Exploring synthetic pathways for nucleosidic derivatives of potent phosphoantigens
Javier Alguacil¹, David Reyes¹, Yoann Aubin¹, Béatrice Roy¹, Christian Périgaud¹, Eric Champagne²
and Suzanne Peyrottes¹*

¹ IBMM, UMR5247 CNRS- University of Montpellier-ENSCM, Campus Triolet, cc 1704, place E.
Bataillon, 34795 Montpellier, France
² Centre de Physiopathologie of Purpan, Toulouse, France
* Corresponding author: peyrottes@um2.fr

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Compound 1  (2E)-2-Methyl-2-butene-1,4-diol
Compound 2: (2E)-4-Hydroxy-2-methyl-2-butenyl acetate
Regioisomer: (2E)-4-Hydroxy-3-methyl-2-butenyl acetate
Compound 3  Dimethyl-(2E)-2-methyl-2-butenedioate
Compounds 4a and 4b isolated as a mixture
Compound 4a
Compound 5  (2E)-4-Bromo-2-methyl-2-butenyl acetate
Compound 6 Isopentenyl-MonoP
Compound 7 HDAM-MonoP
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**Single Mass Analysis**

Tolerance = 3.0 PPM  /  DBE: min = -50.0, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1178 formula(s) evaluated with 2 results within limits (all results (up to 1000) for each mass)

C: 0-100  H: 0-100  N: 0-10  O: 0-20  P: 1-4

SYNAPDT GD-DRIVER205
Z/CP15110507.4 (0.175) Cm (4)

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<th>Calc. Mass</th>
<th>mDa</th>
<th>ppm</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
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<td>1554.7</td>
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<td>99.01</td>
<td>C2H9N8O6P2</td>
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Supplementary material for review & publication online

Single Mass Analysis
Tolerance = 1.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2123 formula(e) evaluated with 3 results within limits (up to 20 closest results for each mass)
Elements Used:
C: 0-100 H: 0-150 N: 0-30 O: 0-30 P: 3-3
SYNAPT G2-SIMnOSet
X-CP146401658 (0.172) Cm (7.12)

Minimum: 5.0
Maximum: 50.0

Mass Calc. Mass eDa PPM DBE i-FIT Norm Conf(%) Formula
572.0715 572.0712 0.2 0.3 8.5 2935.2 0.003 99.73 C16 H25 N5 O12 P3
572.0715 -0.3 -0.5 1.5 2848.8 13.619 0.00 C17 H27 N7 O13 P3
572.0712 0.3 0.9 19.5 2841.1 5.900 0.07 C14 H19 N9 O2 P3

Javi Report

SAMPLE INFORMATION

Sample Name: JA 2.124212 no cell
Sample Type: Unknown
Sample: 21
Injection Volume: 50.0 µl
Mass Spec: 3.0 mm distance
Sample Set: None

Analysis by: [Name]
Date Analysis: [Date]
Mass Spec: [Instrument]
Processing Method: [Method]

Results

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<td>1.000</td>
<td>0.000</td>
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<td>27.989</td>
<td>149.481</td>
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ApCcppH
Supplementary material for review & publication online

Single Mass Analysis

Tolerance = 1.0 PPM / DBE: min = -50.0, max = 50.0
Element prediction: Off
Number of isotopes peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
9059 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)

Elements Used:
C: 0-100 H: 0-100 N: 0-10 O: 0-20 P: 1-5

ApCoopl IA3.185
06-Nov-2015
1: TOF MS ESI:
5.70e+008

Mass      Calcd. Mass  ppm  DBE  i-FIT  Error  Conf(%)  Formula
588.0665  588.0662  0.3  0.5  8.5  977.6  0.000  99.95  C14 H25 N5 O13 P3
588.0663  588.0662  0.3  0.3 17.5  945.6  9.323  0.03  C21 H33 B9 O2 P5
588.0668  588.0663  0.3  0.3 58.5  981.3  9.747  0.01  C21 H31 N7 O13 P5
588.0649  588.0647  0.4  0.7 22.5  981.5  9.899  0.01  C25 H15 N7 O9 P
588.0660  0.5  0.9 16.5  981.6  10.038  0.00  C26 H26 N7 O7 P4
588.0664  0.1  0.2  0.5  989.7  12.148  0.00  C6 H34 N5 O19 P2
588.0667  0.2  0.3 30.5  991.5  13.936  0.00  C35 H16 O3 N3 P2

Auto-Scaled Chromatogram

Peak Results

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<tr>
<th>Name</th>
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<th>% Area</th>
<th>Height</th>
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UpppH

Supplementary material for review & publication online
**Single Mass Analysis**

- **Tolerance:** 1.0 ppm / DDE: min = -50.0, max = 50.0
- **Element prediction:** Off
- **Number of isotope peaks used for i-FIT:** 3

**Monoisotopic Mass, Even Electron Ions**

5764 formula(e) evaluated with 4 results within limits (all results (up to 1000) for each mass)

**Elements Used:**
- C: 0-100
- H: 0-100
- N: 0-10
- O: 0-20
- P: 2-4

**Synapt G2-SIUEER205**

**ZIF1510628-9 (0.262)**

**UppH - JA 4.234**

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**Auto-Scaled Chromatogram**

**Peak Results**

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Supplementary material for review & publication online

Single Mass Analysis
Tolerance = 1.5 ppm / DBE: min = -50.0, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

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**Synapt G2-SiME2B05**
Z-PF15158061.10 (-0.437) (C10)

### SAMPLE INFORMATION

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<tr>
<td>Sample Set Name</td>
<td>jahi</td>
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**Acquired By:** Nucleide
**Sample Name:** dTppH pure
**Sample Type:** Unknown
**Value:** 0.1
**Injection Volume:** 20.00 µl
**Run Time:** 30.00 Minutes
**Sample Set Name:** jahi

**Acq. Method:** Nucleide
**Method:** Javi 0.100 50.00
**Date Acquired:** 03/07/15 16.46.57
**Date Processed:** 03/07/15 17.31.17
**Processing Method:** Javi
**Channel Name:** PDA Single 254.0 nm
**Proc. Chrl. Descr.:** PDA 254.0 nm

**Nucleide**

**Peak Results**

<table>
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<tr>
<th>Name</th>
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