

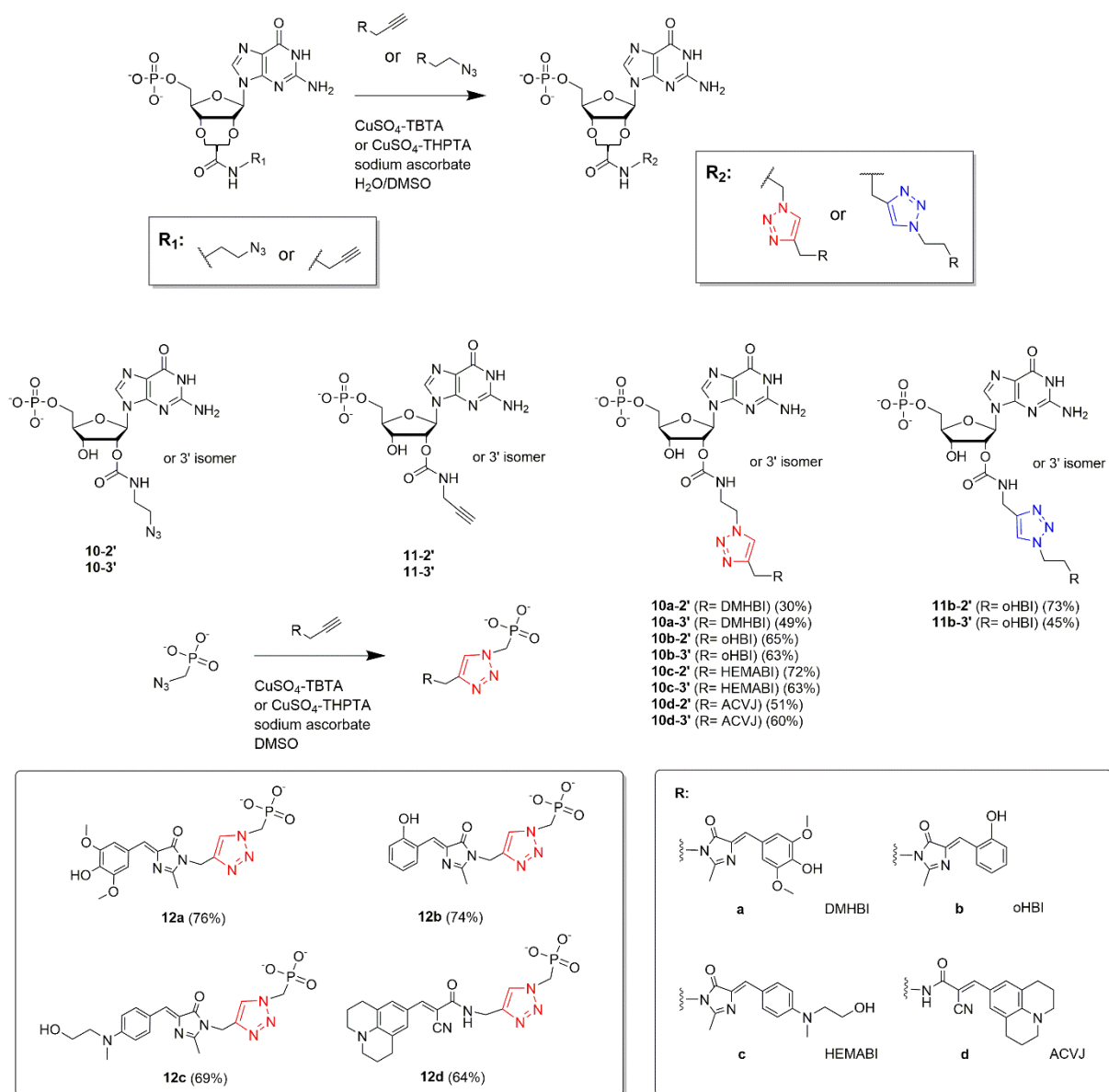
Trimethylguanosine Cap-Fluorescent Molecular Rotor conjugates (TMG-FMR) are potent, specific snurportin1 ligands enabling visualization in living cells

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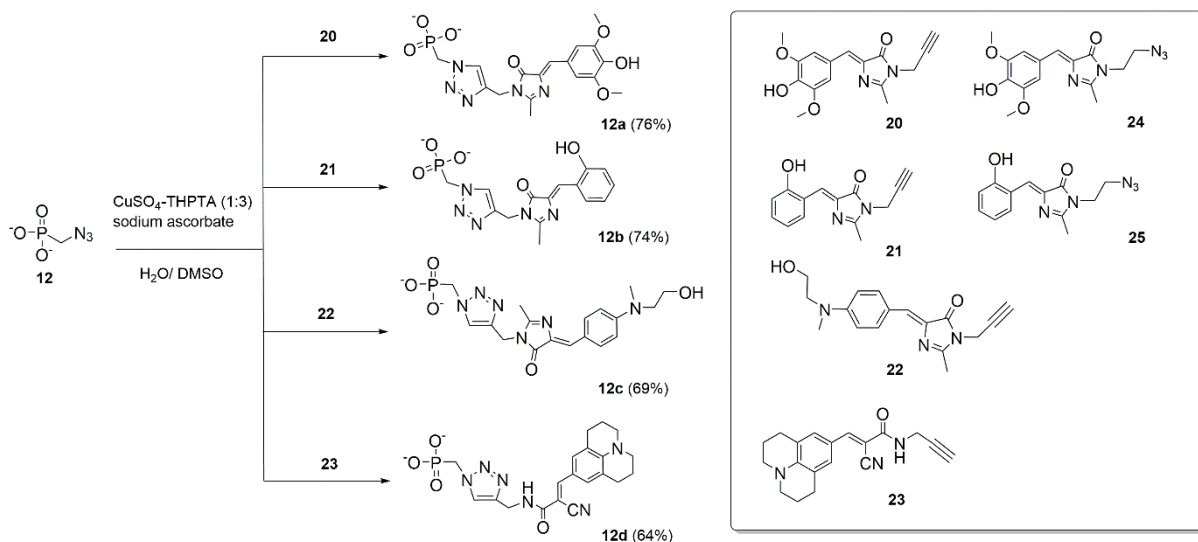
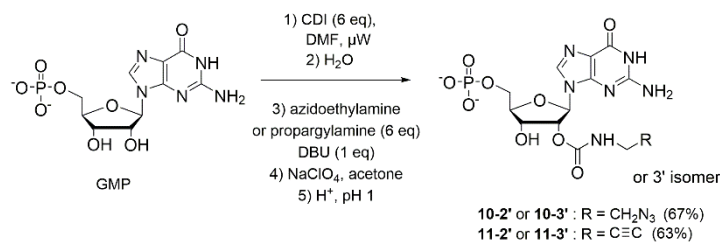
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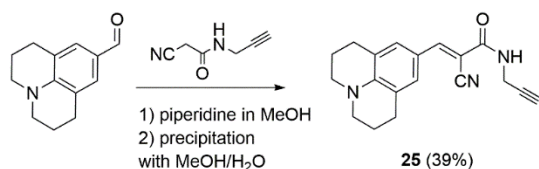
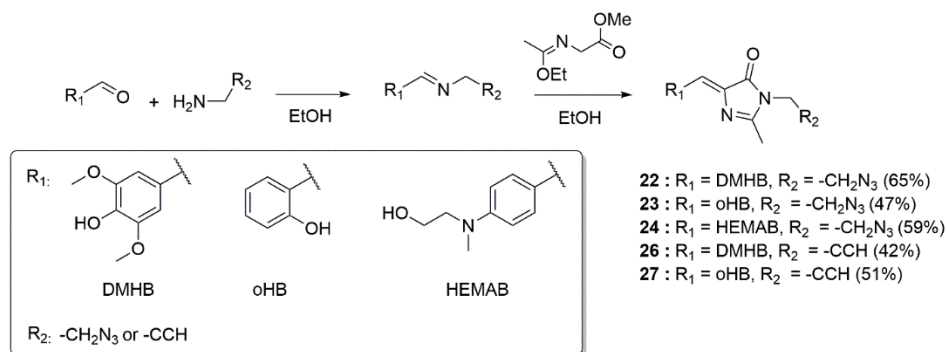
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Scheme S1. General CuAAC schemes and structures of different obtained GMP with linkers (azide/alkyne group) and conjugates with FMR



Scheme S2. Synthesis of functionalized GMP CuAAC reagents **10-** and **11-2'/3'** and FMR conjugates **12a-d**. Compounds **20-25** are FMR derivatives, CuAAC reagents



Scheme S3. Synthesis of FMR derivatives **20-25**

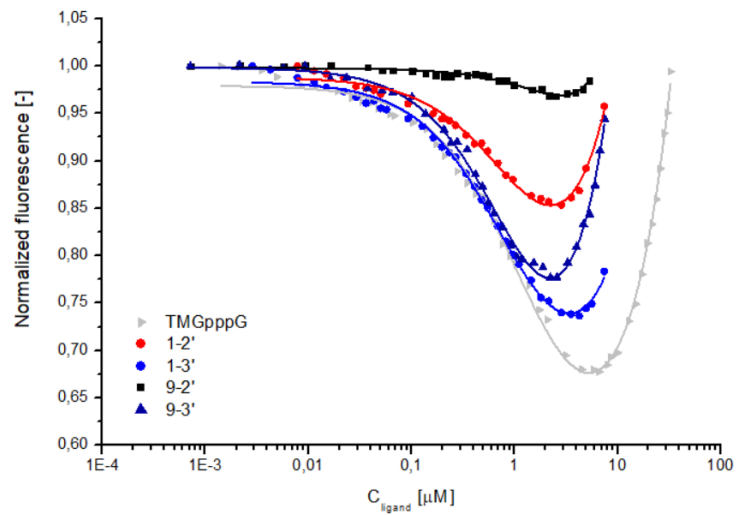


Figure S1. Exemplary FQT curves for TMG cap with linkers either from G or TMG side.

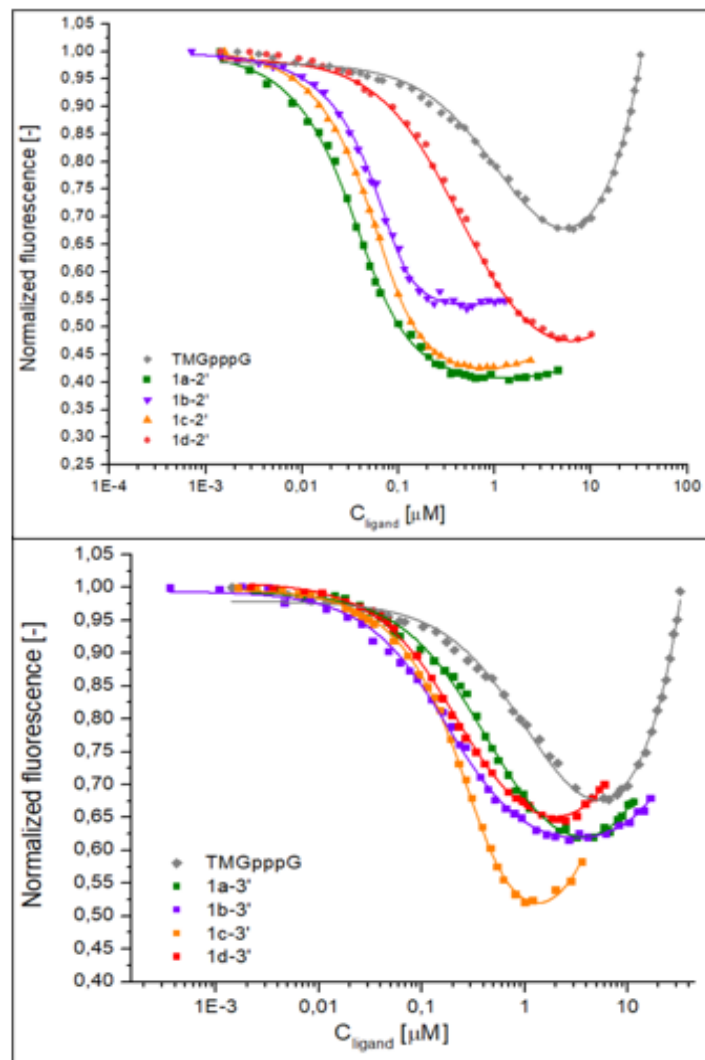


Figure S2. Exemplary FQT curves for complexes of snurportin1 and 2'-O- (top) or 3'-O-substituted (bottom) TMGpppG conjugates with different FMRs, TMGpppG (gray) was a standard.

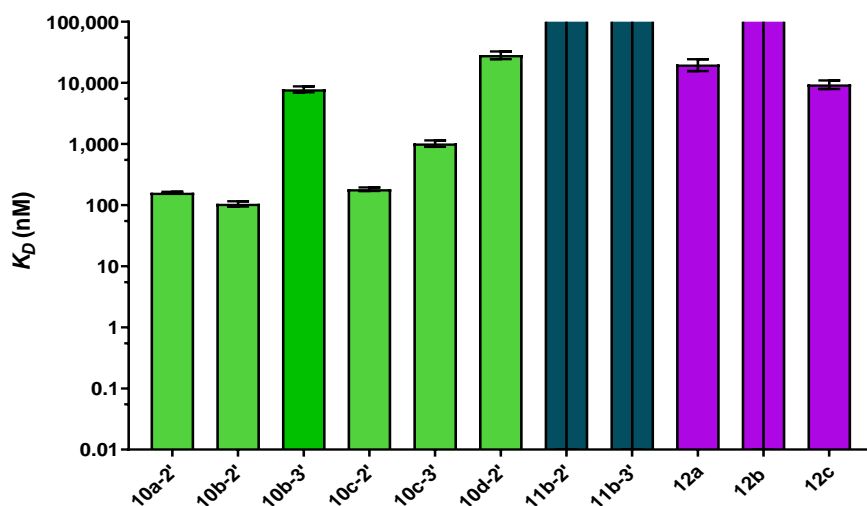


Figure S3. Dissociation constants (K_D) for complexes of snurportin1 and different GMP-FMR conjugates (**10**, **11**) and FMR-CH₂-triazole-CH₂-phosphonates (**12**, **a-c**)

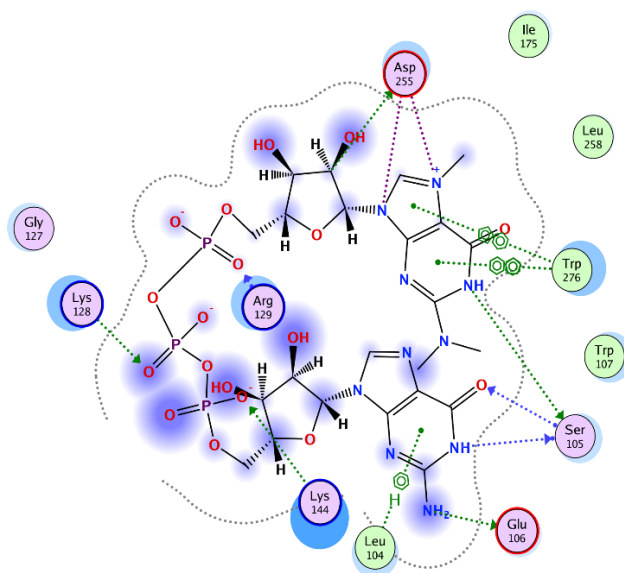


Figure S4: Interaction diagram for the unsubstituted TMGpppG in the snurportin1 binding site with exclusion of water-mediated interactions.

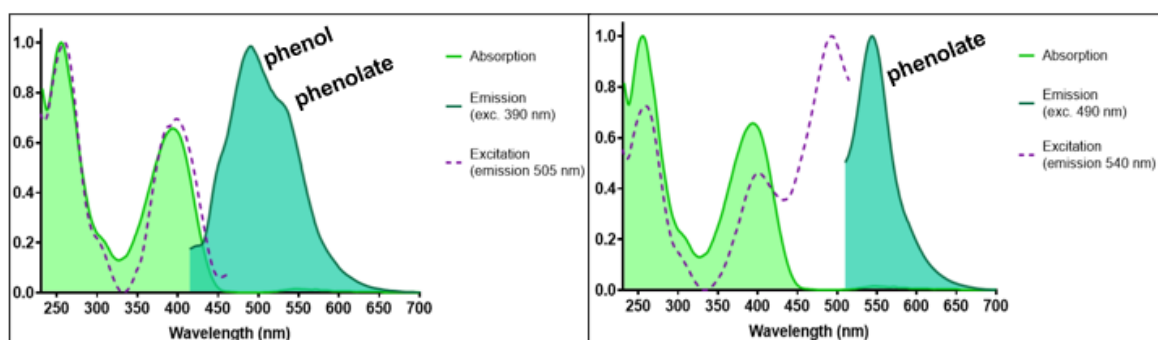


Figure S5. Dual emission for unbound **1a-2'** originating from phenol and phenolate DMHBI forms excited at A. 390 nm, B. 490 nm.

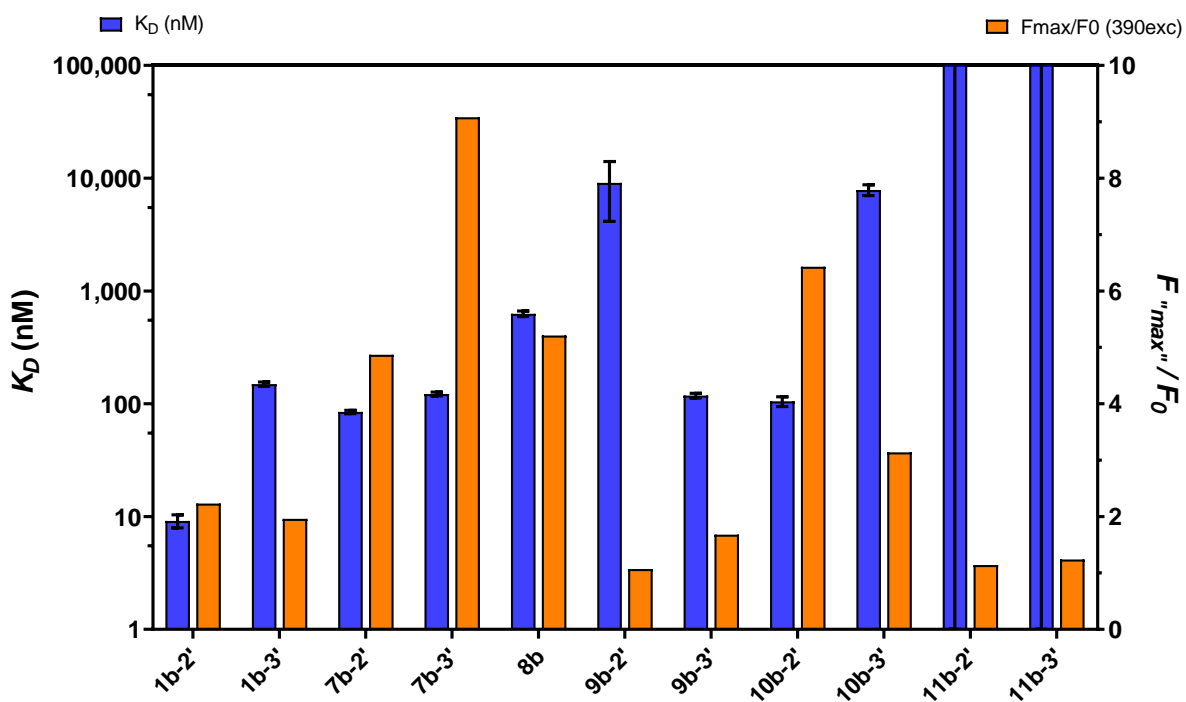
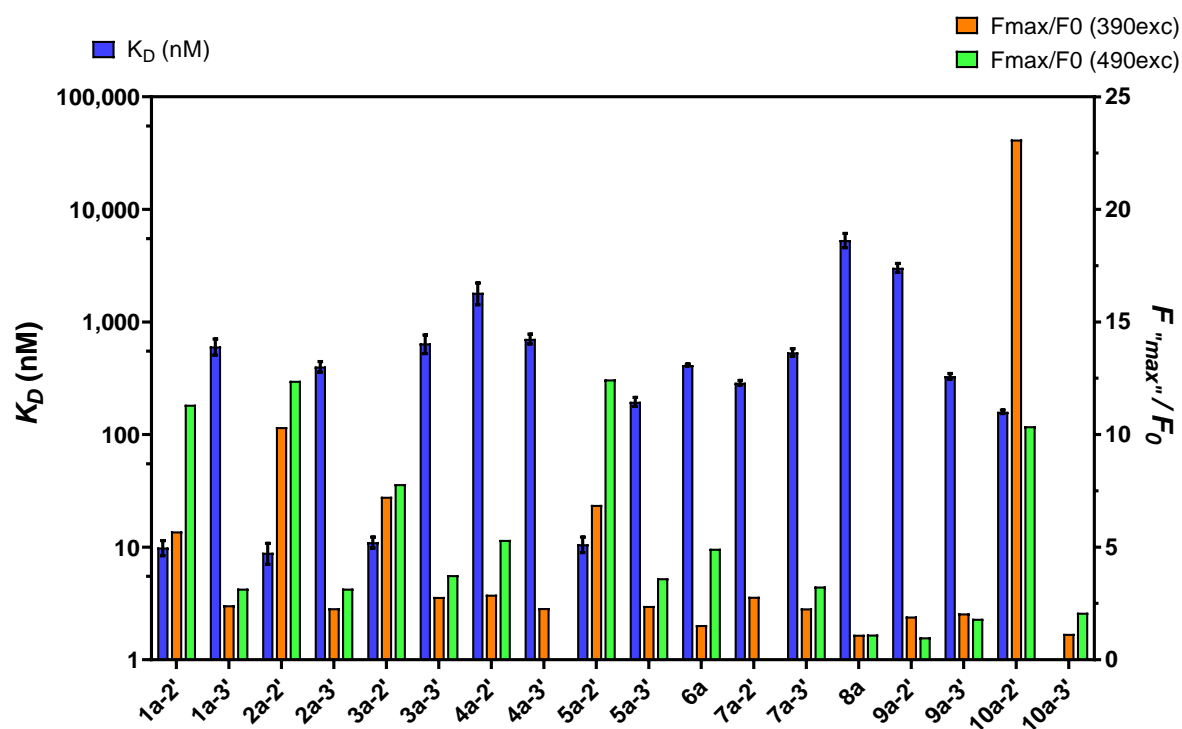


Figure S6. Comparison of dissociation constants and probes responses (F_{max}/F_0) for all A. DMHBI conjugates, B. oHBI conjugates

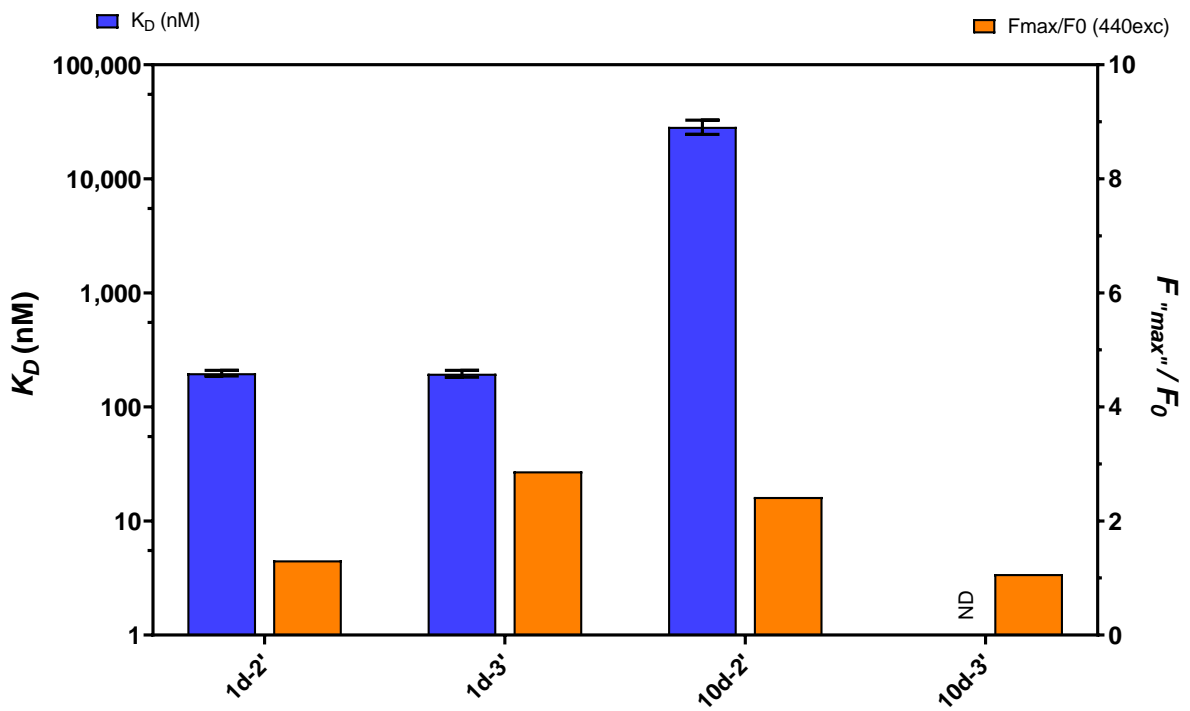
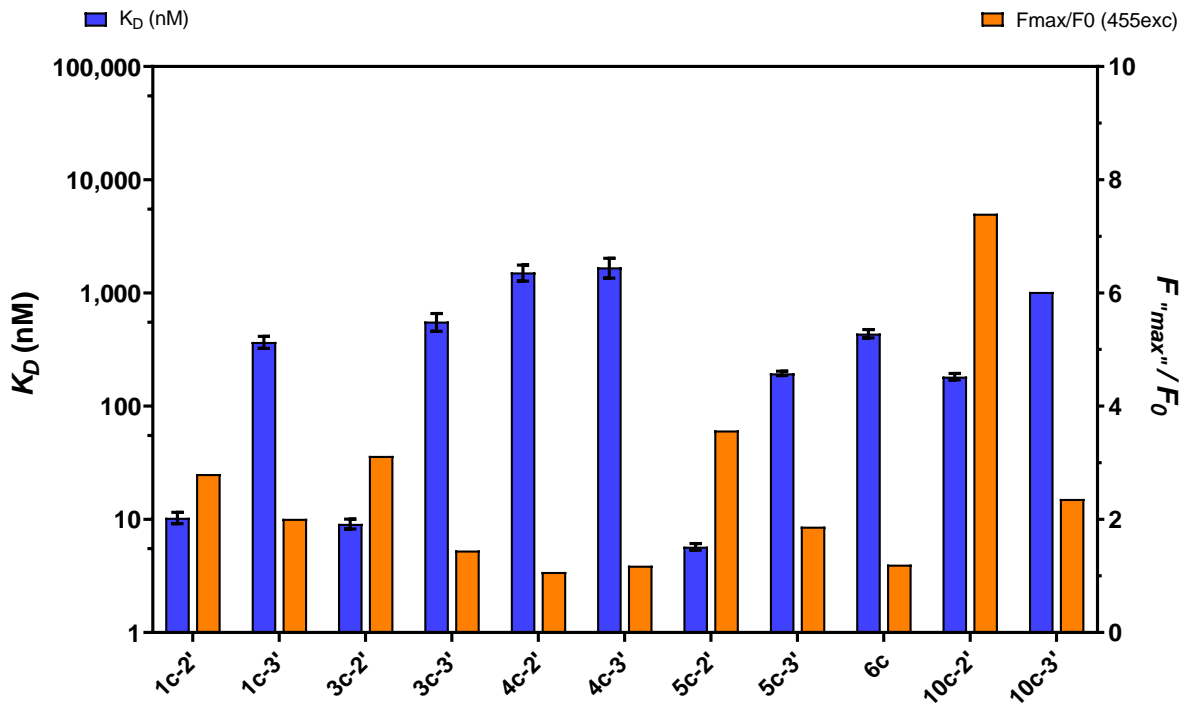


Figure S7. Comparison of dissociation constants and probes responses (F_{max}/F_0) for all A. HEMABI conjugates, B. ACVJ conjugates

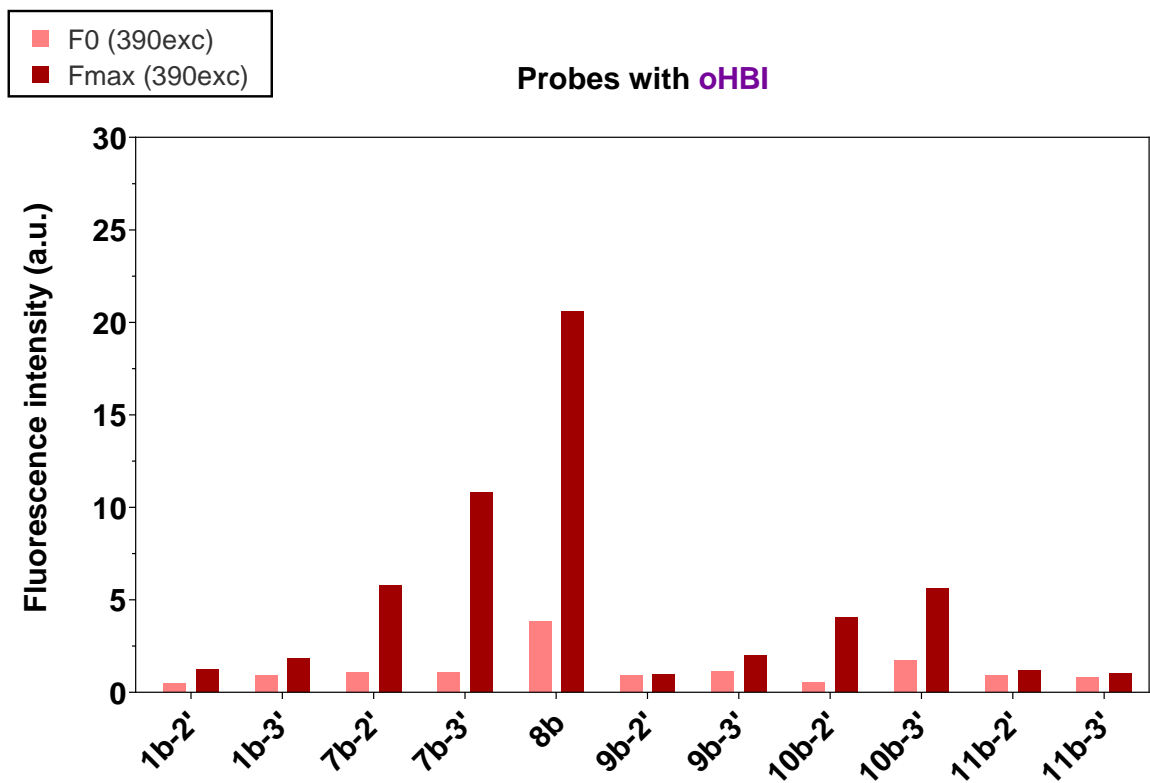
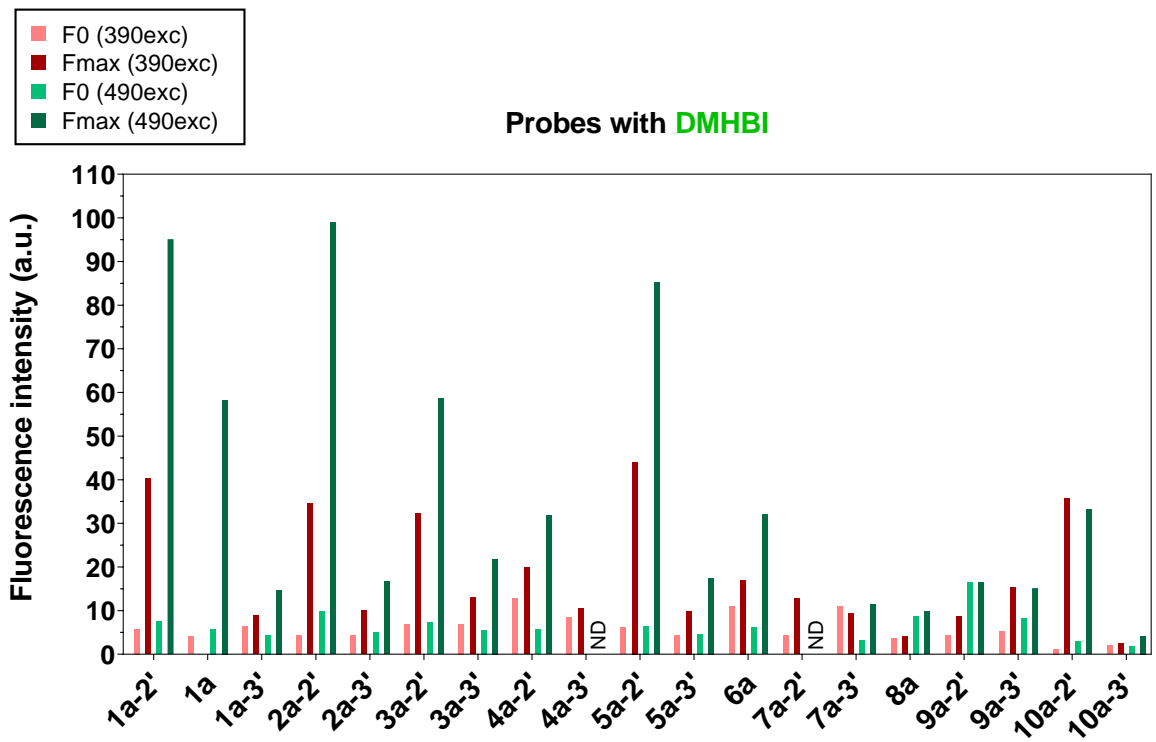


Figure S8. Initial (F0) and partly or fully saturated with snurportin1 (Fmax) normalized to concentration fluorescence intensities, A. DMHBI conjugates| B. oHBI conjugates

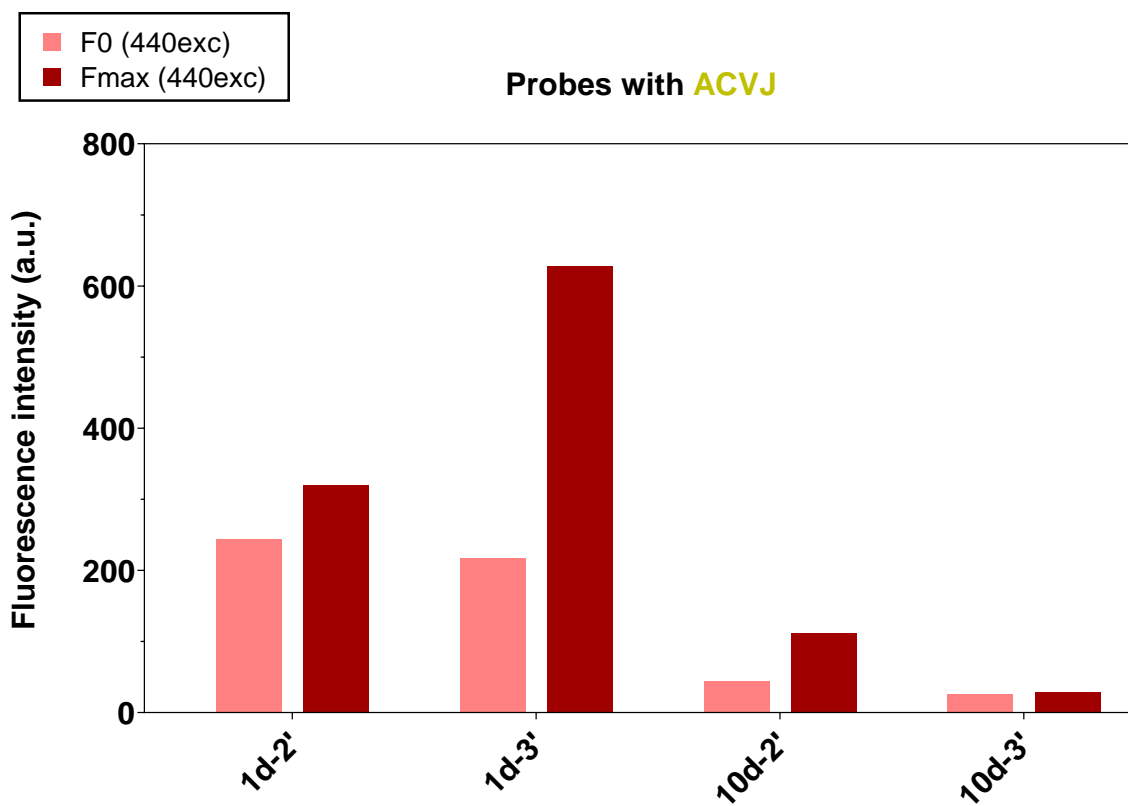
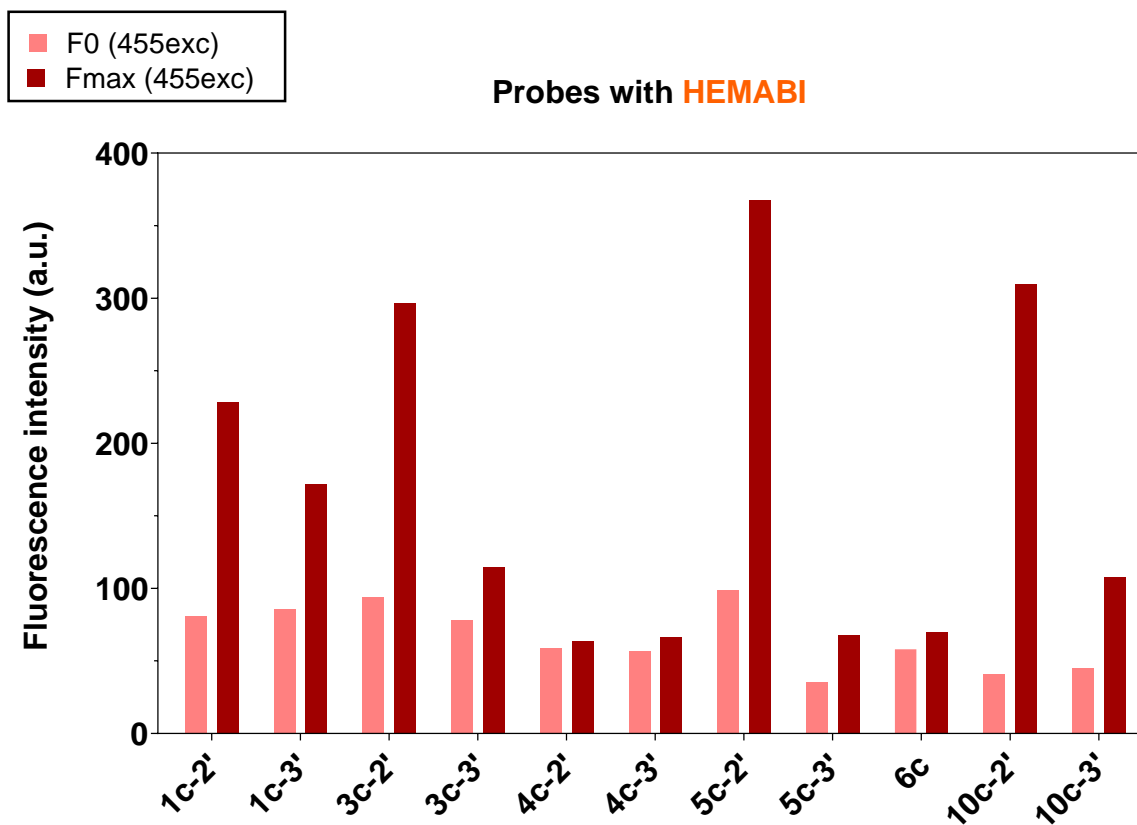


Figure S9. Initial (F0) and partly or fully saturated with snurportin1 (Fmax) normalized to concentration fluorescence intensities. A. HEMABI conjugates. B. ACVJ conjugates

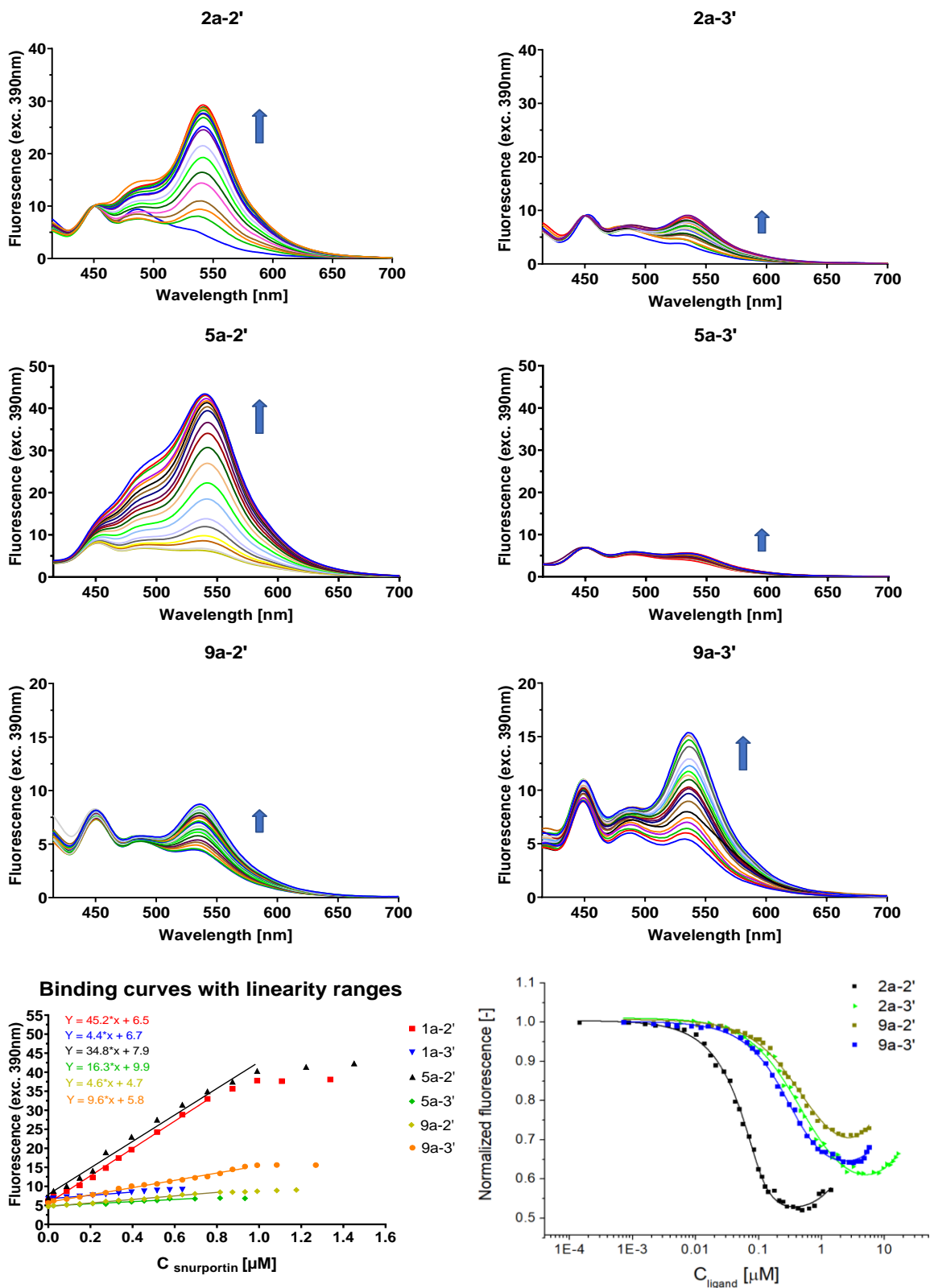


Figure S10. Representative merged emission spectra (excited at 390 nm) for DMHBI conjugates titrated with snurportin, binding curves for ligands titrations with snurportin and FQT curves (titrations with ligand)

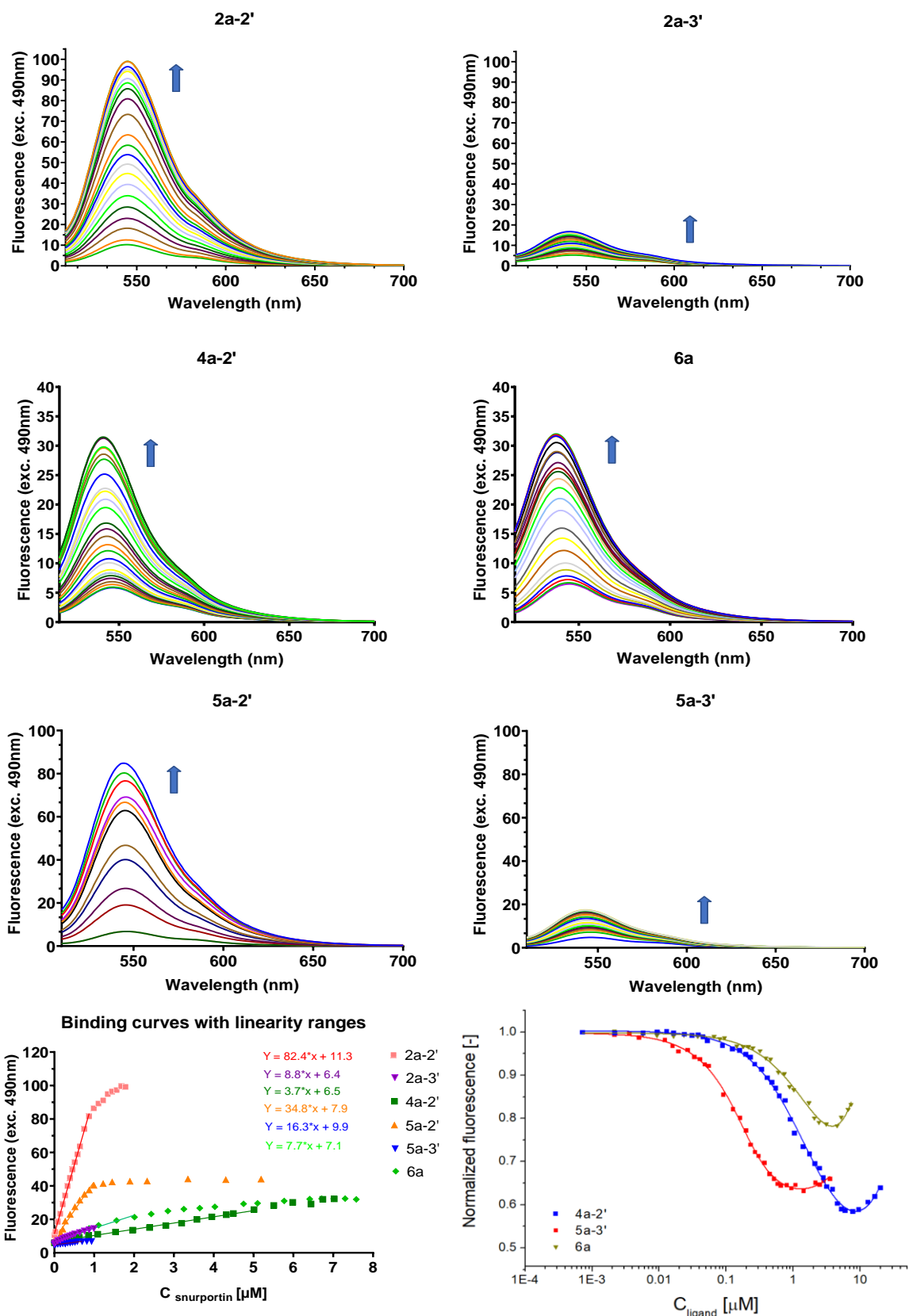


Figure S11. Representative merged emission spectra (excited at 490 nm) for DMHBI conjugates titrated with snurportin, binding curves for titrations with snurportin and FQT curves (titrations with ligand)

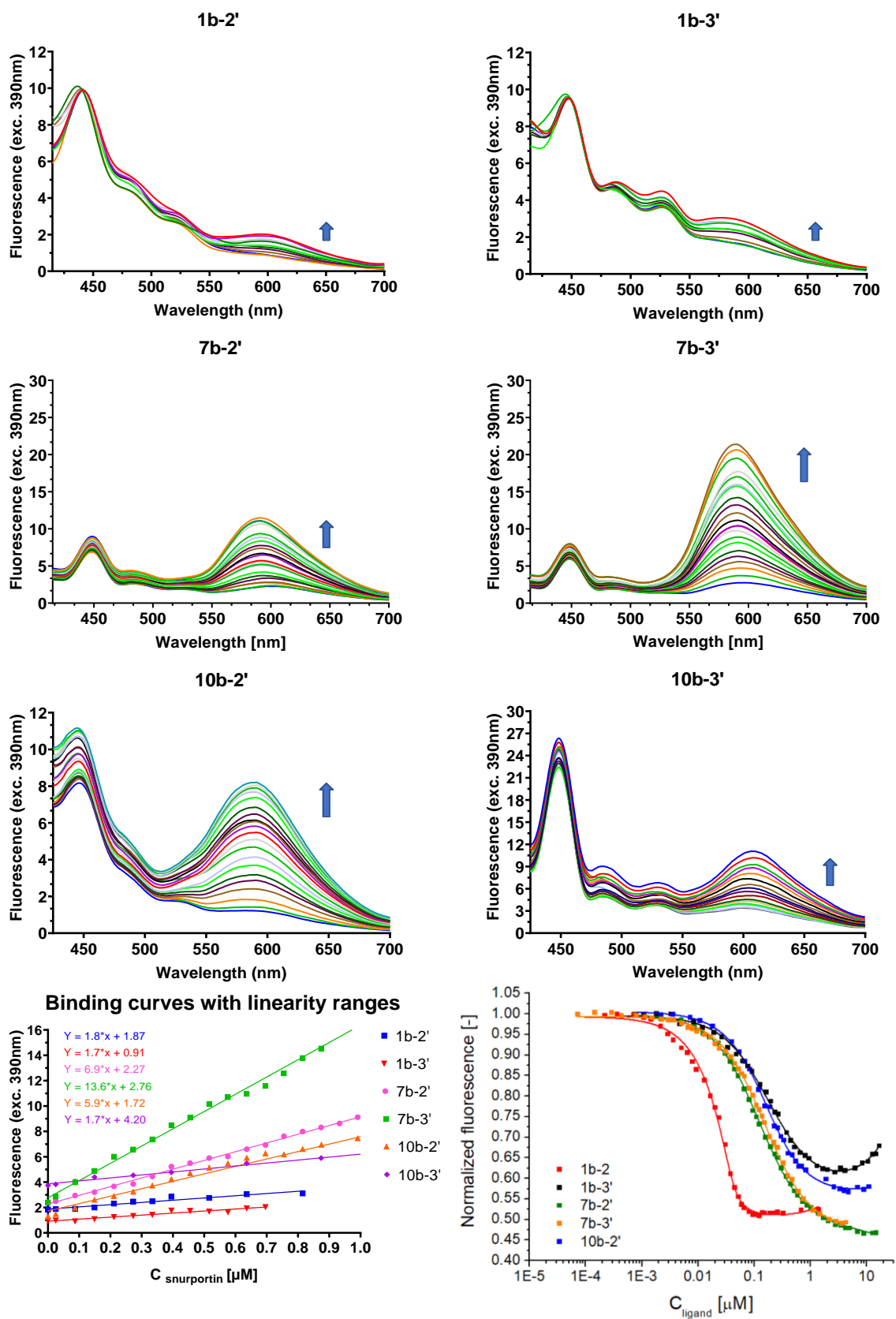


Figure S12. Representative merged emission spectra for oHBI conjugates titrated with snurportin, binding curves for ligands titrations with snurportin and FQT curves (titrations with ligand)

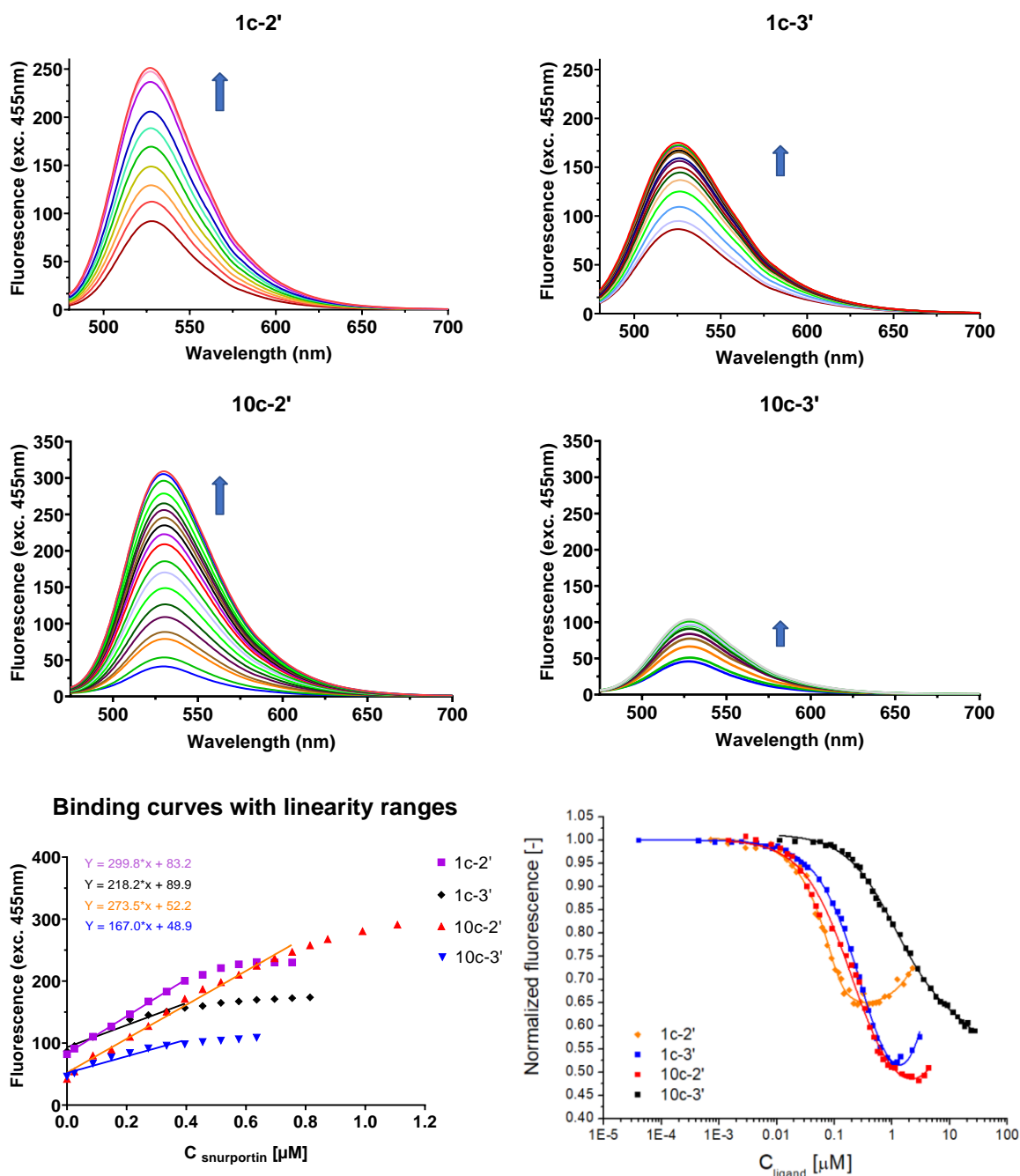


Figure S13. Representative merged emission spectra for HEMABI conjugates titrated with snurportin, binding curves for ligands titrations with snurportin and FQT curves (titrations with ligand)

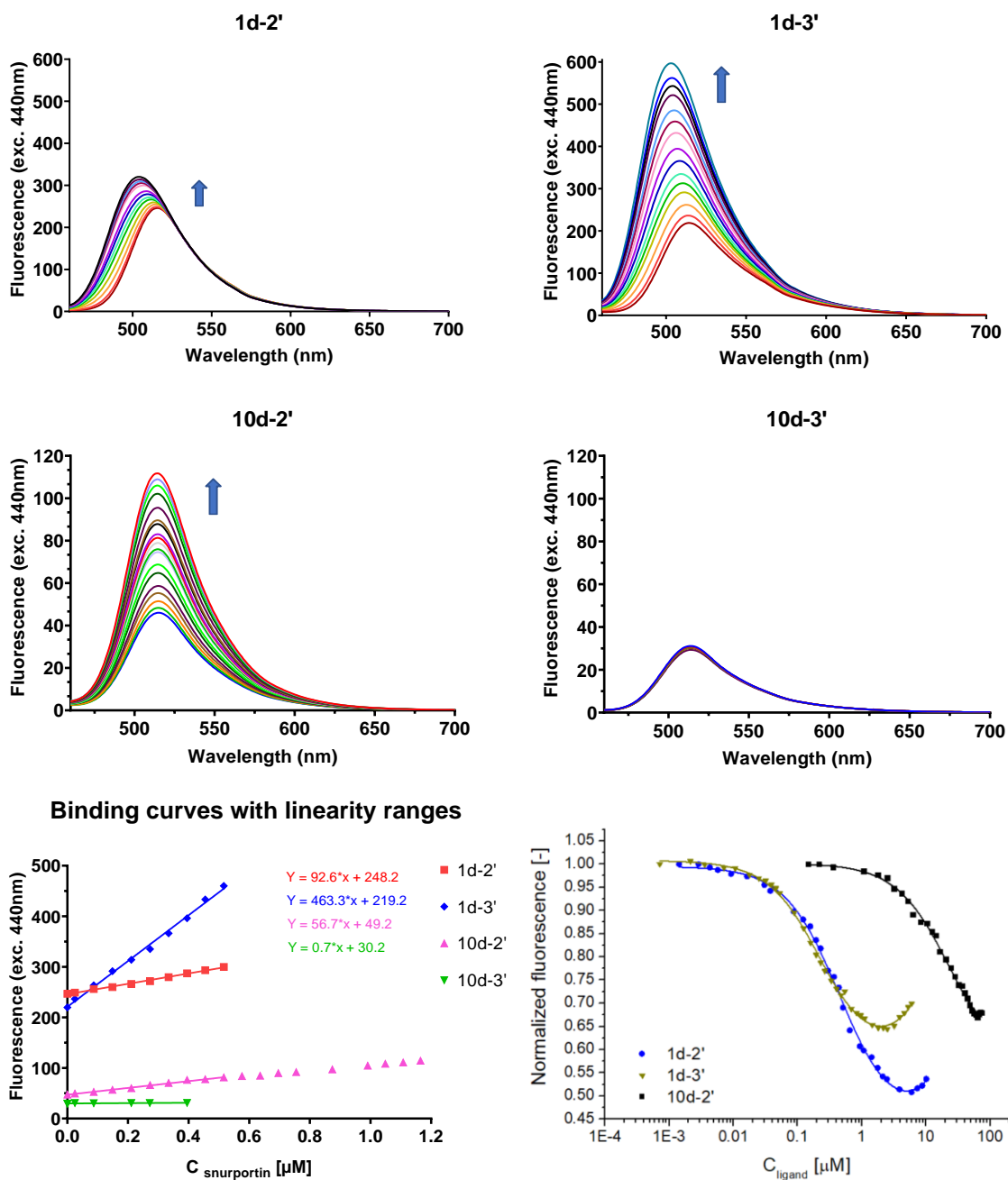


Figure S14. Merged emission spectra for all tested ACVJ conjugates titrated with snurportin binding curves for ligands titrations with snurportin and FQT curves.

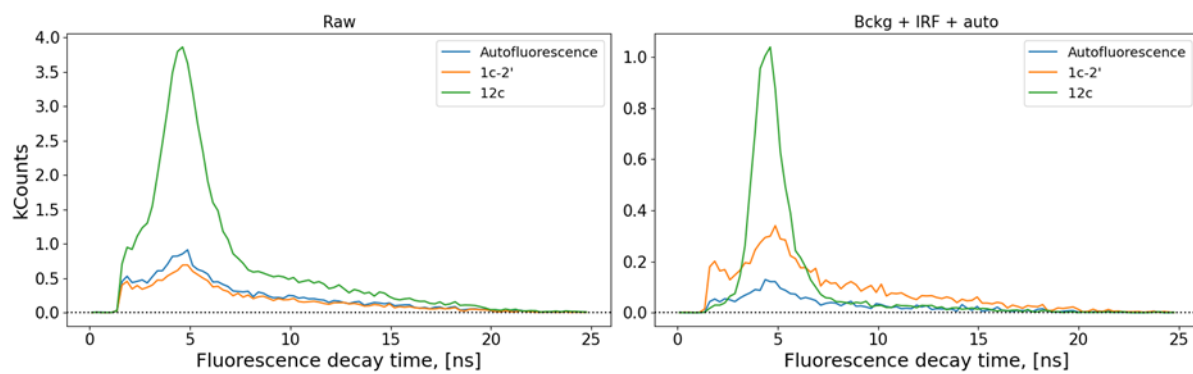


Figure S15. The histograms of the fluorescence lifetimes extracted from the FLIM images depicted in Figure 9.

Table S1. Spectral properties of Fluorescent Molecular Rotors monophosphates derivatives

FMR derivative	$\lambda_{\text{abs}}^{\text{a}}$	$\lambda_{\text{em}}^{\text{b}}$	Stokes Shift (nm)
DMHBI-CH ₂ -triazole-CH ₂ -phosphate (12a)	390 / 490	490 / 525	100 / 35
oHBI-CH ₂ -triazole-CH ₂ -phosphate (12b)	390	605	215
HEMABI-CH ₂ -triazole-CH ₂ -phosphate (12c)	455	535	80
ACVJ-CH ₂ -triazole-CH ₂ -phosphate (12d)	465	535	70

^a – in KH₂PO₄ buffer pH 7 ; ^b – in HEPES buffer pH 7.2

Table S2. Determined K_D for different TMG capped ligands and non TMG-cap-FMR conjugates with snurportin1 based on FQT experiments and fluorescence enhancement values (F_m/F₀) based on saturation experiments paired with maximum emission wavelengths

Compound	K _D (nM)	Compound	K _D (nM)	F _m /F ₀ ($\lambda_{\text{exc}1}$)	$\lambda_{\text{em}1}$ for F _m (nm)	F _m /F ₀ ($\lambda_{\text{exc}2}$)	$\lambda_{\text{em}2}$ for F _m (nm)
TMGpppG	1111 ± 74	10a-2'	159.3 ± 5.6	23.1	549	10.4	545
TMGppCH ₂ pG	1316 ± 17 ^a	10a-3'	NA	1.2	531	2.1	548
TMGpCH ₂ ppG	2564 ± 656 ^a	10b-2'	105 ± 11	6.4	583	-	-
TMGpppA	5263 ± 277 ^a	10b-3'	>10000	3.1	609	-	-
TMGppppG	417 ± 6.9 ^a	10c-2'	182 ± 12	7.4	531	-	-
1-2'	1113 ± 77	10c-3'	1007 ± 46	2.4	527	-	-
1-3'	876 ± 73	10d-2'	>20000	2.4	514	-	-
2-2'	148 ± 12	10d-3'	ND	1.1	512	-	-
2-3'	257 ± 21	11b-2'	>10000	1.1	585	-	-
3-2'	681 ± 32	11b-3'	>10000	1.2	586	-	-
3-3'	780 ± 138	12a	>10000	ND	ND	ND	ND
4-2'	1287 ± 232	12b	>10000	ND	ND	-	-
4-3'	5882 ± 3806	12c	9434 ± 1513	1.0	525	-	-
5-2'	154 ± 5.6	12d	ND	ND	ND	-	-
5-3'	272 ± 18						
6-2'	155 ± 23						
6-3'	343 ± 20						
7-2'	548 ± 129						
7-3'	609 ± 19						
8	No binding						
9-2'	>10000						
9-3'	893 ± 167						

^a M. Waszczuk, Ph.D Thesis, 2017

NA – not applicable, ND – not determined

Table S3. Top 10 poses of 2'-o-HBI in **1b-2'** and 3'-o-HBI in **1b-3'** ranked by docking score, and ligand strain energies (E_strain).

2'-o-HBI (1b-2')			3'-o-HBI (1b-3')		
pose no.	docking score [kcal/mol]	E_strain [kcal/mol]	pose no.	docking score [kcal/mol]	E_strain [kcal/mol]
1	-4.39	11.07	1	-4.11	15.38
2	-4.39	9.14	2	-3.88	17.32
3	-4.07	21.21	3	-3.88	10.37
4	-4.05	10.28	4	-3.87	15.93
5	-4.04	20.61	5	-3.83	11.73
6	-3.99	11.13	6	-3.82	13.55
7	-3.98	15.31	7	-3.8	7.07
8	-3.93	11.68	8	-3.78	14.33
9	-3.84	11.93	9	-3.77	13.22
10	-3.62	23.05	10	-3.71	14.14

DMHBI-methyl-1H-1,2,3-triazol-1-yl)methyl monophosphonate (12a)

Obtained according to GP C starting from 300 μ L (8.16 mg, 60 μ mol) of **12** (200 mM H₂O solution), 300 μ L (9.00 mg, 30 μ mol) of **20** (100 mM DMSO solution), 3.56 mg (6 μ mol, 60 μ L of 100 mM H₂O/DMSO solution) of CuSO₄-THPTA, 2.38 mg (12 μ mol, 120 μ L of 100 mM H₂O solution) of sodium ascorbate. The reaction was quenched by adding 2.23 mg (6 μ mol, 60 μ L of 100 mM H₂O solution) of Na₂EDTA. The RP HPLC (Kinetex C8 column) purification afforded 19.93 mg of **12a** ammonium salt (Yield = 76%). Rt = 14.46 min
HRMS (ESI) m/z, 436.1028 calculated for C₁₇H₁₉N₅O₇P⁻; found 436.1029

o-HBI-methyl-1H-1,2,3-triazol-1-yl)methyl monophosphonate (12b)

Obtained according to GP C starting from 300 μ L (8.16 mg, 60 μ mol) of **12** (200 mM H₂O solution), 300 μ L (7.20 mg, 30 μ mol) of **21** (100 mM DMSO solution), 3.56 mg (6 μ mol, 60 μ L of 100 mM H₂O/DMSO solution) of CuSO₄-THPTA, 2.38 mg (0.012 μ mol, 120 μ L of 100 mM H₂O solution) of sodium ascorbate. The reaction was quenched by adding 2.23 mg (6 μ mol, 60 μ L of 100 mM H₂O solution) of Na₂EDTA. The RP HPLC (Kinetex C8 column) purification afforded 16.74 mg of **12b** ammonium salt (Yield = 74%). Rt = 16.39 min
HRMS (ESI) m/z, 376.0816 calculated for C₁₅H₁₅N₅O₅P⁻; found 376.0820

HEMABI-methyl-1H-1,2,3-triazol-1-yl)methyl monophosphonate (12c)

Obtained according to GP C starting from 300 μ L (8.16 mg, 60 μ mol) of **12** (200 mM H₂O solution), 300 μ L (8.91 mg, 30 μ mol) of **22** (100 mM DMSO solution), 3.56 mg (6 μ mol, 60 μ L of 100 mM H₂O/DMSO solution) of CuSO₄-THPTA, 2.38 mg (12 μ mol, 120 μ L of 100 mM H₂O solution) of sodium ascorbate. The reaction was quenched by adding 2.23 mg (6 μ mol, 60 μ L of 100 mM H₂O solution) of Na₂EDTA. The RP HPLC (Kinetex C8 column) purification afforded 17.98 mg of **12c** ammonium salt (Yield = 69%). Rt = 14.72 min
HRMS (ESI) m/z, 433.1395 calculated for C₁₈H₂₂N₆O₅P⁻; found 433.1396

ACVJ-methyl-1H-1,2,3-triazol-1-yl)methyl monophosphonate (12d)

Obtained according to GP C starting from 300 μ L (8.16 mg, 60 μ mol) of **12** (200 mM H₂O solution), 300 μ L (9.16 mg, 30 μ mol) of **23** (100 mM DMSO solution), 3.56 mg (6 μ mol, 60 μ L

of 100 mM H₂O/DMSO solution) of CuSO₄-THPTA, 2.38 mg (12 μmol, 120 μL of 100 mM H₂O solution) of sodium ascorbate. The reaction was quenched by adding 2.23 mg (6 μmol, 60 μL of 100 mM H₂O solution) of Na₂EDTA. The RP HPLC (Kinetex C8 column) purification afforded 16.98 mg of **12d** ammonium salt (Yield = 64%). Rt = 21.42 min (gradient c)
HRMS (ESI) m/z, 441.1446 calculated for C₂₀H₂₂N₆O₄P⁻; found 441.1450

2'+3'-O-(N-(2-Azidoethyl)carbamoyl) guanosine 5'-diphosphate imidazolide (13)

Obtained according to GP A: GDP triethylammonium salt (98 mg, 0.10 mmol, 1200 mOD) was dissolved in DMSO (2 ml) and CDI (97 mg, 0.600 mmol, 6 equiv) was added. The mixture was stirred and microwaved as described in GP A, then excess of CDI was hydrolyzed by addition of H₂O (22 μL) and after 15 min of stirring, 2-azidoethylamine (54 μL, 0.60 mmol, 6 equiv) and DBU (15 μL, 0.10 mmol, 1 equiv) was added. The reaction mixture was stirred at RT and monitored by HPLC. After 6h the imidazolide was precipitated by addition of NaClO₄ (73 mg, 0.60 mmol, 6 equiv) in 40 ml cold acetone. 26 mg of imidazolide sodium salt was obtained as a mixture of 2' and 3' isomers. (611 mOD, Yield = 51%). Rt = min
HRMS (ESI) m/z, 604.0825 calculated for C₁₆H₂₀N₁₁O₁₁P₂⁻; found 604.0831

2'+3'-O-(N-(2-Azidoethyl)carbamoyl)guanosine 5'-methylene(bisphosphonate) imidazolide (14)

Obtained according to GP A: GpCH₂p triethylammonium salt (98 mg, 0.10 mmol, 1200 mOD) was dissolved in DMSO (2 ml) and CDI (97 mg, 0.600 mmol, 6 equiv) was added. The mixture was stirred and microwaved as described in GP A, then excess of CDI was hydrolyzed by addition of H₂O (22 μL) and after 15 min of stirring, 2-azidoethylamine (54 μL, 0.60 mmol, 6 equiv) and DBU (15 μL, 0.10 mmol, 1 equiv) was added. The reaction mixture was stirred at RT and monitored by HPLC. After 6h the imidazolide was precipitated by addition of NaClO₄ (73 mg, 0.60 mmol, 6 equiv) in 40 ml cold acetone. 40 mg of Imidazolide sodium salt was obtained as a mixture of 2' and 3' isomers based on chromatogram, however, due to aqueous environment, imidazolide hydrolyzed to phosphonate before HRMS analysis. (960 mOD, Yield = 80%). Rt = 6.39 min
HRMS (ESI) m/z, 552.0763 calculated for C₁₄H₂₀N₉O₁₁P₂⁻; found 552.0769

2'+3'-O-(N-(2-Azidoethyl)carbamoyl)adenosine 5'-diphosphate imidazolide (15)

Obtained according to GP A: ADP triethylammonium salt (200 mg, 0.274 mmol) was dissolved in DMSO (5 ml) and CDI (222 mg, 1.37 mmol, 5 equiv) was added. The mixture was stirred at RT for 1h, then excess of CDI was hydrolyzed by addition of H₂O (49 μL) and after 15 min of stirring, 2-azidoethylamine was added (246 μL, 236 mg, 2.73 mmol, 10 equiv). The reaction mixture was stirred at RT and monitored by HPLC. After 24h the imidazolide was precipitated by addition of NaClO₄ (335 mg, 2.73 mmol, 10 equiv) in 50 ml cold acetone. Imidazolide sodium salt was obtained as a mixture of 2' and 3' isomers. (Yield: 91 mg, 52%). Rt = 7.32 min (isomer 2') and 7.93 min (isomer 3')
HRMS (ESI) m/z, 588.0875 calculated for C₁₆H₂₀N₁₁O₁₀P₂⁻; found 588.0881

2'+3'-O-(N-(Propargyl)carbamoyl)guanosine 5'-iodide (16)

5'-I-Guanosine (500 mg, 1.28 mmol) was dissolved in DMSO (20 ml) and CDI (1.03 g, 6.38 mmol, 5 equiv) was added. The mixture was stirred at RT for 1 h, then excess of CDI was hydrolyzed by addition of H₂O (230 μL) and after 15 min of stirring propargylamine was added (702 mg, 12.75 mmol, 10 equiv). The reaction mixture was stirred at RT and monitored by HPLC. After 24 h the crude product was precipitated by addition of 200 ml 1:1 mixture of CH₂Cl₂/H₂O. White precipitate was washed with CH₂Cl₂ and dried in under high vacuum (Yield: 548 mg,

90% as a mixture of 2' and 3' isomers). Rt = 15.58 min (isomer 3') and 16.45 min (isomer 2'). For NMR analysis small amount of isomers were separated and purified on RP-HPLC.

Isomer 2' (Rt = 16.45 min)

^1H NMR (500 MHz, DMSO- d_6) δ [ppm] 7.91 (d, J = 4.9 Hz, 1H), 7.86 (s, 1H), 6.27 (s, 1H), 5.15 (d, J = 14.9 Hz, 1H), 4.92 (dd, J = 5.6, 3.4 Hz, 1H), 4.79 (d, J = 3.3 Hz, 1H), 4.11 (d, J = 5.7 Hz, 1H), 3.78 – 3.74 (m, 2H)

Isomer 3' (Rt = 15.58 min)

^1H NMR (500 MHz, DMSO- d_6) δ [ppm] 7.93 (s, 1H), 5.70 (d, J = 7.6 Hz, 1H), 5.12 (dd, J = 5.4, 2.1 Hz, 1H), 4.93 (dd, J = 7.5, 5.4 Hz, 1H), 4.11 (td, J = 6.7, 2.2 Hz, 1H), 3.76 (d, J = 5.6 Hz, 1H).

HRMS (ESI) m/z , 473.0076 calculated for $\text{C}_{14}\text{H}_{14}\text{IN}_6\text{O}_5^-$; found 473.0080

2'+3'-O-(N-(Propargyl)carbamoyl)guanosine 5'-monothiophosphate (17)

To a suspension of 2'+3'-O-(N-(Propargyl)carbamoyl)guanosine 5'-iodide (**16**) (0.5 g, 1.06 mmol) in 10 mL of DMF, trisodium thiophosphate (0.53 g, 1.27 mmol) was added followed by addition of Et₃N (0.43 g, 728 μL, 4.23 mmol). The reaction mixture was stirred for 6 h at 5°C. The reaction mixture was dissolved in 50 mL of water and purified by AIEC on Sephadex. The fractions containing the desired product were collected and freeze-dried. Yield: 6186 mOD, 0.51 mmol (Yield = 64%). Rt = 6.44 min

¹H NMR (500 MHz, DMSO-*d*₆) δ [ppm] 7.99 (s, 1H), 7.96 (s, 1H), 5.91 (d, *J* = 6.2 Hz, 1H), 5.81 (d, *J* = 3.8 Hz, 1H), 5.68 (d, *J* = 7.5 Hz, 1H), 5.63 (d, *J* = 7.6 Hz, 1H), 5.48 (t, *J* = 5.8 Hz, 1H), 5.35 (dd, *J* = 5.6, 3.7 Hz, 1H), 5.24 (d, *J* = 5.2 Hz, 1H), 5.13 (dd, *J* = 5.4, 2.2 Hz, 1H), 5.03 (dd, *J* = 7.7, 5.0 Hz, 1H), 4.87 (dd, *J* = 7.6, 5.5 Hz, 1H), 4.75 (t, *J* = 5.8 Hz, 1H), 4.40 (dd, *J* = 5.3, 3.6 Hz, 1H), 4.19 (d, *J* = 7.4 Hz, 1H), 4.05 (td, *J* = 6.2, 2.1 Hz, 1H), 3.93 (td, *J* = 6.1, 3.6 Hz, 1H), 3.13 (d, *J* = 2.5 Hz, 1H), 3.09 (d, *J* = 2.4 Hz, 1H)

³¹P NMR (203 MHz, DMSO-*d*₆) δ [ppm] 12.09 (s, 1P), 11.72 (s, 1P)

HRMS (ESI) *m/z*, 459.0493 calculated for C₁₄H₁₆N₆O₈PS⁻; found 459.0501

2'+3'-O-(N-(Propargyl)carbamoyl)guanosine 5'-monothiophosphate imidazolide (18)

Compound **18** was prepared according to Mukaiyama protocol^{1,2}. 2'+3'-O-(N-(Propargyl)carbamoyl)guanosine 5'-monothiophosphate (**17**) (TEA⁺ salt, 1 g, 1.51 mmol), imidazole (1.03 g, 15.09 mmol, 10 equiv), 2,2'-dithiodipyridine (DTDP) (997.25 mg, 4.53 mmol, 3 equiv) were mixed in DMF (10 mL) before addition of triethylamine (458.06 mg, 4.53 mmol, 3 equiv) and triphenylphosphine (PPh₃) (1.19 g, 4.53 mmol, 3 equiv). The mixture was stirred for 6 h or overnight at room temperature and progress was monitored by HPLC. Addition of a solution of anhydrous NaClO₄ (1.84 g) in 100 mL dry acetone resulted in precipitation of the product as sodium salt. The suspension was cooled at 4 °C and the precipitate was filtered off, washed repeatedly with cold, dry acetone and dried in vacuum over P₄O₁₀. (Yield: 914 mg, 87%). Rt = 9.65 min (isomer 2') and 10.58 min (isomer 3')

HRMS (ESI) *m/z*, 509.0762 calculated for C₁₇H₁₈N₈O₇PS⁻; found 509.0764

2'+3'-O-(N-(2-Azidoethyl)carbamoyl)-2,2,7-trimethylguanosine monophosphate imidazolide (19)

Obtained according to GP A: TMGMP triethylammonium salt (25 mg, 0.052 mmol, 622 mOD) was dissolved in DMSO (1 ml) and CDI (51 mg, 0.310 mmol, 6 equiv) was added. The mixture was stirred and microwaved as described in GP A, then excess of CDI was hydrolyzed by addition of H₂O (14 μL) and after 15 min of stirring, 2-azidoethylamine (20 μL, 0.310 mmol, 6 equiv) and DBU (20 μL, 0.052 mmol, 1 equiv) was added. The reaction mixture was stirred at RT and monitored by HPLC. After 6h the imidazolide was precipitated by addition of LiClO₄ (33 mg, 0.310 mmol, 6 equiv) in 40 ml cold acetonitrile. Imidazolide lithium salt was obtained as a mixture of 2' and 3' isomers. (Yield: 19 mg, 387 mOD, 62%).

HRMS (ESI) *m/z*, 566.1631 calculated for C₁₉H₂₅N₁₁O₈P⁻; found 566.1633

References

1. T. Mukaiyama and M. Hashimoto, *J. Am. Chem. Soc.*, 1972, **94** (24), 8528–8532.
2. T. Mukaiyama and M. Hashimoto, *Bulletin of the Chemical Society of Japan*, 1971, **44** (8), 2284.

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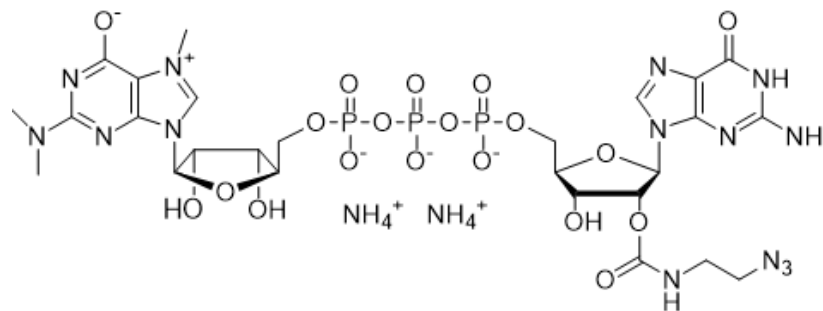
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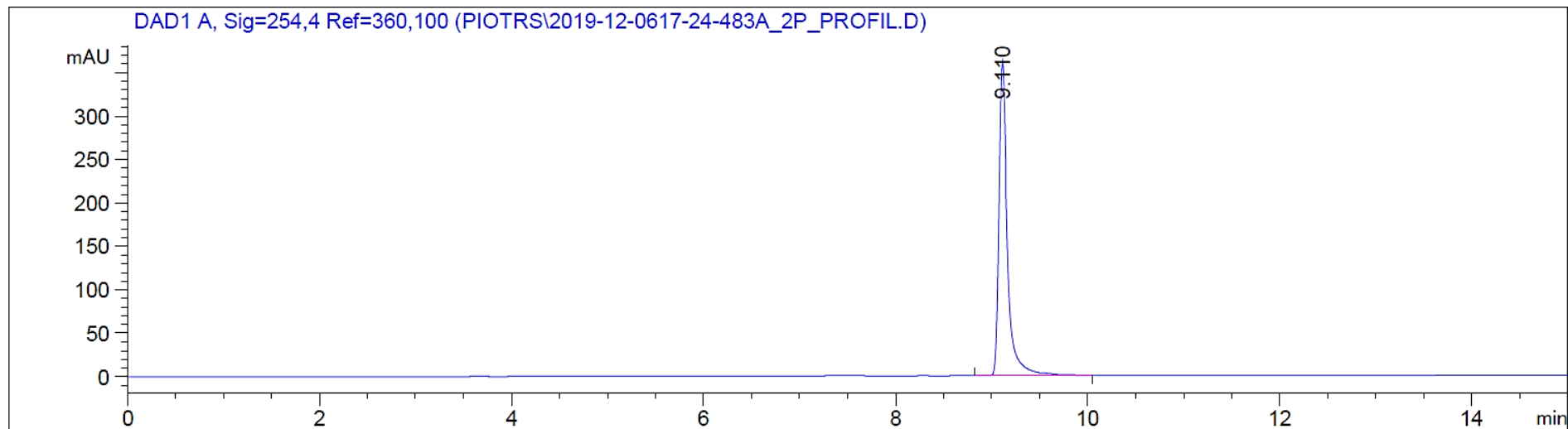
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Compound 1-2': TMGpppG-2'-O-C(O)-NH-CH₂-CH₂-N₃ (NH₄⁺ salt)

Chemical structure

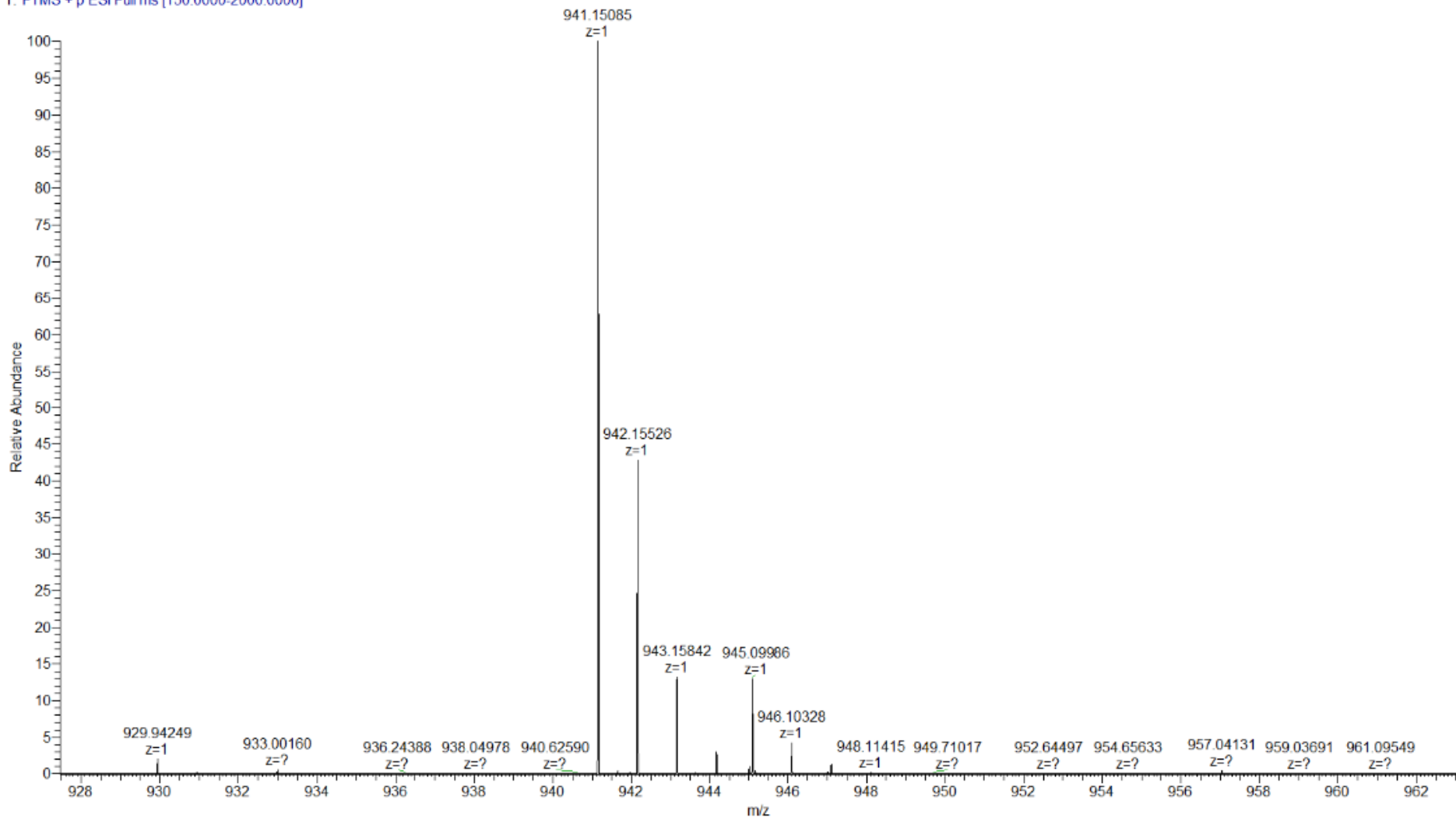


RP-HPLC (conditions c)

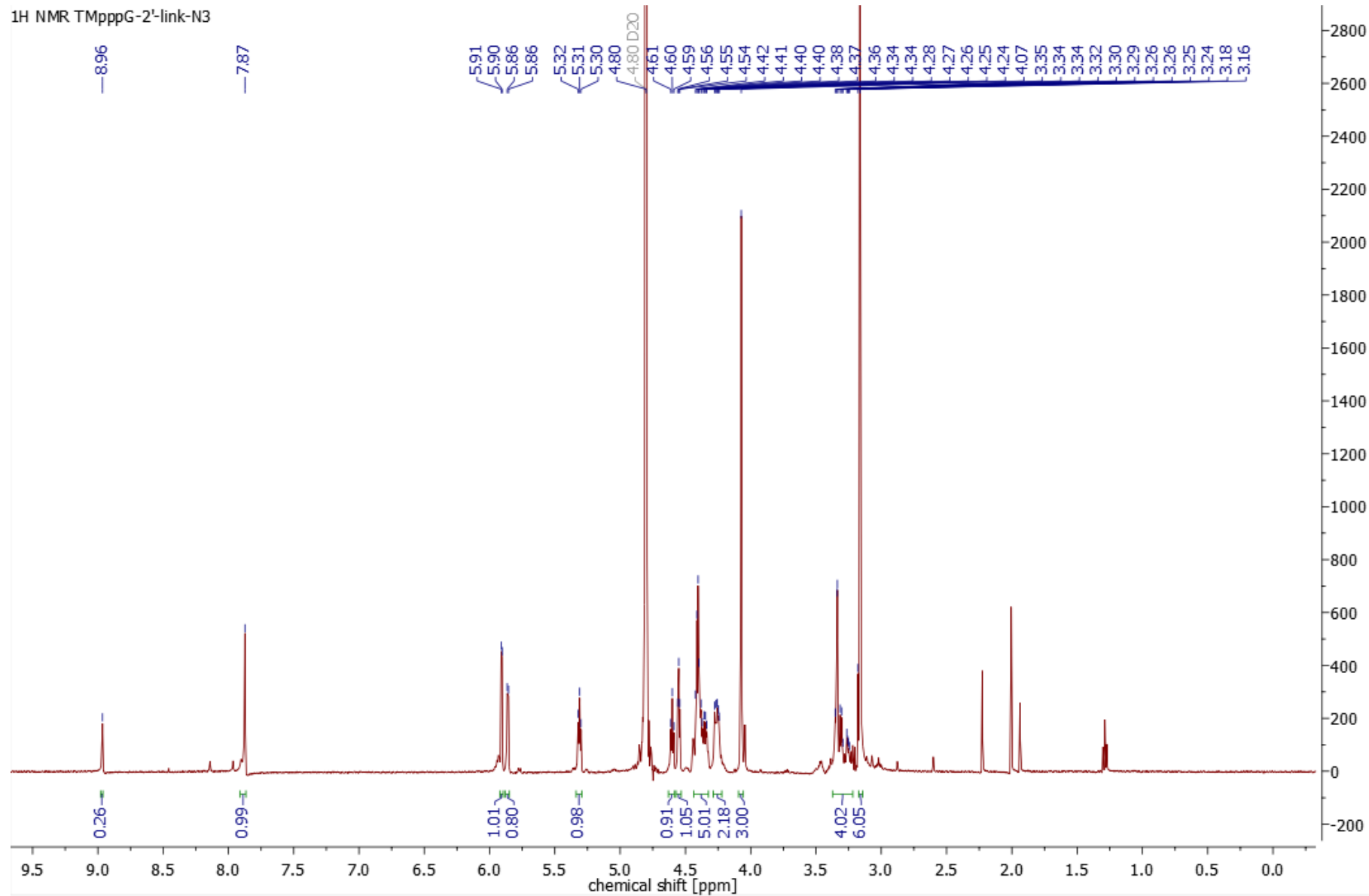


MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₆N₁₄O₁₉P₃ : 941.1500, found: 941.15085)

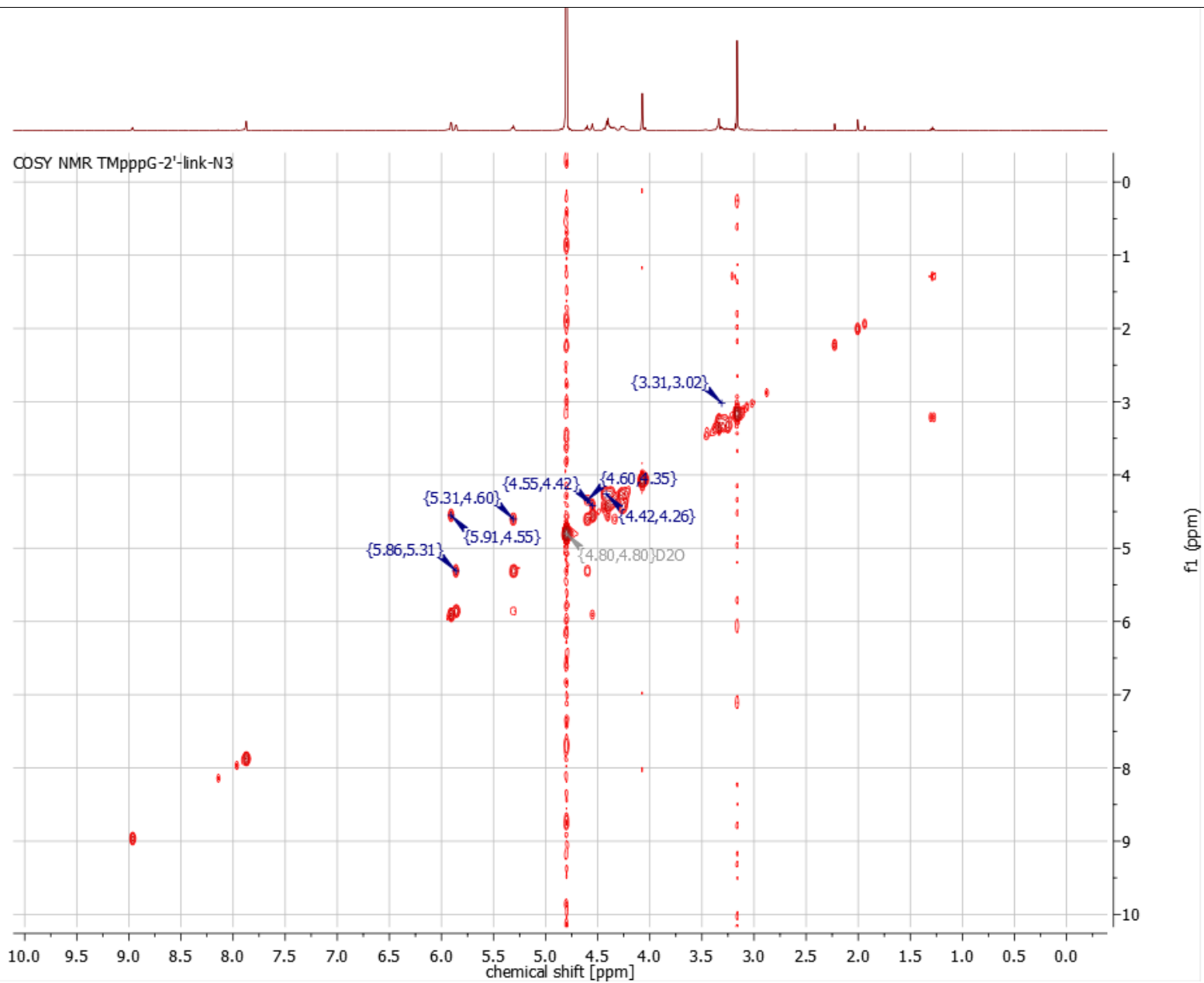
191220_PSu_30 #130-219 RT: 1.25-2.11 AV: 90 NL: 2.33E6
T: FTMS + p ESI Full ms [150.0000-2000.0000]



¹H NMR (500 Hz, D₂O, 25°C)

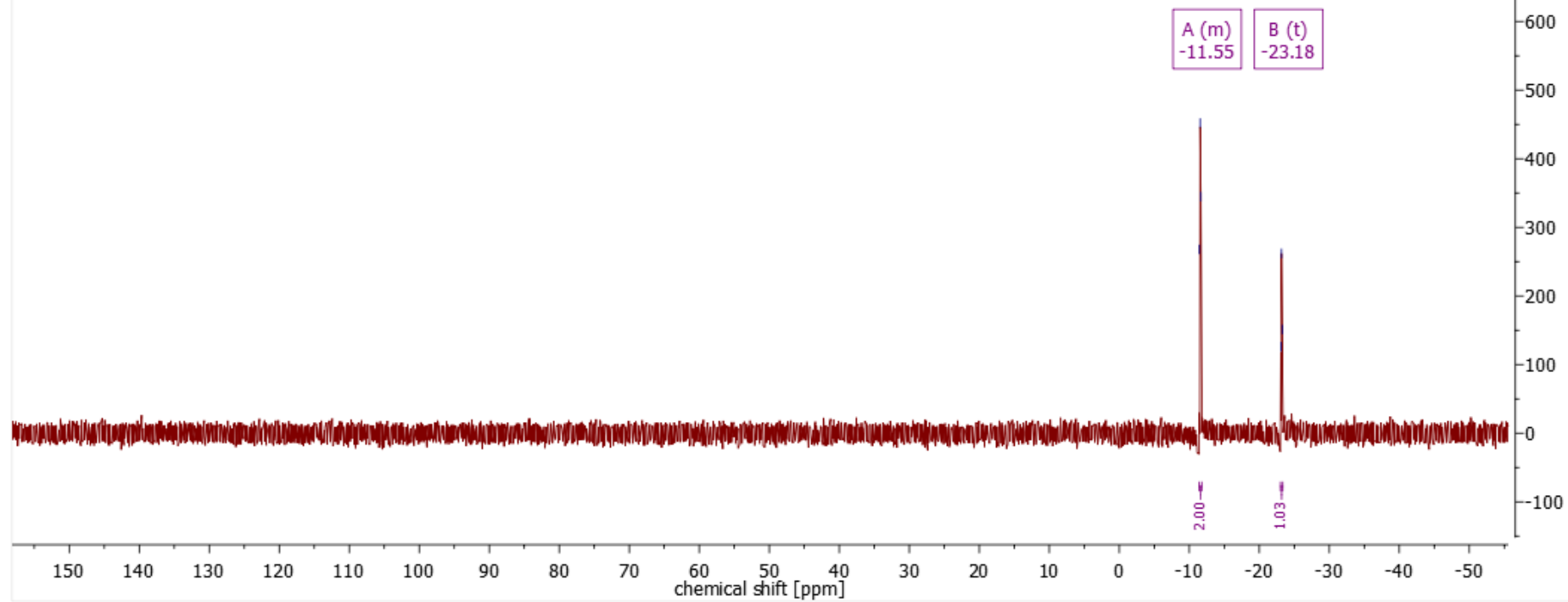
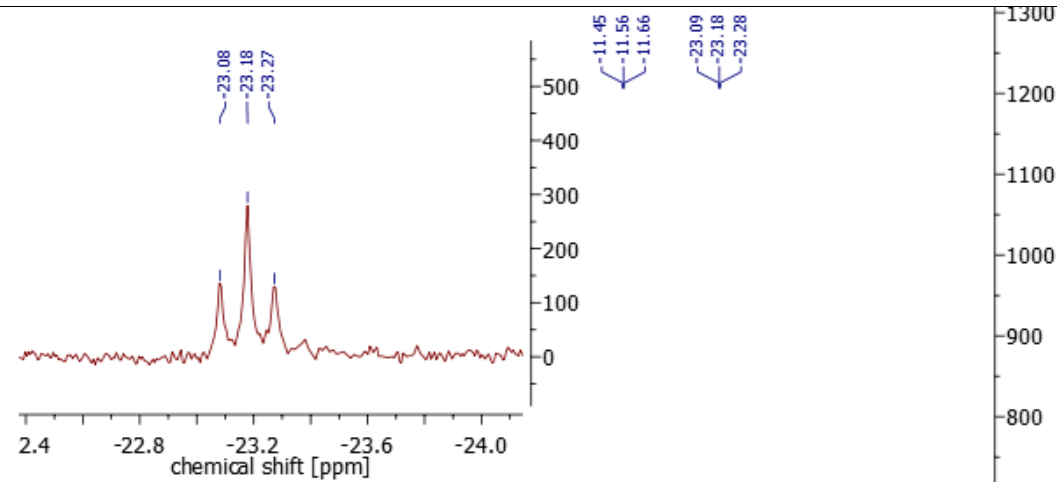
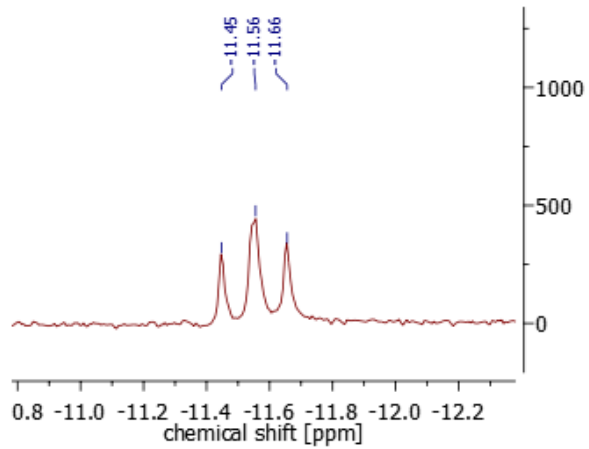


COSY NMR



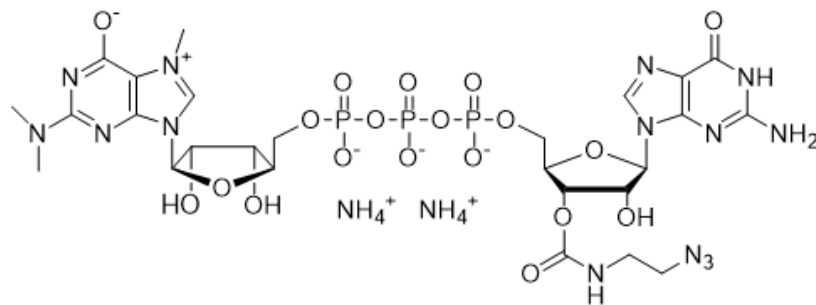
^{31}P NMR (203 MHz, D_2O , H_3PO_4 , 25°C)

^{31}P NMR TMpppG-2'-link-N3

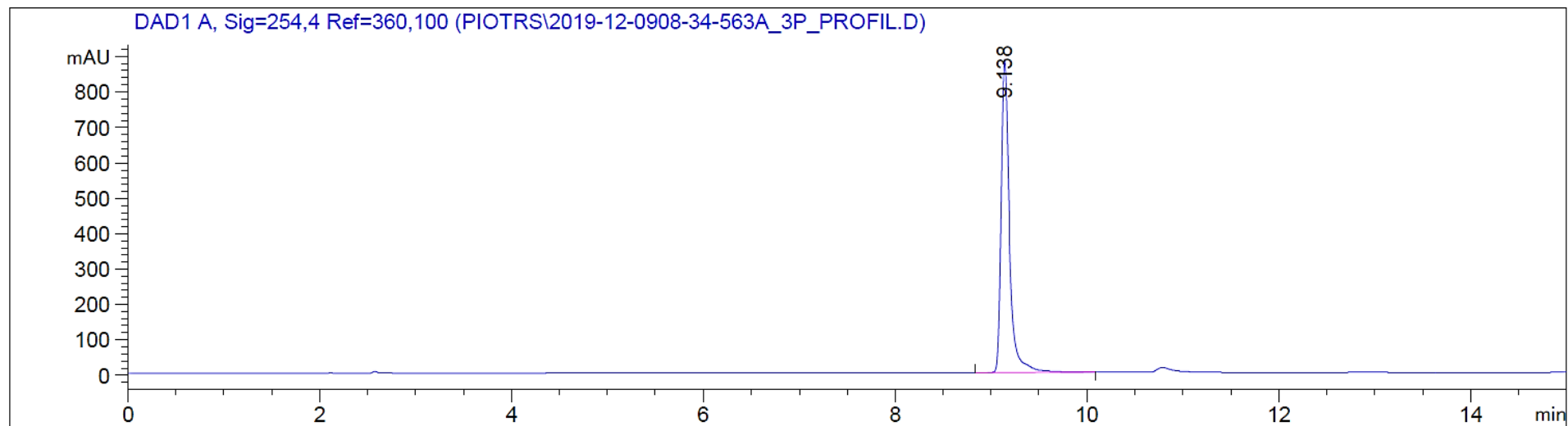


Compound 1-3': TMGpppG-3'-O-C(O)-NH-CH₂-CH₂-N₃ (NH₄⁺ salt)

Chemical structure

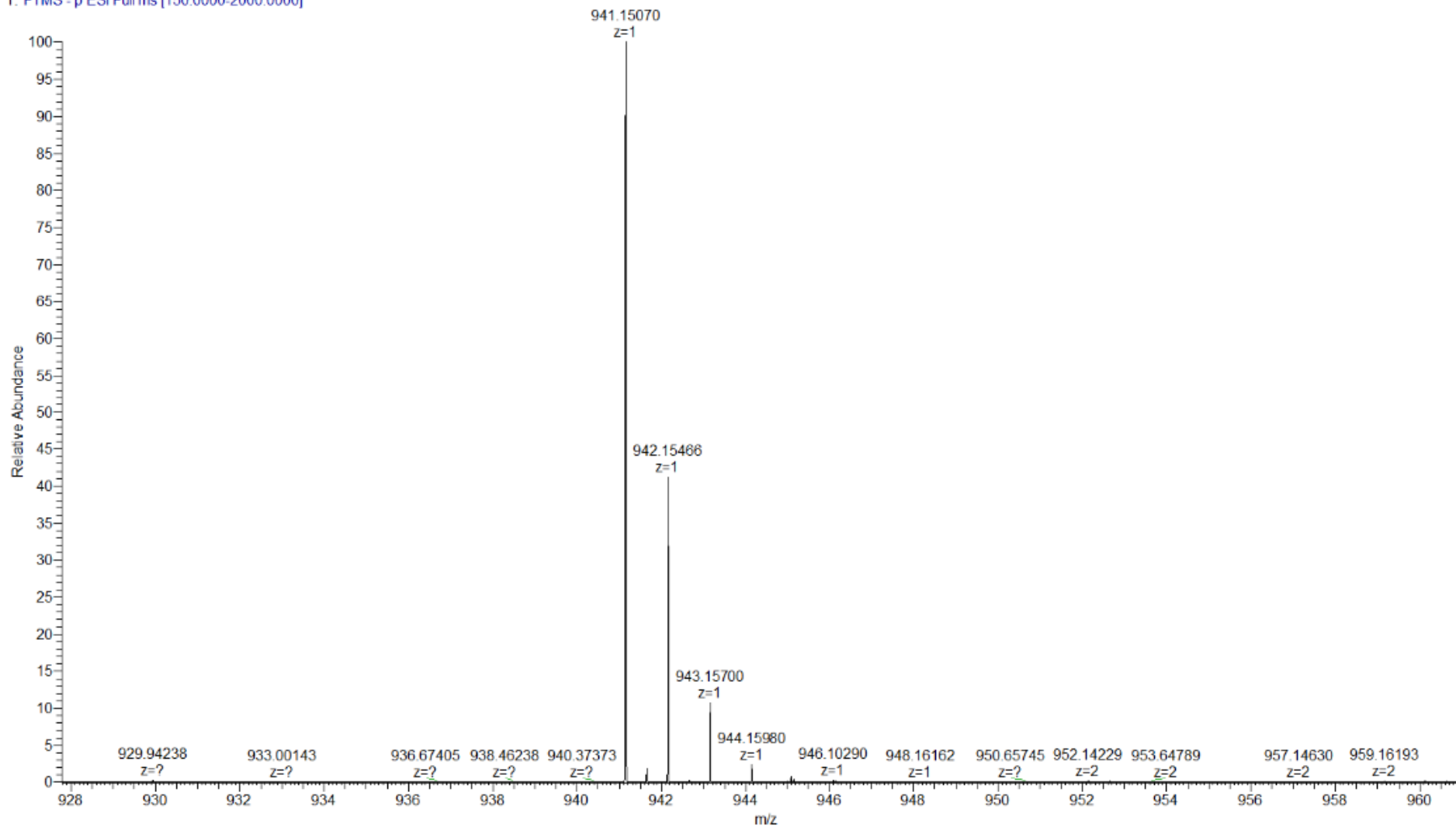


RP-HPLC (conditions c)

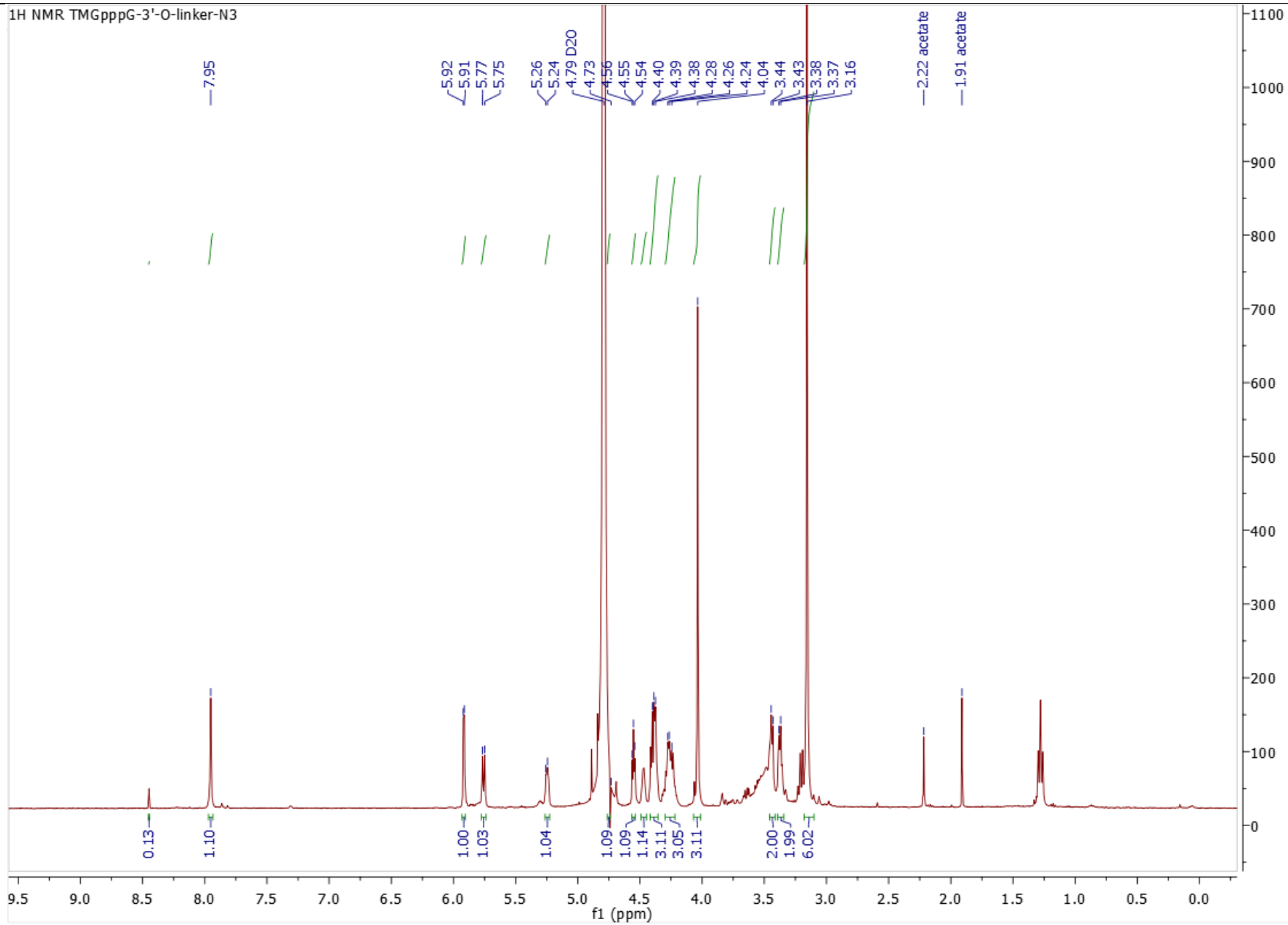


MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₆N₁₄O₁₉P₃ : 941.1500, found: 941.15070)

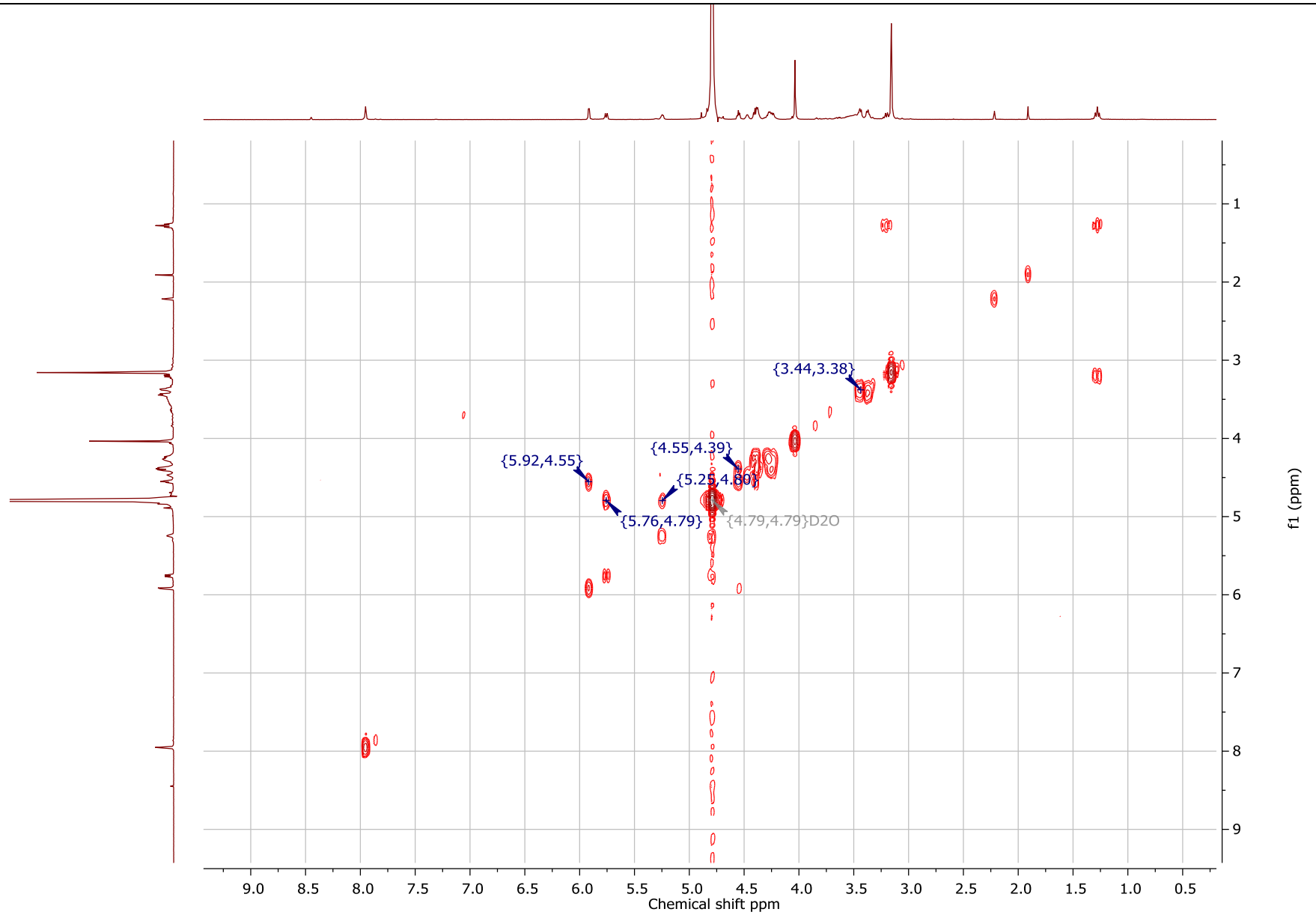
191220_PSu_31#6-102 RT: 0.06-0.98 AV: 97 NL: 1.04E7
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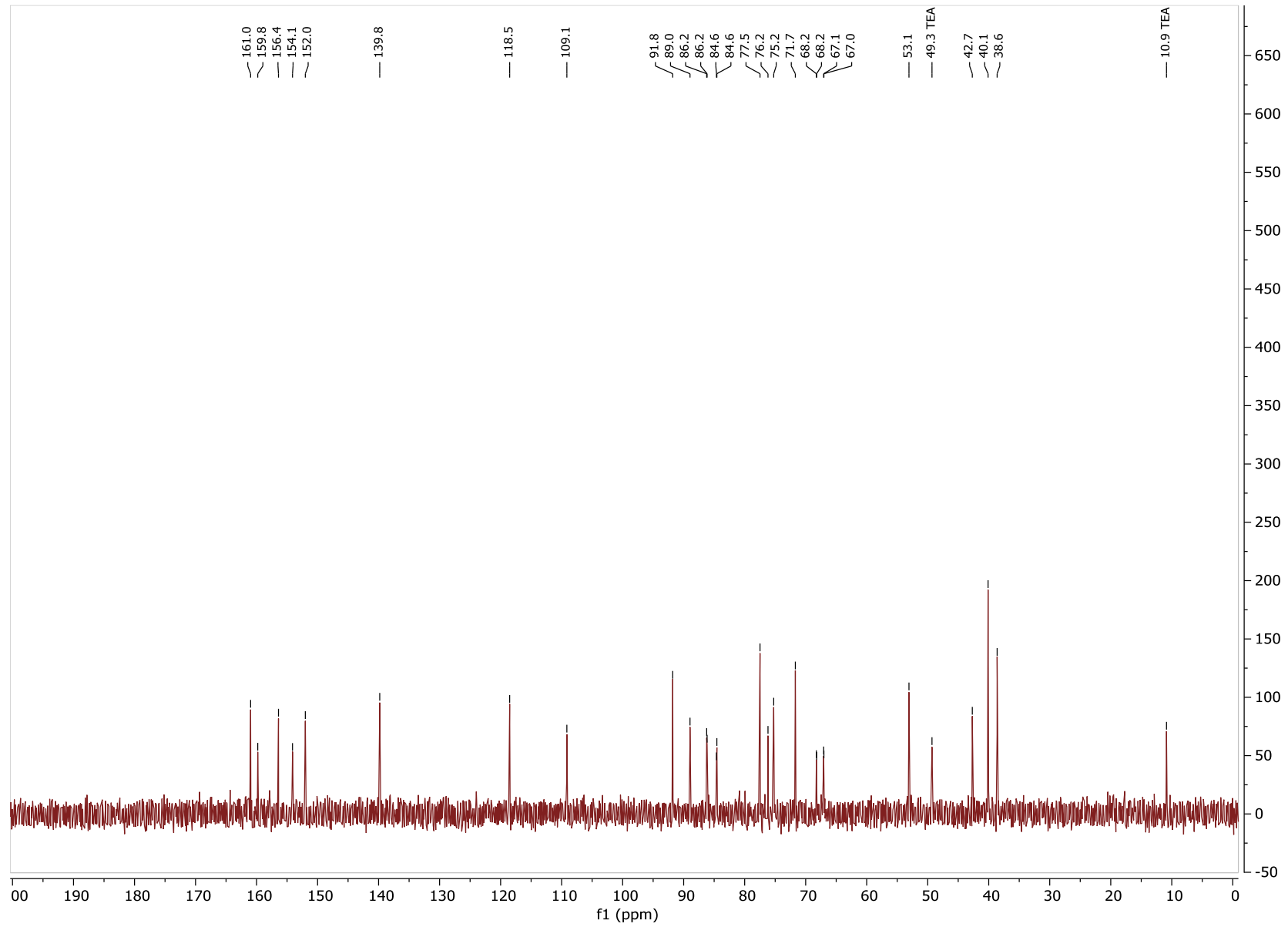
¹H NMR (400 MHz, D₂O, 25°C)



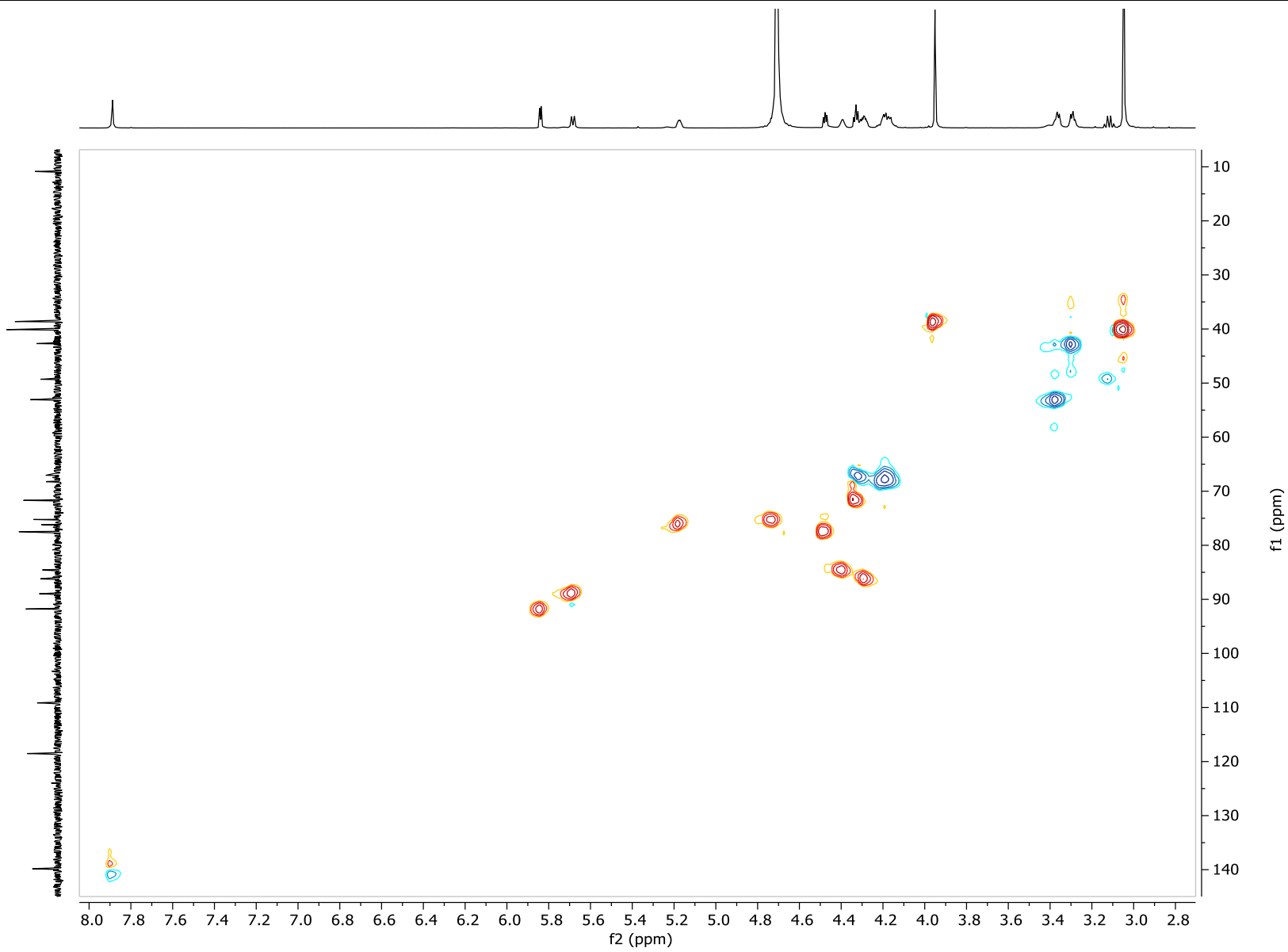
COSY NMR



¹³C NMR (400 MHz, D₂O, 25°C)

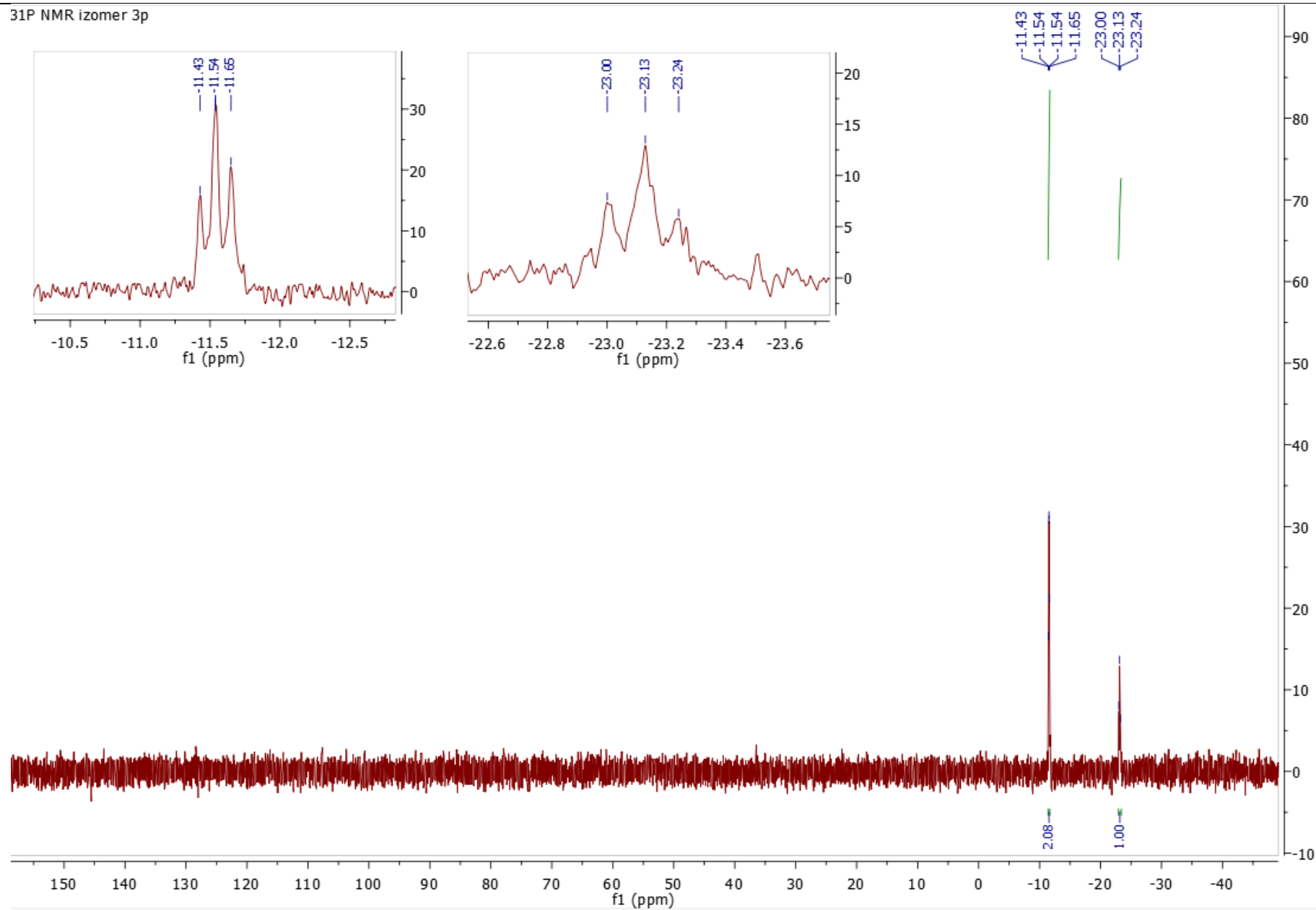


HSQC NMR



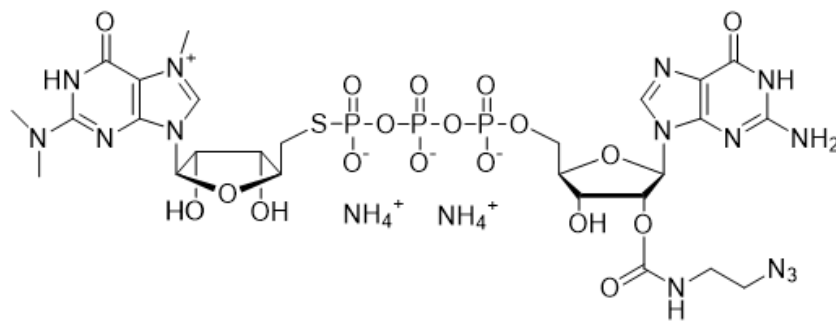
^{31}P NMR (162 MHz, D_2O , H_3PO_4 , 25°C)

^{31}P NMR izomer 3p

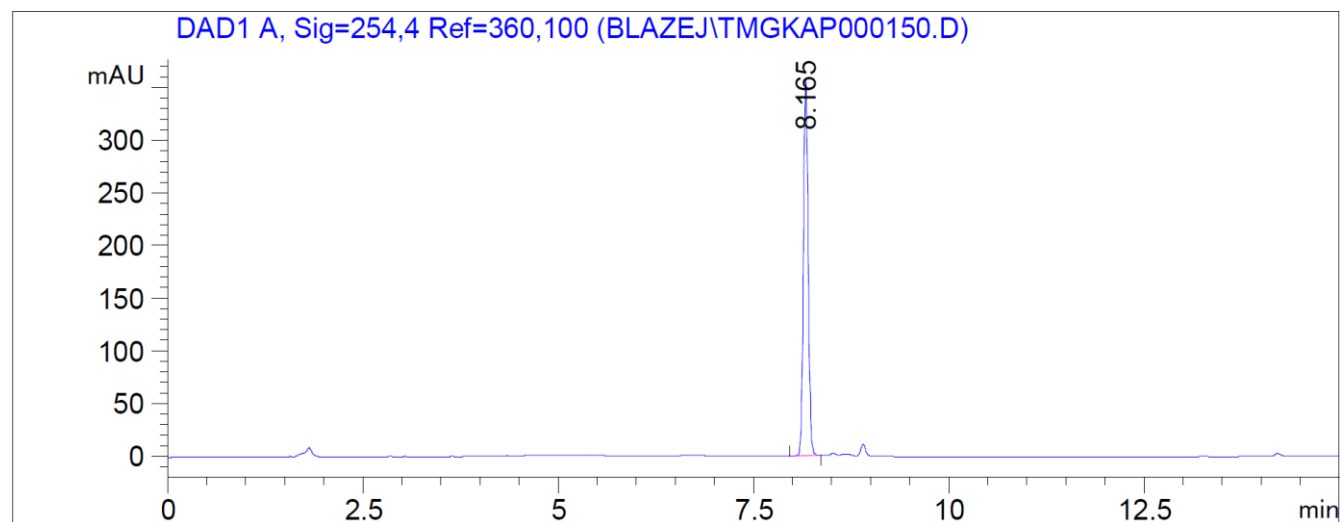


Compound 2-2': TMG-5'-S-pppG-2'-O-C(O)NH-CH₂CH₂N₃ (NH₄⁺ salt)

Chemical structure

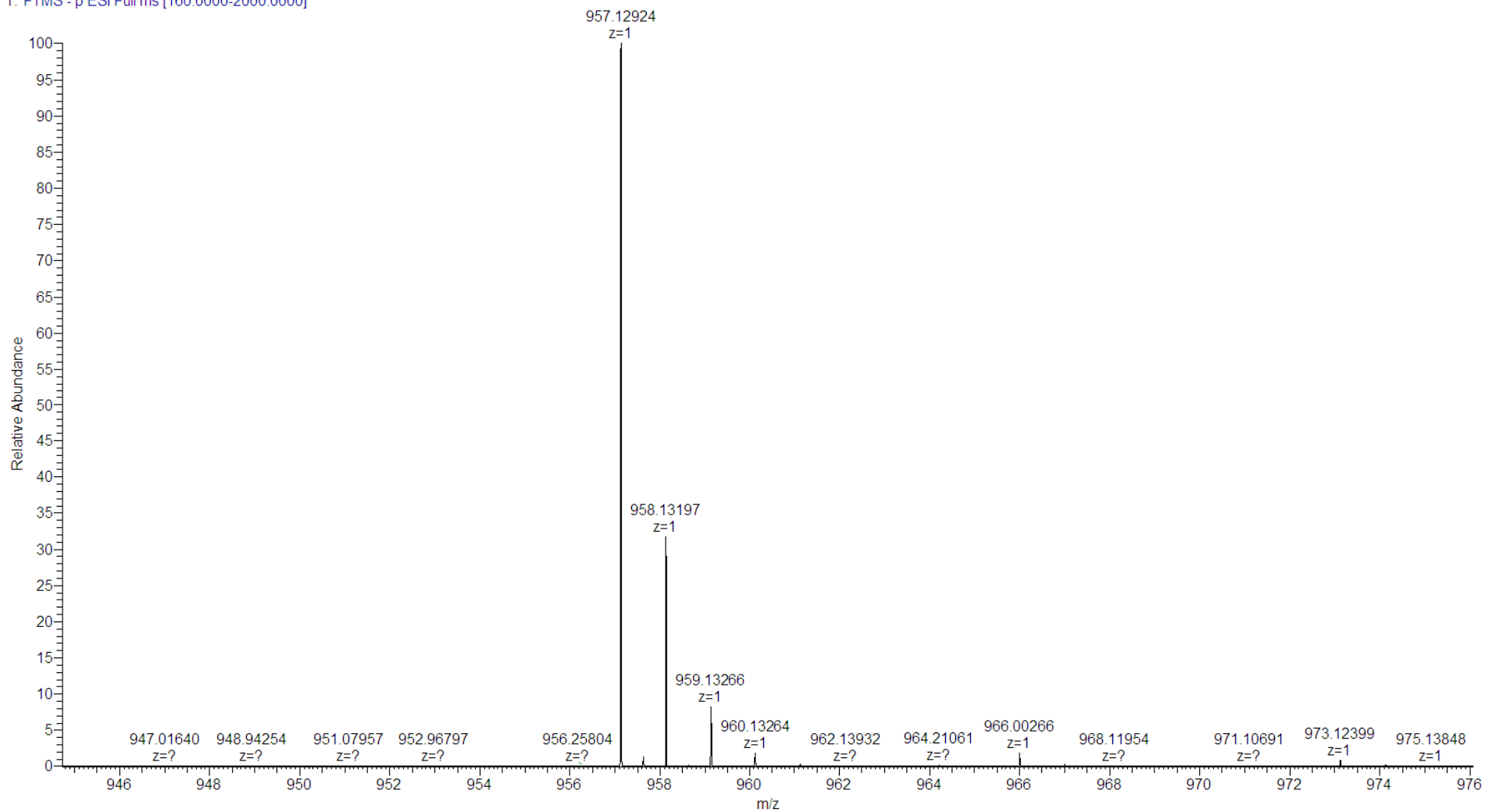


RP-HPLC (conditions c)

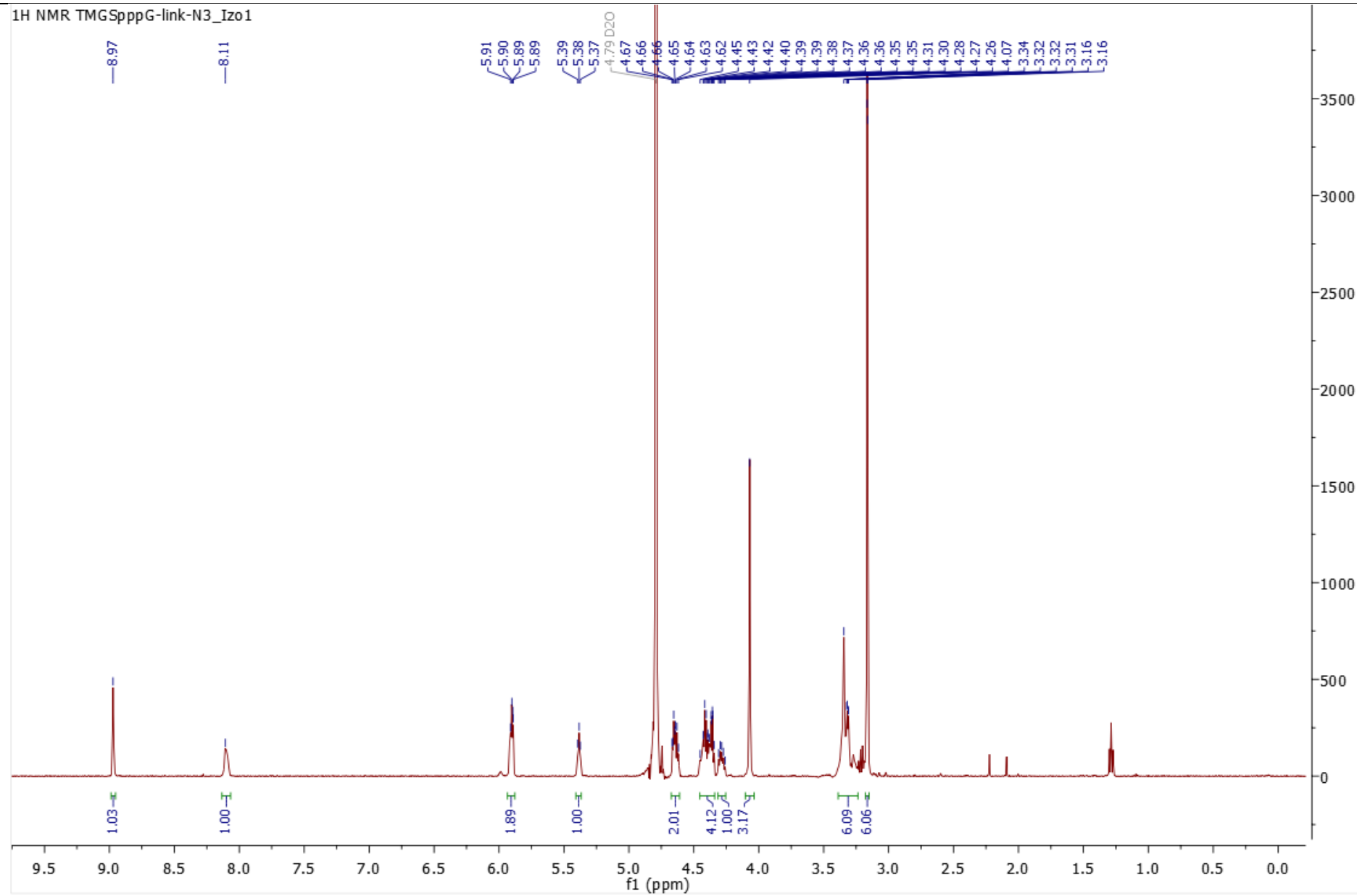


220329_PSu_08 #340-467 RT: 2.98-4.09 AV: 128 NL: 6.71E5
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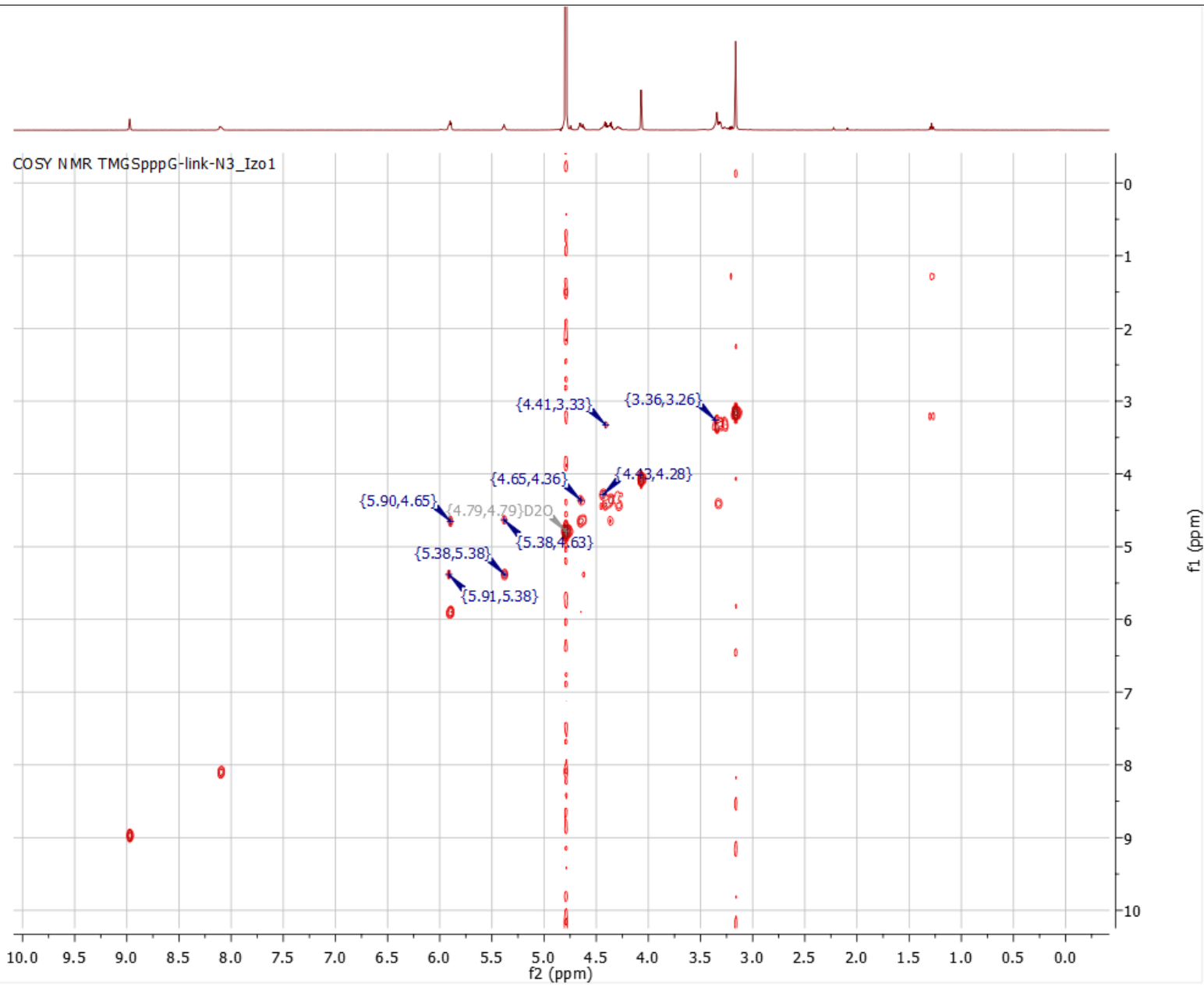
MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₆N₁₄O₁₈P₃S⁻ : 957.1271, found: 957.12924)

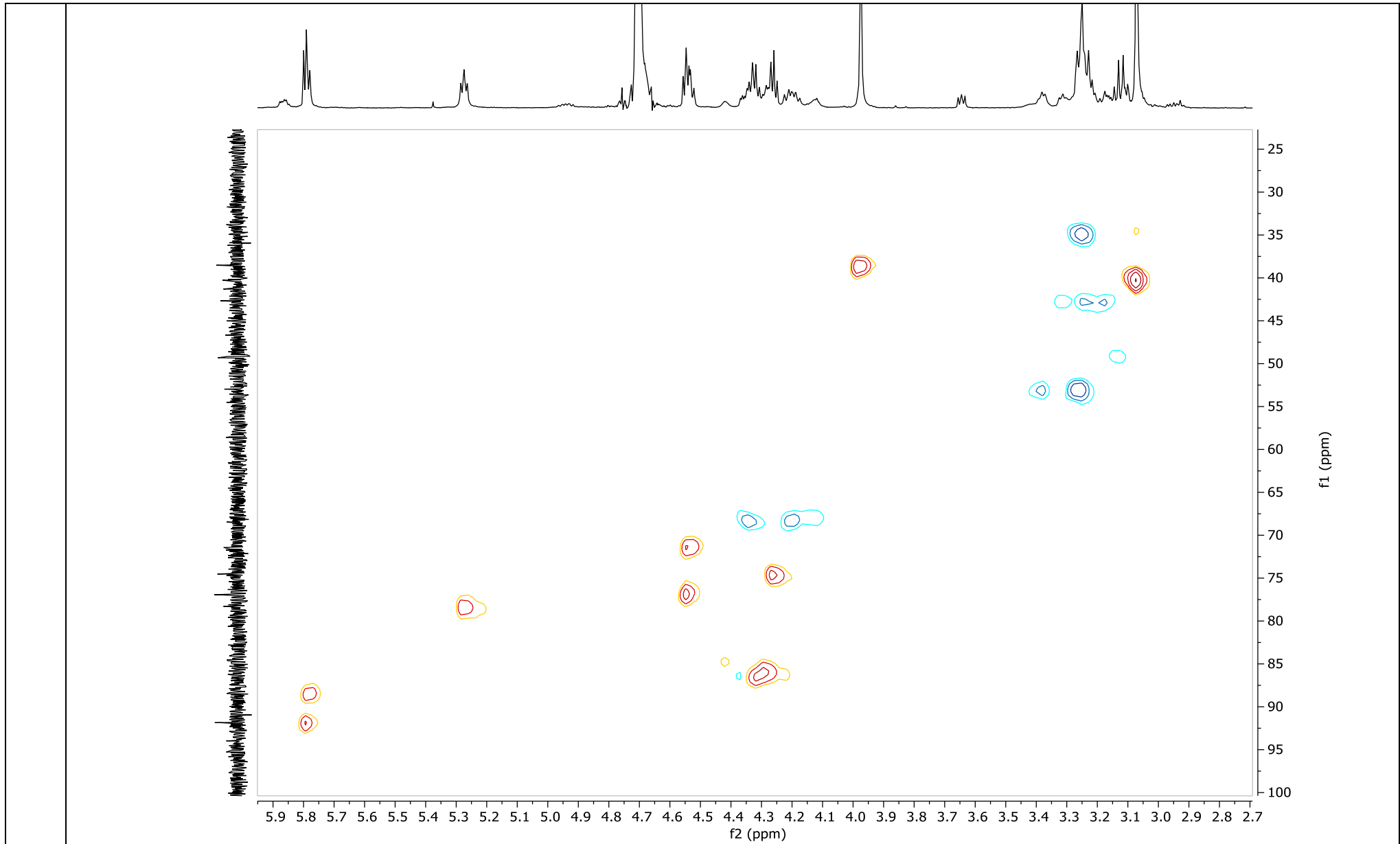


¹H NMR (500 MHz, D₂O, 25°C)

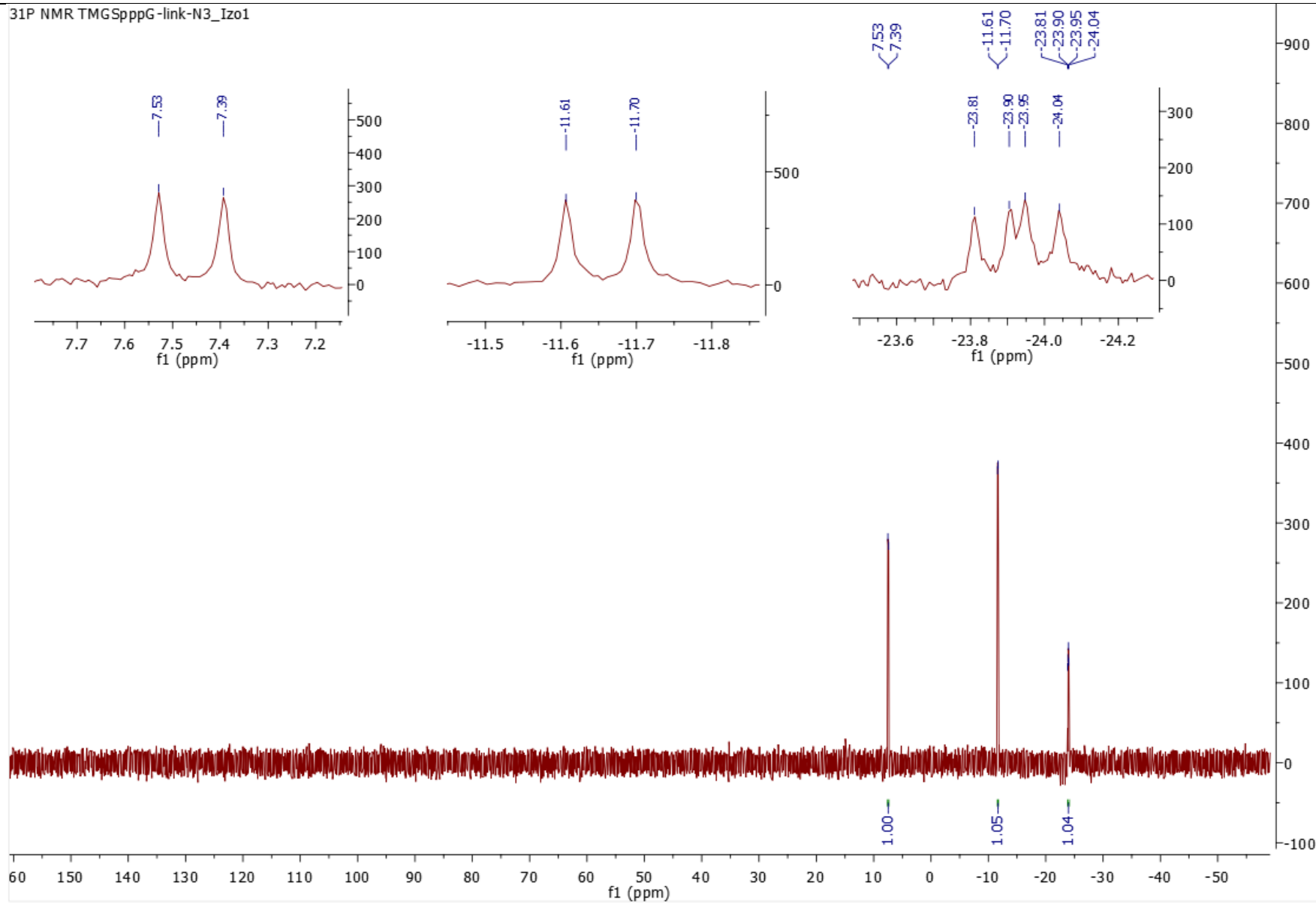


COSY NMR



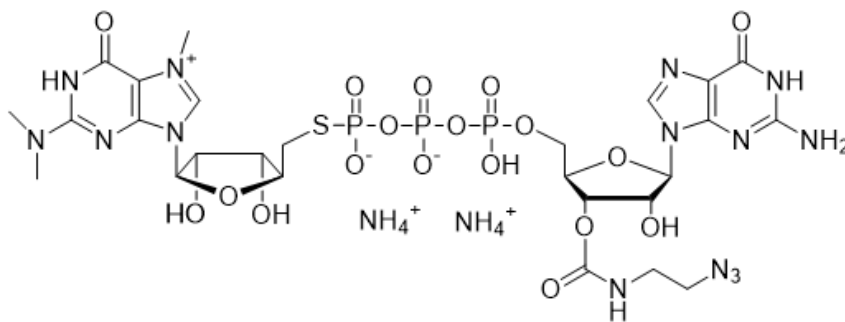


^{31}P NMR (203 MHz, D_2O , H_3PO_4 , 25°C)

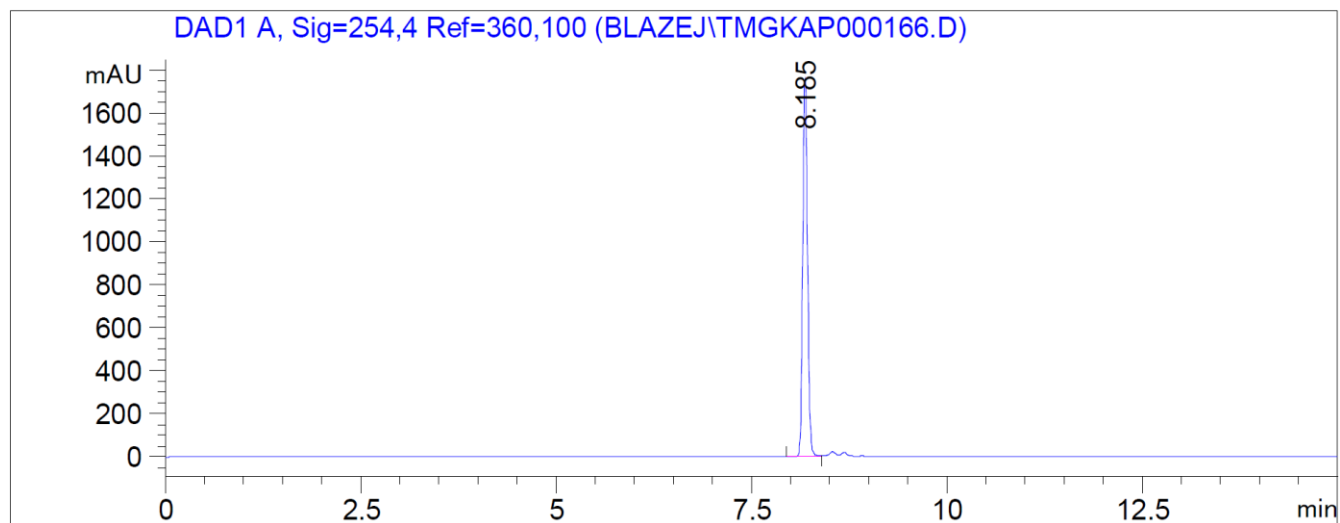


Compound 2-3': TMG-5'-S-pppG-3'-O-C(O)NH-CH₂CH₂N₃ (NH₄⁺ salt)

Chemical structure

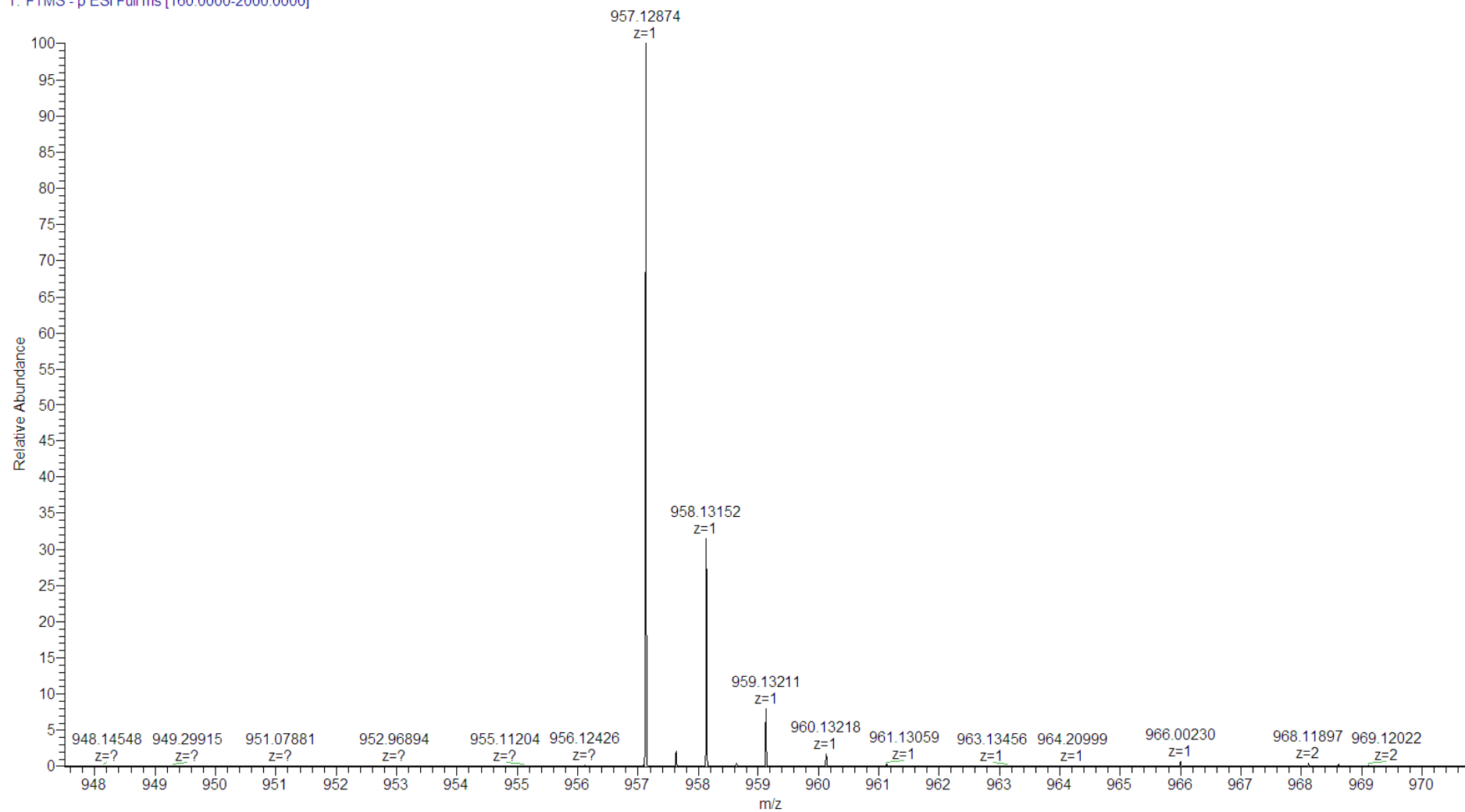


RP-HPLC (conditions c)

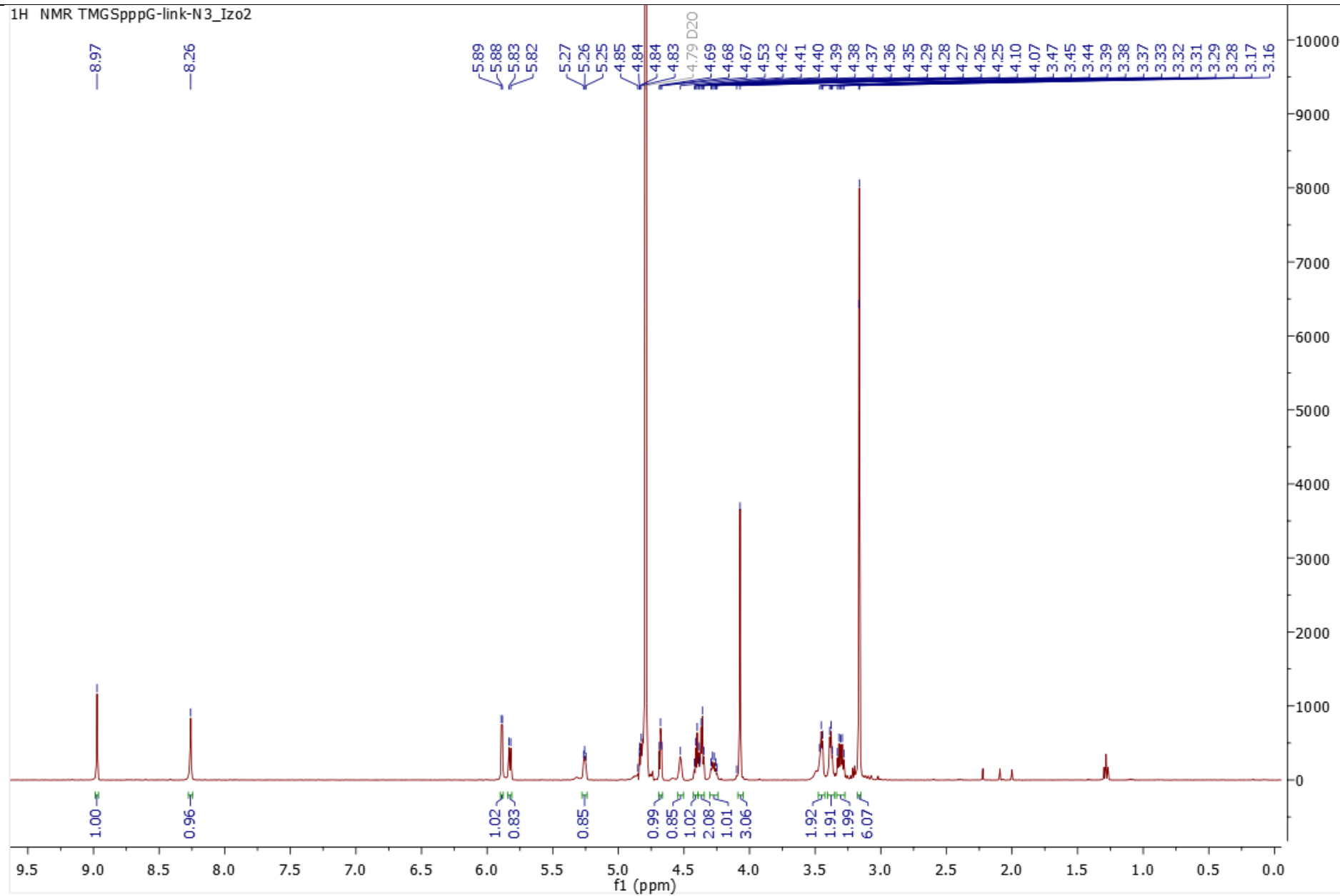


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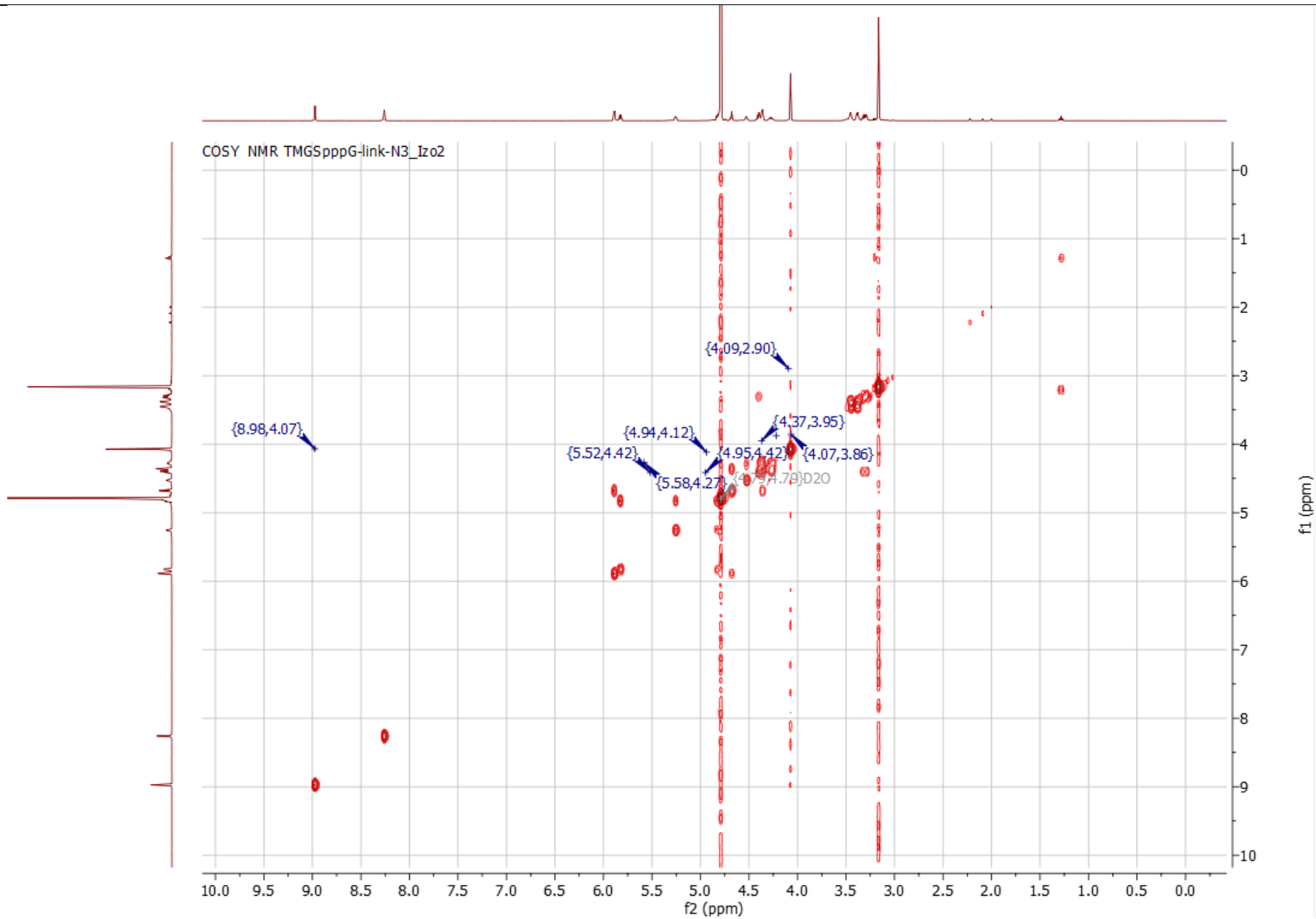
MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₆N₁₄O₁₈P₃S₃: 957.1271, found: 957.12874)



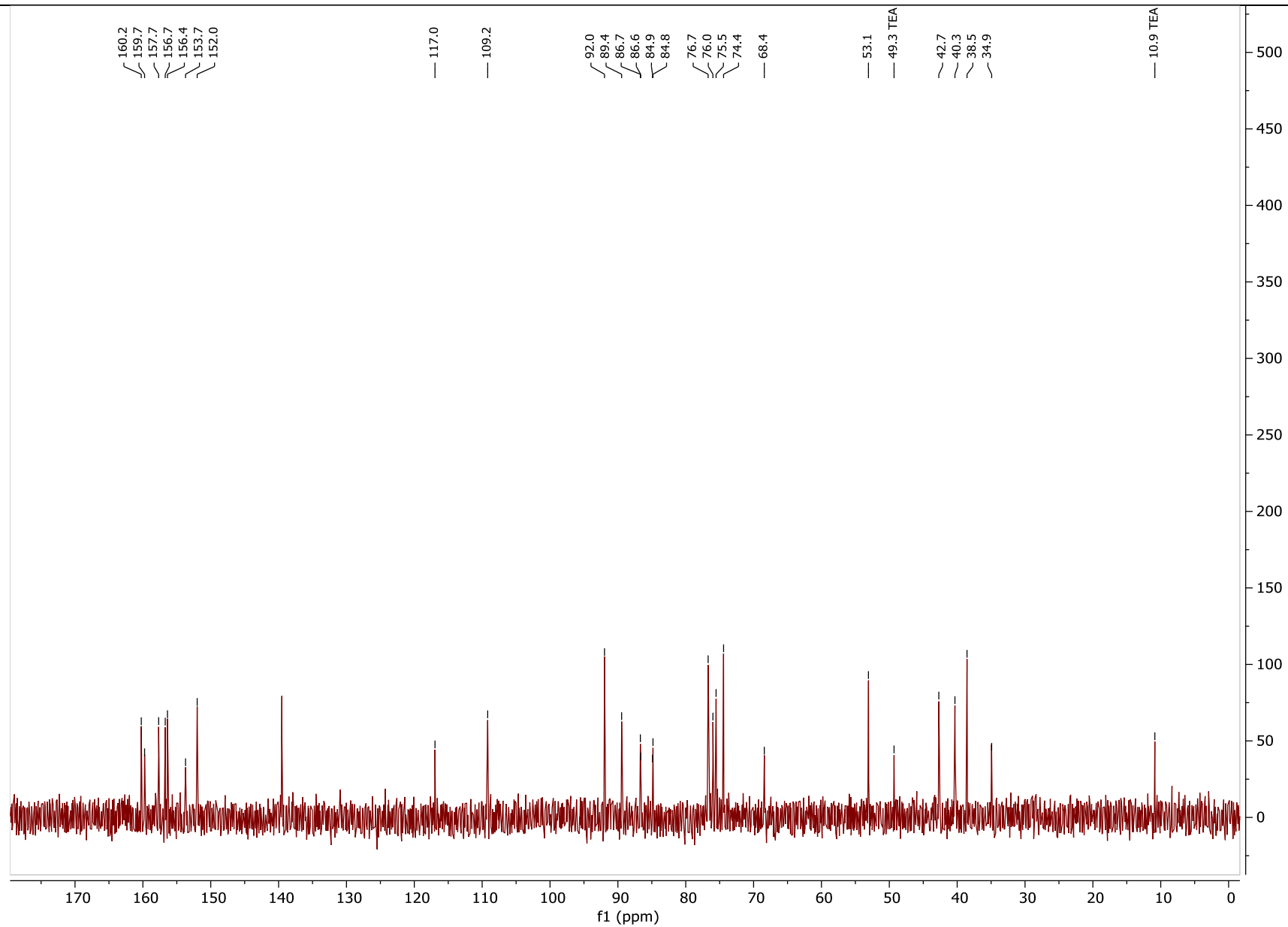
¹H NMR (500 MHz, D₂O, 25°C)



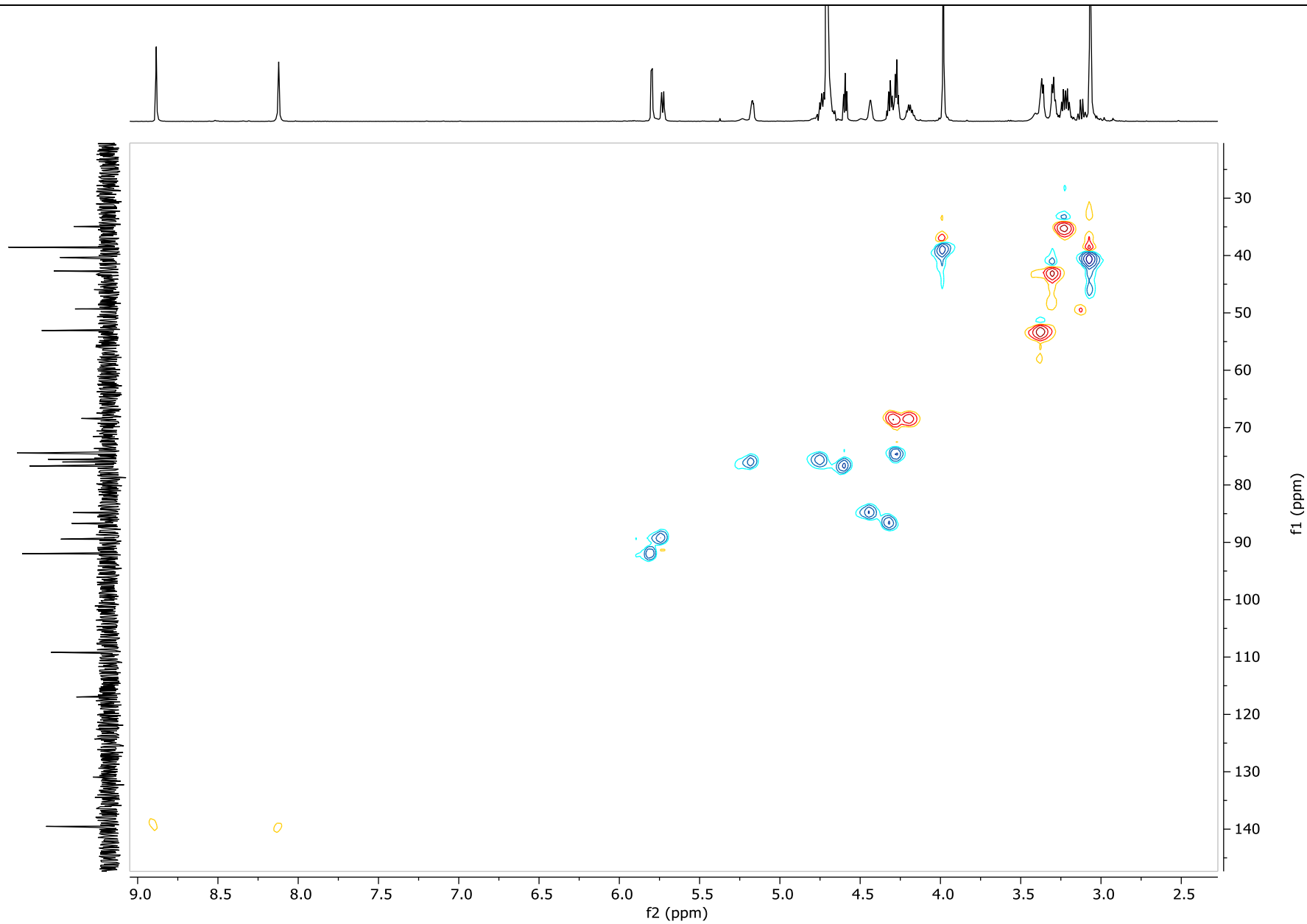
COSY NMR



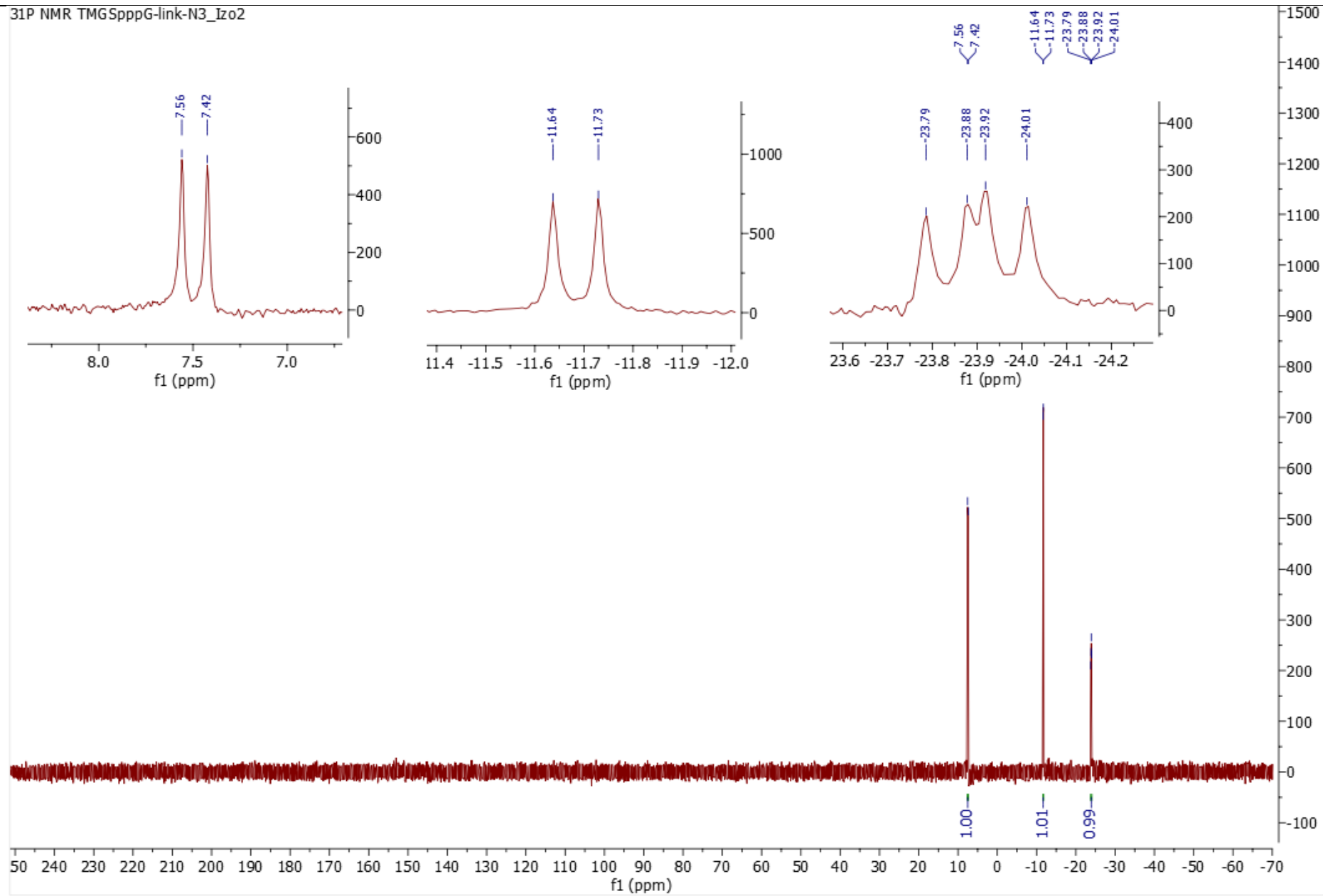
^{13}C NMR (500 MHz, D_2O , 25°C)



HSQC NMR

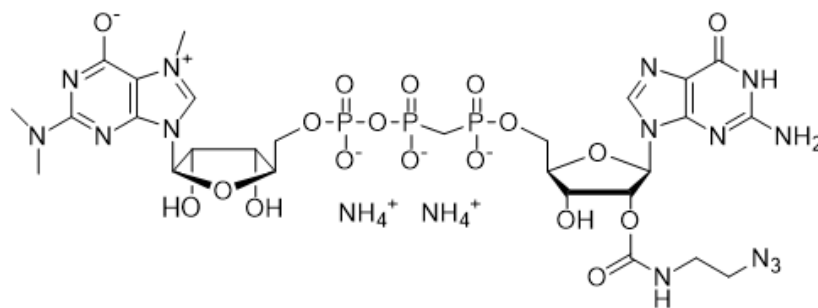


^{31}P NMR (203 MHz, D_2O , H_3PO_4 , 25°C)

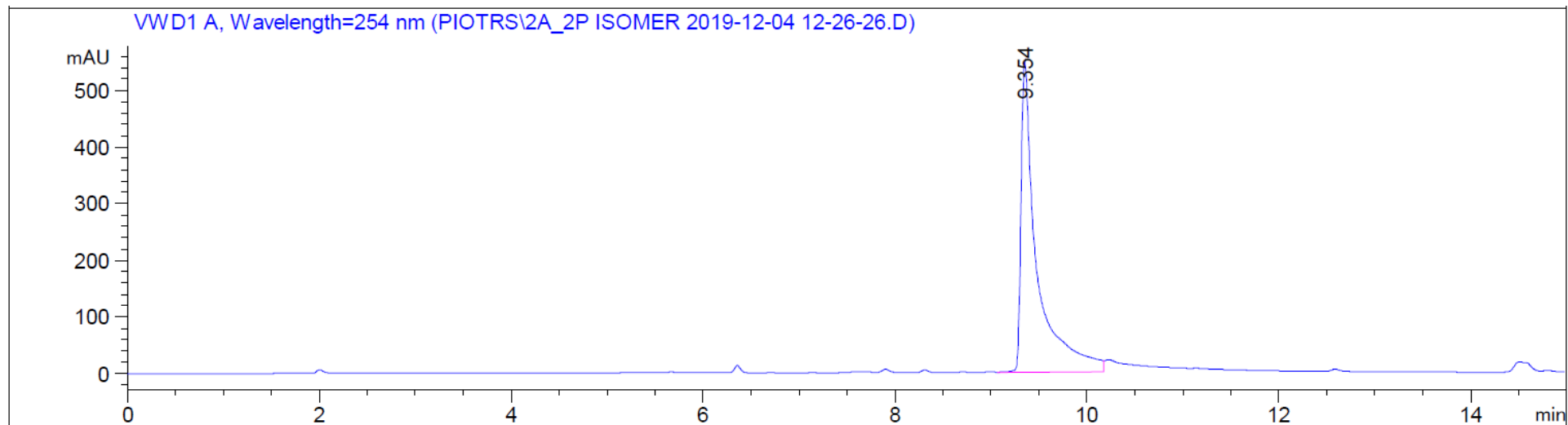


Compound 3-2': TMGppCH₂pG-2'-O-C(O)NH-CH₂CH₂N₃ (NH₄⁺ salt)

Chemical structure

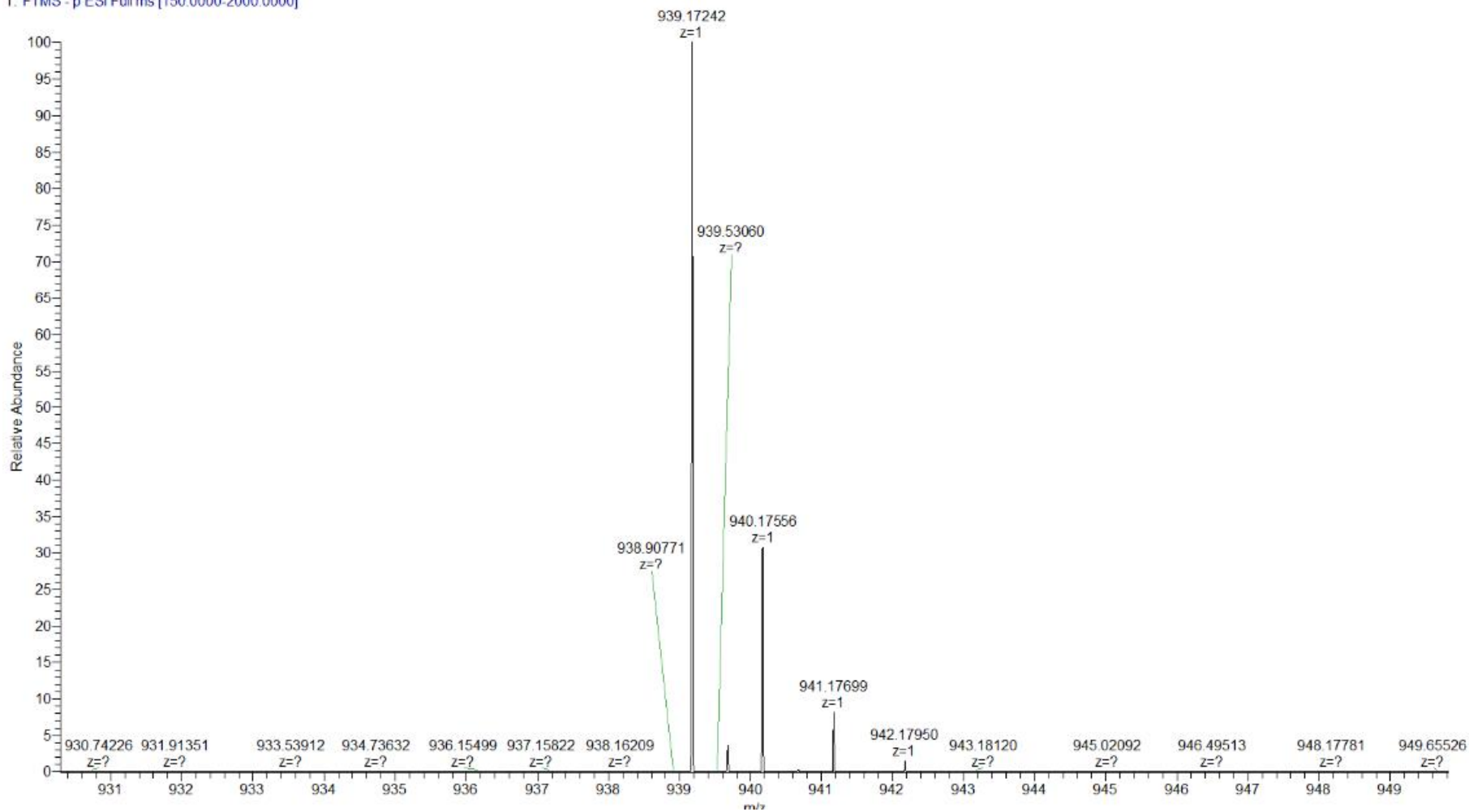


RP-HPLC (conditions c)



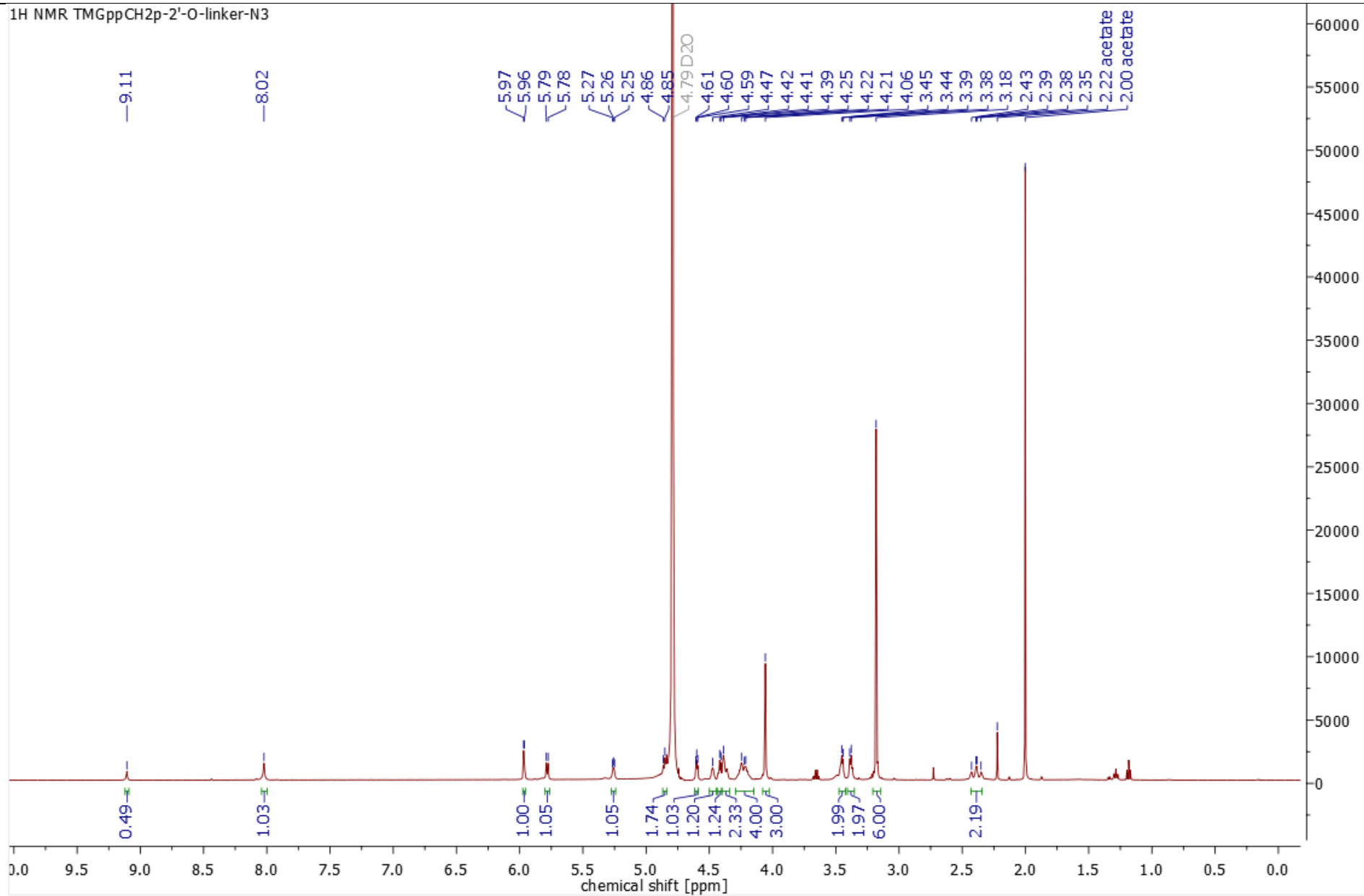
MS (-) ESI (Calc. [M-H]⁻ C₂₇H₃₈N₁₄O₁₈P₃ : 939.1707, found: 939.17242)

190528_PSU_12 #99-152 RT: 0.95-1.46 AV: 54 NL: 3.63E6
190528_PSU_12 #99-152 RT: 0.95-1.46 AV: 54 NL: 3.63E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

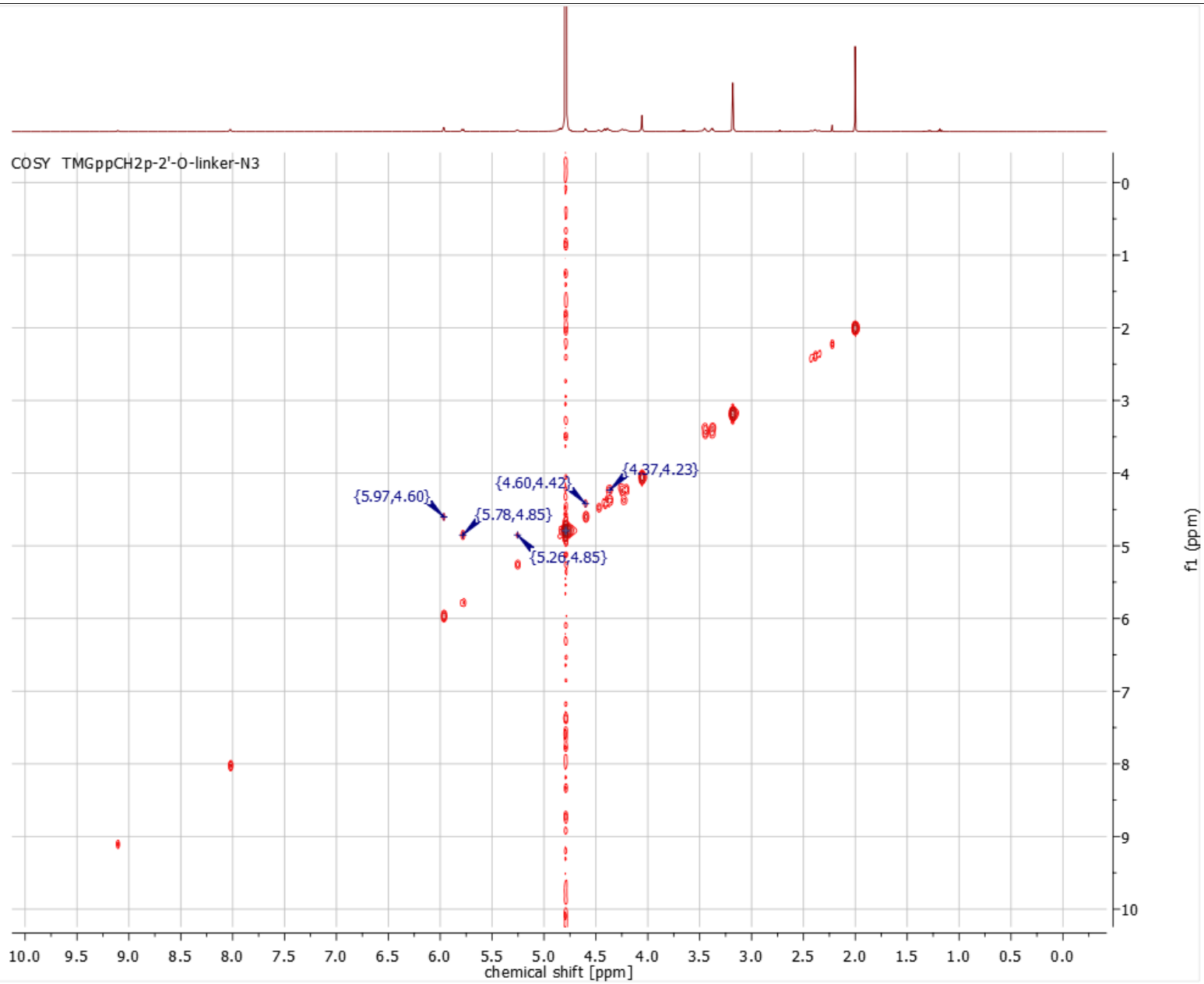


¹H NMR (400 MHz, D₂O, 25°C)

¹H NMR TMGppCH₂p-2'-O-linker-N3

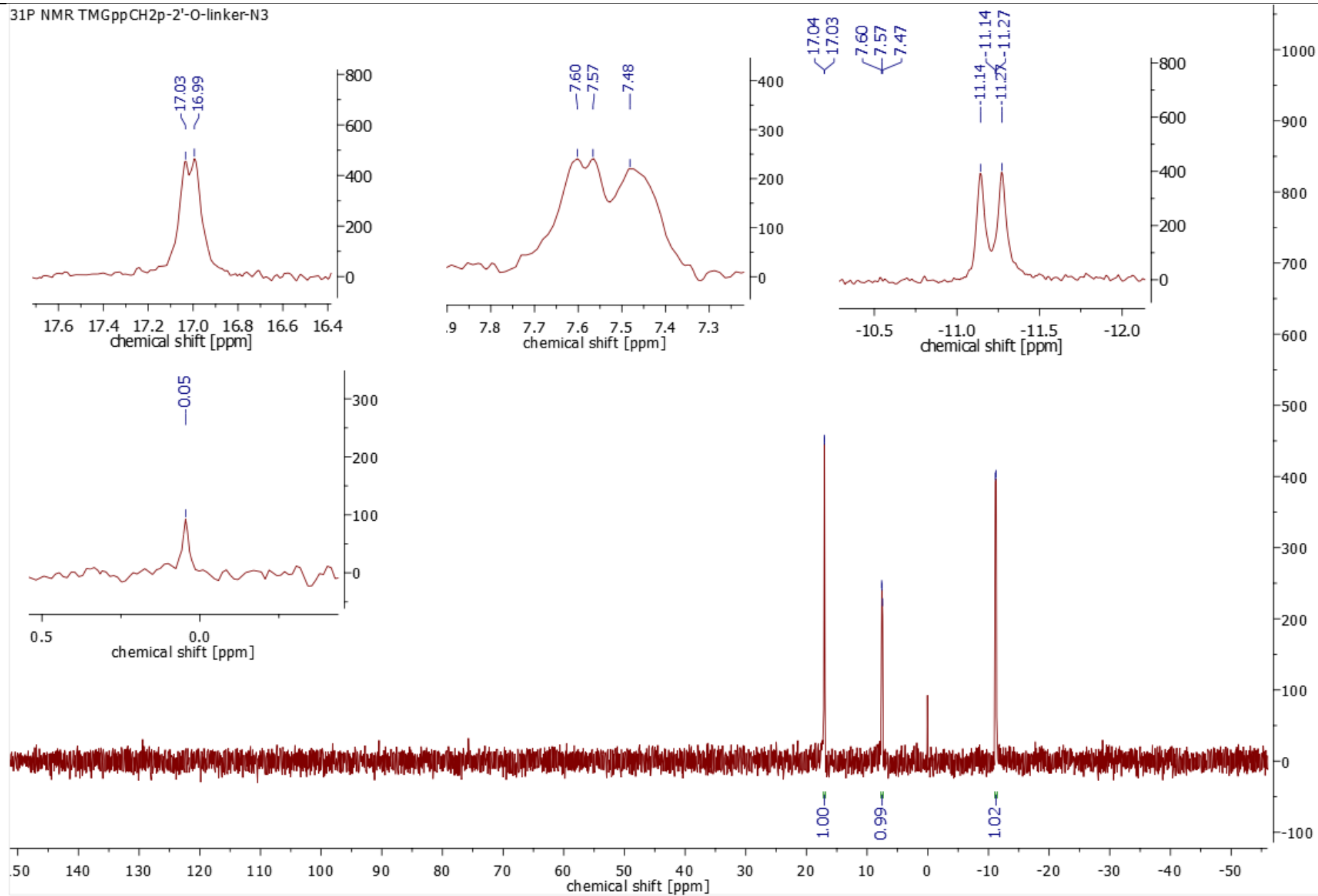


COSY NMR



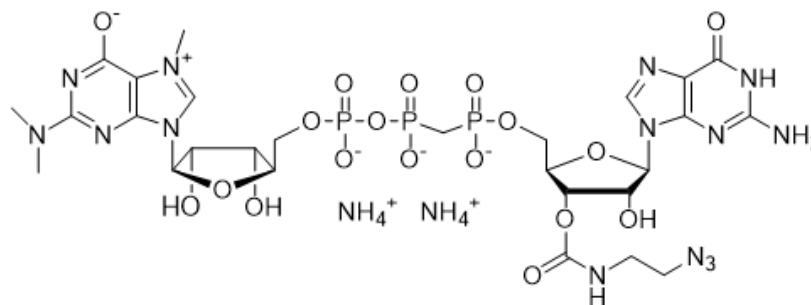
^{31}P NMR (202 MHz, D_2O , H_3PO_4 , 25°C)

31P NMR TMGppCH2p-2'-O-linker-N3

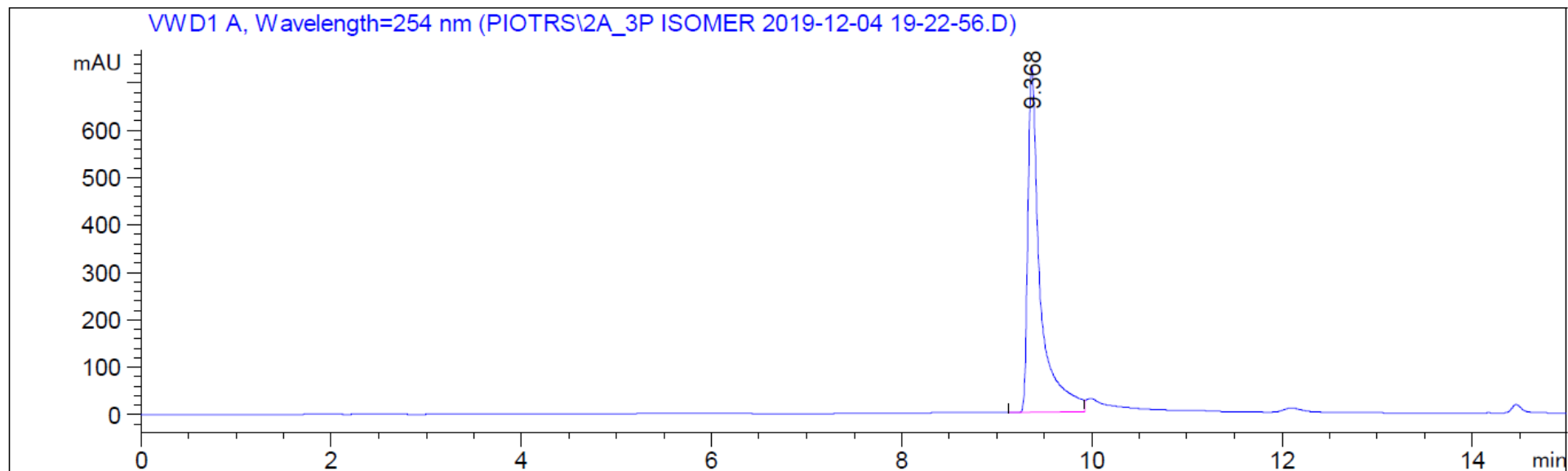


Compound 3-3': TMGppCH₂pG-3'-O-C(O)NH-CH₂CH₂N₃ (NH₄⁺ salt)

Chemical structure

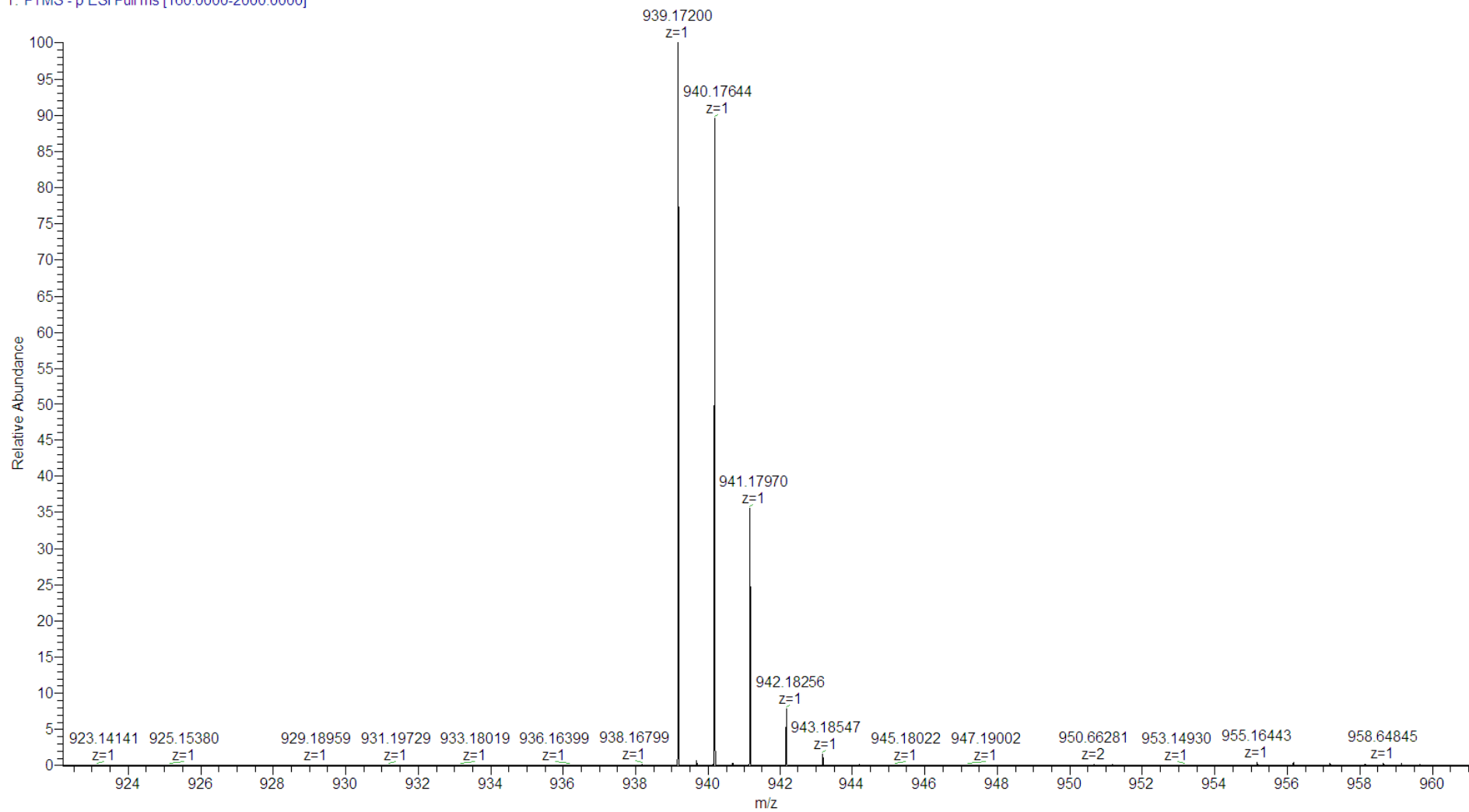


RP-HPLC (conditions c)

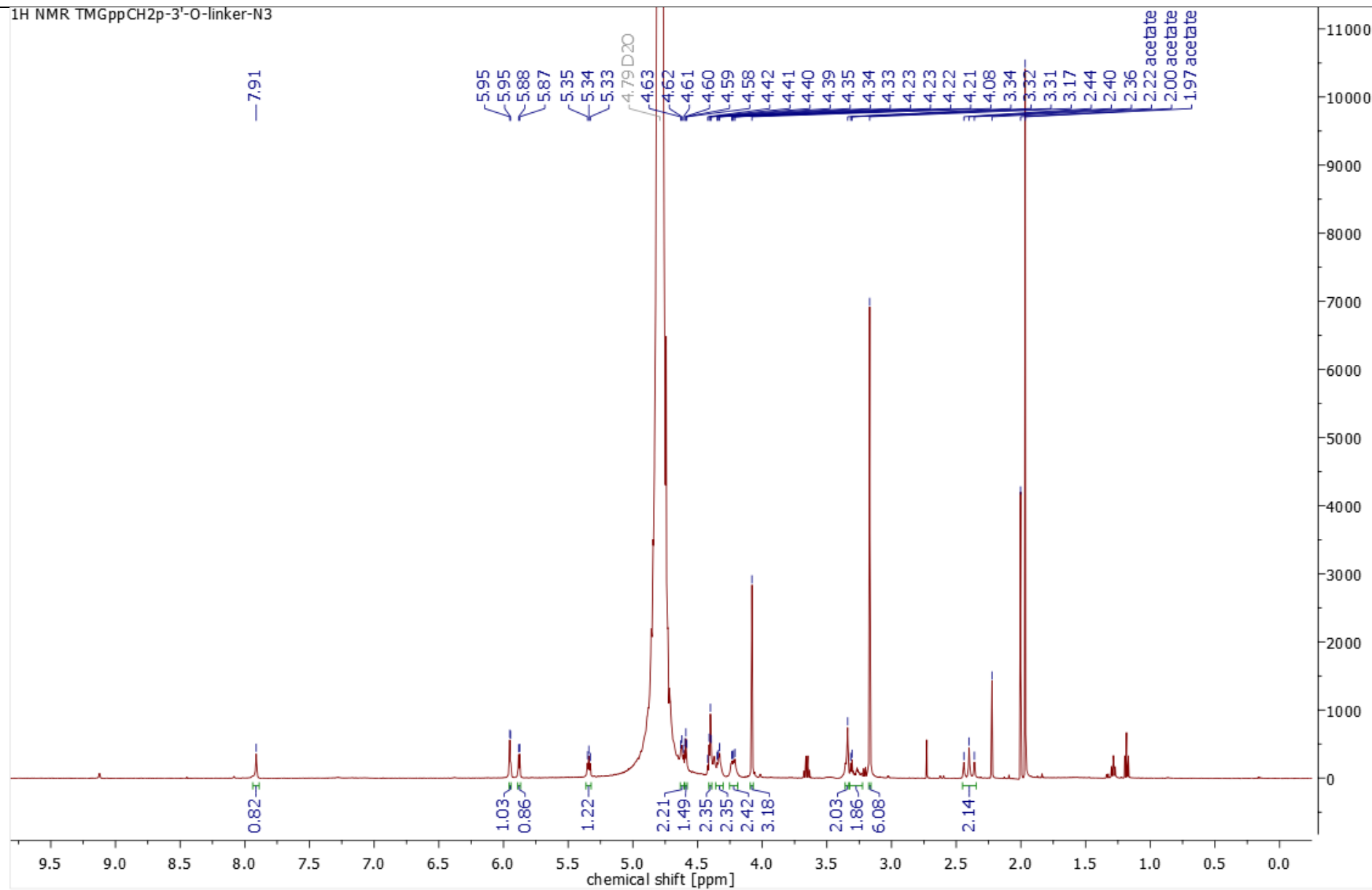


MS (-) ESI (Calc. [M-H]⁻ C₂₇H₃₈N₁₄O₁₈P₃ : 939.1707, found: 939.17200)

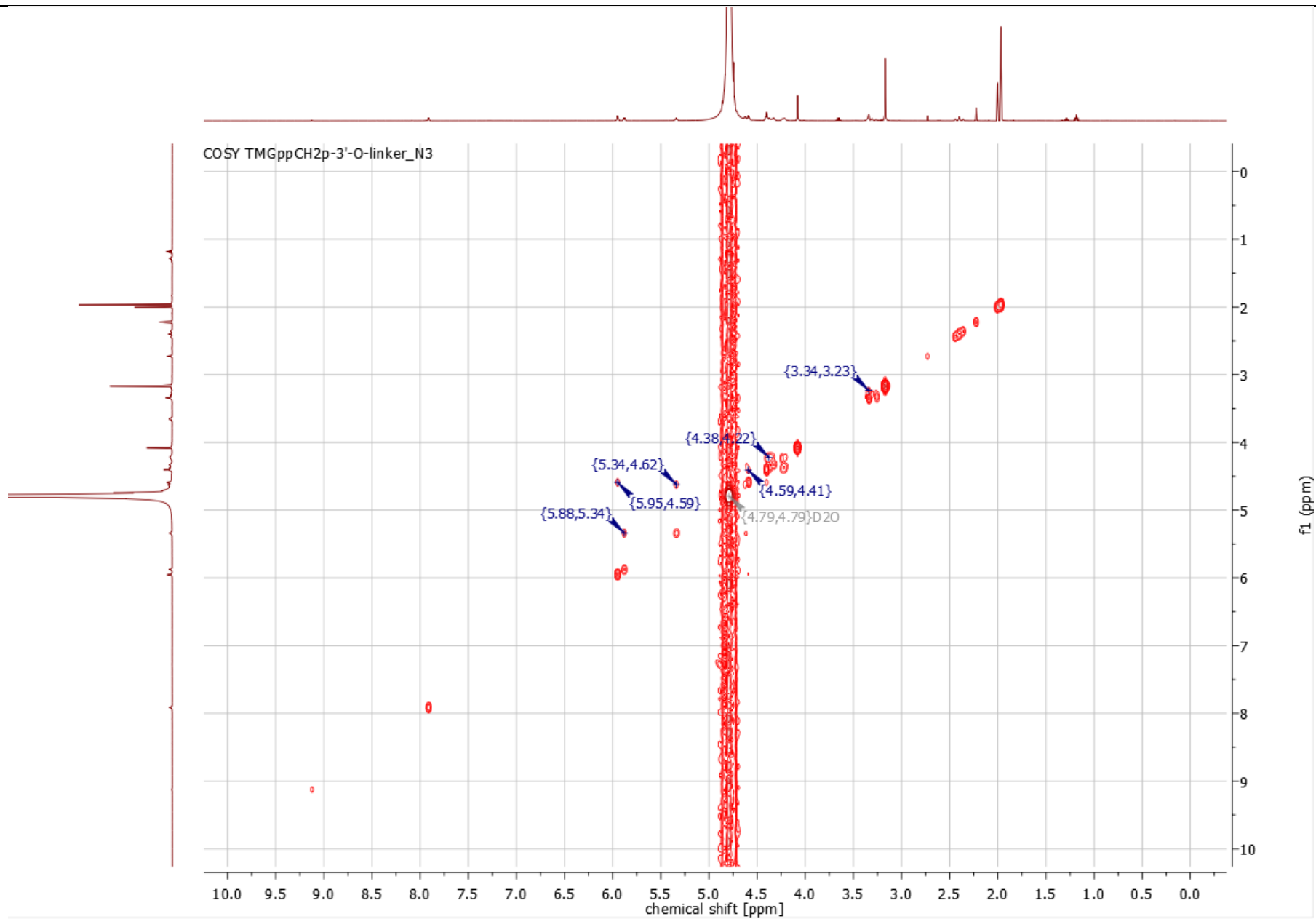
220407_PSu_01 #18-90 RT: 0.16-0.78 AV: 73 NL: 2.73E7
T: FTMS - p ESI Full ms [160.0000-2000.0000]



¹H NMR (400 MHz, D₂O, 25°C)

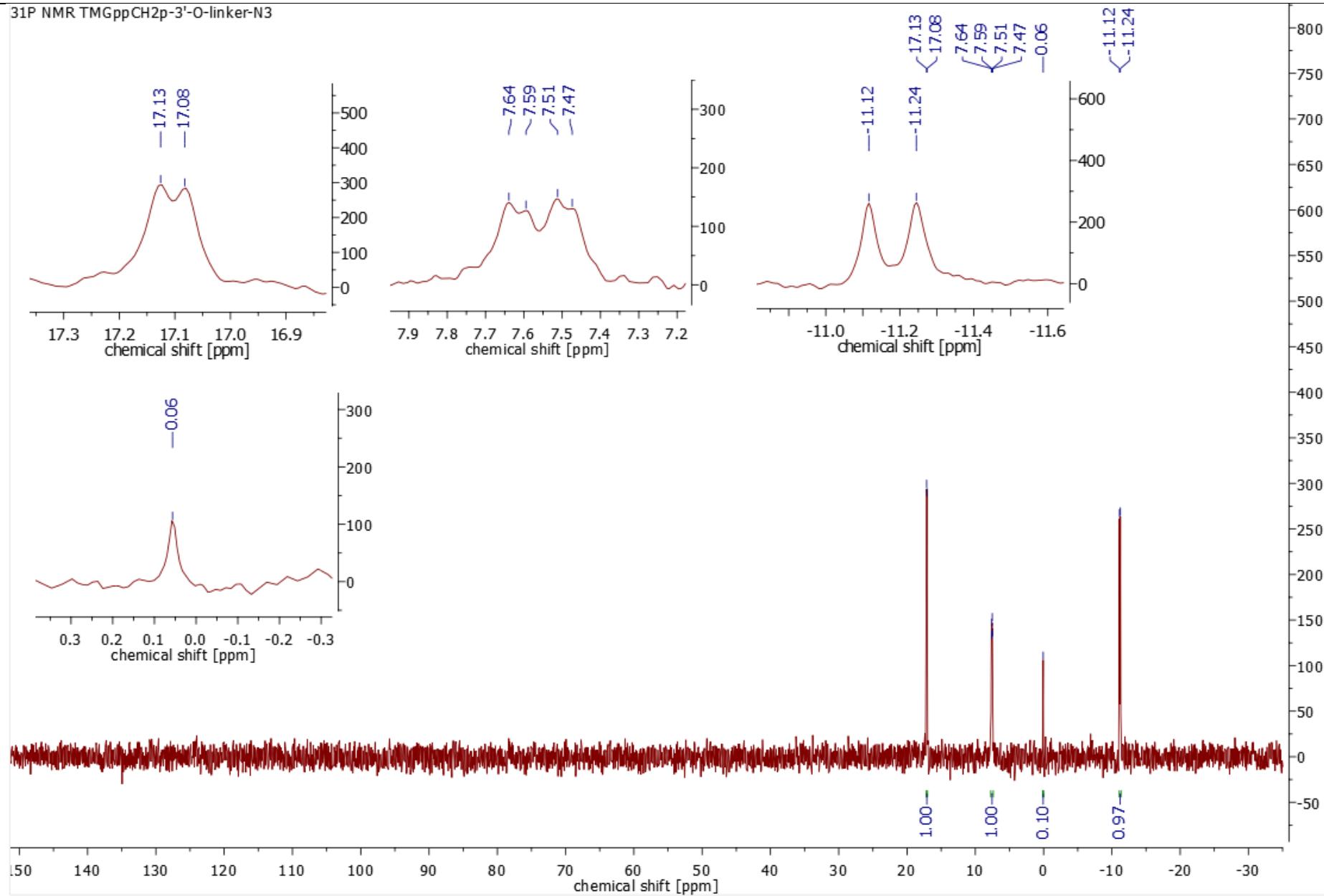


COSY NMR



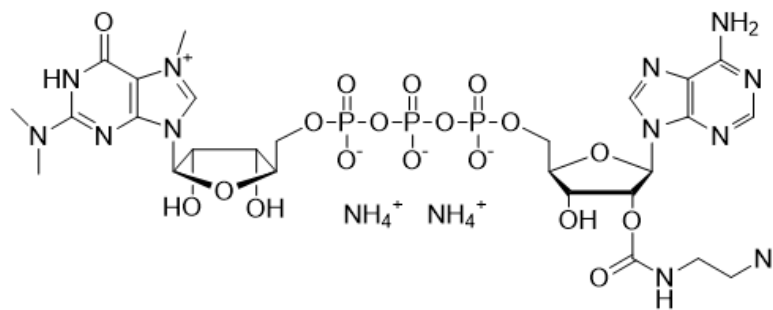
^{31}P NMR (202 MHz, D_2O , H_3PO_4 , 25°C)

^{31}P NMR TMGppCH2p-3'-O-linker-N3

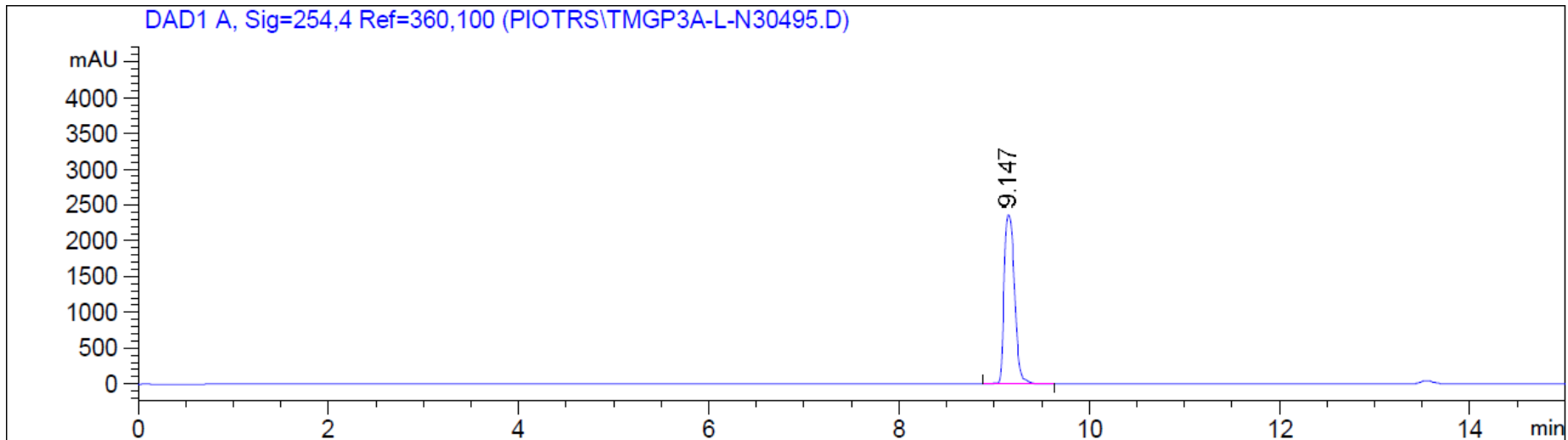


Compound 4-2': TMGpppA-2'-O-C(O)-NH-CH₂-CH₂-N₃ (NH₄⁺ salt)

Chemical structure

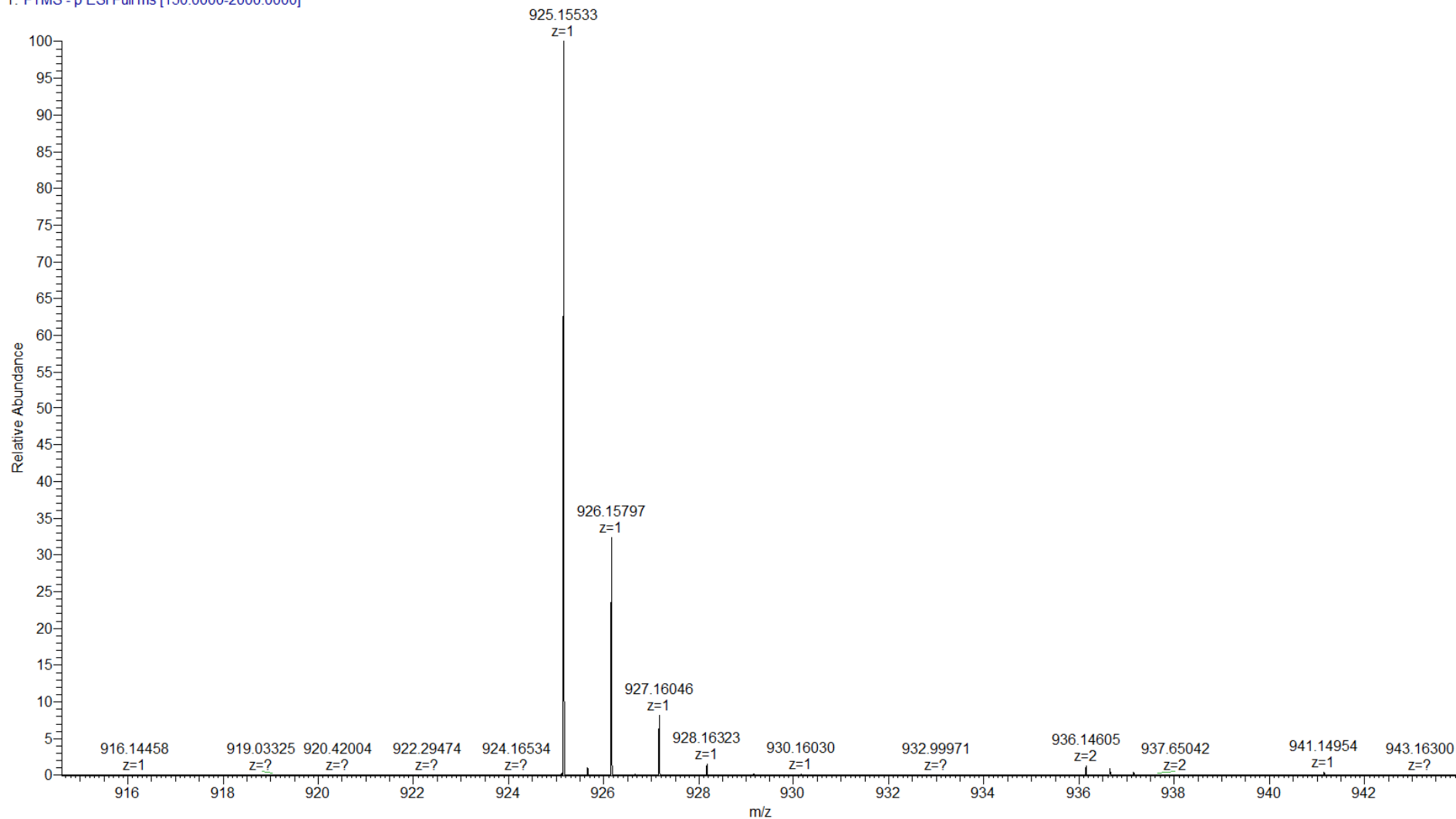


RP-HPLC (conditions c)

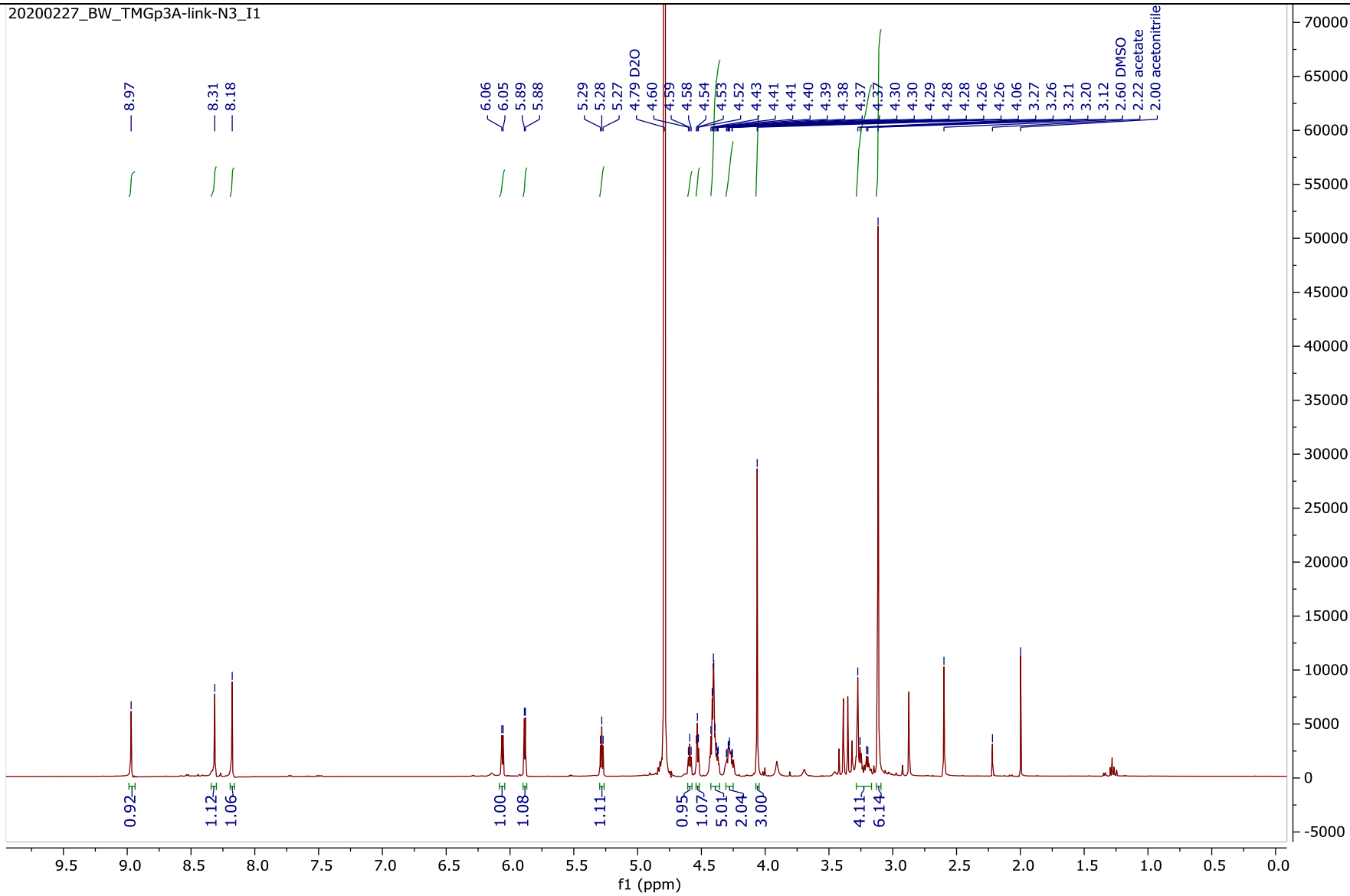


MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₆N₁₄O₁₈P₃: 925.1550, found: 925.15533)

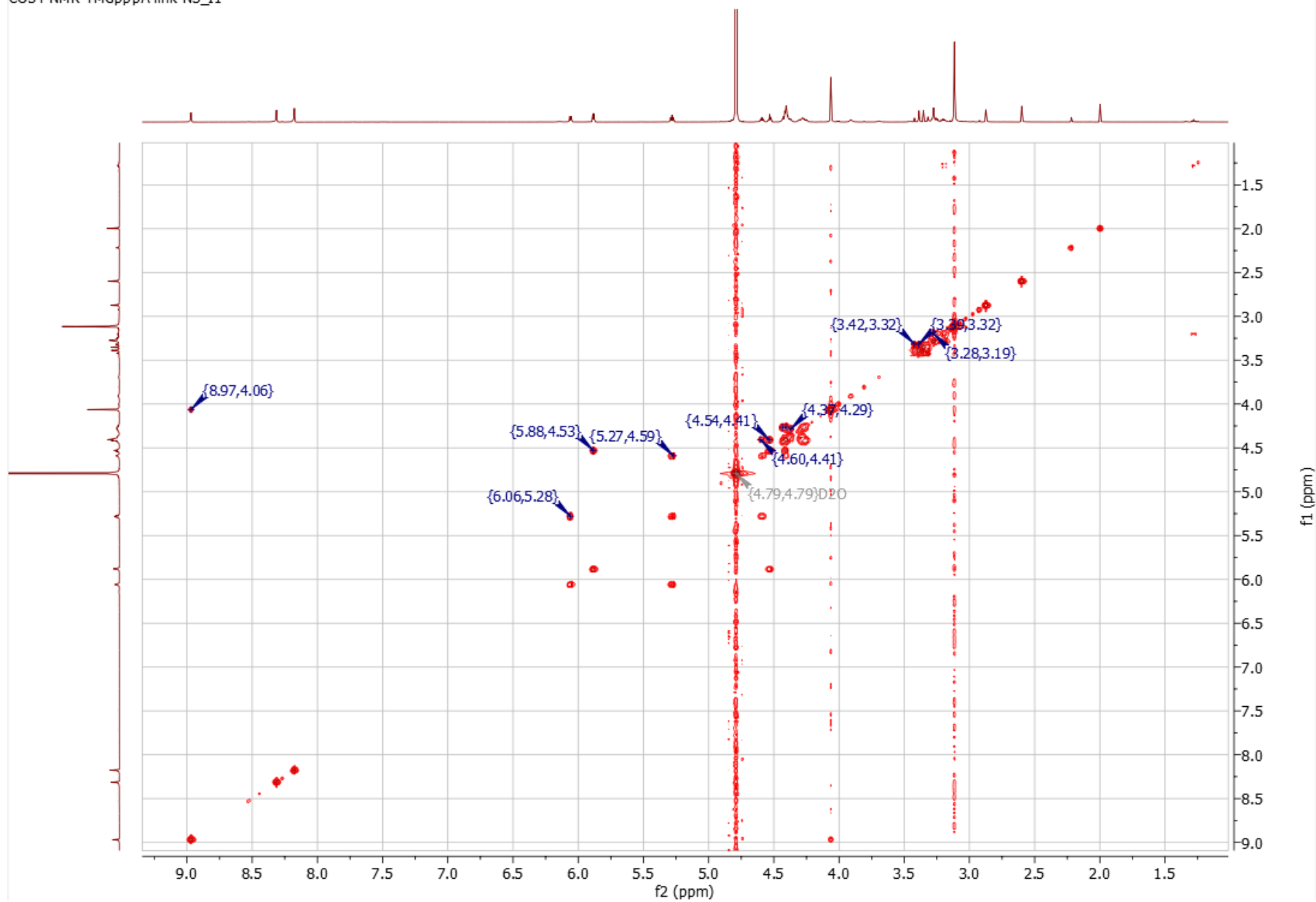
200522_BW_66a #52-97 RT: 0.52-0.99 AV: 46 NL: 2.14E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]



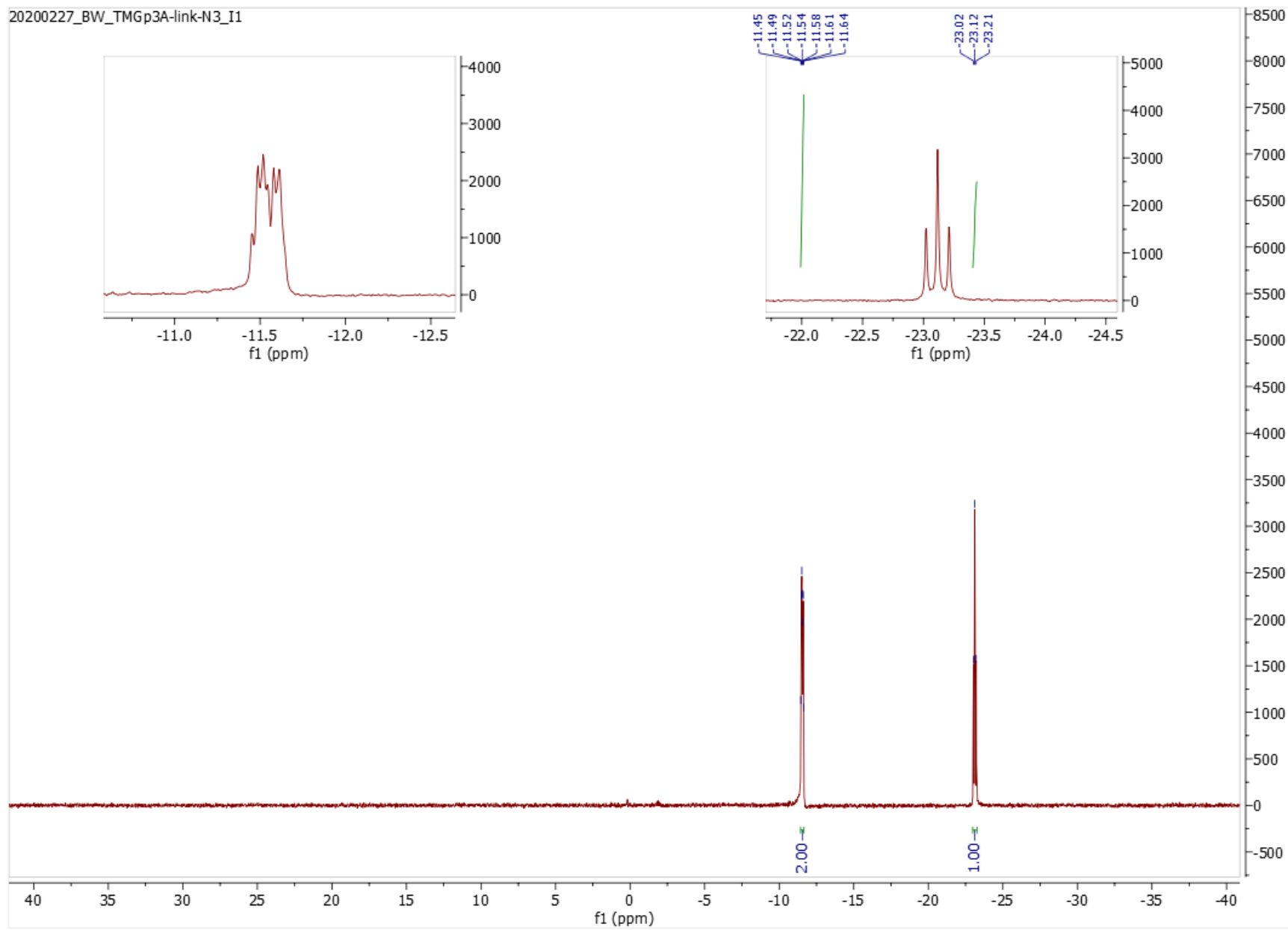
¹H NMR (500 MHz, D₂O, 25°C)



COSY NMR

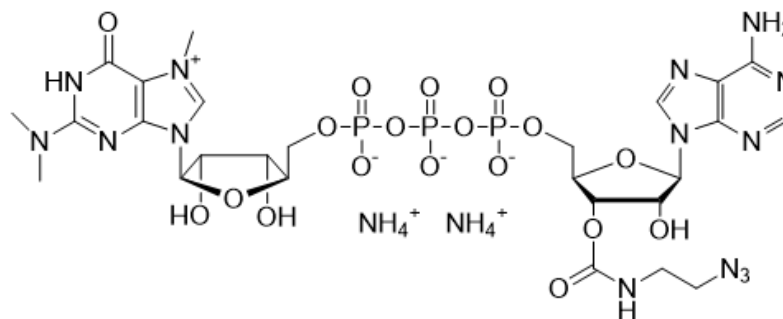


^{31}P NMR (202 MHz, D_2O , H_3PO_4 , 25°C)

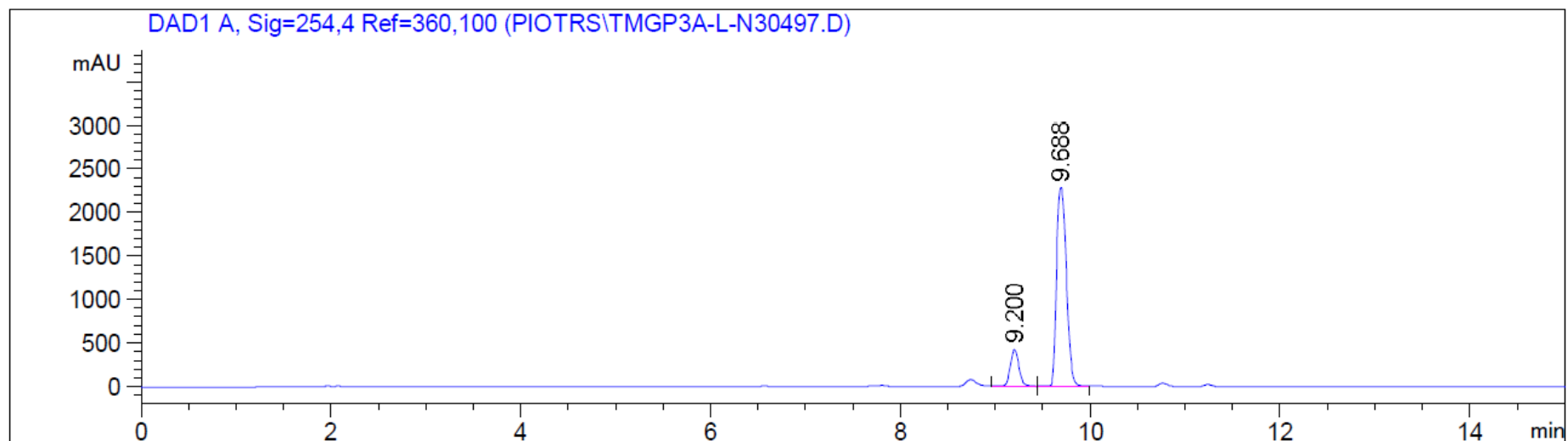


Compound 4-3': TMGpppA-3'-O-C(O)-NH-CH₂-CH₂-N₃ (NH₄⁺ salt)

Chemical structure

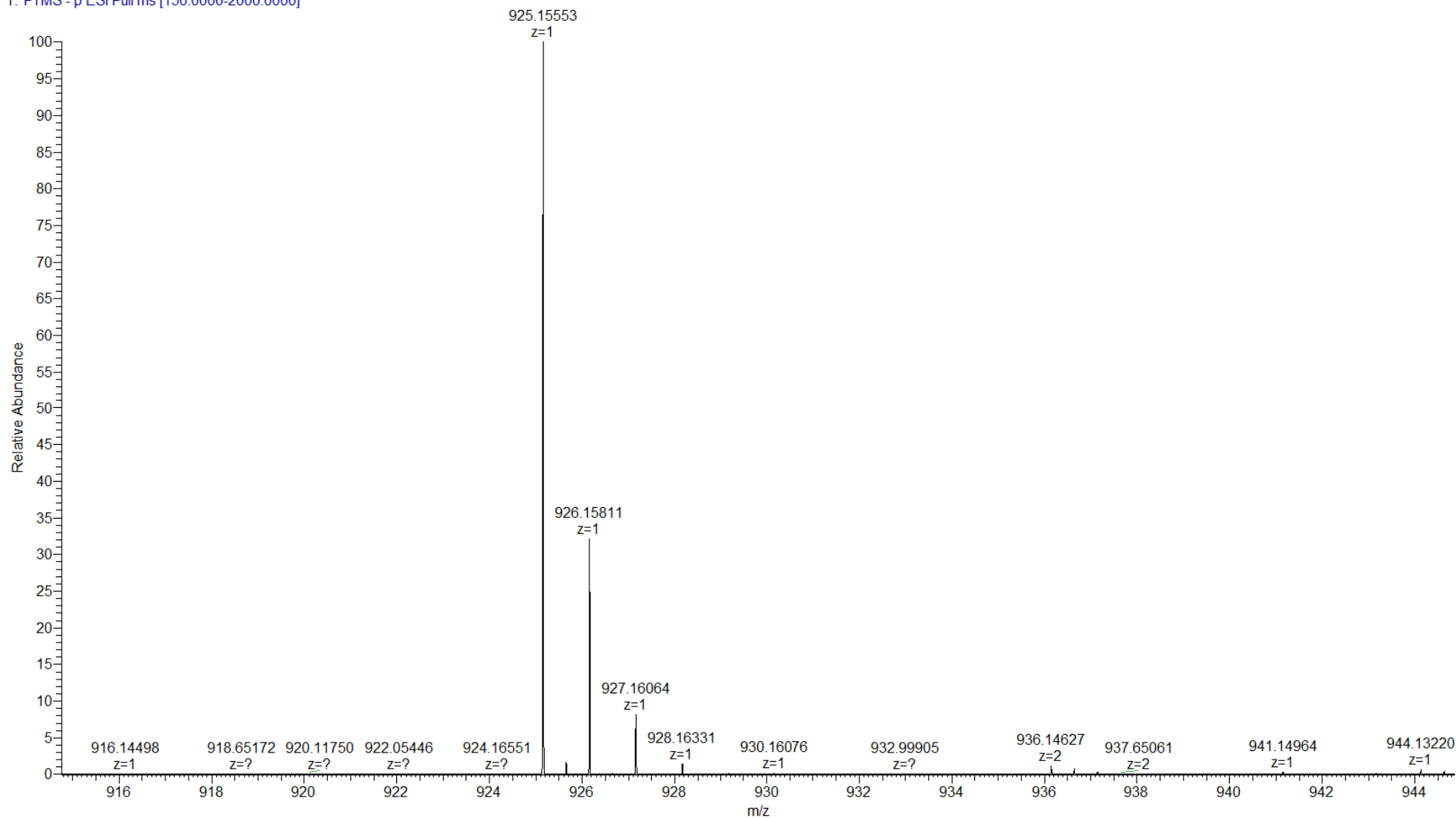


RP-HPLC (conditions c)



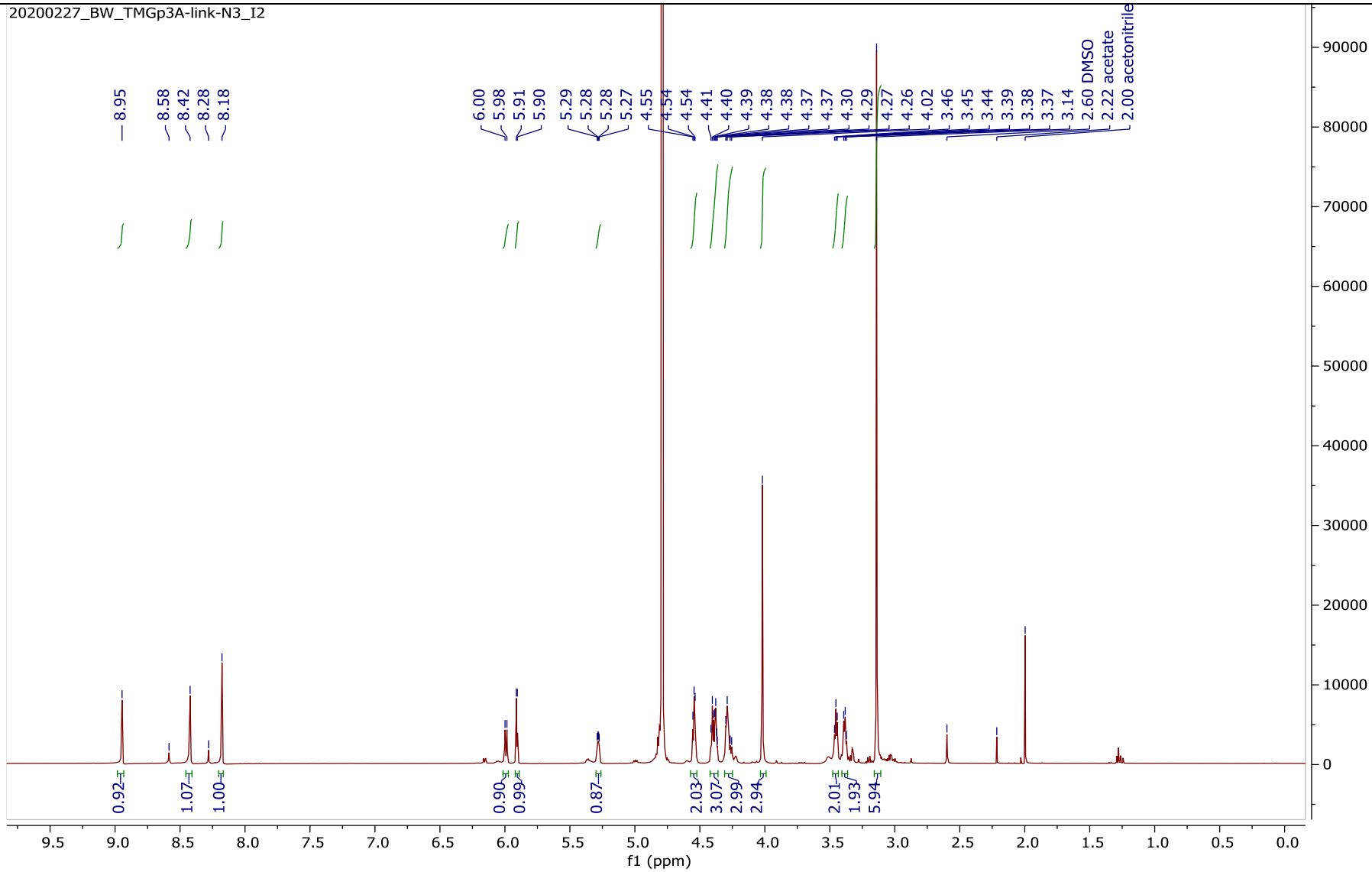
MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₆N₄O₁₈P₃⁻: 925.5758, found: 925.15553)

200522_BW_66b #95-138 RT: 0.96-1.41 AV: 44 NL: 2.40E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

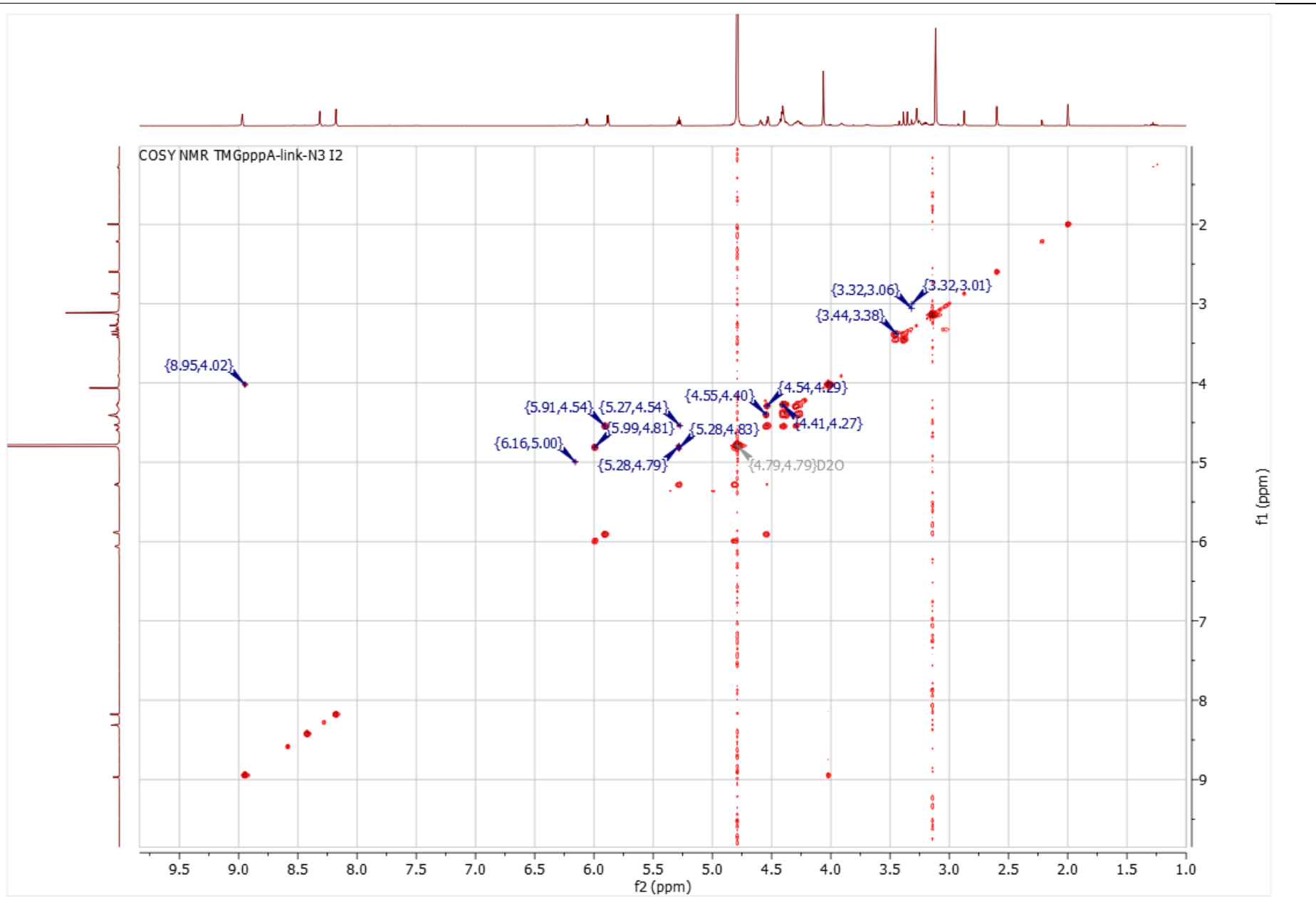


¹H NMR (500 MHz, D₂O, 25°C)

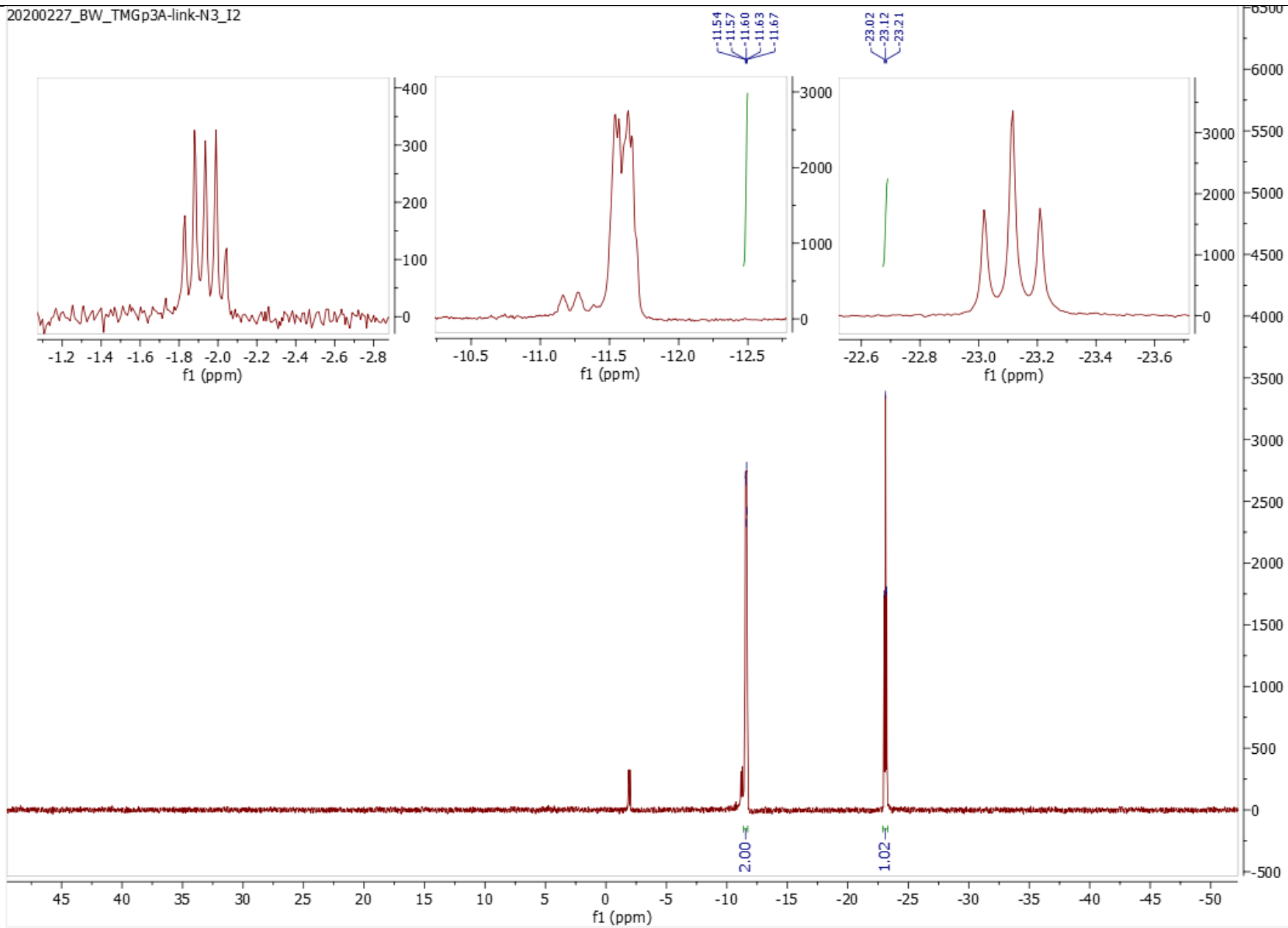
20200227_BW_TMgp3A-link-N3_I2



COSY NMR

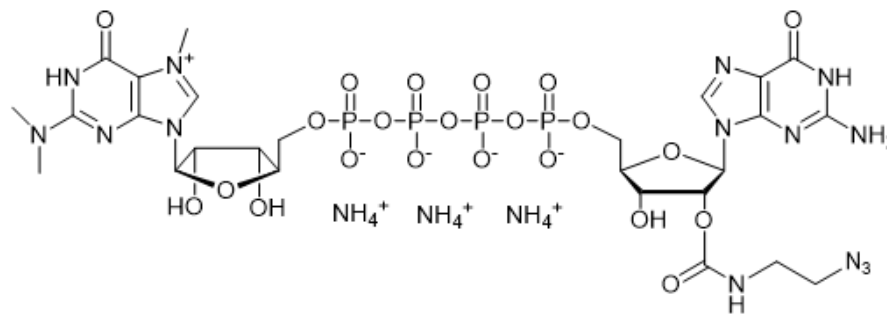


^{31}P NMR (202 MHz, D_2O , H_3PO_4 , 25°C)

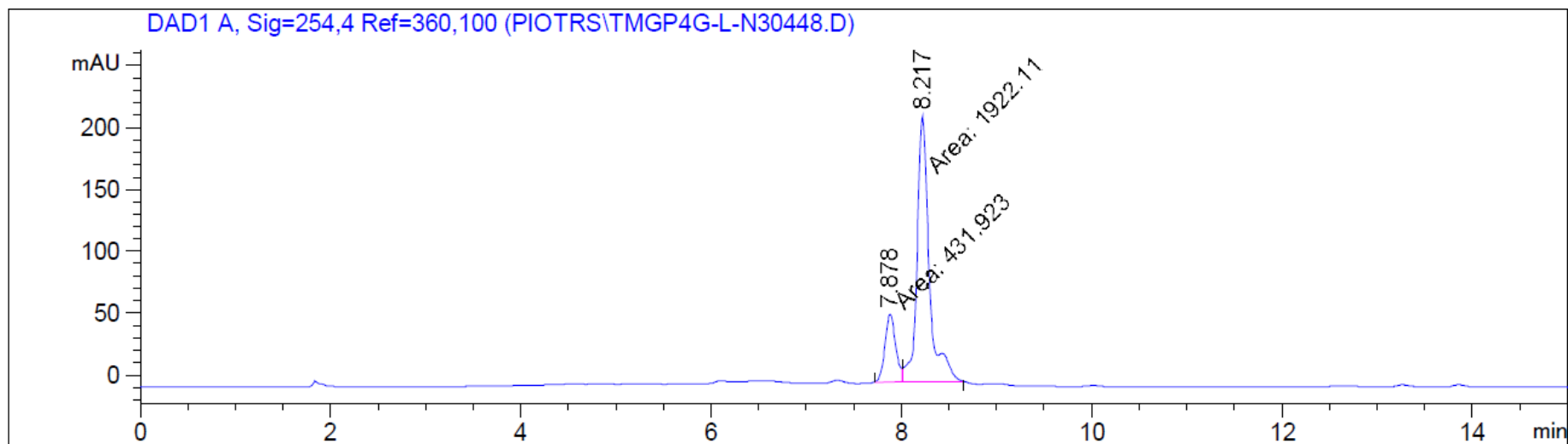


Compound 5-2': TMGppppG-2'-O-C(O)-NH-CH₂CH₂-N₃ (NH₄⁺ salt)

Chemical structure

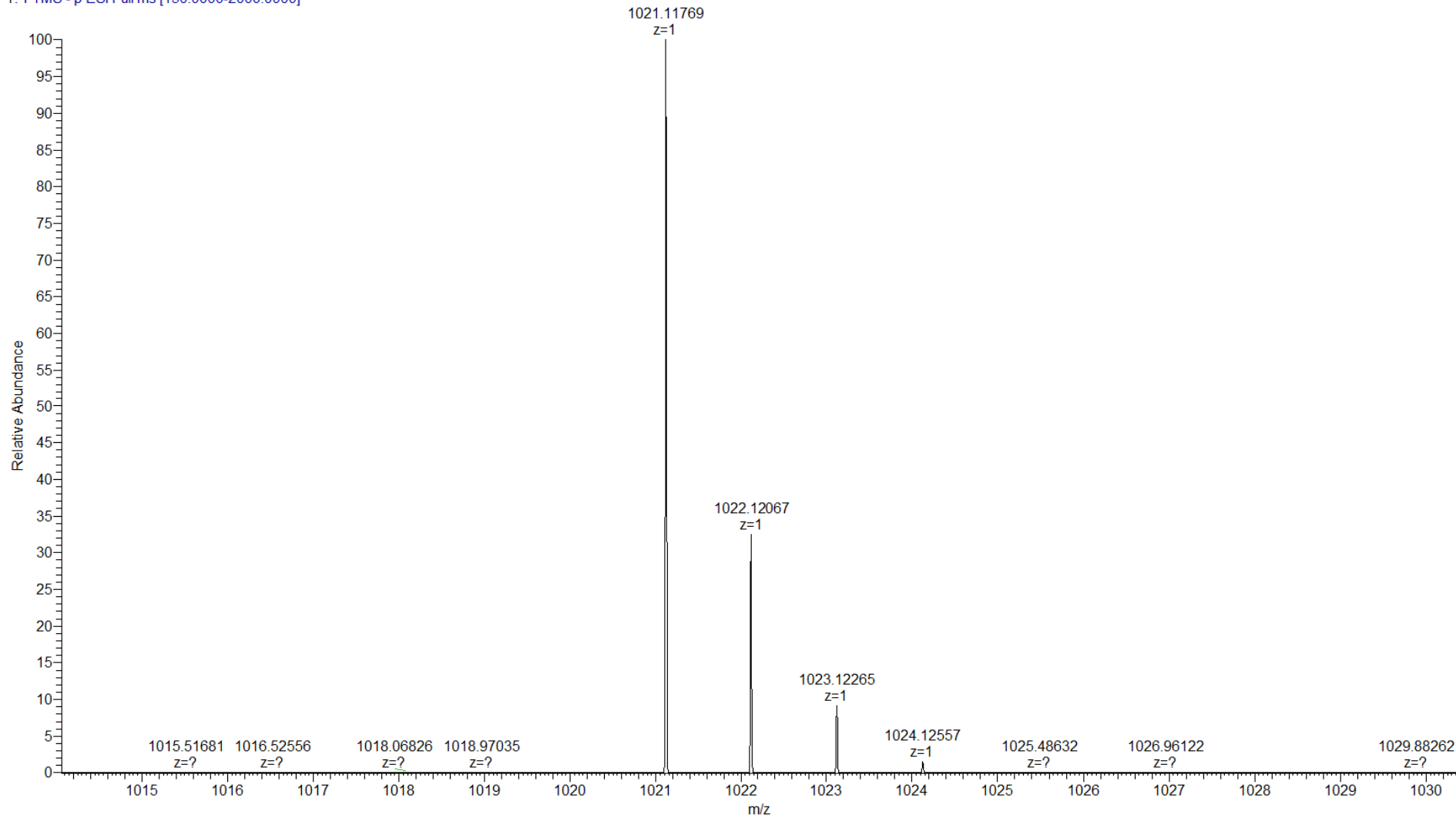


RP-HPLC (conditions c)

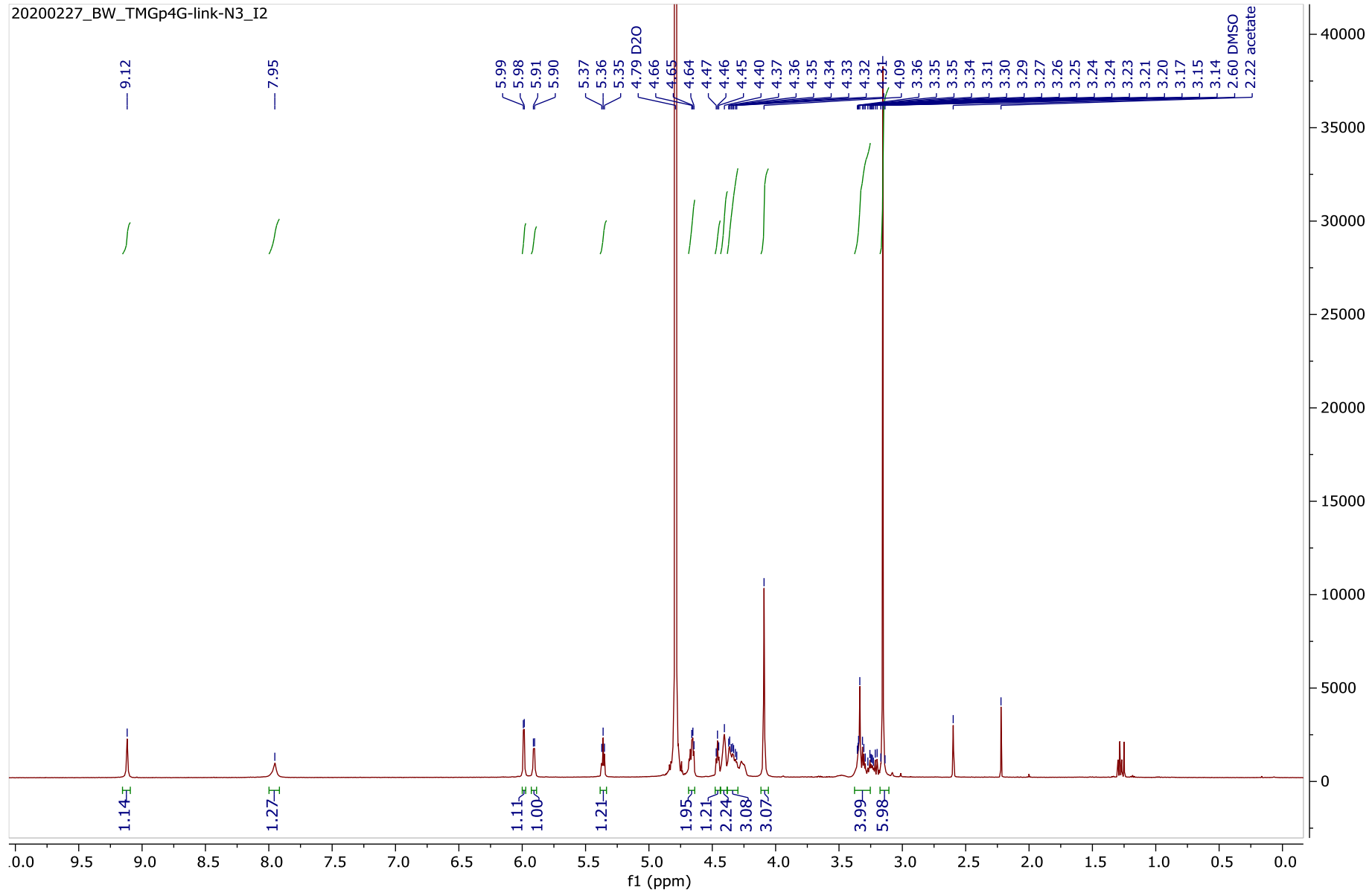


MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₇N₁₄O₂₂P₄; 1021.1163, found: 1021.11769)

200702_PSU_01 #5-51 RT: 0.05-0.51 AV: 47 NL: 2.74E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

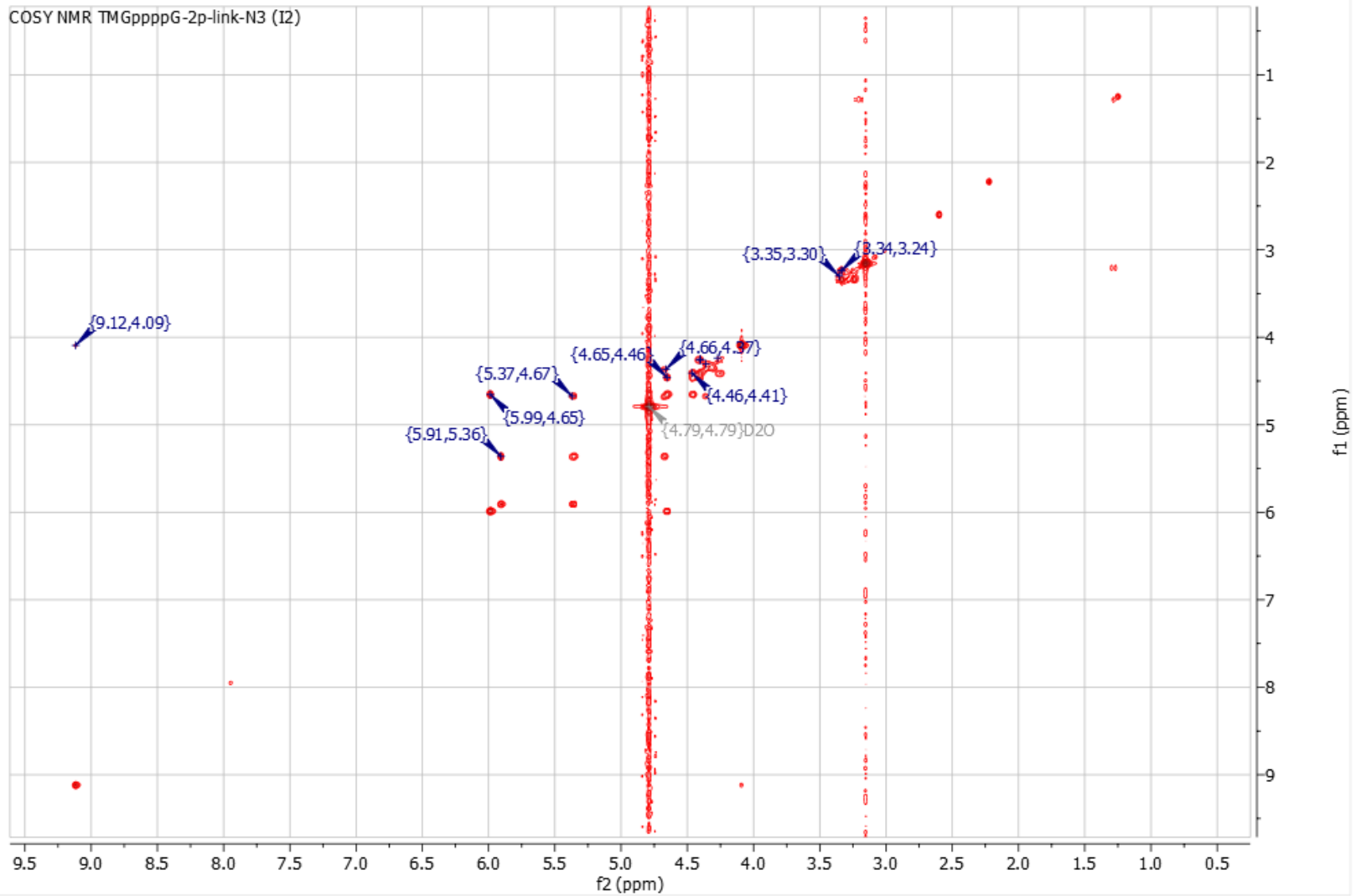


¹H NMR (500 MHz, D₂O, 25°C)

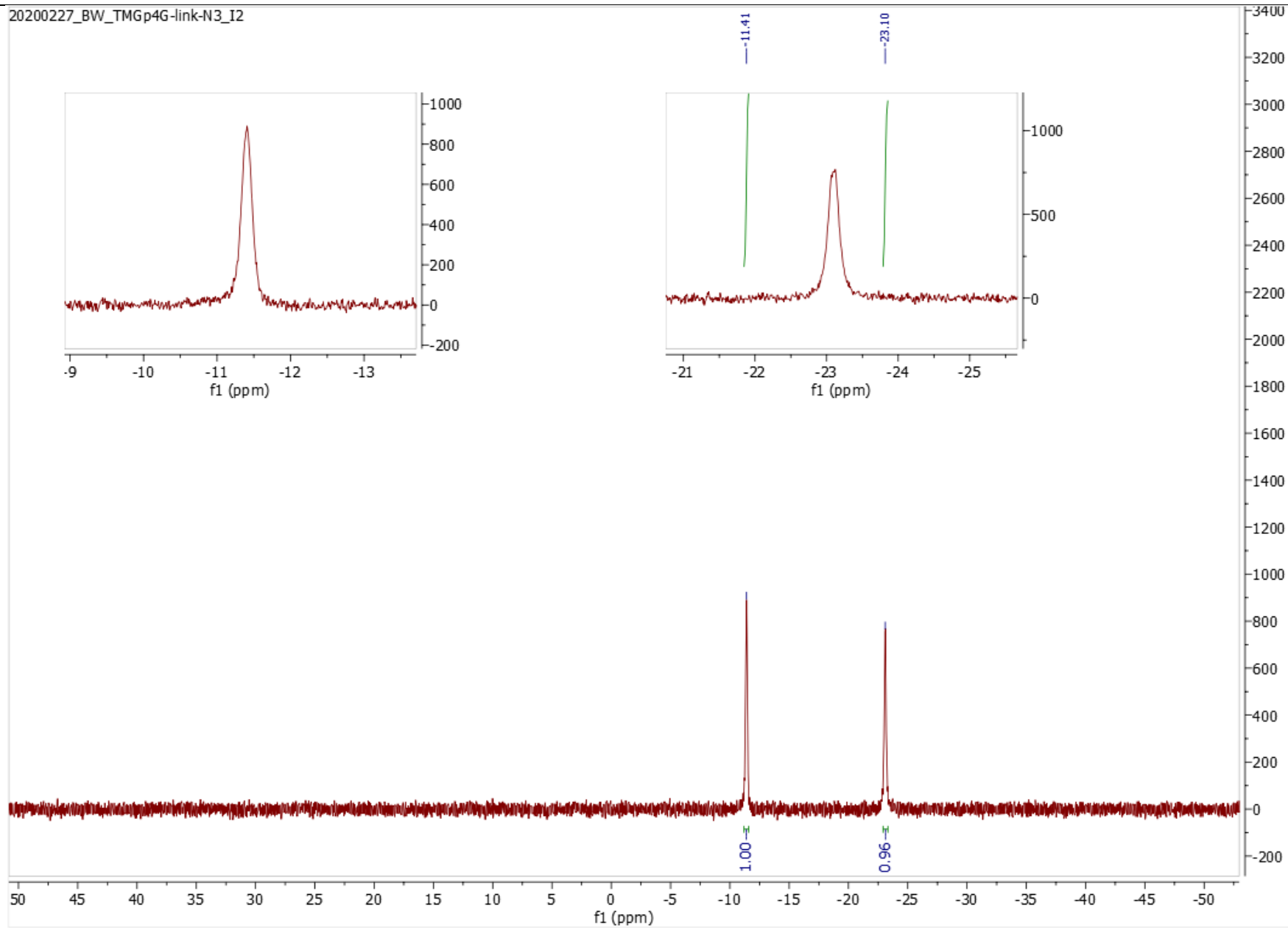


COSY NMR

COSY NMR TMGppppG-2p-link-N3 (I2)

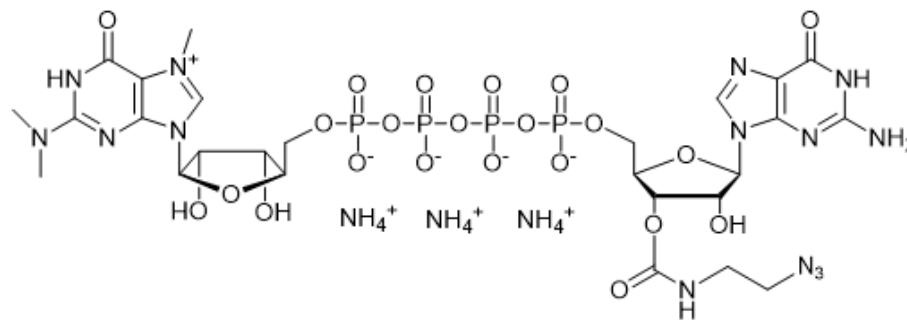


^{31}P NMR (203 MHz, D_2O , H_3PO_4 , 25°C)

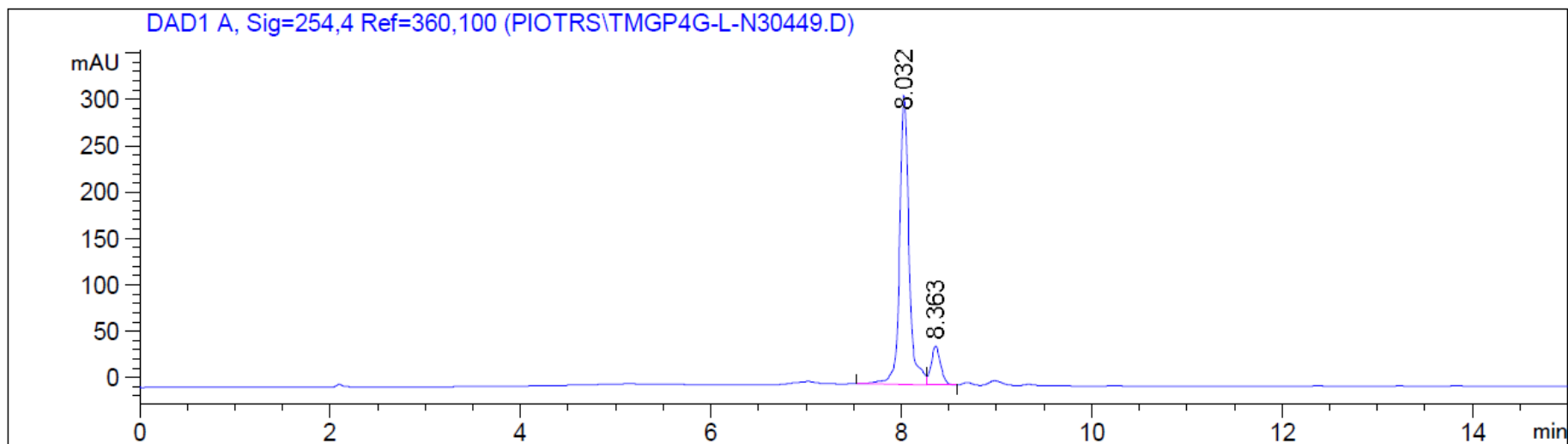


Compound 5-3': TMGppppG-3'-O-C(O)-NH-CH₂CH₂-N₃ (NH₄⁺ salt)

Chemical structure

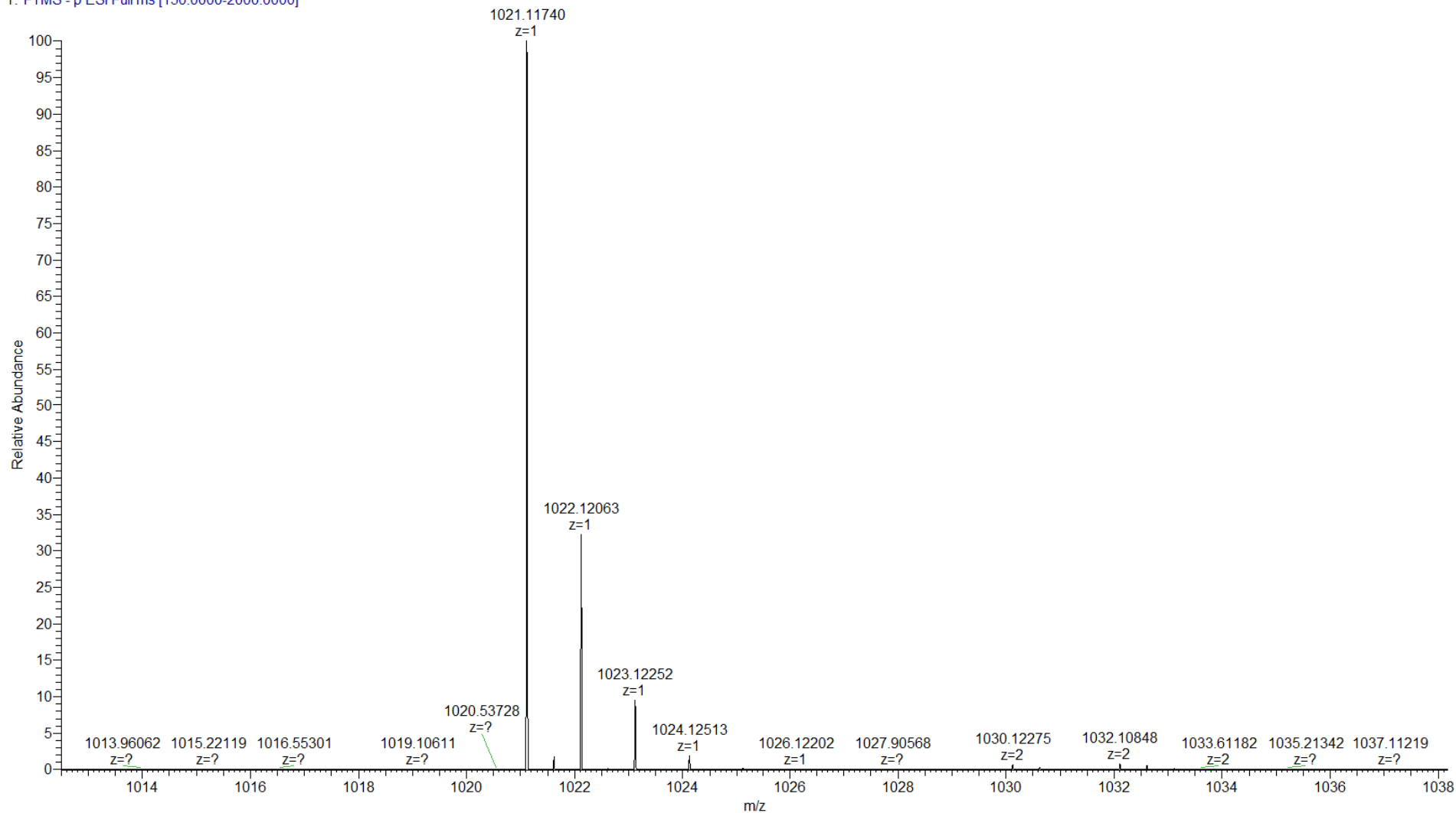


RP-HPLC (conditions c)

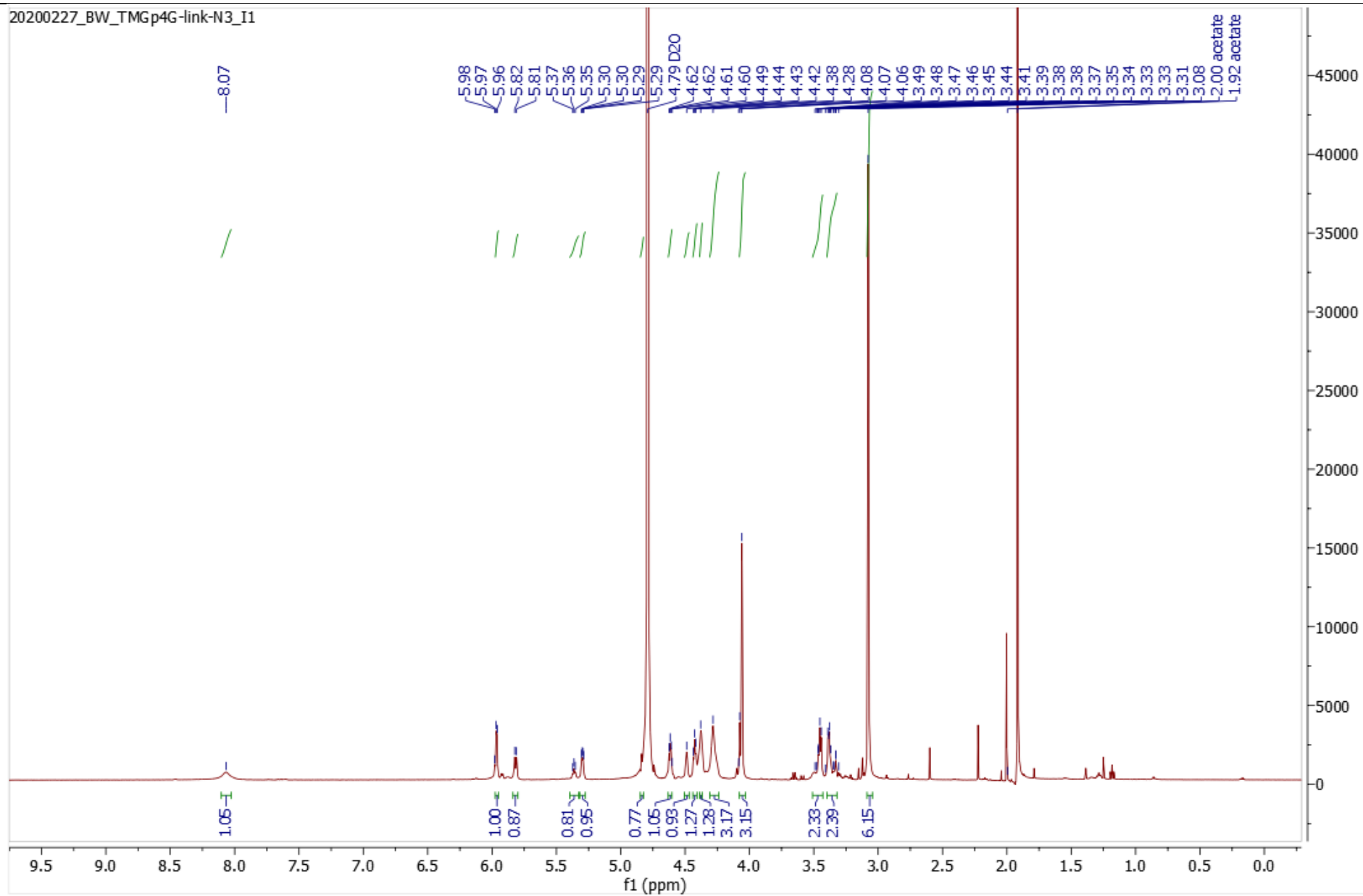


MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₇N₁₄O₂₂P₄; 1021.1163, found: 1021.11740)

200702_PSU_02#26-106 RT: 0.25-1.06 AV: 81 NL: 7.21E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

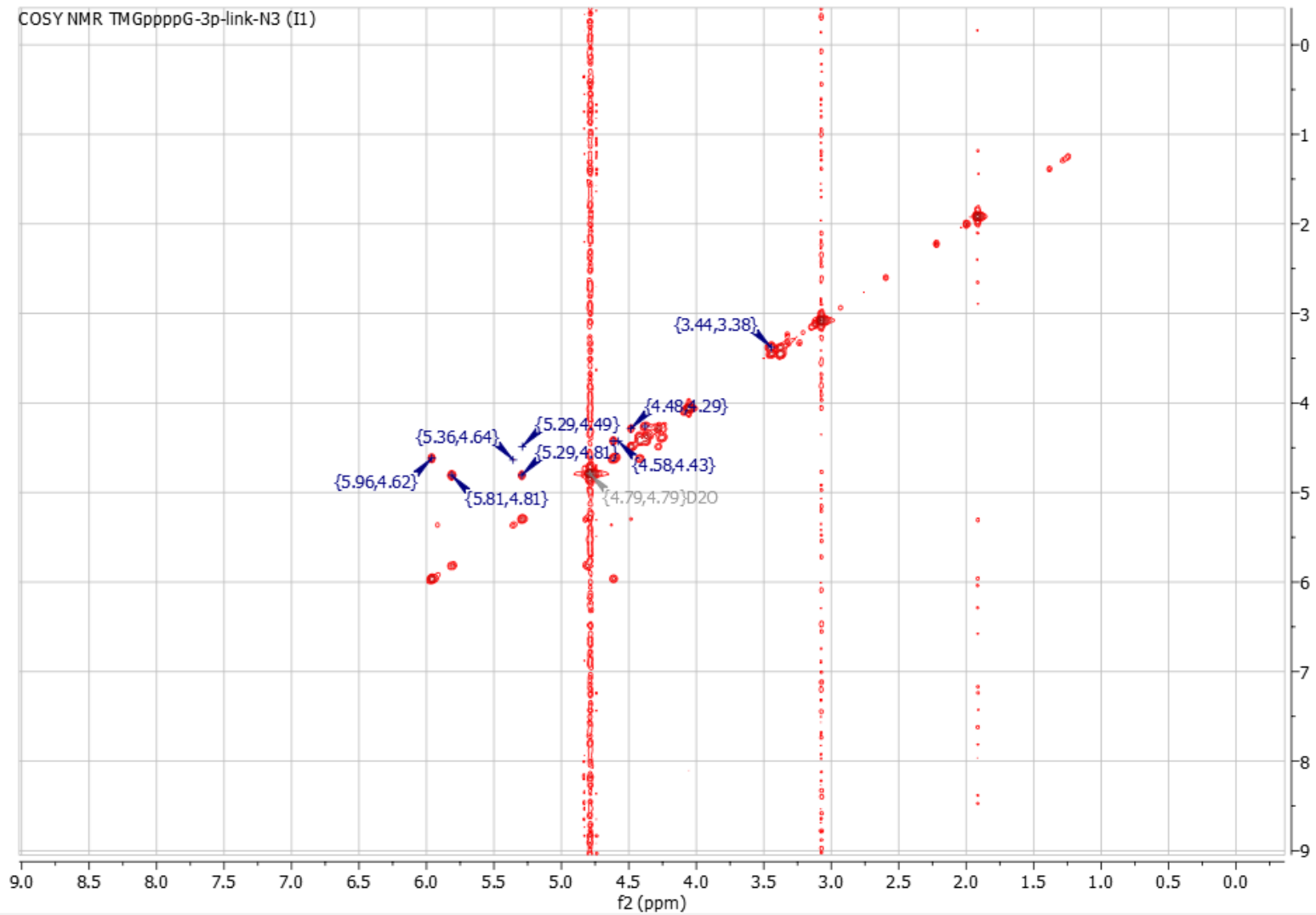


¹H NMR (500 MHz, D₂O, 25°C)



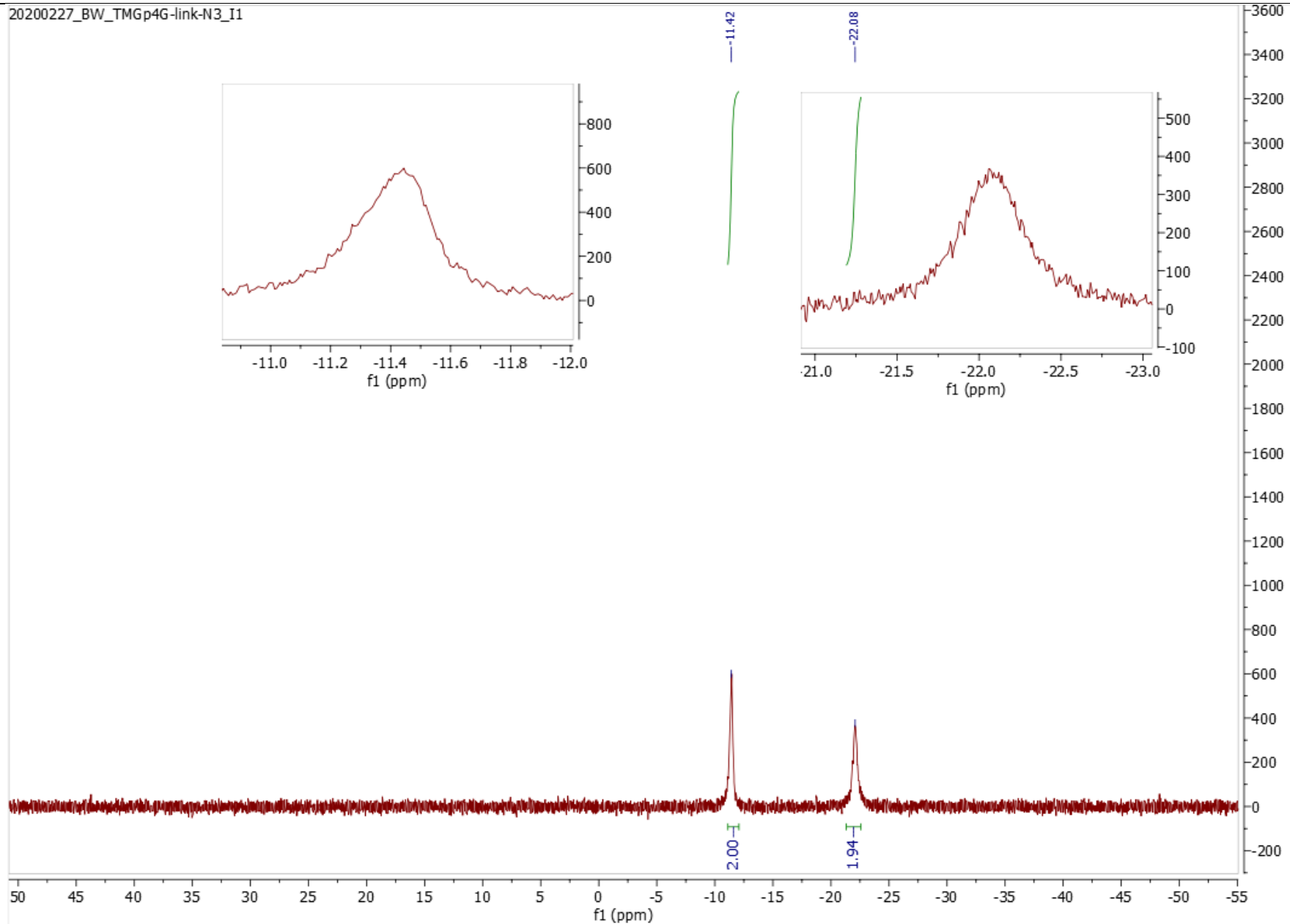
COSY NMR

COSY NMR TMGppppG-3p-link-N3 (I1)



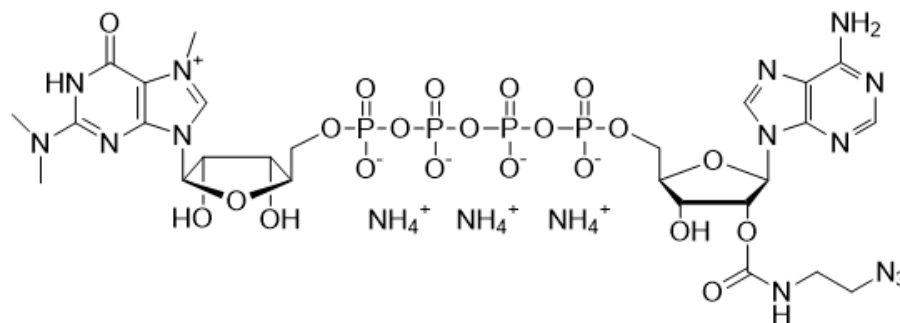
³¹P NMR (203 MHz, D₂O, H₃PO₄, 25°C)

20200227_BW_TMgp4G-link-N3_I1

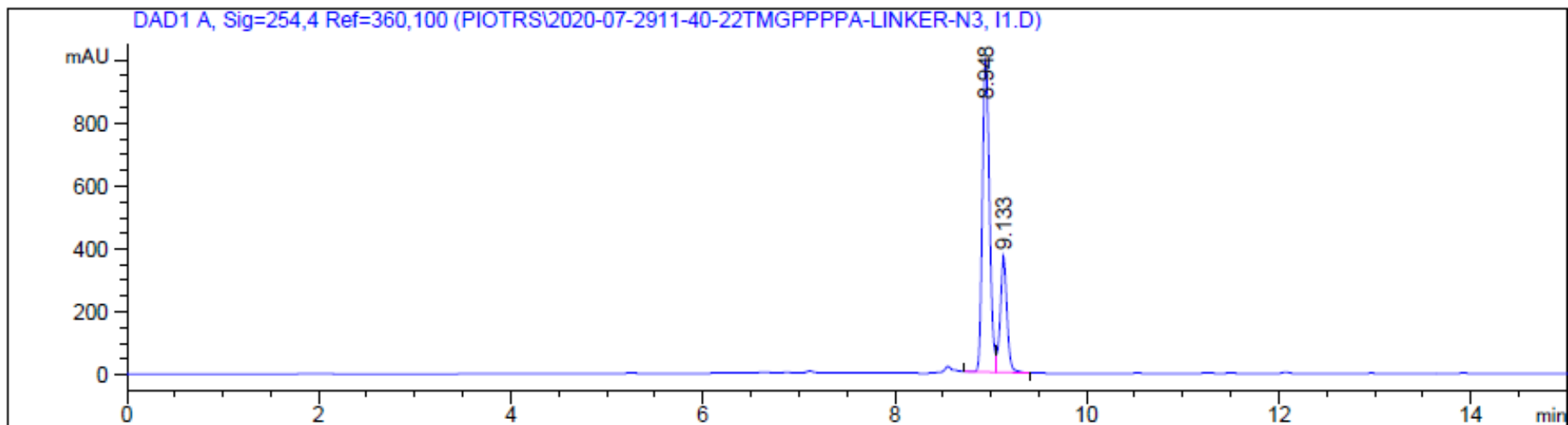


Compound 6: TMGppppA-2'+3'-O-C(O)-NH-CH₂CH₂-N₃ (NH₄⁺ salt)

Chemical structure

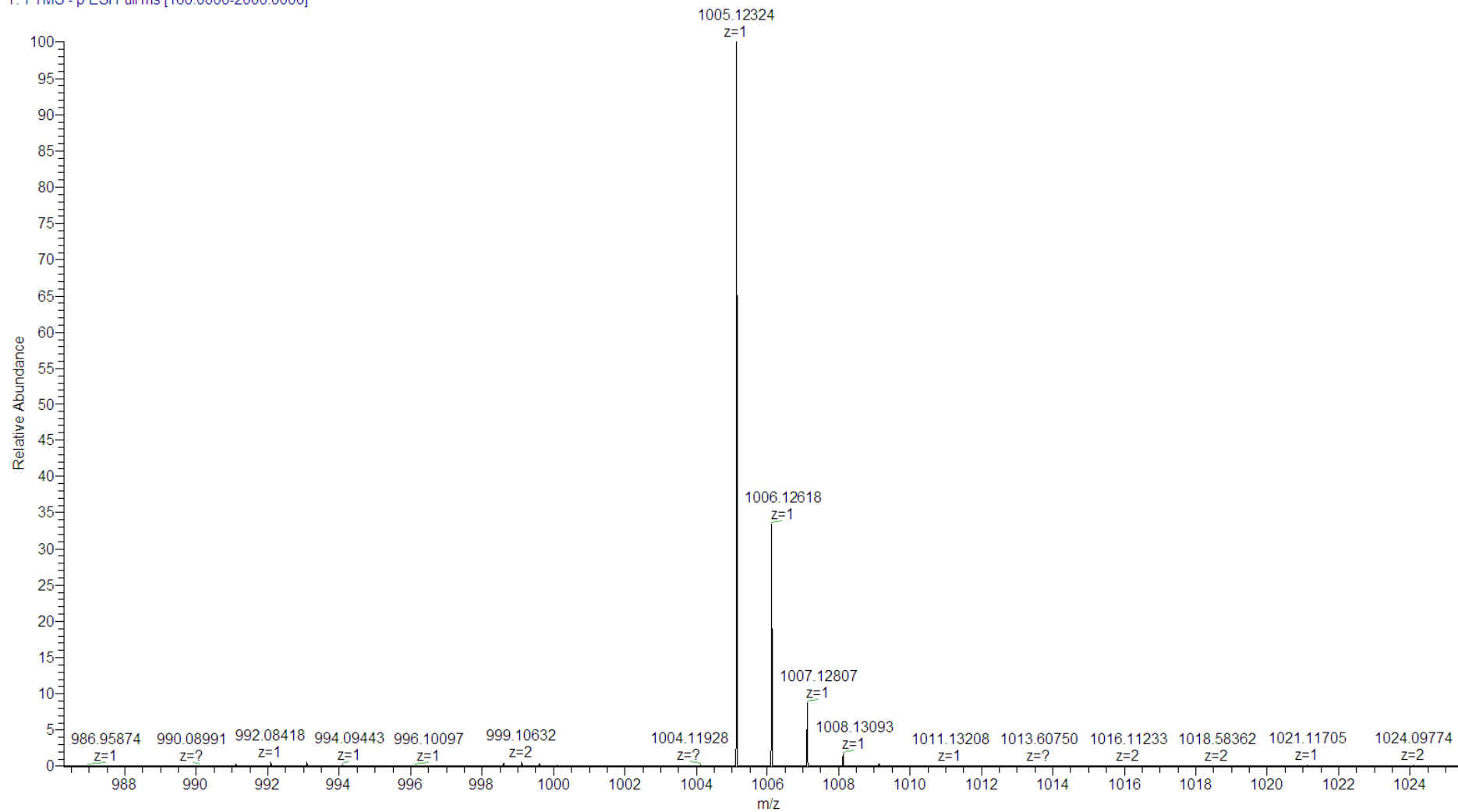


RP-HPLC (conditions c)

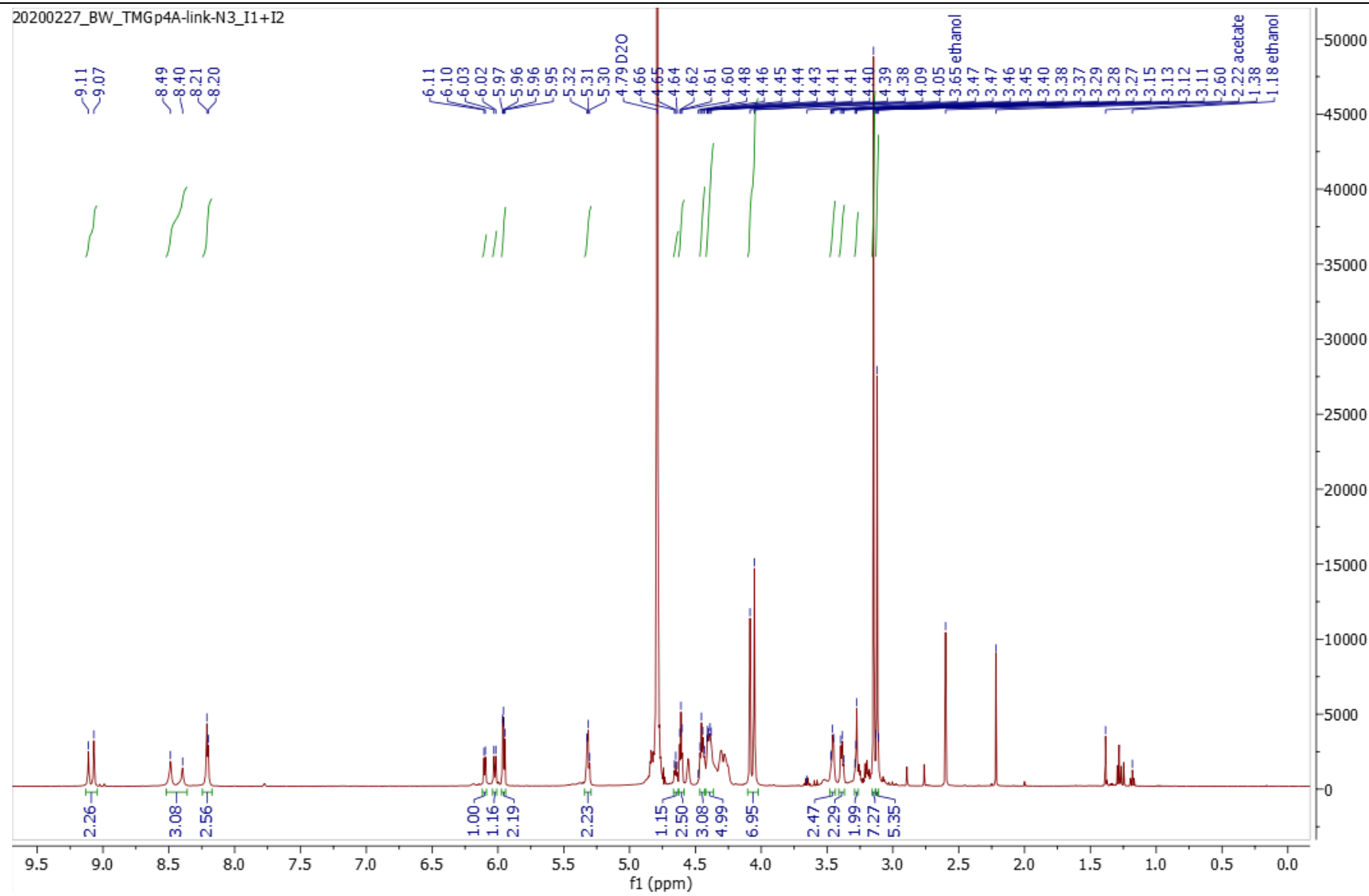


220407_PSu_02#203-267 RT: 1.77-2.33 AV: 65 NL: 3.76E6
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₇N₁₄O₂₁P₄⁻ : 1005.1214, found: 1005.12324)

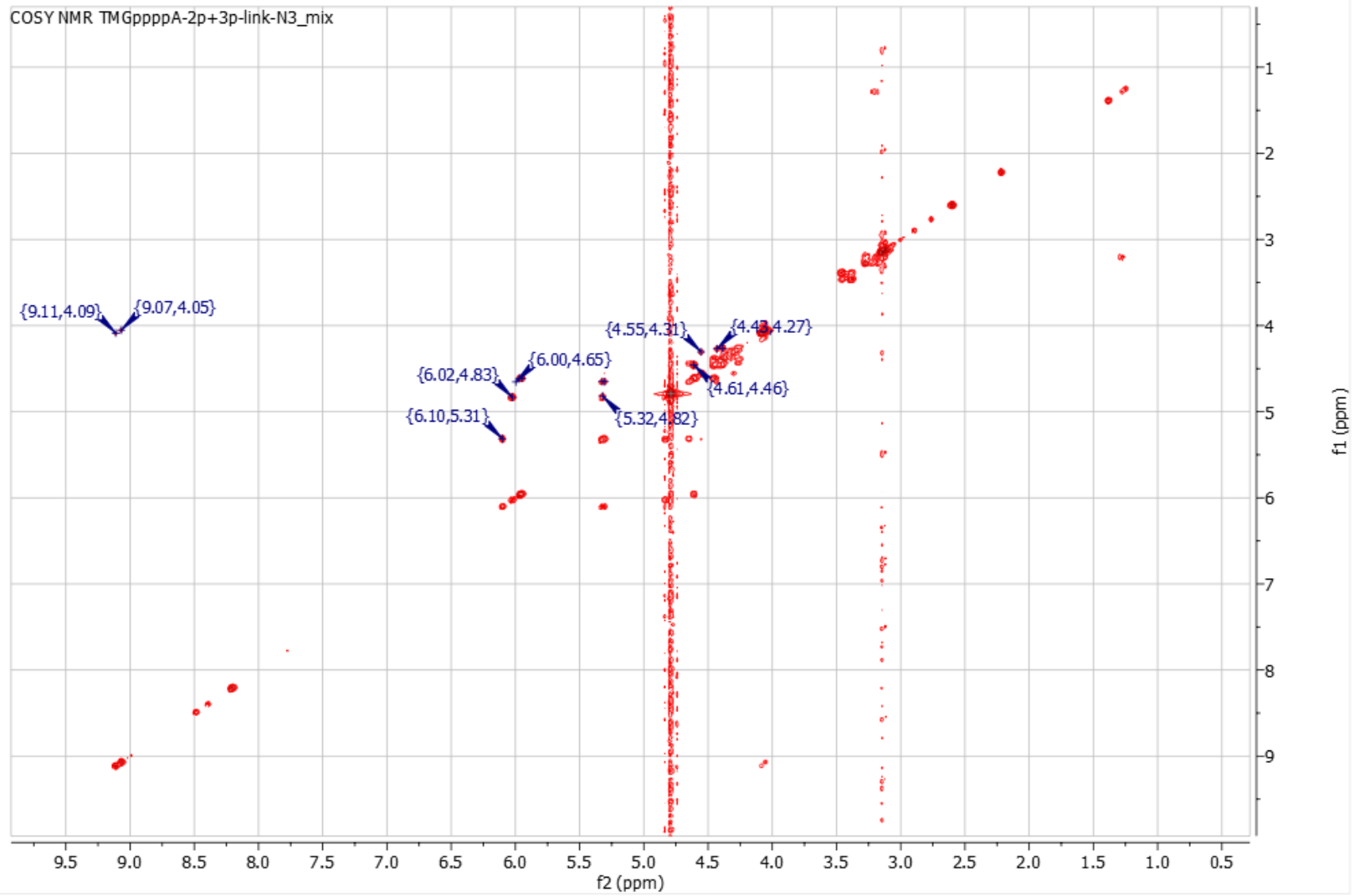


¹H NMR (500 MHz, D₂O, 25°C)

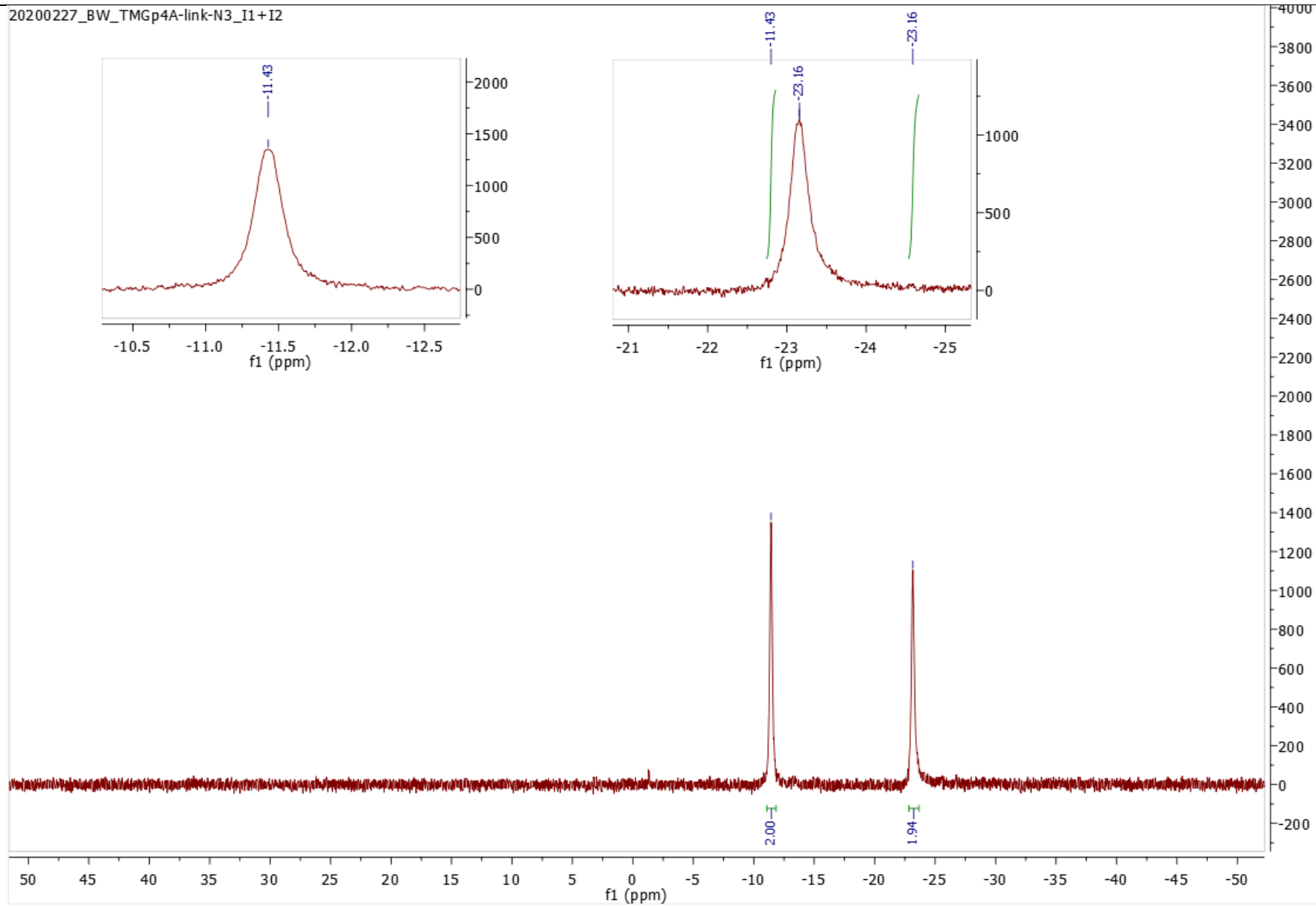


COSY NMR

COSY NMR TMGppppA-2p+3p-link-N3_mix

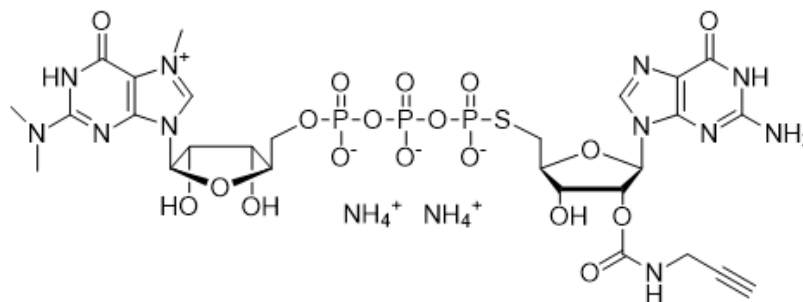


^{31}P NMR (203 MHz, D_2O , H_3PO_4 , 25°C)

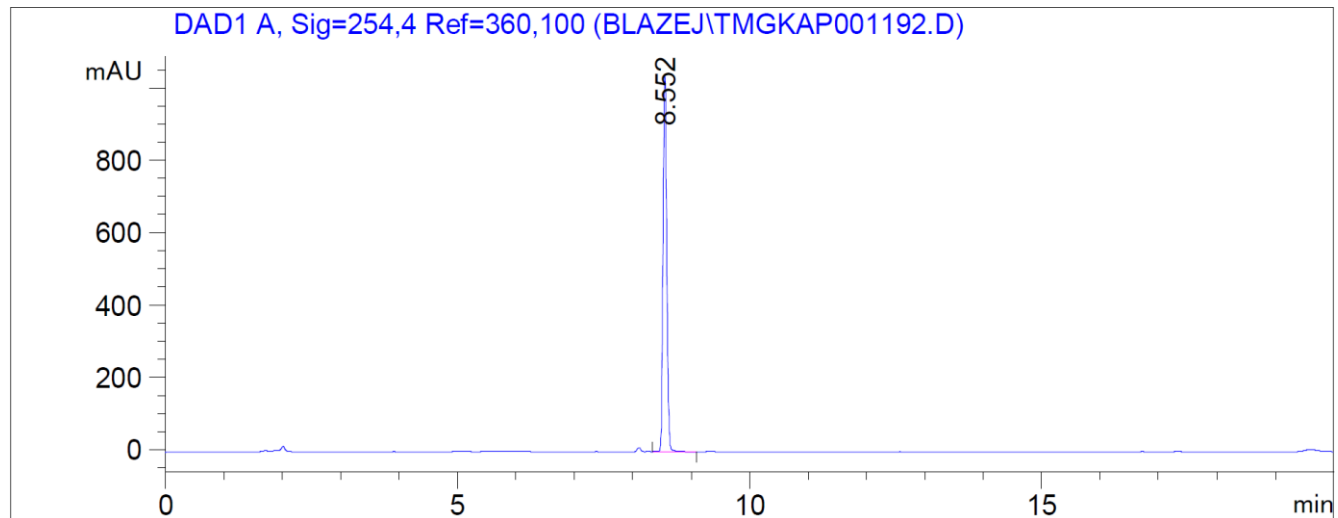


Compound 7-2': TMGppp-5'-SG-2'-O-C(O)-NH-C₃H₃ (NH₄⁺ salt)

Chemical structure

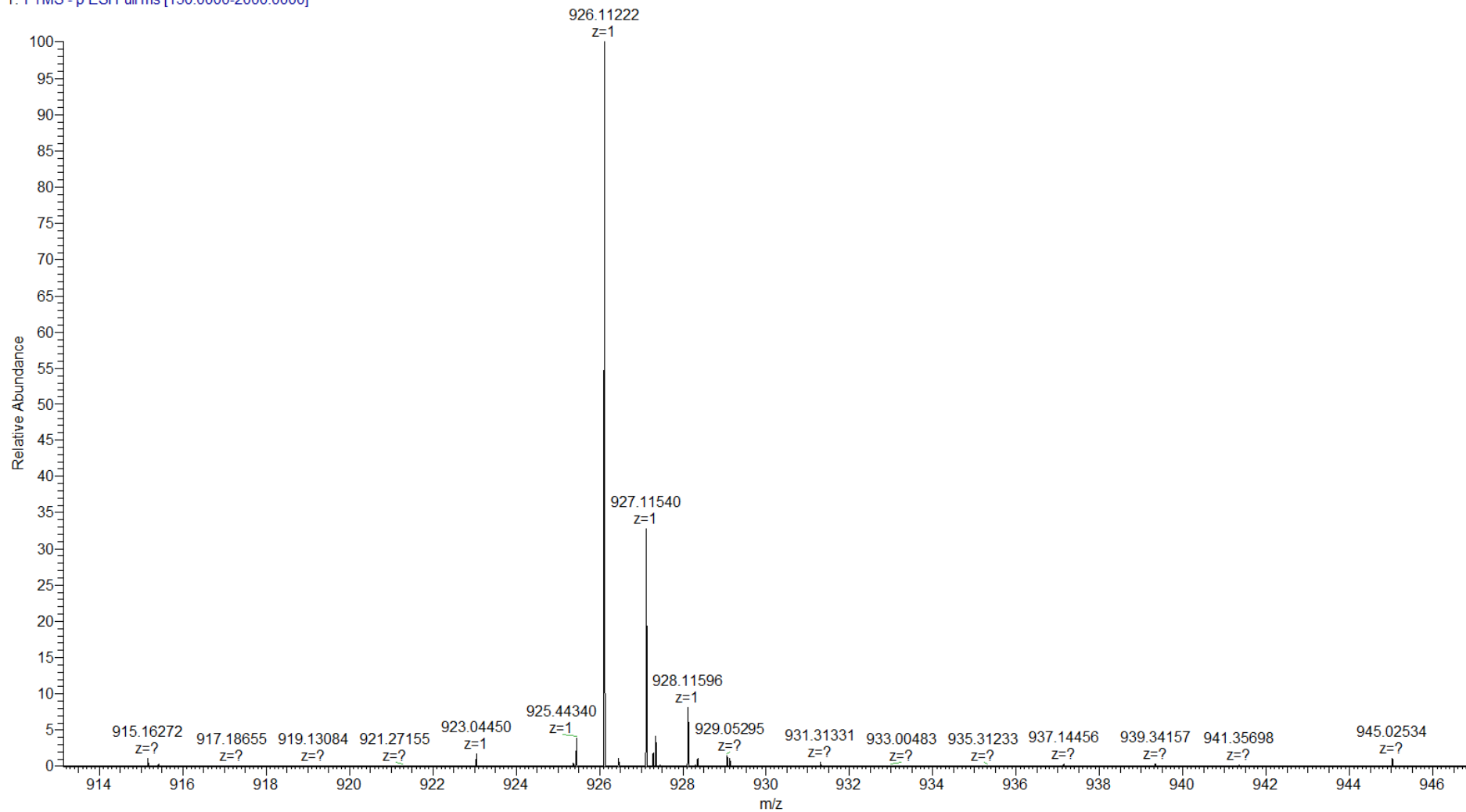


RP-HPLC (conditions c)



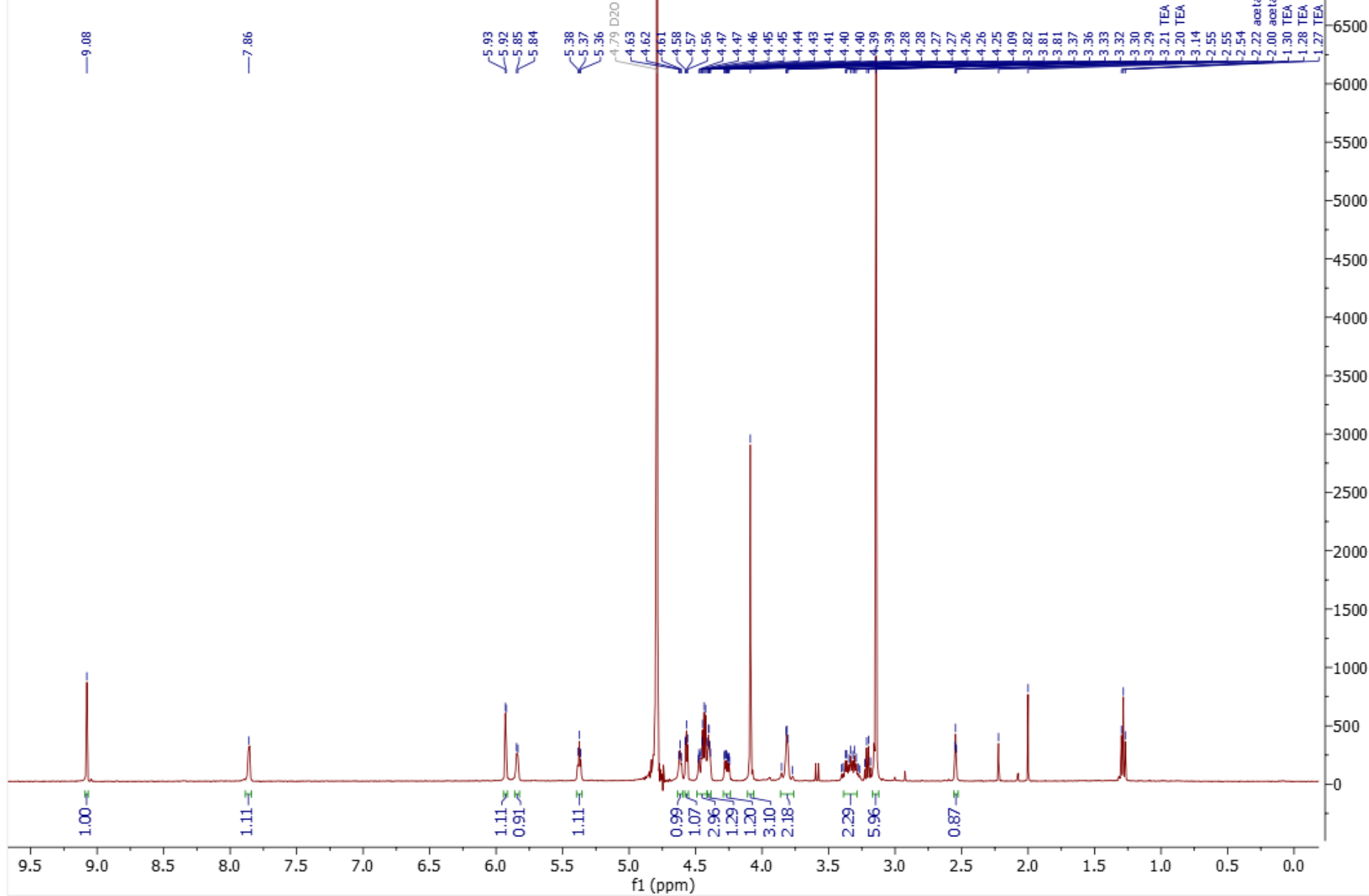
201119_PSu_10 #147-231 RT: 1.42-2.23 AV: 85 NL: 5.25E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₂₇H₃₅N₁₁O₁₈P₃S⁻ : 926.1101; found 926.11222)

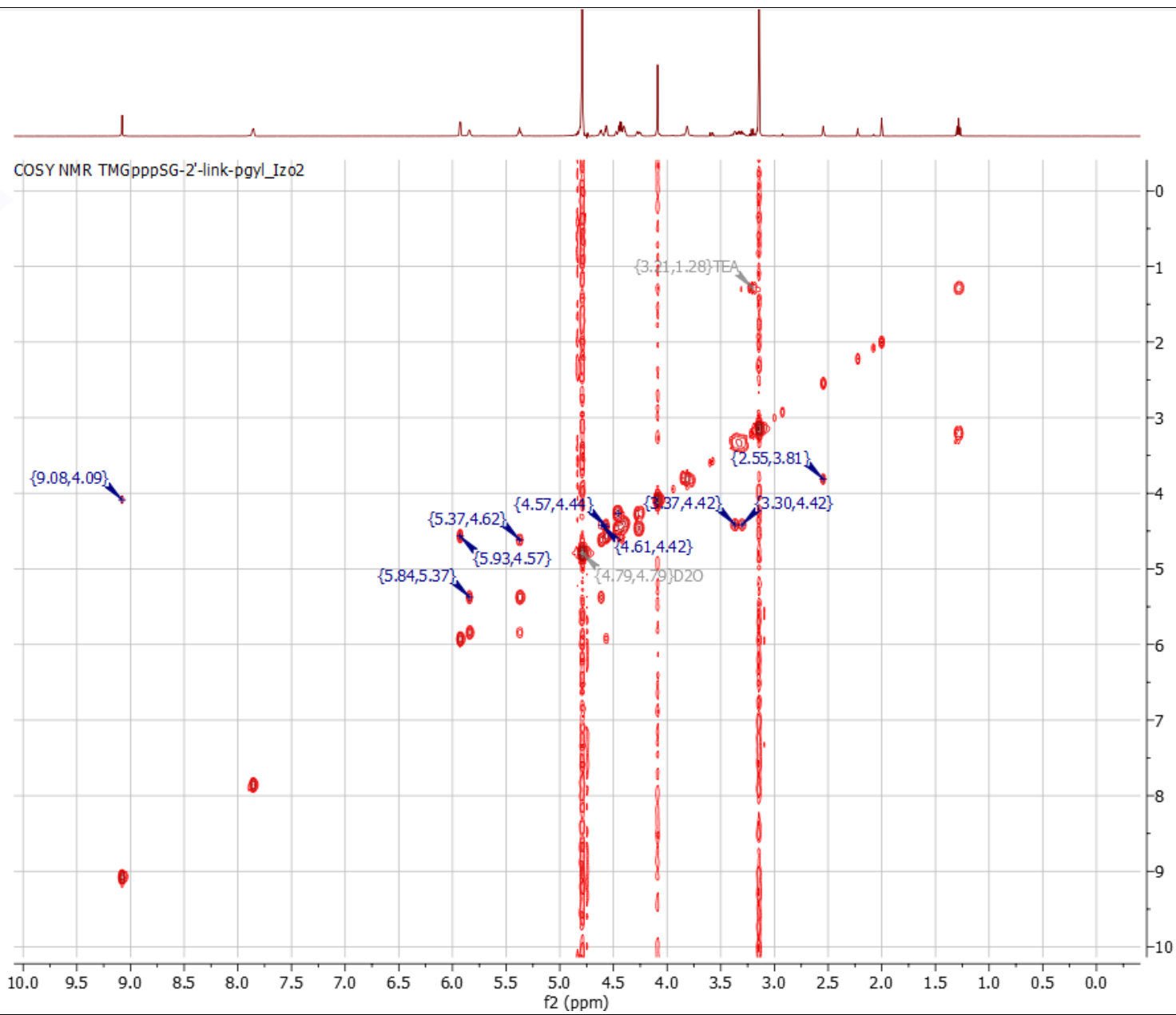


¹H NMR (500 MHz, D₂O, 25°C)

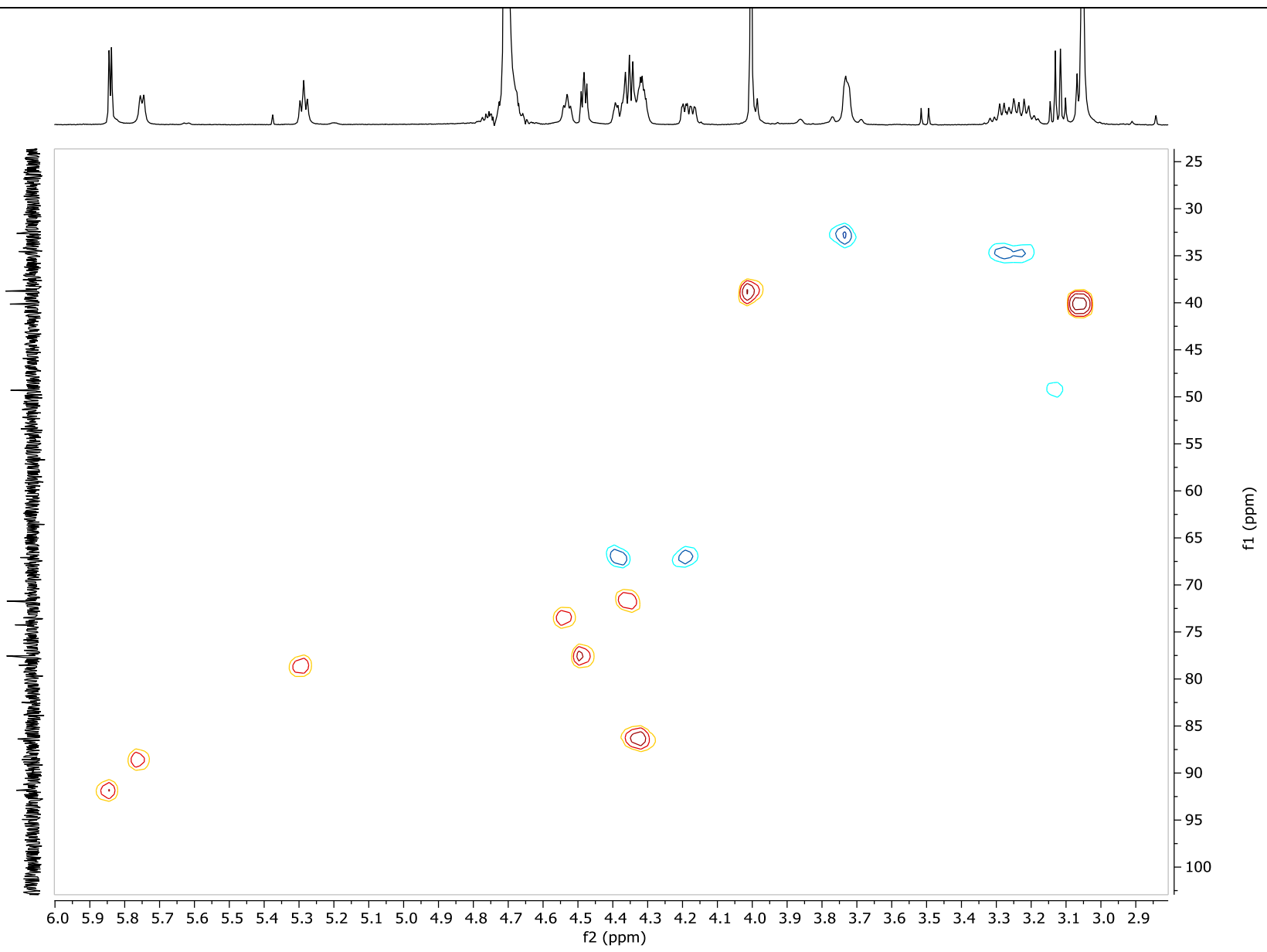
1H NMR TMGpppSG-2'-link-pgyl_Izo2



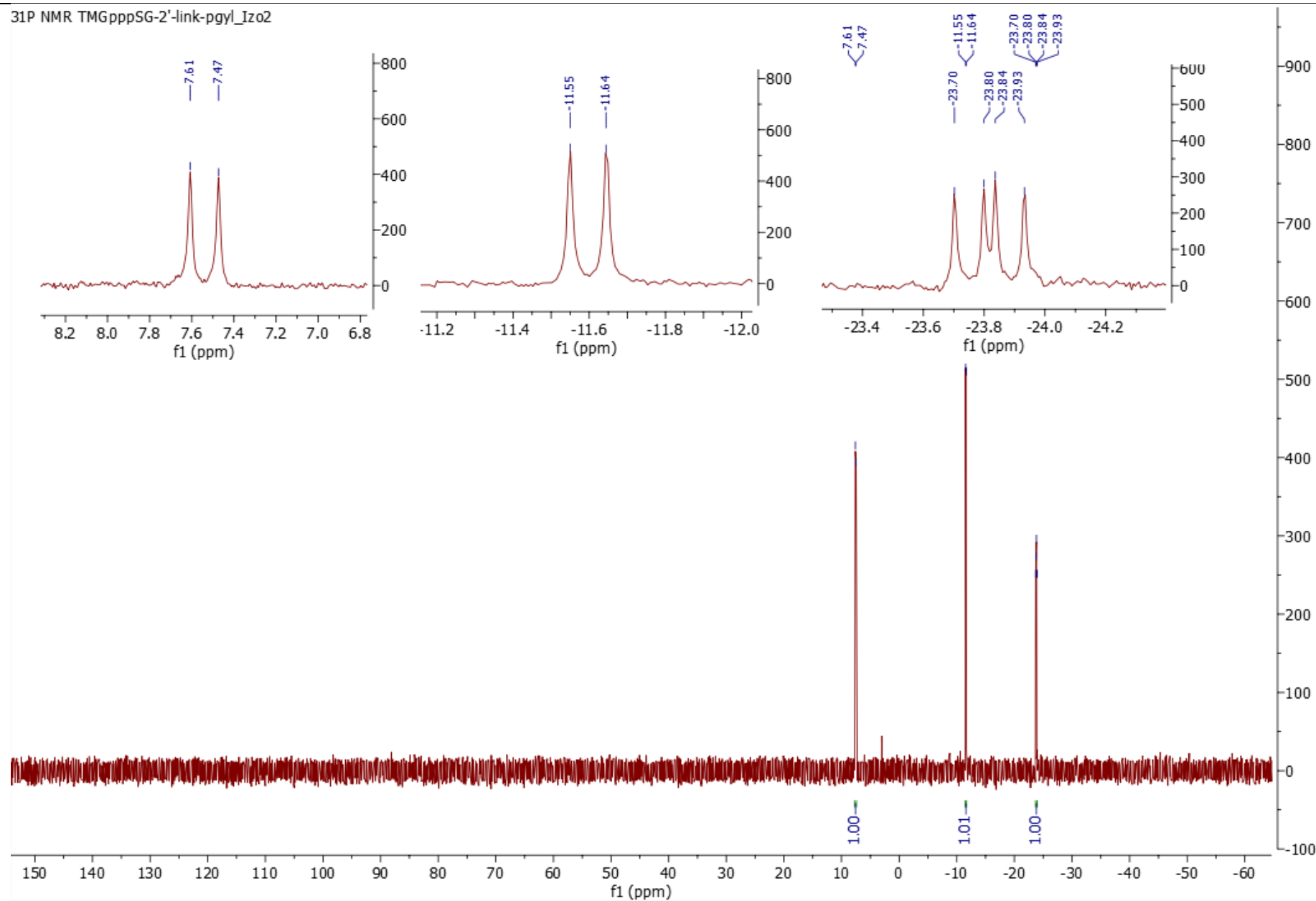
COSY NMR



HSQC NMR

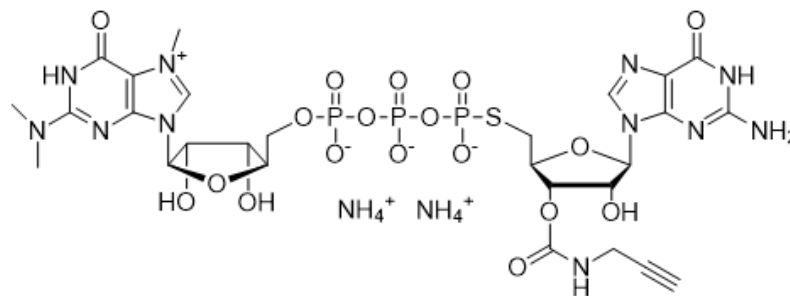


³¹P NMR (203 MHz, D₂O, H₃PO₄, 25°C)

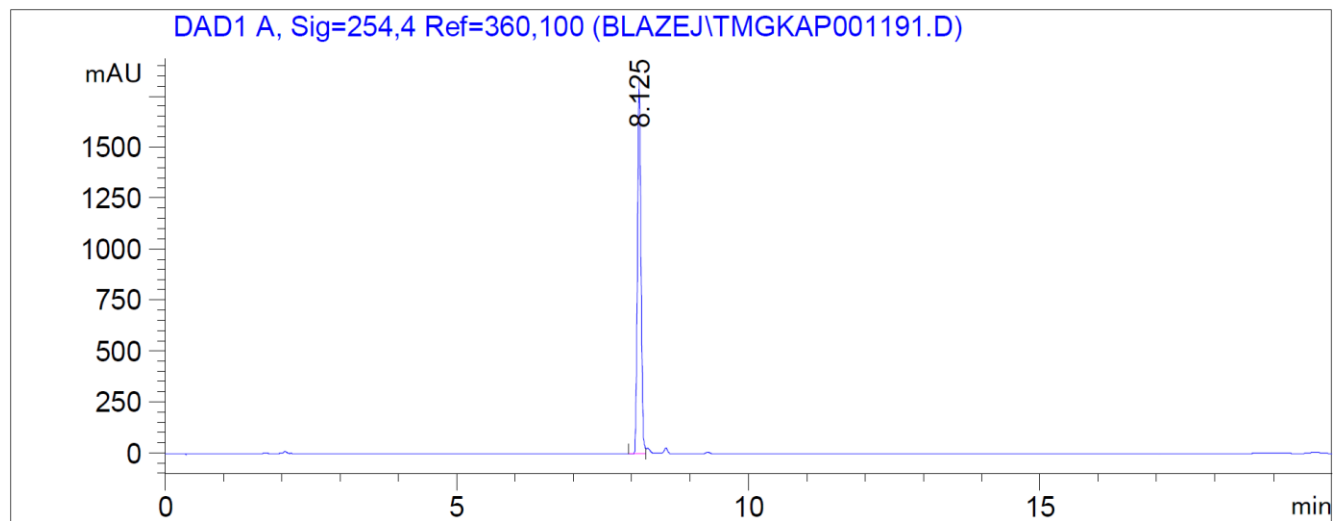


Compound 7-3': TMGppp-5'-SG-3'-O-C(O)-NH-C₃H₃ (NH₄⁺ salt)

Chemical structure

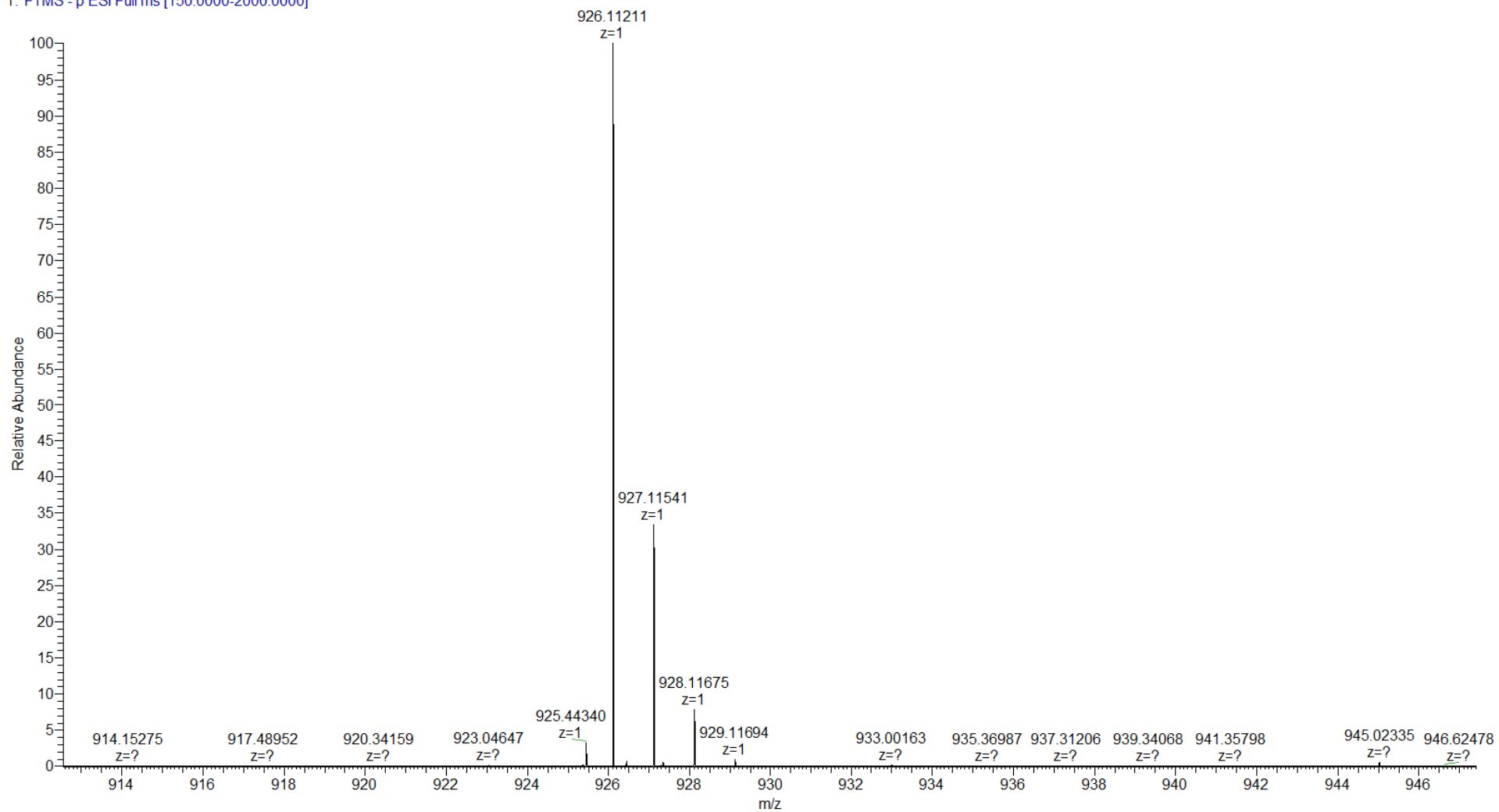


RP-HPLC (conditions c)

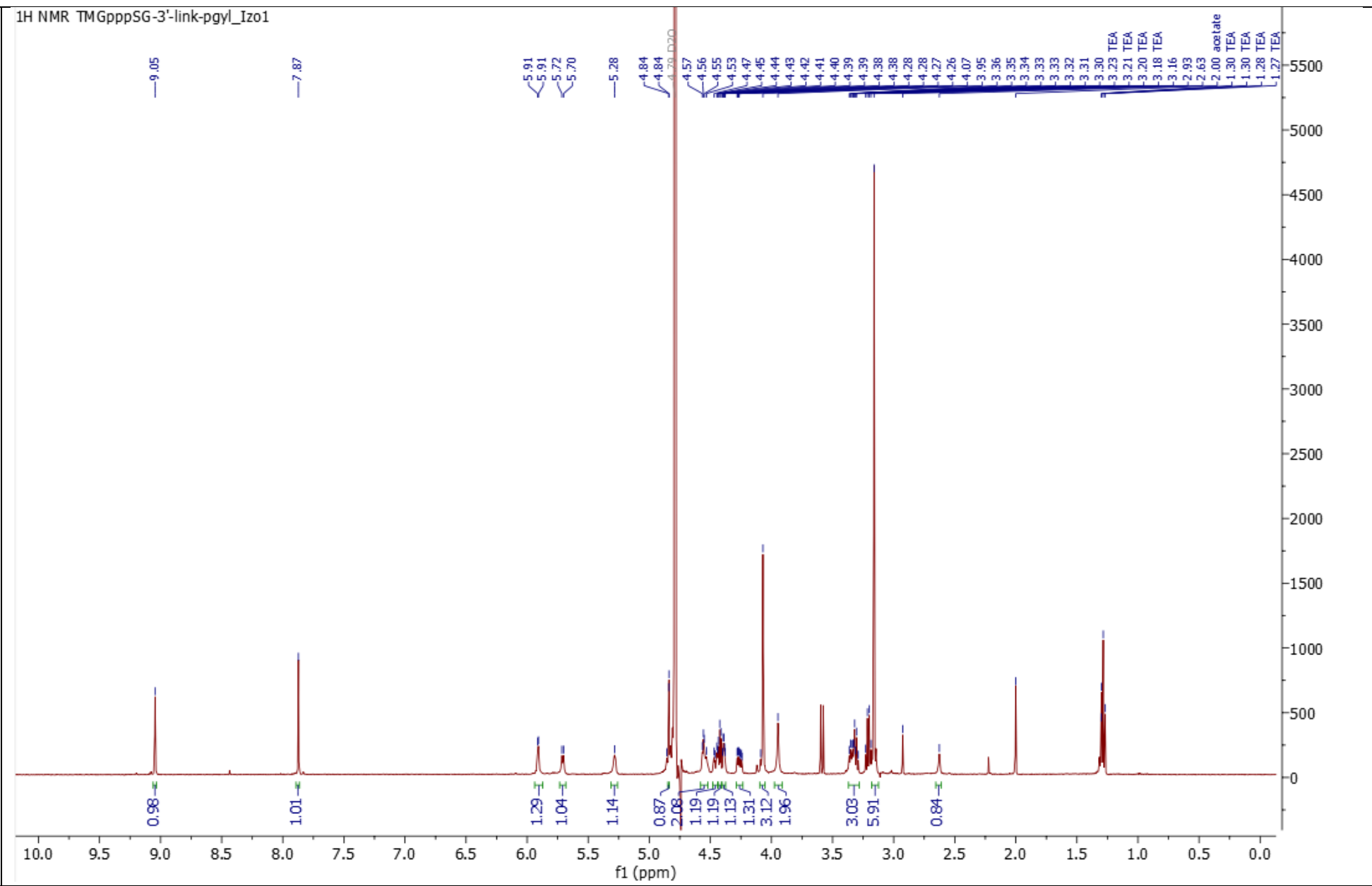


201119_PSu_09 #131-201 RT: 1.28-1.97 AV: 71 NL: 2.37E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

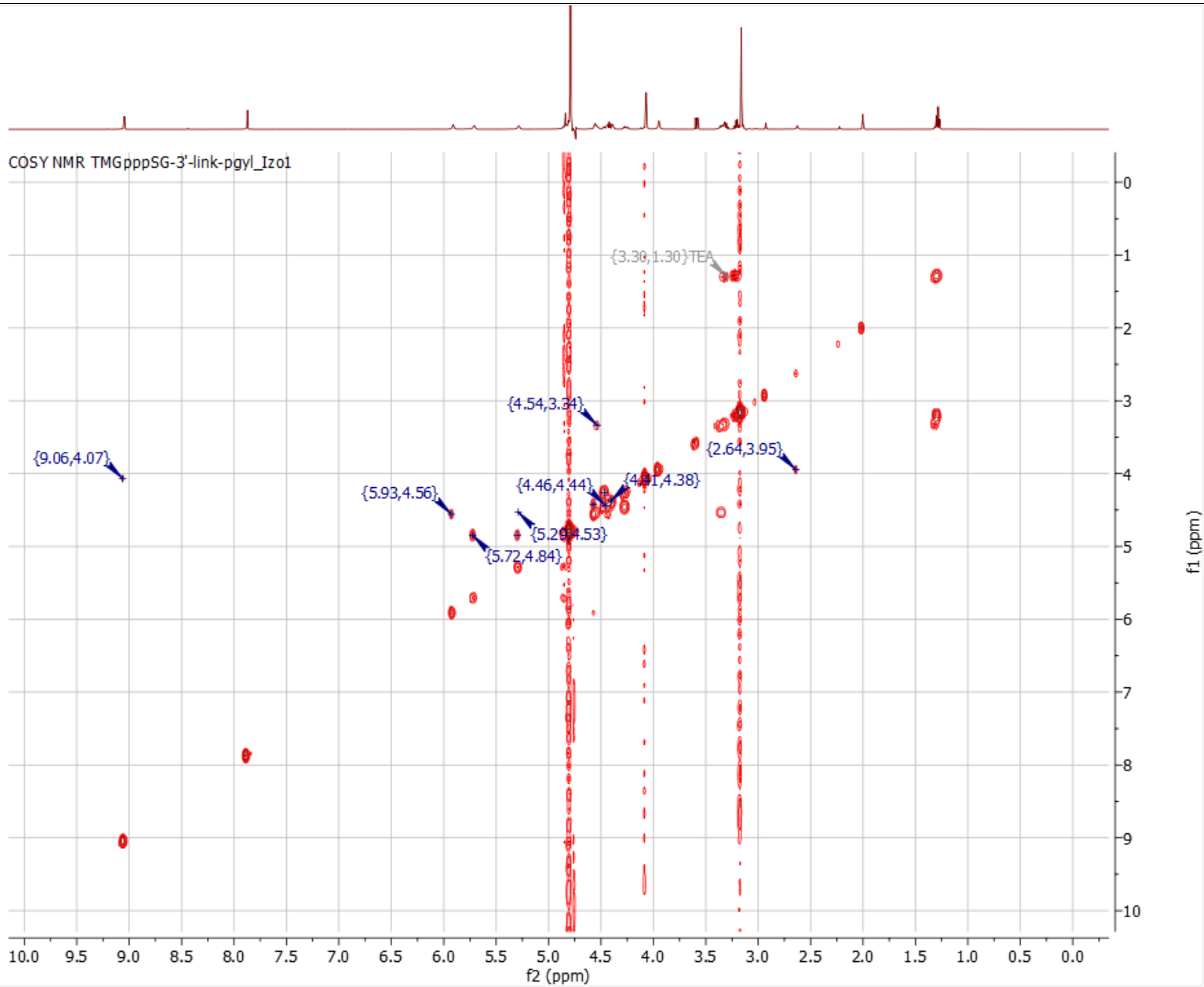
MS (-) ESI (Calc. [M-H]⁻ C₂₇H₃₅N₁₁O₁₈P₃S⁻ : 926.1101; found 926.11211)



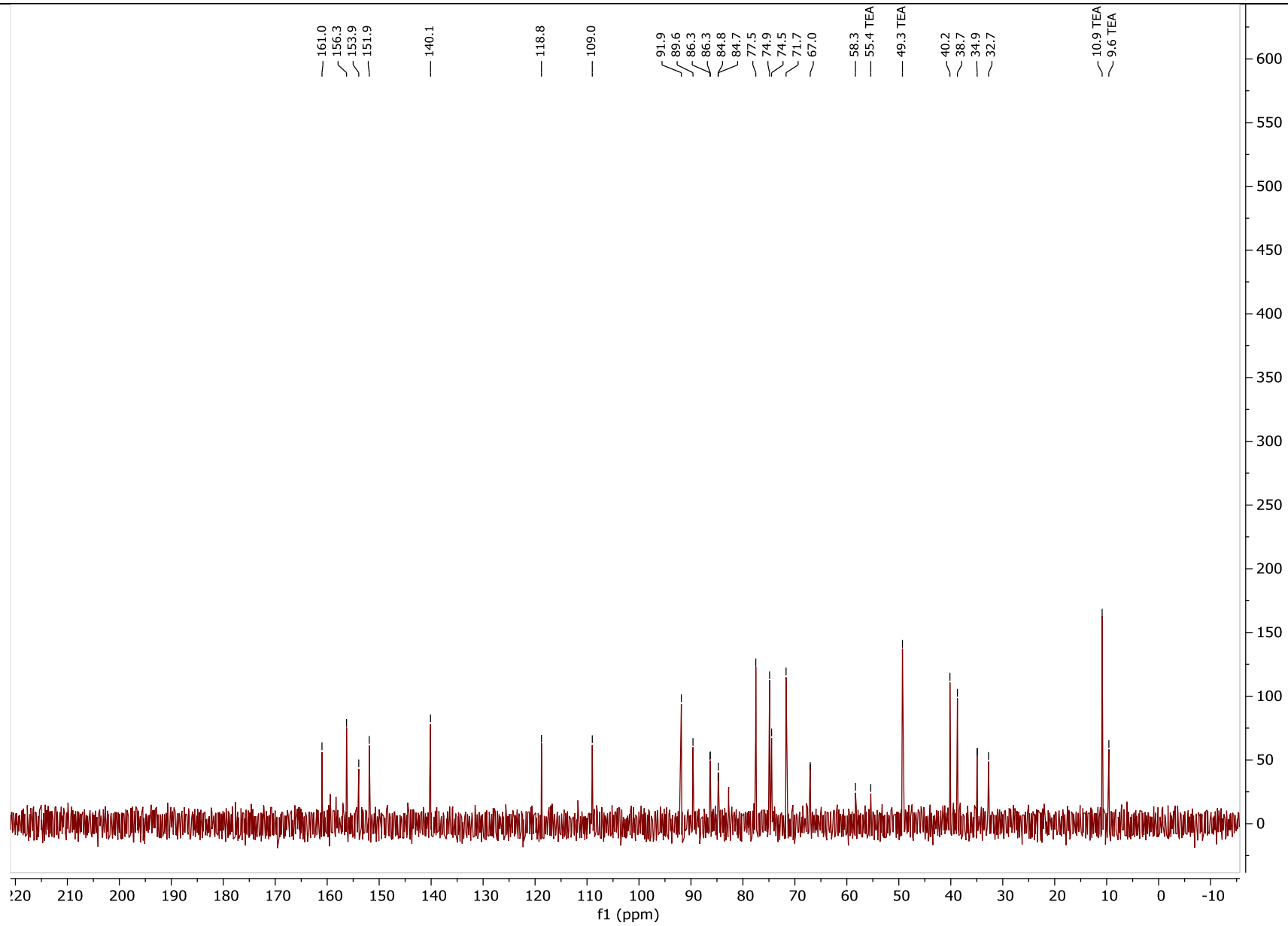
¹H NMR (500 MHz, D₂O, 25°C)



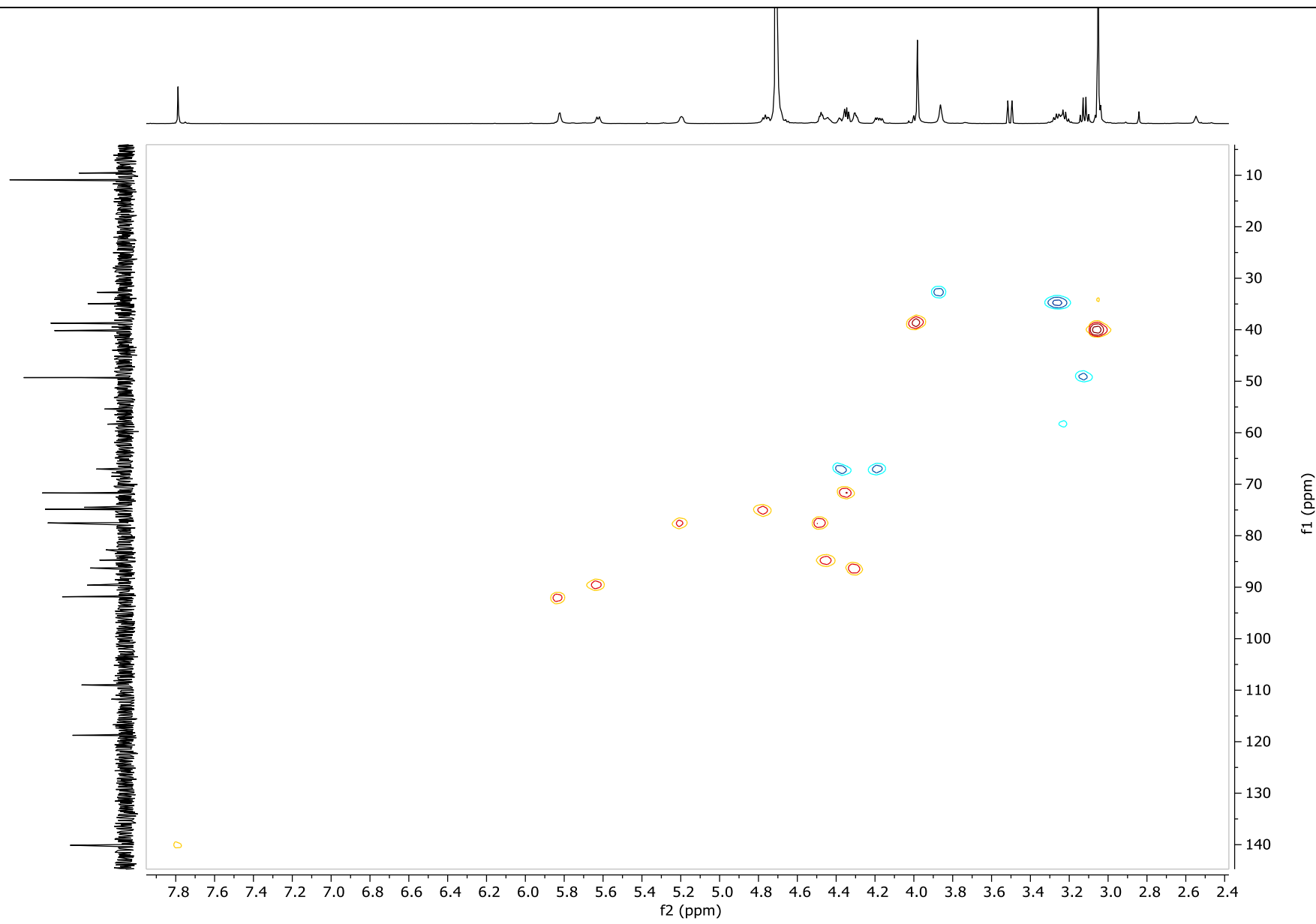
COSY NMR



¹³C NMR (500 MHz, D₂O, 25°C)

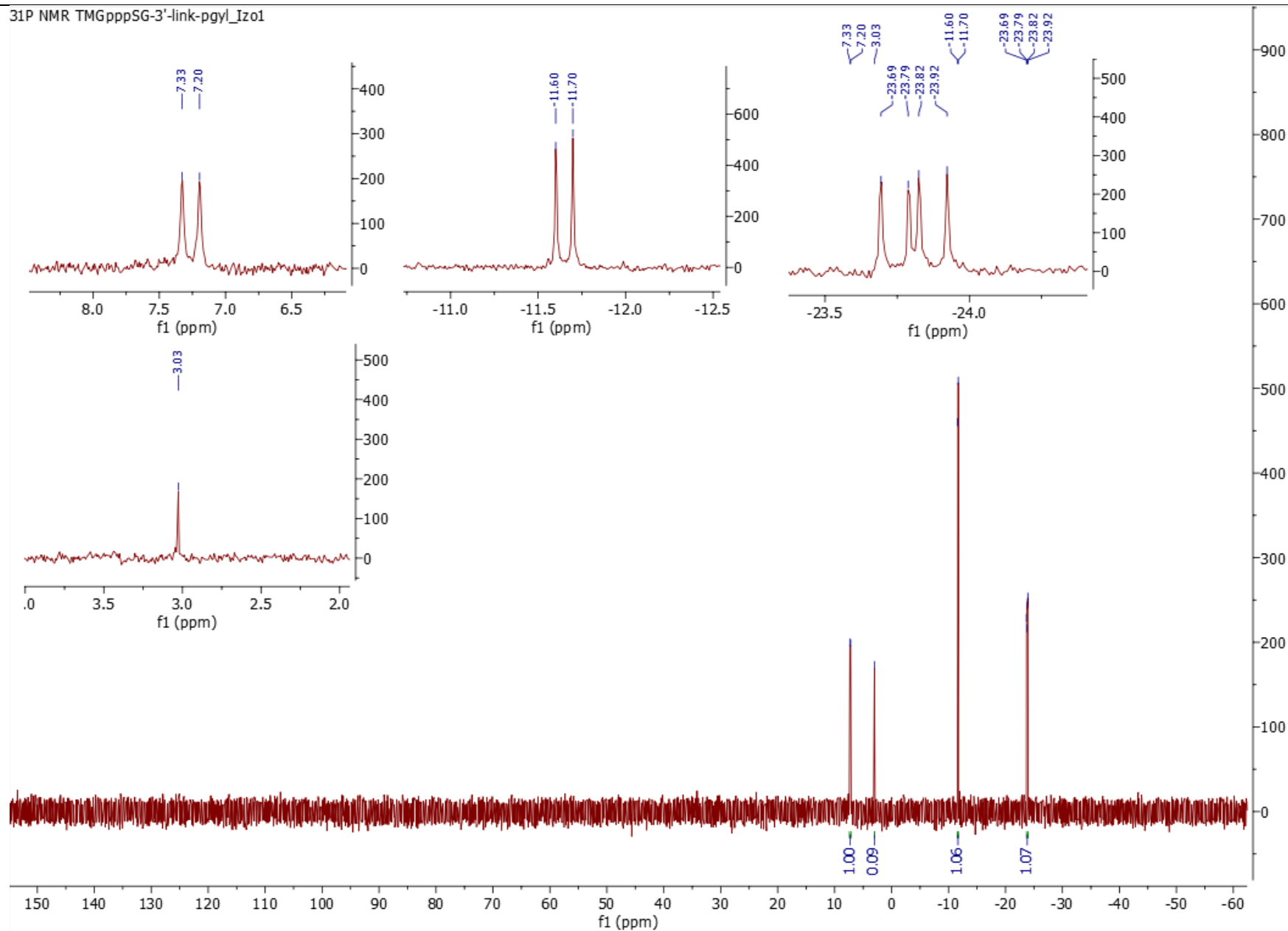


HSQC NMR



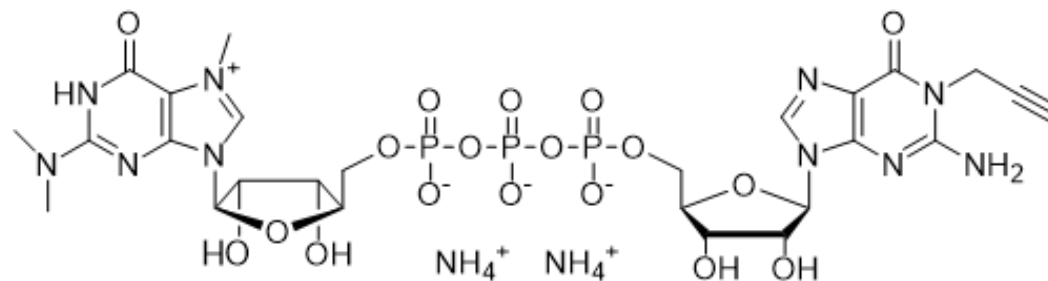
³¹P NMR (203 MHz, D₂O, H₃PO₄, 25°C)

31P NMR TMGpppSG-3'-link-pgyl_Izo1

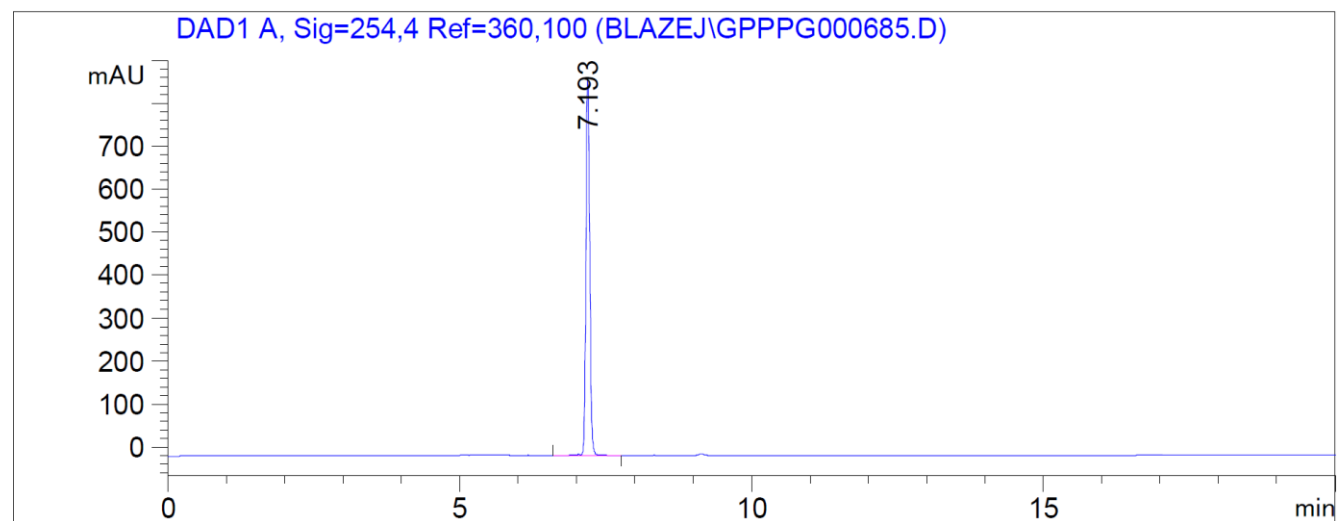


Compound 8: TMGpppG-N1-C₃H₃ (NH₄⁺ salt)

Chemical structure

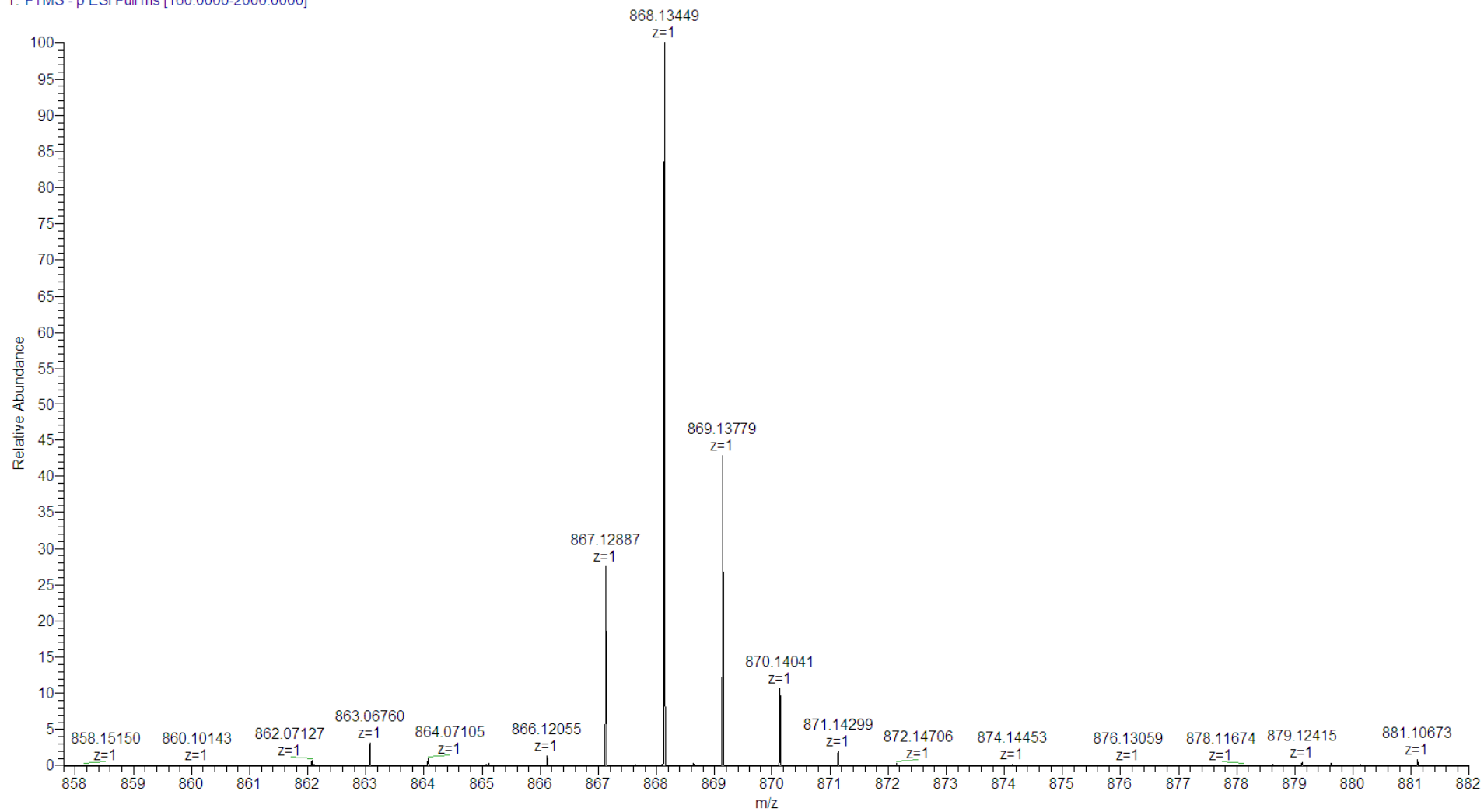


RP-HPLC (conditions c)

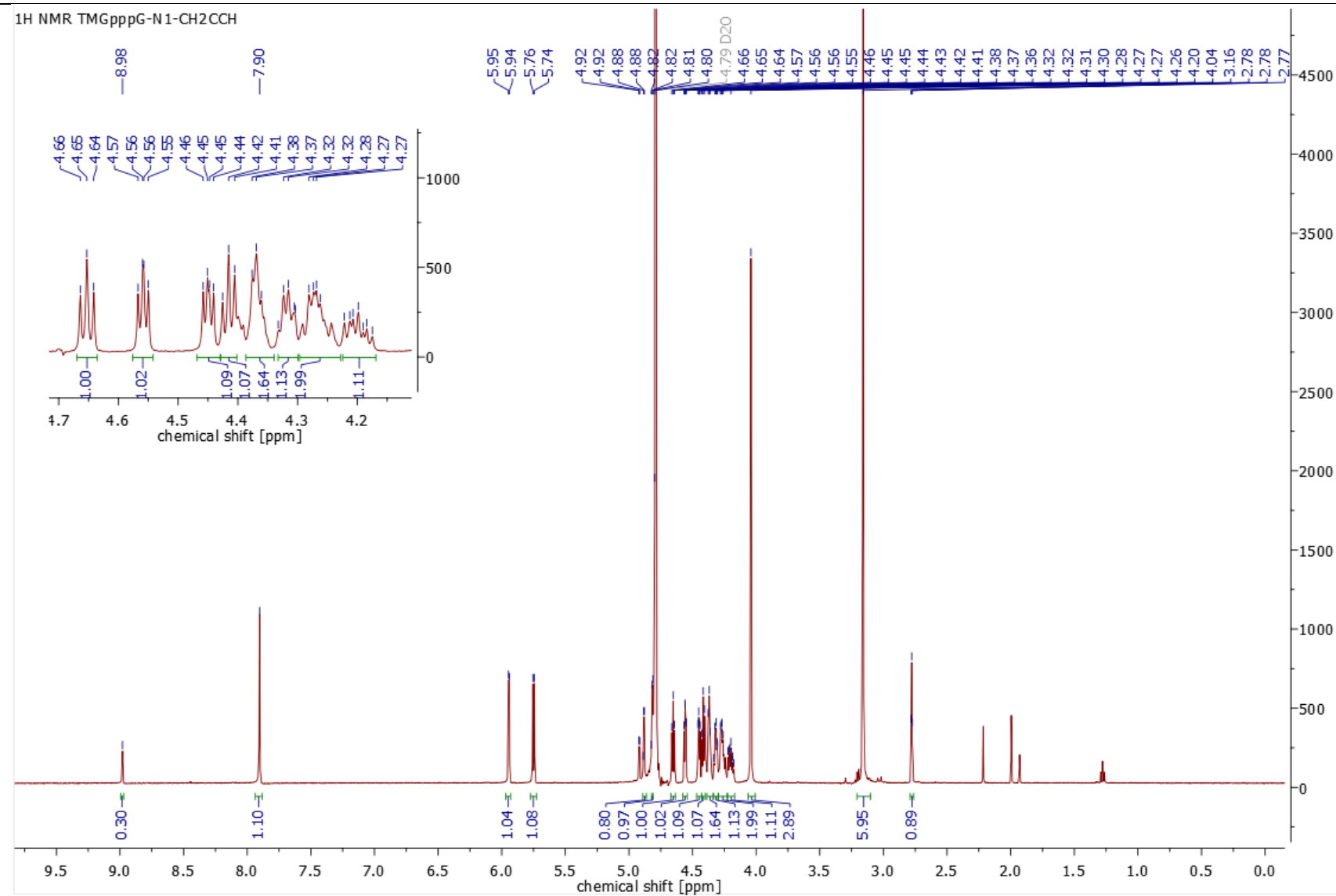


220407_PSu_08 #133-181 RT: 1.16-1.58 AV: 49 NL: 1.23E7
T: FTMS - p ESI Full ms [160.0000-2000.0000]

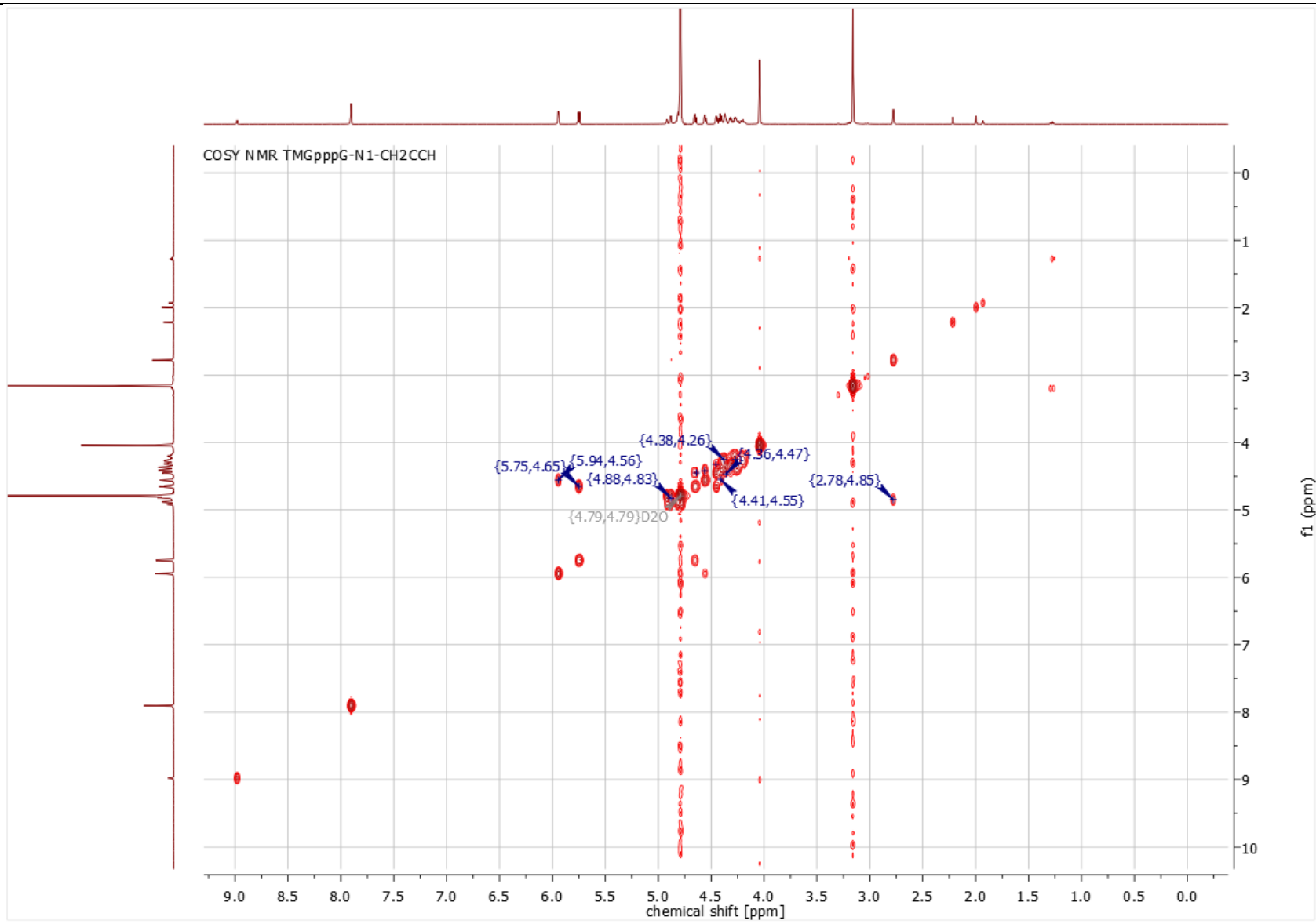
MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₄N₁₀O₁₈P₃⁻ : 867.1271, found 867.12887)



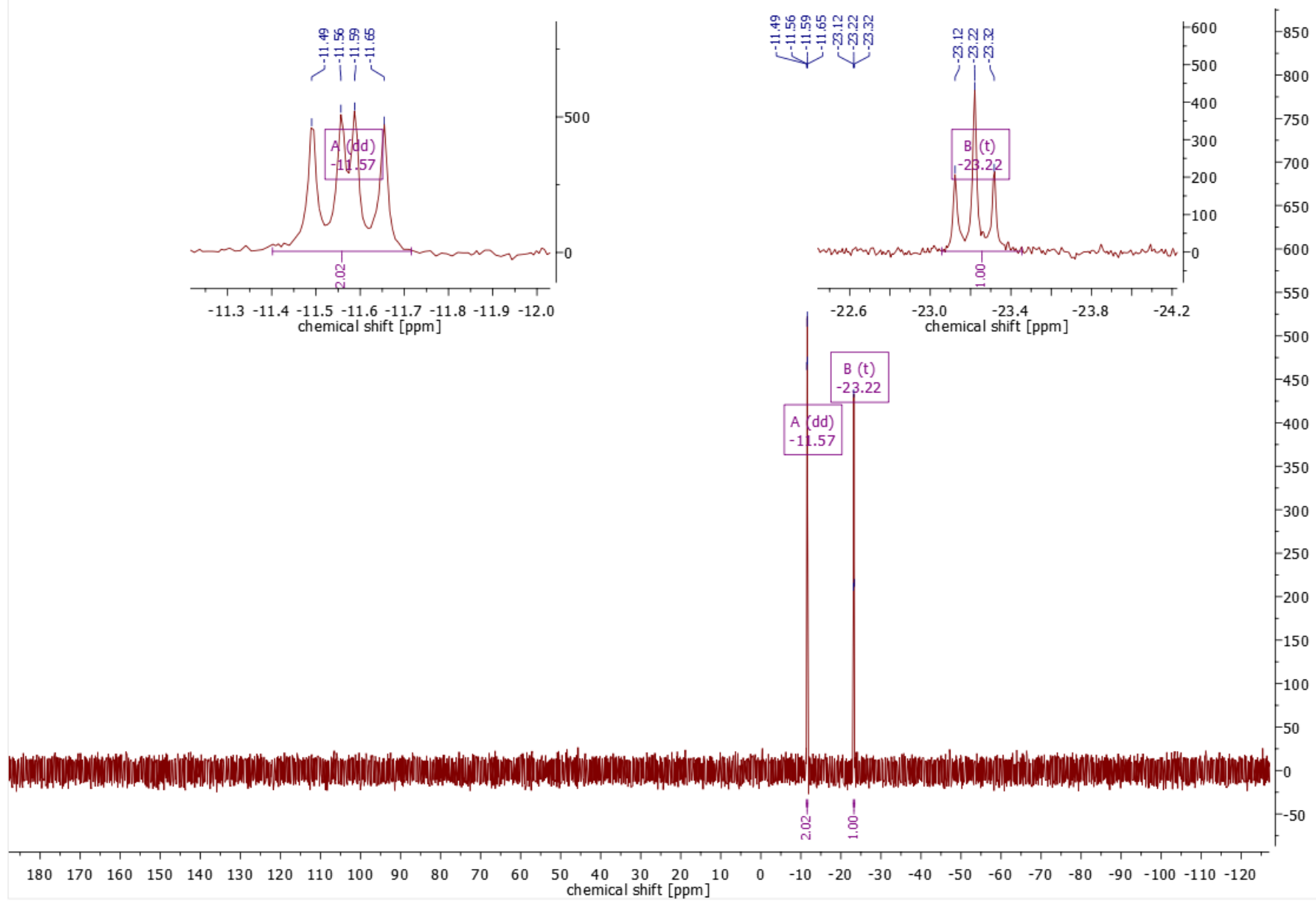
¹H NMR (500 MHz, D₂O, 25°C)



COSY NMR

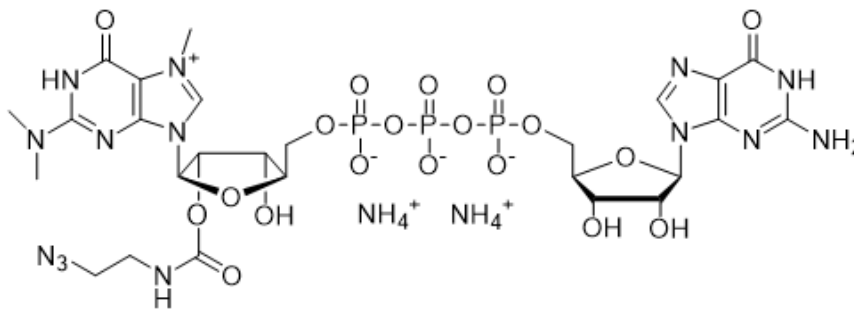


³¹P NMR (203 MHz, D₂O, H₃PO₄, 25°C)

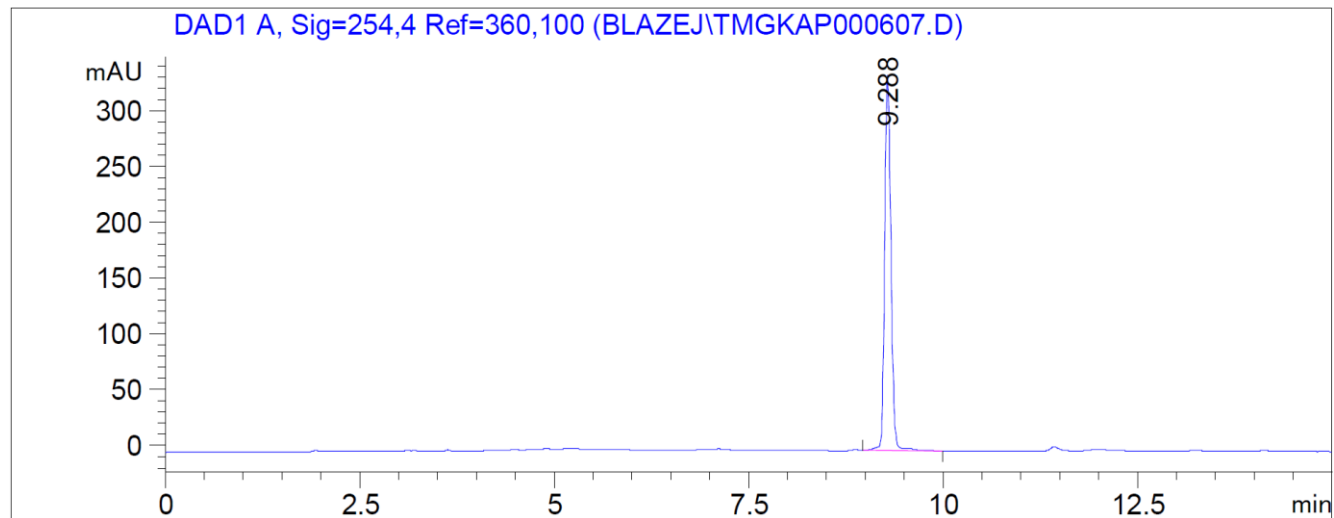


Compound 9-2': TMG(-2'-O-C(O)-NH-CH₂CH₂-N₃)pppG (NH₄⁺ salt)

Chemical structure

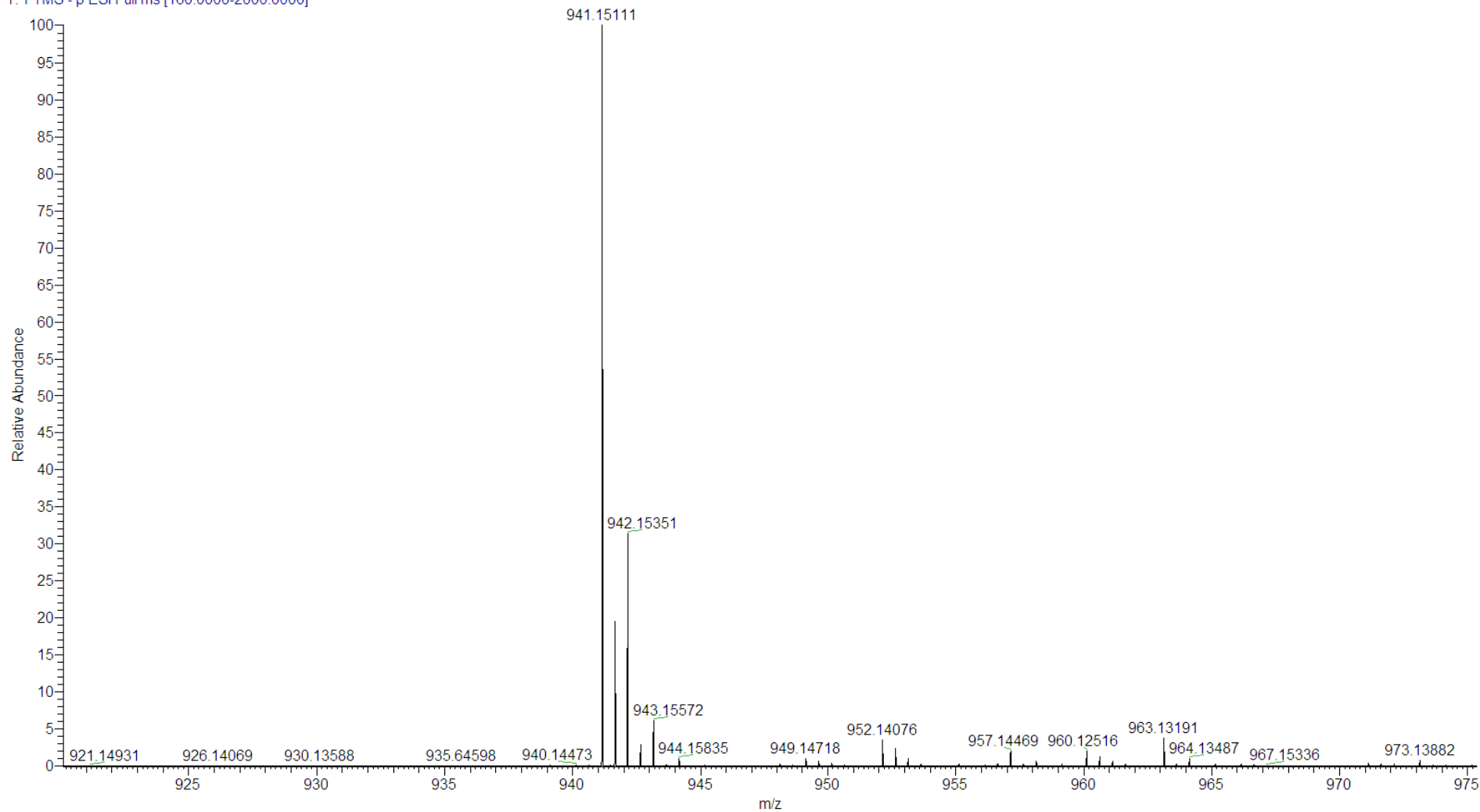


RP-HPLC (conditions c)

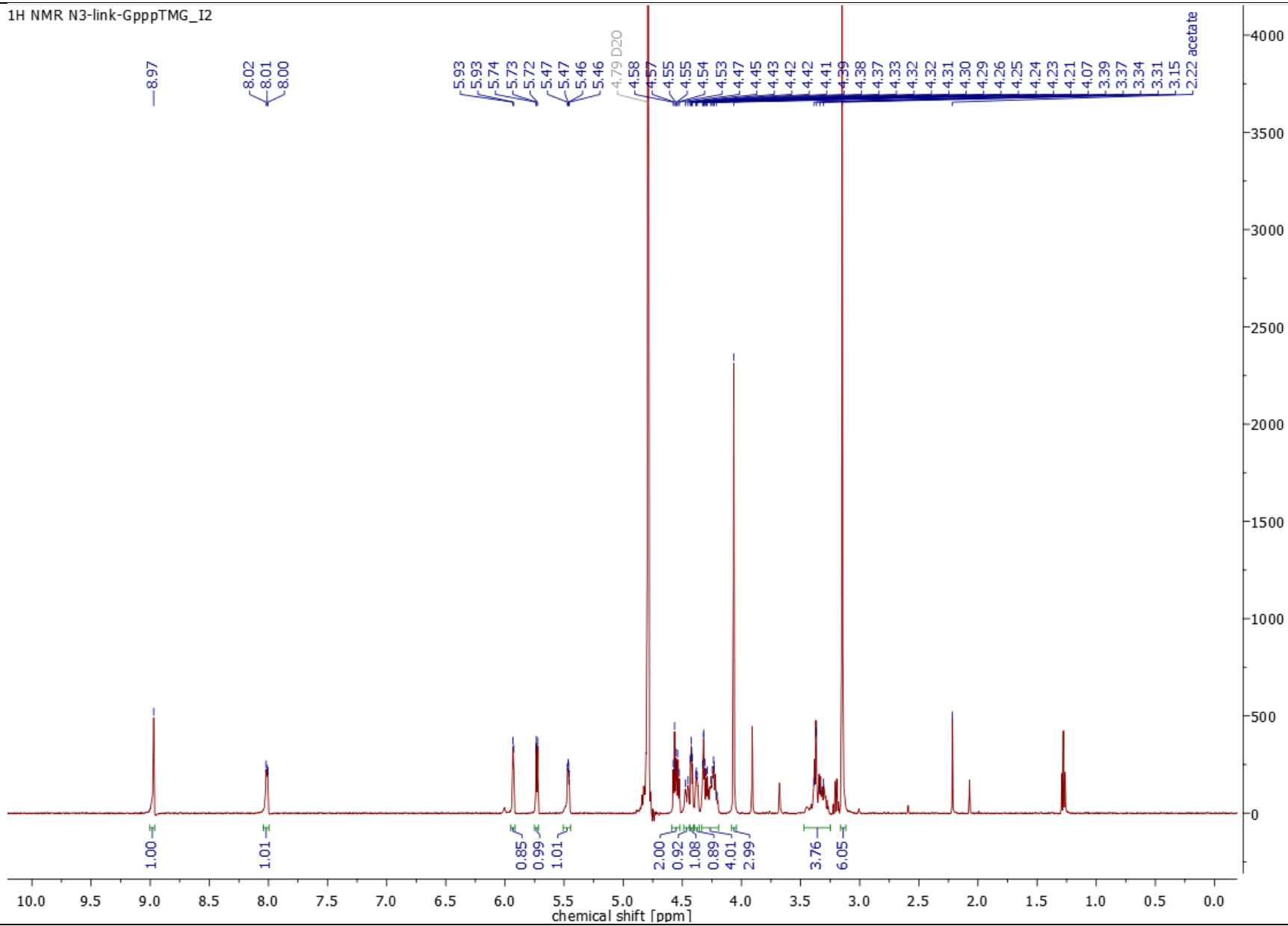


MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₆N₄O₁₉P₃⁻ : 941.1500, found: 941.15111)

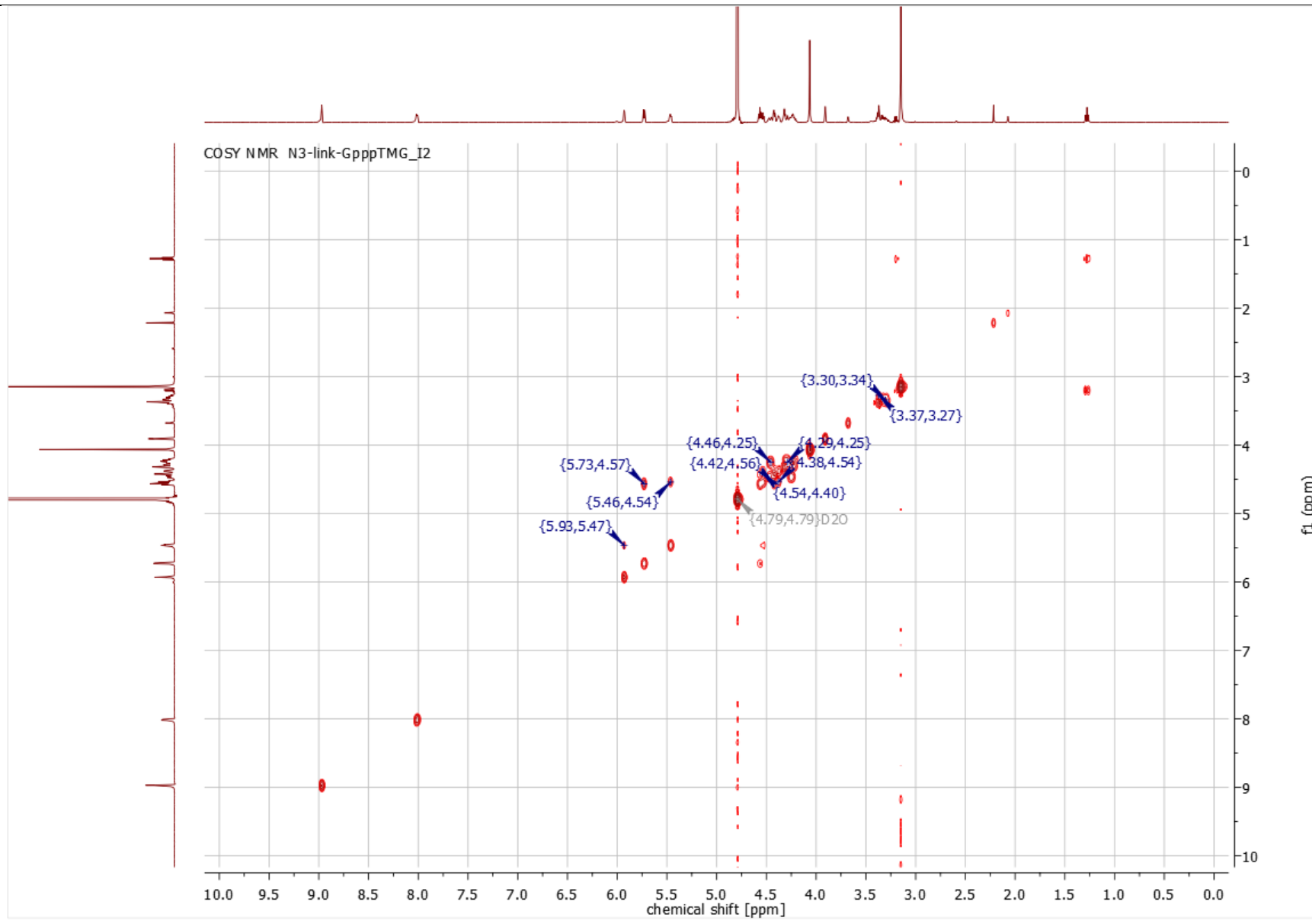
220329_PSu_16 #167-255 RT: 1.46-2.22 AV: 89 NL: 1.67E8
T: FTMS - p ESI Full ms [160.0000-2000.0000]



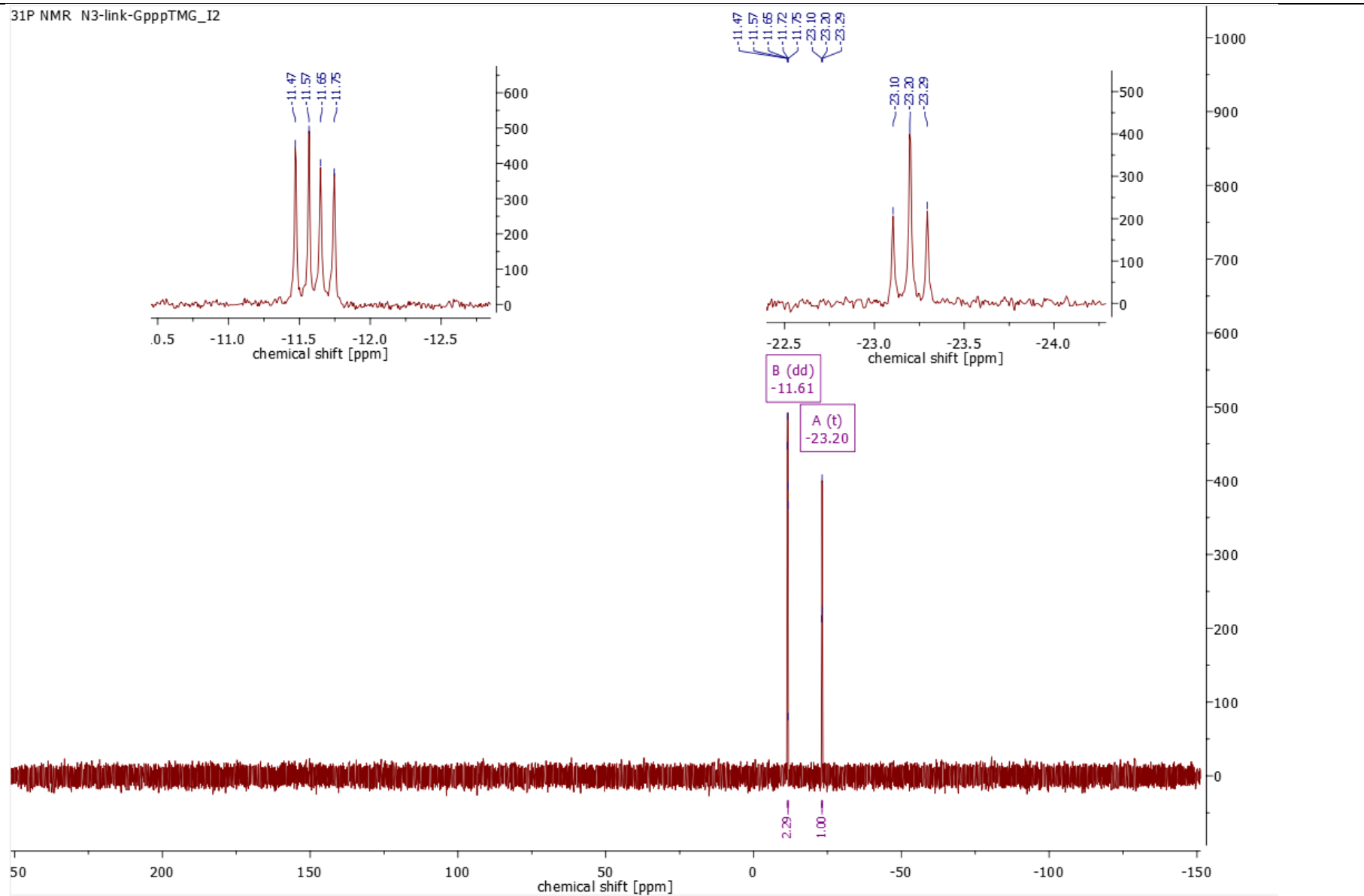
¹H NMR (500 MHz, D₂O, 25°C)



COSY NMR

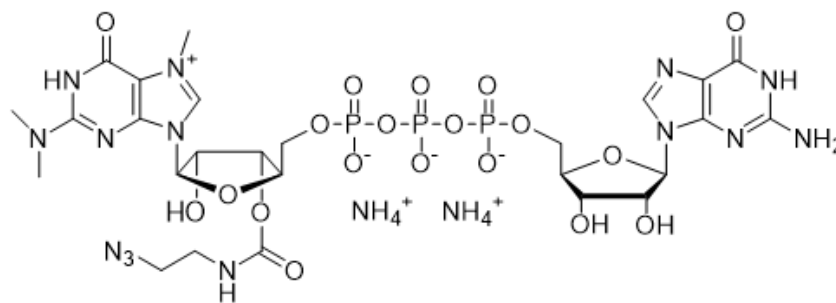


^{31}P NMR (203 MHz, D_2O , H_3PO_4 , 25°C)

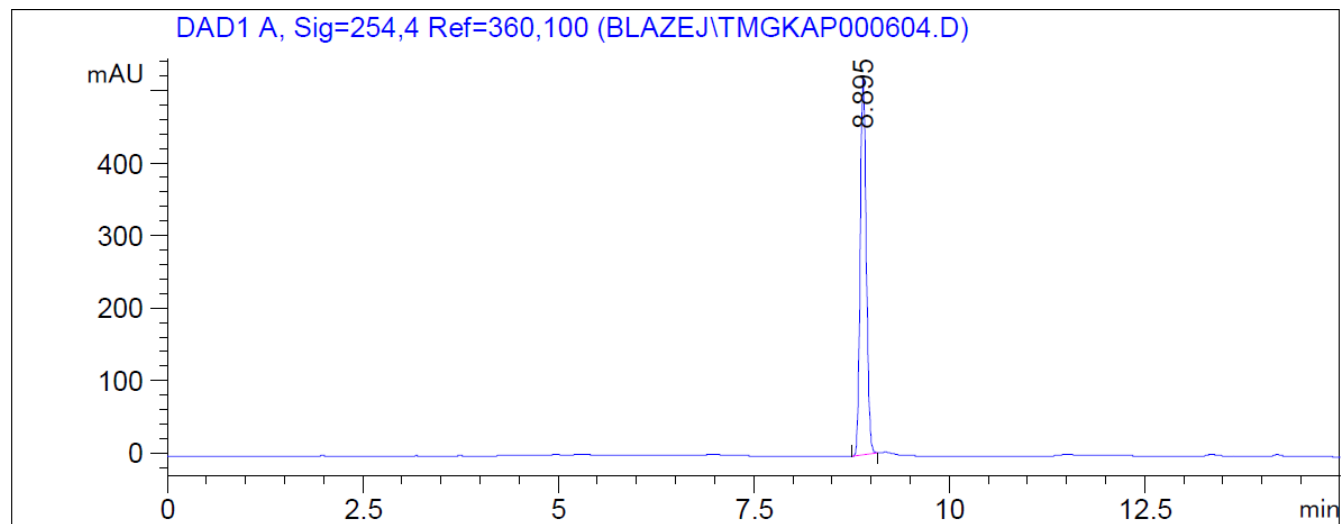


Compound 9-3': TMG(-3'-O-C(O)-NH-CH₂CH₂-N₃)pppG (NH₄⁺ salt)

Chemical structure

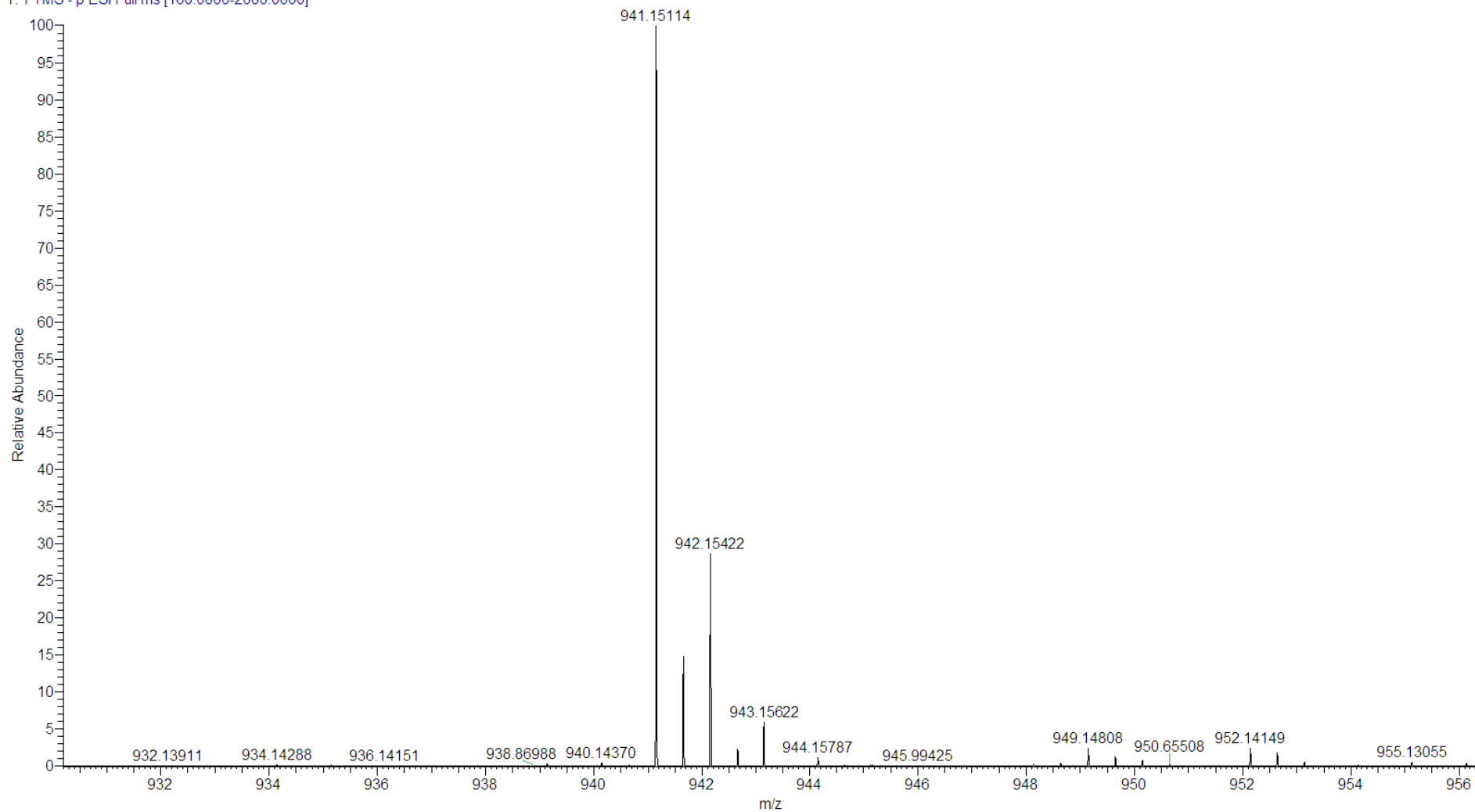


RP-HPLC (conditions c)

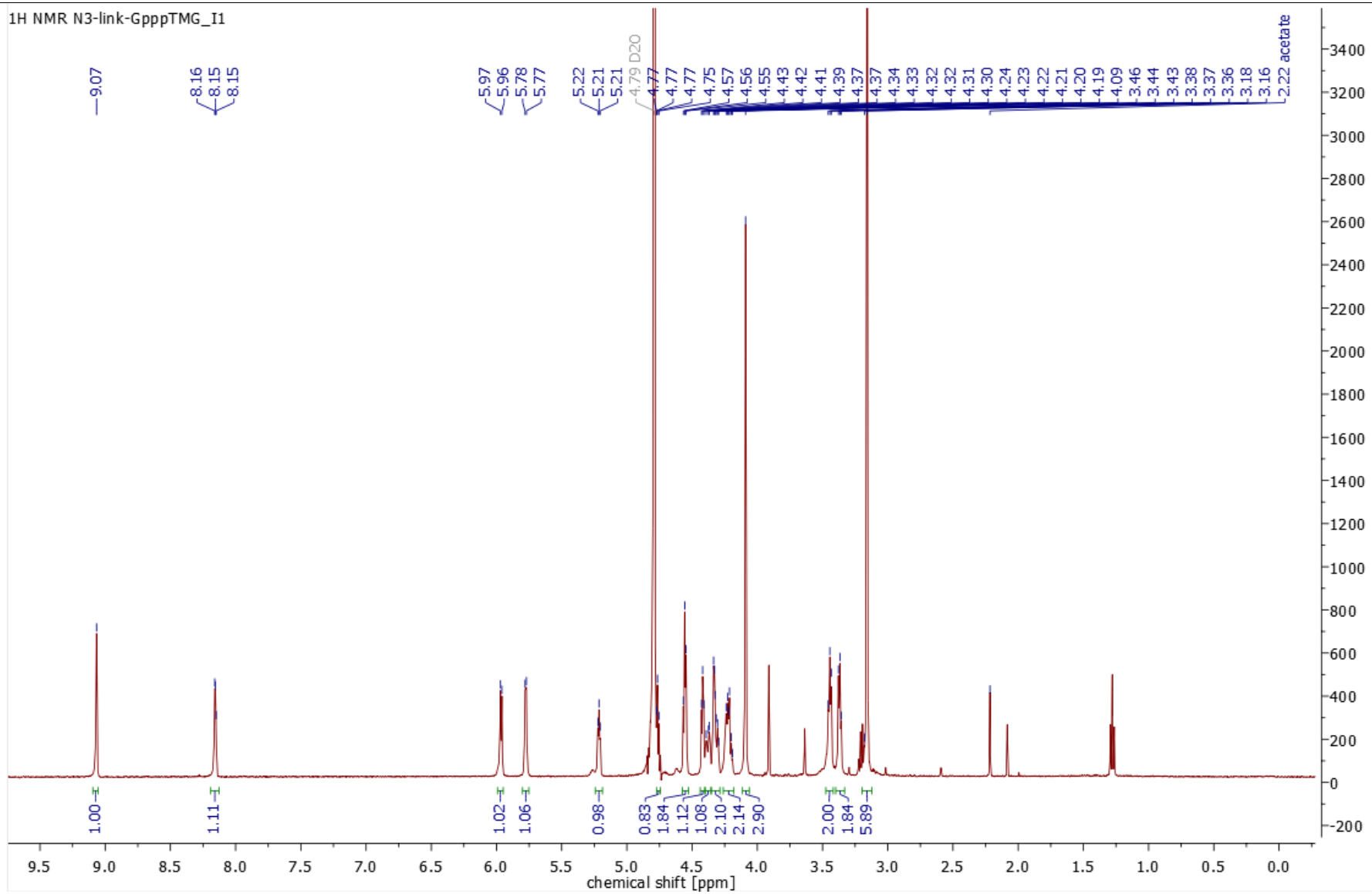


220329_PSu_17 #194-314 RT: 1.69-2.74 AV: 121 NL: 2.10E4
T: FTMS - p ESI Full ms [160.0000-2000.0000]

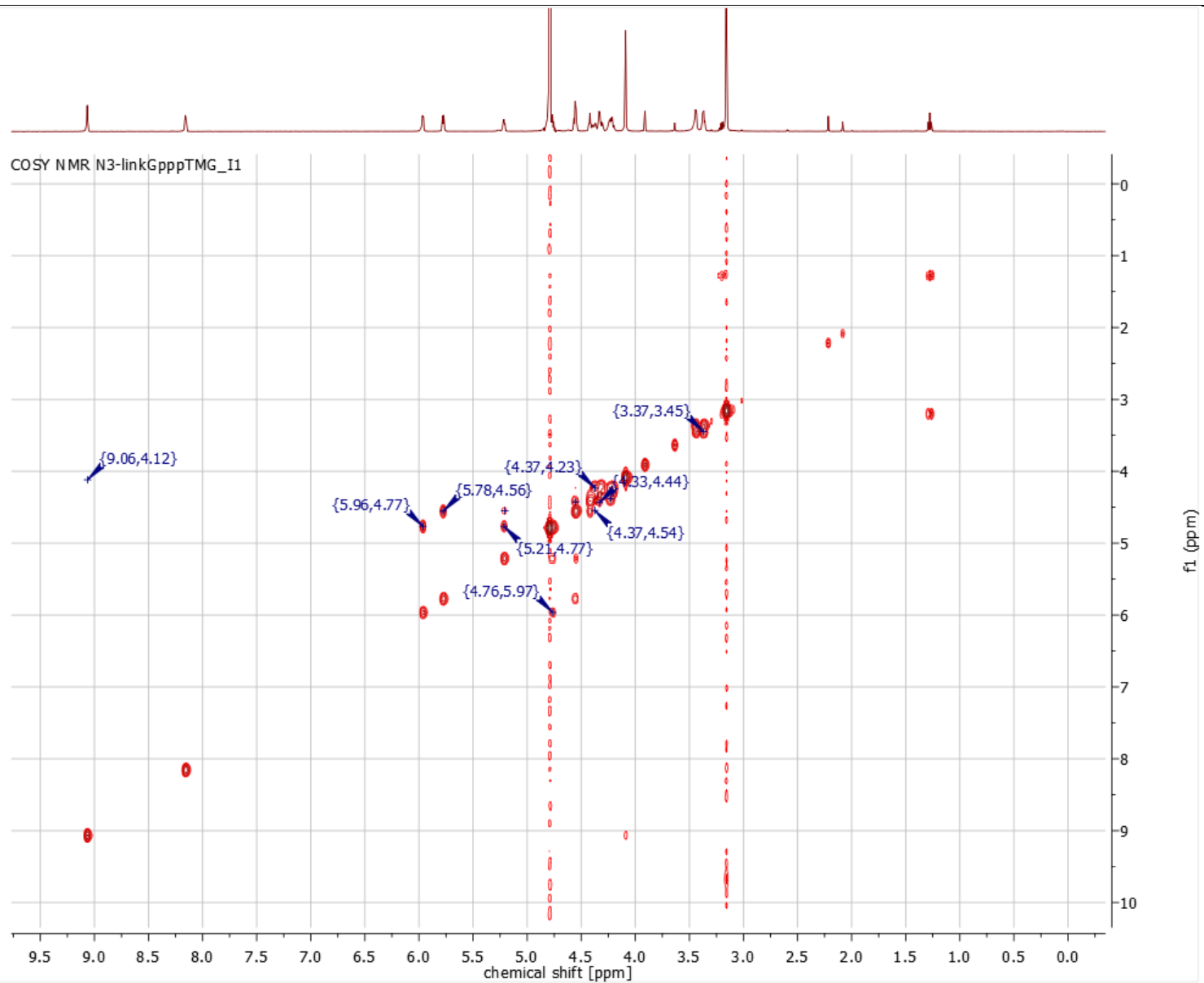
MS (-) ESI (Calc. [M-H]⁻ C₂₆H₃₆N₁₄O₁₉P₃⁻ : 941.1500, found: 941.15114)



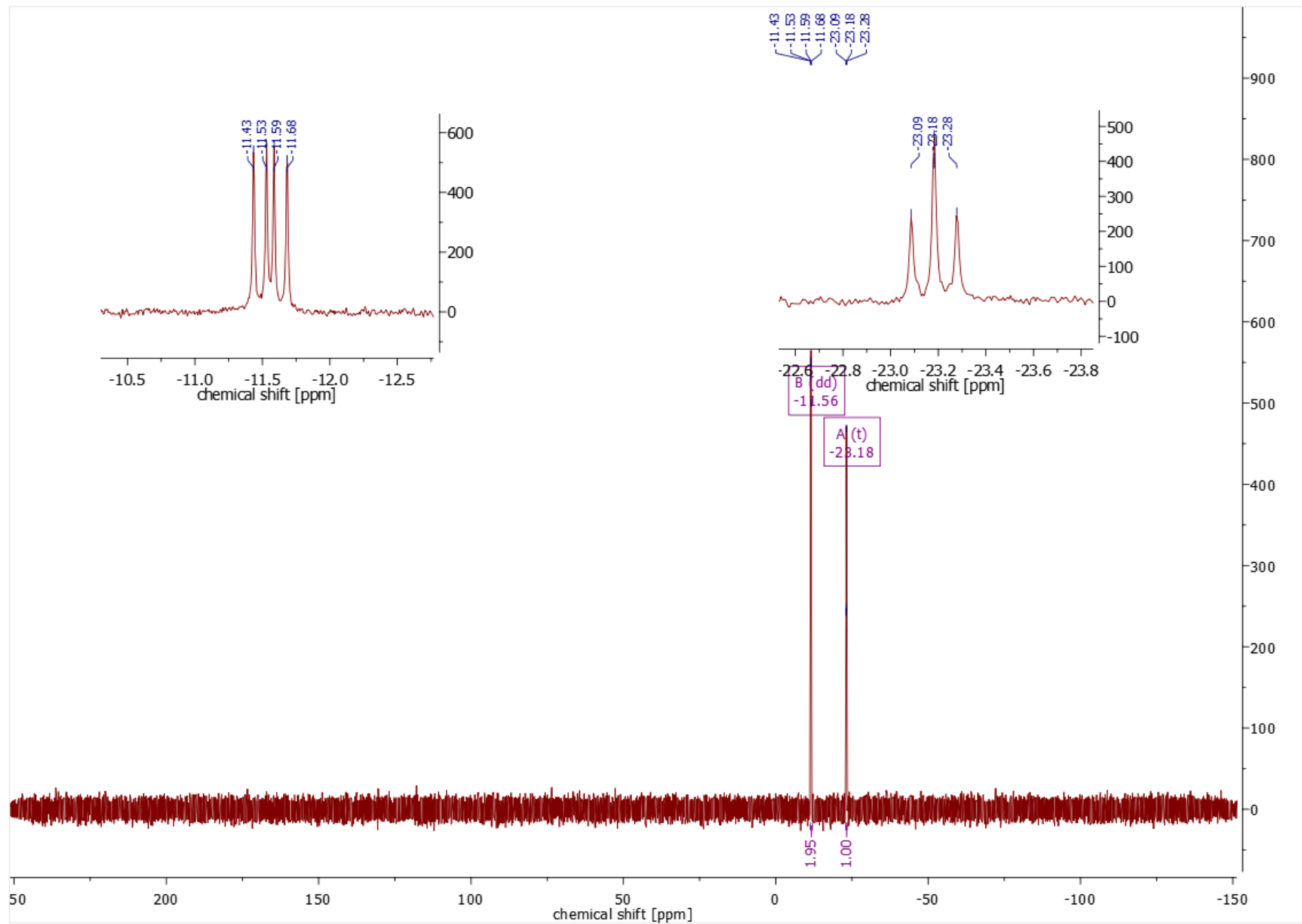
¹H NMR (500 MHz, D₂O, 25°C)



COSY NMR

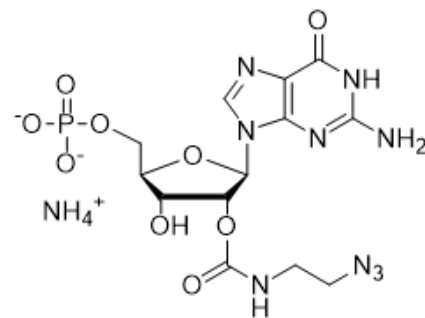


³¹P NMR (203 MHz, D₂O, H₃PO₄, 25°C)

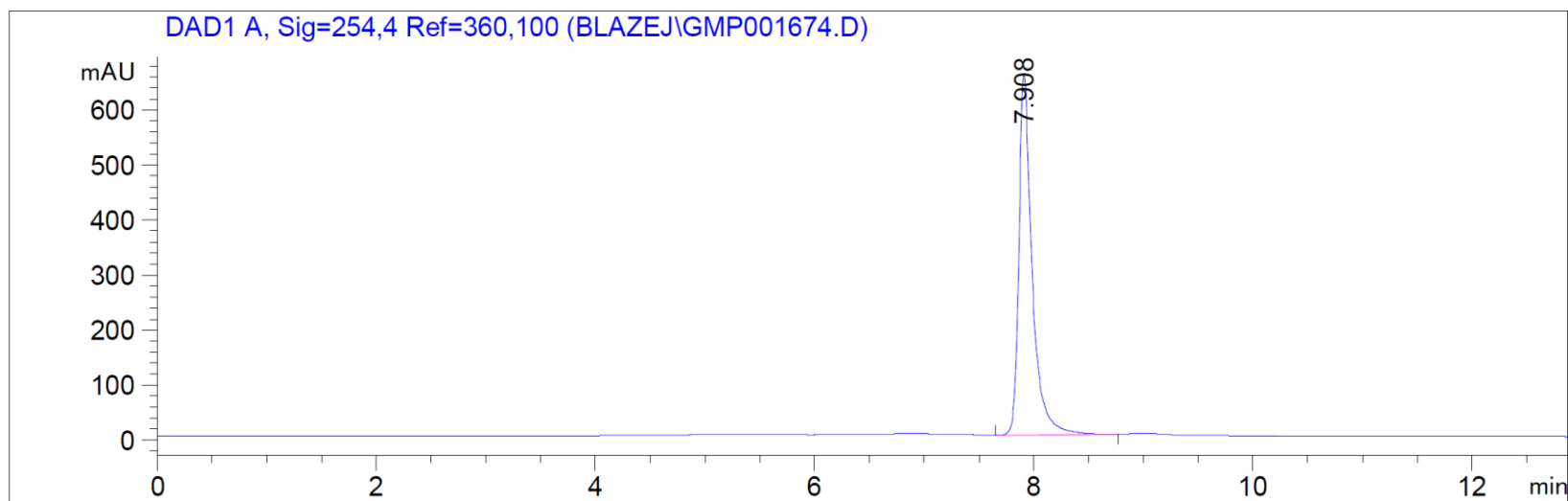


Compound 10-2': GMP-2'-O-C(O)-NH-CH₂CH₂-N₃ (NH₄⁺ salt)

Chemical structure

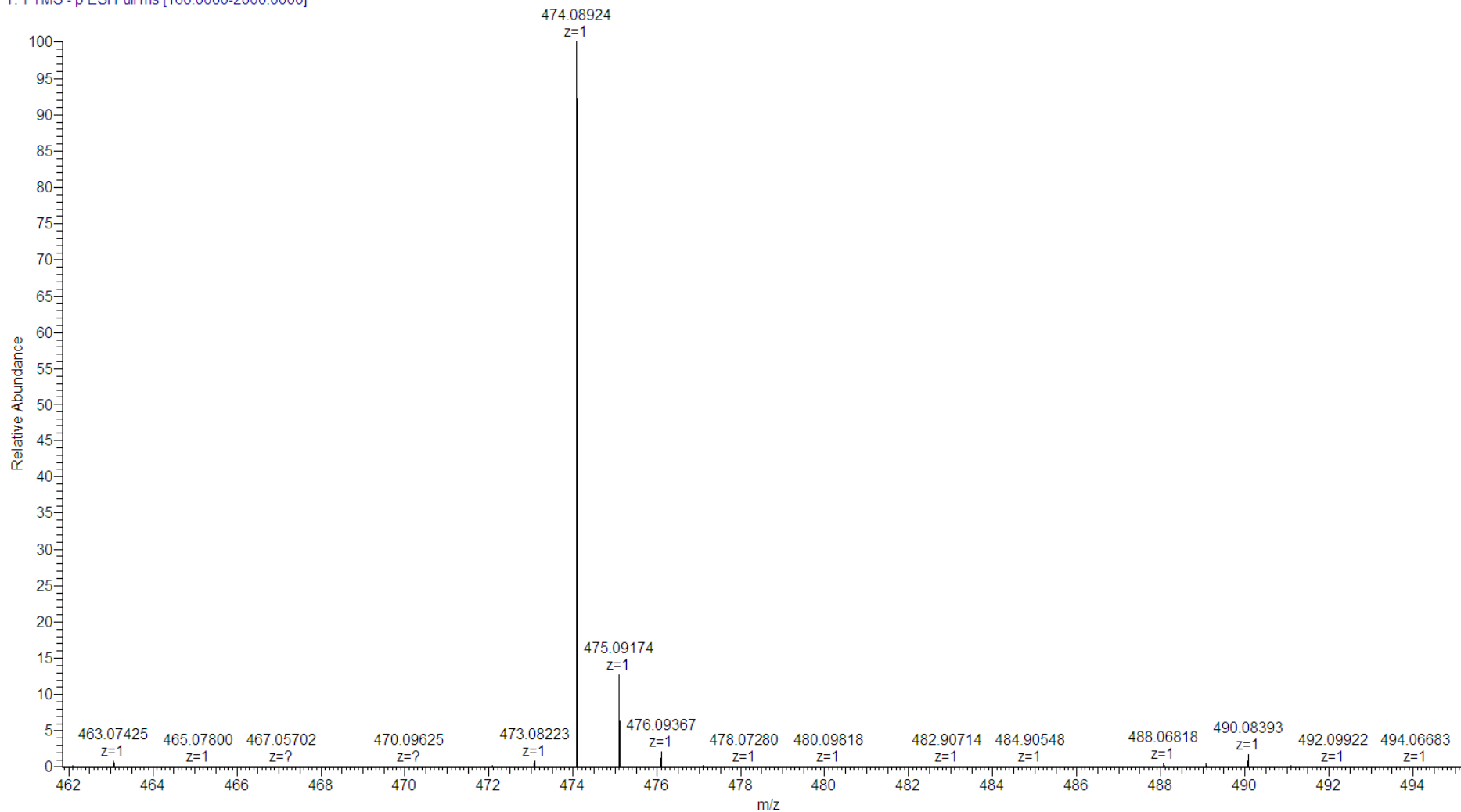


RP-HPLC (conditions c)

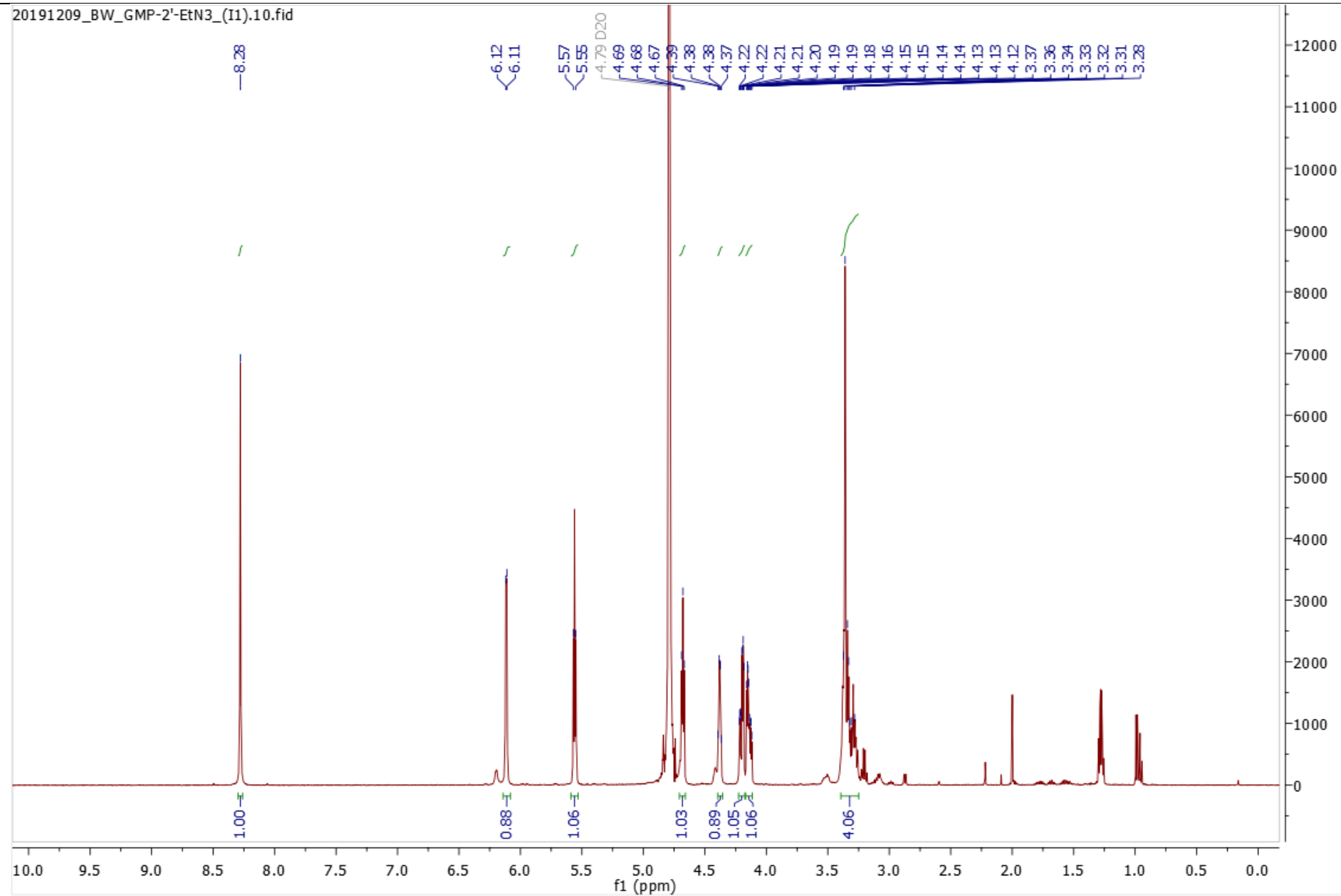


220331_PSu_04 #194-269 RT: 1.70-2.35 AV: 76 NL: 2.04E8
T: FTMS - p ESI Full ms [160.0000-2000.0000]

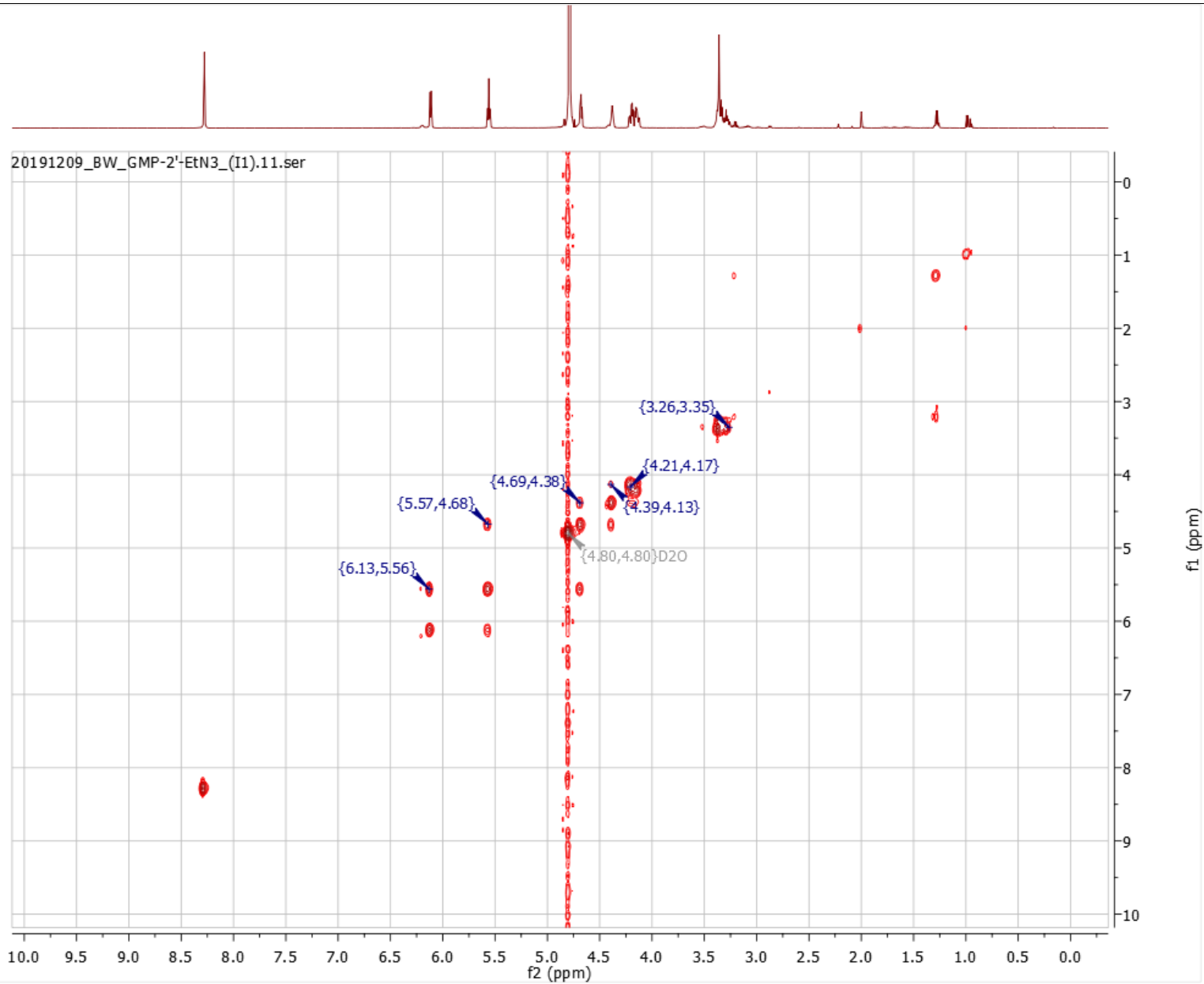
MS (-) ESI (Calc. [M-H]⁻ C₁₃H₁₇N₉O₉P⁻ : 474.0892, found: 474.08924)



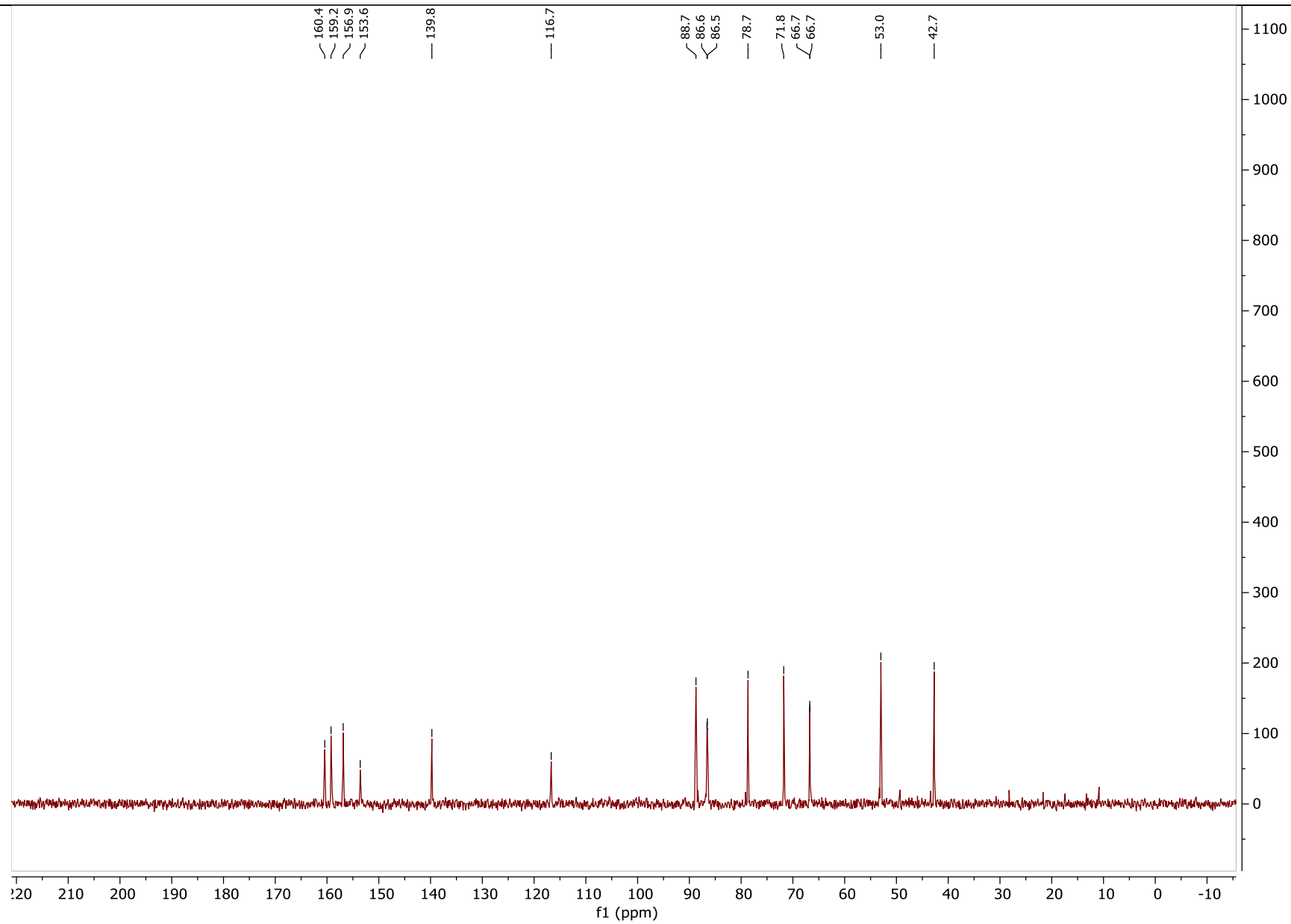
¹H NMR (500 MHz, D₂O, 25°C)

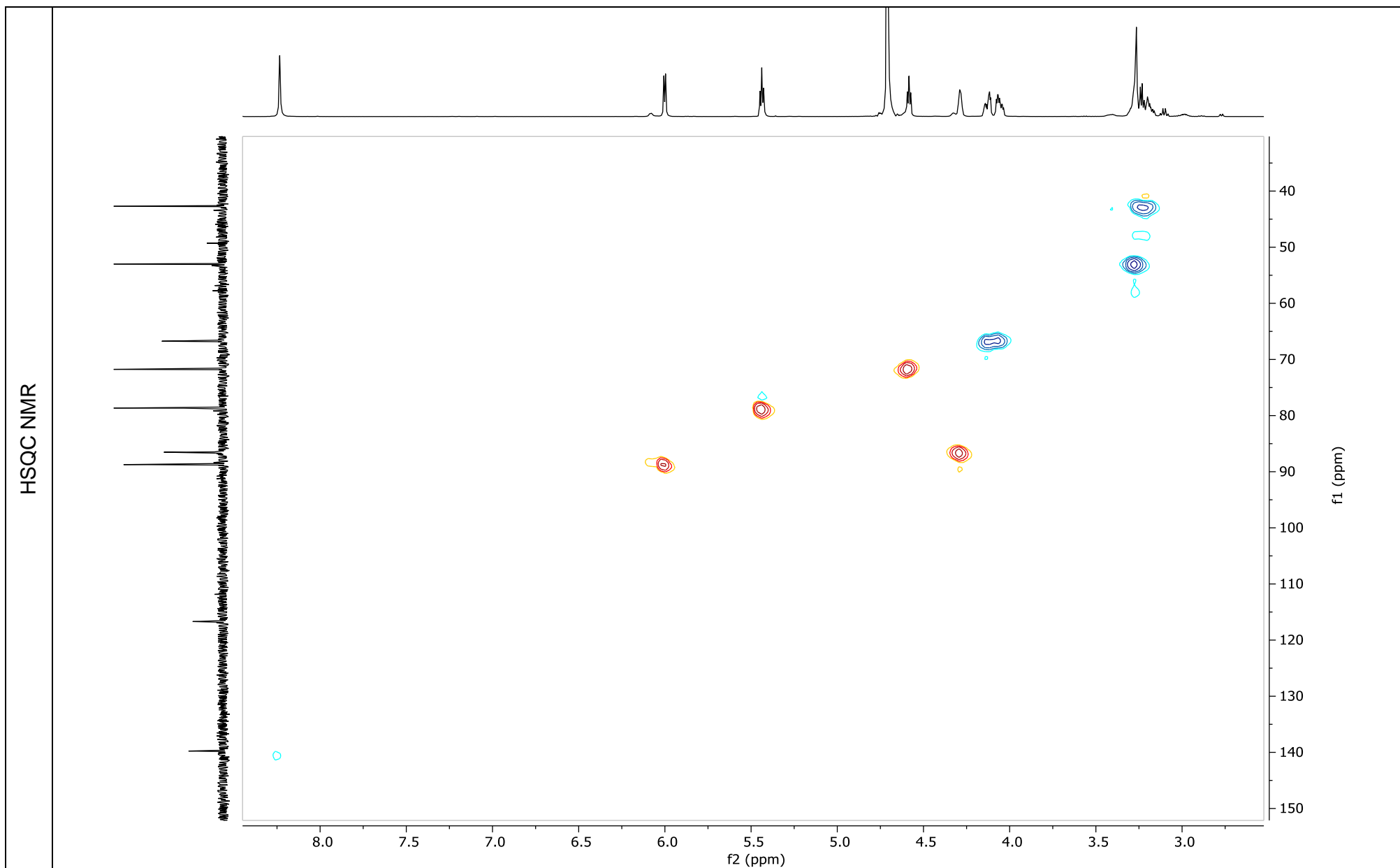


COSY NMR

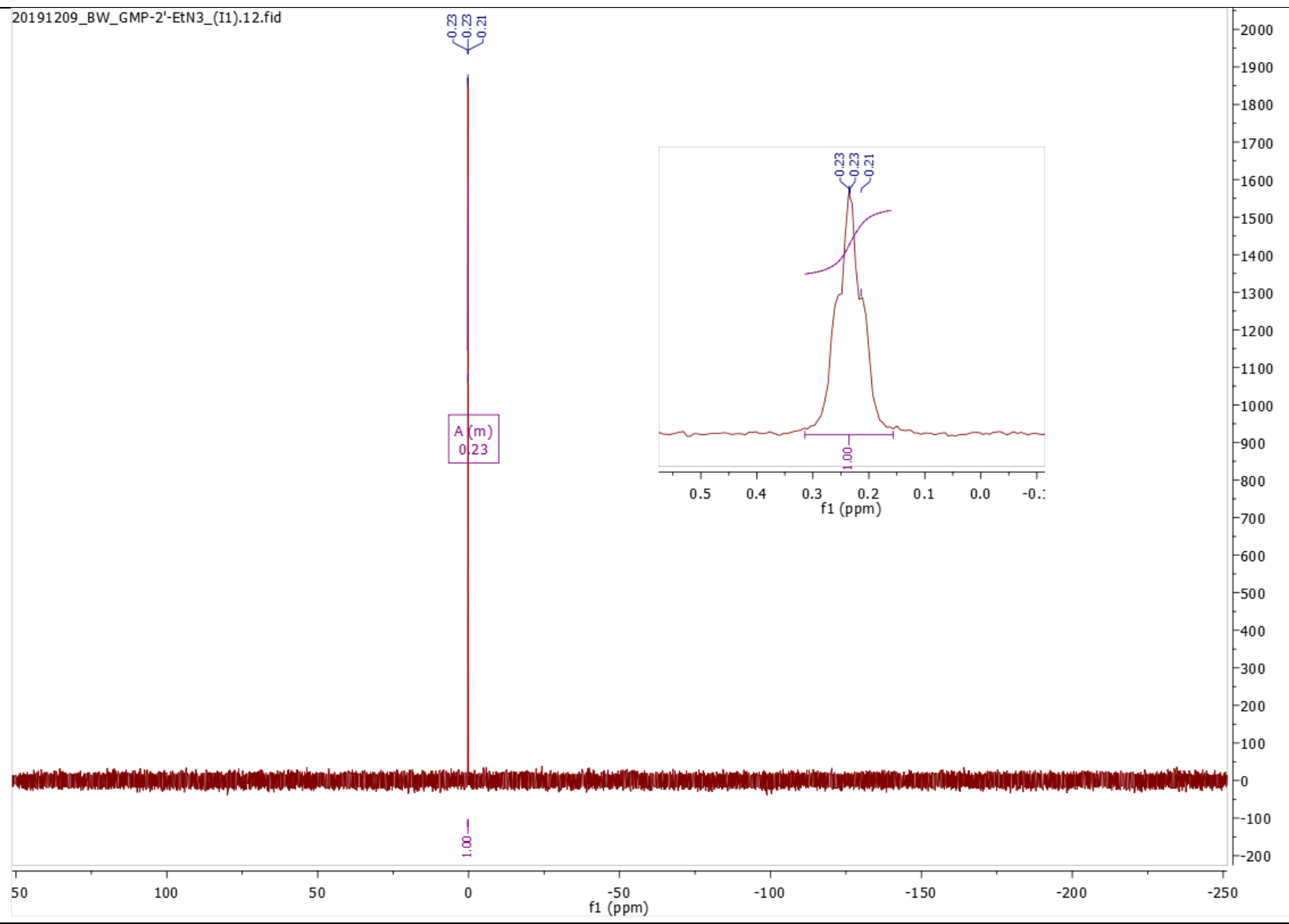


¹³C NMR (500 MHz, D₂O, 25°C)



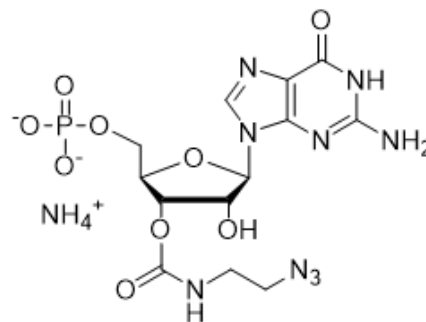


³¹P NMR (203 MHz, D₂O, H₃PO₄, 25°C)

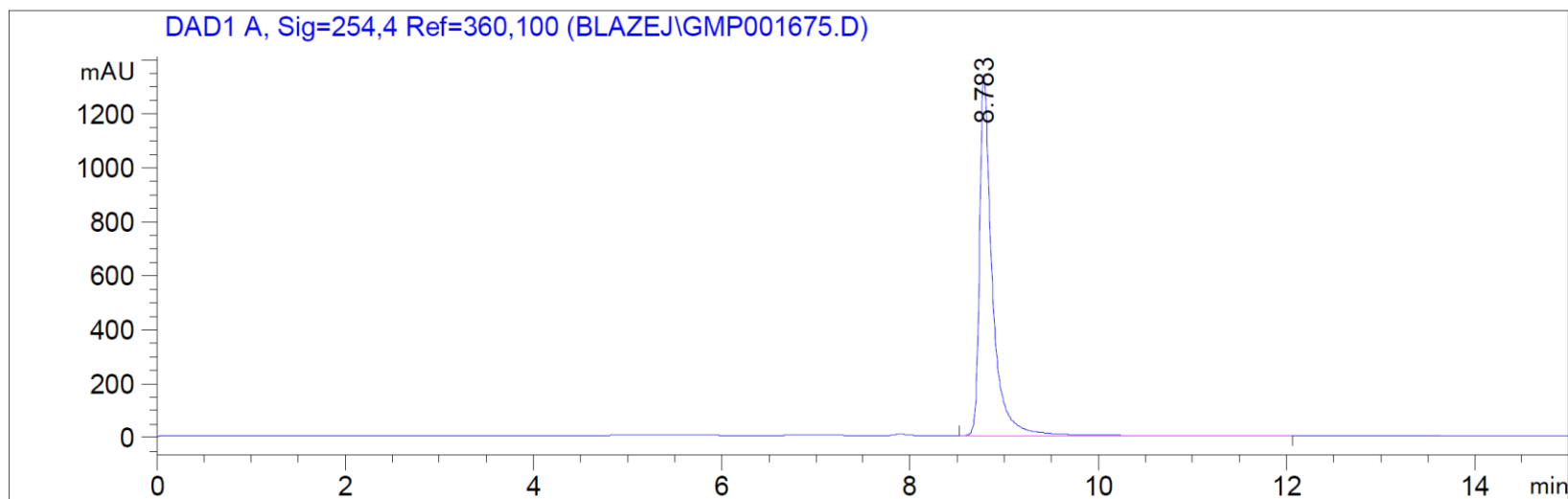


Compound 10-3': GMP-3'-O-C(O)-NH-CH₂CH₂-N₃ (NH₄⁺ salt)

Chemical structure

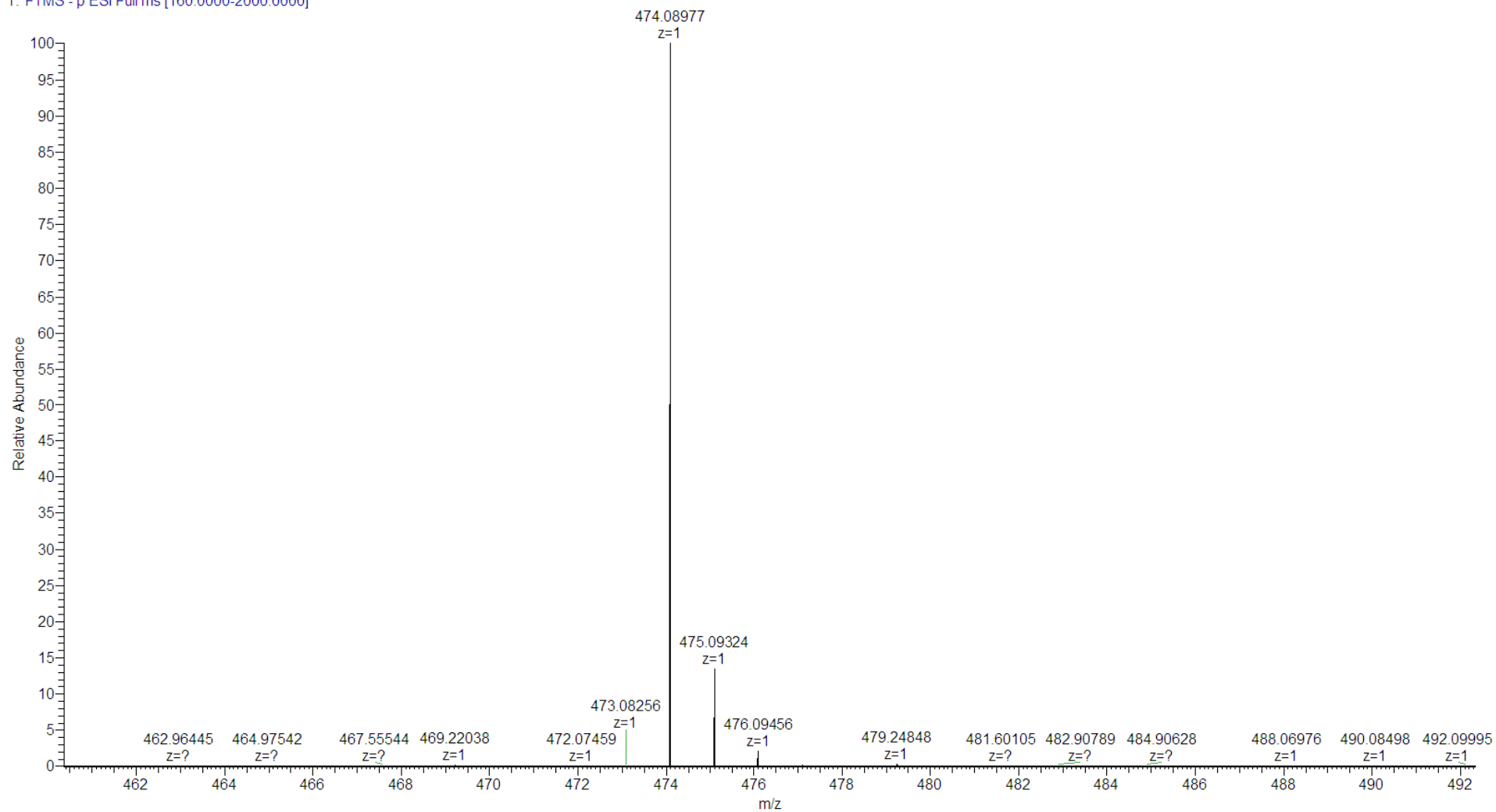


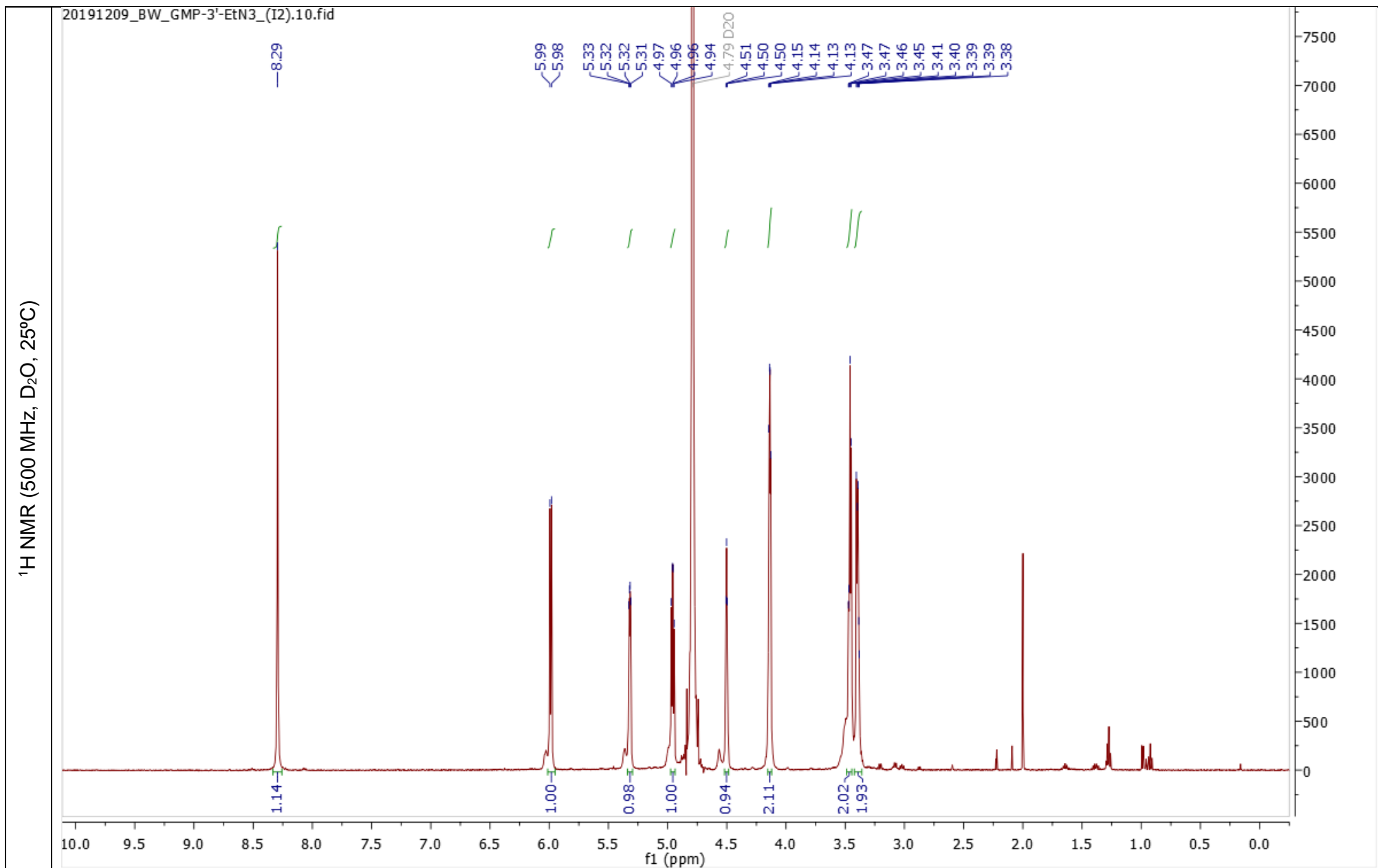
RP-HPLC (conditions c)



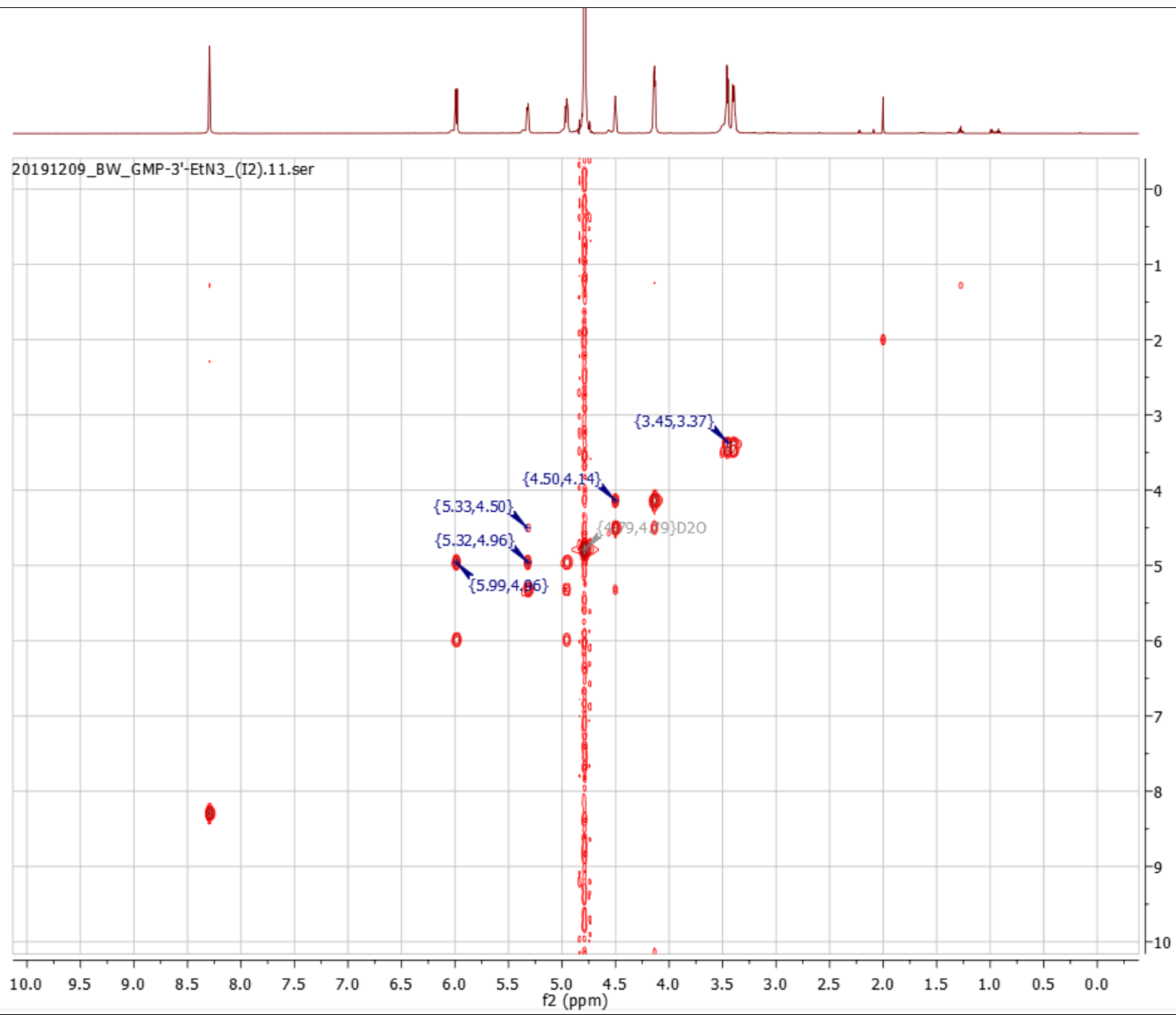
220329_PSu_01 #15-86 RT: 0.13-0.75 AV: 72 NL: 3.19E7
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₁₃H₁₇N₉O₉P⁻ : 474.0892, found: 474.08977)

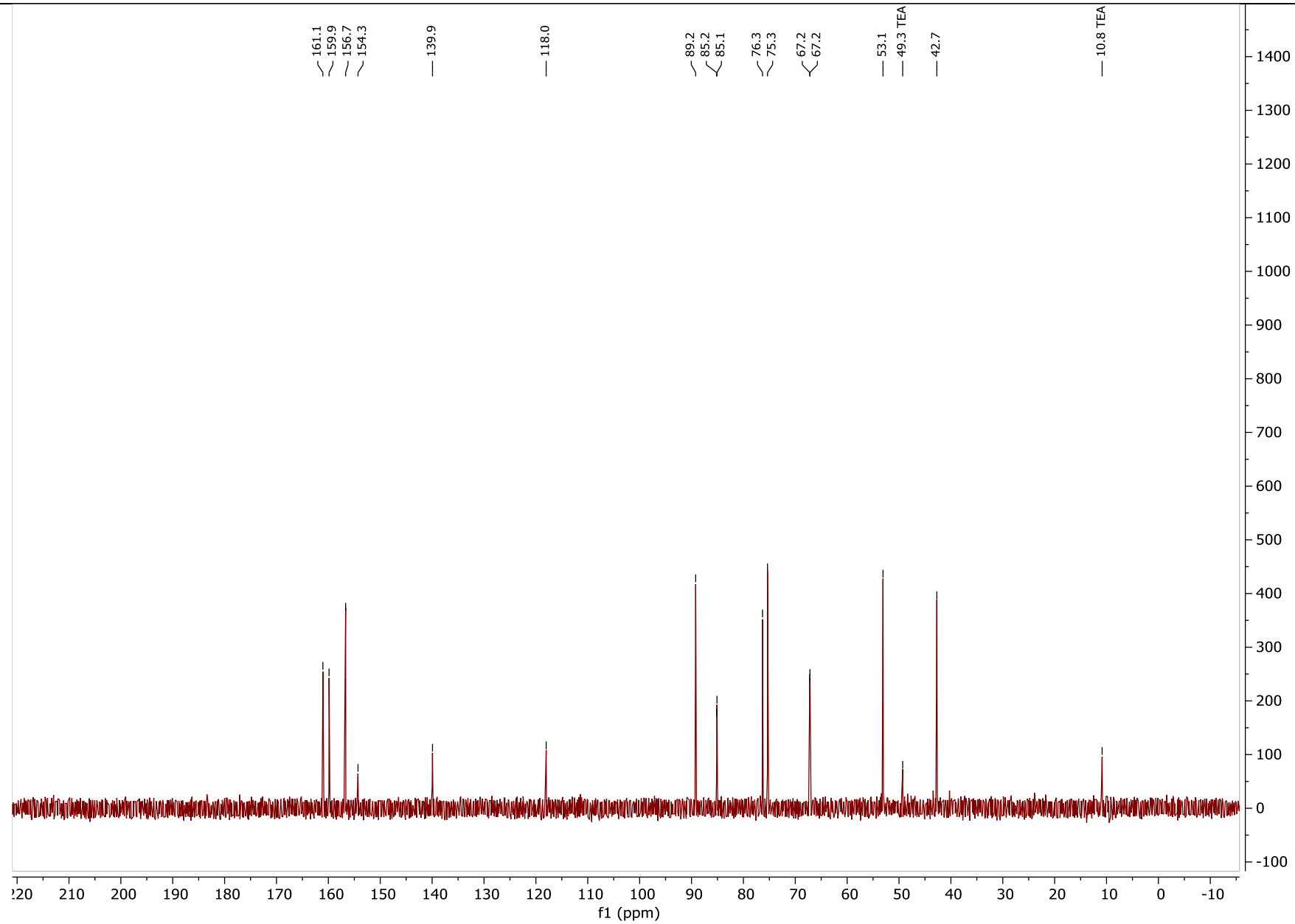




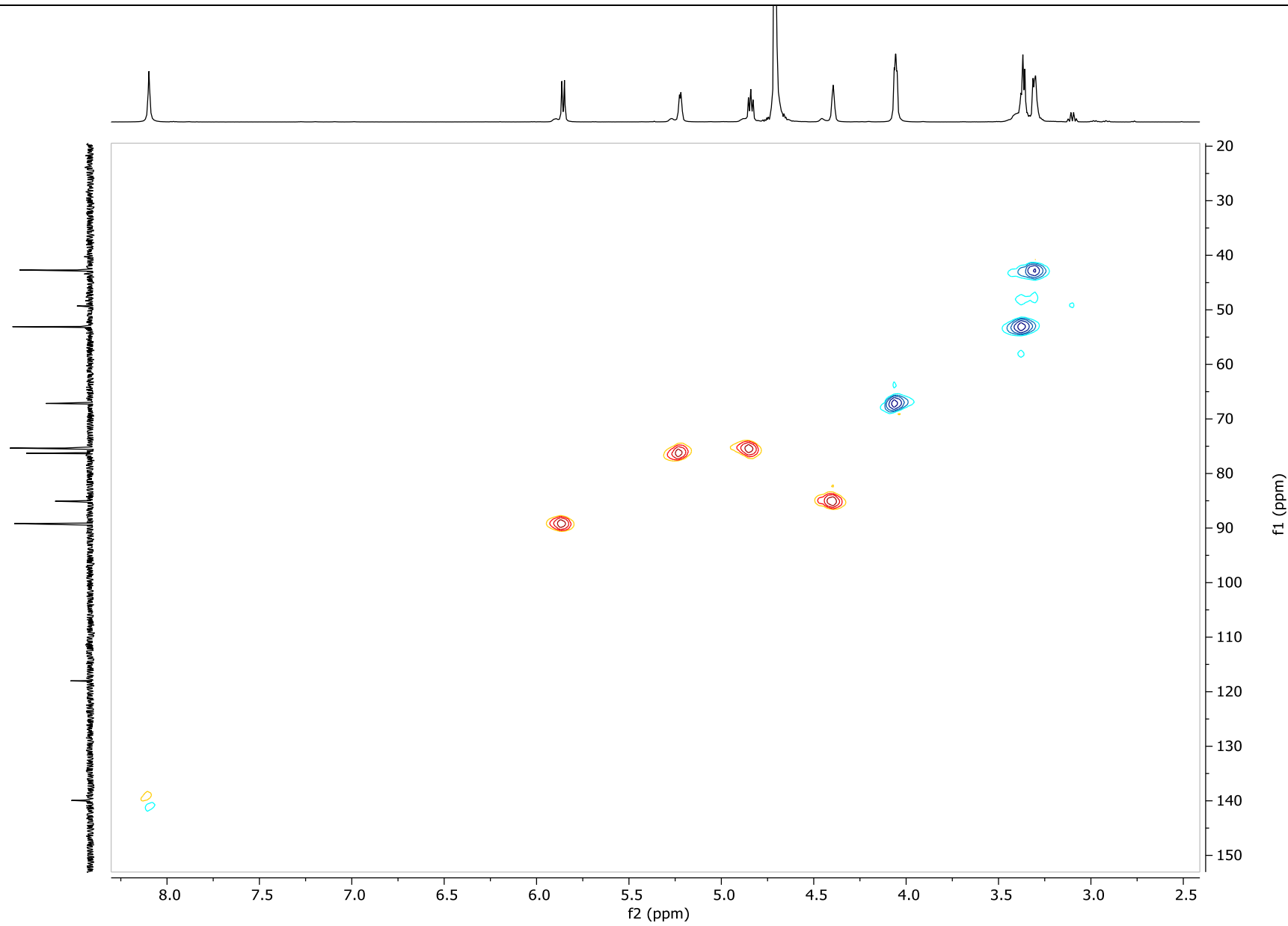
COSY NMR



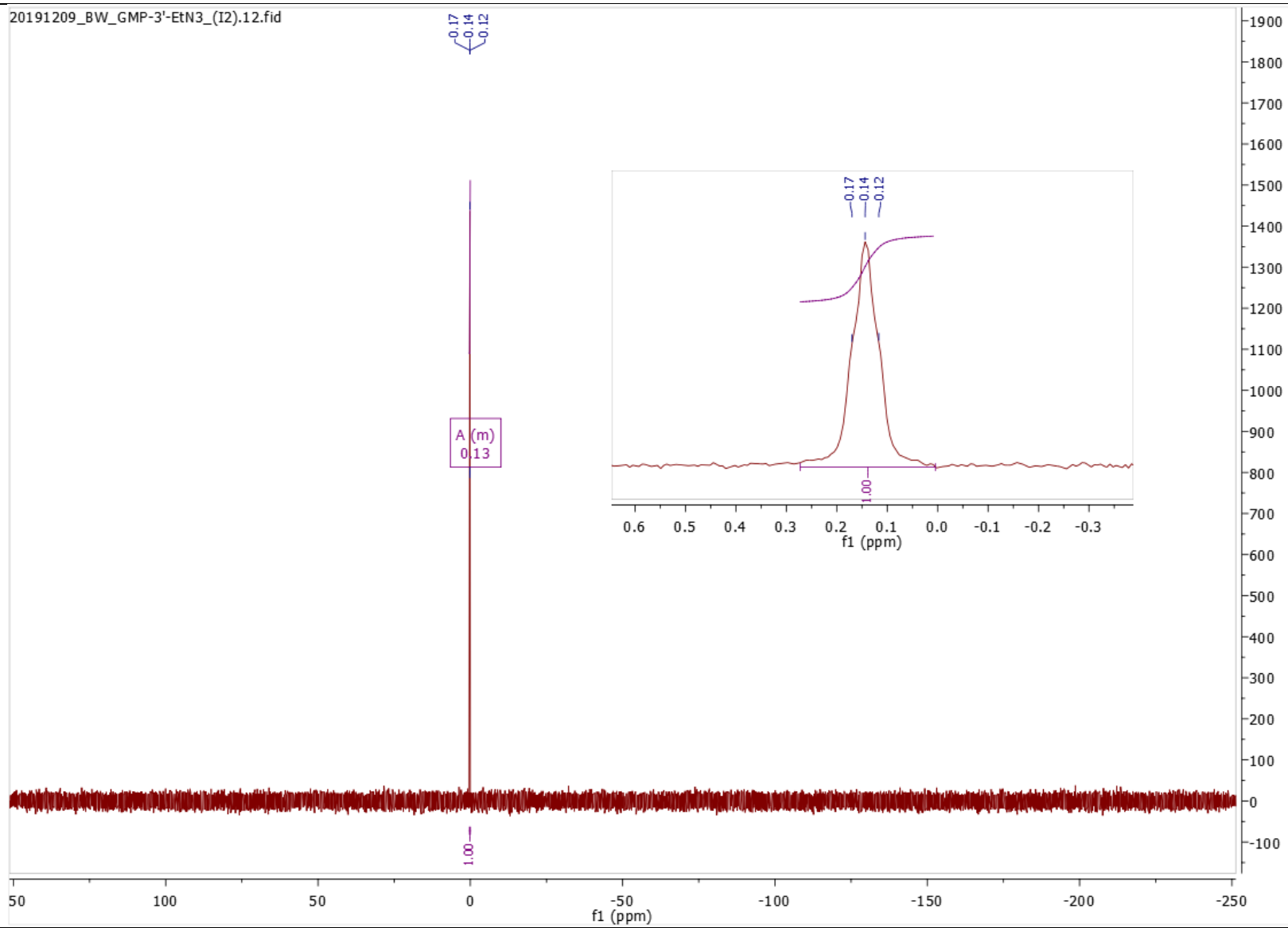
¹³C NMR (500 MHz, D₂O, 25°C)



HSQC NMR

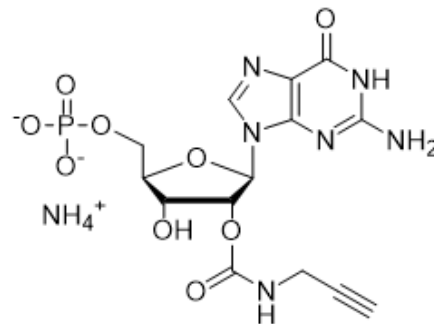


^{31}P NMR (203 MHz, D_2O , H_3PO_4 , 25°C)

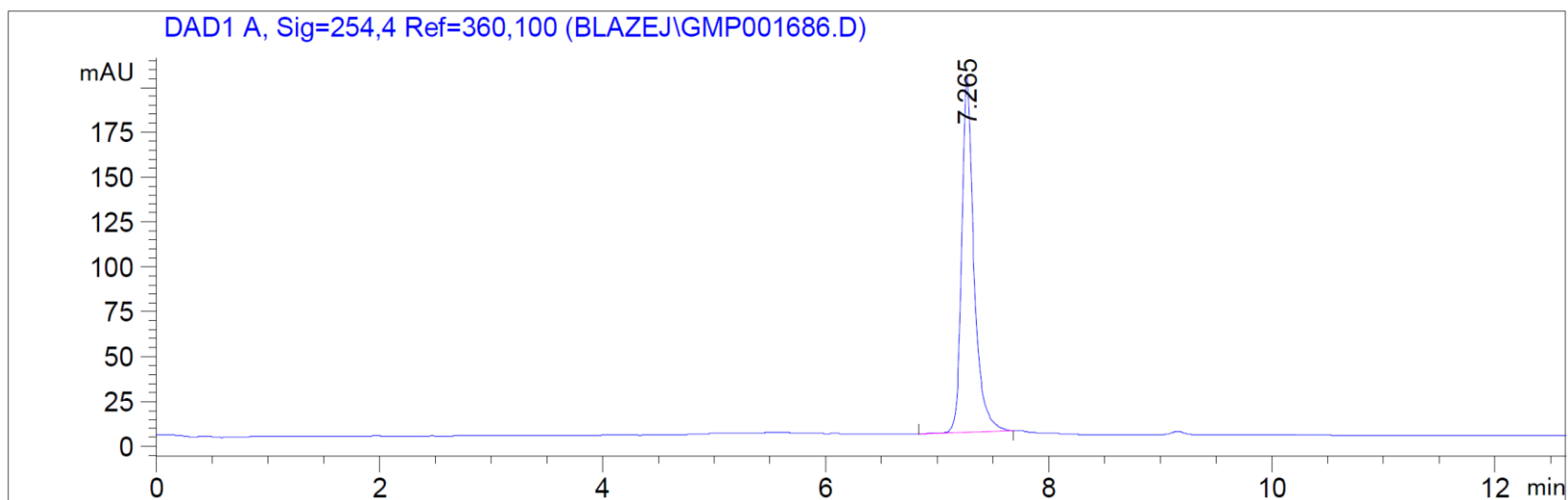


Compound 11-2': GMP-2'-O-C(O)-NH-C₃H₃ (NH₄⁺ salt)

Chemical structure

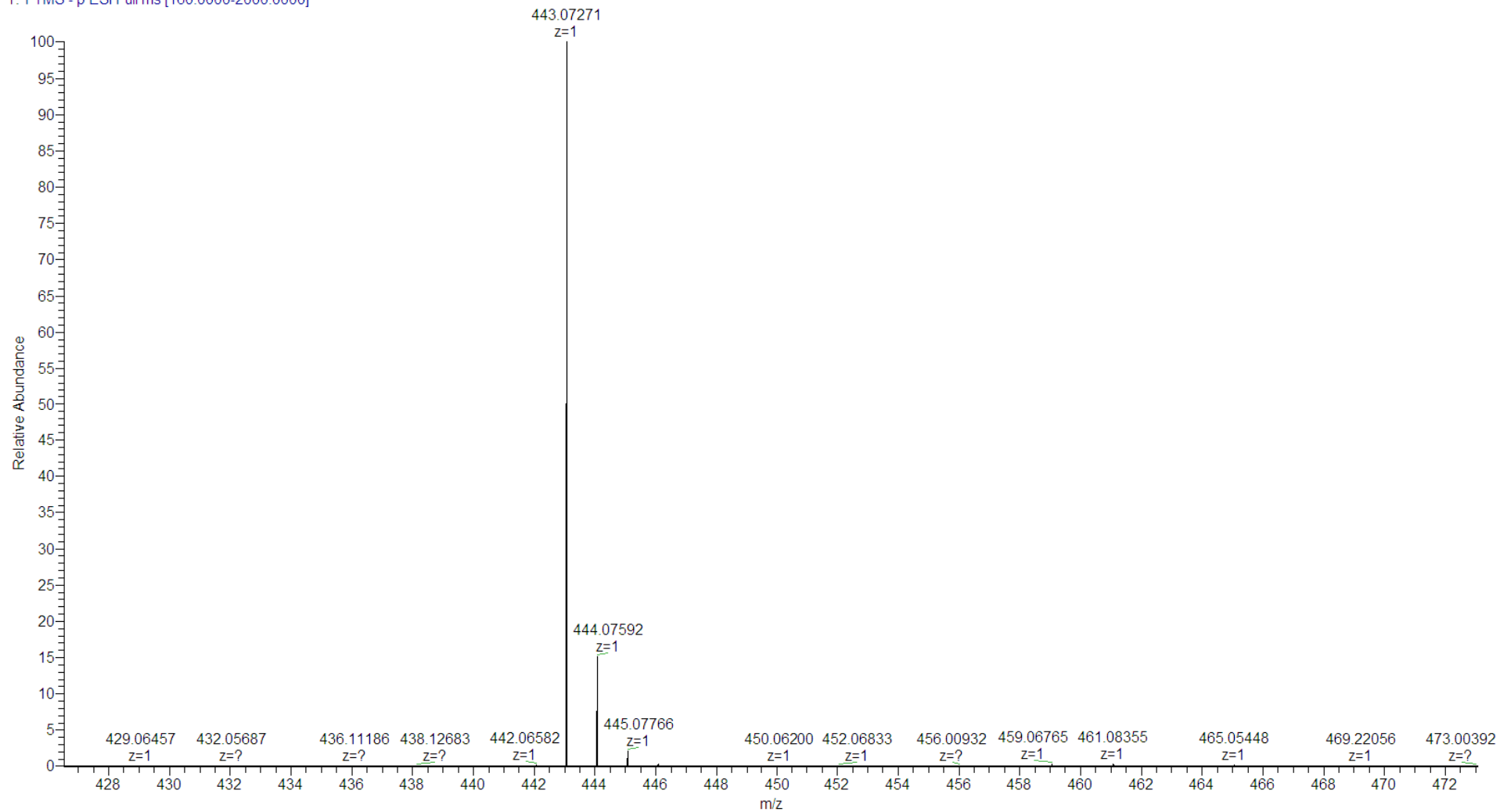


RP-HPLC (conditions c)

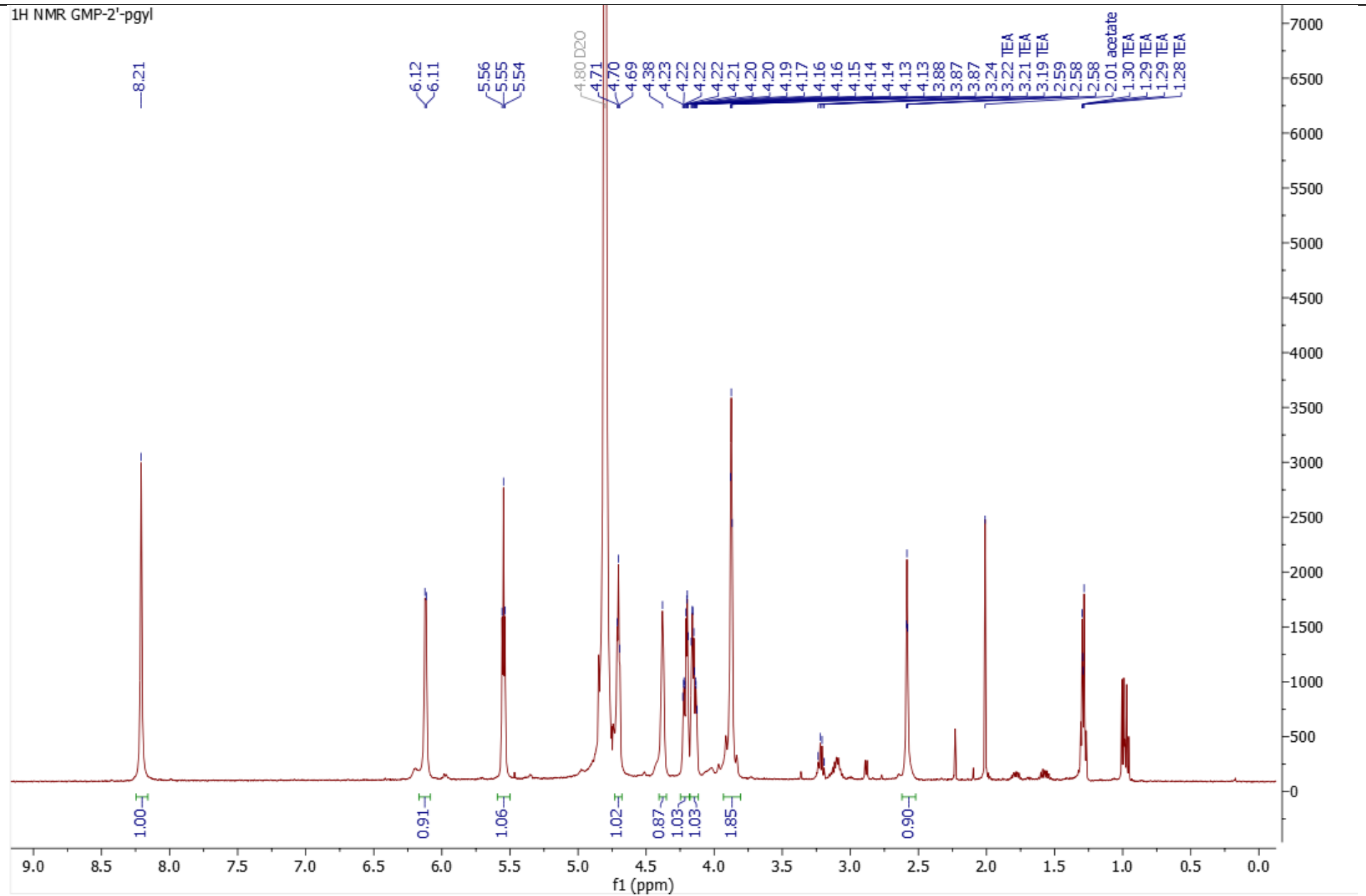


220329_PSu_02#19-76 RT: 0.17-0.66 AV: 58 NL: 1.70E7
T: FTMS - p ESI Full ms [160.0000-2000.0000]

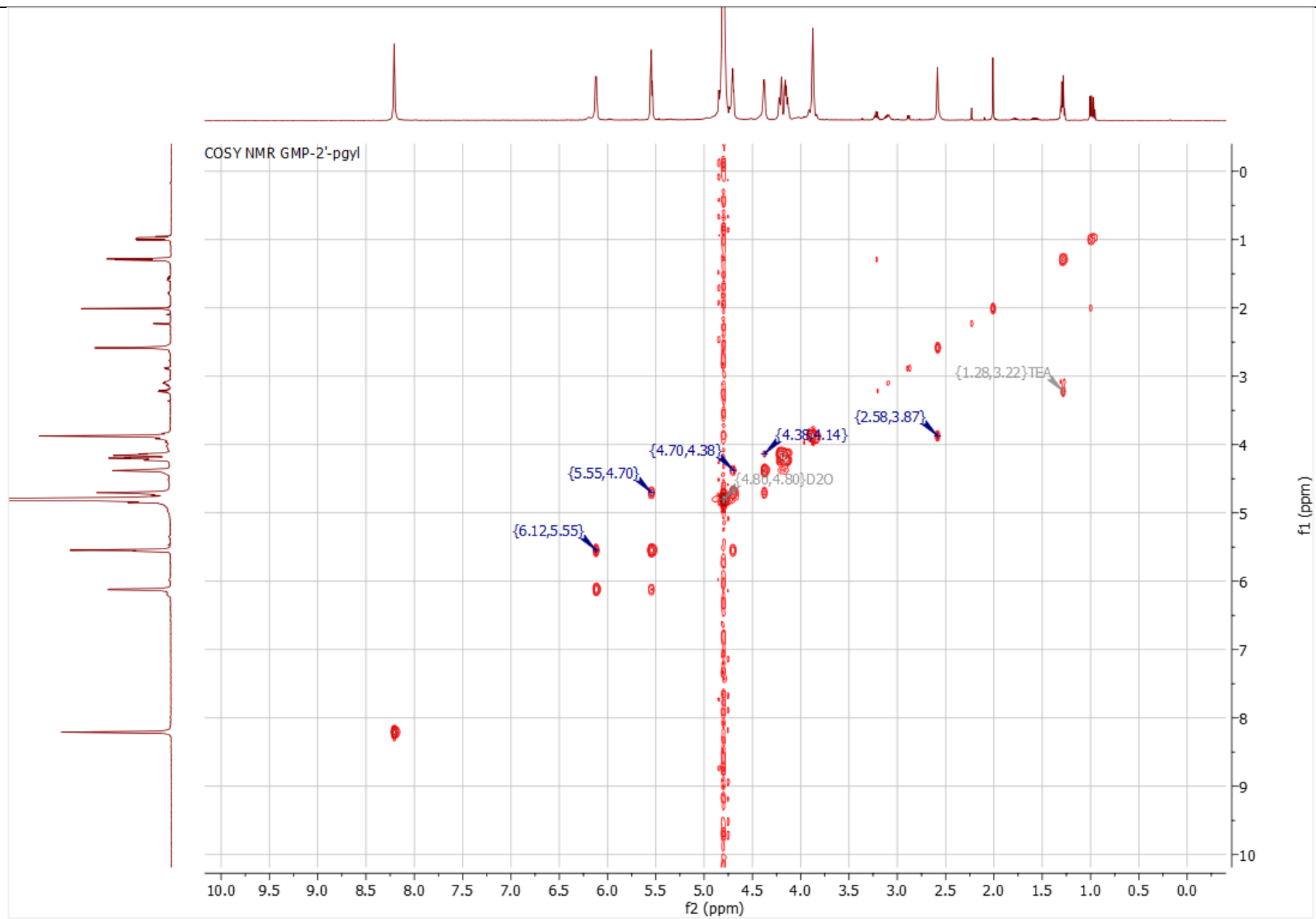
MS (-) ESI (Calc. [M-H]⁻ C₁₄H₁₆N₆O₉P⁻ : 443.0722, found: 443.07271)



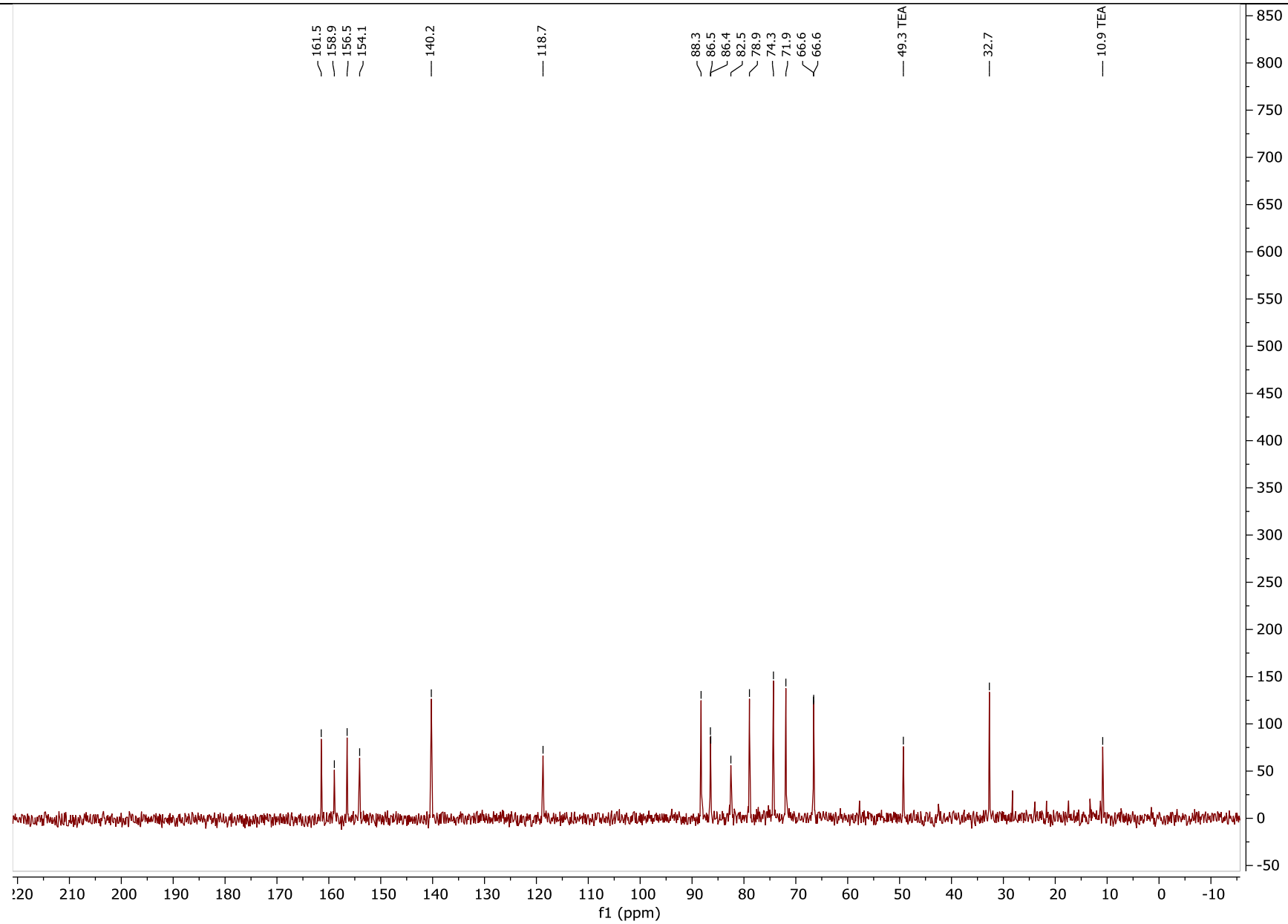
¹H NMR (500 MHz, D₂O, 25°C)



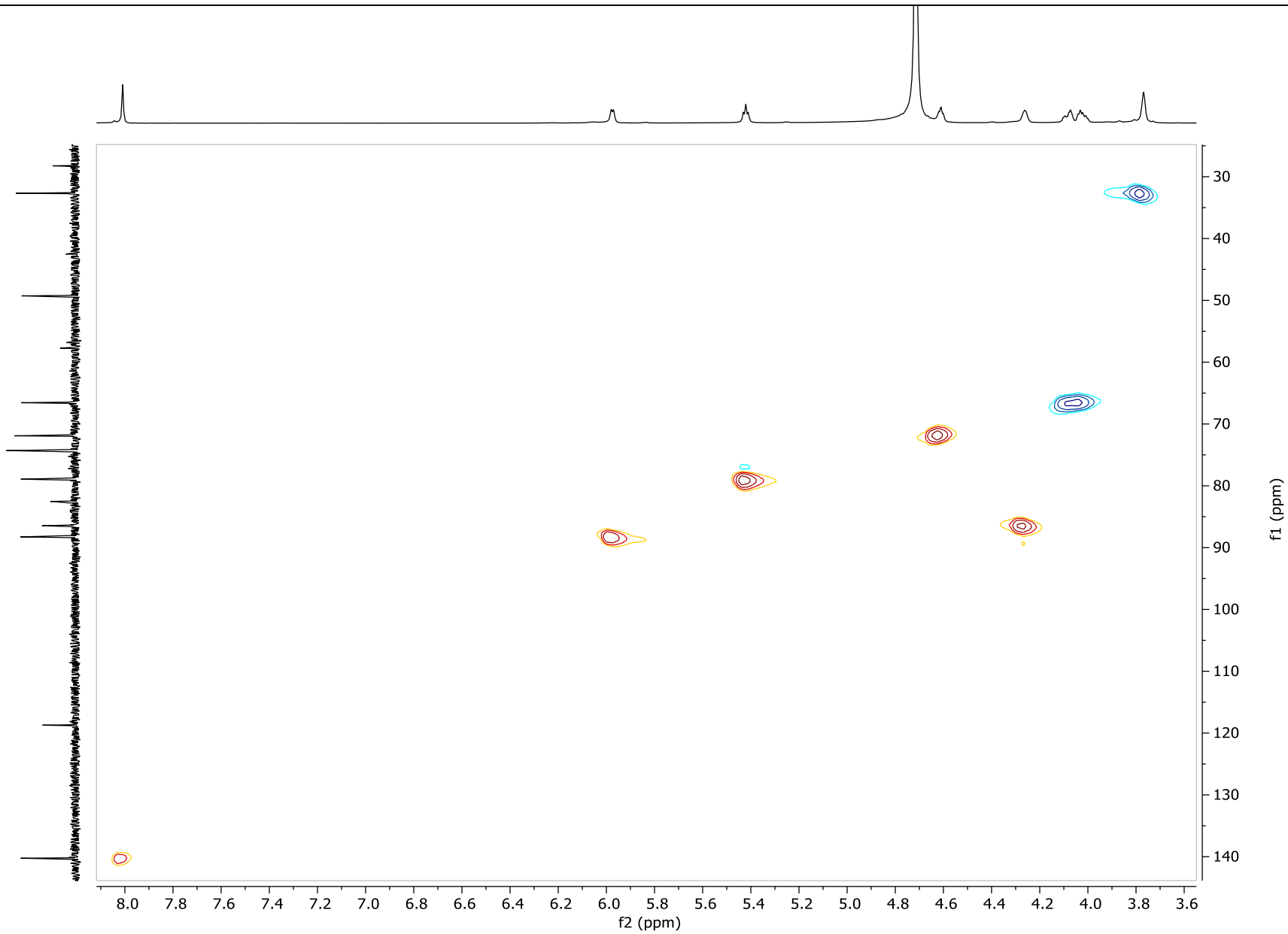
COSY NMR



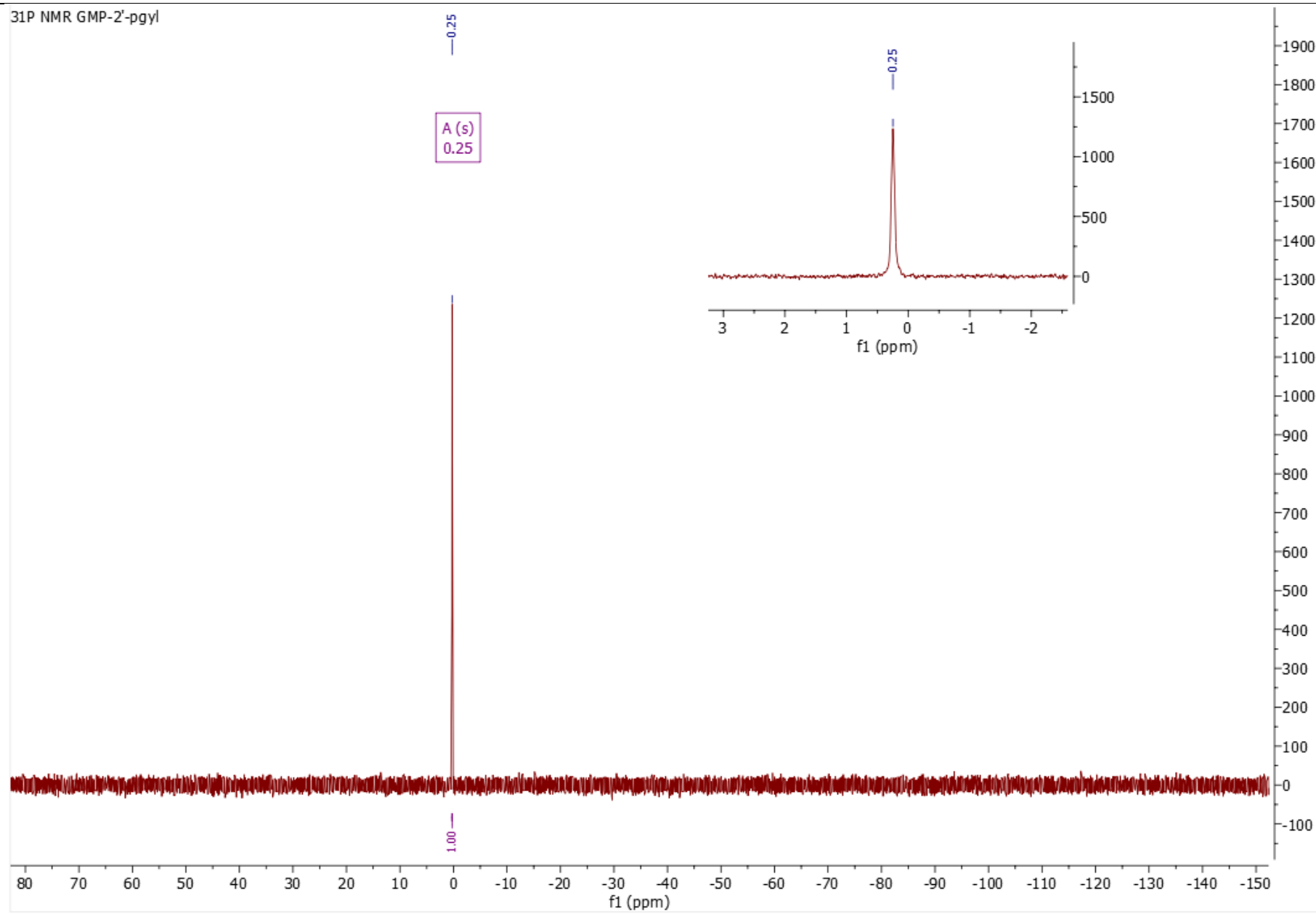
¹³C NMR (500 MHz, D₂O, 25°C)



HSQC NMR

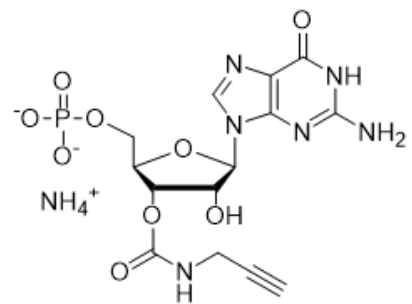


³¹P NMR (203 MHz, D₂O, H₃PO₄, 25°C)

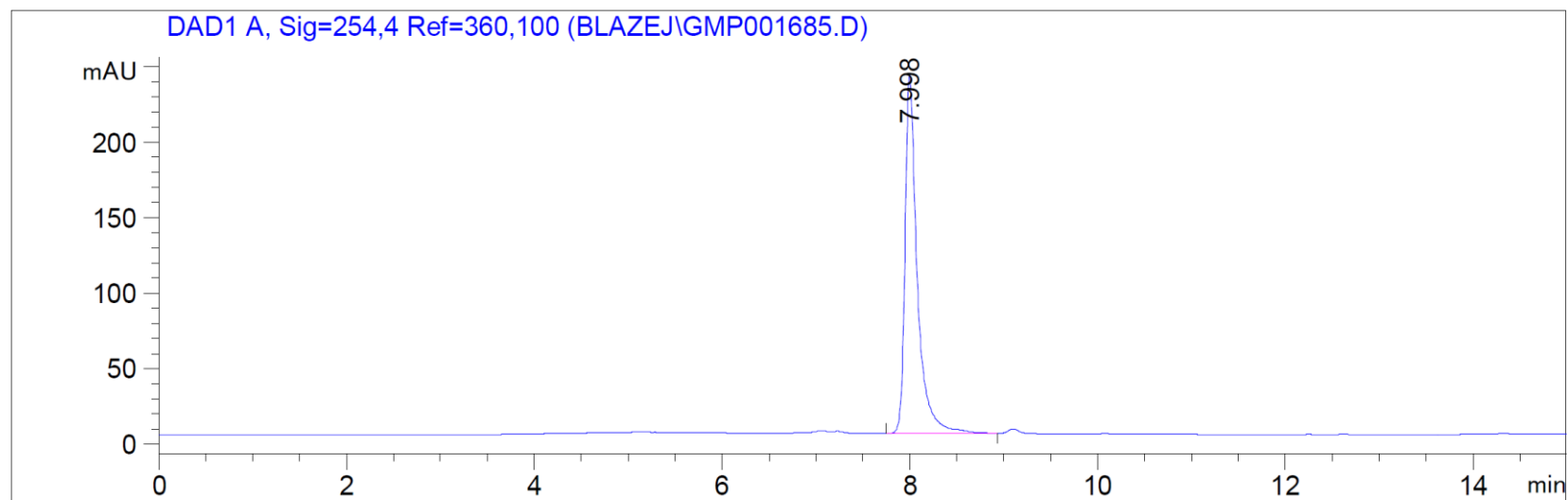


Compound 11-3': GMP-3'-O-C(O)-NH-C₃H₃ (NH₄⁺ salt)

Chemical structure

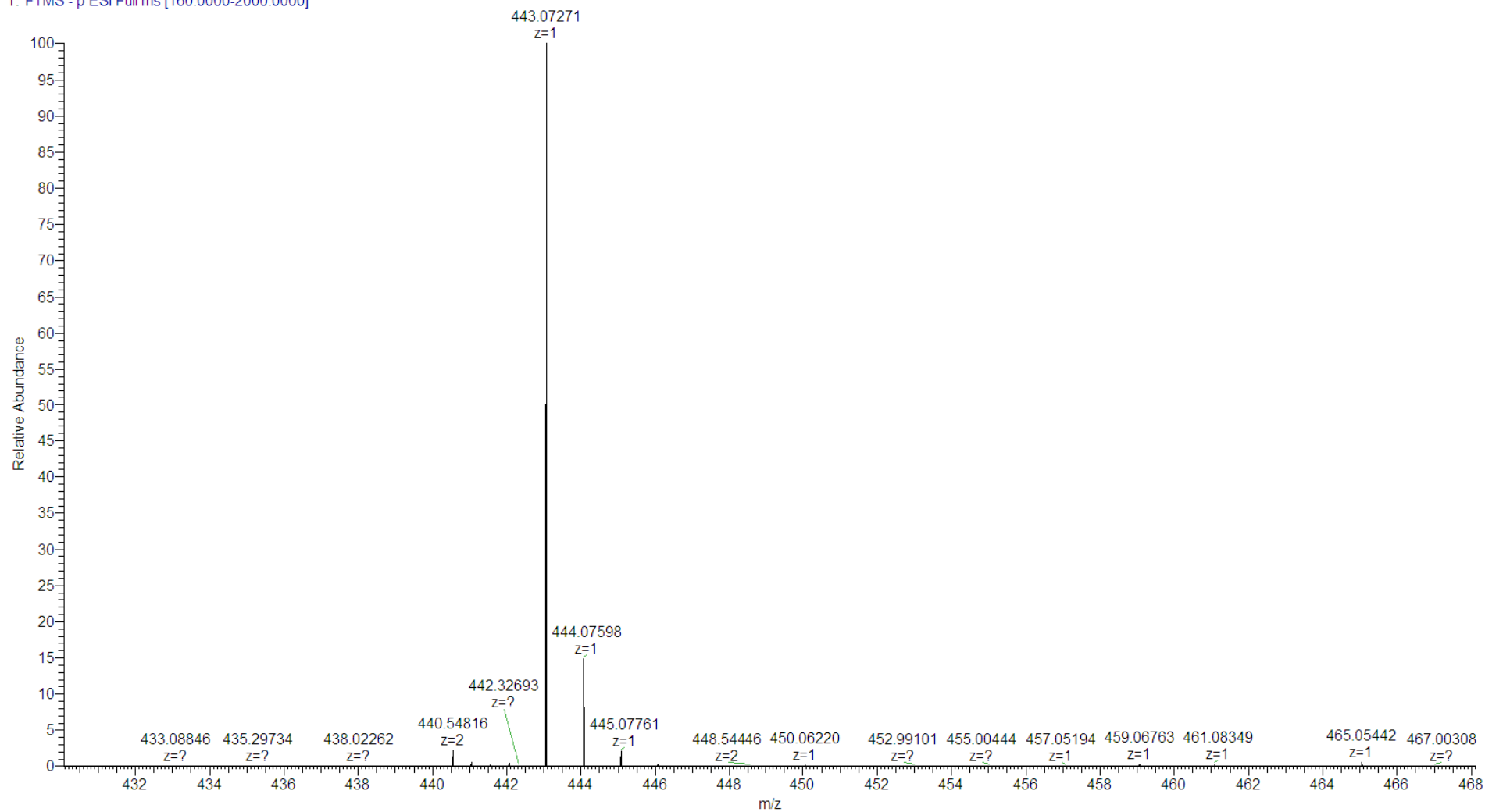


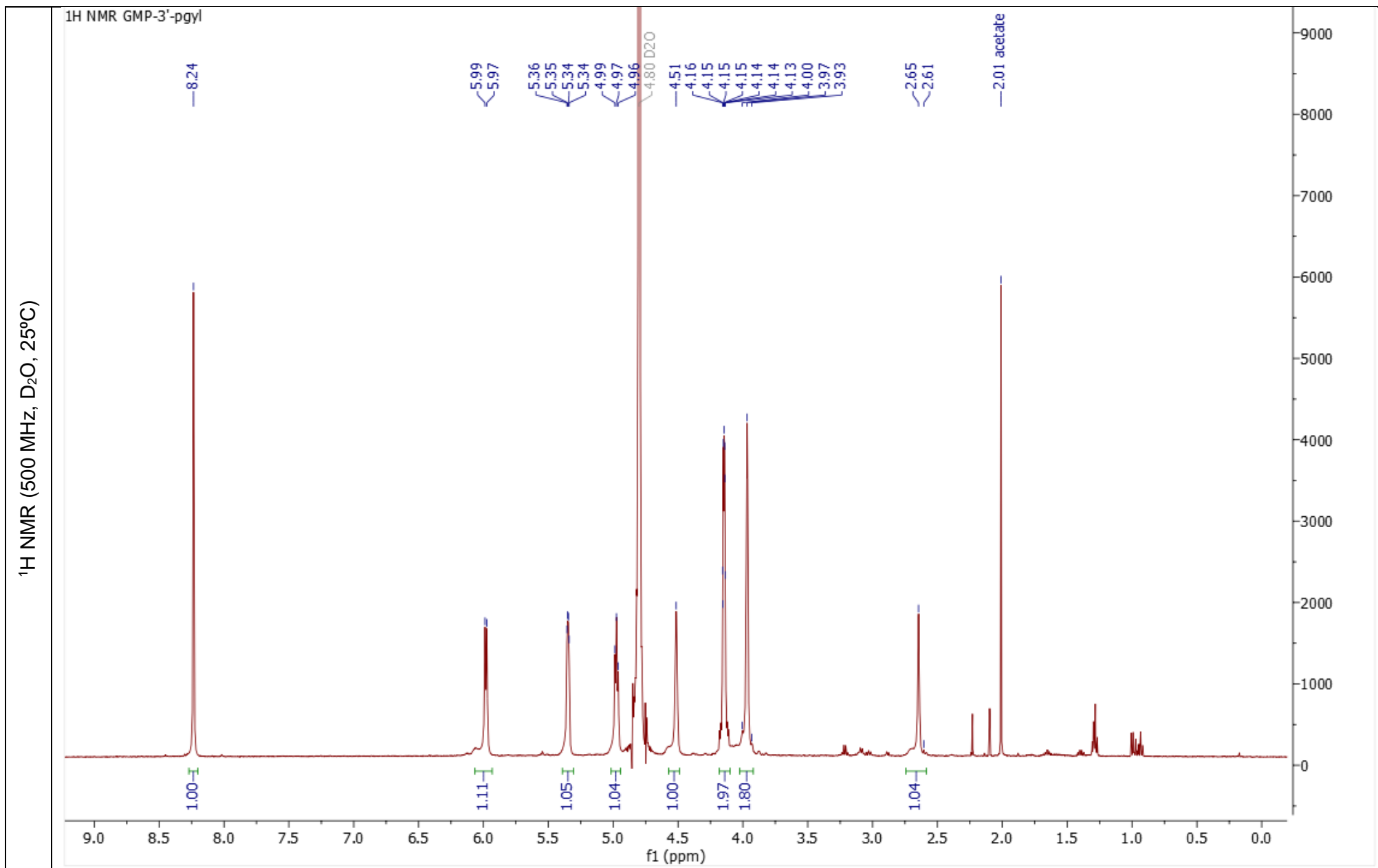
RP-HPLC (conditions c)



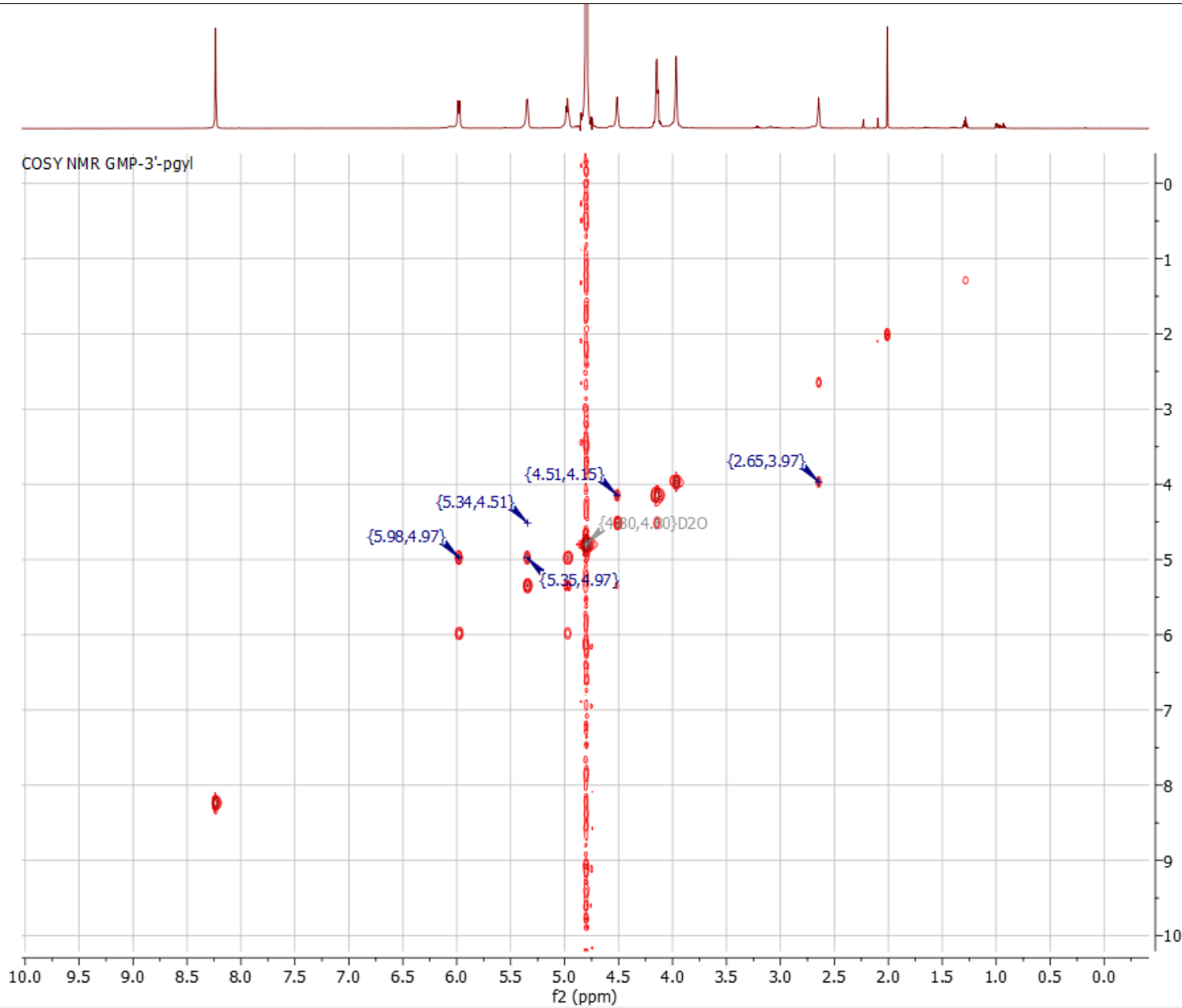
220329_PSu_03 #43-103 RT: 0.37-0.90 AV: 61 NL: 9.05E6
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₁₄H₁₆N₆O₉P⁻ : 443.0722, found: 443.07271)

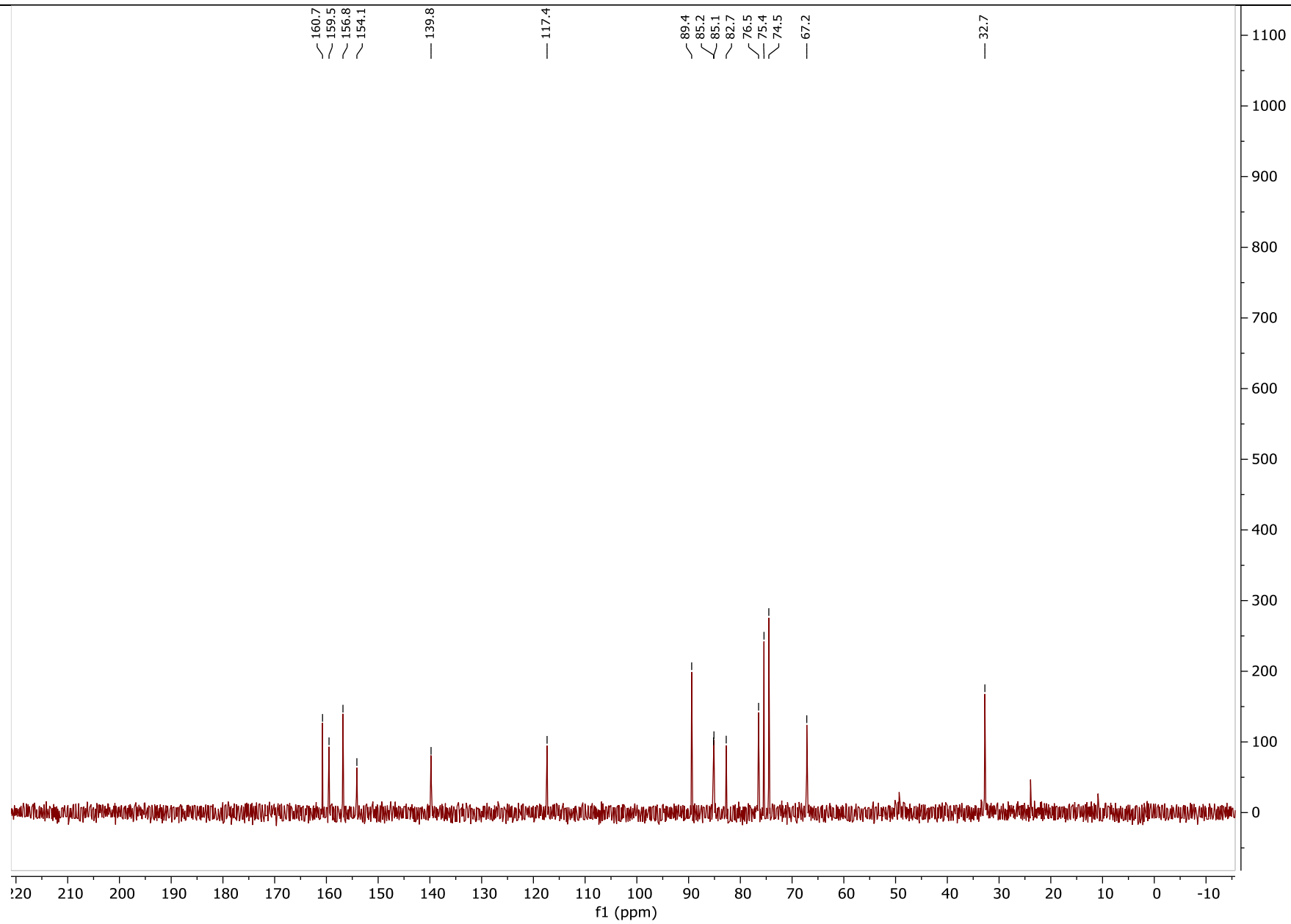




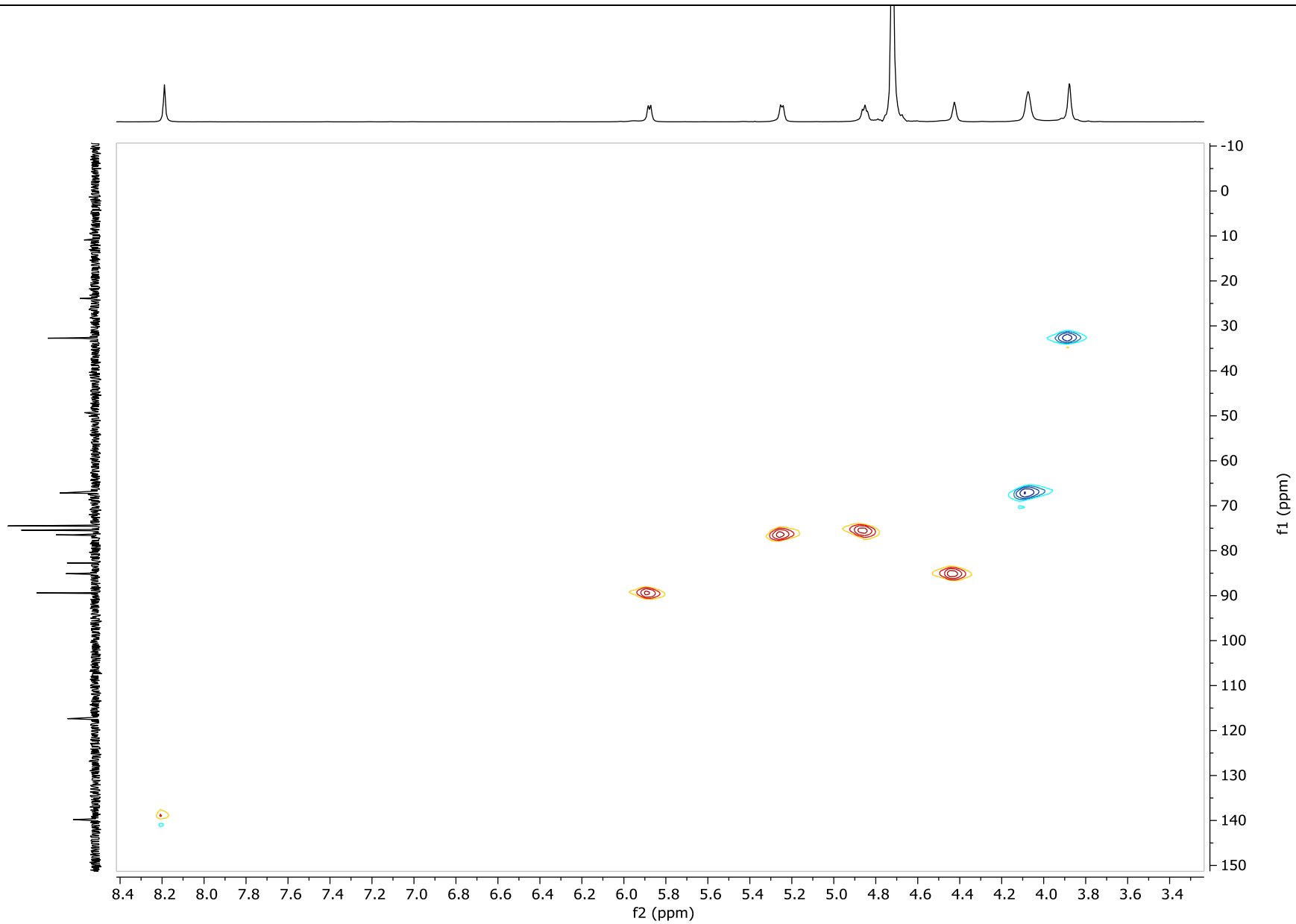
COSY NMR



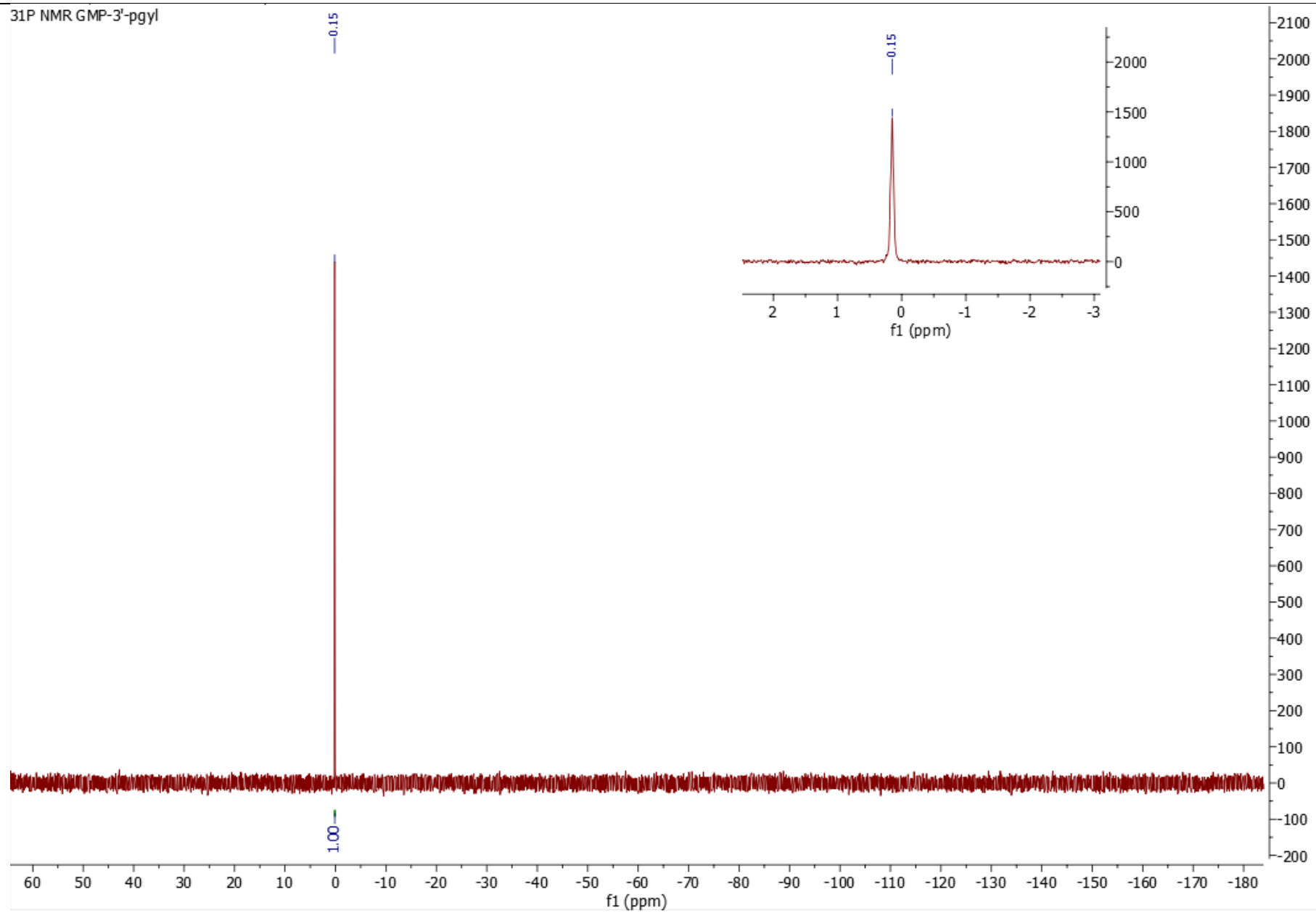
¹³C NMR (500 MHz, D₂O, 25°C)



HSQC NMR

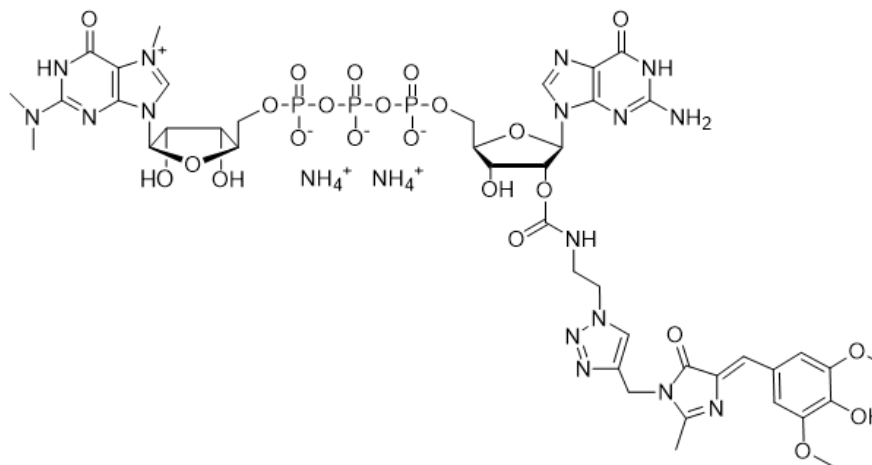


³¹P NMR (203 MHz, D₂O, H₃PO₄, 25°C)

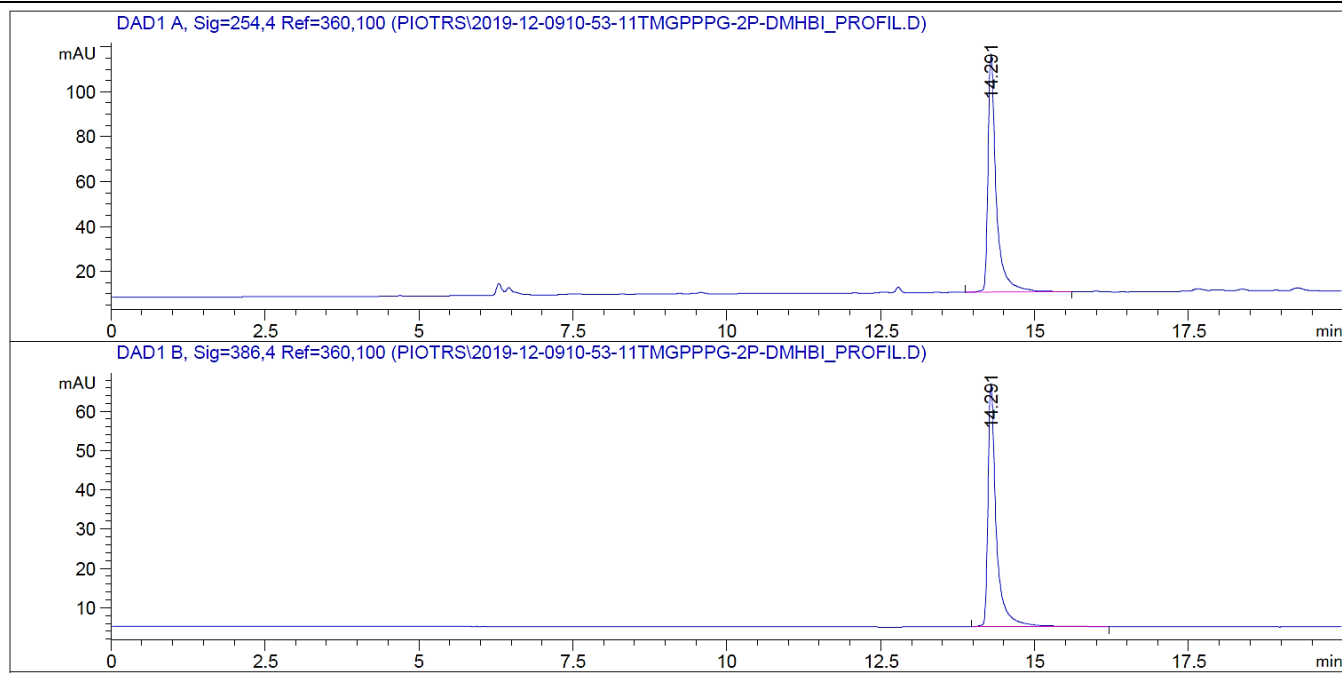


Compound 1a-2': TMGpppG-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

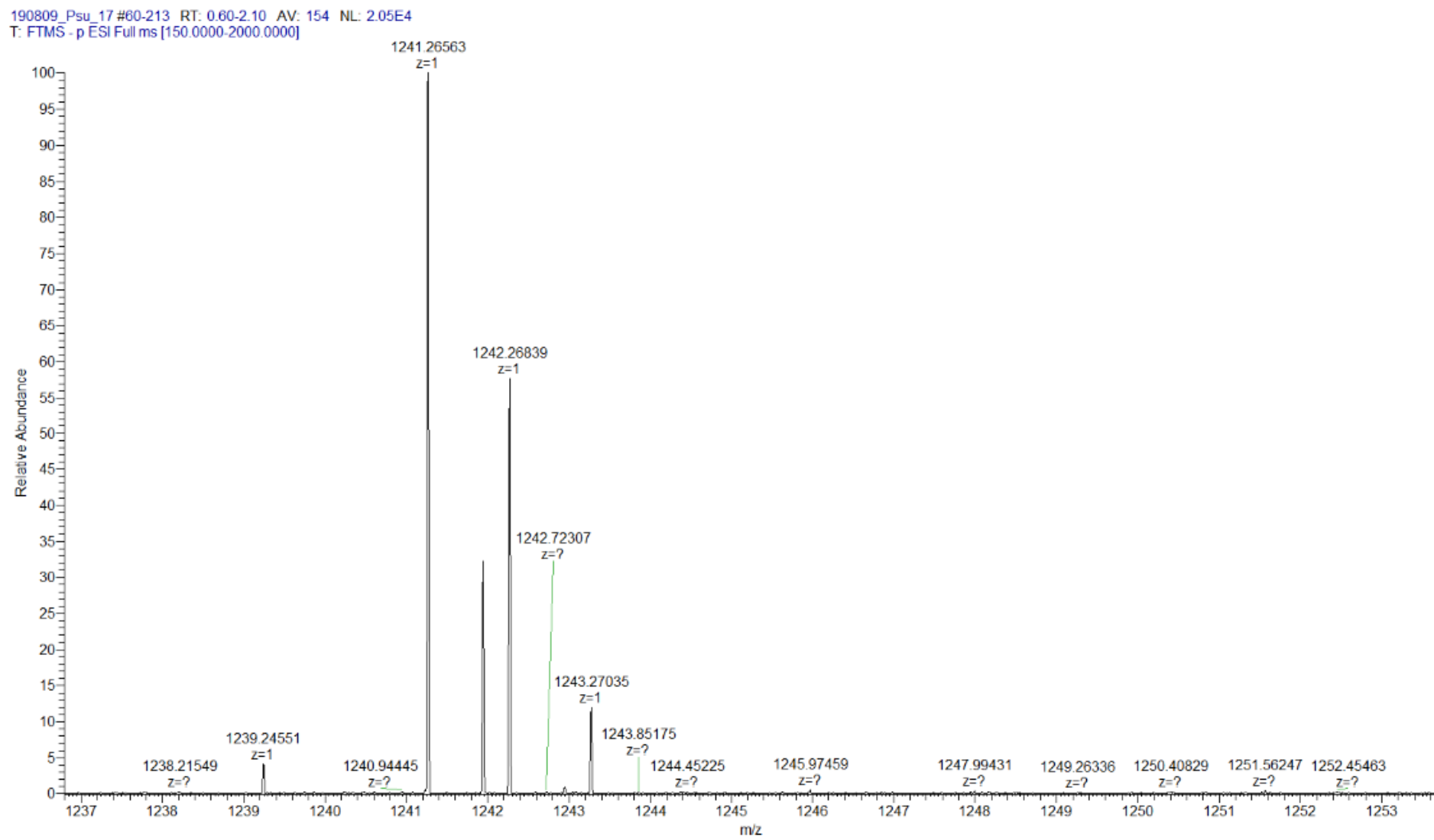
Chemical structure



RP-HPLC (conditions c)

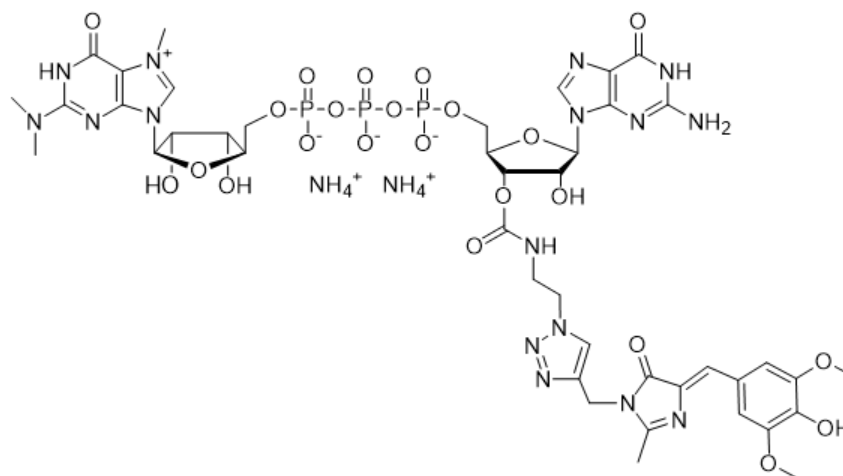


MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₂N₁₆O₂₃P₃ : 1241.2610, found: 1241.26563)

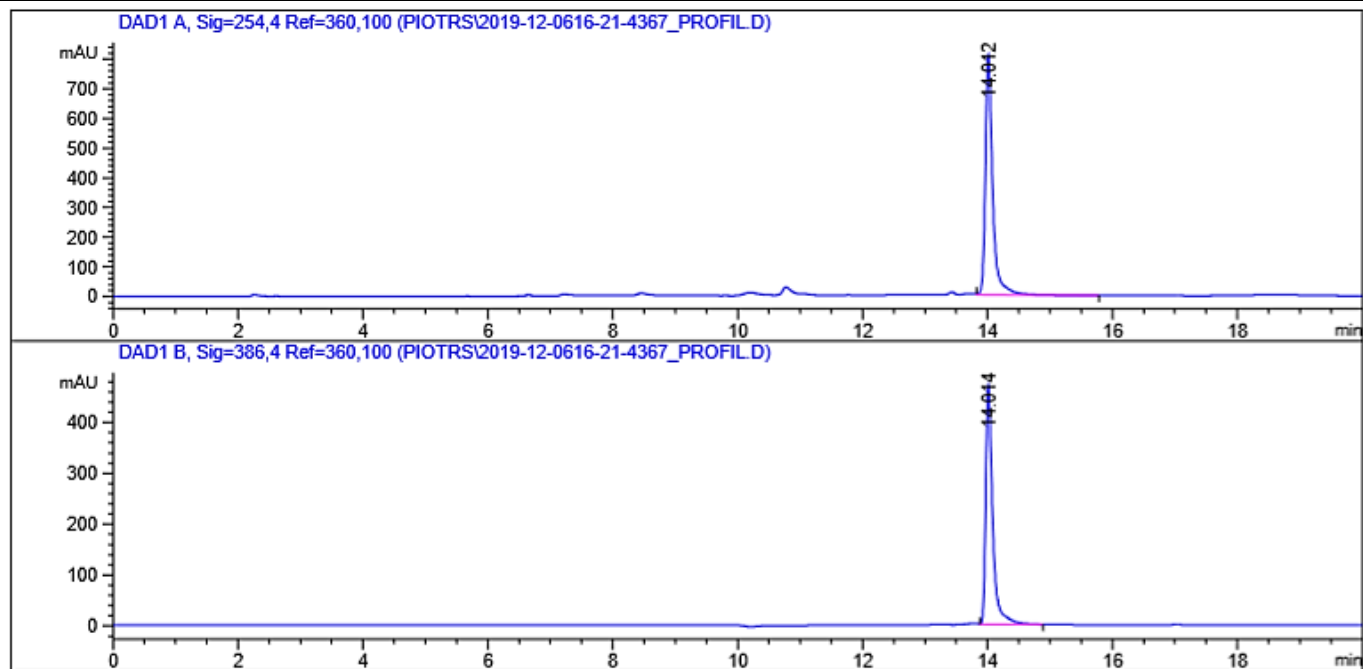


Compound 1a-3': TMGpppG-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

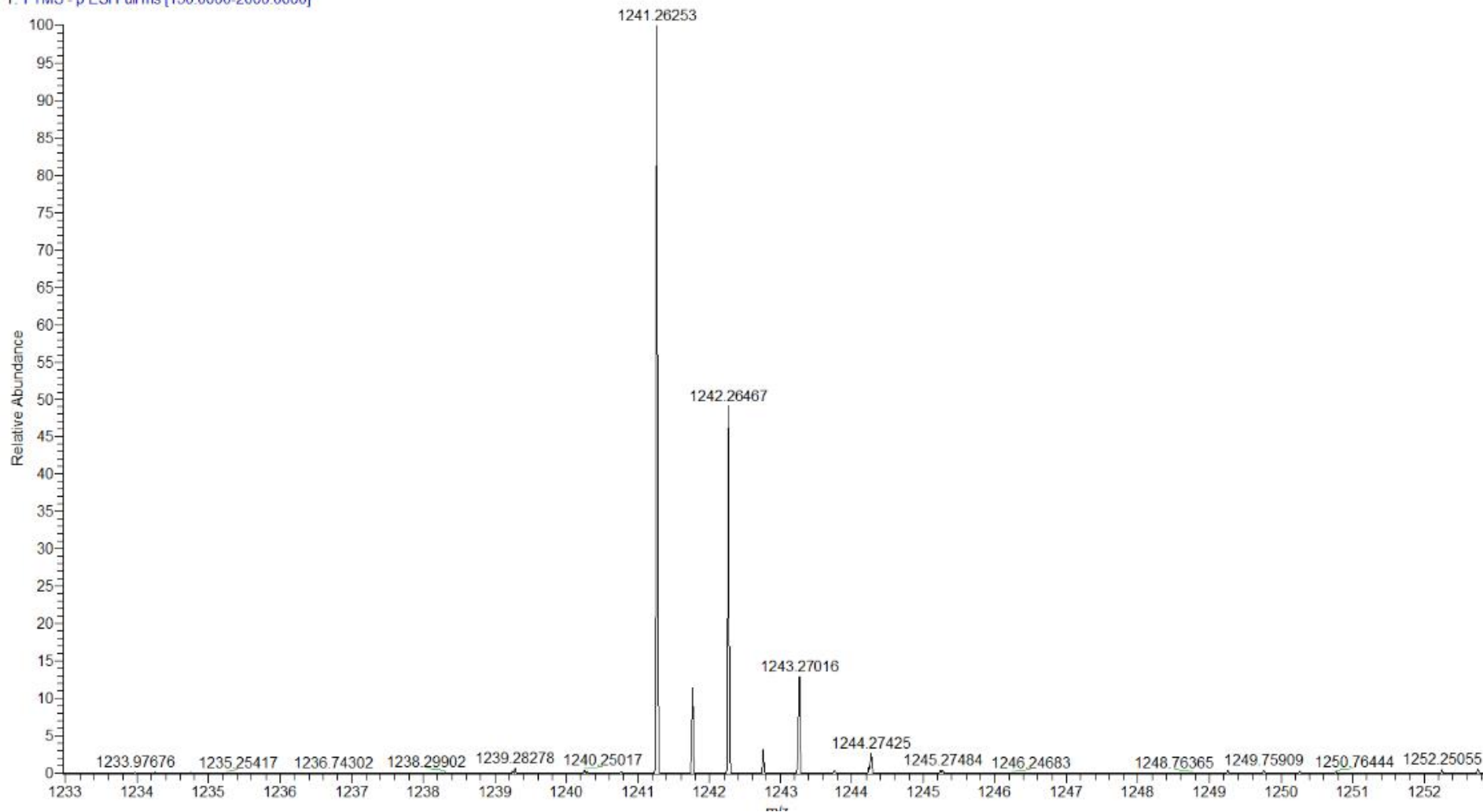


RP-HPLC (conditions c)



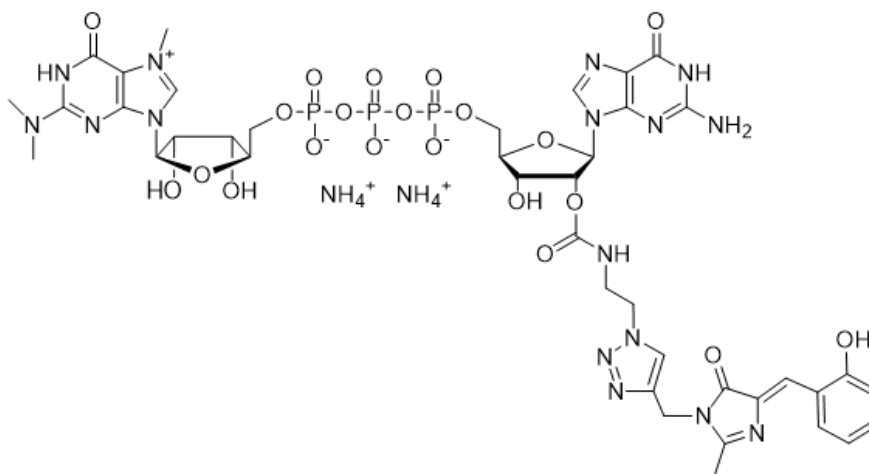
MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₂N₁₆O₂₃P₃ : 1241.2610, found: 1241.26253)

191107_PSu_29#2-74 RT: 0.02-0.75 AV: 73 NL: 3.44E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

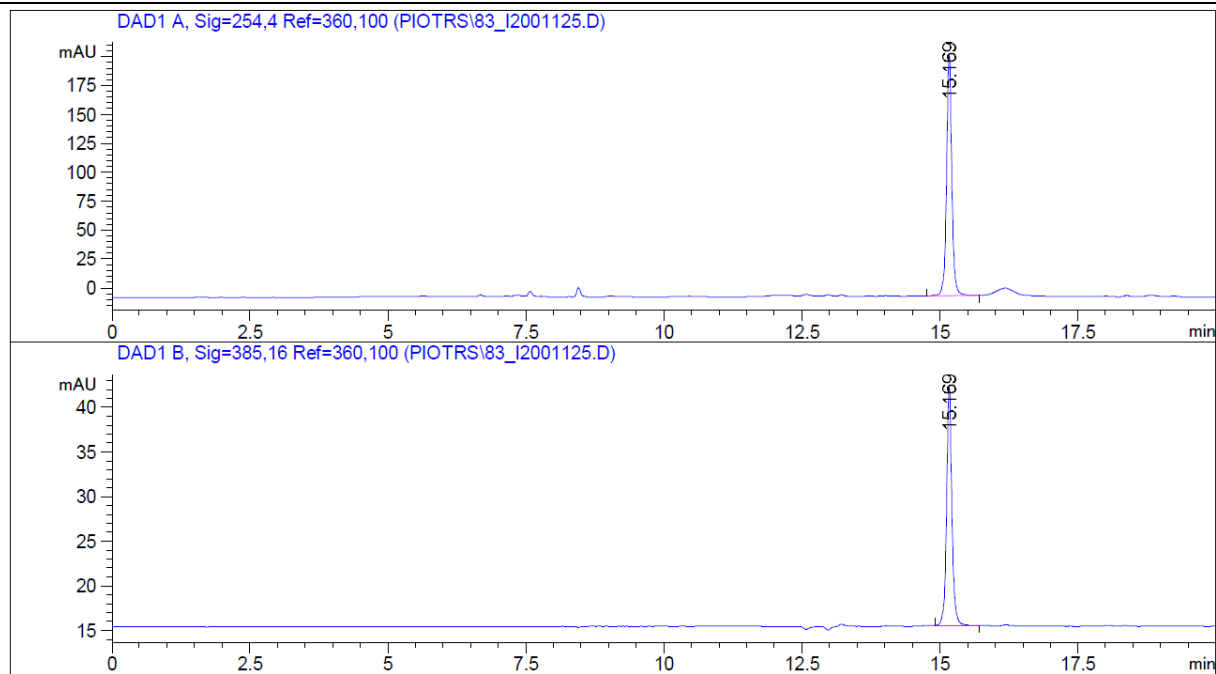


Compound 1b-2': TMGpppG-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-oHBI (NH₄⁺ salt)

Chemical structure

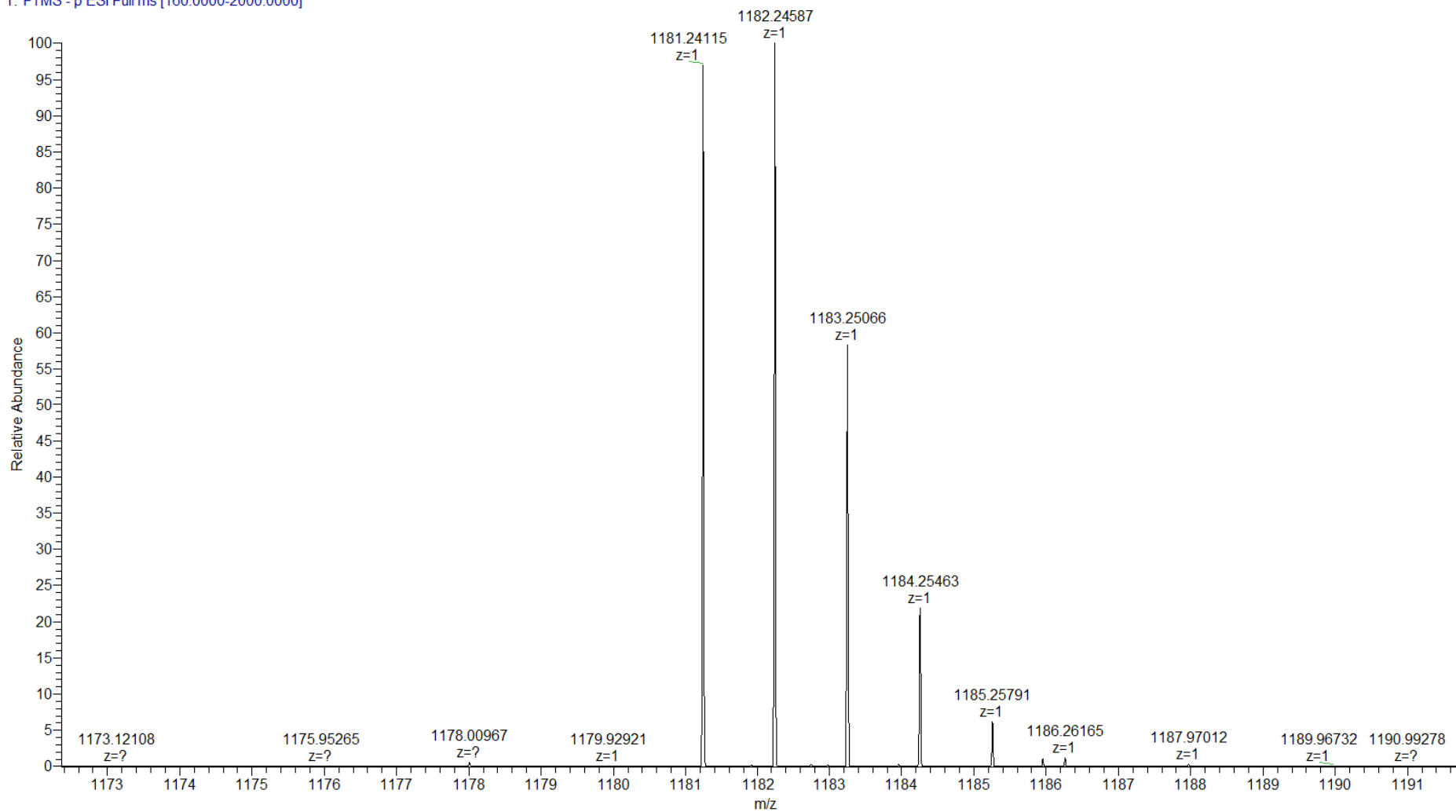


RP-HPLC (conditions b)



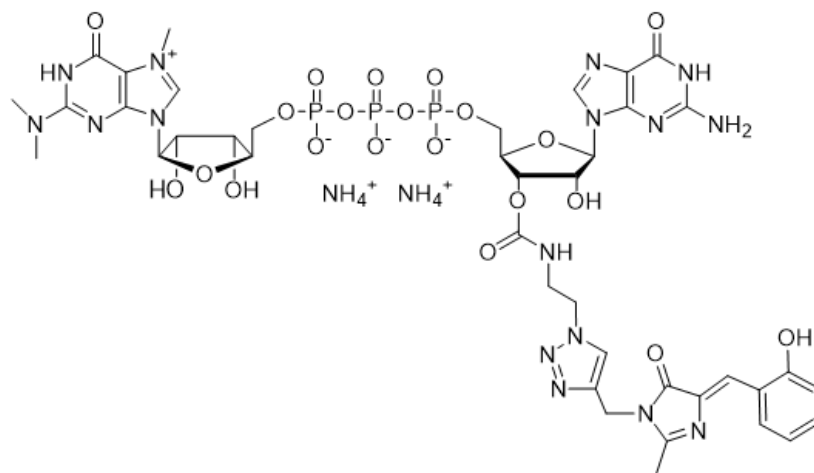
MS (-) ESI (Calc. [M-H]⁻ C₄₀H₄₈N₁₆O₂₁P₃⁻ : 1181.2398, found: 1181.24115)

220214_PSu_63b #7-61 RT: 0.06-0.54 AV: 55 NL: 3.02E5
T: FTMS - p ESI Full ms [160.0000-2000.0000]

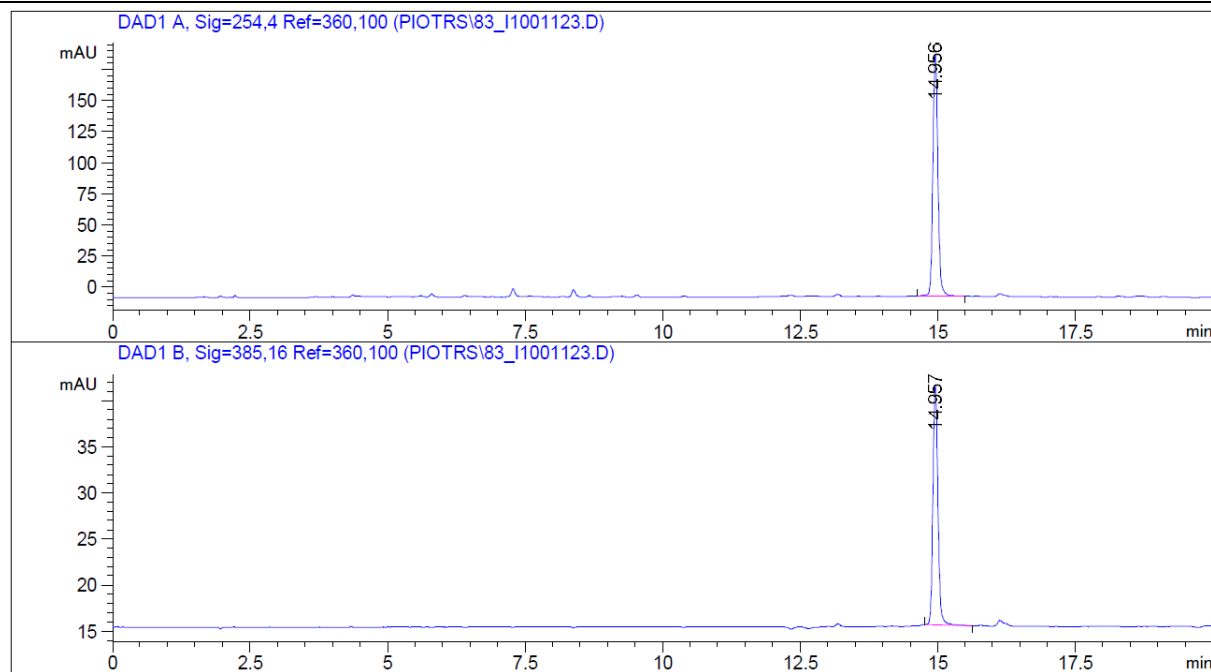


Compound 1b-3': TMGpppG-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-oHBI (NH₄⁺ salt)

Chemical structure

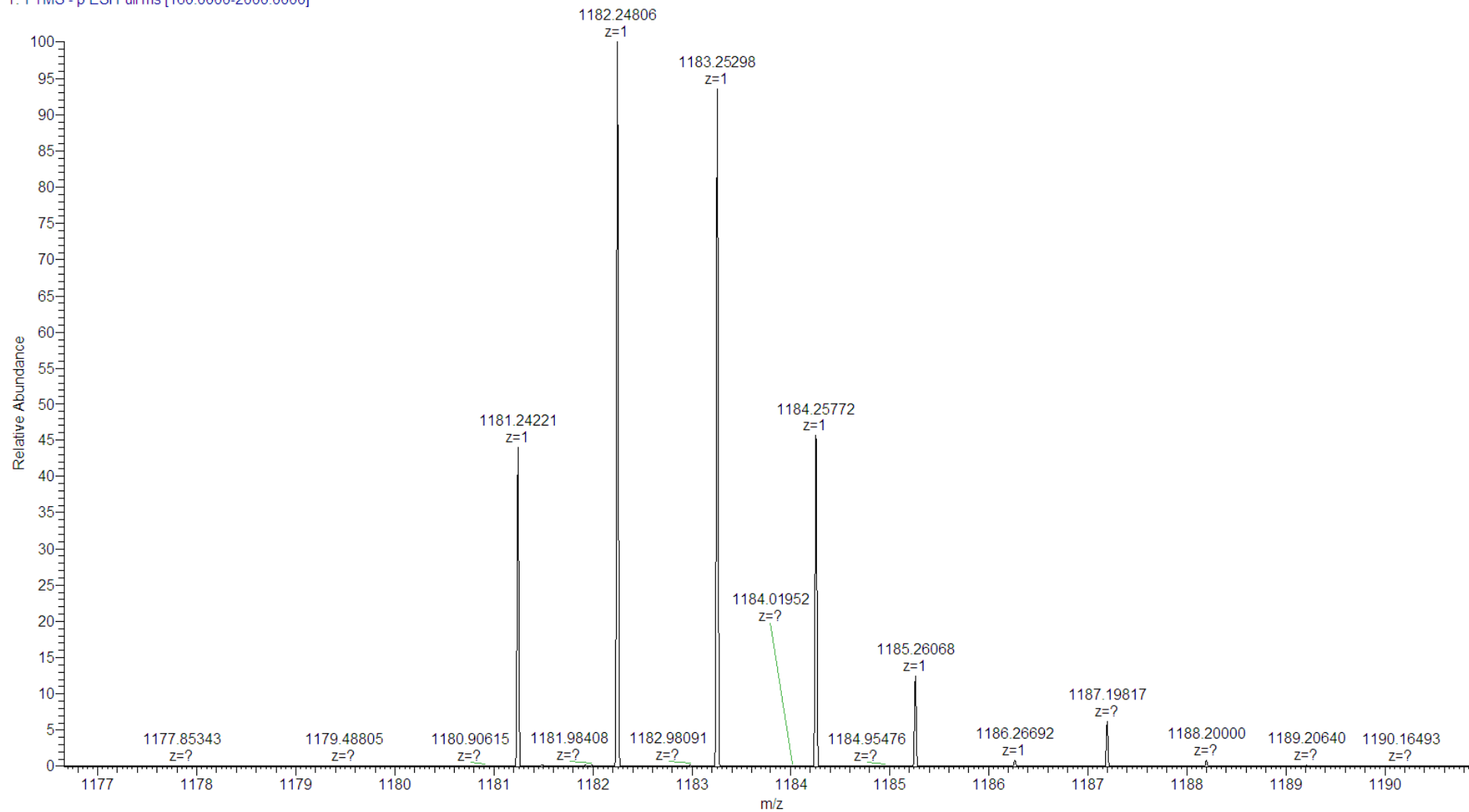


RP-HPLC (conditions b)



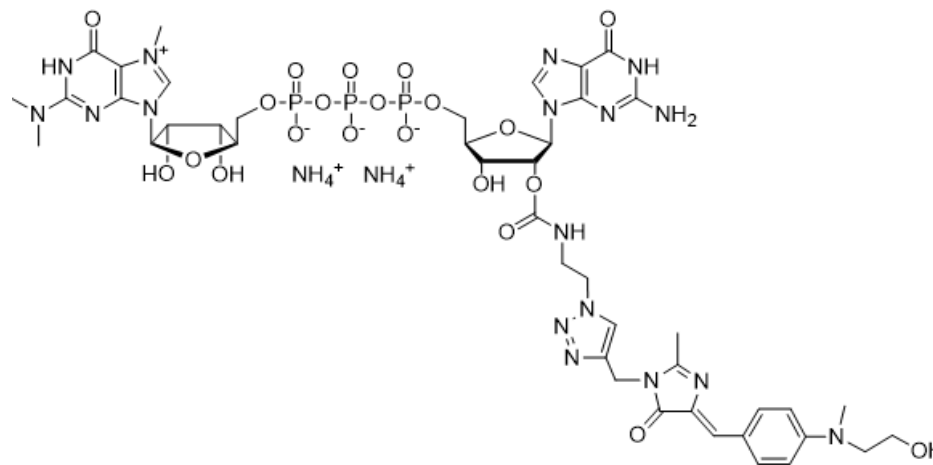
210629_PSu_83-12 #20-203 RT: 0.17-1.77 AV: 184 NL: 9.64E4
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₀H₄₈N₁₆O₂₁P₃⁻ : 1181.2398, found: 1181.24221)

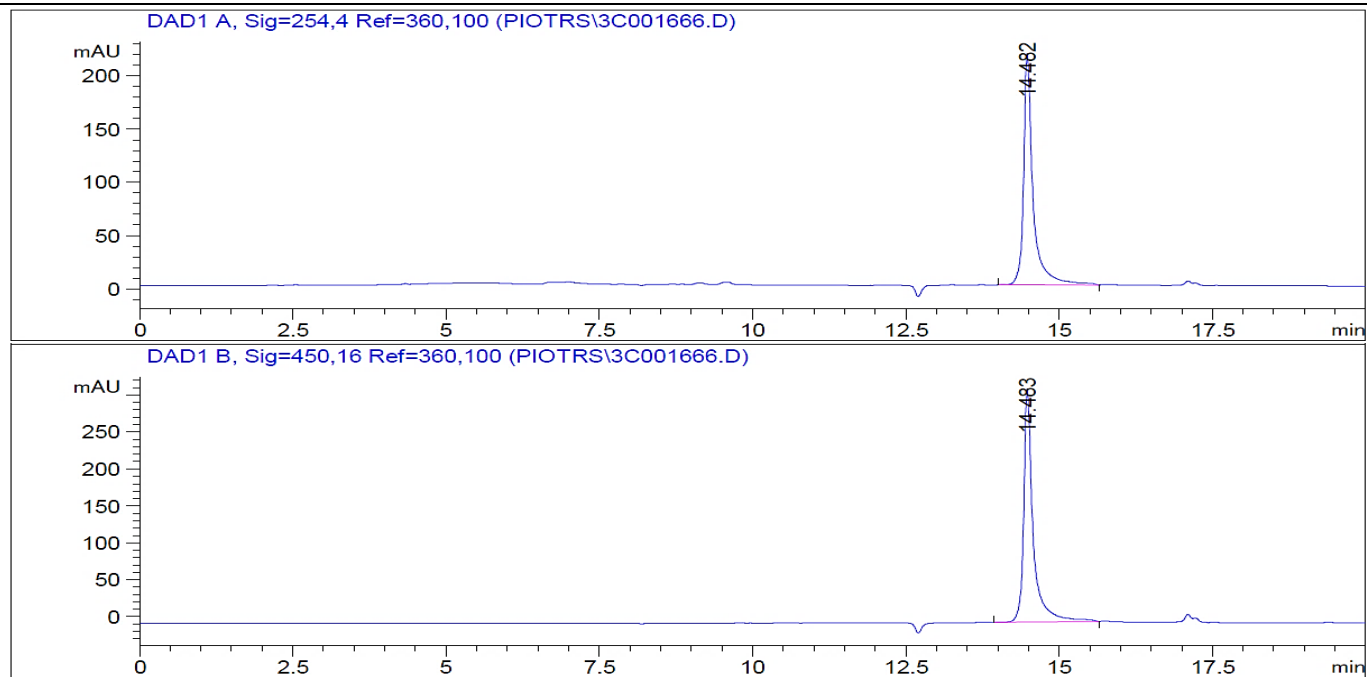


Compound 1c-2': TMGpppG-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

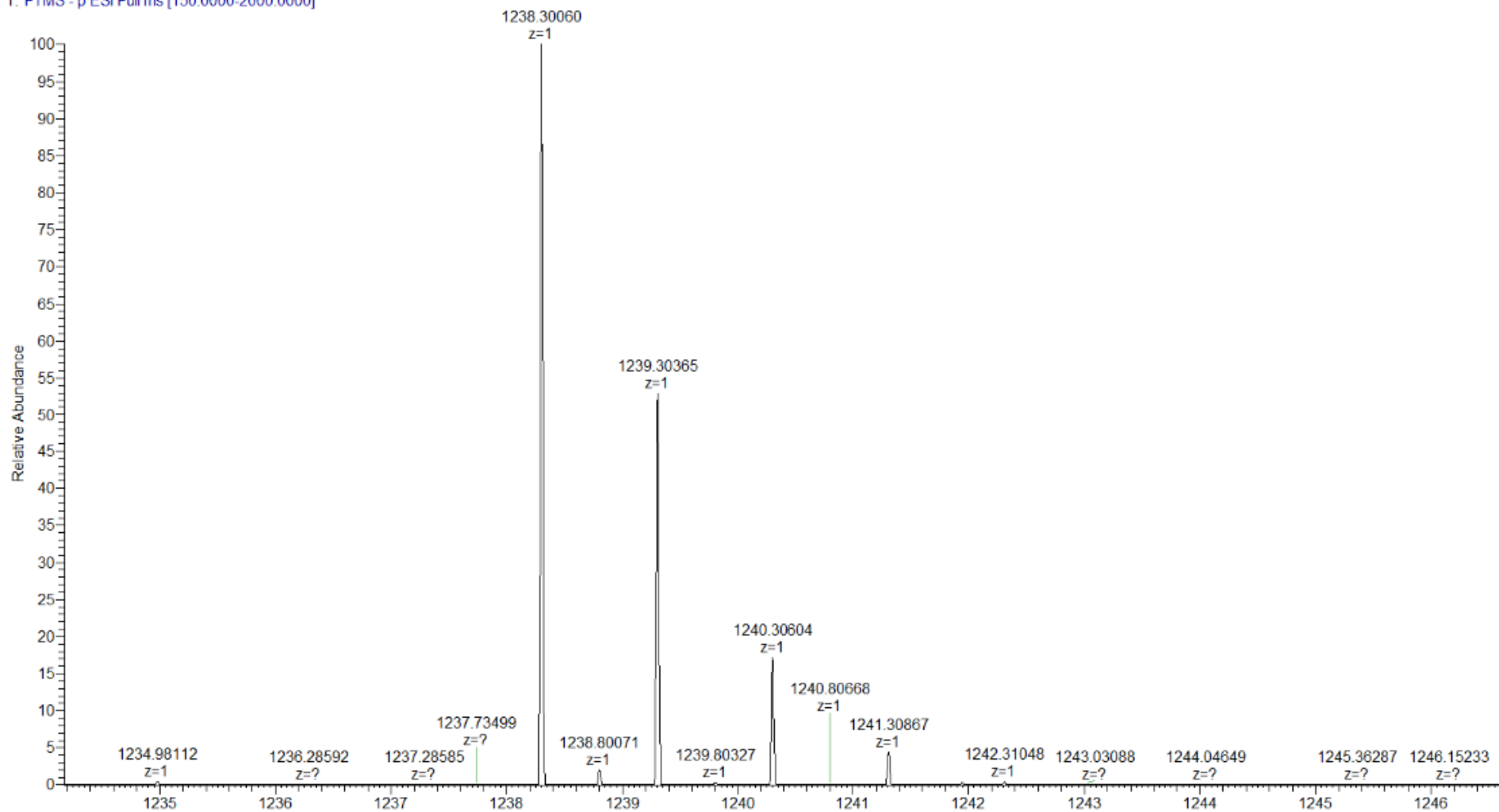


RP-HPLC (conditions c)



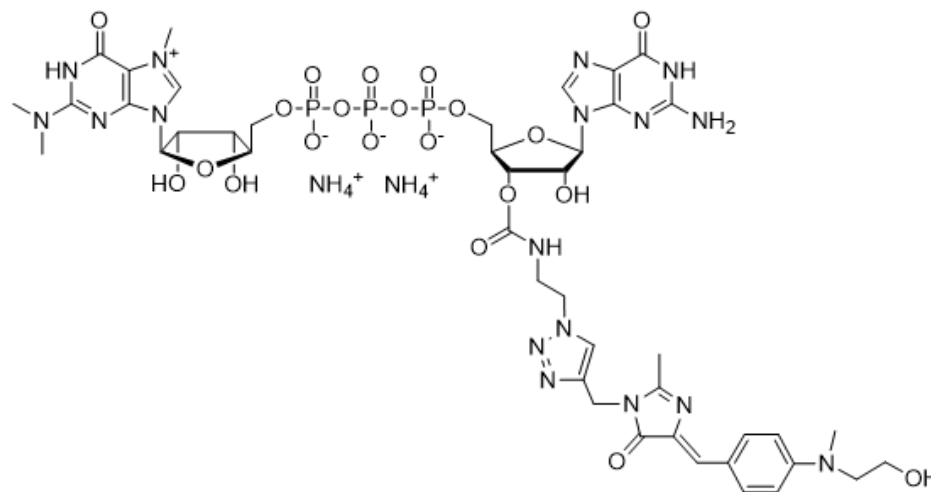
MS (-) ESI (Calc. [M-H]⁻ C₄₃H₅₅N₁₇O₂₁P₃ : 1238.2977, found: 1238.30060)

191107_PSu_26 #133-268 RT: 1.27-2.66 AV: 136 NL: 2.43E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

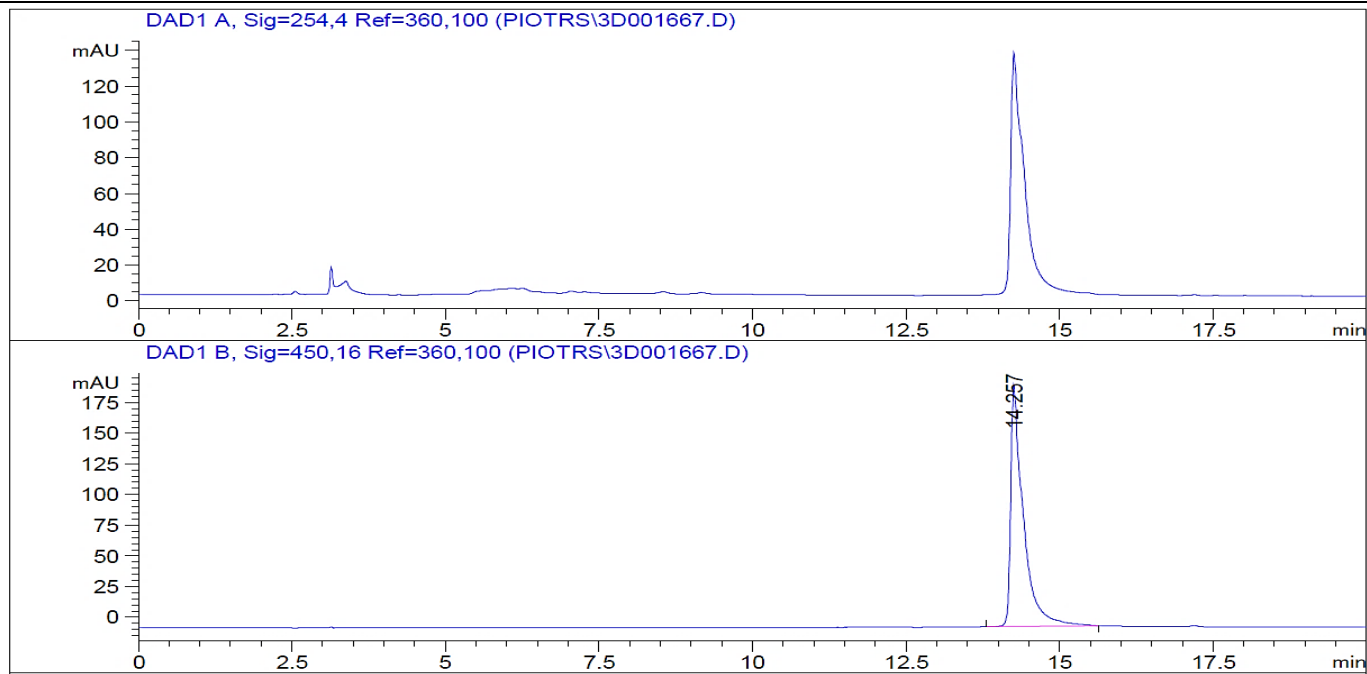


Compound 1c-3': TMGpppG-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

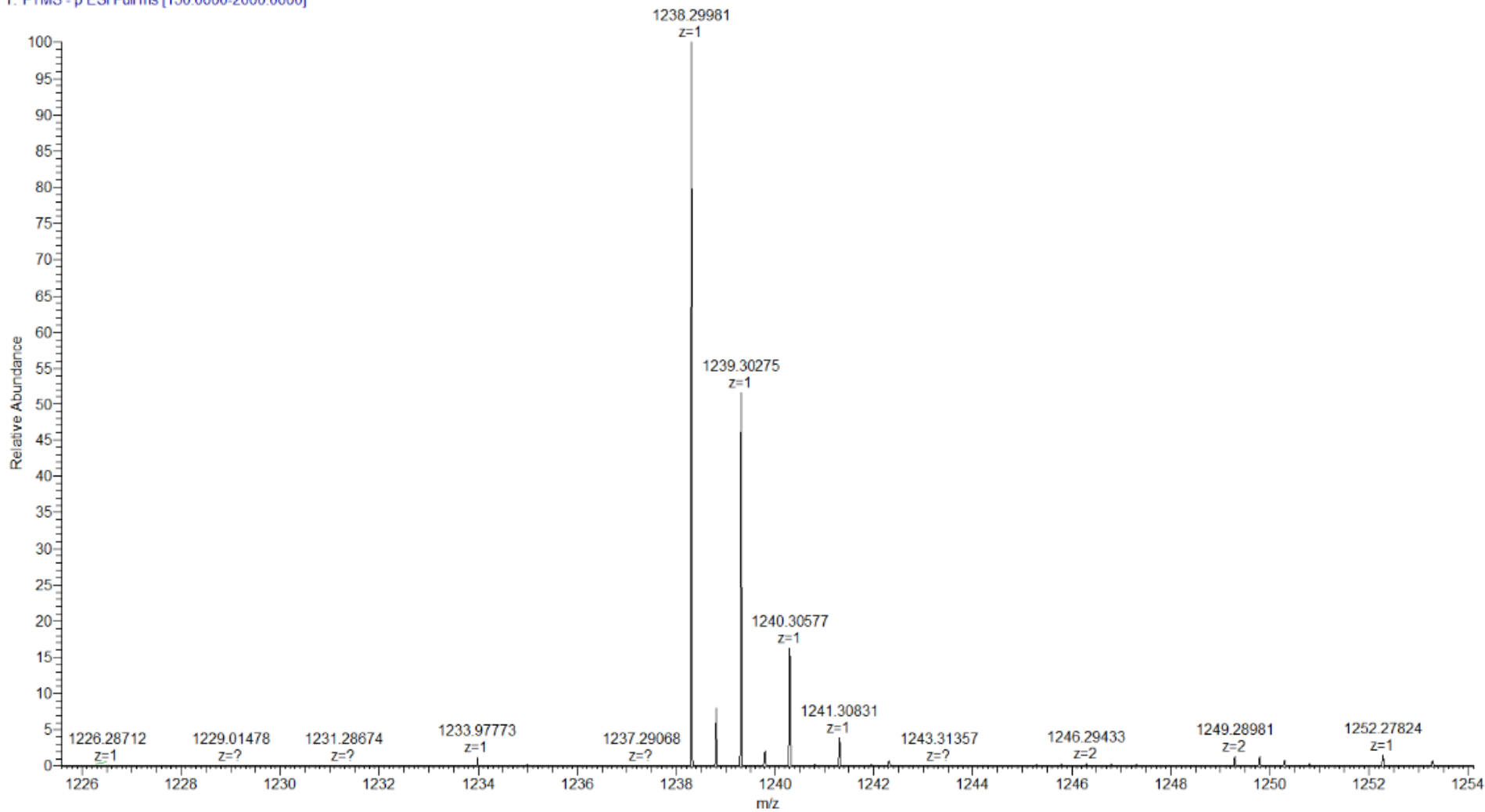


RP-HPLC (conditions c)



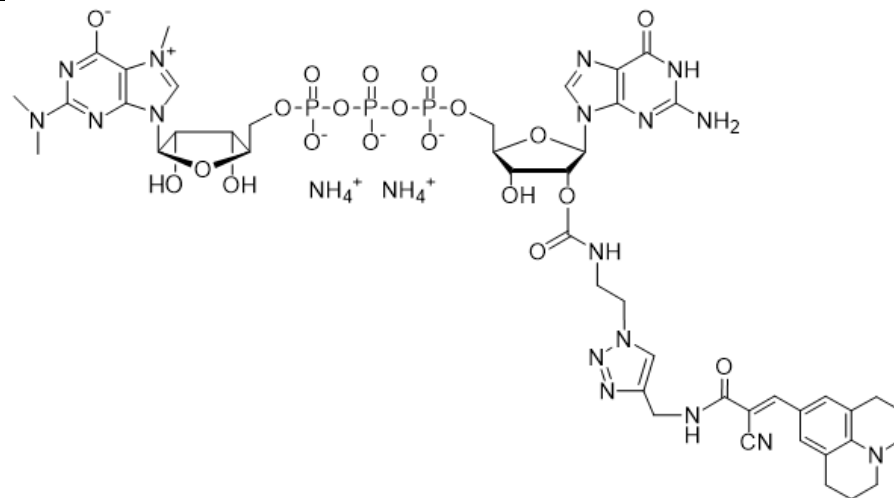
MS (-) ESI (Calc. [M-H]⁻ C₄₃H₅₅N₁₇O₂₁P₃ : 1238.2977, found: 1238.29981)

191107_PSu_27 #2-103 RT: 0.02-1.07 AV: 102 NL: 7.30E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

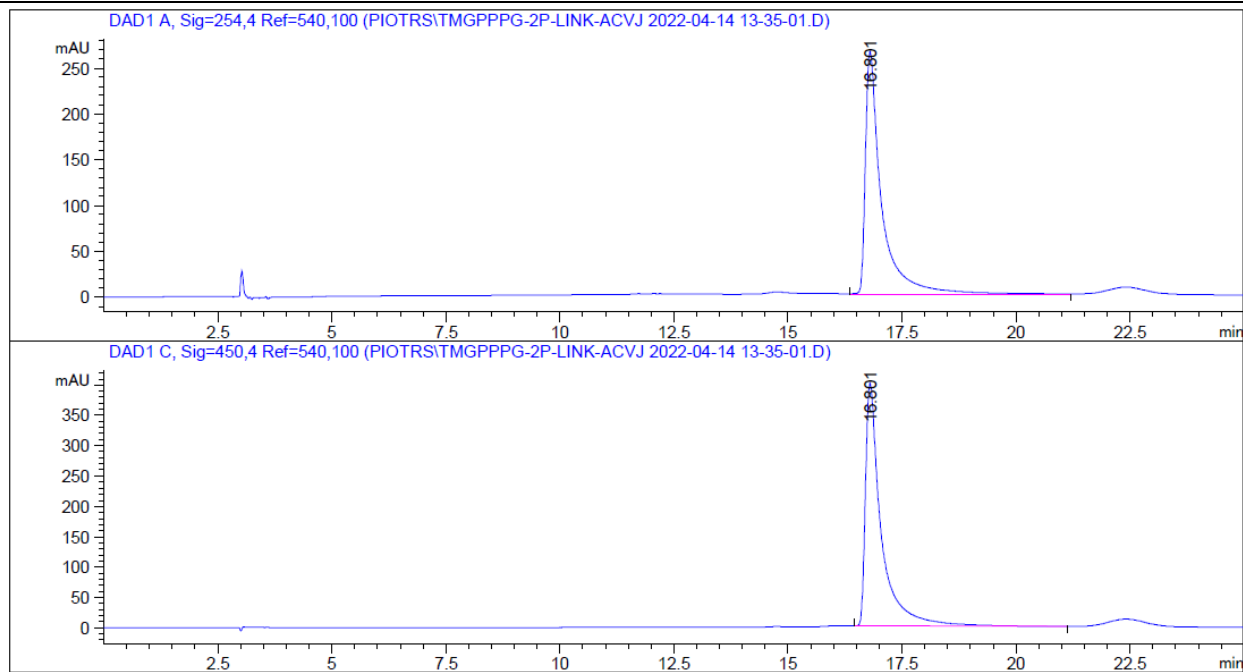


Compound 1d-2': TMGpppG-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-ACVJ (NH₄⁺ salt)

Chemical structure

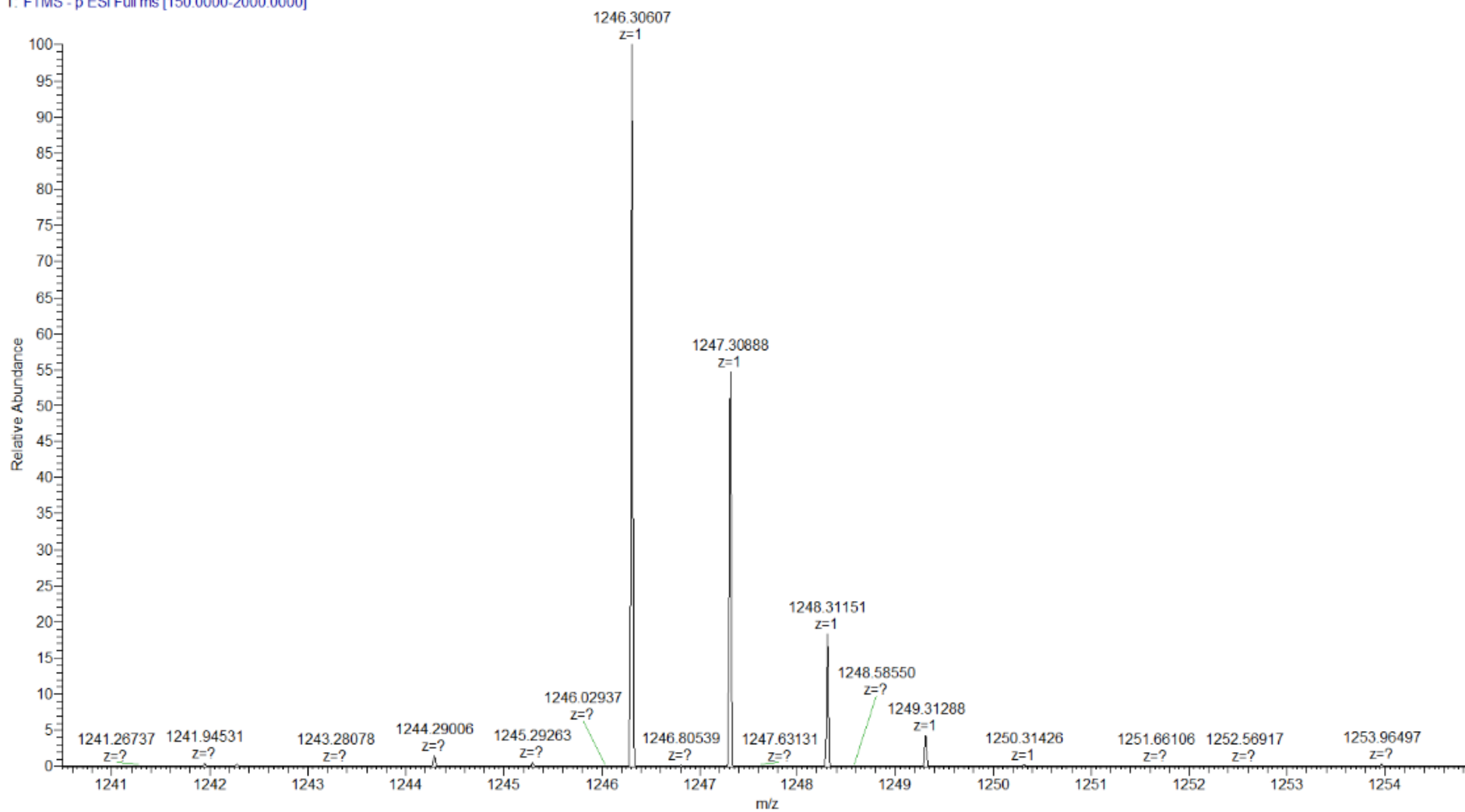


RP-HPLC (conditions b)



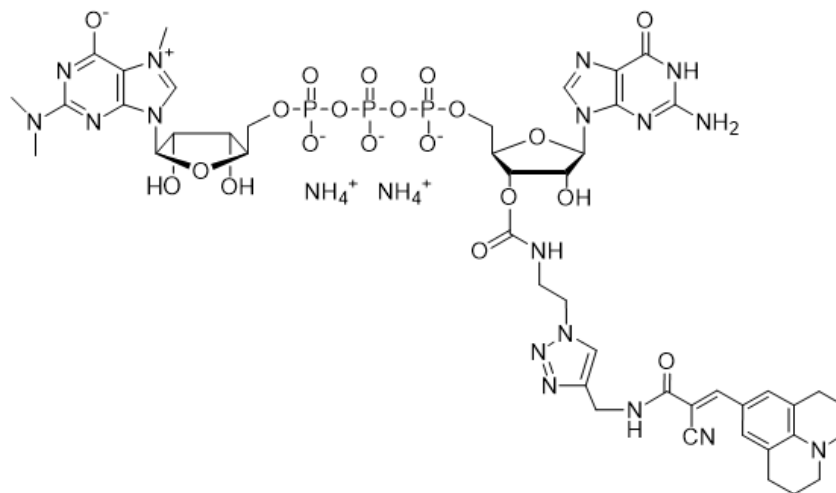
MS (-) ESI (Calc. [M-H]⁻ C₄₅H₅₅N₁₇O₂₀P₃⁻ : 1246.3028, found: 1246.30607)

191107_PSu_28 #166-321 RT: 1.59-3.13 AV: 156 NL: 2.27E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

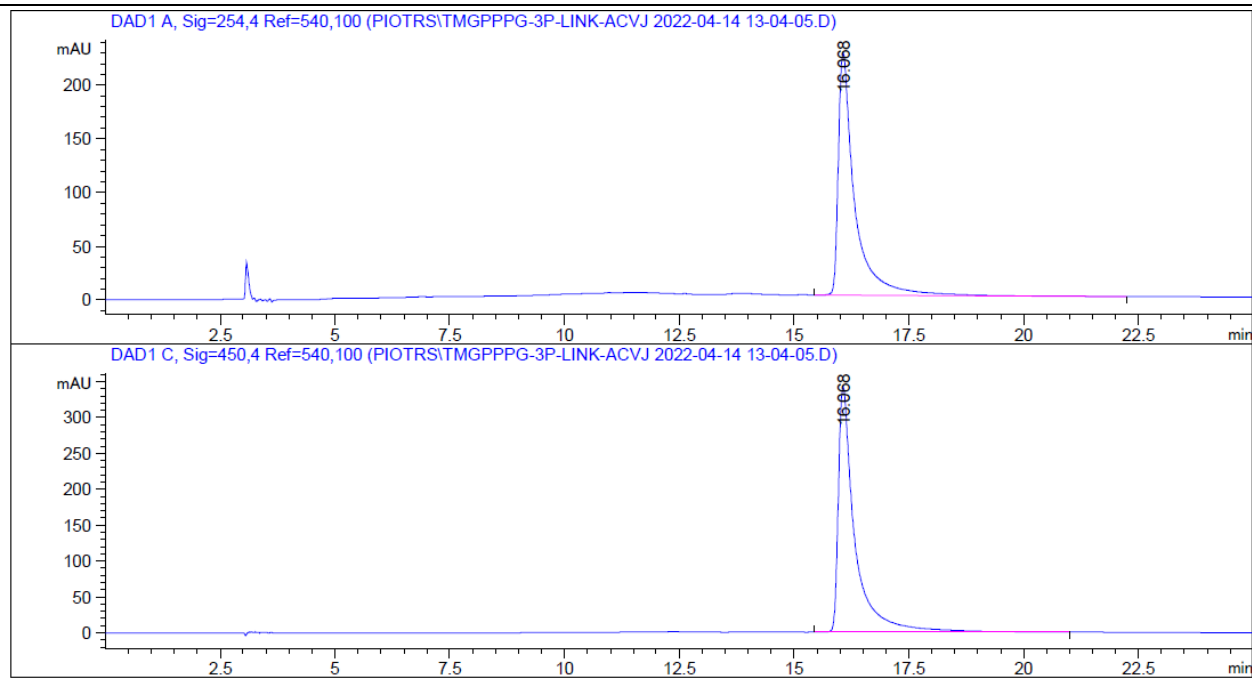


Compound 1d-3': TMGpppG-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-ACVJ (NH₄⁺ salt)

Chemical structure

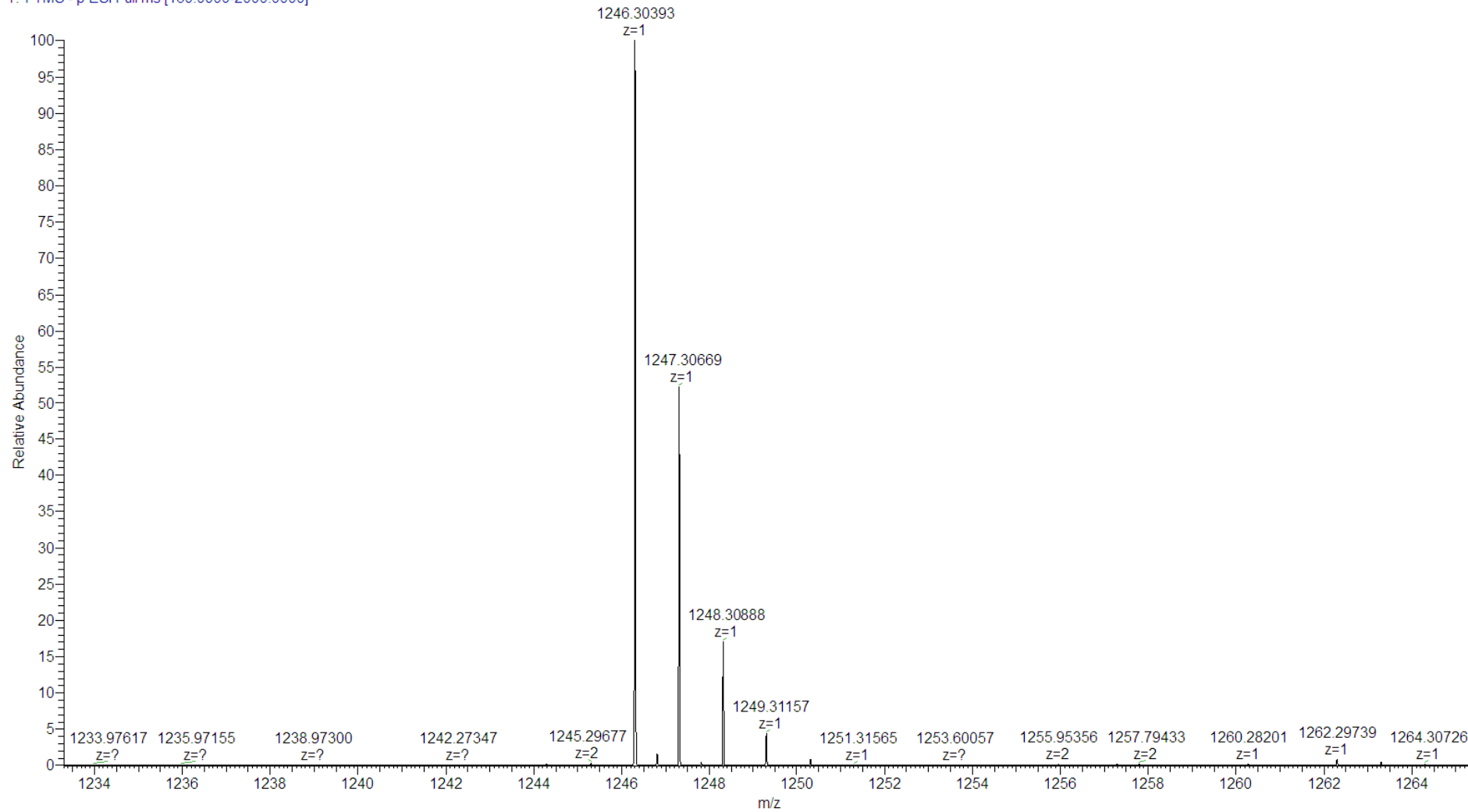


RP-HPLC (conditions b)



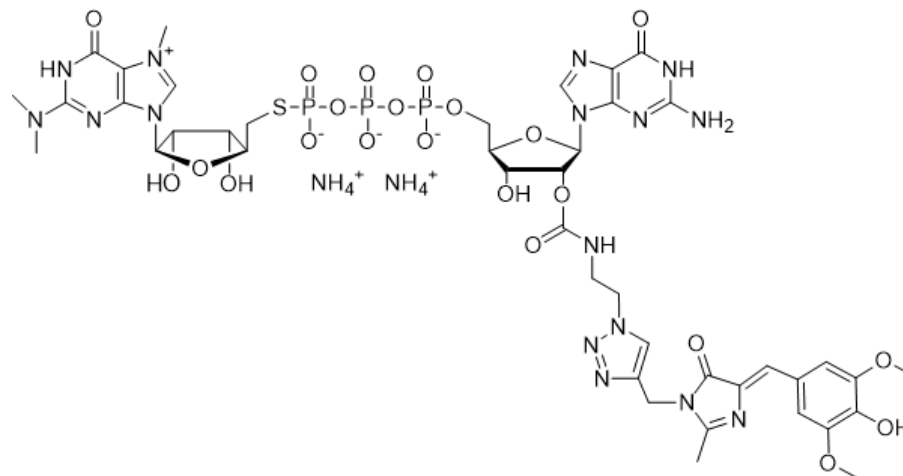
MS (-) ESI (Calc. [M-H]⁻ C₄₅H₅₅N₁₇O₂₀P₃ : 1246.3028, found: 1246.30393)

220407_PSu_03 #59-87 RT: 0.53-0.77 AV: 29 NL: 5.91E6
T: FTMS - p ESI Full ms [160.0000-2000.0000]

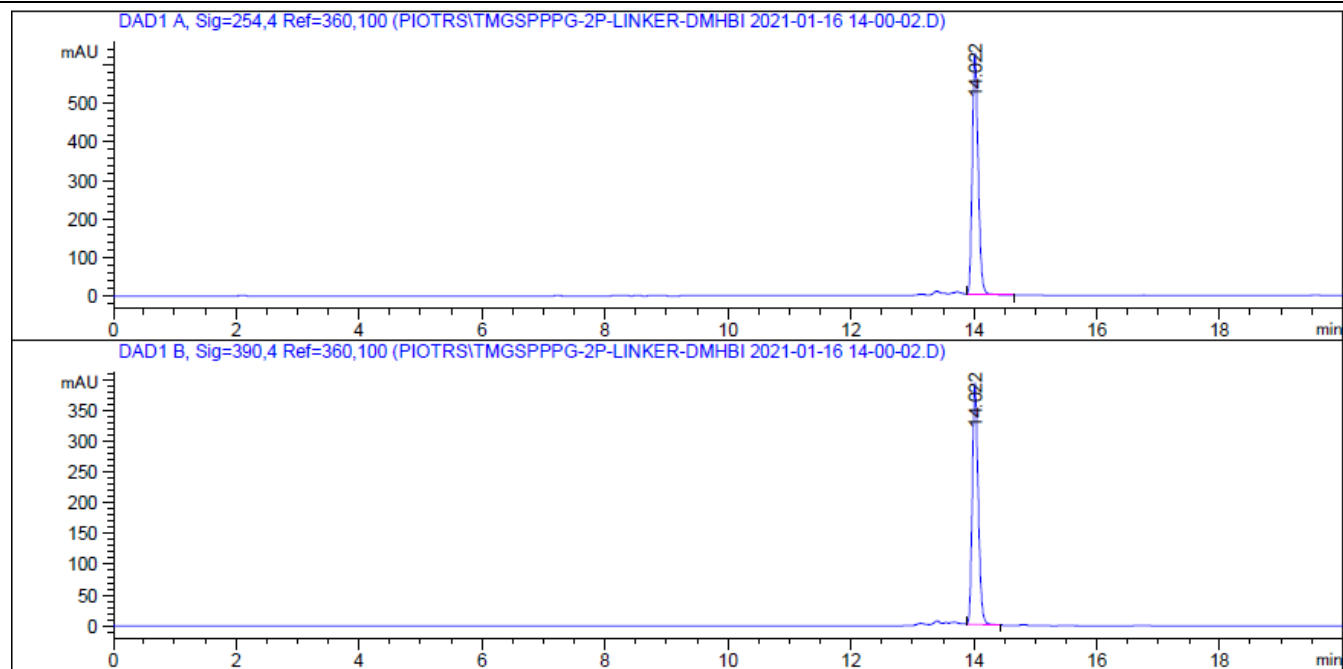


Compound 2a-2': TMG-5'-SpppG-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

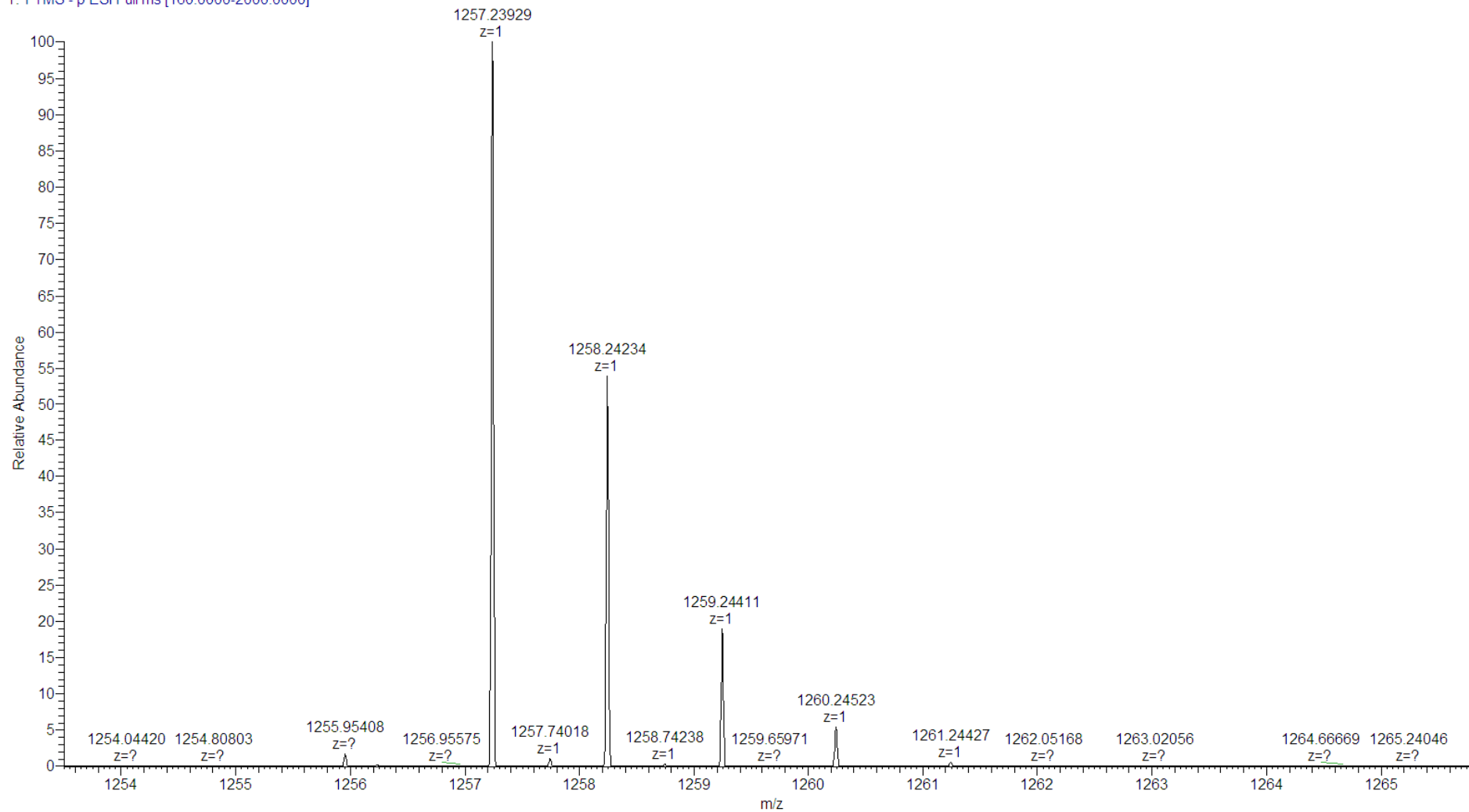


RP-HPLC (conditions c)



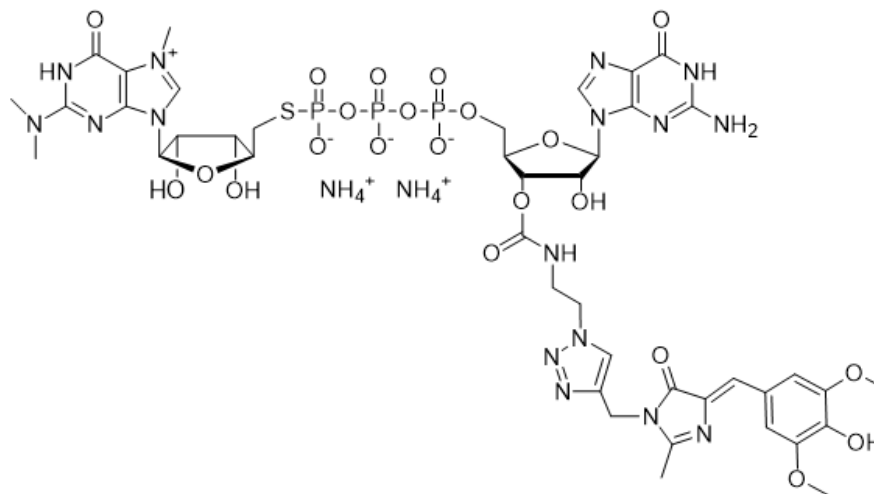
210629_PSu_6a #115-207 RT: 1.00-1.81 AV: 93 NL: 6.22E5
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₂N₁₆O₂₂P₃S₃ : 1257.23811, 1257.23929)

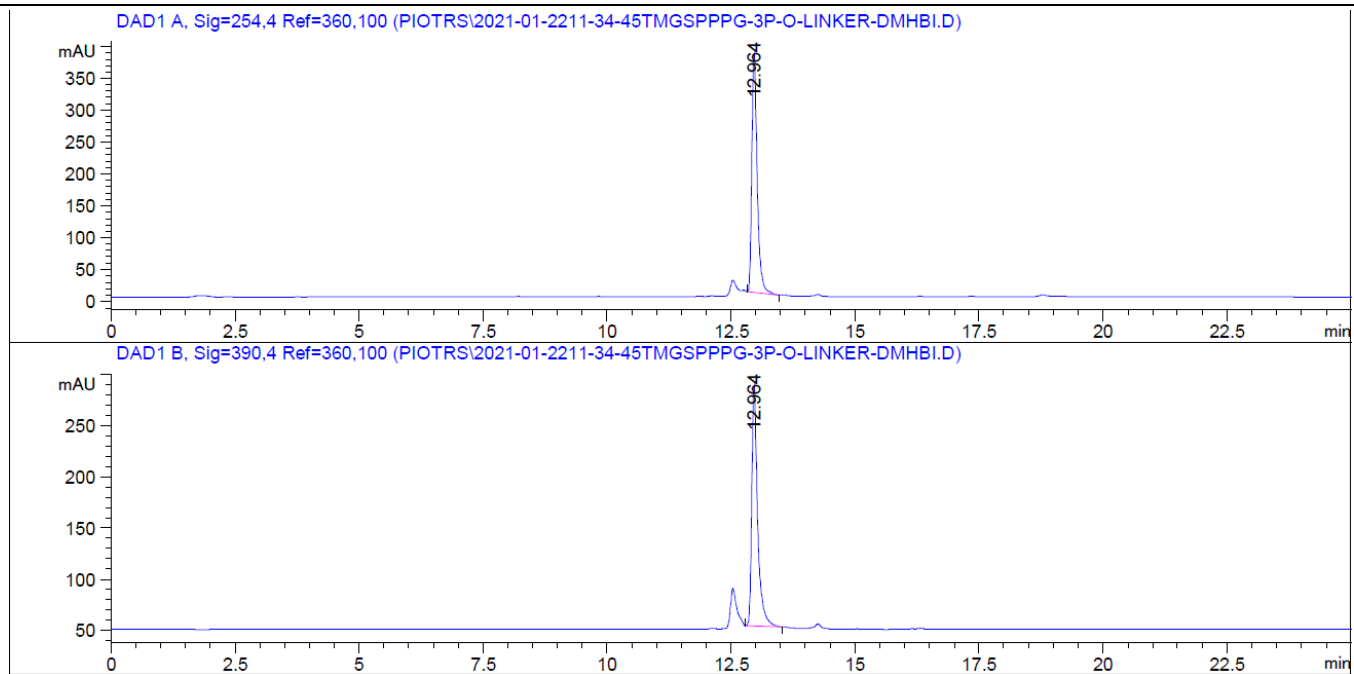


Compound 2a-3': TMG-5'-SpppG-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

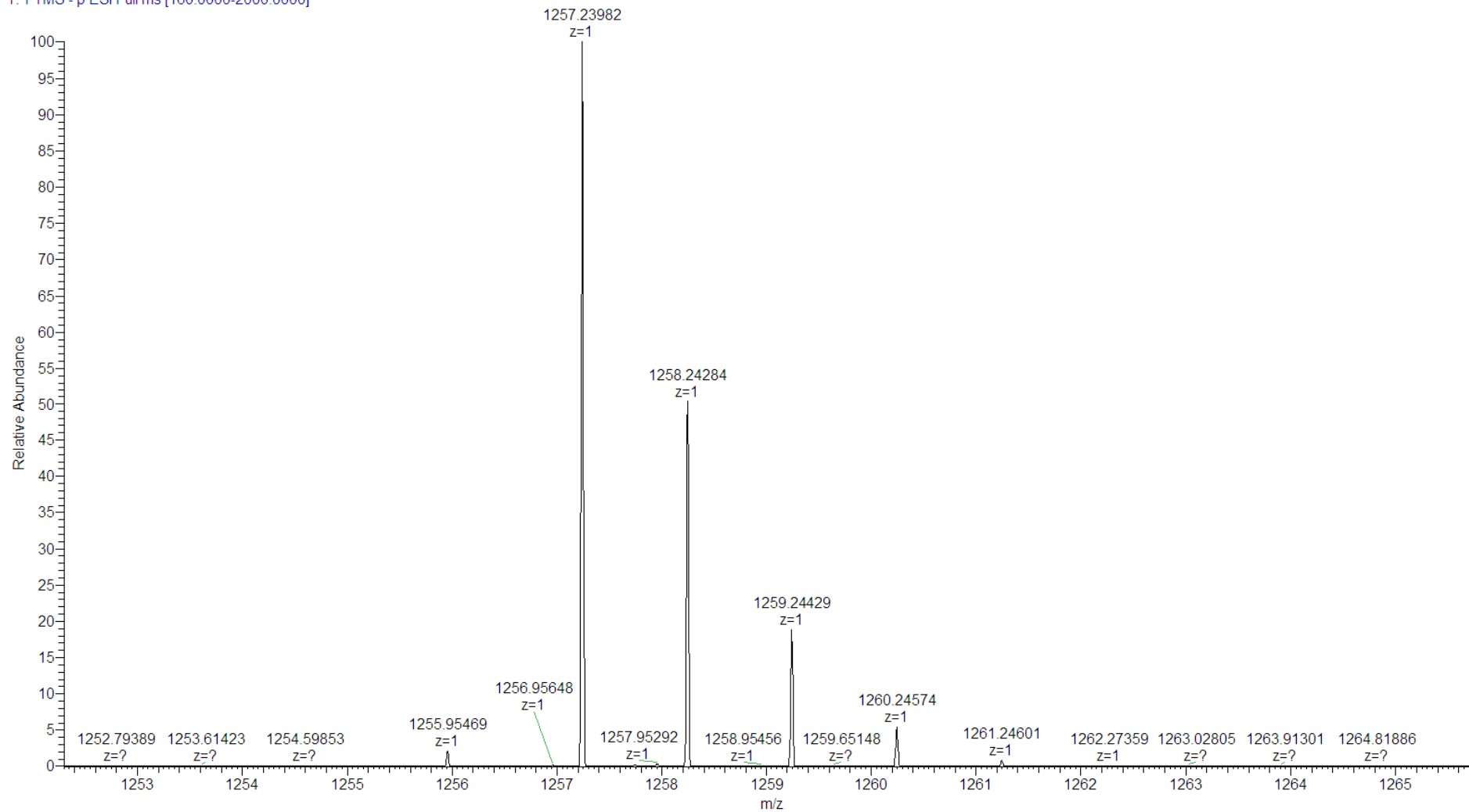


RP-HPLC (conditions c)



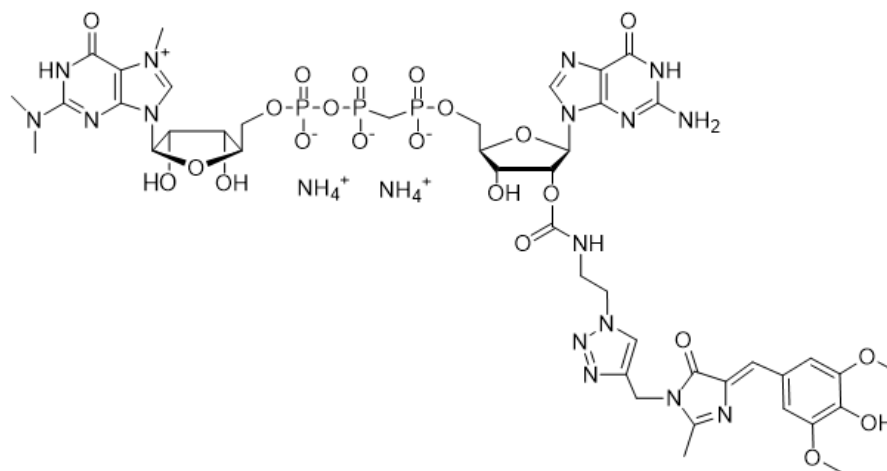
210629_PSu_6b #23-103 RT: 0.20-0.90 AV: 81 NL: 4.30E5
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₂N₁₆O₂₂P₃S⁻ : 1257.23811, found: 1257.23982)

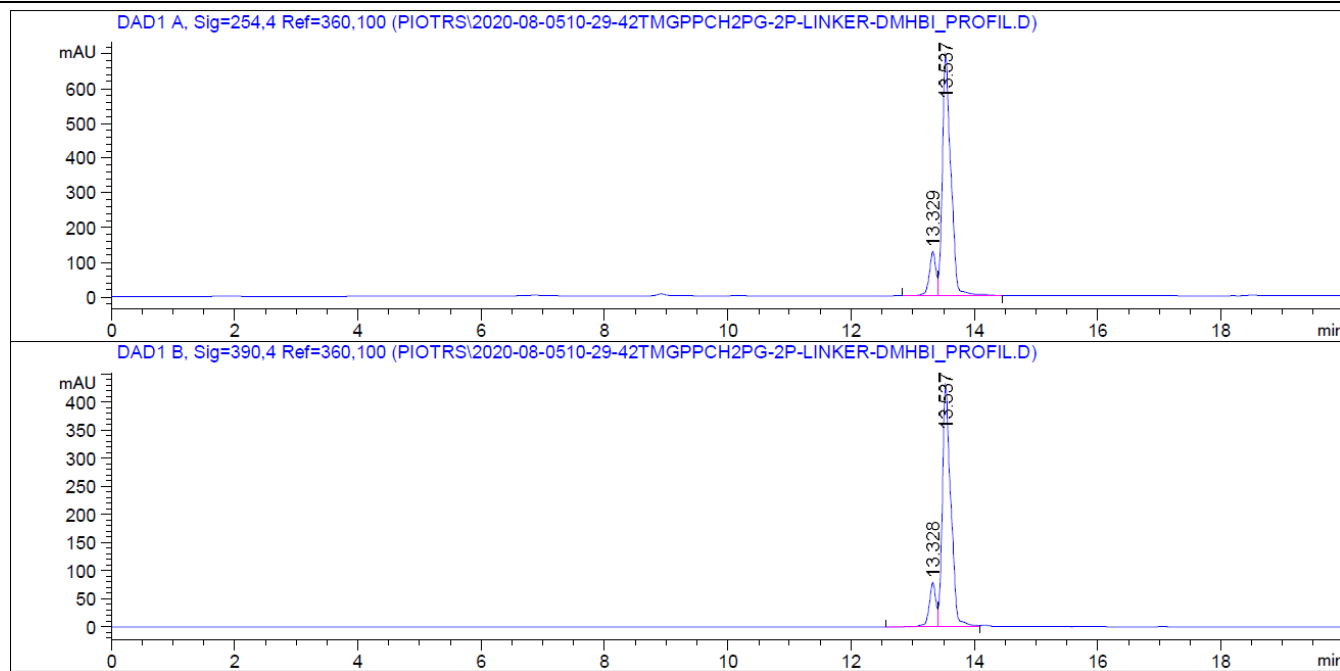


Compound 3a-2': TMGppCH₂pG-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

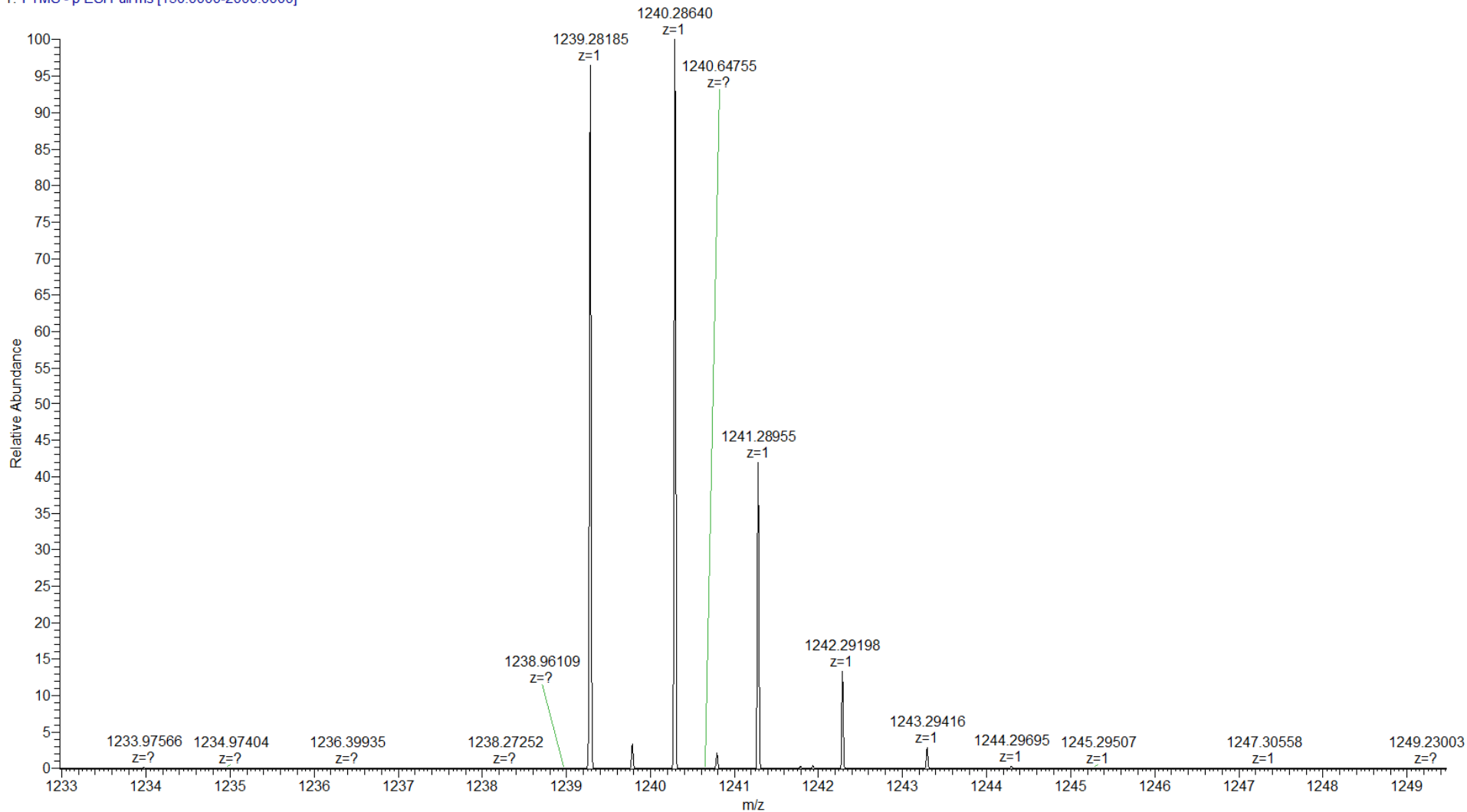


RP-HPLC (conditions c)



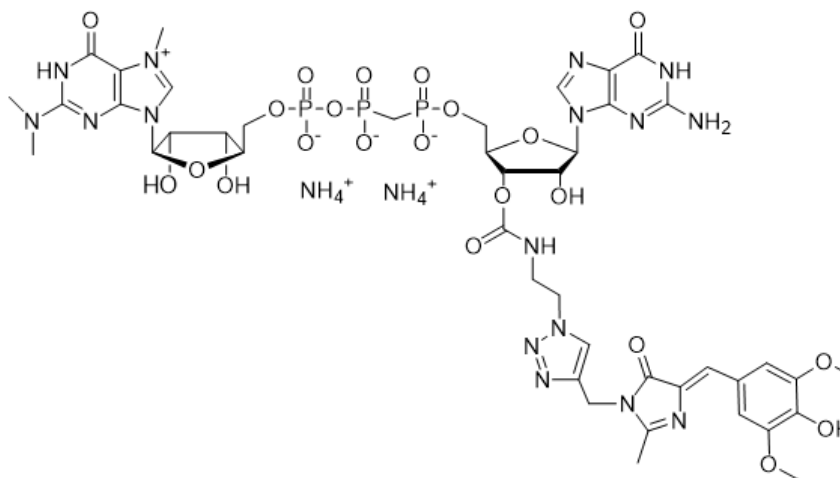
MS (-) ESI (Calc. [M-H]⁻ C₄₃H₅₄N₁₆O₂₂P₃ : 1239.2817, found: 1239.28185)

200812_PSu_01 #10-124 RT: 0.10-1.26 AV: 115 NL: 2.78E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

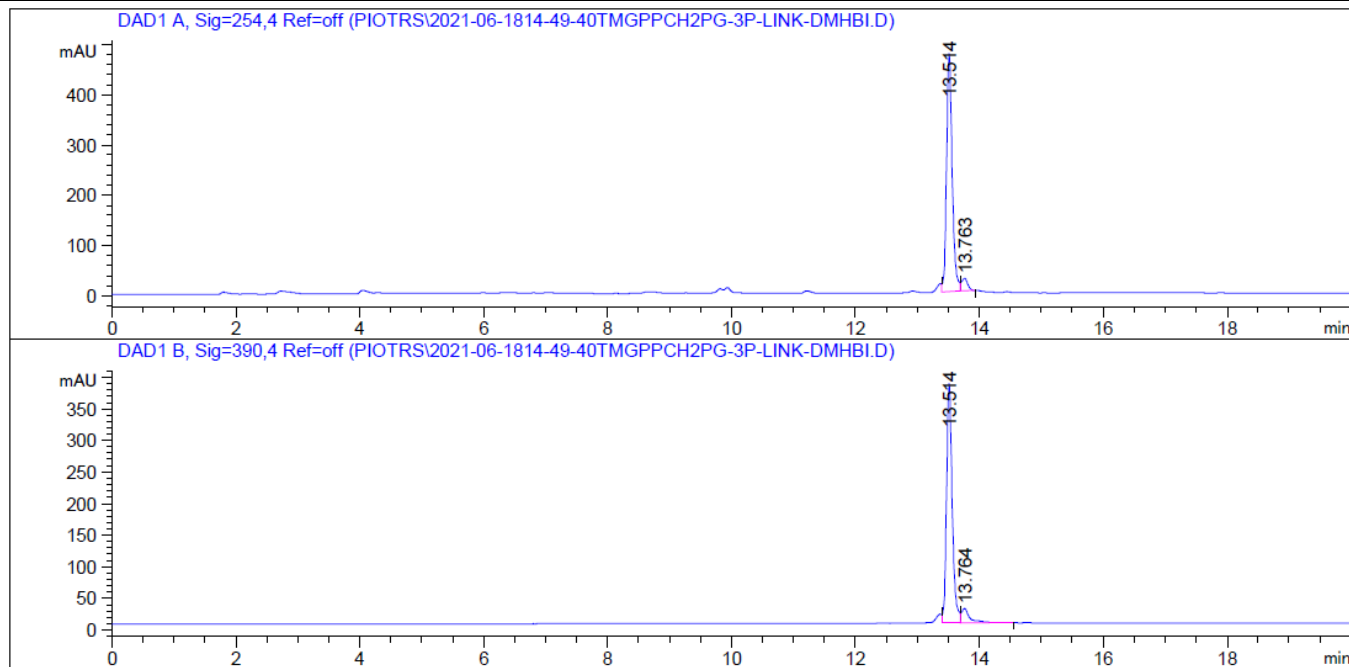


Compound 3a-3': TMGppCH₂pG-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

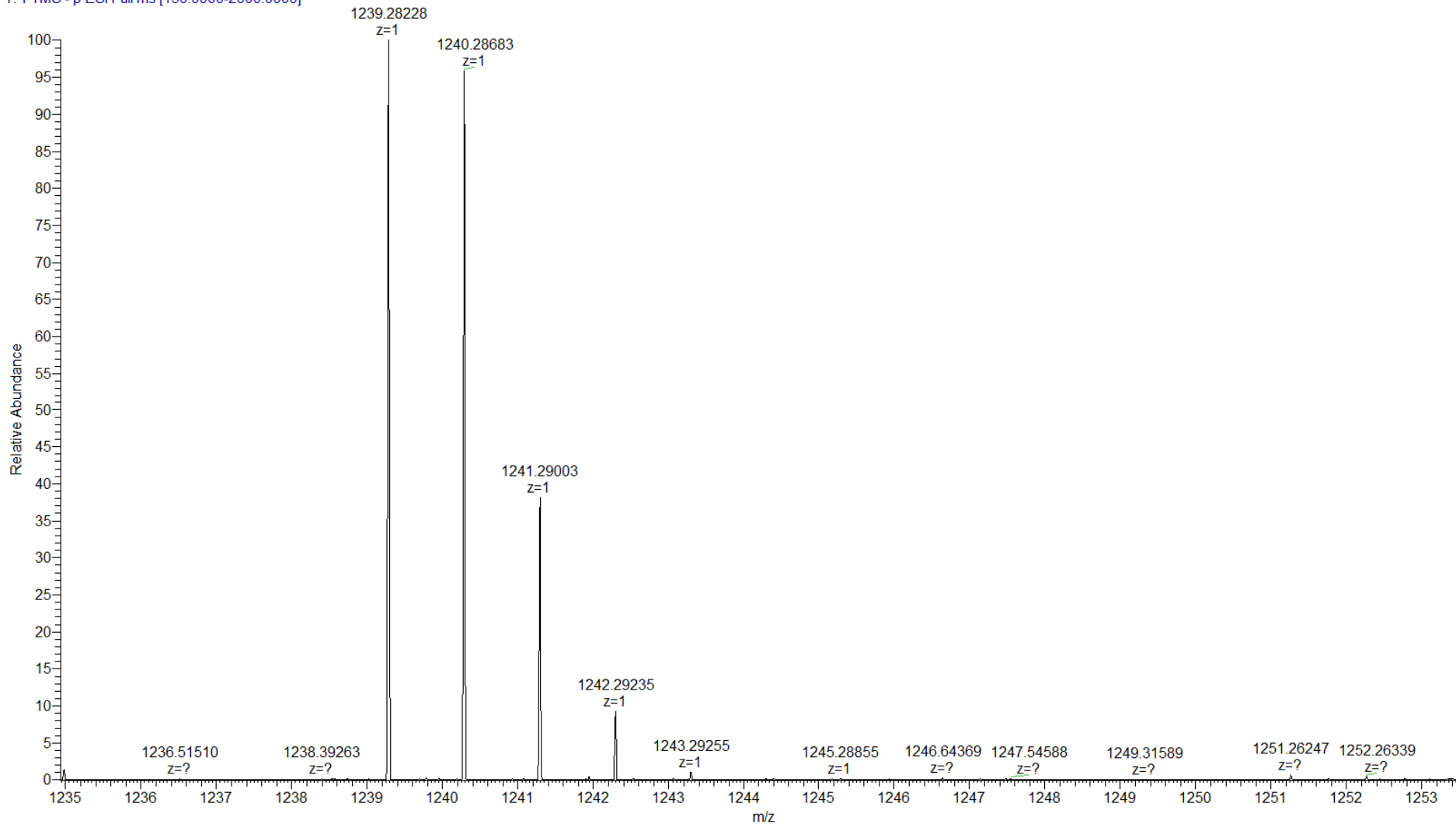


RP-HPLC (conditions c)



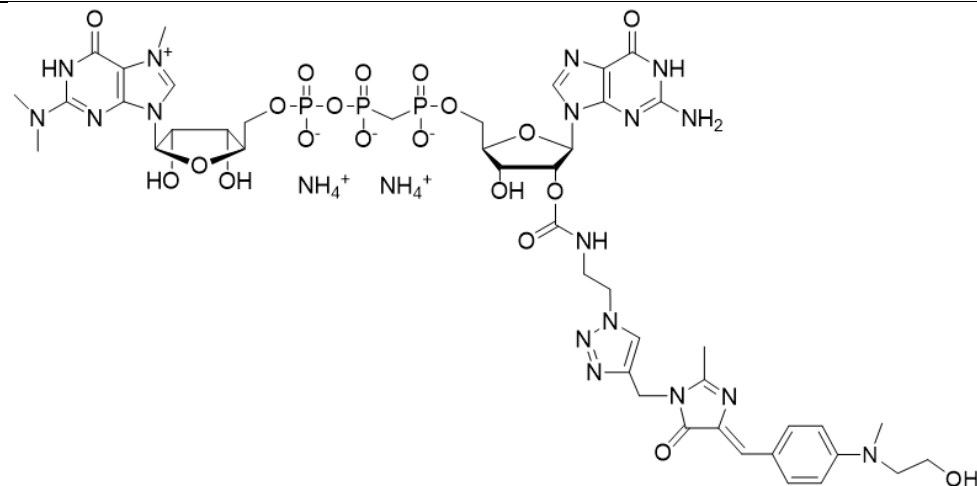
MS (-) ESI (Calc. [M-H]⁻ C₄₃H₅₄N₁₆O₂₂P₃ : 1239.2817, found: 1239.28228)

200812_PSu_02#122-198 RT: 1.24-1.99 AV: 77 NL: 5.48E4
T: FTMS - p ESI Full ms [150.0000-2000.0000]

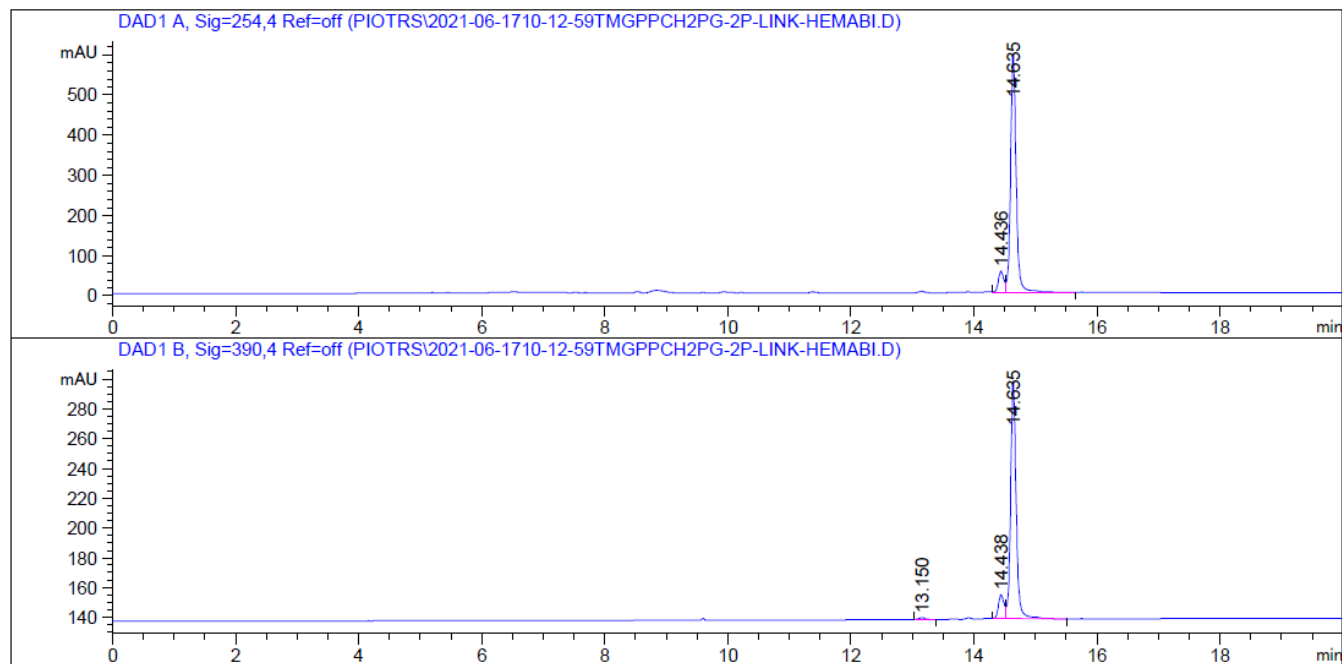


Compound 3c-2': TMGppCH₂pG-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

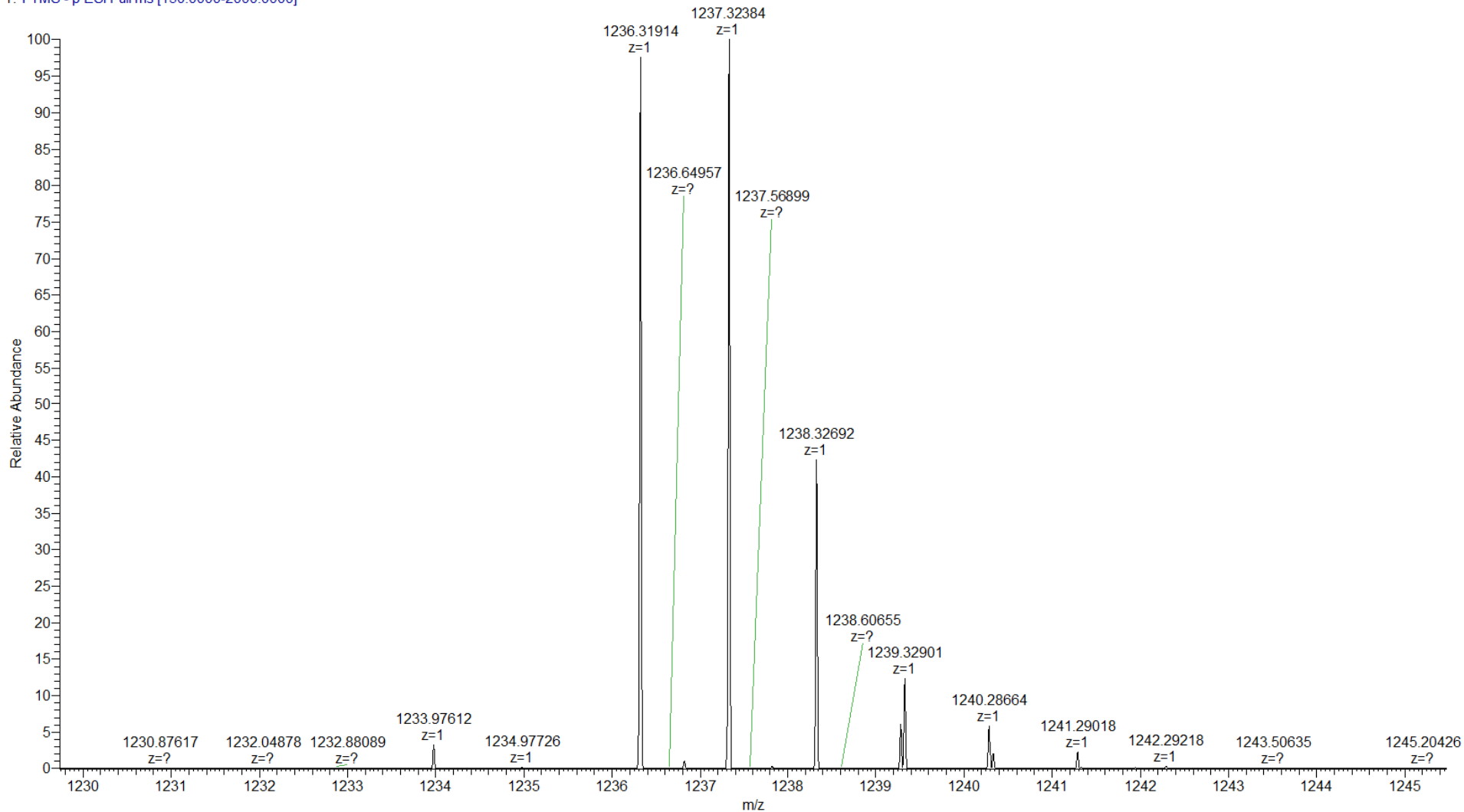


RP-HPLC (conditions c)



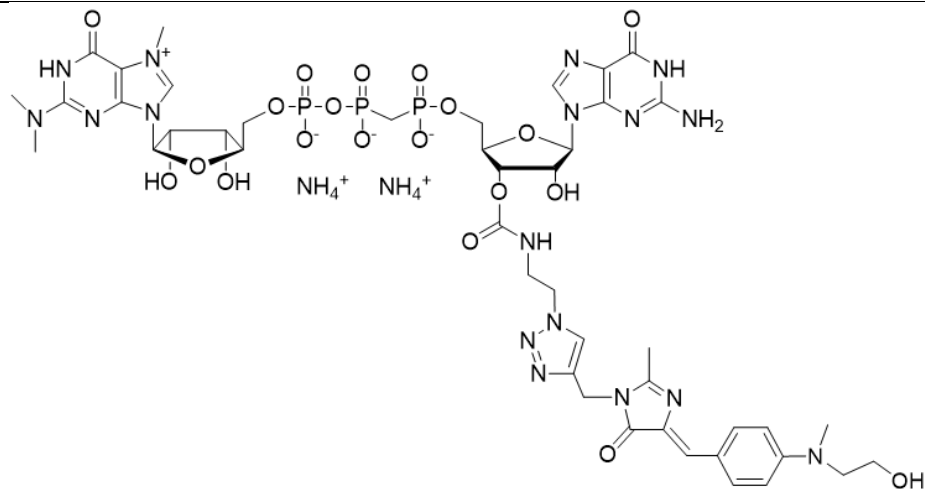
MS (-) ESI (Calc. [M-H]⁻ C₄₄H₅₇N₁₇O₂₀P₃ : 1236.3184, found: 1236.31914)

200812_PSu_03 #6-102 RT: 0.06-1.00 AV: 97 NL: 1.99E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

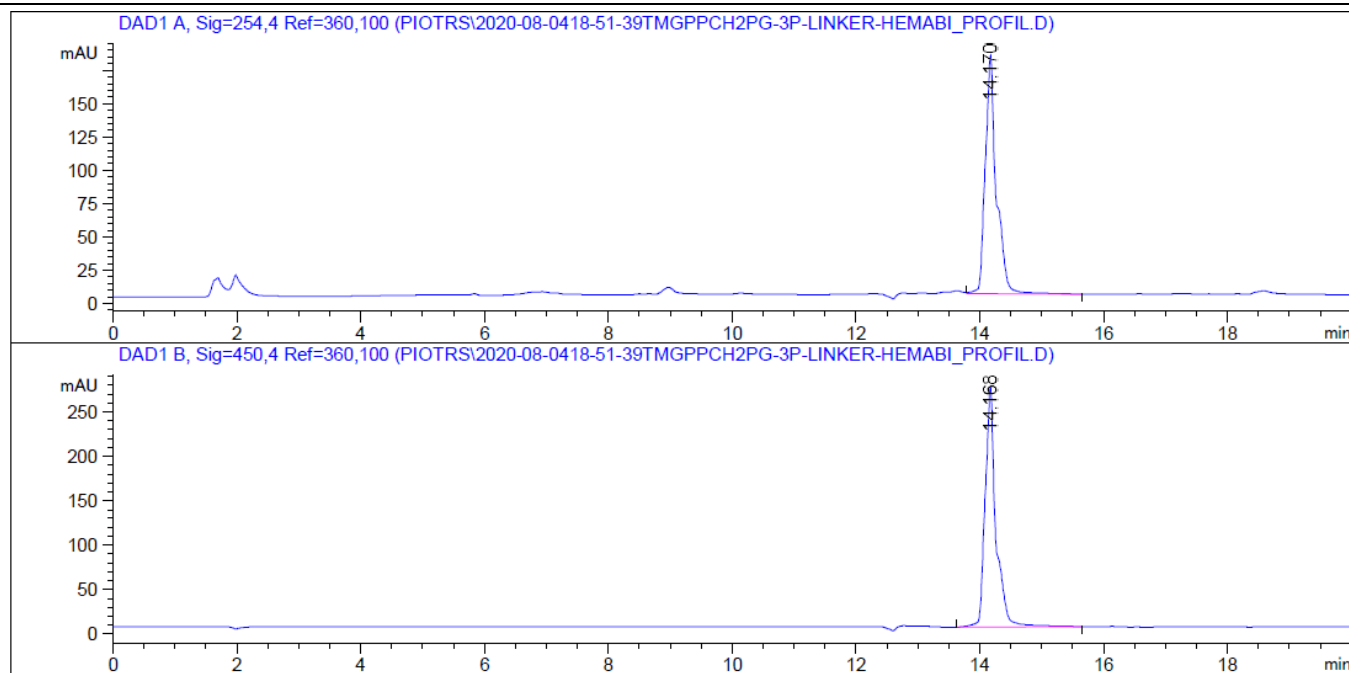


Compound 3c-3': TMGppCH₂pG-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

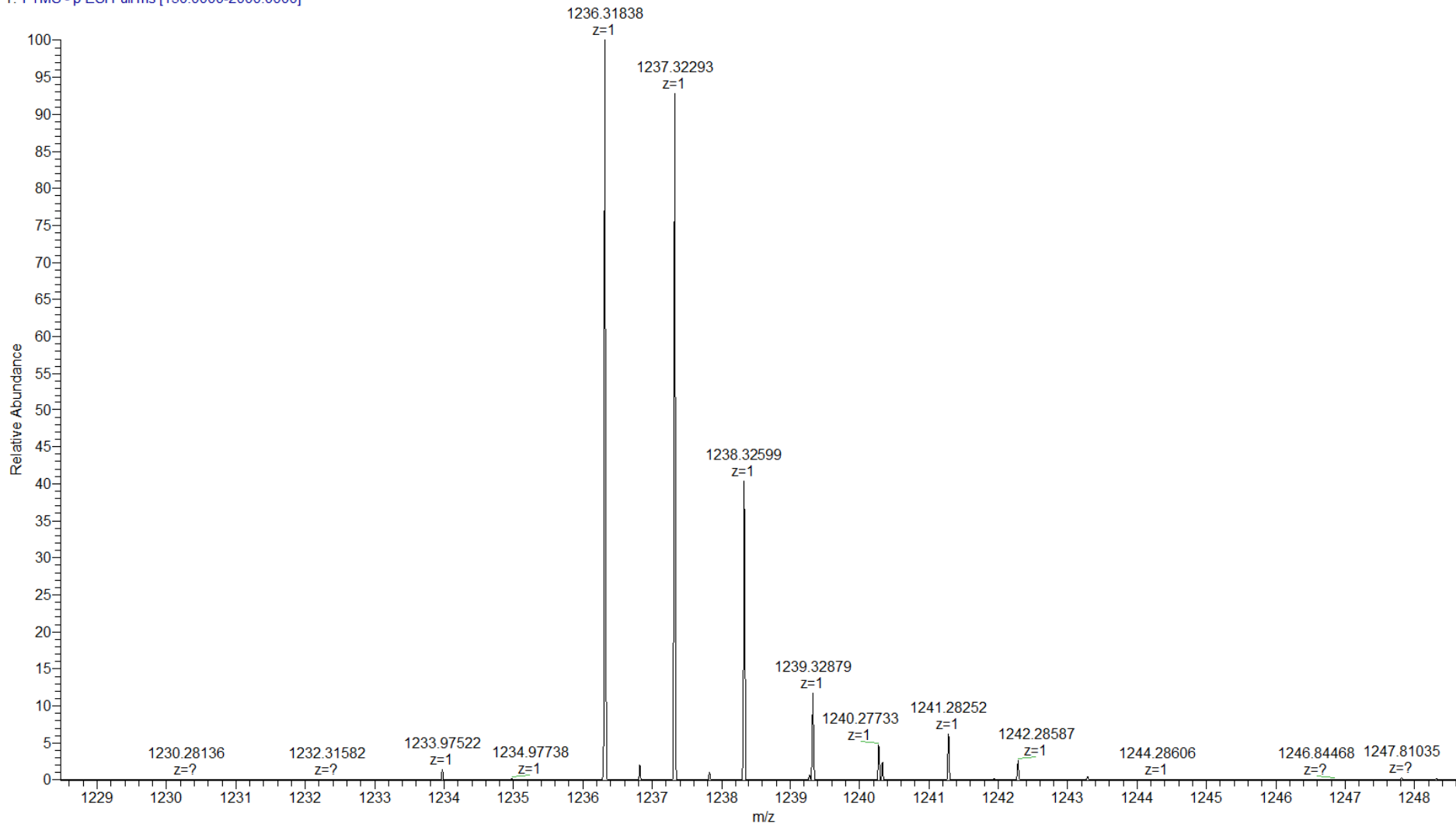


RP-HPLC (conditions c)



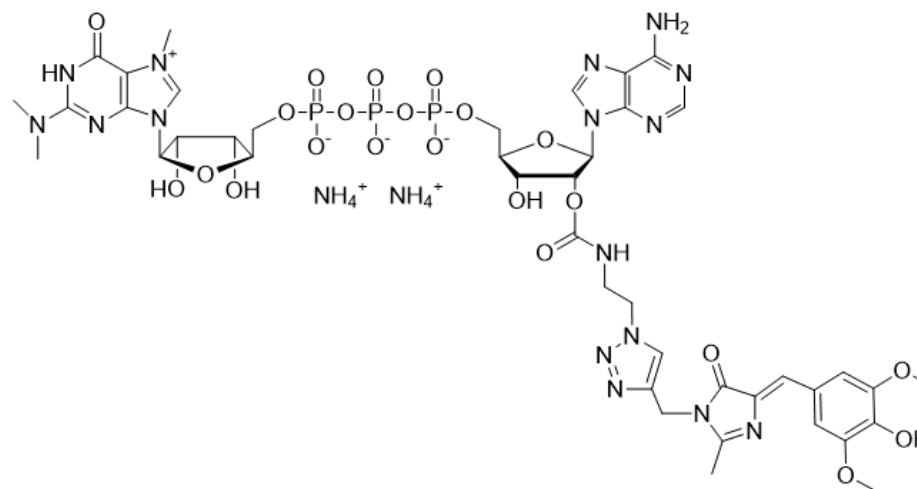
MS (-) ESI (Calc. [M-H]⁻ C₄₄H₅₇N₁₇O₂₀P₃ : 1236.3184, found: 1236.31838)

200812_PSu_04 #4-81 RT: 0.04-0.82 AV: 78 NL: 2.29E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

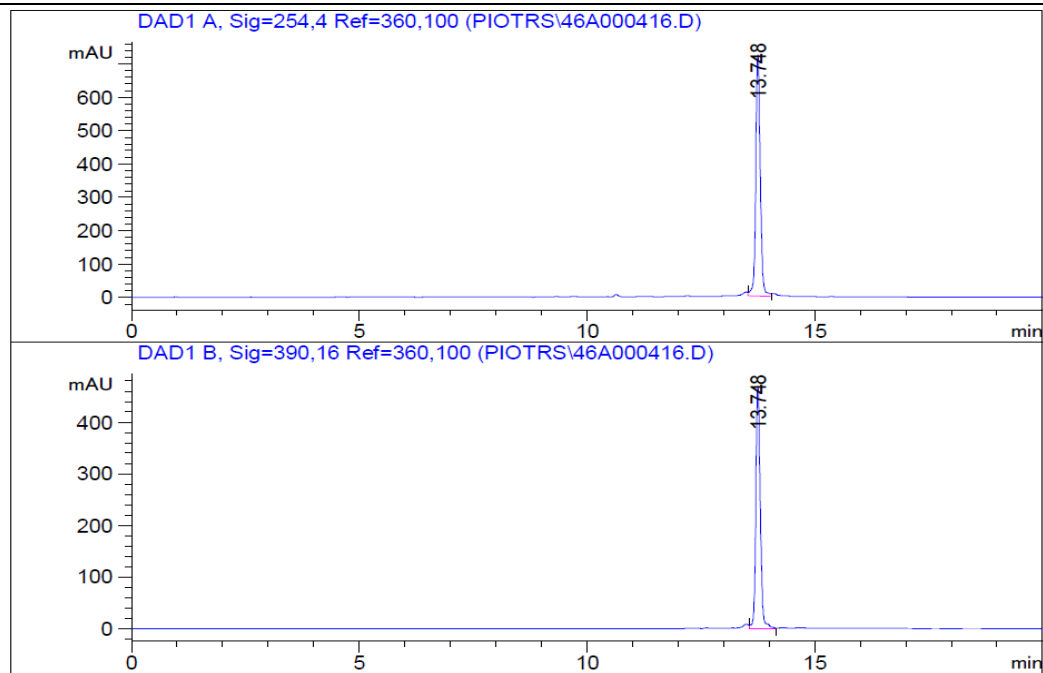


Compound 4a-2': TMGpppA-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

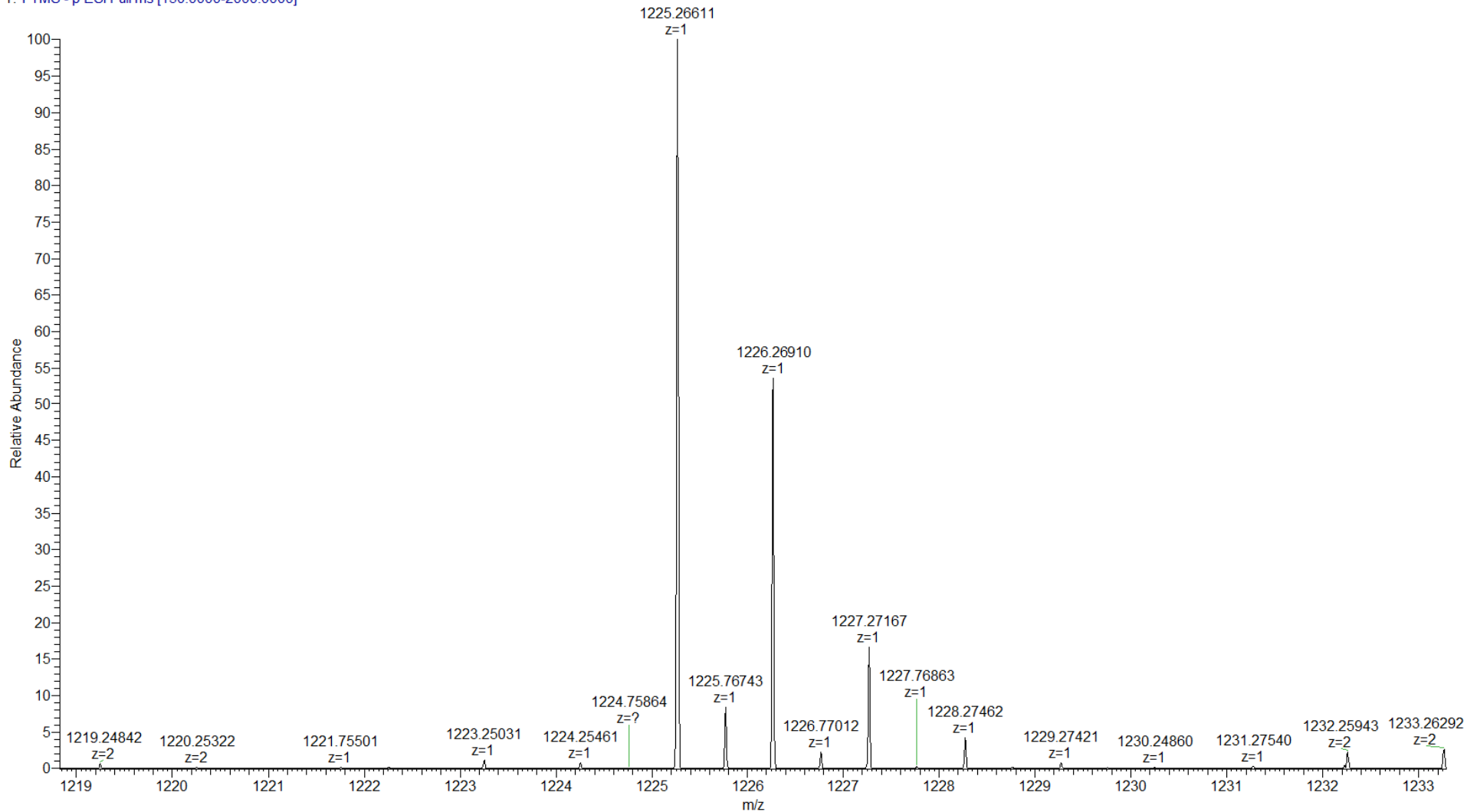


RP-HPLC (conditions c)



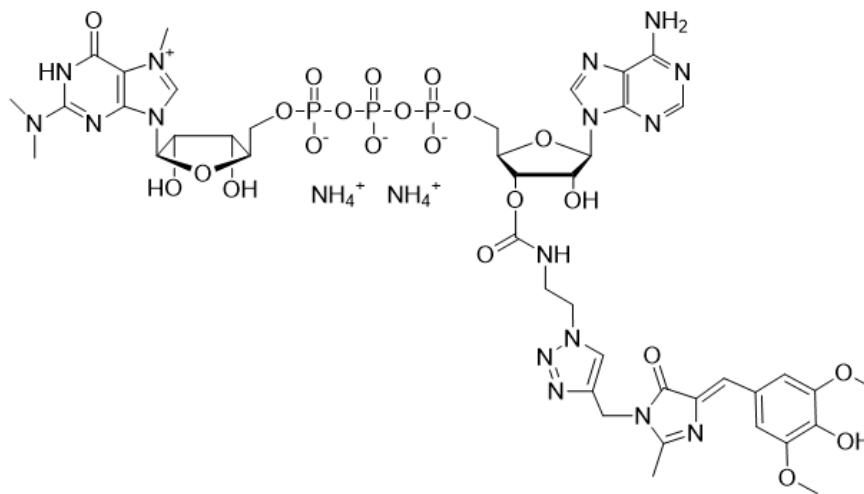
MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₂N₁₆O₂₂P₃ : 1225.2660, found: 1225.26611)

200702_PSU_04 #129-238 RT: 1.24-2.29 AV: 110 NL: 3.89E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

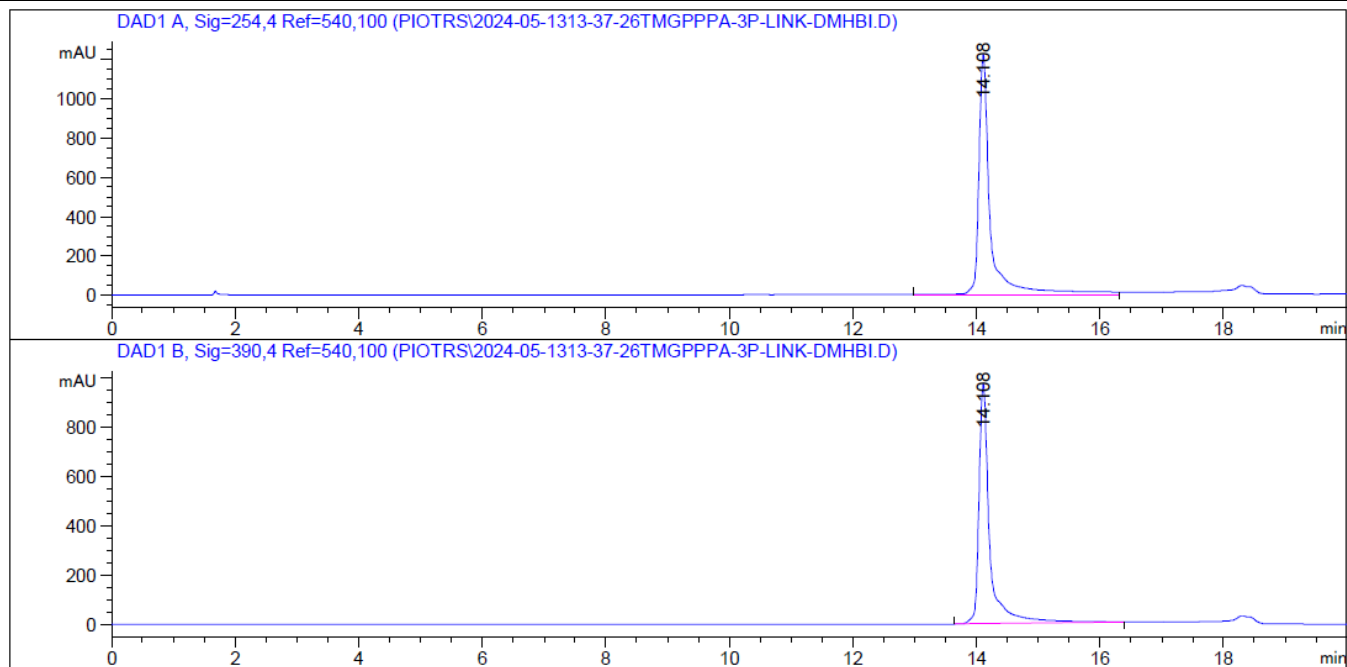


Compound 4a-3': TMGpppA-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

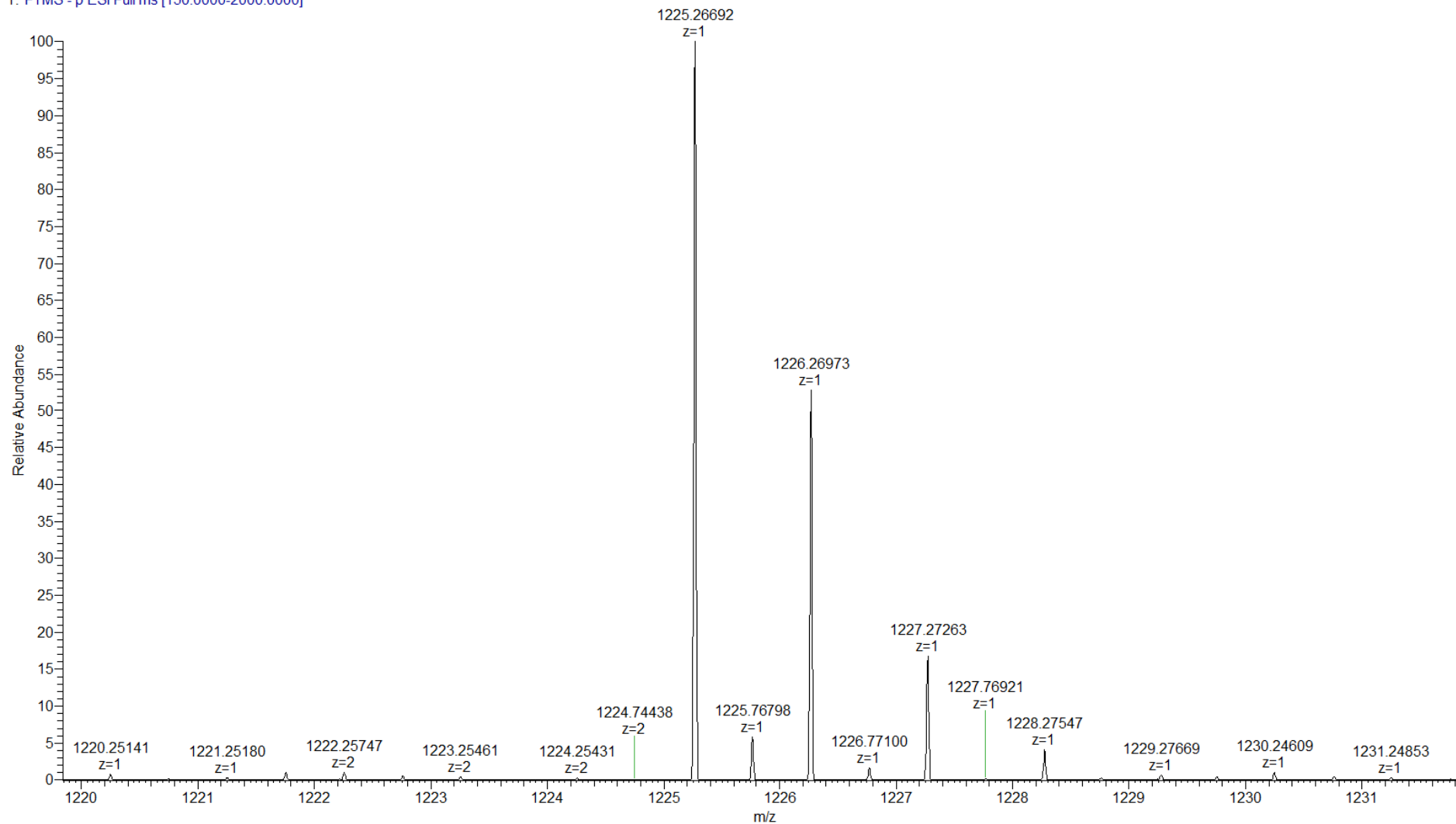


RP-HPLC (conditions c)



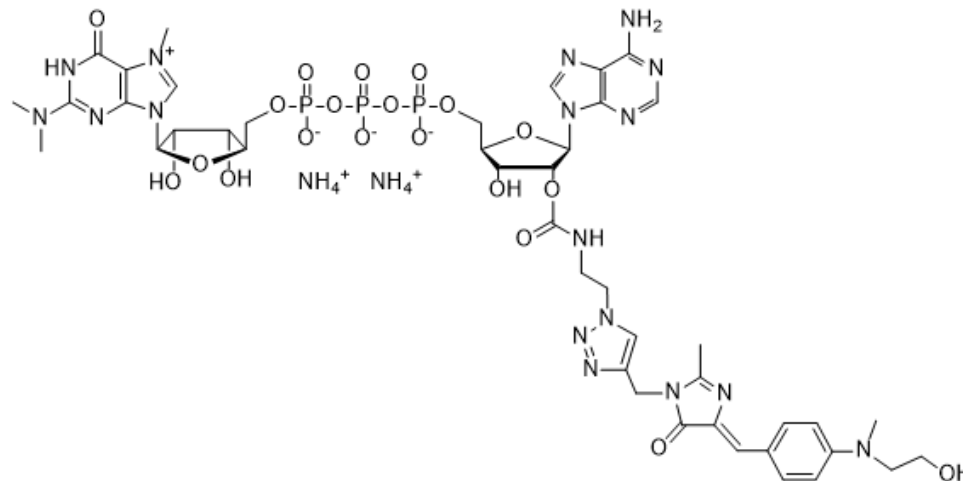
MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₂N₁₆O₂₂P₃ : 1225.2660, found: 1225.26692)

200702_PSU_05 #18-115 RT: 0.17-1.12 AV: 98 NL: 3.05E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

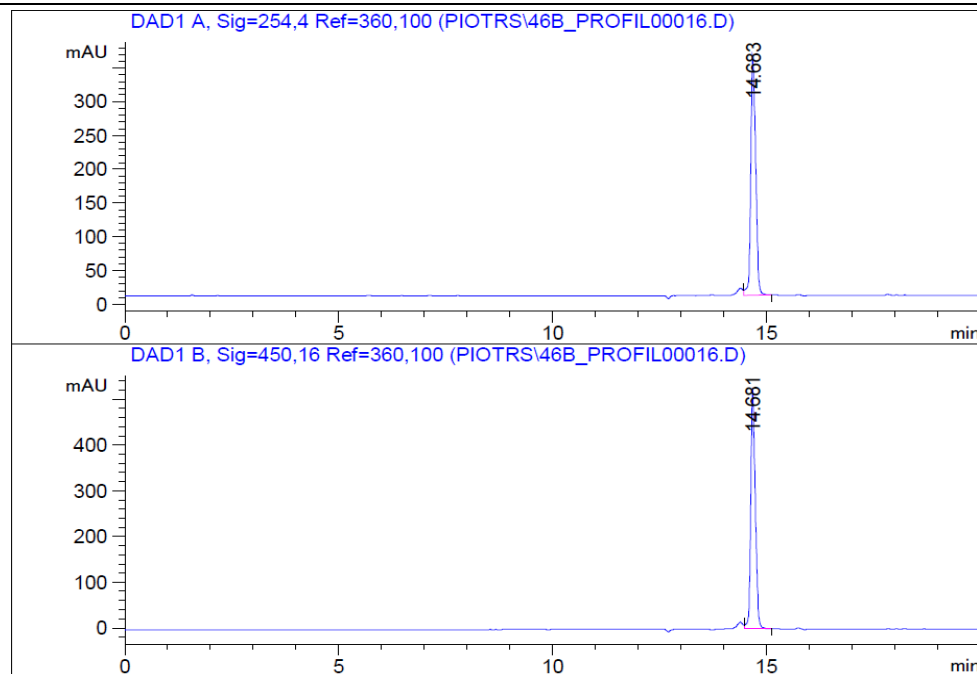


Compound 4c-2': TMGpppA-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

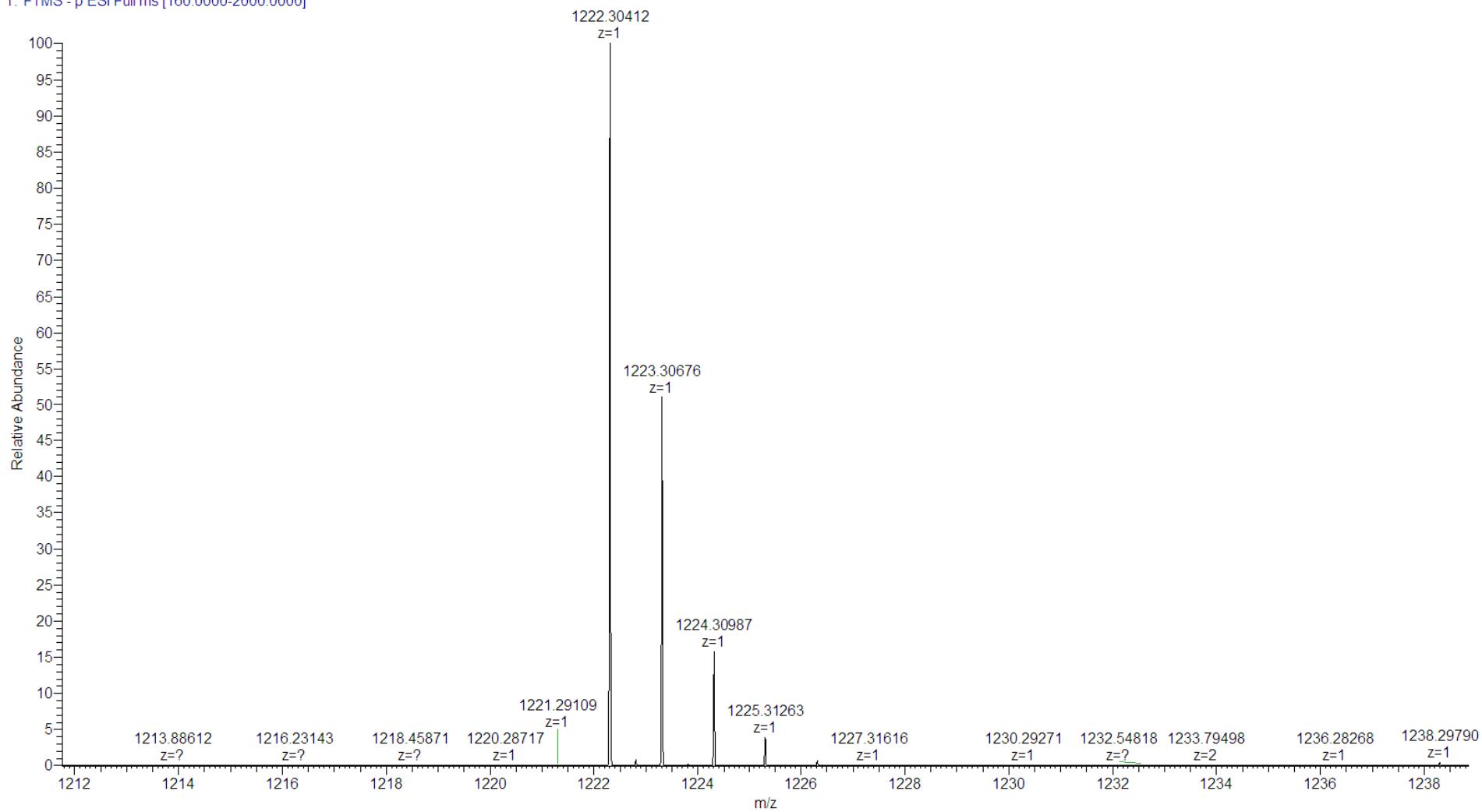


RP-HPLC (conditions c)



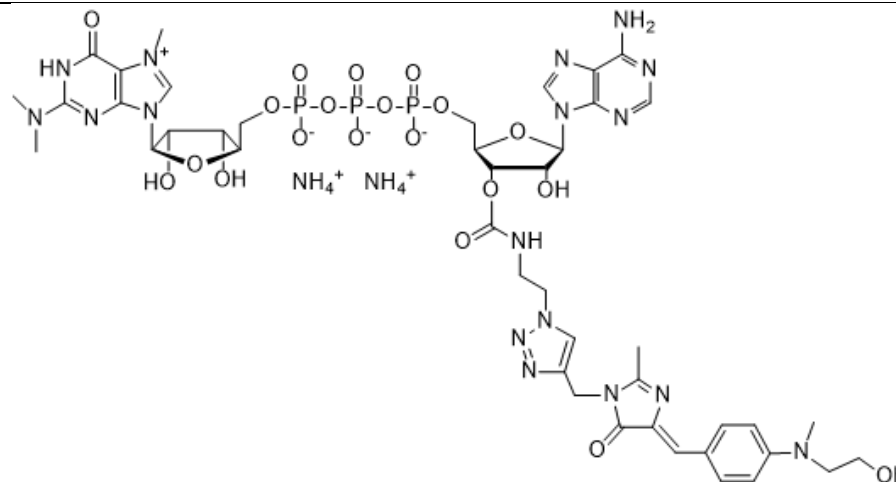
220331_PSu_06 #10-79 RT: 0.09-0.69 AV: 70 NL: 5.13E6
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₃H₅₅N₁₇O₂₀P₃ : 1222.3028, found: 1222.30412)

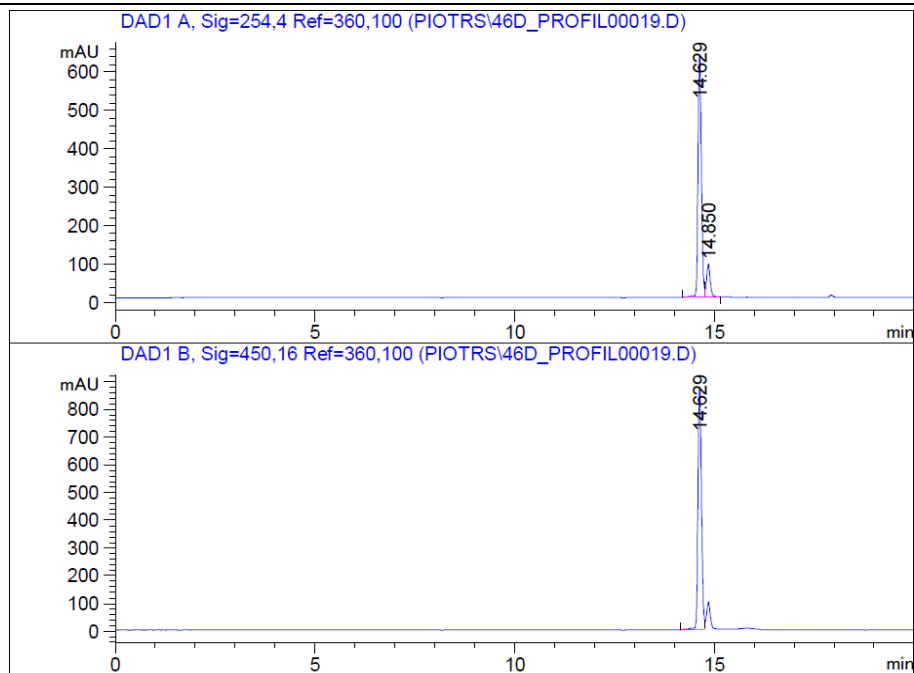


Compound 4c-3': TMGpppA-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

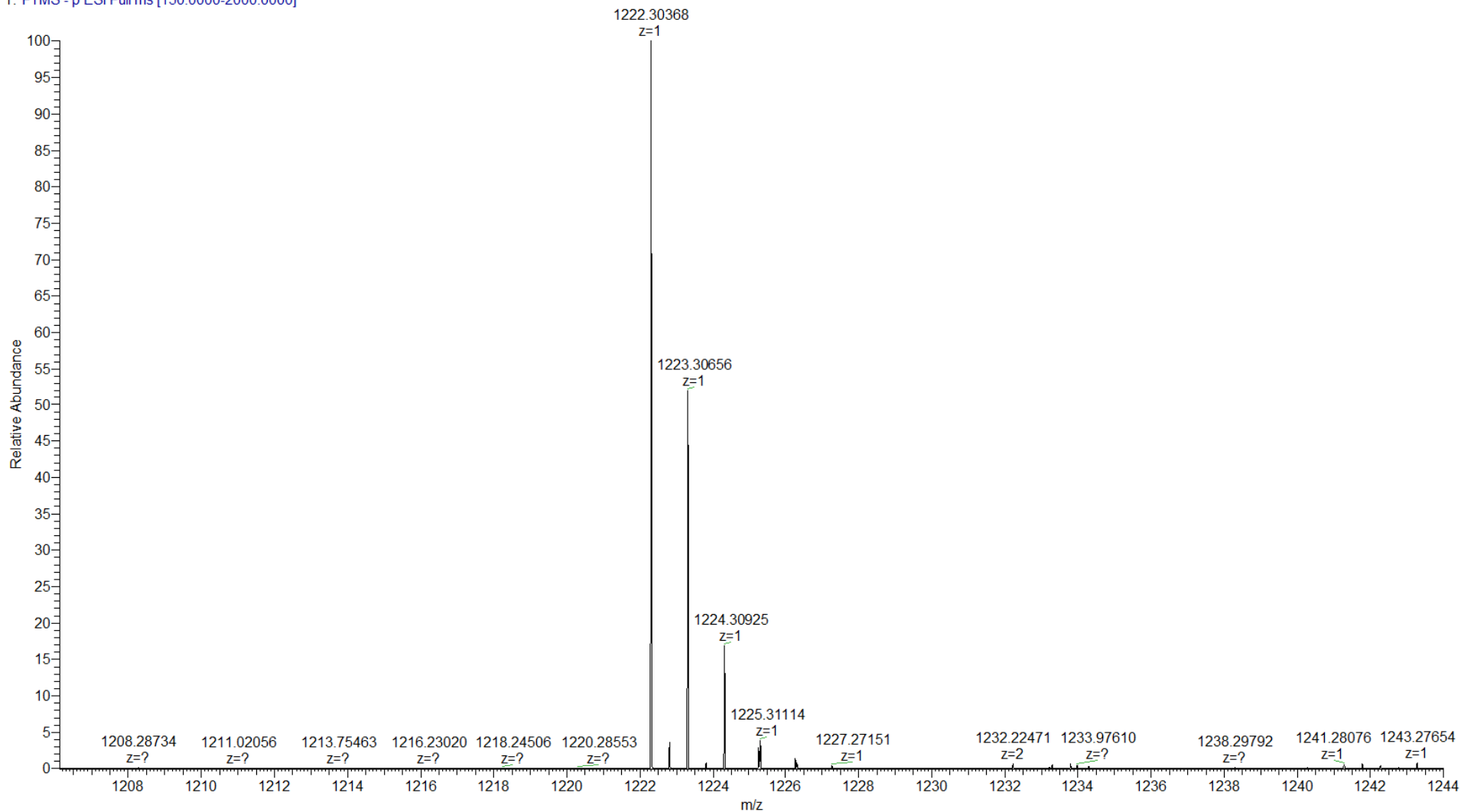


RP-HPLC (conditions c)



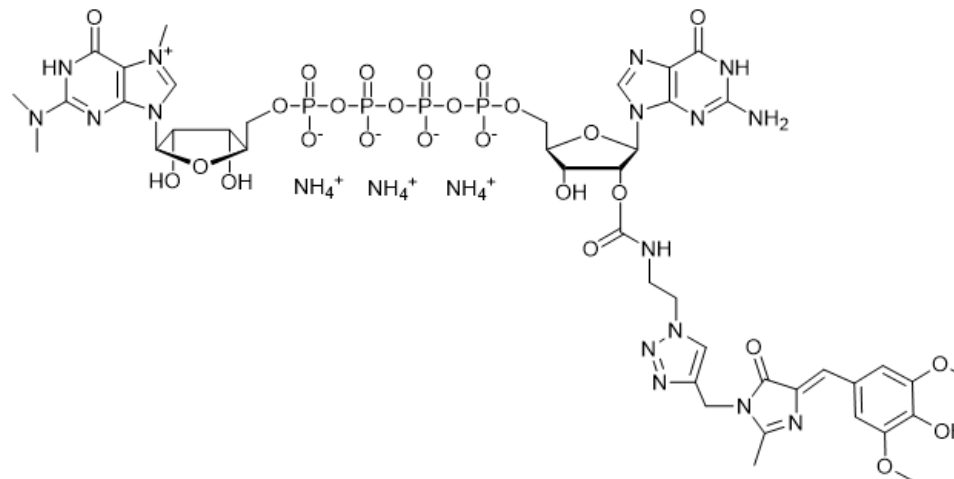
MS (-) ESI (Calc. [M-H]⁻ C₄₃H₅₅N₁₇O₂₀P₃ : 1222.3028, found: 1222.30368)

200702_PSU_06 #15-89 RT: 0.15-0.88 AV: 75 NL: 1.45E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

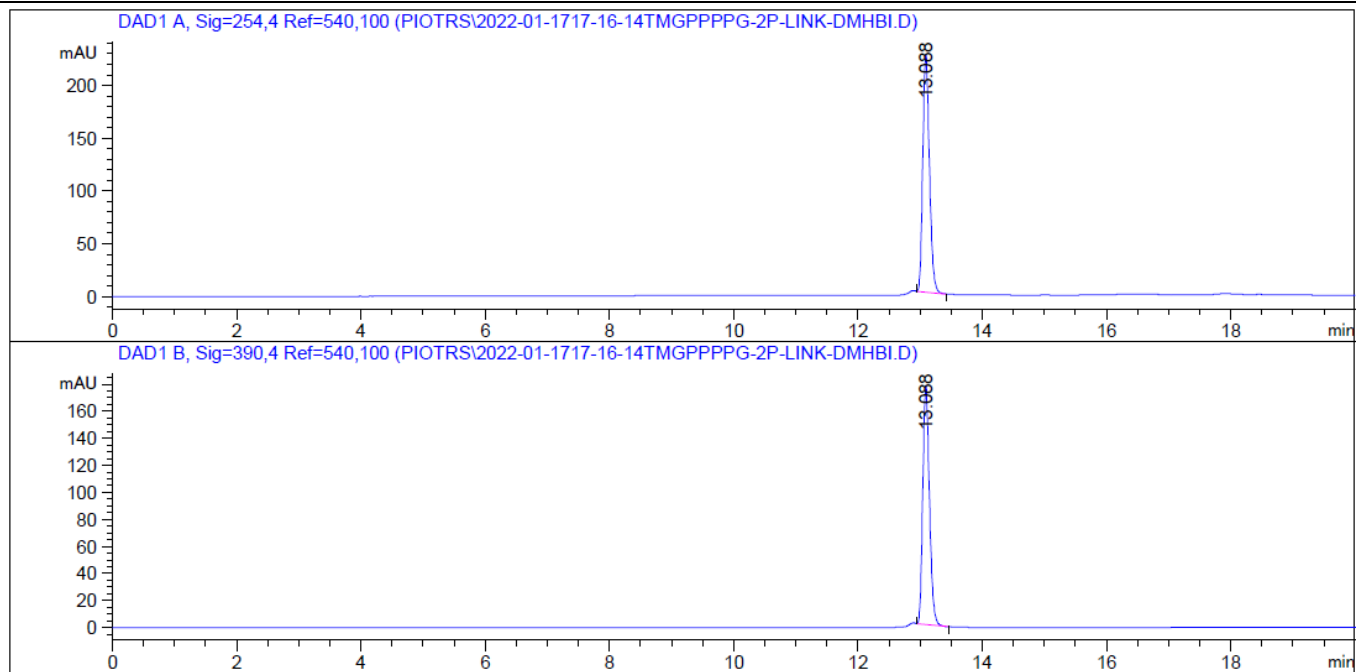


Compound 5a-2': TMGppppG-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

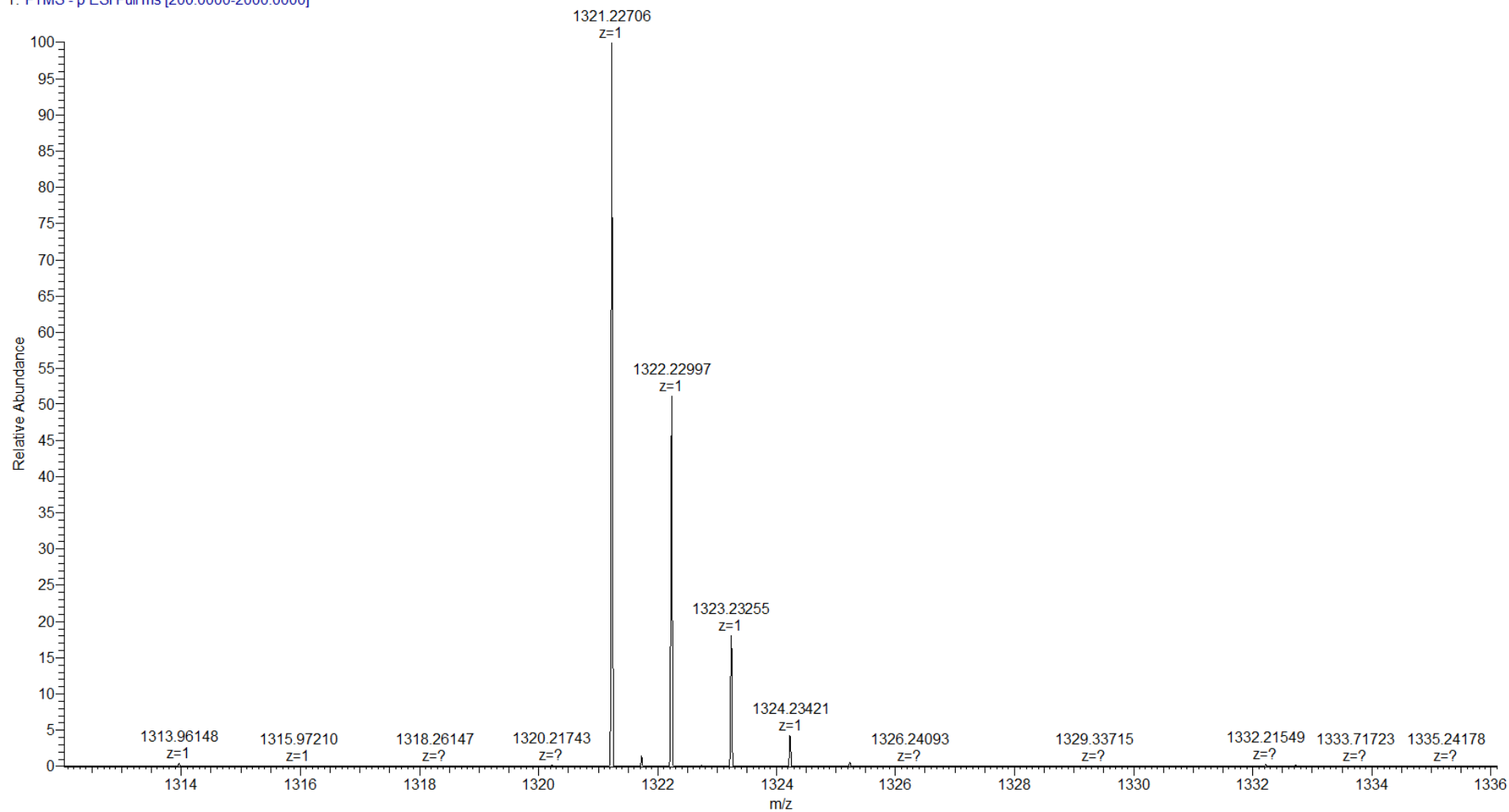


RP-HPLC (conditions c)



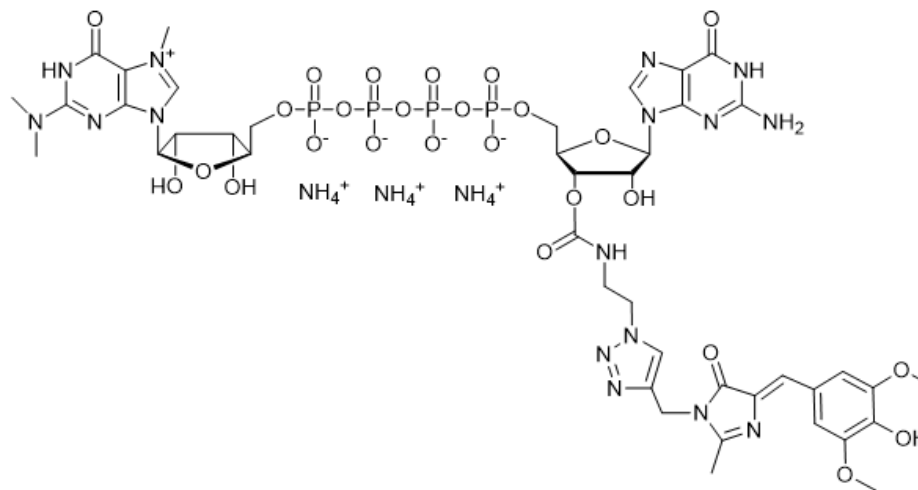
220114_PSU_10 #9-215 RT: 0.08-1.88 AV: 207 NL: 8.49E5
T: FTMS - p ESI Full ms [200.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₃N₁₆O₂₆P₄ : 1321.2273, found : 1321.22706)

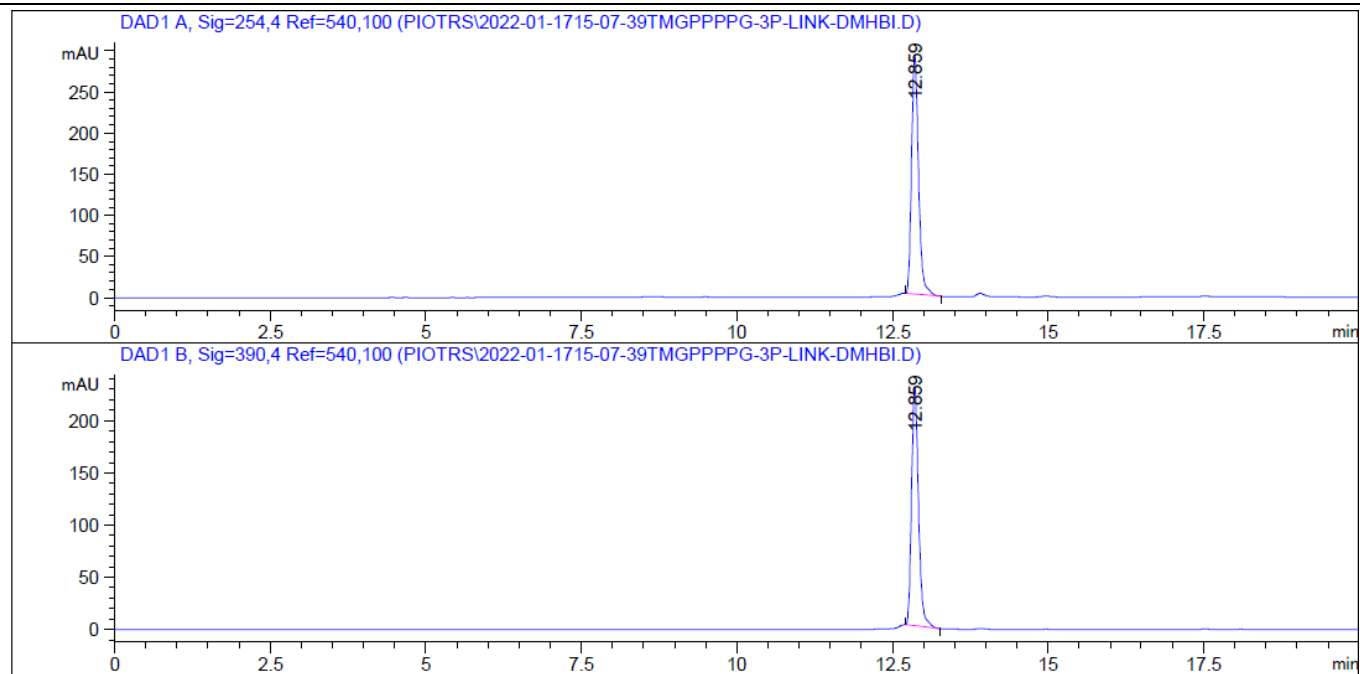


Compound 5a-3': TMGppppG-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

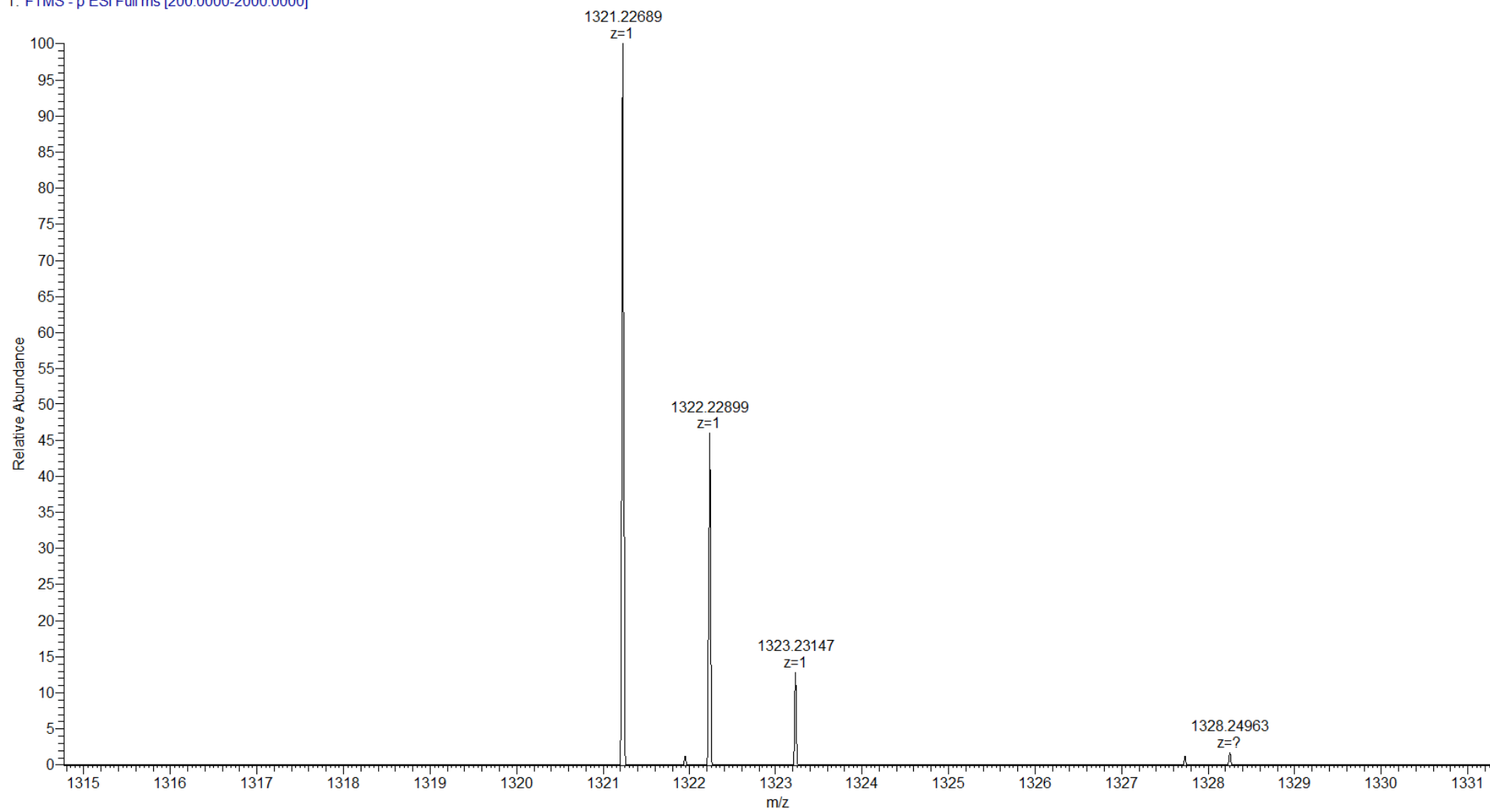


RP-HPLC (conditions c)



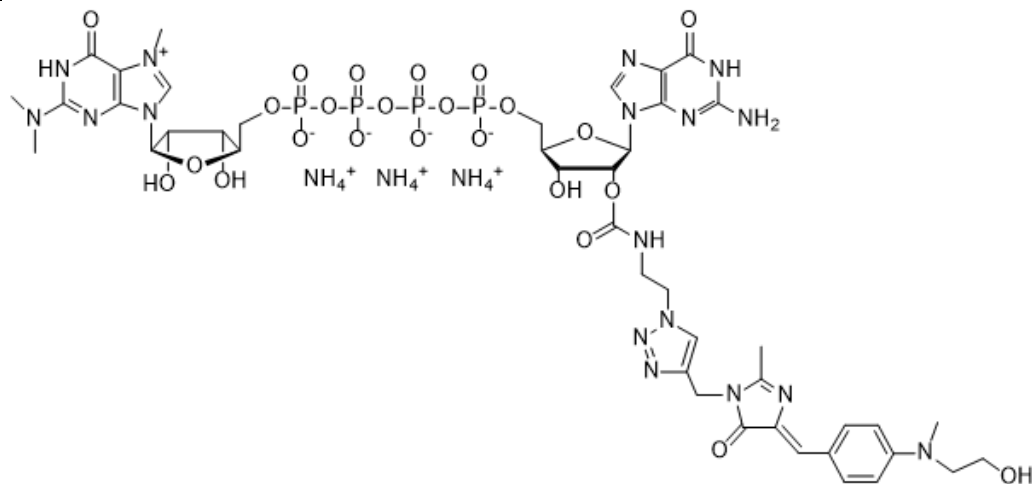
220114_PSU_11 #6-36 RT: 0.05-0.31 AV: 31 NL: 9.80E4
T: FTMS - p ESI Full ms [200.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₃N₁₆O₂₆P₄ : 1321.2273, found : 1321.22689)

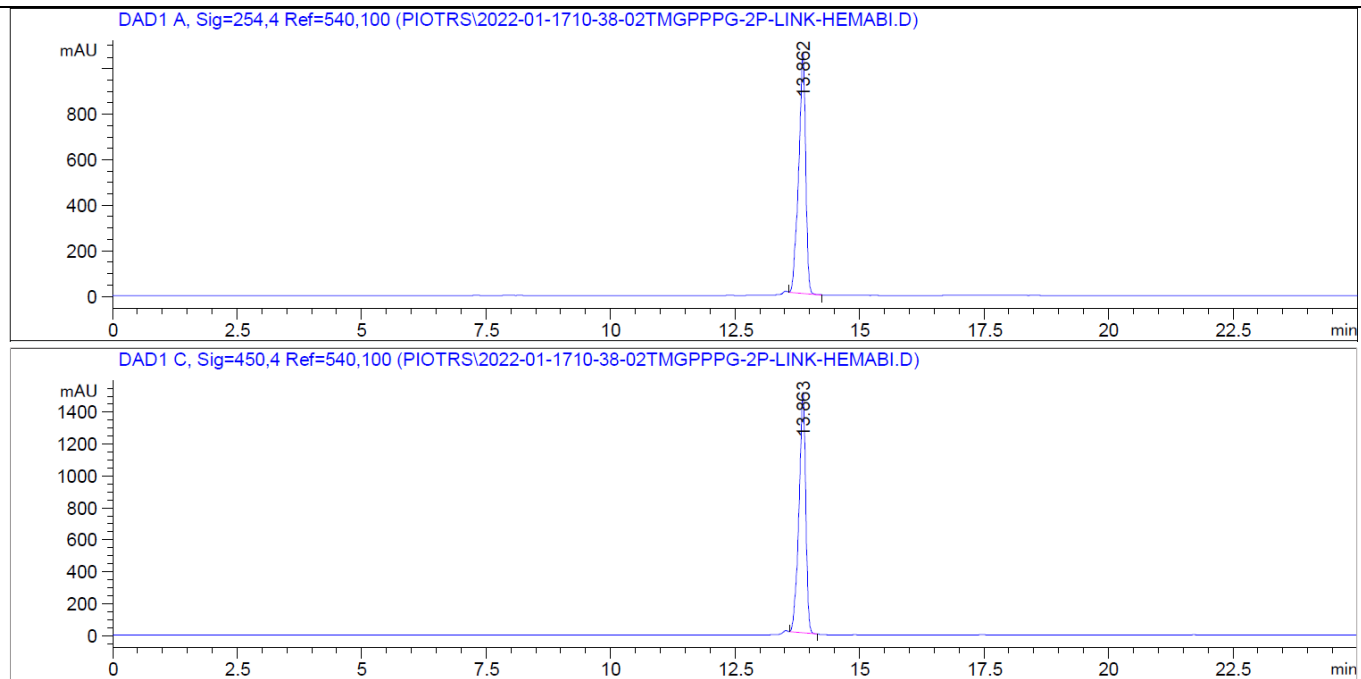


Compound 5c-2': TMGppppG-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

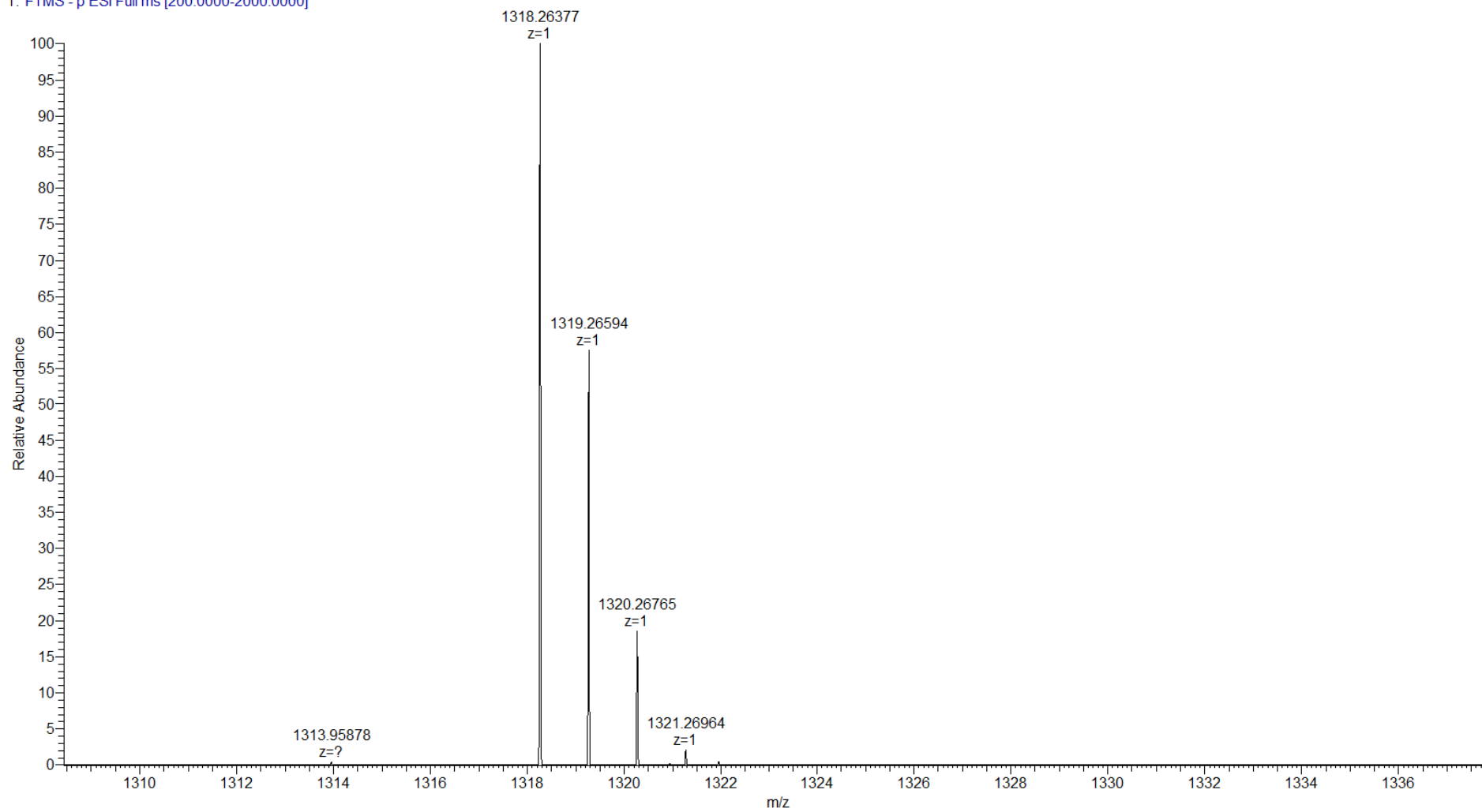


RP-HPLC (conditions c)



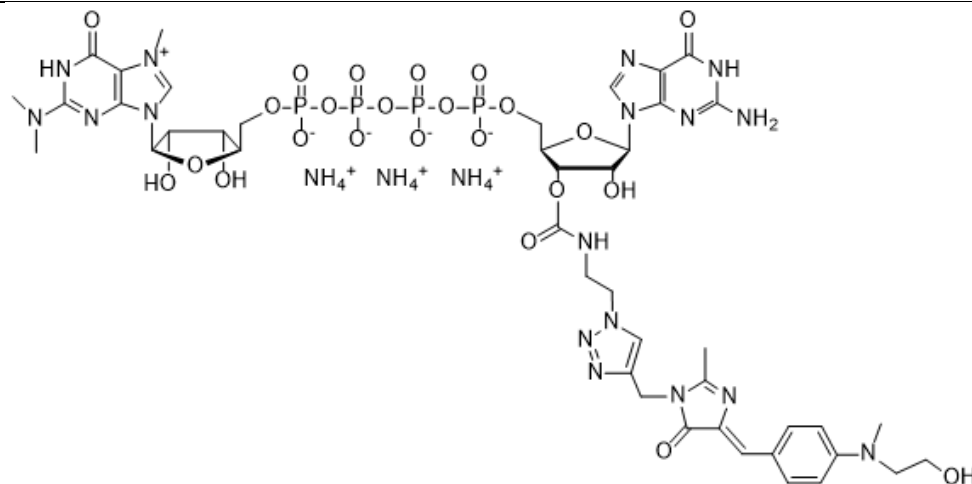
220114_PSU_08 #6-40 RT: 0.05-0.35 AV: 35 NL: 7.11E5
T: FTMS - p ESI Full ms [200.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₃H₅₆N₁₇O₂₄P₄ : 1318.2640, found : 1318.26377)

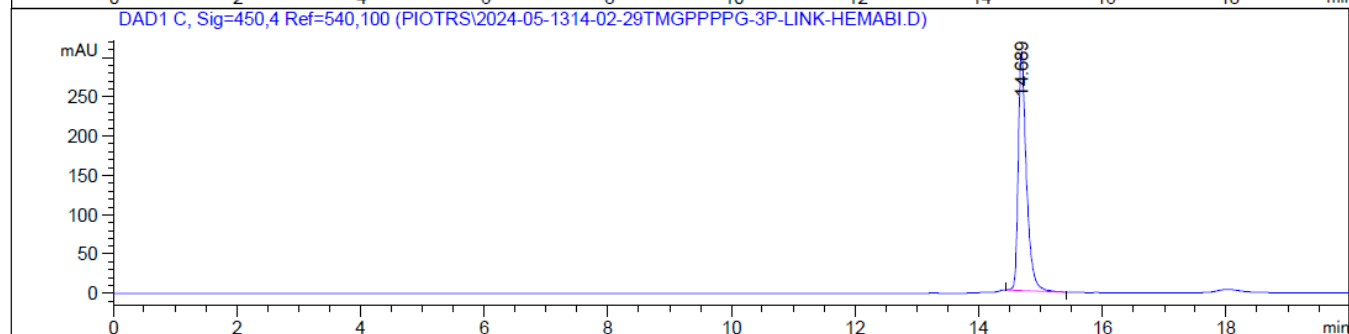
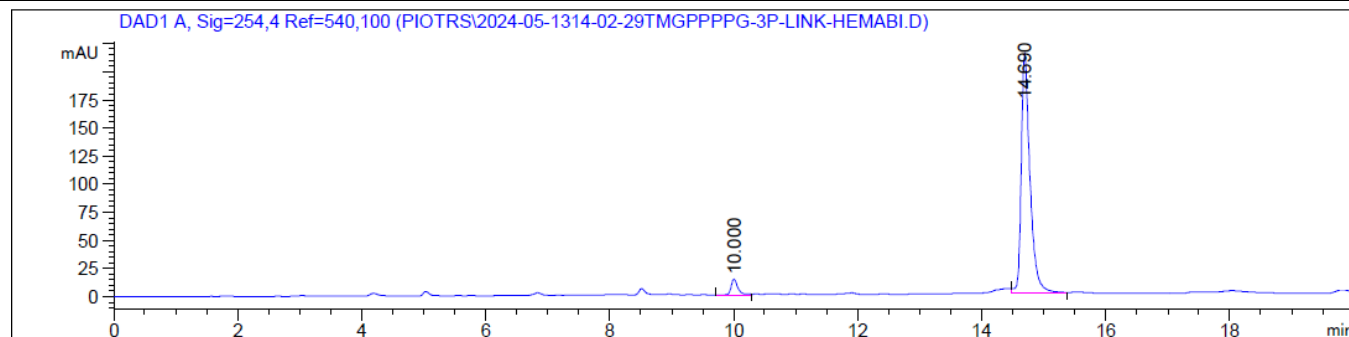


Compound 5c-3': TMGppppG-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

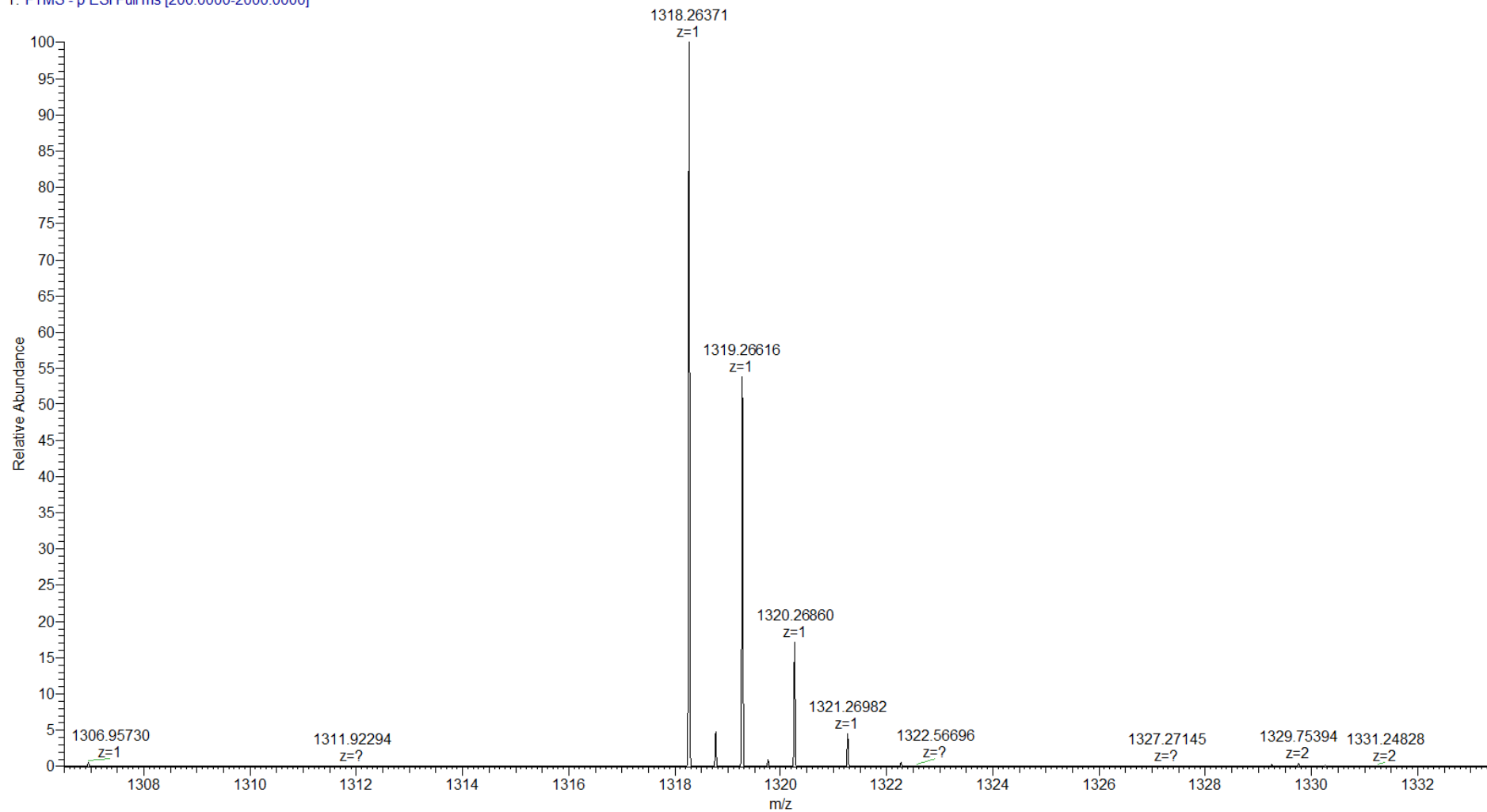


RP-HPLC (conditions c)



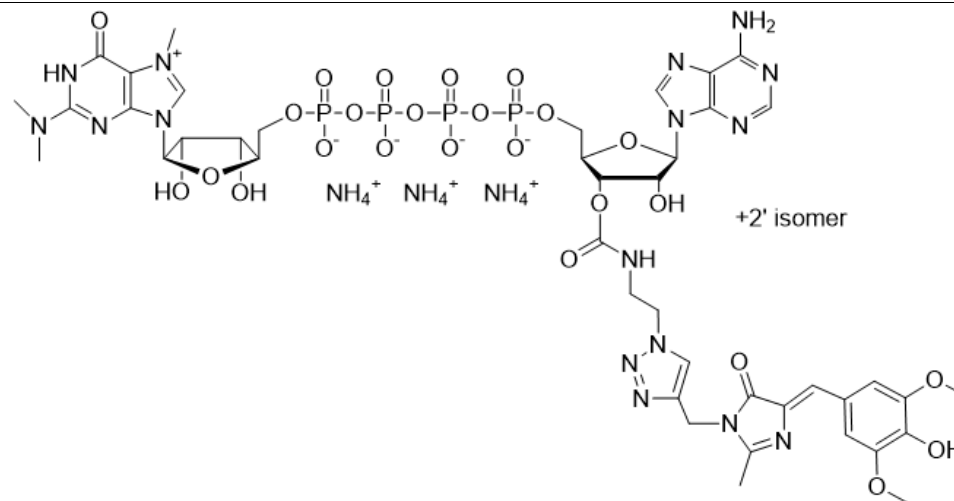
220114_PSU_09 #156-246 RT: 1.36-2.15 AV: 91 NL: 1.10E6
T: FTMS - p ESI Full ms [200.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₃H₅₆N₁₇O₂₄P₄ : 1318.2640, found : 1318.26371)

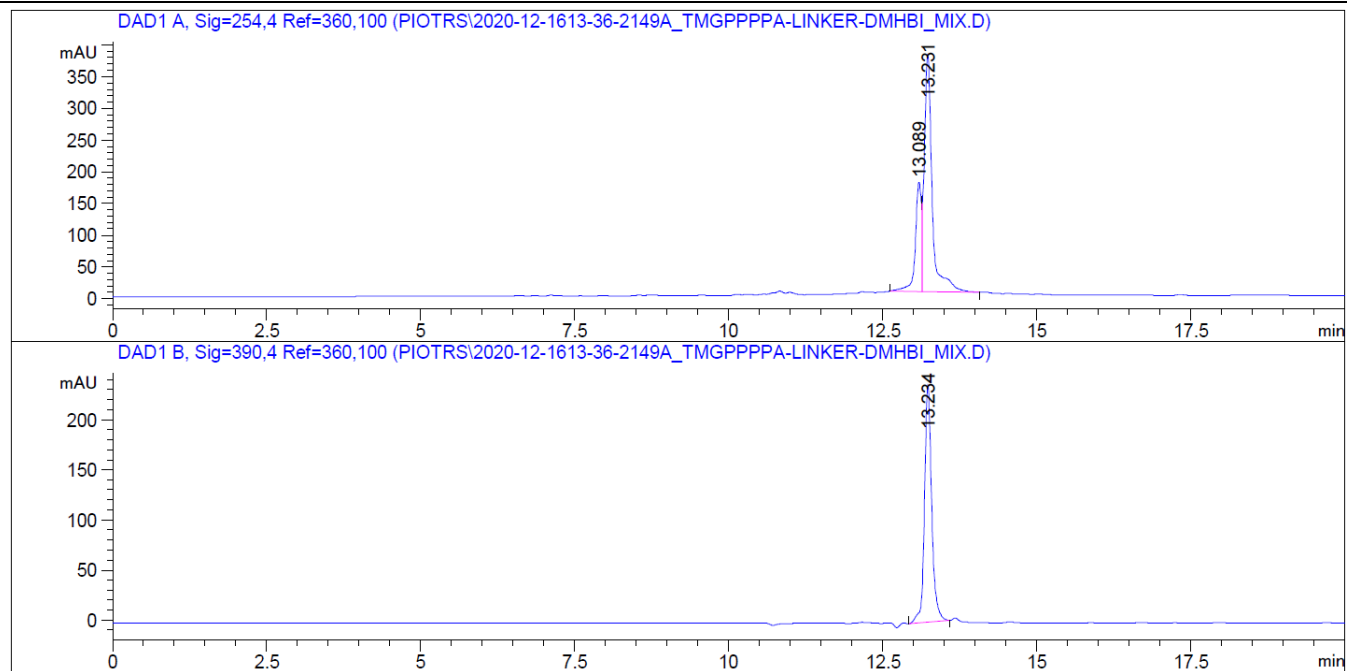


Compound 6a: TMGppppA-2'+3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

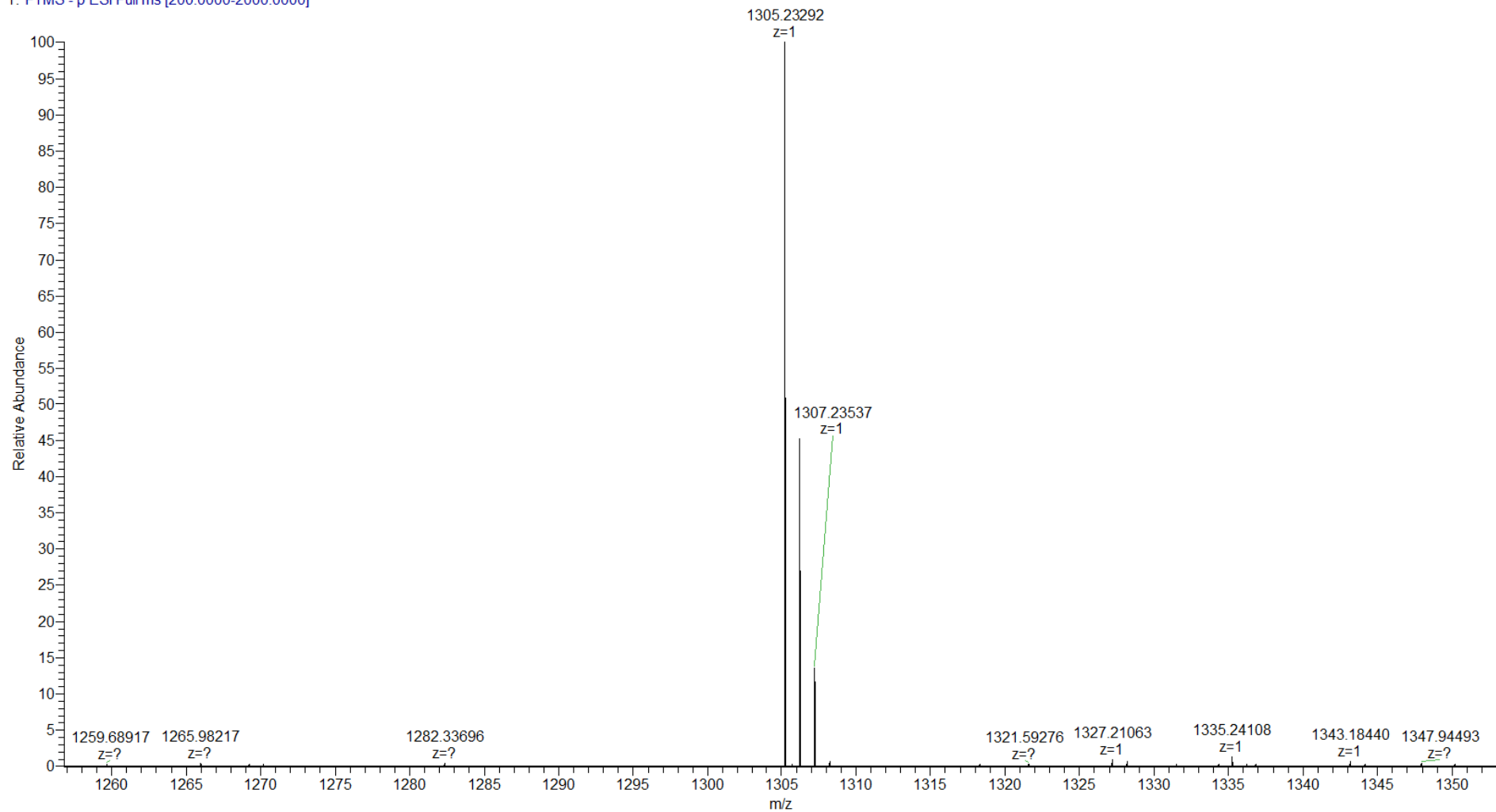


RP-HPLC (conditions c)



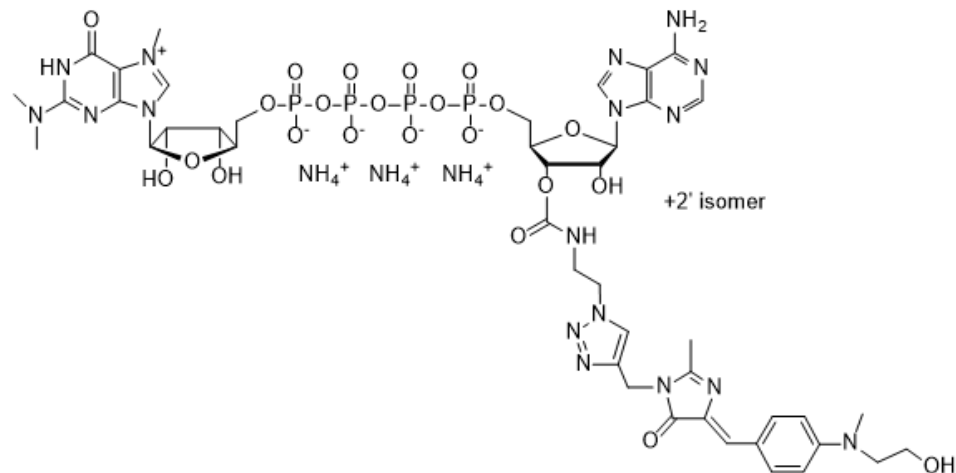
220114_PSU_18b #26-79 RT: 0.23-0.70 AV: 54 NL: 3.61E5
T: FTMS - p ESI Full ms [200.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₃N₁₆O₂₅P₄; 1305.2330, found: 1305.23292)

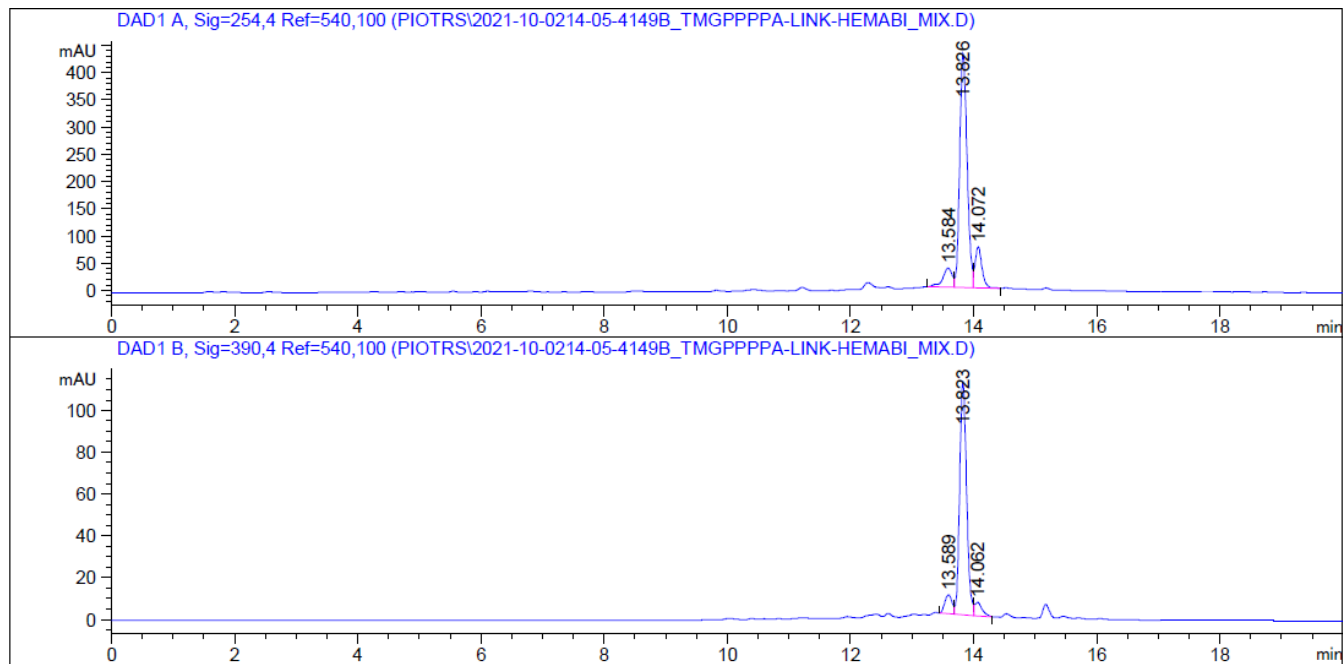


Compound 6c: TMGppppA-2'+3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

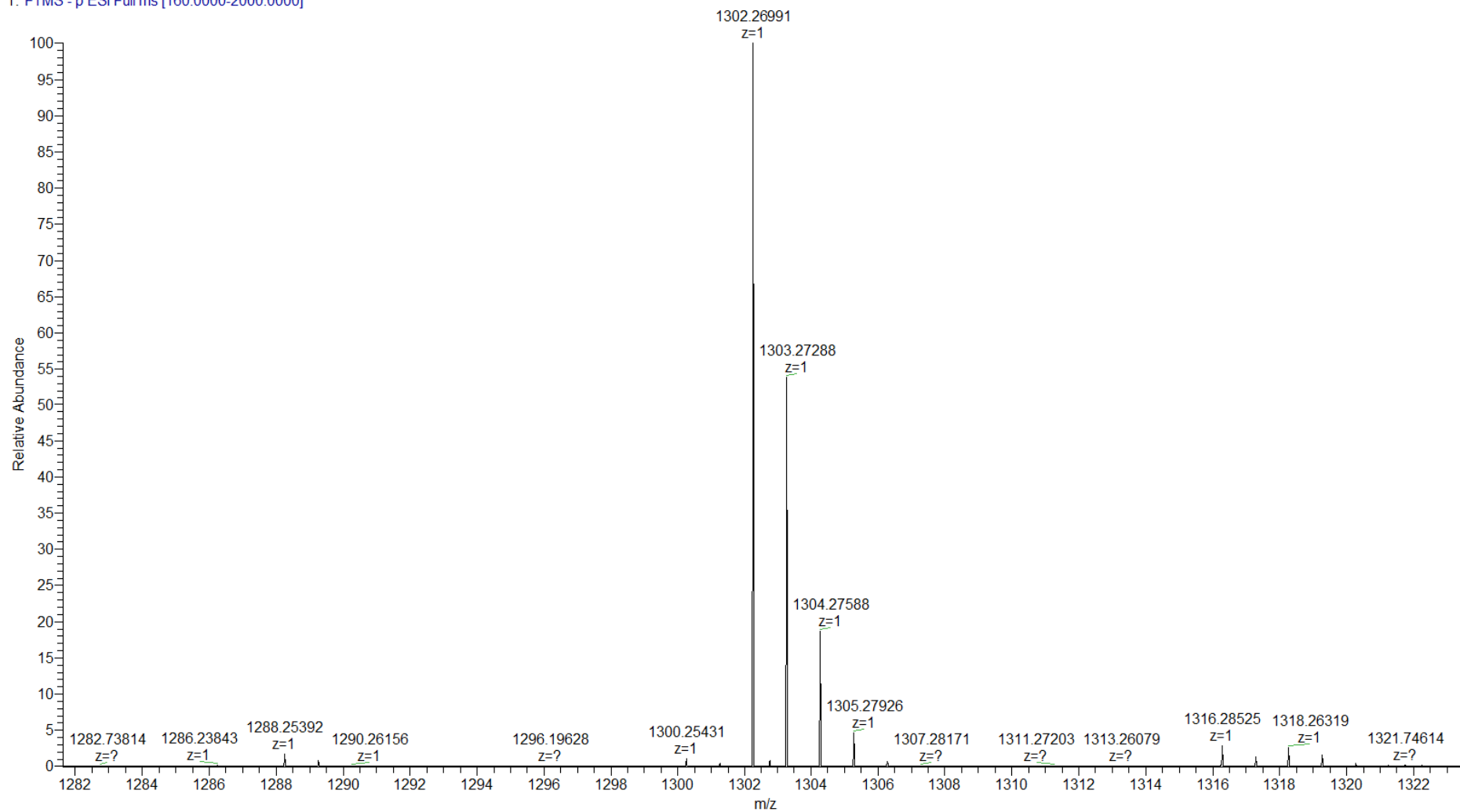


RP-HPLC (conditions c)



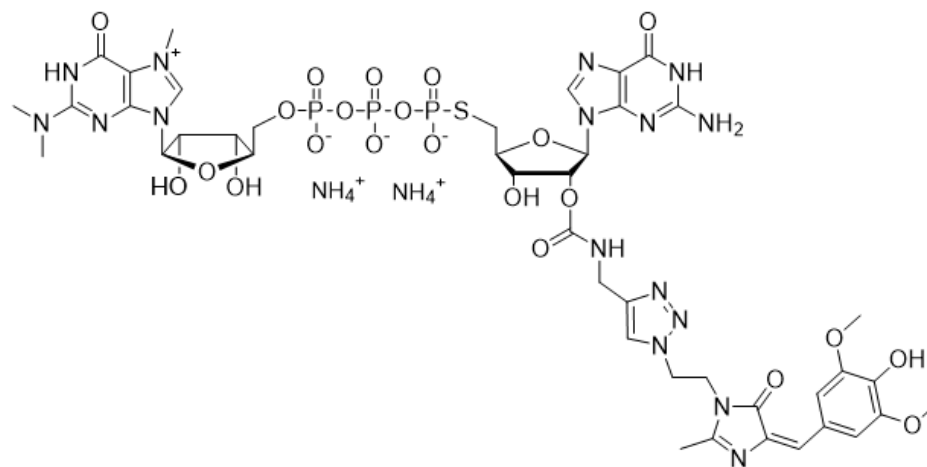
220214_PSu_49c #101-174 RT: 0.89-1.53 AV: 74 NL: 1.49E6
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₃H₅₆N₁₇O₂₃P₄ : 1302.2691, found: 1302.26991)

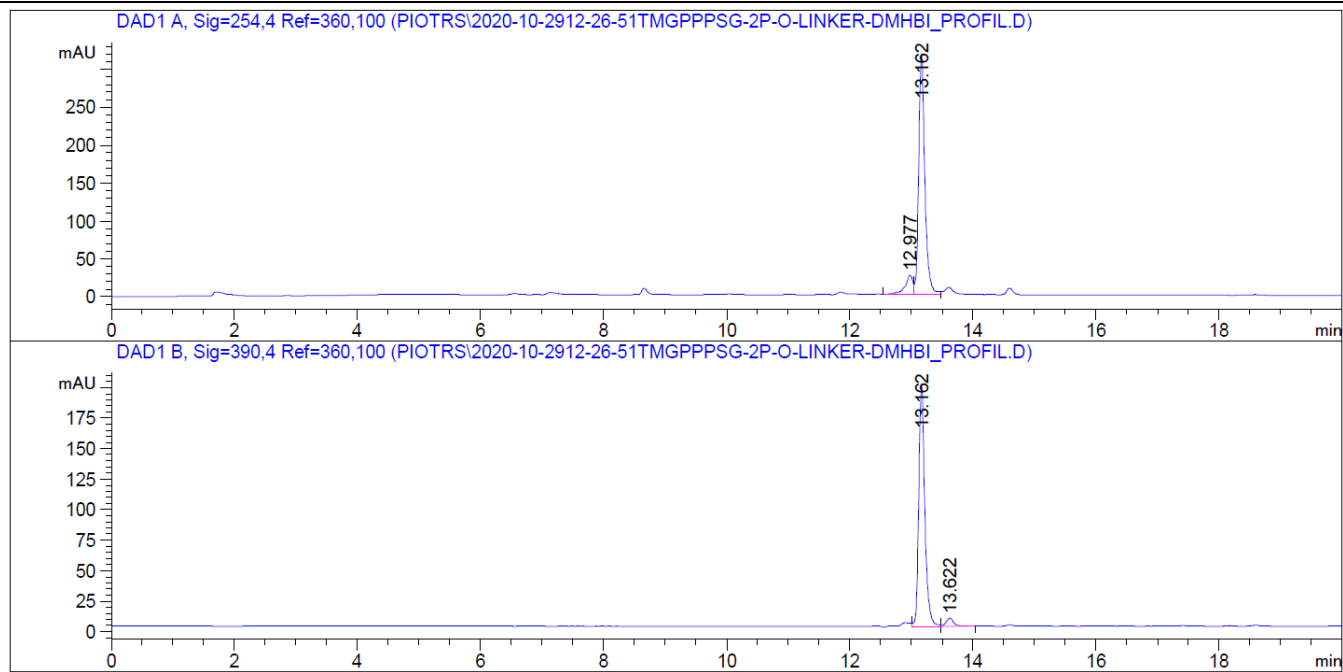


Compound 7a-2': TMGppp-5'-SG-2'-O-C(O)-NH-CH₂-triazole-CH₂CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

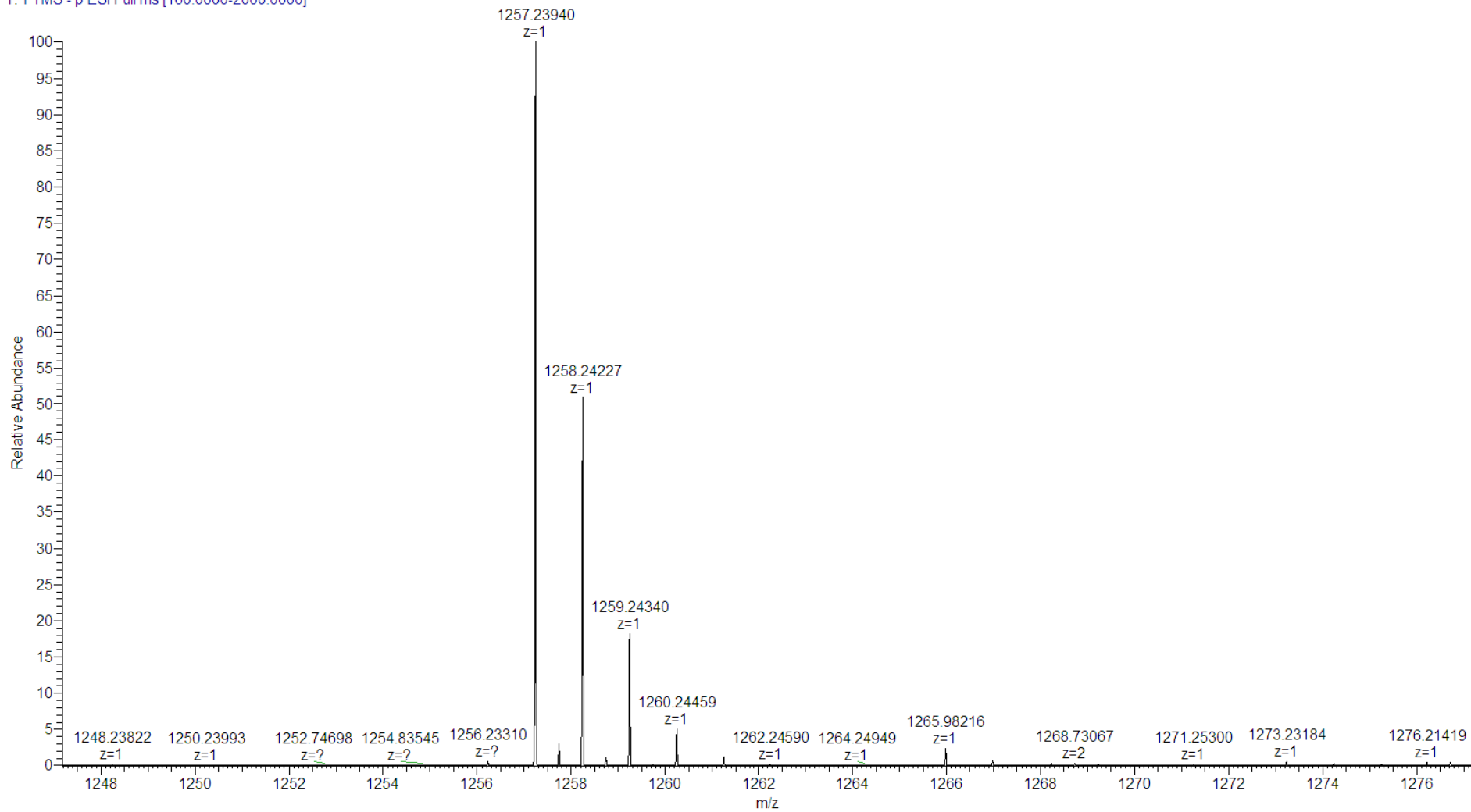


RP-HPLC (conditions c)



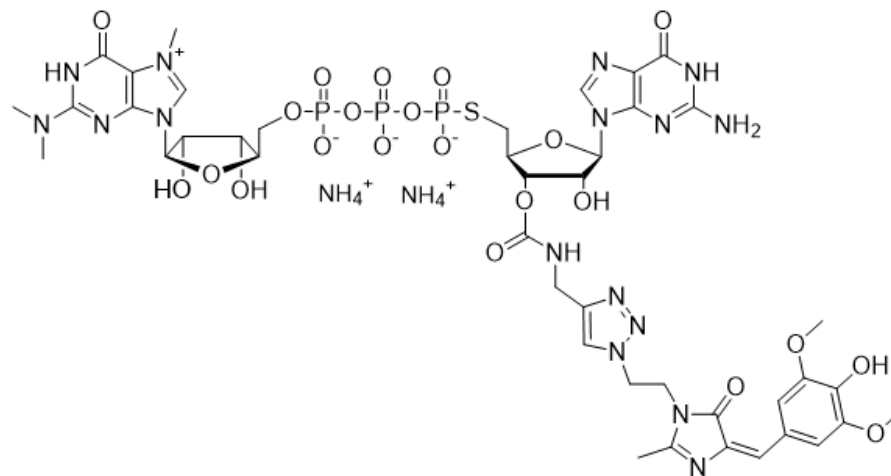
220331_PSu_07 #198-251 RT: 1.73-2.19 AV: 54 NL: 1.12E7
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₂N₁₆O₂₂P₃S⁻ : 1257.23811, found: 1257.23940)

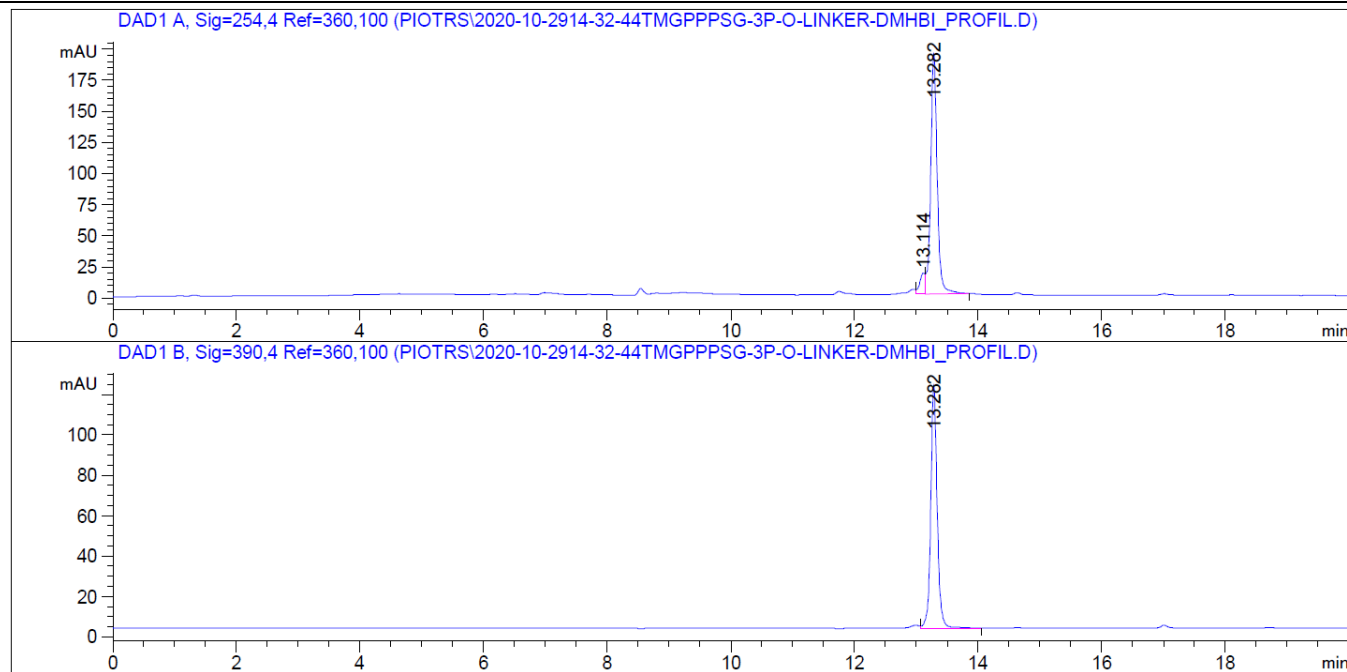


Compound 7a-3': TMGppp-5'-SG-3'-O-C(O)-NH-CH₂-triazole-CH₂CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

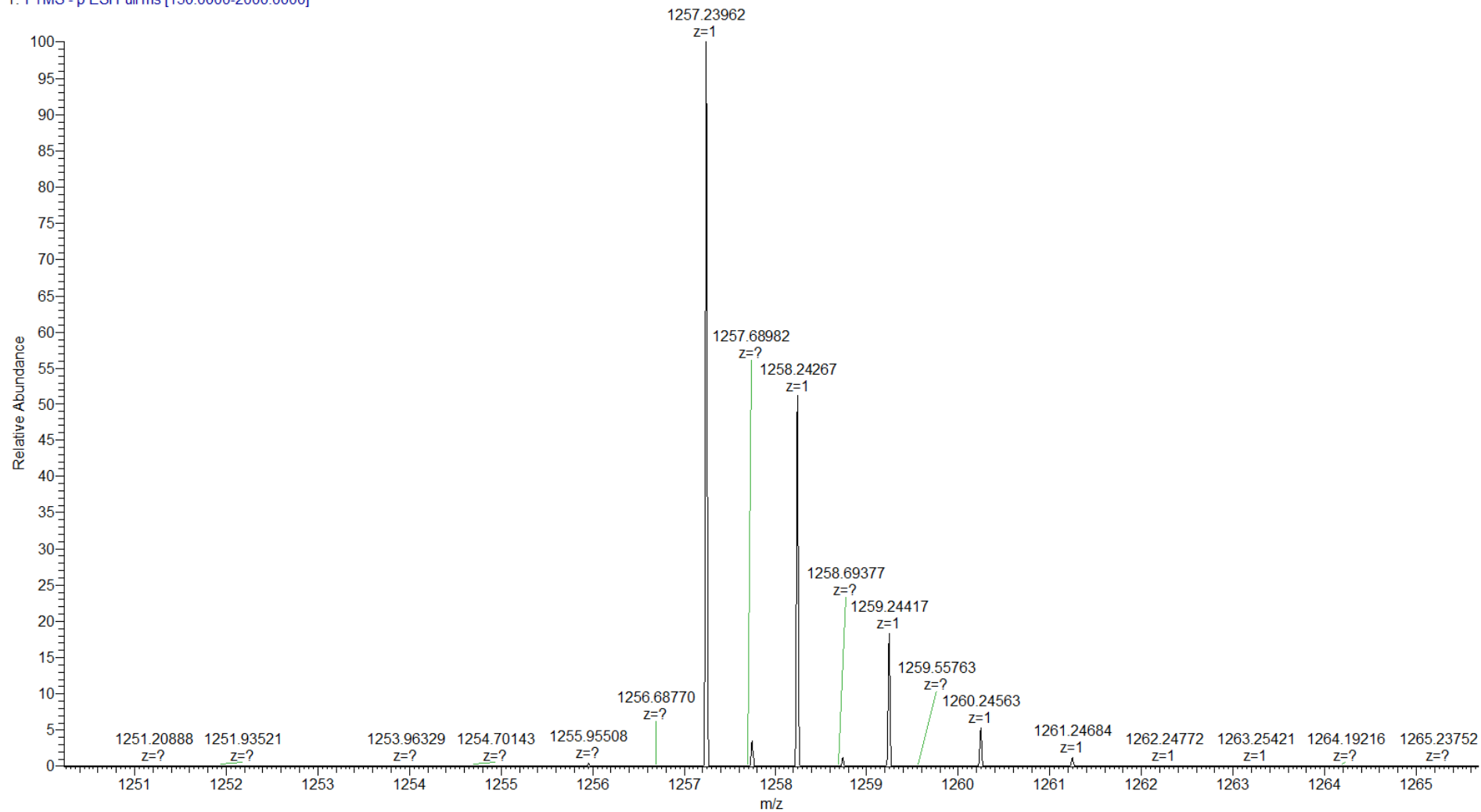


RP-HPLC (conditions c)



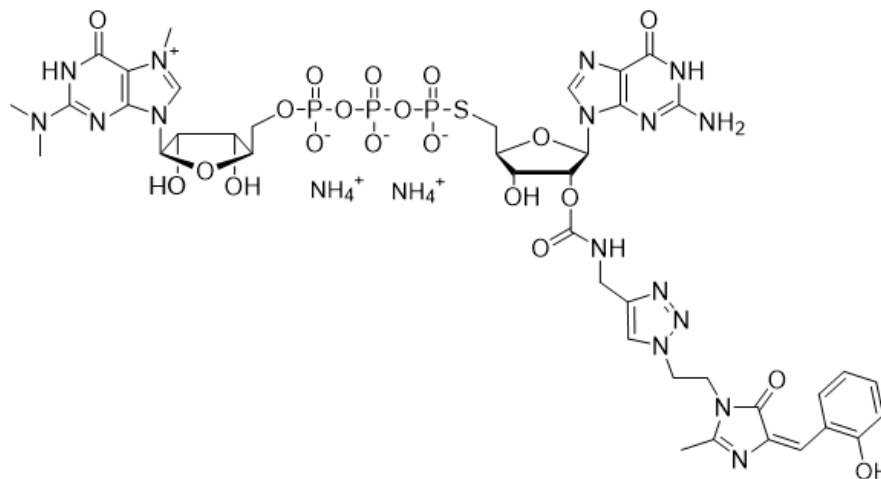
201119_PSu_05 #57-194 RT: 0.58-1.93 AV: 138 NL: 1.39E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₂N₁₆O₂₂P₃S⁻ : 1257.23811, found: 1257.23962)

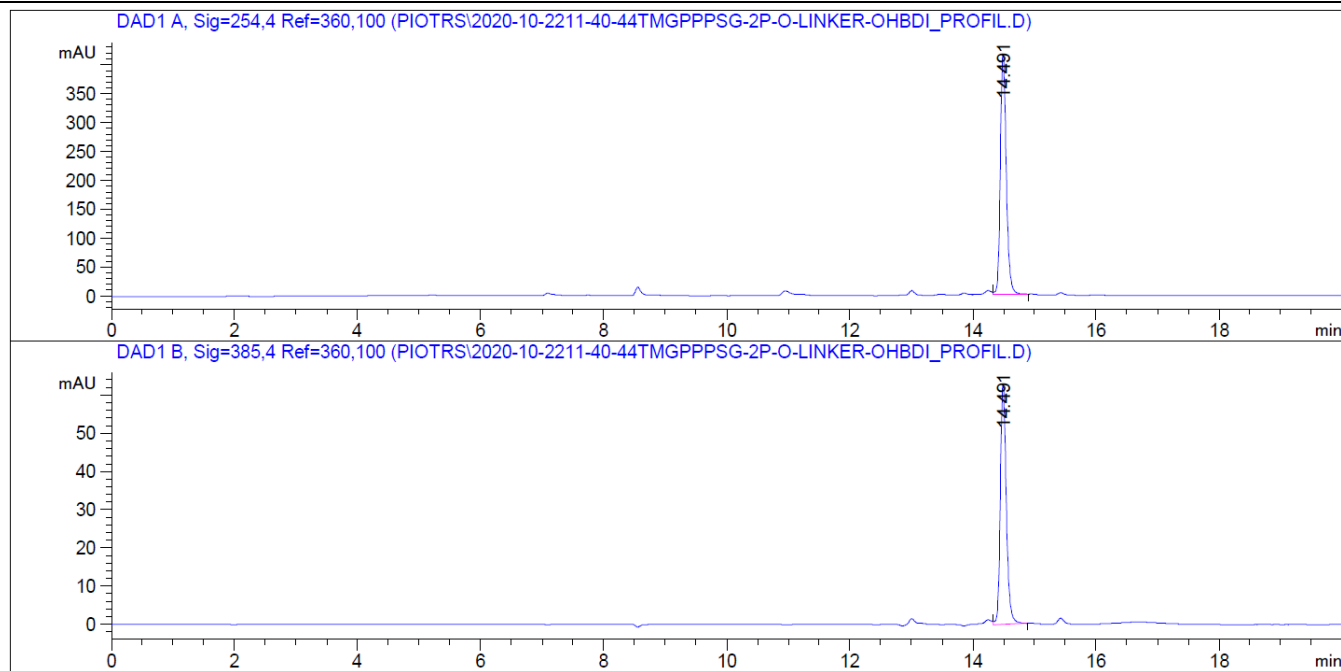


Compound 7b-2': TMGppp-5'-SG-2'-O-C(O)-NH-CH₂-triazole-CH₂CH₂-oHBI (NH₄⁺ salt)

Chemical structure

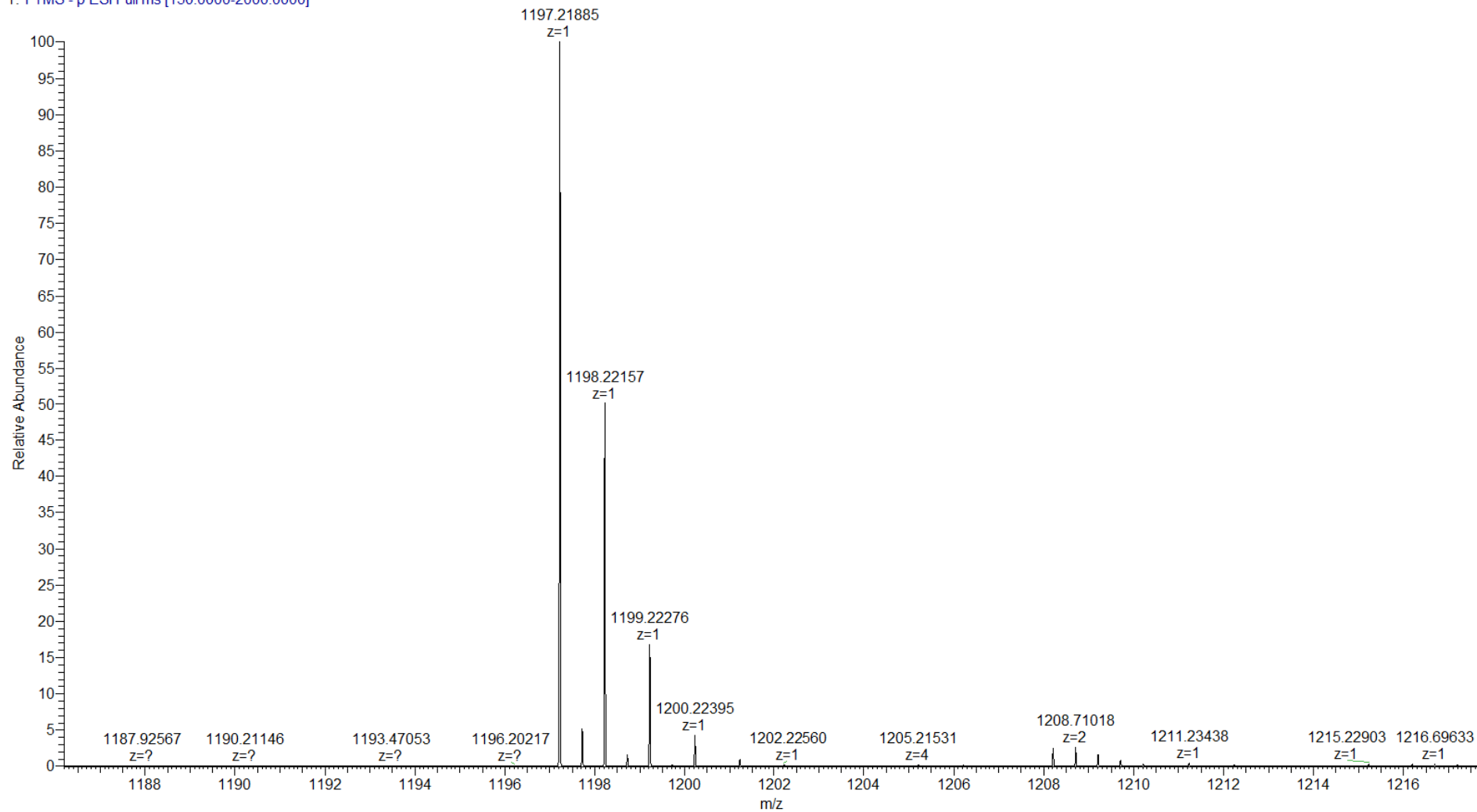


RP-HPLC (conditions c)



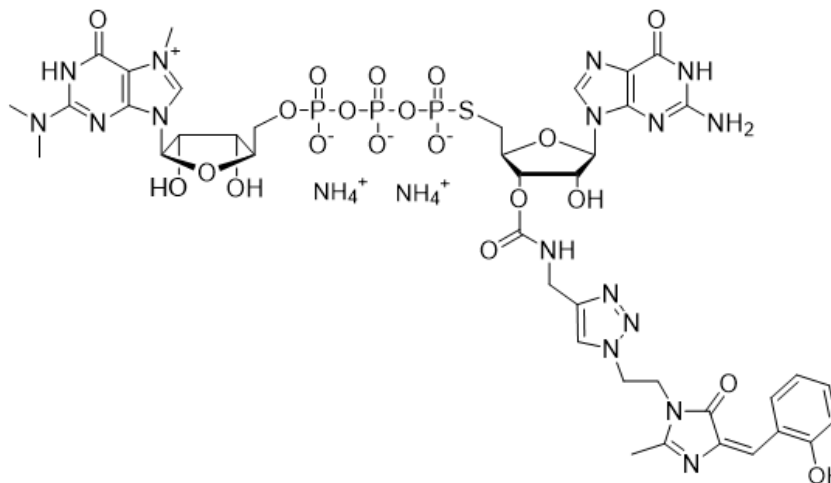
201119_PSu_08 #44-72 RT: 0.42-0.69 AV: 29 NL: 1.47E7
T: FTMS - p ESI Full ms [150.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₀H₄₈N₁₆O₂₀P₃S⁻ : 1197.21698, found: 1197.21885)

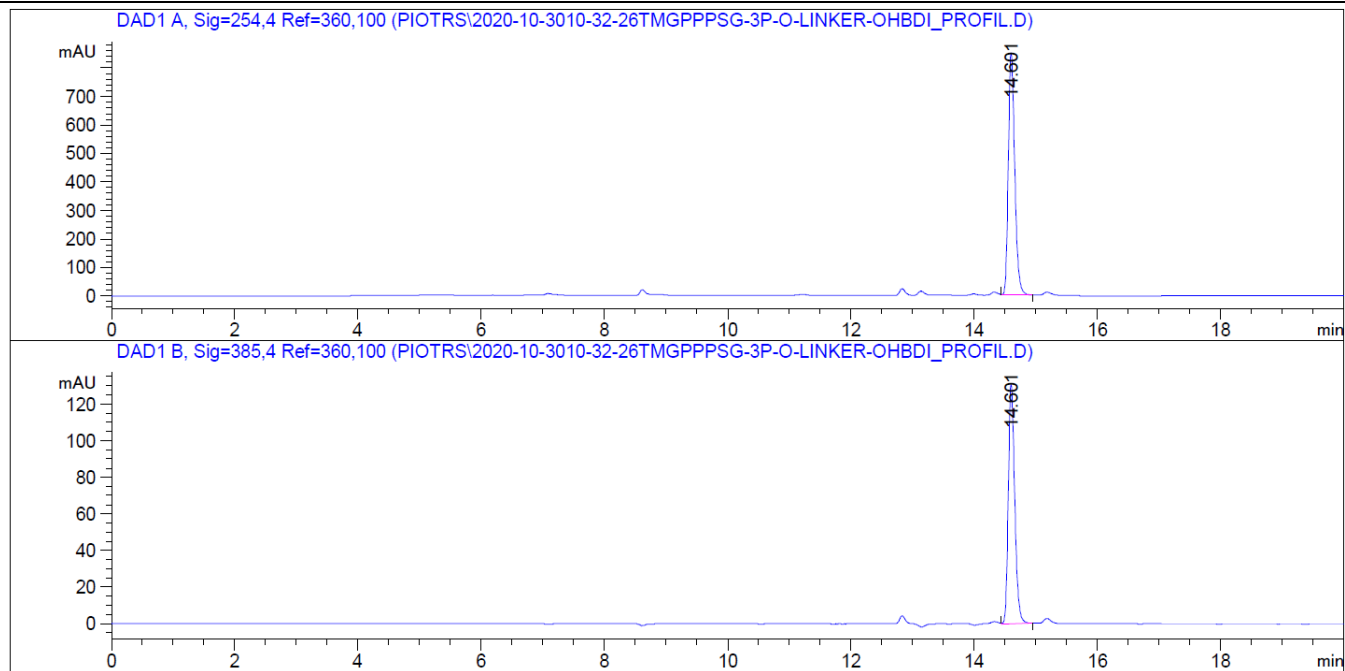


Compound 7b-3': TMGppp-5'-SG-3'-O-C(O)-NH-CH₂-triazole-CH₂CH₂-oHBI (NH₄⁺ salt)

Chemical structure

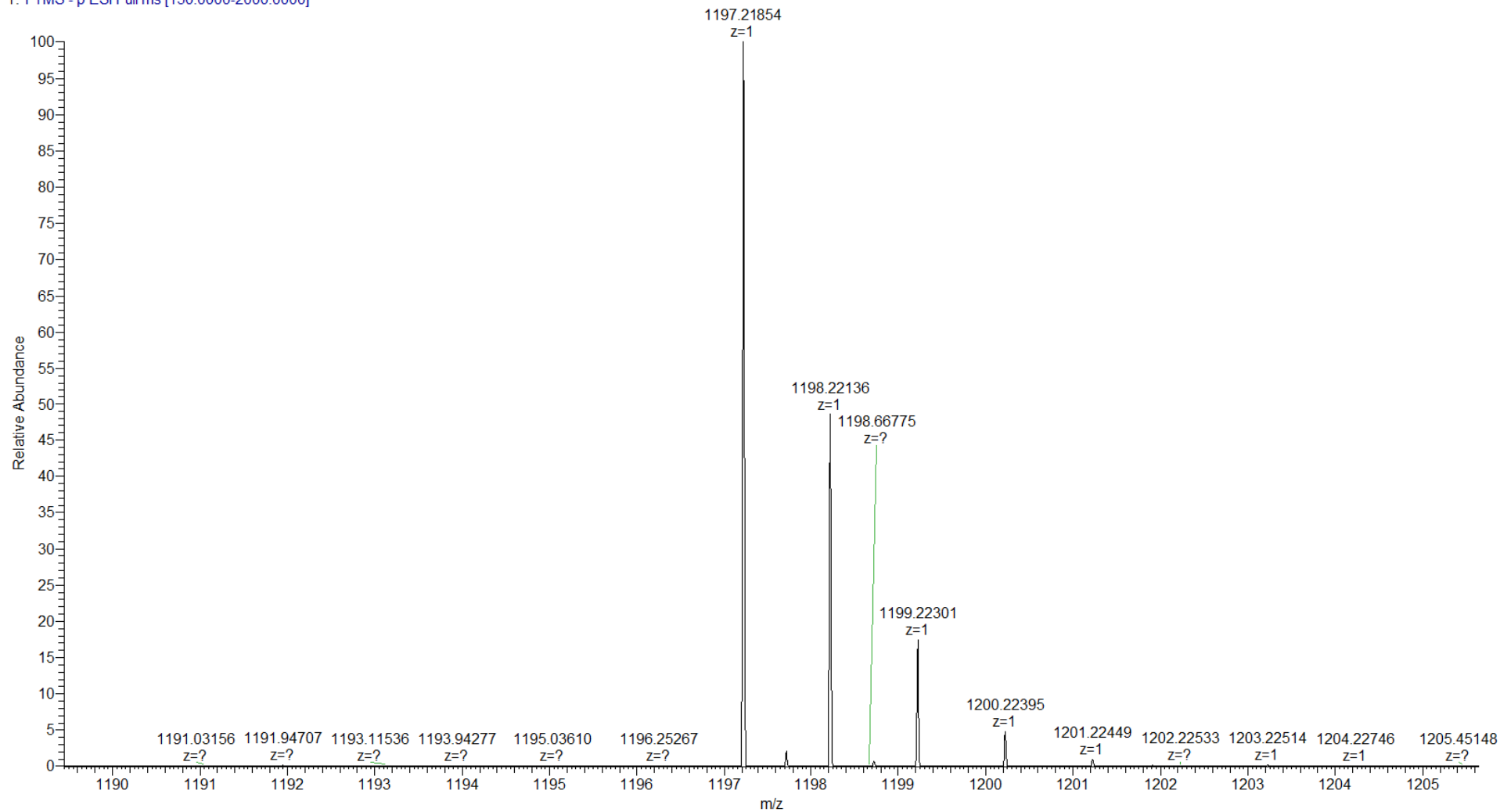


RP-HPLC (conditions c)



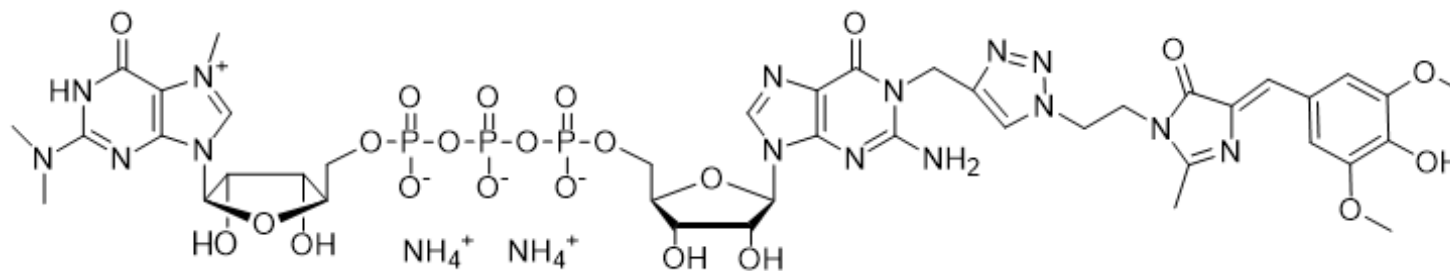
201119_PSu_07 #29-84 RT: 0.30-0.83 AV: 56 NL: 1.79E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₀H₄₈N₁₆O₂₀P₃S⁻ : 1197.21698, found: 1197.21854)

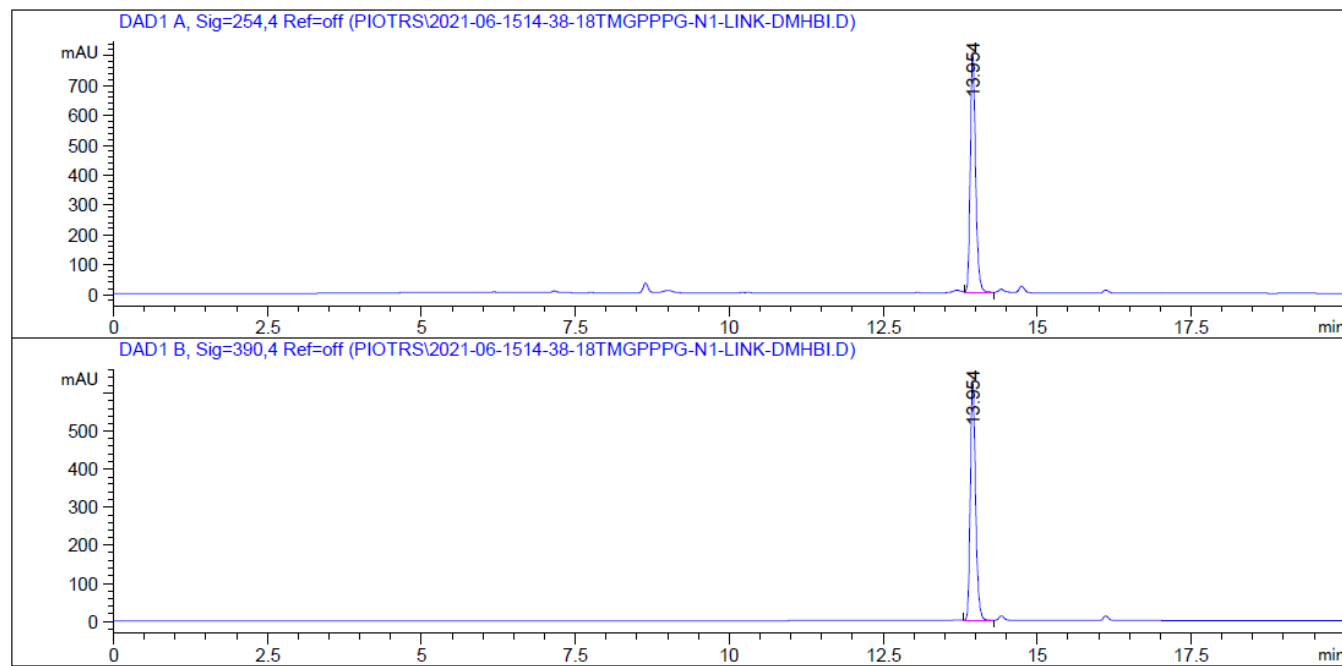


Compound 8a: TMGpppG-N1-CH₂-triazole-CH₂CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

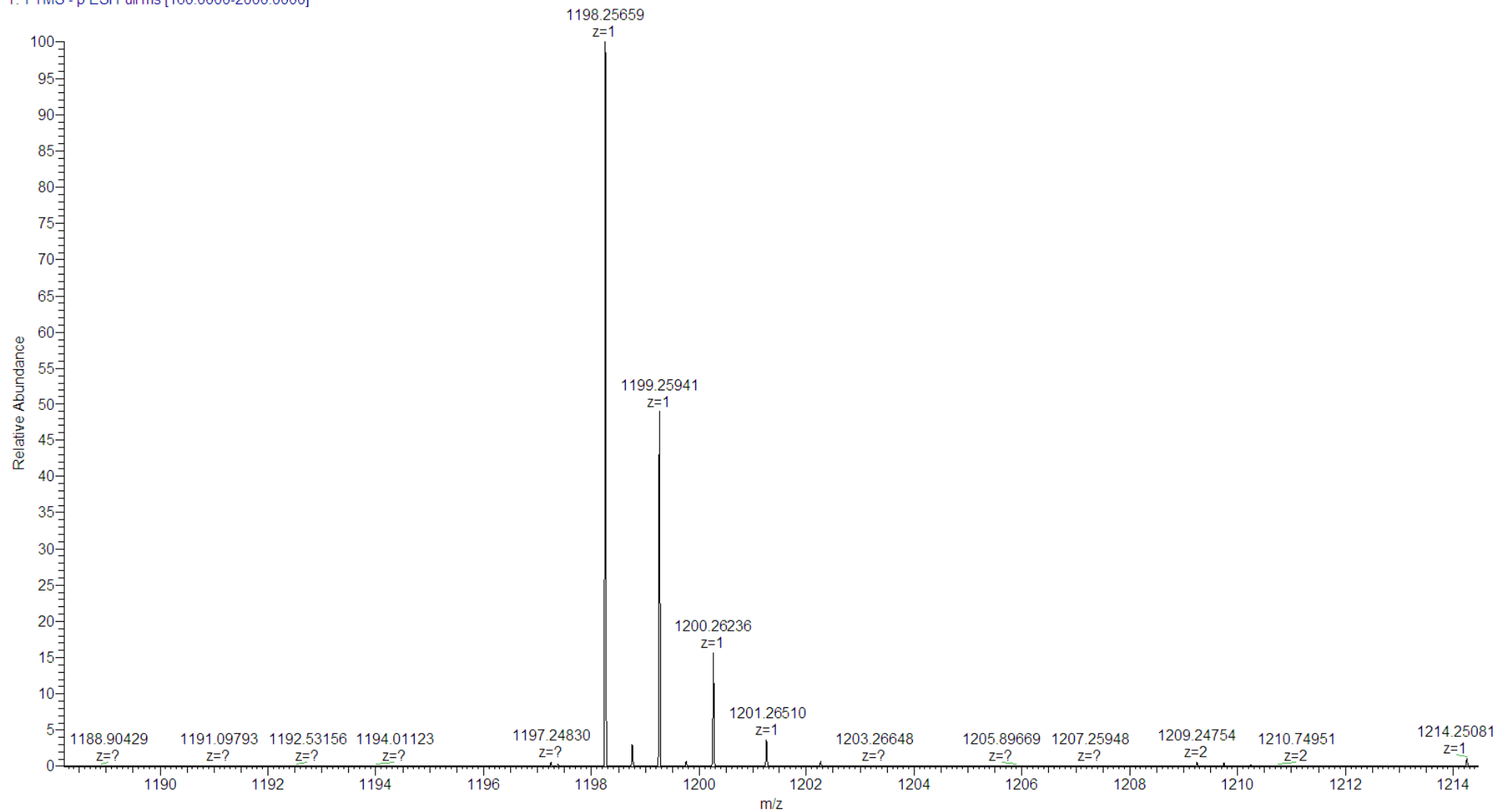


RP-HPLC (conditions c)



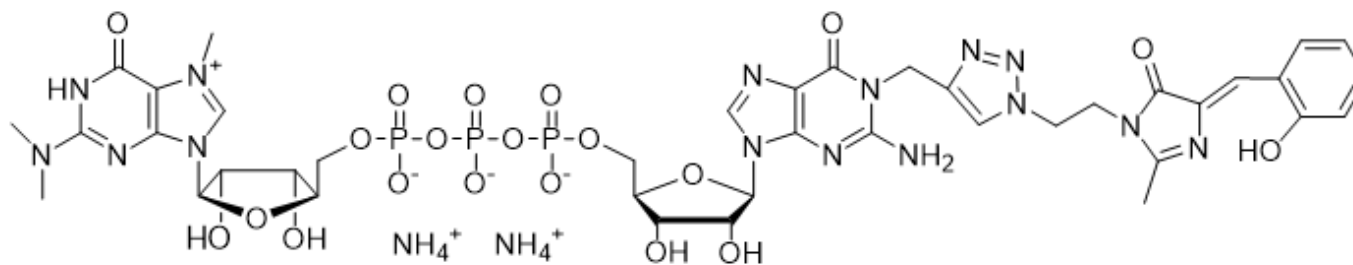
210629_PSu_79a #148-229 RT: 1.29-2.00 AV: 82 NL: 2.95E6
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₁H₅₁N₁₅O₂₂P₃ : 1198.25514, found: 1198.25659)

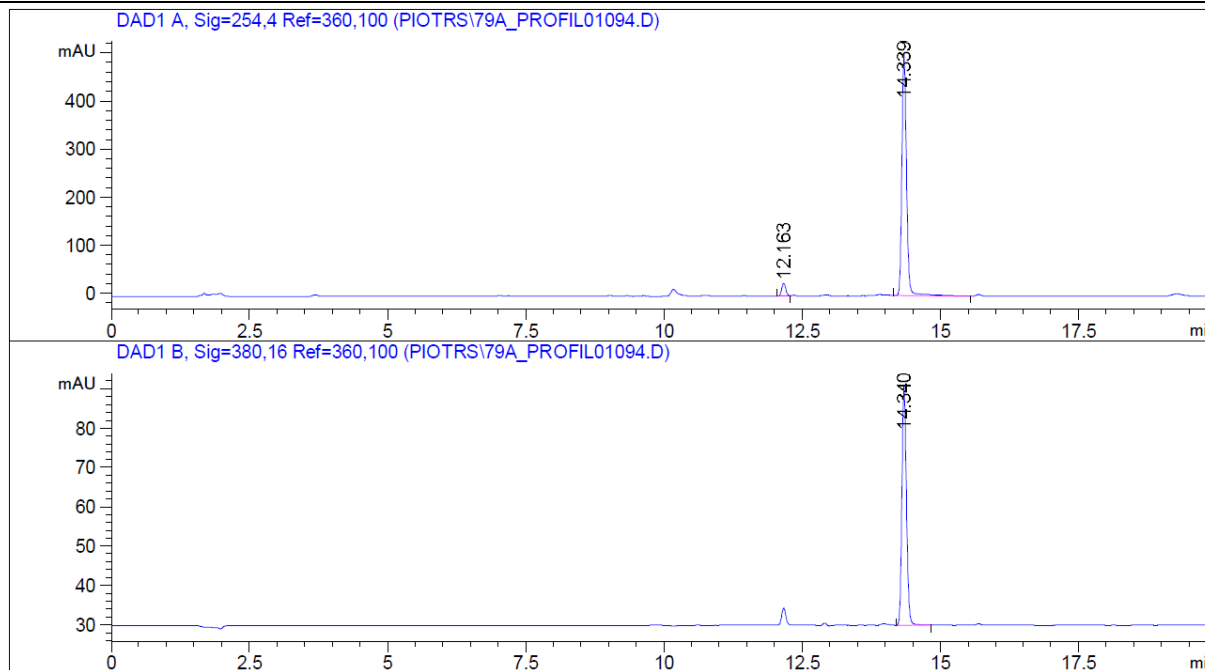


Compound 8b: TMGpppG-N1-CH₂-triazole-CH₂CH₂-oHBI (NH₄⁺ salt)

Chemical structure

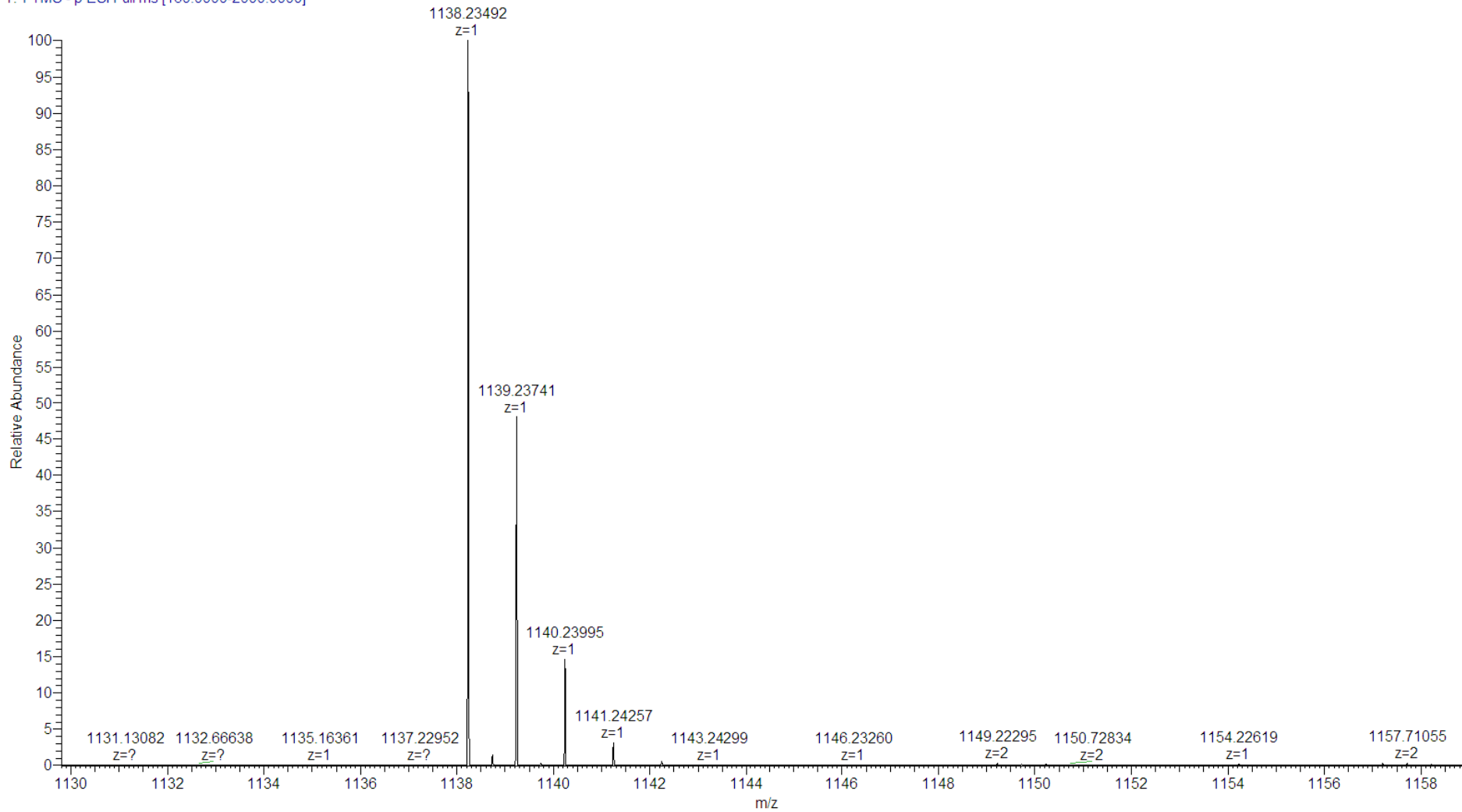


RP-HPLC (conditions c)



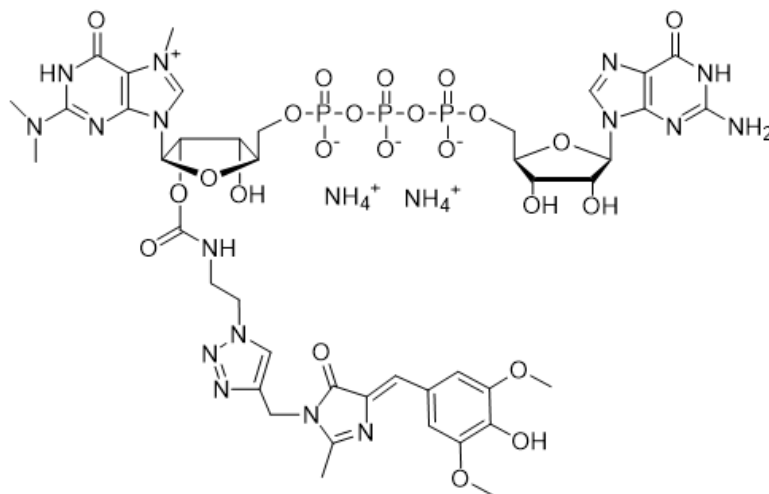
MS (-) ESI (Calc. [M-H]⁻ C₃₉H₄₇N₁₅O₂₀P₃ : 1138.23401, found: 1138.23492)

220407_PSu_04 #249-295 RT: 2.18-2.58 AV: 47 NL: 3.90E7
T: FTMS - p ESI Full ms [160.0000-2000.0000]

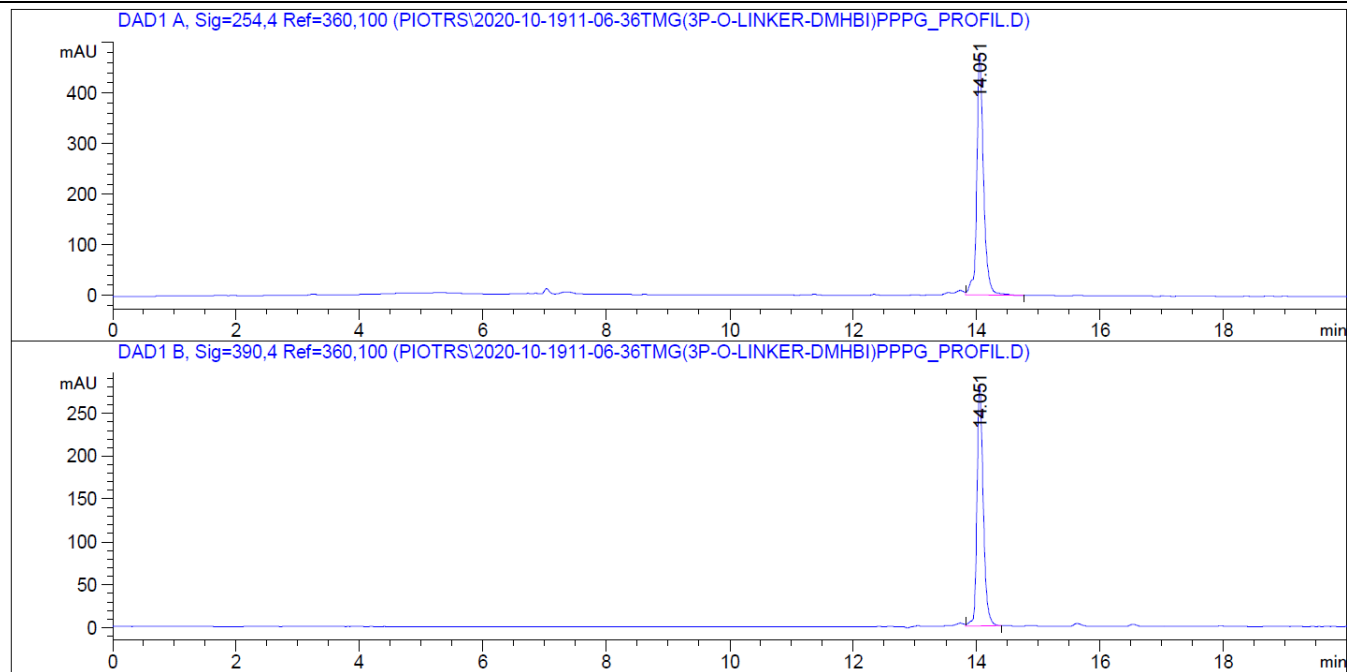


Compound 9a-2': TMG(-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI)pppG (NH₄⁺ salt)

Chemical structure

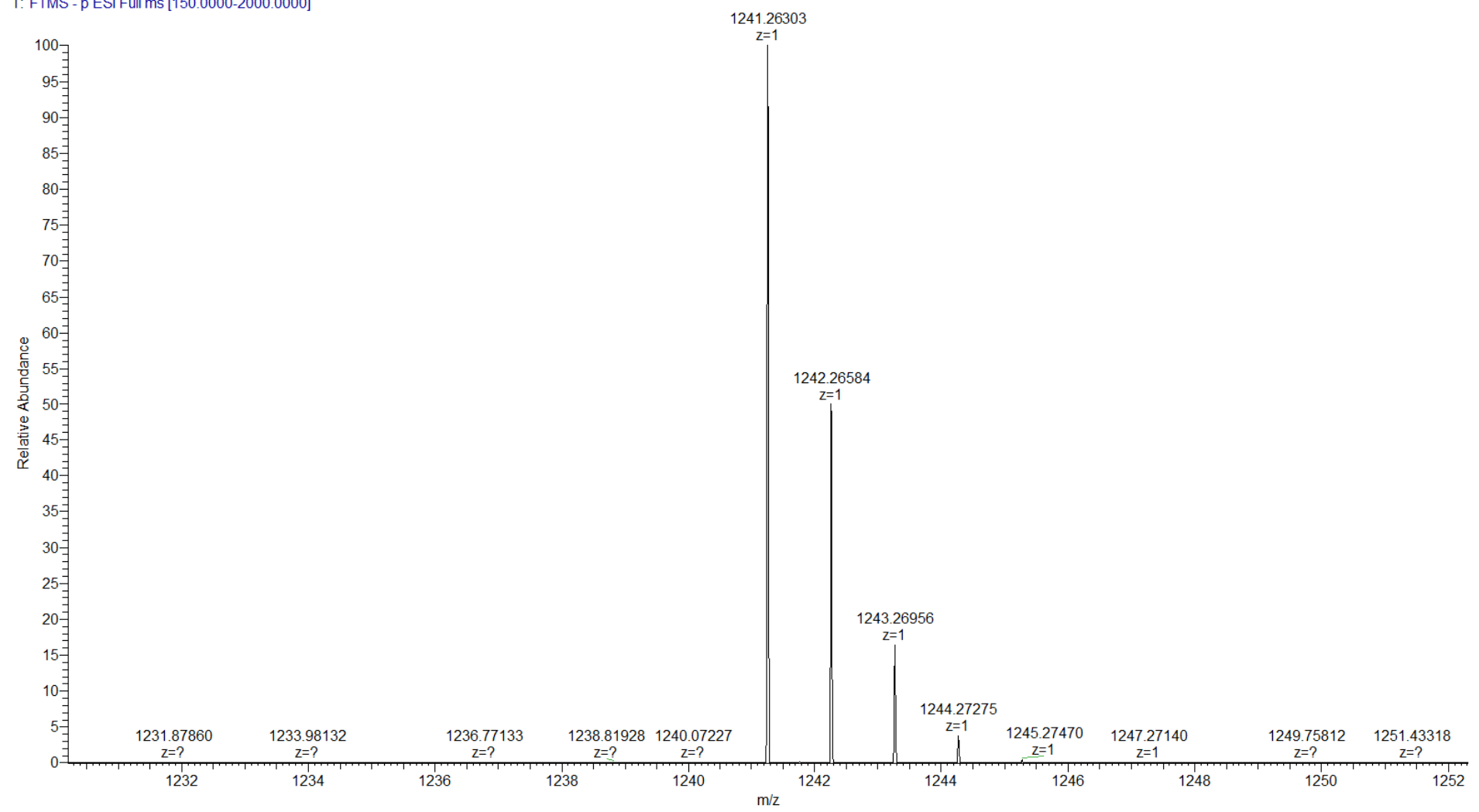


RP-HPLC (conditions c)



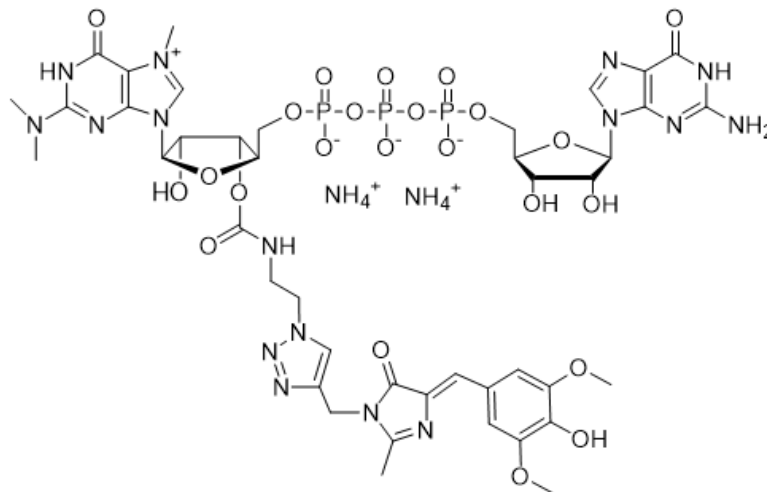
201119_PSu_01 #314-381 RT: 3.23-3.93 AV: 68 NL: 1.95E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₂N₁₆O₂₃P₃ : 1241.26096, found: 1241.26303)

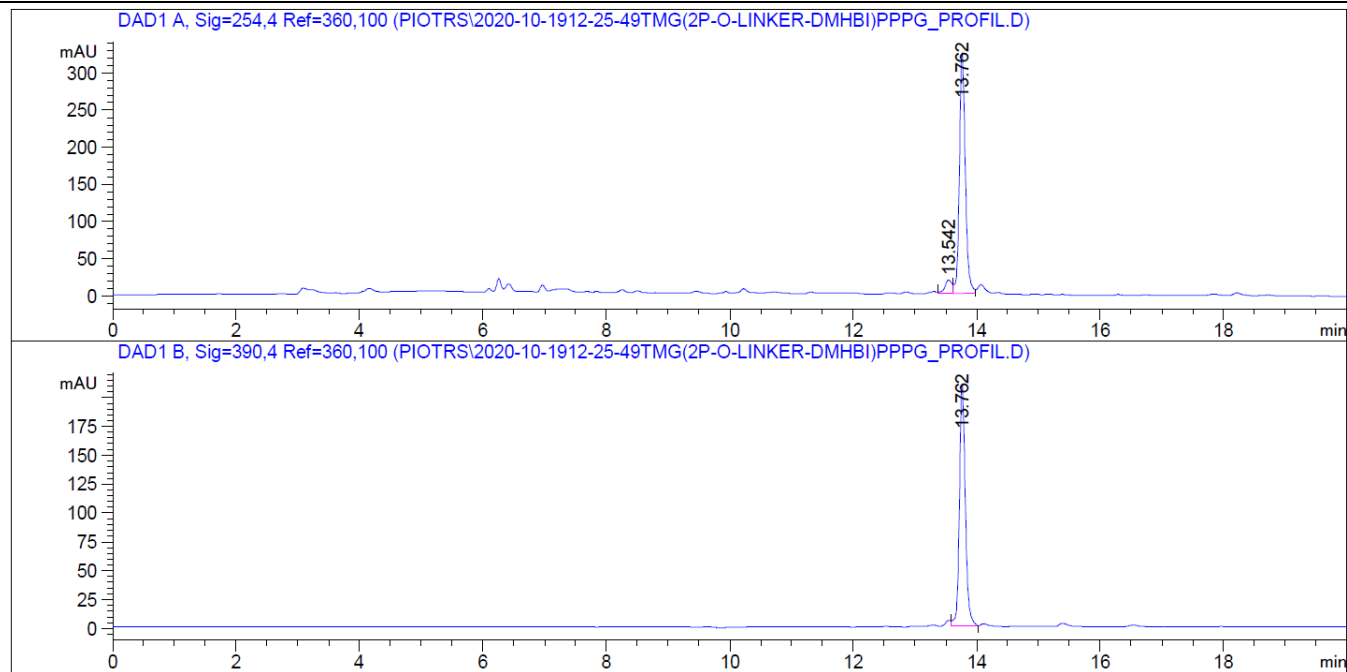


Compound 9a-3': TMG(-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI)pppG (NH₄⁺ salt)

Chemical structure

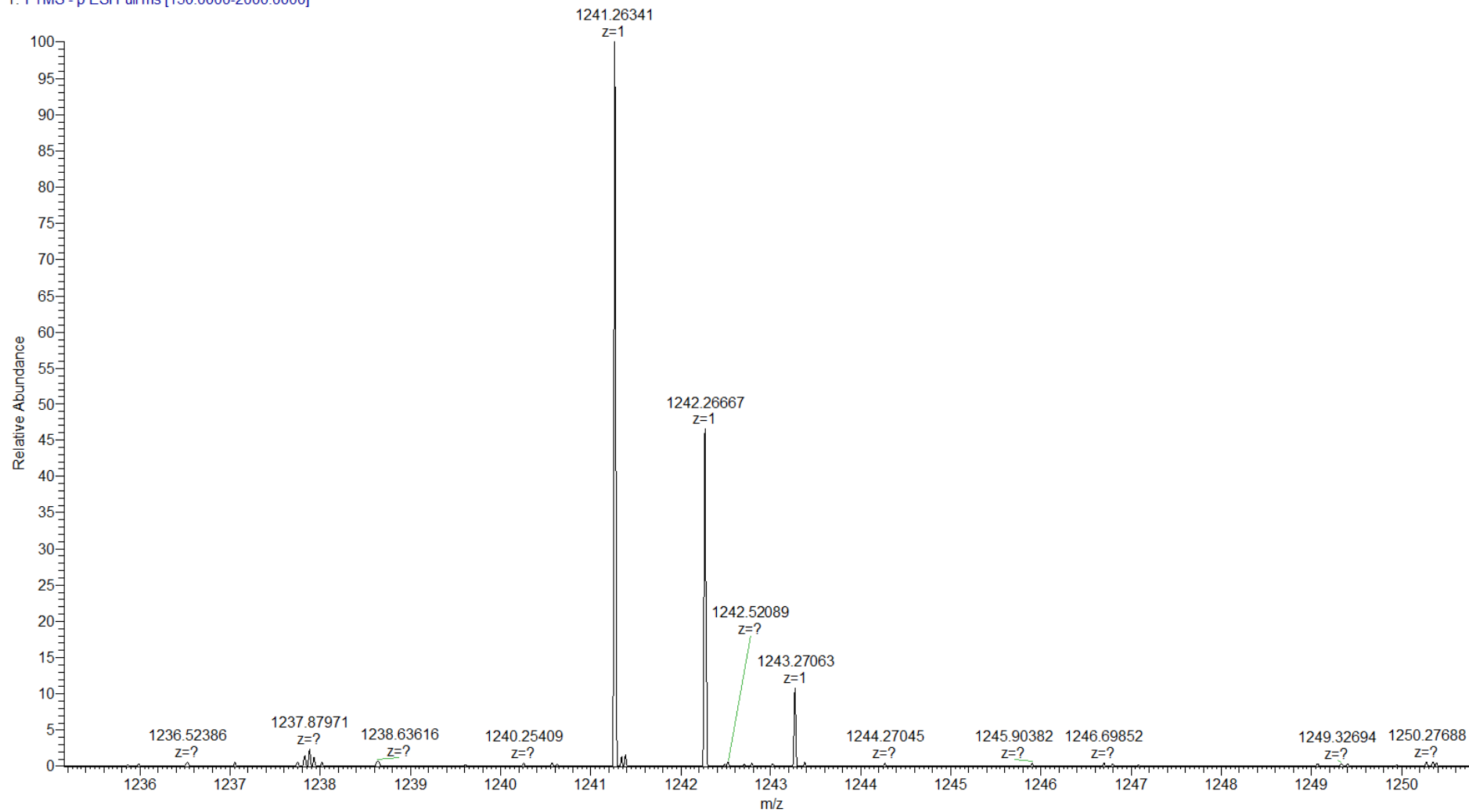


RP-HPLC (conditions c)



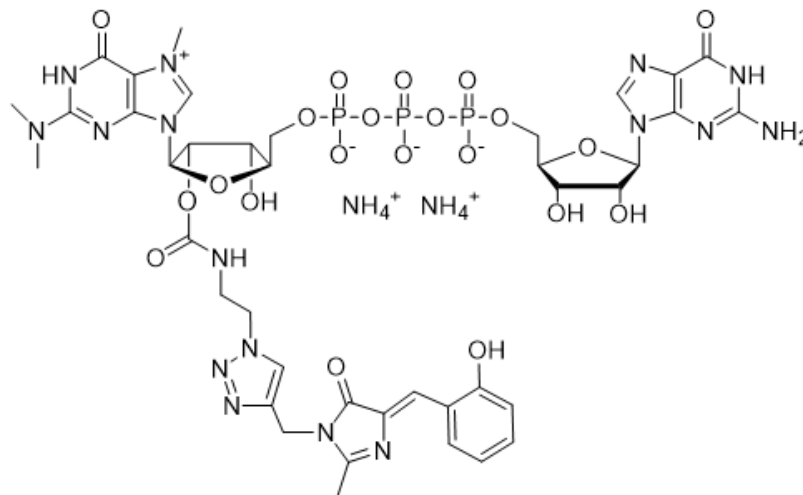
201119_PSu_02 #134-186 RT: 1.35-1.86 AV: 53 NL: 3.56E4
T: FTMS - p ESI Full ms [150.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₂H₅₂N₁₆O₂₃P₃ : 1241.26096, found: 1241.26341)

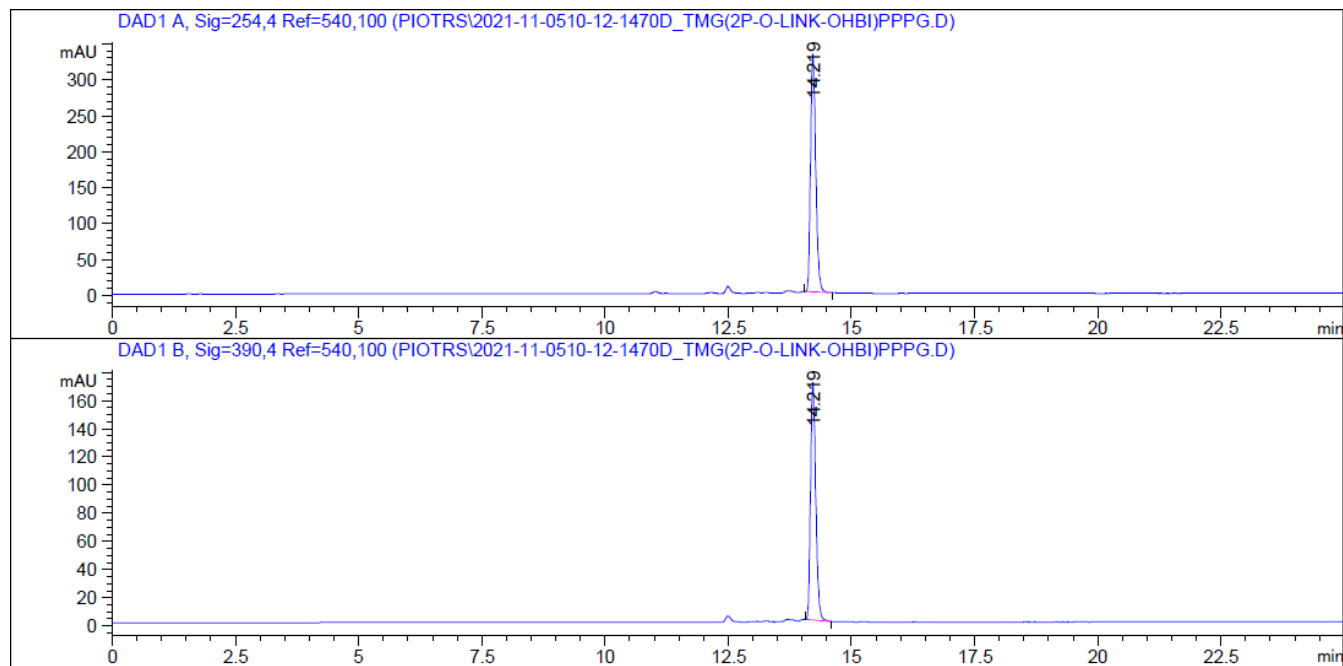


Compound 9b-2': TMG(-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-oHBI)pppG (NH₄⁺ salt)

Chemical structure

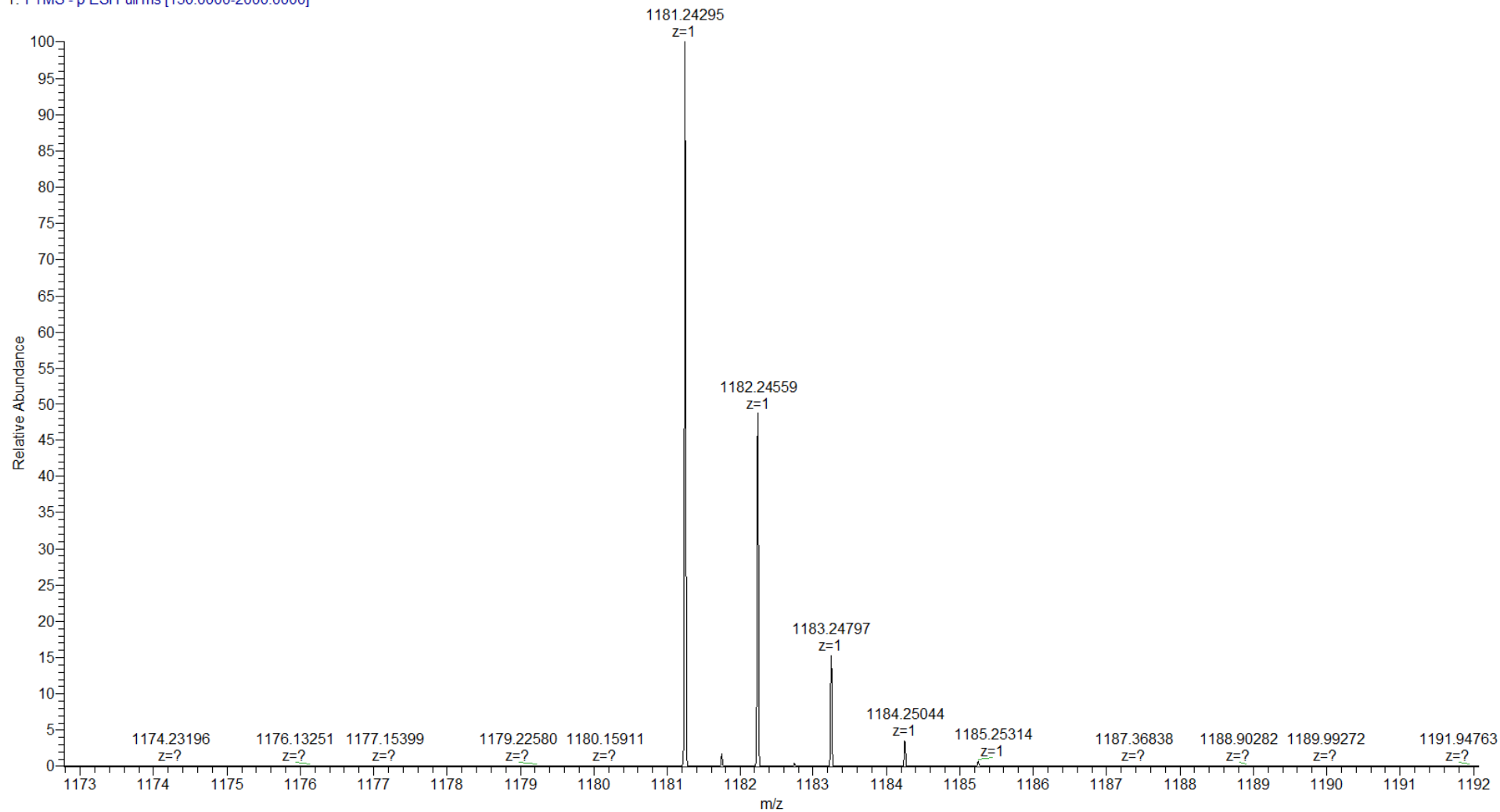


RP-HPLC (conditions c)



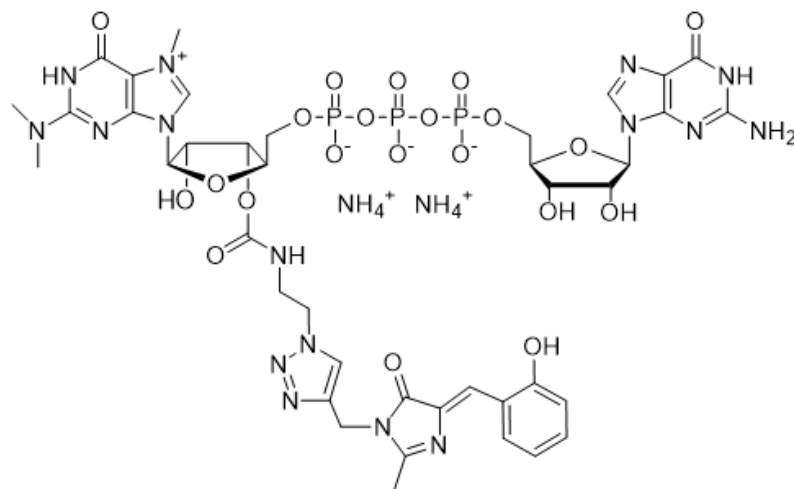
201119_PSu_03 #39-107 RT: 0.40-1.08 AV: 69 NL: 1.37E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₄₀H₄₈N₁₆O₂₁P₃ : 1181.23983, found: 1181.24295)

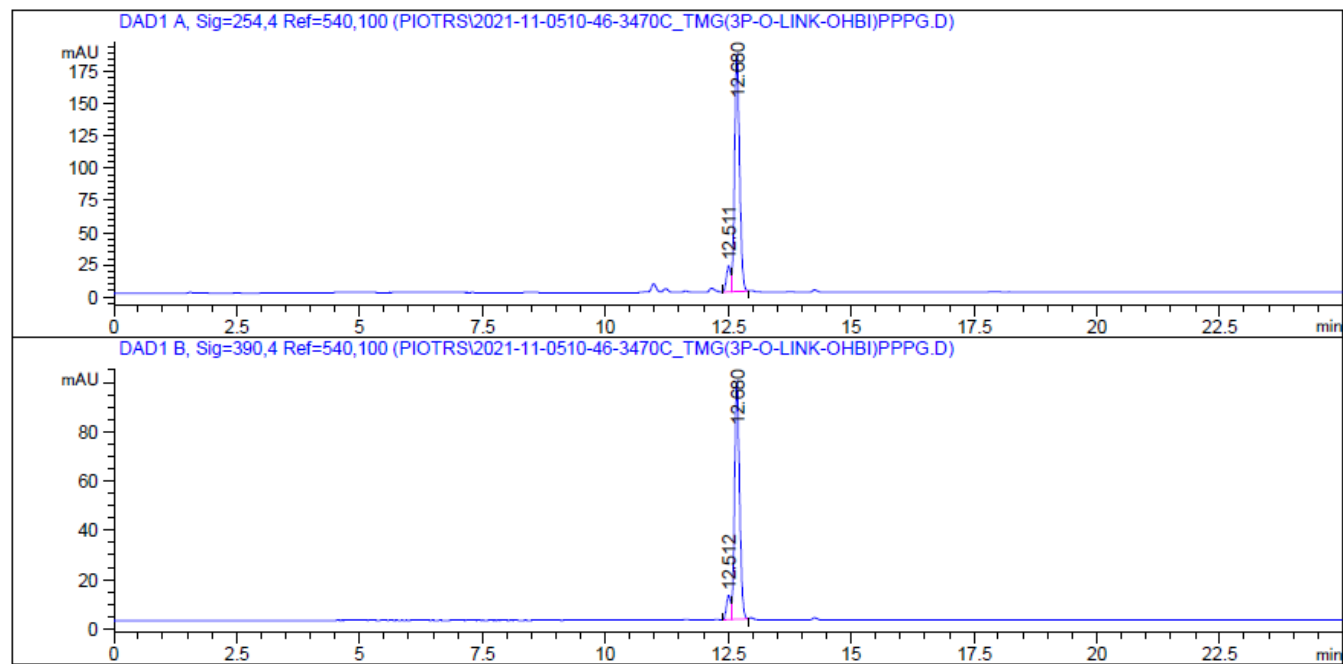


Compound 9b-3': TMG(-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-oHBI)pppG (NH₄⁺ salt)

Chemical structure

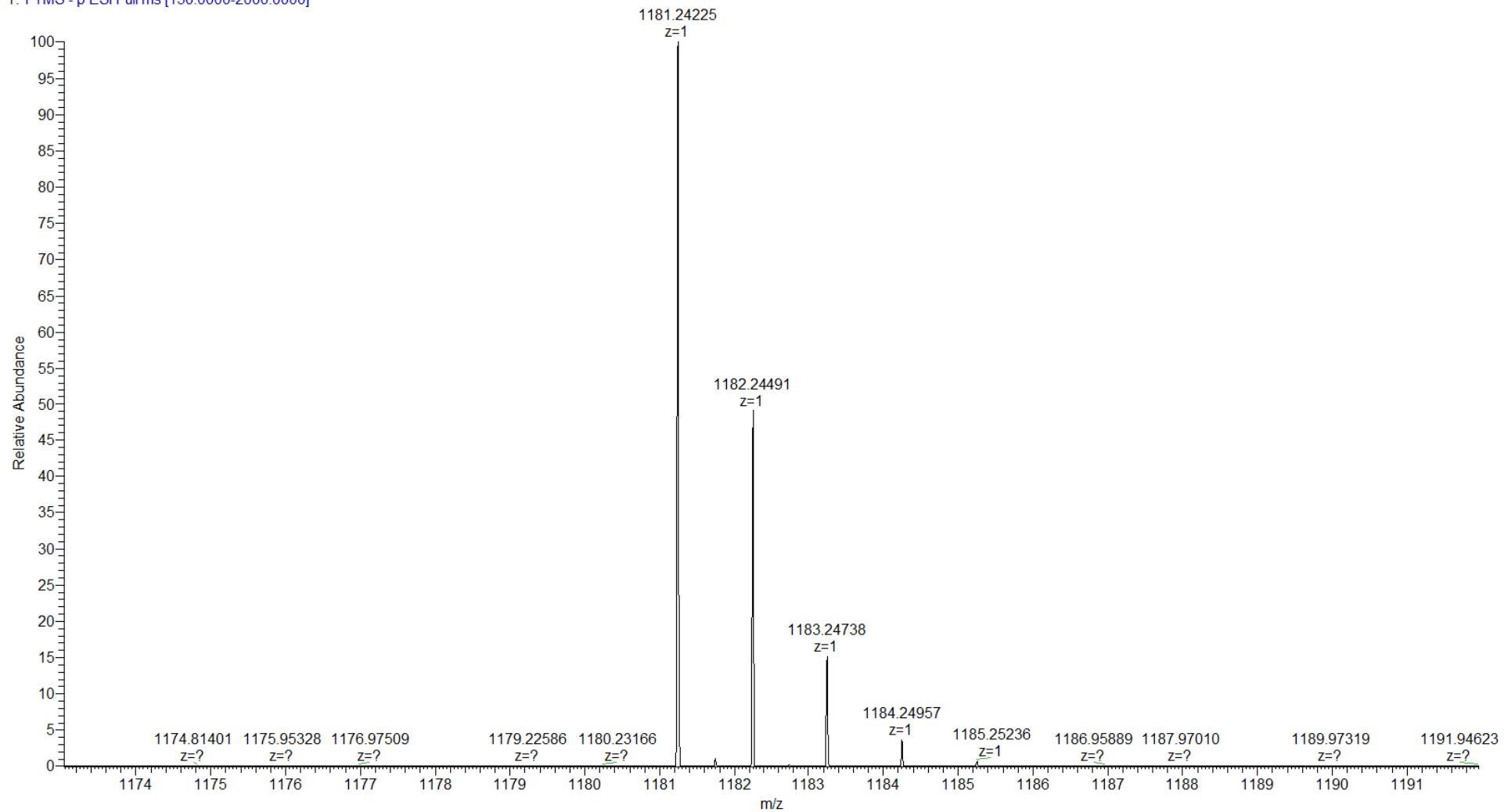


RP-HPLC (conditions c)



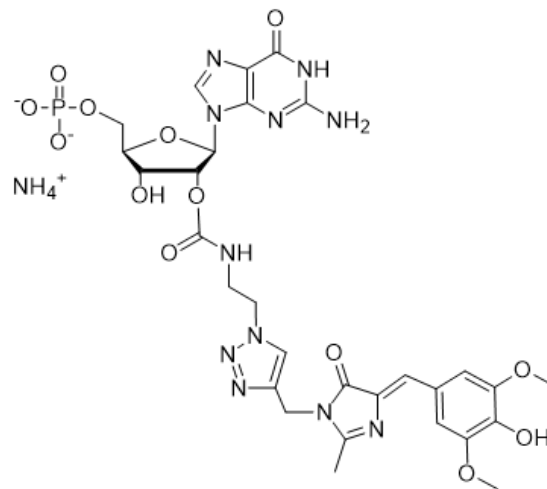
MS (-) ESI (Calc. [M-H]⁻ C₄₀H₄₈N₁₆O₂₁P₃ : 1181.23983, found: 1181.24225)

201119_PSu_04 #27-85 RT: 0.28-0.86 AV: 59 NL: 1.91E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

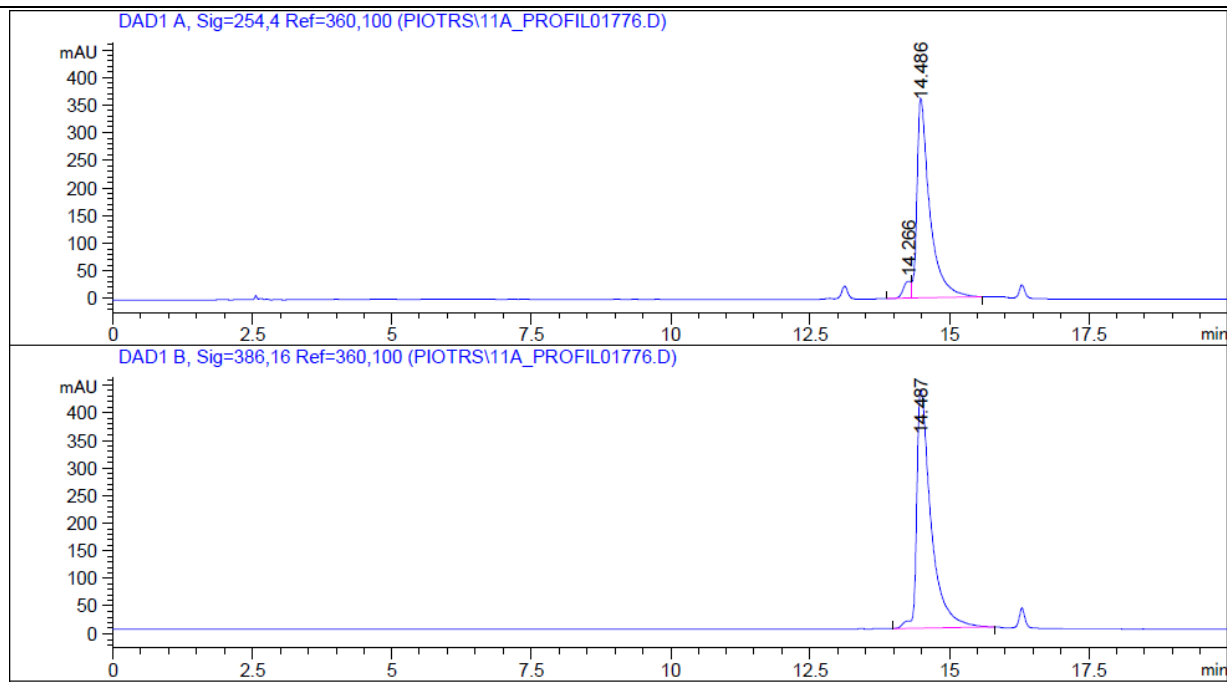


Compound 10a-2': GMP-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

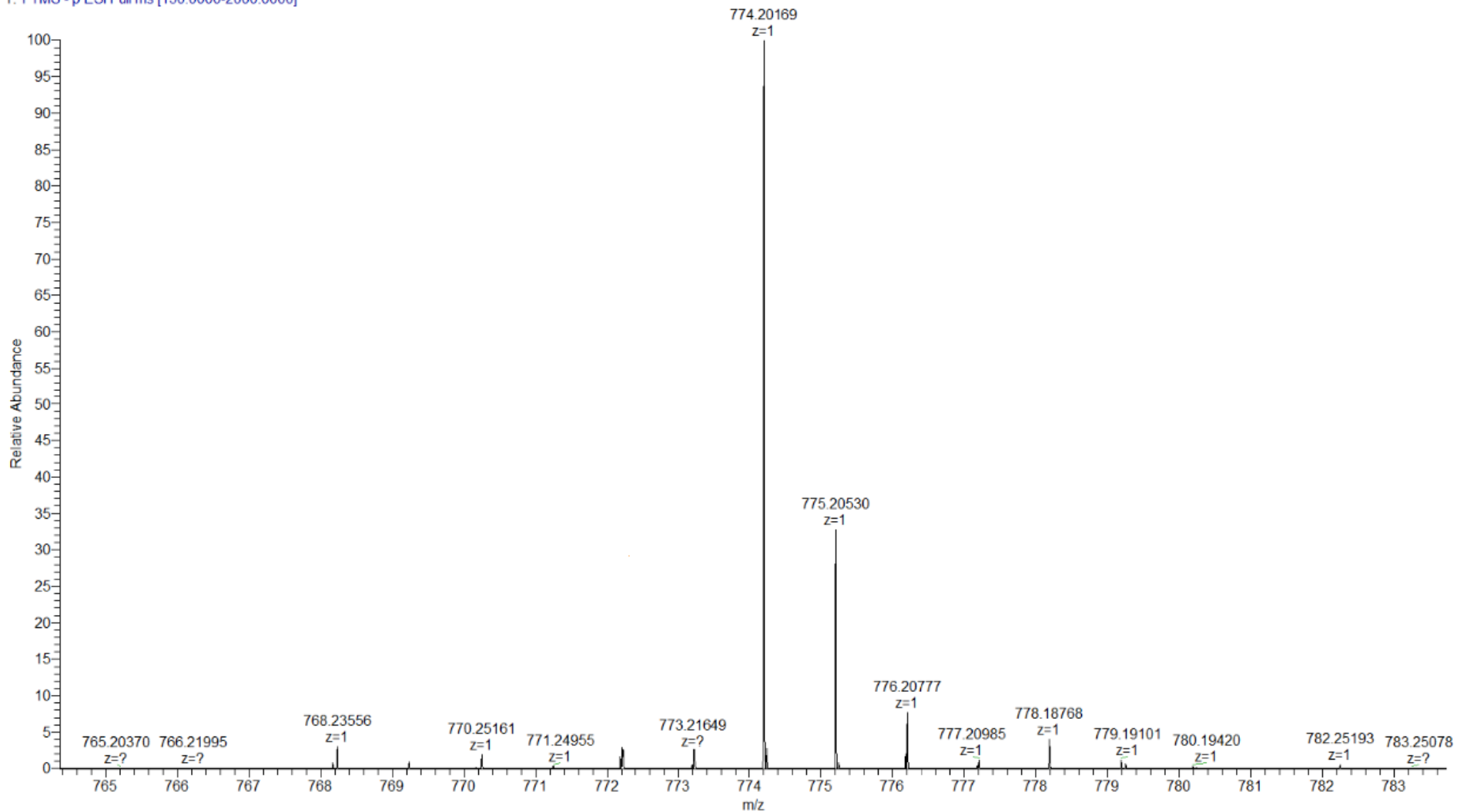


RP-HPLC (conditions c)



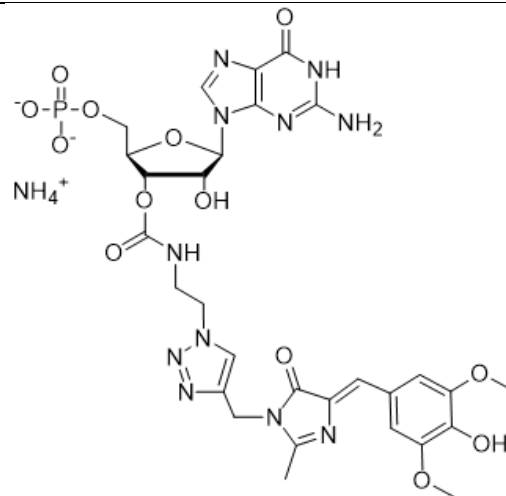
MS (-) ESI (Calc. [M-H]⁻ C₂₉H₃₃N₁₁O₁₃P⁻ : 774.2002, found: 774.20169)

200213_Psu_42 #41-105 RT: 0.43-1.07 AV: 65 NL: 4.42E5
T: FTMS - p ESI Full ms [150.0000-2000.0000]

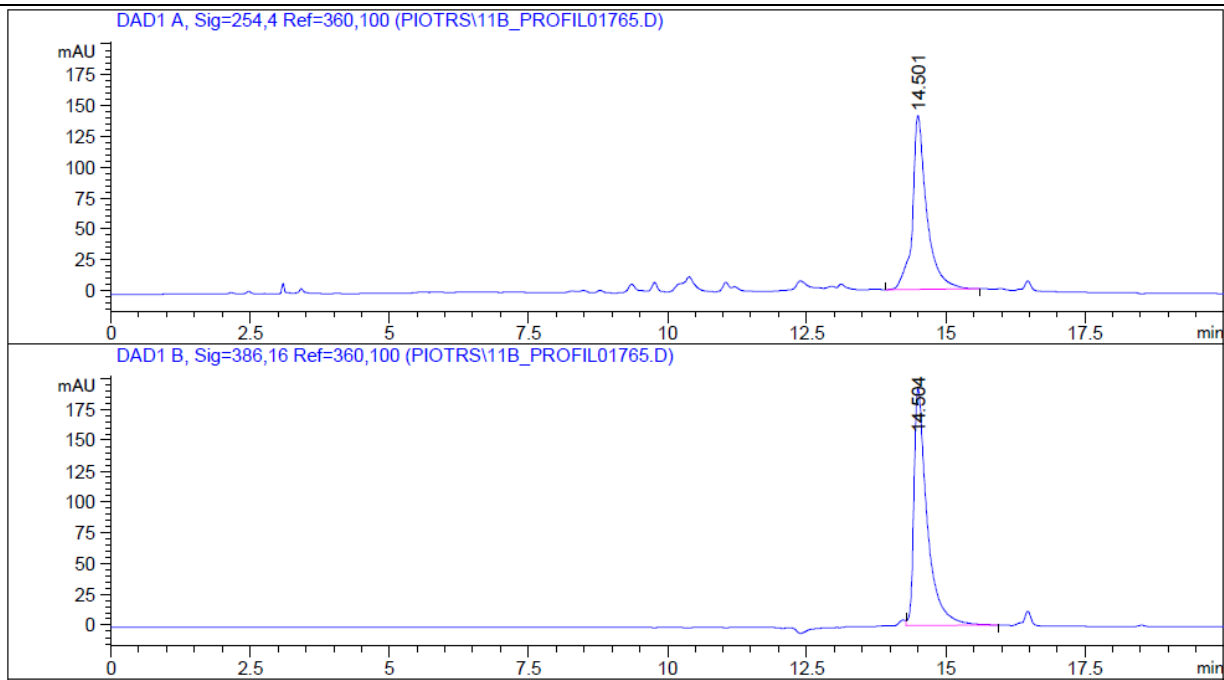


Compound 10a-3': GMP-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

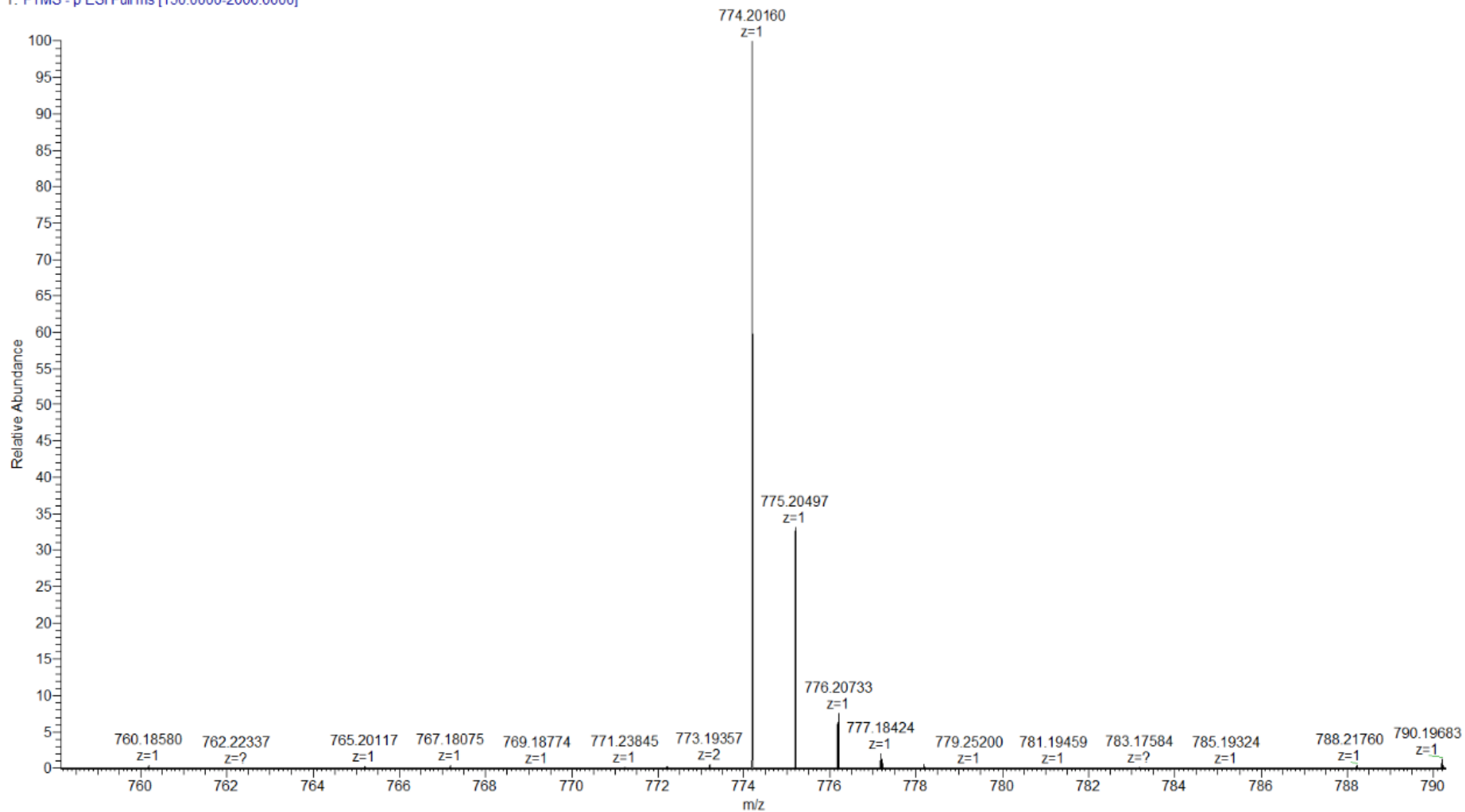


RP-HPLC (conditions c)



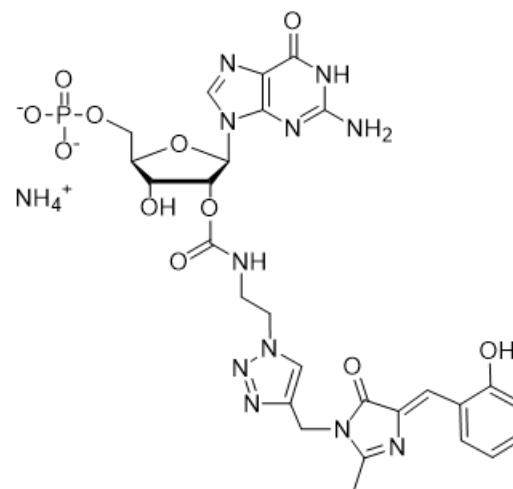
MS (-) ESI (Calc. [M-H]⁻ C₂₉H₃₃N₁₁O₁₃P⁻ : 774.20024, found: 774.20160)

200213_Psu_43#32.139 RT: 0.33-1.38 AV: 108 NL: 6.75E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

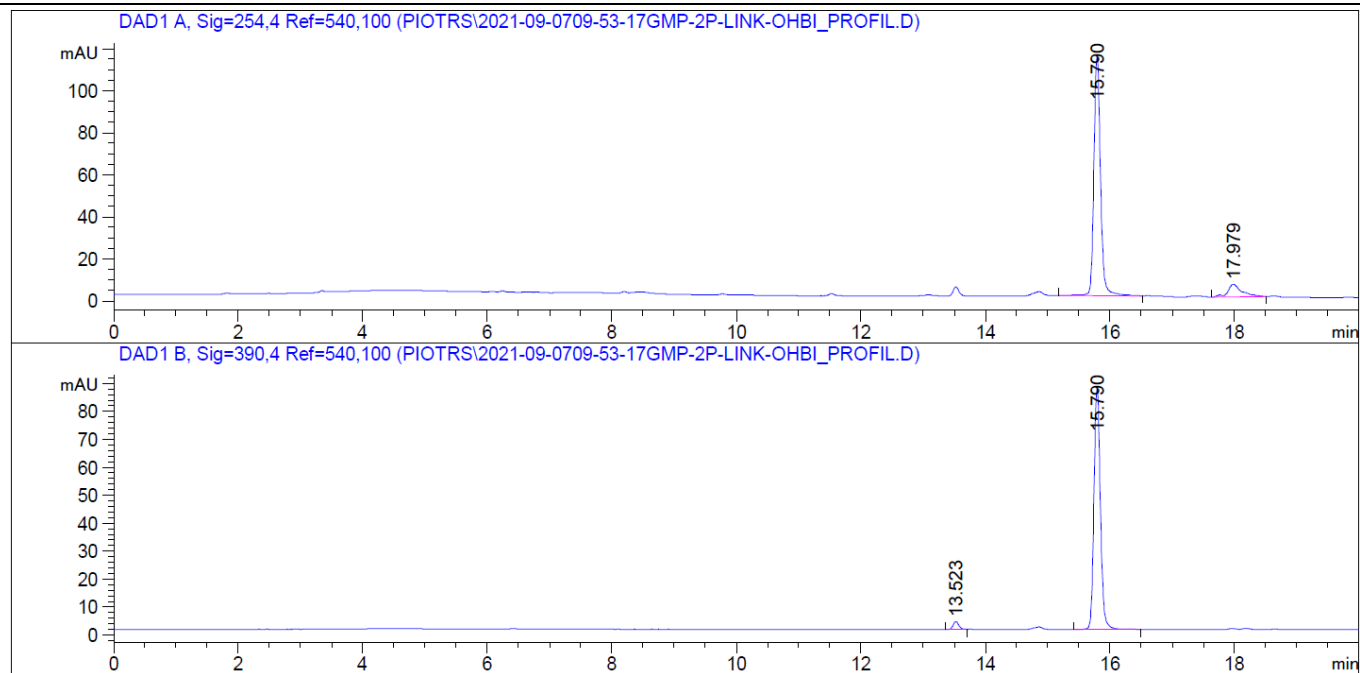


Compound 10b-2': GMP-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-oHBI (NH₄⁺ salt)

Chemical structure

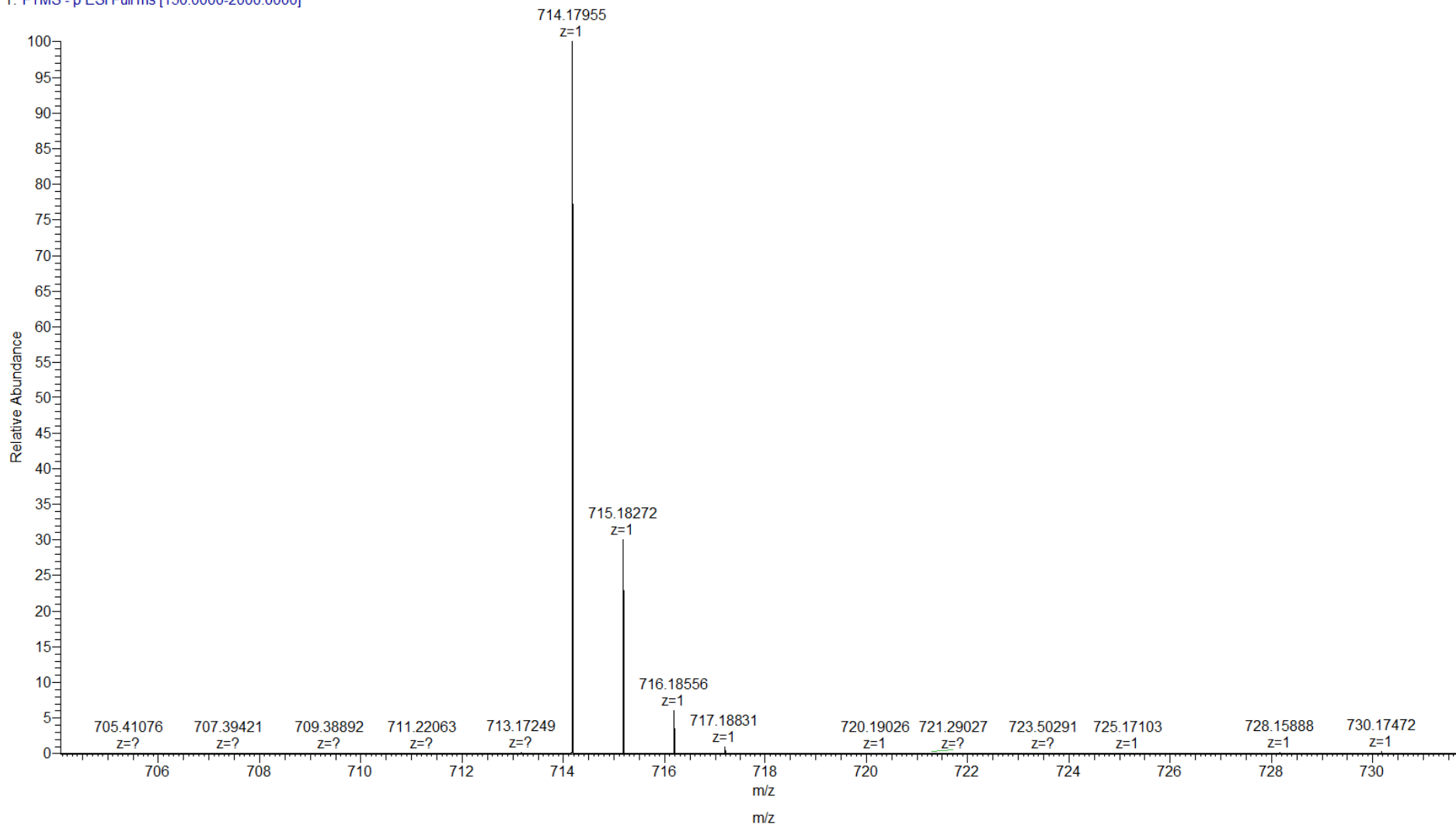


RP-HPLC (conditions c)



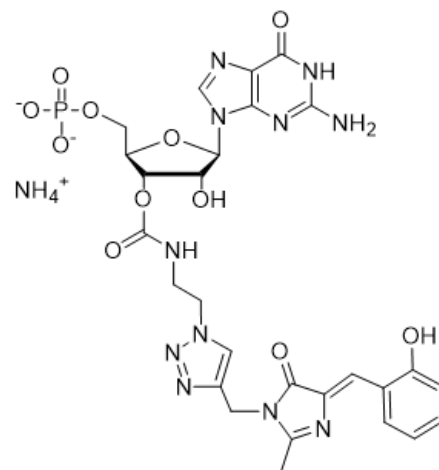
MS (-) ESI (Calc. [M-H]⁻C₂₇H₂₉N₁₁O₁₁P⁻ : 714.1791, found: 714.17955)

210504_PSu_16_c #60-155 RT: 0.57-1.48 AV: 96 NL: 2.89E7
T: FTMS - p ESI Full ms [150.0000-2000.0000]

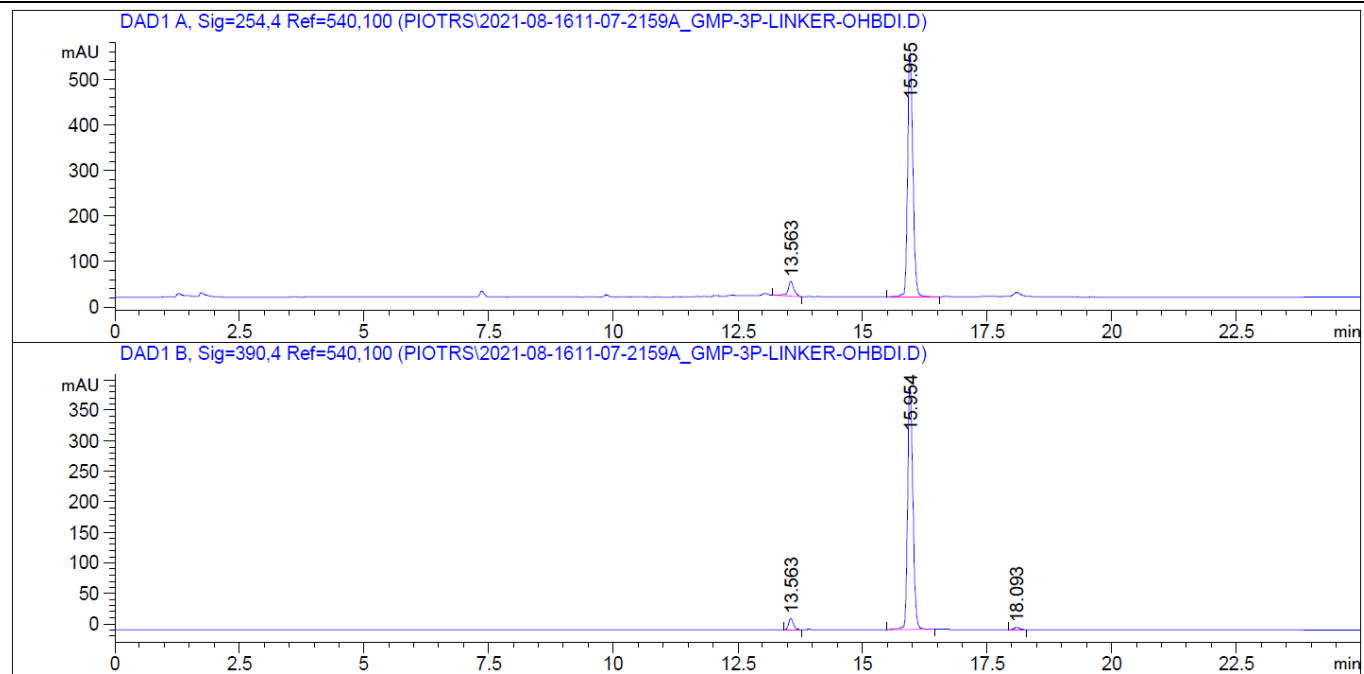


Compound 10b-3': GMP-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-oHBI (NH₄⁺ salt)

Chemical structure

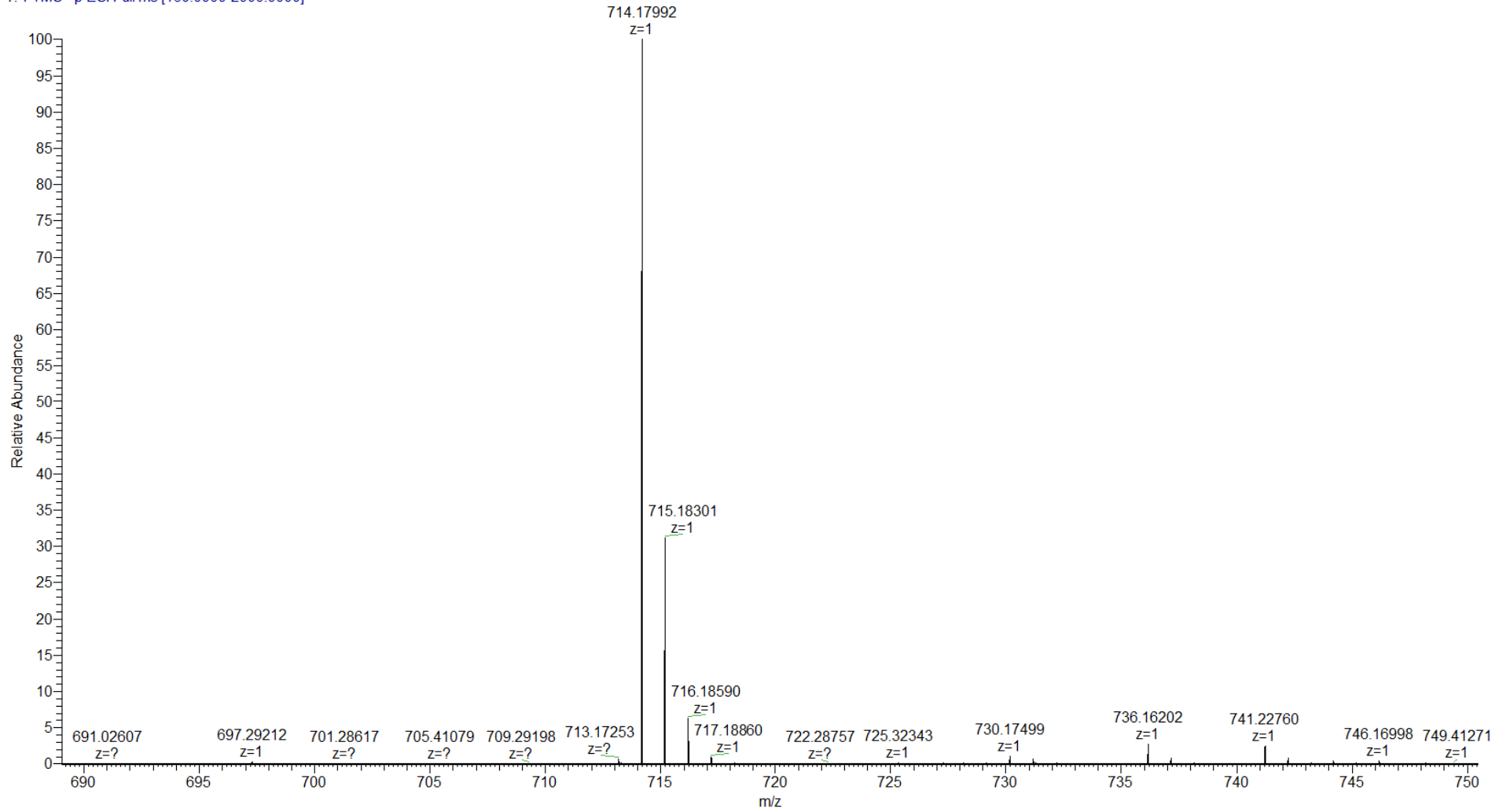


RP-HPLC (conditions c)



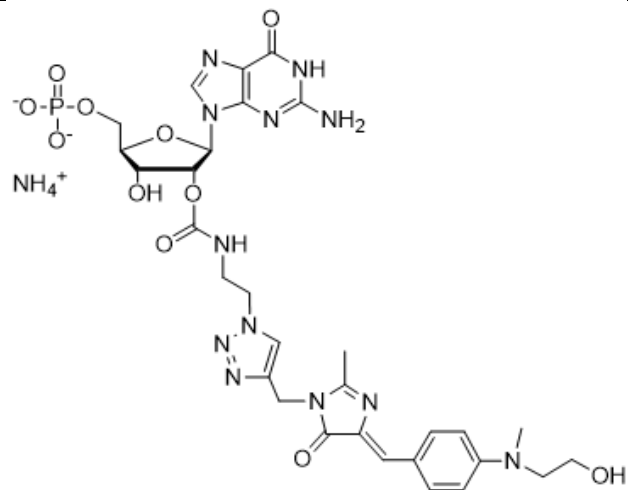
220214_PSu_59a #88-180 RT: 0.77-1.57 AV: 93 NL: 1.41E7
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₂₇H₂₉N₁₁O₁₁P⁻ : 714.1791, found: 714.17992)

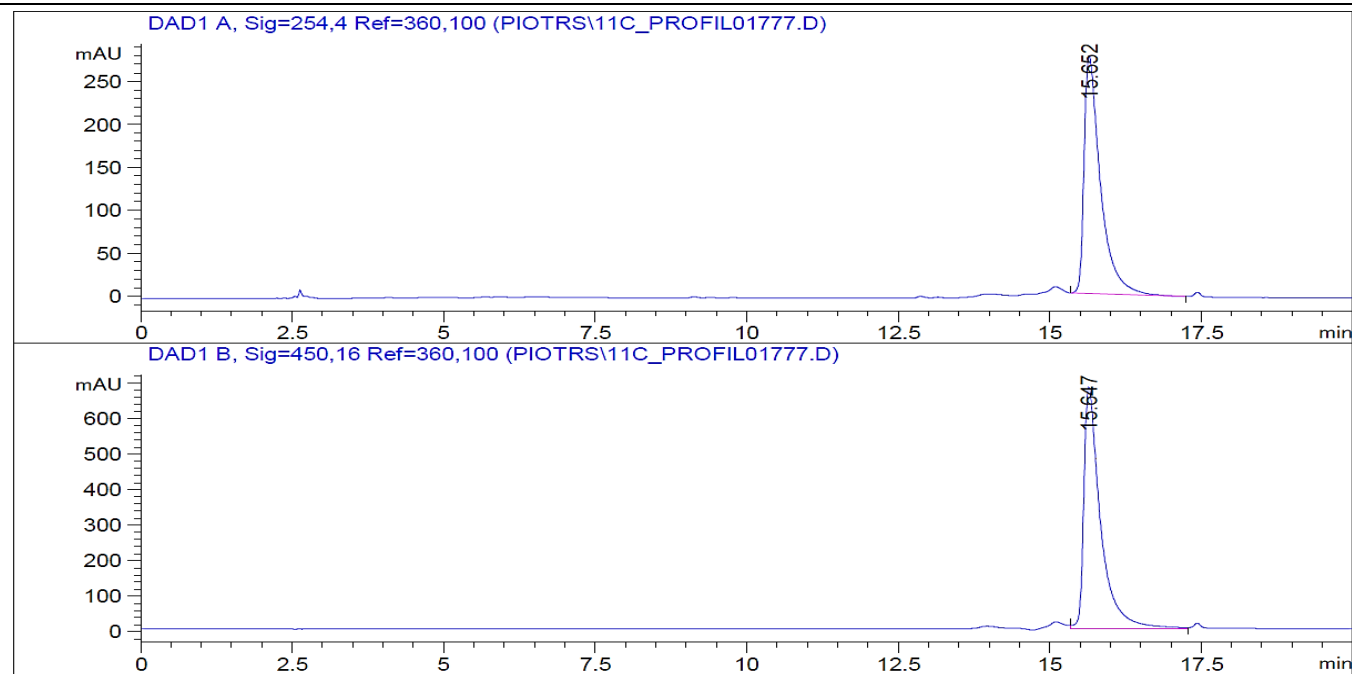


Compound 10c-2': GMP-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

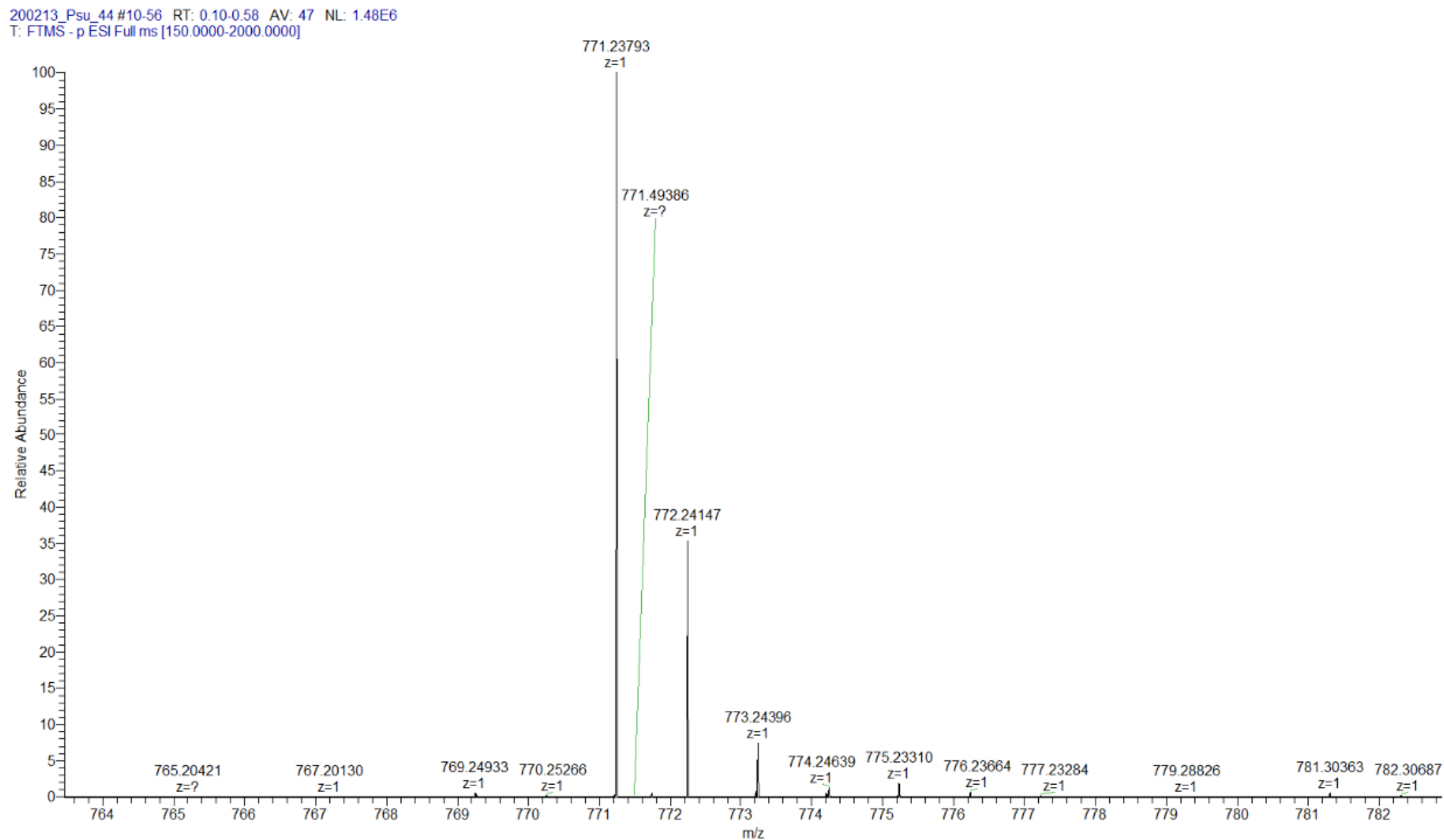
Chemical structure



RP-HPLC (conditions c)

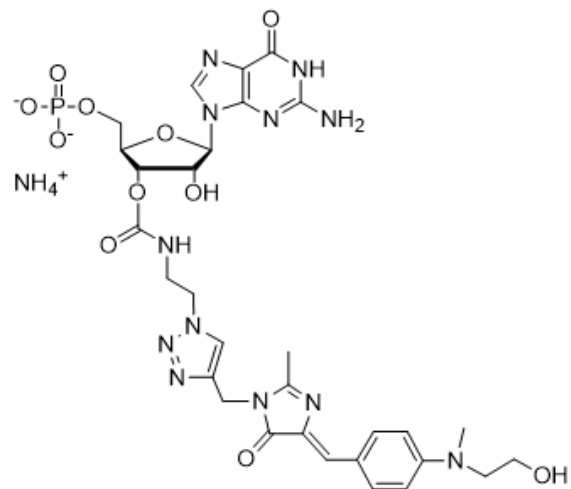


MS (-) ESI (Calc. [M-H]⁻ C₃₀H₃₆N₁₂O₁₁P⁻ : 771.2370, found: 771.23793)

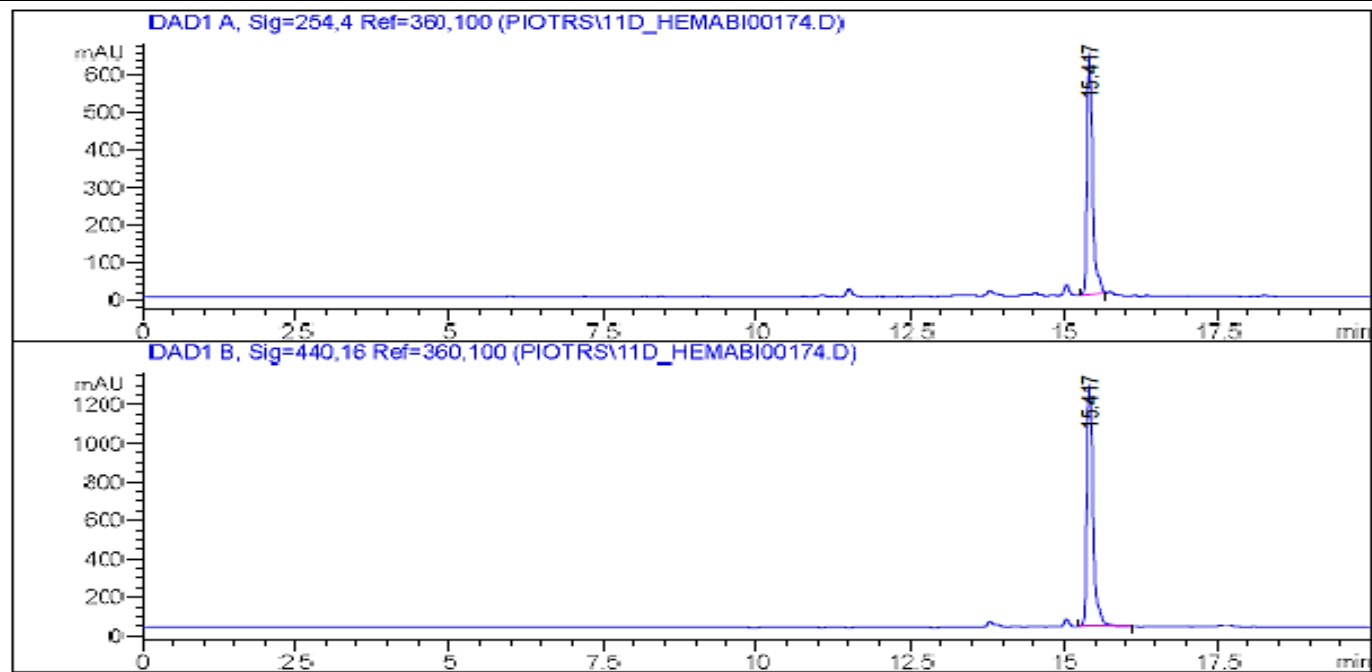


Compound 10c-3': GMP-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

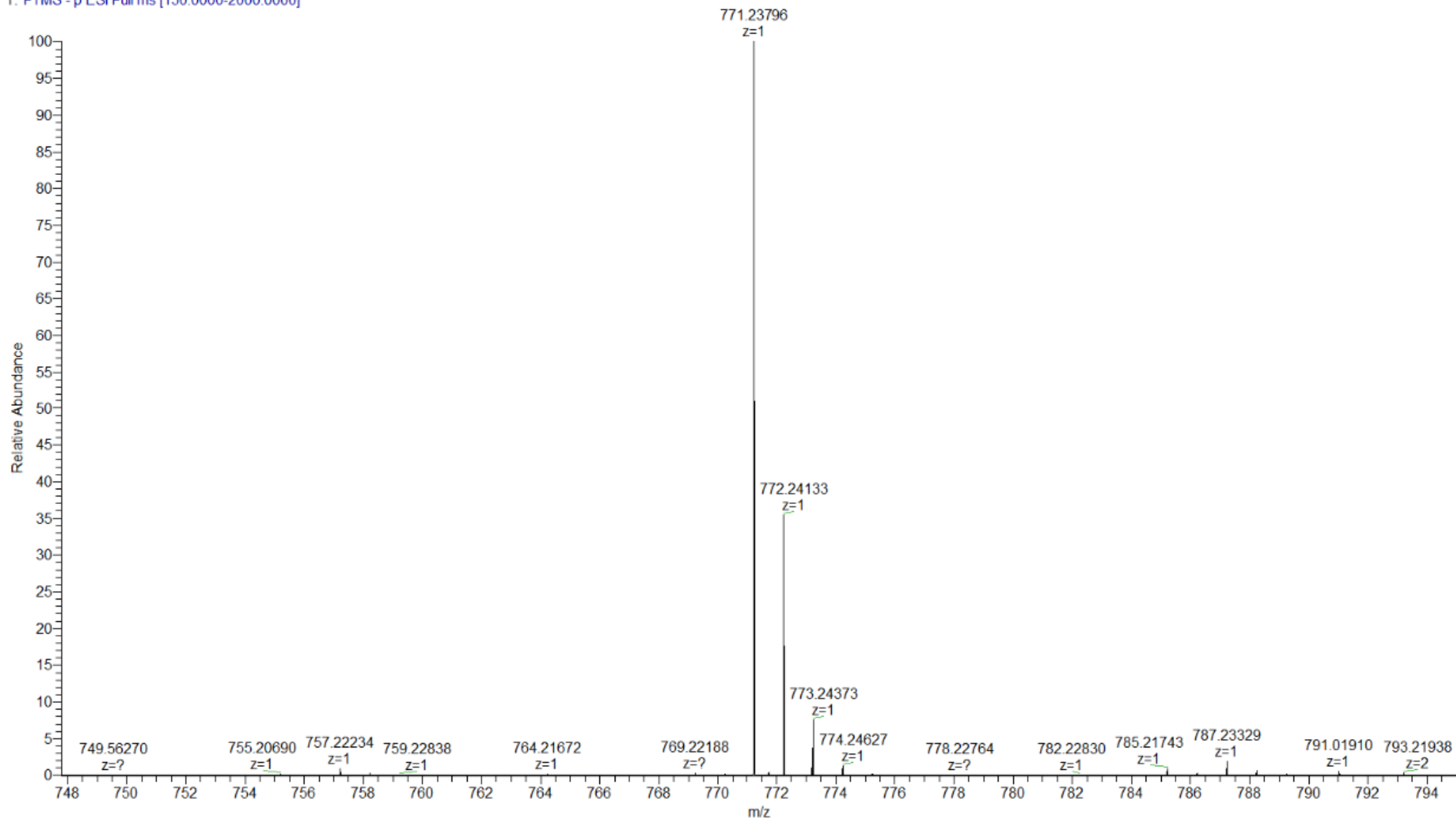


RP-HPLC (conditions c)



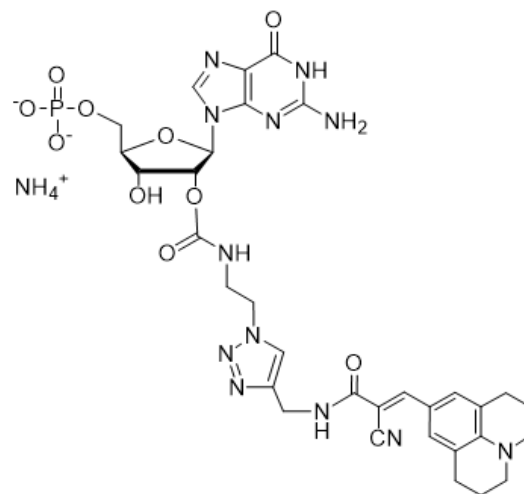
MS (-) ESI (Calc. [M-H]⁻ C₃₀H₃₆N₁₂O₁₁P⁻ : 771.2370, found: 771.23796)

200213_Psu_45 #2-64 RT: 0.02-0.68 AV: 63 NL: 1.11E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

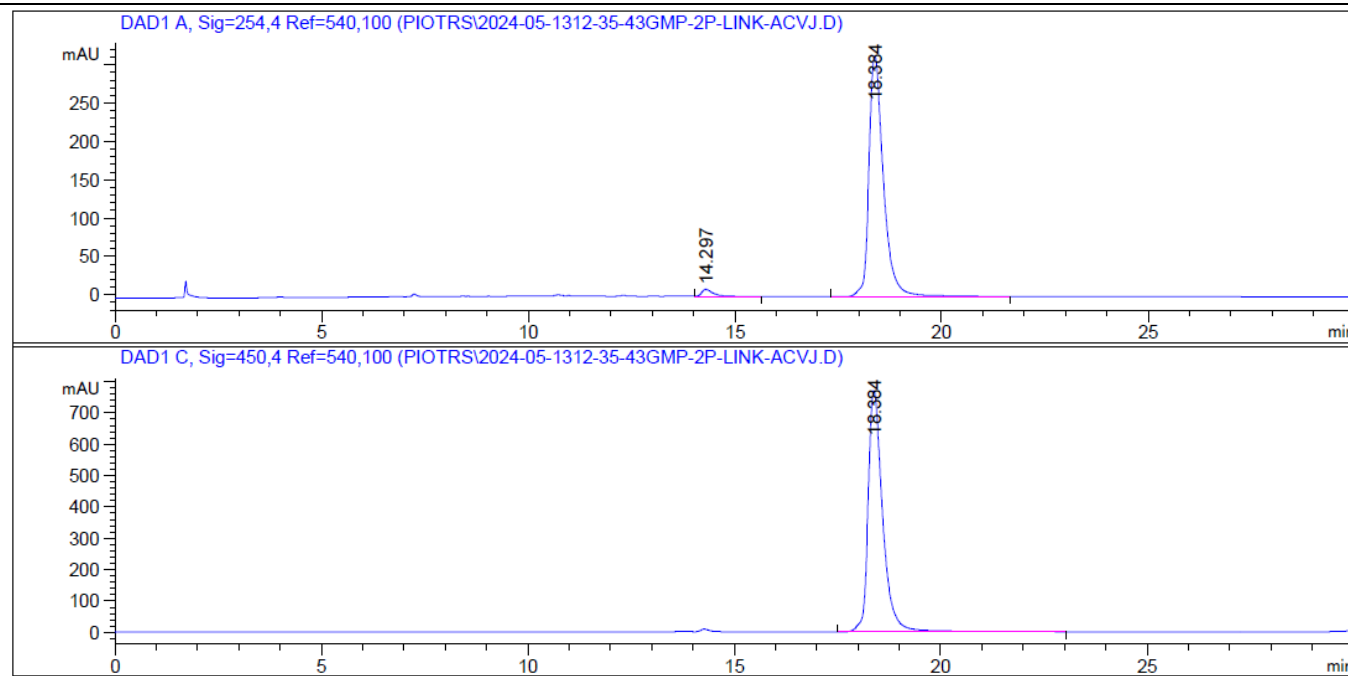


Compound 10d-2': GMP-2'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-ACVJ (NH₄⁺ salt)

Chemical structure

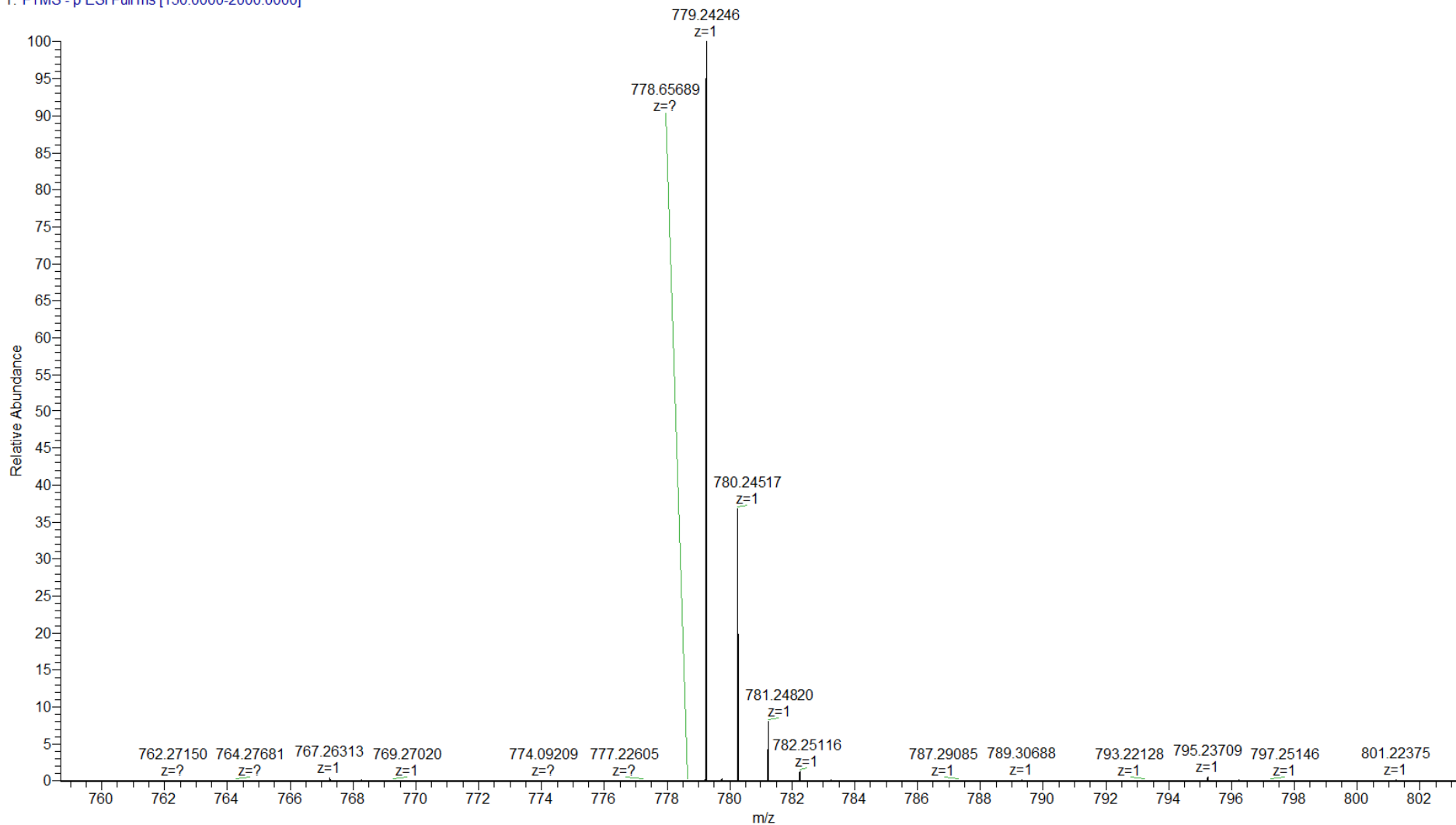


RP-HPLC (conditions c)



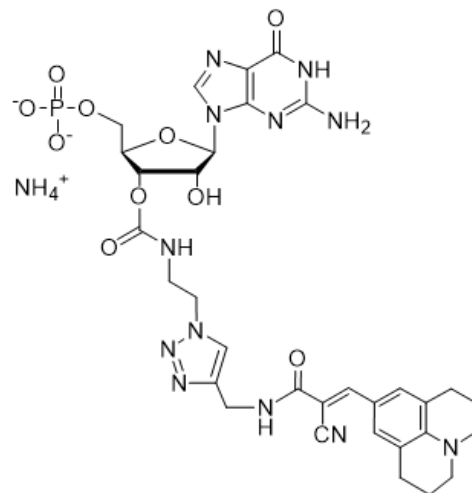
MS (-) ESI (Calc. [M-H]⁻ C₃₂H₃₆N₁₂O₁₀P⁻ : 779.2421, found: 779.24246)

200702_PSU_03 #6-50 RT: 0.06-0.48 AV: 45 NL: 2.12E7
T: FTMS - p ESI Full ms [150.0000-2000.0000]

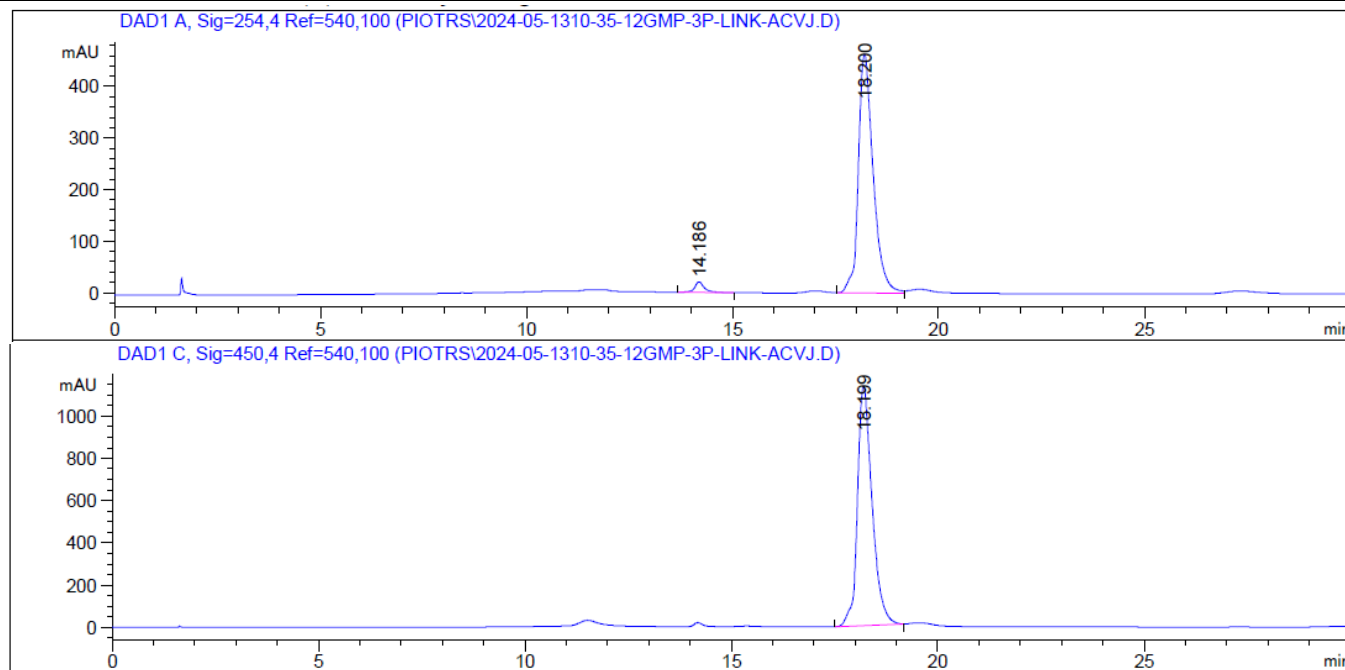


Compound 10d-3': GMP-3'-O-C(O)-NH-CH₂-CH₂-triazole-CH₂-ACVJ (NH₄⁺ salt)

Chemical structure

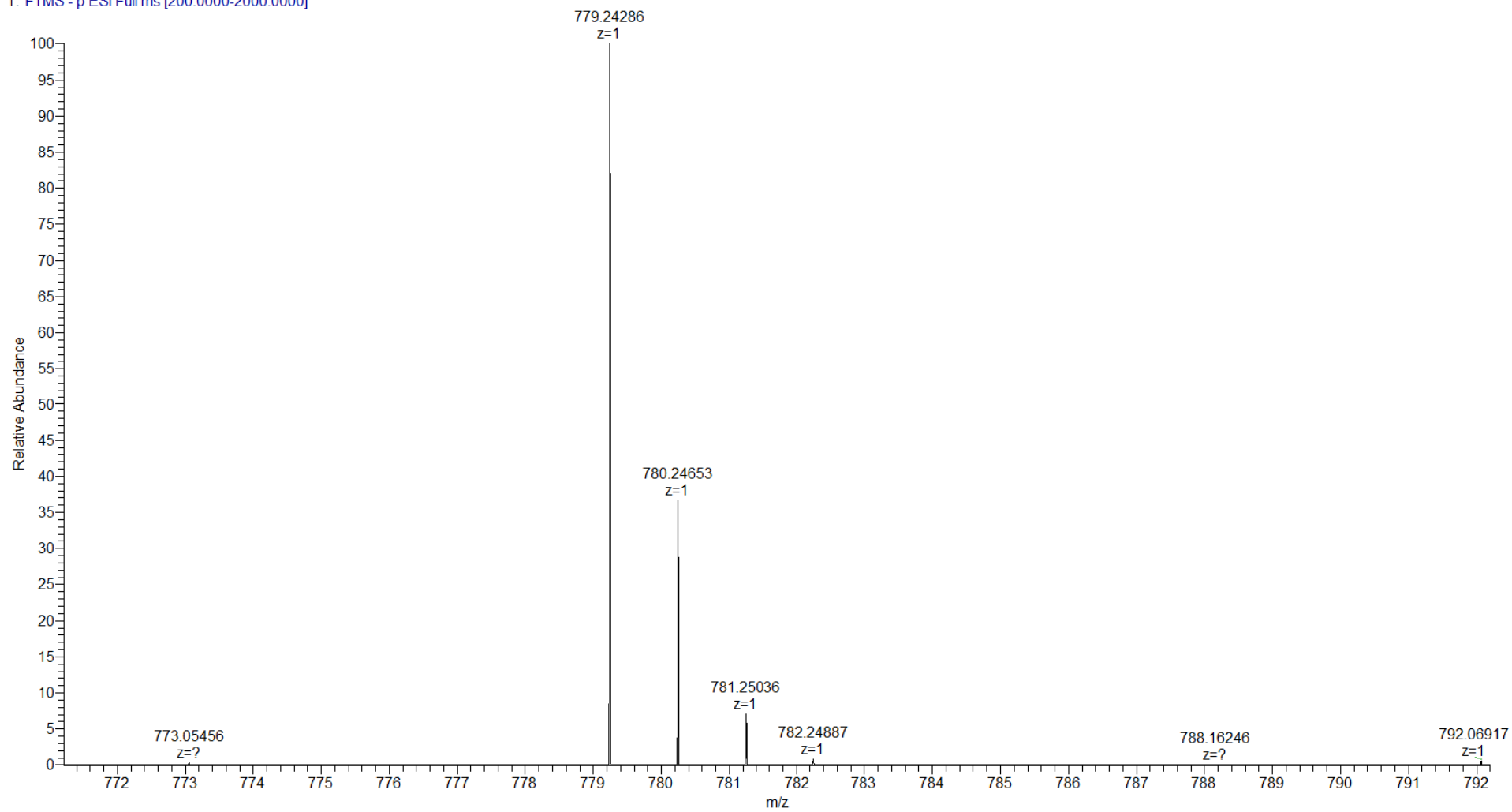


RP-HPLC (conditions c)



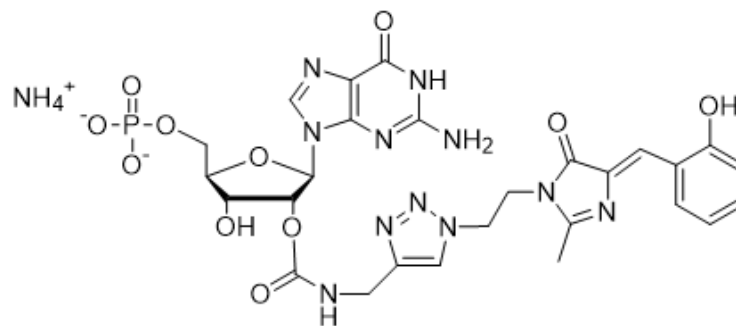
220114_PSU_16 #3-26 RT: 0.03-0.23 AV: 24 NL: 2.80E6
T: FTMS - p ESI Full ms [200.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₃₂H₃₆N₂O₁₀P⁻ : 779.2421, found: 779.24286)

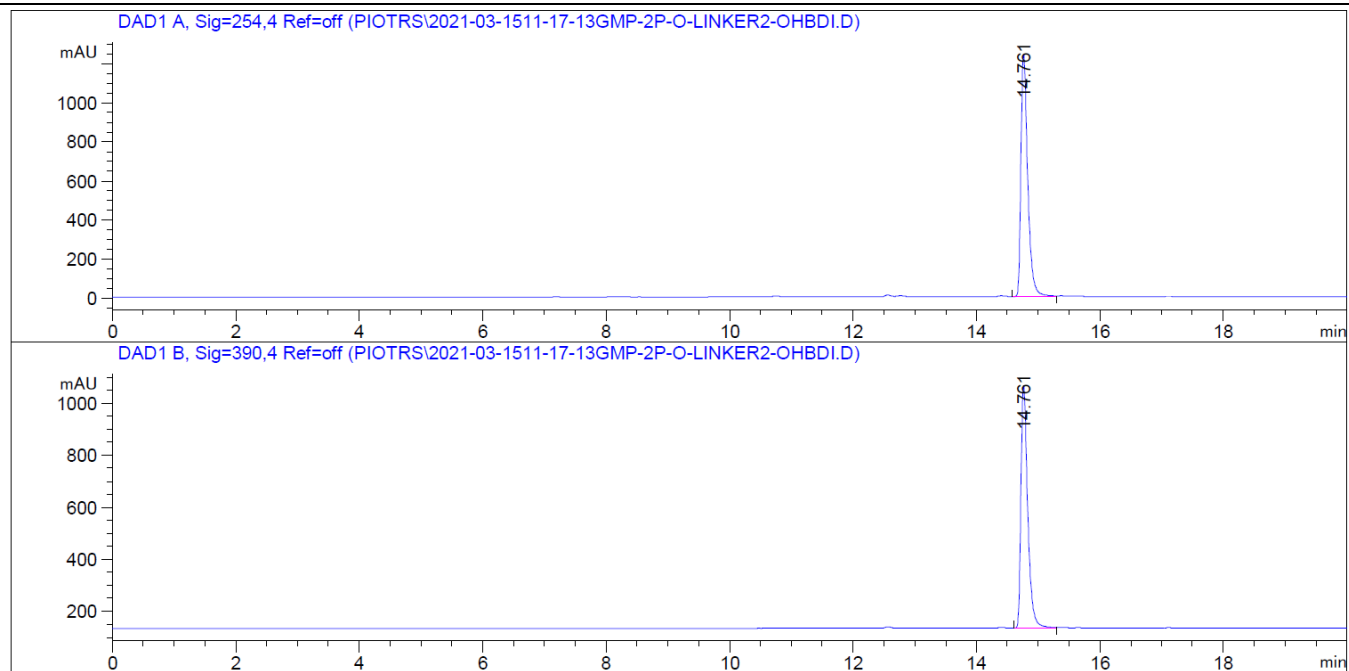


Compound 11b-2': GMP-2'-O-C(O)-NH-CH₂-triazole-CH₂CH₂-oHBI (NH₄⁺ salt)

Chemical structure

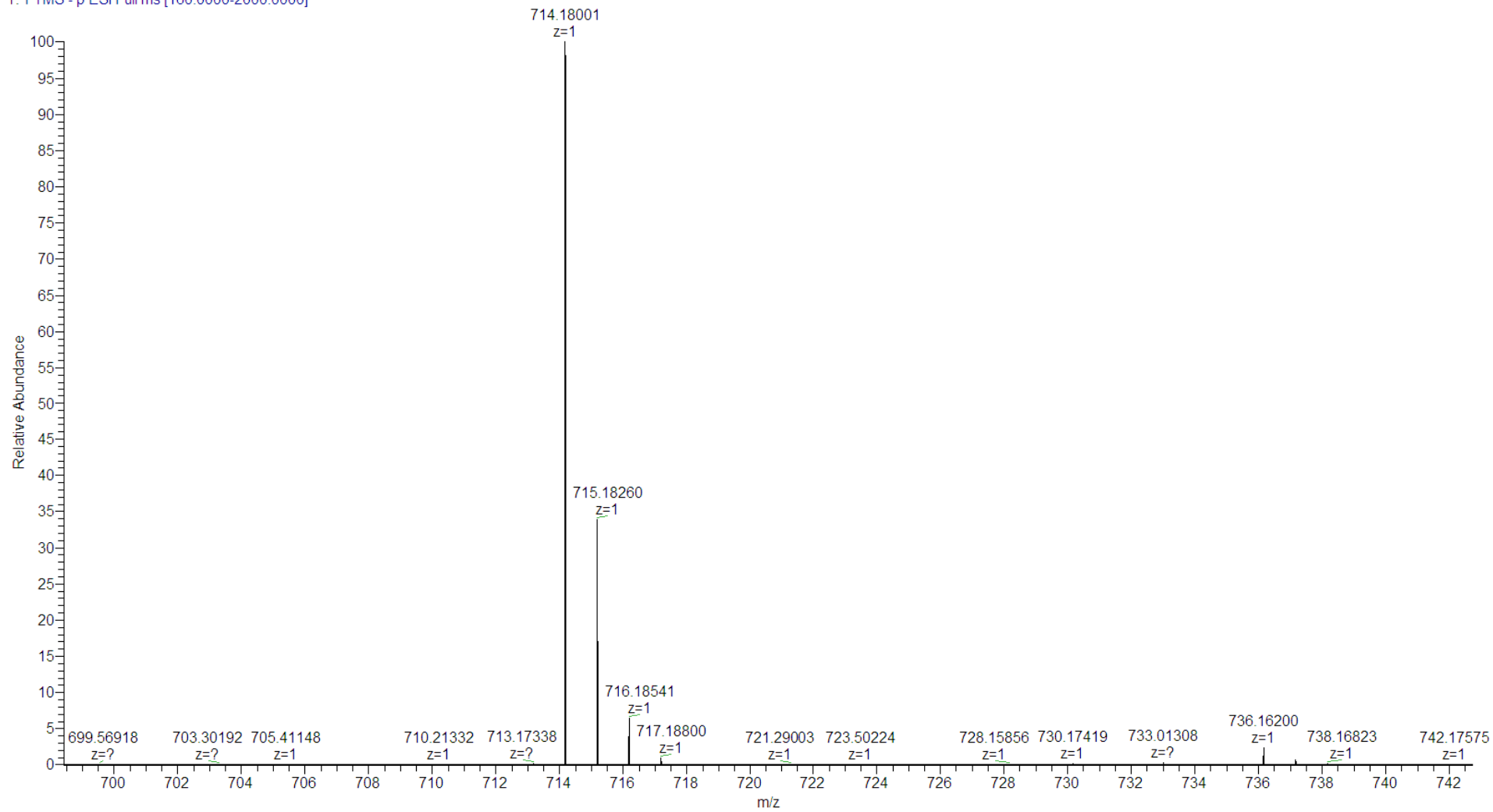


RP-HPLC (conditions c)



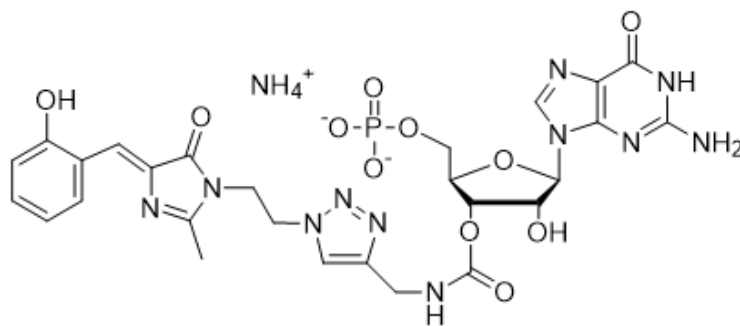
MS (-) ESI (Calc. [M-H]⁻ C₂₇H₂₉N₁₁O₁₁P⁻ : 714.1791, found: 714.18001)

220331_PSu_09 #10-54 RT: 0.09-0.47 AV: 45 NL: 2.76E7
T: FTMS - p ESI Full ms [160.0000-2000.0000]

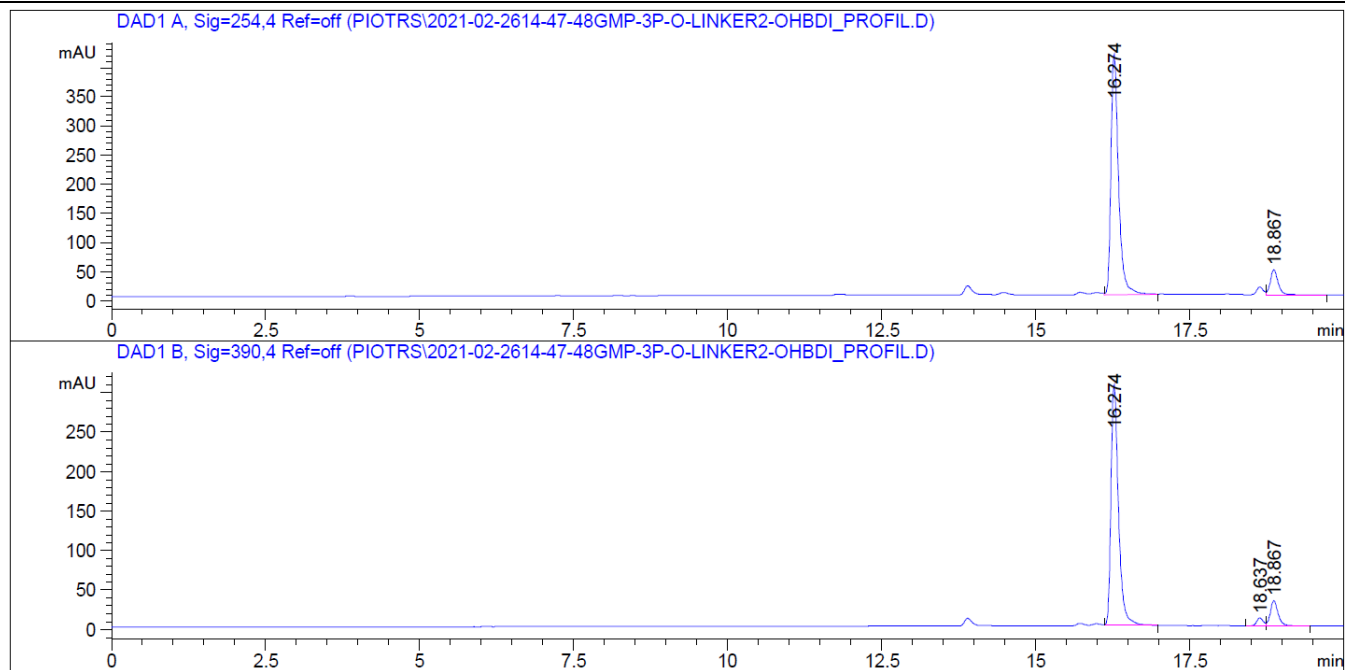


Compound 11b-3': GMP-3'-O-C(O)-NH-CH₂-triazole-CH₂CH₂-oHBI (NH₄⁺ salt)

Chemical structure

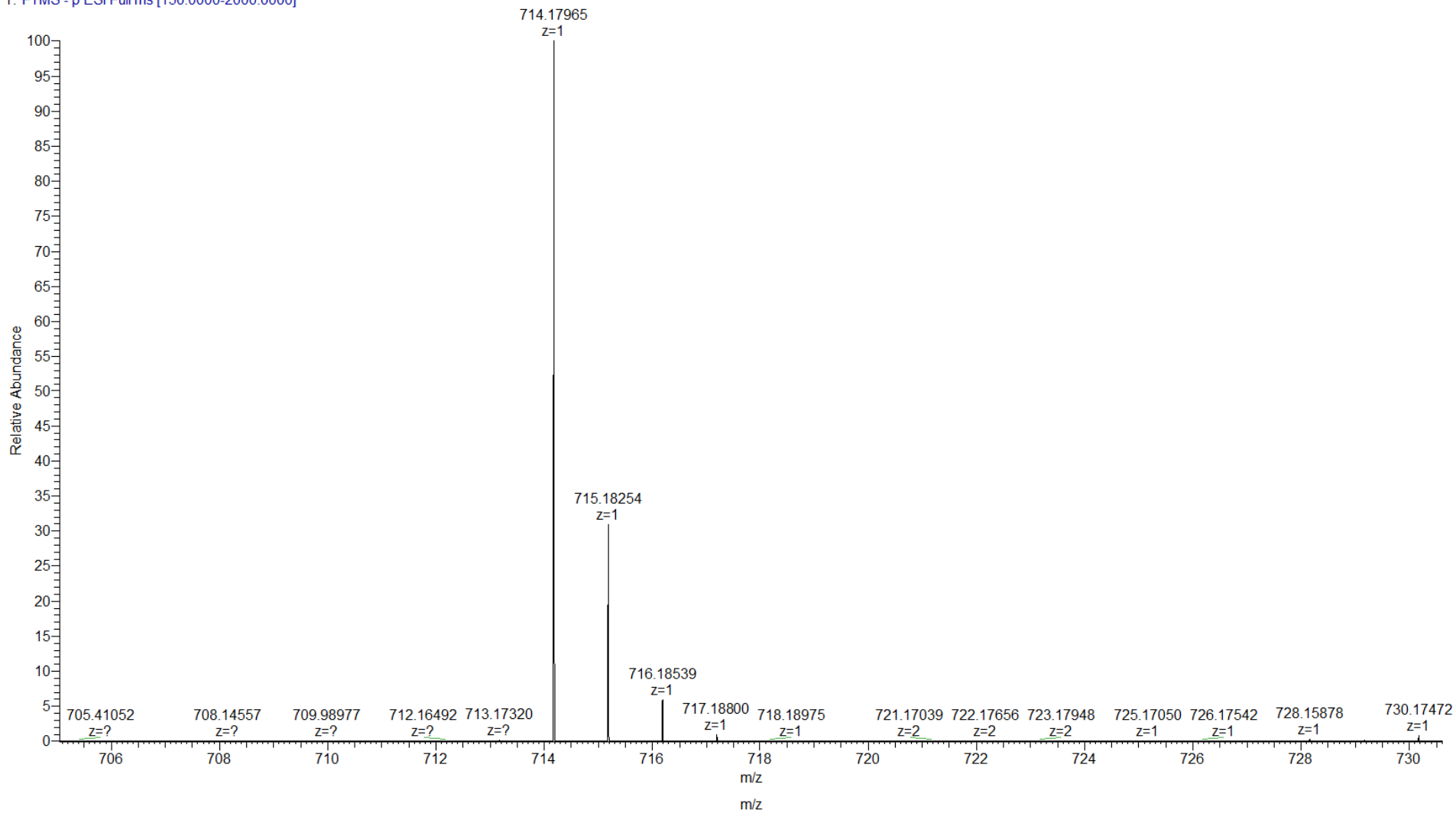


RP-HPLC (conditions c)



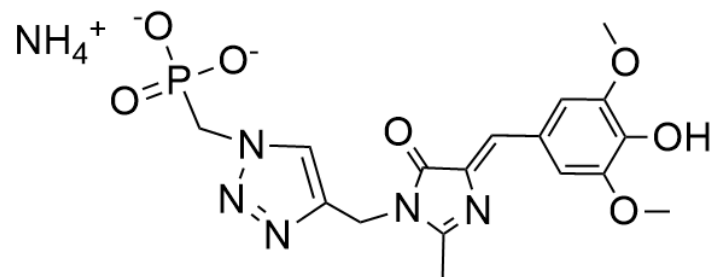
MS (-) ESI (Calc. [M-H]⁻ C₂₇H₂₉N₁₁O₁₁P⁻ : 714.1791, found: 714.17965)

210504_PSu_16_b #4-92 RT: 0.04-0.87 AV: 89 NL: 7.66E7
T: FTMS - p ESI Full ms [150.0000-2000.0000]

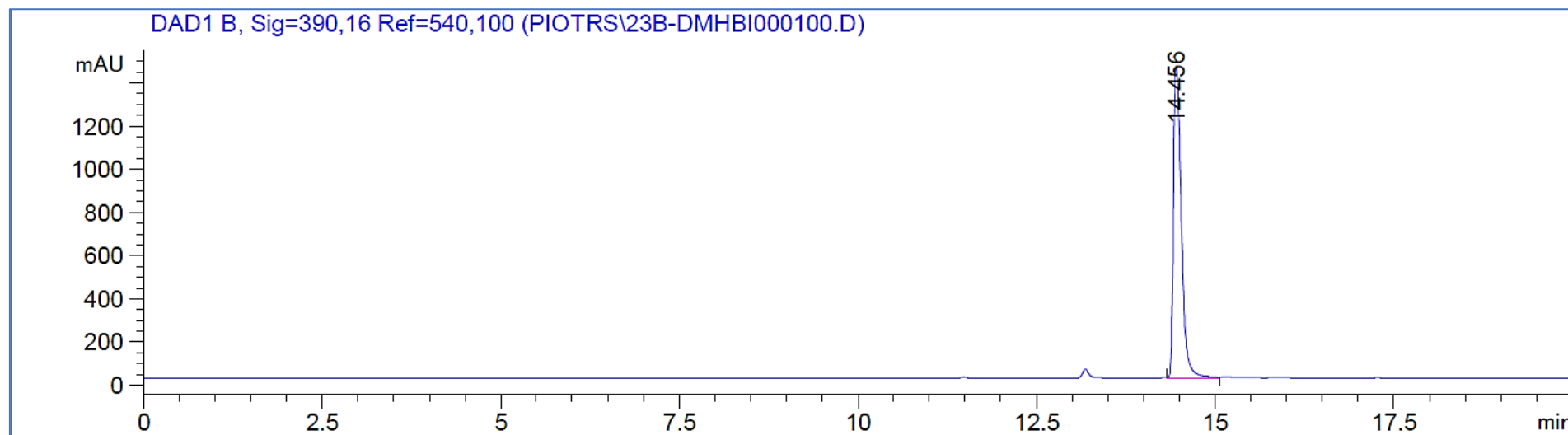


Compound 12a: phosphonate-CH₂-triazole-CH₂-DMHBI (NH₄⁺ salt)

Chemical structure

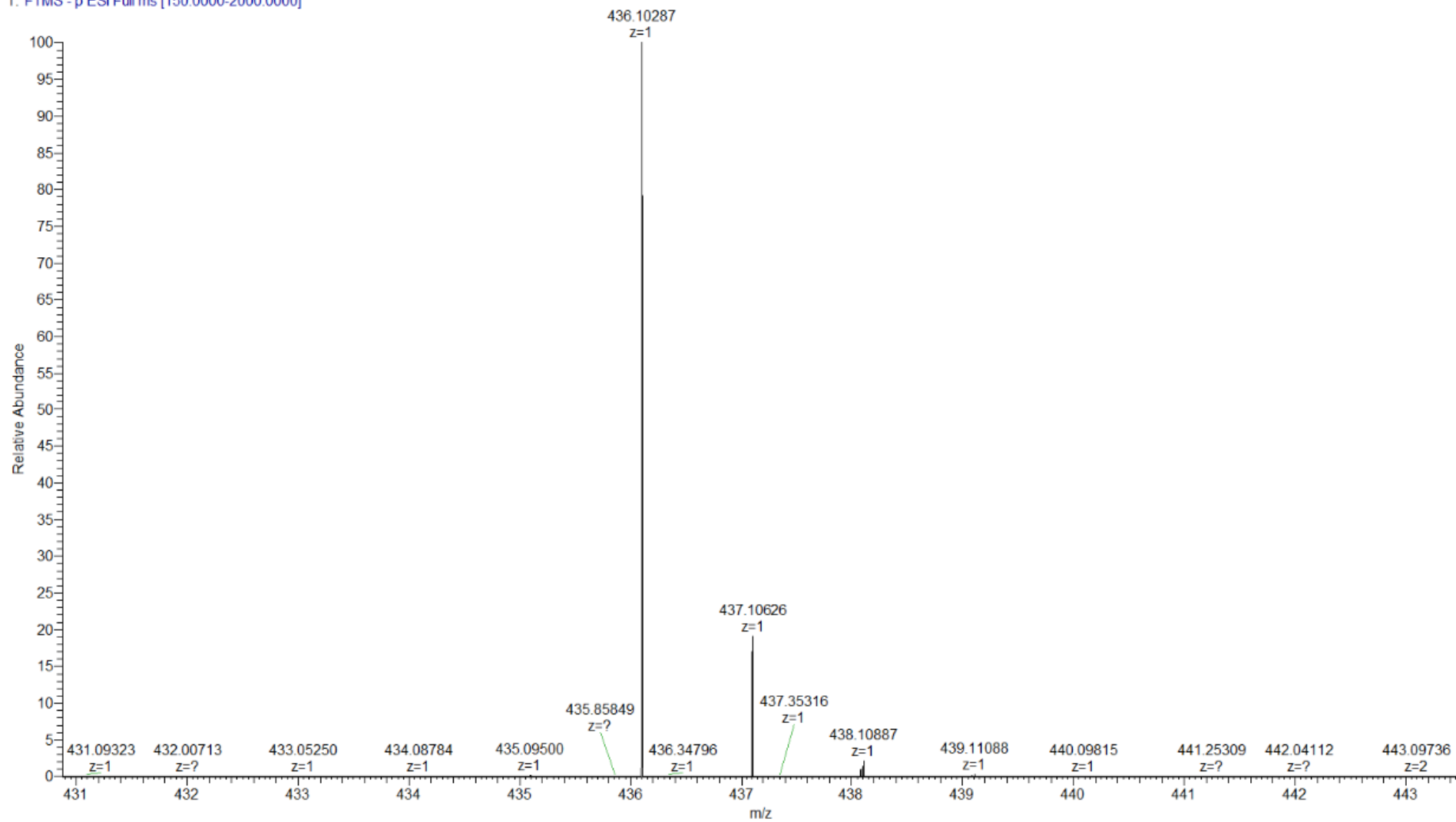


RP-HPLC (conditions c)



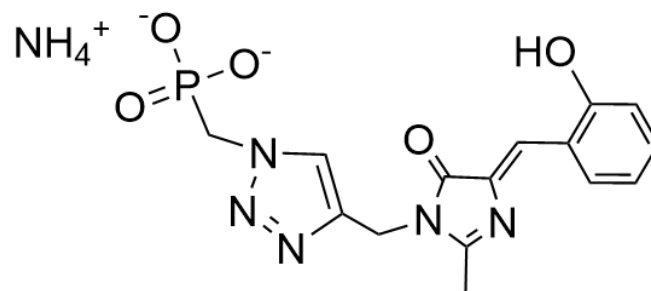
MS (-) ESI (Calc. [M-H]⁻ C₁₇H₁₉N₅O₇P⁻ : 436.1028, found: 436.10287)

200213_Psu_39 #12-89 RT: 0.12-0.91 AV: 78 NL: 1.06E7
T: FTMS - p ESI Full ms [150.0000-2000.0000]

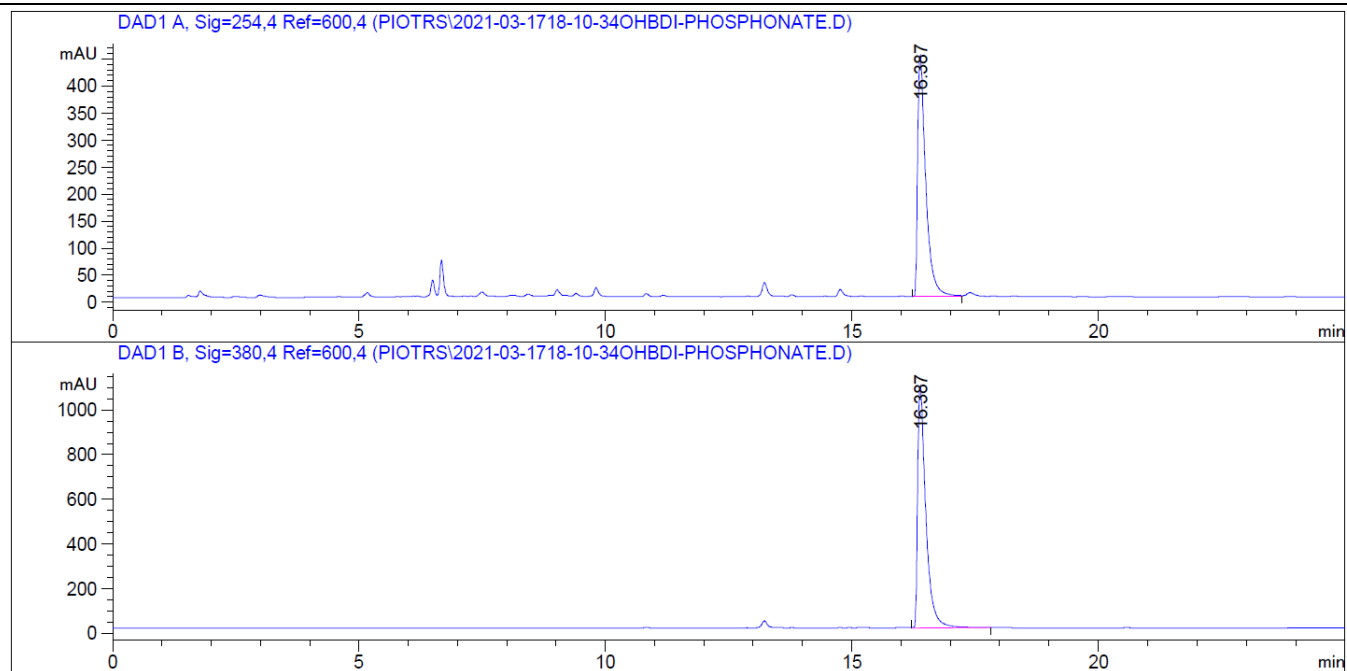


Compound 12b: phosphonate-CH₂-triazole-CH₂-oHBI (NH₄⁺ salt)

Chemical structure

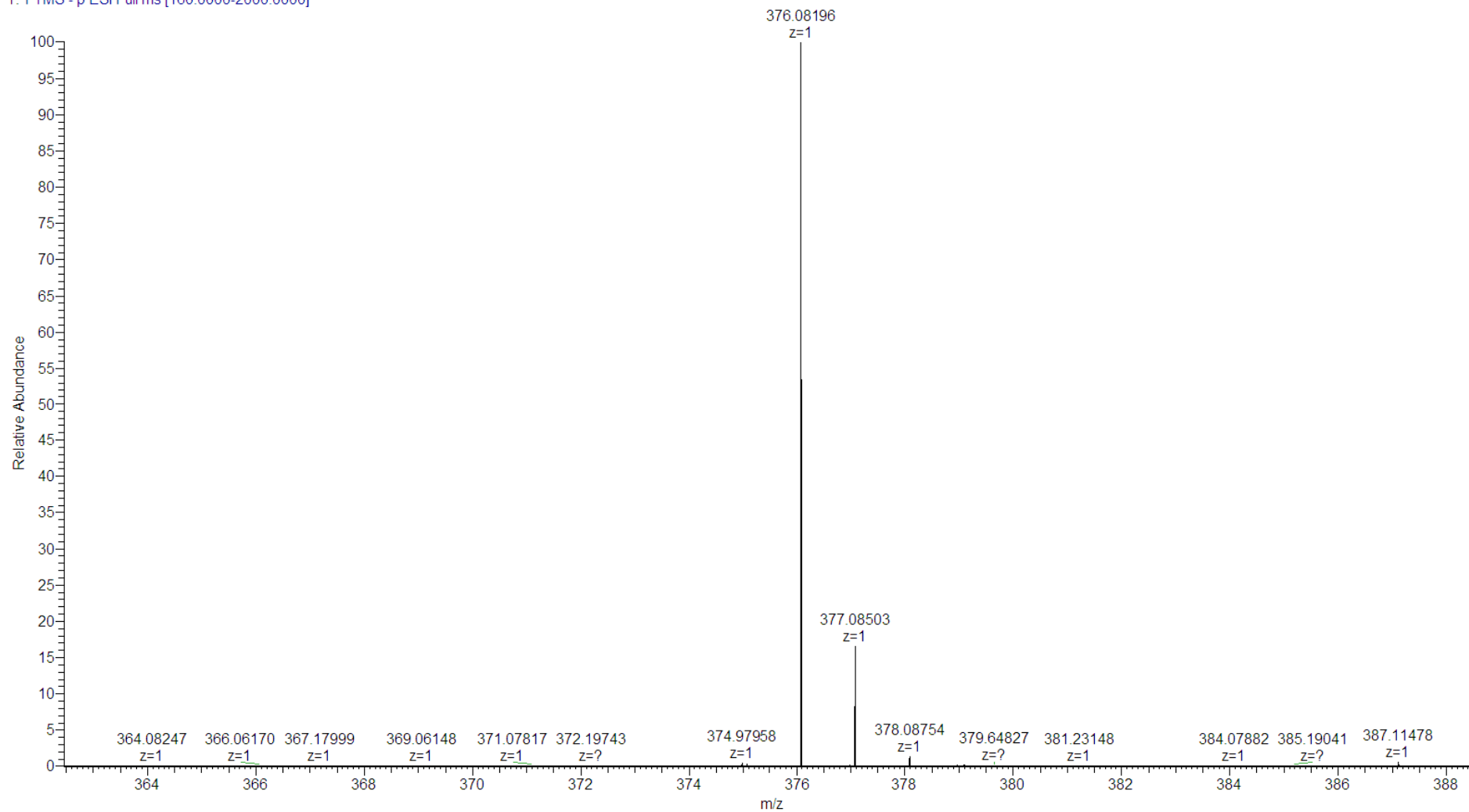


RP-HPLC (conditions c)



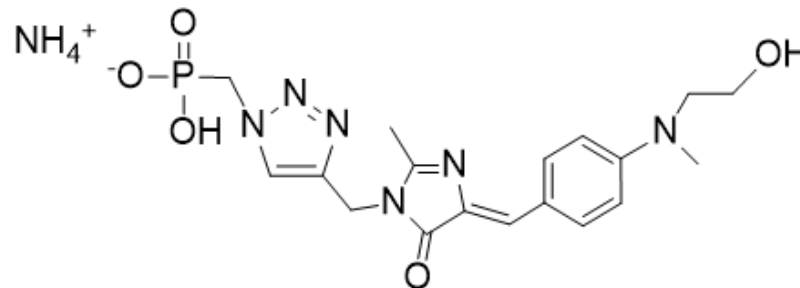
210629_PSu_7 #9-44 RT: 0.08-0.38 AV: 36 NL: 1.84E8
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₁₅H₁₅N₅O₅P⁻ : 376.0816, found: 376.08196)

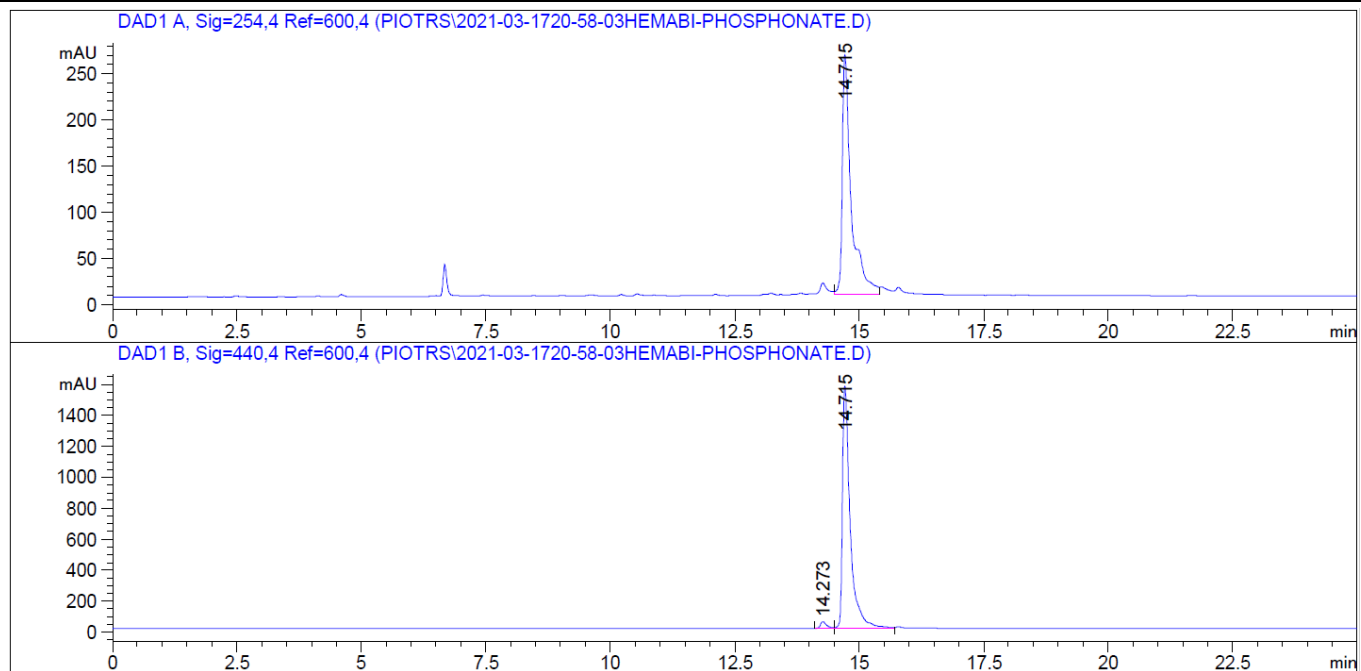


Compound 12c: phosphonate-CH₂-triazole-CH₂-HEMABI (NH₄⁺ salt)

Chemical structure

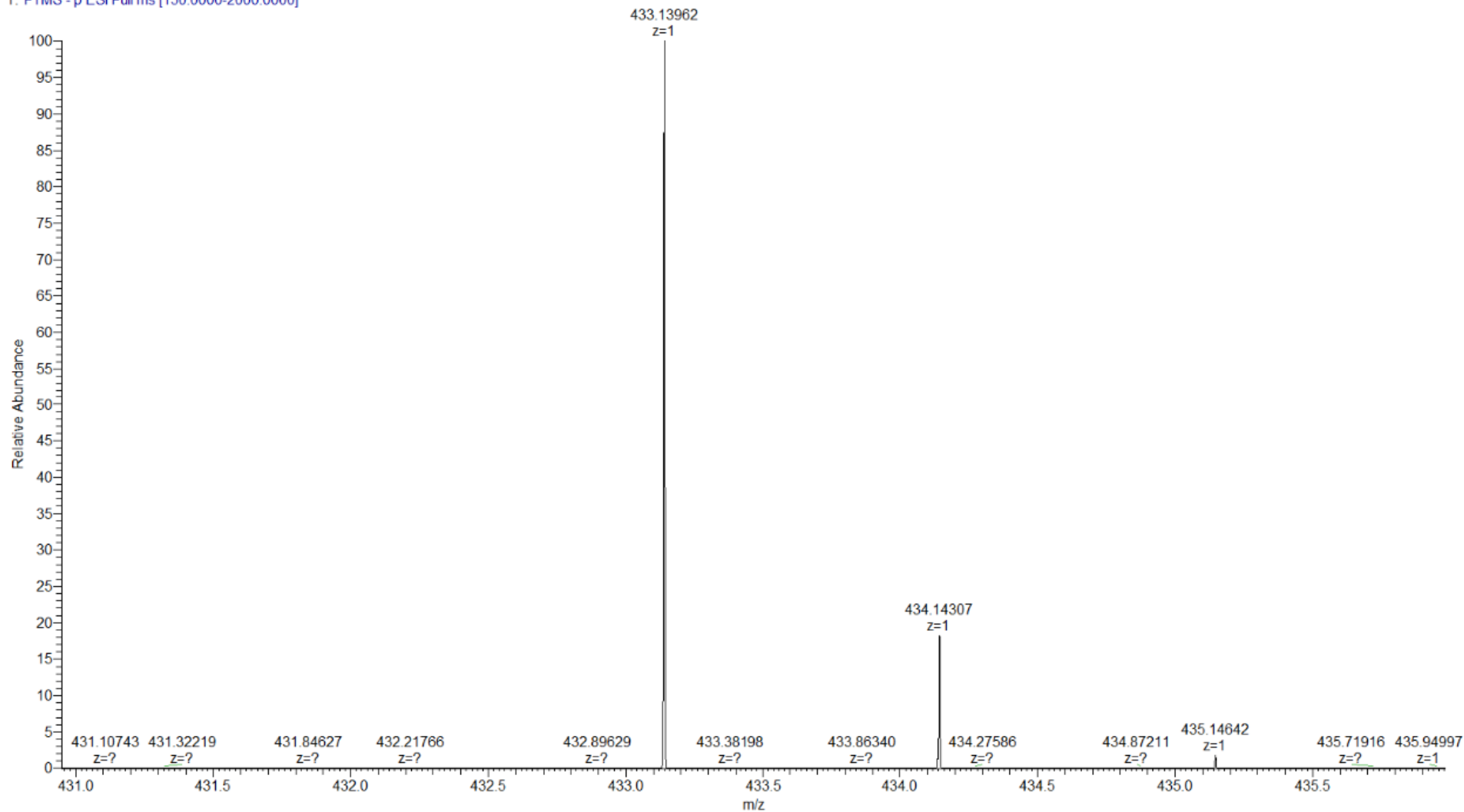


RP-HPLC (conditions c)



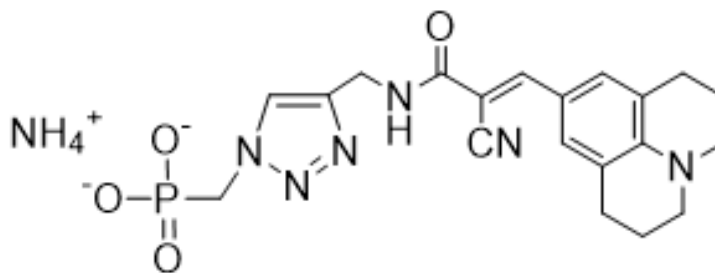
MS (-) ESI (Calc. [M-H]⁻ C₁₈H₂₂N₆O₅P⁻ : 433.1395, found: 433.13962)

200213_Psu_40 #6-50 RT: 0.06-0.51 AV: 45 NL: 2.33E6
T: FTMS -p ESI Full ms [150.0000-2000.0000]

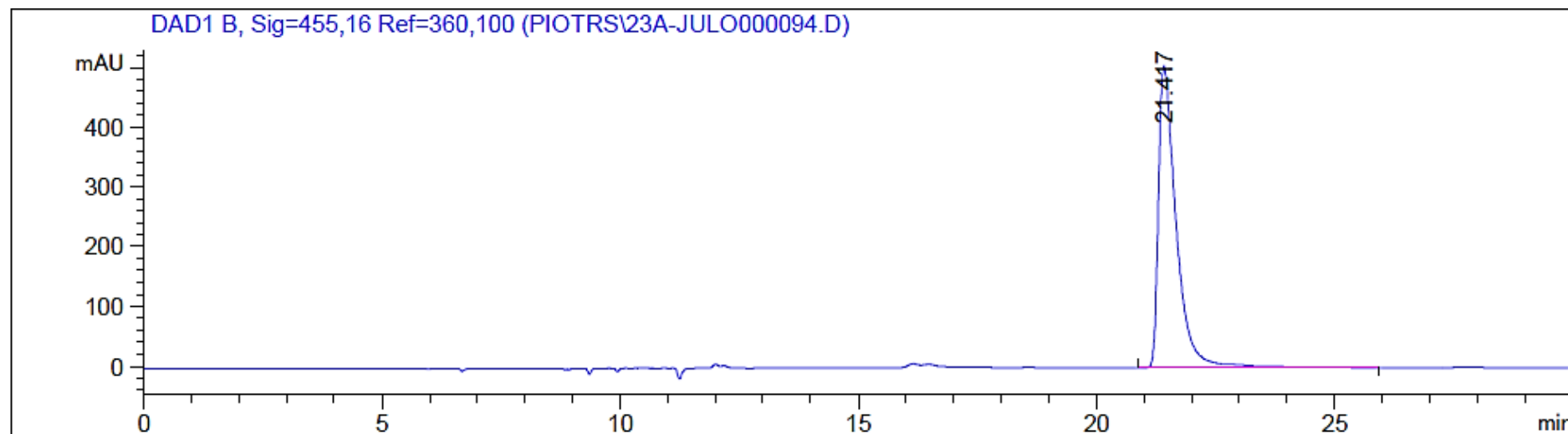


Compound 12d: phosphonate-CH₂-triazole-CH₂-ACVJ (NH₄⁺ salt)

Chemical structure

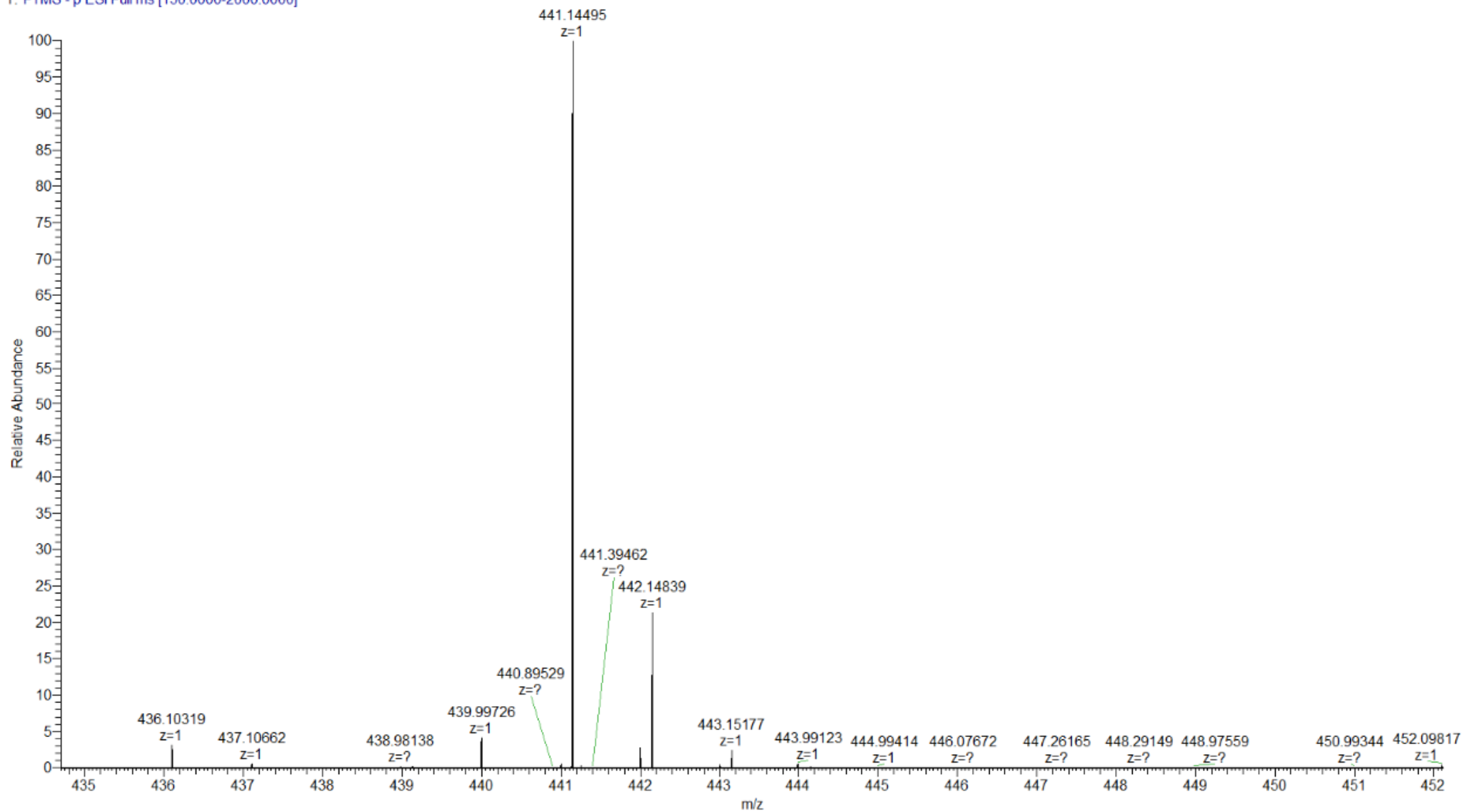


RP-HPLC (conditions b)



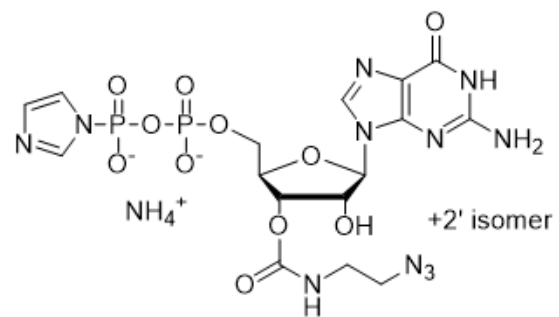
MS (-) ESI (Calc. [M-H]⁻ C₂₀H₂₂N₆O₄P⁻: 441.1446, found: 441.14495)

200213_Psu_41 #5-42 RT: 0.05-0.44 AV: 38 NL: 1.42E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]



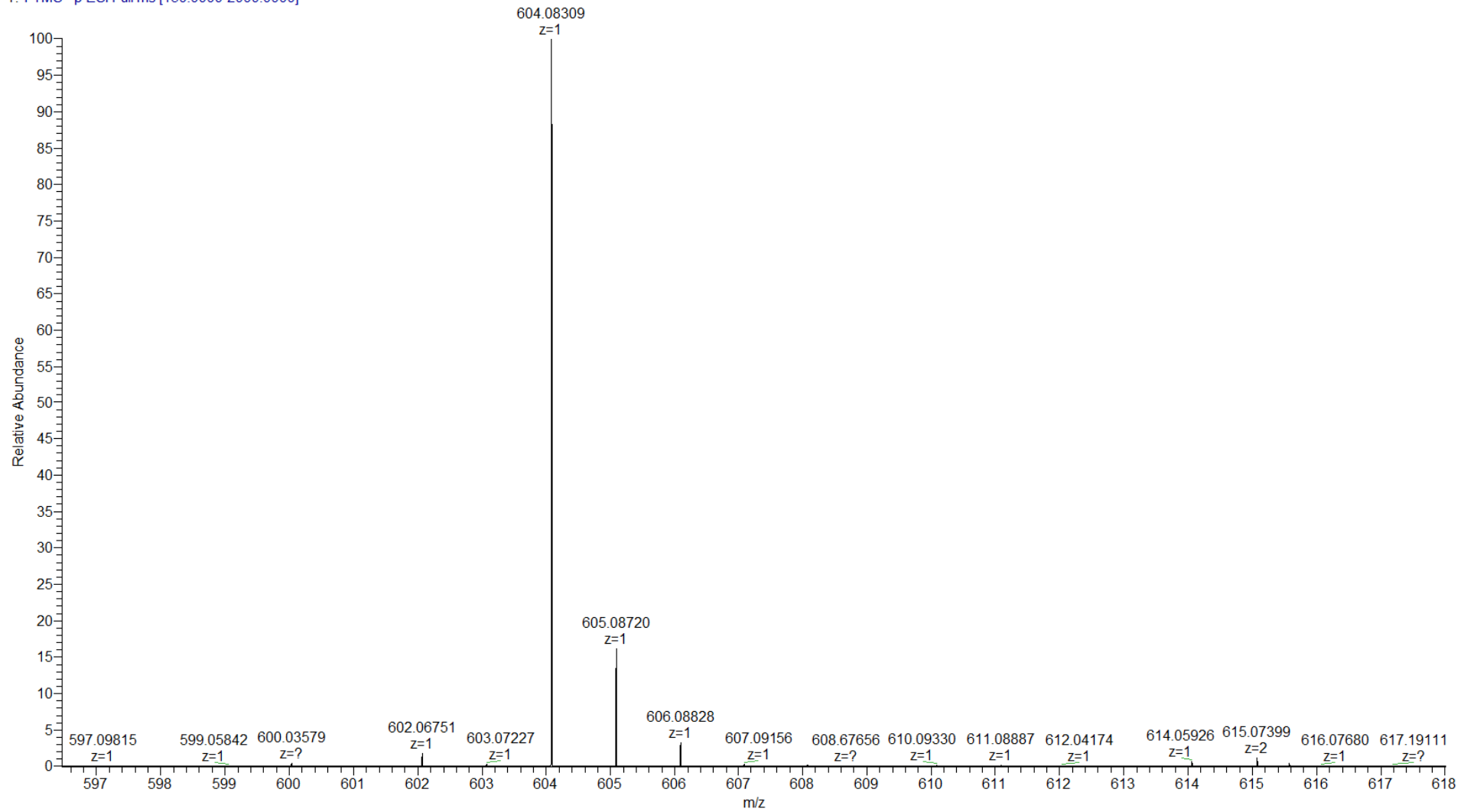
Compound 13: Im-GDP-2'+3'-O-C(O)-NH-CH₂CH₂-N₃ (NH₄⁺ salt)

Chemical structure



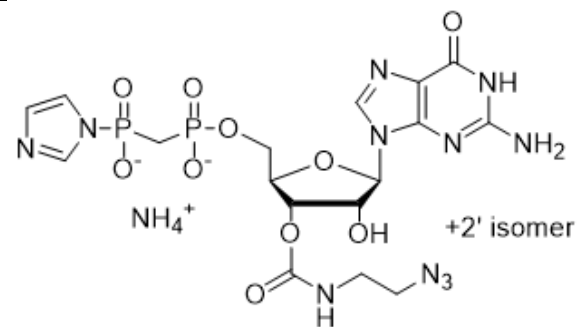
MS (-) ESI (Calc. [M-H]⁻ C₁₆H₂₀N₁₁O₁₁P₂: 604.0825, found: 604.08309)

90415_Psu-4 #7-46 RT: 0.07-0.44 AV: 40 NL: 2.46E7
T: FTMS - p ESI Full ms [150.0000-2000.0000]



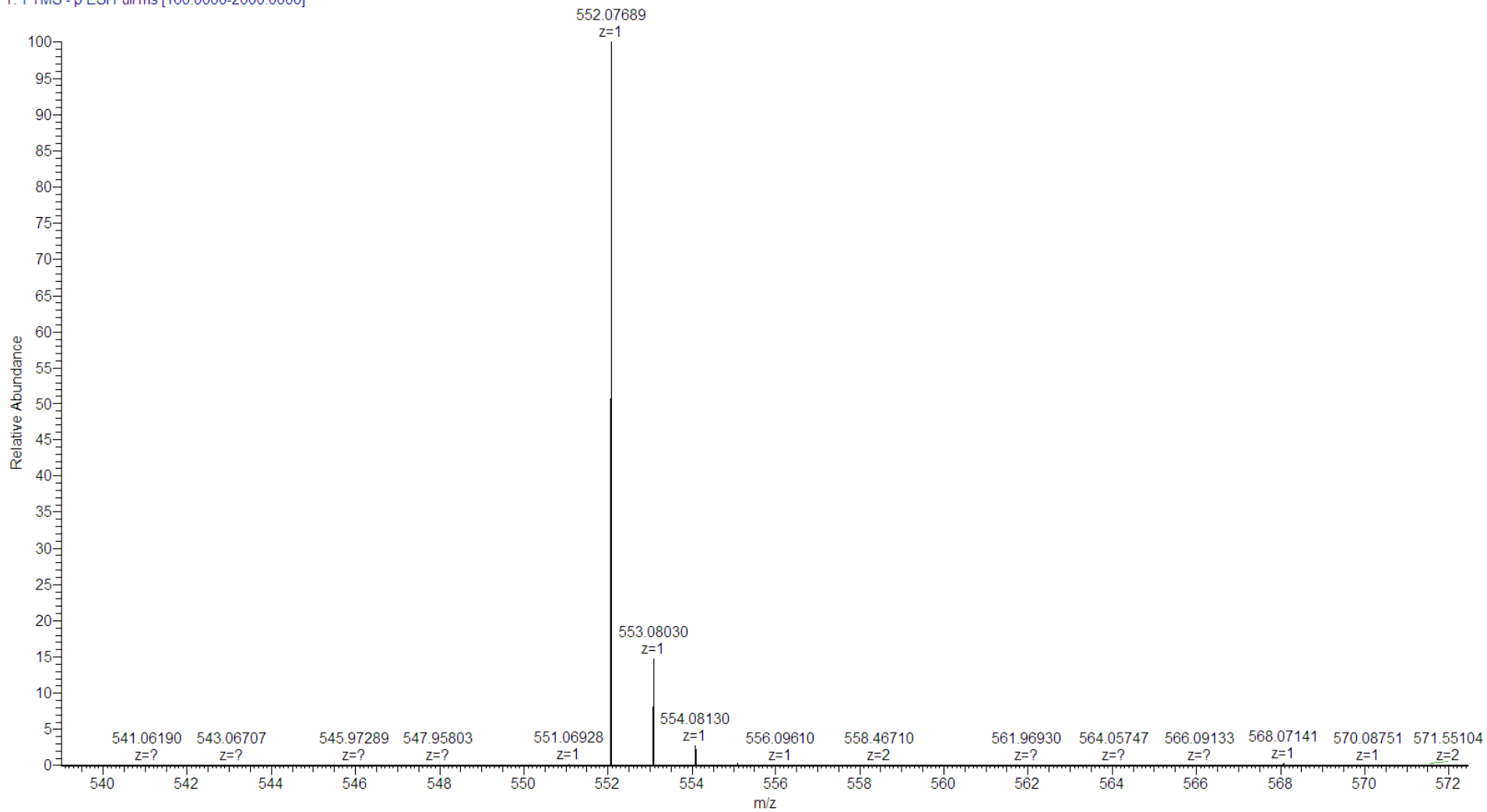
Compound 14: Im-GpCH₂p-2'+3'-O-C(O)-NH-CH₂CH₂-N₃ (NH₄⁺ salt)

Chemical structure



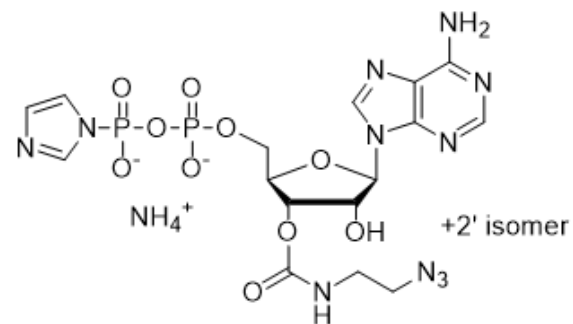
MS (-) ESI (Calc. [M-H]⁻ C₁₄H₂₀N₉O₁₁P₂: 552.0763, found: 552.07689)

220407_PSu_09 #132-212 RT: 1.15-1.85 AV: 81 NL: 7.95E6
T: FTMS - p ESI Full ms [160.0000-2000.0000]

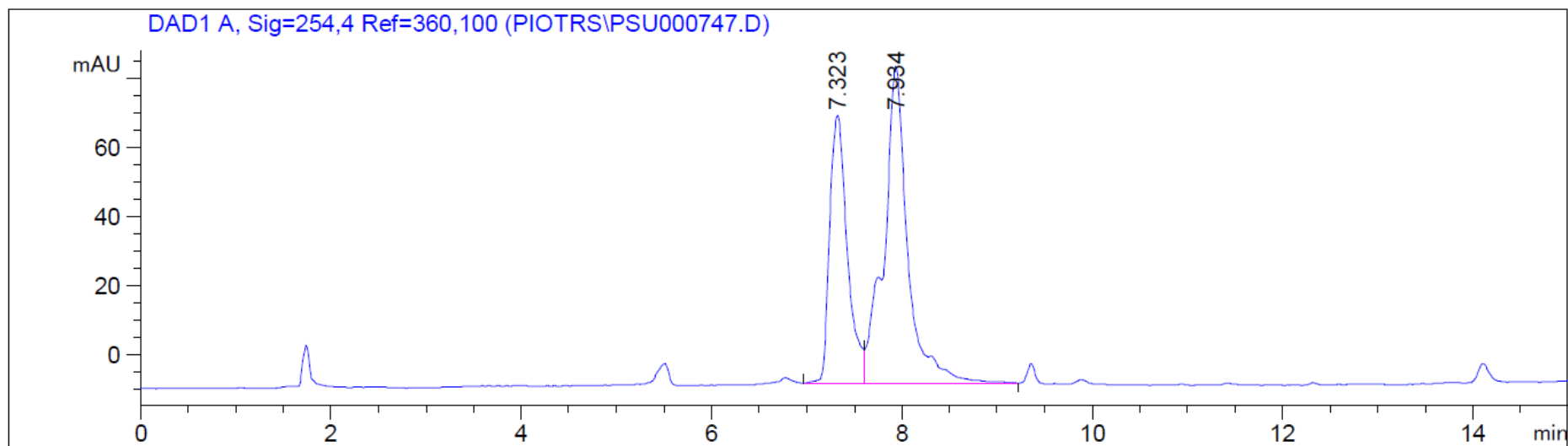


Compound 15: Im-ADP-2'+3'-O-C(O)-NH-CH₂CH₂-N₃ (NH₄⁺ salt)

Chemical structure

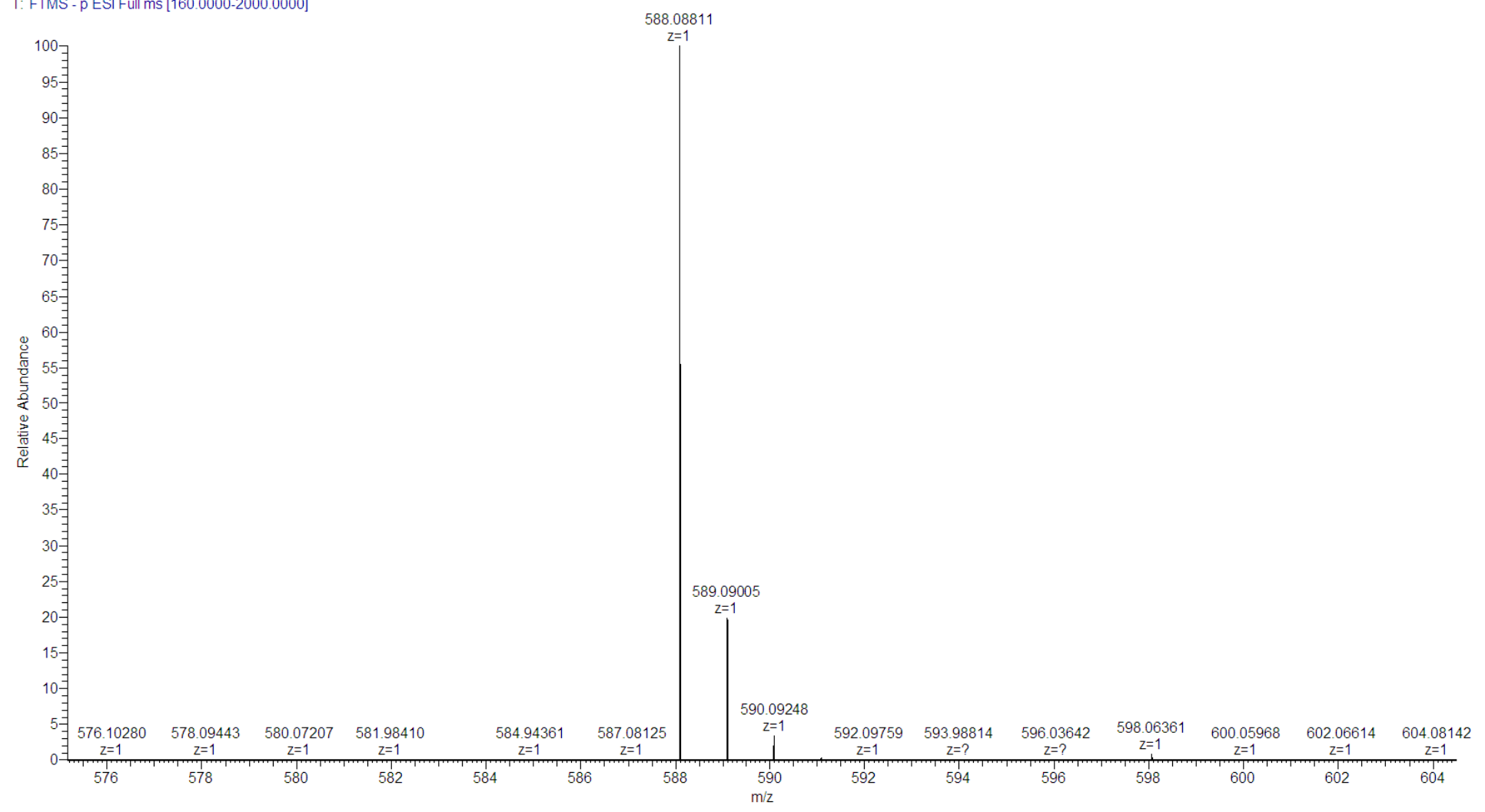


RP-HPLC (conditions c)



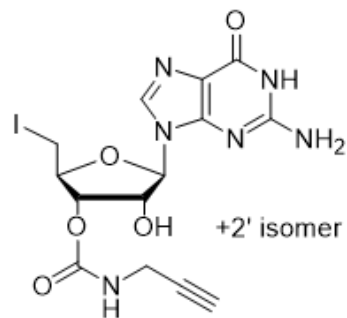
220407_PSu_07 #13-82 RT: 0.11-0.72 AV: 70 NL: 3.87E7
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₁₆H₂₀N₁₁O₁₀P₂: 588.0875, found: 588.08811)

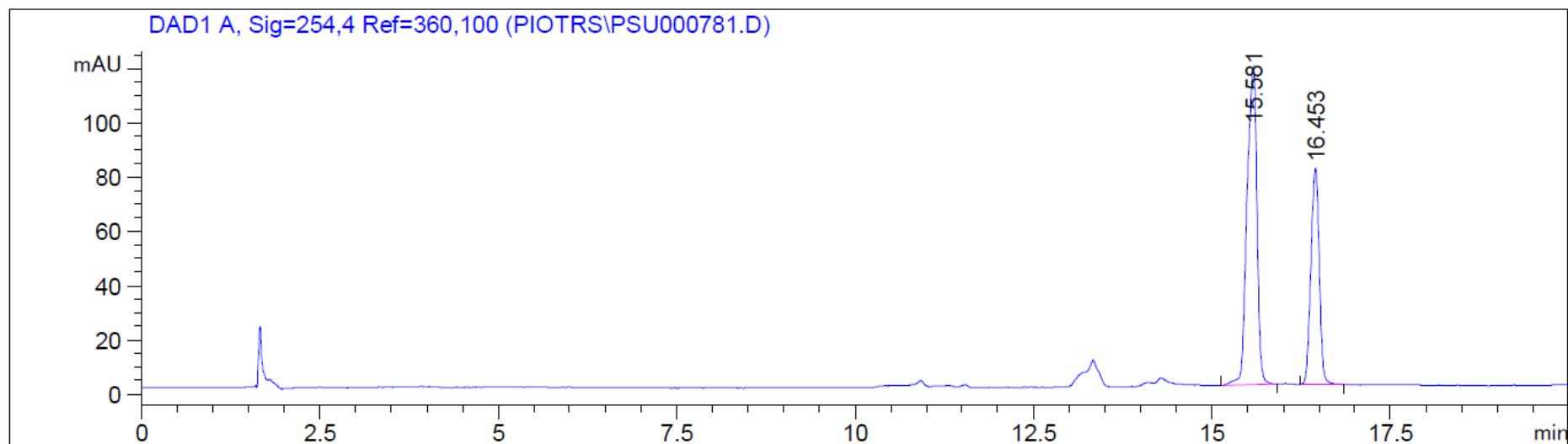


Compound 16: 5'-I-Guo-2'+3'-O-C(O)-NH-C₃H₃

Chemical structure

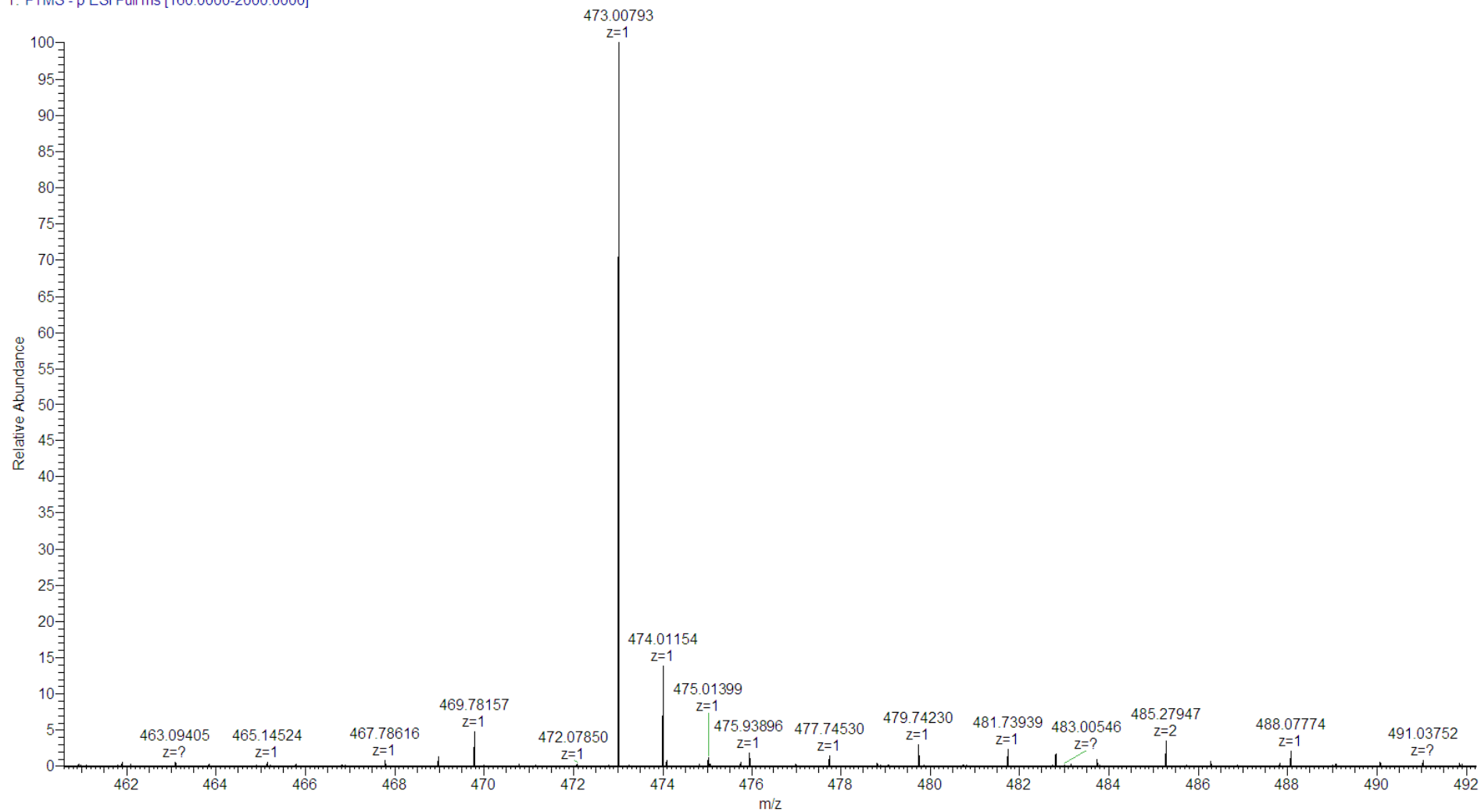


RP-HPLC (conditions c)



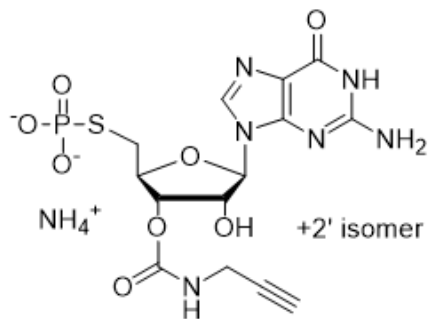
220413_PSu_01 #32-127 RT: 0.28-1.11 AV: 96 NL: 2.50E6
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₁₄H₁₄IN₆O₅ : 473.0076, found: 473.00793)

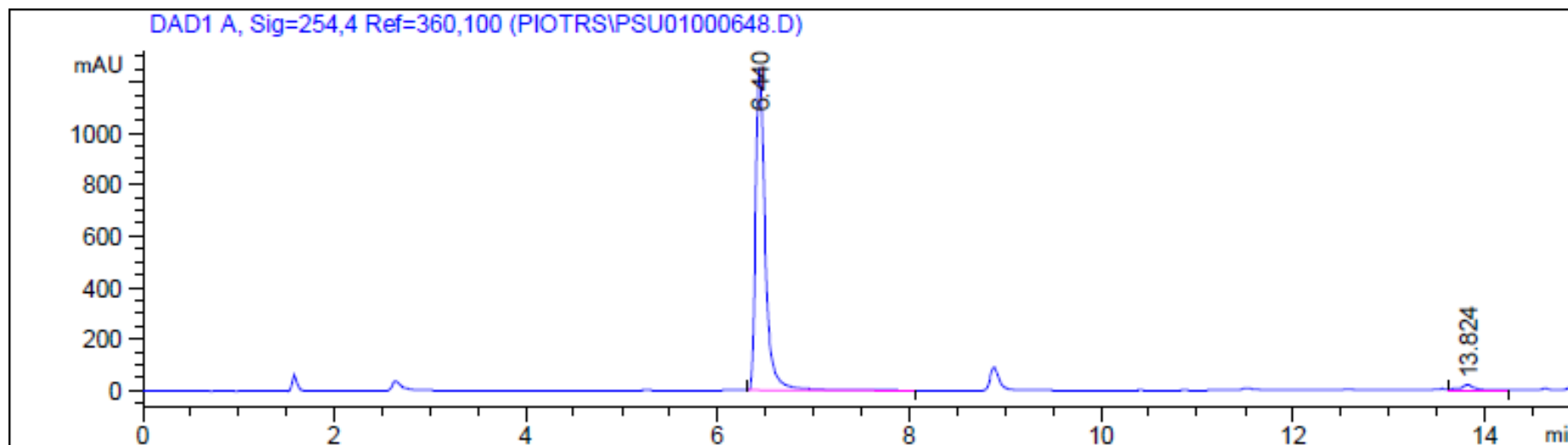


Compound 17: 5'-S-GMP-2'+3'-O-C(O)-NH-C₃H₃ (NH₄⁺ salt)

Chemical structure

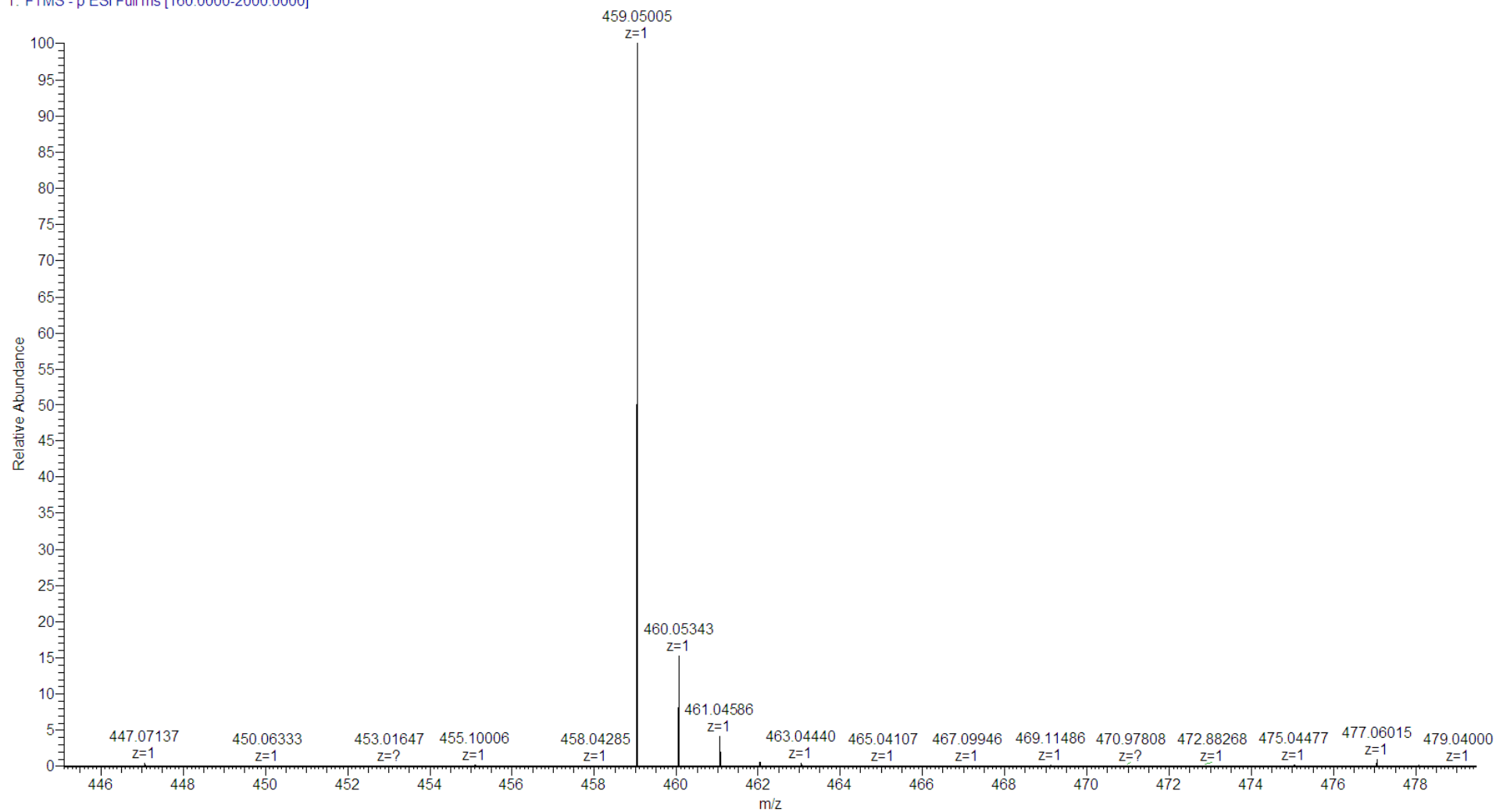


RP-HPLC (conditions c)



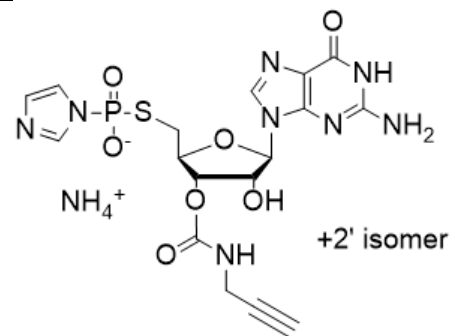
220329_PSu_13 #139-210 RT: 1.21-1.83 AV: 72 NL: 7.57E6
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₁₄H₁₆N₆O₈PS : 459.0493, found: 459.05005)

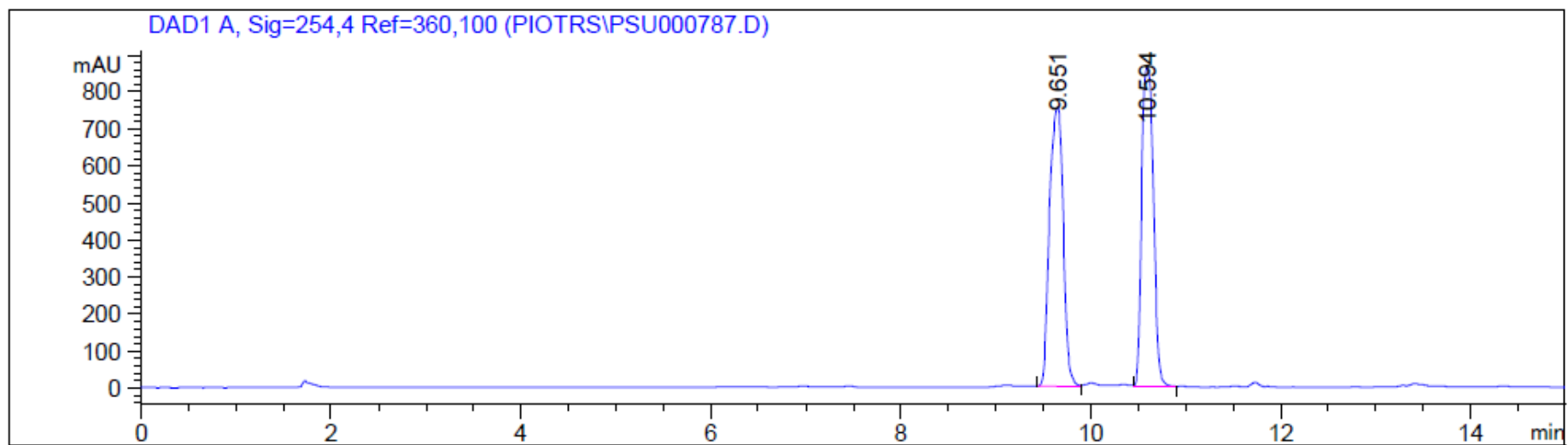


Compound 18: Im-5'-S-GMP-2'+3'-O-C(O)-NH-C₃H₃ (NH₄⁺ salt)

Chemical structure

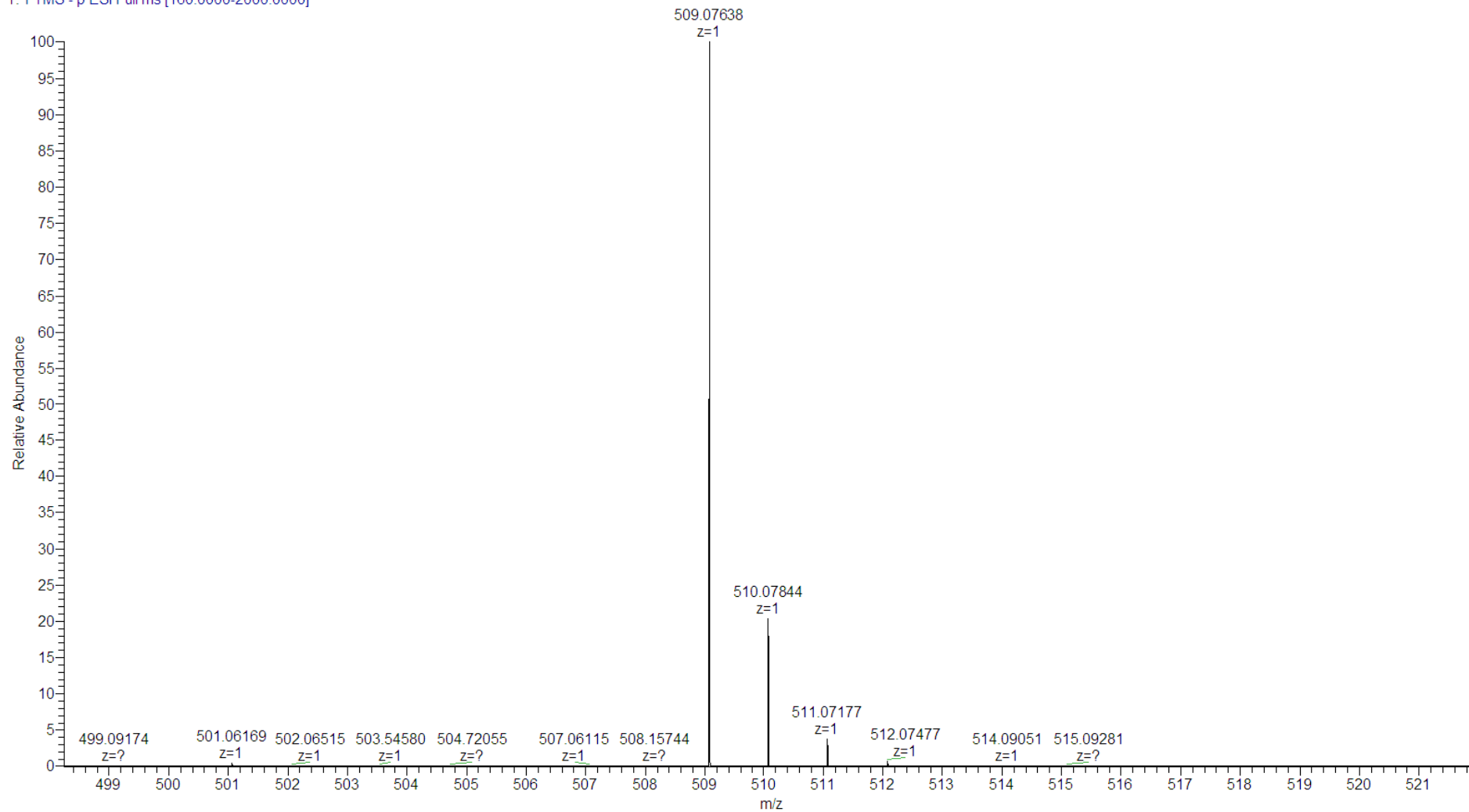


RP-HPLC (conditions c)



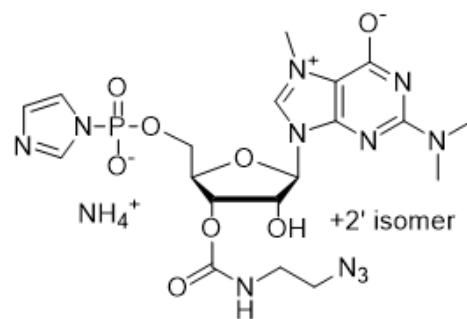
220329_PSu_15 #12-60 RT: 0.10-0.52 AV: 49 NL: 4.82E8
T: FTMS - p ESI Full ms [160.0000-2000.0000]

MS (-) ESI (Calc. [M-H]⁻ C₁₇H₁₈N₈O₇PS : 509.0762, found: 509.07638)



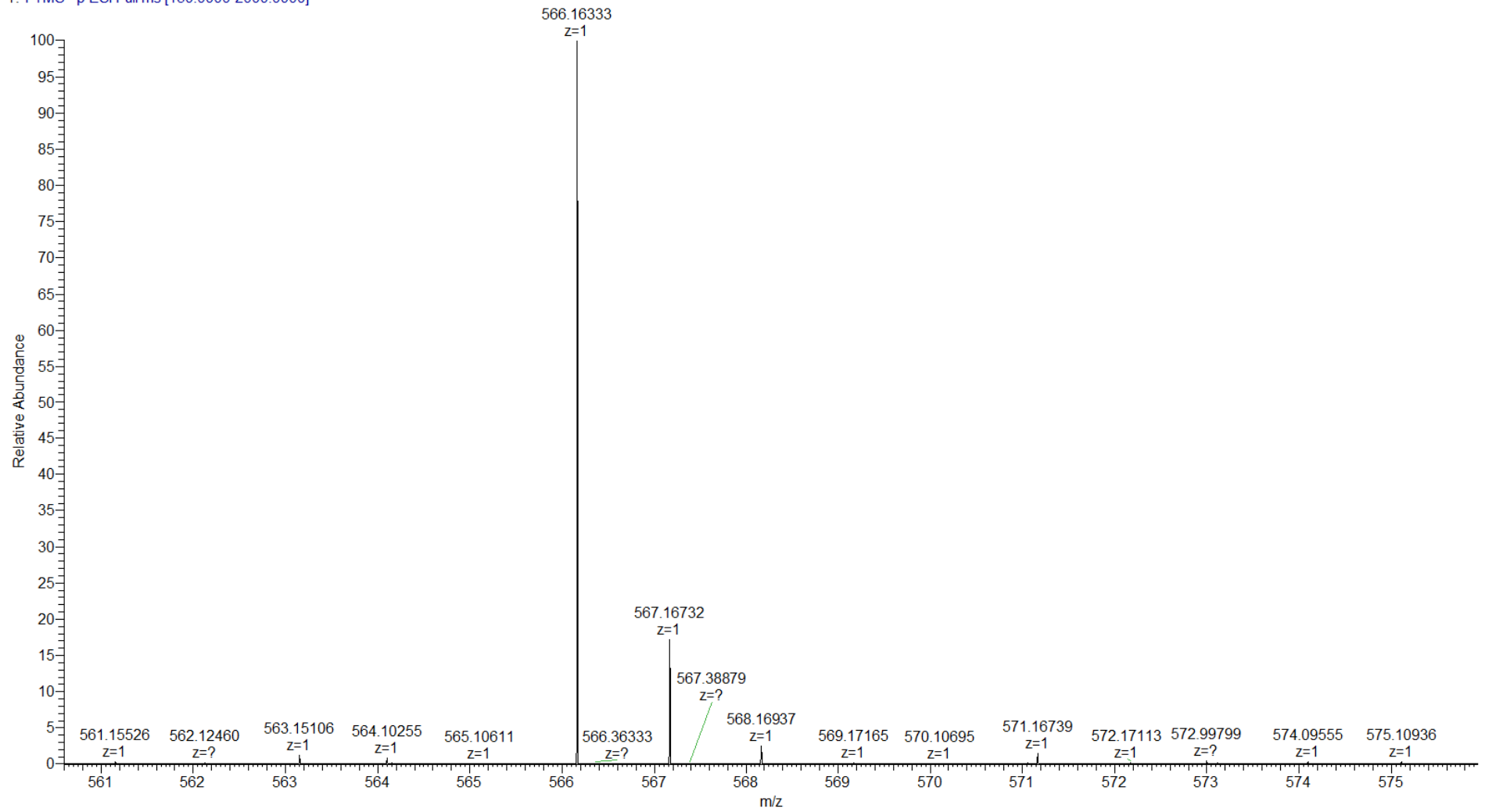
Compound 19: Im-TMGMP-2'+3'-O-C(O)-NH-CH₂CH₂-N₃ (NH₄⁺ salt)

Chemical structure



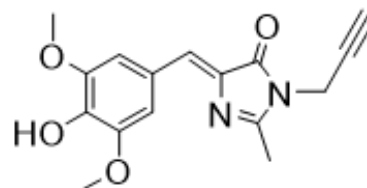
MS (-) ESI (Calc. [M-H]⁻ C₁₉H₂₅N₁₁O₈P⁻; 566.16307, found: 566.16333)

191107_PSu_23 #3-102 RT: 0.03-0.98 AV: 100 NL: 5.35E6
T: FTMS - p ESI Full ms [150.0000-2000.0000]

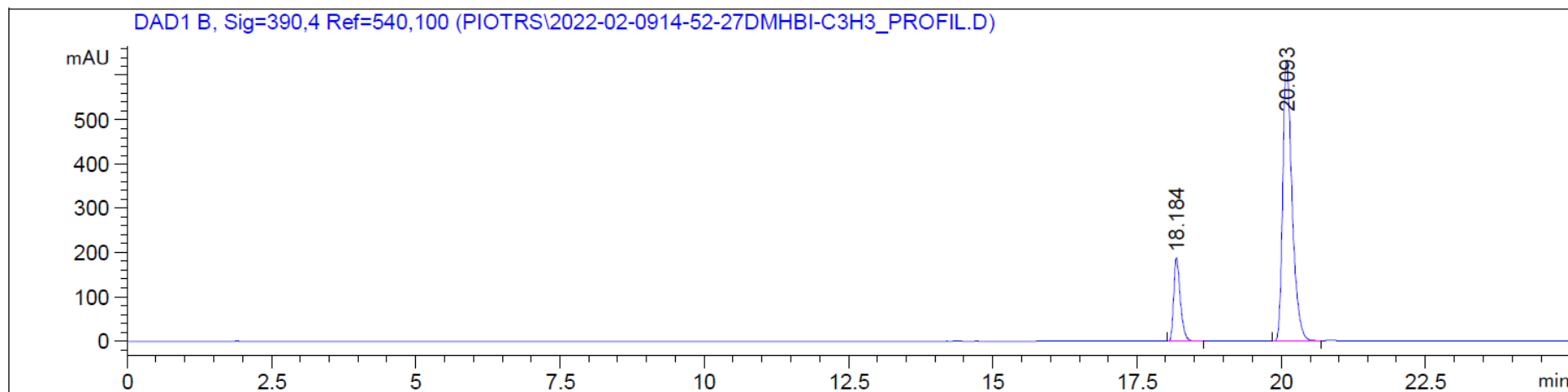


Compound 20: DMHBI-C₃H₃

Chemical structure

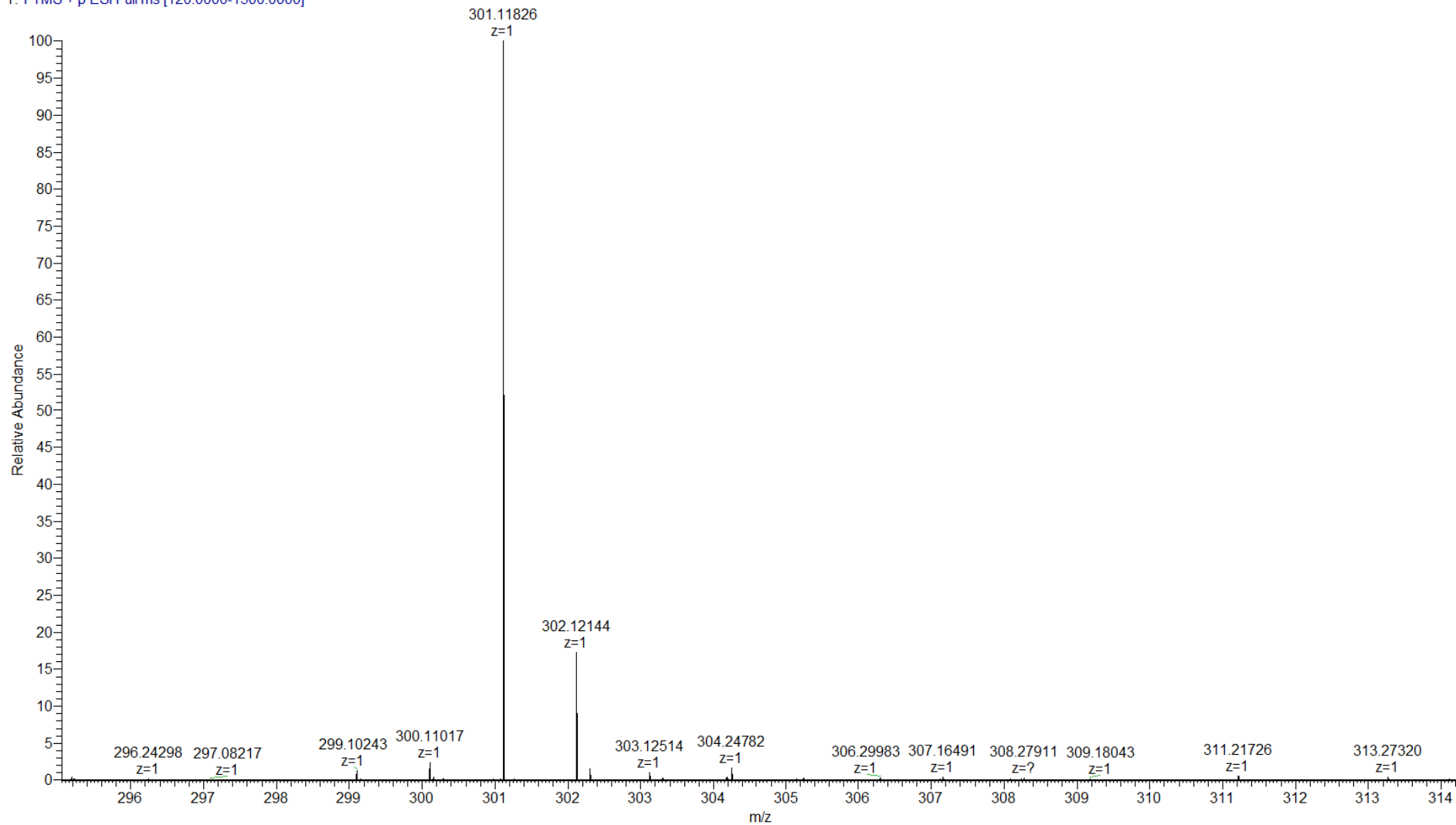


RP-HPLC (conditions c)



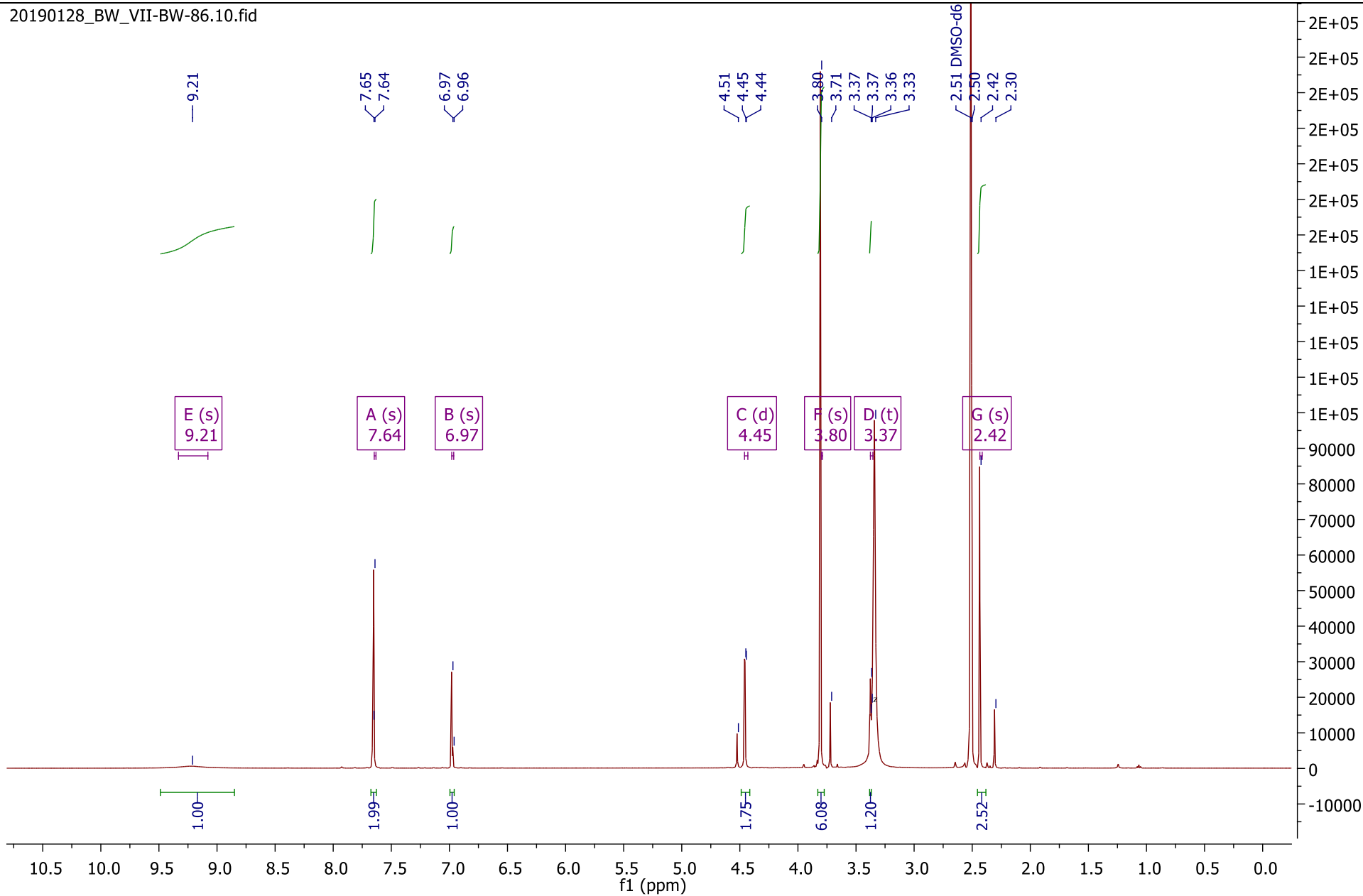
MS (-) ESI (Calc. $[M-H]^-$ $C_{16}H_{17}N_2O_4^+$: 301.1183, found: 301.11826)

90218_VIII_BW_86 #31-129 RT: 0.30-1.23 AV: 99 NL: 1.09E8
T: FTMS + p ESI Full ms [120.0000-1500.0000]

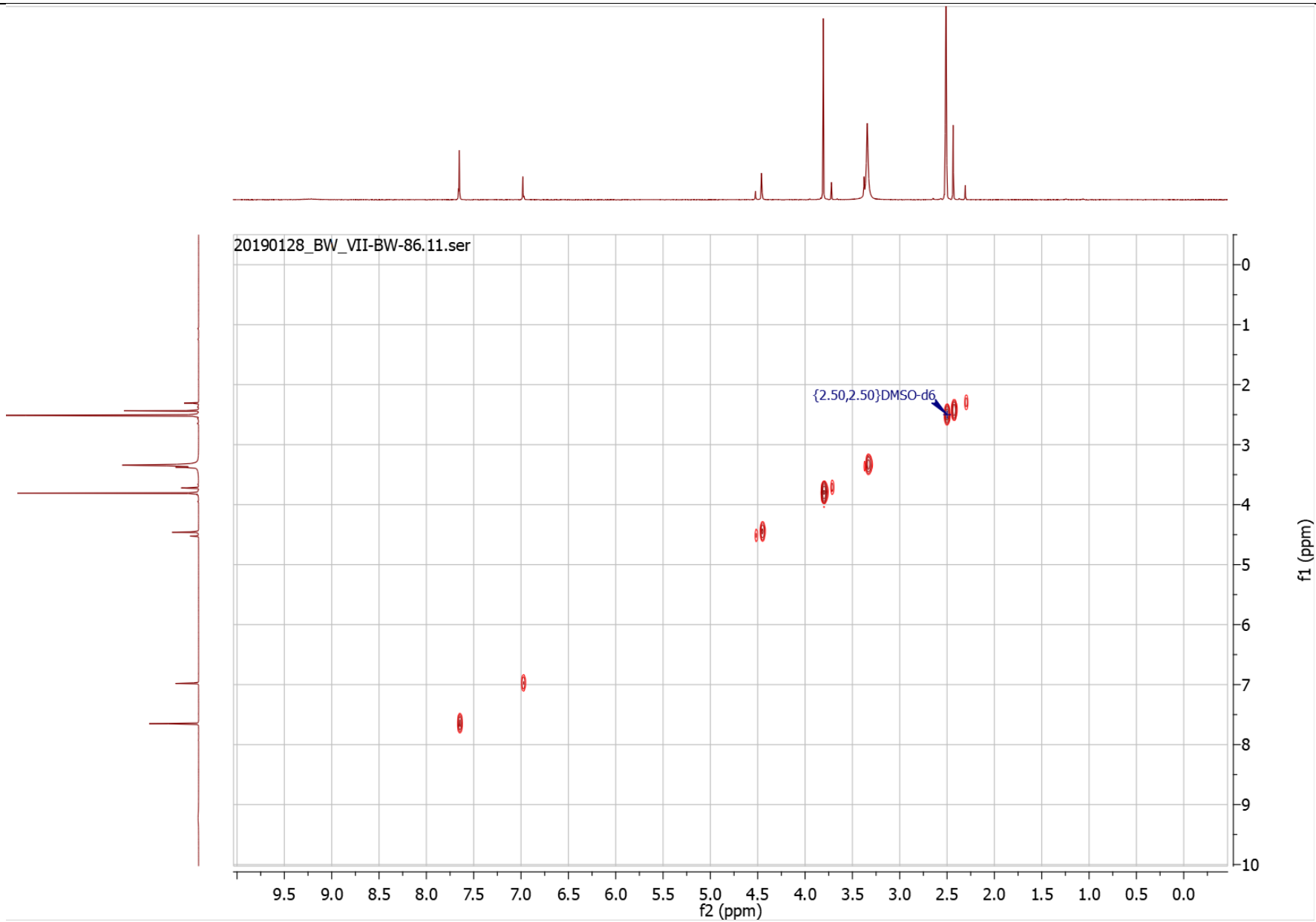


¹H NMR (500 MHz, DMSO-d₆, 25°C)

20190128_BW_VII-BW-86.10.fid

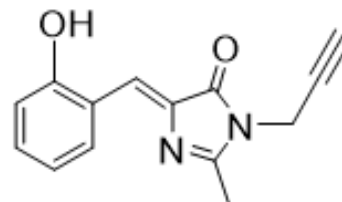


COSY NMR

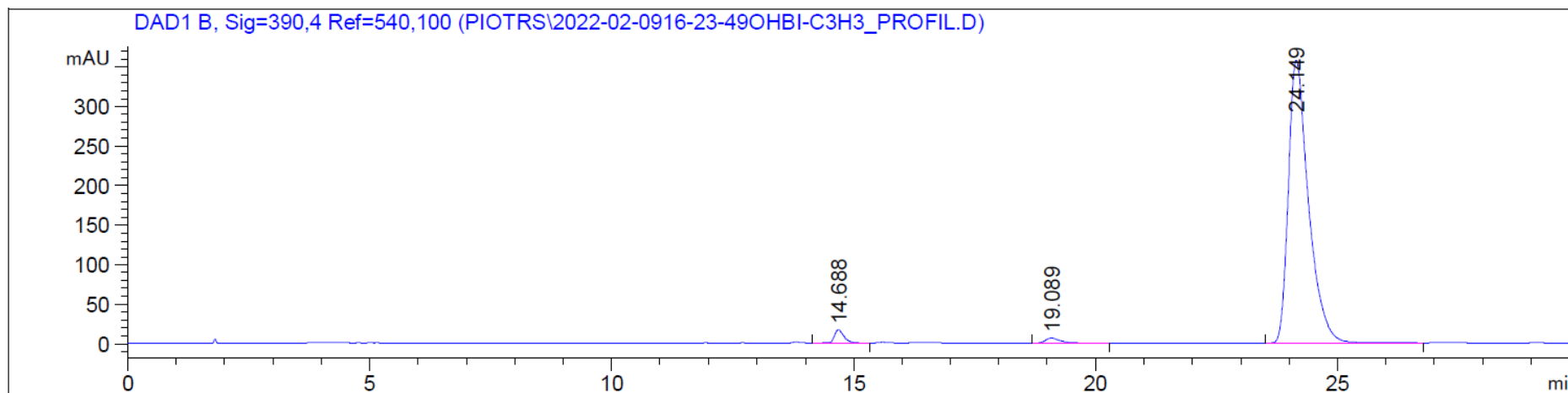


Compound 21: oHBI-C₃H₃

Chemical structure

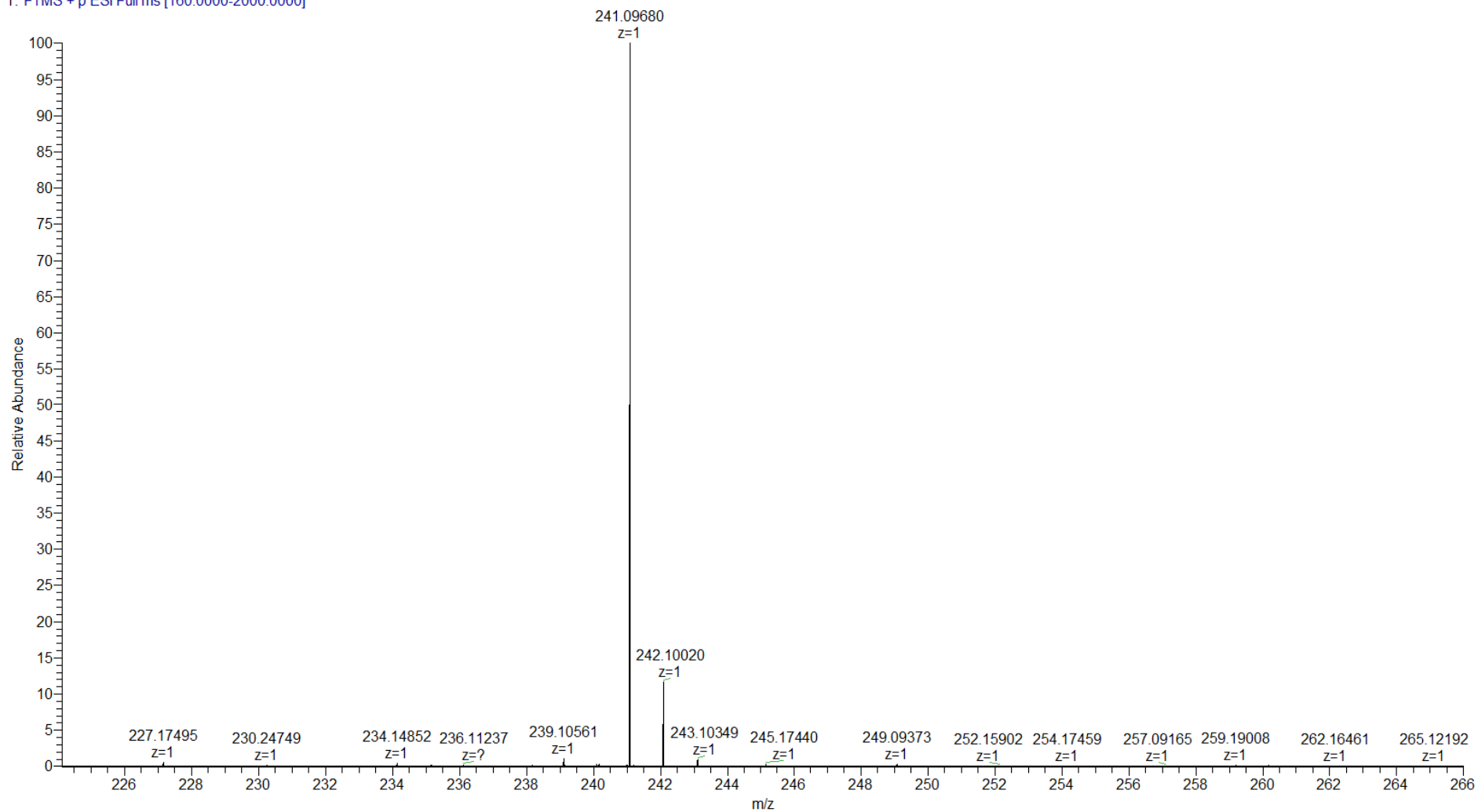


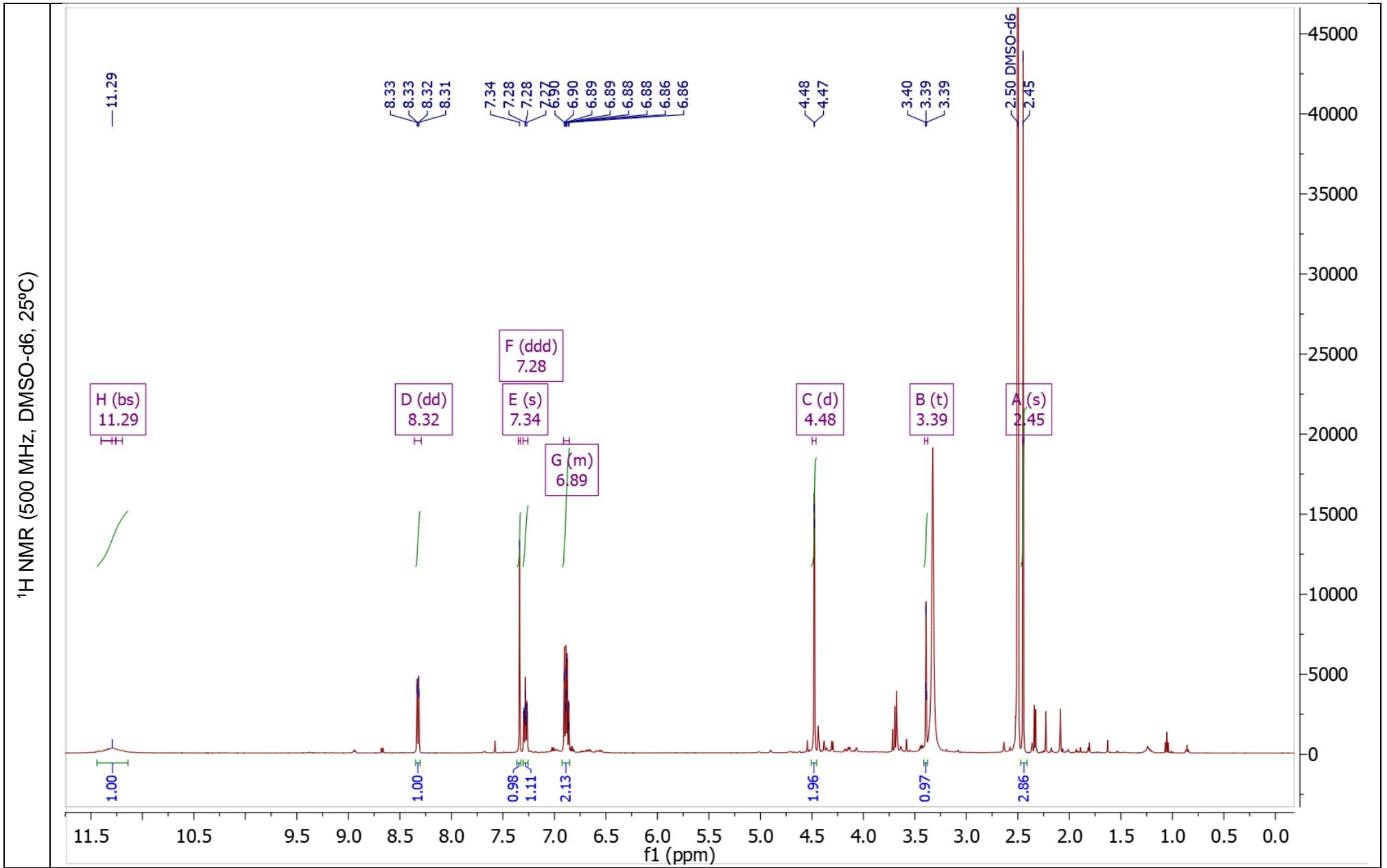
RP-HPLC (conditions b)



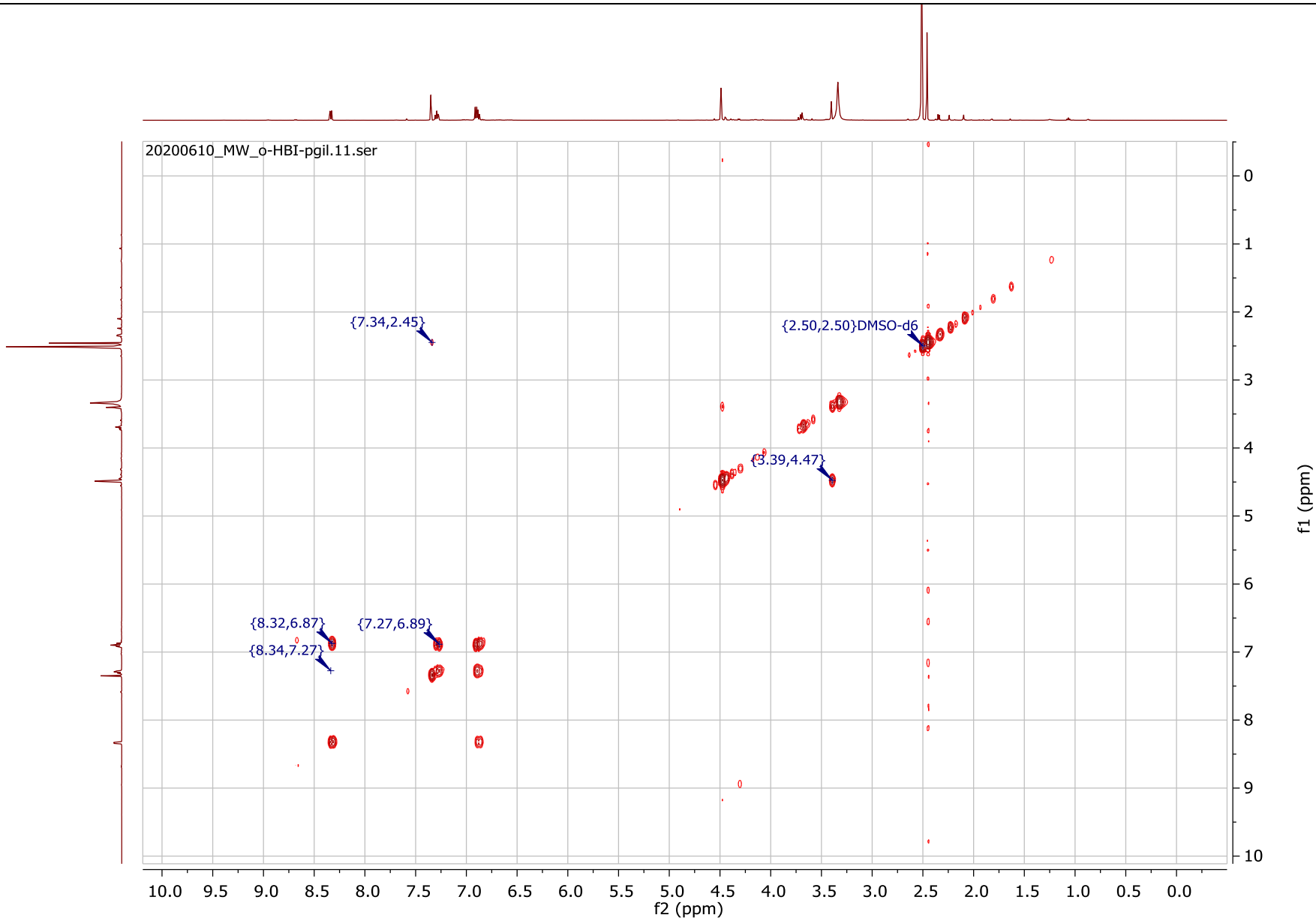
220214_PSu_23 #30-108 RT: 0.27-0.95 AV: 79 NL: 1.54E8
T: FTMS + p ESI Full ms [160.0000-2000.0000]

MS (+) ESI (Calc. $[M+H]^+ C_{14}H_{13}N_2O_2^+$: 241.09715, found : 241.09680)

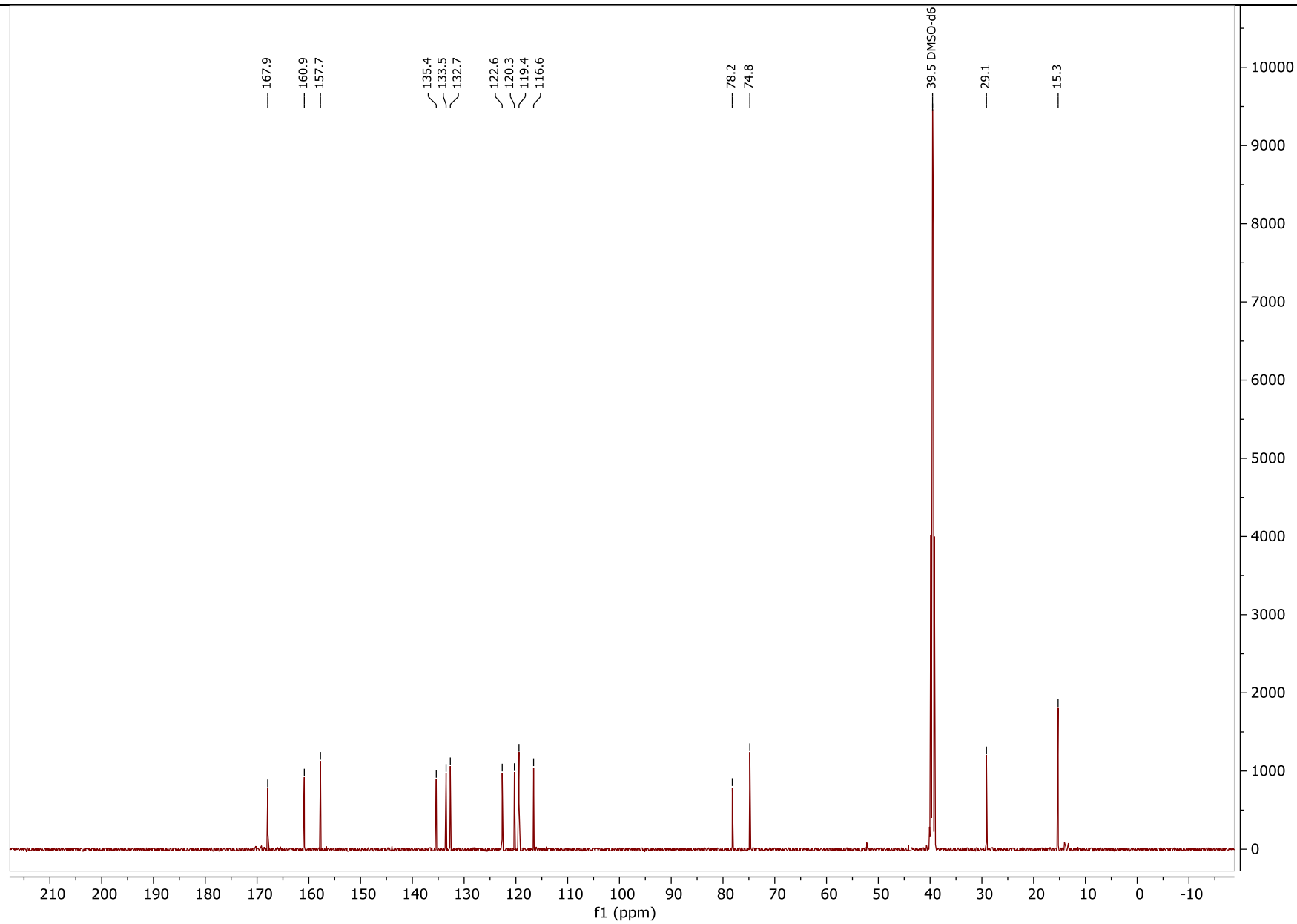




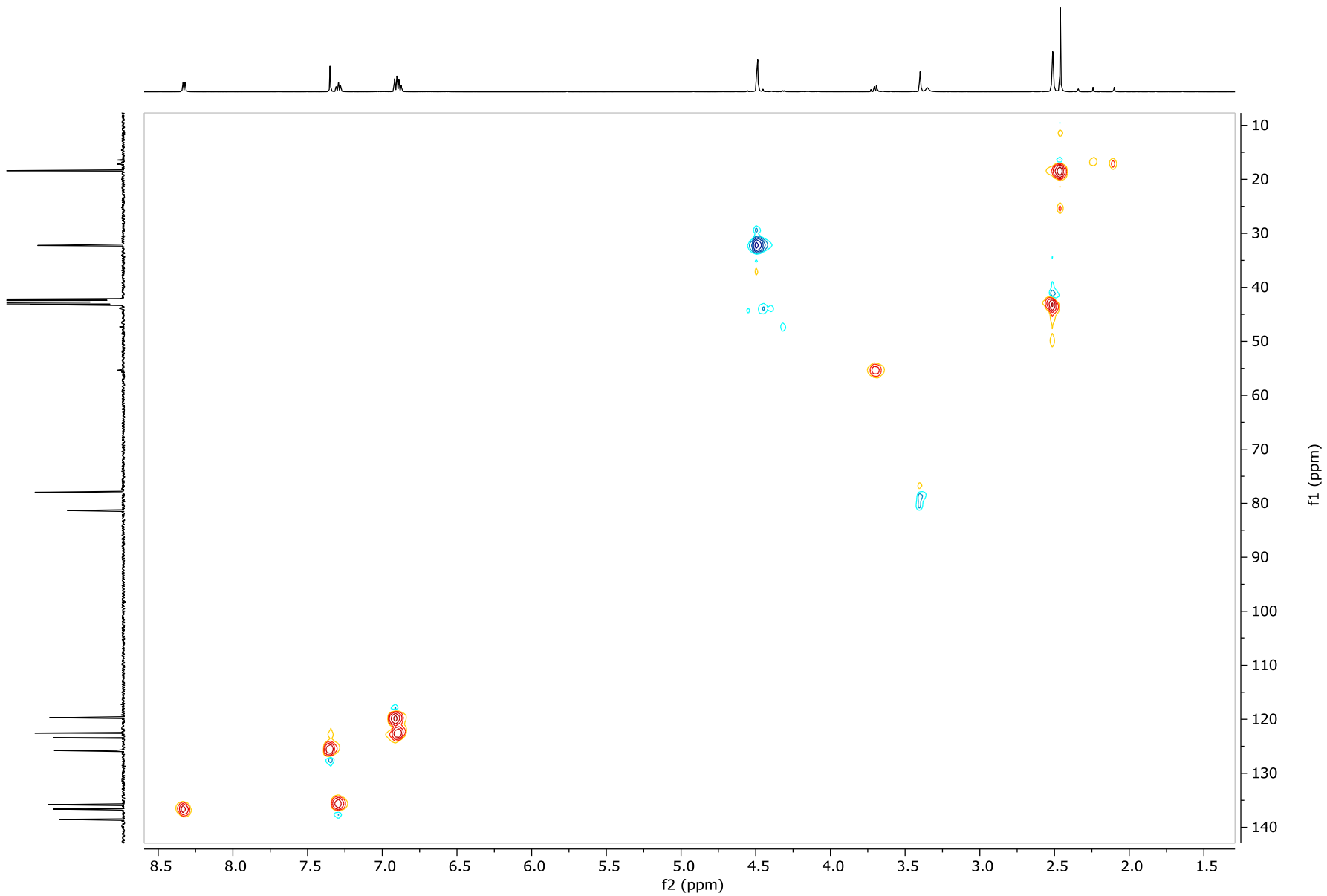
COSY NMR



¹³C NMR (500 MHz, D₂O, 25°C)

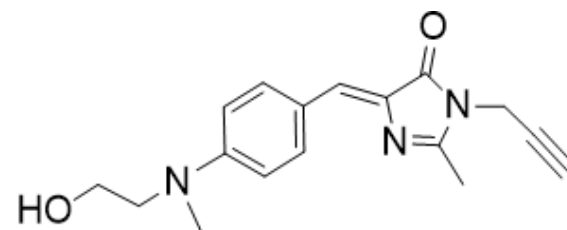


HSQC NMR

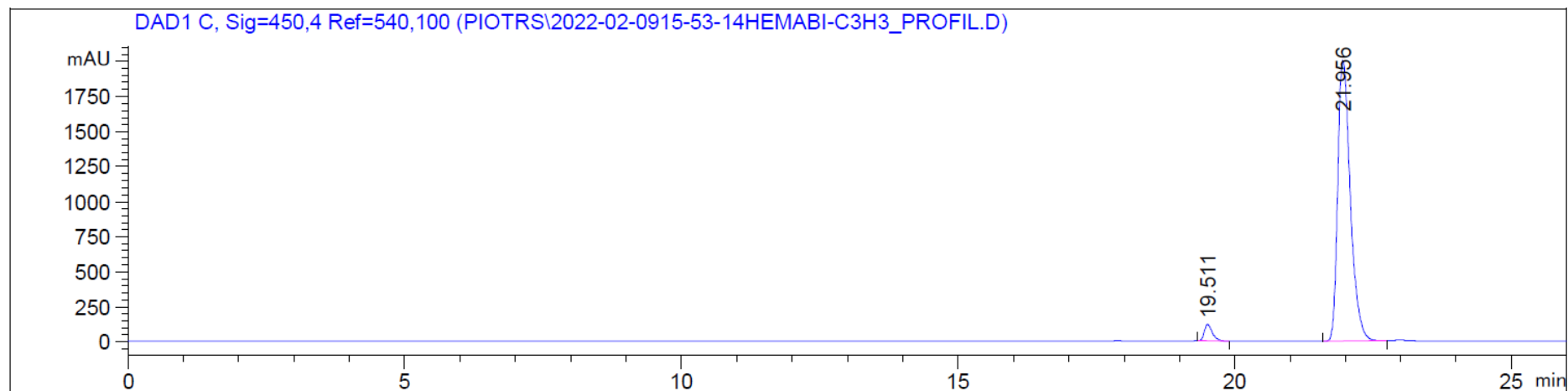


Compound 22: HEMABI-C₃H₃

Chemical structure

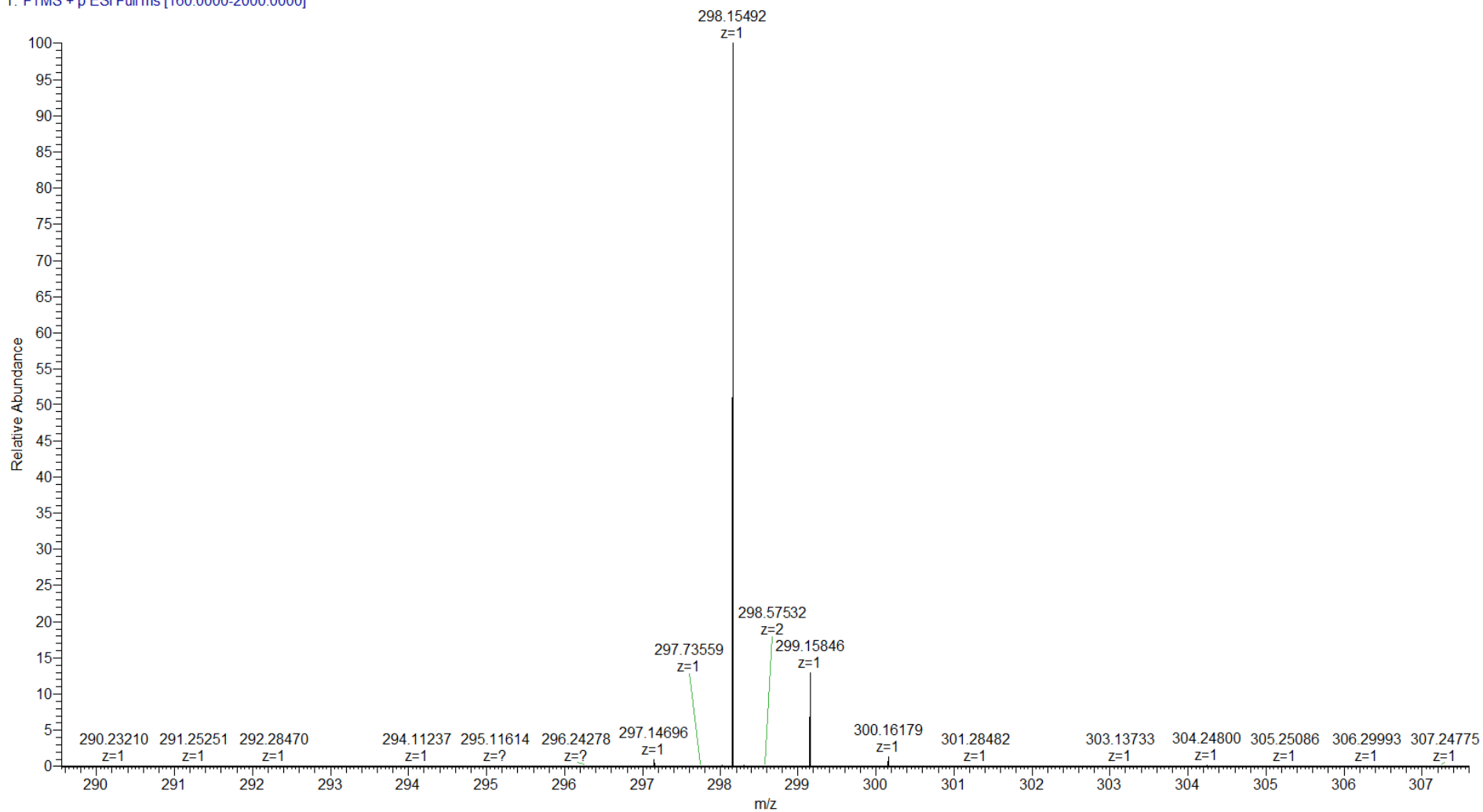


RP-HPLC (conditions c)

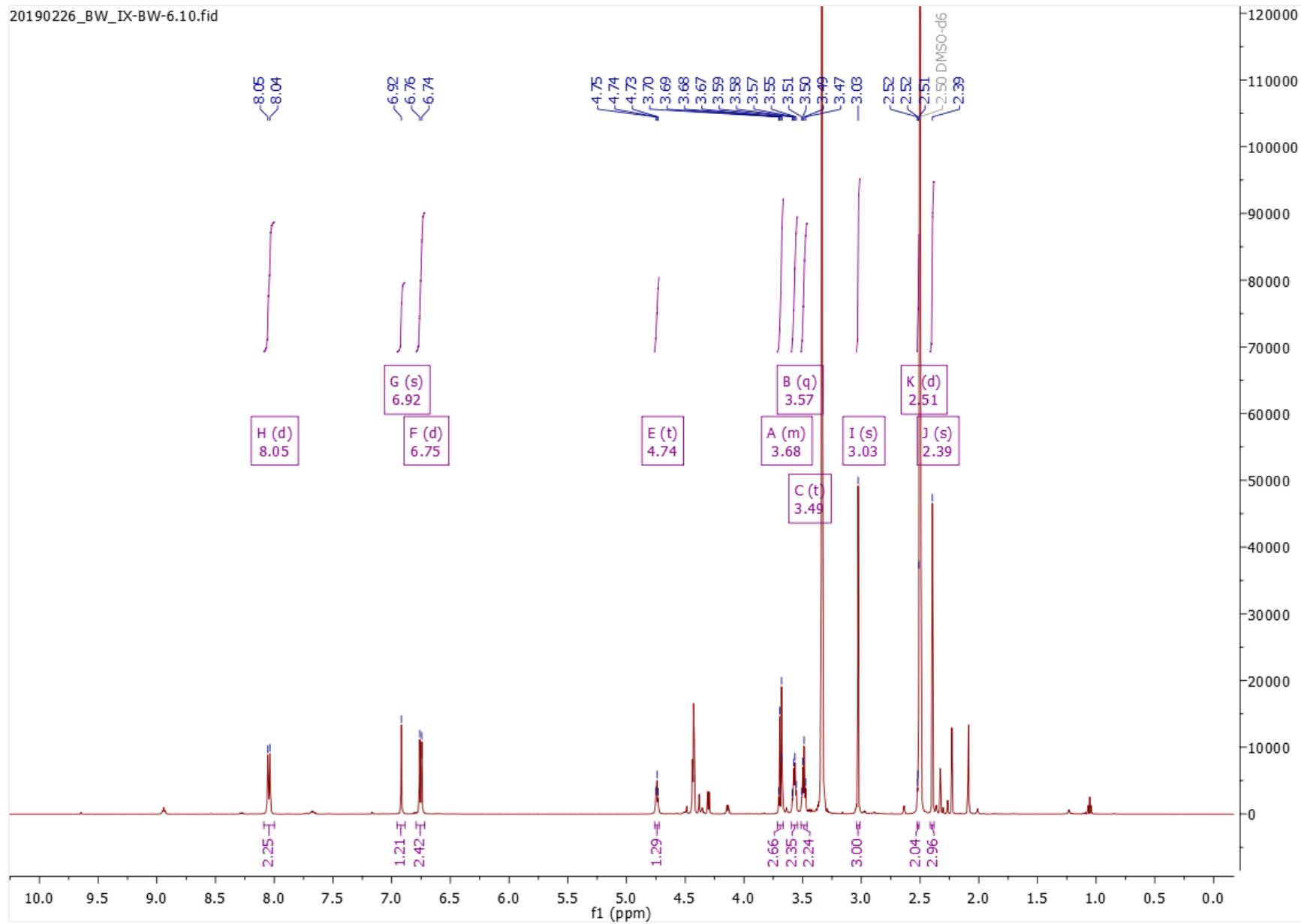


220214_PSu_24 #71-106 RT: 0.62-0.93 AV: 36 NL: 7.72E8
T: FTMS + p ESI Full ms [160.0000-2000.0000]

MS (+) ESI (Calc. [M+H]⁺ C₁₇H₂₀N₃O₂⁺: 298.1550, found : 298.15492)

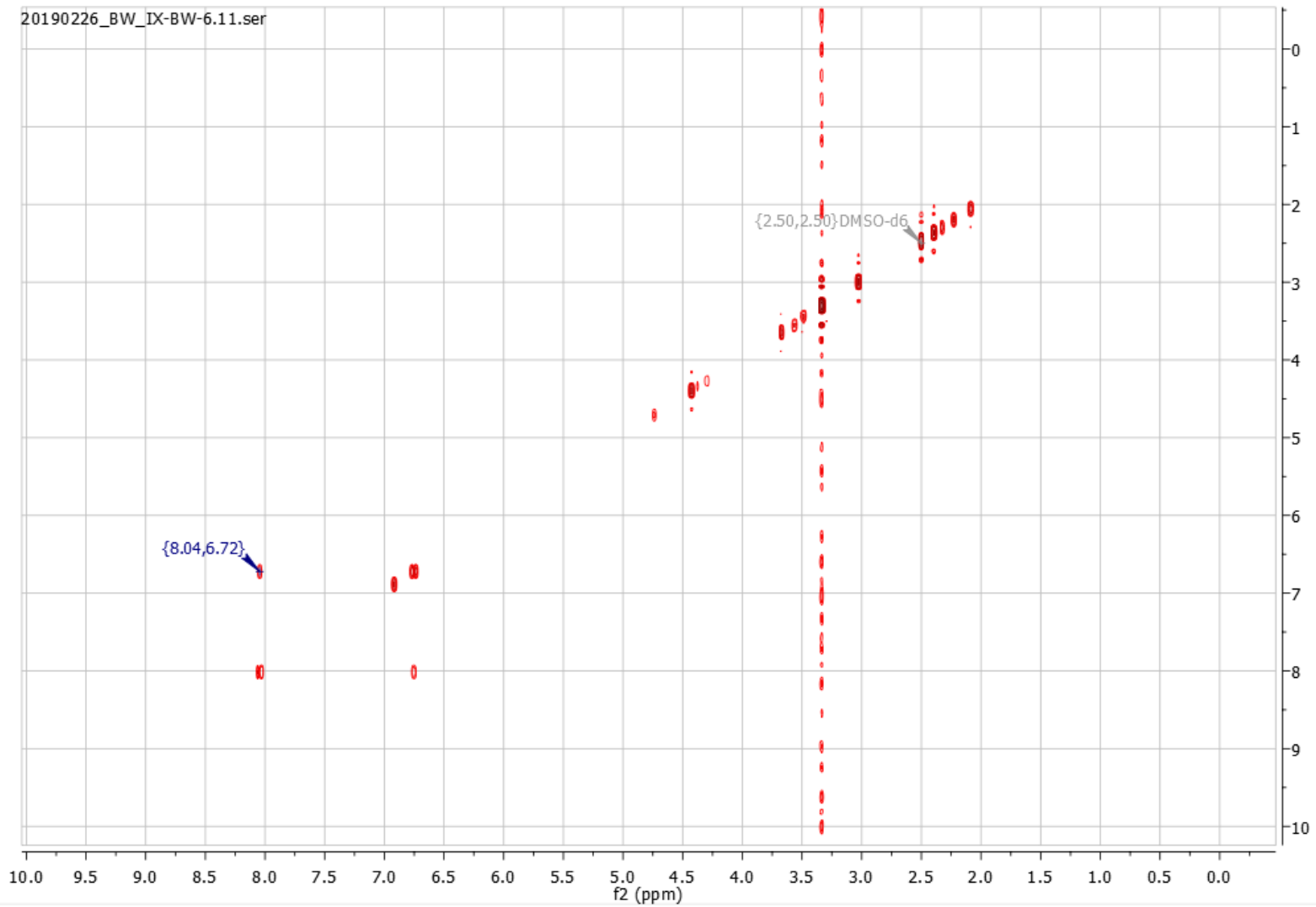


¹H NMR (500 MHz, DMSO-d₆, 25°C)



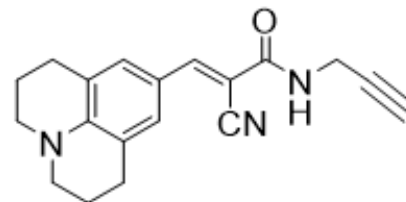
COSY NMR

20190226_BW_IX-BW-6.11.ser

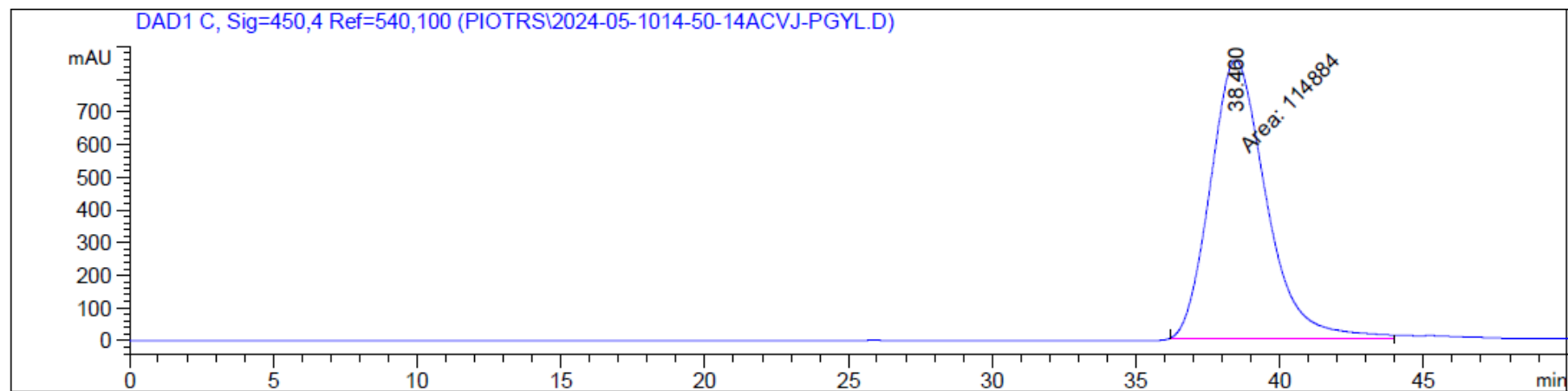


Compound 23: ACVJ-C₃H₃

Chemical structure

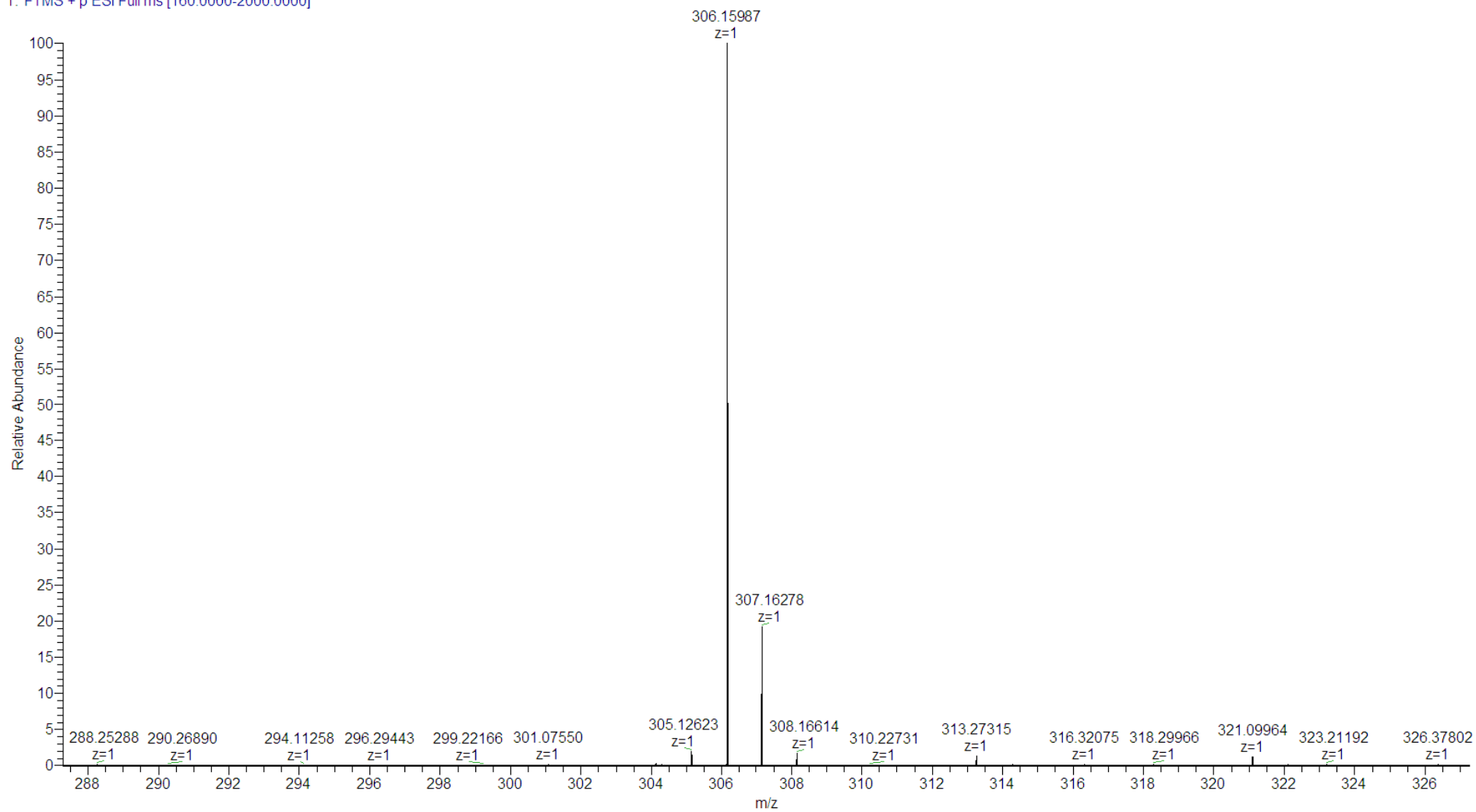


RP-HPLC (conditions b)

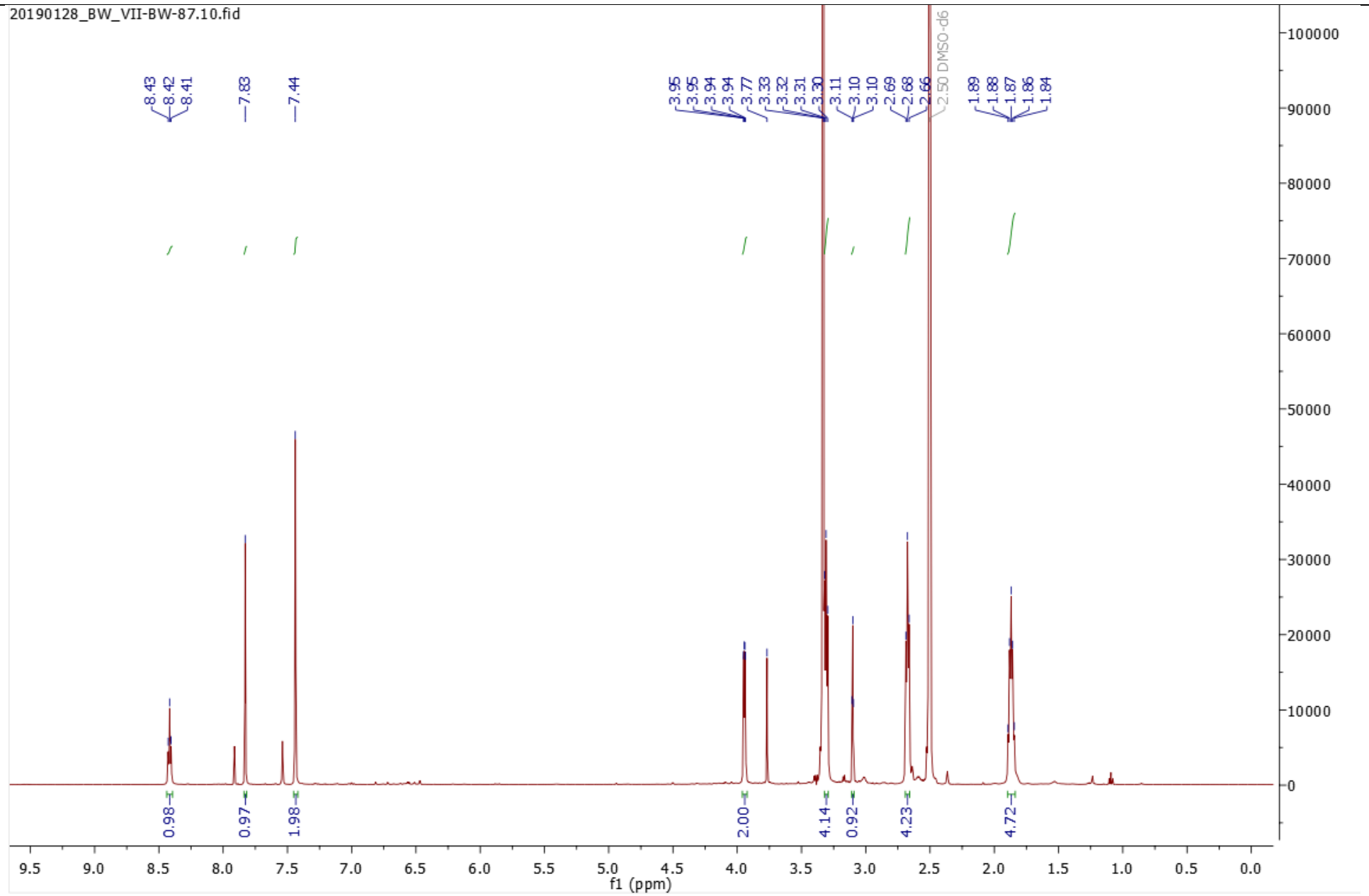


220331_PSu_01 #767-866 RT: 6.55-7.41 AV: 100 NL: 1.78E8
T: FTMS + p ESI Full ms [160.0000-2000.0000]

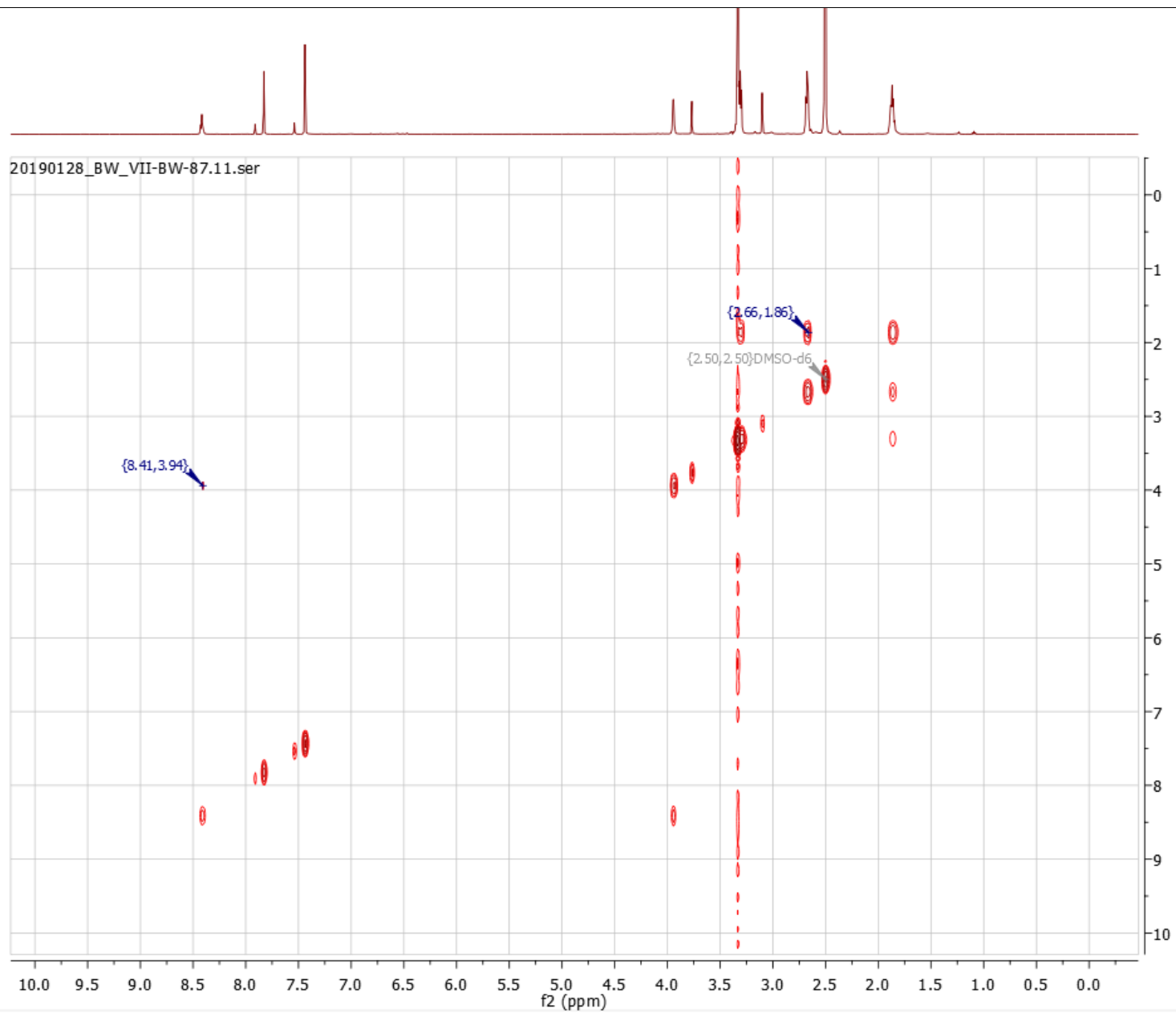
MS (+) ESI (Calc. [M+H]⁺ C₁₉H₂₀N₃O⁺ : 306.1601, found : 306.15987)



¹H NMR (500 MHz, DMSO-d₆, 25°C)

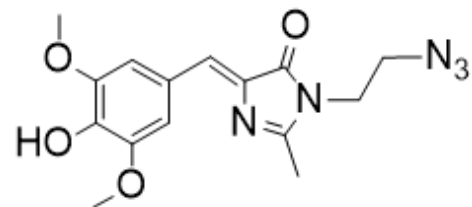


COSY NMR

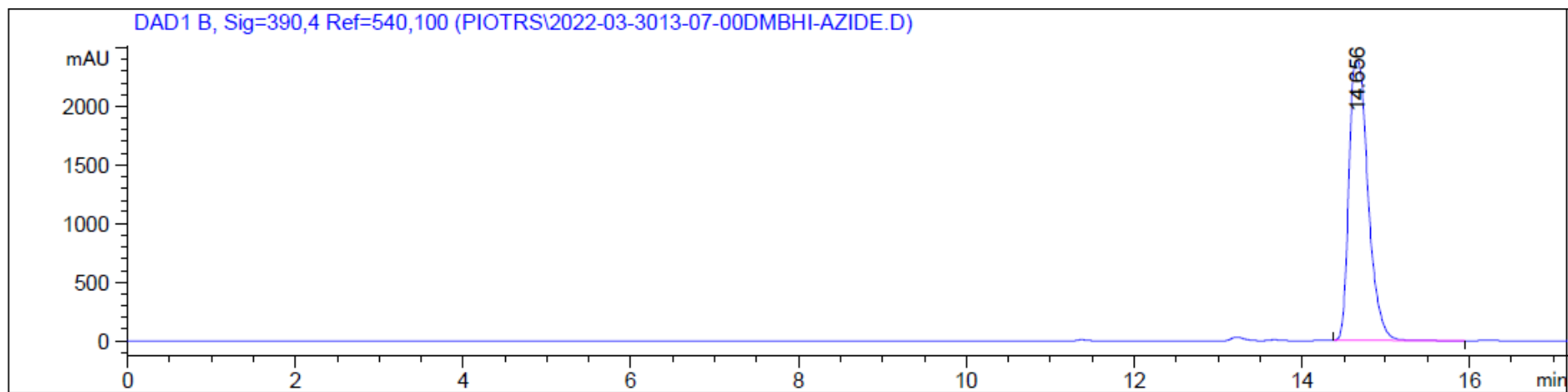


Compound 24: DMHBI-CH₂CH₂-N₃

Chemical structure

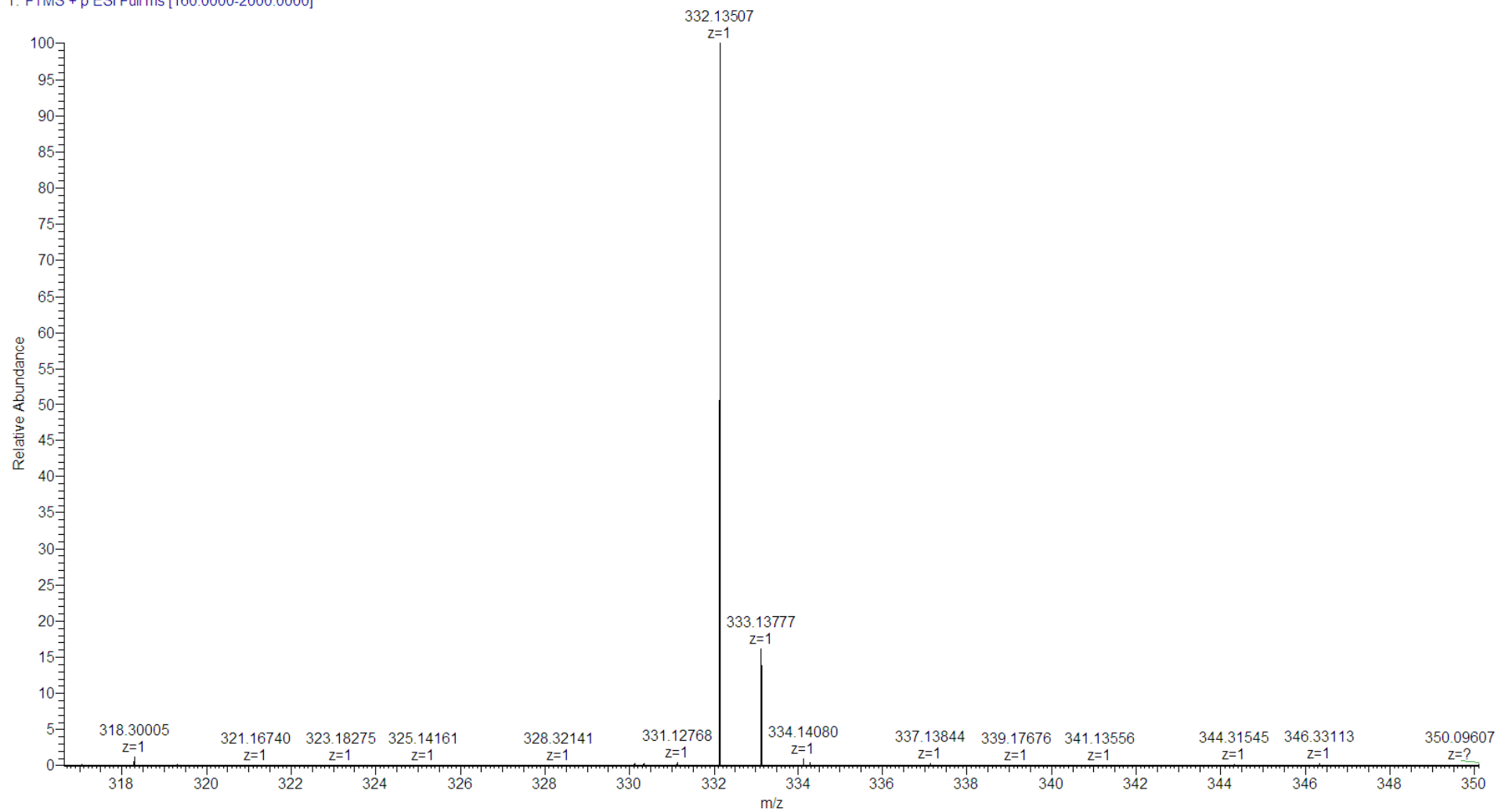


RP-HPLC (conditions c)

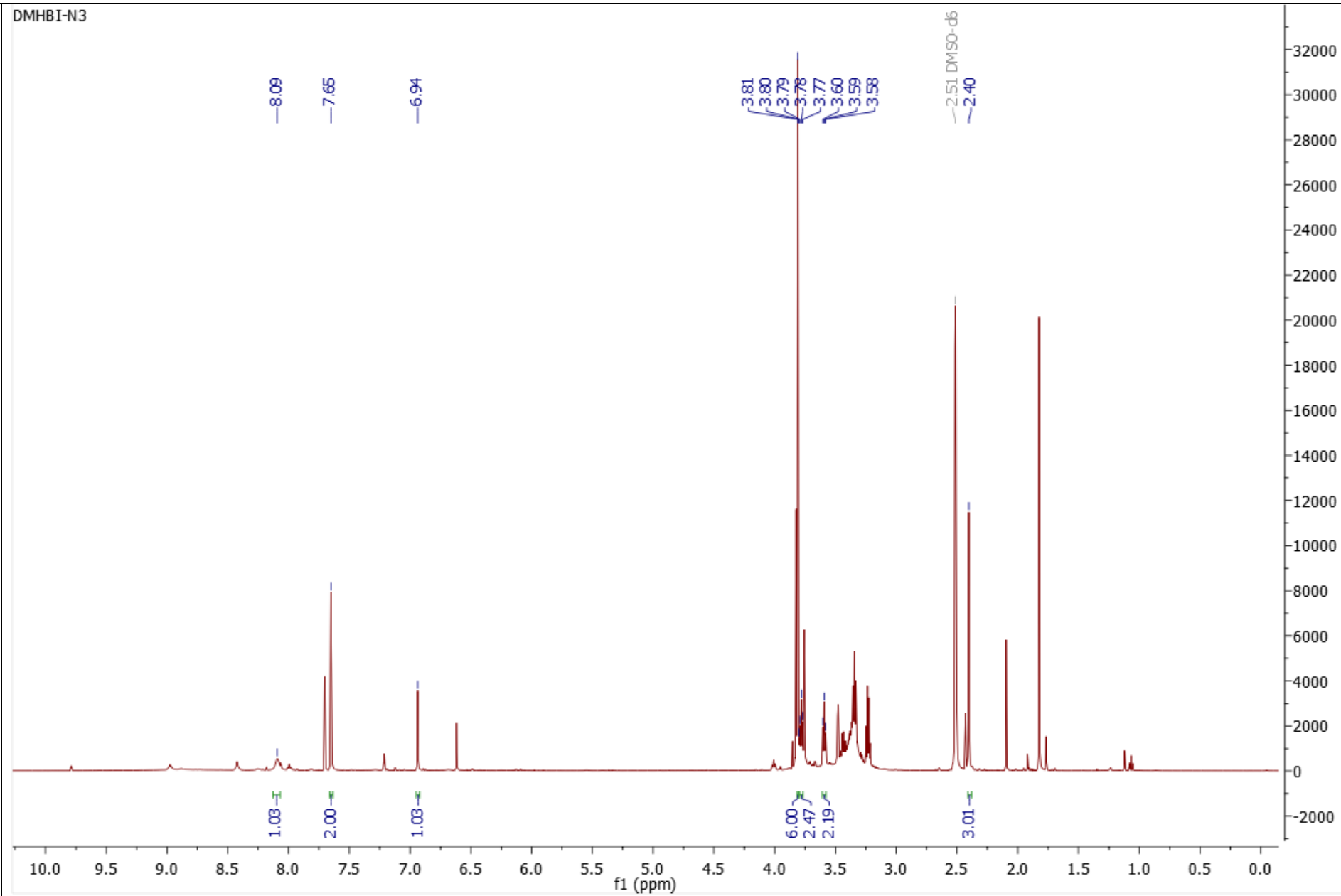


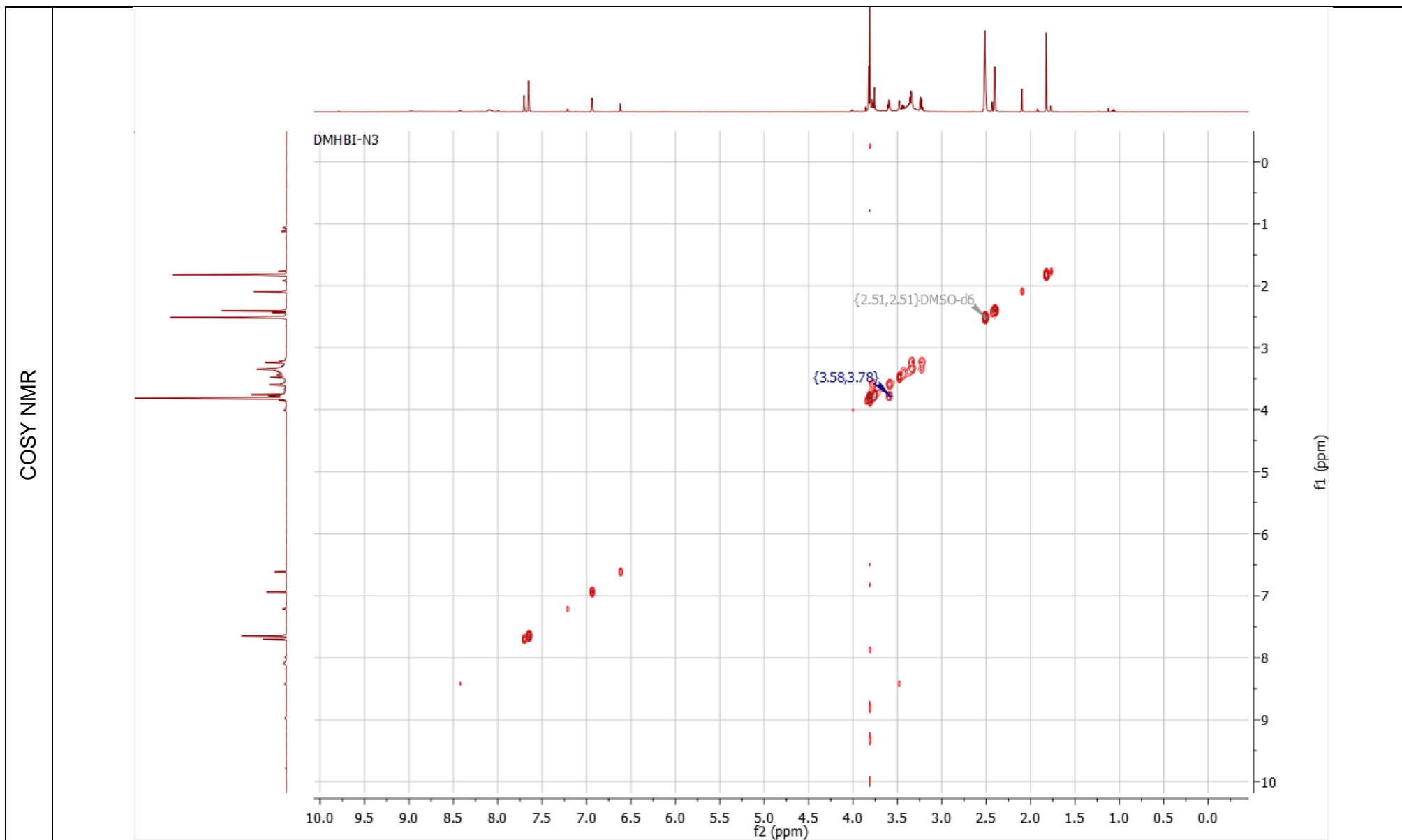
220331_PSu_02 #49-73 RT: 0.43-0.64 AV: 25 NL: 2.65E8
T: FTMS + p ESI Full ms [160.0000-2000.0000]

MS (+) ESI (Calc. $[M-H]^+ C_{15}H_{18}N_5O_4^+$: 332.1353, found : 332.13507)



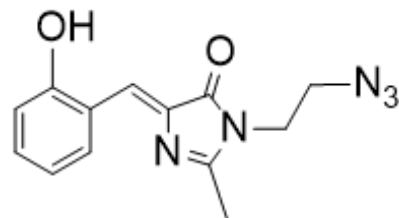
¹H NMR (500 MHz, DMSO-d₆, 25°C)



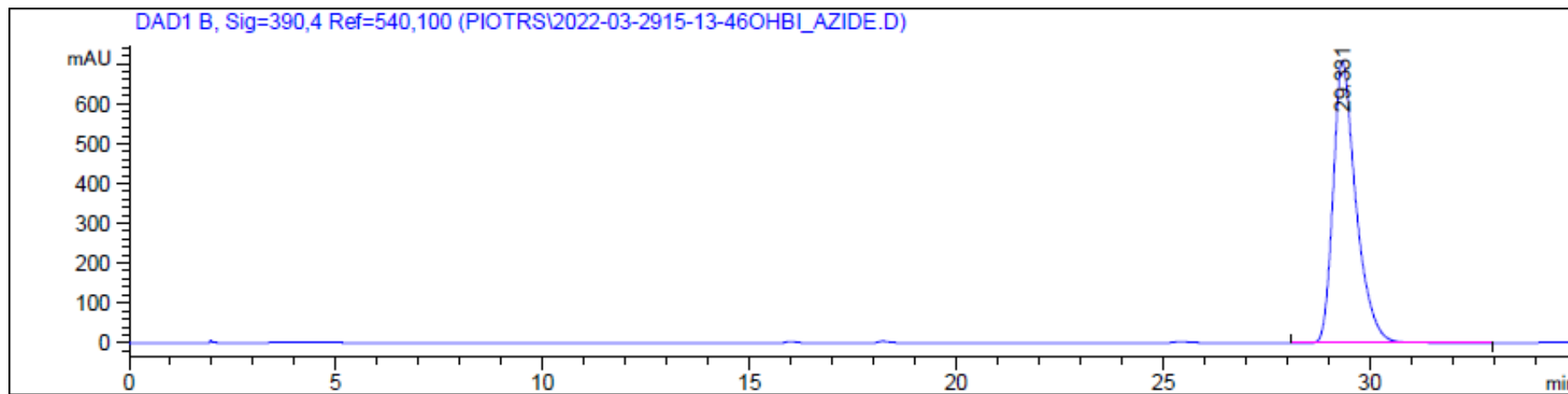


Compound 25: oHBI-CH₂CH₂-N₃

Chemical structure

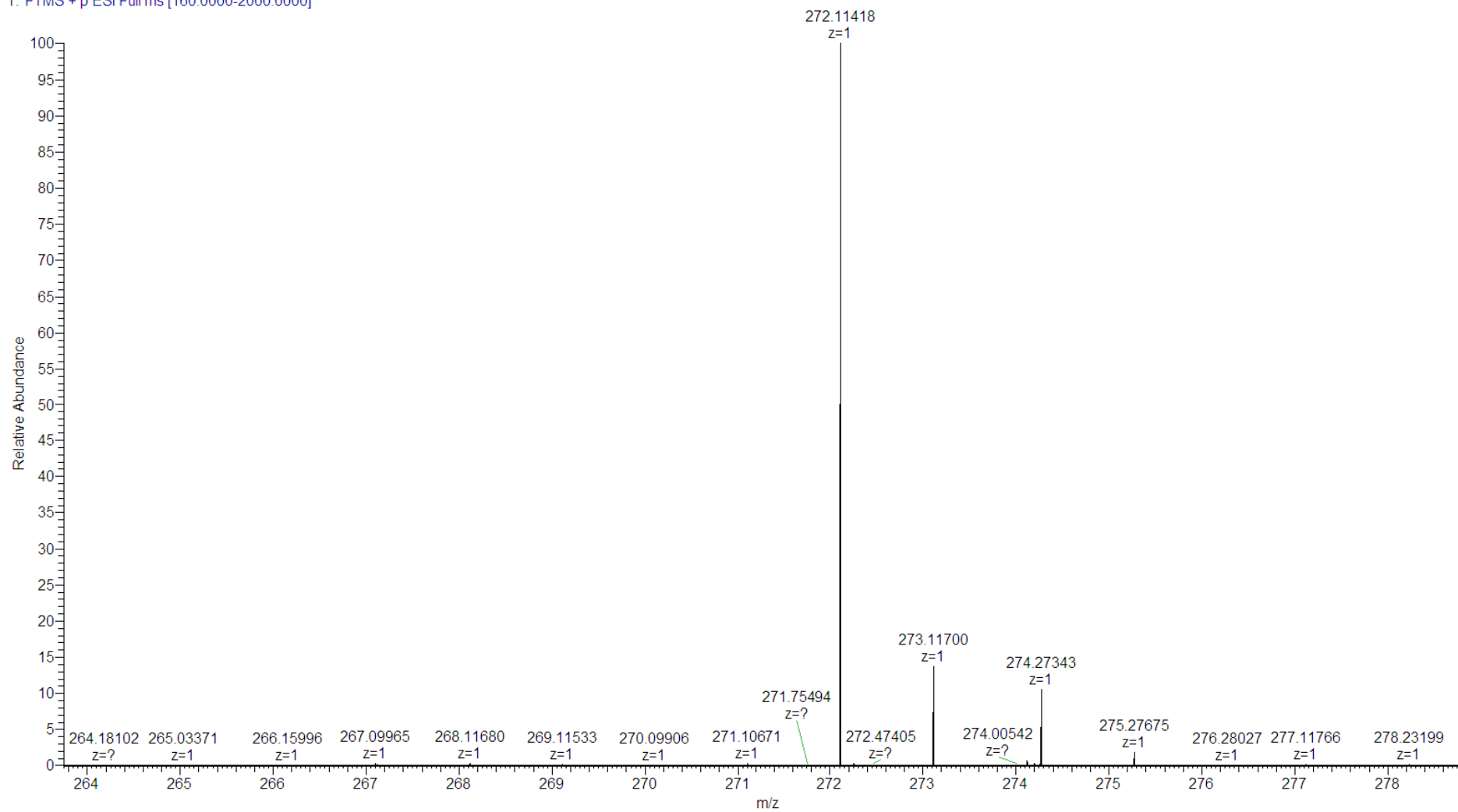


RP-HPLC (conditions b)

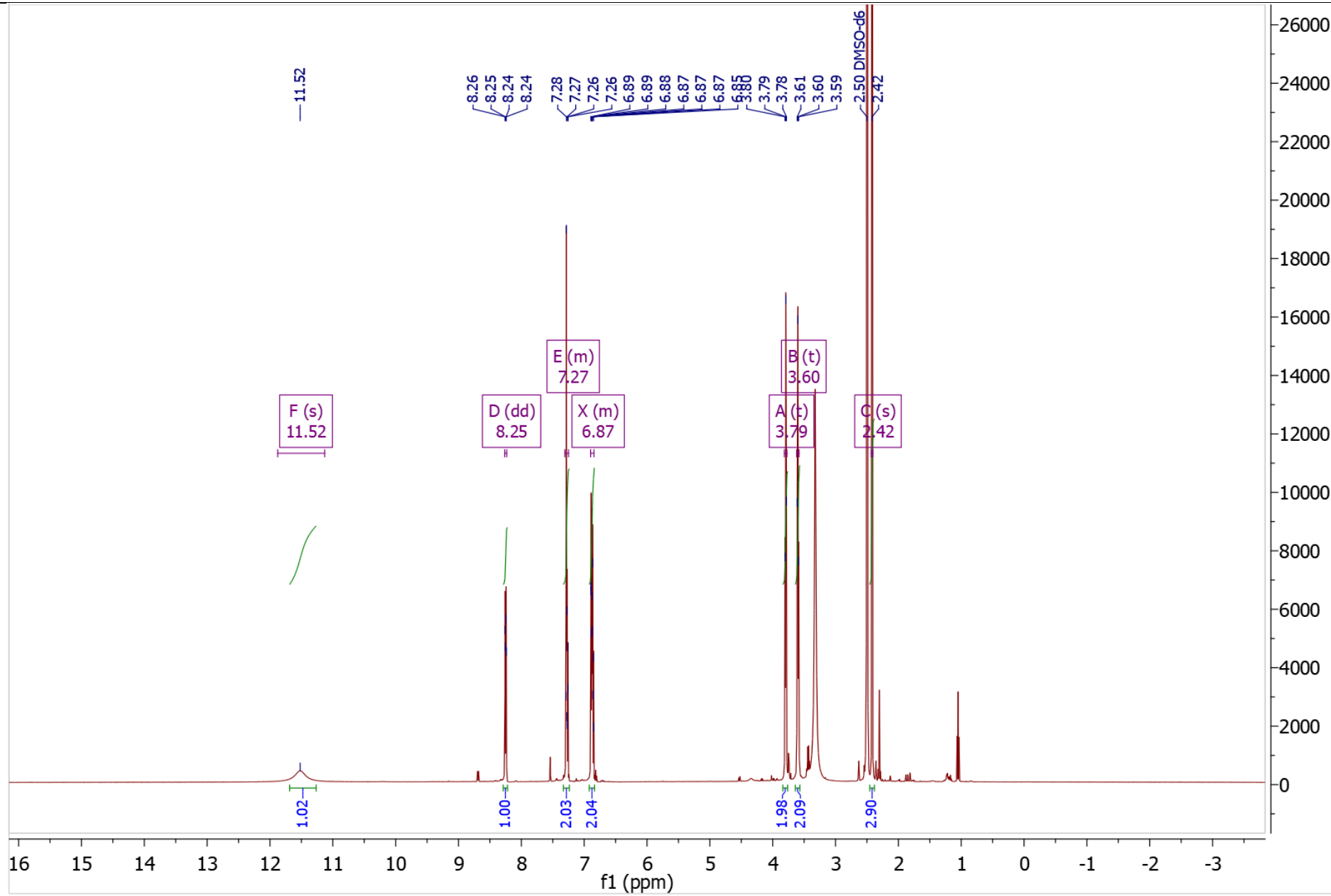


220331_PSu_03 #110-162 RT: 0.96-1.42 AV: 53 NL: 2.87E8
T: FTMS + p ESI Full ms [160.0000-2000.0000]

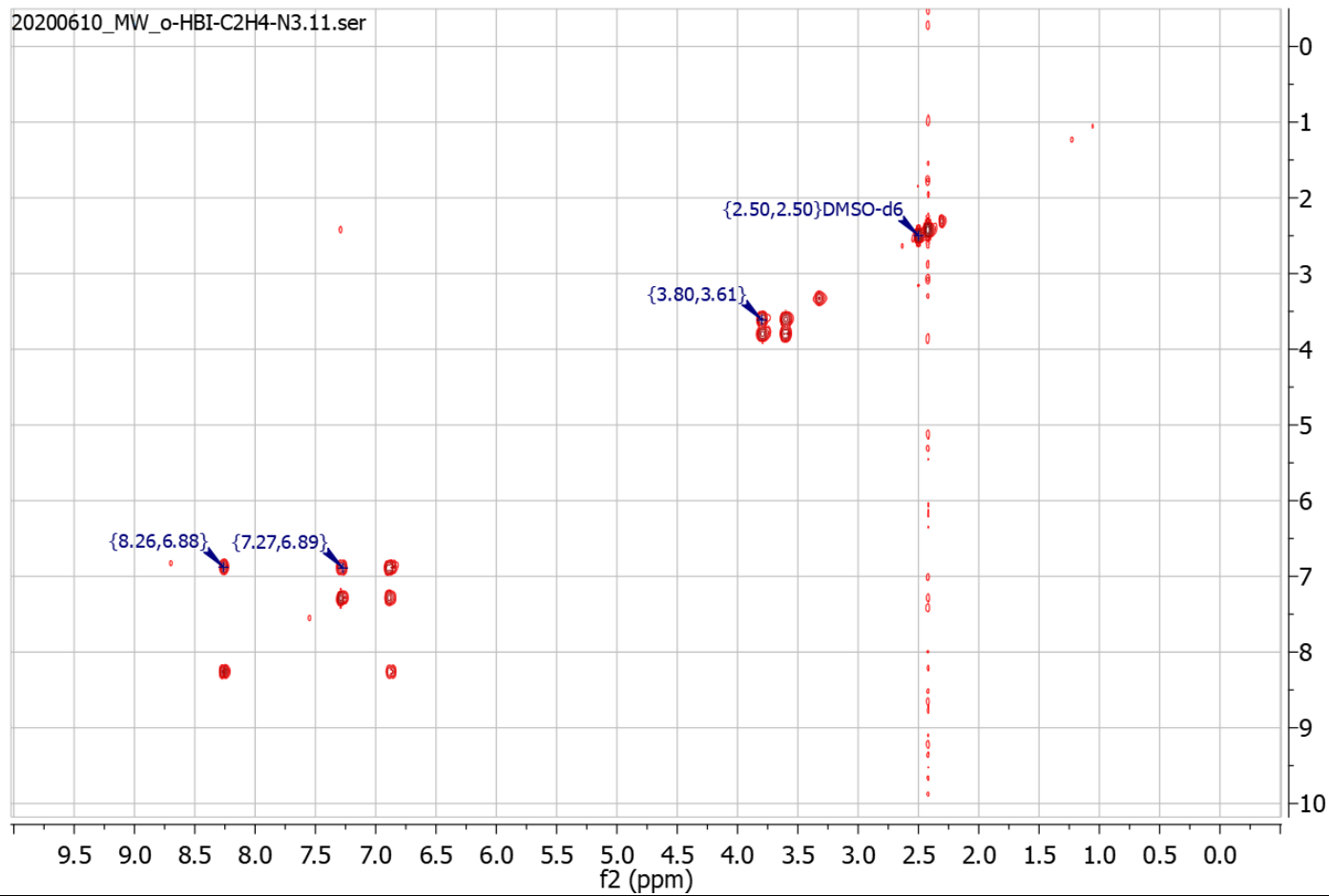
MS (+) ESI (Calc. $[M+H]^+$ C₁₃H₁₄N₅O₂⁺ : 272.1142, found: 272.11418)



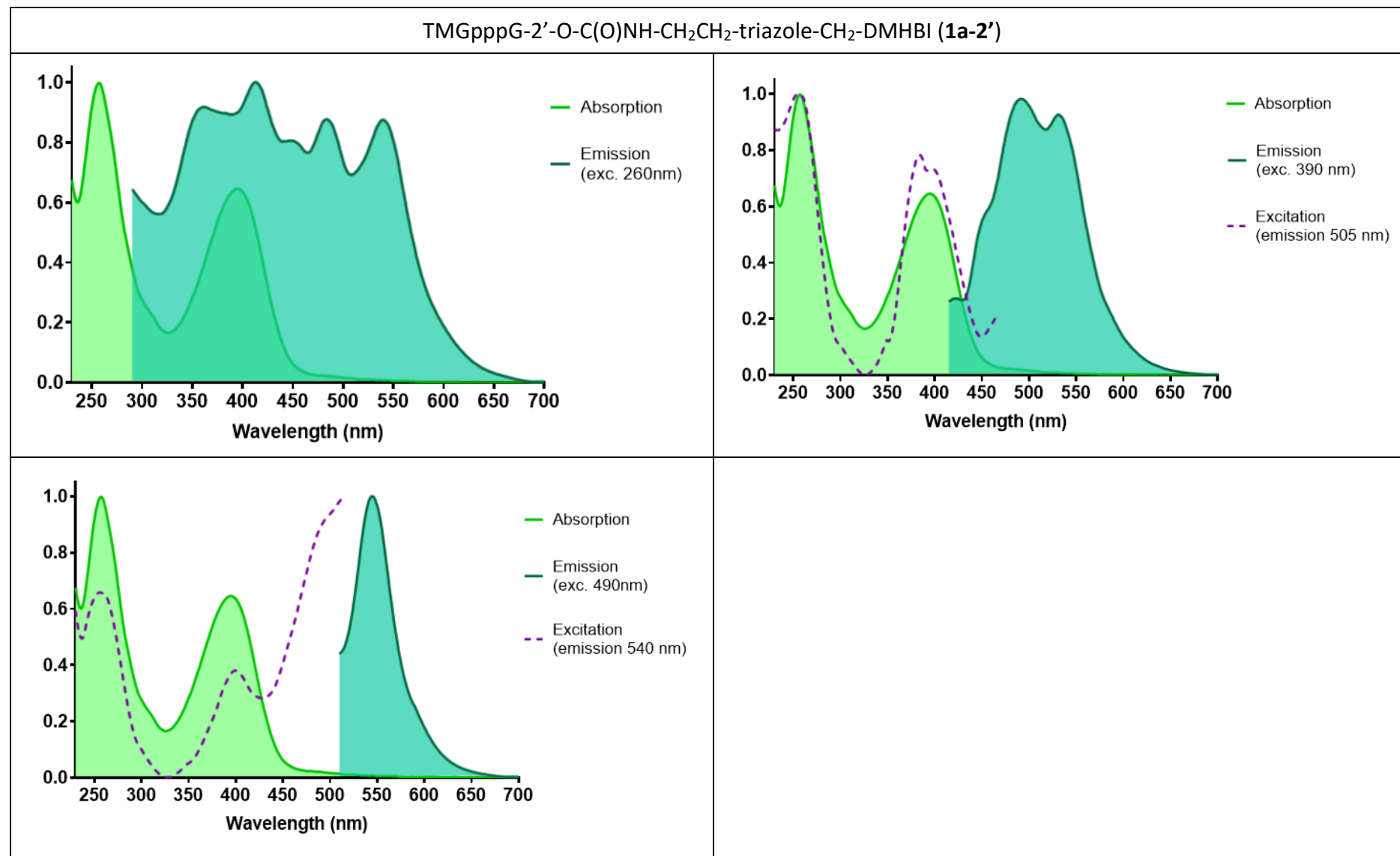
¹H NMR (500 MHz, DMSO-d₆, 25°C)



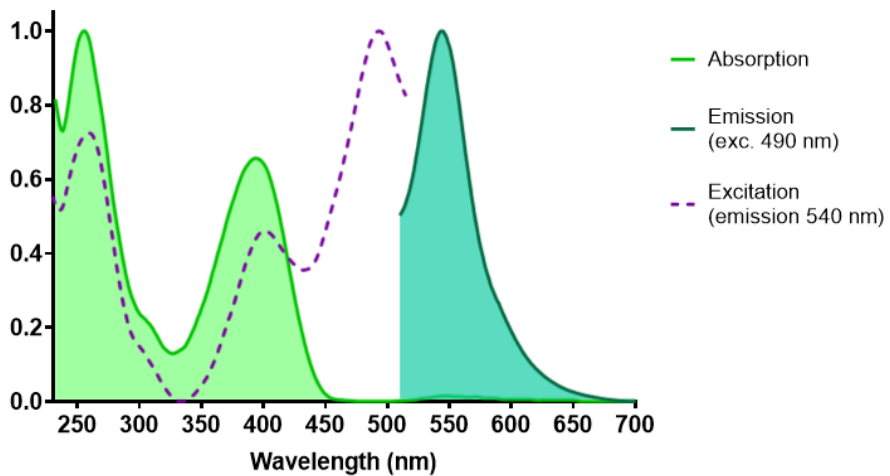
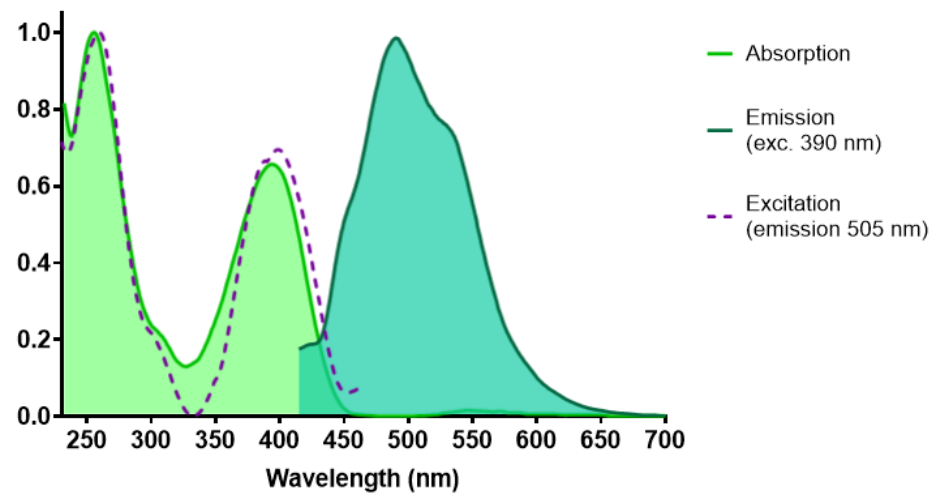
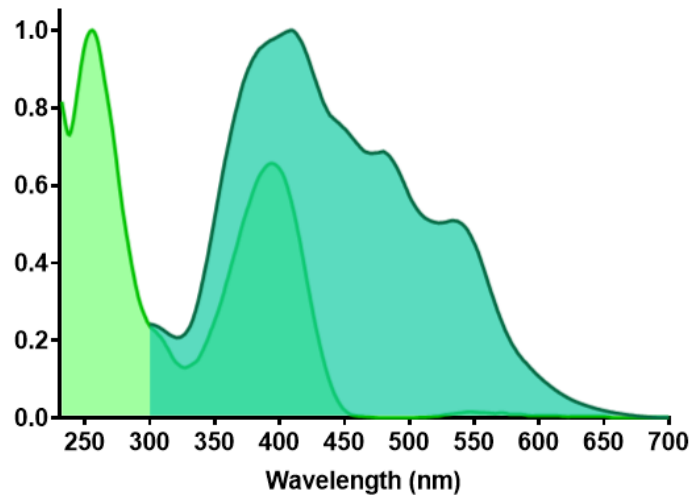
COSY NMR



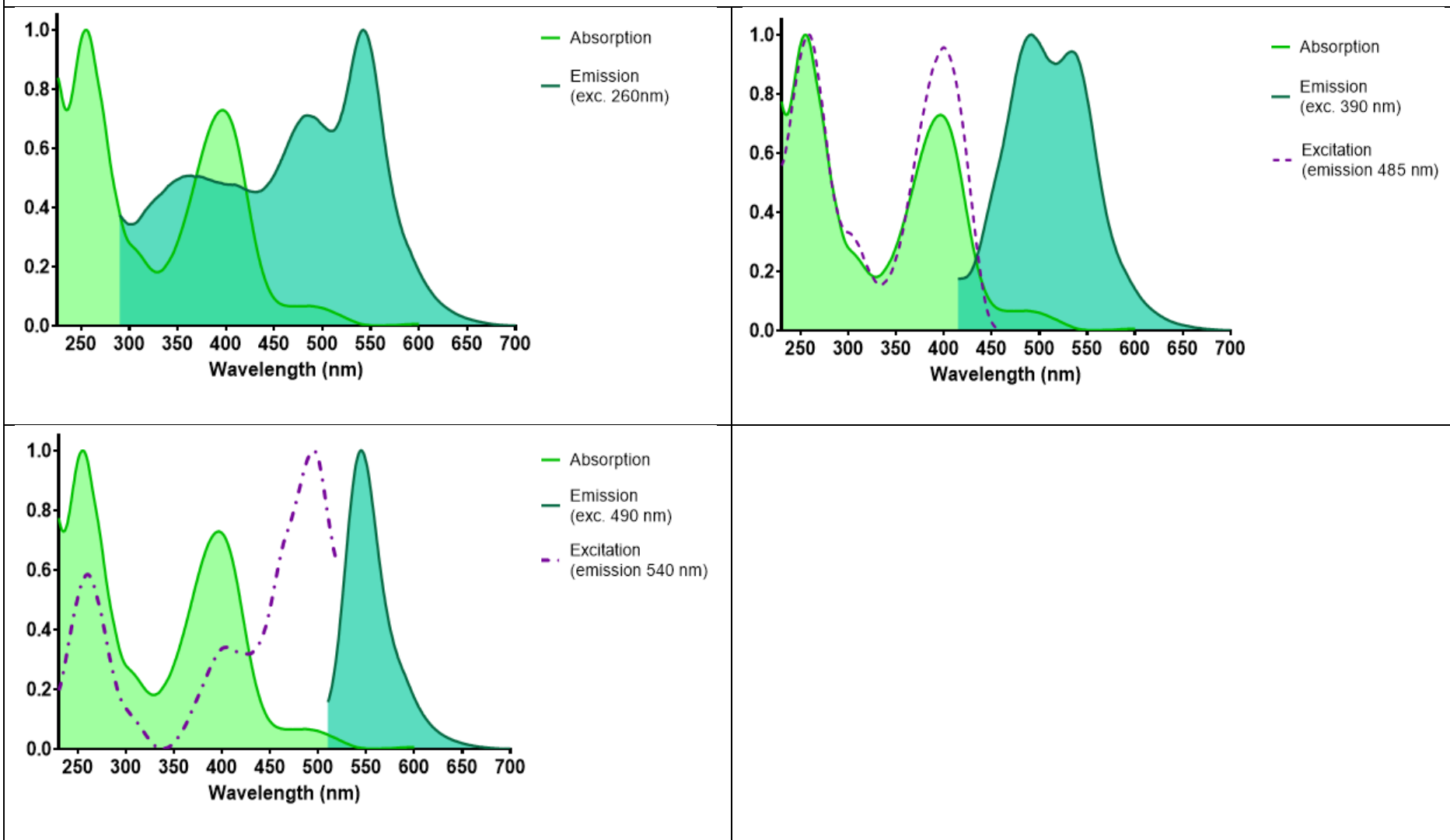
UV-VIS, excitation and emission spectra



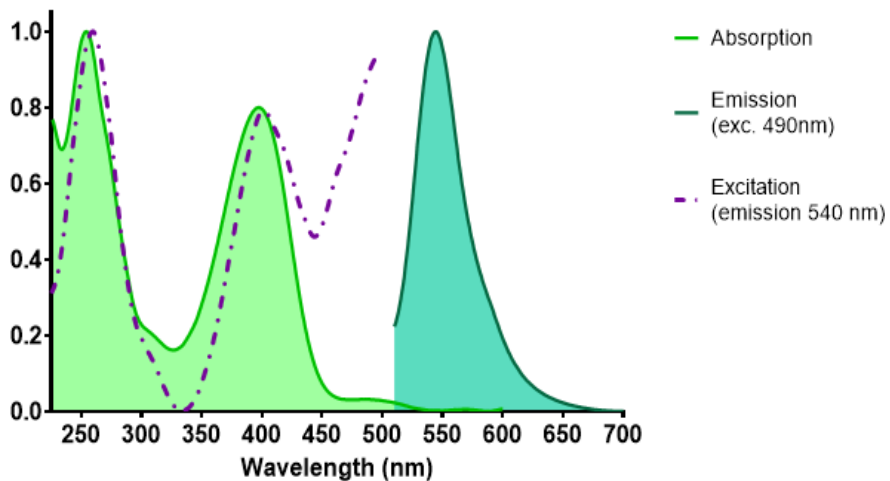
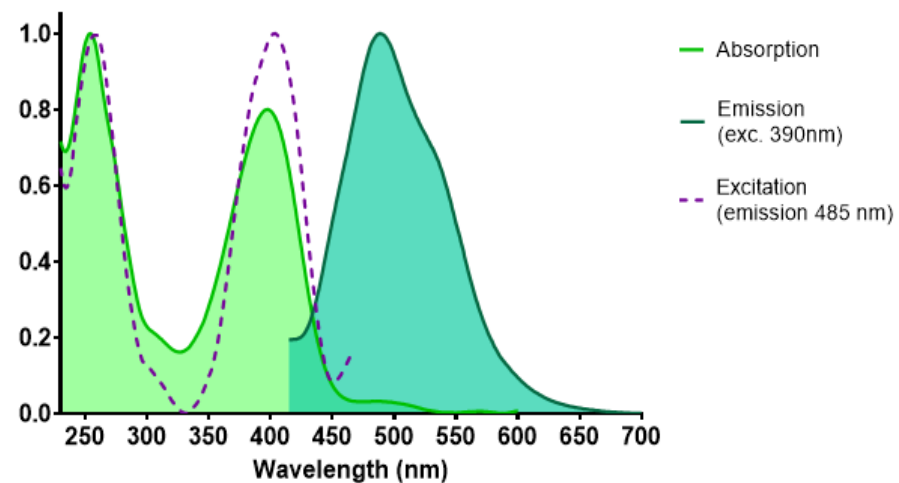
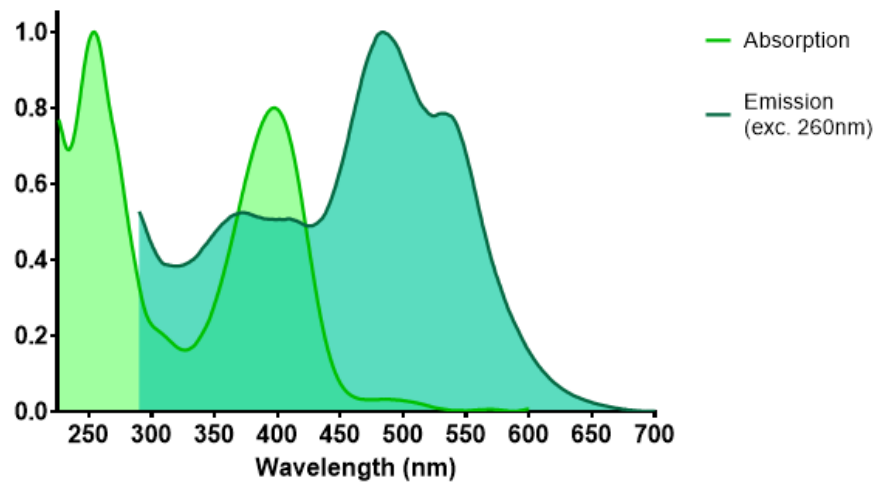
TMGpppG-3'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (1a-3')



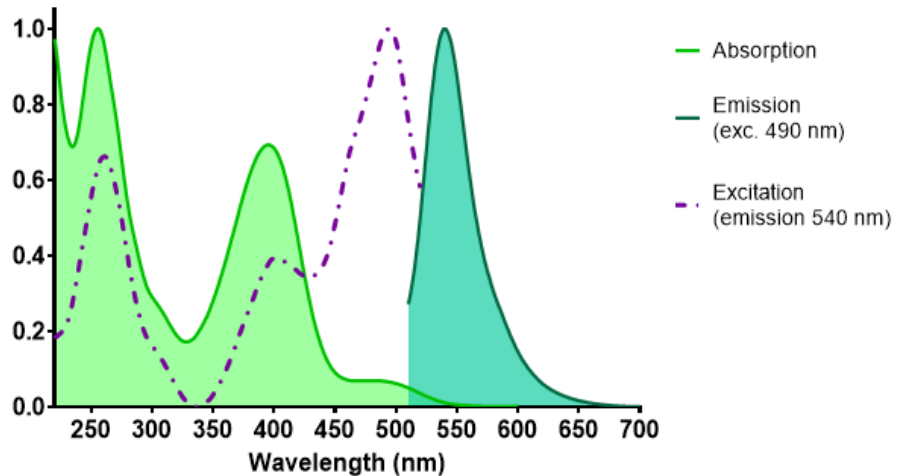
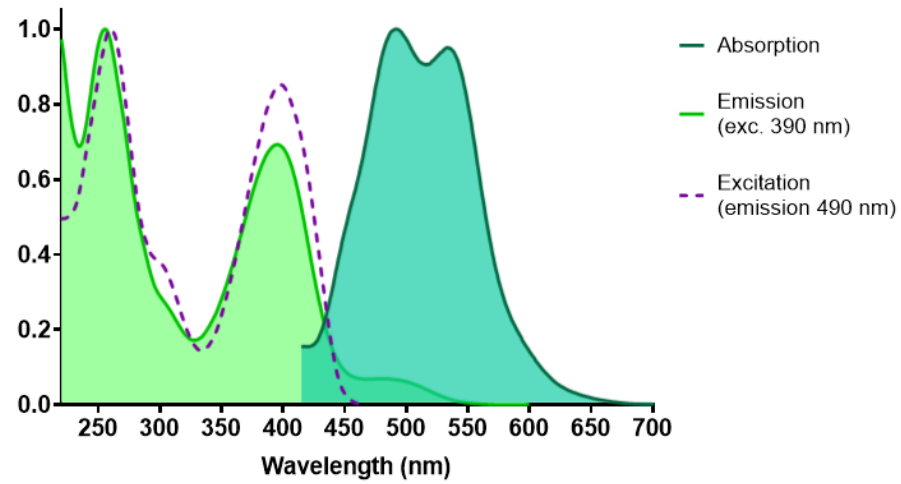
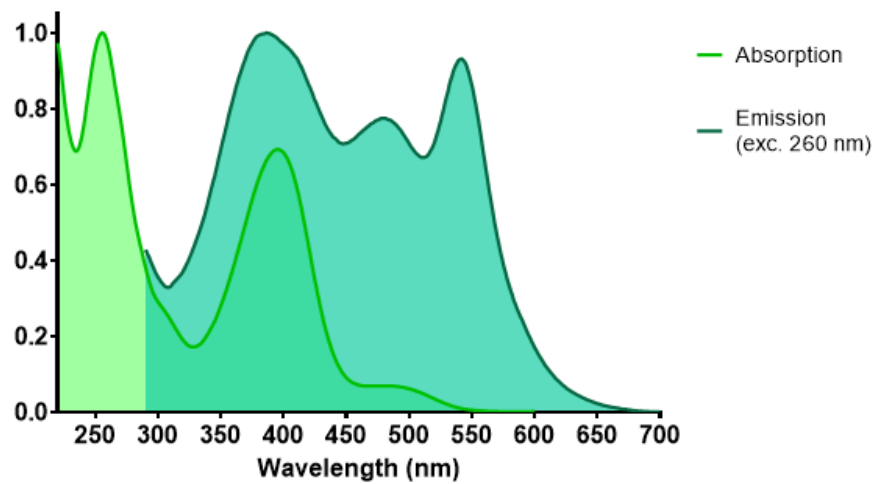
TMG-5'-S-pppG-2'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (2a-2')



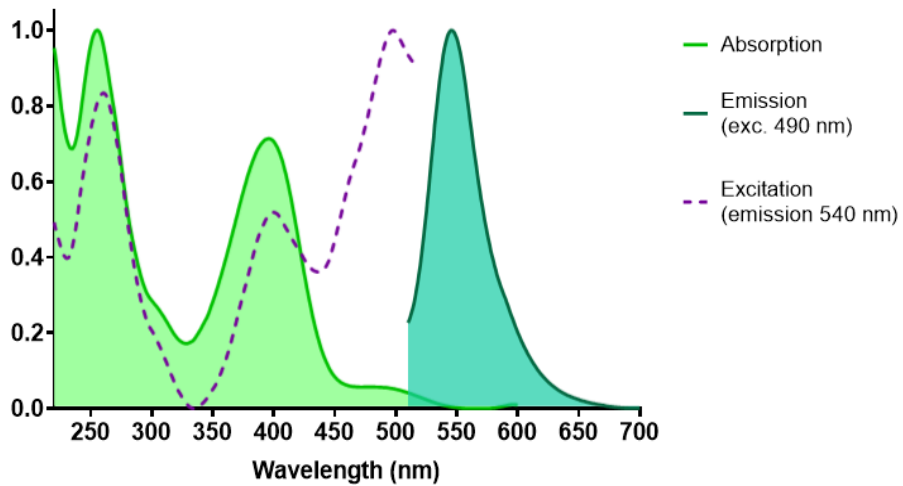
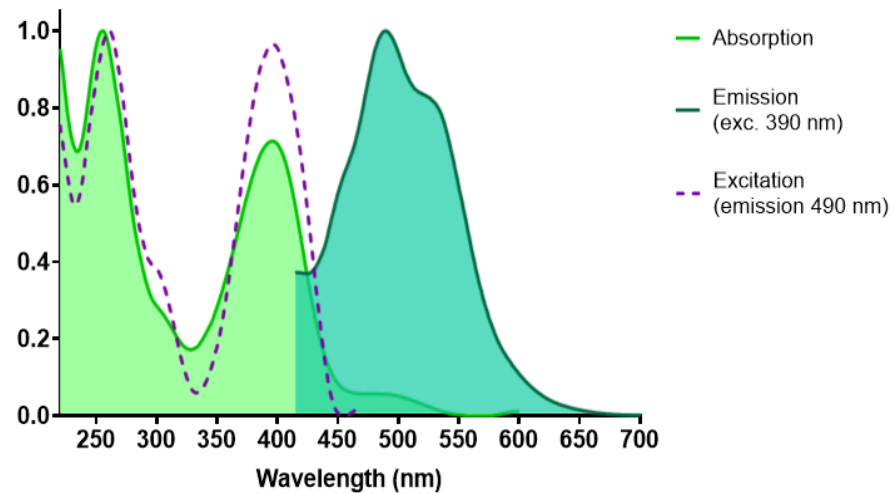
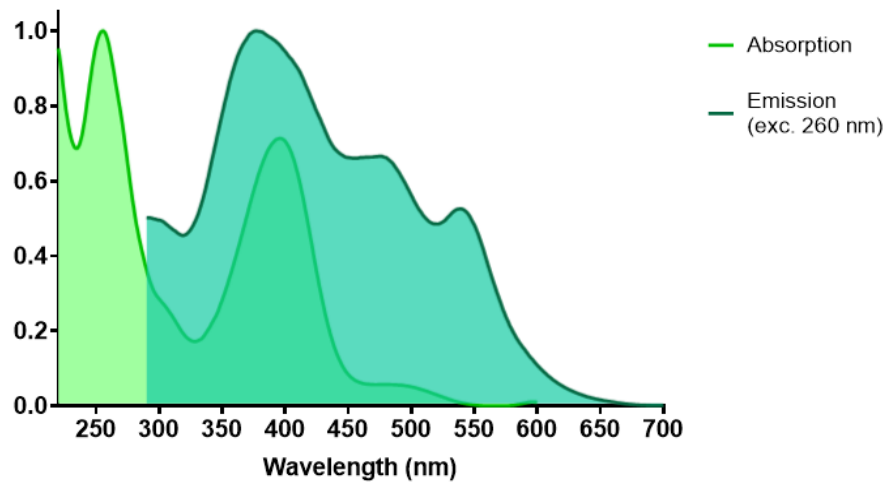
TMG-5'-S-pppG-3'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (2a-3')



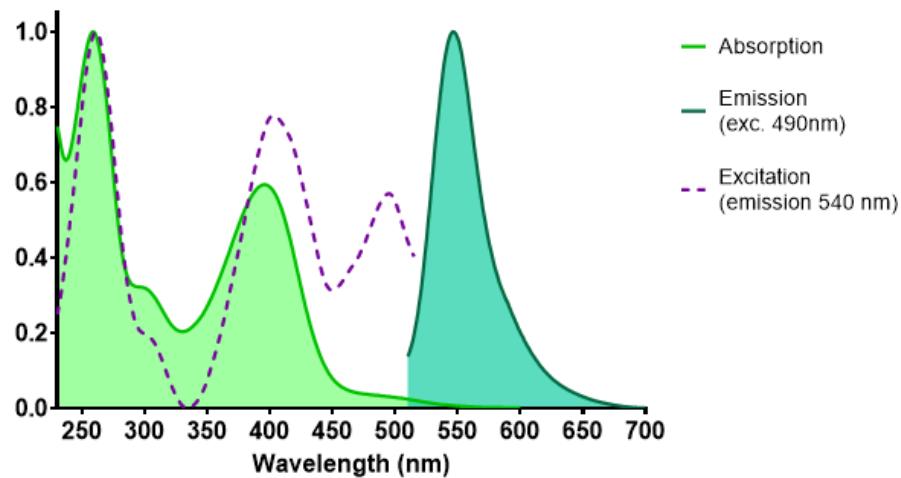
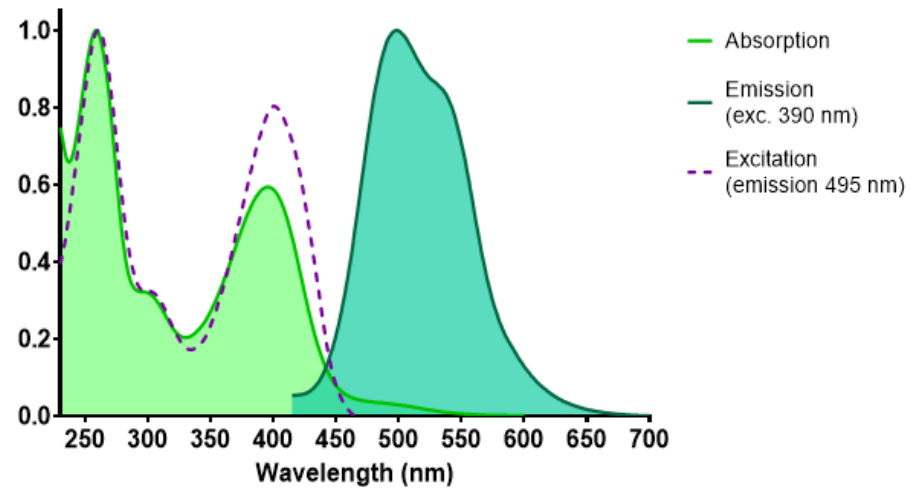
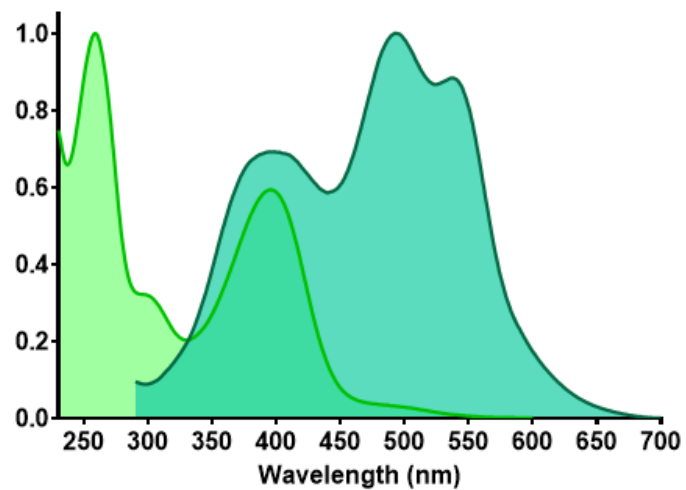
TMGppCH₂pG-2'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (3a-2')



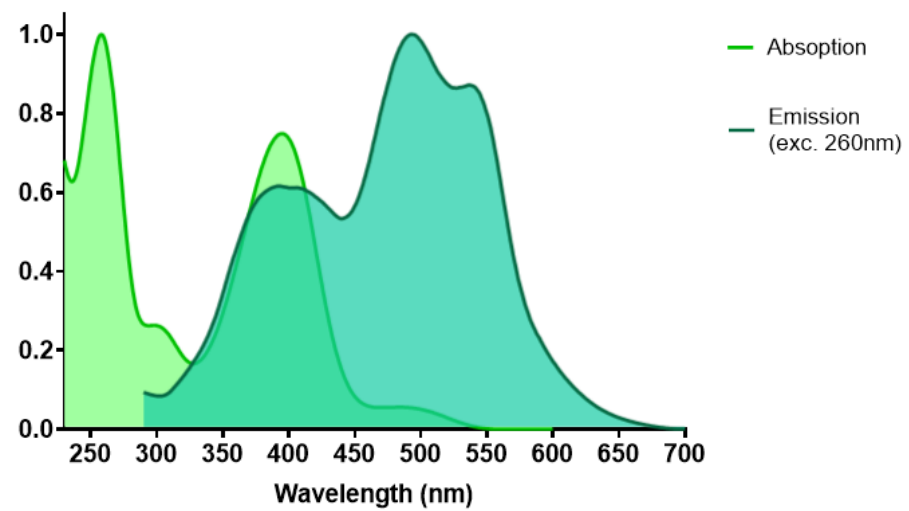
TMGppCH₂pG-3'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (3a-3')



TMGpppA-2'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (**4a-2'**)

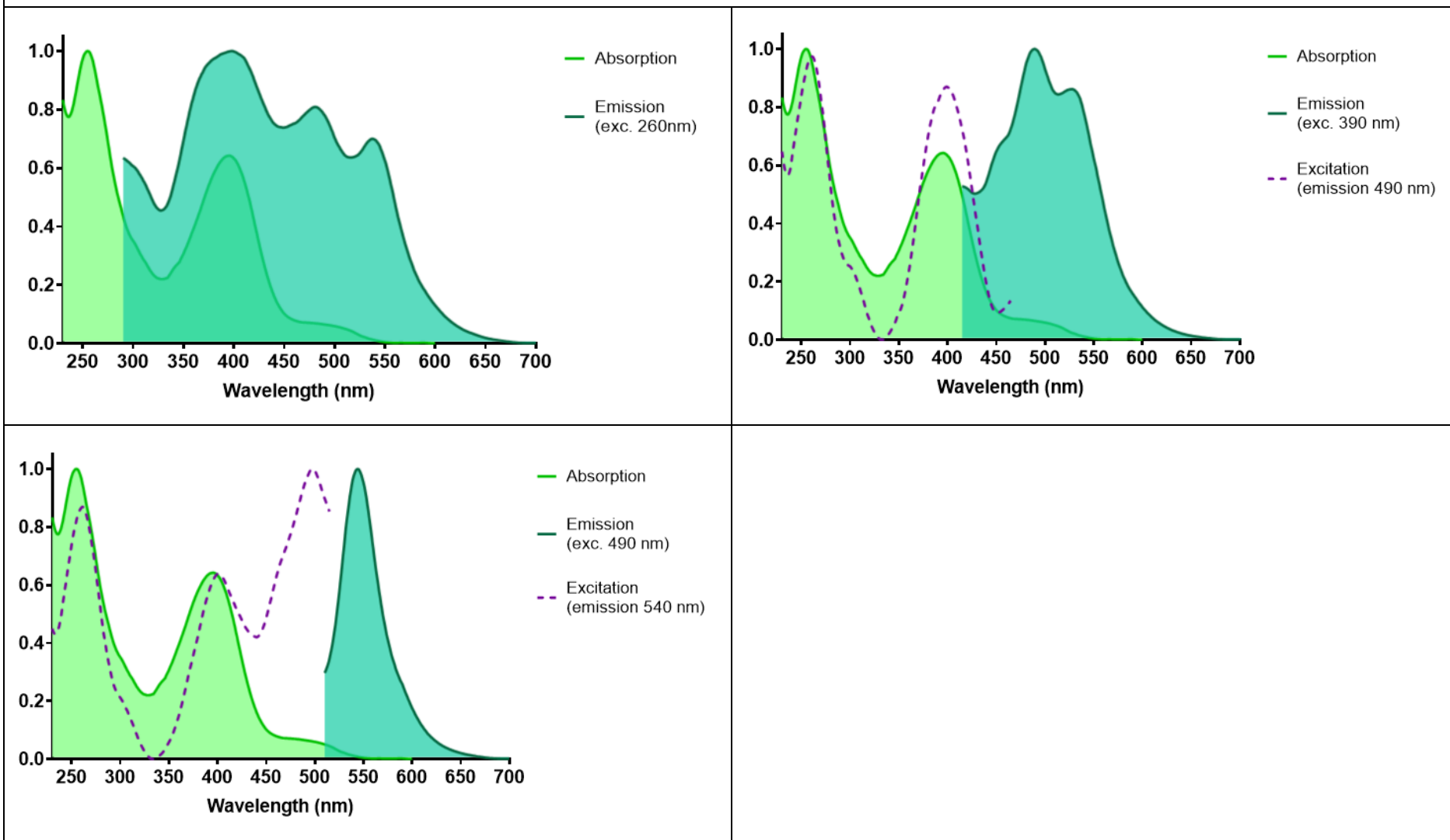


TMGpppA-3'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (4a-3')

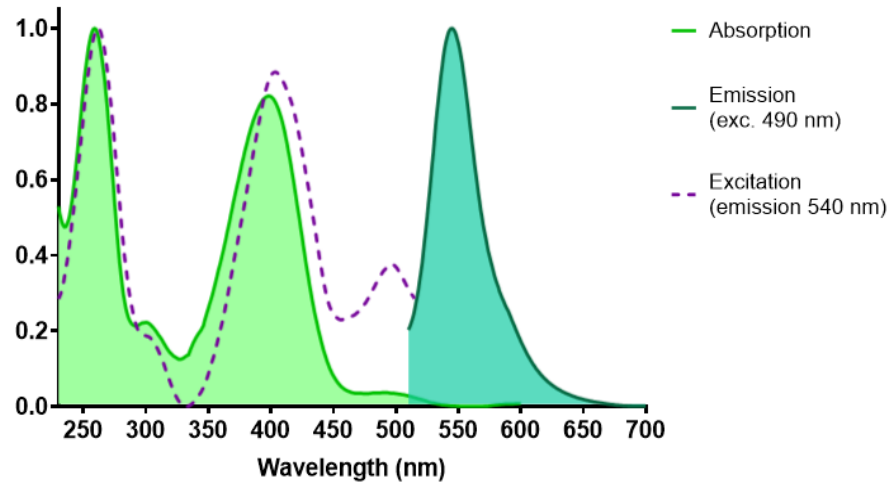
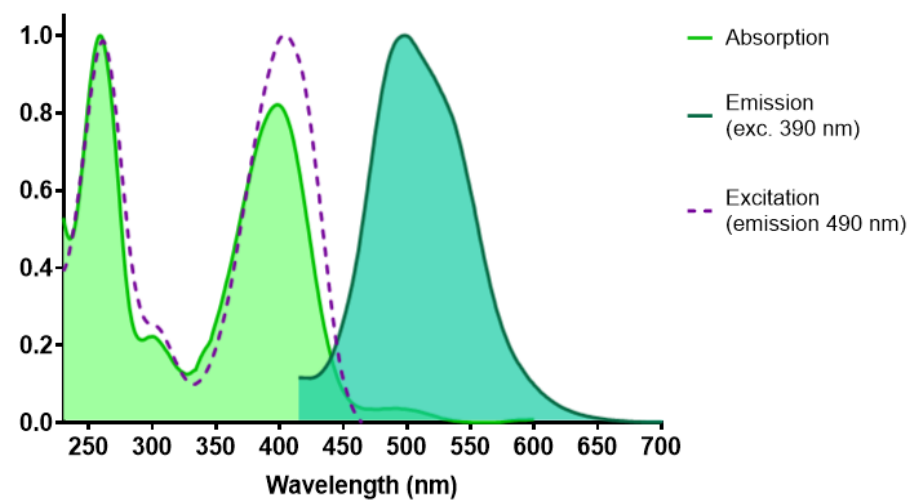
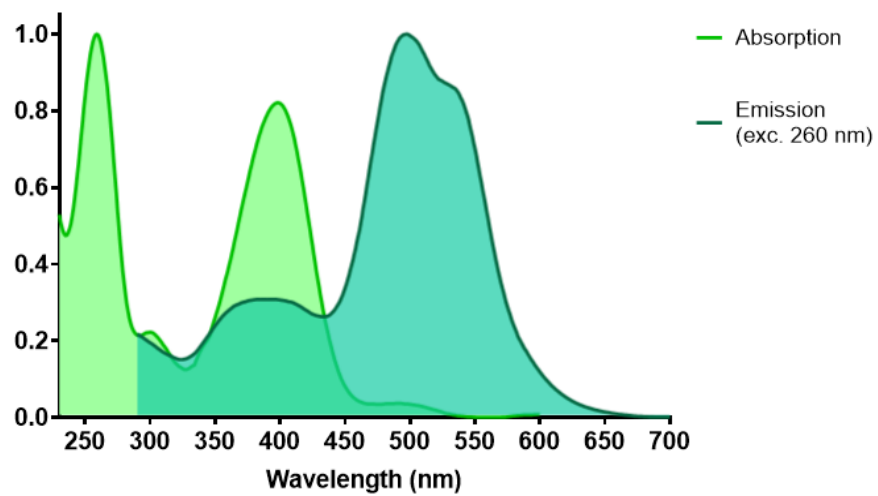


DODAJ

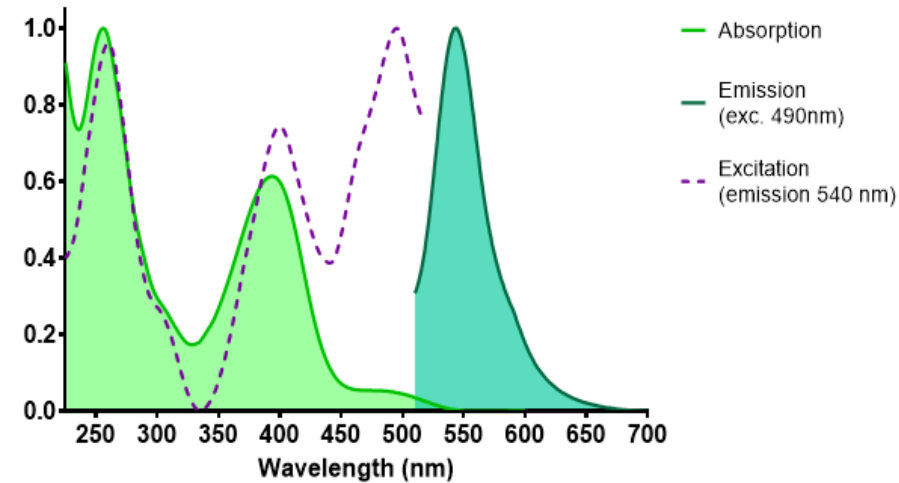
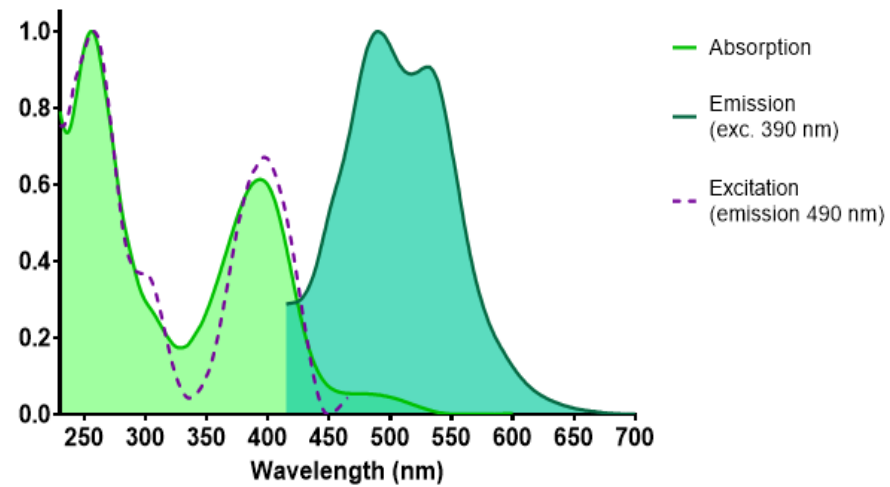
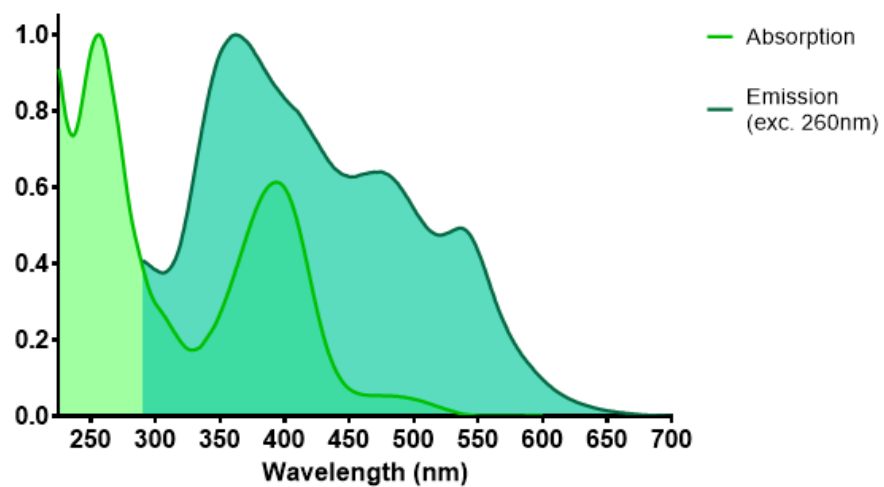
TMGppppG-3'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (5a-3')



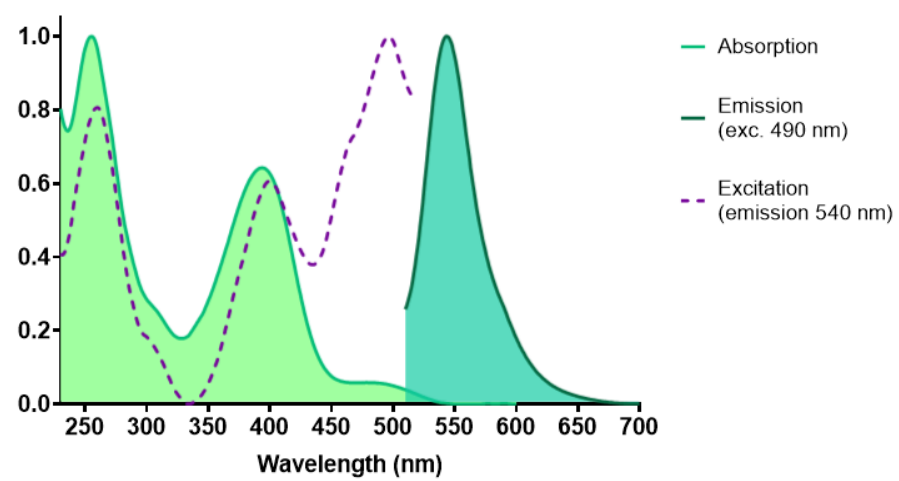
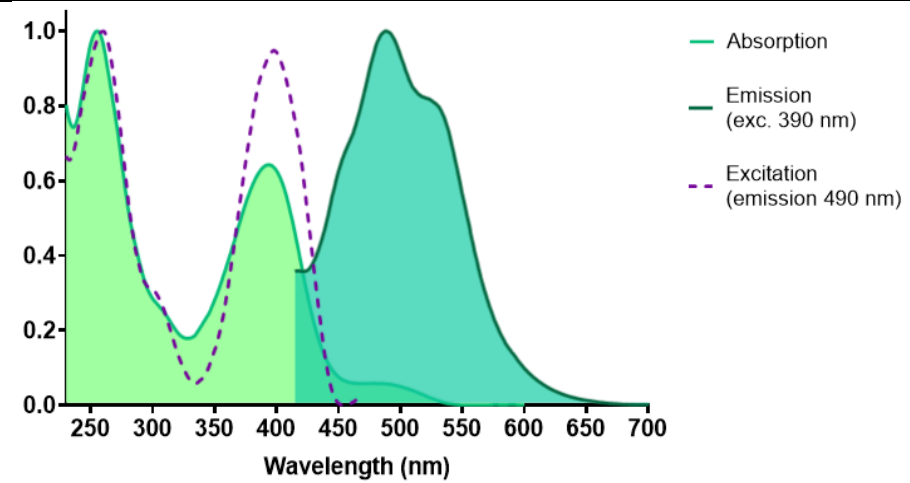
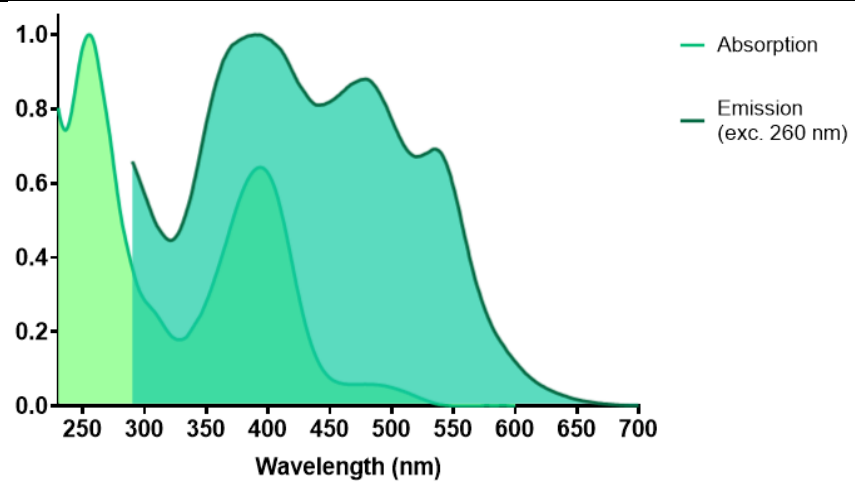
TMGpppA-2'+3'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (6a)



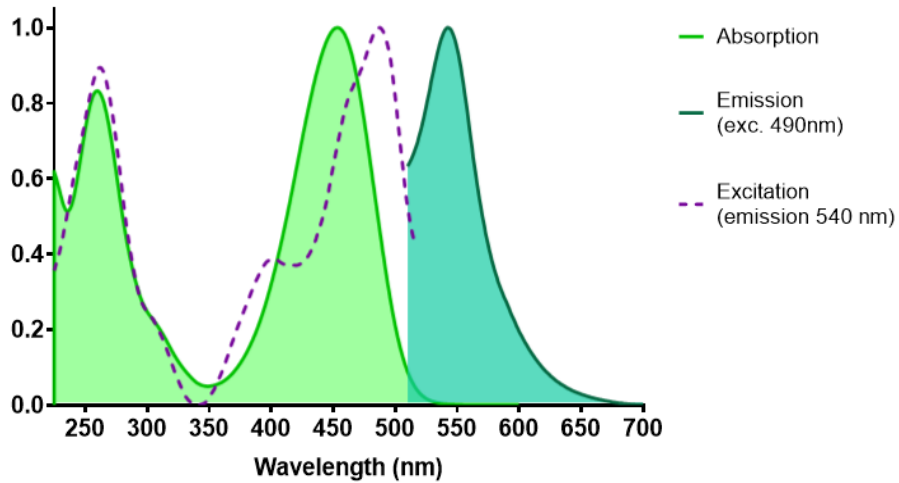
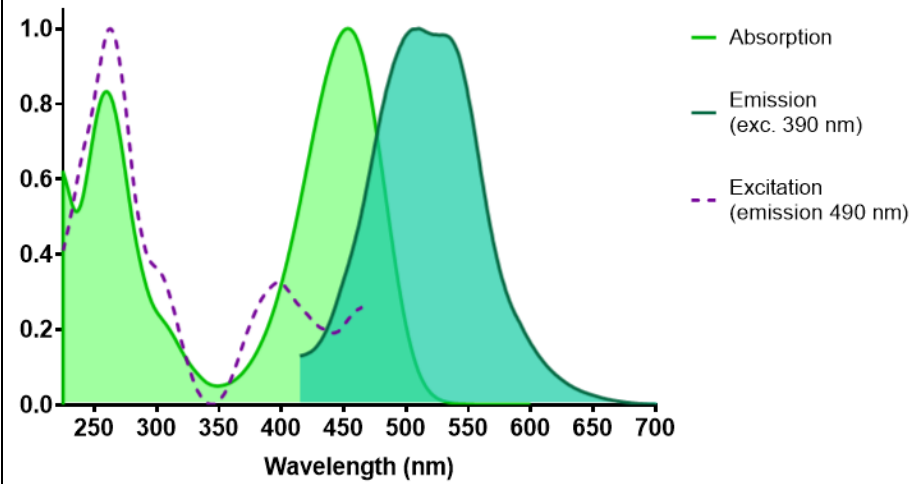
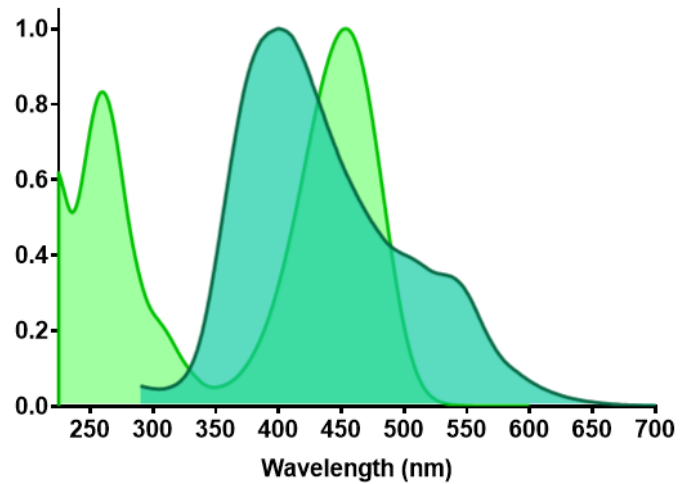
TMGppp-5'-SG-2'-O-C(O)NH-CH₂-triazole-CH₂CH₂-DMHBI (7a-2')



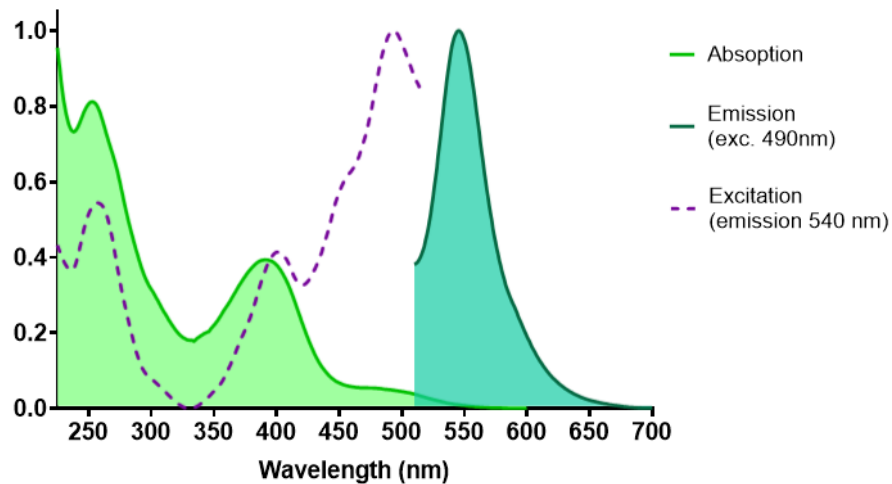
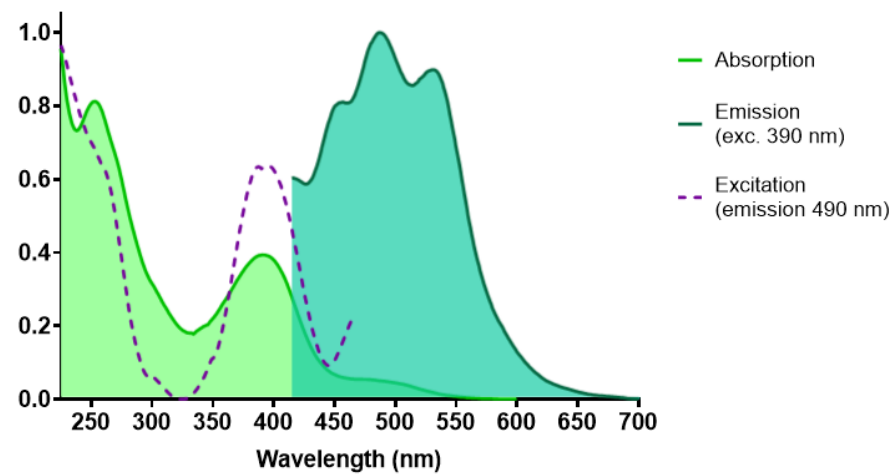
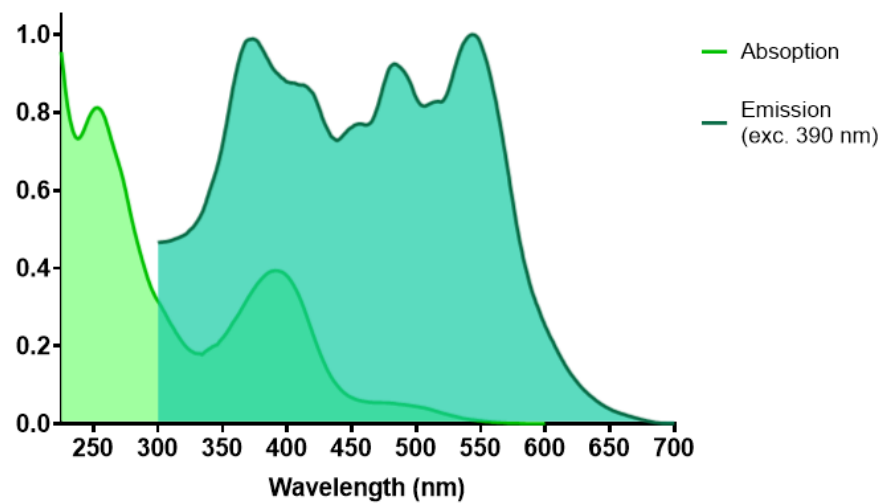
TMGppp-5'-SG-3'-O-C(O)NH-CH₂-triazole-CH₂CH₂-DMHBI (7a-3')



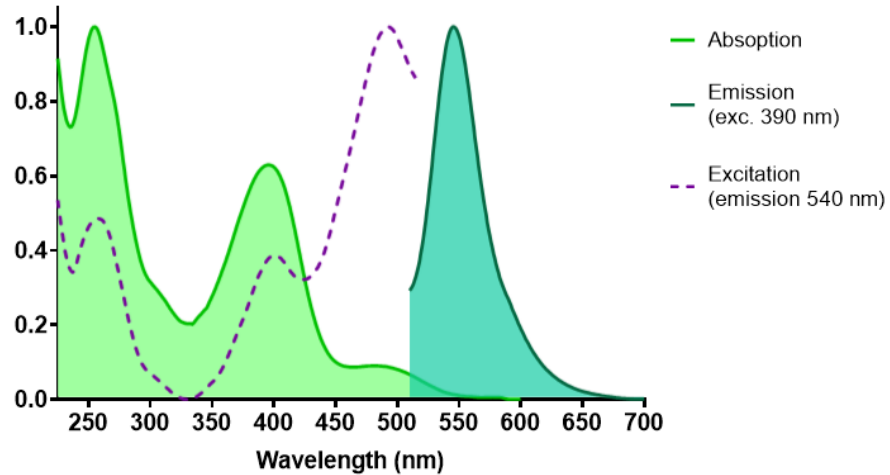
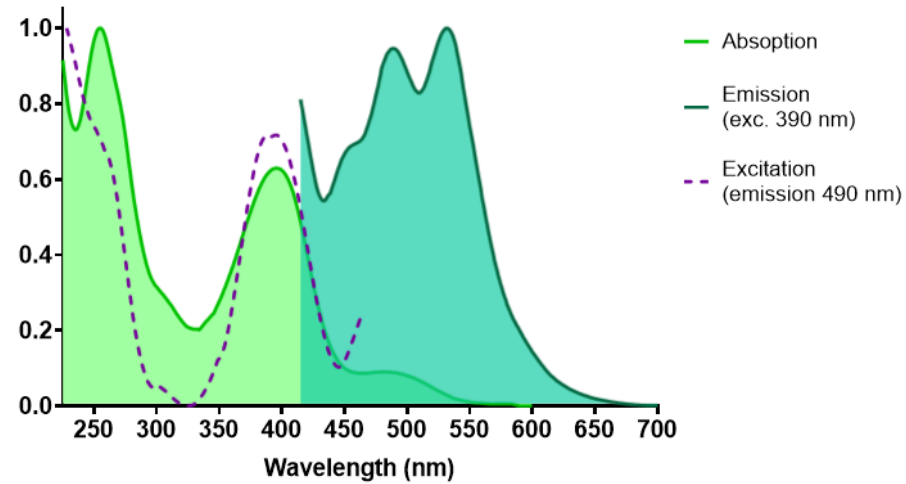
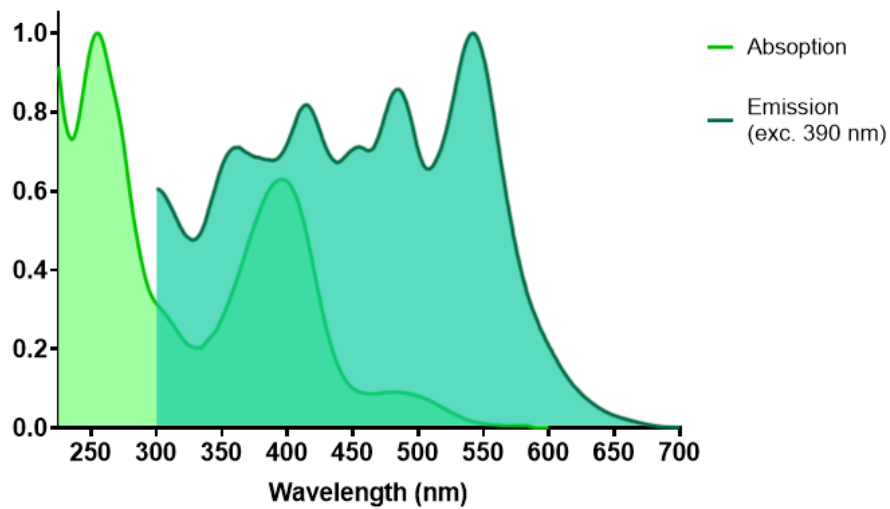
TMGpppG-N1-CH₂-triazole-CH₂CH₂-DMHBI (8a)



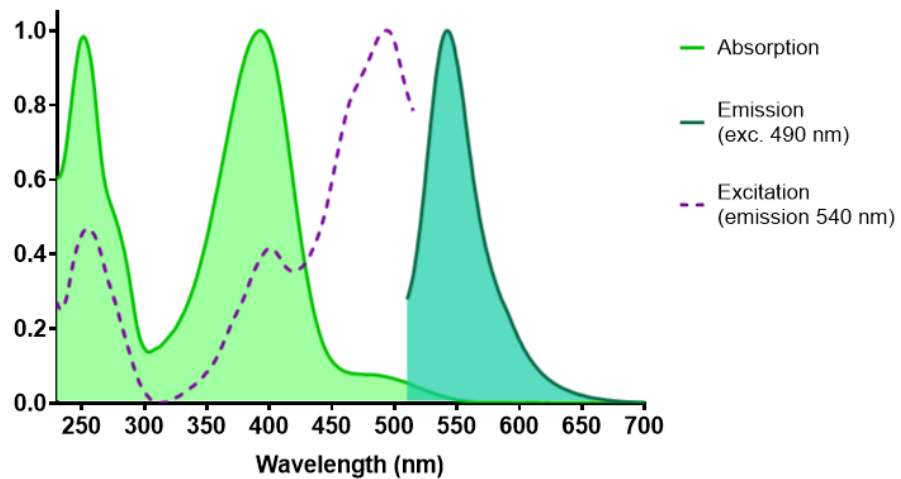
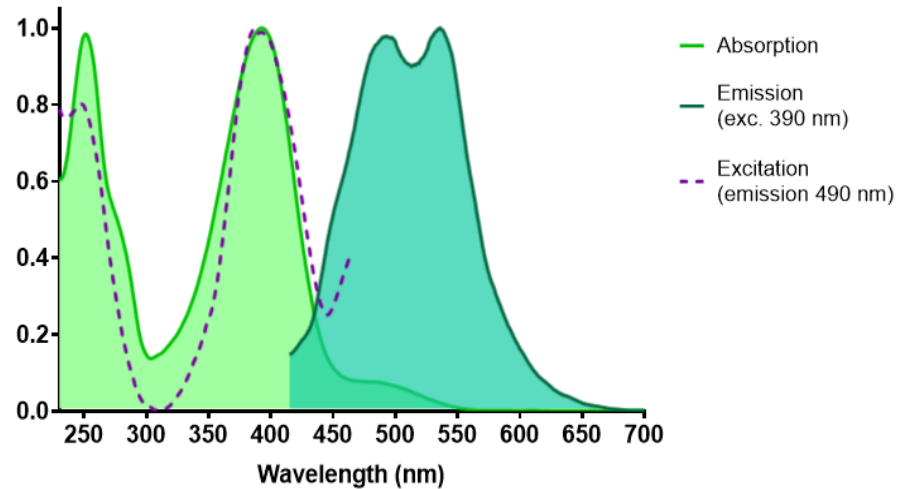
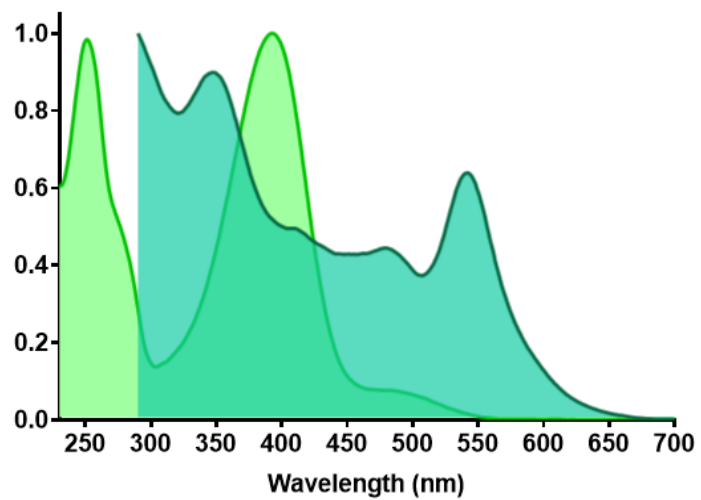
TMG(-2'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI)pppG (9a-2')



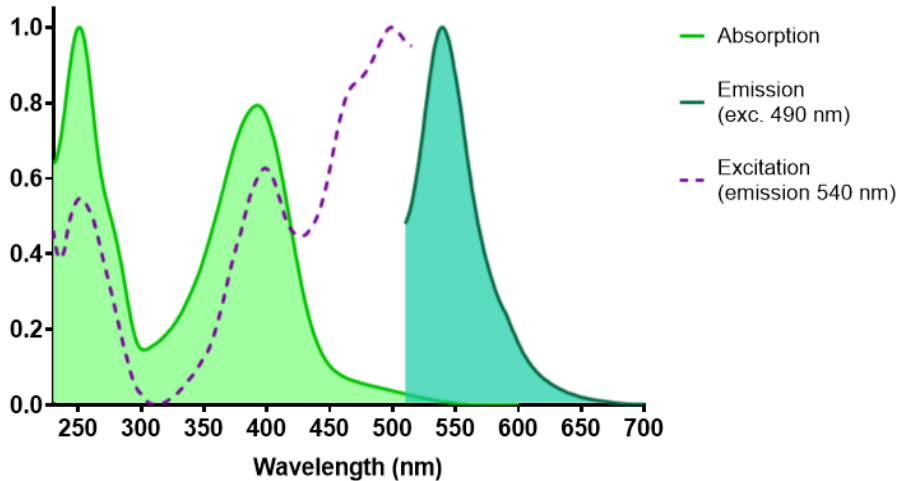
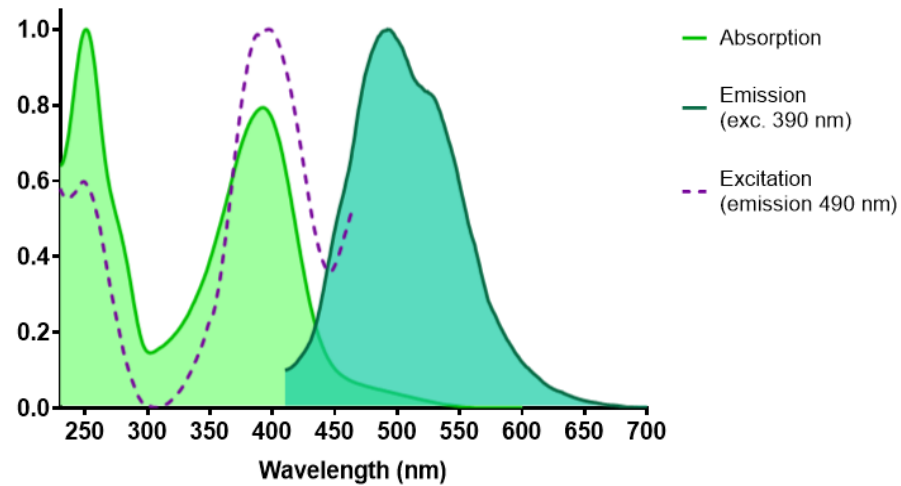
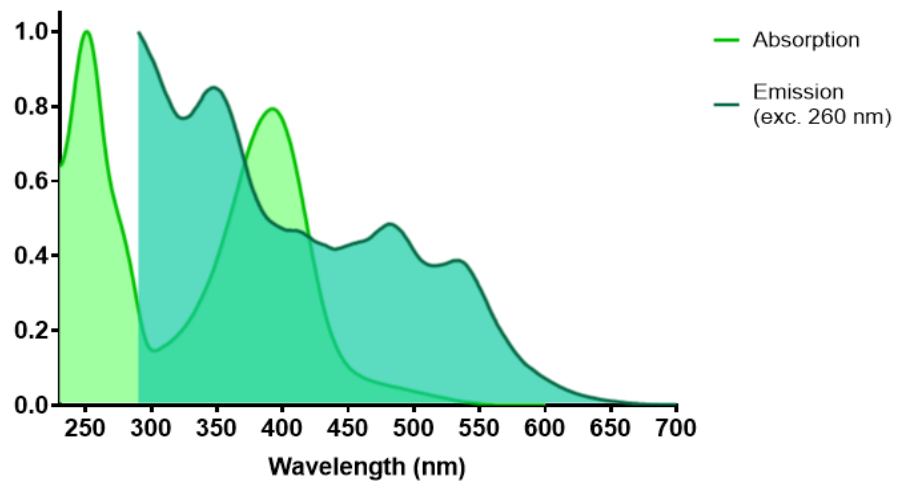
TMG(-3'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI)pppG (9a-3')



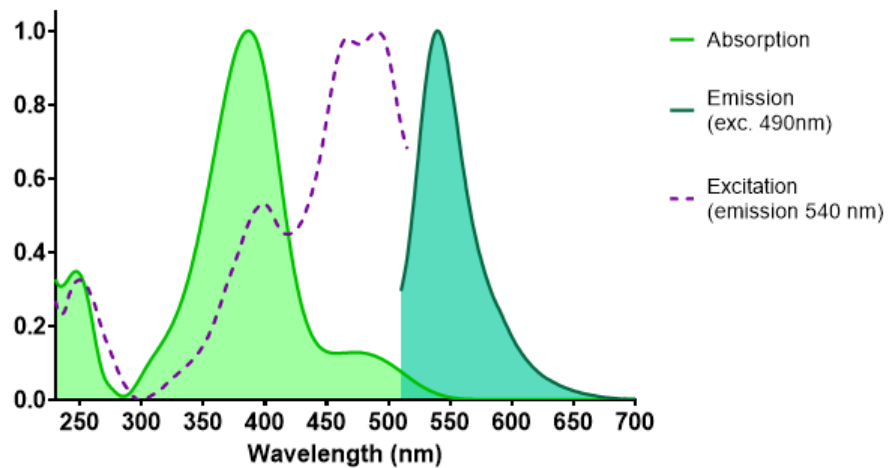
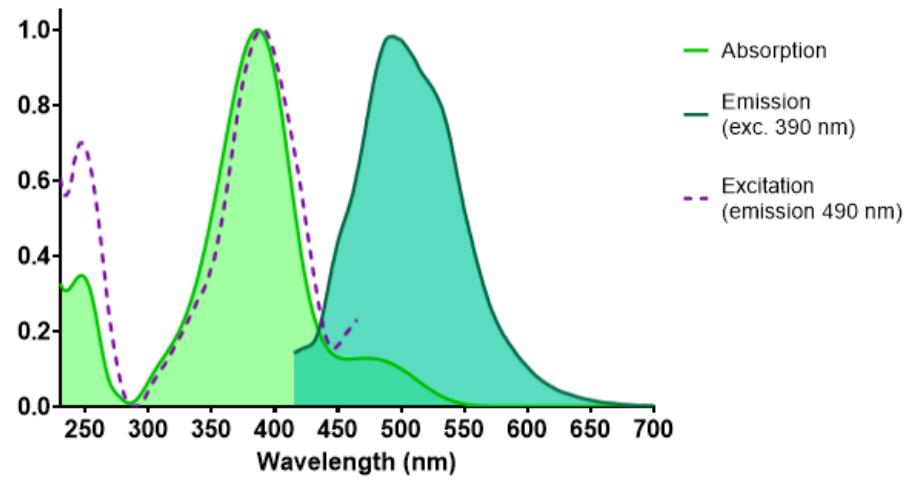
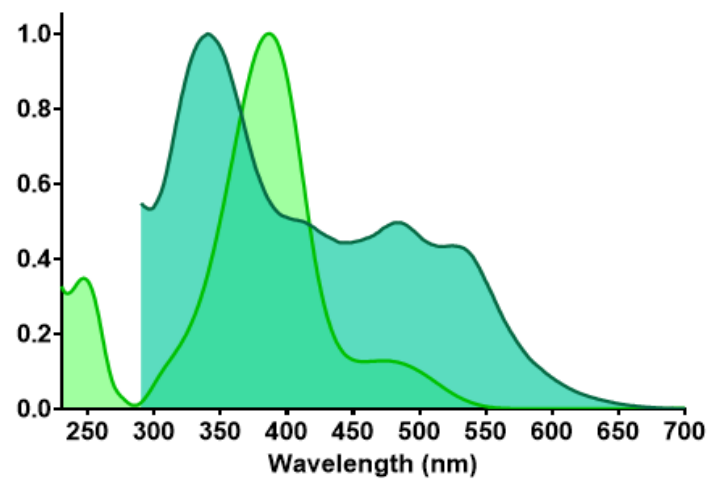
GMP-2'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (**10a-2'**)

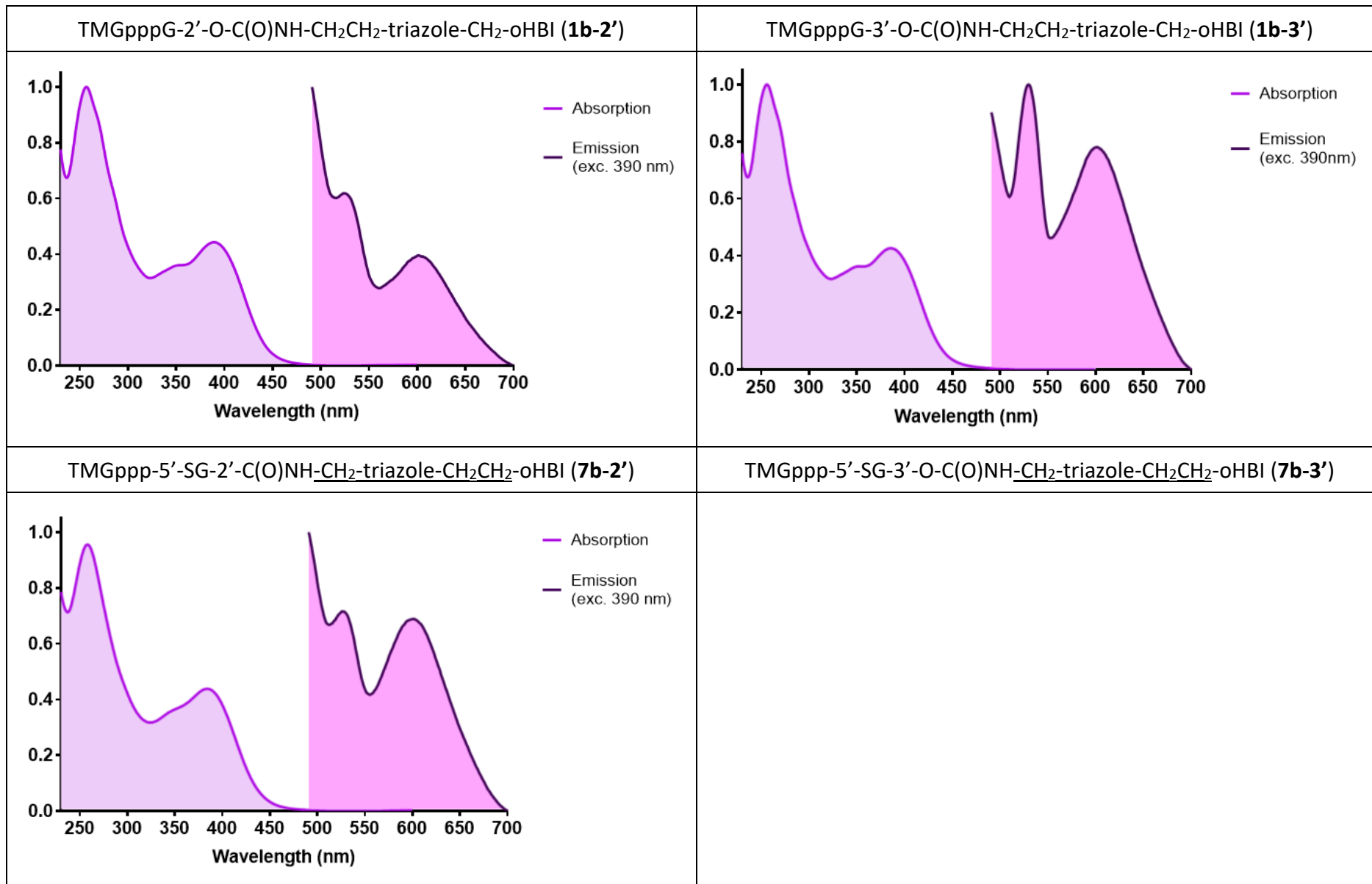


GMP-3'-O-C(O)NH-CH₂CH₂-triazole-CH₂-DMHBI (**10a-3'**)

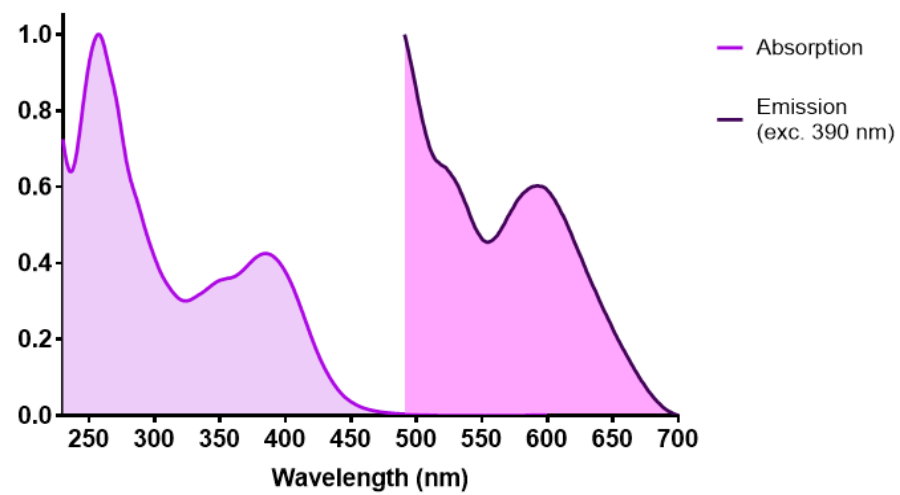


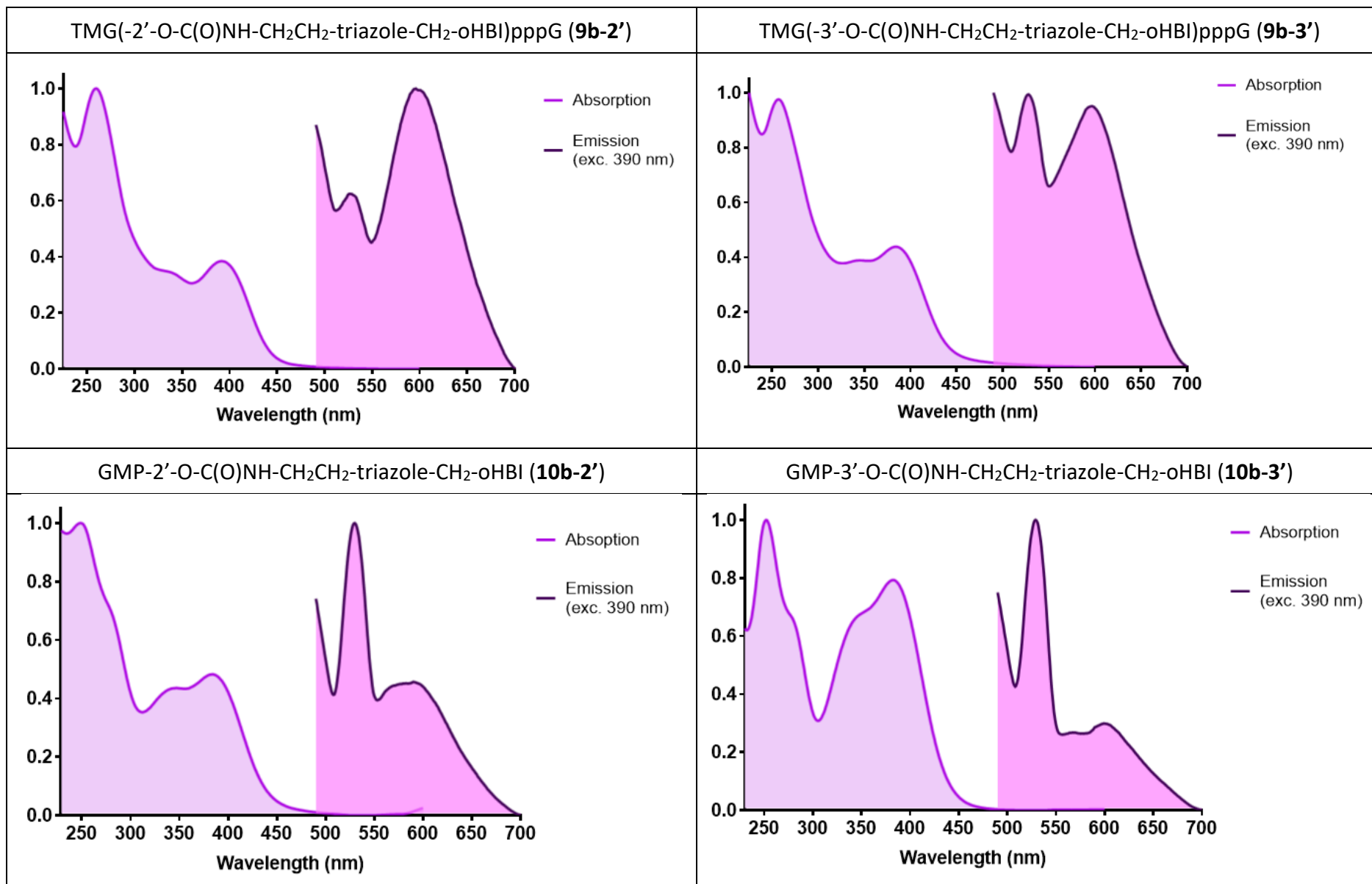
DMHBI-CH₂-triazole-CH₂-phosphonate (12a)

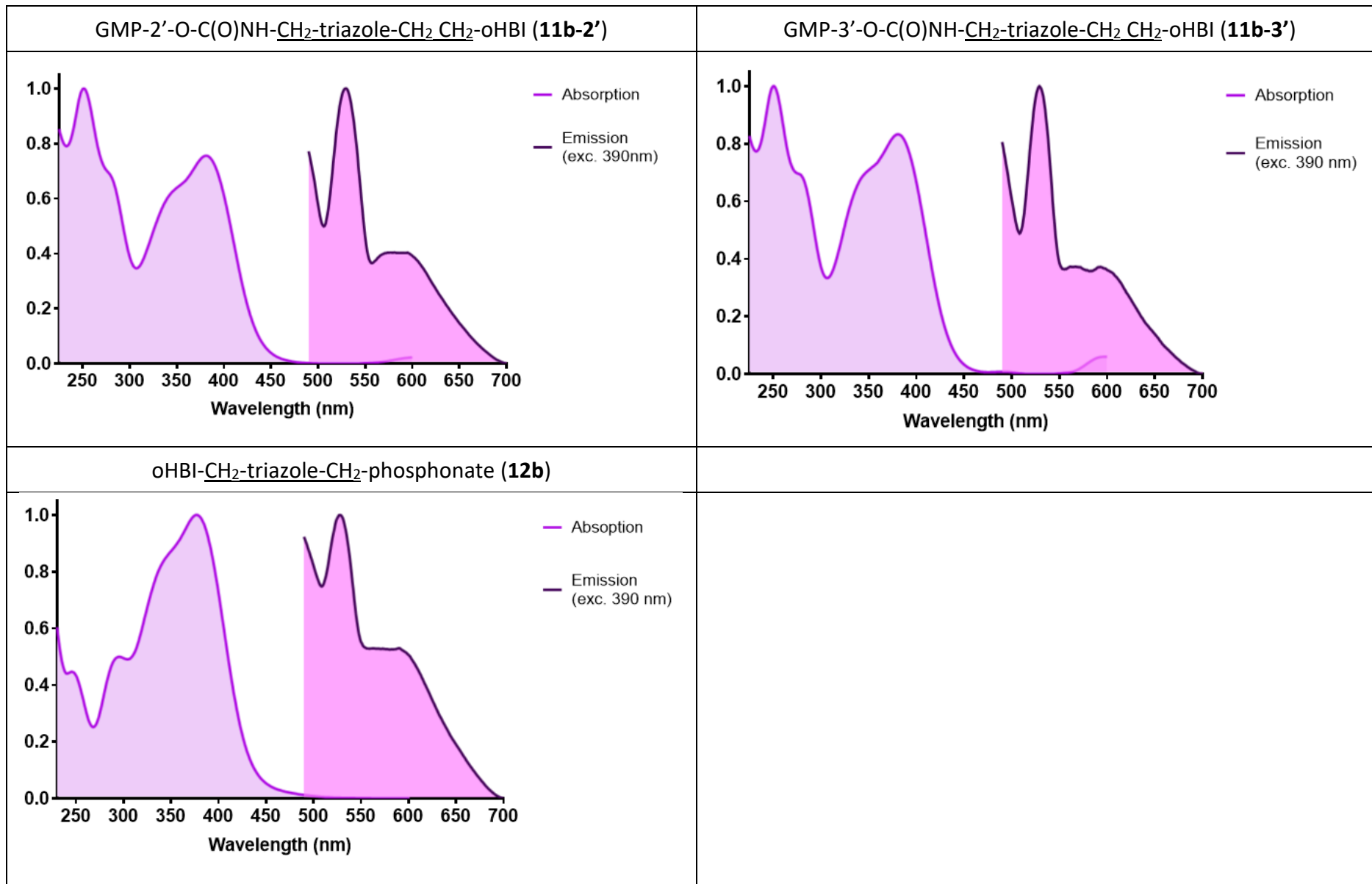


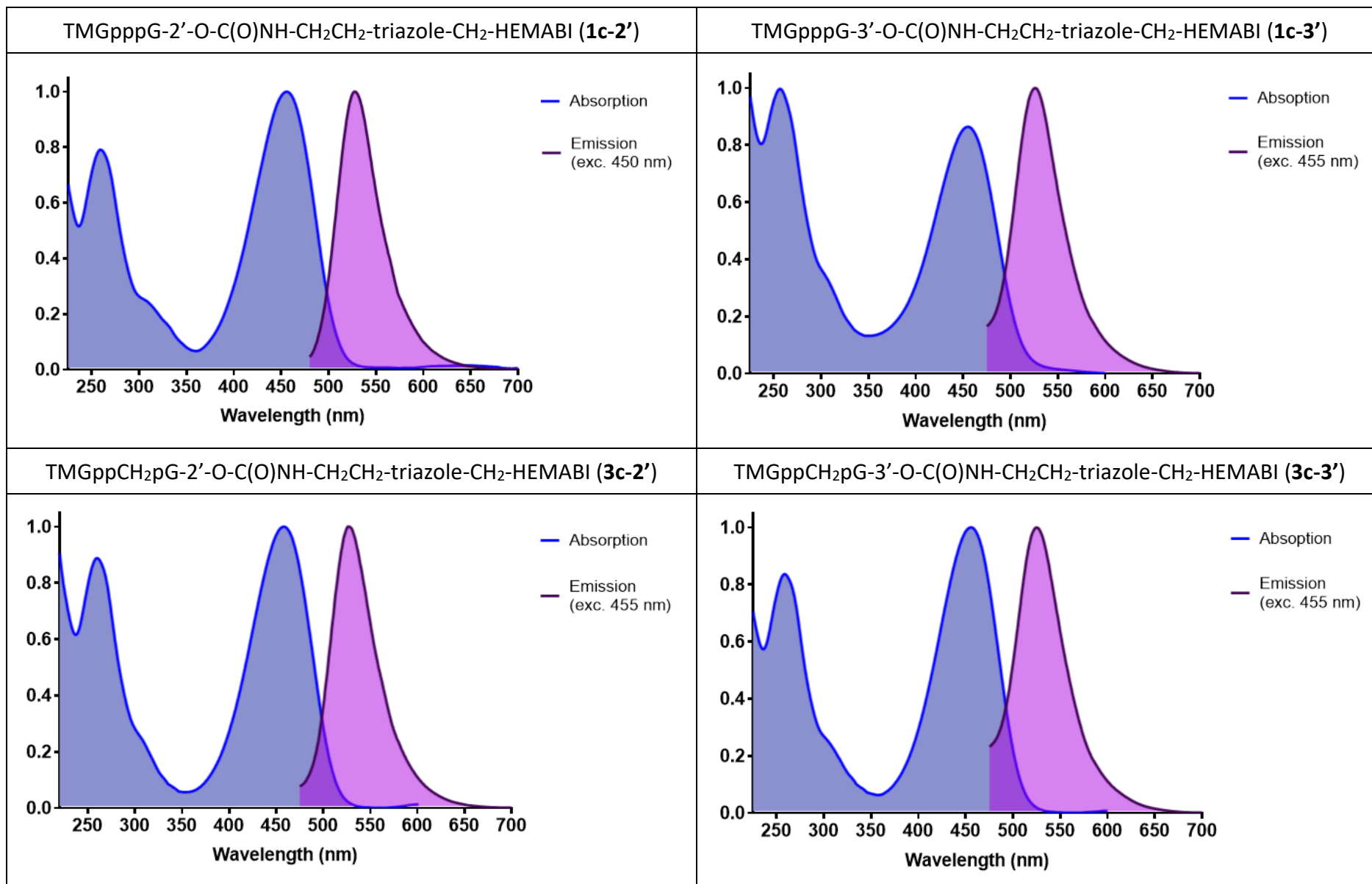


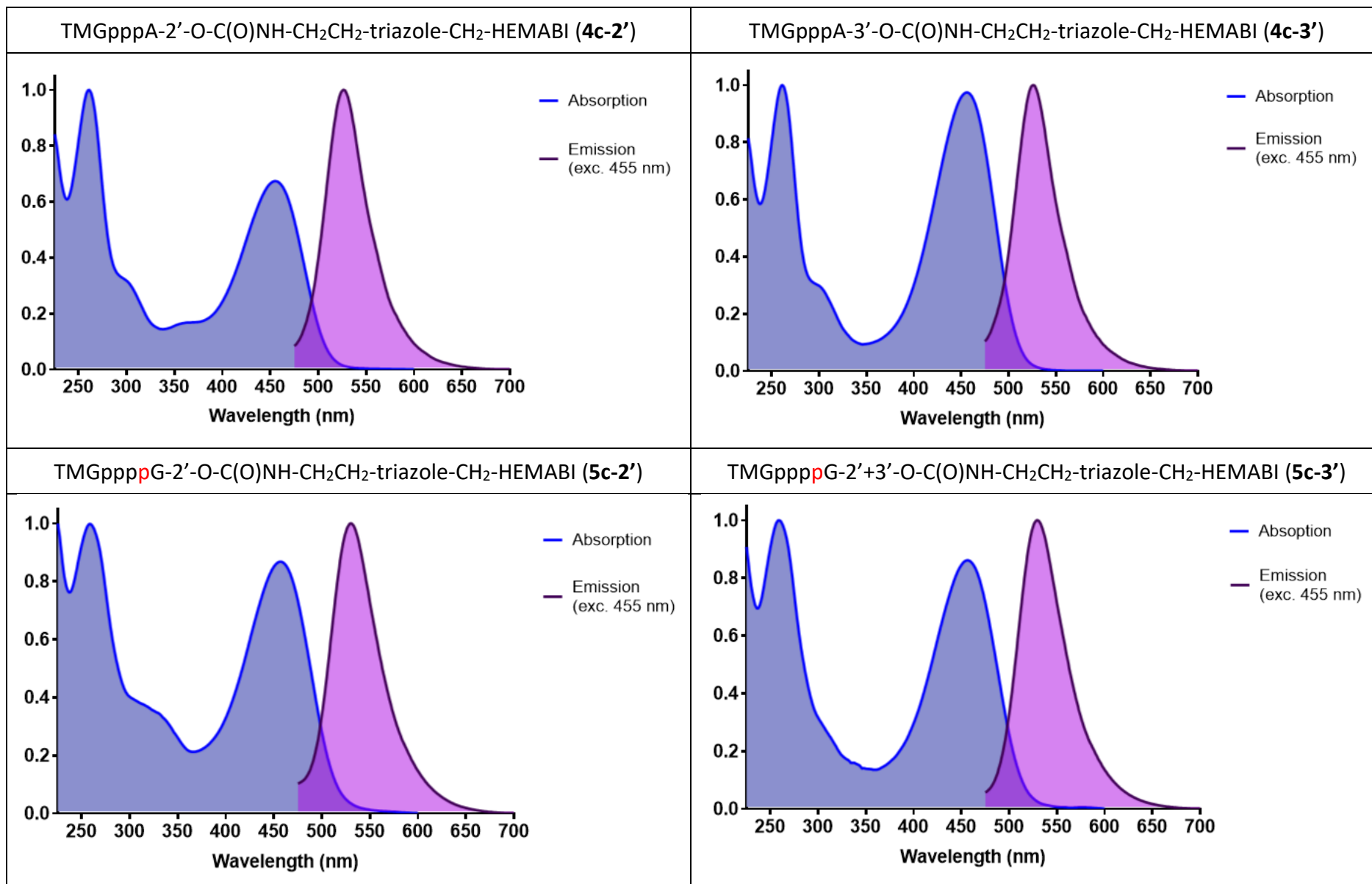
TMGpppG-N1-CH₂-triazole-CH₂CH₂-oHBI (**8b**)

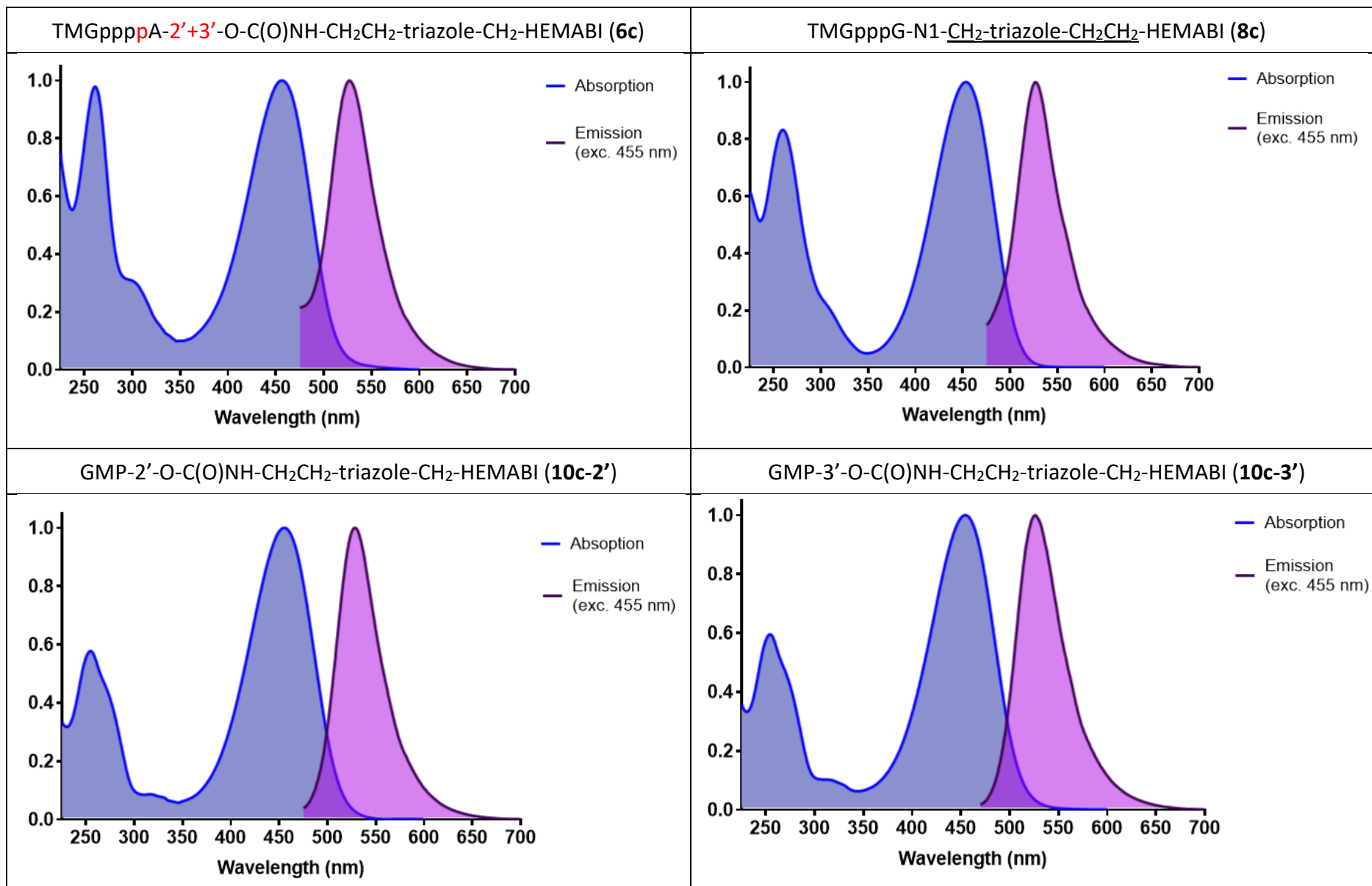




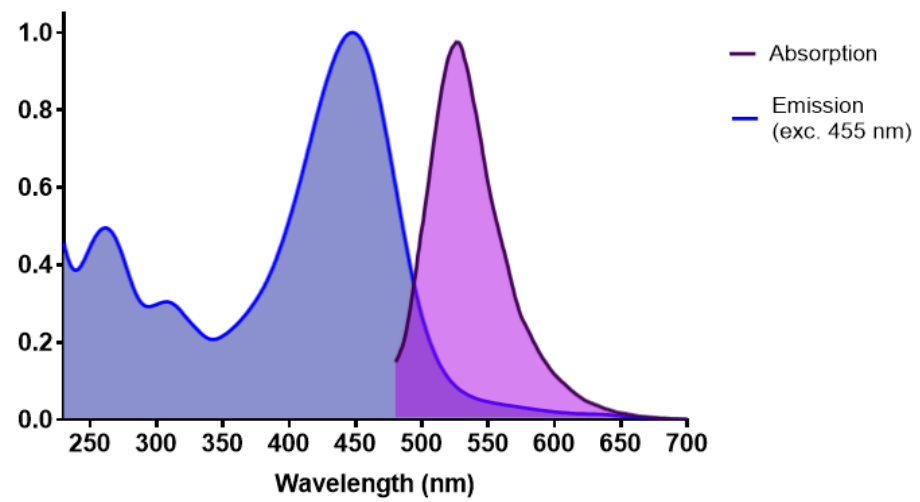


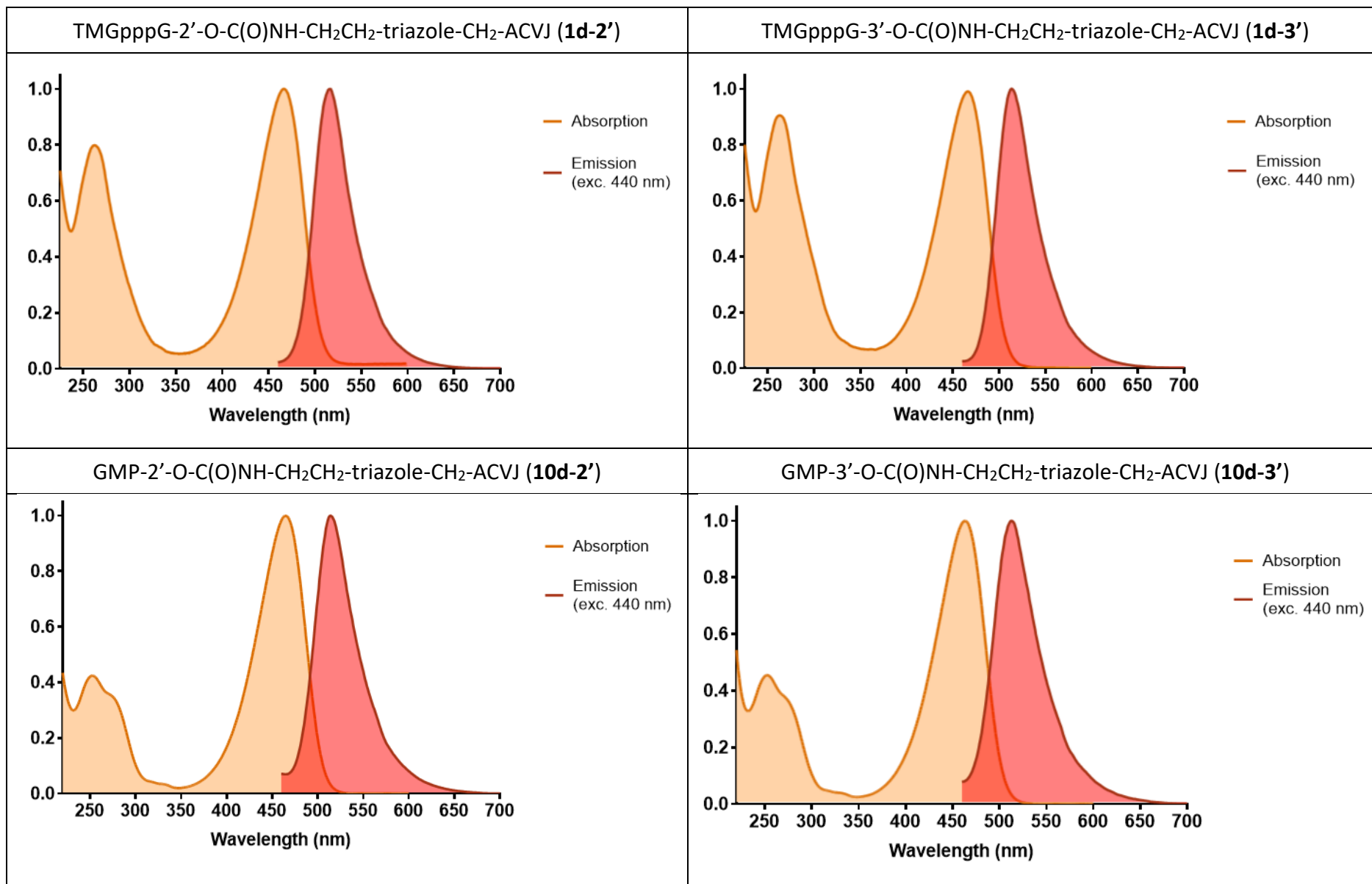






HEMABI-CH₂-triazole-CH₂-phosphonate (**12c**)





ACVJ-CH₂-triazole-CH₂-phosphonate (**12d**)

