Supplementary Information (SI) for Analytical Methods.
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Supplementary material

Strategic Immobilization of α-Amylase on ZIF-8 Nanoplatform for Targeted Bioactivity Screening in Gynura medica Extracts

Ke Ma*, Yuying An, Yu-qing Zhang, Gui-fang Zhong

School of Food and Biological Engineering, Key Laboratory of Industrial Biotechnology in the Tobacco Industry, Zhengzhou University of Light Industry, 136 Kexuedadao Road, 450008, Zhengzhou, China

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Figure 7S: Liquid chromatography-mass spectrometry analysis of mixed sample total ion chromatogram

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Table 2S: Effect of zinc nitrate concentration on the activity of immobilized enzyme

Table 3S: The comprehensive chemical analysis of affinity extraction eluates

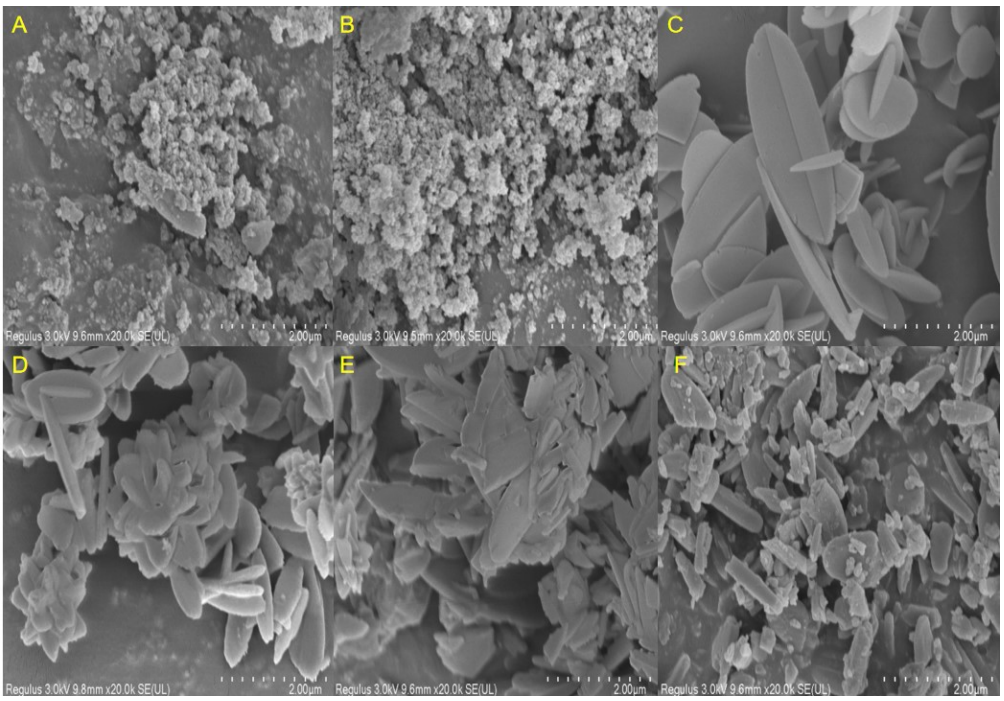

Figure 1S Scanning electron microscopy images of ZIF-8 @ α-amylase immobilized materials synthesized with different concentrations of 2-methylimidazole (A: 0.1 M, B: 0.2 M, C: 0.4 M, D: 0.6 M, E: 0.8 M, F:1.0 M)

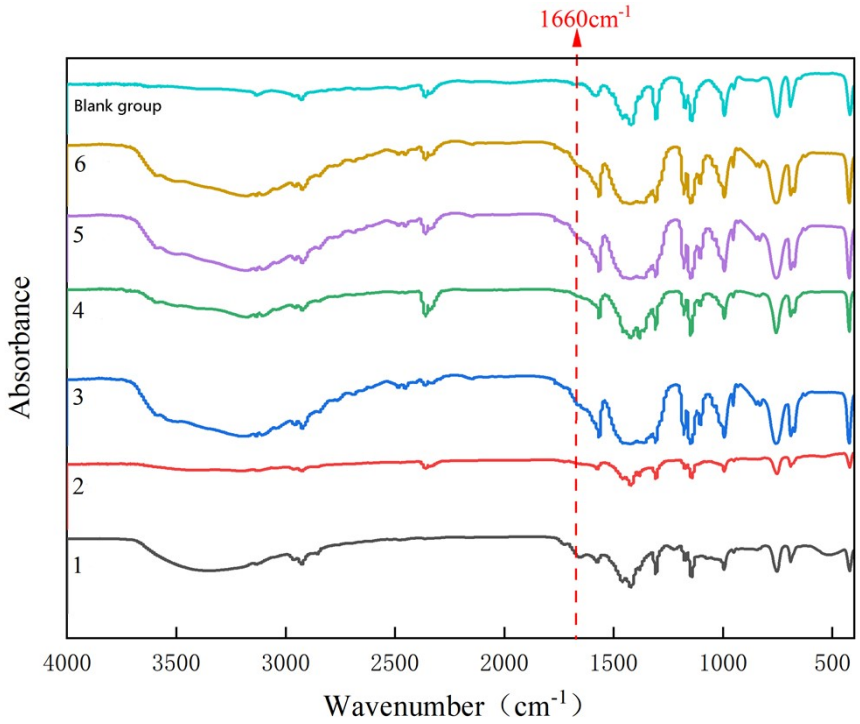

Figure 2S FTIR spectra of ZIF-8@ α-amylase immobilized materials synthesized by α-amylase at different 2-methylimidazole concentration (1: 0.1 M, 2: 0.2 M, 3: 0.4 M, 4: 0.6 M, 5: 0.8 M, 6:1.0 M)

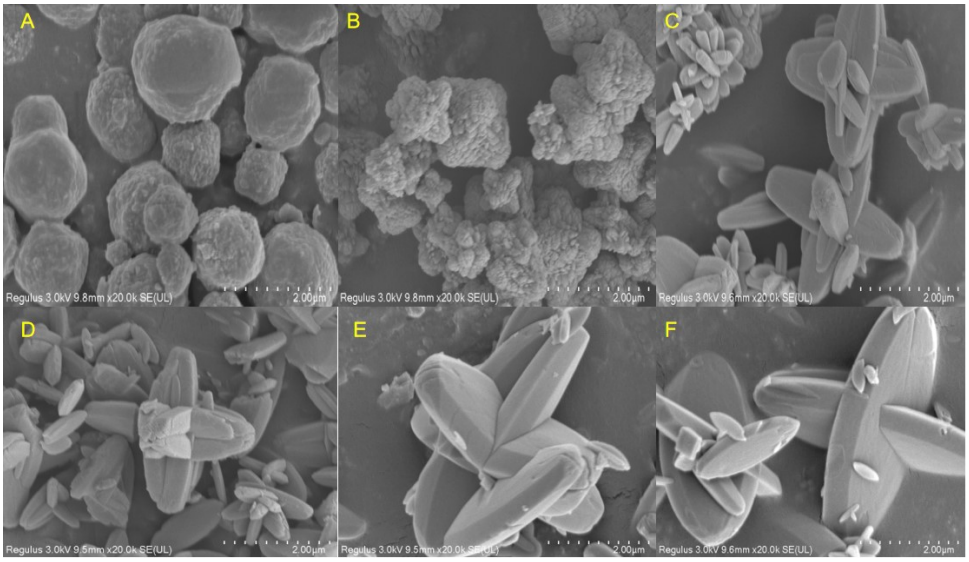

Figure 3S Scanning electron microscopy of ZIF-8@ α-amylase immobilized materials synthesized with different zinc nitrate concentrations (A: 0.1 M, B: 0.2 M, C: 0.3 M, D: 0.4 M, E: 0.5 M, F: 0.6 M)

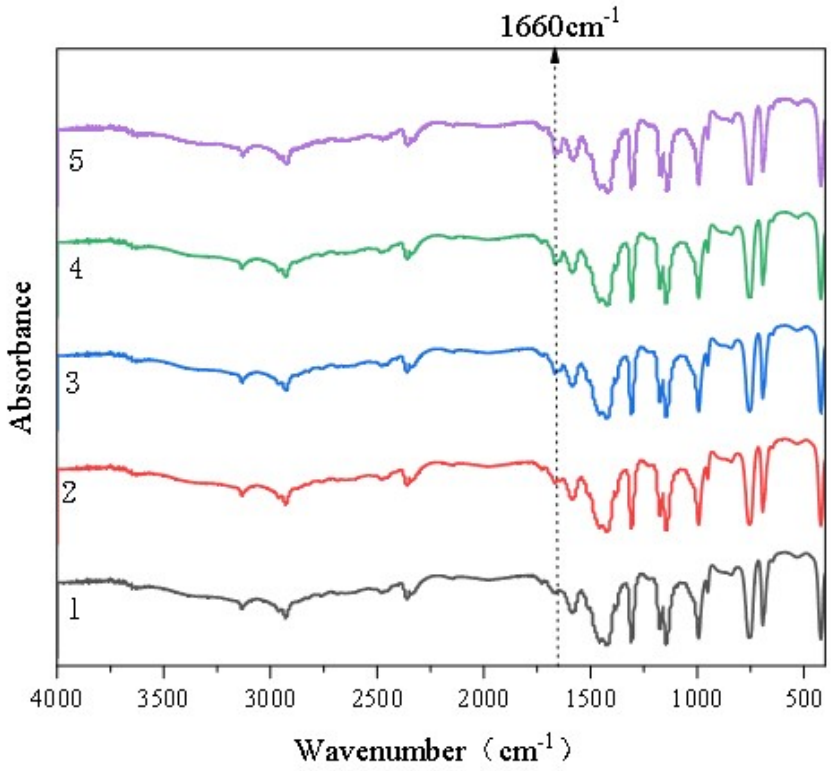

Figure 4S FTIR spectra of ZIF-8@ α-amylase immobilized materials synthesized by α-amylase at different concentrations （1: 5 mg/mL, 2: 10 mg/mL, 3: 20 mg/mL, 3: 30 mg/mL, 4: 40 mg/mL, 5: 50 mg/mL）

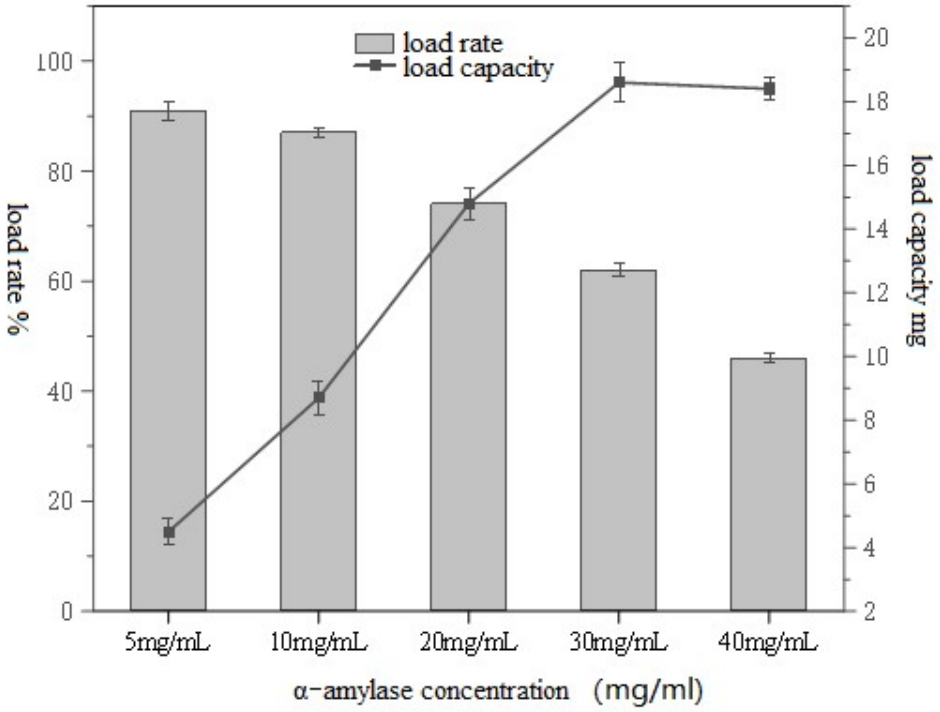

Figure 5S Variation trend of enzyme loading rate and amount with α-amylase concentration in ZIF-8@ α-amylase immobilized material

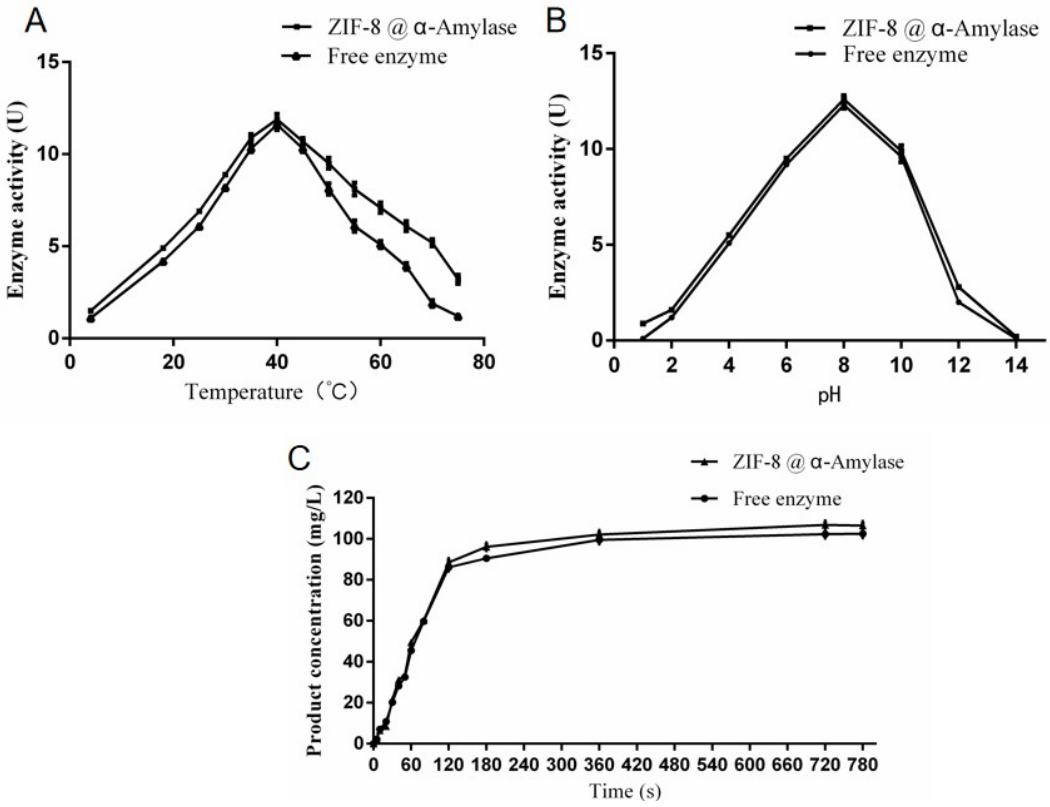

Figure 6S Enzymatic properties of ZIF-8@ α-amylase (A: The effect of temperature on enzyme activity; B: The effect of pH on enzyme activity; C: Comparison of reaction kinetics curves before and after immobilization)

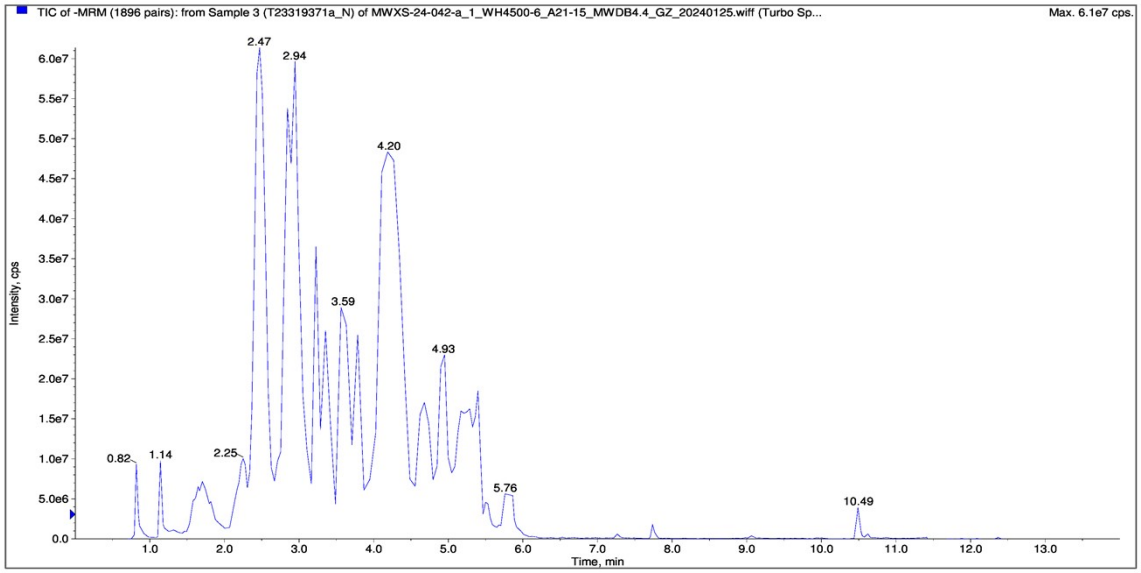

Figure 7S: Liquid chromatography-mass spectrometry analysis of mixed sample total ion chromatogram

Table 1S: Effects of 2-methylimidazole concentration changes on enzyme activity

No.	2-methylimidazole concentration/M	Immobilized enzyme activity/U
1	0.1	0.029
2	0.2	0.056
3	0.4	0.078
4	0.6	0.128
5	0.8	0.204
6	1.0	0.015

Table 2S Effect of zinc nitrate concentration on the activity of immobilized enzyme

No.	Zinc nitrate concentration/M	Immobilized enzyme activity/U
1	0.3	0.128
2	0.4	0.144
3	0.5	0.204
4	0.6	0.218
5	0.7	0.224
6	0.8	0.231

Table 3S The comprehensive chemical analysis of affinity extraction eluates

PeakID	Title	Adduct	Formula	Superclass	Class
582	dioctylamine	[M+H]+	C16H35N	Organic nitrogen compounds	Organonitrogen compounds
209	Alpha-cyclodextrin	[M+H]+	C36H60O30	Organic oxygen compounds	Organooxygen compounds
237	Amarogentin	[M+H]+	C29H30O13	Benzenoids	Benzene and substituted derivatives
449	N-Methylnuciferine	[M+H]+	C20H24NO2	Alkaloids and derivatives	Aporphines
87	3-Methylpyrazole	[M+H]+	C4H6N2	Organoheterocyclic compounds	Azoles
587	Tetradecyldiethanolamine	[M+H]+	C18H39NO2	Organic nitrogen compounds	Organonitrogen compounds
815	Diphenylphosphate	[M+H]+	C12H11O4P	Organic acids and derivatives	Organic phosphoric acids and derivatives
617	N-Methyldioctylamine	[M+H]+	C17H37N	Organic nitrogen compounds	Organonitrogen compounds
201	Phenylacetaldehyde	[M+H]+	C8H8O	Benzenoids	Benzene and substituted derivatives
564	Dicyclohexylurea	[M+H]+	C13H24N2O	Organic acids and derivatives	Organic carbonic acids and derivatives
910	Phthalic anhydride	[M+H]+	C8H4O3	Organoheterocyclic compounds	Benzofurans
507	Coptisine	[M+H]+	C19H14NO4	Alkaloids and derivatives	Protoberberine alkaloids and derivatives
857	Stearamide	[M+H]+	C18H37NO	Organic acids and derivatives	Carboximidic acids and derivatives
589	N,N-Dimethyltetradecylamine-N-oxide	[M+H]+	C16H35NO	Organic nitrogen compounds	Organonitrogen compounds
65	Choline	[M+H]+	C5H13NO	Organic nitrogen compounds	Organonitrogen compounds
234	2"-Rhamnosylvitexin	[M+H]+	C27H30O14	Phenylpropanoids and polyketides	Flavonoids
608	5-O-methylvisammioside	[M+H]+	C22H28O10	Organoheterocyclic compounds	Benzopyrans
261	Pterostilbene	[M+H]+	C16H16O3	Phenylpropanoids and polyketides	Stilbenes
683	Diethyl-phthalate	[M+H]+	C12H14	Benzenoids	Benzene and

PeakID	Title	Adduct	Formula	Superclass	Class
			O4		substituted derivatives
829	13Z-Docosenamide	[M+H]+	C22H43NO	Organic nitrogen compounds	Organic nitrogen compounds
117	Cyclo-prolylglycine	[M+H]+	C7H10N2O2	Organic acids and derivatives	Carboxylic acids and derivatives
580	N,N-Dimethyldodecylamine	[M+H]+	C14H31N	Organic nitrogen compounds	Organonitrogen compounds
408	Imidocarb	[M+H]+	C19H20N6O	Benzenoids	Benzene and substituted derivatives
178	PYROGLUTAMATE	[M+H]+	C5H7NO3	Organic acids and derivatives	Carboxylic acids and derivatives
645	1-Octadecylamine	[M+H]+	C18H39N	Organic nitrogen compounds	Organonitrogen compounds
94	Proline betaine	[M+H]+	C7H13NO2	Organic acids and derivatives	Carboxylic acids and derivatives
161	3-Acetylphenanthrene	[M+H]+	C16H12O	Benzenoids	Phenanthrenes and derivatives
462	(Z)-Guggulsterone	[M+H]+	C21H28O2	Lipids and lipid-like molecules	Steroids and steroid derivatives
366	1-(3-(Trifluoromethyl)phenyl)piperazine	[M+H]+	C11H13F3N2	Organoheterocyclic compounds	Diazinanes
675	alpha-Cyperone	[M+H]+	C15H22O	Lipids and lipid-like molecules	Prenol lipids
646	Triphenyl phosphate (TPP)	[M+H]+	C18H15O4P	Organic acids and derivatives	Organic phosphoric acids and derivatives
291	Indoline	[M+H]+	C8H9N	Organoheterocyclic compounds	Indoles and derivatives
256	Piperidine	[M+H]+	C5H11N	Organoheterocyclic compounds	Piperidines
904	NKH477	[M+H]+	C27H43NO8	Lipids and lipid-like molecules	Prenol lipids
697	Corynoxeine	[M+H]+	C22H26N2O4	Organoheterocyclic compounds	Indolizidines
569	Stearic acid	[M+H]+	C18H36O2	Lipids and lipid-like molecules	Fatty Acyls
263	ANABASAMINE	[M+H]+	C16H19N3	Mixed metal/non-metal compounds	Alkali metal salts
453	Cyclo(proline-leucine)	[M+H]+	C11H18N2O2	Organic acids and derivatives	Carboxylic acids and derivatives
185	Guanine	[M+H]+	C5H5N5O	Organoheterocyclic compounds	Imidazopyrimidines
446	Harmane	[M+H]+	C12H10N2	Alkaloids and derivatives	Harmala alkaloids

PeakID	Title	Adduct	Formula	Superclass	Class
557	Brevicarine	[M+H]+	C17H21N3	Alkaloids and derivatives	Harmala alkaloids
520	4-Hydroxycoumarin	[M+H]+	C9H6O3	Phenylpropanoids and polyketides	Coumarins and derivatives
879	Asarone	[M+H]+	C12H16O3	Benzenoids	Phenol ethers
191	p-Coumaric acid	[M+H]+	C9H8O3	Phenylpropanoids and polyketides	Cinnamic acids and derivatives
5	benzylazanium	[M+H]+	C7H9N	Benzenoids	Benzene and substituted derivatives
7	KOJIC ACID	[M+H]+	C6H6O4	Benzenoids	Naphthalenes
11	4-Methylpyrazole	[M+H]+	C4H6N2	Organoheterocyclic compounds	Azoles
14	Piperazine	[M+H]+	C4H10N2	Organoheterocyclic compounds	Diazinanes
15	Hypotaurine	[M+H]+	C2H7NO2S	Organic acids and derivatives	Sulfinic acids and derivatives
18	4-amino-2-chloropyridine	[M+H]+	C5H5ClN2	Organoheterocyclic compounds	Pyridines and derivatives
21	Ectoine	[M+H]+	C6H10N2O2	Organic acids and derivatives	Carboxylic acids and derivatives
22	OROTATE	[M+H]+	C5H4N2O4	Organoheterocyclic compounds	Diazines
25	Methiocarb-sulfoxide phenol	[M+H]+	C9H12O2S	Benzenoids	Benzene and substituted derivatives
26	1-Naphthoic acid methyl ester	[M+H]+	C12H10O2	Benzenoids	Naphthalenes
28	Splitomicin	[M+H]+	C13H10O2	Organoheterocyclic compounds	Naphthopyrans
30	ETANIDAZOLE	[M+H]+	C7H10N4O4	Organic nitrogen compounds	Organonitrogen compounds
31	Anserine	[M+H]+	C10H16N4O3	Organic acids and derivatives	Peptidomimetics
67	4-Amino-5-hydroxymethyl-2-methylpyrimidine	[M+H]+	C6H9N3O	Organoheterocyclic compounds	Diazines
77	Spectra matches to compound Tolaasin E	[M+H]+	C92H159N21O24	Organic acids and derivatives	Peptidomimetics
88	1,3-DIMETHYLURACIL	[M+H]+	C6H8N2O2	Organoheterocyclic compounds	Diazines
89	Justicidin B	[M+H]+	C21H16O6	Lignans, neolignans and related compounds	Arylnaphthalene lignans
92	Dimethyl sulfone	[M+H]+	C2H6O2S	Organosulfur compounds	Sulfonyls

PeakID	Title	Adduct	Formula	Superclass	Class
93	Ortophosphate	[M+H]+	H3O4P	Homogeneous non-metal compounds	Non-metal oxoanionic compounds
95	ACECLIDINE	[M+H]+	C9H15NO2	Organoheterocyclic compounds	Quinuclidines
114	N-Acetyl-L-Histidine	[M+H]+	C8H11N3O3	Organic acids and derivatives	Carboxylic acids and derivatives
121	1-Hexylamine	[M+H]+	C6H15N	Organic nitrogen compounds	Organonitrogen compounds
122	2,4-Heptadienal	[M+H]+	C7H10O	Organic oxygen compounds	Organooxygen compounds
124	Histamine	[M+H]+	C5H9N3	Organic nitrogen compounds	Organonitrogen compounds
137	Piperine	[M+H]+	C17H19NO3	Alkaloids and derivatives	
139	1-Naphthonitrile	[M+H]+	C11H7N	Benzenoids	Naphthalenes
140	1-Isothiocyanato-8-(methylsulfinyl)-octane	[M+H]+	C10H19NOS2	Organosulfur compounds	Sulfoxides
144	DMPO	[M+H]+	C6H11NO	Organoheterocyclic compounds	Pyrrolines
145	Pyrazinamide	[M+NH4]+	C5H5N3O	Organoheterocyclic compounds	Diazines
147	Trans-4-Hydroxy-L-proline	[M+H]+	C5H9NO3	Organic acids and derivatives	Carboxylic acids and derivatives
149	Trigonelline	[M+H]+	C7H7NO2	Alkaloids and derivatives	
150	Methionine	[M+NH4]+	C5H11NO2S	Organic acids and derivatives	Carboxylic acids and derivatives
151	Xanthine	[M+H]+	C5H4N4O2	Organoheterocyclic compounds	Imidazopyrimidines
152	2,5-dihydroxy benzoic acid	[M+H]+	C7H6O4	Benzenoids	Benzene and substituted derivatives
153	Pyridoxamine	[M+H]+	C8H12N2O2	Organoheterocyclic compounds	Pyridines and derivatives
620	Dodecylbenzenesulfonic acid	325.178	[M-H]-	C18H30O3S	Benzenoids
218	(S)-MALATE	133.0117	[M-H]-	C4H6O5	Organic acids and derivatives
633	Canrenone	339.193	[M-H]-	C22H28O3	Lipids and lipid-like molecules
614	Tocotrienol	423.3191	[M-H]-	C29H44O2	Lipids and lipid-like molecules
103	Pyrophosphate	176.9323	[M-H]-	H4O7P2	Homogeneous non-metal compounds
122	BETA-GLYCEROPHOSPHAT	170.9964	[M-H]-	C3H9O6P	Lipids and lipid-like molecules

PeakID	Title	Adduct	Formula	Superclass	Class
	E				
246	3-Furoic acid	111.0062	[M-H]-	C5H4O3	Organoheterocyclic compounds
575	13-OxoODE	293.2058	[M-H]-	C18H30O3	Lipids and lipid-like molecules
352	L-Phenylalanine	164.0683	[M-H]-	C9H11NO2	Organic acids and derivatives
234	Itaconic acid	129.0171	[M-H]-	C5H6O4	Lipids and lipid-like molecules
465	Fenbufen	253.0888	[M-H]-	C16H14O3	Organic oxygen compounds
508	5-HYDROXY DICLOFENAC	310.0029	[M-H]-	C14H11Cl2NO3	Benzenoids
599	Triptophenolide	311.1624	[M-H]-	C20H24O3	Lipids and lipid-like molecules
2	Acrylate	70.99739	[M-H]-	C3H4O2	Organic acids and derivatives
4	Oxalacetic acid	130.9633	[M-H]-	C4H4O5	Organic acids and derivatives
20	Acetylenedicarboxylic acid	112.9832	[M-H]-	C4H2O4	Organic acids and derivatives
88	B-(4-Fluorobenzoyl)propionic acid	195.0463	[M-H]-	C10H9FO3	Organic oxygen compounds
102	4-Fluorocinnamic acid	165.0365	[M-H]-	C9H7FO2	Phenylpropanoids and polyketides
118	sulfite (Sodium sulfite)	80.96158	[M-H]-	H2O3S	Homogeneous non-metal compounds
121	Decanoate	170.9947	[M-H]-	C10H20O2	Lipids and lipid-like molecules
128	(E)-C-HDMAPP	259.015	[M-H]-	C6H14O7P2	Organic acids and derivatives
165	L-Thyroxine	775.6833	[M-H]-	C15H11I4NO4	Organic acids and derivatives
182	9-Fluorenone	179.0518	[M-H]-	C13H8O	Benzenoids
183	D-SACCHARIC ACID	209.0254	[M-H]-	C6H10O8	Organic oxygen compounds
184	2-Hydroxyanthraquinone	223.0406	[M-H]-	C14H8O3	Benzenoids
210	Maleamic acid	114.0171	[M-H]-	C4H5NO3	Lipids and lipid-like molecules
211	3,4-DIHYDROXY-L-PHENYLALANINE	196.0687	[M-H]-	C9H11NO4	Organic acids and derivatives
213	URIDINE-5-MONOPHOSPHATE	323.0222	[M-H]-	C9H13N2O9P	Nucleosides, nucleotides, and analogues
217	MALEIC ACID	115.0013	[M-H]-	C4H4O4	Organic acids and

PeakID	Title	Adduct	Formula	Superclass	Class
					derivatives
219	Fluroxypyr	252.9663	[M-H]-	C7H5Cl2FN2O3	Organoheterocyclic compounds
221	6-PHOSPHOGLUCONIC ACID	275.0162	[M-H]-	C6H13O10P	Organic oxygen compounds
233	1,4-Butynediol	85.02721	[M-H]-	C4H6O2	Organic oxygen compounds
235	Citramalate	147.026	[M-H]-	C5H8O5	Lipids and lipid-like molecules
237	trans-Aconitate	173.0059	[M-H]-	C6H6O6	Organic acids and derivatives
238	1-Hydroxy-2-naphthoic acid	187.0383	[M-H]-	C11H8O3	Benzenoids
239	N-1-Desalkylflurazepam	287.0381	[M-H]-	C15H10ClFN2O	Organoheterocyclic compounds
240	Naptalam	290.0822	[M-H]-	C18H13NO3	Benzenoids
242	3',5'-CYCLIC AMP	328.037	[M-H]-	C10H12N5O6P	Nucleosides, nucleotides, and analogues
243	AMP	346.0479	[M-H]-	C10H14N5O7P	Nucleosides, nucleotides, and analogues
248	5-OXO-D-PROLINE	128.0327	[M-H]-	C5H7NO3	Organic acids and derivatives
249	N-Methyl-L-glutamate	160.0583	[M-H]-	C6H11NO4	Organic acids and derivatives
251	CITRATE	191.0158	[M-H]-	C6H8O7	Organic acids and derivatives
253	lipoamide	204.0464	[M-H]-	C8H15NOS2	Organoheterocyclic compounds
254	Uridine	243.0568	[M-H]-	C9H12N2O6	Nucleosides, nucleotides, and analogues
259	Caffeoyl-N-tyrosine	341.9016	[M-H]-	C18H17NO6	Organic acids and derivatives
260	GUANOSINE 5'-MONOPHOSPHATE	362.0415	[M-H]-	C10H14N5O8P	Nucleosides, nucleotides, and analogues
264	L-Tyrosine	180.062	[M-H]-	C9H11NO3	Organic acids and derivatives
265	3-Methyluridine	257.0728	[M-H]-	C10H14N2O6	Nucleosides, nucleotides, and analogues
266	Guanosine-3',5'-cyclic monophosphate	344.0334	[M-H]-	C10H12N5O7P	Nucleosides, nucleotides, and analogues

PeakID	Title	Adduct	Formula	Superclass	Class
278	Carbonyl cyanide chlorophenylhydrazone	203.0151	[M-H]-	C9H5ClN4	Benzenoids
279	Fluorescein	331.063	[M-H]-	C20H12O5	Organoheterocyclic compounds
281	Betadex	1133.341	[M-2H]2-	C42H70O35	Organic oxygen compounds
334	Norleucine	130.0845	[M-H]-	C6H13NO2	Organic acids and derivatives
335	Phosphotyrosine	260.0391	[M-H]-	C9H12NO6P	Organic acids and derivatives
338	alpha-guaiaconic acid	339.123	[M-H]-	C20H20O5	Organoheterocyclic compounds
339	Placodiolic acid	375.0983	[M-H]-	C19H20O8	Benzenoids
340	Samidin	385.1271	[M-H]-	C21H22O7	Phenylpropanoids and polyketides
357	Porphobilinogen	225.0833	[M-H]-	C10H14N2O4	Organic nitrogen compounds
358	Ginnalin B	315.0674	[M-H]-	C13H16O9	Benzenoids
359	Traumatic Acid	227.1347	[M-H]-	C12H20O4	Lipids and lipid-like molecules
360	ADIPIC ACID	145.047	[M-H]-	C6H10O4	Lipids and lipid-like molecules
361	Resveratrol	227.0991	[M-H]-	C14H12O3	Phenylpropanoids and polyketides
362	Isobavachin	323.1283	[M-H]-	C20H20O4	Phenylpropanoids and polyketides
363	Climbazol	291.0936	[M-H]-	C15H17ClN2O2	Benzenoids
365	Coumaroyl quinic acid	337.0865	[M-H]-	C16H18O8	Organic oxygen compounds
366	2-NBDG	341.0806	[M-H]-	C12H14N4O8	Organoheterocyclic compounds
367	PRIM-O-GLUCOSYLCIMIFUGIN	467.1472	[M-H]-	C22H28O11	Organoheterocyclic compounds
368	p-Acetaminobenzaldehyde	162.0529	[M-H]-	C9H9NO2	Benzenoids
369	Coumaroyl Hexoside	325.0864	[M-H]-	C15H18O8	Phenylpropanoids and polyketides
370	Axitinib	385.1101	[M-H]-	C22H18N4OS	Organosulfur compounds
371	2-Acrylamido-2-methyl-1-propanesulfonic acid	206.041	[M-H]-	C7H13NO4S	Organic acids and derivatives
373	agnuside	465.1349	[M-H]-	C22H26O11	Lipids and lipid-like molecules
374	Mesaconic acid	129.0518	[M-H]-	C5H6O4	Lipids and lipid-like molecules

PeakID	Title	Adduct	Formula	Superclass	Class
376	Besonprodil	401.1374	[M-H]-	C21H23FN2O3S	Organoheterocyclic compounds
378	Isosakuranin	447.1423	[M-H]-	C22H24O10	Phenylpropanoids and polyketides
379	Pyroglutamyl-Isoleucine	241.1152	[M-H]-	C11H18N2O4	Organic acids and derivatives
380	Oxytetracycline	459.141	[M-H]-	C22H24N2O9	Phenylpropanoids and polyketides
381	7-Hydroxymethotrexat	469.166	[M-H]-	C20H22N8O6	Organoheterocyclic compounds
382	4,4'-Sulfonylbis[2-(prop-2-en-1-yl)phenol]	329.0857	[M-H]-	C18H18O4S	Benzenoids
383	methyl asterrate	361.0892	[M-H]-	C18H18O8	Benzenoids
385	Cetirizine	387.1581	[M-H]-	C21H25ClN2O3	Benzenoids
386	Oxycarboxin	266.0445	[M-H]-	C12H13NO4S	Benzenoids
388	BENZOATE	121.0271	[M-H]-	C7H6O2	Benzenoids
391	RHODOMYRTOXIN	427.1726	[M-H]-	C24H28O7	Organoheterocyclic compounds
392	Gallocatechin	305.064	[M-H]-	C15H14O7	Phenylpropanoids and polyketides
393	Betamethasone 21	433.1994	[M-H]-	C24H31FO6	Lipids and lipid-like molecules
394	Jasmonic acid	209.1251	[M-H]-	C12H18O3	Lipids and lipid-like molecules
395	O-Acetylcarnitine	202.104	[M-H]-	C9H17NO4	Lipids and lipid-like molecules
396	Clobenpropit	307.0789	[M-H]-	C14H17ClN4S	Benzenoids
401	3-(5-methoxy-2,2-dimethylchromen-8-yl)-3-oxopropanoic acid	275.0982	[M-H]-	C15H16O5	Organoheterocyclic compounds
402	Methyl Haematommate	209.0409	[M-H]-	C10H10O5	Benzenoids
405	Flufenamic acid	280.0596	[M-H]-	C14H10F3NO2	Benzenoids
408	4-Vinylphenol	119.047	[M-H]-	C8H8O	Benzenoids
409	2-Hydroxycinnamic acid	163.0376	[M-H]-	C9H8O3	Phenylpropanoids and polyketides
410	N-Acetyl-L-phenylalanine	206.0776	[M-H]-	C11H13NO3	Organic acids and derivatives
412	Tuckolide Decarestrictine D	215.0885	[M-H]-	C10H16O5	
414	Ethopabate	236.088	[M-H]-	C12H15NO4	Benzenoids
416	1,4-Cyclohexanedicarboxylic acid	171.063	[M-H]-	C8H12O4	Organic acids and derivatives
417	3,7,3',4',5'-Pentahydroxyflavone	301.0297	[M-H]-	C15H10O7	Phenylpropanoids and polyketides

PeakID	Title	Adduct	Formula	Superclass	Class
418	ferulic acid	193.0474	[M-H]-	C10H10O4	Phenylpropanoids and polyketides
420	Methyl Jasmonic acid	223.1411	[M-H]-	C13H20O3	Lipids and lipid-like molecules
421	coumarin-SAHA	345.148	[M-H]-	C18H22N2O5	Phenylpropanoids and polyketides
422	Methotrexate	453.17	[M-H]-	C20H22N8O5	Organoheterocyclic compounds
423	Closone butyrate	477.1834	[M-H]-	C26H32ClFO5	
424	Maltotriose	503.1671	[M-H]-	C18H32O16	Organic oxygen compounds
425	Azelaic acid	187.0938	[M-H]-	C9H16O4	Lipids and lipid-like molecules
426	1,3,7-Trimethyluric acid	209.0745	[M-H]-	C8H10N4O3	Organoheterocyclic compounds
427	15-keto Fluprostenol isopropyl ester	497.2127	[M-H]-	C26H33F3O6	
429	Etomidate	243.1191	[M-H]-	C14H16N2O2	Organoheterocyclic compounds
430	Luteolin	285.0345	[M-H]-	C15H10O6	Phenylpropanoids and polyketides
432	Carapin	467.2048	[M-H]-	C27H32O7	Lipids and lipid-like molecules
435	FKGK 11	279.0847	[M-H]-	C13H13F5O	Benzenoids
439	4-hydroxynonenoic acid	171.0993	[M-H]-	C9H16O3	
446	-Mevalonic acid 5-phosphate	227.0301	[M-H]-	C6H13O7P	
449	sinapaldehyde glucoside	369.1153	[M-H]-	C17H22O9	Organic oxygen compounds
454	Sebacic acid	201.1083	[M-H]-	C10H18O4	Lipids and lipid-like molecules
455	Thiopental	241.1034	[M-H]-	C11H18N2O2S	Organoheterocyclic compounds
457	Ilicic acid	251.1705	[M-H]-	C15H24O3	Lipids and lipid-like molecules
461	(-)-12-hydroxyjasmonic acid	225.1084	[M-H]-	C12H18O4	Lipids and lipid-like molecules
464	2',3'-Dideoxyinosine	235.0789	[M-H]-	C10H12N4O3	Nucleosides, nucleotides, and analogues
468	Catechin	289.0636	[M-H]-	C15H14O6	Phenylpropanoids and polyketides
469	Farrerol	299.0931	[M-H]-	C17H16O5	Phenylpropanoids and polyketides
474	syringin	371.1308	[M-H]-	C17H24O9	Organic oxygen compounds

PeakID	Title	Adduct	Formula	Superclass	Class
480	Undecanedioic acid	215.1254	[M-H]-	C11H20O4	Lipids and lipid-like molecules
481	(10E,15Z)-9,12,13-trihydroxyoctadeca-10,15-dienoic acid	327.2109	[M-H]-	C18H32O5	Lipids and lipid-like molecules
482	Tetranor-12(R)-HETE	265.1856	[M-H]-	C16H26O3	
487	Virensic acid	357.0548	[M-H]-	C18H14O8	Phenylpropanoids and polyketides
489	(Z)-5,8,11-trihydroxyoctadec-9-enoic acid	329.2272	[M-H]-	C18H34O5	Lipids and lipid-like molecules
491	gmelinol	401.0805	[M-H]-	C22H26O7	Lignans, neolignans and related compounds
492	Oenin	491.1118	[M-H]-	C23H24O12	Phenylpropanoids and polyketides
498	Glucoibarin	478.0913	[M-H]-	C15H29NO10S3	Organic oxygen compounds
507	Picrotin	309.0881	[M-H]-	C15H18O7	Organoheterocyclic compounds
518	e-64	356.0068	[M-H]-	C15H27N5O5	Organoheterocyclic compounds
527	Monoisobutyl phthalate	221.0781	[M-H]-	C12H14O4	Benzenoids
528	ORTHOTHYMOTINIC ACID	193.0833	[M-H]-	C11H14O3	Lipids and lipid-like molecules
529	EPIAFZELECHIN TRIMETHYL ETHER	315.117	[M-H]-	C18H20O5	Phenylpropanoids and polyketides
530	CEHC	249.1084	[M-H]-	C14H18O4	
531	Methyl jasmonate	223.1291	[M-H]-	C13H20O3	Lipids and lipid-like molecules
532	1,11-Undecanedicarboxylic acid	243.1553	[M-H]-	C13H24O4	Lipids and lipid-like molecules
537	7-(2-aminophenyl)heptanoic acid	220.1425	[M-H]-	C13H19NO2	
538	3-(8-hydroxyoctyl)phenol	221.1502	[M-H]-	C14H22O2	Lipids and lipid-like molecules
539	N-acetyl-O-methyltyrosine	236.1012	[M-H]-	C12H15NO4	Organic acids and derivatives
540	[6]-Gingerol	293.1702	[M-H]-	C17H26O4	Benzenoids
542	Thyrotropin releasing hormone	361.1555	[M-H]-	C16H22N6O4	Organic acids and derivatives
543	AN-7	449.1421	[M-H]-	C19H34N2O2S4	
545	C12-AE1S (TENTATIVE)	309.1652	[M-H]-	C14H30O5S	Organic acids and derivatives

PeakID	Title	Adduct	Formula	Superclass	Class
546	13S-HpOTrE(gamma)	309.2007	[M-H]-	C18H30O4	
547	Chrysanthemic Acid, Ethyl Ester	195.1352	[M-H]-	C12H20O2	Lipids and lipid-like molecules
548	Anserine	239.1243	[M-H]-	C10H16N4O3	Organic acids and derivatives
553	Prostaglandin D2-d9	360.2696	[M-H]-	C20H23D9O5	Lipids and lipid-like molecules
558	N-Methyltyrosine	194.0782	[M-H]-	C10H13NO3	Organic acids and derivatives
559	(9Z,12E)-15,16-dihydroxyoctadeca-9,12-dienoic acid	311.2168	[M-H]-	C18H32O4	Lipids and lipid-like molecules
562	12-OPDA	291.1901	[M-H]-	C18H28O3	Lipids and lipid-like molecules
566	Lacosamide	249.1302	[M-H]-	C13H18N2O3	Organic acids and derivatives
567	PLATYPHYLLENONE	295.135	[M-H]-	C19H20O3	Phenylpropanoids and polyketides
570	9,10-DiHOME	313.2316	[M-H]-	C18H34O4	
574	Curcumenol	233.1492	[M-H]-	C15H22O2	Lipids and lipid-like molecules
576	Ricinoleic acid	297.2362	[M-H]-	C18H34O3	Lipids and lipid-like molecules
578	9-hydroxy-10,12-octadecadienoic acid	295.2224	[M-H]-	C18H32O3	Lipids and lipid-like molecules
579	2,6-Di-tert-butyl-4-nitrophenol	250.14	[M-H]-	C14H21NO3	Benzenoids
580	OSELTAMIVIR PHOSPHATE	311.1945	[M-H]-	C16H28N2O4	Organic acids and derivatives
581	Lauryl sulfate	265.1429	[M-H]-	C12H26O4S	Organic acids and derivatives
582	3,5-Dicarbethoxy-1,4-dihydrocollidine	266.1466	[M-H]-	C14H21NO4	
583	Iso-Olomoucine	297.1474	[M-H]-	C15H18N6O	Organoheterocyclic compounds
586	hirsutanone	327.1202	[M-H]-	C19H20O5	Phenylpropanoids and polyketides
593	Pseudoyohimbine	353.1948	[M-H]-	C21H26N2O3	Alkaloids and derivatives
596	Misoprostol	367.2574	[M-H]-	C21H36O5	Lipids and lipid-like molecules
597	[12]-Gingerol	377.265	[M-H]-	C23H38O4	
598	HYCANTHONE	355.1517	[M-H]-	C20H24N2O2S	Organoheterocyclic compounds
658	Chlorpyrifos-methyl	319.8836	[M-H]-	C7H7Cl3NO3PS	Organic acids and derivatives