

Supporting Information

Beta-Hydroxy- and beta-aminophosphonate acyclonucleosides as potent inhibitors of *Plasmodium falciparum* growth

Thomas Cheviet, Sharon Wein, Gabriel Bourchenin, Manon Lagacherie, Christian Périgaud, Rachel Cerdan* and Suzanne Peyrottes*

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Copies of ^1H NMR, ^{13}C NMR, ^{31}P NMR, ESI-MS or HR-MS, and HPLC	

Preparation of NMR samples.

10mM of the studied compound were dissolved in 100mM α -cyclodextrin solution in D₂O (ratio substrate/CSA was 1/10). NMR spectra were recorded at different temperatures ranging from 15 to 75°C. Small amount of NaOD or DCl were used to reach the pD of interest.

Figure S1. ^{31}P δ variation of racemic mixture of β -hydroxyphosphonates according to the temperature of analysis, at pD 11.7. Separation of enantiomers were visible at 25°C and 15°C, the best separation was observed for 15°C.

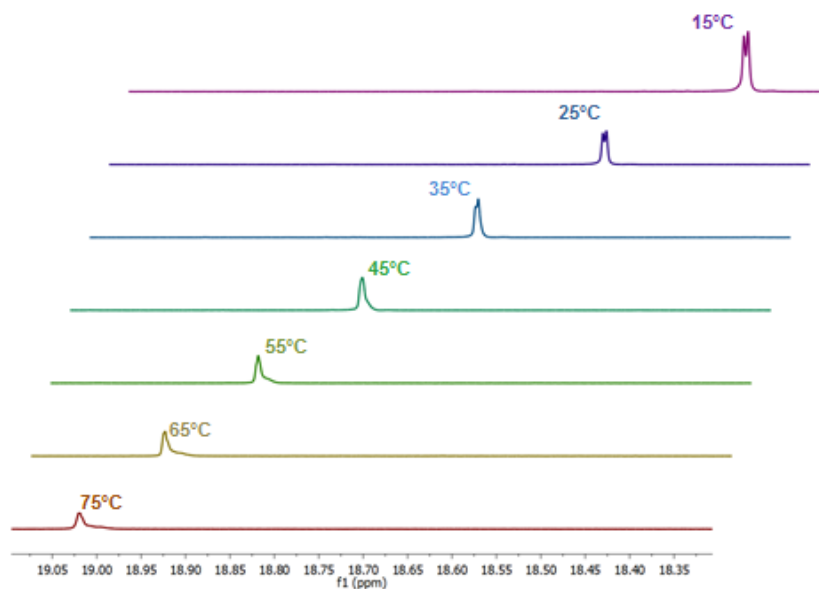


Figure S2. ^{31}P δ variation of racemic mixture of β -hydroxyphosphonates according to pD value, at 15°C. Separation of enantiomers was observed at pD 11.75, but not at higher or lower pD.

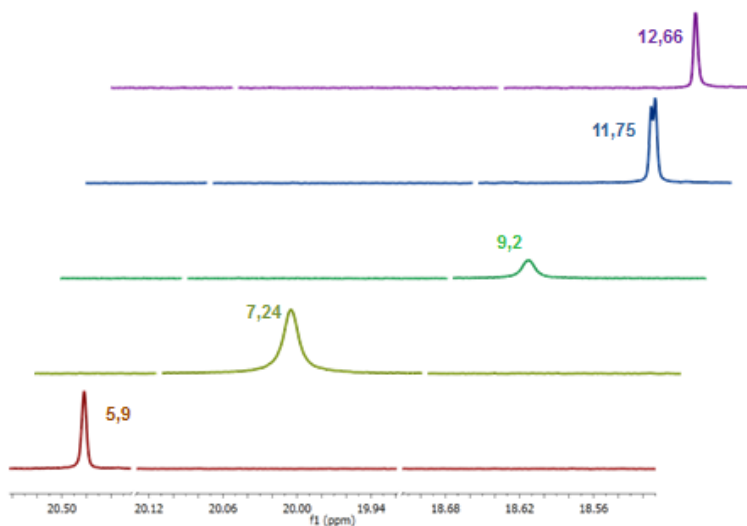
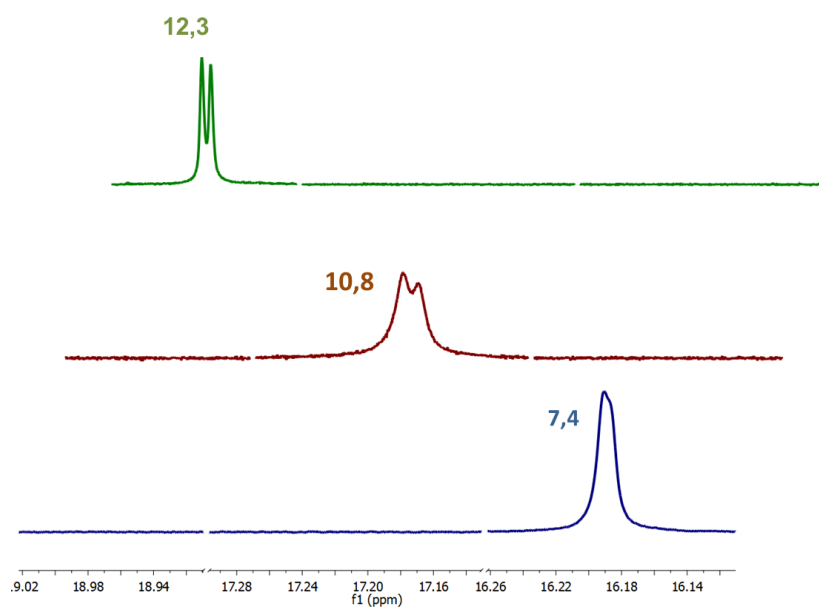
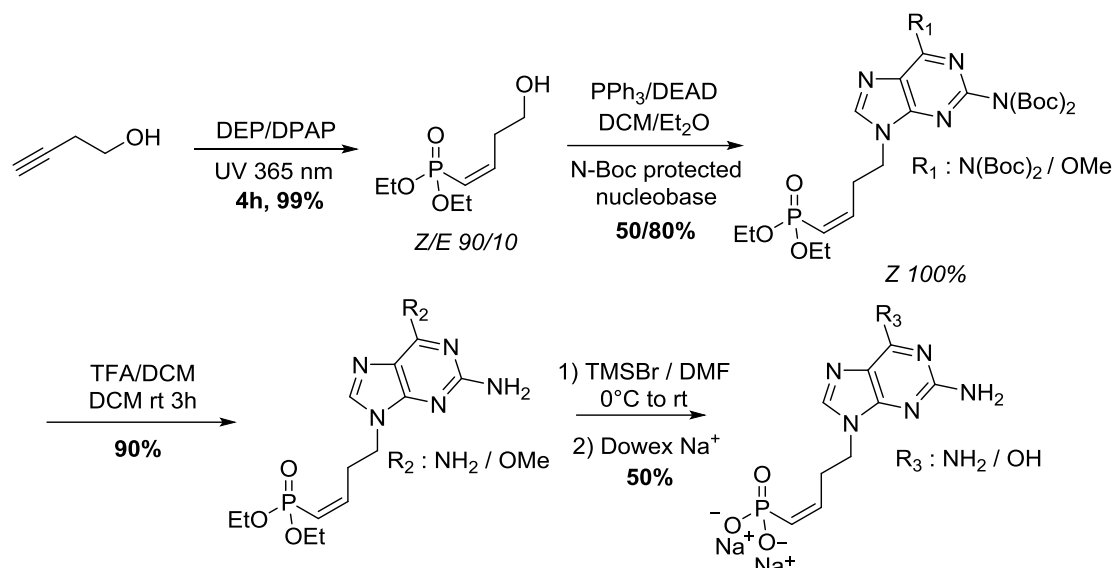


Figure S3. ^{31}P δ variation of racemic mixture of β -aminophosphonates according to pD value, at 15°C. Separation of the two isomers are visible at pD 10.8 but the best result was observed at pD 12.3.



Synthetic pathway for compound 11b



Diethyl-(4-hydroxy)-but-1-en-1-yl-phosphonate.

3-Butyn-1-ol (20 mg) was dissolved in a glass vial (diameter : 1 cm, thickness : 0.65 mm) with diethylphosphite (100 eq). Then, 2,2-dimethoxy-2-phenylacetophenone (DPAP, 0.5 eq) was added and the reaction mixture was stirred under UV activation (UV-A lamp, λ_{max} = 365 nm, 4 x 15W tubes; vial located 2.5 cm away from the lamp) for 30 min. The reaction mixture was diluted in ethyl acetate and the resulting solution was washed with aqueous saturated NaHCO₃. The organic layer was dried over MgSO₄ and concentrated in vacuo. The crude was purified by flash chromatography on silica gel (CH₂Cl₂/MeOH gradient) to obtain the desired compound (59 mg) in quantitative yield and as a 9:1 mixture of Z:E isomers. ¹H NMR (500 MHz, CDCl₃) δ 6.78 (ddt, J = 22.0, 17.2, 6.8 Hz, 1H, CHCH₂, *E*-isomer), 6.61 (ddt, J = 52.8, 13.0, 8.2 Hz, 1H, CHCH₂, *Z*-isomer), 5.75 (ddt, J = 19.0, 13.0, 1.2 Hz, 1H, CHP, *Z*-isomer), 4.24 – 3.96 (m, 4H, OCH₂CH₃), 3.74 (t, J = 5.9 Hz, 2H, CH₂OH), 2.79 (ddd, J = 12.0, 5.6, 1.9 Hz, 2H, CH₂CH), 1.33 (t, J = 7.1 Hz, 6H, CH₃CH₂). ¹³C NMR (126 MHz, CDCl₃) δ 150.7 (d, J = 4.4 Hz, CHCH₂), 119.3 (d, J = 182.2 Hz, CHP), 61.9 (d, J = 5.6 Hz, CH₂CH₃), 60.9 (d, J = 2.2 Hz, CH₂OH), 33.9 (d, J = 8.5 Hz, CH₂CH), 16.5 (CH₃CH₂). ³¹P NMR (202 MHz, CDCl₃) δ 18.1 (s, *E*-isomer), 17.8 (s, *Z*-isomer). HMRS TOF ESI⁺ Found : 209.0943; Calculated for C₈H₁₈O₄P : 209.0943 (M+H)⁺.

Diethyl-(Z)-(4-(2-(bis(*tert*-butoxycarbonyl)amino)-6-methoxy-9*H*-purin-9-yl)-but-1-en-1-yl) phosphonate

Diethyl-(4-hydroxy)-but-1-en-1-yl-phosphonate (300 mg, 1 eq.) was dissolved in anhydrous CH₂Cl₂/Et₂O (2/1, v/v) at 25°C. The nucleobase (1.5 eq.) was added, then triphenylphosphine (PPh₃, 1.6 eq.) and diethylazodicarboxylate (DEAD, 1.6 eq.) dropwise. The reaction mixture was stirred for 24 hours and reaction progress was monitored by TLC (CH₂Cl₂/MeOH 95/5 v/v). The reaction mixture was concentrated in vacuo and purified by flash chromatography on silica gel (CH₂Cl₂/MeOH gradient), which allowed to separate *Z* and *E*-isomers. The title compound (440 mg) was obtained in 55% yield. ¹H NMR (500 MHz, CDCl₃) δ 8.04 (s, 1H, H-8), 6.41 (ddt, J = 51.6, 13.0, 7.6 Hz, 1H, CHCH₂), 5.69 (ddt, J = 17.8, 13.0, 1.4 Hz, 1H, CHP), 4.37 (t, J = 7.0 Hz, 2H, CH₂N), 4.14 (s, 3H, OCH₃), 4.09 – 3.97 (m, 4H, OCH₂CH₃), 3.30 – 3.09 (m, 2H, CH₂CH), 1.45 (s, 18H, CH₃), 1.30 (t, J = 7.0 Hz, 6H, CH₃CH₂). ¹³C NMR (126 MHz, CDCl₃) δ 161.6 (C-6), 152.5 (d, J = 116.3 Hz, C-2), 151.2 (s, C-4), 147.6 (d, J = 3.5 Hz, CHCH₂), 143.1 (CH-8), 121.0 (d, J = 182.4 Hz, CHP), 120.0 (C-5), 83.2 (C(CH₃)₃), 61.8 (d, J = 5.5 Hz, CH₂CH₃), 54.7 (OCH₃), 43.0 (CH₂N), 30.8 (d, J

= 8.0 Hz, $\underline{\text{CH}_2\text{CH}}$), 28.1 (CH_3), 16.5 (d, $J = 6.3$ Hz, $\underline{\text{CH}_3\text{CH}_2}$). ^{31}P NMR (202 MHz, CDCl_3) δ 15.5. HMRS TOF ESI+ Found : 556.2535; Calculated for $\text{C}_{24}\text{H}_{39}\text{N}_5\text{O}_8\text{P}$: 556.2536 ($\text{M}+\text{H}$) $^+$.

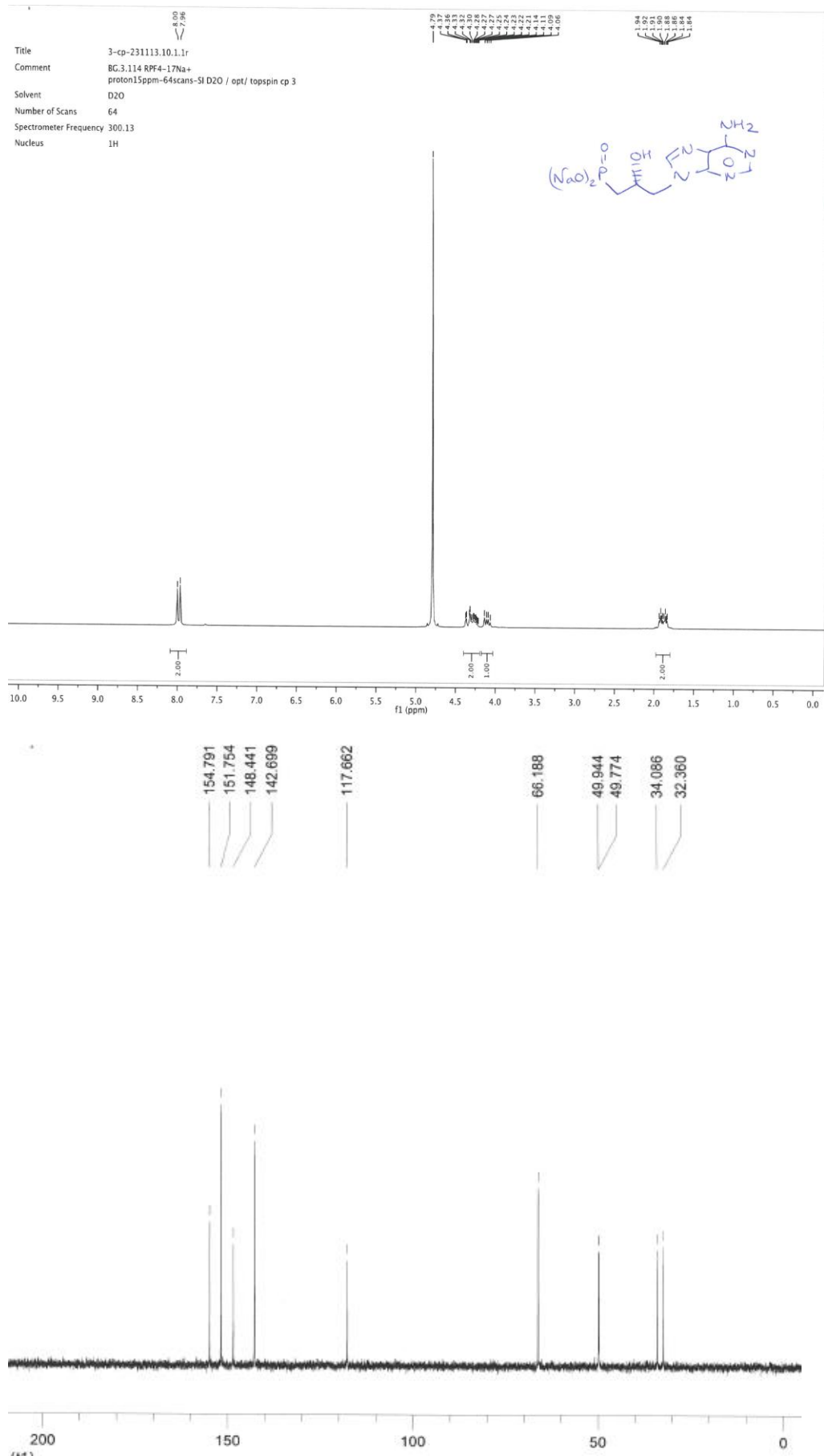
Diethyl-(Z)-(4-(2-amino-6-methoxy-9H-purin-9-yl)-but-1-en-1-yl)phosphonate

To a solution of diethyl-(Z)-(4-(2-(bis(*tert*-butoxycarbonyl)amino)-6-methoxy-9H-purin-9-yl)-but-1-en-1-yl)phosphonate (261 mg, 1 eq.) in anhydrous dichloromethane (3 mL/mmol) was added at room temperature a solution of TFA (8 mL/mmol) in anhydrous dichloromethane (3 mL/mmol). The reaction mixture was stirred for 3h with TLC monitoring (DCM/MeOH, 9/1, v/v). Then, the reaction mixture was diluted with CH_2Cl_2 , concentrated under vacuum and the crude oil was purified on silica gel by flash chromatography (DCM/MeOH gradient, 0 to 10% MeOH) to obtain quantitatively the desired compound (167 mg). ^1H NMR (500 MHz, CDCl_3) δ 7.90 (s, 1H, H_{-8}), 6.37 (ddt, $J = 51.7$, 13.0, 7.7 Hz, 1H, $\underline{\text{CHCH}_2}$), 5.67 – 5.61 (m, 1H, CHP), 4.35 (t, $J = 6.7$ Hz, 2H, CH_2N), 4.06 (s, 3H, OCH_3), 3.90 (m, 4H, $\underline{\text{CH}_2\text{CH}_3}$), 3.10 (tdd, $J = 6.9$, 5.0, 2.4 Hz, 2H, $\underline{\text{CH}_2\text{CH}}$), 1.22 (t, $J = 7.1$ Hz, 6H, $\underline{\text{CH}_3\text{CH}_2}$). ^{13}C NMR (126 MHz, CDCl_3) δ 158.9 (d, $J = 6.8$ Hz, C_{-6}), 157.8 (C_{-5}), 147.6 (d, $J = 3.8$ Hz, $\underline{\text{CHCH}_2}$), 145.0 (CH_{-8}), 128.6 (d, $J = 83.6$ Hz, C_{-2}), 120.7 (d, $J = 182.2$ Hz, CHP), 106.8 (C_{-4}), 61.7 (d, $J = 5.1$ Hz, OCH_2CH_3), 54.7 (OCH_3), 46.5 (CH_2N), 31.4 (d, $J = 7.7$ Hz, $\underline{\text{CH}_2\text{CH}}$), 16.3 (d, $J = 6.0$ Hz, $\underline{\text{CH}_3\text{CH}_2}$). ^{31}P NMR (202 MHz, CDCl_3) δ 15.33. HMRS TOF ESI+ Found : 356.1489; Calculated for $\text{C}_{14}\text{H}_{23}\text{N}_5\text{O}_4\text{P}$: 356.1488 ($\text{M}+\text{H}$) $^+$

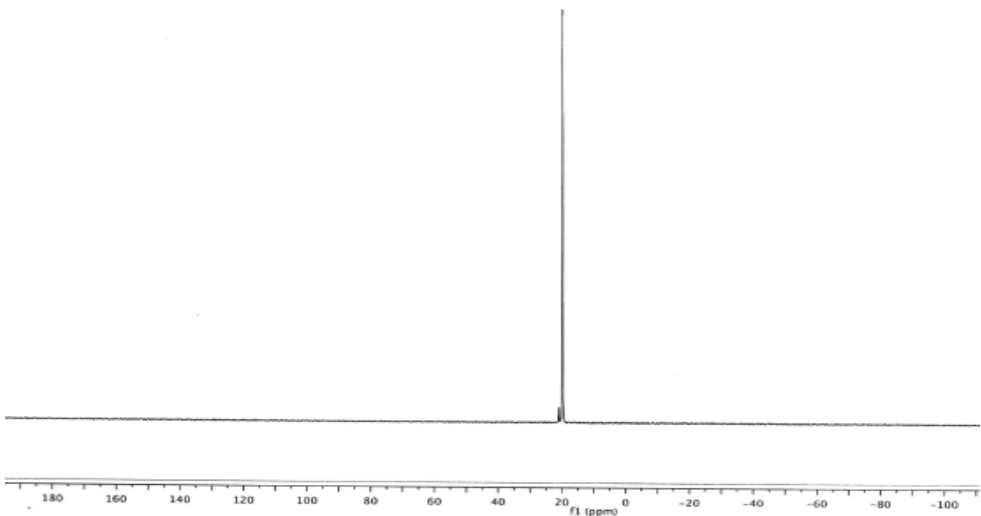
(Z)-(4-(2-amino-6-hydroxy-9H-purin-9-yl)-but-1-en-1-yl)phosphonic acid disodic salt 11b

The diethyl-(Z)-(4-(2-amino-6-methoxy-9H-purin-9-yl)-but-1-en-1-yl)phosphonate (261 mg, 1 eq.) was dissolved under argon atmosphere in anhydrous DMF (20 mL/mmol) at 0°C. TMSBr (6.6 eq.) was added dropwise to the solution, and the mixture was kept at 0°C for 5 min, then allowed to slowly warm to room temperature and stirred for 3 days. The reaction progress was followed by TLC monitoring (isopropanol/water/ammoniac 7/2/1 v/v/v). The reaction was quenched by addition of a triethylbutylammonium solution (1M, pH 7). The volatiles were removed under vacuum and the resulting aqueous solution was freeze-dried. The crude was purified on reverse phase flash chromatography (water/methanol gradient, 0 to 100% methanol), leading to the phosphonate triethylammonium salts as a white powder. The compound was percolated through a Na^+ Dowex resin and after freeze-dried of the require fractions the sodium salts were obtained as a white lyophilizate. The desired compound (130 mg) was obtained in 54% yield. ^1H NMR (500 MHz, D_2O) δ 7.82 (s, 1H, H_{-8}), 6.11 (ddt, $J = 45.8$, 13.0, 7.4 Hz, 1H, $\underline{\text{CHCH}_2}$), 5.83 (ddt, $J = 17.7$, 13.1, 1.6 Hz, 1H, CHP), 4.15 (t, $J = 7.1$ Hz, 2H, CH_2N), 2.93 (qdd, $J = 7.0$, 2.8, 1.5 Hz, 2H, $\underline{\text{CH}_2\text{CH}}$). ^{13}C NMR (126 MHz, D_2O) δ 158.9 (C_{-6}), 153.5 (C_{-2}), 151.4 (C_{-5}), 141.1 ($\underline{\text{CHCH}_2}$), 140.1 (CH_{-8}), 126.3 (d, $J = 171.7$ Hz, CHP), 115.9 (C_{-4}), 42.8 (CH_2N), 30.2 (d, $J = 21.8$ Hz, 1C, $\underline{\text{CH}_2\text{CH}}$). ^{31}P NMR (202 MHz, D_2O) δ 10.5. HMRS TOF ESI+ Found : 286.0708; Calculated for $\text{C}_9\text{H}_{13}\text{N}_5\text{O}_4\text{P}$: 286.0705 ($\text{M}+\text{H}$) $^+$.

(R)-(3-(6-amino-9H-purin-9-yl)-2-hydroxypropyl)phosphonic acid (R)-1



Title 3-cp-231113.11.1.1r
 Comment BG.3.114 RPF4-17Na+
 P31dec1H-SI D2O / opt/ topspin cp 3
 Solvent D2O
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

363 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-50 O: 0-50 P: 1-1

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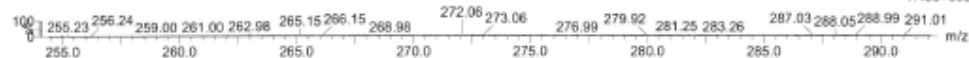
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ACQUAP

31-May-2013

1: TOF MS ES-

1.43e+005

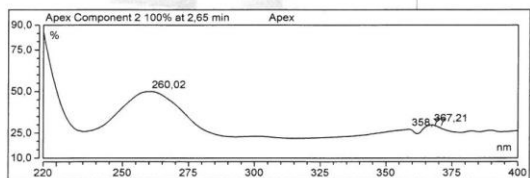
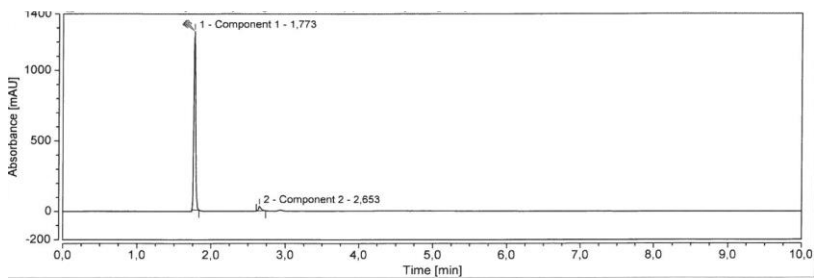


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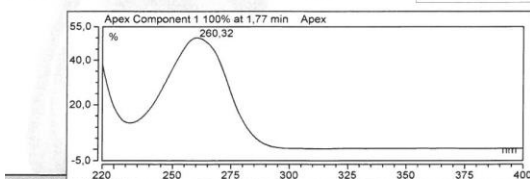
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 50.0

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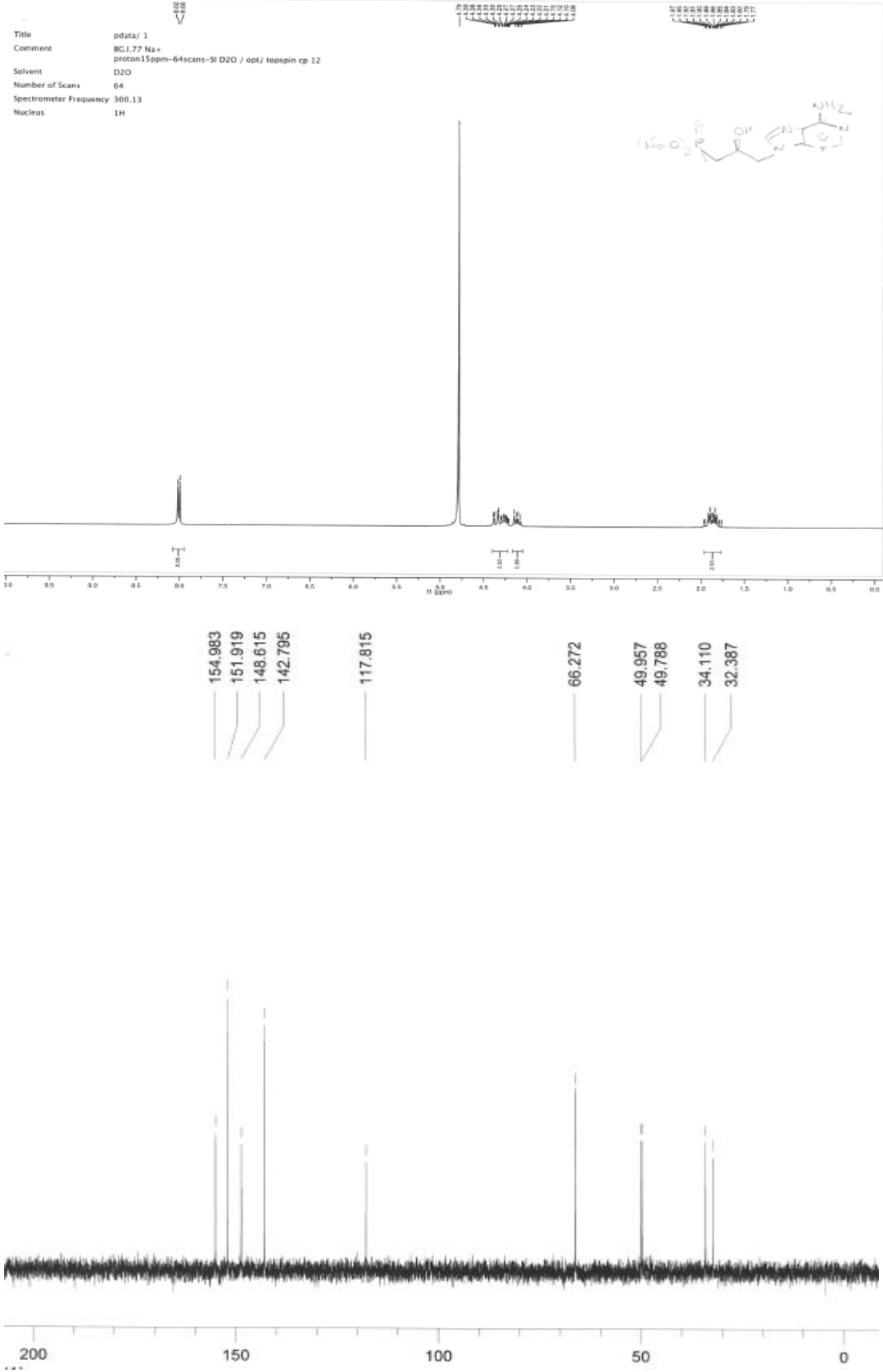


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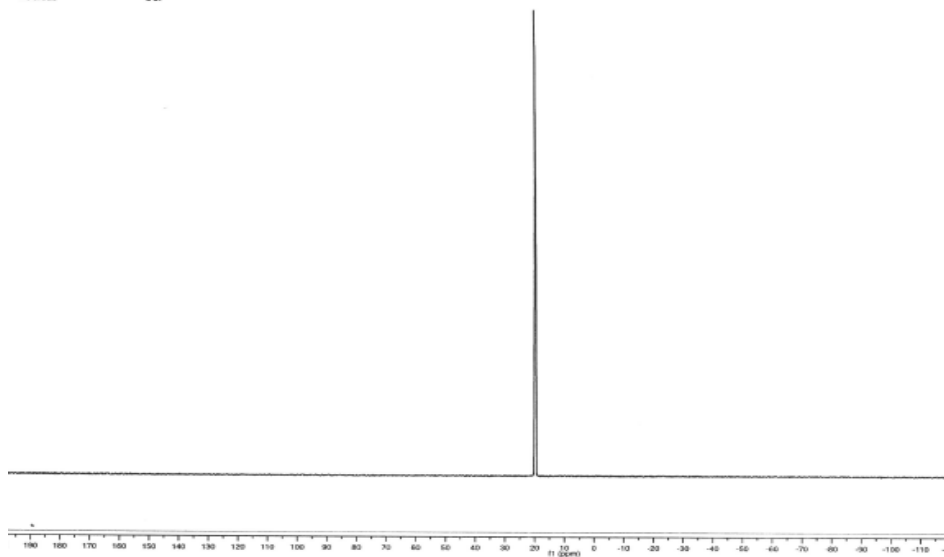


Integration results						
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
1	Component 1	1.773	37,404	1267,116	96.74	97.43
2	Component 2	2.653	1,262	33,457	3.26	2.57
						n.a.

(S)-(3-(6-amino-9H-purin-9-yl)-2-hydroxypropyl)phosphonic acid (S)-1



Title pdata/ 1
 Comment BG1.77 Na+
 P31dec1H-Si D2O / opt/ topspin cp 12
 Solvent D2O
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

342 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: 0-50 O: 0-50 Na: 2-2 P: 1-1

SYNAPT G2-S#UEB205

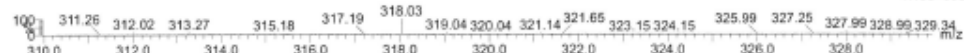
BGI77RPF7-10Na+

Y-CP13091608 14 (0.263) AM2 (Ar,30000.0,0.00,0.00)

16-Sep-2013

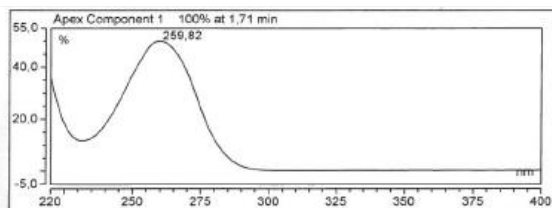
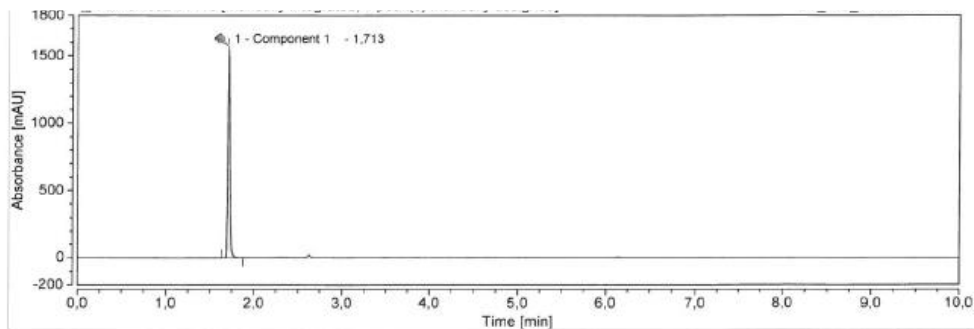
1: TOF MS ES+

1.19e+005



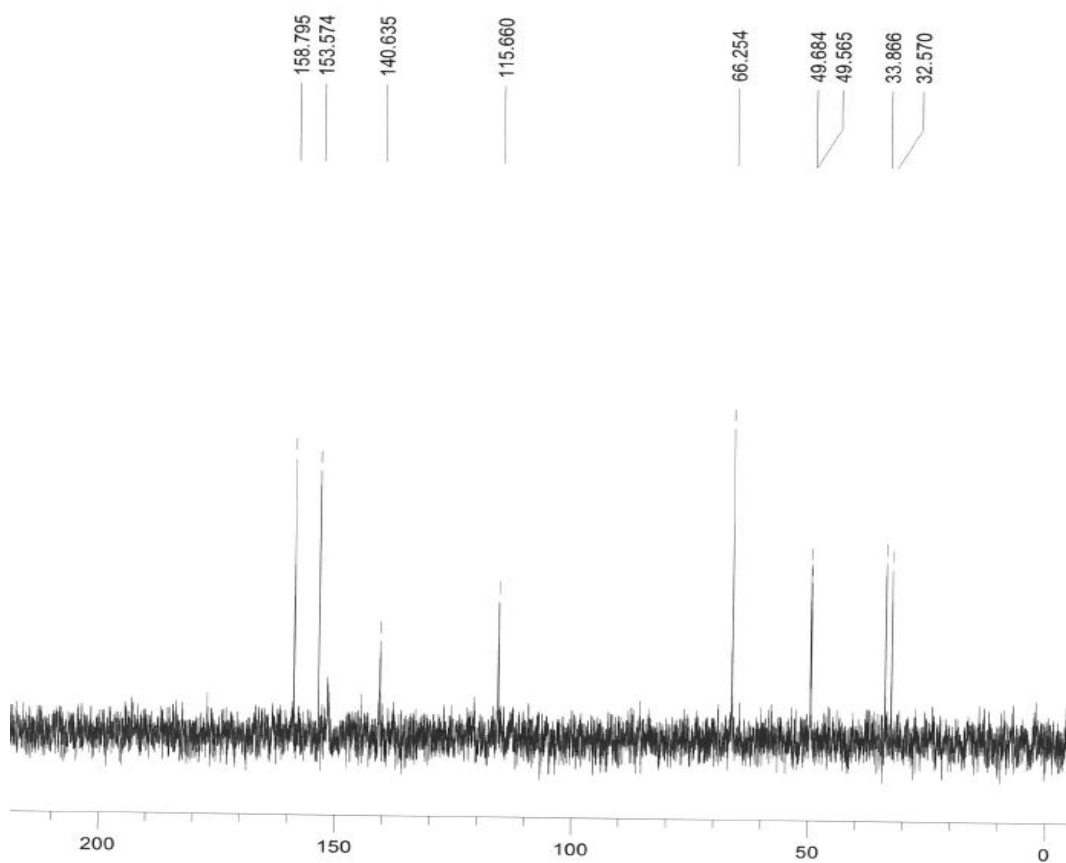
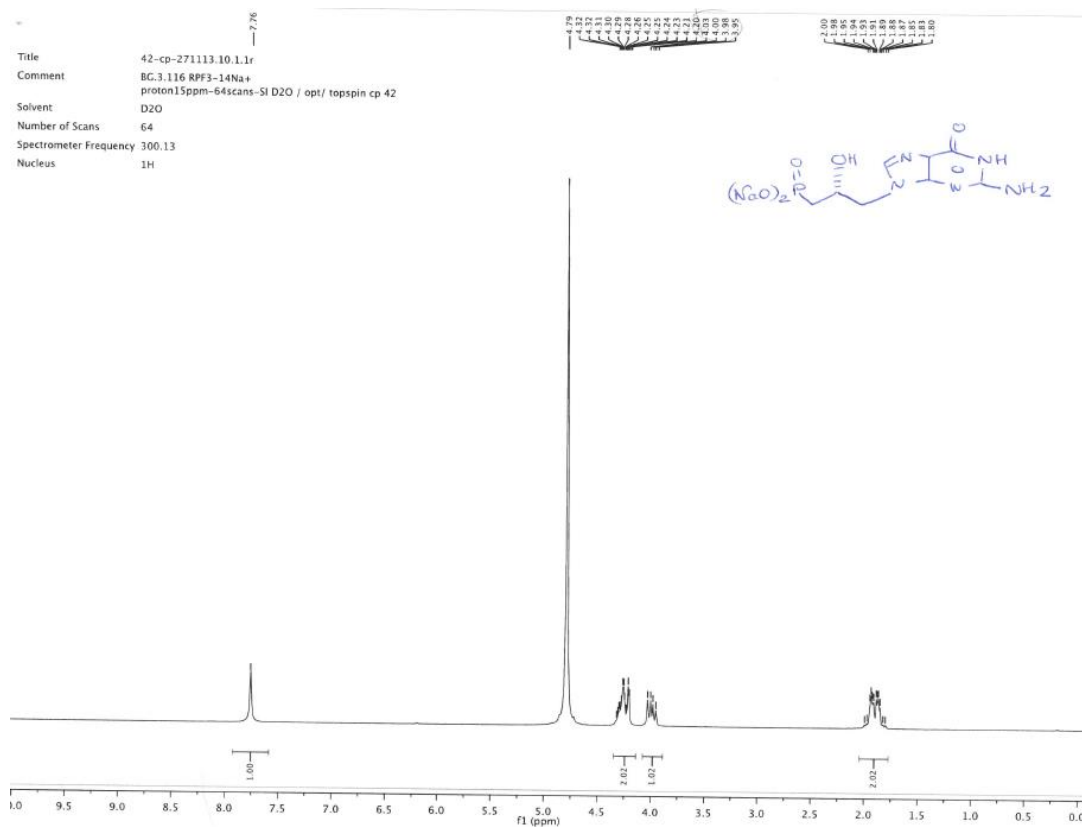
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 Maximum: 5.0 10.0 50.0

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318.0331	318.0331	1.8	5.7	0.5	1264.3	1.251	28.62	C7 H15 N O8 Na2 P
318.0357	318.0357	-0.8	-2.5	10.5	1264.7	1.664	18.93	C9 H7 N9 Na2 P

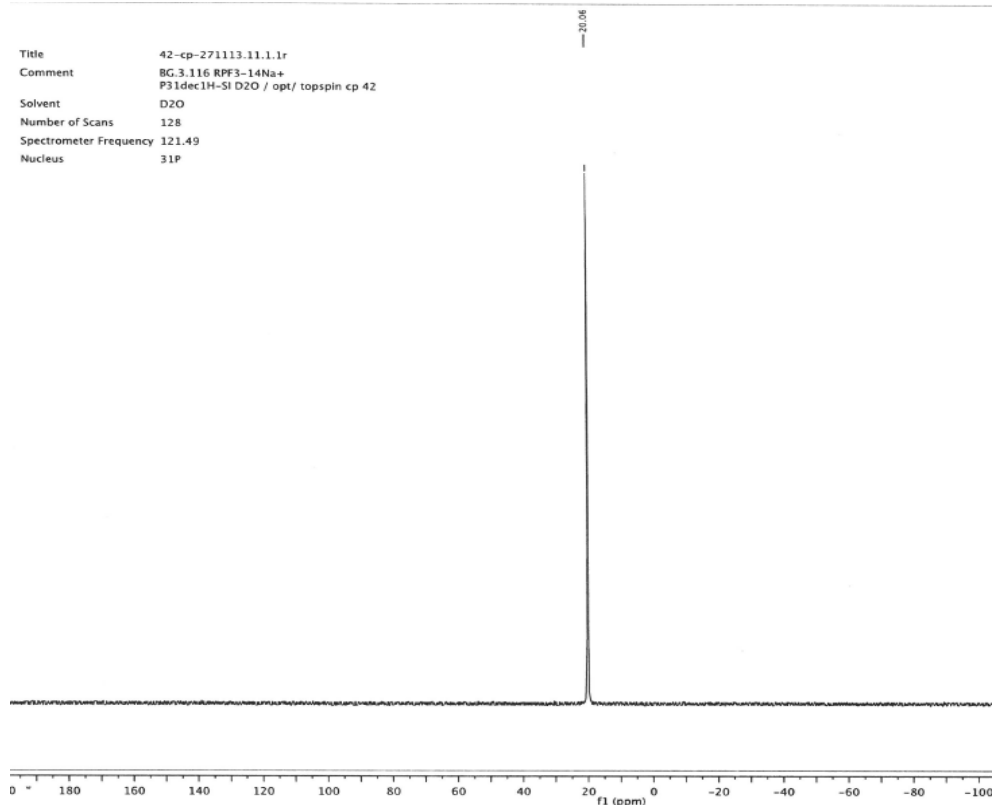


Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1	Component 1	1.713	46,130	1566,763	100,00	100,00	n.a.

(R)-(3-(2-amino-6-oxo-9H-purin-9-yl)-2-hydroxypropyl)phosphonic acid (R)-2



Title 42-cp-271113.11.1.1r
 Comment BG.3.116 RPF3-14Na+
 P31dec1H-SI D2O / opt/ topspin cp 42
 Solvent D2O
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P



Monoisotopic Mass, Even Electron Ions
 424 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

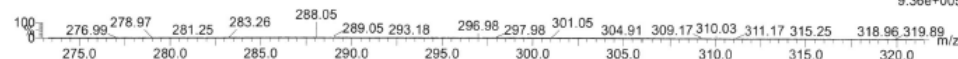
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SYNAPT G2-S#UEB205

Y-CP13053105 23 (0.465) AM2 (Ar.30000.0,0.00,0.00); Cm (23.32)

BGI71 (RPF1)

31-May-2013
 1: TOF MS ES-
 9.36e+005



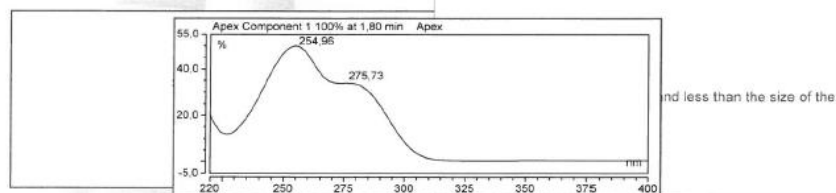
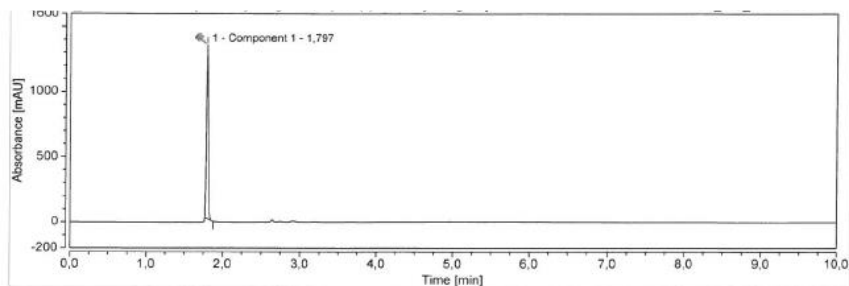
Minimum:

Maximum:

5.0 2.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(%) Formula

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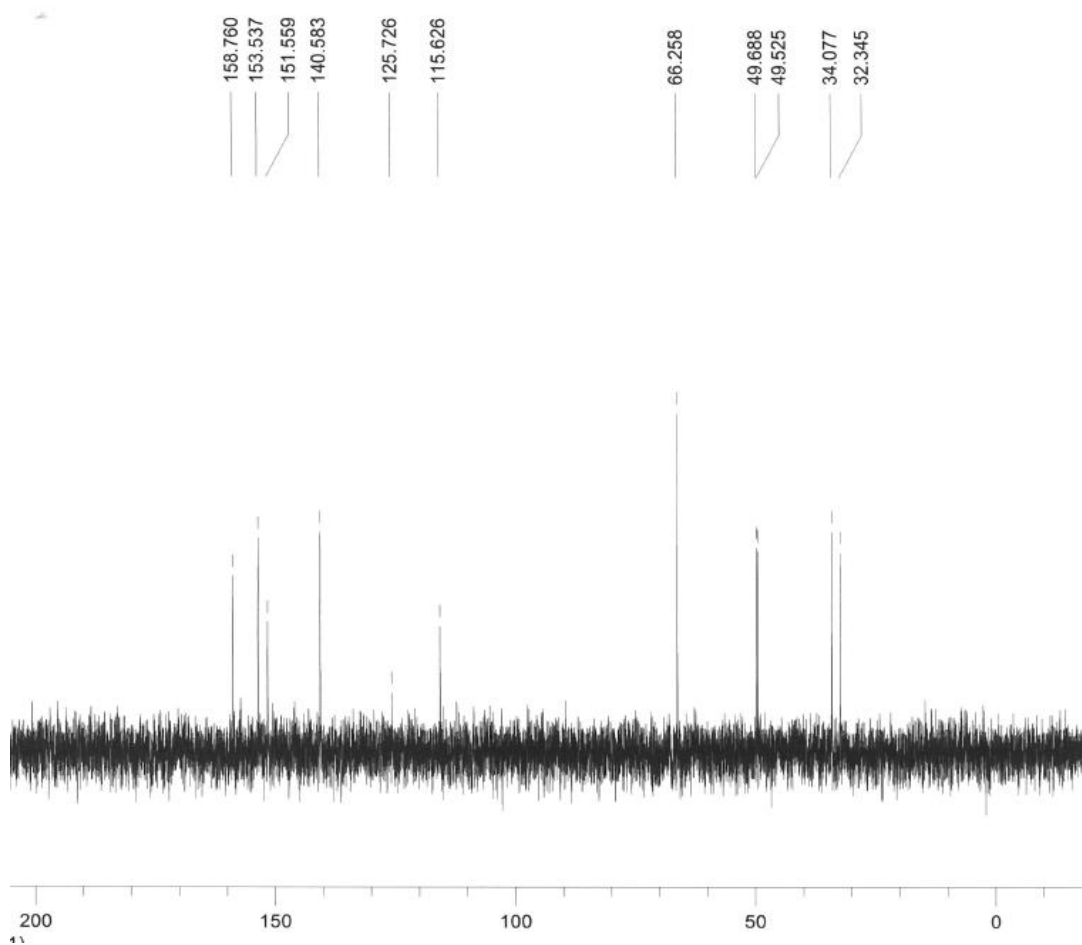
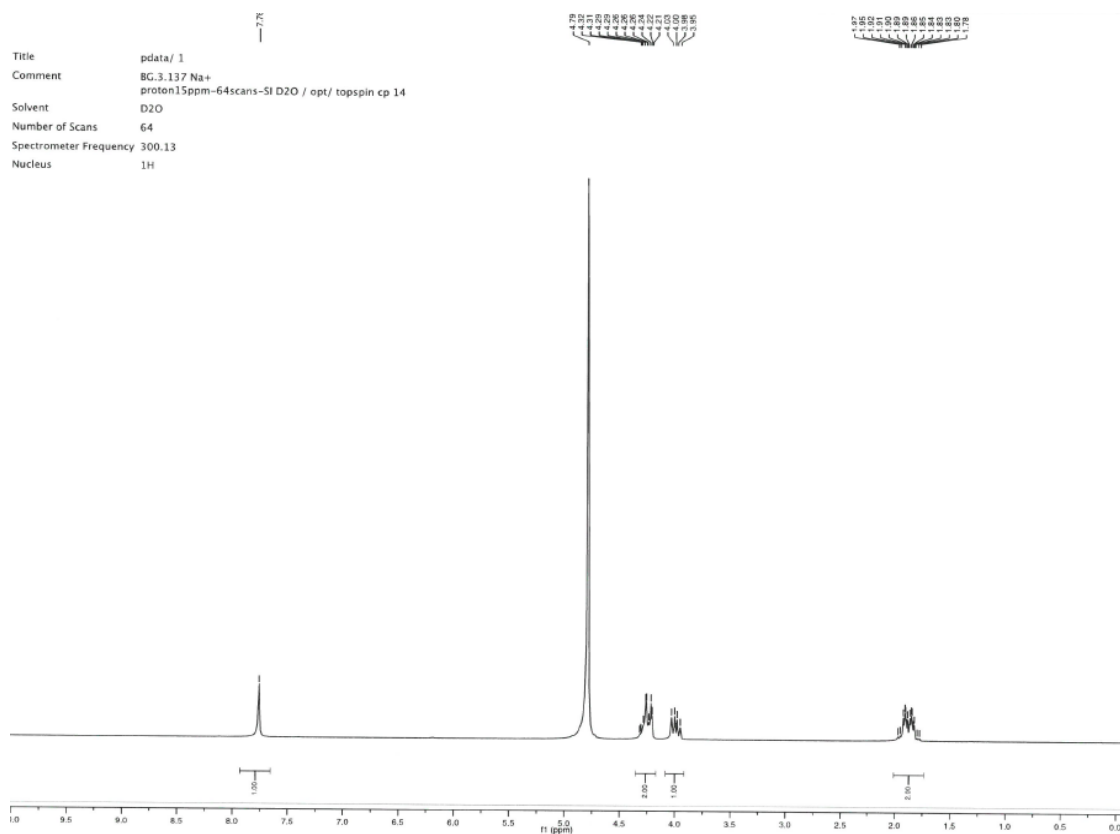


and less than the size of the

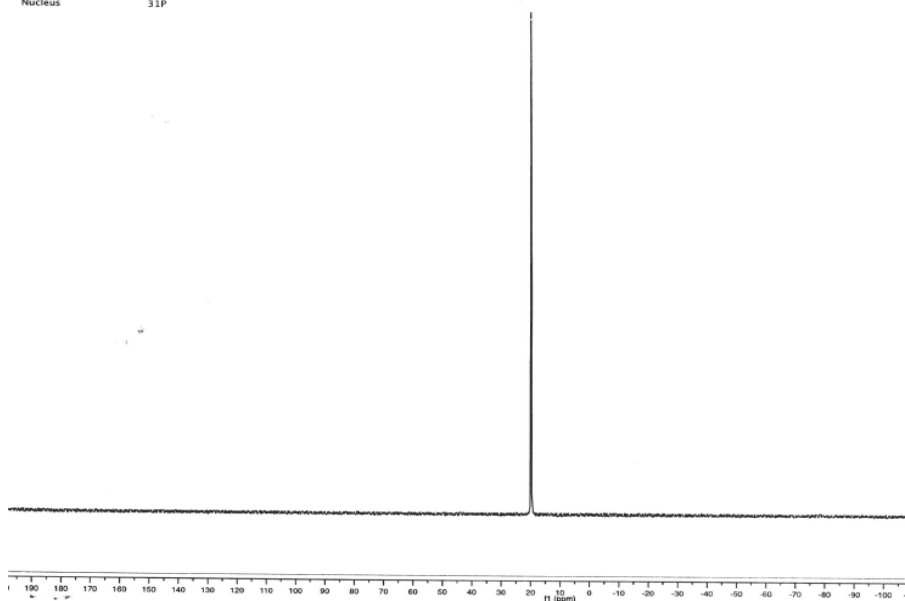
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1	Component 1	1.797	38,749	1335,498	100,00	100,00	n.a.

(S)-(3-(2-amino-6-oxo-9H-purin-9-yl)-2-hydroxypropyl) phosphonic acid (S)-2



Title pdata/ 1
 Comment BG.3.137 Na+
 P31dec1H-Si D2O / opt/ topspin cp 14
 Solvent D2O
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

401 formula(e) evaluated with 4 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-50 O: 0-50 Na: 2-2 P: 1-1

SYNAPT G2-S#UEB205

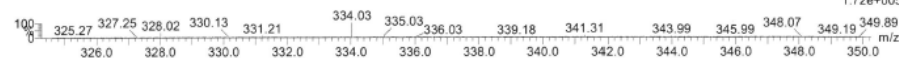
BGI78RPF4-5Na+

Y-CP13091609 11 (0.213) AM2 (Ar,30000.0,0.00,0.00)

16-Sep-2013

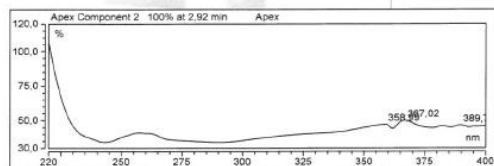
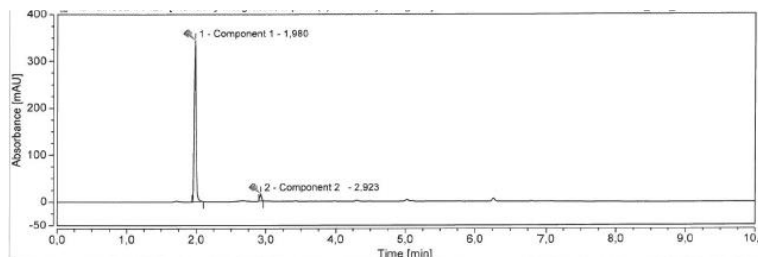
1: TOF MS ES+

1.72e+005

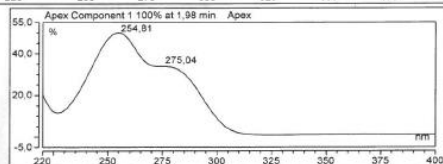


Minimum: -1.5
 Maximum: 5.0 10.0 50.0

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334.0307	-0.5	-1.5	10.5	1227.6	2.832	5.89		C9 H7 N9 O Na2 P
334.0333	-3.1	-9.3	9.5	1228.8	3.991	1.85		C13 H11 N3 O3 Na2 P
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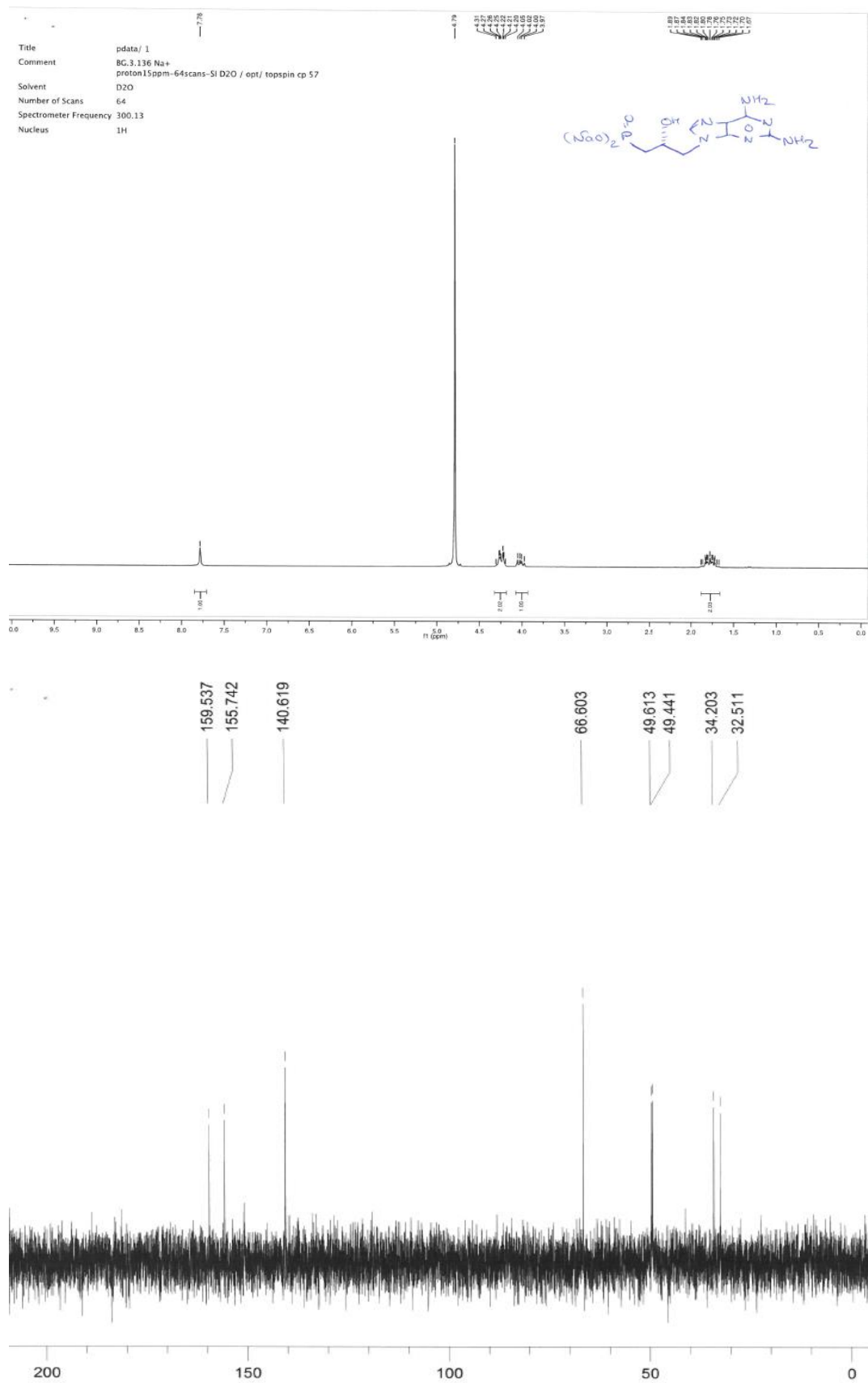


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 No spectra selected.

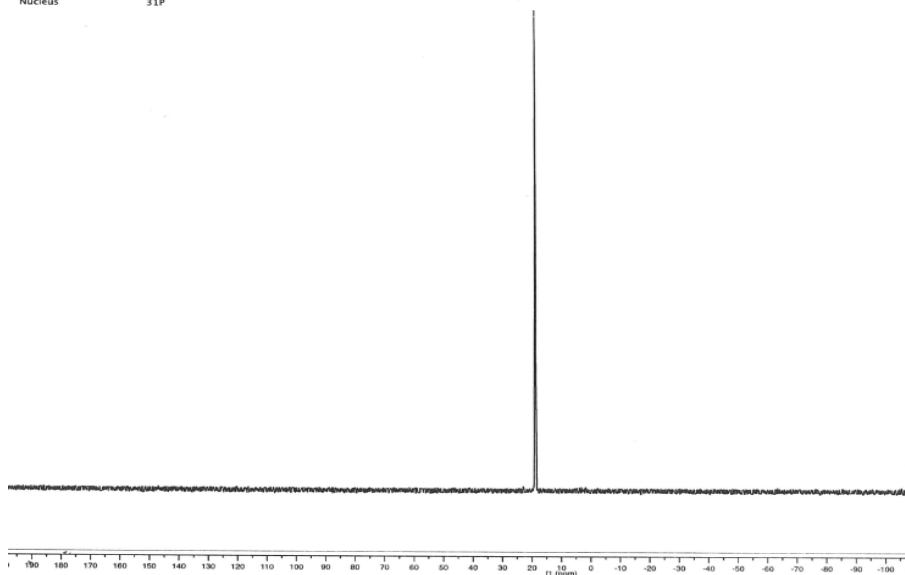


No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1	Component 1	1.980	10.921	344.675	96.45	95.77	n.a.
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
2	Component 2	2.923	0.402	15.231	3.55	4.23	n.a.

(R)-(3-(2,6-diamino-9H-purin-9-yl)-2-hydroxypropyl) phosphonic acid (R)-3



Title pdata/ 1
 Comment BG.3.136 Na+
 P31dec1H-SI D2O / opt/ topspin cp 10
 Solvent D2O
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

386 formula(e) evaluated with 5 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-50 O: 0-50 Na: 2-2 P: 1-1

SYNAPT G2-S#UEB205

BGI95RPF5-12Na+

Y-CP13091610 12 (0.229) AM2 (Ar.30000.0.0.0.0.0.0)

16-Sep-2013

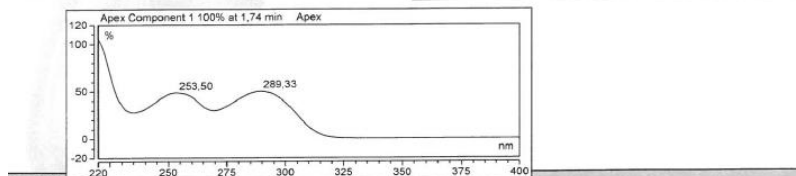
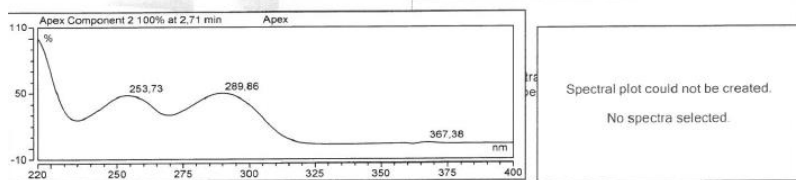
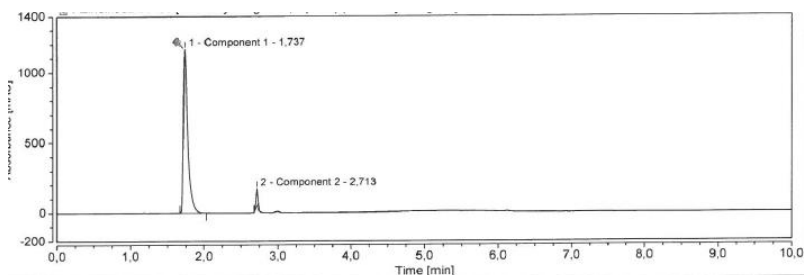
1: TOF MS ES+

3.88e+006



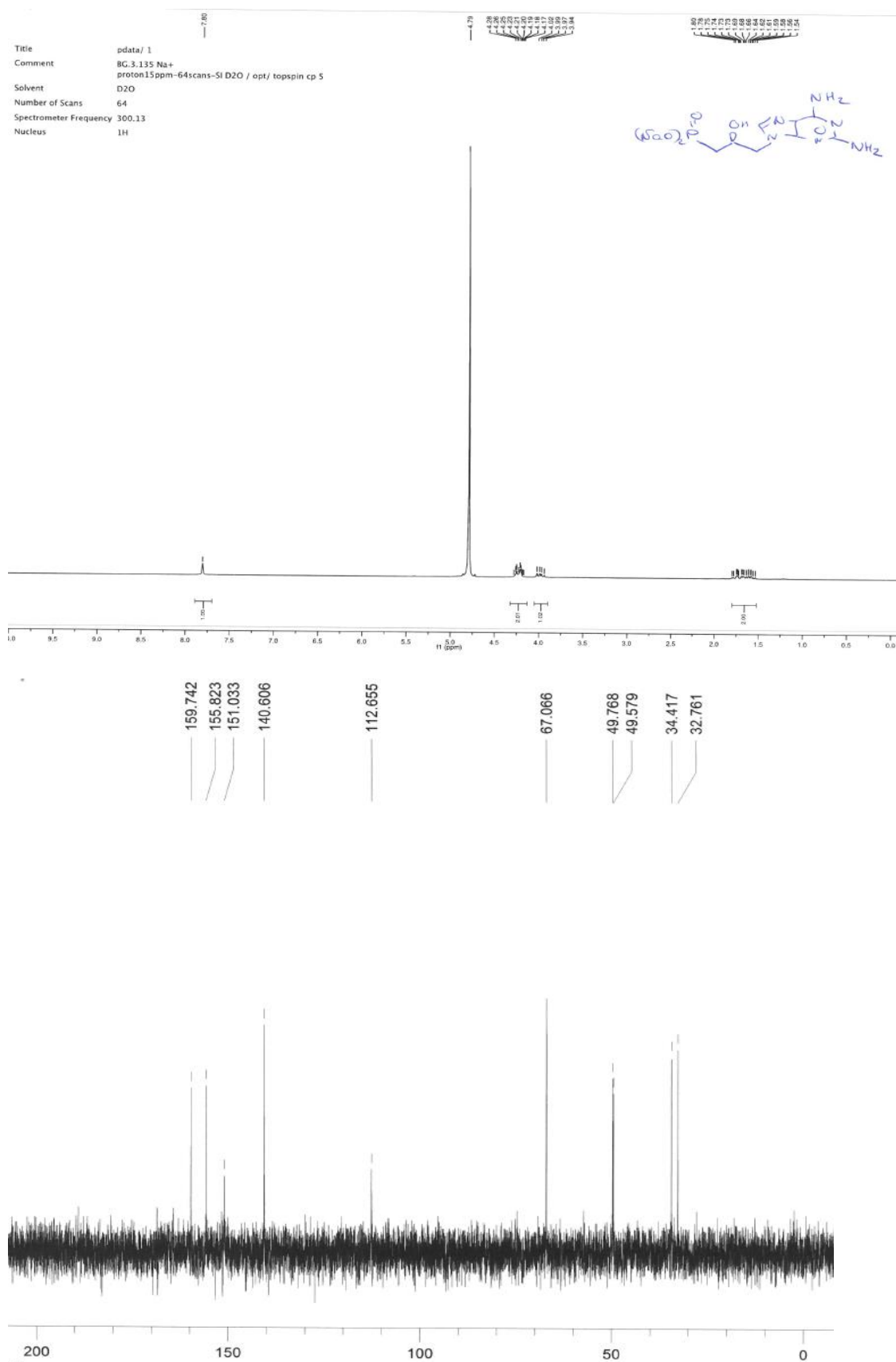
Minimum: -1.5
 Maximum: 50.0

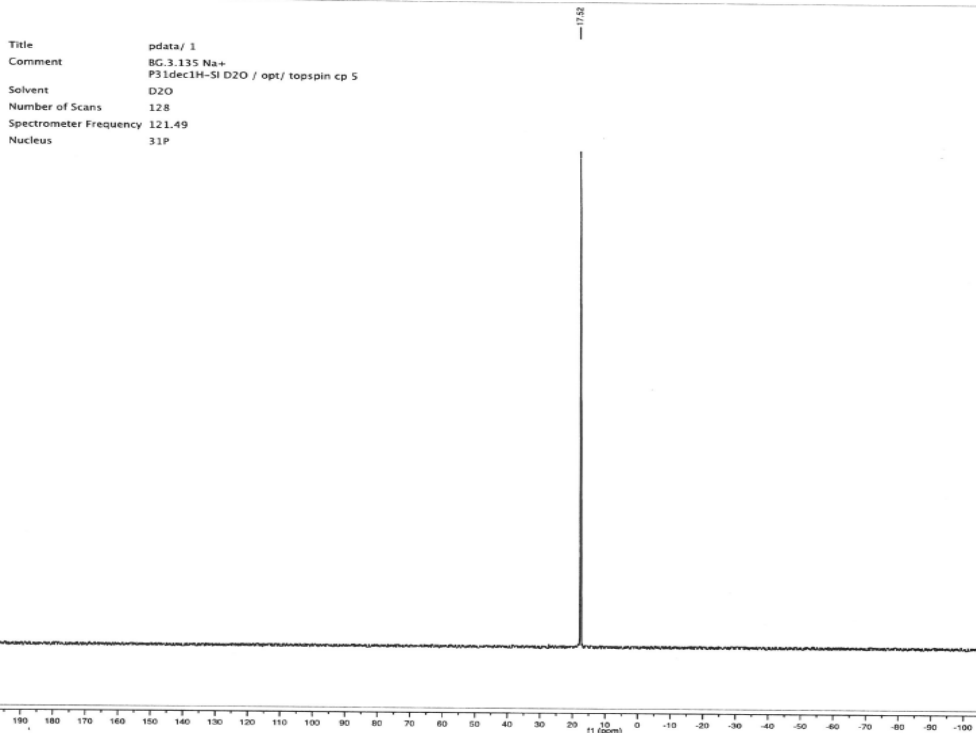
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
333.0460	333.0453	0.7	2.1	5.5	1198.7	0.013	98.69	C8 H12 N6 O4 Na2 P
	333.0440	2.0	6.0	0.5	1203.5	4.798	0.82	C7 H16 N2 O8 Na2 P
	333.0480	-2.0	-6.0	4.5	1204.2	5.529	0.40	C12 H16 O6 Na2 F
	333.0466	-0.6	-1.8	10.5	1206.3	7.585	0.05	C9 H8 N10 Na2 P
	333.0493	-3.3	-9.9	9.5	1206.7	7.983	0.03	C13 H12 N4 O2 Na2 P



Integration Results							
lo.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
	Component 1	1,737	76,497	1168,777	95,97	90,28	n.a.
	Component 2	2,713	3,212	125,814	4,03	9,72	n.a.

(S)-(3-(2,6-diamino-9H-purin-9-yl)-2-hydroxypropyl) phosphonic acid (S)-3





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

386 formula(e) evaluated with 6 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-50 O: 0-50 Na: 2-2 P: 1-1

SYNAPT G2-S#UEB205

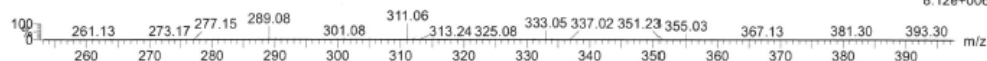
BGI94RPF4-12Na+

Y-CP13091611 8 (0.157) AM2 (At.30000.0,0.00,0.00), Cm (8.16)

16-Sep-2013

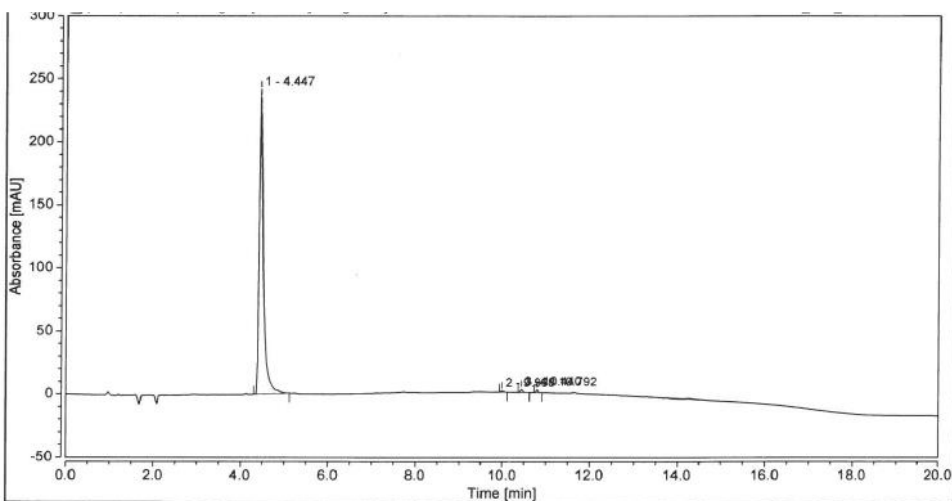
1: TOP MS ES+

8.12e+006



Minimum: -1.5
Maximum: 5.0 10.0 50.0

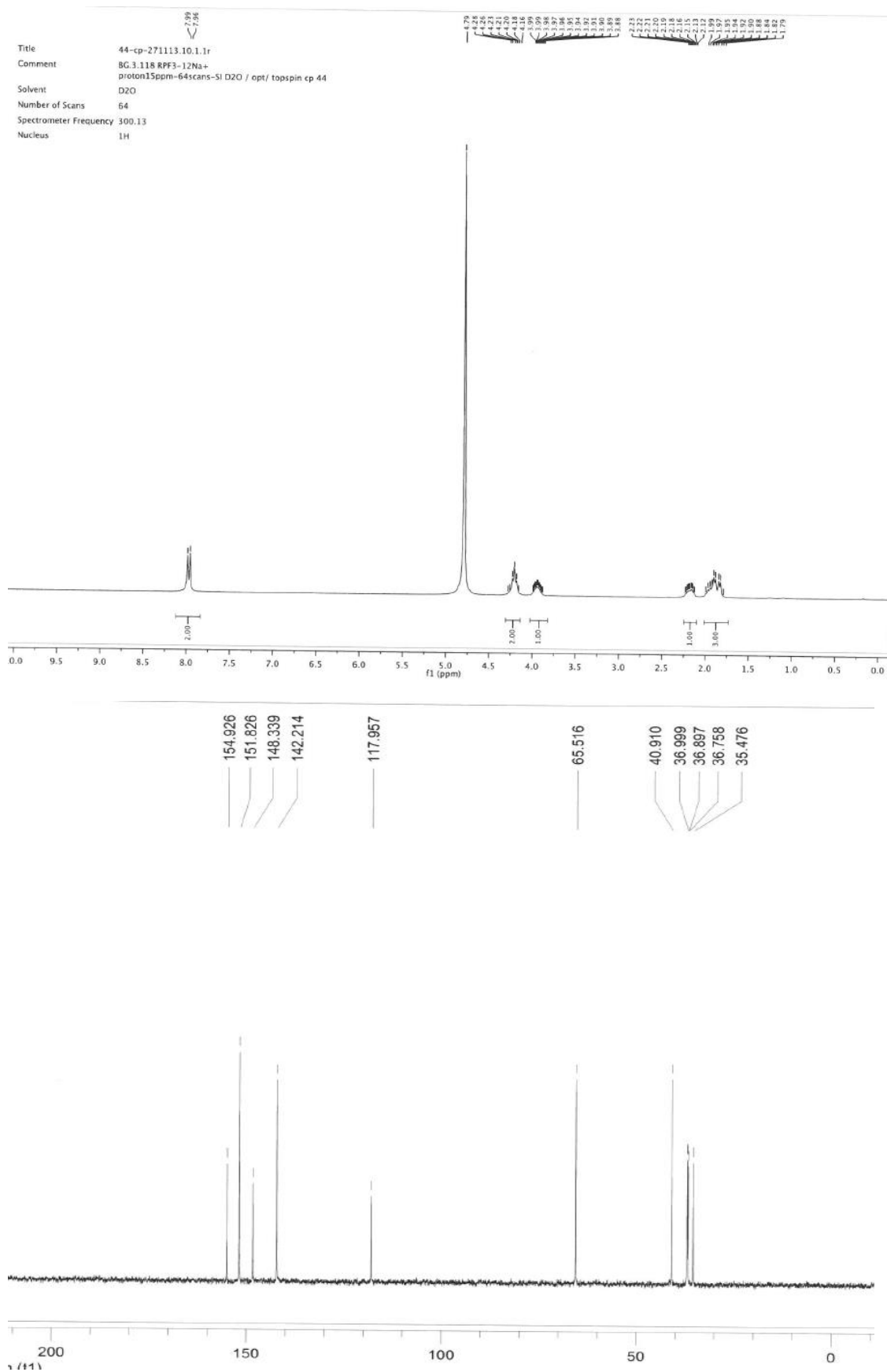
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
333.0450	333.0453	-0.3	-0.9	5.5	1752.5	0.001	99.94	C8 H12 N6 O4 Na2 P
333.0440	1.0	3.0	0.5	1760.0	7.502	0.06		C7 H16 N2 O8 Na2 P
333.0480	-3.0	-9.0	4.5	1763.2	10.693	0.00		C12 H16 O6 Na2 P
333.0466	-1.6	-4.8	10.5	1765.7	13.140	0.00		C9 H8 N10 Na2 P
333.0426	2.4	7.2	6.5	1766.2	13.703	0.00		C4 H8 N12 O2 Na2 P
333.0421	2.9	8.7	13.5	1769.9	17.402	0.00		C19 H12 O Na2 P



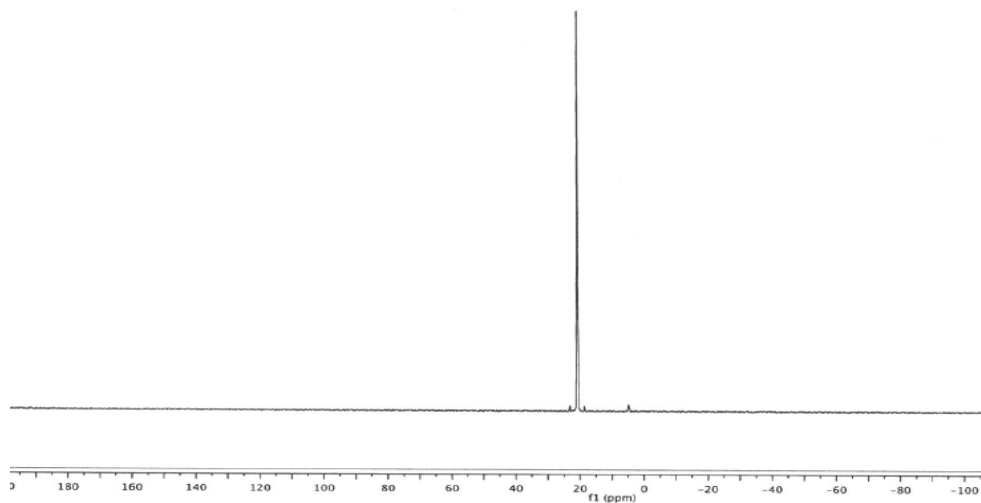
Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		4.447	25.454	241.913	98.50	97.38	n.a.
2		9.998	0.086	1.366	0.33	0.55	n.a.
3		10.440	0.166	2.698	0.64	1.09	n.a.
4		10.792	0.137	2.446	0.53	0.98	n.a.

(R)-(4-(6-amino-9H-purin-9-yl)-2-hydroxybutyl)phosphonic acid (R)-4



Title 44-cp-271113.11.1.1r
 Comment BG.3.118 RPF3-12Na+
 P31dec1H-SI D2O / opt/ topspin cp 44
 Solvent D2O
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

422 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-50 O: 0-50 P: 1-1

SYNAPT G2-S#NotSet

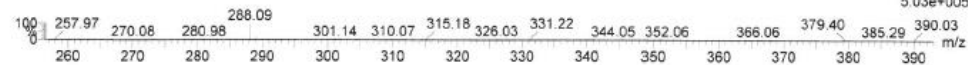
Y-CP14091902 17 (0.329) Cm (17)

BG3.118

19-Sep-2014

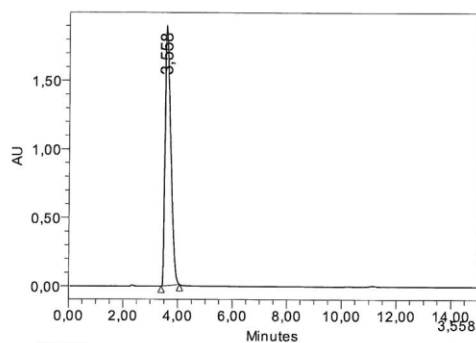
1: TOF MS ES+

5.03e+005

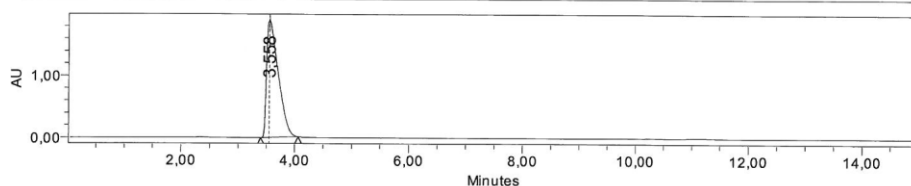
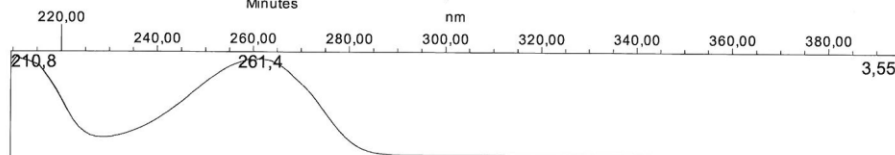


Minimum: -1.5
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
288.0867	288.0862	0.5	1.7	5.5	2642.5	n/a	n/a	C9 H15 N5 O4 P



	RT	Area	% Area	Height
1	3,558	27201874	100,00	1912409

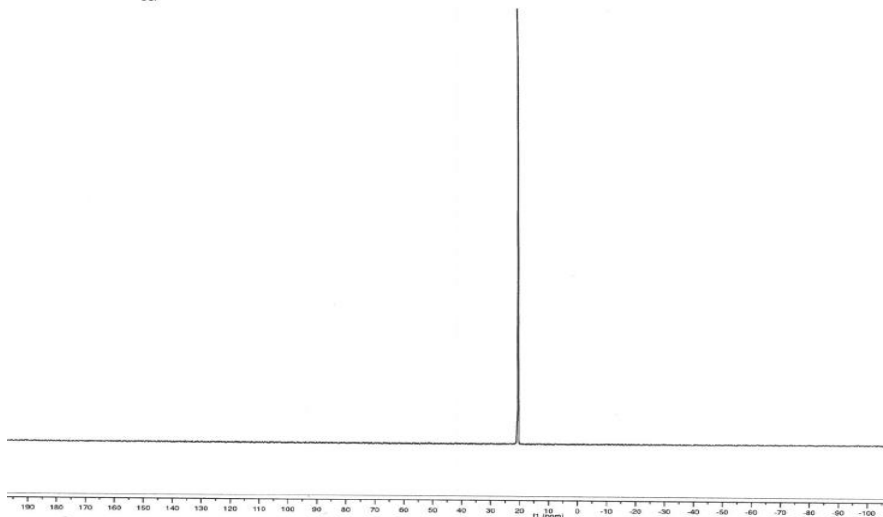


Title pdata/ 1
Comment BG-3.147 Na+
proton15ppm-64scans-SI D2O / opt/ topspin cp 9
Solvent D2O
Number of Scans 64
Spectrometer Frequency 300.13
Nucleus 1H

Chemical structure of compound 15 is shown above the spectrum:

N[C@@H]1CNC(=N)[C@H](N1)CCOP(=O)([O-])[O-]

Title pdata/ 1
 Comment BG 3.147 Na+
 Solvent P11dec1H-SI D2O / opt/ topspin cp 9
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

422 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-50 O: 0-50 P: 1-1

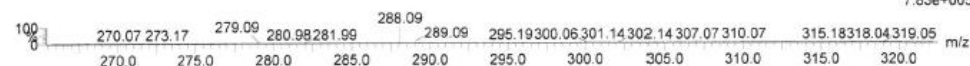
SYNAPT G2-S#NotSet

BG3.147

19-Sep-2014

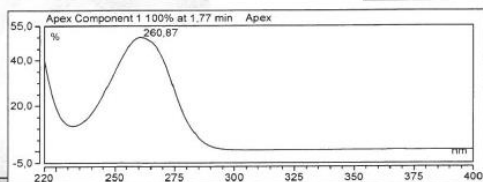
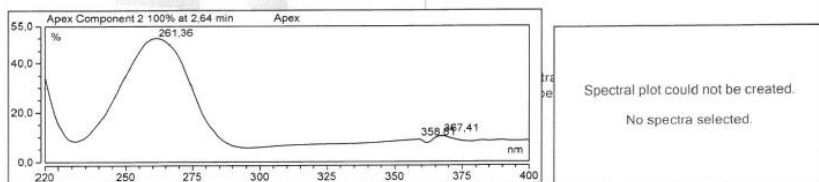
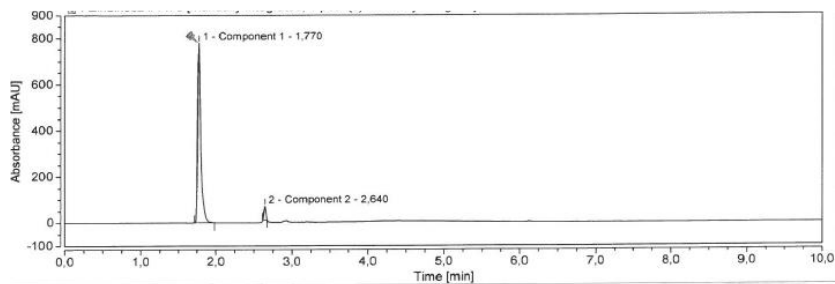
1: TOF MS ES+

7.83e+005



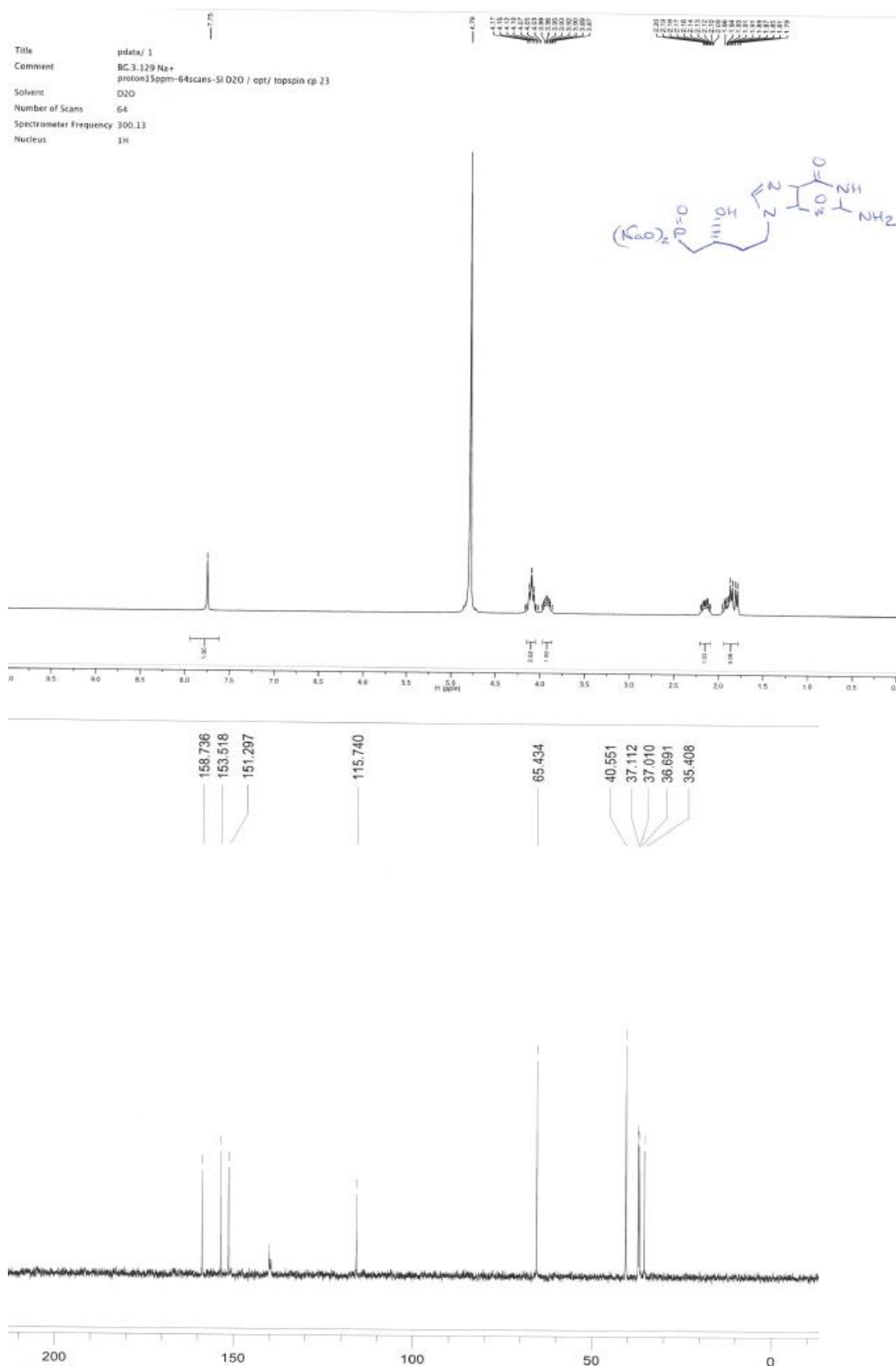
Minimum: -1.5
 Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
288.0860	288.0862	-0.2	-0.7	5.5	3401.7	n/a	n/a	C9 H15 N5 O4 P

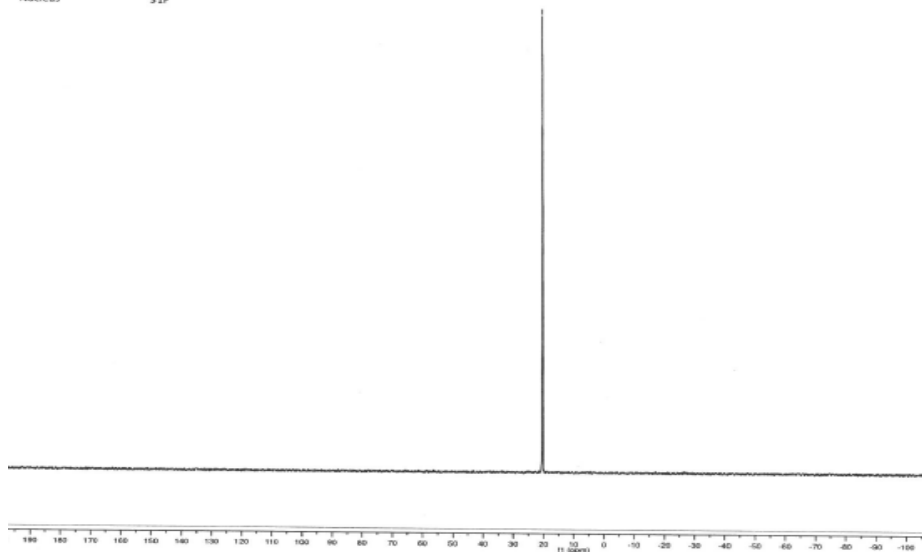


Integration results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1	Component 1	1.770	35.223	779.205	96.37	92.87	n.a.
2	Component 2	2.640	1.712	59.831	4.63	7.13	n.a.
n.a.	Component 3	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.

(R)-4-(2-amino-6-oxo-9H-purin-9-yl)-2-hydroxybutyl phosphonic acid (R)-5



Title pdata/ 1
 Comment BG3.129 Na+
 P31dec1H-SI D2O / opt/ topspin cp 23
 Solvent D2O
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

489 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

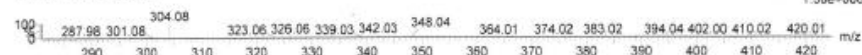
Elements Used:

C: 0-100 H: 0-150 N: 0-50 O: 0-50 P: 1-1

SYNAPT G2-SAMNotSet
 Y-CP14091712 9 (0.185)

BG3.129

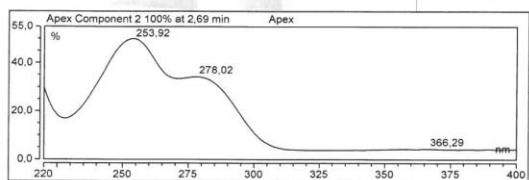
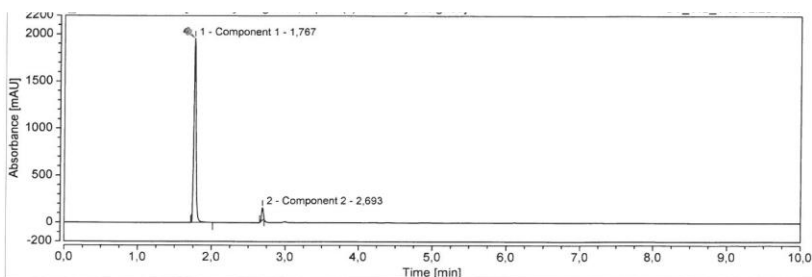
17-Sep-2014
 1: TOF MS ES+
 1.58e+006



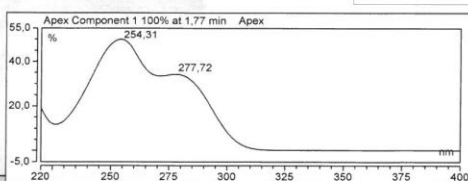
Minimum: -1.5
 Maximum: 5.0 2.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(%) Formula

304.0808 304.0811 -0.3 -1.0 5.5 2937.7 n/a n/a C9 H15 N5 O5 P



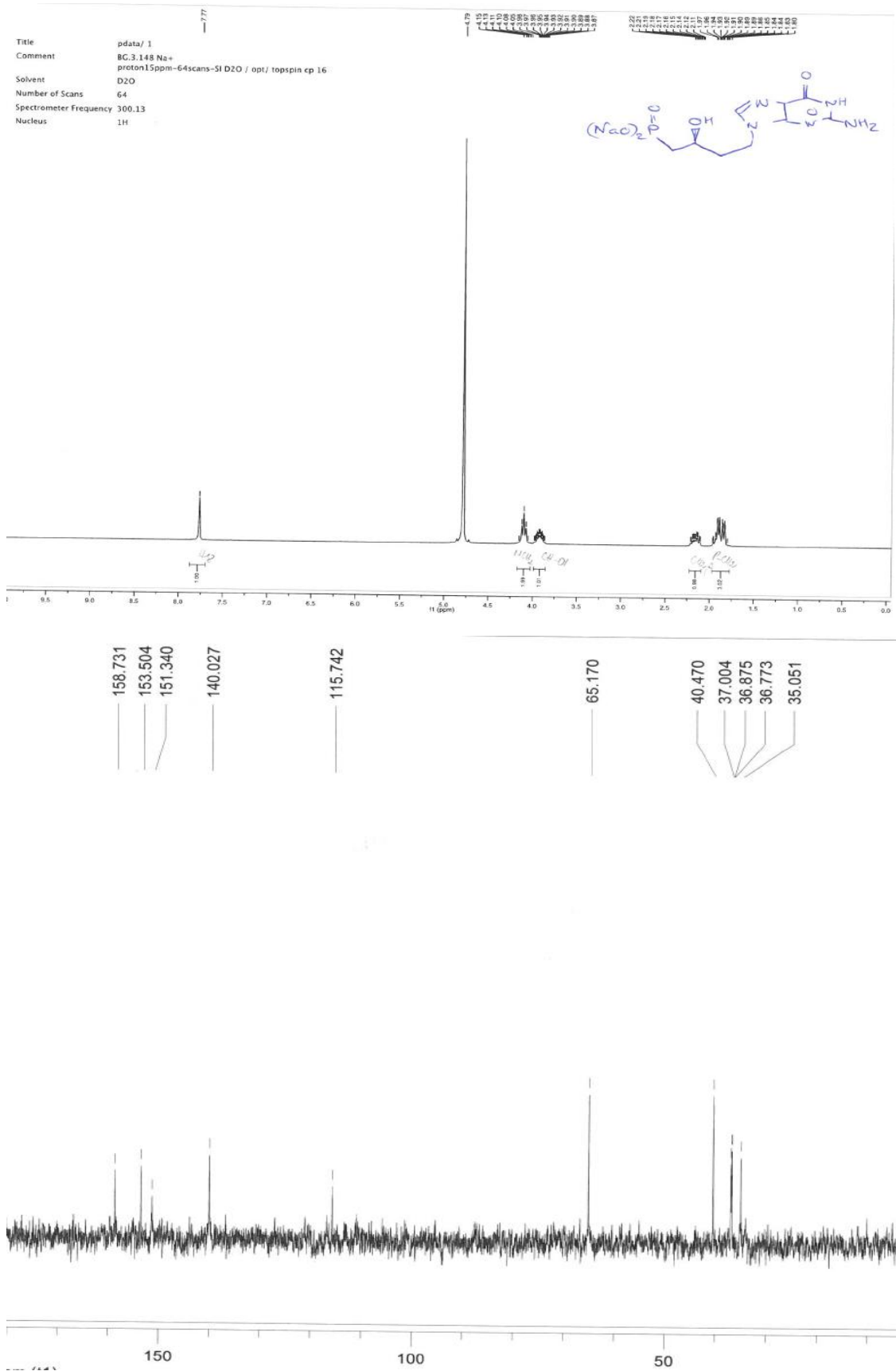
Spectral plot could not be created.
 No spectra selected.



Integration Results

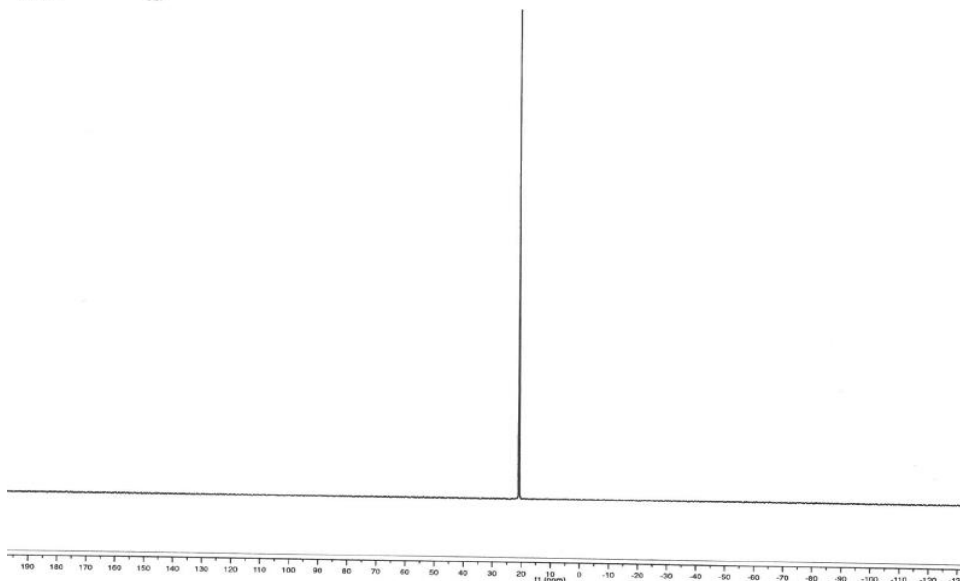
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1	Component 1	1.767	67,869	1957,506	95.45	93.57	n.a.
2	Component 2	2.693	3,236	134,497	4.55	6.43	n.a.

(S)-4-(2-amino-6-oxo-9H-purin-9-yl)-2-hydroxybutyl phosphonic acid (S)-5



Title pdata/ 1
 Comment BG3.148 Na+
 P31dec1H-SI D2O / opt/ topspin cp 16
 Solvent D2O
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P

3
 12
 1



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

489 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-50 O: 0-50 P: 1-1

SYNAPT G2-S#NotSet

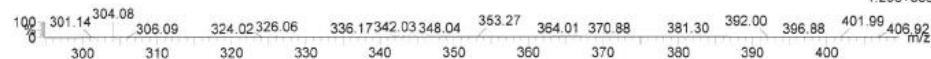
BG3.148

17-Sep-2014

Y-CP14091713 7 (0.143) Cm (7:8)

1. TOF MS ES+

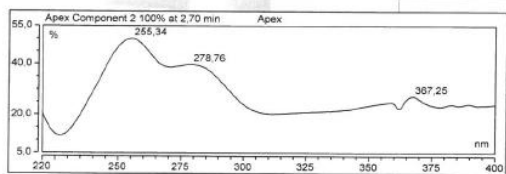
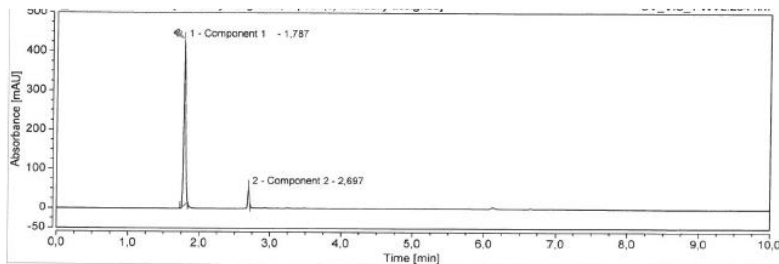
1.29e+006



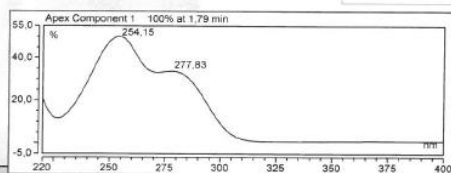
Minimum: -1.5
 Maximum: 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(%) Formula

304.0813 304.0811 0.2 0.7 5.5 3667.7 n/a n/a C9 H15 N5 O5 P

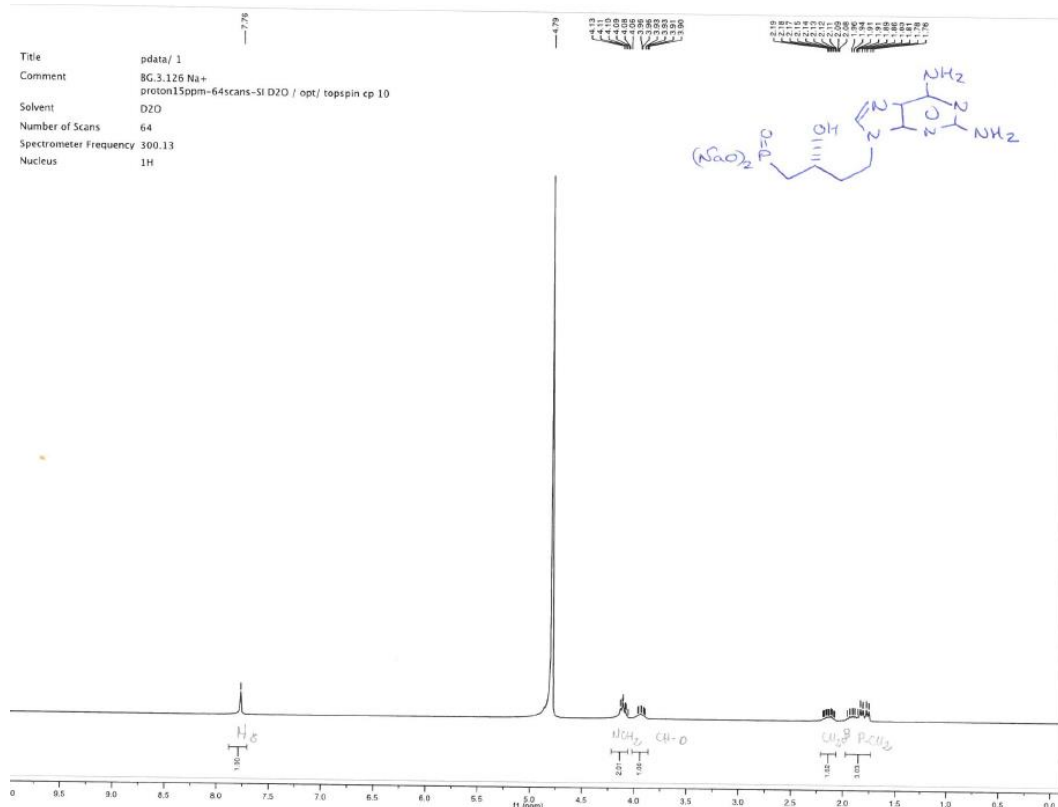


Spectral plot could not be created.
 No spectra selected.



Integration results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1	Component 1	1.787	14,129	422.531	99.07	98.23	n.a.
2	Component 2	2.697	0,132	7,592	0,93	1,77	n.a.

(R)-(4-(2,6-diamino-9H-purin-9-yl)-2-hydroxybutyl) phosphonic acid (R)-6



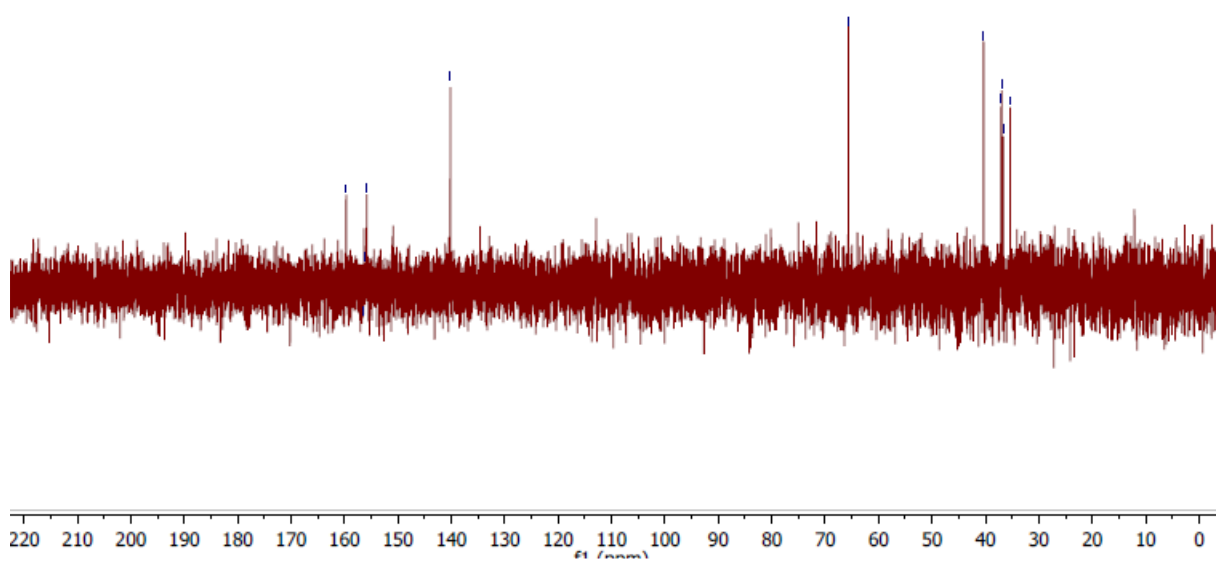
-BG3-113

159.68
 156.50
 156.34
 155.83

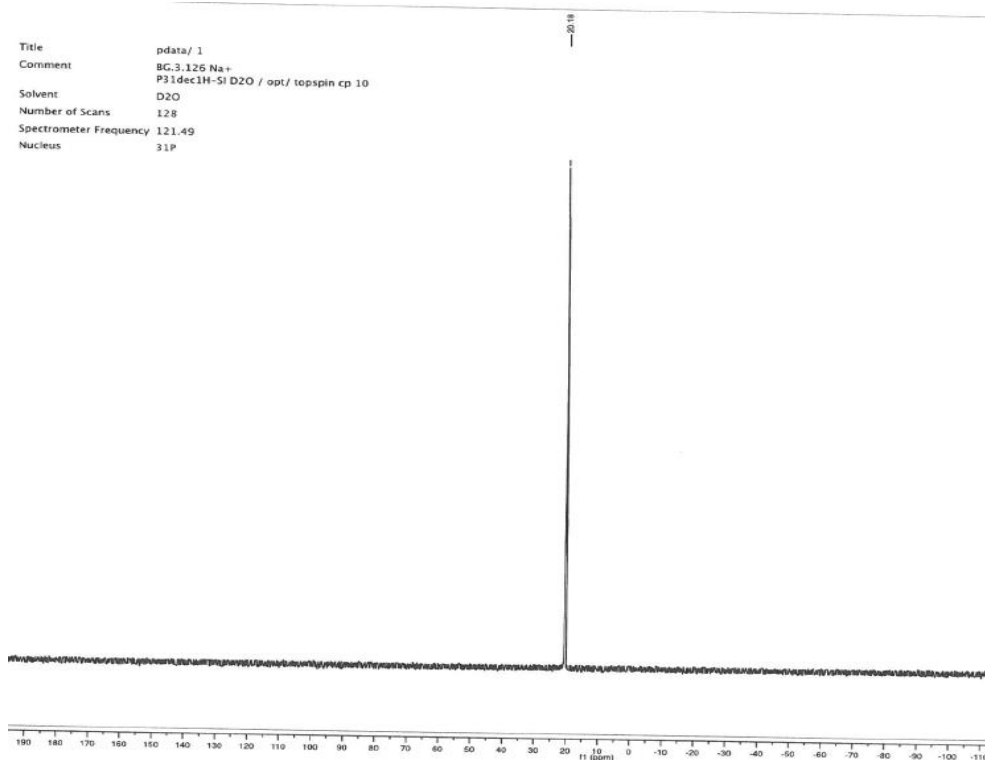
140.18

65.65

40.34
 37.06
 36.96
 36.64
 35.37



Title pdata/ 1
 Comment BG 3.126 Na+
 P31dec1H-SI D2O / opt/ topspin cp 10
 Solvent D2O
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 2.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 4

Monoisotopic Mass, Even Electron Ions

472 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-150 N: 0-50 O: 0-50 P: 1-1

SYNAPT G2-S#NotSet

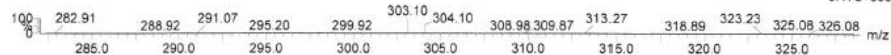
BG3.126

17-Sep-2014

Y-CP14091714 7 (0.143) Cm (6.8)

1: TOF MS ES+

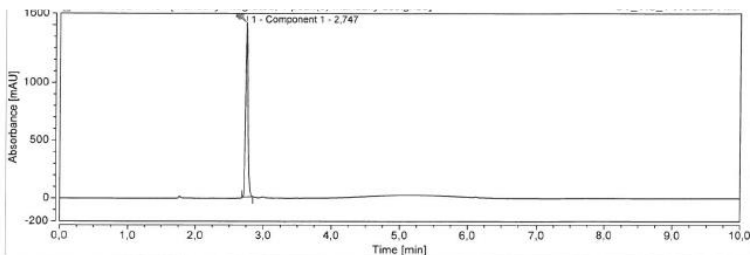
9.17e+005



Minimum: -1.5
 Maximum: 50.0

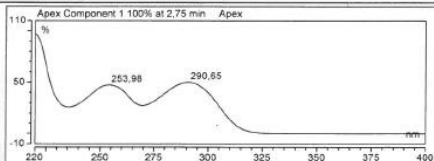
Mass Calc. Mass mDa FPM DBE i-FIT Norm Conf(%) Formula

303.0968 303.0971 -0.3 -1.0 5.5 4192.1 n/a n/a C9 H16 N6 O4 P



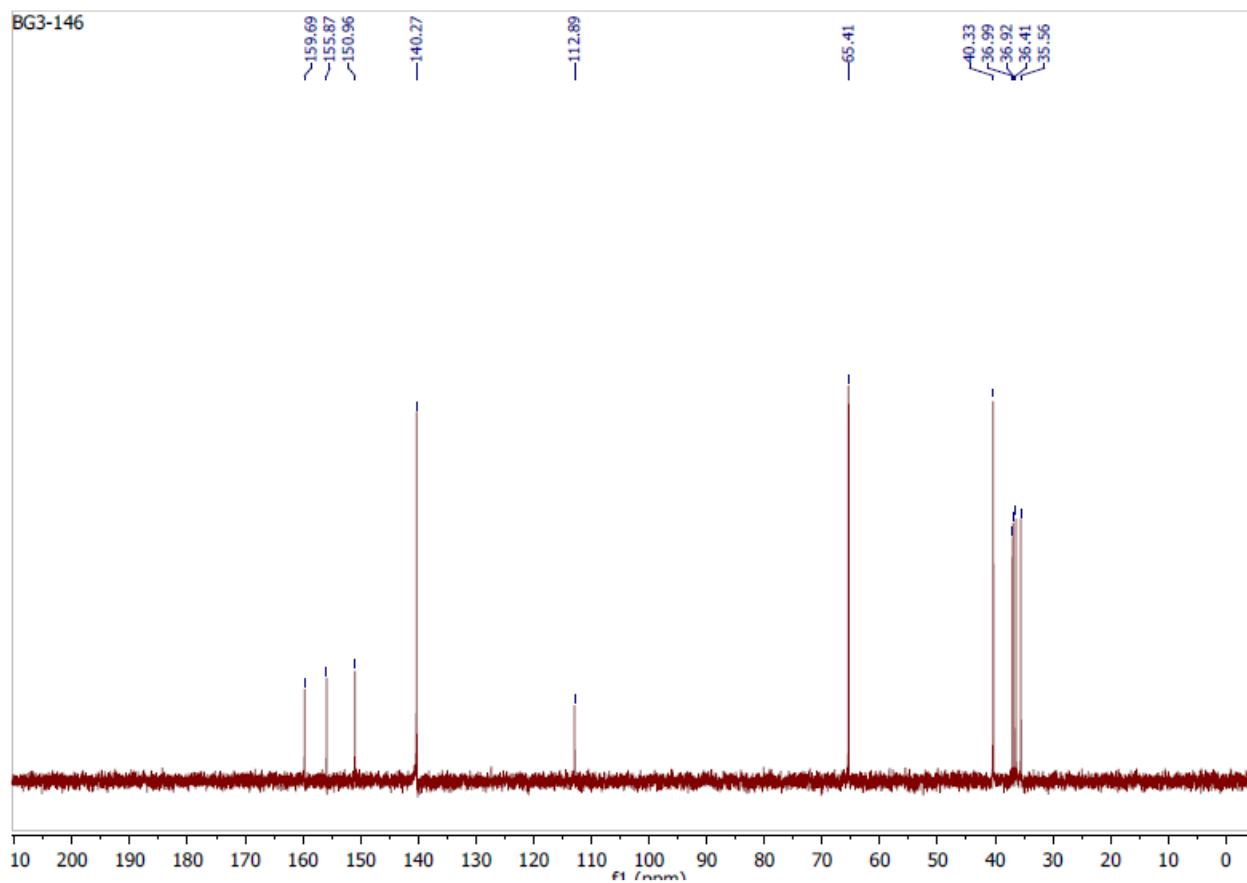
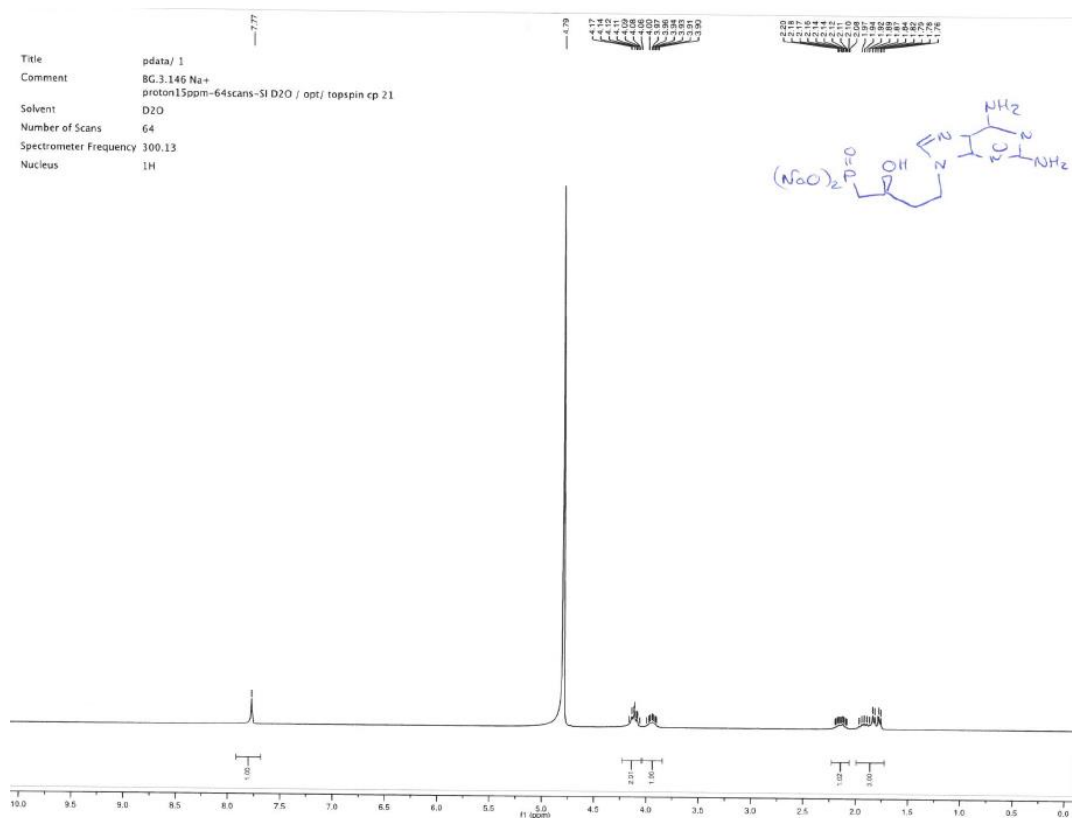
Spectral plot could not be created.
 No spectra selected.

Spectral plot could not be created.
 No spectra selected.

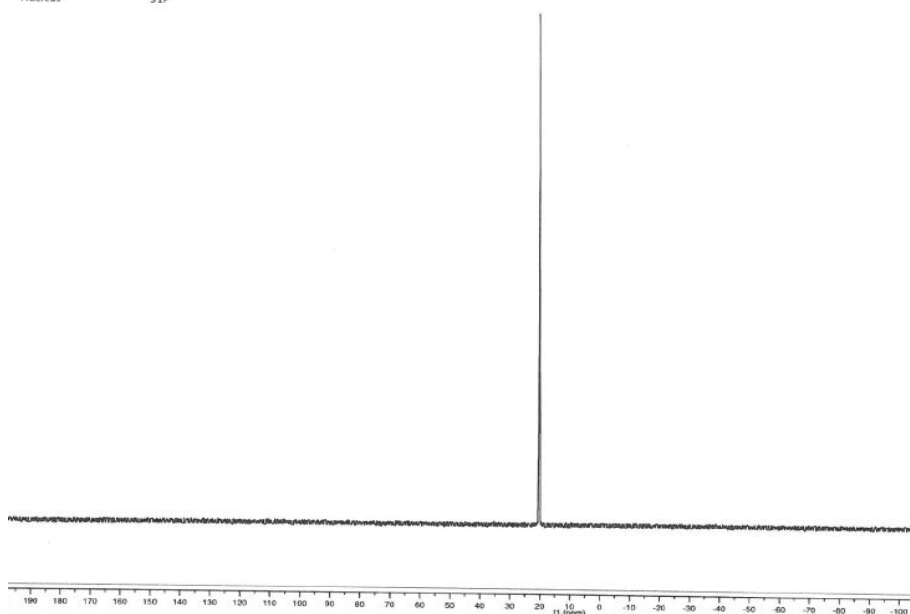


Integration Results						
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.
1	Component 1	2.747	57.007	1511.888	100.00	100.00
						Amount
						n.a.

(S)-4-(2,6-diamino-9H-purin-9-yl)-2-hydroxybutyl phosphonic acid (S)-6



Title pdata/ 1
 Comment BG 3.146 Na+
 P31dec1H-SI D2O / opt/ topspin cp 21
 Solvent D2O
 Number of Scans 128
 Spectrometer Frequency 121.49
 Nucleus 31P



Elemental Composition Report

Page 1

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 = 4

Monoisotopic Mass, Odd and Even Electron Ions

472 formula(e) evaluated with 1 results within limits (up to 20 closest results for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-50 O: 0-50 P: 1-1

SYNAPT G2-S#NotSet

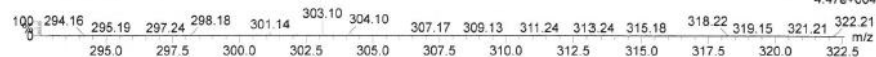
BQ3.146

24-Sep-2014

1: TOF MS ES+

4.47e+004

Y-CP14092401 17 (0.329)



Minimum:

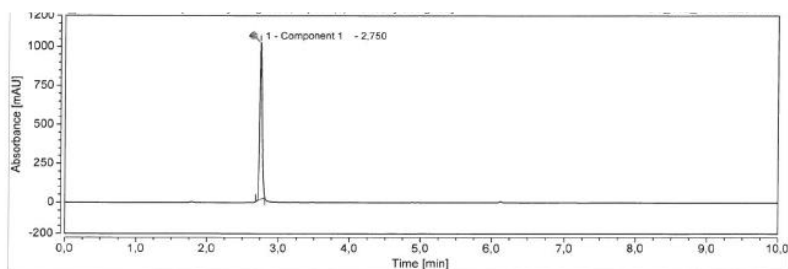
-1.5

Maximum:

1.0 1.0 50.0

Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(%) Formula

303.0971 303.0971 0.0 0.0 5.5 2146.2 n/a n/a C9 H16 N6 O4 P

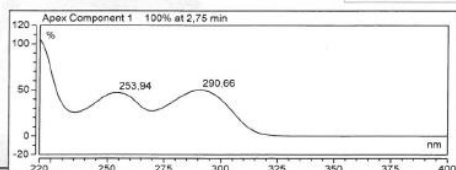


Spectral plot could not be created.

No spectra selected.

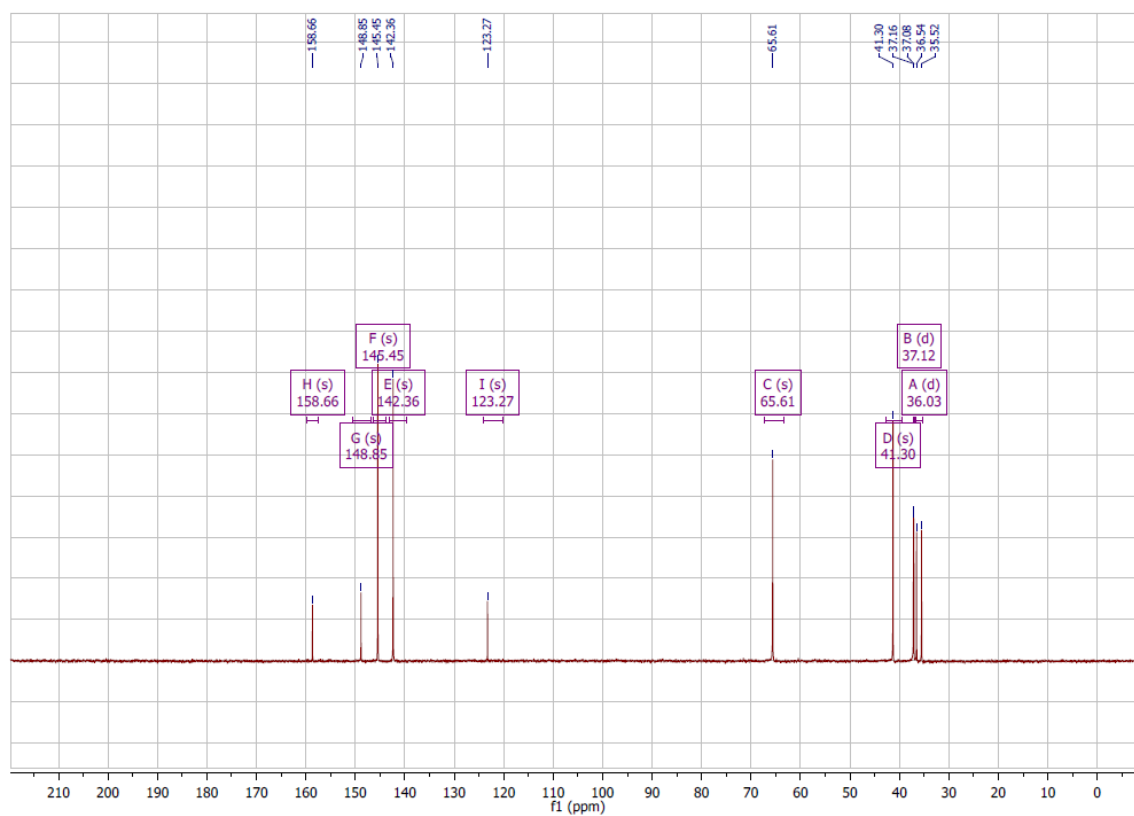
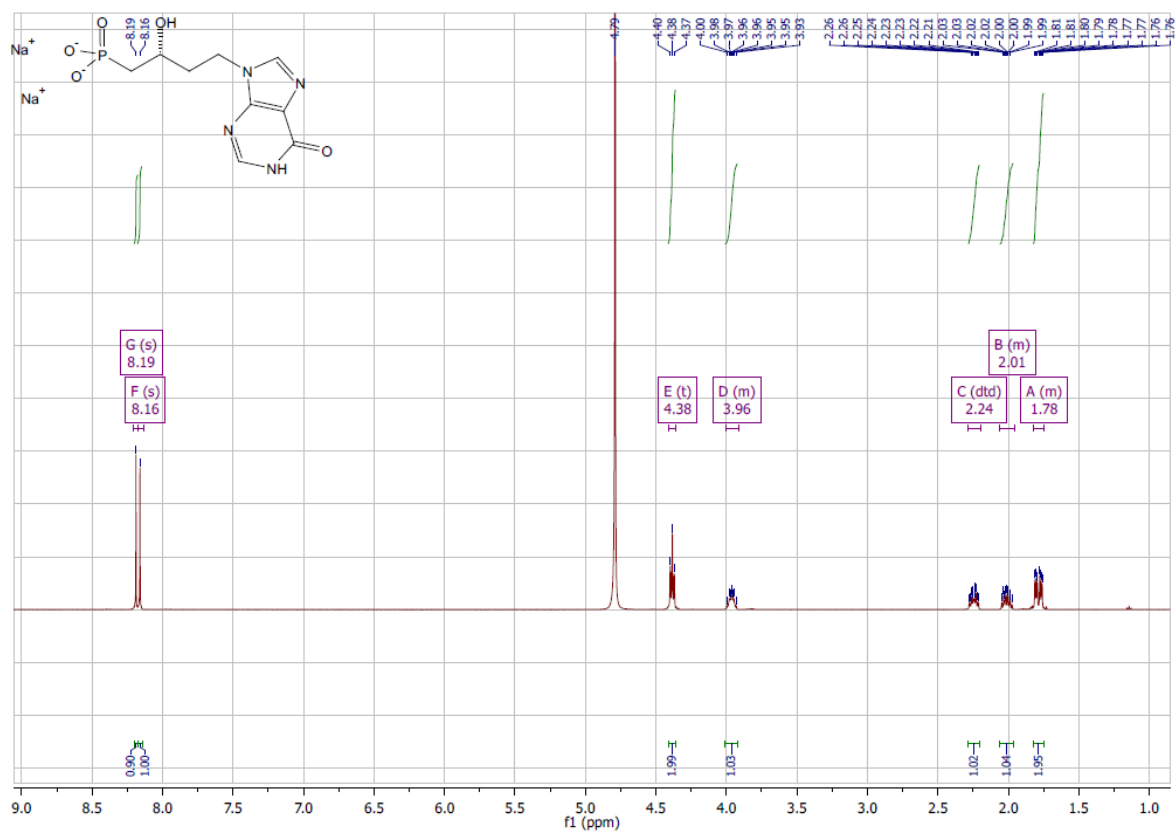
Spectral plot could not be created.

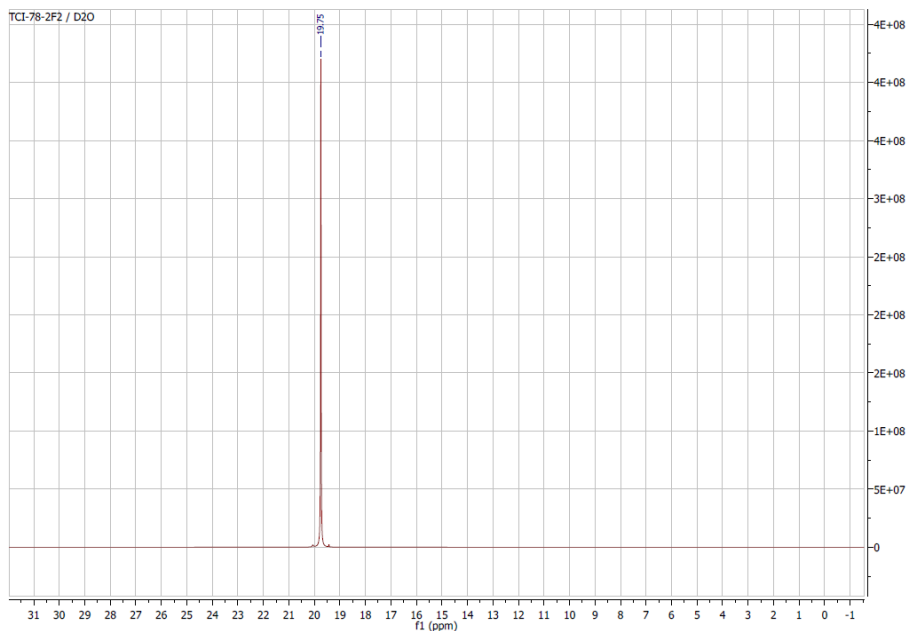
No spectra selected.



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
n.a.	Component 2	n.a.	n.a.	n.a.	n.a.	n.a.	n.a.
1	Component 1	2.750	35,985	1007,402	100,00	100,00	n.a.

(R)-(2-hydroxy-4-(6-oxo-1,6-dihydro-9H-purin-9-yl)butyl)phosphonic acid disodic salt (R)-7





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 PPM / DBE: min = -10.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1299 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-100 H: 0-100 N: 0-20 O: 0-20 Na: 0-2 P: 1-1

SYNAPT G2-SiUEB205

Y-CP17040502 3 (0.161) Cm (3.4)

TCI-78-2f2

05-Apr-2017

1: TOF MS ES-

2.36e+005



Minimum:

Maximum:

10.0

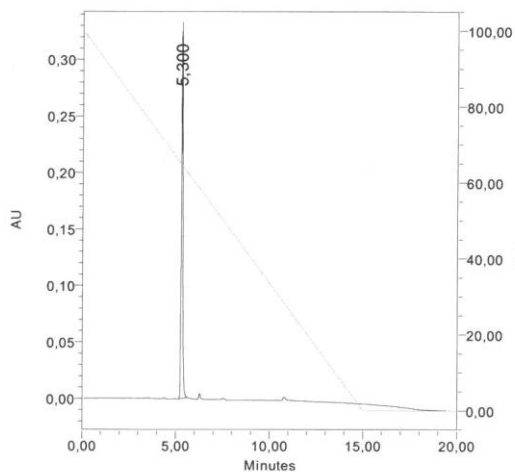
1.0

-10.0

100.0

Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(%) Formula

287.0547 287.0545 0.2 0.7 6.5 1018.4 n/a n/a C⁹ H¹² N⁴ O⁵ P



Acq Method Set grad 20mn T3

Processing Method grad 20mn T3

SampleName: tc1-78-2f2 dowex

Lambda Extract Wvln Ch1

Injection Volume 3.00 ul

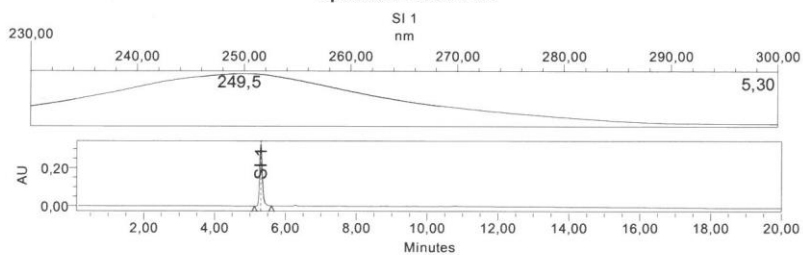
Vial 74

Run Time 20.0 Minutes

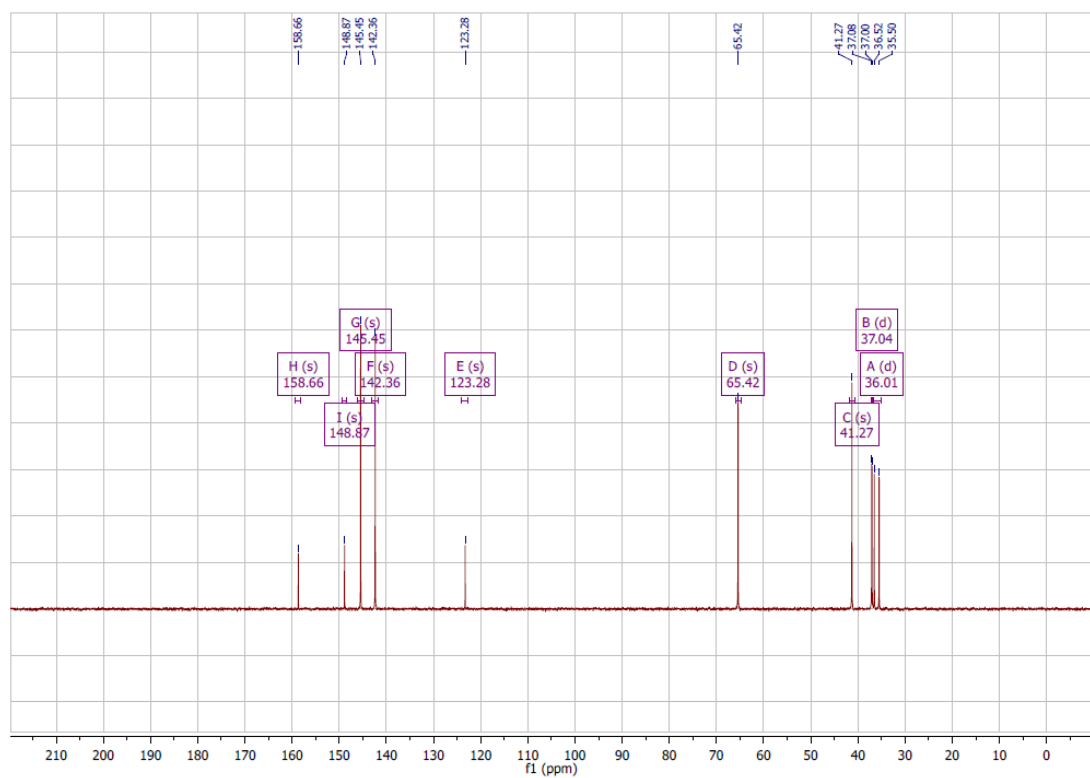
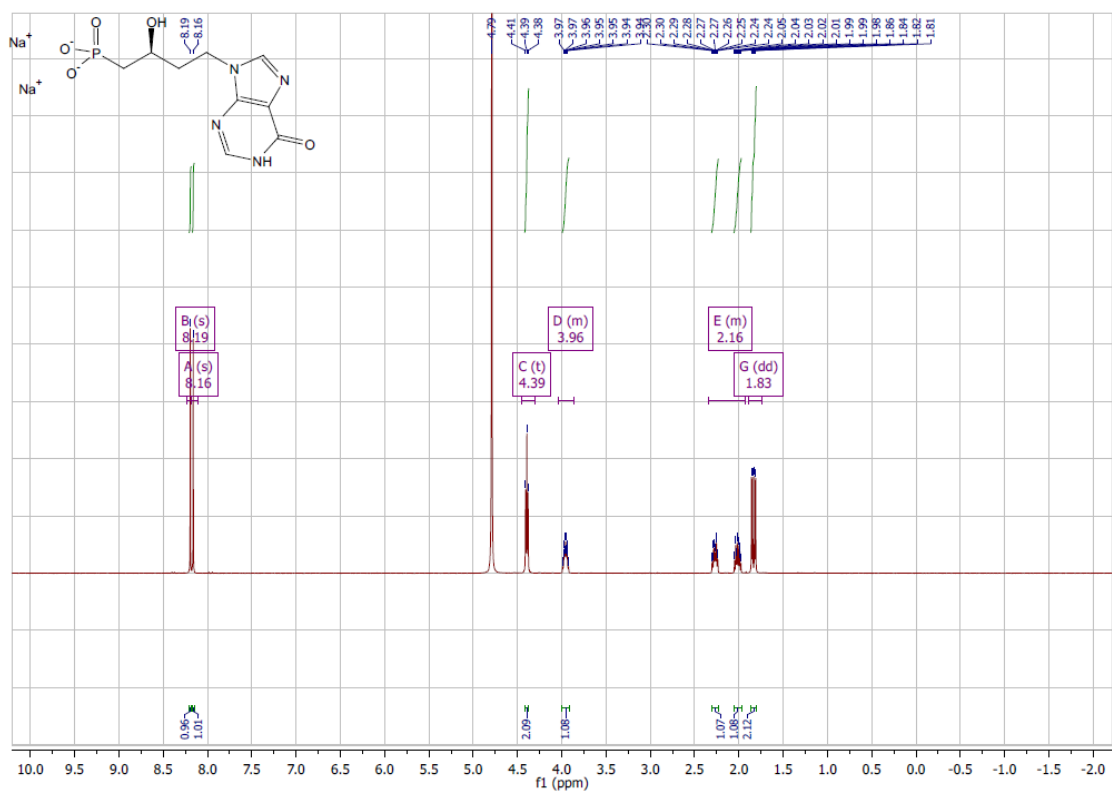
Processed Results

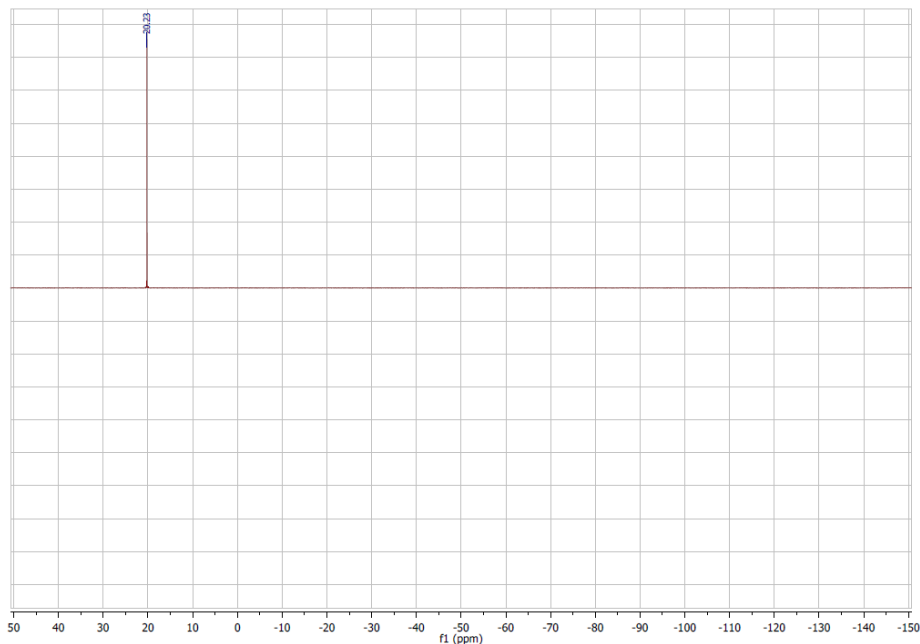
RT	Area	% Area	Height	% Height
1 5.3	1821874	100.0	325350	100.00

Spectrum Index Plot



(S)-(2-hydroxy-4-(6-oxo-1,6-dihydro-9H-purin-9-yl)butyl) phosphonic acid disodic salt (S)-7





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -10.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

548 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

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

SYNAPT G2-S#UEB205

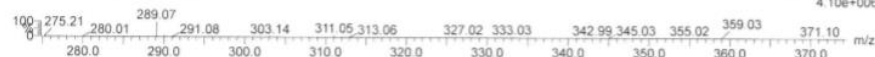
Y-JM17032901 3 (0.141) Cm (3)

TCI-72F1

29-Mar-2017

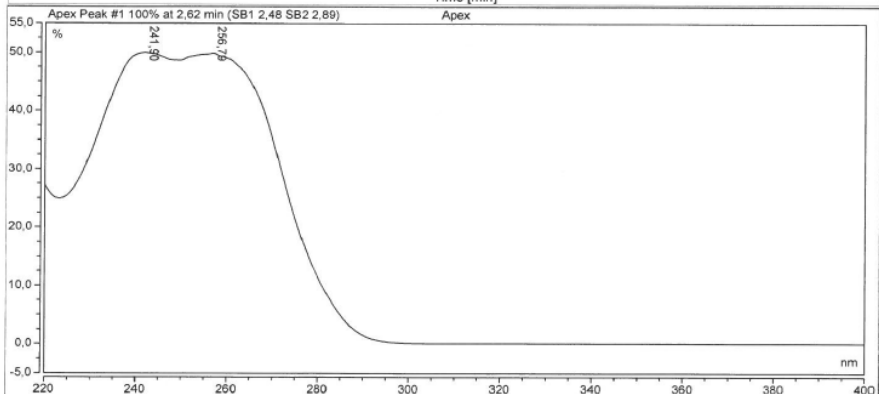
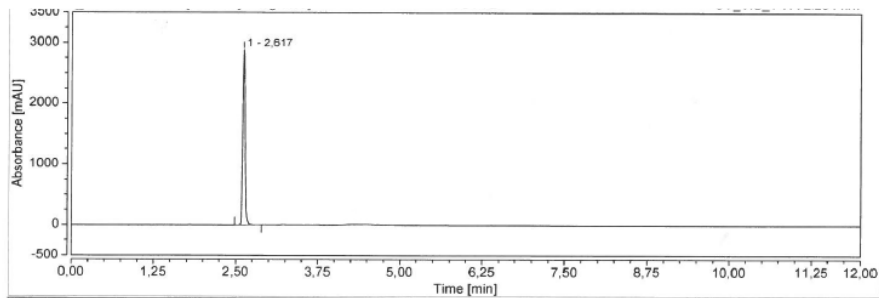
1: TOF MS ES+

4.10e+006



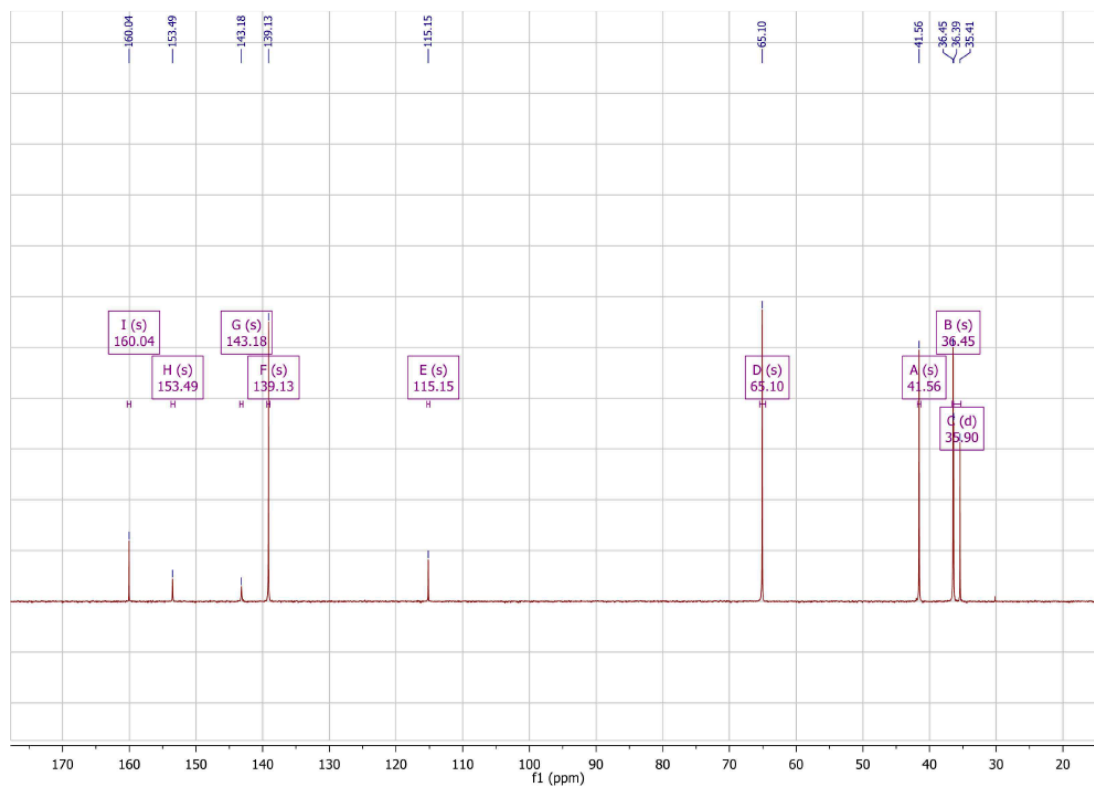
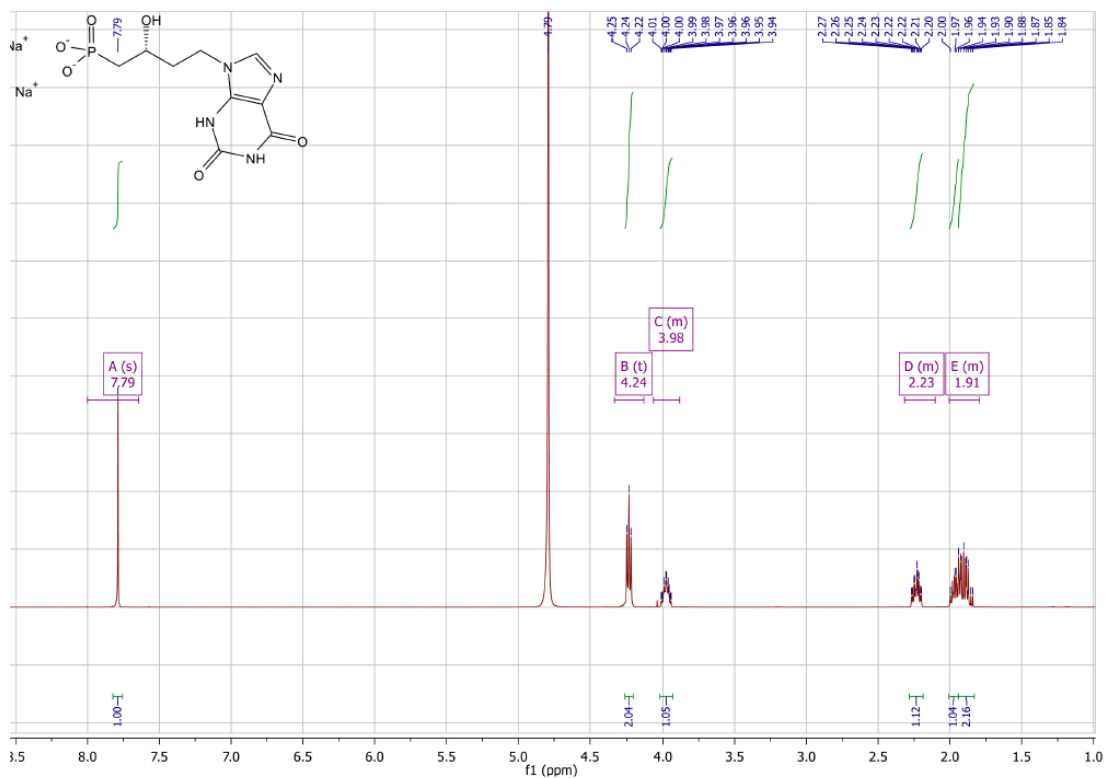
Minimum: -10.0
Maximum: 1.0 1.0 100.0

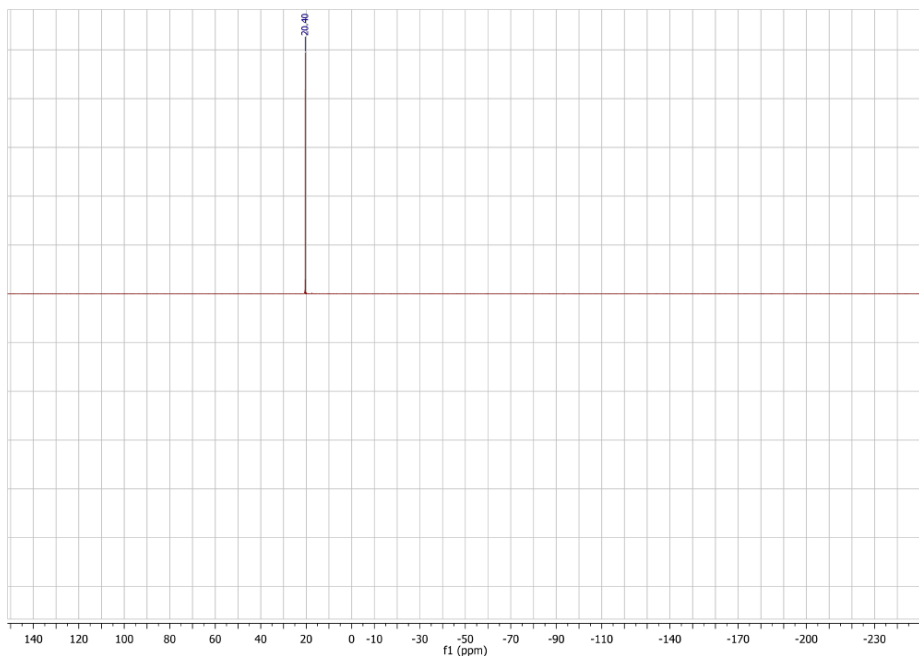
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
289.0703	289.0702	0.1	0.3	5.5	1988.3	n/a	n/a	C9 H14 N4 O5 P



No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		2.617	127.623	2885.441	100.00	100.00	n.a.

(R)-(4-(2,6-dioxo-1,2,3,6-tetrahydro-9H-purin-9-yl)-2-hydroxybutyl)phosphonic acid disodic salt (R)-8





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -10.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

642 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20 P: 1-1 Na: 2-2

SYNAPT G2-S#UEB205

TCI-67

10-Mar-2017

Y-CP17031001 4 (0.175) Cm (4.5-(1.2+8.11))

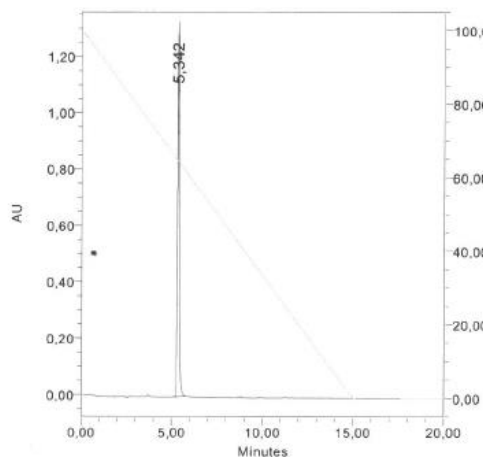
1: TOF MS ES+

1.35e+006



Minimum: -10.0
Maximum: 1.0 1.0 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
349.0289	349.0290	-0.1	-0.3	5.5	890.7	n/a	n/a	C9 H12 N4 O6 F Na2



Acq Method Set grad 20mn T3

Processing Method grad 20mn T3

SampleName: tc1-67f3c

Lambda Extract Wvln Ch1

Injection Volume 10.00 ul

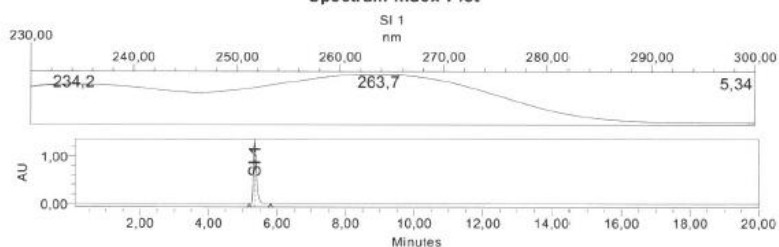
Vial 44

Run Time 20.0 Minutes

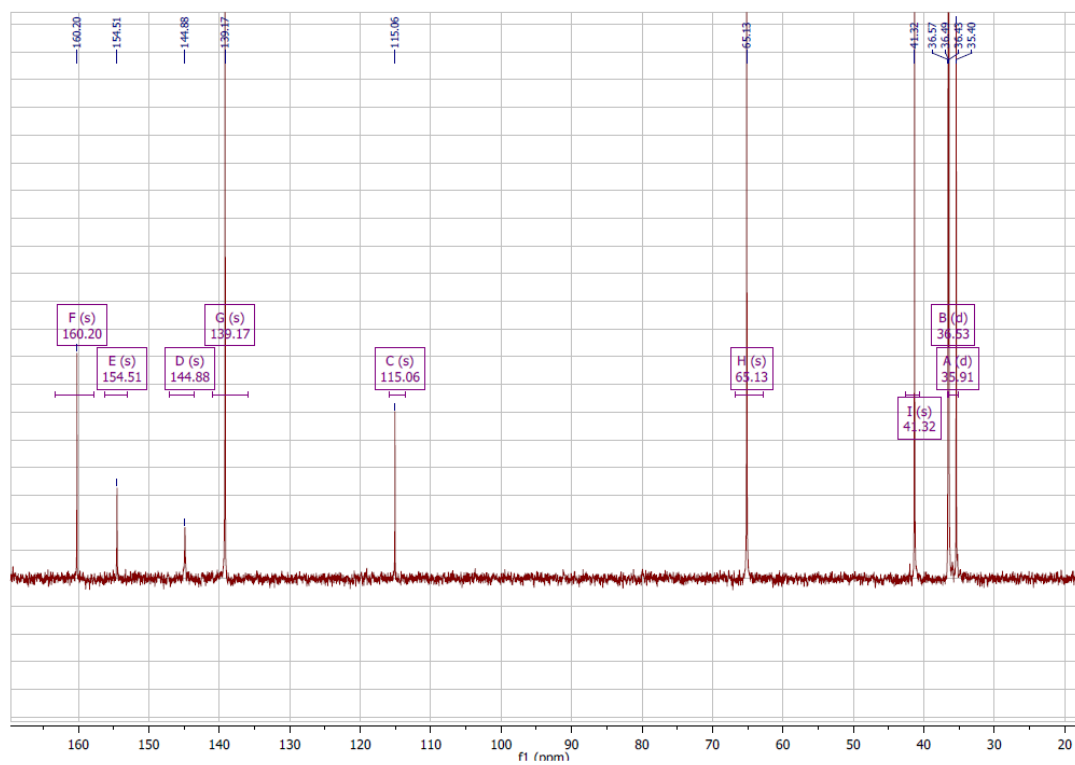
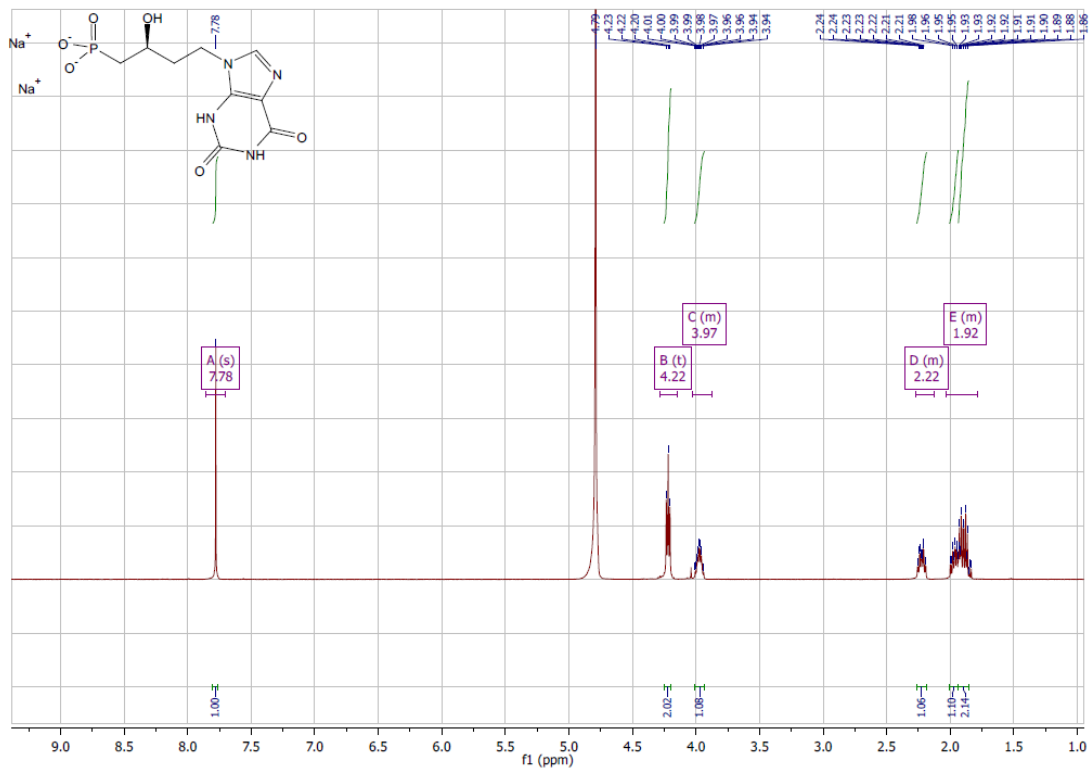
Processed Results

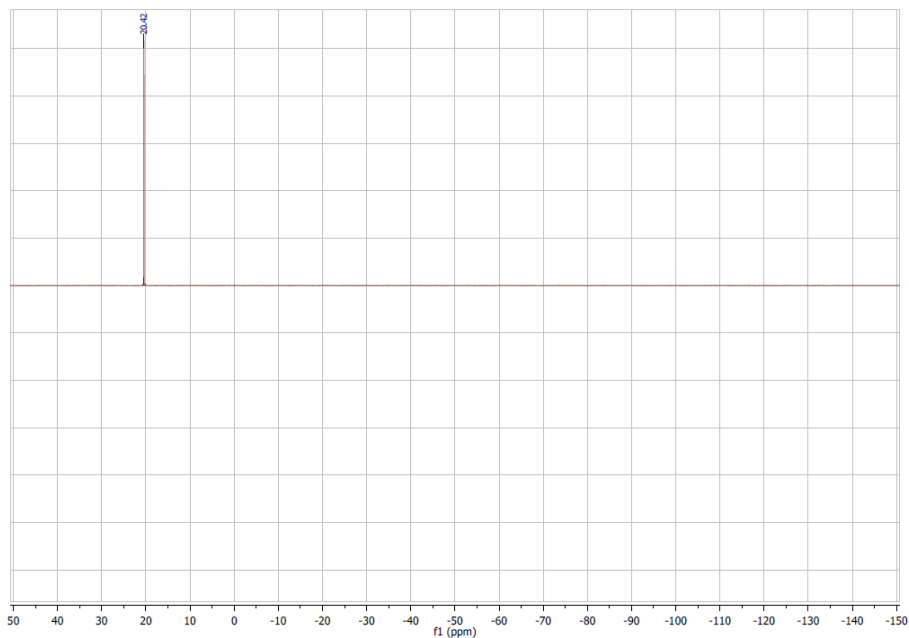
RT	Area	% Area	Height	% Height
1 5.3	8233273	100.0	1298974	100.00

Spectrum Index Plot



(S)-(4-(2,6-dioxo-1,2,3,6-tetrahydro-9H-purin-9-yl)-2-hydroxybutyl)phosphonic acid disodium salt (S)-8





Final Composition Report

Page 1

Mass Analysis

Mass = 1.0 mDa / DBE: min = -10.0, max = 100.0

Isotope prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

05 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:

C: 1-100 H: 0-100 N: 0-20 O: 0-20 Na: 2-2 P: 1-1

SYNAPT G2-S#UEB205

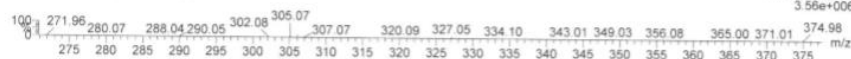
TCI-70-2 F3

Y-CP17033101 3 (0.141) Cm (3)

31-Mar-2017

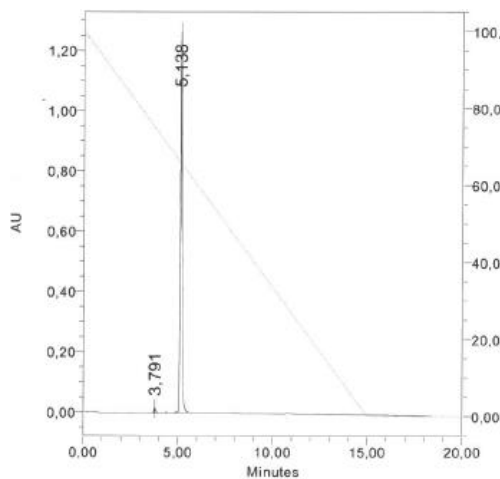
1: TOF MS ES+

3.56e+006



Minimum: -10.0
Maximum: 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
349.0291	349.0290	0.1	0.3	5.5	948.0	n/a	n/a	C9 H12 N4 O6 Na2 P



Acq Method Set grad 20mn T3

Processing Method grad 20mn T3

SampleName: tc1-70-2f3b

Lambda Extract Wvin Ch1

Injection Volume 2.00 ul

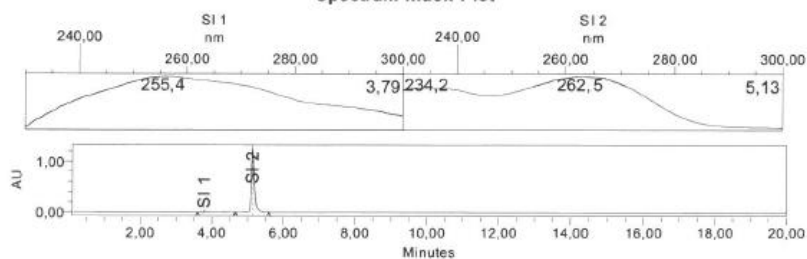
Vial 10

Run Time 20.0 Minutes

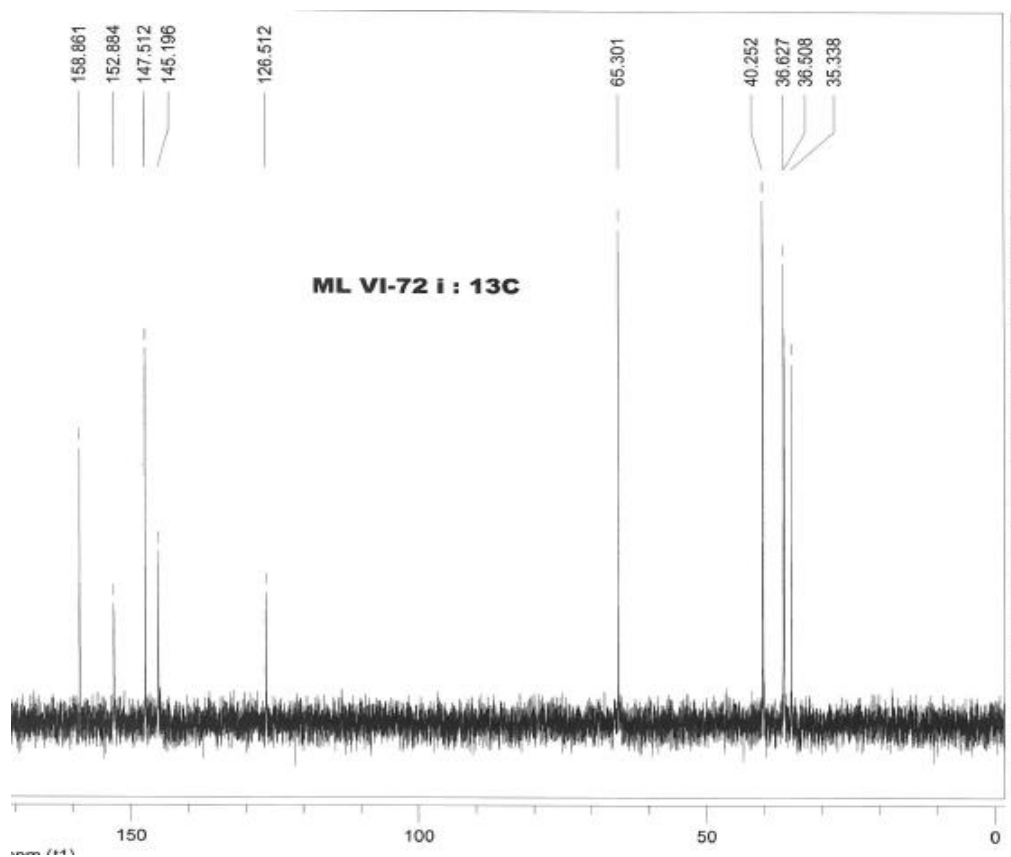
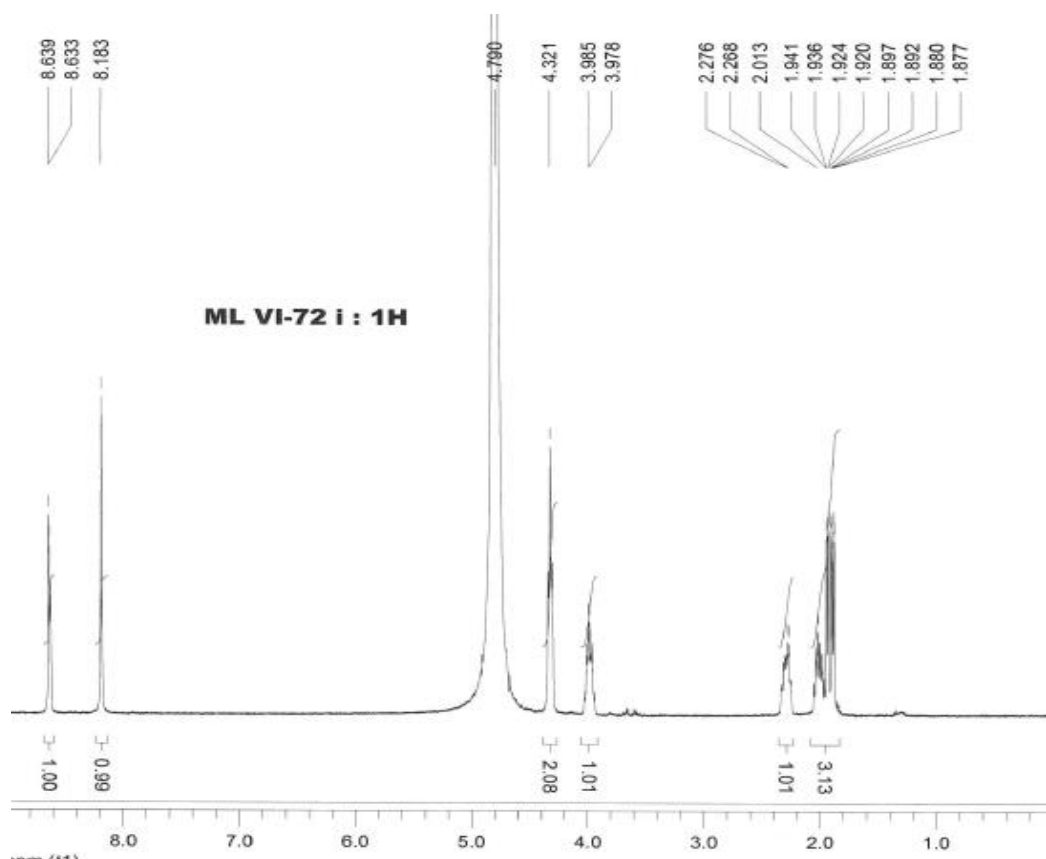
Processed Results

RT	Area	% Area	Height	% Height
1 3.8	147006	1.8	15220	1.18
2 5.1	7873144	98.2	1274073	98.82

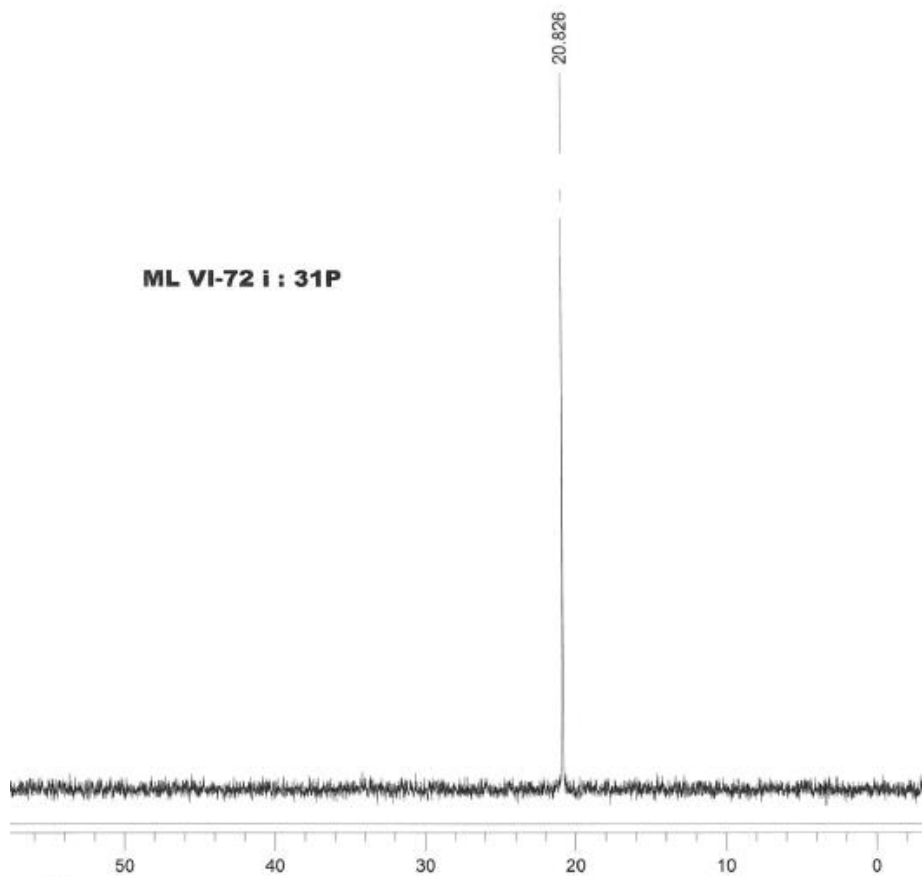
Spectrum Index Plot



(R)-(4-(2-amino-9H-purin-9-yl)-2-hydroxybutyl) phosphonic acid (R)-9



ML VI-72 i : 31P



Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 3.0 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

917 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

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

SYNAPT G2-SNUEB205

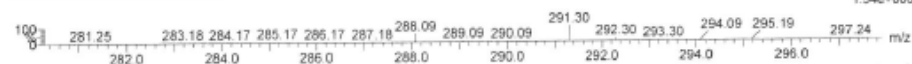
Y-SP18030601 9 (0.403) Cm (4.9)

ML VI 72i

06-Mar-2018

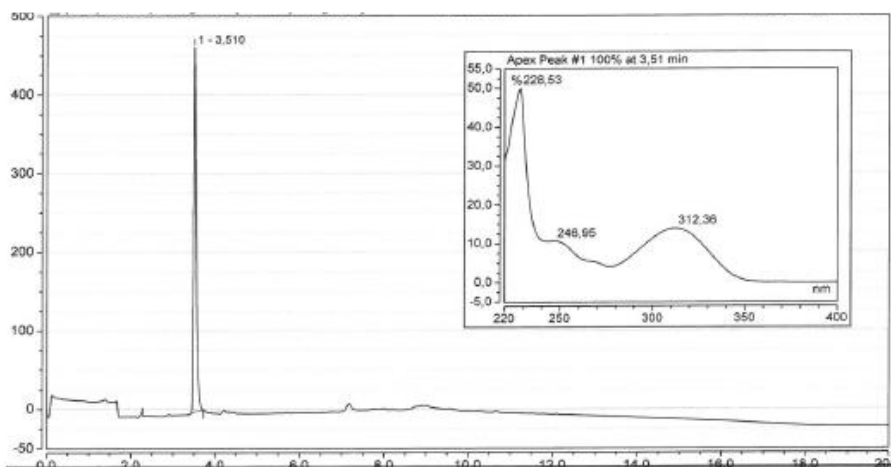
1: TOF MS ES+

1.54e+006



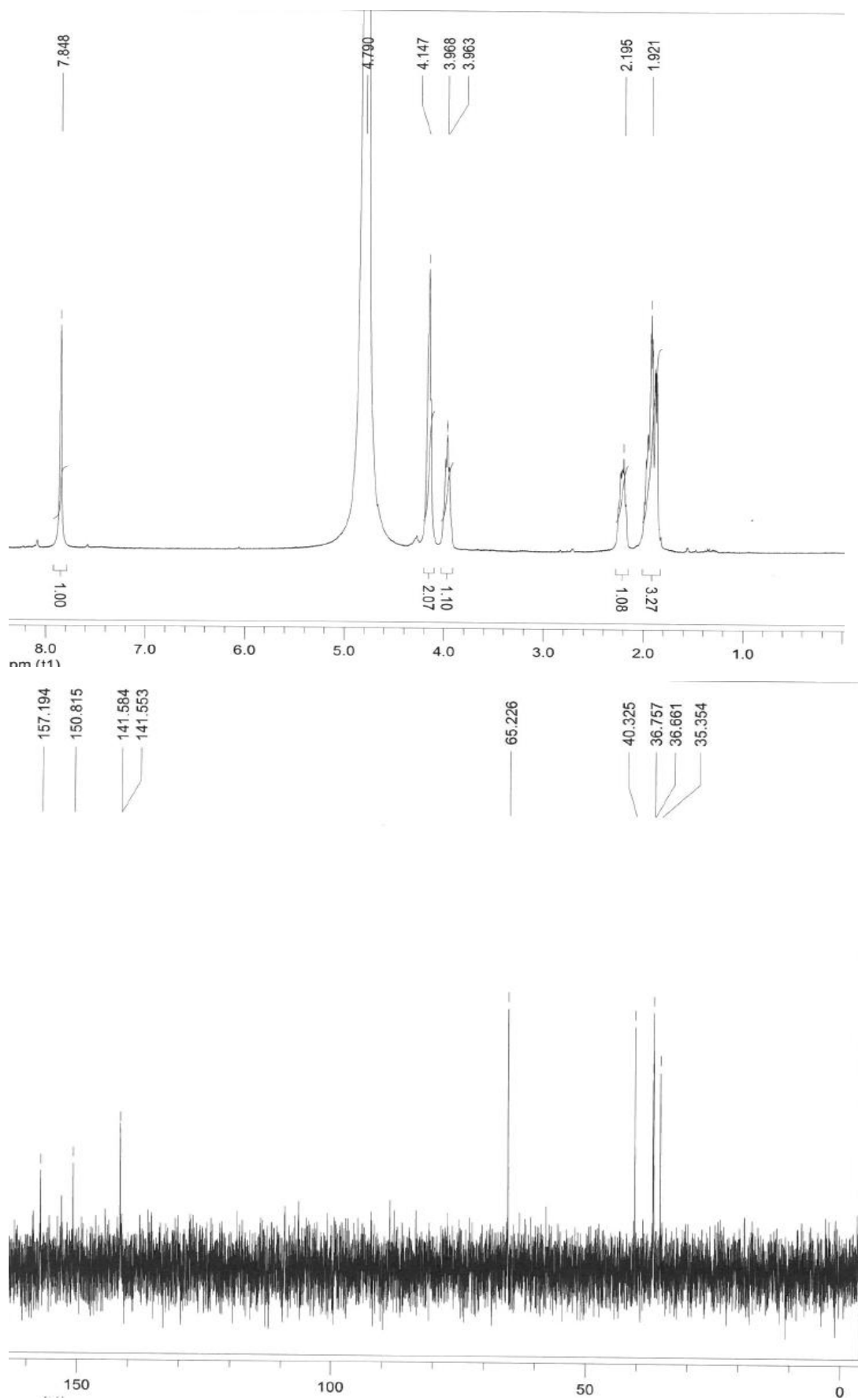
Minimum: -1.5
Maximum: 50.0

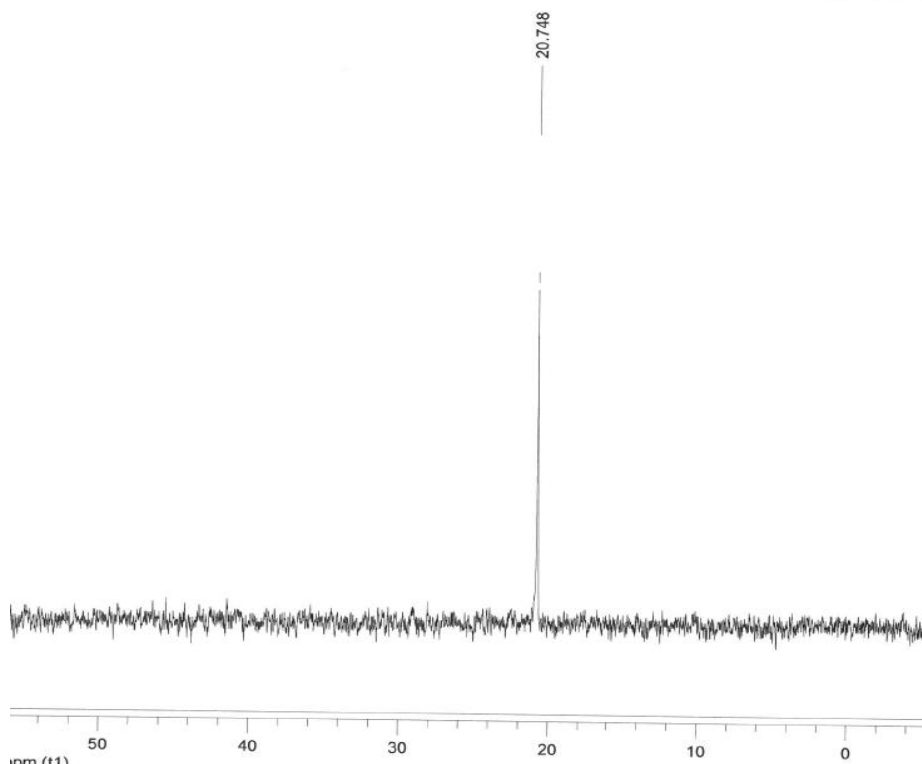
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
288.0861	288.0862	-0.1	-0.3	5.5	1706.2	n/a	n/a	C9 H15 N5 O4 P



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		3.510	32.385	463.771	100.00	100.00	n.a.

(R)-(4-(6-amino-2-fluoro-9H-purin-9-yl)-2-hydroxybutyl) phosphonic acid (R)-10





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1384 formula(e) evaluated with 5 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-10 O: 0-10 F: 0-1 P: 0-1

SYNAPT G2-S#UEB205

Y-CP17100602 4 (0.175)

ML VI-61 i

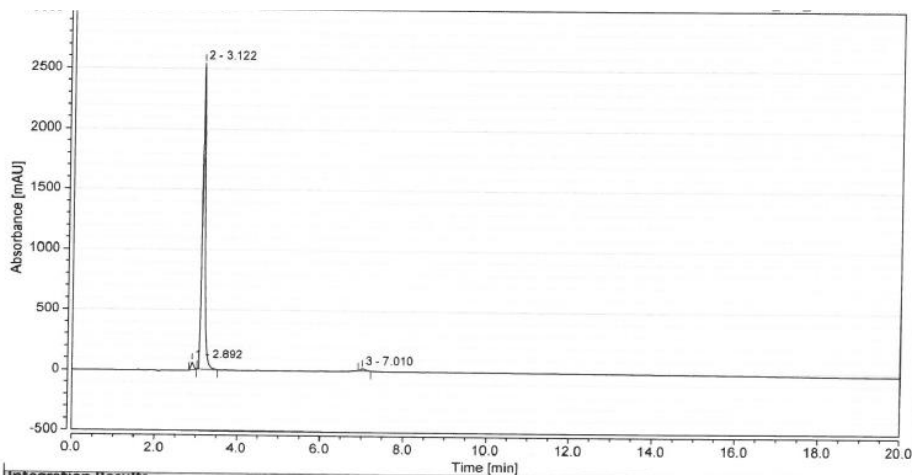
1: TOF MS ES+

3.98e+006



Minimum: -1.5
Maximum: 50.0

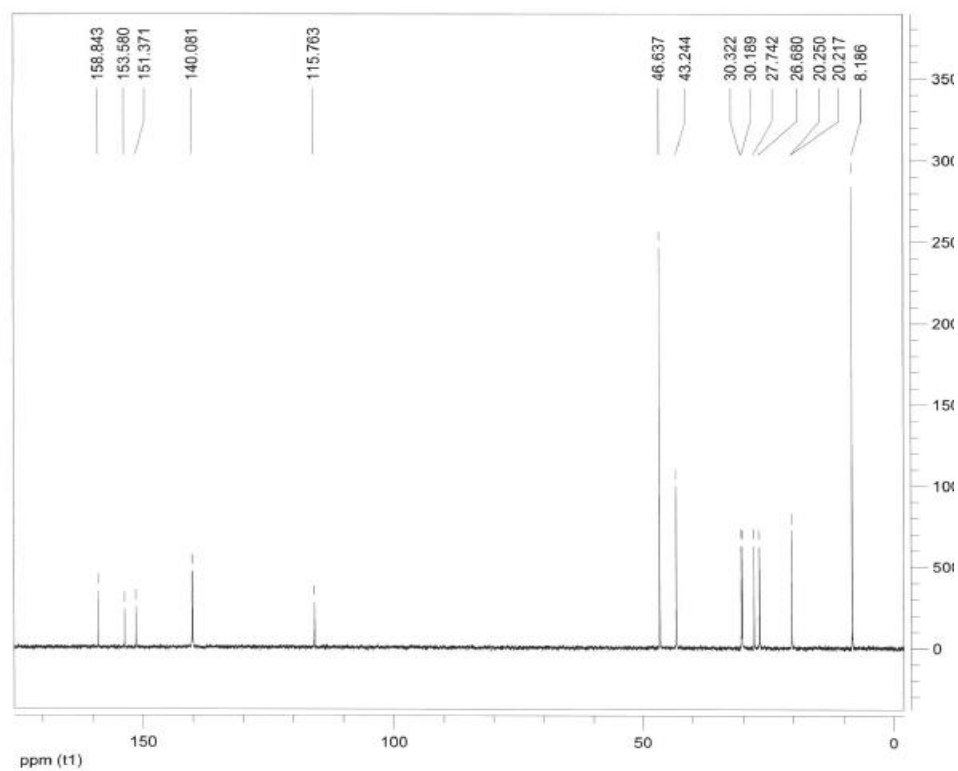
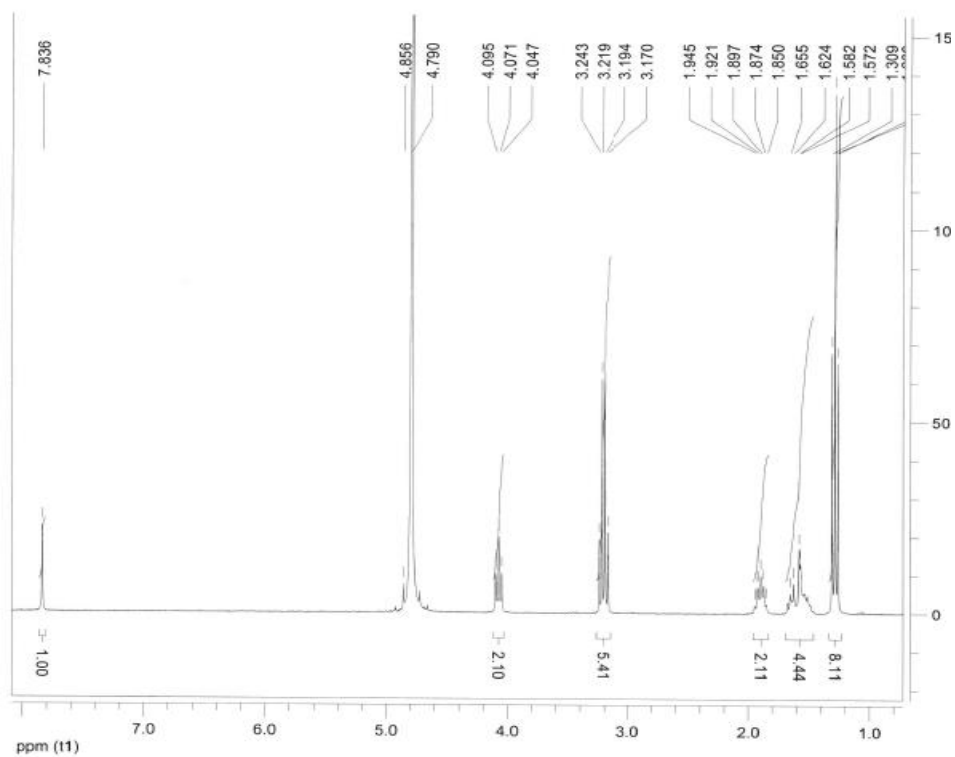
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
304.0815	304.0806	0.9	3.0	6.5	2217.8	0.947	38.79	C8 H11 N7 O5 F
	304.0822	-0.7	-2.3	1.5	2218.0	1.214	29.70	C6 H16 N5 O6 F P
	304.0811	0.4	1.3	5.5	2218.1	1.298	27.30	C9 H15 N5 O5 P
	304.0824	-0.9	-3.0	10.5	2220.2	3.369	3.44	C10 H11 N9 O P
	304.0821	-0.6	-2.0	9.5	2221.7	4.866	0.77	C15 H14 N O6

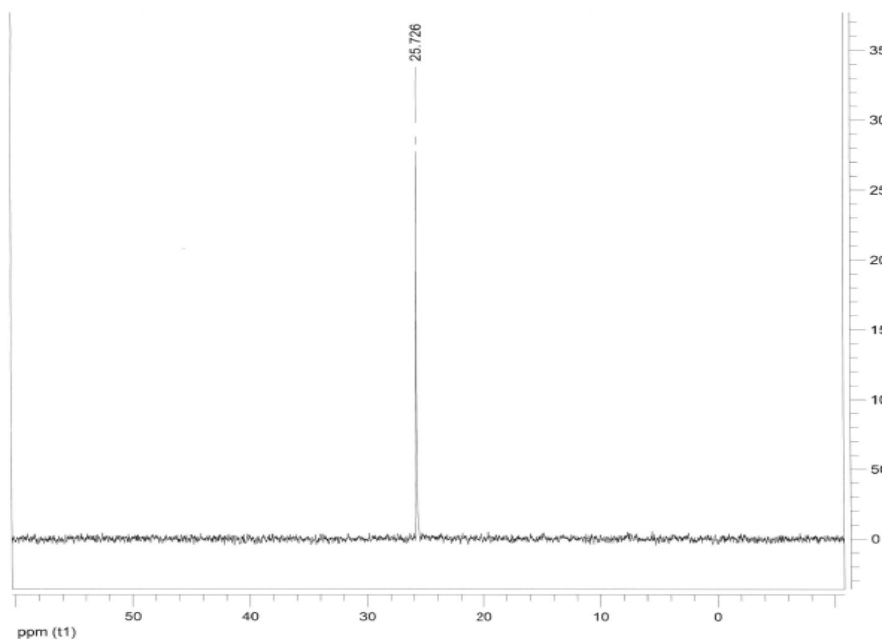


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		2.892	5.043	65.479	2.63	2.50	n.a.
2		3.122	184.044	2537.409	96.14	96.84	n.a.
3		7.010	2.345	17.254	1.23	0.66	n.a.

N-9-[4-phosphonic acid-butyl]guanine, 11a





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -10.0, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1337 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

Elements Used:

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

SYNAPT G2-S#UEB205

MLA V-38b

06-Jun-2017

Y-JV17060601 3 (0.141) Cm (3)

1: TOF MS ES+

2.42e+006



Minimum:

Maximum:

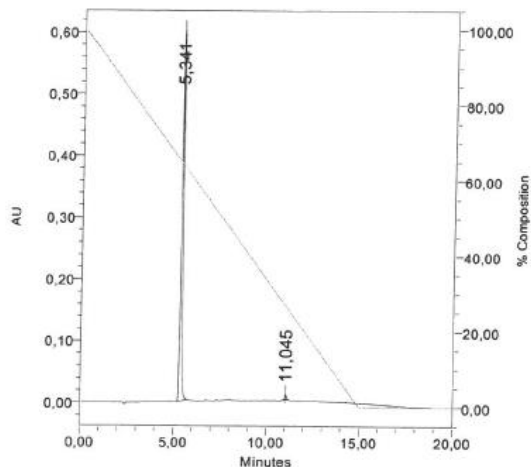
1.0 1.0

-10.0 100.0

Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(%) Formula

288.0864 288.0872 -0.8 -2.8 9.5 2110.7 0.000 99.99 C15 H14 N O5

288.0862 288.0862 0.2 0.7 5.5 2120.1 9.423 0.01 C9 H15 N5 O4 P



Acq Method Set grad 20mn T3

Processing Method grad 20mn T3

SampleName: ML V-38b

Lambda Extract Wvln Ch1

Injection Volume 50.00 ul

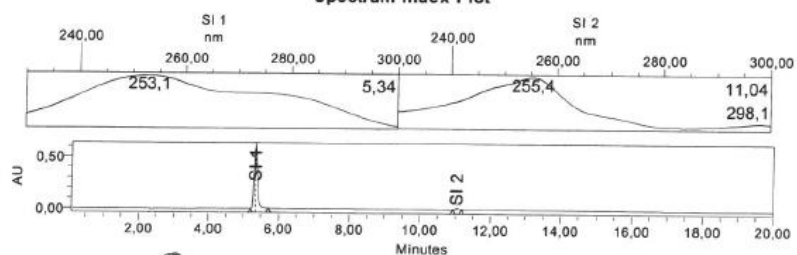
Vial 13

Run Time 20.0 Minutes

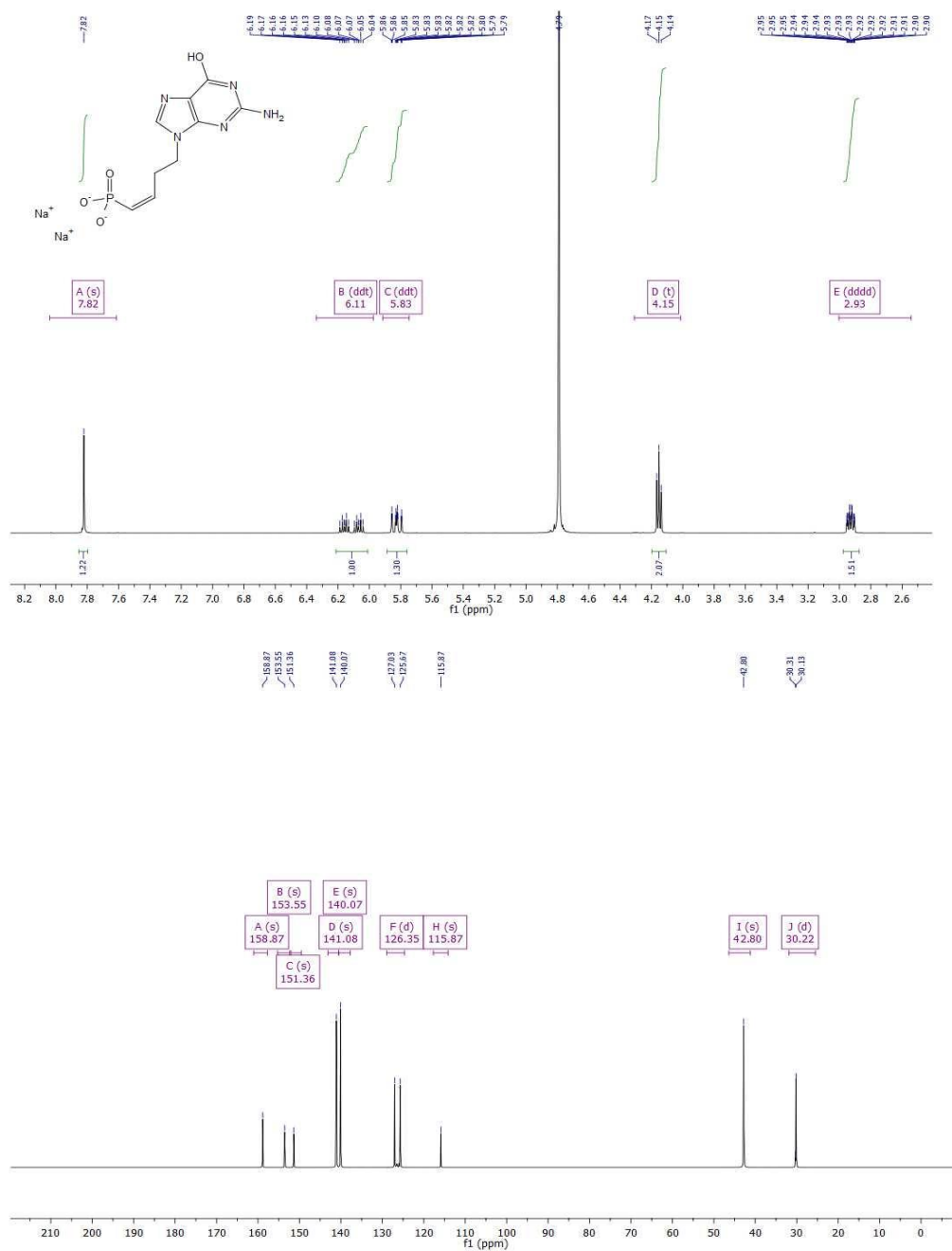
Processed Results

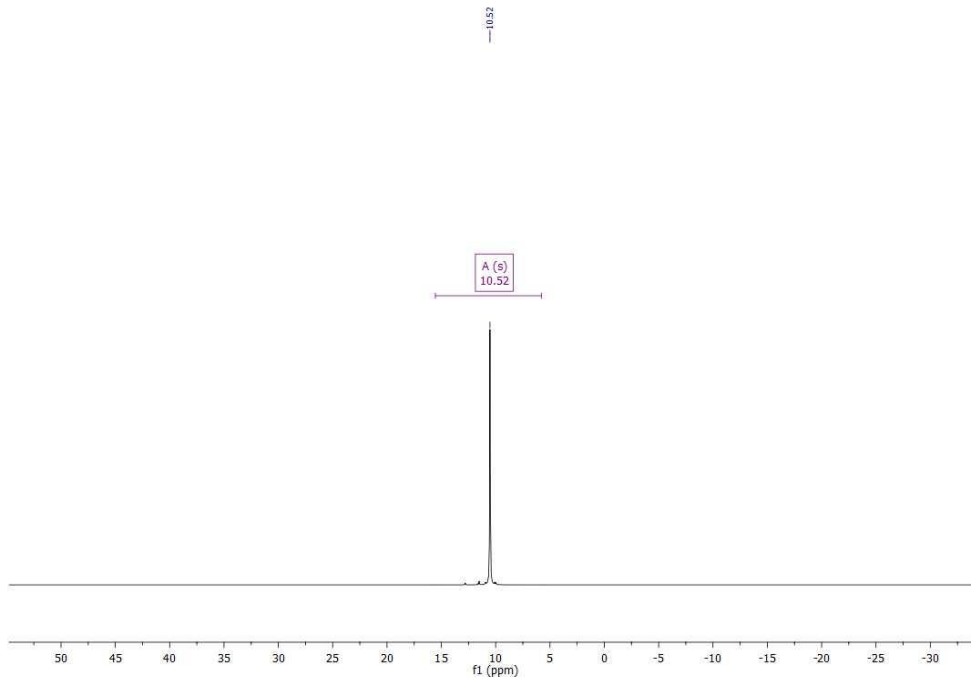
RT	Area	% Area	Height	% Height
1 5.3	3622707	98.3	601709	98.47
2 11.0	63879	1.7	9343	1.53

Spectrum Index Plot



(Z)-(4-(2-amino-6-hydroxy-9H-purin-9-yl)-but-1-en-1-yl)phosphonic acid disodic salt 11b





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 100.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

322 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

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

SYNAPT G2-SHUEB205
 Y-CP17120404 5 (0.228)

TC3-196-1F1

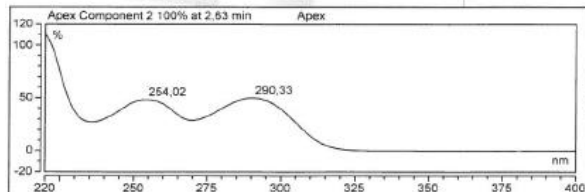
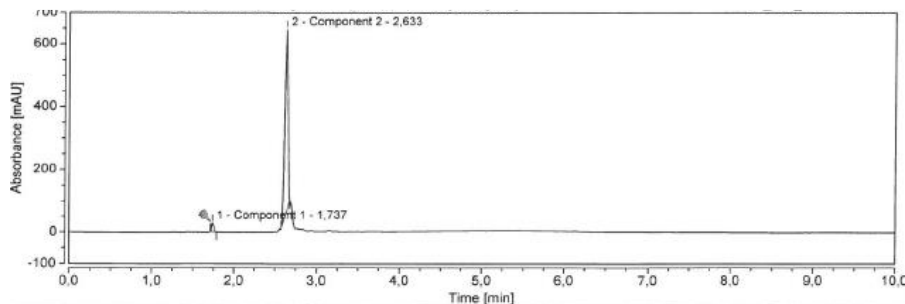
04-Dec-2017
 1: TOF MS ES+
 1.14e+005



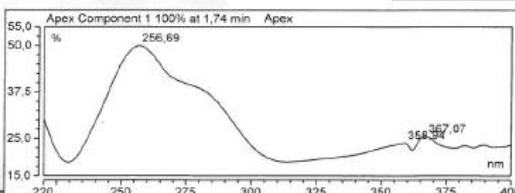
Minimum:

Maximum: 1.0 1.0 -1.5 100.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
286.0708	286.0705	0.3	1.0	6.5	1906.8	n/a	n/a	C9 H13 N5 O4 P



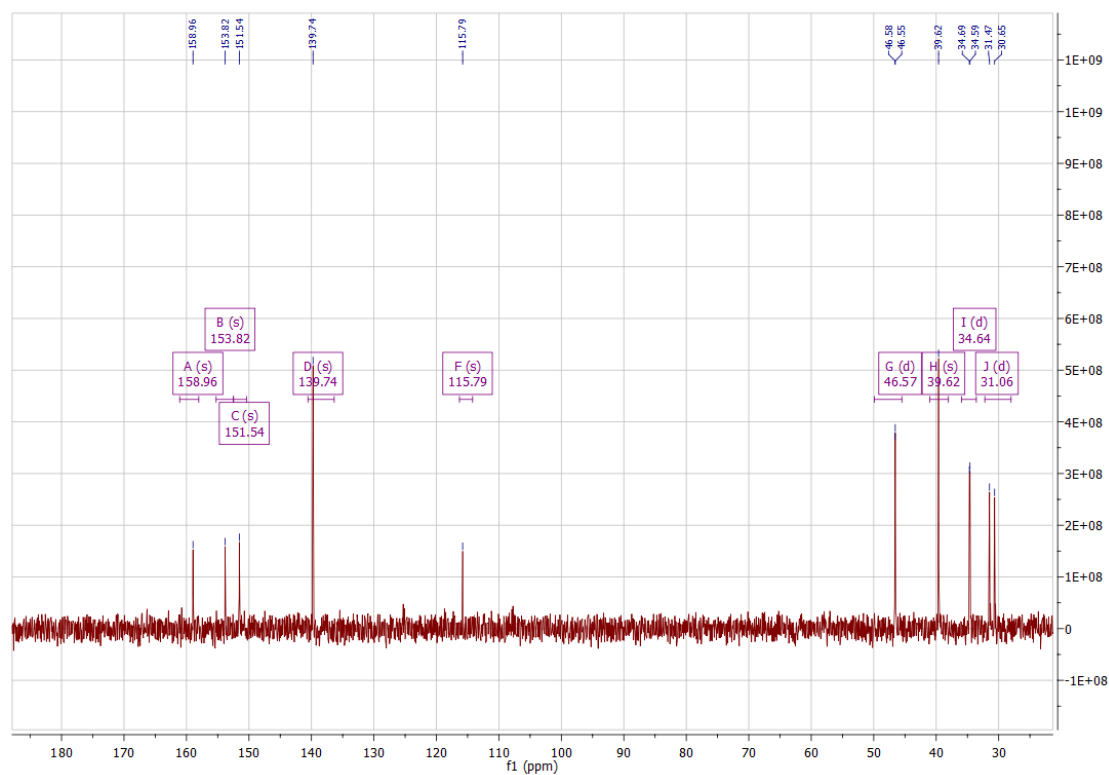
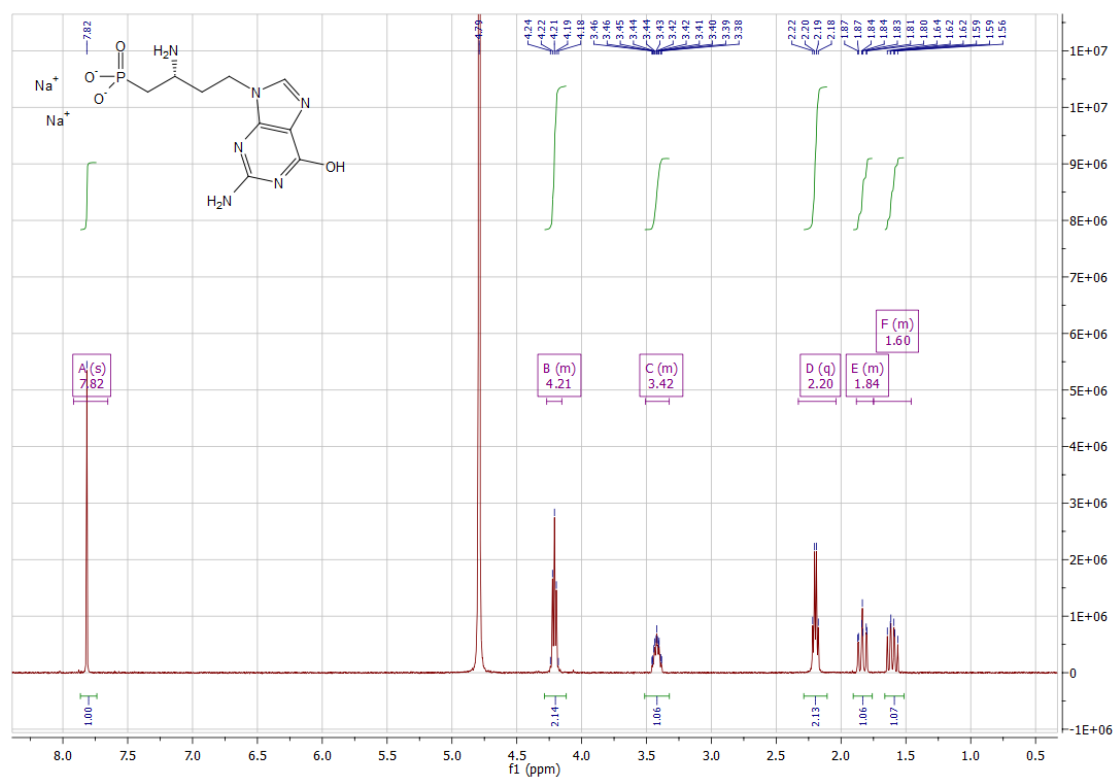
Spectral plot could not be created.
 No spectra selected.

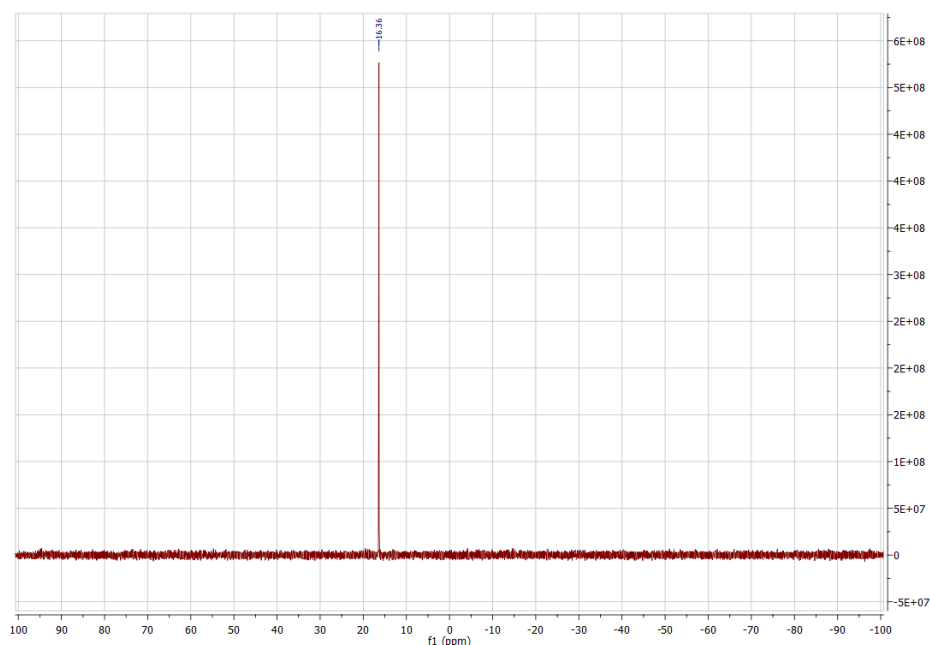


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1	Component 1	1.737	0.893	29.374	3.30	4.79	n.a.
2	Component 2	2.633	26.178	583.221	96.70	95.21	n.a.

(*R*)-(4-(2-amino-6-oxo-9*H*-purin-9-yl)-2-aminobutyl) phosphonic acid (*R*)-12





Initial Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.5 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

439 formula(e) evaluated with 3 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20 P: 1-1 Na: 2-2

SYNAPT G2-S#UEB205

TC3-241

01-Feb-2018

1: TOF MS ES+

3.02e+006



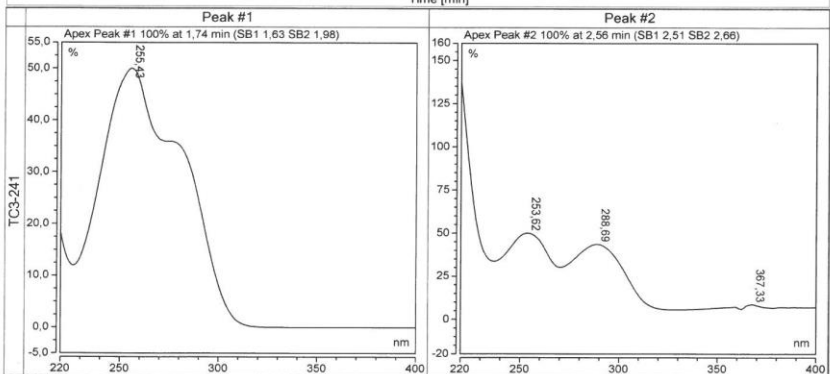
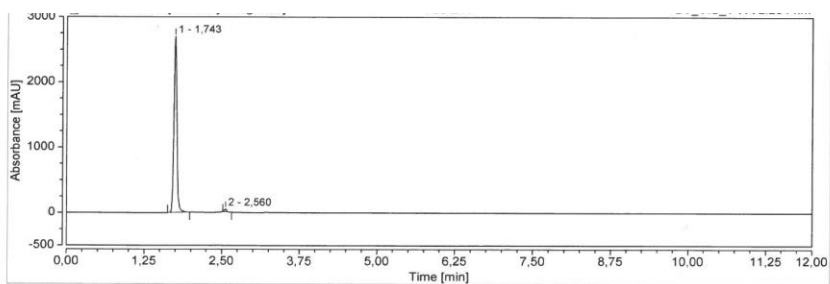
Minimum:

Maximum:

1.5 1.0 -1.5

100.0

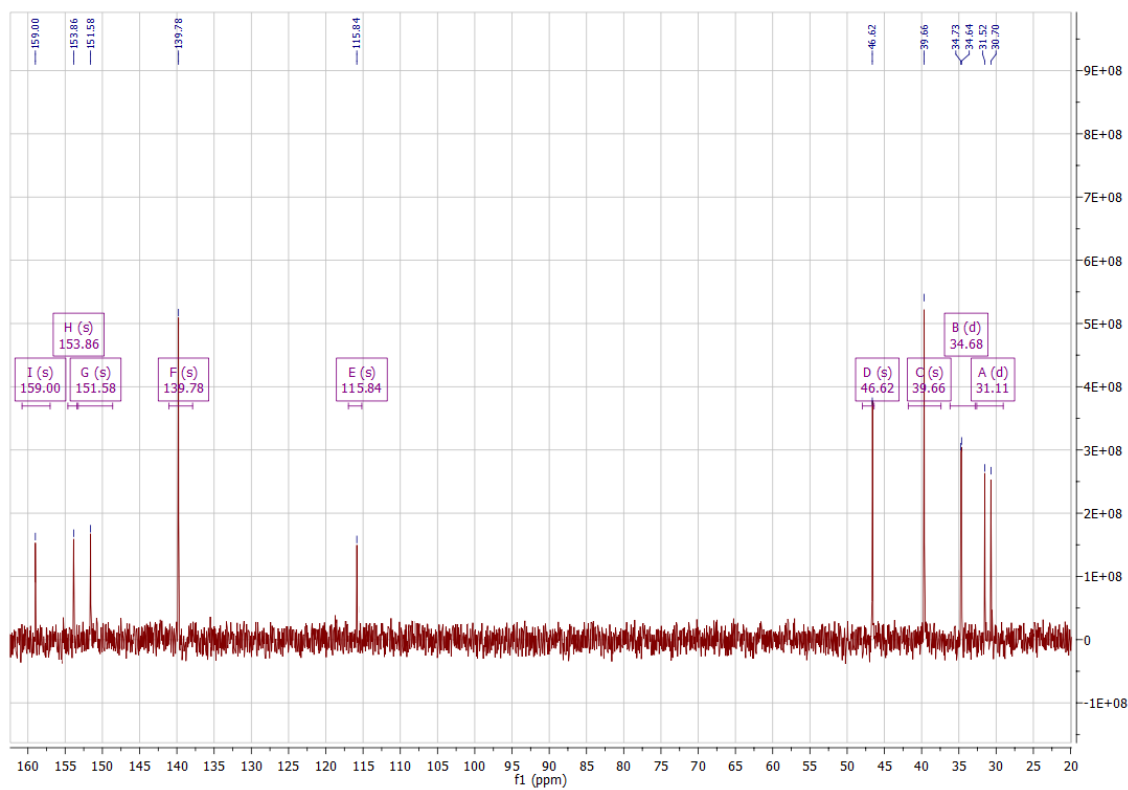
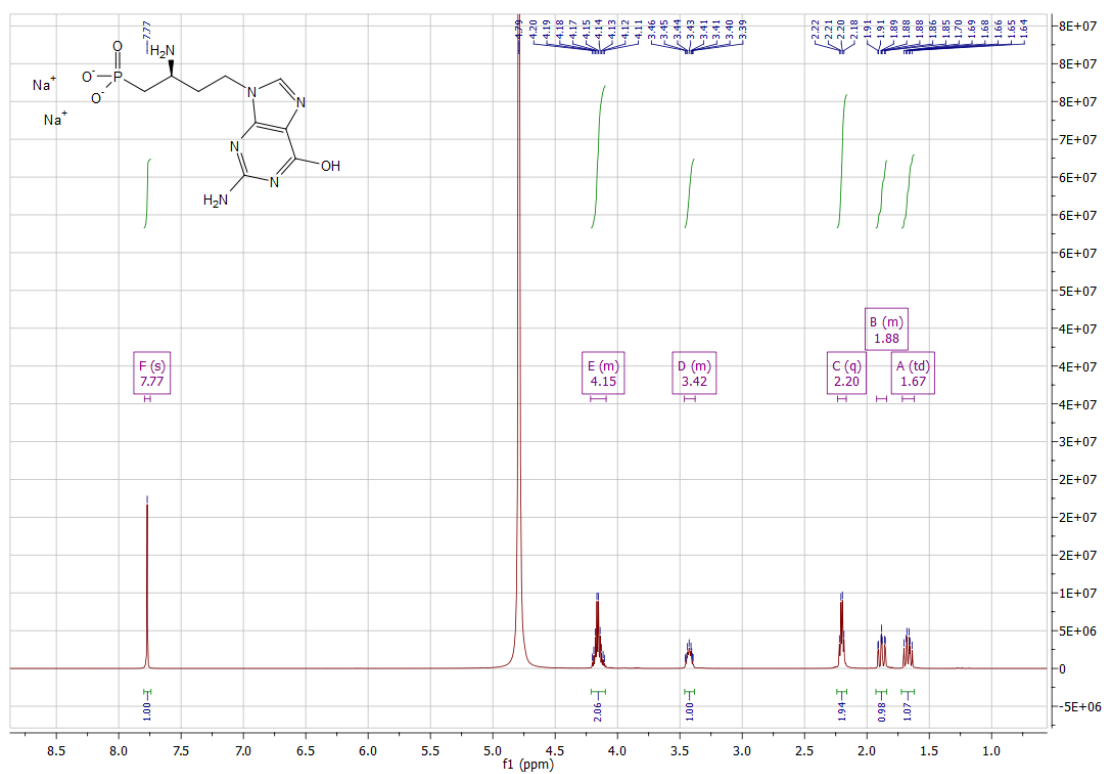
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
347.0611	347.0610	0.1	0.3	5.5	1077.2	0.000	99.97	C9 H14 N6 O4 P Na2
347.0596	347.0596	1.5	4.3	0.5	1085.5	8.303	0.02	C8 H18 N2 O8 P Na2
347.0623	347.0623	-1.2	-3.5	10.5	1086.8	9.682	0.01	C10 H10 N10 P Na2

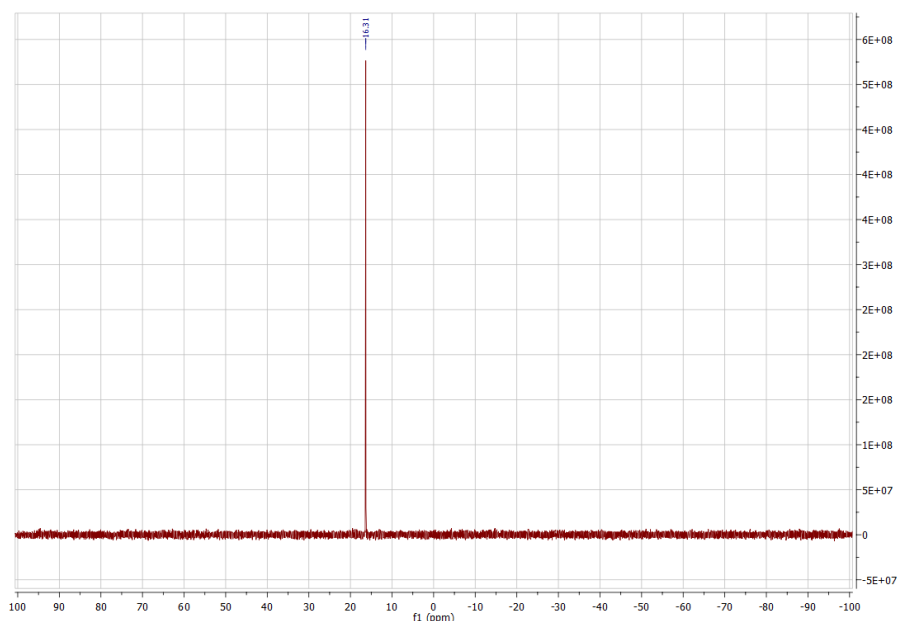


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		1.743	150,702	2700,527	98.87	98.37	n.a.
2		2.560	1,719	44,883	1.13	1.63	n.a.

(S)-(4-(2-amino-6-oxo-9H-purin-9-yl)-2-aminobutyl) phosphonic acid (S)-12





Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 1.0 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1693 formula(e) evaluated with 6 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20 Na: 0-2 P: 1-1

SYNAPT G2-S#UEB205

TC3-218

Y-NuEP18011702 11 (0.491) Cm (10:11)

17-Jan-2018

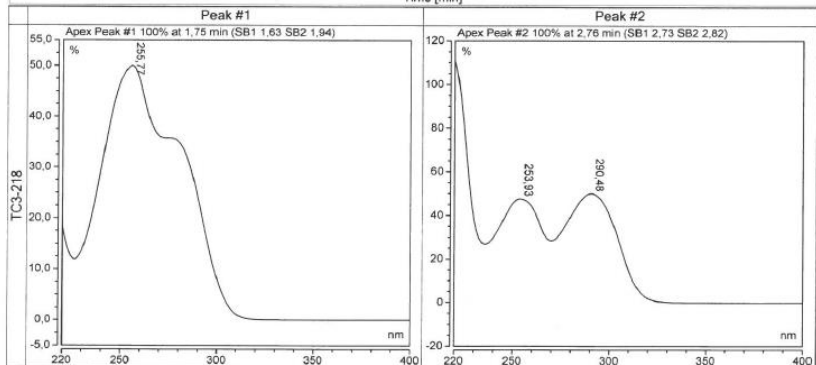
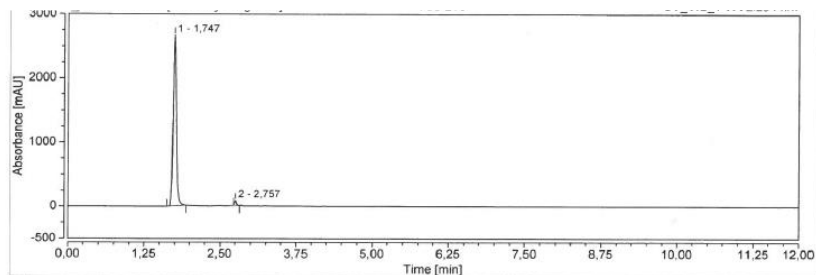
1: TOF MS ES+

1.03e+006



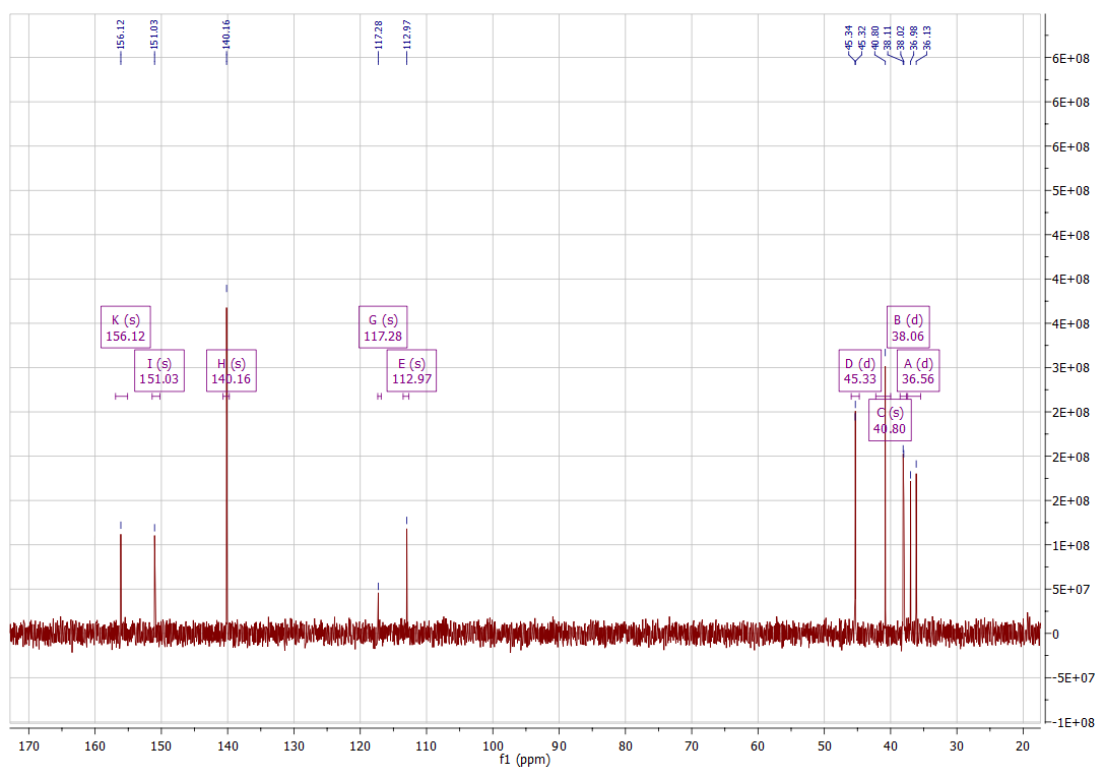
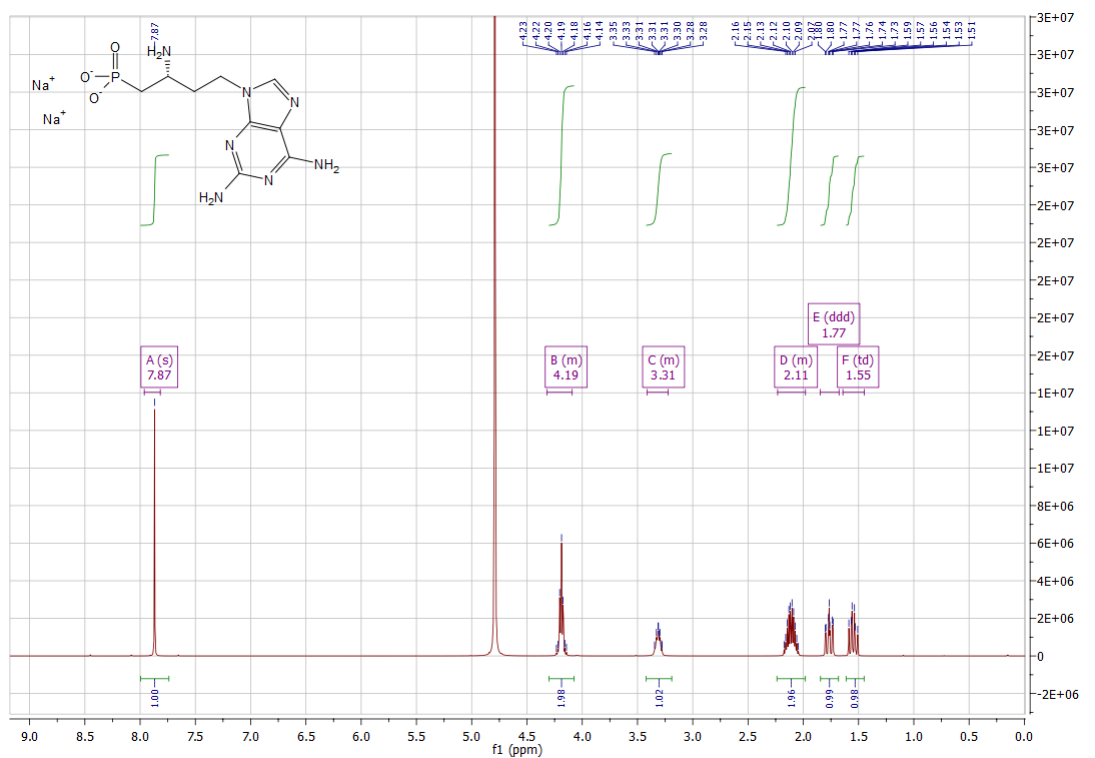
Minimum: -1.5
Maximum: 100.0

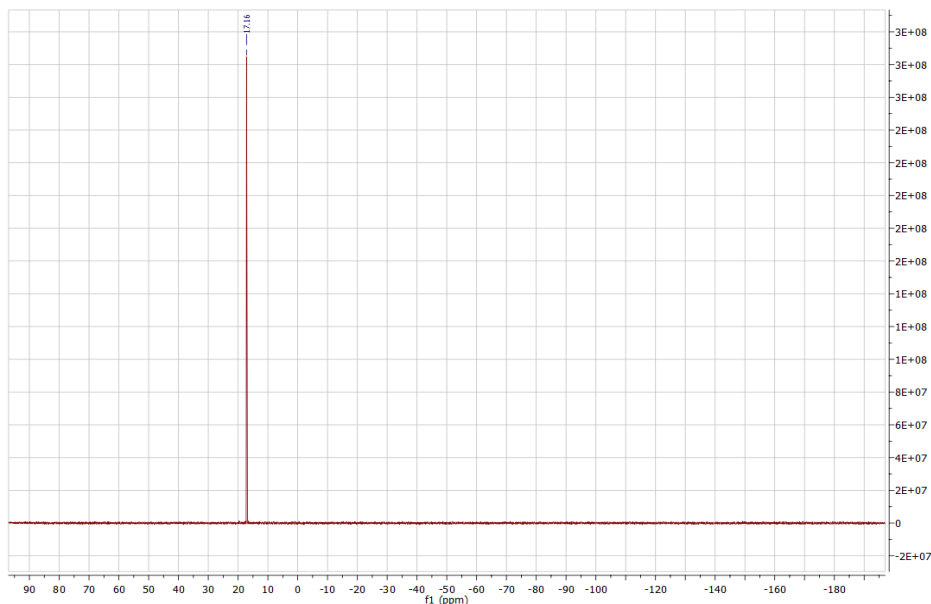
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
347.0605	347.0602	0.3	0.9	16.5	724.0	0.006	100.00	C22 H13 O Na P
	347.0610	-0.5	-1.4	5.5	735.2	11.164	0.00	C9 H14 N6 O4 Na2 F
	347.0604	0.1	0.3	2.5	736.0	12.022	0.00	C7 H16 N4 O10 P
	347.0596	0.9	2.6	0.5	736.3	12.269	0.00	C8 H18 N2 O8 Na2 F
	347.0607	-0.2	-0.6	9.5	737.8	13.922	0.00	C7 H9 N12 O2 Na P
	347.0604	0.1	0.3	13.5	740.4	16.413	0.00	C5 H4 N18 P



No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		1.747	161,910	2666,631	98.43	97.14	n.a.
2		2.757	2,586	78,560	1.57	2.86	n.a.

(*R*)-(4-(2,6-diamino-9*H*-purin-9-yl)-2-aminobutyl) phosphonic acid (*R*)-13





Elemental Composition Report

Page 1

Sample Mass Analysis

Mass tolerance = 1.5 mDa / DBE: min = -1.5, max = 100.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

447 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20 P: 1-1 Na: 2-2

SYNAPT G2-S#UEB205

Y-NuEP18020106 5 (0.228) Cm (3.6)

TC3-240

01-Feb-2018

1: TOF MS ES+

3.01e+006

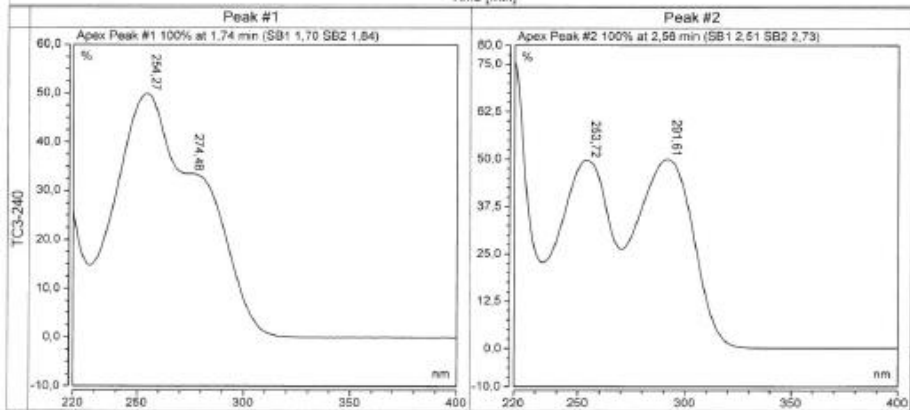
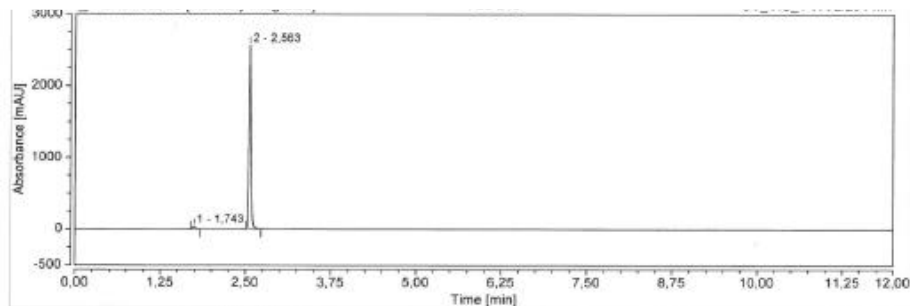


Minimum:

Maximum: 1.5 1.0 -1.5

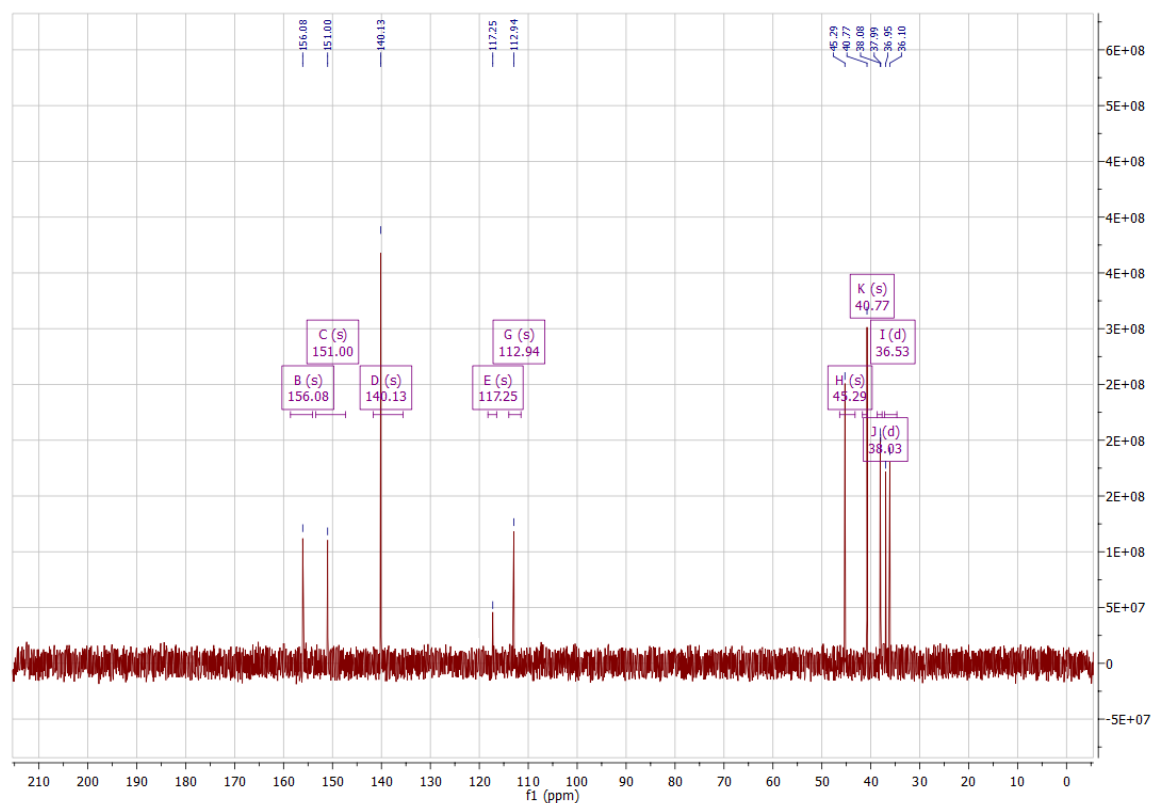
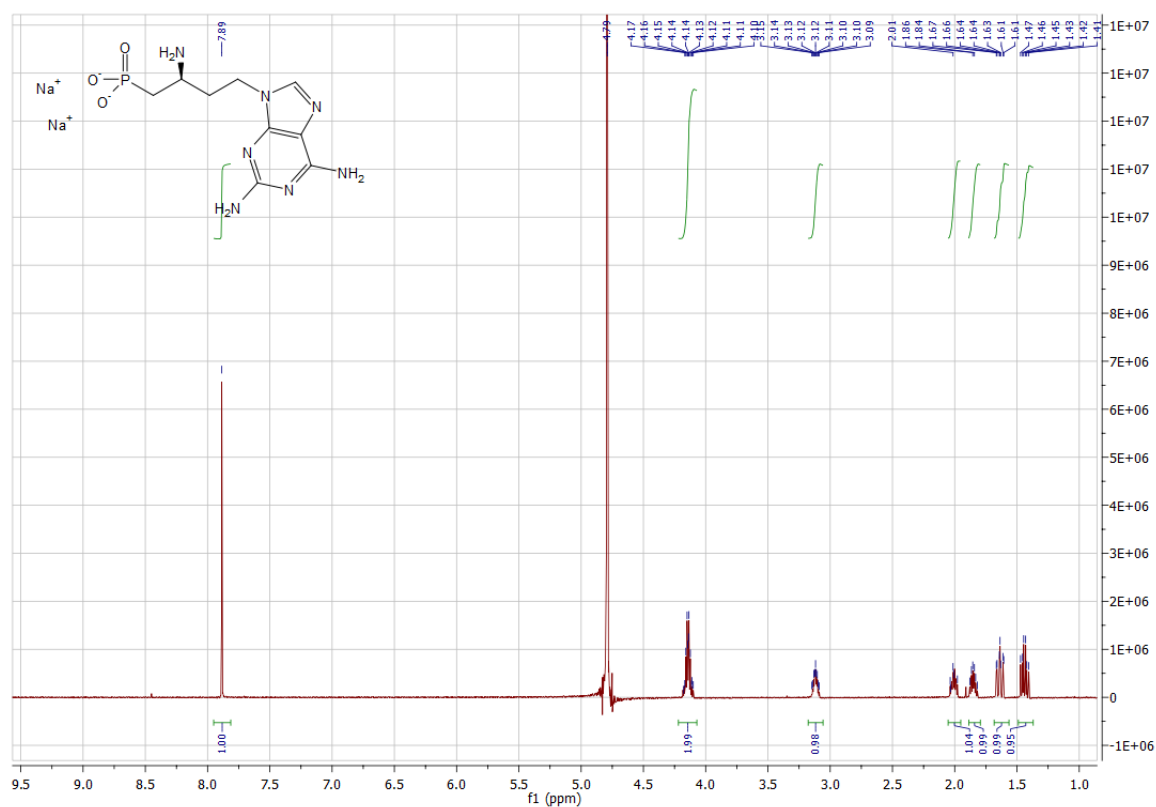
Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(%) Formula

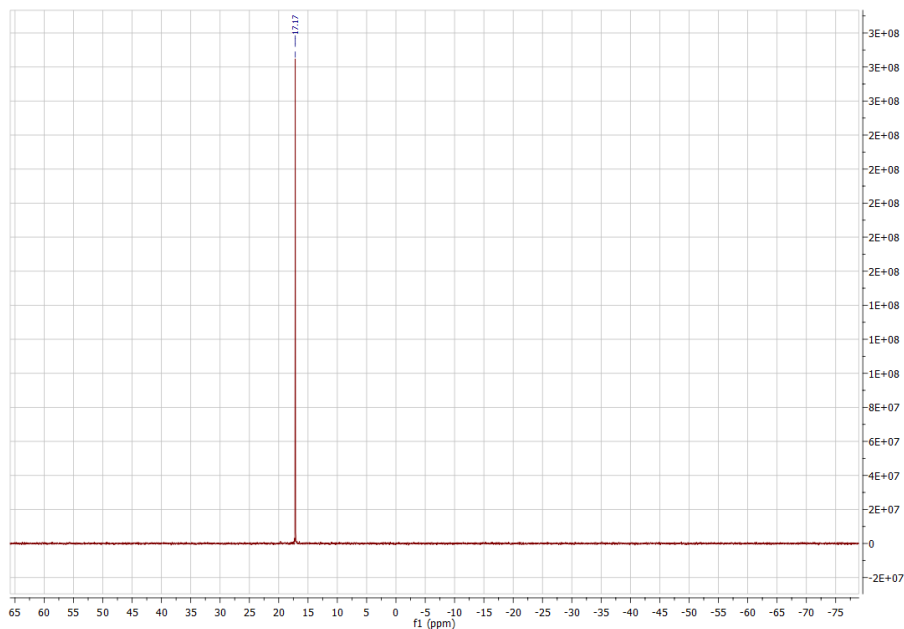
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf(%)	Formula
346.0770	346.0769	0.1	0.3	5.5	1104.8	0.001	99.94	C9 H15 N7 O3 P Na2
	346.0756	1.4	4.0	0.5	1112.3	7.484	0.06	C8 H19 N3 O7 P Na2



No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount
1		1.743	2,106	39,662	2.16	1.52	n.s.
2		2.563	95,293	2563,936	97.84	98.48	n.s.

(S)-(4-(2,6-diamino-9H-purin-9-yl)-2-aminobutyl) phosphonic acid (S)-13





ental Composition Report

Page 1

ngle Mass Analysis

olerance = 1.5 mDa / DBE: min = -1.5, max = 100.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

447 formula(e) evaluated with 2 results within limits (up to 50 best isotopic matches for each mass)

Elements Used:

C: 0-100 H: 0-100 N: 0-20 O: 0-20 P: 1-1 Na: 2-2

SYNAPT G2-S#UEB205

TC3-239

Y-NuEP18020109 5 (0.229) Cm (5)

01-Feb-2018

1: TOF MS ES+

6.80e+005



Minimum:

Maximum:

1.5

1.0

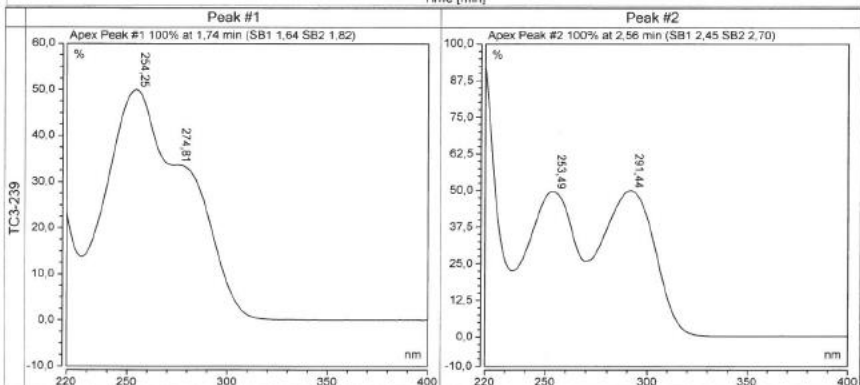
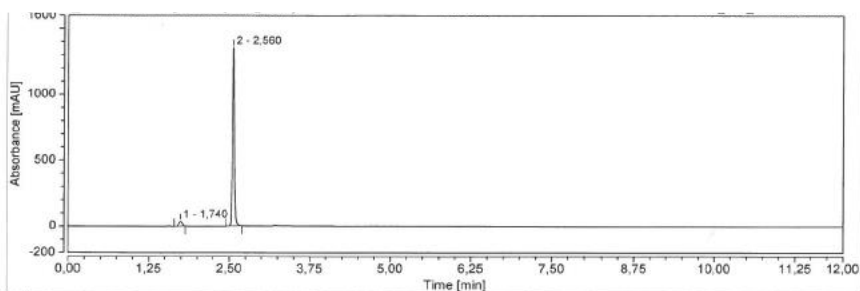
-1.5

100.0

Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf(%) Formula

346.0769 346.0769 0.0 0.0 5.5 482.3 0.036 96.50 C9 H15 N7 O3 P Na2

346.0756 1.3 3.8 0.5 485.6 3.352 3.50 C8 H19 N3 O7 P Na2



Integration Results							
No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		1,740	1,980	36,495	3.84	2.62	n.a.
2		2,560	49,530	1355,695	96.16	97.38	n.a.