protona tion	b'[2-[(9Z)-hexadec-9-enoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(18:1(11Z)/16:1(9Z))'	HMDB01 13114	C40H76NO8 P	
		729.5308554	0.0006 446	Protona tion	b'[2-[(9Z)-hexadec-9-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(18:1(9Z)/16:1(9Z))'	HMDB01 13141	C40H76NO8 P	
		729.5308554	0.0006 446	Protona tion	b'[2-(hexadecanoyloxy)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(18:2(9Z,12Z)/16:0)'	HMDB01 13167	C40H76NO8 P	
		729.5308554	0.0006 446	Protona tion	b'[3-[(11Z)-icos-11-enoyloxy]-2-[(9Z)-tetradec-9-enoyloxy]propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(20:1(11Z)/14:1(9Z))'	HMDB01 13309	C40H76NO8 P	
		729.5308554	0.0006 446	Protona tion	b'[3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-(tetradecanoyloxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(20:2(11Z,14Z)/14:0)'	HMDB01 13337	C40H76NO8 P	
		729.5308554	0.0006 446	Protona tion	b'[2-(dimethylamino)ethoxy]({2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-3-(pentadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(15:0/18:2(9Z,12Z))'	HMDB01 13920	C40H76NO8 P	
		729.5308554	0.0006 446	Protona tion	b'[2-(dimethylamino)ethoxy]({3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-2-(pentadecanoyloxy)propoxy})phosphinic acid'	b'PE-NMe2(18:2(9Z,12Z)/15:0)'	HMDB01 14067	C40H76NO8 P	
34	728.55	729.5672404	0.0029 404	Protona tion	b'trimethyl[2-({2-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]-3-(pentadecanoyloxy)propyl phosphonato}oxy)ethyl]azanium'	b'PC(15:0/P-18:1(11Z))'	HMDB00 07963	C41H80NO7 P	
5	65	729.5672404	0.0029	Protona	b'trimethyl[2-({2-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]-3-(pentadecanoyloxy)propyl phosphonato}oxy)ethyl]azanium'	b'PC(15:0/P-18:1(9Z))'	HMDB00	C41H80NO7	C001

		404	tion			07964	P	57
729.5672404	0.0029 404	Protone tion	b'(2-aminoethoxy)[(2R)-2-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/P-18:1(11Z))'	HMDB00 09017	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'(2-aminoethoxy)[(2R)-2-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/P-18:1(9Z))'	HMDB00 09018	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'(2-aminoethoxy)[(2R)-2-[(1Z)-octadec-1-en-1-yloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(11Z)/P-18:0)'	HMDB00 09049	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'(2-aminoethoxy)[(2R)-2-[(1Z)-octadec-1-en-1-yloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)/P-18:0)'	HMDB00 09082	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'(2-aminoethoxy)[(2R)-2-[(1Z)-hexadec-1-en-1-yloxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/P-16:0)'	HMDB00 09279	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'trimethyl[2-[(2R)-3-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]-2-(pentadecanoyloxy)propyl phosphonato]oxy]ethyl]azanium'	b'PC(P-18:1(11Z)/15:0)'	HMDB00 11271	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'trimethyl[2-[(3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]-2-(pentadecanoyloxy)propyl phosphonato]oxy]ethyl]azanium'	b'PC(P-18:1(9Z)/15:0)'	HMDB00 11304	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'(2-aminoethoxy)[(2R)-3-[(1Z)-hexadec-1-en-1-yloxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(P-16:0/20:1(11Z))'	HMDB00 11348	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'(2-aminoethoxy)[(2R)-3-[(1Z)-octadec-1-en-1-yloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(P-18:0/18:1(11Z))'	HMDB00 11374	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'(2-aminoethoxy)[(2R)-3-[(1Z)-octadec-1-en-1-yloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(P-18:0/18:1(9Z))'	HMDB00 11375	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'(2-aminoethoxy)[(2R)-3-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(P-18:1(11Z)/18:0)'	HMDB00 11406	C41H80NO7 P		
729.5672404	0.0029 404	Protone tion	b'(2-aminoethoxy)[(2R)-3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(P-18:1(9Z)/18:0)'	HMDB00 11439	C41H80NO7 P		
728.5591048	0.0026	Redox	b'(2S)-1-[[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy]-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'	b'DG(11D3/11D5/0:0)'	HMDB01	C45H76O7		

			048					16370		
728.5591048	0.0026 048	Redox	b'(2S)-1-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoate'				b'DG(11D5/11D3/0:0)'	HMDB01 16378	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-2-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-hydroxypropyl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'				b'DG(11D5/9D5/0:0)'	HMDB01 16385	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-1-hydroxy-3-{{11-(3-methyl-5-propylfuran-2-yl)undecanoyl}oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate'				b'DG(11M3/13M5/0:0)'	HMDB01 16392	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-1-hydroxy-3-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propan-2-yl 11-(3-methyl-5-pentylfuran-2-yl)undecanoate'				b'DG(11M5/11M5/0:0)'	HMDB01 16399	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-hydroxypropyl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate'				b'DG(13D5/9D3/0:0)'	HMDB01 16411	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-3-hydroxy-2-{{11-(3-methyl-5-propylfuran-2-yl)undecanoyl}oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate'				b'DG(13M5/11M3/0:0)'	HMDB01 16416	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-3-hydroxy-2-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}propyl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate'				b'DG(13M5/9M5/0:0)'	HMDB01 16421	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-1-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-hydroxypropan-2-yl 13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoate'				b'DG(9D3/13D5/0:0)'	HMDB01 16426	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-1-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-hydroxypropan-2-yl 11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoate'				b'DG(9D5/11D5/0:0)'	HMDB01 16432	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-1-hydroxy-3-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}propan-2-yl 13-(3-methyl-5-pentylfuran-2-yl)tridecanoate'				b'DG(9M5/13M5/0:0)'	HMDB01 16445	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-1-hydroxy-3-(icosanoyloxy)propan-2-yl (5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'				b'DG(20:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/0:0)'	HMDB02 96367	C45H76O7	
728.5591048	0.0026 048	Redox	b'(2S)-3-hydroxy-2-(icosanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'				b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/20:0/0:0)'	HMDB02 96368	C45H76O7	
728.5591048	0.0026	Redox	b'(2R)-2-hydroxy-3-(icosanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'				b'DG(20:0/0:0/22:6(5Z,8E,10Z,13Z,15E	HMDB02	C45H76O7	

			048				,19Z)-2OH(7S, 17S))'	96369		
728.5591048	0.0026 048	Redox		b'(2S)-2-hydroxy-3-(icosanoyloxy)propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S))0:0/20:0)'	HMDB02 96370	C45H76O7			
728.5591048	0.0026 048	Redox		b'(2S)-1-hydroxy-3-(icosanoyloxy)propan-2-yl (4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(20:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/0:0)'	HMDB02 96399	C45H76O7			
728.5591048	0.0026 048	Redox		b'(2S)-3-hydroxy-2-(icosanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/20:0/0:0)'	HMDB02 96400	C45H76O7			
728.5591048	0.0026 048	Redox		b'(2R)-2-hydroxy-3-(icosanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(20:0/0:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17))'	HMDB02 96401	C45H76O7			
728.5591048	0.0026 048	Redox		b'(2S)-2-hydroxy-3-(icosanoyloxy)propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/0:0/20:0)'	HMDB02 96402	C45H76O7			
728.5591048	0.0026 048	Redox		b'(2S)-1-hydroxy-3-[(18-methylnonadecanoyl)oxy]propan-2-yl (5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(i-20:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/0:0)'	HMDB03 00106	C45H76O7			
728.5591048	0.0026 048	Redox		b'(2S)-3-hydroxy-2-[(18-methylnonadecanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/i-20:0/0:0)'	HMDB03 00107	C45H76O7			
728.5591048	0.0026 048	Redox		b'(2R)-2-hydroxy-3-[(18-methylnonadecanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(i-20:0/0:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S))'	HMDB03 00108	C45H76O7			
728.5591048	0.0026 048	Redox		b'(2S)-2-hydroxy-3-[(18-methylnonadecanoyl)oxy]propyl (5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoate'	b'DG(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/0:0/i-20:0)'	HMDB03 00109	C45H76O7			
728.5591048	0.0026 048	Redox		b'(2S)-1-hydroxy-3-[(18-methylnonadecanoyl)oxy]propan-2-yl (4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(i-20:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/0:0)'	HMDB03 00138	C45H76O7			
728.5591048	0.0026 048	Redox		b'(2S)-3-hydroxy-2-[(18-methylnonadecanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/i-20:0/0:0)'	HMDB03 00139	C45H76O7			

34		728.5591048	0.0026 048	Redox	b'(2R)-2-hydroxy-3-[(18-methylnonadecanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(i- 20:0/0:0/22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17))'	HMDB03 00140	C45H76O7	
		728.5591048	0.0026 048	Redox	b'(2S)-2-hydroxy-3-[(18-methylnonadecanoyl)oxy]propyl (4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoate'	b'DG(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/0:0/i-20:0)'	HMDB03 00141	C45H76O7	
	729.54 07	730.5512565	0.0027 565	Protona tion	b'[(2R)-2-[(15Z)-tetracos-15-enoyloxy]-3-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(14:0/24:1(15Z))'	HMDB01 14794	C41H79O8P	
		730.5512565	0.0027 565	Protona tion	b'[(2R)-2-(tetracosanoyloxy)-3-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(14:1(9Z)/24:0)'	HMDB01 14810	C41H79O8P	
		730.5512565	0.0027 565	Protona tion	b'[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-(hexadecanoyloxy)propoxy]phosphonic acid'	b'PA(16:0/22:1(13Z))'	HMDB01 14844	C41H79O8P	
		730.5512565	0.0027 565	Protona tion	b'[(2R)-2-(docosanoyloxy)-3-[(9Z)-hexadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(16:1(9Z)/22:0)'	HMDB01 14864	C41H79O8P	
		730.5512565	0.0027 565	Protona tion	b'[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/20:1(11Z))'	HMDB01 14882	C41H79O8P	
		730.5512565	0.0027 565	Protona tion	b'[(2R)-2-(icosanoyloxy)-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(11Z)/20:0)'	HMDB01 14906	C41H79O8P	
		730.5512565	0.0027 565	Protona tion	b'[(2R)-2-(icosanoyloxy)-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(18:1(9Z)/20:0)'	HMDB01 14931	C41H79O8P	
		730.5512565	0.0027 565	Protona tion	b'[(2R)-3-(icosanoyloxy)-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PA(20:0/18:1(11Z))'	HMDB01 15068	C41H79O8P	
		730.5512565	0.0027 565	Protona tion	b'[(2R)-3-(icosanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(20:0/18:1(9Z))'	HMDB01 15069	C41H79O8P	
		730.5512565	0.0027 565	Protona tion	b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(20:1(11Z)/18:0)'	HMDB01 15096	C41H79O8P	
		730.5512565	0.0027	Protona	b'[(2R)-3-(docosanoyloxy)-2-[(9Z)-hexadec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(22:0/16:1(9Z))'	HMDB01	C41H79O8P	

34	7	746.51		565	tion			15244		
			730.5512565	0.0027 565	Protona tion	b'[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-(hexadecanoyloxy)propoxy]phosphonic acid'	b'PA(22:1(13Z)/16:0)'	HMDB01 15273	C41H79O8P	
			730.5512565	0.0027 565	Protona tion	b'[(2R)-3-(tetracosanoyloxy)-2-[(9Z)-tetradec-9-enoyloxy]propoxy]phosphonic acid'	b'PA(24:0/14:1(9Z))'	HMDB01 15429	C41H79O8P	
			730.5512565	0.0027 565	Protona tion	b'[(2R)-3-[(15Z)-tetracos-15-enoyloxy]-2-(tetradecanoyloxy)propoxy]phosphonic acid'	b'PA(24:1(15Z)/14:0)'	HMDB01 15455	C41H79O8P	
			730.5512565	0.0027 565	Protona tion	b'butoxy[3-(hexadecanoyloxy)-2-(octadec-9-enoyloxy)propoxy]phosphonic acid'	b'phosphatidylbutanol'	HMDB02 56466	C41H79O8P	
	7	746.51	747.5202902	0.0016 902	Protona tion		b'PE(P- 16:0/22:6(4Z,7Z,10Z,13Z,16Z,19Z))'	HMDB00 05780	C43H74NO7 P	C003 50
			747.5202902	0.0016 902	Protona tion	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-2-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphonic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,17Z)/P- 18:1(11Z))'	HMDB00 09479	C43H74NO7 P	
			747.5202902	0.0016 902	Protona tion	b'(2-aminoethoxy)[(2R)-3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-2-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphonic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,17Z)/P- 18:1(9Z))'	HMDB00 09480	C43H74NO7 P	
			747.5202902	0.0016 902	Protona tion	b'(2-aminoethoxy)[(2R)-3-[(4Z,7Z,10Z,13Z,16Z,19Z)-docosa-4,7,10,13,16,19-hexaenoyloxy]-2-[(1Z)-hexadec-1-en-1-yloxy]propoxy]phosphonic acid'	b'PE(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/P- 16:0)'	HMDB00 09708	C43H74NO7 P	
			747.5202902	0.0016 902	Protona tion	b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-3-[(1Z,11Z)-octadeca-1,11-dien-1-yloxy]propoxy]phosphonic acid'	b'PE(P- 18:1(11Z)/20:5(5Z,8Z,11Z,14Z,17Z))'	HMDB00 11420	C43H74NO7 P	
			747.5202902	0.0016 902	Protona tion	b'(2-aminoethoxy)[(2R)-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]-3-[(1Z,9Z)-octadeca-1,9-dien-1-yloxy]propoxy]phosphonic acid'	b'PE(P- 18:1(9Z)/20:5(5Z,8Z,11Z,14Z,17Z))'	HMDB00 11453	C43H74NO7 P	
			746.5097851	0.0010 149	Redox	b'[(2S)-2,3-dihydroxypropoxy][[(2R)-3-(hexadecanoyloxy)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'	b'PG(16:0/18:2(9Z,12Z))'	HMDB00 10575	C40H75O10 P	
			746.5097851	0.0010 149	Redox	b'[(2S)-2,3-dihydroxypropoxy][[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphonic acid'	b'PG(16:1(9Z)/18:1(11Z))'	HMDB00 10588	C40H75O10 P	
			746.5097851	0.0010	Redox	b'[(2S)-2,3-dihydroxypropoxy][[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphonic acid'	b'PG(16:1(9Z)/18:1(9Z))'	HMDB00	C40H75O10	

			149				10589	P	
		746.5097851	0.0010 149	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(11Z)/16:1(9Z))'	HMDB00 10616	C40H75O10 P	
		746.5097851	0.0010 149	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)/16:1(9Z))'	HMDB00 10631	C40H75O10 P	
		746.5097851	0.0010 149	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(18:2(9Z,12Z)/16:0)'	HMDB00 10645	C40H75O10 P	
34 8	748.52 35	748.5254352	0.0019 352	Redox		b'PG(16:0/18:1(11Z))'	HMDB00 10573	C40H77O10 P	
		748.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(16:0/18:1(9Z))'	HMDB00 10574	C40H77O10 P	
		748.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(16:1(9Z)/18:0)'	HMDB00 10587	C40H77O10 P	
		748.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(18:0/16:1(9Z))'	HMDB00 10601	C40H77O10 P	
		748.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(11Z)/16:0)'	HMDB00 10615	C40H77O10 P	
		748.5254352	0.0019 352	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)/16:0)'	HMDB00 10630	C40H77O10 P	
		748.5254357	0.0019 357	Redox	b'(2,3-dihydroxypropoxy)[3-(hexadecanoyloxy)-2-(octadec-9-enoyloxy)propoxy]phosphinic acid'	b'1-Palmitoyl-2-oleoylglycerol-3-phosphoglycerol'	HMDB02 44000	C40H77O10 P	
		748.5254357	0.0019 357	Redox	b'[(2R)-2-[[[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-3-(nonadecanoyloxy)propoxy]phosphonic acid'	b'PA(19:0/18:1(12Z)-2OH(9,10))'	HMDB02 64462	C40H77O10 P	
		748.5254357	0.0019 357	Redox	b'[(2R)-3-[[[(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-2-(nonadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:1(12Z)-2OH(9,10)/19:0)'	HMDB02 64463	C40H77O10 P	
		748.5254357	0.0019	Redox	b'[(2R)-2-[[[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-3-[(17-methyloctadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-19:0/18:1(12Z)-2OH(9,10))'	HMDB02	C40H77O10	

			357				68092	P	
		748.5254357	0.0019 357	Redox	b'[(2R)-3-[(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-2-[(17-methyloctadecanoyl)oxy]propoxy]phosphonic acid'	b'PA(18:1(12Z)-2OH(9,10)/i-19:0)'	HMDB02 68093	C40H77O10 P	
34 9	750.53 98	750.5410853	0.0012 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-(hexadecanoyloxy)-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(16:0/18:0)'	HMDB00 10572	C40H79O10 P	
		750.5410853	0.0012 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(18:0/16:0)'	HMDB00 10600	C40H79O10 P	
		750.5410857	0.0012 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(10-methyldodecanoyl)oxy]-2-[(18-methylcosanoyl)oxy]propoxy]phosphinic acid'	b'PG(a-13:0/a-21:0)'	HMDB01 16640	C40H79O10 P	
		750.5410857	0.0012 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(10-methyldodecanoyl)oxy]-2-[(19-methylcosanoyl)oxy]propoxy]phosphinic acid'	b'PG(a-13:0/i-21:0)'	HMDB01 16651	C40H79O10 P	
		750.5410857	0.0012 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(20-methylhenicosanoyl)oxy]-3-[(10-methylundecanoyl)oxy]propoxy]phosphinic acid'	b'PG(i-12:0/i-22:0)'	HMDB01 16670	C40H79O10 P	
		750.5410857	0.0012 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(11-methyldodecanoyl)oxy]-2-[(18-methylcosanoyl)oxy]propoxy]phosphinic acid'	b'PG(i-13:0/a-21:0)'	HMDB01 16676	C40H79O10 P	
		750.5410857	0.0012 857	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(11-methyldodecanoyl)oxy]-2-[(19-methylcosanoyl)oxy]propoxy]phosphinic acid'	b'PG(i-13:0/i-21:0)'	HMDB01 16687	C40H79O10 P	
35 0	751.52 55	752.5356064	0.0023 064	Protona tion	b'[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(18:0/22:4(7Z,10Z,13Z,16Z))'	HMDB01 14890	C43H77O8P	
		752.5356064	0.0023 064	Protona tion	b'[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'	b'PA(18:2(9Z,12Z)/22:2(13Z,16Z))'	HMDB01 14966	C43H77O8P	
		752.5356064	0.0023 064	Protona tion	b'[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphonic acid'	b'PA(18:3(6Z,9Z,12Z)/22:1(13Z))'	HMDB01 14992	C43H77O8P	
		752.5356064	0.0023 064	Protona tion	b'[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphonic acid'	b'PA(18:3(9Z,12Z,15Z)/22:1(13Z))'	HMDB01 15019	C43H77O8P	
		752.5356064	0.0023	Protona	b'[(2R)-2-(docosanoyloxy)-3-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphonic acid'	b'PA(18:4(6Z,9Z,12Z,15Z)/22:0)'	HMDB01	C43H77O8P	

		064	tion				15045		
752.5356064	0.0023 064	Protona tion		b'[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-3-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:0/20:4(5Z,8Z,11Z,14Z))'	HMDB01 15078	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-3-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:0/20:4(8Z,11Z,14Z,17Z))'	HMDB01 15079	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/20:3(5Z,8Z,11Z))'	HMDB01 15105	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:3(5Z,8Z,11Z)/20:1(11Z))'	HMDB01 15131	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:4(5Z,8Z,11Z,14Z)/20:0)'	HMDB01 15156	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-(icosanoyloxy)propoxy]phosphonic acid'	b'PA(20:4(8Z,11Z,14Z,17Z)/20:0)'	HMDB01 15183	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-3-(docosanoyloxy)-2-[(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy]propoxy]phosphonic acid'	b'PA(22:0/18:4(6Z,9Z,12Z,15Z))'	HMDB01 15251	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(6Z,9Z,12Z)-octadeca-6,9,12-trienoyloxy]propoxy]phosphonic acid'	b'PA(22:1(13Z)/18:3(6Z,9Z,12Z))'	HMDB01 15279	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(9Z,12Z,15Z)-octadeca-9,12,15-trienoyloxy]propoxy]phosphonic acid'	b'PA(22:1(13Z)/18:3(9Z,12Z,15Z))'	HMDB01 15280	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphonic acid'	b'PA(22:2(13Z,16Z)/18:2(9Z,12Z))'	HMDB01 15304	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphonic acid'	b'PA(22:4(7Z,10Z,13Z,16Z)/18:0)'	HMDB01 15328	C43H77O8P		
752.5356064	0.0023 064	Protona tion		b'[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphonic acid'	b'PA(20:1(11Z)/20:3(8Z,11Z,14Z))'	HMDB01 15531	C43H77O8P		
752.5356064	0.0023	Protona		b'[(2R)-2,3-bis[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphonic acid'	b'PA(20:2(11Z,14Z)/20:2(11Z,14Z))'	HMDB01	C43H77O8P		

			064	tion			15545		
		752.5356064	0.0023 064	Protone tion	b'[(2R)-2-((11Z)-icos-11-enoyloxy)-3-((8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy)propoxy]phosphonic acid'	b'PA(20:3(8Z,11Z,14Z)/20:1(11Z))'	HMDB01 15573	C43H77O8P	
35	757.58	758.59379	0.0023 1	Protone tion	b'(2-(((2S,3R)-3-hydroxy-2-(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl} octanamido)nonadecyl phosphono)oxy) ethyl)trimethylazanium'	b'SM(d19:0/18:1(12Z)-O(9S,10R))'	HMDB02 90636	C42H83N2O 7P	
1	83	758.59379	0.0023 1	Protone tion	b'(2-(((2S,3R)-3-hydroxy-2-((9Z)-11-(3-pentylloxiran-2-yl)undec-9-enamido)nonadecyl phosphono)oxy) ethyl)trimethylazanium'	b'SM(d19:0/18:1(9Z)-O(12,13))'	HMDB02 90637	C42H83N2O 7P	
35	762.50	762.5047002	0.0027 002	Redox	b'[(2R)-2-((7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)cyclopentyl]heptanoyl)oxy)-2-(heptadecanoyloxy)propoxy]phosphonic acid'	b'PA(17:0/PGF1alpha)'	HMDB02 63569	C40H75O11 P	
		762.5047002	0.0027 002	Redox	b'[(2R)-3-((7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)cyclopentyl]heptanoyl)oxy)-2-(heptadecanoyloxy)propoxy]phosphonic acid'	b'PA(PGF1alpha/17:0)'	HMDB02 63570	C40H75O11 P	
		762.5047002	0.0027 002	Redox	b'[(2R)-2-((7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)cyclopentyl]heptanoyl)oxy)-2-((14-methylhexadecanoyl)oxy)propoxy]phosphonic acid'	b'PA(a-17:0/PGF1alpha)'	HMDB02 67099	C40H75O11 P	
		762.5047002	0.0027 002	Redox	b'[(2R)-3-((7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)cyclopentyl]heptanoyl)oxy)-2-((14-methylhexadecanoyl)oxy)propoxy]phosphonic acid'	b'PA(PGF1alpha/a-17:0)'	HMDB02 67100	C40H75O11 P	
		762.5047002	0.0027 002	Redox	b'[(2R)-2-((7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)cyclopentyl]heptanoyl)oxy)-3-((15-methylhexadecanoyl)oxy)propoxy]phosphonic acid'	b'PA(i-17:0/PGF1alpha)'	HMDB02 67926	C40H75O11 P	
		762.5047002	0.0027 002	Redox	b'[(2R)-3-((7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)cyclopentyl]heptanoyl)oxy)-2-((15-methylhexadecanoyl)oxy)propoxy]phosphonic acid'	b'PA(PGF1alpha/i-17:0)'	HMDB02 67927	C40H75O11 P	
		762.5047002	0.0027 002	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-(hexadecanoyloxy)-2-((8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl} octanoyl)oxy)propoxy]phosphonic acid'	b'PG(16:0/18:1(12Z)-O(9S,10R))'	HMDB02 68611	C40H75O11 P	
		762.5047002	0.0027 002	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-((8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl} octanoyl)oxy)propoxy]phosphonic acid'	b'PG(18:1(12Z)-O(9S,10R)/16:0)'	HMDB02 68612	C40H75O11 P	
		762.5047002	0.0027 002	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-(hexadecanoyloxy)-2-((9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl)oxy]propoxy]phosphonic acid'	b'PG(16:0/18:1(9Z)-O(12,13))'	HMDB02 68613	C40H75O11 P	
		762.5047002	0.0027	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(hexadecanoyloxy)-3-((9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl)oxy]propoxy]phosphonic acid'	b'PG(18:1(9Z)-O(12,13)/16:0)'	HMDB02	C40H75O11	

			002					68614	P	
		762.5047002	0.0027 002	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(14-methylpentadecanoyl)oxy]-2-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphinic acid'	b'PG(i-16:0/18:1(12Z)-O(9S,10R))'	HMDB02 71520	C40H75O11 P		
		762.5047002	0.0027 002	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(14-methylpentadecanoyl)oxy]-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphinic acid'	b'PG(18:1(12Z)-O(9S,10R)/i-16:0)'	HMDB02 71521	C40H75O11 P		
		762.5047002	0.0027 002	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(14-methylpentadecanoyl)oxy]-2-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphinic acid'	b'PG(i-16:0/18:1(9Z)-O(12,13))'	HMDB02 71522	C40H75O11 P		
		762.5047002	0.0027 002	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(14-methylpentadecanoyl)oxy]-3-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)-O(12,13)/i-16:0)'	HMDB02 71523	C40H75O11 P		
35 3	773.93 86	774.9483145	0.0019 145	Protona tion	b'[dichloro({(((2R,3S,4R,5R)-3,4-dihydroxy-5-(6-[[2-(methylsulfonyl)ethyl]amino)-2-[(3,3,3-trifluoropropyl)sulfonyl]-9H-purin-9-yl)oxolan-2-yl]methoxy)(hydroxy)phosphoryl)oxy)(hydroxy)phosphoryl)methyl]phosphonic acid'	b'Cangrelor'	HMDB02 40386	C17H25Cl2F3N5O12P 3S2		
35 4	774.53 87	774.5410853	0.0023 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(18:0/18:2(9Z,12Z))'	HMDB00 10605	C42H79O10 P		
		774.5410857	0.0023 857	Redox	b'[(2R)-2,3-bis[(11Z)-octadec-11-enoyloxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(18:1(11Z)/18:1(11Z))'	HMDB00 10618	C42H79O10 P		
		774.5410853	0.0023 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(11Z)-octadec-11-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(11Z)/18:1(9Z))'	HMDB00 10619	C42H79O10 P		
		774.5410853	0.0023 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(11Z)-octadec-11-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(18:1(9Z)/18:1(11Z))'	HMDB00 10633	C42H79O10 P		
		774.5410857	0.0023 857	Redox	b'[(2R)-2,3-bis[(9Z)-octadec-9-enoyloxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(18:1(9Z)/18:1(9Z))'	HMDB00 10634	C42H79O10 P		
		774.5410853	0.0023 853	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(18:2(9Z,12Z)/18:0)'	HMDB00 10647	C42H79O10 P		
		774.5410857	0.0023 857	Redox	b'[2,3-bis(octadec-9-enoyloxy)propoxy](2,3-dihydroxypropoxy)phosphinic acid'	b'1,2-Dioleoyl-sn-glycero-3-phosphoglycerol'	HMDB02 44089	C42H79O10 P		
35	776.54	776.5468398	0.0024	Redox	b'(2-[[[(2S,3R,4E)-3-hydroxy-2-[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenamido]heptadec-4-en-1-yl phosphono]oxy]ethyl)trimethylazanium']	b'SM(d17:1/22:6(5Z,7Z,10Z,13Z,16Z,1	HMDB02	C44H77N2O		

36	792.54	790.5360004	0.0009 004	Redox	b'[(2R)-3-((7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)cyclopentyl)heptanoyl)oxy)-2-((17-methyloctadecanoyl)oxy)propoxy]phosphonic acid'	b'PA(PGF1alpha/i-19:0)'	HMDB02 68135	C42H79O11 P	
		790.5360004	0.0009 004	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-((8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy)-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(18:0/18:1(12Z)-O(9S,10R))'	HMDB02 68819	C42H79O11 P	
		790.5360004	0.0009 004	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-((8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy)-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PG(18:1(12Z)-O(9S,10R)/18:0)'	HMDB02 68820	C42H79O11 P	
		790.5360004	0.0009 004	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(octadecanoyloxy)-2-(((9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl)oxy)propoxy]phosphinic acid'	b'PG(18:0/18:1(9Z)-O(12,13))'	HMDB02 68821	C42H79O11 P	
		790.5360004	0.0009 004	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-(octadecanoyloxy)-3-(((9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl)oxy)propoxy]phosphinic acid'	b'PG(18:1(9Z)-O(12,13)/18:0)'	HMDB02 68822	C42H79O11 P	
		790.5360004	0.0009 004	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-((16-methylheptadecanoyl)oxy)-2-((8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy)propoxy]phosphinic acid'	b'PG(i-18:0/18:1(12Z)-O(9S,10R))'	HMDB02 71728	C42H79O11 P	
		790.5360004	0.0009 004	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-((16-methylheptadecanoyl)oxy)-3-((8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy)propoxy]phosphinic acid'	b'PG(18:1(12Z)-O(9S,10R)/i-18:0)'	HMDB02 71729	C42H79O11 P	
		790.5360004	0.0009 004	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-((16-methylheptadecanoyl)oxy)-2-(((9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl)oxy)propoxy]phosphinic acid'	b'PG(i-18:0/18:1(9Z)-O(12,13))'	HMDB02 71730	C42H79O11 P	
		790.5360004	0.0009 004	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-((16-methylheptadecanoyl)oxy)-3-(((9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl)oxy)propoxy]phosphinic acid'	b'PG(18:1(9Z)-O(12,13)/i-18:0)'	HMDB02 71731	C42H79O11 P	
0	56	793.5526397	0.0007 603	Protone tion	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-(((2S)-1-hydroxy-3-(nonadecanoyloxy)propan-2-yl)oxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(19:0/LTE4/0:0)'	HMDB02 96091	C45H79NO8 S	
		793.5526397	0.0007 603	Protone tion	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-((2S)-3-hydroxy-2-(nonadecanoyloxy)propoxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(LTE4/19:0/0:0)'	HMDB02 96092	C45H79NO8 S	
		793.5526397	0.0007 603	Protone tion	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-((2R)-2-hydroxy-3-(nonadecanoyloxy)propoxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(19:0/0:0/LTE4)'	HMDB02 96093	C45H79NO8 S	
		793.5526397	0.0007 603	Protone tion	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-((2S)-2-hydroxy-3-(nonadecanoyloxy)propoxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(LTE4/0:0/19:0)'	HMDB02 96094	C45H79NO8 S	

		793.5526397	0.0007 603	Protona tion	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-((17-methyloctadecanoyl)oxy)propan-2-yl)oxy)-3-oxopropyl)sulfanyl]-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(i-19:0/LTE4/0:0)'	HMDB02 99831	C45H79NO8 S	
		793.5526397	0.0007 603	Protona tion	b'(5S,6R,7E,9E,11Z,14Z)-6-((2R)-2-amino-3-((2S)-3-hydroxy-2-((17-methyloctadecanoyl)oxy)propoxy)-3-oxopropyl)sulfanyl]-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(LTE4/i-19:0/0:0)'	HMDB02 99832	C45H79NO8 S	
		793.5526397	0.0007 603	Protona tion	b'(5S,6R,7E,9E,11Z,14Z)-6-((2R)-2-amino-3-((2R)-2-hydroxy-3-((17-methyloctadecanoyl)oxy)propoxy)-3-oxopropyl)sulfanyl]-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(i-19:0/0:0/LTE4)'	HMDB02 99833	C45H79NO8 S	
		793.5526397	0.0007 603	Protona tion	b'(5S,6R,7E,9E,11Z,14Z)-6-((2R)-2-amino-3-((2S)-3-hydroxy-3-((17-methyloctadecanoyl)oxy)propoxy)-3-oxopropyl)sulfanyl]-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'DG(LTE4/0:0/i-19:0)'	HMDB02 99834	C45H79NO8 S	
36 1	793.51 31	794.5213987	0.0004 987	Protona tion	b' {6-[2,3-bis(hexadecanoyloxy)propoxy]-3,4,5-trihydroxyoxan-2-yl}methanesulfonic acid'	b'1,2-Di-O-palmitoyl-3-O-(6-sulfoquinovopyranosyl)glycerol'	HMDB00 41202	C41H78O12 S	
		794.521019	0.0001 19	Protona tion	b'(2-(((2S,3R,4E,14Z)-3-hydroxy-2-((5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenamido)octadeca-4,14-dien-1-yl phosphono)oxy)ethyl)trimethylazanium'	b'SM(d18:2(4E,14Z)/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 90591	C43H75N2O 9P	
		793.5105139	0.0025 861	Redox	b'(2S)-2-amino-3-(((2R)-2-(((9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl)oxy)-3-(hexadecanoyloxy)propoxy)(hydroxy)phosphoryl)oxy)propanoic acid'	b'PS(16:0/18:1(12Z)-2OH(9,10))'	HMDB02 81164	C40H76NO1 2P	
		793.5105139	0.0025 861	Redox	b'(2S)-2-amino-3-(((2R)-3-(((9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl)oxy)-2-(hexadecanoyloxy)propoxy)(hydroxy)phosphoryl)oxy)propanoic acid'	b'PS(18:1(12Z)-2OH(9,10)/16:0)'	HMDB02 81165	C40H76NO1 2P	
36 2	796.52 82	796.5254352	0.0027 648	Redox	b'((2S)-2,3-dihydroxypropoxy)((2R)-2-((4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy)-3-(hexadecanoyloxy)propoxy)phosphinic acid'	b'PG(16:0/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB00 10582	C44H77O10 P	
		796.5254352	0.0027 648	Redox	b'((2S)-2,3-dihydroxypropoxy)((2R)-2-((7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy)-3-(hexadecanoyloxy)propoxy)phosphinic acid'	b'PG(16:0/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB00 10583	C44H77O10 P	
		796.5254352	0.0027 648	Redox	b'((2S)-2,3-dihydroxypropoxy)((2R)-2-((7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy)-3-((9Z)-hexadec-9-enoyloxy)propoxy)phosphinic acid'	b'PG(16:1(9Z)/22:4(7Z,10Z,13Z,16Z))'	HMDB00 10596	C44H77O10 P	
		796.5254352	0.0027 648	Redox	b'((2S)-2,3-dihydroxypropoxy)((2R)-2-((5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy)-3-((11Z)-octadec-11-enoyloxy)propoxy)phosphinic acid'	b'PG(18:1(11Z)/20:4(5Z,8Z,11Z,14Z))'	HMDB00 10625	C44H77O10 P	
		796.5254352	0.0027 648	Redox	b'((2S)-2,3-dihydroxypropoxy)((2R)-2-((5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy)-3-((9Z)-octadec-9-enoyloxy)propoxy)phosphinic acid'	b'PG(18:1(9Z)/20:4(5Z,8Z,11Z,14Z))'	HMDB00 10640	C44H77O10 P	

		796.5254352	0.0027 648	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(18:2(9Z,12Z)/20:3(5Z,8Z,11Z))'	HMDB00 10653	C44H77O10 P	
		796.5254352	0.0027 648	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(18:2(9Z,12Z)/20:3(8Z,11Z,14Z))'	HMDB00 10654	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(20:3(5Z,8Z,11Z)/18:2(9Z,12Z))'	HMDB01 16578	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]phosphinic acid'	b'PG(20:3(8Z,11Z,14Z)/18:2(9Z,12Z))'	HMDB01 16581	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PG(20:4(5Z,8Z,11Z,14Z)/18:1(11Z))'	HMDB01 16609	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PG(20:4(5Z,8Z,11Z,14Z)/18:1(9Z))'	HMDB01 16610	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-(hexadecanoyloxy)propoxy]phosphinic acid'	b'PG(22:5(7Z,10Z,13Z,16Z,19Z)/16:0)'	HMDB01 16621	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-(hexadecanoyloxy)propoxy]phosphinic acid'	b'PG(22:5(4Z,7Z,10Z,13Z,16Z)/16:0)'	HMDB01 16743	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2R)-3-(hencosanoyloxy)-2-([(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy)propoxy]phosphonic acid'	b'PA(21:0/PGJ2)'	HMDB02 65479	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2R)-2-(hencosanoyloxy)-3-([(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy)propoxy]phosphonic acid'	b'PA(PGJ2/21:0)'	HMDB02 65480	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2R)-2-([(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy)-3-[(18-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(a-21:0/PGJ2)'	HMDB02 67139	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2R)-3-([(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy)-3-[(18-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(PGJ2/a-21:0)'	HMDB02 67140	C44H77O10 P	
		796.5254357	0.0027 643	Redox	b'[(2R)-2-([(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy)-3-[(19-methylcosanoyl)oxy]propoxy]phosphonic acid'	b'PA(i-21:0/PGJ2)'	HMDB02 68278	C44H77O10 P	

		796.5254357	0.0027 643	Redox	b'[(2R)-3-{{(5Z)-7-{{(1S,5R)-5-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}}-4-oxocyclopent-2-en-1-yl}}hept-5-enoyl}oxy}-2-{{(19-methylcosanoyl}oxy)propoxy}]phosphonic acid'	b'PA(PGJ2/i-21:0)'	HMDB02 68279	C44H77O10 P	
36 3	806.54 13	806.541832	0.0005 32	Redox	b'N-{{1,6-dicyclohexyl-3,4-dihydroxy-5-{{3-methyl-2-{{(methyl[(pyridin-2-yl)methyl]carbamoyl}amino)butanamido]hexan-2-yl}}-3-methyl-2-{{(methyl[(pyridin-2-yl)methyl]carbamoyl}amino)butanamide}'	b'Inhibitor CC'	HMDB02 60354	C44H70N8O 6	
36 4	807.54 4	807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 61166	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy}-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/18:0)'	HMDB02 61167	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 61168	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy}-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/18:0)'	HMDB02 61169	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy}-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 61170	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy}-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/18:0)'	HMDB02 61171	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy}-3-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(18:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 61172	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy}-2-(octadecanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/18:0)'	HMDB02 61173	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-(octadecanoyloxy)-2-{{(4Z,7Z,10Z,13Z)-15-{{3-{{(2Z)-pent-2-en-1-yl}oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl}oxy}propoxy}]phosphinic acid'	b'PE(18:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 61176	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-(octadecanoyloxy)-3-{{(4Z,7Z,10Z,13Z)-15-{{3-{{(2Z)-pent-2-en-1-yl}oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl}oxy}propoxy}]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/18:0)'	HMDB02 61177	C45H78NO9 P	
		807.5414201	0.0025 799	Redox		b'PE(20:1(11Z)/20:4(6E,8Z,11Z,14Z)+=O(5))'	HMDB02 61968	C45H78NO9 P	

		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[[{(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z))+=O(5)/20:1(11Z))'	HMDB02 61969	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[(11Z)-icos-11-enoyloxy]-2-[[{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl]oxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(5Z,8Z,11Z,13E))+=O(15))'	HMDB02 61970	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[(11Z)-icos-11-enoyloxy]-3-[[{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E))+=O(15)/20:1(11Z))'	HMDB02 61971	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 61982	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/20:1(11Z))'	HMDB02 61983	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	HMDB02 61984	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)-OH(18)/20:1(11Z))'	HMDB02 61985	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:5(5Z,8Z,10E,14Z,17Z)-OH(12))'	HMDB02 61986	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)-OH(12)/20:1(11Z))'	HMDB02 61987	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[[{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 61988	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[[{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/20:1(11Z))'	HMDB02 61989	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]-2-[[{(5Z,8Z,11Z)-13-(3-pentyloxiran-2-yl)trideca-5,8,11-trienoyl]oxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:3(5Z,8Z,11Z)-O(14R,15S))'	HMDB02 62022	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]-3-[[{(5Z,8Z,11Z)-13-(3-pentyloxiran-2-yl)trideca-5,8,11-trienoyl]oxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)-O(14R,15S)/20:2(11Z,14Z))'	HMDB02 62023	C45H78NO9 P	

		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[(11Z,14Z)-icosa-11,14-dienyloxy]-2-[[{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyl}oxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:3(5Z,8Z,14Z)- O(11S,12R))'	HMDB02 62024	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[(11Z,14Z)-icosa-11,14-dienyloxy]-3-[[{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyl}oxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,14Z)- O(11S,12R)/20:2(11Z,14Z))'	HMDB02 62025	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[(11Z,14Z)-icosa-11,14-dienyloxy]-2-[[{(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl}oxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:3(5Z,11Z,14Z)- O(8,9))'	HMDB02 62026	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[(11Z,14Z)-icosa-11,14-dienyloxy]-3-[[{(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl}oxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,11Z,14Z)- O(8,9)/20:2(11Z,14Z))'	HMDB02 62027	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[(11Z,14Z)-icosa-11,14-dienyloxy]-2-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl}oxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:3(8Z,11Z,14Z)- O(5,6))'	HMDB02 62028	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[(11Z,14Z)-icosa-11,14-dienyloxy]-3-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl}oxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)- O(5,6)/20:2(11Z,14Z))'	HMDB02 62029	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoyl}oxy]-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14 Z)-OH(20))'	HMDB02 62030	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoyl}oxy]-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(20)/20:2(11Z,14Z))'	HMDB02 62031	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[[{(5R,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoyl}oxy]-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(6E,8Z,11Z,14 Z)-OH(5S))'	HMDB02 62032	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[[{(5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoyl}oxy]-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)- OH(5S)/20:2(11Z,14Z))'	HMDB02 62033	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,14Z,19S)-19-hydroxyicosa-5,8,11,14-tetraenoyl}oxy]-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14 Z)-OH(19S))'	HMDB02 62034	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[[{(5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoyl}oxy]-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(19S)/20:2(11Z,14Z))'	HMDB02 62035	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[[{(5Z,8Z,11Z,14Z,18R)-18-hydroxyicosa-5,8,11,14-tetraenoyl}oxy]-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14 Z)-OH(18R))'	HMDB02 62036	C45H78NO9 P	

		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,14Z,18S)-18-hydroxyicosa-5,8,11,14-tetraenyl}oxy}-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(18R)/20:2(11Z,14Z))'	HMDB02 62037	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenyl}oxy}-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14 Z)-OH(17))'	HMDB02 62038	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenyl}oxy}-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(17)/20:2(11Z,14Z))'	HMDB02 62039	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,14Z,16R)-16-hydroxyicosa-5,8,11,14-tetraenyl}oxy}-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,14 Z)-OH(16R))'	HMDB02 62040	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,14Z,16S)-16-hydroxyicosa-5,8,11,14-tetraenyl}oxy}-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(16R)/20:2(11Z,14Z))'	HMDB02 62041	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,13E,15S)-15-hydroxyicosa-5,8,11,13-tetraenyl}oxy}-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(5Z,8Z,11Z,13 E)-OH(15S))'	HMDB02 62042	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,13E,15R)-15-hydroxyicosa-5,8,11,13-tetraenyl}oxy}-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)- OH(15S)/20:2(11Z,14Z))'	HMDB02 62043	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,10E,12S,14Z)-12-hydroxyicosa-5,8,10,14-tetraenyl}oxy}-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(5Z,8Z,10E,14 Z)-OH(12S))'	HMDB02 62044	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenyl}oxy}-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,10E,14Z)- OH(12S)/20:2(11Z,14Z))'	HMDB02 62045	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5E,8Z,11R,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenyl}oxy}-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(5E,8Z,12Z,14 Z)-OH(11R))'	HMDB02 62046	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5E,8Z,11S,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenyl}oxy}-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:4(5E,8Z,12Z,14Z)- OH(11R)/20:2(11Z,14Z))'	HMDB02 62047	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenyl}oxy}-3-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:4(5Z,7E,11Z,14 Z)-OH(9))'	HMDB02 62048	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenyl}oxy}-2-[(11Z,14Z)-icosa-11,14-dienyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,7E,11Z,14Z)- OH(9)/20:2(11Z,14Z))'	HMDB02 62049	C45H78NO9 P	

		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{{(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl}oxy}-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)/20:3(6,8,11)-OH(5))'	HMDB02 62228	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{{(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl}oxy}-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(6,8,11)-OH(5)/20:3(5Z,8Z,11Z))'	HMDB02 62229	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{{(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl}oxy}-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)/20:3(6,8,11)-OH(5))'	HMDB02 62332	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{{(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl}oxy}-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(6,8,11)-OH(5)/20:3(8Z,11Z,14Z))'	HMDB02 62333	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphinic acid'	b'PE(22:4(7Z,10Z,13Z,16Z)/18:1(12Z)-O(9S,10R))'	HMDB02 84082	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl)oxy]propoxy]phosphinic acid'	b'PE(18:1(12Z)-O(9S,10R)/22:4(7Z,10Z,13Z,16Z))'	HMDB02 84083	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-{{{(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl}oxy}propoxy]phosphinic acid'	b'PE(22:4(7Z,10Z,13Z,16Z)/18:1(9Z)-O(12,13))'	HMDB02 84084	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-{{{(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl}oxy}propoxy]phosphinic acid'	b'PE(18:1(9Z)-O(12,13)/22:4(7Z,10Z,13Z,16Z))'	HMDB02 84085	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{{(5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S))'	HMDB02 85342	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{{(5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/P-18:0)'	HMDB02 85343	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-2-{{{(4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl}oxy}-3-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(P-18:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17))'	HMDB02 85358	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-aminoethoxy)[(2R)-3-{{{(4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl}oxy}-2-[(1E)-octadec-1-en-1-yloxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/P-18:0)'	HMDB02 85359	C45H78NO9 P	

		807.5414201	0.0025 799	Redox	b'(2-){[(2R)-2-]{[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy}-3-(pentadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(15:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 85868	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-){[(2R)-3-]{[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy}-2-(pentadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/15:0)'	HMDB02 85869	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-){[(2R)-2-]{[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy}-3-(pentadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(15:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 85870	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-){[(2R)-3-]{[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy}-2-(pentadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/15:0)'	HMDB02 85871	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-){[(2R)-2-]{[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl]oxy}-3-(pentadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(15:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 85872	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-){[(2R)-3-]{[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl]oxy}-2-(pentadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/15:0)'	HMDB02 85873	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-){[(2R)-2-]{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl]oxy}-3-(pentadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(15:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 85874	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'(2-){[(2R)-3-]{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl]oxy}-2-(pentadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/15:0)'	HMDB02 85875	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'trimethyl(2-){[(2R)-2-]{[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy}-3-(pentadecanoyloxy)propyl phosphono]oxy}ethyl)azanium'	b'PC(15:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 85878	C45H78NO9 P	
		807.5414201	0.0025 799	Redox	b'trimethyl(2-){[(2R)-3-]{[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy}-2-(pentadecanoyloxy)propyl phosphono]oxy}ethyl)azanium'	b'PC(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/15:0)'	HMDB02 85879	C45H78NO9 P	
36 5	808.54 6	808.546565	0.0005 65	Redox	b'[(2R)-2-]{[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-3-(octadecanoyloxy)propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(18:0/18:1(12Z)-2OH(9,10))'	HMDB02 68817	C42H81O12 P	
		808.546565	0.0005 65	Redox	b'[(2R)-3-]{[(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-2-(octadecanoyloxy)propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(18:1(12Z)-2OH(9,10)/18:0)'	HMDB02 68818	C42H81O12 P	
		808.546565	0.0005 65	Redox	b'[(2R)-2-]{[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-3-[(16-methylheptadecanoyl]oxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(i-18:0/18:1(12Z)-2OH(9,10))'	HMDB02 71726	C42H81O12 P	

		808.546565	0.0005 65	Redox	b'[(2R)-3-{{(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl}oxy}-2-[(16-methylheptadecanoyl)oxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(18:1(12Z)-2OH(9,10)/i-18:0)'	HMDB02 71727	C42H81O12 P	
36	821.54	821.541814	0.0002 14	Redox	b'(2S)-2-amino-3-{{(2R)-2-{{(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl}oxy}-3-(octadecanoyloxy)propoxy}(hydroxy)phosphoryl}oxy}propanoic acid'	b'PS(18:0/18:1(12Z)-2OH(9,10))'	HMDB02 81372	C42H80NO1 2P	
		821.541814	0.0002 14	Redox	b'(2S)-2-amino-3-{{(2R)-3-{{(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl}oxy}-2-(octadecanoyloxy)propoxy}(hydroxy)phosphoryl}oxy}propanoic acid'	b'PS(18:1(12Z)-2OH(9,10)/18:0)'	HMDB02 81373	C42H80NO1 2P	
36	824.54	825.5519848	0.0015 152	Protona tion	b'(2-aminoethoxy)[(2R)-2-{{(5Z)-7-{{(1S,5R)-5-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-4-oxocyclopent-2-en-1-yl}hept-5-enoyl}oxy}-3-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:0/PGJ2)'	HMDB02 61850	C45H80NO1 0P	
			0.0015 152	Protona tion	b'(2-aminoethoxy)[(2R)-3-{{(5Z)-7-{{(1S,5R)-5-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-4-oxocyclopent-2-en-1-yl}hept-5-enoyl}oxy}-2-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(PGJ2/20:0)'	HMDB02 61851	C45H80NO1 0P	
		825.5519848	0.0015 152	Protona tion	b'(2-aminoethoxy)[(2R)-2-{{(5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl}oxy}-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(6Z,8E,10E,14Z)- 2OH(5S,12R))'	HMDB02 61958	C45H80NO1 0P	
		825.5519848	0.0015 152	Protona tion	b'(2-aminoethoxy)[(2R)-3-{{(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl}oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6Z,8E,10E,14Z)- 2OH(5S,12R)/20:1(11Z))'	HMDB02 61959	C45H80NO1 0P	
		825.5519848	0.0015 152	Protona tion	b'(2-aminoethoxy)[(2R)-2-{{(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl}oxy}-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(6E,8Z,11Z,13E)- 2OH(5S,15S))'	HMDB02 61994	C45H80NO1 0P	
		825.5519848	0.0015 152	Protona tion	b'(2-aminoethoxy)[(2R)-3-{{(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl}oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/20:1(11Z))'	HMDB02 61995	C45H80NO1 0P	
		825.5519848	0.0015 152	Protona tion	b'(2-aminoethoxy)[(2R)-2-{{(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl}oxy}-3-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:1(11Z)/20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R))'	HMDB02 61996	C45H80NO1 0P	
		825.5519848	0.0015 152	Protona tion	b'(2-aminoethoxy)[(2R)-3-{{(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl}oxy}-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/20:1(11Z))'	HMDB02 61997	C45H80NO1 0P	
		825.5519848	0.0015 152	Protona tion	b'(2-aminoethoxy)[(2R)-2-{{(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl}oxy}-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphinic acid'	b'PE(20:2(11Z,14Z)/20:3(8Z,11Z,14Z)- 2OH(5,6))'	HMDB02 62068	C45H80NO1 0P	
		825.5519848	0.0015 152	Protona tion	b'(2-aminoethoxy)[(2R)-3-{{(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl}oxy}-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)- 2OH(5,6)/20:2(11Z,14Z))'	HMDB02 62069	C45H80NO1 0P	

		825.5519848	0.0015 152	Protone	b'(2-aminoethoxy)[(2R)-2-{{(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl}oxy}-3-{{(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy}propoxy}phosphinic acid'	b'PE(22:4(7Z,10Z,13Z,16Z)/18:1(12Z)- 2OH(9,10))'	HMDB02 84080	C45H80NO1 0P	
		825.5519848	0.0015 152	Protone	b'(2-aminoethoxy)[(2R)-3-{{(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl}oxy}-2-{{(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy}propoxy}phosphinic acid'	b'PE(18:1(12Z)- 2OH(9,10)/22:4(7Z,10Z,13Z,16Z))'	HMDB02 84081	C45H80NO1 0P	
		825.5519848	0.0015 152	Protone	b'(2-aminoethoxy)[(2R)-3-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-2-{{8-{{(2Z)-oct-2-en-1-yl}oxiran-2-yl}octanoyl}oxy}propoxy}phosphinic acid'	b'PE(DiMe(11,5)/18:1(12Z)- O(9S,10R))'	HMDB02 84810	C45H80NO1 0P	
		825.5519848	0.0015 152	Protone	b'(2-aminoethoxy)[(2R)-2-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-3-{{8-{{(2Z)-oct-2-en-1-yl}oxiran-2-yl}octanoyl}oxy}propoxy}phosphinic acid'	b'PE(18:1(12Z)- O(9S,10R)/DiMe(11,5))'	HMDB02 84811	C45H80NO1 0P	
		825.5519848	0.0015 152	Protone	b'(2-aminoethoxy)[(2R)-3-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-2-{{(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl}oxy}propoxy}phosphinic acid'	b'PE(DiMe(11,5)/18:1(9Z)-O(12,13))'	HMDB02 84812	C45H80NO1 0P	
		825.5519848	0.0015 152	Protone	b'(2-aminoethoxy)[(2R)-2-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-3-{{(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl}oxy}propoxy}phosphinic acid'	b'PE(18:1(9Z)-O(12,13)/DiMe(11,5))'	HMDB02 84813	C45H80NO1 0P	
		825.5519848	0.0015 152	Protone	b'(2-{{(2R)-3-(heptadecanoyloxy)-2-{{(5Z)-7-{{(1S,5R)-5-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-4-oxocyclopent-2-en-1-yl}hept-5-enoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(17:0/PGJ2)'	HMDB02 86135	C45H80NO1 0P	
		825.5519848	0.0015 152	Protone	b'(2-{{(2R)-2-(heptadecanoyloxy)-3-{{(5Z)-7-{{(1S,5R)-5-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-4-oxocyclopent-2-en-1-yl}hept-5-enoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(PGJ2/17:0)'	HMDB02 86136	C45H80NO1 0P	
		824.5441593	0.0015 407	Redox	b'(3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-2-{{11-(3-methyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(9,3)/MonoMe(11,3))'	HMDB00 61422	C45H79NO1 0P	
		824.5441593	0.0015 407	Redox	b'(3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-2-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(9,3)/MonoMe(9,5))'	HMDB00 61425	C45H79NO1 0P	
		824.5441593	0.0015 407	Redox	b'(2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-{{11-(3-methyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,3)/DiMe(9,3))'	HMDB00 61438	C45H79NO1 0P	
		824.5441593	0.0015 407	Redox	b'(2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(9,5)/DiMe(9,3))'	HMDB00 61465	C45H79NO1 0P	
36 8	830.51 83	831.526164	6.40E- 05	Protone	b'(2-aminoethoxy)[(2R)-2-{{7-{{(1R,2R,3R,5S)-3,5-dihydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}cyclopentyl}-6-oxoheptanoyl}oxy}-3-{{(11Z)-octadec-11- enoyloxy}propoxy}phosphinic acid'	b'PE(18:1(11Z)/6 keto-PGF1alpha)'	HMDB02 61222	C43H78NO1 2P	

36	834.52	831.526164	6.40E-05	Protocation	b'(2-aminoethoxy)[(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]-6-oxoheptanoyl}oxy)-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(6 keto-PGF1alpha/18:1(11Z))'	HMDB02 61223	C43H78NO1 2P	
		831.526164	6.40E-05	Protocation		b'PE(18:1(11Z)/TXB2)'	HMDB02 61232	C43H78NO1 2P	
		831.526164	6.40E-05	Protocation	b'(2-aminoethoxy)[(2R)-3-({(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl}oxy)-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphinic acid'	b'PE(TXB2/18:1(11Z))'	HMDB02 61233	C43H78NO1 2P	
		831.526164	6.40E-05	Protocation	b'(2-aminoethoxy)[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]-6-oxoheptanoyl}oxy)-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)/6 keto-PGF1alpha)'	HMDB02 61326	C43H78NO1 2P	
		831.526164	6.40E-05	Protocation		b'PE(6 keto-PGF1alpha/18:1(9Z))'	HMDB02 61327	C43H78NO1 2P	
		831.526164	6.40E-05	Protocation	b'(2-aminoethoxy)[(2R)-2-({(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl}oxy)-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(18:1(9Z)/TXB2)'	HMDB02 61336	C43H78NO1 2P	
		831.526164	6.40E-05	Protocation	b'(2-aminoethoxy)[(2R)-3-({(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl}oxy)-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphinic acid'	b'PE(TXB2/18:1(9Z))'	HMDB02 61337	C43H78NO1 2P	
	48	834.5258296	0.0010296	Redox	b'[(2R)-3-(hexadecanoyloxy)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]({[(1S,2R,3R,4S,5S,6R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(16:0/18:2(9Z,12Z))'	HMDB00 09784	C43H79O13 P	
		834.5258291	0.0010291	Redox	b'[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(16:1(9Z)/18:1(11Z))'	HMDB00 09800	C43H79O13 P	
		834.5258291	0.0010291	Redox	b'[(2R)-3-[(9Z)-hexadec-9-enoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(16:1(9Z)/18:1(9Z))'	HMDB00 09801	C43H79O13 P	C006 26
		834.5258291	0.0010291	Redox	b'[(2R)-3-[(9Z,12Z)-hexadeca-9,12-dienoyloxy]-2-(octadecanoyloxy)propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(16:2(9Z,12Z)/18:0)'	HMDB00 09803	C43H79O13 P	
		834.5258291	0.0010291	Redox	b'[(2R)-2-[(9Z,12Z)-hexadeca-9,12-dienoyloxy]-3-(octadecanoyloxy)propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:0/16:2(9Z,12Z))'	HMDB00 09807	C43H79O13 P	
		834.5258291	0.0010291	Redox	b'[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy]({[(1S,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(11Z)/16:1(9Z))'	HMDB00 09823	C43H79O13 P	

		834.5258291	0.0010 291	Redox	b'[(2R)-2-[(9Z)-hexadec-9-enoyloxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy]({[(1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:1(9Z)/16:1(9Z))'	HMDB00 09835	C43H79O13 P	
		834.5258291	0.0010 291	Redox	b'[(2R)-2-(hexadecanoyloxy)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy]({[(1s,3R)-2,3,4,5,6-pentahydroxycyclohexyl]oxy})phosphinic acid'	b'PI(18:2(9Z,12Z)/16:0)'	HMDB00 09846	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2R)-2-({[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl]oxy}-3-[(14-methylhexadecanoyl]oxy)propoxy]((2S)-2,3-dihydroxypropoxy)phosphinic acid'	b'PG(a-17:0/PGF2alpha)'	HMDB02 70768	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2R)-3-({[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl]oxy}-2-[(14-methylhexadecanoyl]oxy)propoxy]((2S)-2,3-dihydroxypropoxy)phosphinic acid'	b'PG(PGF2alpha/a-17:0)'	HMDB02 70769	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-2-({[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl]oxy)-3-[(14-methylhexadecanoyl]oxy)propoxy)phosphinic acid'	b'PG(a-17:0/PGE1)'	HMDB02 70829	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-3-({[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl]oxy)-2-[(14-methylhexadecanoyl]oxy)propoxy)phosphinic acid'	b'PG(PGE1/a-17:0)'	HMDB02 70830	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-2-({[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl]oxy)-3-[(14-methylhexadecanoyl]oxy)propoxy)phosphinic acid'	b'PG(a-17:0/PGD1)'	HMDB02 70831	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-3-({[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl]oxy)-2-[(14-methylhexadecanoyl]oxy)propoxy)phosphinic acid'	b'PG(PGD1/a-17:0)'	HMDB02 70832	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2R)-2-({[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl]oxy}-3-[(15-methylhexadecanoyl]oxy)propoxy]((2S)-2,3-dihydroxypropoxy)phosphinic acid'	b'PG(i-17:0/PGF2alpha)'	HMDB02 71598	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2R)-3-({[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl]oxy}-2-[(15-methylhexadecanoyl]oxy)propoxy]((2S)-2,3-dihydroxypropoxy)phosphinic acid'	b'PG(PGF2alpha/i-17:0)'	HMDB02 71599	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-2-({[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl]oxy)-3-[(15-methylhexadecanoyl]oxy)propoxy)phosphinic acid'	b'PG(i-17:0/PGE1)'	HMDB02 71660	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-3-({[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl]oxy)-2-[(15-methylhexadecanoyl]oxy)propoxy)phosphinic acid'	b'PG(PGE1/i-17:0)'	HMDB02 71661	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2S)-2,3-dihydroxypropoxy]((2R)-2-({[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl]oxy)-3-[(15-methylhexadecanoyl]oxy)propoxy)phosphinic acid'	b'PG(i-17:0/PGD1)'	HMDB02 71662	C43H79O13 P	

		834.5258296	0.0010 296	Redox	b'[(2S)-2,3-dihydroxypropoxy][(2R)-3-({17-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-2-[(1S-methylhexadecanoyl)oxy]propoxy]phosphinic acid'	b'PG(PGD1/i-17:0)'	HMDB02 71663	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2R)-2-[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl]oxy]-3-[(17-methyloctadecanoyl)oxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(i-19:0/5-iso PGF2VI)'	HMDB02 71820	C43H79O13 P	
		834.5258296	0.0010 296	Redox	b'[(2R)-3-[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl]oxy]-2-[(17-methyloctadecanoyl)oxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(5-iso PGF2VI/i-19:0)'	HMDB02 71821	C43H79O13 P	
37 0	835.57 49	835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl]oxy]-3-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 61894	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl]oxy]-2-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/20:0)'	HMDB02 61895	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl]oxy]-3-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 61896	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl]oxy]-2-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/20:0)'	HMDB02 61897	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy]-3-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 61898	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy]-2-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/20:0)'	HMDB02 61899	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy]-3-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(20:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 61900	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy]-2-(icosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/20:0)'	HMDB02 61901	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-(icosanoyloxy)-2-[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy]propoxy]phosphinic acid'	b'PE(20:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 61904	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-(icosanoyloxy)-3-[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy]propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/20:0)'	HMDB02 61905	C47H82NO9 P	

		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[[(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(6E,8Z,11Z,14Z)+= O(5))'	HMDB02 83864	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[[(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)+=O(5)/22:1(13Z))'	HMDB02 83865	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,13E)+= O(15))'	HMDB02 83866	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)+=O(15)/22: 1(13Z))'	HMDB02 83867	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[[(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:5(5Z,8Z,11Z,14Z,16 E)-OH(18R))'	HMDB02 83878	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[[(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl]oxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/22:1(13Z))'	HMDB02 83879	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:5(5Z,8Z,11Z,14Z,16 E)-OH(18))'	HMDB02 83880	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl]oxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/22:1(13Z))'	HMDB02 83881	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[[(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:5(5Z,8Z,10E,14Z,17 Z)-OH(12))'	HMDB02 83882	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[[(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl]oxy]propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/22:1(13Z))'	HMDB02 83883	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[[(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:5(6E,8Z,11Z,14Z,17 Z)-OH(5))'	HMDB02 83884	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[[(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl]oxy]propoxy]phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/22:1(13Z))'	HMDB02 83885	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[[(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl]oxy]propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:3(5Z,8Z,11Z)- O(14R,15S))'	HMDB02 83918	C47H82NO9 P	

		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienoyl]oxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)- O(14R,15S)/22:2(13Z,16Z))'	HMDB02 83919	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:3(5Z,8Z,14Z)- O(11S,12R))'	HMDB02 83920	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyl]oxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,14Z)- O(11S,12R)/22:2(13Z,16Z))'	HMDB02 83921	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:3(5Z,11Z,14Z)- O(8,9))'	HMDB02 83922	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl]oxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,11Z,14Z)- O(8,9)/22:2(13Z,16Z))'	HMDB02 83923	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:3(8Z,11Z,14Z)- O(5,6))'	HMDB02 83924	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl]oxy}propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)- O(5,6)/22:2(13Z,16Z))'	HMDB02 83925	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(5Z,8Z,11Z,14 Z)-OH(20))'	HMDB02 83926	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(20)/22:2(13Z,16Z))'	HMDB02 83927	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5R,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(6E,8Z,11Z,14 Z)-OH(5S))'	HMDB02 83928	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)- OH(5S)/22:2(13Z,16Z))'	HMDB02 83929	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5Z,8Z,11Z,14Z,19S)-19-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(5Z,8Z,11Z,14 Z)-OH(19S))'	HMDB02 83930	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(19S)/22:2(13Z,16Z))'	HMDB02 83931	C47H82NO9 P	

		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5Z,8Z,11Z,14Z,18R)-18-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(5Z,8Z,11Z,14Z)-OH(18R))'	HMDB02 83932	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5Z,8Z,11Z,14Z,18S)-18-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)-OH(18R)/22:2(13Z,16Z))'	HMDB02 83933	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(5Z,8Z,11Z,14Z)-OH(17))'	HMDB02 83934	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)-OH(17)/22:2(13Z,16Z))'	HMDB02 83935	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5Z,8Z,11Z,14Z,16R)-16-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(5Z,8Z,11Z,14Z)-OH(16R))'	HMDB02 83936	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5Z,8Z,11Z,14Z,16S)-16-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)-OH(16R)/22:2(13Z,16Z))'	HMDB02 83937	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5Z,8Z,11Z,13E,15S)-15-hydroxyicosa-5,8,11,13-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(5Z,8Z,11Z,13E)-OH(15S))'	HMDB02 83938	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5Z,8Z,11Z,13E,15R)-15-hydroxyicosa-5,8,11,13-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)-OH(15S)/22:2(13Z,16Z))'	HMDB02 83939	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5Z,8Z,10E,12S,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(5Z,8Z,10E,14Z)-OH(12S))'	HMDB02 83940	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,10E,14Z)-OH(12S)/22:2(13Z,16Z))'	HMDB02 83941	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5E,8Z,11R,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(5E,8Z,12Z,14Z)-OH(11R))'	HMDB02 83942	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[{(5E,8Z,11S,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5E,8Z,12Z,14Z)-OH(11R)/22:2(13Z,16Z))'	HMDB02 83943	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[[{(5E,7Z,11Z,14Z)-9-hydroxyicosa-5,7,11,14-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:4(5Z,7E,11Z,14Z)-OH(9))'	HMDB02 83944	C47H82NO9 P	

		835.5727202	0.0021 798	Redox	b'(2-aminoethoxy)((2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[[5E,7Z,11Z,14Z]-9-hydroxyicosa-5,7,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,7E,11Z,14Z)-OH(9)/22:2(13Z,16Z))'	HMDB02 83945	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-[[[(2R)-3-(heptadecanoyloxy)-2-[[5Z,7Z,10Z,13Z,16Z,19Z]-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy]propyl phosphono]oxy]ethyl)trimethylazanium'	b'PC(17:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 86179	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-[[[(2R)-2-(heptadecanoyloxy)-3-[[5Z,7Z,10Z,13Z,16Z,19Z]-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy]propyl phosphono]oxy]ethyl)trimethylazanium'	b'PC(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/17:0)'	HMDB02 86180	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-[[[(2R)-3-(heptadecanoyloxy)-2-[[4Z,8Z,10Z,13Z,16Z,19Z]-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy]propyl phosphono]oxy]ethyl)trimethylazanium'	b'PC(17:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 86181	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-[[[(2R)-2-(heptadecanoyloxy)-3-[[4Z,8Z,10Z,13Z,16Z,19Z]-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy]propyl phosphono]oxy]ethyl)trimethylazanium'	b'PC(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/17:0)'	HMDB02 86182	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-[[[(2R)-3-(heptadecanoyloxy)-2-[[4Z,7Z,10Z,12E,16Z,19Z]-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl]oxy]propyl phosphono]oxy]ethyl)trimethylazanium'	b'PC(17:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 86183	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-[[[(2R)-2-(heptadecanoyloxy)-3-[[4Z,7Z,10Z,12E,16Z,19Z]-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl]oxy]propyl phosphono]oxy]ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/17:0)'	HMDB02 86184	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-[[[(2R)-3-(heptadecanoyloxy)-2-[[4Z,7Z,10Z,13E,15E,19Z]-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl]oxy]propyl phosphono]oxy]ethyl)trimethylazanium'	b'PC(17:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 86185	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-[[[(2R)-2-(heptadecanoyloxy)-3-[[4Z,7Z,10Z,13E,15E,19Z]-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl]oxy]propyl phosphono]oxy]ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/17:0)'	HMDB02 86186	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-[[[(2R)-3-(heptadecanoyloxy)-2-[[4Z,7Z,10Z,13Z]-15-{3-[[2Z]-pent-2-en-1-yl]oxiran-2-yl}]pentadeca-4,7,10,13-tetraenyl]oxy]propyl phosphono]oxy]ethyl)trimethylazanium'	b'PC(17:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 86189	C47H82NO9 P	
		835.5727202	0.0021 798	Redox	b'(2-[[[(2R)-2-(heptadecanoyloxy)-3-[[4Z,7Z,10Z,13Z]-15-{3-[[2Z]-pent-2-en-1-yl]oxiran-2-yl}]pentadeca-4,7,10,13-tetraenyl]oxy]propyl phosphono]oxy]ethyl)trimethylazanium'	b'PC(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/17:0)'	HMDB02 86190	C47H82NO9 P	
37 1	836.58 03	837.5883703	0.0002 703	Protontaion	b'(2-aminoethoxy)((2R)-3-(docosanoyloxy)-2-[[6E,8Z,11Z,14Z]-5-oxoicosa-6,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:0/20:4(6E,8Z,11Z,14Z)+=O(5)) ,	HMDB02 83760	C47H84NO9 P	
		837.5883703	0.0002 703	Protontaion	b'(2-aminoethoxy)((2R)-2-(docosanoyloxy)-3-[[6E,8Z,11Z,14Z]-5-oxoicosa-6,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)+=O(5)/22:0) ,	HMDB02 83761	C47H84NO9 P	

		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-3-(docosanoyloxy)-2-{{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/20:4(5Z,8Z,11Z,13E)+=O(15))'	HMDB02 83762	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-2-(docosanoyloxy)-3-{{(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl}oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)+=O(15)/22:0)'	HMDB02 83763	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-3-(docosanoyloxy)-2-{{(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 83774	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-2-(docosanoyloxy)-3-{{(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/22:0)'	HMDB02 83775	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-3-(docosanoyloxy)-2-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	HMDB02 83776	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-2-(docosanoyloxy)-3-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)-OH(18)/22:0)'	HMDB02 83777	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-3-(docosanoyloxy)-2-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/20:5(5Z,8Z,10E,14Z,17Z)-OH(12))'	HMDB02 83778	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-2-(docosanoyloxy)-3-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)-OH(12)/22:0)'	HMDB02 83779	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-3-(docosanoyloxy)-2-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(22:0/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 83780	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-2-(docosanoyloxy)-3-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl}oxy}propoxy]phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/22:0)'	HMDB02 83781	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-3-[(13Z)-docos-13-enoyloxy]-2-{{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl}oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:3(5Z,8Z,11Z)-O(14R,15S))'	HMDB02 83814	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-2-[(13Z)-docos-13-enoyloxy]-3-{{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl}oxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)-O(14R,15S)/22:1(13Z))'	HMDB02 83815	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)((2R)-3-[(13Z)-docos-13-enoyloxy]-2-{{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienyl}oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:3(5Z,8Z,14Z)-O(11S,12R))'	HMDB02 83816	C47H84NO9 P	

		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienyl]oxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,14Z)- O(11S,12R)/22:1(13Z))'	HMDB02 83817	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:3(5Z,11Z,14Z)- O(8,9))'	HMDB02 83818	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl]oxy]propoxy]phosphinic acid'	b'PE(20:3(5Z,11Z,14Z)- O(8,9)/22:1(13Z))'	HMDB02 83819	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-2-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:3(8Z,11Z,14Z)- O(5,6))'	HMDB02 83820	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl]oxy]propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)- O(5,6)/22:1(13Z))'	HMDB02 83821	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(5Z,8Z,11Z,14Z)-20-hydroxycosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)- OH(20))'	HMDB02 83822	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(5Z,8Z,11Z,14Z)-20-hydroxycosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(20)/22:1(13Z))'	HMDB02 83823	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(5R,6E,8Z,11Z,14Z)-5-hydroxycosa-6,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(6E,8Z,11Z,14Z)- OH(5S))'	HMDB02 83824	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(5S,6E,8Z,11Z,14Z)-5-hydroxycosa-6,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)- OH(5S)/22:1(13Z))'	HMDB02 83825	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(5Z,8Z,11Z,14Z,19S)-19-hydroxycosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)- OH(19S))'	HMDB02 83826	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(5Z,8Z,11Z,14Z,19R)-19-hydroxycosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(19S)/22:1(13Z))'	HMDB02 83827	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(5Z,8Z,11Z,14Z,18R)-18-hydroxycosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)- OH(18R))'	HMDB02 83828	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(5Z,8Z,11Z,14Z,18S)-18-hydroxycosa-5,8,11,14-tetraenyl]oxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(18R)/22:1(13Z))'	HMDB02 83829	C47H84NO9 P	

		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[{(5Z,8Z,11Z,14Z)-17-hydroxyicos-5,8,11,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)- OH(17))'	HMDB02 83830	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(5Z,8Z,11Z,14Z)-17-hydroxyicos-5,8,11,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(17)/22:1(13Z))'	HMDB02 83831	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[{(5Z,8Z,11Z,14Z,16R)-16-hydroxyicos-5,8,11,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,14Z)- OH(16R))'	HMDB02 83832	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(5Z,8Z,11Z,14Z,16S)-16-hydroxyicos-5,8,11,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(16R)/22:1(13Z))'	HMDB02 83833	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[{(5Z,8Z,11Z,13E,15S)-15-hydroxyicos-5,8,11,13-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,11Z,13E)- OH(15S))'	HMDB02 83834	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(5Z,8Z,11Z,13E,15R)-15-hydroxyicos-5,8,11,13-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)- OH(15S)/22:1(13Z))'	HMDB02 83835	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[{(5Z,8Z,10E,12S,14Z)-12-hydroxyicos-5,8,10,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,8Z,10E,14Z)- OH(12S))'	HMDB02 83836	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(5Z,8Z,10E,12R,14Z)-12-hydroxyicos-5,8,10,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,10E,14Z)- OH(12S)/22:1(13Z))'	HMDB02 83837	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[{(5E,8Z,11R,12Z,14Z)-11-hydroxyicos-5,8,12,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5E,8Z,12Z,14Z)- OH(11R))'	HMDB02 83838	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(5E,8Z,11S,12Z,14Z)-11-hydroxyicos-5,8,12,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5E,8Z,12Z,14Z)- OH(11R)/22:1(13Z))'	HMDB02 83839	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[{(5E,7Z,11Z,14Z)-9-hydroxyicos-5,7,11,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(5Z,7E,11Z,14Z)- OH(9))'	HMDB02 83840	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(5E,7Z,11Z,14Z)-9-hydroxyicos-5,7,11,14-tetraenyl]oxy}propoxy]phosphinic acid'	b'PE(20:4(5Z,7E,11Z,14Z)- OH(9)/22:1(13Z))'	HMDB02 83841	C47H84NO9 P	
		837.5883703	0.0002 703	Protone	b'(2-aminoethoxy)[(2R)-3-[(13Z,16Z)-docos-13,16-dienoyloxy]-2-[[{(6E,8E,11E)-5-hydroxyicos-6,8,11-trienyl]oxy}propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/20:3(6,8,11)- OH(5))'	HMDB02 84020	C47H84NO9 P	

		837.5883703	0.0002 703	Protona tion	b'(2-aminoethoxy)[(2R)-2-[(13Z,16Z)-docosa-13,16-dienyloxy]-3-[[[6E,8E,11E]-5-hydroxyicosa-6,8,11-trienoyl]oxy]propoxy]phosphinic acid'	b'PE(20:3(6,8,11)- OH(5)/22:2(13Z,16Z))'	HMDB02 84021	C47H84NO9 P	
		836.5778652	0.0024 348	Redox	b'[(2R)-2-[[[9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-3-[(18-methylnonadecanoyl)oxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(i-20:0/18:1(12Z)-2OH(9,10))'	HMDB02 71934	C44H85O12 P	
		836.5778652	0.0024 348	Redox	b'[(2R)-3-[[[9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-2-[(18-methylnonadecanoyl)oxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(18:1(12Z)-2OH(9,10)/i-20:0)'	HMDB02 71935	C44H85O12 P	
37	849.57 18	849.5731141	0.0013 141	Redox	b'(2S)-2-amino-3-[[[2R)-2-[[[9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-3-(icosanoyloxy)propoxy](hydroxy)phosphoryl]oxy]propanoic acid'	b'PS(20:0/18:1(12Z)-2OH(9,10))'	HMDB02 82099	C44H84NO1 2P	
		849.5731141	0.0013 141	Redox	b'(2S)-2-amino-3-[[[2R)-3-[[[9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy]-2-(icosanoyloxy)propoxy](hydroxy)phosphoryl]oxy]propanoic acid'	b'PS(18:1(12Z)-2OH(9,10)/20:0)'	HMDB02 82100	C44H84NO1 2P	
37	853.58 49	853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-[[[5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy]propoxy]phosphinic acid'	b'PE(22:0/PGJ2)'	HMDB02 83746	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-[[[5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy]propoxy]phosphinic acid'	b'PE(PGJ2/22:0)'	HMDB02 83747	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-2-[[[5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl]oxy]-3-[(13Z)-docos-13-enoyloxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(6Z,8E,10E,14Z)- 2OH(5S,12R))'	HMDB02 83854	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-3-[[[5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl]oxy]-2-[(13Z)-docos-13-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6Z,8E,10E,14Z)- 2OH(5S,12R)/22:1(13Z))'	HMDB02 83855	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-2-[[[5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy]-3-[(13Z)-docos-13-enoyloxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(6E,8Z,11Z,13E)- 2OH(5S,15S))'	HMDB02 83890	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-3-[[[5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy]-2-[(13Z)-docos-13-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/22:1(13Z))'	HMDB02 83891	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-2-[[[5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy]-3-[(13Z)-docos-13-enoyloxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R))'	HMDB02 83892	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-3-[[[5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy]-2-[(13Z)-docos-13-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/22:1(13Z))'	HMDB02 83893	C47H84NO1 0P	

		853.5832849	0.0016 151	Redox		b'PE(22:2(13Z,16Z)/20:3(8Z,11Z,14Z)- 2OH(5,6))'	HMDB02 83964	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-3-{{(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl}oxy}-2-[(13Z,16Z)-docosa-13,16-dienoyl}oxy]propoxy]phosphonic acid'	b'PE(20:3(8Z,11Z,14Z)- 2OH(5,6)/22:2(13Z,16Z))'	HMDB02 83965	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-3-{{[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy}-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl} octanoyl)oxy]propoxy]phosphonic acid'	b'PE(DiMe(13,5)/18:1(12Z)- O(9S,10R))'	HMDB02 84914	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-2-{{[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy}-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl} octanoyl)oxy]propoxy]phosphonic acid'	b'PE(18:1(12Z)- O(9S,10R)/DiMe(13,5))'	HMDB02 84915	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-3-{{[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy}-2-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphonic acid'	b'PE(DiMe(13,5)/18:1(9Z)-O(12,13))'	HMDB02 84916	C47H84NO1 0P	
		853.5832849	0.0016 151	Redox	b'(2-aminoethoxy)[(2R)-2-{{[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy}-3-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]propoxy]phosphonic acid'	b'PE(18:1(9Z)-O(12,13)/DiMe(13,5))'	HMDB02 84917	C47H84NO1 0P	
37 4	854.60 13	854.603686	0.0023 86	Redox	b'[(2R)-2-{{[(5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl]oxy}-3-[(22-methyltracosanoyl)oxy]propoxy]phosphonic acid'	b'PA(a-25:0/20:4(6Z,8E,10E,14Z)- 2OH(5S,12R))'	HMDB02 67247	C48H87O10 P	
		854.603686	0.0023 86	Redox	b'[(2R)-3-{{[(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl]oxy}-2-[(22-methyltracosanoyl)oxy]propoxy]phosphonic acid'	b'PA(20:4(6Z,8E,10E,14Z)- 2OH(5S,12R)/a-25:0)'	HMDB02 67248	C48H87O10 P	
		854.603686	0.0023 86	Redox	b'[(2R)-2-{{[(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy}-3-[(22-methyltracosanoyl)oxy]propoxy]phosphonic acid'	b'PA(a-25:0/20:4(6E,8Z,11Z,13E)- 2OH(5S,15S))'	HMDB02 67283	C48H87O10 P	
		854.603686	0.0023 86	Redox	b'[(2R)-3-{{[(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy}-2-[(22-methyltracosanoyl)oxy]propoxy]phosphonic acid'	b'PA(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/a-25:0)'	HMDB02 67284	C48H87O10 P	
		854.603686	0.0023 86	Redox	b'[(2R)-2-{{[(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy}-3-[(22-methyltracosanoyl)oxy]propoxy]phosphonic acid'	b'PA(a-25:0/20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R))'	HMDB02 67285	C48H87O10 P	
		854.603686	0.0023 86	Redox	b'[(2R)-3-{{[(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy}-2-[(22-methyltracosanoyl)oxy]propoxy]phosphonic acid'	b'PA(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/a-25:0)'	HMDB02 67286	C48H87O10 P	
37 5	856.60 55	857.614585	0.0012 85	Protone tion	b'(2-aminoethoxy)[(2R)-2-{{(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl}oxy}-3-(docosanoyl)oxy]propoxy]phosphonic acid'	b'PE(22:0/20:3(8Z,11Z,14Z)-2OH(5,6))'	HMDB02 83756	C47H88NO1 0P	

		857.614585	0.0012 85	Protone	b'(2-aminoethoxy)[(2R)-3-[[[(8Z,11Z,14Z)-5,6-dihydroxycosa-8,11,14-trienyl]oxy]-2-(docosanoyloxy)propoxy]phosphonic acid'	b'PE(20:3(8Z,11Z,14Z)-2OH(5,6)/22:0)	HMDB02 83757	C47H88NO1 0P	
37	857.51	858.5193049	0.0002 951	Protone	b'(5S,6R,7E,9E,11Z,14Z)-6-[[[(2R)-2-amino-3-[[[(2-aminooethoxy)(hydroxy)phosphoryl]oxy]-3-(hexadec-1-en-1-yloxy)propan-2-yl]oxy]-3-oxopropyl]sulfanyl]-5-hydroxycosa-7,9,11,14-tetraenoic acid'	b'PE(P-16:0/LTE4)	HMDB02 85204	C44H79N2O 10PS	
6	18	858.5193049	0.0002 951	Protone	b'(5S,6R,7E,9E,11Z,14Z)-6-[[[(2R)-2-amino-3-[(2R)-3-[[[(2-aminooethoxy)(hydroxy)phosphoryl]oxy]-2-(hexadec-1-en-1-yloxy)propoxy]-3-oxopropyl]sulfanyl]-5-hydroxycosa-7,9,11,14-tetraenoic acid'	b'PE(LTE4/P-16:0)	HMDB02 85205	C44H79N2O 10PS	
37	857.56	858.5692281	0.0018 719	Protone	b'([[(3,7,11,15,19,23,27,31,35,39-decamethyltetraconta-2,6,10,14,18,22,26,30,34,38-decaen-1-yl)oxy](hydroxy)phosphoryl]oxy]phosphonic acid'	b'all-trans-Decaprenyl diphosphate'	HMDB00 59616	C50H84O7P 2	C174 32
37	858.51	859.5210786	0.0024 214	Protone	b'(2S)-2-amino-3-(hydroxy[(2R)-2-[[[(5Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]hept-5-enoyl]oxy]-3-(octadecanoyloxy)propoxy]phosphoryl]oxy]propanoic acid'	b'PS(18:0/PGE2)	HMDB02 81342	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone	b'(2S)-2-amino-3-(hydroxy[(2R)-3-[[[(5Z)-7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]hept-5-enoyl]oxy]-2-(octadecanoyloxy)propoxy]phosphoryl]oxy]propanoic acid'	b'PS(PGE2/18:0)	HMDB02 81343	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone	b'(2S)-2-amino-3-(hydroxy[(2R)-2-[[[(5Z)-7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]hept-5-enoyl]oxy]-3-(octadecanoyloxy)propoxy]phosphoryl]oxy]propanoic acid'	b'PS(18:0/PGD2)	HMDB02 81344	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone	b'(2S)-2-amino-3-(hydroxy[(2R)-3-[[[(5Z)-7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]hept-5-enoyl]oxy]-2-(octadecanoyloxy)propoxy]phosphoryl]oxy]propanoic acid'	b'PS(PGD2/18:0)	HMDB02 81345	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone	b'(2S)-2-amino-3-(hydroxy[(2R)-3-(octadecanoyloxy)-2-[[[(5S,6S,7E,9E,11Z,13E,15S)-5,6,15-trihydroxycosa-7,9,11,13-tetraenyl]oxy]propoxy]phosphoryl]oxy]propanoic acid'	b'PS(18:0/20:4(7E,9E,11Z,13E)-3OH(5S,6R,15S))	HMDB02 81358	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone	b'(2S)-2-amino-3-(hydroxy[(2R)-2-(octadecanoyloxy)-3-[[[(5R,6R,7E,9E,11Z,13E,15R)-5,6,15-trihydroxycosa-7,9,11,13-tetraenyl]oxy]propoxy]phosphoryl]oxy]propanoic acid'	b'PS(20:4(7E,9E,11Z,13E)-3OH(5S,6R,15S)/18:0)	HMDB02 81359	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone	b'(2S)-2-amino-3-([[(2R)-2-[[[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl]oxy]-3-[(11Z)-octadec-11-enoyloxy]propoxy](hydroxy)phosphoryl]oxy]propanoic acid'	b'PS(18:1(11Z)/PGF2alpha)	HMDB02 81452	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone	b'(2S)-2-amino-3-([[(2R)-3-[[[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl]oxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy](hydroxy)phosphoryl]oxy]propanoic acid'	b'PS(PGF2alpha/18:1(11Z))	HMDB02 81453	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone	b'(2S)-2-amino-3-(hydroxy[(2R)-2-(7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl]oxy)-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphoryl]oxy]propanoic acid'	b'PS(18:1(11Z)/PGE1)	HMDB02 81514	C44H78NO1 3P	

		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({hydroxy[(2R)-3-({7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGE1/18:1(11Z))'	HMDB02 81515	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({hydroxy[(2R)-3-({7-[(1R,2R,3R)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-3-[(11Z)-octadec-11-enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(18:1(11Z)/PGD1))'	HMDB02 81516	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion		b'PS(PGD1/18:1(11Z))'	HMDB02 81517	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({[(2R)-3- {[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl}oxy]-3-[(9Z)-octadec-9-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(18:1(9Z)/PGF2alpha))'	HMDB02 81556	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({[(2R)-3- {[(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]hept-5-enoyl}oxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(PGF2alpha/18:1(9Z))'	HMDB02 81557	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(18:1(9Z)/PGE1))'	HMDB02 81618	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({hydroxy[(2R)-3-({7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGE1/18:1(9Z))'	HMDB02 81619	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-3-[(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(18:1(9Z)/PGD1))'	HMDB02 81620	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({hydroxy[(2R)-3-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGD1/18:1(9Z))'	HMDB02 81621	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(18:2(9Z,12Z)/PGF1alpha))'	HMDB02 81726	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({[(2R)-3-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(9Z,12Z)-octadeca-9,12-dienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(PGF1alpha/18:2(9Z,12Z))'	HMDB02 81727	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({[(2R)-2- {[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy]-3-[(11Z)-icos-11-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:1(11Z)/5-iso PGF2VI))'	HMDB02 82193	C44H78NO1 3P	
		859.5210786	0.0024 214	Protone tion	b'(2S)-2-amino-3-({[(2R)-3- {[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy]-2-[(11Z)-icos-11-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(5-iso PGF2VI/20:1(11Z))'	HMDB02 82194	C44H78NO1 3P	

37	9	858.56	72	859.5727202	0.0022 798	Protone	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienoyloxy)-2-(((5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 83998	C49H82NO9 P	
				859.5727202	0.0022 798	Protone	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienoyloxy)-3-(((5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/22:2(13Z,16Z))'	HMDB02 83999	C49H82NO9 P	
				859.5727202	0.0022 798	Protone	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienoyloxy)-2-(((4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 84000	C49H82NO9 P	
				859.5727202	0.0022 798	Protone	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienoyloxy)-3-(((4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/22:2(13Z,16Z))'	HMDB02 84001	C49H82NO9 P	
				859.5727202	0.0022 798	Protone	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienoyloxy)-2-(((4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 84002	C49H82NO9 P	
				859.5727202	0.0022 798	Protone	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienoyloxy)-3-(((4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/22:2(13Z,16Z))'	HMDB02 84003	C49H82NO9 P	
				859.5727202	0.0022 798	Protone	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienoyloxy)-2-(((4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 84004	C49H82NO9 P	
				859.5727202	0.0022 798	Protone	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienoyloxy)-3-(((4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/22:2(13Z,16Z))'	HMDB02 84005	C49H82NO9 P	
				859.5727202	0.0022 798	Protone	b'(2-aminoethoxy)((2R)-3-((13Z,16Z)-docosa-13,16-dienoyloxy)-2-(((4Z,7Z,10Z,13Z)-15-{3-((2Z)-pent-2-en-1-yl)oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:2(13Z,16Z)/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 84008	C49H82NO9 P	
				859.5727202	0.0022 798	Protone	b'(2-aminoethoxy)((2R)-2-((13Z,16Z)-docosa-13,16-dienoyloxy)-3-(((4Z,7Z,10Z,13Z)-15-{3-((2Z)-pent-2-en-1-yl)oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/22:2(13Z,16Z))'	HMDB02 84009	C49H82NO9 P	
38	0	859.57	02	860.5778652	0.0001 348	Protone	b'[(2R)-2-(((8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl)oxy)-3-((18-methylnonadecanoyl)oxy)propoxy]phosphinic acid'	b'PG(i-20:0/20:3(8Z,11Z,14Z)-2OH(5,6))'	HMDB02 71922	C46H85O12 P	
				860.5778652	0.0001 348	Protone	b'[(2R)-3-(((8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl)oxy)-2-((18-methylnonadecanoyl)oxy)propoxy]phosphinic acid'	b'PG(20:3(8Z,11Z,14Z)-2OH(5,6)/i-20:0)'	HMDB02 71923	C46H85O12 P	
38	1	861.59	04	861.5883703	0.0020 297	Redox	b'(2-aminoethoxy)((2R)-3-((13Z)-docosa-13-enoyloxy)-2-(((5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl)oxy)propoxy]phosphinic acid'	b'PE(22:1(13Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 83894	C49H84NO9 P	

		861.5883703	0.0020 297	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/22:1(13Z))'	HMDB02 83895	C49H84NO9 P	
		861.5883703	0.0020 297	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 83896	C49H84NO9 P	
		861.5883703	0.0020 297	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/22:1(13Z))'	HMDB02 83897	C49H84NO9 P	
		861.5883703	0.0020 297	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 83898	C49H84NO9 P	
		861.5883703	0.0020 297	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/22:1(13Z))'	HMDB02 83899	C49H84NO9 P	
		861.5883703	0.0020 297	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 83900	C49H84NO9 P	
		861.5883703	0.0020 297	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/22:1(13Z))'	HMDB02 83901	C49H84NO9 P	
		861.5883703	0.0020 297	Redox	b'(2-aminoethoxy)[(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[[{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:1(13Z)/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 83904	C49H84NO9 P	
		861.5883703	0.0020 297	Redox	b'(2-aminoethoxy)[(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[[{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/22:1(13Z))'	HMDB02 83905	C49H84NO9 P	
38 2	863.55 71	863.5547477	0.0023 523	Redox	b'8-[3-methoxy-4,8-dimethyl-9-(2-methyl-1,3-oxazol-4-yl)nona-4,6,8-trien-2-yl]-11,16-dimethyl-6,19-dioxo-4,7,12,18-tetraoxatetracyclo[15.3.1.0 ^{3,5} .0 ^{11,13}]benicos-14-en-10-yl hexadecanoate'	b'Palmitoyl rhizoxin'	HMDB02 56089	C51H77NO1 0	
38 3	863.60 67	864.6161783	0.0016 783	Protona tion	b'bis(3-methylbut-2-en-1-yl) {hexakis(3-methylbut-2-en-1-yl)bis[(3-methylbut-2-en-1-yl)oxy]phosphoroso}oxy]phosphonate'	b'All trans decaprenyl diphosphate'	HMDB00 06288	C50H90O7P 2	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-[[{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 83790	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-[[{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenoyl}oxy]propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/22:0)	HMDB02 83791	C49H86NO9 P	

		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 83792	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/22:0)'	HMDB02 83793	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 83794	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/22:0)'	HMDB02 83795	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 83796	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/22:0)'	HMDB02 83797	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-(docosanoyloxy)-2-{{[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:0/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 83800	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-(docosanoyloxy)-3-{{[(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy}propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/22:0)'	HMDB02 83801	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-{{[(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl]oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(6E,8Z,11Z,14Z))+O(5))'	HMDB02 84592	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-{{[(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl]oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z))+O(5)/24:1(15Z))'	HMDB02 84593	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-{{[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl]oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,13E))+O(15))'	HMDB02 84594	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-3-{{[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl]oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E))+O(15)/24:1(15Z))'	HMDB02 84595	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)[(2R)-2-{{[(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoyl]oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 84606	C49H86NO9 P	

		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicos-5,8,11,14,16-pentaenyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/24:1(15Z))'	HMDB02 84607	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)((2R)-2-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicos-5,8,11,13,17-pentaenyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(24:1(15Z)/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	HMDB02 84608	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,11Z,13E,17Z)-16-hydroxyicos-5,8,11,13,17-pentaenyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)-OH(18)/24:1(15Z))'	HMDB02 84609	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)((2R)-2-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicos-5,8,10,14,17-pentaenyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(24:1(15Z)/20:5(5Z,8Z,10E,14Z,17Z)-OH(12))'	HMDB02 84610	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)((2R)-3-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicos-5,8,10,14,17-pentaenyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)-OH(12)/24:1(15Z))'	HMDB02 84611	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)((2R)-2-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicos-6,8,11,14,17-pentaenyl}oxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(24:1(15Z)/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 84612	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-aminoethoxy)((2R)-3-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicos-6,8,11,14,17-pentaenyl}oxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/24:1(15Z))'	HMDB02 84613	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'trimethyl(2-{{(2R)-3-{{(10E,12E)-9-oxooctadeca-10,12-dienyl}oxy}-2-{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)azanium'	b'PC(18:2(10E,12Z)+=O(9)/22:3(10Z,13Z,16Z))'	HMDB02 88125	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'trimethyl(2-{{(2R)-2-{{(9Z,11E)-13-oxooctadeca-9,11-dienyl}oxy}-3-{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/18:2(9Z,11E)+=O(13))'	HMDB02 88126	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'trimethyl(2-{{(2R)-3-{{(9Z,11E)-13-oxooctadeca-9,11-dienyl}oxy}-2-{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)azanium'	b'PC(18:2(9Z,11E)+=O(13)/22:3(10Z,13Z,16Z))'	HMDB02 88127	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-{{(2R)-2-{{(10E,12E,15E)-9-hydroxyoctadeca-10,12,15-trienyl}oxy}-3-{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/18:3(10,12,15)-OH(9))'	HMDB02 88162	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-{{(2R)-3-{{(10E,12E,15E)-9-hydroxyoctadeca-10,12,15-trienyl}oxy}-2-{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(18:3(10,12,15)-OH(9)/22:3(10Z,13Z,16Z))'	HMDB02 88163	C49H86NO9 P	
		863.6040204	0.0026 796	Redox	b'(2-{{(2R)-2-{{(9E,11E,15E)-13-hydroxyoctadeca-9,11,15-trienyl}oxy}-3-{{(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/18:3(9,11,15)-OH(13))'	HMDB02 88164	C49H86NO9 P	

		863.6040204	0.0026 796	Redox	b'(2-([(2R)-3-([(9E,11E,15E)-13-hydroxyoctadeca-9,11,15-trienoyl]oxy)-2-[(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(18:3(9,11,15)-OH(13)/22:3(10Z,13Z,16Z))'	HMDB02 88165	C49H86NO9 P	
38	864.57	865.5832844	0.0012 156	Protone	b'(2-aminoethoxy)[(2R)-3-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)-2-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy]phosphinic acid'	b'PE(DiMe(11,3)/MonoMe(13,5))'	HMDB00 61478	C48H84NO1 OP	
		865.5832844	0.0012 156	Protone	b'(2-aminoethoxy)[(2R)-3-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-2-([13-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy]phosphinic acid'	b'PE(DiMe(11,5)/MonoMe(11,5))'	HMDB00 61486	C48H84NO1 OP	
		865.5832844	0.0012 156	Protone	b'(2-aminoethoxy)[(2R)-3-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy]phosphinic acid'	b'PE(DiMe(13,5)/MonoMe(11,3))'	HMDB00 61494	C48H84NO1 OP	
		865.5832844	0.0012 156	Protone	b'(2-aminoethoxy)[(2R)-3-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propoxy]phosphinic acid'	b'PE(DiMe(13,5)/MonoMe(9,5))'	HMDB00 61497	C48H84NO1 OP	
		865.5832844	0.0012 156	Protone	b'(2-aminoethoxy)[(2R)-3-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-2-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy]phosphinic acid'	b'PE(DiMe(9,5)/MonoMe(13,5))'	HMDB00 61514	C48H84NO1 OP	
		865.5832844	0.0012 156	Protone	b'(2-aminoethoxy)[(2R)-2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy]phosphinic acid'	b'PE(MonoMe(11,3)/DiMe(13,5))'	HMDB00 61518	C48H84NO1 OP	
		865.5832844	0.0012 156	Protone	b'(2-aminoethoxy)[(2R)-2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy]phosphinic acid'	b'PE(MonoMe(11,5)/DiMe(11,5))'	HMDB00 61526	C48H84NO1 OP	
		865.5832844	0.0012 156	Protone	b'(2-aminoethoxy)[(2R)-2-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy]phosphinic acid'	b'PE(MonoMe(13,5)/DiMe(11,3))'	HMDB00 61534	C48H84NO1 OP	
		865.5832844	0.0012 156	Protone	b'(2-aminoethoxy)[(2R)-2-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy]phosphinic acid'	b'PE(MonoMe(13,5)/DiMe(9,5))'	HMDB00 61538	C48H84NO1 OP	
		865.5832844	0.0012 156	Protone	b'(2-aminoethoxy)[(2R)-2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propoxy]phosphinic acid'	b'PE(MonoMe(9,5)/DiMe(13,5))'	HMDB00 61545	C48H84NO1 OP	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-([(2R)-2-([(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-3-(icosanoyloxy)propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(20:0/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB01 12535	C48H84NO1 OP	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-([(2R)-2-([7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-3-(icosanoyloxy)propoxy](hydroxy)phosphoryl]oxy)propanoic acid'	b'PS(20:0/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB01 12536	C48H84NO1 OP	

		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-({(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3-[(11Z)-icos-11-enoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:1(11Z)/22:4(7Z,10Z,13Z,16Z))'	HMDB01 12561	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-({(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:3(5Z,8Z,11Z)/22:2(13Z,16Z))'	HMDB01 12615	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-({(2R)-2-[(13Z)-docos-13-enoyloxy]-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:4(5Z,8Z,11Z,14Z)/22:1(13Z))'	HMDB01 12647	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-({(2R)-2-(docosanoyloxy)-3-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:5(5Z,8Z,11Z,14Z,17Z)/22:0)'	HMDB01 12698	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-({(2R)-3-(docosanoyloxy)-2-[(5Z,8Z,11Z,14Z,17Z)-icosa-5,8,11,14,17-pentaenoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:0/20:5(5Z,8Z,11Z,14Z,17Z))'	HMDB01 12726	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-({(2R)-3-[(13Z)-docos-13-enoyloxy]-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:1(13Z)/20:4(5Z,8Z,11Z,14Z))'	HMDB01 12752	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-({(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:2(13Z,16Z)/20:3(5Z,8Z,11Z))'	HMDB01 12776	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-({(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-[(11Z)-icos-11-enoyloxy]propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:4(7Z,10Z,13Z,16Z)/20:1(11Z))'	HMDB01 12801	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-({(2R)-3-[(4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy]-2-(icosanoyloxy)propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:5(4Z,7Z,10Z,13Z,16Z)/20:0)'	HMDB01 12826	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2S)-2-amino-3-({(2R)-3-[(7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy]-2-(icosanoyloxy)propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:5(7Z,10Z,13Z,16Z,19Z)/20:0)'	HMDB01 12850	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'[(2R)-2-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-3-{{11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11D3/11D5)'	HMDB01 13757	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'[(2R)-3-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-2-{{11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11D5/11D3)'	HMDB01 13765	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'[(2R)-2-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11D5/9D5)'	HMDB01 13772	C48H84NO1 0P	

		865.5832849	0.0012 151	Protona tion	b'[(2R)-2-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMc(11M3/13M5)'	HMDB01 13779	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-2,3-bis([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)]propoxy[2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMc(11M5/11M5)'	HMDB01 13786	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-3-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMc(13D5/9D3)'	HMDB01 13798	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMc(13M5/11M3)'	HMDB01 13803	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-2-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMc(13M5/9M5)'	HMDB01 13809	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMc(9D3/13D5)'	HMDB01 13814	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-3-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMc(9D5/11D5)'	HMDB01 13820	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-3-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)-2-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMc(9M5/13M5)'	HMDB01 13833	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-3-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-2-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(11D3/11M5)'	HMDB01 14663	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-3-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-2-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(11D5/11M3)'	HMDB01 14671	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-3-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-2-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(11D5/9M5)'	HMDB01 14677	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(11M3/11D5)'	HMDB01 14679	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'[(2R)-2-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)-3-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(11M5/11D3)'	HMDB01 14687	C48H84NO1 0P	

		865.5832849	0.0012 151	Protone tion	b'[(2R)-2-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(11M5/9D5)'	HMDB01 14694	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'[(2R)-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-3-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(13M5/9D3)'	HMDB01 14711	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'[(2R)-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}-2-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(9D3/13M5)'	HMDB01 14719	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'[(2R)-3-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(9D5/11M5)'	HMDB01 14726	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'[(2R)-2-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-3-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(9M5/11D5)'	HMDB01 14732	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'(2S)-2-amino-3-({hydroxy[(2R)-3-{{(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy}-2-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphoryl}oxy]propanoic acid'	b'PS(18:4(6Z,9Z,12Z,15Z)/24:1(15Z))'	HMDB01 16760	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'(2S)-2-amino-3-({[(2R)-2-{{(13Z,16Z)-docosa-13,16-dienoyloxy}-3-{{(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy}propoxy}(hydroxy)phosphoryl}oxy]propanoic acid'	b'PS(20:3(8Z,11Z,14Z)/22:2(13Z,16Z))'	HMDB01 16768	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'(2S)-2-amino-3-({[(2R)-2-{{(13Z)-docos-13-enoyloxy}-3-{{(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy}propoxy}(hydroxy)phosphoryl}oxy]propanoic acid'	b'PS(20:4(8Z,11Z,14Z,17Z)/22:1(13Z))'	HMDB01 16772	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'(2S)-2-amino-3-({[(2R)-3-{{(13Z)-docos-13-enoyloxy}-2-{{(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy}propoxy}(hydroxy)phosphoryl}oxy]propanoic acid'	b'PS(22:1(13Z)/20:4(8Z,11Z,14Z,17Z))'	HMDB01 16776	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'(2S)-2-amino-3-({[(2R)-3-{{(13Z,16Z)-docosa-13,16-dienoyloxy}-2-{{(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy}propoxy}(hydroxy)phosphoryl}oxy]propanoic acid'	b'PS(22:2(13Z,16Z)/20:3(8Z,11Z,14Z))'	HMDB01 16779	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'(2S)-2-amino-3-({hydroxy[(2R)-2-{{(6Z,9Z,12Z,15Z)-octadeca-6,9,12,15-tetraenoyloxy}-3-{{(15Z)-tetracos-15-enoyloxy}propoxy}phosphoryl}oxy]propanoic acid'	b'PS(24:1(15Z)/18:4(6Z,9Z,12Z,15Z))'	HMDB01 16793	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'(2-{{[(2R)-2-{{(5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-3-(octadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(18:0/22:6(5Z,8E,10Z,13Z,15E,19Z)- Z)-2OH(7S, 17S))'	HMDB02 86275	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone tion	b'(2-{{[(2R)-3-{{(5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-2-(octadecanoyloxy)propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S, 17S)/18:0)'	HMDB02 86276	C48H84NO1 0P	

		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-2- -{[(4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenyl]oxy}-3-(octadecanoyloxy)propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(18:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17))'	HMDB02 86291	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-2- -{[(4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenyl]oxy}-2-(octadecanoyloxy)propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/18:0))'	HMDB02 86292	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-2- -{[(5Z)-7- -{[(1S,5R)-5- -{[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}-3- -{[(11Z)-icos-11-enoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:1(11Z)/PGJ2))'	HMDB02 87070	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-3- -{[(5Z)-7- -{[(1S,5R)-5- -{[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}-2- -{[(11Z)-icos-11-enoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(PGJ2/20:1(11Z))'	HMDB02 87071	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-2- -{[(5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenyl]oxy}-3- -{[(11Z,14Z)-icosa-11,14-dienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:2(11Z,14Z)/20:4(6Z,8E,10E,14Z)-2OH(5S,12R))'	HMDB02 87178	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-3- -{[(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenyl]oxy}-2- -{[(11Z,14Z)-icosa-11,14-dienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(6Z,8E,10E,14Z)-2OH(5S,12R)/20:2(11Z,14Z))'	HMDB02 87179	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-2- -{[(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenyl]oxy}-3- -{[(11Z,14Z)-icosa-11,14-dienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:2(11Z,14Z)/20:4(6E,8Z,11Z,13E)-2OH(5S,15S))'	HMDB02 87212	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-3- -{[(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenyl]oxy}-2- -{[(11Z,14Z)-icosa-11,14-dienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(6E,8Z,11Z,13E)-2OH(5S,15S)/20:2(11Z,14Z))'	HMDB02 87213	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-2- -{[(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenyl]oxy}-3- -{[(11Z,14Z)-icosa-11,14-dienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:2(11Z,14Z)/20:4(8Z,11Z,14Z,17Z)-2OH(5S,6R))'	HMDB02 87214	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-3- -{[(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenyl]oxy}-2- -{[(11Z,14Z)-icosa-11,14-dienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(8Z,11Z,14Z,17Z)-2OH(5S,6R)/20:2(11Z,14Z))'	HMDB02 87215	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-2- -{[(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl]oxy}-3- -{[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:3(5Z,8Z,11Z)/20:3(8Z,11Z,14Z)-2OH(5,6))'	HMDB02 87285	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-3- -{[(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl]oxy}-2- -{[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:3(8Z,11Z,14Z)-2OH(5,6)/20:3(5Z,8Z,11Z))'	HMDB02 87286	C48H84NO1 0P	
		865.5832849	0.0012 151	Protone	b'(2- -{[(2R)-2- -{[(8Z,11Z,14Z)-5,6-dihydroxyicosa-8,11,14-trienoyl]oxy}-3- -{[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:3(8Z,11Z,14Z)/20:3(8Z,11Z,14Z)-2OH(5,6))'	HMDB02 87389	C48H84NO1 0P	

		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-3-(((8Z,11Z,14Z)-5,6-dihydroxyoctadec-8,11,14-trienoyl)oxy)-2-((8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(20:3(8Z,11Z,14Z)- 2OH(5,6)/20:3(8Z,11Z,14Z))'	HMDB02 87390	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-2-(((9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl)oxy)-3-((4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(22:5(4Z,7Z,10Z,13Z,16Z)/18:1(12 Z)-2OH(9,10))'	HMDB02 88336	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-3-(((9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl)oxy)-2-((4Z,7Z,10Z,13Z,16Z)-docosa-4,7,10,13,16-pentaenoyloxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(18:1(12Z)- 2OH(9,10)/22:5(4Z,7Z,10Z,13Z,16Z))'	HMDB02 88337	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-2-(((9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl)oxy)-3-((7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(22:5(7Z,10Z,13Z,16Z,19Z)/18:1(1 2Z)-2OH(9,10))'	HMDB02 88440	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-3-(((9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl)oxy)-2-((7Z,10Z,13Z,16Z,19Z)-docosa-7,10,13,16,19-pentaenoyloxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(18:1(12Z)- 2OH(9,10)/22:5(7Z,10Z,13Z,16Z,19Z))'	HMDB02 88441	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-3-[[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)-2-(((6E,8E,11E)-5-hydroxyoctadec-6,8,11-trienoyl)oxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(DiMe(11,3)/20:3(6,8,11)-OH(5))'	HMDB02 89004	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-2-[[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)-3-(((6E,8E,11E)-5-hydroxyoctadec-6,8,11-trienoyl)oxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(20:3(6,8,11)-OH(5)/DiMe(11,3))'	HMDB02 89005	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-3-[[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-2-(((10E,12Z)-9-oxooctadeca-10,12-dienoyl)oxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(DiMe(11,5)/18:2(10E,12Z)+=O(9) y)	HMDB02 89060	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-2-[[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-(((10E,12Z)-9-oxooctadeca-10,12-dienoyl)oxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(18:2(10E,12Z)+=O(9)/DiMe(11,5) y)	HMDB02 89061	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-3-[[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-2-(((9Z,11E)-13-oxooctadeca-9,11-dienoyl)oxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(DiMe(11,5)/18:2(9Z,11E)+=O(13) y)	HMDB02 89062	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-2-[[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-(((9Z,11E)-13-oxooctadeca-9,11-dienoyl)oxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(18:2(9Z,11E)+=O(13)/DiMe(11,5) y)	HMDB02 89063	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-3-[[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-2-(((10E,12E,15E)-9-hydroxyoctadeca-10,12,15-trienoyl)oxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(DiMe(11,5)/18:3(10,12,15)- OH(9))'	HMDB02 89097	C48H84NO1 0P	
		865.5832849	0.0012 151	Protona tion	b'(2-(((2R)-2-[[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-(((10E,12E,15E)-9-hydroxyoctadeca-10,12,15-trienoyl)oxy)propyl phosphono)oxy)ethyl)trimethylazanium'	b'PC(18:3(10,12,15)- OH(9)/DiMe(11,5))'	HMDB02 89098	C48H84NO1 0P	

38	5	864.61	865.5832849	0.0012 151	Protone	b'(2-(((2R)-3-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-2-(((9E,11E,15E)-13-hydroxyoctadeca-9,11,15-trienyl]oxy)propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(DiMe(11,5)/18:3(9,11,15)-OH(13))'	HMDB02 89099	C48H84NO1 0P	
			865.5832849	0.0012 151	Protone	b'(2-(((2R)-2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-(((9E,11E,15E)-13-hydroxyoctadeca-9,11,15-trienyl]oxy)propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(18:3(9,11,15)-OH(13)/DiMe(11,5))'	HMDB02 89100	C48H84NO1 0P	
			865.5832849	0.0012 151	Protone	b'(2-(((2R)-3-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-2-(((6E,8E,11E)-5-hydroxyicosa-6,8,11-trienyl]oxy)propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(DiMe(9,5)/20:3(6,8,11)-OH(5))'	HMDB02 89419	C48H84NO1 0P	
			865.5832849	0.0012 151	Protone	b'(2-(((2R)-2-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-(((6E,8E,11E)-5-hydroxyicosa-6,8,11-trienyl]oxy)propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(20:3(6,8,11)-OH(5)/DiMe(9,5))'	HMDB02 89420	C48H84NO1 0P	
	34	864.61	865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)((2R)-2-(((6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl]oxy)-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:4(6E,8Z,11Z,14Z)+=O(5)) ,	HMDB02 84488	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)((2R)-2-(((6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl]oxy)-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)+=O(5)/24:0) ,	HMDB02 84489	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)((2R)-2-(((5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl]oxy)-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:4(5Z,8Z,11Z,13E)+=O(15)))'	HMDB02 84490	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)((2R)-3-(((5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl]oxy)-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)+=O(15)/24:0))'	HMDB02 84491	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)((2R)-2-(((5Z,8Z,11Z,14Z,16E,18E)-18-hydroxyicosa-5,8,11,14,16-pentaenyl]oxy)-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 84502	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)((2R)-3-(((5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl]oxy)-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/24:0))'	HMDB02 84503	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)((2R)-2-(((5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl]oxy)-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	HMDB02 84504	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)((2R)-3-(((5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl]oxy)-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,11Z,14Z,16E)-OH(18)/24:0))'	HMDB02 84505	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)((2R)-2-(((5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl]oxy)-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:5(5Z,8Z,10E,14Z,17Z)-OH(12))'	HMDB02 84506	C49H88NO9 P	

		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-3-{{(5Z,8Z,10E,14Z,17Z)-12-hydroxyicos-5,8,10,14,17-pentaenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(5Z,8Z,10E,14Z,17Z)-OH(12)/24:0)'	HMDB02 84507	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-2-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicos-6,8,11,14,17-pentaenyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 84508	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-3-{{(6E,8Z,11Z,14Z,17Z)-5-hydroxyicos-6,8,11,14,17-pentaenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/24:0)'	HMDB02 84509	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-2-{{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl}oxy}-3-((15Z)-tetracos-15-enoyloxy)propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:3(5Z,8Z,11Z)-O(14R,15S))'	HMDB02 84542	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-3-{{(5Z,8Z,11Z)-13-(3-pentylloxiran-2-yl)trideca-5,8,11-trienyl}oxy}-2-((15Z)-tetracos-15-enoyloxy)propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,11Z)-O(14R,15S)/24:1(15Z))'	HMDB02 84543	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-2-{{(5Z,8Z)-10-{3-((2Z)-oct-2-en-1-yl)oxiran-2-yl}deca-5,8-dienyl}oxy}-3-((15Z)-tetracos-15-enoyloxy)propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:3(5Z,8Z,14Z)-O(11S,12R))'	HMDB02 84544	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-3-{{(5Z,8Z)-10-{3-((2Z)-oct-2-en-1-yl)oxiran-2-yl}deca-5,8-dienyl}oxy}-2-((15Z)-tetracos-15-enoyloxy)propoxy]phosphinic acid'	b'PE(20:3(5Z,8Z,14Z)-O(11S,12R)/24:1(15Z))'	HMDB02 84545	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-3-((15Z)-tetracos-15-enoyloxy)-2-{{(5Z)-7-{3-((2Z,5Z)-undeca-2,5-dien-1-yl)oxiran-2-yl}hept-5-enoyl}oxy}propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:3(5Z,11Z,14Z)-O(8,9))'	HMDB02 84546	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-2-((15Z)-tetracos-15-enoyloxy)-3-{{(5Z)-7-{3-((2Z,5Z)-undeca-2,5-dien-1-yl)oxiran-2-yl}hept-5-enoyl}oxy}propoxy]phosphinic acid'	b'PE(20:3(5Z,11Z,14Z)-O(8,9)/24:1(15Z))'	HMDB02 84547	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-3-((15Z)-tetracos-15-enoyloxy)-2-((4-{3-((2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl)oxiran-2-yl}butanoyl)oxy)propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:3(8Z,11Z,14Z)-O(5,6))'	HMDB02 84548	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-2-((15Z)-tetracos-15-enoyloxy)-3-((4-{3-((2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl)oxiran-2-yl}butanoyl)oxy)propoxy]phosphinic acid'	b'PE(20:3(8Z,11Z,14Z)-O(5,6)/24:1(15Z))'	HMDB02 84549	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-2-{{(5Z,8Z,11Z,14Z)-20-hydroxyicos-5,8,11,14-tetraenyl}oxy}-3-((15Z)-tetracos-15-enoyloxy)propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,14Z)-OH(20))'	HMDB02 84550	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b(2-aminoethoxy)((2R)-3-{{(5Z,8Z,11Z,14Z)-20-hydroxyicos-5,8,11,14-tetraenyl}oxy}-2-((15Z)-tetracos-15-enoyloxy)propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)-OH(20)/24:1(15Z))'	HMDB02 84551	C49H88NO9 P	

		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-2-{{(5R,6E,8Z,11Z,14Z)-5-hydroxyicos-6,8,11,14-tetraenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(6E,8Z,11Z,14Z)- OH(5S))'	HMDB02 84552	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-{{(5S,6E,8Z,11Z,14Z)-5-hydroxyicos-6,8,11,14-tetraenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,14Z)- OH(5S)/24:1(15Z))'	HMDB02 84553	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,14Z,19S)-19-hydroxyicos-5,8,11,14-tetraenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,14Z)- OH(19S))'	HMDB02 84554	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,14Z,19R)-19-hydroxyicos-5,8,11,14-tetraenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(19S)/24:1(15Z))'	HMDB02 84555	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,14Z,18R)-18-hydroxyicos-5,8,11,14-tetraenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,14Z)- OH(18R))'	HMDB02 84556	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,14Z,18S)-18-hydroxyicos-5,8,11,14-tetraenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(18R)/24:1(15Z))'	HMDB02 84557	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,14Z)-17-hydroxyicos-5,8,11,14-tetraenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,14Z)- OH(17))'	HMDB02 84558	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,14Z)-17-hydroxyicos-5,8,11,14-tetraenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(17)/24:1(15Z))'	HMDB02 84559	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,14Z,16R)-16-hydroxyicos-5,8,11,14-tetraenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,14Z)- OH(16R))'	HMDB02 84560	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,14Z,16S)-16-hydroxyicos-5,8,11,14-tetraenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,14Z)- OH(16R)/24:1(15Z))'	HMDB02 84561	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,11Z,13E,15S)-15-hydroxyicos-5,8,11,13-tetraenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,11Z,13E)- OH(15S))'	HMDB02 84562	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-{{(5Z,8Z,11Z,13E,15R)-15-hydroxyicos-5,8,11,13-tetraenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,11Z,13E)- OH(15S)/24:1(15Z))'	HMDB02 84563	C49H88NO9 P	
		865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-2-{{(5Z,8Z,10E,12S,14Z)-12-hydroxyicos-5,8,10,14-tetraenyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,8Z,10E,14Z)- OH(12S))'	HMDB02 84564	C49H88NO9 P	

38	6	875.60	865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-[[[(5Z,8Z,10E,12R,14Z)-12-hydroxyicos-5,8,10,14-tetraenyl]oxy]-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,8Z,10E,14Z)- OH(12S)/24:1(15Z))'	HMDB02 84565	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-[[[(5E,8Z,11R,12Z,14Z)-11-hydroxyicos-5,8,12,14-tetraenyl]oxy]-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5E,8Z,12Z,14Z)- OH(11R))'	HMDB02 84566	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-[[[(5E,8Z,11S,12Z,14Z)-11-hydroxyicos-5,8,12,14-tetraenyl]oxy]-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5E,8Z,12Z,14Z)- OH(11R)/24:1(15Z))'	HMDB02 84567	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-[[[(5E,7Z,11Z,14Z)-9-hydroxyicos-5,7,11,14-tetraenyl]oxy]-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(5Z,7E,11Z,14Z)- OH(9))'	HMDB02 84568	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'(2-aminoethoxy)[(2R)-3-[[[(5E,7Z,11Z,14Z)-9-hydroxyicos-5,7,11,14-tetraenyl]oxy]-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(5Z,7E,11Z,14Z)- OH(9)/24:1(15Z))'	HMDB02 84569	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'trimethyl(2-[[[(2R)-2-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl]oxy]-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono]oxy)ethyl]azanium'	b'PC(22:3(10Z,13Z,16Z)/18:1(12Z)- O(9S,10R))'	HMDB02 88130	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'trimethyl(2-[[[(2R)-3-[(8-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}octanoyl]oxy]-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono]oxy)ethyl]azanium'	b'PC(18:1(12Z)- O(9S,10R)/22:3(10Z,13Z,16Z))'	HMDB02 88131	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'trimethyl(2-[[[(2R)-2-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono]oxy)ethyl]azanium'	b'PC(22:3(10Z,13Z,16Z)/18:1(9Z)- O(12,13))'	HMDB02 88132	C49H88NO9 P	
			865.6196704	0.0015 296	Protone	b'trimethyl(2-[[[(2R)-3-[(9Z)-11-(3-pentylloxiran-2-yl)undec-9-enoyl]oxy]-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono]oxy)ethyl]azanium'	b'PC(18:1(9Z)- O(12,13)/22:3(10Z,13Z,16Z))'	HMDB02 88133	C49H88NO9 P	
6	875.60	49	875.6040204	0.0008 796	Redox	b'(2-[[[(2R)-2-[[[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propyl phosphono]oxy)ethyl]trimethylazanium'	b'PC(20:1(11Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 87114	C50H86NO9 P	
			875.6040204	0.0008 796	Redox	b'(2-[[[(2R)-3-[[[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propyl phosphono]oxy)ethyl]trimethylazanium'	b'PC(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)/20:1(11Z))'	HMDB02 87115	C50H86NO9 P	
			875.6040204	0.0008 796	Redox	b'(2-[[[(2R)-2-[[[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy]-3-[(11Z)-icos-11-enoyloxy]propyl phosphono]oxy)ethyl]trimethylazanium'	b'PC(20:1(11Z)/22:6(4Z,8Z,10Z,13Z,16Z,19Z)- Z,19Z)-OH(7))'	HMDB02 87116	C50H86NO9 P	
			875.6040204	0.0008 796	Redox	b'(2-[[[(2R)-3-[[[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy]-2-[(11Z)-icos-11-enoyloxy]propyl phosphono]oxy)ethyl]trimethylazanium'	b'PC(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/20:1(11Z))'	HMDB02 87117	C50H86NO9 P	

		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-2- -{[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy}-3-[(11Z)-icos-11-enoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:1(11Z)/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 87118	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-3- -{[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenoyl]oxy}-2-[(11Z)-icos-11-enoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/20:1(11Z))'	HMDB02 87119	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-2- -{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy}-3-[(11Z)-icos-11-enoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:1(11Z)/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 87120	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-3- -{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy}-2-[(11Z)-icos-11-enoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/20:1(11Z))'	HMDB02 87121	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-3-[(11Z)-icos-11-enoyloxy]-2- -{[(4Z,7Z,10Z,13Z)-15- -{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:1(11Z)/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 87124	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-2-[(11Z)-icos-11-enoyloxy]-3- -{[(4Z,7Z,10Z,13Z)-15- -{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17)/20:1(11Z))'	HMDB02 87125	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2- -{[(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:2(13Z,16Z)/20:4(6E,8Z,11Z,14Z)-O(5))'	HMDB02 88017	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3- -{[(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:4(6E,8Z,11Z,14Z)-O(5)/22:2(13Z,16Z))'	HMDB02 88018	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2- -{[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:2(13Z,16Z)/20:4(5Z,8Z,11Z,13E)-O(15))'	HMDB02 88019	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3- -{[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,13E)-O(15)/22:2(13Z,16Z))'	HMDB02 88020	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2- -{[(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:2(13Z,16Z)/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 88031	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3- -{[(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/22:2(13Z,16Z))'	HMDB02 88032	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2- -{[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:2(13Z,16Z)/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	HMDB02 88033	C50H86NO9 P	

		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3- -{[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/22:2(13Z,16Z))'	HMDB02 88034	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2- -{[(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:2(13Z,16Z)/20:5(5Z,8Z,10E,14 Z,17Z)-OH(12))'	HMDB02 88035	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3- -{[(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/22:2(13Z,16Z))'	HMDB02 88036	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]-2- -{[(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:2(13Z,16Z)/20:5(6E,8Z,11Z,14 Z,17Z)-OH(5))'	HMDB02 88037	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]-3- -{[(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:5(6E,8Z,11Z,14Z,17Z)- OH(5)/22:2(13Z,16Z))'	HMDB02 88038	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2- -{[(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:4(7Z,10Z,13Z,16Z)/20:3(6,8,11)-OH(5))'	HMDB02 88276	C50H86NO9 P	
		875.6040204	0.0008 796	Redox	b'(2- -{[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-3- -{[(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl]oxy}propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:3(6,8,11)- OH(5)/22:4(7Z,10Z,13Z,16Z))'	HMDB02 88277	C50H86NO9 P	
38	7	877.6044143	0.0013 857	Redox	b'(2S)-2-amino-3- -{[(2R)-2- -{[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-3-(docosanoyloxy)propoxy}(hydroxy)phosphoryl}oxy}propanoic acid'	b'PS(22:0/18:1(12Z)-2OH(9,10))'	HMDB02 82930	C46H88NO1 2P	
		877.6044143	0.0013 857	Redox	b'(2S)-2-amino-3- -{[(2R)-3- -{[(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enoyl]oxy}-2-(docosanoyloxy)propoxy}(hydroxy)phosphoryl}oxy}propanoic acid'	b'PS(18:1(12Z)-2OH(9,10)/22:0)'	HMDB02 82931	C46H88NO1 2P	
38	8	879.60	0.0012 405	Protona tion	b'(3- -{[11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy}-2- -{[11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(11,3)/MonoMe(11,5))'	HMDB00 61396	C49H87NO1 0P	
				Protona tion	b'(3- -{[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-2- -{[11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(11,5)/MonoMe(11,3))'	HMDB00 61404	C49H87NO1 0P	
				Protona tion	b'(3- -{[11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy}-2- -{[9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(11,5)/MonoMe(9,5))'	HMDB00 61407	C49H87NO1 0P	
				Protona tion	b'(3- -{[9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy}-2- -{[13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy}propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(9,3)/MonoMe(13,5))'	HMDB00 61424	C49H87NO1 0P	

		880.6067595	0.0012 405	Protona tion	b'(3-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-2-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(9,5)/MonoMe(11,5))'	HMDB00 61432	C49H87NO1 0P	
		880.6067595	0.0012 405	Protona tion	b'(2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,3)/DiMe(11,5))'	HMDB00 61436	C49H87NO1 0P	
		880.6067595	0.0012 405	Protona tion	b'(2-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)-3-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,5)/DiMe(11,3))'	HMDB00 61444	C49H87NO1 0P	
		880.6067595	0.0012 405	Protona tion	b'(2-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,5)/DiMe(9,5))'	HMDB00 61448	C49H87NO1 0P	
		880.6067595	0.0012 405	Protona tion	b'(2-([9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(13,5)/DiMe(9,3))'	HMDB00 61456	C49H87NO1 0P	
		880.6067595	0.0012 405	Protona tion	b'(2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(9,5)/DiMe(11,5))'	HMDB00 61463	C49H87NO1 0P	
		879.5989345	0.0012 655	Redox	b'(2-aminoethoxy)((2R)-2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy)phosphinic acid'	b'PE(DiMe(11,3)/DiMe(13,5))'	HMDB00 61473	C49H86NO1 0P	
		879.5989345	0.0012 655	Redox	b'(2-aminoethoxy)((2R)-2,3-bis([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)phosphinic acid'	b'PE(DiMe(11,5)/DiMe(11,5))'	HMDB00 61481	C49H86NO1 0P	
		879.5989345	0.0012 655	Redox	b'(2-aminoethoxy)((2R)-3-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy)phosphinic acid'	b'PE(DiMe(13,5)/DiMe(11,3))'	HMDB00 61489	C49H86NO1 0P	
		879.5989345	0.0012 655	Redox	b'(2-aminoethoxy)((2R)-2-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)phosphinic acid'	b'PE(DiMe(13,5)/DiMe(9,5))'	HMDB00 61493	C49H86NO1 0P	
		879.5989345	0.0012 655	Redox	b'(2-aminoethoxy)((2R)-3-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)phosphinic acid'	b'PE(DiMe(9,5)/DiMe(13,5))'	HMDB00 61509	C49H86NO1 0P	
		879.5989345	0.0012 655	Redox	b'(2-aminoethoxy)((2R)-2-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)phosphinic acid'	b'PE(MonoMe(11,5)/MonoMe(13,5))'	HMDB00 61532	C49H86NO1 0P	
		879.5989345	0.0012 655	Redox	b'(2-aminoethoxy)((2R)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)phosphinic acid'	b'PE(MonoMe(13,5)/MonoMe(11,5))'	HMDB00 61540	C49H86NO1 0P	

		879.598935	0.0012 65	Redox	b'[(2R)-3-{{11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl}oxy}-2-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11D3/13M5)'	HMDB01 13761	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-3-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-2-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11D5/11M5)'	HMDB01 13768	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-2-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-{{11-(3-methyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11M3/13D5)'	HMDB01 13778	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-2-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-3-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11M5/11D5)'	HMDB01 13784	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-3-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{11-(3-methyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(13D5/11M3)'	HMDB01 13794	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-3-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(13D5/9M5)'	HMDB01 13800	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-2-{{11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl}oxy}-3-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(13M5/11D3)'	HMDB01 13801	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-2-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(13M5/9D5)'	HMDB01 13808	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-3-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-2-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(9D5/13M5)'	HMDB01 13824	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-2-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(9M5/13D5)'	HMDB01 13832	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-2-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-3-{{11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMe2(11D3/11D5)'	HMDB01 14661	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-3-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-2-{{11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMe2(11D5/11D3)'	HMDB01 14669	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-2-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMe2(11D5/9D5)'	HMDB01 14676	C49H86NO1 0P	

		879.598935	0.0012 65	Redox	b'[2-(dimethylamino)ethoxy][(2R)-2-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-{{11-(3-methyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy]phosphinic acid'	b'PE-NMc2(11M3/13M5)'	HMDB01 14683	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-2,3-bis({11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy})propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(11M5/11M5)'	HMDB01 14690	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-3-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(13D5/9D3)'	HMDB01 14702	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[2-(dimethylamino)ethoxy][(2R)-3-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{11-(3-methyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy]phosphinic acid'	b'PE-NMc2(13M5/11M3)'	HMDB01 14707	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[2-(dimethylamino)ethoxy][(2R)-2-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy]phosphinic acid'	b'PE-NMc2(13M5/9M5)'	HMDB01 14713	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-2-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(9D3/13D5)'	HMDB01 14718	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[(2R)-3-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-2-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMc2(9D5/11D5)'	HMDB01 14724	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'[2-(dimethylamino)ethoxy][(2R)-3-{{9-(3-methyl-5-pentylfuran-2-yl)nonanoyl}oxy}-2-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy]phosphinic acid'	b'PE-NMc2(9M5/13M5)'	HMDB01 14736	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-3-(docosanoyloxy)propoxy]phosphinic acid'	b'PE(22:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S))'	HMDB02 83782	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-2-(docosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/22:0)'	HMDB02 83783	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'(2-aminoethoxy)[(2R)-2-{{(4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl}oxy}-3-(docosanoyloxy)propoxy]phosphinic acid'	b'PE(22:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17))'	HMDB02 83798	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl}oxy}-2-(docosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/22:0)'	HMDB02 83799	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl}oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/PGJ2)'	HMDB02 84578	C49H86NO1 0P	

		879.598935	0.0012 65	Redox	b'(2-aminoethoxy)[(2R)-3-{{[(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(PGJ2/24:1(15Z))'	HMDB02 84579	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'(2-aminoethoxy)[(2R)-3-{{[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy}-2-{{[(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl]oxy}propoxy]phosphinic acid'	b'PE(DiMe(13,5)/20:3(6,8,11)-OH(5))'	HMDB02 84956	C49H86NO1 0P	
		879.598935	0.0012 65	Redox	b'(2-aminoethoxy)[(2R)-2-{{[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy}-3-{{[(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienoyl]oxy}propoxy]phosphinic acid'	b'PE(20:3(6,8,11)-OH(5)/DiMe(13,5))'	HMDB02 84957	C49H86NO1 0P	
38 9	880.60 79	881.614585	0.0011 15	Protona tion	b'(2-aminoethoxy)[(2R)-2-{{[(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/PJG2)	HMDB02 84474	C49H88NO1 0P	
		881.614585	0.0011 15	Protona tion	b'(2-aminoethoxy)[(2R)-3-{{[(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl]oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(PGJ2/24:0)'	HMDB02 84475	C49H88NO1 0P	
		881.614585	0.0011 15	Protona tion		b'PE(24:1(15Z)/20:4(6Z,8E,10E,14Z)- 2OH(5S,12R))'	HMDB02 84582	C49H88NO1 0P	
		881.614585	0.0011 15	Protona tion	b'(2-aminoethoxy)[(2R)-3-{{[(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxyicosa-6,8,10,14-tetraenoyl]oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6Z,8E,10E,14Z)- 2OH(5S,12R)/24:1(15Z))'	HMDB02 84583	C49H88NO1 0P	
		881.614585	0.0011 15	Protona tion	b'(2-aminoethoxy)[(2R)-2-{{[(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(6E,8Z,11Z,13E)- 2OH(5S,15S))'	HMDB02 84618	C49H88NO1 0P	
		881.614585	0.0011 15	Protona tion	b'(2-aminoethoxy)[(2R)-3-{{[(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxyicosa-6,8,11,13-tetraenoyl]oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/24:1(15Z))'	HMDB02 84619	C49H88NO1 0P	
		881.614585	0.0011 15	Protona tion	b'(2-aminoethoxy)[(2R)-2-{{[(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R))'	HMDB02 84620	C49H88NO1 0P	
		881.614585	0.0011 15	Protona tion	b'(2-aminoethoxy)[(2R)-3-{{[(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxyicosa-8,11,14,17-tetraenoyl]oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/24:1(15Z))'	HMDB02 84621	C49H88NO1 0P	
39 0	883.52 75	884.534955	0.0003 45	Protona tion	b'(5S,6R,7E,9E,11Z,14Z)-6-{{[(2R)-2-amino-3-{{[(2R)-1-{{[(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-3-[(11Z)-octadeca-1,11-dien-1-yloxy]propan-2-yl]oxy}-3-oxopropyl]sulfonyl}-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'PE(P-18:1(11Z)/LTE4)	HMDB02 85412	C46H81N2O 10PS	
		884.534955	0.0003 45	Protona tion	b'(5S,6R,7E,9E,11Z,14Z)-6-{{[(2R)-2-amino-3-{{[(2R)-3-{{[(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-[(11Z)-octadeca-1,11-dien-1-yloxy]propoxy]-3-oxopropyl]sulfonyl}-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'PE(LTE4/P-18:1(11Z))'	HMDB02 85413	C46H81N2O 10PS	

		884.534955	0.0003 45	Protone tion	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-(((2R)-1-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-3-((9Z)-octadeca-1,9-dien-1-yloxy)propan-2-yl)oxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'PE(P-18:1(9Z)/LTE4)	HMDB02 85513	C46H81N2O 10PS	
		884.534955	0.0003 45	Protone tion	b'(5S,6R,7E,9E,11Z,14Z)-6-(((2R)-2-amino-3-(((2R)-3-(((2-aminoethoxy)(hydroxy)phosphoryl)oxy)-2-((9Z)-octadeca-1,9-dien-1-yloxy)propoxy)-3-oxopropyl)sulfanyl)-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'PE(LTE4/P-18:1(9Z))'	HMDB02 85514	C46H81N2O 10PS	
39 1	884.53 09	885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(hydroxy((2R)-3-(icosanoyloxy)-2-(((5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenyl)oxy)propoxy)phosphoryl)oxy)propanoic acid'	b'PS(20:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB02 82115	C46H80NO1 3P	
		885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(hydroxy((2R)-2-(icosanoyloxy)-3-(((5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenyl)oxy)propoxy)phosphoryl)oxy)propanoic acid'	b'PS(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/20:0))'	HMDB02 82116	C46H80NO1 3P	
		885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(hydroxy((2R)-2-(((5Z)-7-((1R,2R,3R)-3-hydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)-5-oxocyclopentyl)hept-5-enoyl)oxy)-3-((11Z)-icos-11-enoyloxy)propoxy)phosphoryl)oxy)propanoic acid'	b'PS(20:1(11Z)/PGE2))'	HMDB02 82173	C46H80NO1 3P	
		885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(hydroxy((2R)-3-(((5Z)-7-((1R,2R,3R)-3-hydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)-5-oxocyclopentyl)hept-5-enoyl)oxy)-2-((11Z)-icos-11-enoyloxy)propoxy)phosphoryl)oxy)propanoic acid'	b'PS(PGE2/20:1(11Z))'	HMDB02 82174	C46H80NO1 3P	
		885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(hydroxy((2R)-2-(((5Z)-7-((1R,2R,5S)-5-hydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)-3-oxocyclopentyl)hept-5-enoyl)oxy)-3-((11Z)-icos-11-enoyloxy)propoxy)phosphoryl)oxy)propanoic acid'	b'PS(20:1(11Z)/PGD2))'	HMDB02 82175	C46H80NO1 3P	
		885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(hydroxy((2R)-3-(((5Z)-7-((1R,2R,5S)-5-hydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)-3-oxocyclopentyl)hept-5-enoyl)oxy)-2-((11Z)-icos-11-enoyloxy)propoxy)phosphoryl)oxy)propanoic acid'	b'PS(PGD2/20:1(11Z))'	HMDB02 82176	C46H80NO1 3P	
		885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(hydroxy((2R)-3-((11Z)-icos-11-enoyloxy)-2-(((5S,6S,7E,9E,11Z,13E,15S)-5,6,15-trihydroxyicosa-7,9,11,13-tetraenyl)oxy)propoxy)phosphoryl)oxy)propanoic acid'	b'PS(20:1(11Z)/20:4(7E,9E,11Z,13E)-3OH(5S,6R,15S))'	HMDB02 82189	C46H80NO1 3P	
		885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(hydroxy((2R)-2-((11Z)-icos-11-enoyloxy)-3-(((5R,6R,7E,9E,11Z,13E,15R)-5,6,15-trihydroxyicosa-7,9,11,13-tetraenyl)oxy)propoxy)phosphoryl)oxy)propanoic acid'	b'PS(20:4(7E,9E,11Z,13E)-3OH(5S,6R,15S)/20:1(11Z))'	HMDB02 82190	C46H80NO1 3P	
		885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(((2R)-2-(((5E)-7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)cyclopentyl)hept-5-enoyl)oxy)-3-((11Z,14Z)-icosa-11,14-dienoyloxy)propoxy)(hydroxy)phosphoryl)oxy)propanoic acid'	b'PS(20:2(11Z,14Z)/PGF2alpha))'	HMDB02 82283	C46H80NO1 3P	
		885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(((2R)-3-(((5E)-7-((1R,2R,3R,5S)-3,5-dihydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)cyclopentyl)hept-5-enoyl)oxy)-2-((11Z,14Z)-icosa-11,14-dienoyloxy)propoxy)(hydroxy)phosphoryl)oxy)propanoic acid'	b'PS(PGF2alpha/20:2(11Z,14Z))'	HMDB02 82284	C46H80NO1 3P	
		885.5367286	0.0019 714	Protone tion	b'(2S)-2-amino-3-(hydroxy((2R)-2-((7-((1R,2R,3R)-3-hydroxy-2-((1E,3S)-3-hydroxyoct-1-en-1-yl)-5-oxocyclopentyl)heptanoyl)oxy)-3-((11Z,14Z)-icosa-11,14-dienoyloxy)propoxy)phosphoryl)oxy)propanoic acid'	b'PS(20:2(11Z,14Z)/PGE1))'	HMDB02 82345	C46H80NO1 3P	

		885.5367286	0.0019 714	Protona tion	b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-[(1R,2R,3R)-3-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-5-oxocyclopentyl]heptanoyl}oxy)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGE1/20:2(11Z,14Z))'	HMDB02 82346	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-3-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:2(11Z,14Z)/PGD1)'	HMDB02 82347	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-2-[(11Z,14Z)-icosa-11,14-dienoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGD1/20:2(11Z,14Z))'	HMDB02 82348	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2S)-2-amino-3-({[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:3(5Z,8Z,11Z)/PGF1alpha)'	HMDB02 82453	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2S)-2-amino-3-({[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(PGF1alpha/20:3(5Z,8Z,11Z))'	HMDB02 82454	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2S)-2-amino-3-({[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:3(8Z,11Z,14Z)/PGF1alpha)'	HMDB02 82557	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2S)-2-amino-3-({[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(PGF1alpha/20:3(8Z,11Z,14Z))'	HMDB02 82558	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2S)-2-amino-3-({[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy)-3-[(13Z,16Z)-docosa-13,16-dienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:2(13Z,16Z)/5-iso PGF2VI)'	HMDB02 83128	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2S)-2-amino-3-({[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy)-2-[(13Z,16Z)-docosa-13,16-dienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(5-iso PGF2VI/22:2(13Z,16Z))'	HMDB02 83129	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2--{[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]-6-oxoheptanoyl}oxy)-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(9,3)/6 keto-PGF1alpha)'	HMDB02 89245	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2--{[(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]-6-oxoheptanoyl}oxy)-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(6 keto-PGF1alpha/DiMe(9,3))'	HMDB02 89246	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2--{[(2R)-2-{{[(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl}oxy}-3-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(DiMe(9,3)/TXB2)'	HMDB02 89255	C46H80NO1 3P	
		885.5367286	0.0019 714	Protona tion	b'(2--{[(2R)-2-{{[(5Z)-7-[(2R,3S,4S)-4,6-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]oxan-3-yl]hept-5-enoyl}oxy}-2-{{9-(3,4-dimethyl-5-propylfuran-2-yl)nonanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(TXB2/DiMe(9,3))'	HMDB02 89256	C46H80NO1 3P	

39	885.54	886.5506051	0.0014 949	Protona tion	b'(5S,6R,7E,9E,11Z,14Z)-6-{{(2R)-2-amino-3-{{(2R)-1-{{(2-aminoethoxy)(hydroxy)phosphoryl}oxy}-3-(octadec-1-en-1-yloxy)propan-2-yl}oxy}-3-oxopropyl}sulfanyl}-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'PE(P-18:0/LTE4)'	HMDB02 85308	C46H83N2O 10PS	
		886.5506051	0.0014 949	Protona tion	b'(5S,6R,7E,9E,11Z,14Z)-6-{{(2R)-2-amino-3-{{(2R)-3-{{(2-aminoethoxy)(hydroxy)phosphoryl}oxy}-2-(octadec-1-en-1-yloxy)propoxy}-3-oxopropyl}sulfanyl}-5-hydroxyicosa-7,9,11,14-tetraenoic acid'	b'PE(LTE4/P-18:0)'	HMDB02 85309	C46H83N2O 10PS	
39 3	887.55 23	887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2- {{(5Z)-7-[(1R,2R,3R)-3-hydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-5-oxocyclopentyl]hept-5-enoyl}oxy}]-3-(icosanoyloxy)propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:0/PGE2)'	HMDB02 82069	C46H82NO1 3P	
		887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-3- {{(5Z)-7-[(1R,2R,3R)-3-hydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-5-oxocyclopentyl]hept-5-enoyl}oxy}]-2-(icosanoyloxy)propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGE2/20:0)'	HMDB02 82070	C46H82NO1 3P	
		887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2- {{(5Z)-7-[(1R,2R,5S)-5-hydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-3-oxocyclopentyl]hept-5-enoyl}oxy}]-3-(icosanoyloxy)propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:0/PGD2)'	HMDB02 82071	C46H82NO1 3P	
		887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-3- {{(5Z)-7-[(1R,2R,5S)-5-hydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-3-oxocyclopentyl]hept-5-enoyl}oxy}]-2-(icosanoyloxy)propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGD2/20:0)'	HMDB02 82072	C46H82NO1 3P	
		887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-3-(icosanoyloxy)-2- {{(5S,6S,7E,9E,11Z,13E,15S)-5,6,15-trihydroxyicosa-7,9,11,13-tetraenoyl}oxy}propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:0/20:4(7E,9E,11Z,13E)- 3OH(5S,6R,15S))'	HMDB02 82085	C46H82NO1 3P	
		887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2-(icosanoyloxy)-3- {{(5R,6R,7E,9E,11Z,13E,15R)-5,6,15-trihydroxyicosa-7,9,11,13-tetraenoyl}oxy}propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:4(7E,9E,11Z,13E)- 3OH(5S,6R,15S)/20:0)'	HMDB02 82086	C46H82NO1 3P	
		887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({(2R)-2- {{(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}cyclopentyl]hept-5-enoyl}oxy}]-3-{{(11Z)-icos-11-enoyloxy}propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:1(11Z)/PGF2alpha)'	HMDB02 82179	C46H82NO1 3P	
		887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({(2R)-3- {{(5E)-7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}cyclopentyl]hept-5-enoyl}oxy}]-2-{{(11Z)-icos-11-enoyloxy}propoxy}(hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(PGF2alpha/20:1(11Z))'	HMDB02 82180	C46H82NO1 3P	
		887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-[(1R,2R,3R)-3-hydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-5-oxocyclopentyl]heptanoyl}oxy)-3-{{(11Z)-icos-11-enoyloxy}propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:1(11Z)/PGE1)'	HMDB02 82241	C46H82NO1 3P	
		887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-3-({7-[(1R,2R,3R)-3-hydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-5-oxocyclopentyl]heptanoyl}oxy)-2-{{(11Z)-icos-11-enoyloxy}propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGE1/20:1(11Z))'	HMDB02 82242	C46H82NO1 3P	
		887.5523787	7.87E- 05	Redox	b'(2S)-2-amino-3-({hydroxy[(2R)-2-({7-[(1R,2R,5S)-5-hydroxy-2-{{(1E,3S)-3-hydroxyoct-1-en-1-yl}-3-oxocyclopentyl]heptanoyl}oxy)-3-{{(11Z)-icos-11-enoyloxy}propoxy]phosphoryl}oxy)propanoic acid'	b'PS(20:1(11Z)/PGD1)'	HMDB02 82243	C46H82NO1 3P	

39	887.60	887.5523787	7.87E-05	Redox	b'(2S)-2-amino-3-((hydroxy[(2R)-3-({7-[(1R,2R,5S)-5-hydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-3-oxocyclopentyl]heptanoyl}oxy)-2-[(11Z)-icos-11-enoyloxy]propoxy]phosphoryl}oxy)propanoic acid'	b'PS(PGD1/20:1(11Z))'	HMDB02 82244	C46H82NO1 3P	
		887.5523787	7.87E-05	Redox	b'(2S)-2-amino-3-(([(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-3-[(11Z,14Z)-icos-11,14-dienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(20:2(11Z,14Z)/PGF1alpha)'	HMDB02 82349	C46H82NO1 3P	
		887.5523787	7.87E-05	Redox	b'(2S)-2-amino-3-(([(2R)-2-({7-[(1R,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3S)-3-hydroxyoct-1-en-1-yl]cyclopentyl]heptanoyl}oxy)-2-[(11Z,14Z)-icos-11,14-dienoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(PGF1alpha/20:2(11Z,14Z))'	HMDB02 82350	C46H82NO1 3P	
		887.5523787	7.87E-05	Redox	b'(2S)-2-amino-3-(([(2R)-2-({[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy)-3-[(13Z)-docos-13-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(22:1(13Z)/5-iso PGF2VI)'	HMDB02 83024	C46H82NO1 3P	
		887.5523787	7.87E-05	Redox	b'(2S)-2-amino-3-(([(2R)-2-({[(3Z)-5-[(1S,2R,3R,5S)-3,5-dihydroxy-2-[(1E,3R)-3-hydroxyoct-1-en-1-yl]cyclopentyl]pent-3-enoyl}oxy)-2-[(13Z)-docos-13-enoyloxy]propoxy](hydroxy)phosphoryl}oxy)propanoic acid'	b'PS(5-iso PGF2VI/22:1(13Z))'	HMDB02 83025	C46H82NO1 3P	
	56	887.6040204	0.0015796	Redox	b'trimethyl(2- {[(2R)-2- {[(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl}oxy]-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy)ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(6E,8Z,11Z,14Z))+=O(5))'	HMDB02 88121	C51H86NO9 P	
		887.6040204	0.0015796	Redox	b'trimethyl(2- {[(2R)-2- {[(6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenoyl}oxy]-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy)ethyl)azanium'	b'PC(20:4(6E,8Z,11Z,14Z))+=O(5)/22:3(10Z,13Z,16Z))'	HMDB02 88122	C51H86NO9 P	
		887.6040204	0.0015796	Redox	b'trimethyl(2- {[(2R)-2- {[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl}oxy]-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy)ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(5Z,8Z,11Z,13E))+=O(15))'	HMDB02 88123	C51H86NO9 P	
		887.6040204	0.0015796	Redox	b'trimethyl(2- {[(2R)-2- {[(5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenoyl}oxy]-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy)ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/18:2(10E,12Z))+=O(9))'	HMDB02 88124	C51H86NO9 P	
		887.6040204	0.0015796	Redox	b'(2- {[(2R)-2- {[(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenoyl}oxy]-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy)ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	HMDB02 88134	C51H86NO9 P	
		887.6040204	0.0015796	Redox	b'(2- {[(2R)-3- {[(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenoyl}oxy]-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy)ethyl)trimethylazanium'	b'PC(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/22:3(10Z,13Z,16Z))'	HMDB02 88135	C51H86NO9 P	
		887.6040204	0.0015796	Redox	b'(2- {[(2R)-2- {[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoyl}oxy]-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy)ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	HMDB02 88136	C51H86NO9 P	
		887.6040204	0.0015796	Redox	b'(2- {[(2R)-3- {[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenoyl}oxy]-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy)ethyl)trimethylazanium'	b'PC(20:5(5Z,8Z,11Z,14Z,16E)-OH(18)/22:3(10Z,13Z,16Z))'	HMDB02 88137	C51H86NO9 P	

39	5	889.6205	887.6040204	0.0015 796	Redox	b'(2-([(2R)-2-([(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl]oxy)-3-[(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:5(5Z,8Z,10E,14Z,17Z)-OH(12))'	HMDB02 88138	C51H86NO9 P	
			887.6040204	0.0015 796	Redox	b'(2-([(2R)-3-([(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl]oxy)-2-[(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(20:5(5Z,8Z,10E,14Z,17Z)-OH(12)/22:3(10Z,13Z,16Z))'	HMDB02 88139	C51H86NO9 P	
			887.6040204	0.0015 796	Redox	b'(2-([(2R)-2-([(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl]oxy)-3-[(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 88140	C51H86NO9 P	
			887.6040204	0.0015 796	Redox	b'(2-([(2R)-3-([(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl]oxy)-2-[(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy)ethyl)trimethylazanium'	b'PC(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/22:3(10Z,13Z,16Z))'	HMDB02 88141	C51H86NO9 P	
	5	889.6205	889.6196704	0.0008 296	Redox	b'(2-aminoethoxy)[(2R)-2-([(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy)-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 84622	C51H88NO9 P	
			889.6196704	0.0008 296	Redox	b'(2-aminoethoxy)[(2R)-3-([(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy)-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/24:1(15Z))'	HMDB02 84623	C51H88NO9 P	
			889.6196704	0.0008 296	Redox	b'(2-aminoethoxy)[(2R)-2-([(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy)-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 84624	C51H88NO9 P	
			889.6196704	0.0008 296	Redox	b'(2-aminoethoxy)[(2R)-3-([(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy)-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/24:1(15Z))'	HMDB02 84625	C51H88NO9 P	
			889.6196704	0.0008 296	Redox	b'(2-aminoethoxy)[(2R)-2-([(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl]oxy)-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 84626	C51H88NO9 P	
			889.6196704	0.0008 296	Redox	b'(2-aminoethoxy)[(2R)-3-([(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl]oxy)-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/24:1(15Z))'	HMDB02 84627	C51H88NO9 P	
			889.6196704	0.0008 296	Redox	b'(2-aminoethoxy)[(2R)-2-([(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl]oxy)-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 84628	C51H88NO9 P	
			889.6196704	0.0008 296	Redox	b'(2-aminoethoxy)[(2R)-3-([(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl]oxy)-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/24:1(15Z))'	HMDB02 84629	C51H88NO9 P	
			889.6196704	0.0008 296	Redox	b'(2-aminoethoxy)[(2R)-2-([(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl]oxy)-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 84632	C51H88NO9 P	

		889.6196704	0.0008 296	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/24:1(15Z))'	HMDB02 84633	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'trimethyl(2-{{(2R)-2-{{(5Z,8Z,11Z)-13-(3-pentyloxiran-2-yl)trideca-5,8,11-trienoyl}oxy}-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy} ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/20:3(5Z,8Z,11 Z)-O(14R,15S))'	HMDB02 88071	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'trimethyl(2-{{(2R)-3-{{(5Z,8Z,11Z)-13-(3-pentyloxiran-2-yl)trideca-5,8,11-trienoyl}oxy}-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy} ethyl)azanium'	b'PC(20:3(5Z,8Z,11Z)- O(14R,15S)/22:3(10Z,13Z,16Z))'	HMDB02 88072	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'trimethyl(2-{{(2R)-2-{{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyl}oxy}-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy} ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/20:3(5Z,8Z,14 Z)-O(11S,12R))'	HMDB02 88073	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'trimethyl(2-{{(2R)-3-{{(5Z,8Z)-10-{3-[(2Z)-oct-2-en-1-yl]oxiran-2-yl}deca-5,8-dienoyl}oxy}-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy} ethyl)azanium'	b'PC(20:3(5Z,8Z,14Z)- O(11S,12R)/22:3(10Z,13Z,16Z))'	HMDB02 88074	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'trimethyl(2-{{(2R)-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]-2-{{(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl}oxy}propyl phosphono}oxy} ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/20:3(5Z,11Z,1 4Z)-O(8,9))'	HMDB02 88075	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'trimethyl(2-{{(2R)-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]-3-{{(5Z)-7-{3-[(2Z,5Z)-undeca-2,5-dien-1-yl]oxiran-2-yl}hept-5-enoyl}oxy}propyl phosphono}oxy} ethyl)azanium'	b'PC(20:3(5Z,11Z,14Z)- O(8,9)/22:3(10Z,13Z,16Z))'	HMDB02 88076	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'trimethyl(2-{{(2R)-2-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl}oxy)-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy} ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/20:3(8Z,11Z,1 4Z)-O(5,6))'	HMDB02 88077	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'trimethyl(2-{{(2R)-3-[(4-{3-[(2Z,5Z,8Z)-tetradeca-2,5,8-trien-1-yl]oxiran-2-yl}butanoyl}oxy)-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy} ethyl)azanium'	b'PC(20:3(8Z,11Z,14Z)- O(5,6)/22:3(10Z,13Z,16Z))'	HMDB02 88078	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2-{{(2R)-2-{{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenyl}oxy}-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy} ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(5Z,8Z,11 Z,14Z)-OH(20))'	HMDB02 88079	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2-{{(2R)-3-{{(5Z,8Z,11Z,14Z)-20-hydroxyicosa-5,8,11,14-tetraenyl}oxy}-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy} ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)- OH(20)/22:3(10Z,13Z,16Z))'	HMDB02 88080	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2-{{(2R)-2-{{(5R,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenyl}oxy}-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy} ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(6E,8Z,11 Z,14Z)-OH(5S))'	HMDB02 88081	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2-{{(2R)-3-{{(5S,6E,8Z,11Z,14Z)-5-hydroxyicosa-6,8,11,14-tetraenyl}oxy}-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono}oxy} ethyl)trimethylazanium'	b'PC(20:4(6E,8Z,11Z,14Z)- OH(5S)/22:3(10Z,13Z,16Z))'	HMDB02 88082	C51H88NO9 P	

		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-2- -{[(5Z,8Z,11Z,14Z,19S)-19-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}-3- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(5Z,8Z,11Z,14Z)-OH(19S))'	HMDB02 88083	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-3- -{[(5Z,8Z,11Z,14Z,19R)-19-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}-2- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)-OH(19S)/22:3(10Z,13Z,16Z))'	HMDB02 88084	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-2- -{[(5Z,8Z,11Z,14Z,18R)-18-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}-3- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(5Z,8Z,11Z,14Z)-OH(18R))'	HMDB02 88085	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-3- -{[(5Z,8Z,11Z,14Z,18S)-18-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}-2- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)-OH(18R)/22:3(10Z,13Z,16Z))'	HMDB02 88086	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-2- -{[(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}-3- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(5Z,8Z,11Z,14Z)-OH(17))'	HMDB02 88087	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-3- -{[(5Z,8Z,11Z,14Z)-17-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}-2- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)-OH(17)/22:3(10Z,13Z,16Z))'	HMDB02 88088	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-2- -{[(5Z,8Z,11Z,14Z,16R)-16-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}-3- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(5Z,8Z,11Z,14Z)-OH(16R))'	HMDB02 88089	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-3- -{[(5Z,8Z,11Z,14Z,16S)-16-hydroxyicosa-5,8,11,14-tetraenoyl]oxy}-2- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,14Z)-OH(16R)/22:3(10Z,13Z,16Z))'	HMDB02 88090	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-2- -{[(5Z,8Z,11Z,13E,15S)-15-hydroxyicosa-5,8,11,13-tetraenoyl]oxy}-3- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(5Z,8Z,11Z,13E)-OH(15S))'	HMDB02 88091	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-3- -{[(5Z,8Z,11Z,13E,15R)-15-hydroxyicosa-5,8,11,13-tetraenoyl]oxy}-2- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,11Z,13E)-OH(15S)/22:3(10Z,13Z,16Z))'	HMDB02 88092	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-2- -{[(5Z,8Z,10E,12S,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoyl]oxy}-3- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(5Z,8Z,10E,14Z)-OH(12S))'	HMDB02 88093	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-3- -{[(5Z,8Z,10E,12R,14Z)-12-hydroxyicosa-5,8,10,14-tetraenoyl]oxy}-2- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(20:4(5Z,8Z,10E,14Z)-OH(12S)/22:3(10Z,13Z,16Z))'	HMDB02 88094	C51H88NO9 P	
		889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-2- -{[(5E,8Z,11R,12Z,14Z)-11-hydroxyicosa-5,8,12,14-tetraenoyl]oxy}-3- -{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono]oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(5E,8Z,12Z,14Z)-OH(11R))'	HMDB02 88095	C51H88NO9 P	

39	6	891.63	889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-3- -{[(5E,8Z,11S,12Z,14Z)-11-hydroxyicosano-5,8,12,14-tetraenyl]oxy}-2- -{(10Z,13Z,16Z)-tricosano-10,13,16-trienyloxy]propyl phosphono}oxy} ethyl)trimethylazanium'	b'PC(20:4(5E,8Z,12Z,14Z)-OH(11R)/22:3(10Z,13Z,16Z))'	HMDB02 88096	C51H88NO9 P	
			889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-3- -{[(5E,7Z,11Z,14Z)-9-hydroxyicosano-5,7,11,14-tetraenyl]oxy}-3- -{(10Z,13Z,16Z)-tricosano-10,13,16-trienyloxy]propyl phosphono}oxy} ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(5Z,7E,11Z,14Z)-OH(9))'	HMDB02 88097	C51H88NO9 P	
			889.6196704	0.0008 296	Redox	b'(2- -{[(2R)-3- -{[(5E,7Z,11Z,14Z)-9-hydroxyicosano-5,7,11,14-tetraenyl]oxy}-2- -{(10Z,13Z,16Z)-tricosano-10,13,16-trienyloxy]propyl phosphono}oxy} ethyl)trimethylazanium'	b'PC(20:4(5Z,7E,11Z,14Z)-OH(9)/22:3(10Z,13Z,16Z))'	HMDB02 88098	C51H88NO9 P	
	55	891.63	892.6404654	0.0028 346	Protonation	b'[(2R)-2- -{[(9S,10S,12Z)-9,10-dihydroxyoctadec-12-enyl]oxy}-3- -{(22-methyltricosanoyl)oxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(i-24:0/18:1(12Z)-2OH(9,10))'	HMDB02 72245	C48H93O12 P	
			892.6404654	0.0028 346	Protonation	b'[(2R)-3- -{[(9R,10R,12Z)-9,10-dihydroxyoctadec-12-enyl]oxy}-2- -{(22-methyltricosanoyl)oxy]propoxy][(2S)-2,3-dihydroxypropoxy]phosphinic acid'	b'PG(18:1(12Z)-2OH(9,10)/i-24:0)'	HMDB02 72246	C48H93O12 P	
			891.6353205	0.0001 795	Redox	b'(2-aminoethoxy)[(2R)-2- -{[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy}-3- -{(tetracosanoyl)oxy]propoxy]phosphinic acid'	b'PE(24:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 84518	C51H90NO9 P	
			891.6353205	0.0001 795	Redox	b'(2-aminoethoxy)[(2R)-3- -{[(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl]oxy}-2- -{(tetracosanoyl)oxy]propoxy]phosphinic acid'	b'PE(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/24:0)'	HMDB02 84519	C51H90NO9 P	
			891.6353205	0.0001 795	Redox	b'(2-aminoethoxy)[(2R)-2- -{[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy}-3- -{(tetracosanoyl)oxy]propoxy]phosphinic acid'	b'PE(24:0/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 84520	C51H90NO9 P	
			891.6353205	0.0001 795	Redox	b'(2-aminoethoxy)[(2R)-3- -{[(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl]oxy}-2- -{(tetracosanoyl)oxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/24:0)'	HMDB02 84521	C51H90NO9 P	
			891.6353205	0.0001 795	Redox	b'(2-aminoethoxy)[(2R)-2- -{[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl]oxy}-3- -{(tetracosanoyl)oxy]propoxy]phosphinic acid'	b'PE(24:0/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 84522	C51H90NO9 P	
			891.6353205	0.0001 795	Redox	b'(2-aminoethoxy)[(2R)-3- -{[(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl]oxy}-2- -{(tetracosanoyl)oxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/24:0)'	HMDB02 84523	C51H90NO9 P	
			891.6353205	0.0001 795	Redox	b'(2-aminoethoxy)[(2R)-2- -{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl]oxy}-3- -{(tetracosanoyl)oxy]propoxy]phosphinic acid'	b'PE(24:0/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 84524	C51H90NO9 P	
			891.6353205	0.0001 795	Redox	b'(2-aminoethoxy)[(2R)-3- -{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl]oxy}-2- -{(tetracosanoyl)oxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/24:0)'	HMDB02 84525	C51H90NO9 P	

		891.6353205	0.0001 795	Redox	b'(2-aminoethoxy)[(2R)-2-{{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17))'	HMDB02 84528	C51H90NO9 P	
		891.6353205	0.0001 795	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10Z,13Z)-15-{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/24:0)'	HMDB02 84529	C51H90NO9 P	
		891.6353205	0.0001 795	Redox	b'(2-{{(2R)-2-{{(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienyl}oxy}-3-[(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:3(6,8,11)- OH(5))'	HMDB02 88172	C51H90NO9 P	
		891.6353205	0.0001 795	Redox	b'(2-{{(2R)-3-{{(6E,8E,11E)-5-hydroxyicosa-6,8,11-trienyl}oxy}-2-[(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:3(6,8,11)- OH(5)/22:3(10Z,13Z,16Z))'	HMDB02 88173	C51H90NO9 P	
39	7	903.598935	0.0016 65	Redox	b'(2-{{(2R)-2-{{(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl}oxy}-3-[(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/PGJ2)'	HMDB02 88107	C51H86NO1 0P	
		903.598935	0.0016 65	Redox	b'(2-{{(2R)-3-{{(5Z)-7-[(1S,5R)-5-[(1E,3S)-3-hydroxyoct-1-en-1-yl]-4-oxocyclopent-2-en-1-yl]hept-5-enoyl}oxy}-2-[(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy]propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(PGJ2/22:3(10Z,13Z,16Z))'	HMDB02 88108	C51H86NO1 0P	
39	8	903.6353205	0.0008 205	Redox	b'(2-{{(2R)-3-[(13Z)-docos-13-enoyloxy]-2-{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:1(13Z)/22:6(5Z,7Z,10Z,13Z,16 Z,19Z)-OH(4))'	HMDB02 87943	C52H90NO9 P	
		903.6353205	0.0008 205	Redox	b'(2-{{(2R)-2-[(13Z)-docos-13-enoyloxy]-3-{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:6(5Z,7Z,10Z,13Z,16Z,19Z)- OH(4)/22:1(13Z))'	HMDB02 87944	C52H90NO9 P	
		903.6353205	0.0008 205	Redox	b'(2-{{(2R)-3-[(13Z)-docos-13-enoyloxy]-2-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:1(13Z)/22:6(4Z,8Z,10Z,13Z,16 Z,19Z)-OH(7))'	HMDB02 87945	C52H90NO9 P	
		903.6353205	0.0008 205	Redox	b'(2-{{(2R)-2-[(13Z)-docos-13-enoyloxy]-3-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,8Z,10Z,13Z,16Z,19Z)- OH(7)/22:1(13Z))'	HMDB02 87946	C52H90NO9 P	
		903.6353205	0.0008 205	Redox	b'(2-{{(2R)-3-[(13Z)-docos-13-enoyloxy]-2-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:1(13Z)/22:6(4Z,7Z,10Z,12E,16 Z,19Z)-OH(14))'	HMDB02 87947	C52H90NO9 P	
		903.6353205	0.0008 205	Redox	b'(2-{{(2R)-2-[(13Z)-docos-13-enoyloxy]-3-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,12E,16Z,19Z)- OH(14)/22:1(13Z))'	HMDB02 87948	C52H90NO9 P	
		903.6353205	0.0008 205	Redox	b'(2-{{(2R)-3-[(13Z)-docos-13-enoyloxy]-2-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:1(13Z)/22:6(4Z,7Z,10Z,13E,15 E,19Z)-OH(17))'	HMDB02 87949	C52H90NO9 P	

39	905.61	903.6353205	0.0008 205	Redox	b'(2- -{[(2R)-2-[(13Z)-docos-13-enoyloxy]-3- -{[(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenoyl]oxy}propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,13E,15E,19Z)- OH(17)/22:1(13Z))'	HMDB02 87950	C52H90NO9 P	
		903.6353205	0.0008 205	Redox	b'(2- -{[(2R)-3-[(13Z)-docos-13-enoyloxy]-2- -{[(4Z,7Z,10Z,13Z)-15- -{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy}propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(22:1(13Z)/22:5(4Z,7Z,10Z,13Z,19 Z)-O(16,17))'	HMDB02 87953	C52H90NO9 P	
		903.6353205	0.0008 205	Redox	b'(2- -{[(2R)-2-[(13Z)-docos-13-enoyloxy]-3- -{[(4Z,7Z,10Z,13Z)-15- -{3-[(2Z)-pent-2-en-1-yl]oxiran-2-yl}pentadeca-4,7,10,13-tetraenoyl]oxy}propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/22:1(13Z))'	HMDB02 87954	C52H90NO9 P	
	56	905.614585	0.0010 15	Redox	b'(2-aminoethoxy)[(2R)-2- -{[(5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl]oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/22:6(5Z,8E,10Z,13Z,15 E,19Z)-2OH(7S,17S))'	HMDB02 84614	C51H88NO1 OP	
		905.614585	0.0010 15	Redox	b'(2-aminoethoxy)[(2R)-3- -{[(5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl]oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(22:6(5Z,8E,10Z,13Z,15E,19Z)- 2OH(7S,17S)/24:1(15Z))'	HMDB02 84615	C51H88NO1 OP	
		905.614585	0.0010 15	Redox	b'(2-aminoethoxy)[(2R)-2- -{[(4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl]oxy}-3-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(24:1(15Z)/22:6(4Z,7Z,11E,13Z,15 E,19Z)-2OH(10S,17))'	HMDB02 84630	C51H88NO1 OP	
		905.614585	0.0010 15	Redox	b'(2-aminoethoxy)[(2R)-3- -{[(4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenoyl]oxy}-2-[(15Z)-tetracos-15-enoyloxy]propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,11E,13Z,15E,19Z)- 2OH(10S,17)/24:1(15Z))'	HMDB02 84631	C51H88NO1 OP	
		905.614585	0.0010 15	Redox	b'(2- -{[(2R)-2- -{[(5R,6Z,8E,10E,12S,14Z)-5,12-dihydroxydocosa-6,8,10,14-tetraenoyl]oxy}-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(6Z,8E,10 E,14Z)-2OH(5S,12R))'	HMDB02 88111	C51H88NO1 OP	
		905.614585	0.0010 15	Redox	b'(2- -{[(2R)-3- -{[(5S,6Z,8E,10E,12R,14Z)-5,12-dihydroxydocosa-6,8,10,14-tetraenoyl]oxy}-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(6Z,8E,10E,14Z)- 2OH(5S,12R)/22:3(10Z,13Z,16Z))'	HMDB02 88112	C51H88NO1 OP	
		905.614585	0.0010 15	Redox	b'(2- -{[(2R)-2- -{[(5S,6E,8Z,11Z,13E,15R)-5,15-dihydroxydocosa-6,8,11,13-tetraenoyl]oxy}-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(6E,8Z,11 Z,13E)-2OH(5S,15S))'	HMDB02 88146	C51H88NO1 OP	
		905.614585	0.0010 15	Redox	b'(2- -{[(2R)-3- -{[(5R,6E,8Z,11Z,13E,15S)-5,15-dihydroxydocosa-6,8,11,13-tetraenoyl]oxy}-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(6E,8Z,11Z,13E)- 2OH(5S,15S)/22:3(10Z,13Z,16Z))'	HMDB02 88147	C51H88NO1 OP	
		905.614585	0.0010 15	Redox	b'(2- -{[(2R)-2- -{[(5R,6R,8Z,11Z,14Z,17Z)-5,6-dihydroxydocosa-8,11,14,17-tetraenoyl]oxy}-3-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:4(8Z,11Z,1 4Z,17Z)-2OH(5S,6R))'	HMDB02 88148	C51H88NO1 OP	
		905.614585	0.0010 15	Redox	b'(2- -{[(2R)-3- -{[(5S,6S,8Z,11Z,14Z,17Z)-5,6-dihydroxydocosa-8,11,14,17-tetraenoyl]oxy}-2-[(10Z,13Z,16Z)-tricos-10,13,16-trienoyloxy]propyl phosphono]oxy} ethyl)trimethylazanium'	b'PC(20:4(8Z,11Z,14Z,17Z)- 2OH(5S,6R)/22:3(10Z,13Z,16Z))'	HMDB02 88149	C51H88NO1 OP	

40 0	907.63 06	908.6380596	0.0003 404	Protona tion	b'(3-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)-2-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(11,3)/MonoMe(13,5))'	HMDB00 61397	C51H91NO1 0P	
		908.6380596	0.0003 404	Protona tion	b'(3-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-2-([11-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(11,5)/MonoMe(11,5))'	HMDB00 61405	C51H91NO1 0P	
		908.6380596	0.0003 404	Protona tion	b'(3-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(13,5)/MonoMe(11,3))'	HMDB00 61413	C51H91NO1 0P	
		908.6380596	0.0003 404	Protona tion	b'(3-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(13,5)/MonoMe(9,5))'	HMDB00 61416	C51H91NO1 0P	
		908.6380596	0.0003 404	Protona tion	b'(3-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-2-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(DiMe(9,5)/MonoMe(13,5))'	HMDB00 61433	C51H91NO1 0P	
		908.6380596	0.0003 404	Protona tion	b'(2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([11-(3-methyl-5-propylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,3)/DiMe(13,5))'	HMDB00 61437	C51H91NO1 0P	
		908.6380596	0.0003 404	Protona tion	b'(2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(11,5)/DiMe(11,5))'	HMDB00 61445	C51H91NO1 0P	
		908.6380596	0.0003 404	Protona tion	b'(2-([11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(13,5)/DiMe(11,3))'	HMDB00 61453	C51H91NO1 0P	
		908.6380596	0.0003 404	Protona tion	b'(2-([9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl]oxy)-3-([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(13,5)/DiMe(9,5))'	HMDB00 61457	C51H91NO1 0P	
		908.6380596	0.0003 404	Protona tion	b'(2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([9-(3-methyl-5-pentylfuran-2-yl)nonanoyl]oxy)propoxy)[2-(trimethylazaniumyl)ethoxy]phosphinic acid'	b'PC(MonoMe(9,5)/DiMe(13,5))'	HMDB00 61464	C51H91NO1 0P	
		907.6302346	0.0003 654	Redox	b'(2-aminoethoxy)[(2R)-2-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-3-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy]phosphinic acid'	b'PE(DiMe(11,5)/DiMe(13,5))'	HMDB00 61482	C51H90NO1 0P	
		907.6302346	0.0003 654	Redox	b'(2-aminoethoxy)[(2R)-3-([13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)-2-([11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl]oxy)propoxy]phosphinic acid'	b'PE(DiMe(13,5)/DiMe(11,5))'	HMDB00 61490	C51H90NO1 0P	
		907.6302346	0.0003 654	Redox	b'(2-aminoethoxy)[(2R)-2,3-bis([13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl]oxy)]propoxy]phosphinic acid'	b'PE(MonoMe(13,5)/MonoMe(13,5))'	HMDB00 61541	C51H90NO1 0P	

		907.6302351	0.0003 649	Redox	b'[(2R)-3-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-2-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11D5/13M5)'	HMDB01 13770	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'[(2R)-2-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(11M5/13D5)'	HMDB01 13787	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'[(2R)-3-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(13D5/11M5)'	HMDB01 13795	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'[(2R)-2-{{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy}-3-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(methylamino)ethoxy]phosphinic acid'	b'PE-NMe(13M5/11D5)'	HMDB01 13802	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'[(2R)-2-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-{{11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMe2(11D3/13D5)'	HMDB01 14664	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'[(2R)-2,3-bis({{11-(3,4-dimethyl-5-pentylfuran-2-yl)undecanoyl}oxy})propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMe2(11D5/11D5)'	HMDB01 14670	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'[2-(dimethylamino)ethoxy][(2R)-2-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-3-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy]phosphinic acid'	b'PE-NMe2(11M5/13M5)'	HMDB01 14692	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'[(2R)-3-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{11-(3,4-dimethyl-5-propylfuran-2-yl)undecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMe2(13D5/11D3)'	HMDB01 14696	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'[(2R)-2-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-3-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMe2(13D5/9D5)'	HMDB01 14703	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'[2-(dimethylamino)ethoxy][(2R)-3-{{13-(3-methyl-5-pentylfuran-2-yl)tridecanoyl}oxy}-2-{{11-(3-methyl-5-pentylfuran-2-yl)undecanoyl}oxy}propoxy]phosphinic acid'	b'PE-NMe2(13M5/11M5)'	HMDB01 14708	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'[(2R)-3-{{9-(3,4-dimethyl-5-pentylfuran-2-yl)nonanoyl}oxy}-2-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propoxy][2-(dimethylamino)ethoxy]phosphinic acid'	b'PE-NMe2(9D5/13D5)'	HMDB01 14727	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'(2-aminoethoxy)[(2R)-2-{{(5Z,7R,8E,10Z,13Z,15E,17S,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-3-(tetracosanoyl)oxy]propoxy]phosphinic acid'	b'PE(24:0/22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S))'	HMDB02 84510	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'(2-aminoethoxy)[(2R)-3-{{(5Z,7S,8E,10Z,13Z,15E,17R,19Z)-7,17-dihydroxydocosa-5,8,10,13,15,19-hexaenoyl}oxy}-2-(tetracosanoyl)oxy]propoxy]phosphinic acid'	b'PE(22:6(5Z,8E,10Z,13Z,15E,19Z)-2OH(7S, 17S)/24:0)'	HMDB02 84511	C51H90NO1 0P	

40	1	907.6302351	0.0003 649	Redox	b'(2-aminoethoxy)[(2R)-2-{{(4Z,7Z,10R,11E,13Z,15E,17S,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenyl}oxy}-3-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(24:0/22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17))'	HMDB02 84526	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'(2-aminoethoxy)[(2R)-3-{{(4Z,7Z,10S,11E,13Z,15E,17R,19Z)-10,17-dihydroxydocosa-4,7,11,13,15,19-hexaenyl}oxy}-2-(tetracosanoyloxy)propoxy]phosphinic acid'	b'PE(22:6(4Z,7Z,11E,13Z,15E,19Z)-2OH(10S,17)/24:0)'	HMDB02 84527	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'(2-{{(2R)-2-{{(8Z,11Z,14Z)-5,6-dihydroxydocosa-8,11,14-trienyl}oxy}-3-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/20:3(8Z,11Z,14Z)-2OH(5,6))'	HMDB02 88117	C51H90NO1 0P	
		907.6302351	0.0003 649	Redox	b'(2-{{(2R)-3-{{(8Z,11Z,14Z)-5,6-dihydroxydocosa-8,11,14-trienyl}oxy}-2-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(20:3(8Z,11Z,14Z)-2OH(5,6)/22:3(10Z,13Z,16Z))'	HMDB02 88118	C51H90NO1 0P	
	35	913.6196704	0.0016 296	Protontion	b'(2-{{(2R)-2-{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl}oxy}-3-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))'	HMDB02 88150	C53H88NO9 P	
		913.6196704	0.0016 296	Protontion	b'(2-{{(2R)-3-{{(5Z,7Z,10Z,13Z,16Z,19Z)-4-hydroxydocosa-5,7,10,13,16,19-hexaenyl}oxy}-2-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4)/22:3(10Z,13Z,16Z))'	HMDB02 88151	C53H88NO9 P	
		913.6196704	0.0016 296	Protontion	b'(2-{{(2R)-2-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl}oxy}-3-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7))'	HMDB02 88152	C53H88NO9 P	
		913.6196704	0.0016 296	Protontion	b'(2-{{(2R)-3-{{(4Z,8Z,10Z,13Z,16Z,19Z)-7-hydroxydocosa-4,8,10,13,16,19-hexaenyl}oxy}-2-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,8Z,10Z,13Z,16Z,19Z)-OH(7)/22:3(10Z,13Z,16Z))'	HMDB02 88153	C53H88NO9 P	
		913.6196704	0.0016 296	Protontion	b'(2-{{(2R)-2-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl}oxy}-3-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14))'	HMDB02 88154	C53H88NO9 P	
		913.6196704	0.0016 296	Protontion	b'(2-{{(2R)-3-{{(4Z,7Z,10Z,12E,16Z,19Z)-14-hydroxydocosa-4,7,10,12,16,19-hexaenyl}oxy}-2-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,12E,16Z,19Z)-OH(14)/22:3(10Z,13Z,16Z))'	HMDB02 88155	C53H88NO9 P	
		913.6196704	0.0016 296	Protontion	b'(2-{{(2R)-2-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl}oxy}-3-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:3(10Z,13Z,16Z)/22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17))'	HMDB02 88156	C53H88NO9 P	
		913.6196704	0.0016 296	Protontion	b'(2-{{(2R)-3-{{(4Z,7Z,10Z,13E,15E,19Z)-17-hydroxydocosa-4,7,10,13,15,19-hexaenyl}oxy}-2-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(22:6(4Z,7Z,10Z,13E,15E,19Z)-OH(17)/22:3(10Z,13Z,16Z))'	HMDB02 88157	C53H88NO9 P	
		913.6196704	0.0016 296	Protontion	b'trimethyl(2-{{(2R)-2-{{(4Z,7Z,10Z,13Z)-15-3-{{(2Z)-pent-2-en-1-yl}oxiran-2-yl}pentadeca-4,7,10,13-tetraenyl}oxy}-3-{{(10Z,13Z,16Z)-tricoso-10,13,16-trienoyloxy}propyl phosphono}oxy}ethyl)azanium'	b'PC(22:3(10Z,13Z,16Z)/22:5(4Z,7Z,10Z,13Z,19Z)-O(16,17))'	HMDB02 88160	C53H88NO9 P	

		913.6196704	0.0016 296	Protone tion	b'trimethyl(2-((2R)-3-((4Z,7Z,10Z,13Z)-15-{3-((2Z)-pent-2-en-1-yl)oxiran-2-yl)pentadeca-4,7,10,13-tetraenyl}oxy)-2-((10Z,13Z,16Z)-tricoso-10,13,16-trienyloxy)propyl phosphono)oxy)ethyl)azanium'	b'PC(22:5(4Z,7Z,10Z,13Z,19Z)- O(16,17)/22:3(10Z,13Z,16Z))'	HMDB02 88161	C53H88NO9 P	
40 2	933.52 7	934.5336314	0.0011 686	Protone tion	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-3-((18-methylcosanoyl)oxy)-2-((6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl)oxy)propoxy)phosphoryl)oxy]propoxy]phosphonic acid'	b'PGP(a- 21:0/20:4(6E,8Z,11Z,14Z)+=O(5))'	HMDB02 74623	C47H84O14 P2	
		934.5336314	0.0011 686	Protone tion	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-2-((18-methylcosanoyl)oxy)-3-((6E,8Z,11Z,14Z)-5-oxoicosa-6,8,11,14-tetraenyl)oxy)propoxy)phosphoryl)oxy]propoxy]phosphonic acid'	b'PGP(20:4(6E,8Z,11Z,14Z)+=O(5))a- 21:0)'	HMDB02 74624	C47H84O14 P2	
		934.5336314	0.0011 686	Protone tion	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-3-((18-methylcosanoyl)oxy)-2-((5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl)oxy)propoxy)phosphoryl)oxy]propoxy]phosphonic acid'	b'PGP(a- 21:0/20:4(5Z,8Z,11Z,13E)+=O(15))'	HMDB02 74625	C47H84O14 P2	
		934.5336314	0.0011 686	Protone tion	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-2-((18-methylcosanoyl)oxy)-3-((5Z,8Z,11Z,13E)-15-oxoicosa-5,8,11,13-tetraenyl)oxy)propoxy)phosphoryl)oxy]propoxy]phosphonic acid'	b'PGP(20:4(5Z,8Z,11Z,13E)+=O(15))a- 21:0)'	HMDB02 74626	C47H84O14 P2	
		934.5336314	0.0011 686	Protone tion	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-2-((5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosa-5,8,11,14,16-pentaenyl)oxy)-3-((18- methylcosanoyl)oxy)propoxy)phosphoryl)oxy]propoxy]phosphonic acid'	b'PGP(a- 21:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18R))'	HMDB02 74637	C47H84O14 P2	
		934.5336314	0.0011 686	Protone tion	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-3-((5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosa-5,8,11,14,16-pentaenyl)oxy)-2-((18- methylcosanoyl)oxy)propoxy)phosphoryl)oxy]propoxy]phosphonic acid'	b'PGP(20:5(5Z,8Z,11Z,14Z,16E)- OH(18R)/a-21:0)'	HMDB02 74638	C47H84O14 P2	
		934.5336314	0.0011 686	Protone tion	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-2-((5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl)oxy)-3-((18- methylcosanoyl)oxy)propoxy)phosphoryl)oxy]propoxy]phosphonic acid'	b'PGP(a- 21:0/20:5(5Z,8Z,11Z,14Z,16E)- OH(18))'	HMDB02 74639	C47H84O14 P2	
		934.5336314	0.0011 686	Protone tion	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-3-((5Z,8Z,11Z,13E,17Z)-16-hydroxyicosa-5,8,11,13,17-pentaenyl)oxy)-2-((18- methylcosanoyl)oxy)propoxy)phosphoryl)oxy]propoxy]phosphonic acid'	b'PGP(20:5(5Z,8Z,11Z,14Z,16E)- OH(18)/a-21:0)'	HMDB02 74640	C47H84O14 P2	
		934.5336314	0.0011 686	Protone tion	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-2-((5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl)oxy)-3-((18- methylcosanoyl)oxy)propoxy)phosphoryl)oxy]propoxy]phosphonic acid'	b'PGP(a- 21:0/20:5(5Z,8Z,10E,14Z,17Z)- OH(12))'	HMDB02 74641	C47H84O14 P2	
		934.5336314	0.0011 686	Protone tion	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-3-((5Z,8Z,10E,14Z,17Z)-12-hydroxyicosa-5,8,10,14,17-pentaenyl)oxy)-2-((18- methylcosanoyl)oxy)propoxy)phosphoryl)oxy]propoxy]phosphonic acid'	b'PGP(20:5(5Z,8Z,10E,14Z,17Z)- OH(12)/a-21:0)'	HMDB02 74642	C47H84O14 P2	
		934.5336314	0.0011	Protone	b'[(2S)-2-hydroxy-3-(hydroxy((2R)-2-((6E,8Z,11Z,14Z,17Z)-5-hydroxyicosa-6,8,11,14,17-pentaenyl)oxy)-3-((18-	b'PGP(a-	HMDB02	C47H84O14	

		686	tion	methylicosanoyl}oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	21:0/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	74643	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-3-[[[(6E,8Z,11Z,14Z,17Z)-5-hydroxyicosan-6,8,11,14,17-pentaenyl]oxy]-2-[(18-methylicosanoyl}oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/a-21:0))'	74644	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-3-[(19-methylicosanoyl}oxy]-2-[[[(6E,8Z,11Z,14Z)-5-oxoicosan-6,8,11,14-tetraenyl]oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(i-21:0/20:4(6E,8Z,11Z,14Z)+=O(5))'	75764	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-2-[(19-methylicosanoyl}oxy]-3-[[[(6E,8Z,11Z,14Z)-5-oxoicosan-6,8,11,14-tetraenyl]oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(20:4(6E,8Z,11Z,14Z)+=O(5)/i-21:0))'	75765	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-3-[(19-methylicosanoyl}oxy]-2-[[[(5Z,8Z,11Z,13E)-15-oxoicosan-5,8,11,13-tetraenyl]oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(i-21:0/20:4(5Z,8Z,11Z,13E)+=O(15))'	75766	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-2-[(19-methylicosanoyl}oxy]-3-[[[(5Z,8Z,11Z,13E)-15-oxoicosan-5,8,11,13-tetraenyl]oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(20:4(5Z,8Z,11Z,13E)+=O(15)/i-21:0))'	75767	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-2-[[[(5Z,8Z,11Z,14Z,16E,18R)-18-hydroxyicosan-5,8,11,14,16-pentaenyl]oxy]-3-[(19-methylicosanoyl}oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(i-21:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18R))'	75778	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-3-[[[(5Z,8Z,11Z,14Z,16E,18S)-18-hydroxyicosan-5,8,11,14,16-pentaenyl]oxy]-2-[(19-methylicosanoyl}oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/i-21:0))'	75779	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-2-[[[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosan-5,8,11,13,17-pentaenyl]oxy]-3-[(19-methylicosanoyl}oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(i-21:0/20:5(5Z,8Z,11Z,14Z,16E)-OH(18))'	75780	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-3-[[[(5Z,8Z,11Z,13E,17Z)-16-hydroxyicosan-5,8,11,13,17-pentaenyl]oxy]-2-[(19-methylicosanoyl}oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(20:5(5Z,8Z,11Z,14Z,16E)-OH(18)/i-21:0))'	75781	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-2-[[[(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosan-5,8,10,14,17-pentaenyl]oxy]-3-[(19-methylicosanoyl}oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(i-21:0/20:5(5Z,8Z,10E,14Z,17Z)-OH(12))'	75782	P2	
934.5336314	0.0011	686	Protontion	b'[(2S)-2-hydroxy-3-(hydroxy{(2R)-3-[[[(5Z,8Z,10E,14Z,17Z)-12-hydroxyicosan-5,8,10,14,17-pentaenyl]oxy]-2-[(19-methylicosanoyl}oxy}propoxy}phosphoryl}oxy}propoxy}phosphonic acid'	b'PGP(20:5(5Z,8Z,10E,14Z,17Z)-OH(12)/i-21:0))'	75783	P2	

		934.5336314	0.0011 686	Protone	b'[(2S)-2-hydroxy-3-(hydroxy[(2R)-2-[(6E,8Z,11Z,14Z,17Z)-5-hydroxyicos-6,8,11,14,17-pentaenyl]oxy)-3-[(19-methylicosanoyl]oxy)propoxy]phosphoryl]oxy)propoxy]phosphonic acid'	b'PGP(i-21:0/20:5(6E,8Z,11Z,14Z,17Z)-OH(5))'	HMDB02 75784	C47H84O14 P2	
		934.5336314	0.0011 686	Protone	b'[(2S)-2-hydroxy-3-(hydroxy[(2R)-3-[(6E,8Z,11Z,14Z,17Z)-5-hydroxyicos-6,8,11,14,17-pentaenyl]oxy)-2-[(19-methylicosanoyl]oxy)propoxy]phosphoryl]oxy)propoxy]phosphonic acid'	b'PGP(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/i-21:0)'	HMDB02 75785	C47H84O14 P2	
40 3	965.51 57	966.5234597	4.03E-05	Protone	b'[(1R,3S)-3-[(2R)-2-[(10Z,13Z,16Z,19Z)-docosa-10,13,16,19-tetraenyl]oxy)-3-(hexadecanoyl)oxy]propoxy]phosphoryl]oxy)-2,4,5,6-tetrahydroxycyclohexyl]oxy]phosphonic acid'	b'PIP(16:0/22:4(10Z,13Z,16Z,19Z))'	HMDB00 09922	C47H84O16 P2	
		966.5234597	4.03E-05	Protone	b'[(1R,3S)-3-[(2R)-2-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenyl]oxy)-3-(hexadecanoyl)oxy]propoxy]phosphoryl]oxy)-2,4,5,6-tetrahydroxycyclohexyl]oxy]phosphonic acid'	b'PIP(16:0/22:4(7Z,10Z,13Z,16Z))'	HMDB00 09936	C47H84O16 P2	
		966.5234597	4.03E-05	Protone	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-2-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenyl]oxy)-3-(octadecanoyl)oxy]propoxy]phosphoryl]oxy)cyclohexyl]oxy]phosphonic acid'	b'PIP(18:0/20:4(5Z,8Z,11Z,14Z))'	HMDB00 09956	C47H84O16 P2	
		966.5234597	4.03E-05	Protone	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-2-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenyl]oxy)-3-(octadecanoyl)oxy]propoxy]phosphoryl]oxy)cyclohexyl]oxy]phosphonic acid'	b'PIP(18:0/20:4(8Z,11Z,14Z,17Z))'	HMDB00 09957	C47H84O16 P2	
		966.5234597	4.03E-05	Protone	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienyl]oxy)-3-(11Z)-octadec-11-enyl]oxy]propoxy]phosphoryl]oxy)cyclohexyl]oxy]phosphonic acid'	b'PIP(18:1(11Z)/20:3(5Z,8Z,11Z))'	HMDB00 09965	C47H84O16 P2	C006 26
		966.5234597	4.03E-05	Protone	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienyl]oxy)-3-(11Z)-octadec-11-enyl]oxy]propoxy]phosphoryl]oxy)cyclohexyl]oxy]phosphonic acid'	b'PIP(18:1(11Z)/20:3(8Z,11Z,14Z))'	HMDB00 09966	C47H84O16 P2	C006 26
		966.5234597	4.03E-05	Protone	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-2-[(5Z,8Z,11Z)-icosa-5,8,11-trienyl]oxy)-3-(9Z)-octadec-9-enyl]oxy]propoxy]phosphoryl]oxy)cyclohexyl]oxy]phosphonic acid'	b'PIP(18:1(9Z)/20:3(5Z,8Z,11Z))'	HMDB00 09978	C47H84O16 P2	
		966.5234597	4.03E-05	Protone	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-2-[(8Z,11Z,14Z)-icosa-8,11,14-trienyl]oxy)-3-(9Z)-octadec-9-enyl]oxy]propoxy]phosphoryl]oxy)cyclohexyl]oxy]phosphonic acid'	b'PIP(18:1(9Z)/20:3(8Z,11Z,14Z))'	HMDB00 09979	C47H84O16 P2	
		966.5234597	4.03E-05	Protone	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-2-[(11Z,14Z)-icosa-11,14-dienyl]oxy)-3-(9Z,12Z)-octadeca-9,12-dienyl]oxy]propoxy]phosphoryl]oxy)cyclohexyl]oxy]phosphonic acid'	b'PIP(18:2(9Z,12Z)/20:2(11Z,14Z))'	HMDB00 09990	C47H84O16 P2	C006 26
		966.5234597	4.03E-05	Protone	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(11Z,14Z)-icosa-11,14-dienyl]oxy)-2-(9Z,12Z)-octadeca-9,12-dienyl]oxy]propoxy]phosphoryl]oxy)cyclohexyl]oxy]phosphonic acid'	b'PIP(20:2(11Z,14Z)/18:2(9Z,12Z))'	HMDB00 10004	C47H84O16 P2	C006 26
		966.5234597	4.03E-05	Protone	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienyl]oxy)-2-(11Z)-octadec-11-enyl]oxy]propoxy]phosphoryl]oxy)cyclohexyl]oxy]phosphonic acid'	b'PIP(20:3(5Z,8Z,11Z)/18:1(11Z))'	HMDB00 10007	C47H84O16 P2	C006 26

		966.5234597	4.03E-05	Protocation	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(5Z,8Z,11Z)-icosa-5,8,11-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl)oxy)cyclohexyl]oxy}phosphonic acid'	b'PIP(20:3(5Z,8Z,11Z)/18:1(9Z))'	HMDB0010008	C47H84O16P2	C00626
		966.5234597	4.03E-05	Protocation	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(11Z)-octadec-11-enoyloxy]propoxy]phosphoryl)oxy)cyclohexyl]oxy}phosphonic acid'	b'PIP(20:3(8Z,11Z,14Z)/18:1(11Z))'	HMDB0010012	C47H84O16P2	C00626
		966.5234597	4.03E-05	Protocation	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(8Z,11Z,14Z)-icosa-8,11,14-trienoyloxy]-2-[(9Z)-octadec-9-enoyloxy]propoxy]phosphoryl)oxy)cyclohexyl]oxy}phosphonic acid'	b'PIP(20:3(8Z,11Z,14Z)/18:1(9Z))'	HMDB0010013	C47H84O16P2	C00626
		966.5234597	4.03E-05	Protocation	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(5Z,8Z,11Z,14Z)-icosa-5,8,11,14-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphoryl)oxy)cyclohexyl]oxy}phosphonic acid'	b'PIP(20:4(5Z,8Z,11Z,14Z)/18:0)'	HMDB0010016	C47H84O16P2	C00626
		966.5234597	4.03E-05	Protocation	b'[(1R,5S)-2,3,4,6-tetrahydroxy-5-(hydroxy[(2R)-3-[(8Z,11Z,14Z,17Z)-icosa-8,11,14,17-tetraenoyloxy]-2-(octadecanoyloxy)propoxy]phosphoryl)oxy)cyclohexyl]oxy}phosphonic acid'	b'PIP(20:4(8Z,11Z,14Z,17Z)/18:0)'	HMDB0010020	C47H84O16P2	C00626
		966.5234597	4.03E-05	Protocation	b'[(1R,3S)-3-([(2R)-3-[(10Z,13Z,16Z,19Z)-docosa-10,13,16,19-tetraenoyloxy]-2-(hexadecanoyloxy)propoxy](hydroxy)phosphoryl)oxy)-2,4,5,6-tetrahydroxycyclohexyl]oxy}phosphonic acid'	b'PIP(22:4(10Z,13Z,16Z,19Z)/16:0)'	HMDB0010027	C47H84O16P2	
		966.5234597	4.03E-05	Protocation	b'[(1R,3S)-3-([(2R)-3-[(7Z,10Z,13Z,16Z)-docosa-7,10,13,16-tetraenoyloxy]-2-(hexadecanoyloxy)propoxy](hydroxy)phosphoryl)oxy)-2,4,5,6-tetrahydroxycyclohexyl]oxy}phosphonic acid'	b'PIP(22:4(7Z,10Z,13Z,16Z)/16:0)'	HMDB0010028	C47H84O16P2	C00626
		966.5234606	3.94E-05	Protocation	b'[(2S)-2-hydroxy-3-(hydroxy[(2R)-3-[(18-methylicosanoyl)oxy]-2-[(5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl]oxy)propoxy]phosphoryl)oxy)propoxy]phosphonic acid'	b'PGP(a-21:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB0274647	C47H84O16P2	
		966.5234606	3.94E-05	Protocation	b'[(2S)-2-hydroxy-3-(hydroxy[(2R)-2-[(18-methylicosanoyl)oxy]-3-[(5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl]oxy)propoxy]phosphoryl)oxy)propoxy]phosphonic acid'	b'PGP(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/a-21:0)'	HMDB0274648	C47H84O16P2	
		966.5234606	3.94E-05	Protocation	b'[(2S)-2-hydroxy-3-(hydroxy[(2R)-3-[(19-methylicosanoyl)oxy]-2-[(5R,6R,7Z,9Z,11E,13E,15S,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl]oxy)propoxy]phosphoryl)oxy)propoxy]phosphonic acid'	b'PGP(i-21:0/20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15))'	HMDB0275788	C47H84O16P2	
		966.5234606	3.94E-05	Protocation	b'[(2S)-2-hydroxy-3-(hydroxy[(2R)-2-[(19-methylicosanoyl)oxy]-3-[(5S,6S,7Z,9Z,11E,13E,15R,17Z)-5,6,15-trihydroxyicosa-7,9,11,13,17-pentaenoyl]oxy)propoxy]phosphoryl)oxy)propoxy]phosphonic acid'	b'PGP(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/i-21:0)'	HMDB0275789	C47H84O16P2	
404	1037.6277	1038.634335	0.001165	Protocation	b(2-([(2R)-2-[(2R)-2-amino-3-[(4S,5R,6E,8E,10Z,13Z)-1-carboxy-4-hydroxynonadeca-6,8,10,13-tetraen-5-yl]sulfonyl)propanoyl]oxy)-3-[13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl]oxy)propyl phosphonoxy)ethyl)trimethylazanium'	b'PC(DiMe(13,5)/LTE4)	HMDB0289147	C55H95N2O12PS	

		1038.634335	0.0011 65	Protona tion	b'(2-{{(2R)-3-{{(2R)-2-amino-3-{{(4S,5R,6E,8E,10Z,13Z)-1-carboxy-4-hydroxynonadeca-6,8,10,13-tetraen-5-yl}sulfanyl}propanoyl}oxy)-2-{{13-(3,4-dimethyl-5-pentylfuran-2-yl)tridecanoyl}oxy}propyl phosphono}oxy}ethyl)trimethylazanium'	b'PC(LTE4/DiMe(13,5))'	HMDB02 89148	C55H95N2O 12PS	

3.3.Table S3. Metal ions and isotopes detected in 4T1 tumor-bearing BALB/c mouse brain with iohexol on ITO slide. In order to avoid interferences of Au and iodide, Au sputtered ITO glass slides were not used for metal ion analysis.

Table S3. Metal ions and isotopes detected in 4T1 tumor-bearing BALB/c mouse brain with iohexol on ITO slide. In order to avoid interferences of Au and iodide, Au sputtered ITO glass slides were not used for metal ion analysis.				
Metal ions	Detected species	Expected (<i>m/z</i>)	Observed (<i>m/z</i>)	Errors (Da)
Na	NaI ₂ ⁻	276.7987	276.7989	0.0002
K	³⁹ KI ₂ ⁻	292.7726	292.7733	0.0007
	⁴¹ KI ₂ ⁻	294.7707	294.7717	0.0010
Ca	⁴⁰ CaI ₃ ⁻	420.6760	420.6761	0.0001
	⁴⁴ CaI ₃ ⁻	424.6689	/	/
Mg	²⁴ MgI ₃ ⁻	404.6984	404.6989	0.0005
	²⁵ MgI ₃ ⁻	405.6992	405.6997	0.0005
	²⁶ MgI ₃ ⁻	406.6960	406.6959	0.0001

Zn	$^{64}\text{ZnI}_3^-$	444.6426	444.6425	0.0001
	$^{66}\text{ZnI}_3^-$	446.6395	446.6401	0.0006
	$^{67}\text{ZnI}_3^-$	447.6406	447.6406	0.0000
	$^{68}\text{ZnI}_3^-$	448.6383	448.6388	0.0005
Cu	$^{63}\text{CuI}_2^-$	316.7385	316.7391	0.0006
	$^{65}\text{CuI}_2^-$	318.7367	318.7369	0.0002
Fe	$^{56}\text{FeI}_3^-$	436.6484	436.6484	0.0000
	$^{54}\text{FeI}_3^-$	434.6531	434.6531	0.0000
	$^{57}\text{FeI}_3^-$	437.6489	437.6494	0.0005
Mn	MnI_3^-	435.6515	435.6518	0.0003
Ni	$^{58}\text{NiI}_3^-$	438.6488	438.6384	0.0004
	$^{60}\text{NiI}_3^-$	440.6443	/	/
	$^{61}\text{NiI}_3^-$	441.6446	/	/
	$^{62}\text{NiI}_3^-$	442.6418	/	/
	$^{64}\text{NiI}_3^-$	444.6415	/	/
Co	CoI_3^-	439.6466	/	/
Mo	MoO_3I^-	266.7960	/	/

Mo	MoOI_3^-	488.6151	/	/
Cr	CrI_3^-	432.6540	/	/