SUPPORTING INFORMATION

Trojan Horse siderophore conjugates induce *P. aeruginosa* suicide and qualify the TonB protein as a novel antibiotic target

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General chemical information

Unless otherwise mentioned, reagents were purchased and used without further purification. All employed solvents for workups and purifications were HPLC purity grade. Solid-phase peptide synthesis (SPPS) was performed on an automated Syro Multiple Peptide Synthesizer (MultiSynTech, Witten, Germany) with a Rapp TentaGel® S RAM resin (Rapp Polymere, Tübingen, Germany). Centrifugations were performed on a Universal 32 R centrifuge (Hettich).

With the exception of biphasic reactions or reactions in water, all reactions were carried out in anhydrous solvents. Moisture-sensitive reactions were carried out oven-dried glassware under argon atmosphere. Reaction progress was monitored by TLC (silica gel 60 F_{254}, on aluminum/glass, Merck®).

Automatic preparative column chromatography was performed on a Grace Reveleris® X2 instrument (Büchi®) with disposable columns (Reveleris® Flash Cartridges Silica 40 µm, Büchi).

Purifications by RP-HPLC were performed on a Pure C-850 (Büchi) or Dionex Ultimate (Thermo Fisher Scientific) on a Phenomenex Gemini C18 RP-column 00G-4436-NO, 10 µm, 110 A, 250×10.00 mm (5 mL/min) or Phenomenex Gemini C18 RP-column 00G-4435-PO-AX, 5 µm, 110 A, 250×21.20 mm (10 mL/min). Substances were subsequently freeze-dried on an Alpha 2-4 LSCbasic (Christ) instrument.

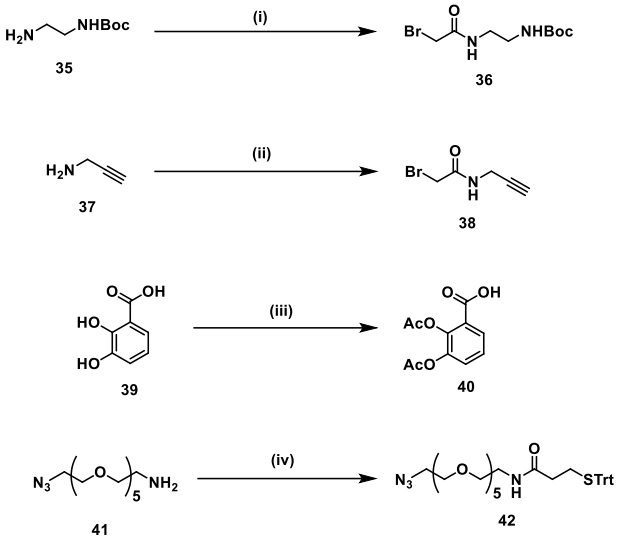
High resolution mass spectrometry (HRMS) was performed using a Dionex Ultimate 3000 HPLC system equipped with a DAD detector and a Bruker maxis HD QTOF mass detector with electrospray ionization (ESI). Samples were injected directly *via* an Ultimate 3000RS autosampler (Thermo Fisher Scientific). The mass-to-charge ratios (m/z) are indicated.

All isolated compounds were characterized by ^{1}H-, ^{13}C-NMR spectra, and/or ESI-HRMS.

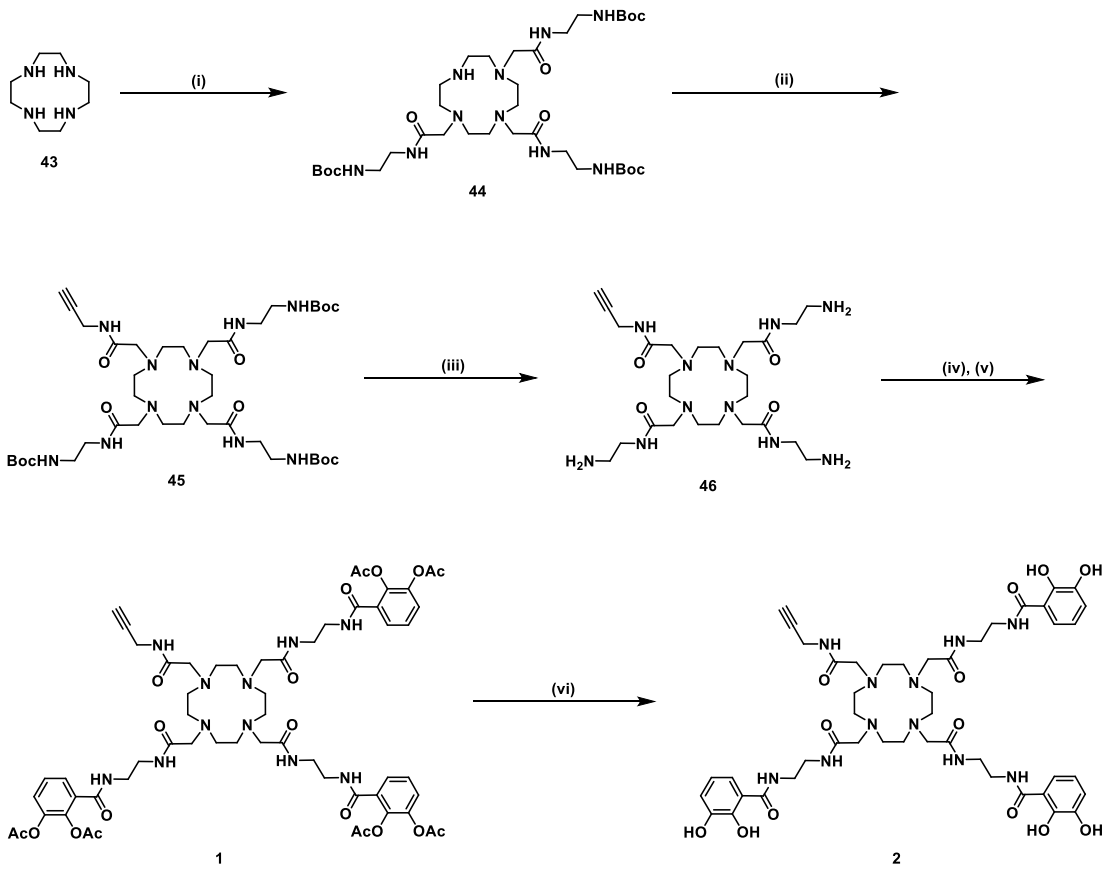
Yields are calculated based on substance purity ≥95% as confirmed by NMR and MS.

NMR spectra were acquired on Advance III 500 with the probe head PABBO BB/19F-1H/D Z-GRD (500 MHz for ^{1}H, 125 MHz for ^{13}C), and Advance III HD 700 with cryo platform and the probe head CPTCI 1H-13C/15N/D Z-GRD (700 MHz for ^{1}H, 176 MHz for ^{13}C) from Bruker. The measured substances were dissolved in the respective deuterated solvent and the chemical shifts δ are given in ppm. Multiplicities of the individual signals are as follows: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet) and combinations thereof, dd (doublet of doublet), tt (triplet of triplet), dt (doublet of triplet), td (triplet of doublet), etc. Others include: bs (broad singlet) and m (multiplet). All spectra were interpreted as first order spectra. The coupling constants *J* are given in hertz (Hz) and refer to ^{1}H-^{1}H couplings.

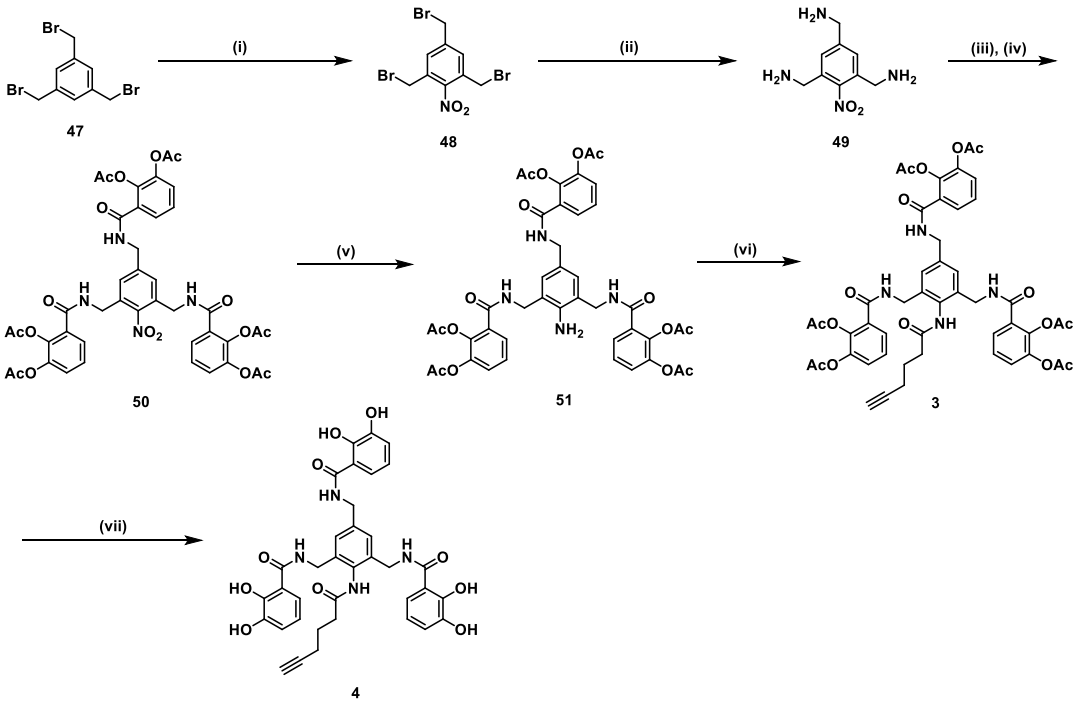
Chemistry figures, schemes and tables



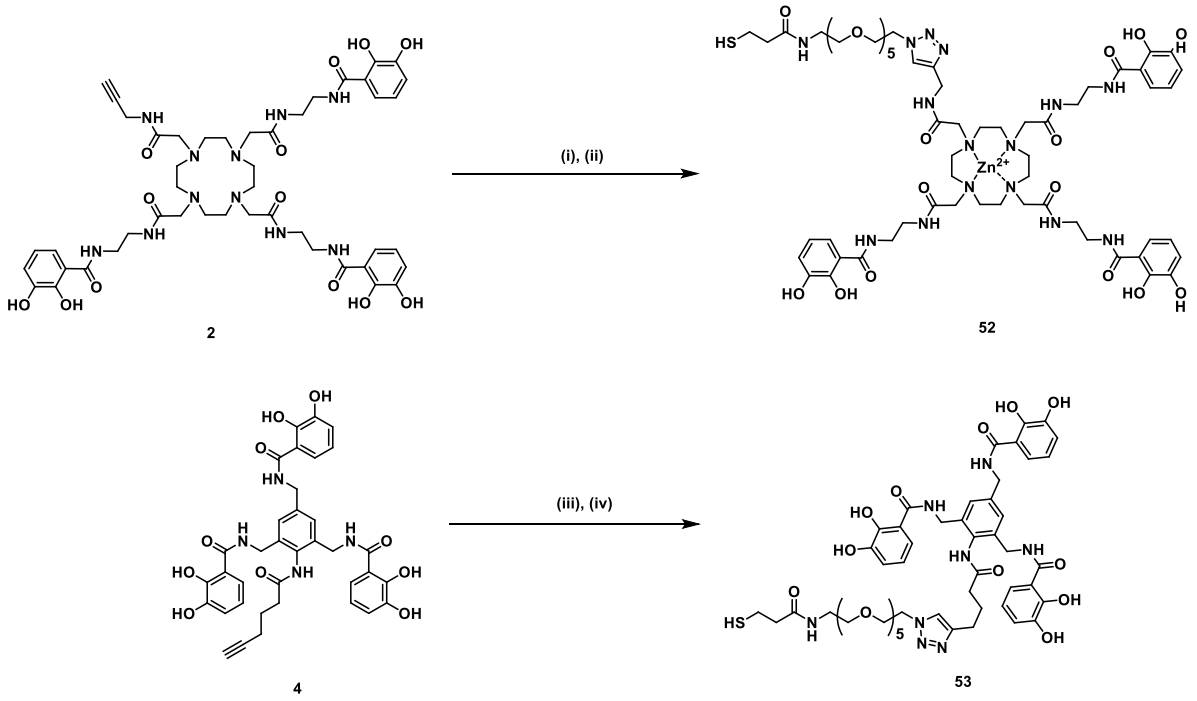
Scheme S1: Synthesis of siderophore building blocks **36**, **38**, **40** and **42**. (i) $BrCH_2COBr$, K_2CO_3, H_2O/CH_2Cl_2, 0-23 °C, 2 h, 95% (ii) $BrCH_2COBr$, K_2CO_3, H_2O/CH_2Cl_2, 0-23 °C, 2 h, 81%, (iii) Ac_2O, TEA, DMAP, THF, 23-60 °C, 2h 96%, (iv) $(C_6H_5)_3CS(CH_2)_2COOH$, HATU, TEA, CH_2Cl_2/DMF, 23 °C, 21 h, 76%.



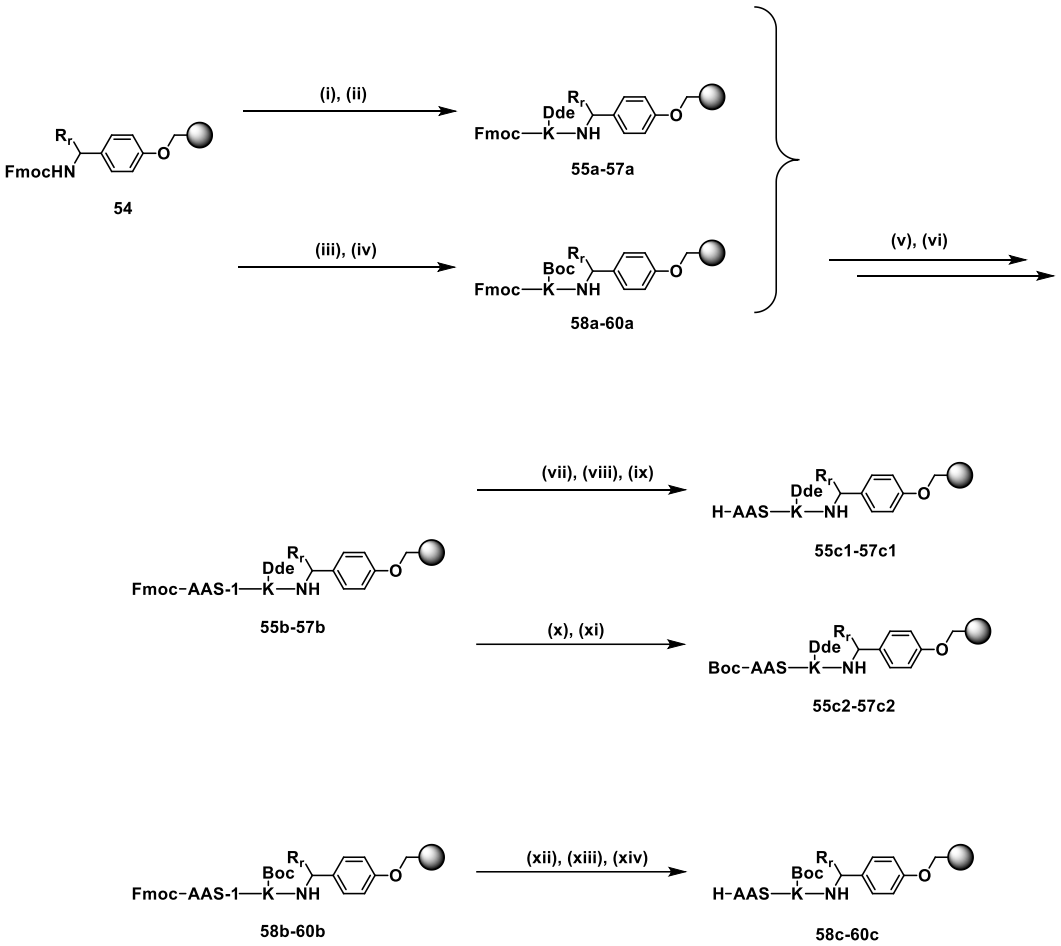
Scheme S2: Synthesis of DOTAM siderophores **1** and **2**. (i) **36**, NaOAc, ACN, 23 °C, 21 h, (ii) **38**, K_2CO_3, ACN, 23 °C, 21 h, (iii) 25% TFA, DCM, 0-23 °C, 4 h, 82% over 3 steps, (iv) **40**, $(COCl)_2$, DCM/DMF, 0-23 °C, 3 h, (v) $NaHCO_3$, H_2O/1,4-dioxane, 0-23 °C, 6 h, (vi) 20% DIPEA, MeOH, 0-23 °C, 4 h, 80% over two steps.



Scheme S3: Synthesis of MECAM siderophores **3** and **4**. (i) HNO_3 (50%), H_2SO_4, 0-23 °C, 48 h, 98%, (ii) NH_4OH (30%), THF/EtOH, 23 °C, 21 h, (iii) **40**, $(COCl)_2$, DCM/DMF, 0-23 °C, 3 h, (iv) $NaHCO_3$, H_2O/1,4-dioxane, 0-23 °C, 6 h, over two steps 68%, (v) Zn dust, AcOH, THF/EtOH, 0-23 °C, 1 h, (vi) 5-hexynoic acid, iBuCF, NMM, THF, 0-23 °C, 6 h, over two steps 56%, (vii) 20% DIPEA, MeOH, 0-23 °C, 4 h, 90%.

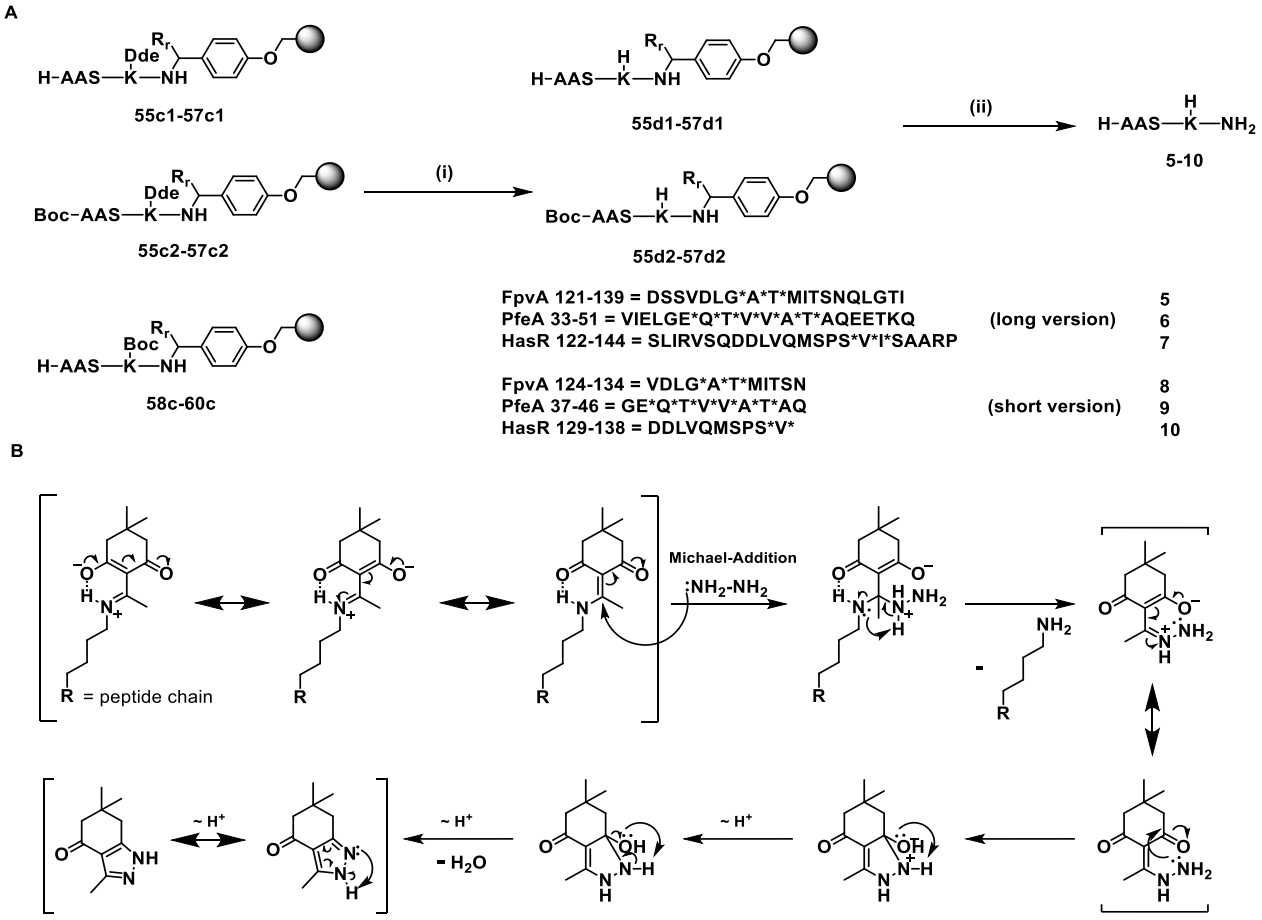


Scheme S4: Synthesis of thio-DOTAM (**52**) and MECAM (**53**) derivatives. (i) $Zn(CH_3COO)_2$, DMSO/H_2O, 23 °C, 5 min, then **44**, DMSO, 23 °C, 5 min, then $CuSO_4$, sodium ascorbate, THPTA, PBS pH 7.4, 23 °C, 1 h, 76%, (ii) 25% TFA, TIPS, DCM, 0-23 °C, 2 h, 94%. (iii) **44**, DMSO/H_2O, 23 °C, 5 min, then $CuSO_4$, sodium ascorbate, THPTA, PBS pH 7.4, 23 °C, 1 h, 82%, (iv) 25% TFA, TIPS, DCM, 0-23 °C, 2 h, 90%.



FpvA 121-139 = DSSVDLG*A*T*MITSNQLGTI		5
PfeA 33-51 = VIELGE*Q*T*V*V*A*T*AQEETKQ	(long version)	6
HasR 122-144 = SLIRVSQDDLVQMSPS*V*I*SAARP		7
FpvA 124-134 = VDLG*A*T*MITSN		8
PfeA 37-46 = GE*Q*T*V*V*A*T*AQ	(short version)	9
HasR 129-138 = DDLVQMSPS*V*		10

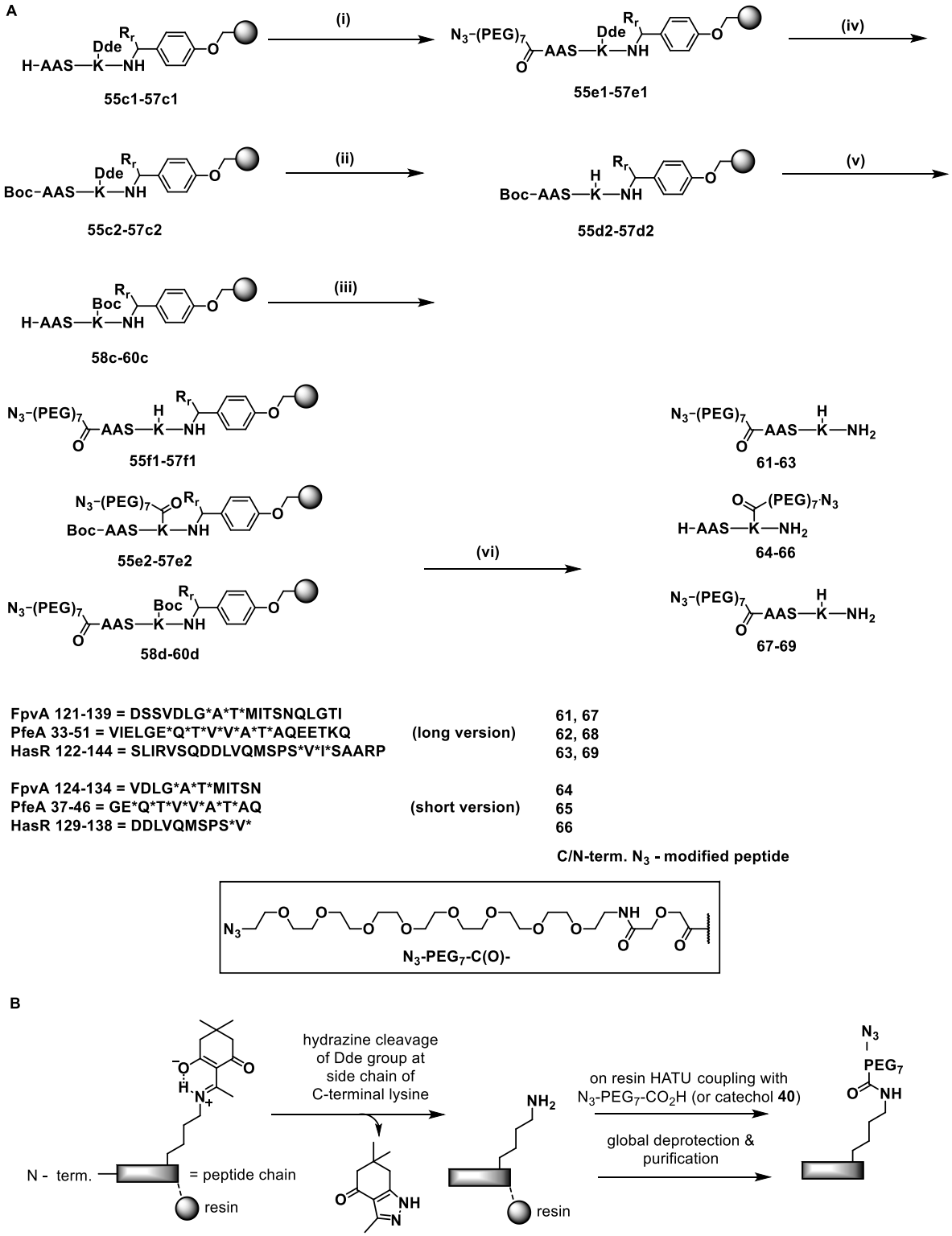
Scheme S5: Synthesis of (unmodified) peptide precursors *via* SPPS. * = mark complicated couplings determined by *Peptide Companion* (1.25 CoshiSoft/PeptiSearch, 2000) and were performed with double coupling and capping. For the long peptide sequences, an Fmoc- or Boc-protected amino acid at the *α*-amino group was introduced as the terminal amino acid. (i) piperidine, DMF, 23 °C, 10 min, (ii) Fmoc-Lys(Dde)-OH, HATU, DIPEA, DMF, 23 °C, 1 h, (iii) piperidine, DMF, 23 °C, 10 min, (iv) Fmoc-Lys(Boc)-OH, HATU, DIPEA, DMF, 23 °C, 1 h, (v) piperidine, DMF, 23 °C, 10 min, (vi) protected Fmoc-aa, HCTU, DIPEA, DMF, 23 °C, 1 h, (vii) piperidine, DMF, 23 °C, 10 min, (viii) protected Fmoc-aa, HCTU, DIPEA, DMF, 23 °C, 1 h, (ix) piperidine, DMF, 23 °C, 10 min, (x) piperidine, DMF, 23 °C, 10 min, (xi) protected Boc-aa, HATU, DIPEA, DMF, 23 °C, 1 h, (xii) piperidine, DMF, 23 °C, 10 min, (xiii) protected Fmoc-aa, HCTU, DIPEA, DMF, 23 °C, 1 h, (xiv) piperidine, DMF, 23 °C, 10 min.



Scheme S6: Synthesis of unmodified peptides **5-10**. * = mark complicated couplings determined by Peptide Companion (1.25 CoshiSoft/PeptiSearch, 2000) and were performed with double coupling and capping. For the long peptide sequences, a Fmoc- or Boc-protected amino acid at the *α*-amino group was introduced as the terminal amino acid. (i) 1.0 M hydrazine in THF, 23 C, 3 h, (ii) 95% TFA, 3% TIPS, 2% H_2O, 23 °C, 3 h, over 12 to 26 steps 12-52%. (B) Cleavage mechanism of Dde protecting group based on findings by Bradley et al.[1]

Table S1: Synthesis characteristics of the unmodified peptides **5-10**. aa = amino acid, (l) = long peptide, (s) = short peptide.

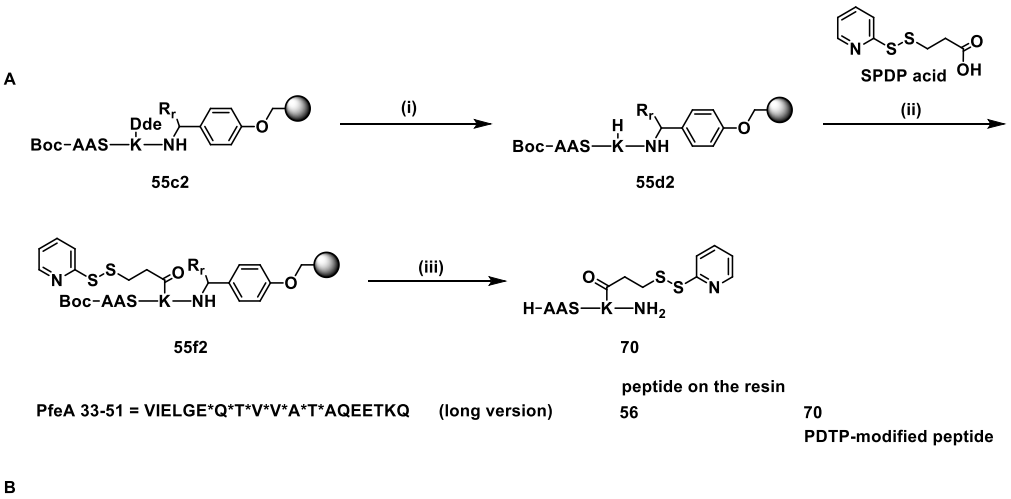
#	Peptides	aa	Cycles	Time *t* [h]	Steps	Yield [%]	Yield/step [%]
5	*FpvA* (l)	20	23	34	22	16	92
6	*PfeA* (l)	20	27	39	22	27	94
7	*HasR* (l)	24	27	38	26	12	92
8	*FpvA* (s)	12	15	21	13	33	92
9	*PfeA* (s)	11	18	25	12	52	95
10	*HasR* (s)	11	13	19	12	36	92



Scheme S7: Syntheses of *N*- & C-terminal PEG-modified peptides **61-69**. (i) N_3-PEG_7-CO_2H, HOBt, HATU, NMM, DMF, 23 °C, 21 h, (ii) 1.0 M hydrazine in THF, DMF, 23 °C, 3 h, (iii) N_3-PEG_7-CO_2H, HOBt, HATU, NMM, DMF, 23 °C, 21 h, (iv) 1.0 M hydrazine in THF, DMF, 23 °C, 3 h, (v) N_3-PEG_7-CO_2H, HOBt, HATU, NMM, DMF, 23 °C, 21 h, (vi) 95% TFA; 3% TIPS, 2% H_2O, 23 °C, 3 h, over 13 to 27 steps with 10-33%. (B) Schematic strategy for C-terminal modification of peptides, also employed for PTDP-peptides **70** and for monocatechol conjugates **33** and **34**.

Table S2. Synthesis characteristics of the PEG-modified peptides **61-69**. aa = amino acid, (l) = long peptide, (s) = short peptide.

#	Peptides	aa	Cycles	time *t* [h]	Steps	Yield [%]	Yield/step [%]
61	*FpvA* (l) *N*-term	20	23	55	23	11	91
62	*PfeA* (l) *N*-term	20	27	60	23	21	93
63	*HasR* (l) *N*-term	24	27	59	27	10	92
64	*FpvA* (l) *C*-term	20	23	55	23	12	91
65	*PfeA* (l) *C*-term	20	27	60	23	23	94
66	*HasR* (l) *C*-term	24	27	59	27	12	92
67	*FpvA* (s) *N*-term	12	15	42	14	24	90
68	*PfeA* (s) *N*-term	11	18	46	13	33	92
69	*HasR* (s) *N*-term	11	13	40	13	15	86

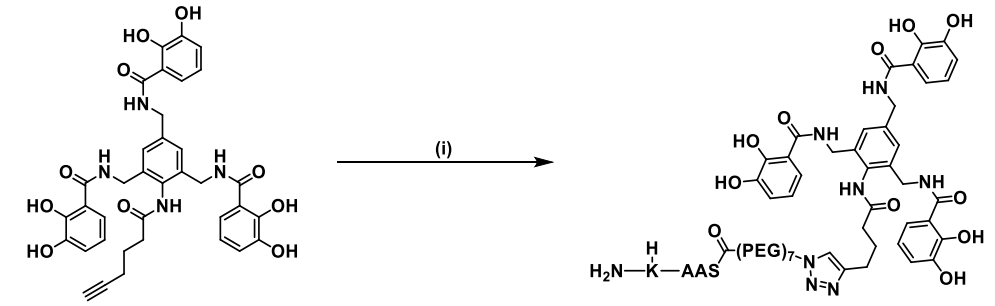


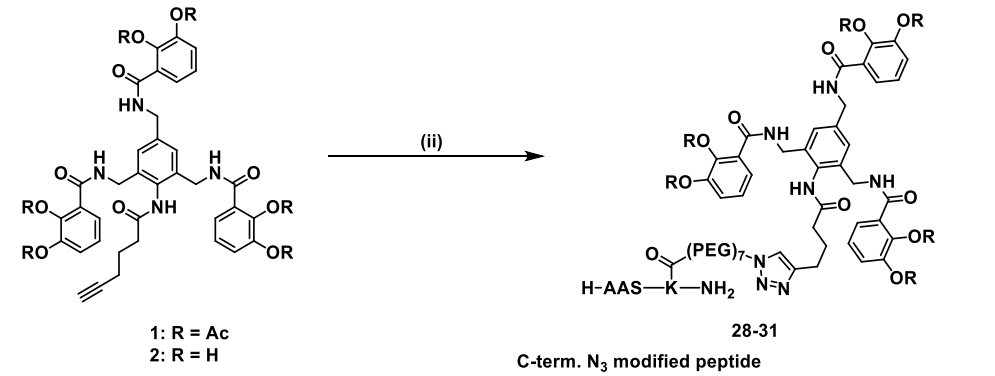
Scheme S8: (A) Synthesis of *C*-terminal PDTP-modified *PfeA* 33-51 peptide **70**. (i) 1.0 M hydrazine, in THF, DMF, 23 °C, 3 h, (ii) 3-(pyridin-2-yldisulfaneyl)propanoic acid (SPDP acid), HOBt, HATU, NMM, DMF, 23 °C, 21 h, (iii) 95% TFA, 3% TIPS, 2% H_2O, 23 °C, 3 h, over 23 steps 11%.

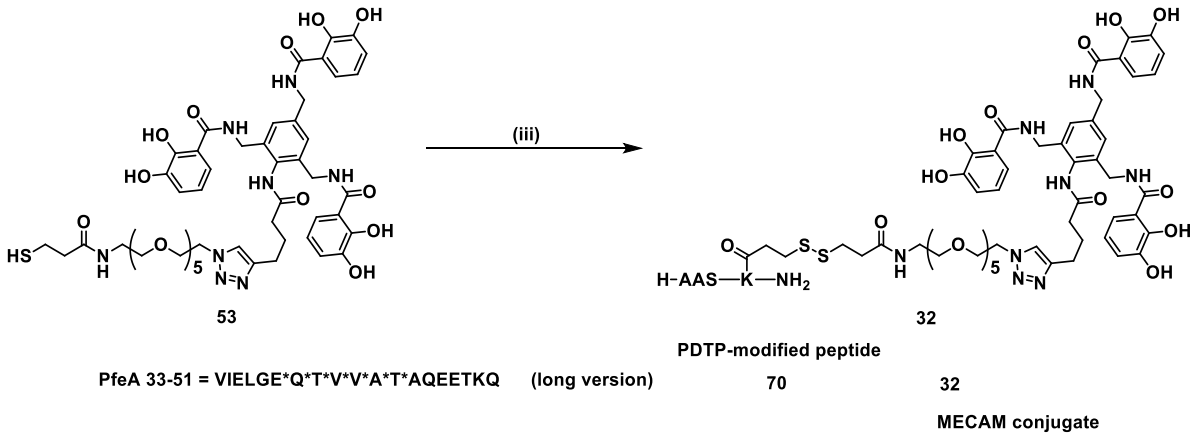
Conjugate synthesis

Table S3: Overview over the yields of the peptide DOTAM siderophore conjugates **11**-**21** for the final CuAAC. l = long, s = short peptide.

#	Peptide	Siderophore	Conjugation	Yield [%]
11	*FpvA* (l)	DOTAM-OH	*N*-term PEG	91
12	*PfeA* (l)	DOTAM-OH	*N*-term PEG	99
13	*HasR* (l)	DOTAM-OH	*N*-term PEG	87
14	*FpvA* (s)	DOTAM-OH	*N*-term PEG	91
15	*PfeA* (s)	DOTAM-OH	*N*-term PEG	96
16	*HasR* (s)	DOTAM-OH	*N*-term PEG	81
17	*FpvA* (l)	DOTAM-OH	*C*-term PEG	94
18	*PfeA* (l)	DOTAM-OH	*C*-term PEG	99
19	*HasR* (l)	DOTAM-OH	*C*-term PEG	79
20	*PfeA* (l)	DOTAM-OAc	*C*-term PEG	82
21	*PfeA* (l)	DOTAM-OH	*C*-term disulfide	76



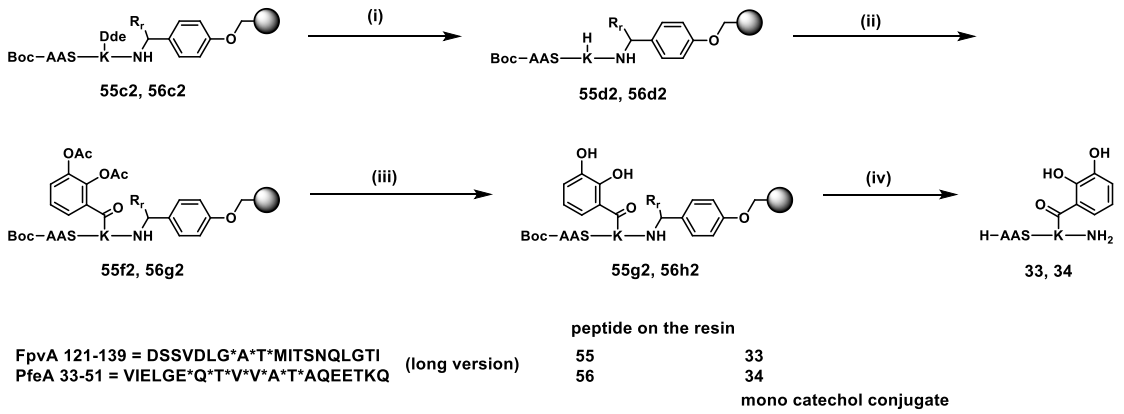




Scheme S9: Conjugation of the TonB box containing peptides to the MECAM siderophores. (i) **61**/**62**/**63**/**67**/**68**/**69**, DMSO, H_2O, 23 °C, 5 min, $CuSO_4$, sodium ascorbate, THPTA, PBS pH 7.4, 23 °C, 1 h, 86-97%, (ii) **64**/**65**/**66**, DMSO, H_2O, 23 °C, 5 min, $CuSO_4$, sodium ascorbate, THPTA, PBS pH 7.4, 23 °C, 1 h, 85-95%, (iii) **70**, HEPES buffer pH 7.4, DMF, DMSO, 23 °C, 48 , 78%.* indicates a complicated coupling.

Table S4: Overview over the yields of peptide MECAM siderophore conjugates **22-32** for the final CuAAC. l = long, s = short peptide.

#	Peptide	Siderophore	Conjugation	Yield [%]
22	*FpvA* (l)	MECAM-OH	*N*-term PEG	95
23	*PfeA* (l)	MECAM-OH	*N*-term PEG	97
24	*HasR* (l)	MECAM-OH	*N*-term PEG	86
25	*FpvA* (s)	MECAM-OH	*N*-term PEG	88
26	*PfeA* (s)	MECAM-OH	*N*-term PEG	96
27	*HasR* (s)	MECAM-OH	*N*-term PEG	86
28	*FpvA* (l)	MECAM-OH	*C*-term PEG	95
29	*PfeA* (l)	MECAM-OH	*C*-term PEG	96
30	*HasR* (l)	MECAM-OH	*C*-term PEG	85
31	*PfeA* (l)	MECAM-OAc	*C*-term PEG	80
32	*PfeA* (l)	MECAM-OH	*C*-term disulfide	78



Scheme S10: Syntheses of *C*-terminal mono catechol-modified peptides **33** and **34**. (i) 1.0 M hydrazine in THF, DMF, 23 °C, 3 h, (ii) **40**, HOBt, HATU, NMM, DMF, 0-23 °C, 21 h, (iii) 20% DIPEA, MeOH, 0-23 °C, 4 h, (iv) 95% TFA, 3% TIPS, 2% H_2O, 23 °C, 3 h, over 24 steps 9-15%.

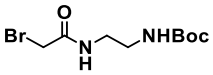
Table S5: Comparison of yields of the mono catechol-modified peptides **33** and **34**. aa = amino acids, (l) = long peptide.

#	Peptides	aa	Cycles	Time *t* [h]	Steps	Yield [%]	Yield/step [%]
33	*FpvA* (l) *C*-term	20	23	59	24	9	90
34	*PfeA* (l) *C*-term	20	27	64	24	15	92

Structures of synthetized intermediates and final compounds

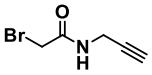
The compounds are given in the same order as the experimental in the main text.

Compound 36[2, 3]



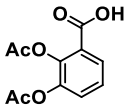
Chemical Formula: $C_9H_{17}BrN_2O_3$
Exact Mass: 280,0423
Molecular Weight: 281,1500

Compound 38[2]



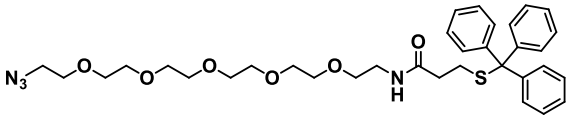
Chemical Formula: C_5H_6BrNO
Exact Mass: 174,9633
Molecular Weight: 176,0130

Compound 40[2]



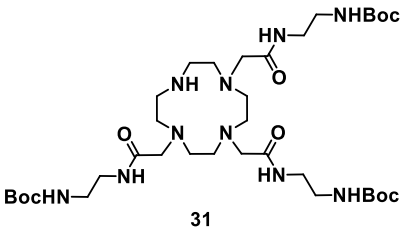
Chemical Formula: $C_{11}H_{10}O_6$
Exact Mass: 238,0477
Molecular Weight: 238,1950

Compound 42[4, 5]



Chemical Formula: $C_{34}H_{44}N_4O_6S$
Exact Mass: 636,2982
Molecular Weight: 636,8080

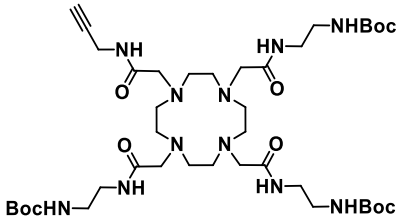
Compound 44[2, 3]



31

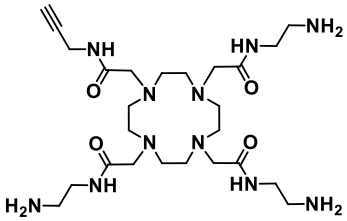
Chemical Formula: $C_{35}H_{68}N_{10}O_9$
Exact Mass: 772,5171
Molecular Weight: 772,9900

Compound 45[2, 3]



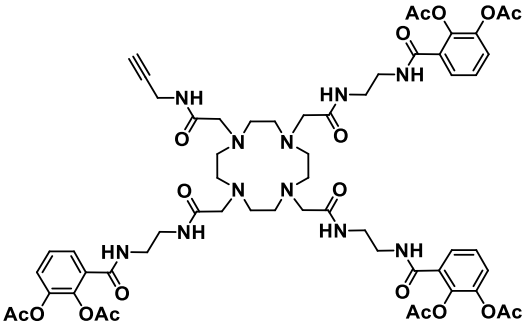
Chemical Formula: $C_{40}H_{73}N_{11}O_{10}$
Exact Mass: 867,5542
Molecular Weight: 868,0910

Compound 46[2, 3]



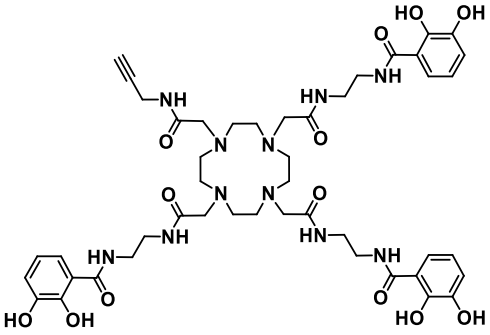
Chemical Formula: $C_{25}H_{49}N_{11}O_4$
Exact Mass: 567,3969
Molecular Weight: 567,7400

Compound 1[2, 3]



Chemical Formula: $C_{58}H_{73}N_{11}O_{19}$
Exact Mass: 1227,5084
Molecular Weight: 1228,2800

Compound 2[2, 3]

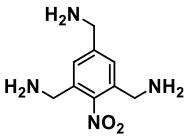


Chemical Formula: $C_{46}H_{61}N_{11}O_{13}$
Exact Mass: 975,4450
Molecular Weight: 976,0580

Compound 48[6]

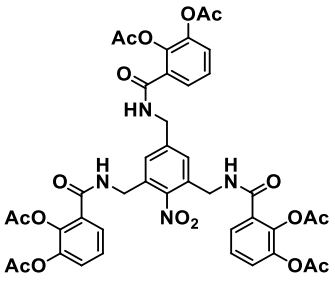
Chemical Formula: $C_9H_8Br_3NO_2$
Exact Mass: 398,8105
Molecular Weight: 401,8800

Compound 49[6]



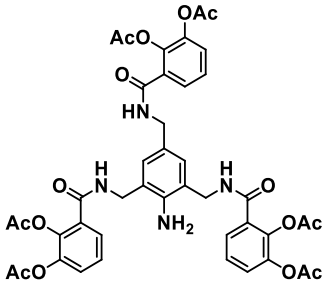
Chemical Formula: $C_9H_{14}N_4O_2$
Exact Mass: 210,1117
Molecular Weight: 210,2370

Compound 50[6]



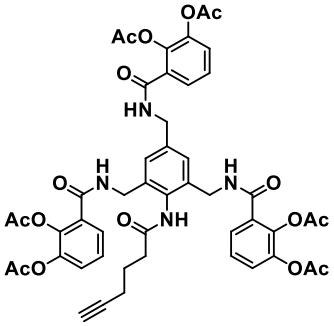
Chemical Formula: $C_{42}H_{38}N_4O_{17}$
Exact Mass: 870,2232
Molecular Weight: 870,7770

Compound 51[6]



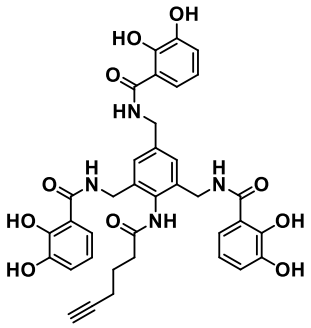
Chemical Formula: $C_{42}H_{40}N_4O_{15}$
Exact Mass: 840,2490
Molecular Weight: 840,7950

Compound 3[6]



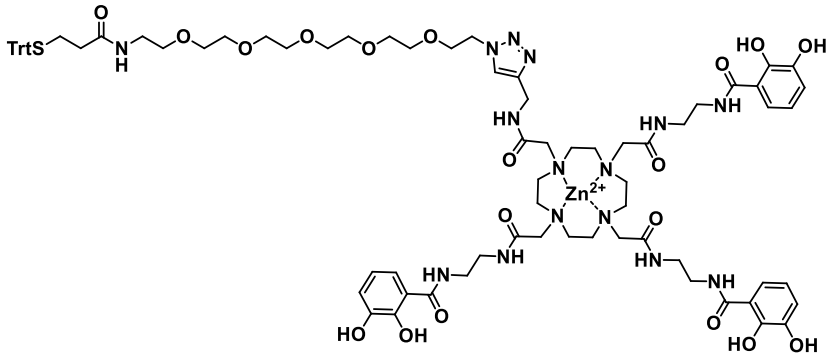
Chemical Formula: $C_{48}H_{46}N_4O_{16}$
Exact Mass: 934,2909
Molecular Weight: 934,9080

Compound 4[6]



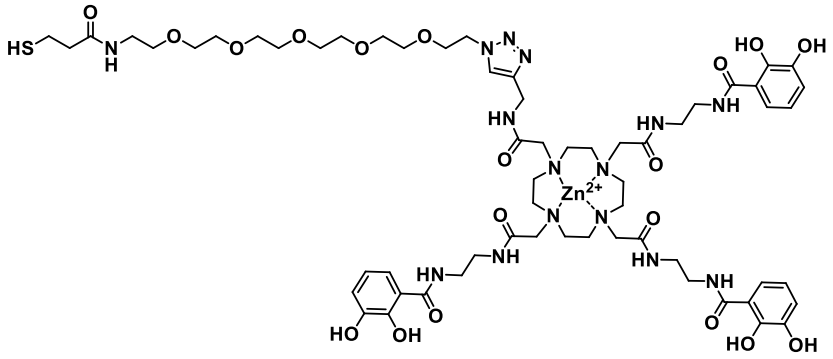
Chemical Formula: $C_{36}H_{34}N_4O_{10}$
Exact Mass: 682,2275
Molecular Weight: 682,6860

Compound 52a



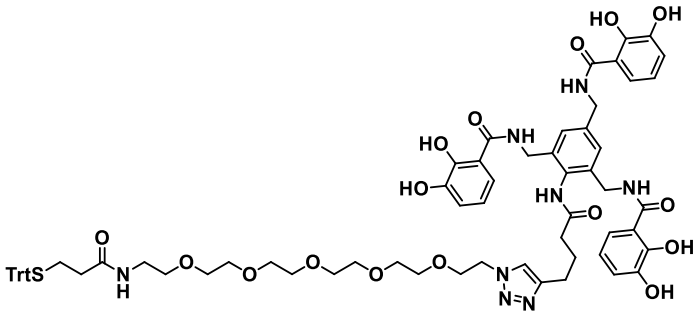
Chemical Formula: $C_{80}H_{105}N_{15}O_{19}SZn^{2+}$
Exact Mass: 1675,6712
Molecular Weight: 1678,2449

Compound 52



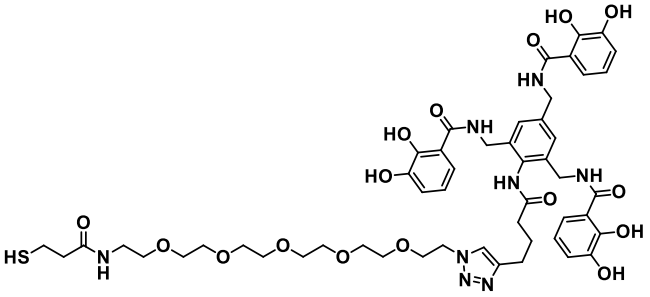
Chemical Formula: $C_{61}H_{91}N_{15}O_{19}SZn^{2+}$
Exact Mass: 1433,5617
Molecular Weight: 1435,9239

Compound 53a



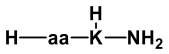
Chemical Formula: $C_{70}H_{78}N_8O_{16}S$
Exact Mass: 1318,5256
Molecular Weight: 1319,4940

Compound 53



Chemical Formula: $C_{51}H_{64}N_8O_{16}S$
Exact Mass: 1076,4161
Molecular Weight: 1077,1730

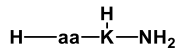
FpvA 121-139 peptide 5



aa: DSSVDLG*A*T*MITSNQLGTI

Chemical Formula: $C_{85}H_{148}N_{24}O_{32}S$
Exact Mass: 2049,04122
Molecular Weight: 2050,31500

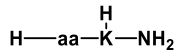
PfeA 33-51 peptide 6



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{94}H_{162}N_{26}O_{34}$
Exact Mass: 2199,17468
Molecular Weight: 2200,47800

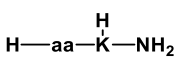
HasR 122-144 peptide 7



aa: SLIRVSQDDLVQMSPS*V*I*SAARP

Chemical Formula: $C_{111}H_{194}N_{34}O_{35}S$
Exact Mass: 2595,41665
Molecular Weight: 2597,03600

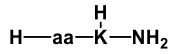
FpvA 124-134 peptide 8



aa: VDLG*A*T*MITSN

Chemical Formula: $C_{52}H_{93}N_{15}O_{18}S$
Exact Mass: 1247,65437
Molecular Weight: 1248,46300

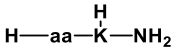
PfeA 37-46 peptide 9



aa: GE*Q*T*V*V*A*T*AQ

Chemical Formula: $C_{47}H_{83}N_{15}O_{17}$
Exact Mass: 1129,60914
Molecular Weight: 1130,26900

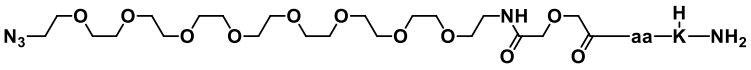
HasR 129-138 peptide 10



aa: DDLVQMSPS*V*

Chemical Formula: $C_{51}H_{88}N_{14}O_{18}S$
Exact Mass: 1216,61217
Molecular Weight: 1217,40500

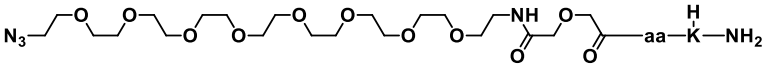
Compound 61



aa: DSSVDLG*A*T*MITSNQLGTI

Chemical Formula: $C_{107}H_{188}N_{28}O_{43}S$
Exact Mass: 2585,31058
Molecular Weight: 2586,89400

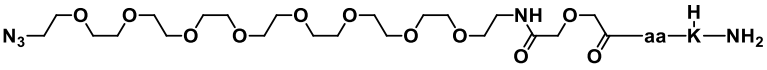
Compound 62



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{116}H_{202}N_{30}O_{45}$
Exact Mass: 2735,44403
Molecular Weight: 2737,05700

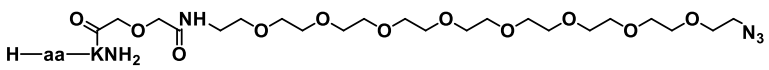
Compound 63



aa: SLIRVSQDDLVQMSPS*V*I*SAARP

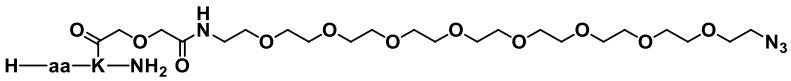
Chemical Formula: $C_{133}H_{234}N_{38}O_{46}S$
Exact Mass: 3131,68601
Molecular Weight: 3133,61500

Compound 64



aa: DSSVDLG*A*T*MITSNQLGTI
Chemical Formula: $C_{107}H_{188}N_{28}O_{43}S$
Exact Mass: 2585,31058
Molecular Weight: 2586,89400

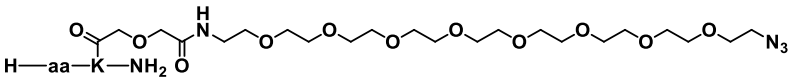
Compound 65



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{116}H_{202}N_{30}O_{45}$
Exact Mass: 2735,44403
Molecular Weight: 2737,05700

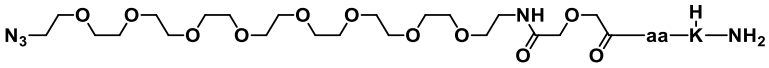
Compound 66



aa: SLIRVSQDDLVQMSPS*V*I*SAARP

Chemical Formula: $C_{133}H_{234}N_{38}O_{46}S$
Exact Mass: 3131,68601
Molecular Weight: 3133,61500

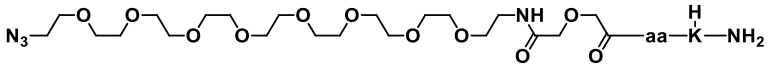
Compound 67



aa: VDLG*A*T*MITSN

Chemical Formula: $C_{74}H_{133}N_{19}O_{29}S$
Exact Mass: 1783,92373
Molecular Weight: 1785,04200

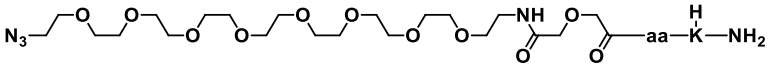
Compound 68



aa: GE*Q*T*V*V*A*T*AQ

Chemical Formula: $C_{69}H_{123}N_{19}O_{28}$
Exact Mass: 1665,87849
Molecular Weight: 1666,84800

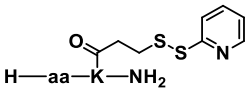
Compound 69



aa: DDLVQMSPS*V*

Chemical Formula: $C_{73}H_{128}N_{18}O_{29}S$
Exact Mass: 1752,88153
Molecular Weight: 1753,98400

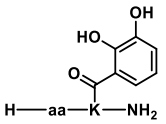
Compound 70



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{102}H_{169}N_{27}O_{35}S_2$
Exact Mass: 2396,17158
Molecular Weight: 2397,74800

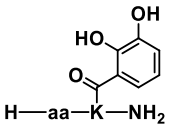
Compound *C*33



aa: DSSVDLG*A*T*MITSNQLGTI

Chemical Formula: $C_{92}H_{152}N_{24}O_{35}S$
Exact Mass: 2185,05726
Molecular Weight: 2186,42100

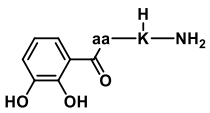
Compound *C*34



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{101}H_{166}N_{26}O_{37}$
Exact Mass: 2335,19072
Molecular Weight: 2336,58400

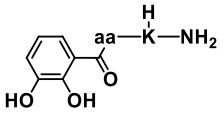
Compound *N*33$_L$



aa: DSSVDLG*A*T*MITSNQLGTI

Chemical Formula: $C_{92}H_{152}N_{24}O_{35}S$
Exact Mass: 2185,05726
Molecular Weight: 2186,42100

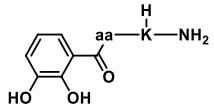
Compound *N*34$_L$



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{101}H_{166}N_{26}O_{37}$
Exact Mass: 2335,19072
Molecular Weight: 2336,58400

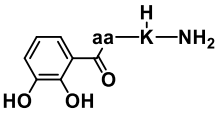
Compound *N*33$_D$



aa: DSSVDLG*A*T*MITSNQLGTI
D-amino acids

Chemical Formula: $C_{92}H_{152}N_{24}O_{35}S$
Exact Mass: 2185,05726
Molecular Weight: 2186,42100

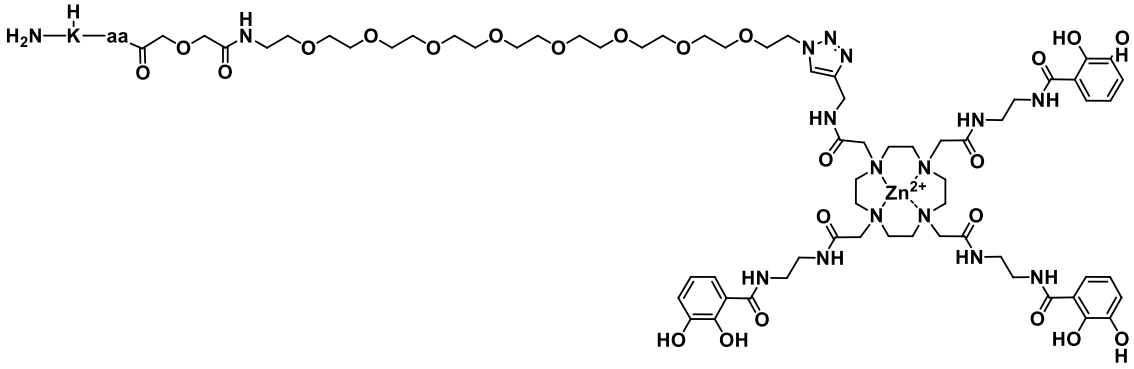
Compound *N*34$_D$



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ
D-amino acids

Chemical Formula: $C_{101}H_{166}N_{26}O_{37}$
Exact Mass: 2335,19072
Molecular Weight: 2336,58400

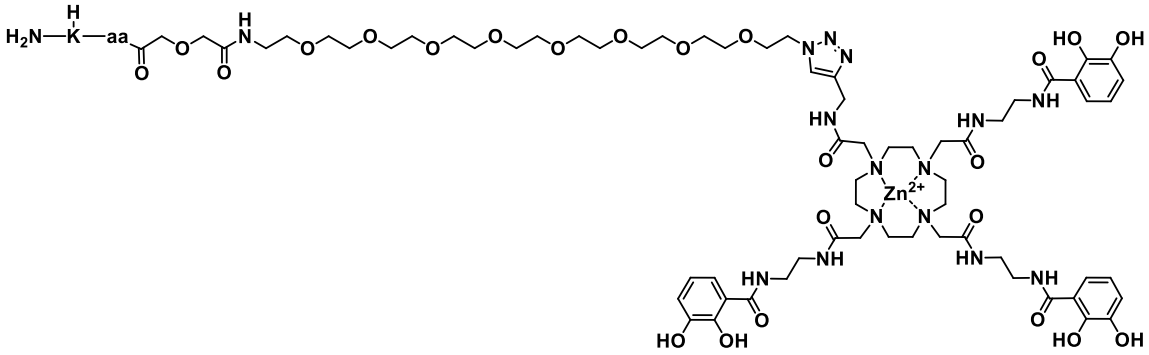
Compound 11 (*FpvA* 121-139 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)



aa: DSSVDLG*A*T*MITSNQLGTI

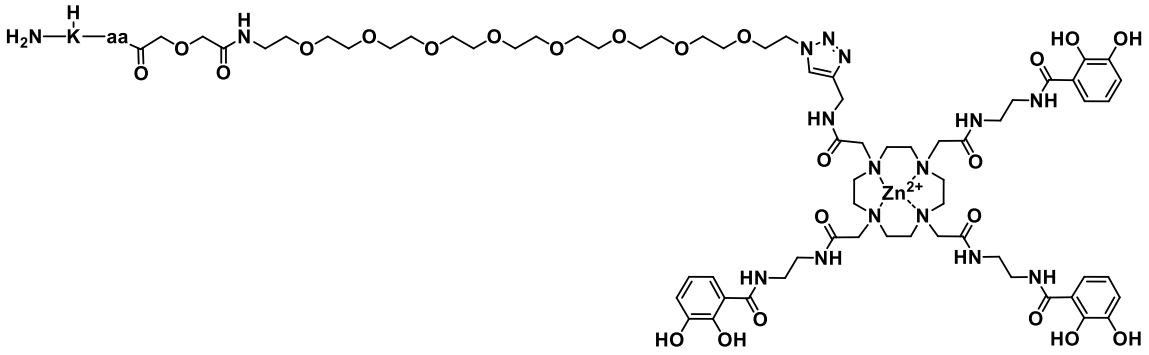
Chemical Formula: $C_{153}H_{249}N_{39}O_{56}SZn^{2+}$
Exact Mass: 3624,68366
Molecular Weight: 3628,33090

Compound 12 (*PfeA* 33-51 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ
Chemical Formula: $C_{162}H_{263}N_{41}O_{58}Zn^{2+}$
Exact Mass: 3774,81712
Molecular Weight: 3778,49390

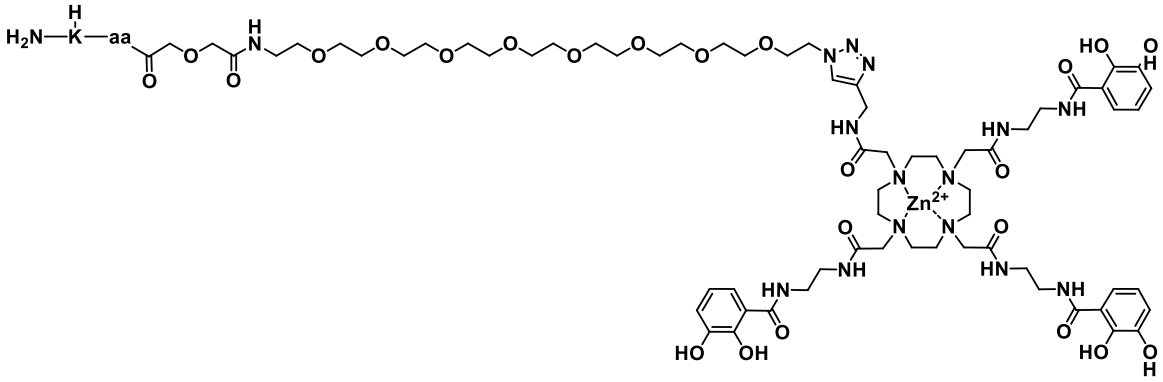
Compound 13 (*HasR* 122-144 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)



aa: SLIRVSQDDLVQMSPS*V*I*SAARP

Chemical Formula: $C_{179}H_{295}N_{49}O_{59}SZn^{2+}$
Exact Mass: 4171,05909
Molecular Weight: 4175,05190

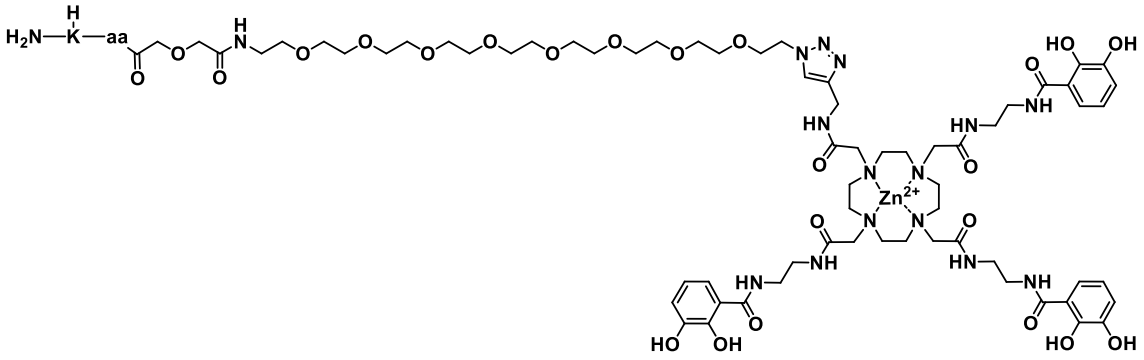
Compound 14 (*FpvA* 124-134 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)



aa: VDLG*A*T*MITSN

Chemical Formula: $C_{120}H_{194}N_{30}O_{42}SZn^{2+}$
Exact Mass: 2823,29681
Molecular Weight: 2826,47890

Compound 15 (*PfeA* 37-46 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)



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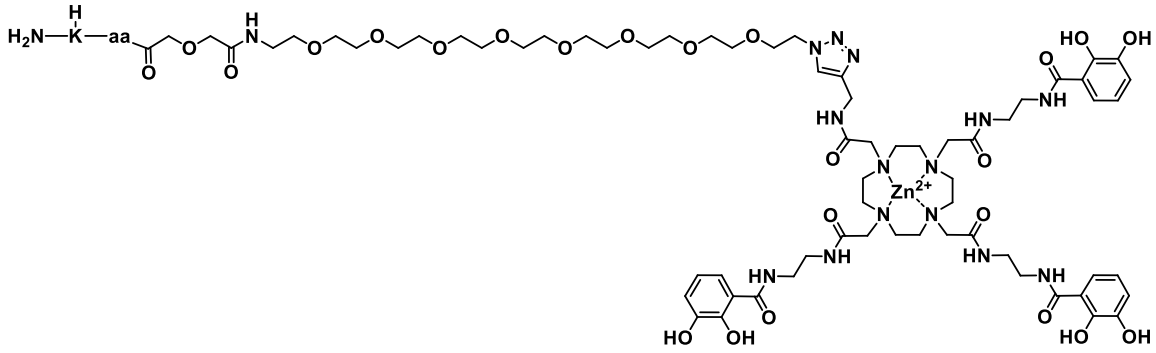
aa: GE*Q*T*V*V*A*T*AQ

Chemical Formula: $C_{115}H_{184}N_{30}O_{41}Zn^{2+}$
Exact Mass: 2705,25158
Molecular Weight: 2708,28490

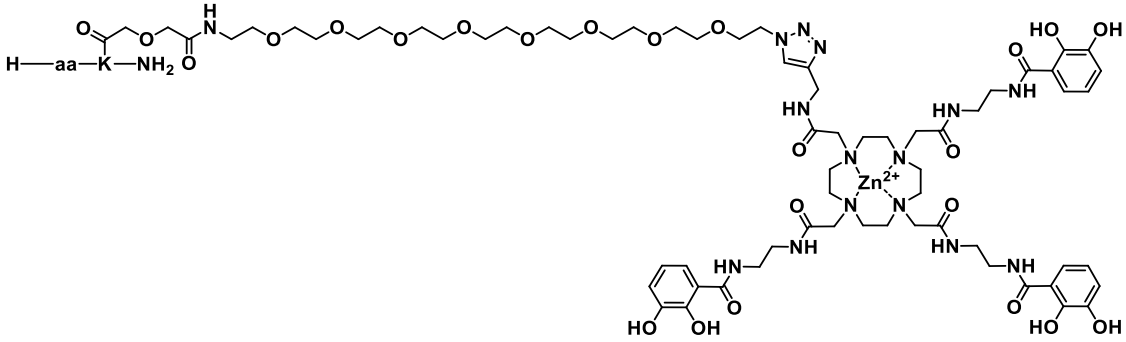
Compound 16 (*HasR* 129-138 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)



aa: DDLVQMSPS*V*

Chemical Formula: $C_{119}H_{189}N_{29}O_{42}SZn^{2+}$
Exact Mass: 2792,25461
Molecular Weight: 2795,42090

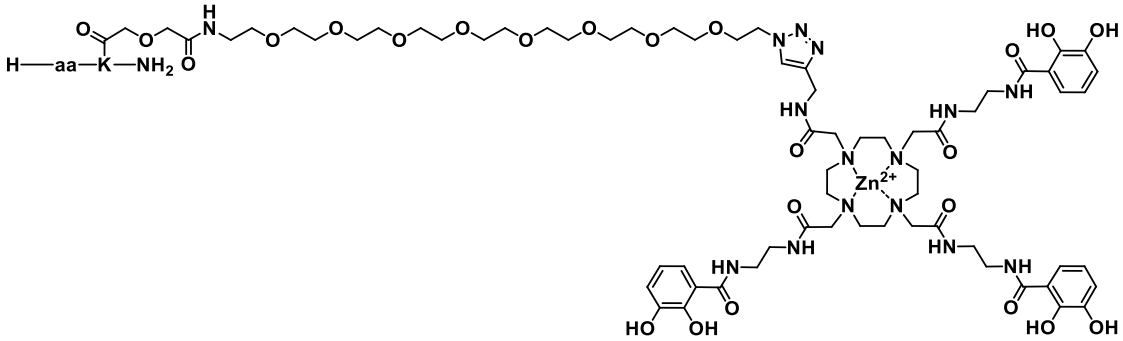
Compound 17 (*FpvA* 121-139 C-term $(PEG)_7$-Zn^{2+}-DOTAM)



aa: DSSVDLG*A*T*MITSNQLGTI

Chemical Formula: $C_{153}H_{249}N_{39}O_{56}SZn^{2+}$
Exact Mass: 3624,68366
Molecular Weight: 3628,33090

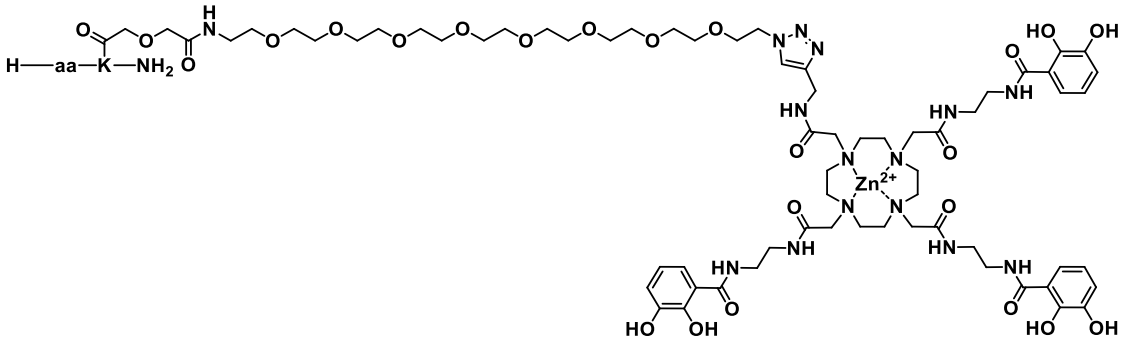
Compound 18 (*PfeA* 33-51 C-term $(PEG)_7$-Zn^{2+}-DOTAM)



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{162}H_{263}N_{41}O_{58}Zn^{2+}$
Exact Mass: 3774,81712
Molecular Weight: 3778,49390

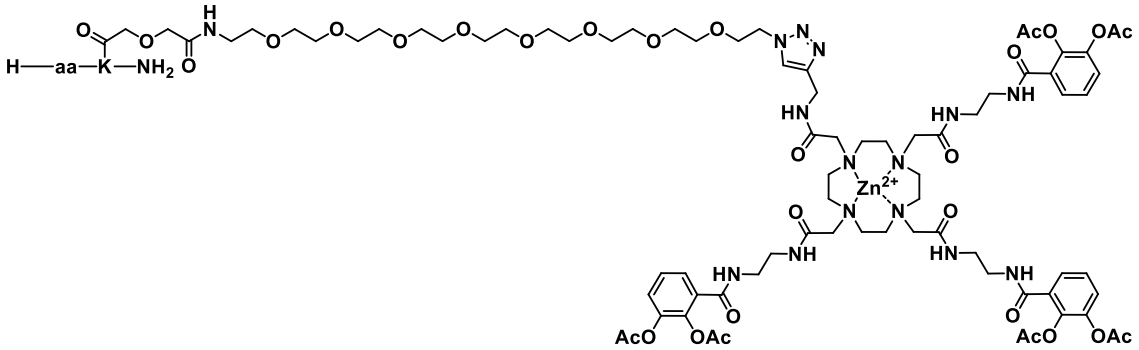
Compound 19 (*HasR* 122-144 C-term $(PEG)_7$-Zn^{2+}-DOTAM)



aa: SLIRVSQDDLVQMSPS*V*I*SAARP

Chemical Formula: $C_{179}H_{295}N_{49}O_{59}SZn^{2+}$
Exact Mass: 4171,05909
Molecular Weight: 4175,05190

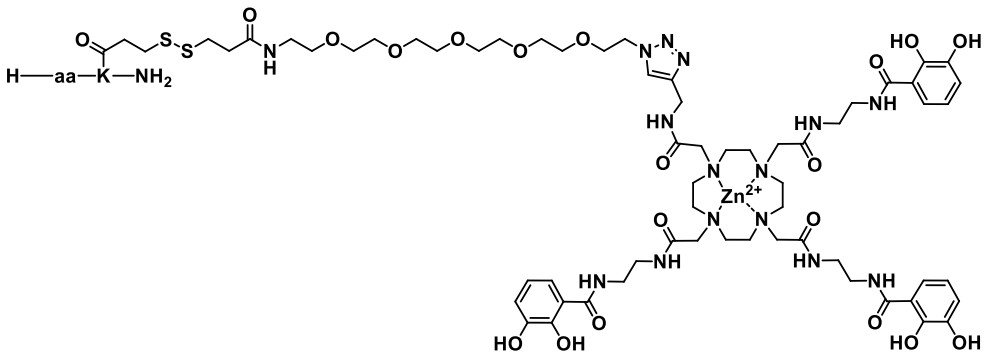
Compound 20 (*PfeA* 33-51 C-term $(PEG)_7$-Zn^{2+}-DOTAM-OAc)



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{174}H_{275}N_{41}O_{64}Zn^{2+}$
Exact Mass: 4026,88050
Molecular Weight: 4030,71590

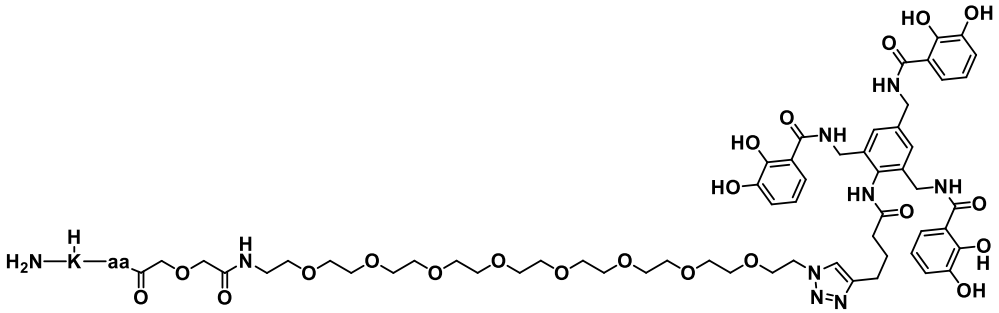
Compound 21 (*PfeA* 33-51 C-term disulfide-$(PEG)_5$-Zn^{2+}-DOTAM)



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{158}H_{255}N_{41}O_{54}S_2Zn^{2+}$
Exact Mass: 3718,71900
Molecular Weight: 3722,50990

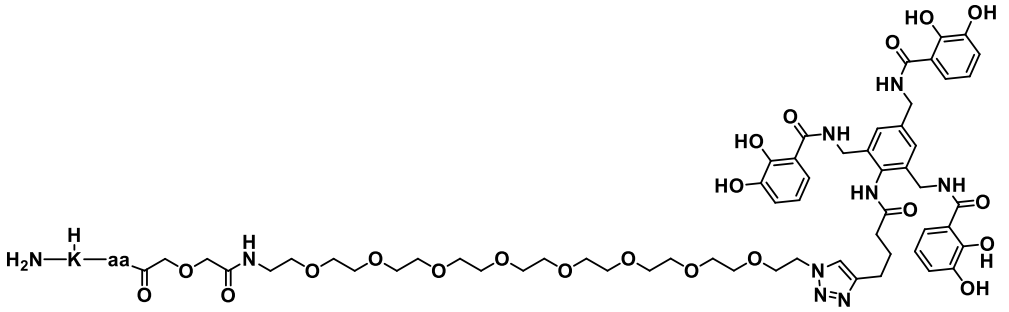
Compound 22 (*FpvA* 121-139 *N*-term-$(PEG)_7$-MECAM)



aa: DSSVDLG*A*T*MITSNQLGTI

Chemical Formula: $C_{143}H_{222}N_{32}O_{53}S$
Exact Mass: 3267,53807
Molecular Weight: 3269,58000

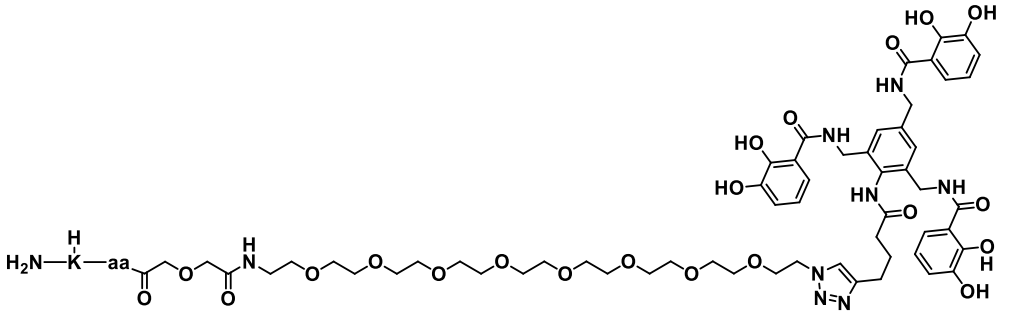
Compound 23 (*PfeA* 33-51 *N*-term $(PEG)_7$-MECAM)



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{152}H_{236}N_{34}O_{55}$
Exact Mass: 3417,67153
Molecular Weight: 3419,74300

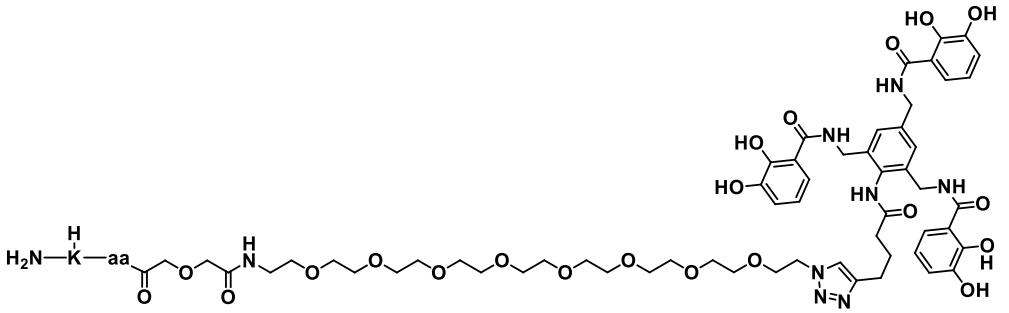
Compound 24 (*HasR* 122-144 *N*-term $(PEG)_7$-MECAM)



aa: SLIRVSQDDLVQMSPS*V*I*SAARP

Chemical Formula: $C_{169}H_{268}N_{42}O_{56}S$
Exact Mass: 3813,91351
Molecular Weight: 3816,30100

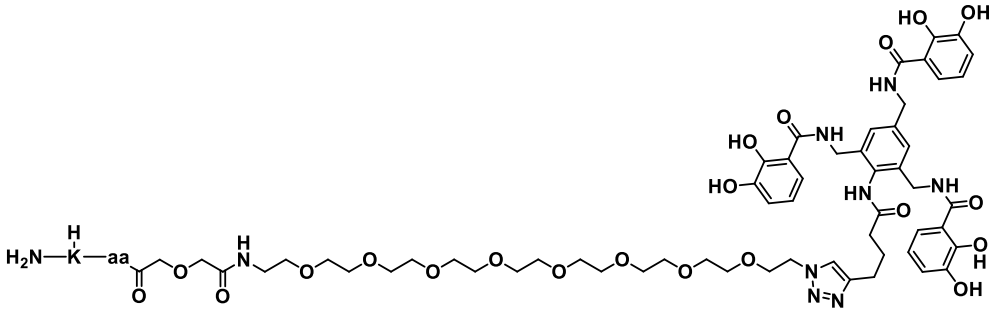
Compound 25 (*FpvA* 124-134 *N*-term $(PEG)_7$-MECAM)



aa: VDLG*A*T*MITSN

Chemical Formula: $C_{110}H_{167}N_{23}O_{39}S$
Exact Mass: 2466,15122
Molecular Weight: 2467,72800

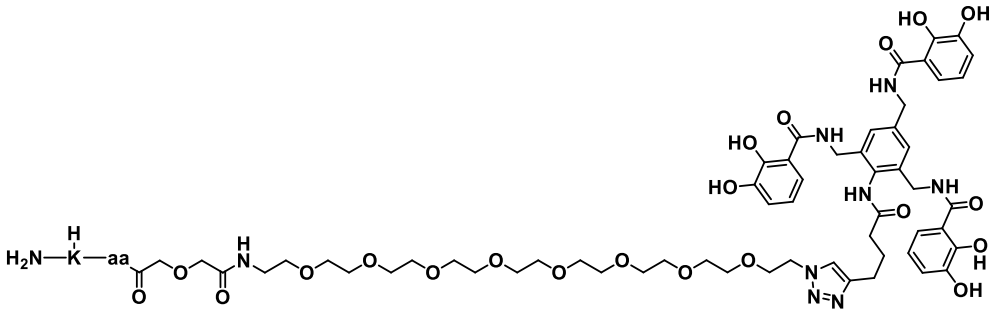
Compound 26 (*PfeA* 37-46 *N*-term $(PEG)_7$-MECAM)



aa: GE*Q*T*V*V*A*T*AQ

Chemical Formula: $C_{105}H_{157}N_{23}O_{38}$
Exact Mass: 2348,10599
Molecular Weight: 2349,53400

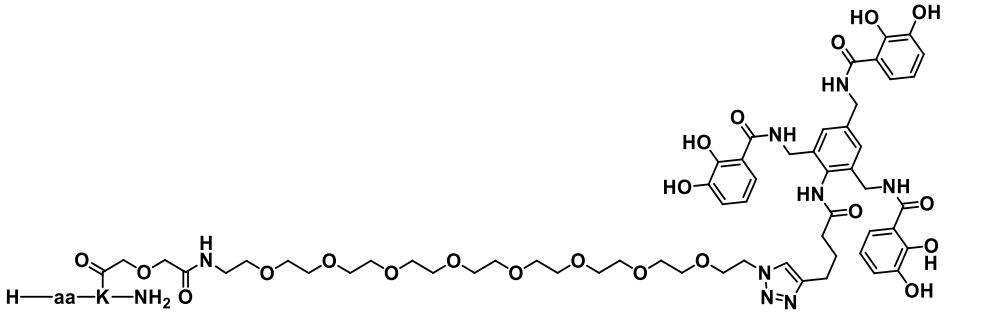
Compound 27 (*HasR* 129-138 *N*-term $(PEG)_7$-MECAM)



aa: DDLVQMSPS*V*

Chemical Formula: $C_{109}H_{162}N_{22}O_{39}S$
Exact Mass: 2435,10902
Molecular Weight: 2436,67000

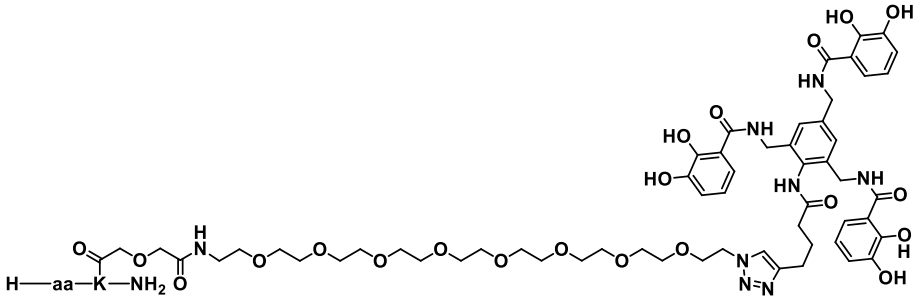
Compound 28 (*FpvA* 121-139 C-term $(PEG)_7$-MECAM)



aa: DSSVDLG*A*T*MITSNQLGTI

Chemical Formula: $C_{143}H_{222}N_{32}O_{53}S$
Exact Mass: 3267,53807
Molecular Weight: 3269,58000

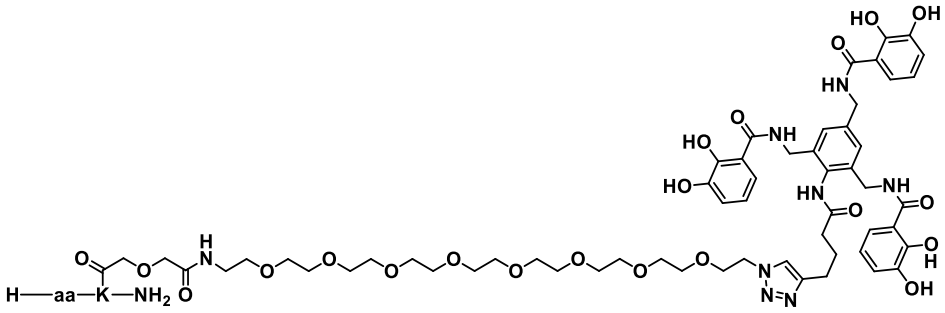
Compound 29 (*PfeA* 33-51 C-term $(PEG)_7$-MECAM)



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{152}H_{236}N_{34}O_{55}$
Exact Mass: 3417,67153
Molecular Weight: 3419,74300

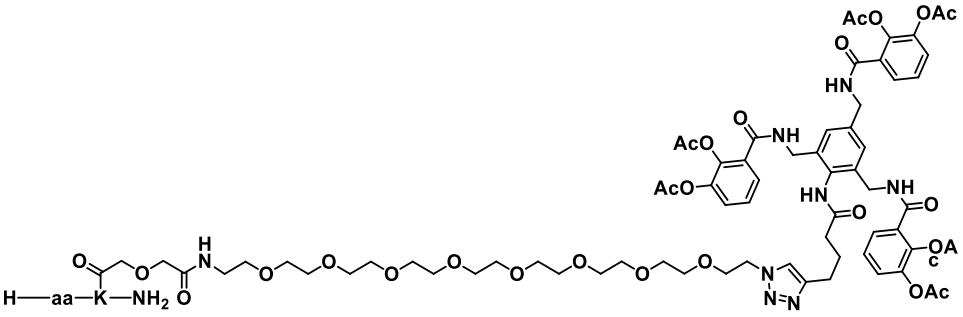
Compound 30 (*HasR* 122-144 C-term $(PEG)_7$-MECAM)



aa: SLIRVSQDDLVQMSPS*V*I*SAARP

Chemical Formula: $C_{169}H_{268}N_{42}O_{56}S$
Exact Mass: 3813,91351
Molecular Weight: 3816,30100

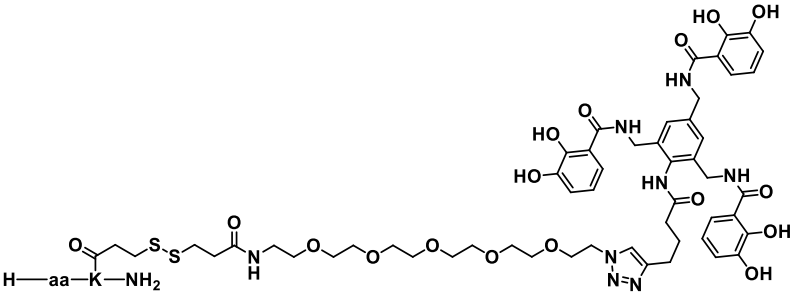
Compound 31 (*PfeA* 33-51 C-term $(PEG)_7$-MECAM-OAc)



aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{164}H_{248}N_{34}O_{61}$
Exact Mass: 3669,73492
Molecular Weight: 3671,96500

Compound 32 (*PfeA* 33-51 C-term disulfide-$(PEG)_5$-MECAM)

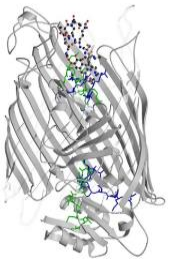


aa: VIELGE*Q*T*V*V*A*T*AQEETKQ

Chemical Formula: $C_{148}H_{228}N_{34}O_{51}S_2$
Exact Mass: 3361,57341
Molecular Weight: 3363,75900

Supplementary biological information

Literature information on *P. aeruginosa's* TBDTs



FpvA

PfeA

no crystal structure

HasR

Name	Ferripyoverdine receptor	Ferric enterobactin receptor	Heme assimilation system receptor
UniProt #	P48632 (FPVA_PSEAE)	Q05098 (PFEA_PSEAE)	Q9HYJ7 (Q9HYJ7_PSEAE)
Genome DB tag	PA2398 (fpvA)	PA2688 (pfeA)	PA3408 (hasR)
Gene	*fpvA*	*pfeA*	*hasR*
MW [kDa]	91.2	81.0	97.9
Location	OM	OM	OM
Organism	PAO1 DSM 22644	PAO1 DSM 22644	PAO1 DSM 22644
Induction	pyoverdine, under iron starvation conditions	enterobactin, iron	-
***TonB* box & framing aa**	^{121}DSSVDLGATMITSNQLGTI^{139}	^{33}VIELGEQTVVATAQEETKQ^{51}	^{122}SLIRVSQDDLVQMSPSVISAARP^{144}

Figure S1: (Top) Crystal structures of *FpvA*-PYO-Fe (PDB 2W6T) and *PfeA*-ENT-Fe (PDB 5M9B) of *P. aeruginosa*, no crystal structure determined for *HasR*.[7 8] (Bottom) Summary on the three selected OMRs FpvA, PfeA and HasR regarding their name, UniProt accession numbers, Genome DB tag, gene, MW = molecular weight [kDa], location = outer membrane (OM), organism, induction of TBDT expression, the TonB box and framing amino acid (aa) sequences.

Table S6: Natural and synthetic siderophores and the corresponding TBDTs of *P. aeruginosa*. PYO: pyoverdine, PCH: pyochelin, ENT: enterobactin.[9, 10, 11, 12, 13, 14].

Siderophore	PYO	PCH	ENT	DOTAM	MECAM	Heme
P. aeruginosa	*FpvA*	*FptA*	*PfeA*, *PirA*	*PirA*	*PfeA*, *PirA*	*HasR*, *PhuR*

Figure S2: Clustal alignment of reviewed *P. aeruginosa* TonB box sequences from FpvA (FPVA_PSEAE), PfeA (PFEA_PSEAE) and HasR (Q9HYJ7_PSEAE) from the Uniprot database with ClustalΩ.

Biology methods

Fe-Chrome Azurol S (CAS) assay

The Fe-chrome azurol S (FeCAS) assay was conducted following a known procedure.[15, 2] All glassware needed for the assay was cleaned with concentrated hydrochloric acid and milliQ water. Water and aqueous solutions of iron(III) chloride (1 mM in 10 mM HCl, 150 µL) and Chrome Azurol S (50 µL, CAS) were added to an aqueous solution of hexadecyltrimethylammonium bromide (600 µL HDTMA 10 mM). A buffer solution consisting of piperazine (431 mg, 5 mmol) and concentrated hydrochloric acid (625 µL) in water (5 mL) was added. The resulting solution was diluted with dH_2O to a total volume of 10 mL. The stock solution used for the assay was generated by further addition of 5-sulfosalicylic acid dihydrate (10.2 mg, 40 µmol). Solutions of the test compounds (15 µM, 120 µL each), as well as water (40 µL) were added to 40 µL of stock solution. The assay was conducted in technical triplicates in transparent, untreated 96-well plates. Absorbance from 300 to 800 nm was determined after 17 h using a plate reader, the curves were plotted and evaluated using Microsoft Excel 2016 and GraphPad Prism 9.

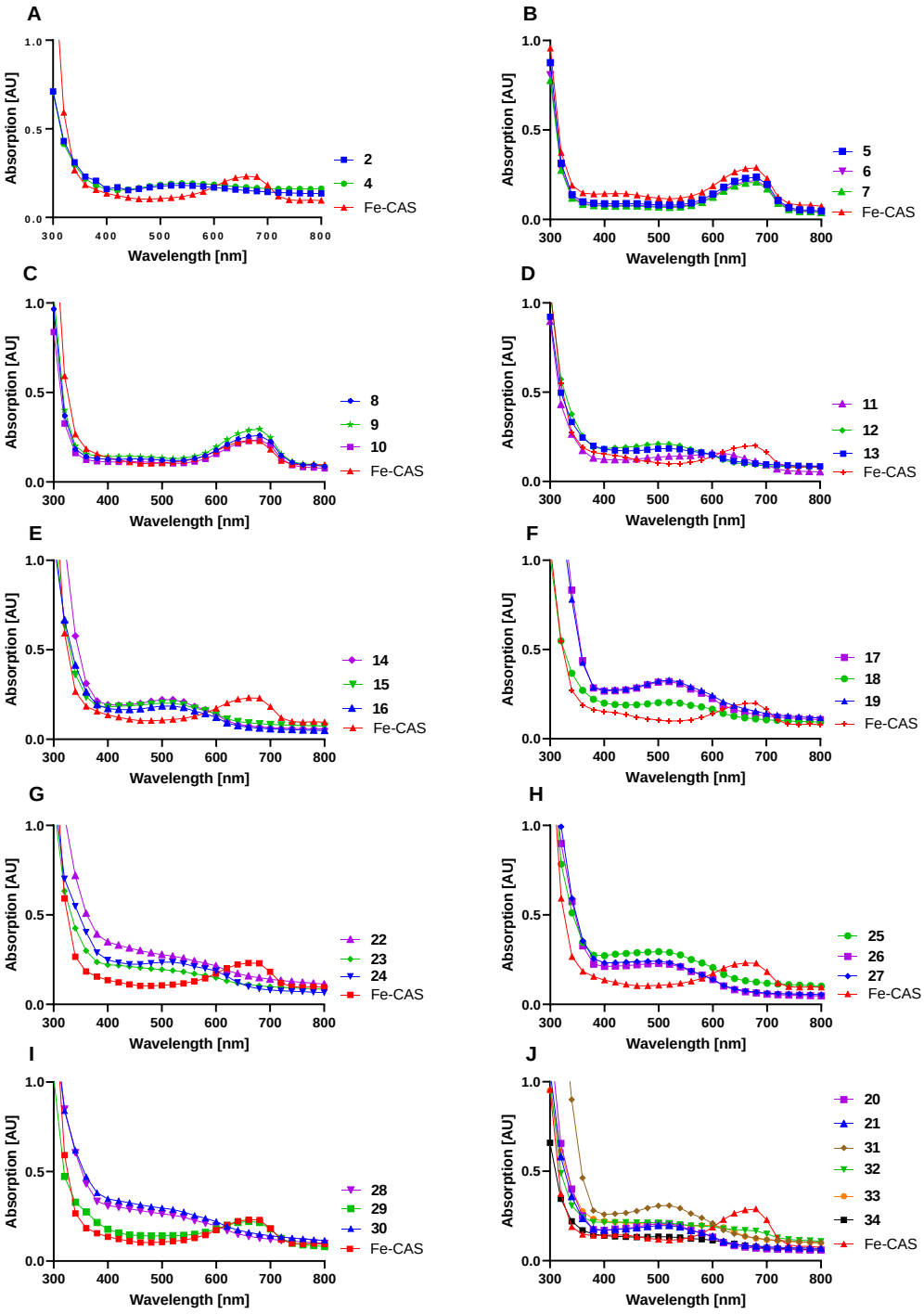


Figure S3: Absorbance spectra from 300-800 nm of Fe-CAS, the free unmodified TonB box peptides **5-10** and siderophore conjugates **11-34** upon incubation with the Fe-CAS complex for 17 hours. (**A**) DOTAM **2** and MECAM **4** (**B**) long, free peptides **5**-**7**, (**C**) short, free peptides **8**-**10**, (**D**) long, *N*-term. DOTAM conjugates **11**-**13**, (E) short, *N*-term. DOTAM conjugates **14**-**16**, (**F**) long *C*-term. DOTAM conjugates **17**-**18**, (**G**) long, *N*-term. MECAM conjugates 22-24, (**H**) short, *N*-term. MECAM conjugates **25**-**27**, (**I**) long, *C*-term. MECAM conjugates **28**-**30**, (**J**) special conjugates **20**, **21**, **31**-**34**. All plots with a FeCAS reference curve, (n = 3).

Table S7: Iron-binding capability measured by the Fe-CAS assay and antimicrobial activity in mutant *P. aeruginosa* strains.

#	Name	Fe-CAS result
2	DOTAM	P
4	MECAM	P
5	FpvA (l)	N
6	PfeA (l)	N
7	HasR (l)	N
8	FpvA (s)	N
9	PfeA (s)	N
10	HasR (s)	N
11	FpvA (l)-N-D	P
12	PfeA (l)-N-D	P
13	HasR (l)-N- D	P
14	FpvA (s)-N-D	P
15	PfeA (s)-N-D	P
16	HasR (s)-N- D	P
17	FpvA (l)-C-D	P
18	PfeA (l)-C-D	P
19	HasR (l)-C-D	P
20	PfeA (l)-C-D-Ac	P
21	PfeA (l)-DS-C-D	P
22	FpvA (l)-N-M	P
23	PfeA (l)-N-M	P
24	HasR (l)-N-M	P
25	FpvA (s)-N-M	P
26	PfeA (s)-N-M	P
27	HasR (s)-N- M	P
28	FpvA (l)-C-M	P
29	PfeA (l)-C-M	P
30	HasR (l)-C-M	P
31	PfeA (l)-C-M-Ac	P
32	PfeA (l)-DS-C-M	P
33	FpvA-C-catechol	P
34	PfeA-C-catechol	P

P = positive FeCAS result, absorbance shift (blue to red), N = negative. (l) = long, (s) = short, D = DOTAM and M = MECAM, Ac = acetyl, DS = disulfide.

Antimicrobial susceptibility assays

The *P. aeruginosa* strains used in this study are listed in Table S1. Evaluation of the different compounds activities was carried out in the iron-deficient CAA medium (casamino acid medium, composition: 5 g l^{-1} low-iron CAA (Difco), 1.46 g l^{-1} K_2HPO_4 $3H_2O$, 0.25 g l^{-1} $MgSO_4$ $7H_2O$) using the two-fold serial dilution method with an inoculum of 10^5 bacteria per mL. *P. aeruginosa* Δ*pvdF*Δ*pchA* strains were first grown overnight at 37 °C in LB broth, then washed and resuspended in CAA medium. The strains were grown for two successive overnight cultures at 30 °C in iron-deficient CAA medium, with a dilution of the cells of 1/10. Data were reported as MIC, which reflects the lowest concentration of antibiotic or test compound that inhibits the visible cell growth after a 24 h or 48 h incubation at 30 °C.

RT-qPCR analysis in PAO1 wildtype and mutant strains

qRT-PCR was used to follow specific gene transcription as previously described.[1] Bacteria (PAO1 or Δ*pvdF*Δ*pchA*) were grown in CAA medium and in 50 mL Falcons, for 8 h, at 30 °C, in the presence or absence of 10 µM of the tested compounds and with vigorous shaking. Aliquot of 2.5 x 10^8 cells from these cultures were added to two volumes of RNAprotect Bacteria Reagent (Qiagen) and exactly the same protocol was used as previously described (Perraud *et al.*, 2020). Primers efficiency were determined using serially diluted genomic DNA and the double ΔC_T method was used to analyze qPCR data. The primers used are summarized in Table S8.

Growth kinetic in function of time in the absence and presence of vectors and conjugates

Bacteria were first grown overnight in LB, washed and then grown in CAA at 30 °C. This culture was washed and resuspended in CAA medium at an $OD_{600\ nm}$ of 0.02 and 200 µL was distributed in 96 well U-shaped plates (Greiner). Fresh, sterile-filtered aqueous solutions of the tested compounds were added to the different strains tested, at a final concentration of 10 µM. $OD_{600\ nm}$ was monitored in an Infinite M200 (TECAN, Austria) plate reader for 48 h, with regular agitation and incubation temperature set to 30 °C. More information on the bacterial strains, especially the knockouts, can be found in our previous, recent publication Fritsch et al.

Table S8: Primers used for the RT-qPCR assays.

Primer ID	Target	Sequence
uvrD F	*uvrD*	CTACGGTAGCGAGACCTACAACAA
uvrD R	*uvrD*	GCGGCTGACGGTATTGGA
pfeA F	*pfeA*	GCCGAGACCAGCGTGAAC
pfeA R	*pfeA*	GGCCGGATTCGATCTTGTT
pirA F	*pirA*	GCCTGAACGCTTCCCAAA
pirA R	*pirA*	TGAAGGCCCGTGCGATA
fpvA F	*fpvA*	AGCCGCCTACCAGGATAAGC
fpvA R	*fpvA*	TGCCGTAATAGACGCTGGTTT
fptA F	*fptA*	GCGCCTGGGCTACAAGATC
fptA R	*fptA*	CCGTAGCGGTTGTTCCAGTT

Table S9. MIC values in *P. aeruginosa ΔpvdFΔpchA* strain for siderophores **2** and **4**, peptides **5-10** and peptide-siderophore conjugates **11-34** µM and µg/ml.

Compound	MIC 24 h [µM]	MIC 24 h [µg/ml]	MIC 48 h [µM]	MIC 48 h [µg/ml]
1	-	-	-	-
2	64	62.47	64	62.47
3	-	-	-	-
4	>64	>43.69	>64	>43.69
5	>64	>131.2	>64	>131,2
6	>64	>140.8	>64	>140.8
7	>64	>166.2	>64	>166.2
8	>64	>79,90	>64	>79.90
9	>64	>72.34	>64	>72.34
10	>64	>77.91	>64	>77.91
11	0.5	1.814	1	3.628
12	0.5	1.889	1	3.778
13	4	16.70	32	133.6
14	32	90.45	>64	>180.9
15	32	86.67	32	86.67
16	>64	>178.9	>64	>178.9
17	0.1	0.363	>64	>232.2
18	>64	>241.8	>64	>241.8
19	>64	>267.2	>64	>267.2
20	>64	>258.0	>64	>258.0
21	8	29.78	>64	>238.2
22	>64	>209.3	>64	>209.3
23	>64	>218.9	>64	>218.9
24	>64	>244.2	>64	>244.2
25	>64	>157.9	>64	>157.9
26	>64	>150.4	>64	>150.4
27	>64	>156.0	>64	>156.0
28	>64	>209.3	>64	>209.3
29	>64	>218.9	>64	>218.9
30	>64	>244.2	>64	>244.2
31	>64	>235.0	>64	>235.0
32	>64	>215.3	>64	>215.3
C33	>64	>139.9	>64	>139.9
C34	>64	>149.5	>64	>149.5
$N33_L$	>64	>139.9	>64	>139.9
$N34_L$	>64	>149.5	>64	>149.5
$N33_D$	>64	>139.9	>64	>139.9
$N34_D$	>64	>149.5	>64	>149.5
Gentamicin	1	0.478	4	1.91

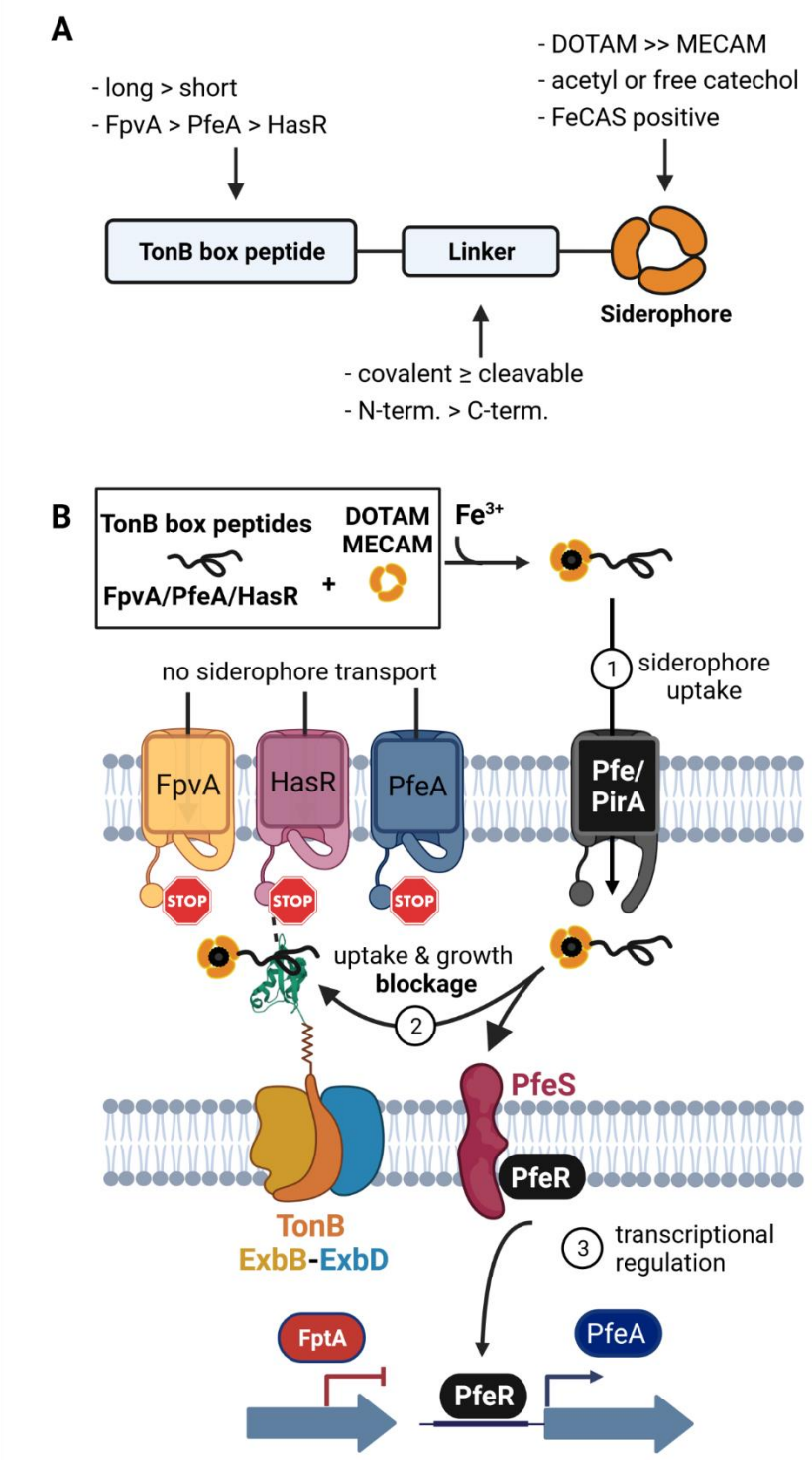
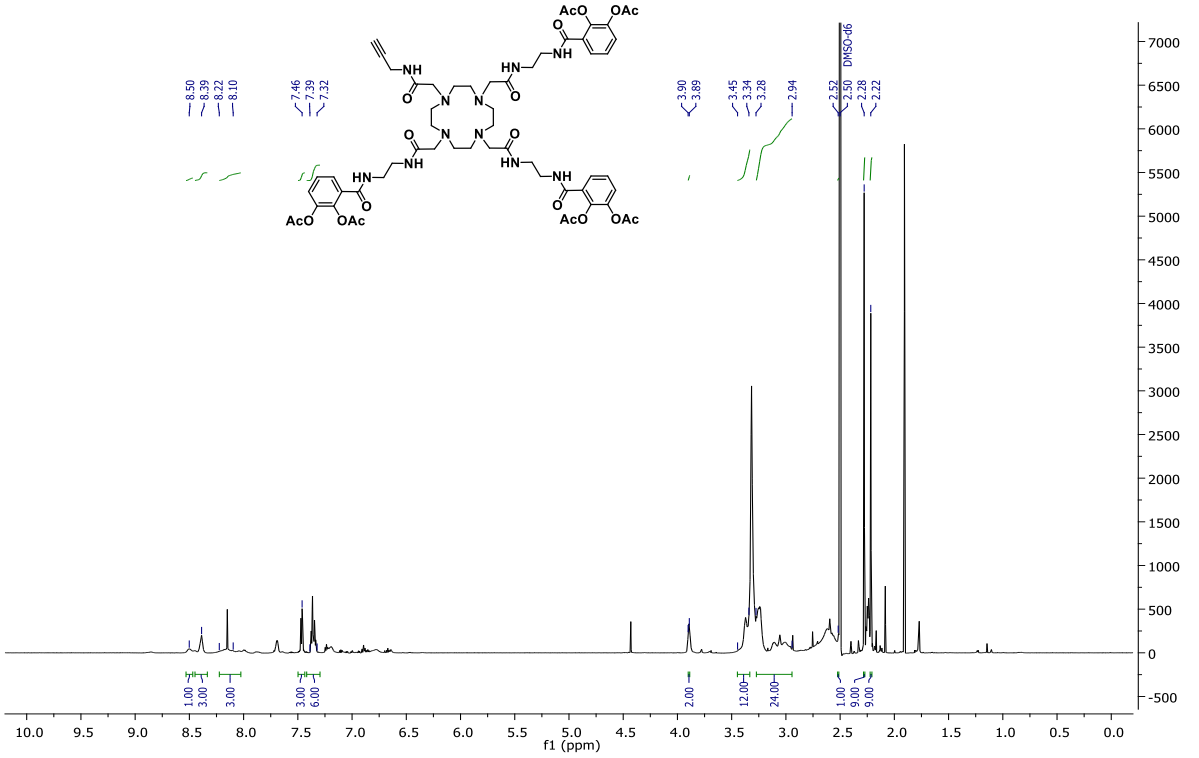


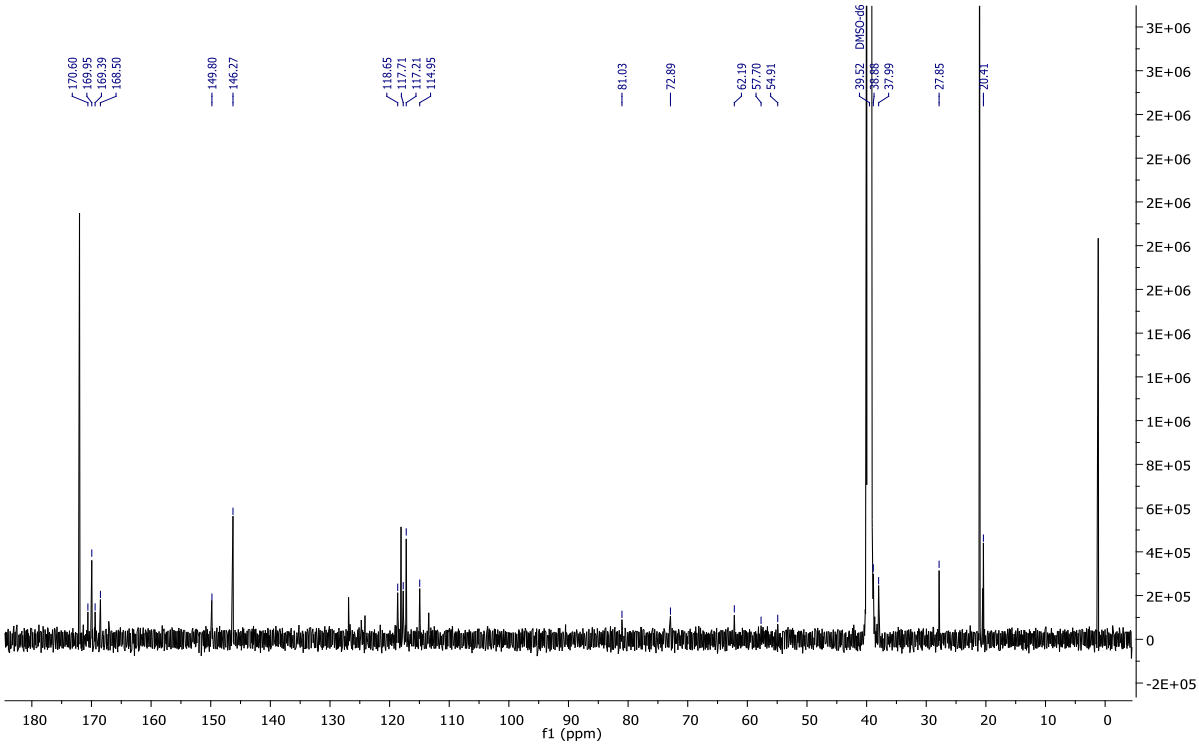
Figure S4: Rough structure-activity-relationships (A) and mechanistic summary (B) on TonB box peptide-siderophore conjugates.

Appendix

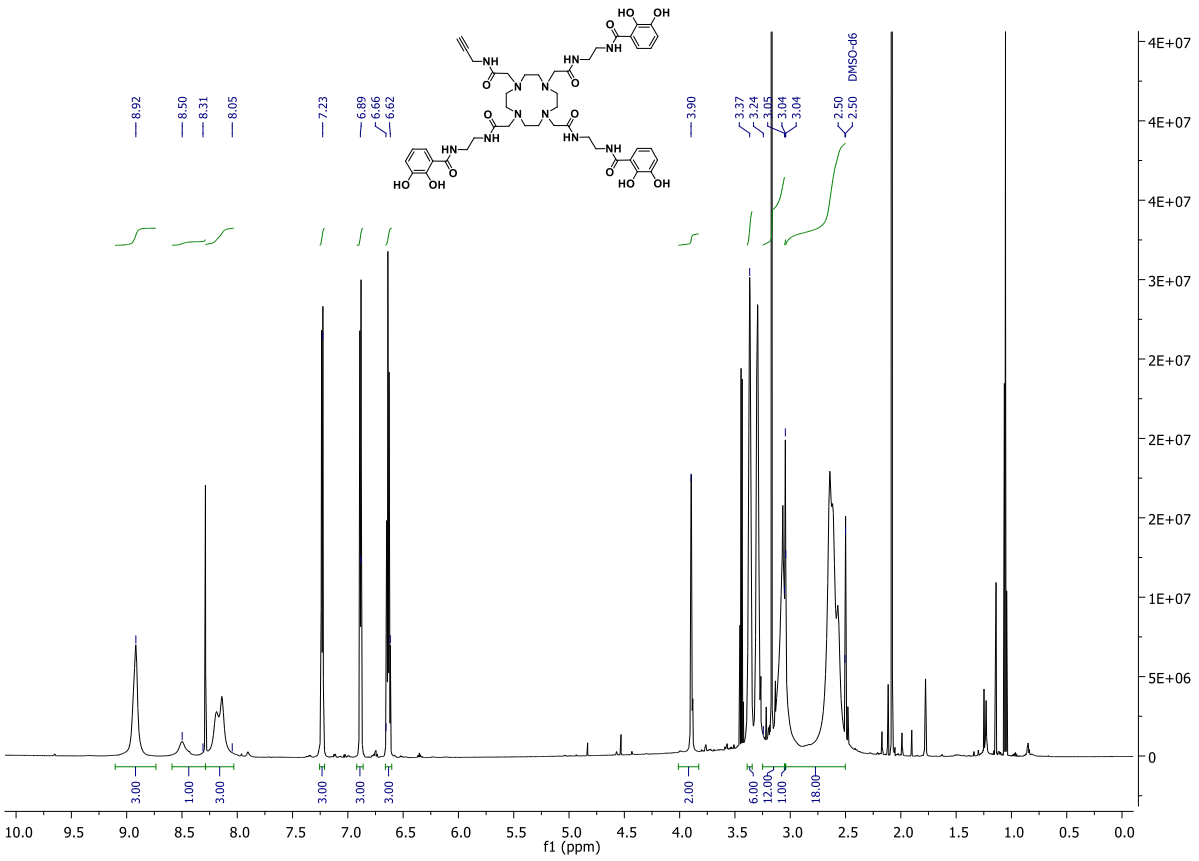
NMR and MS spectra

Compound 1





Compound 2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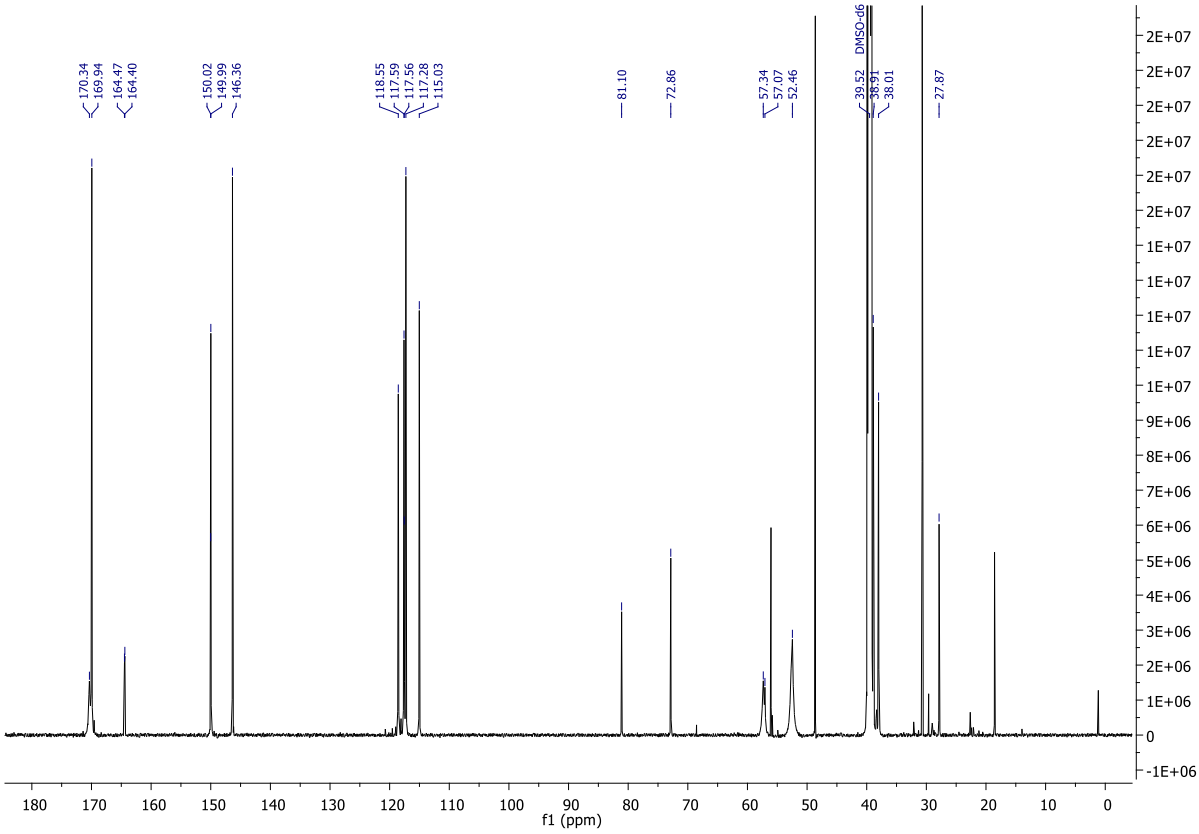
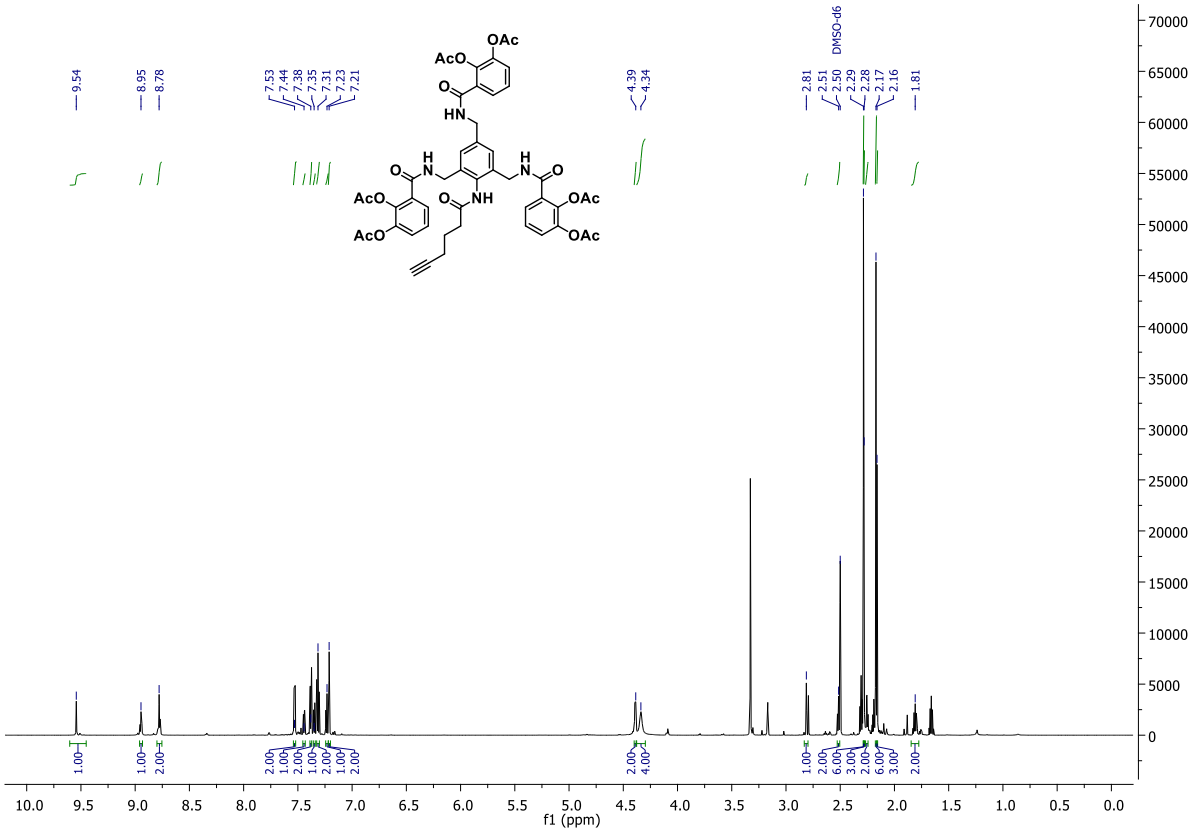
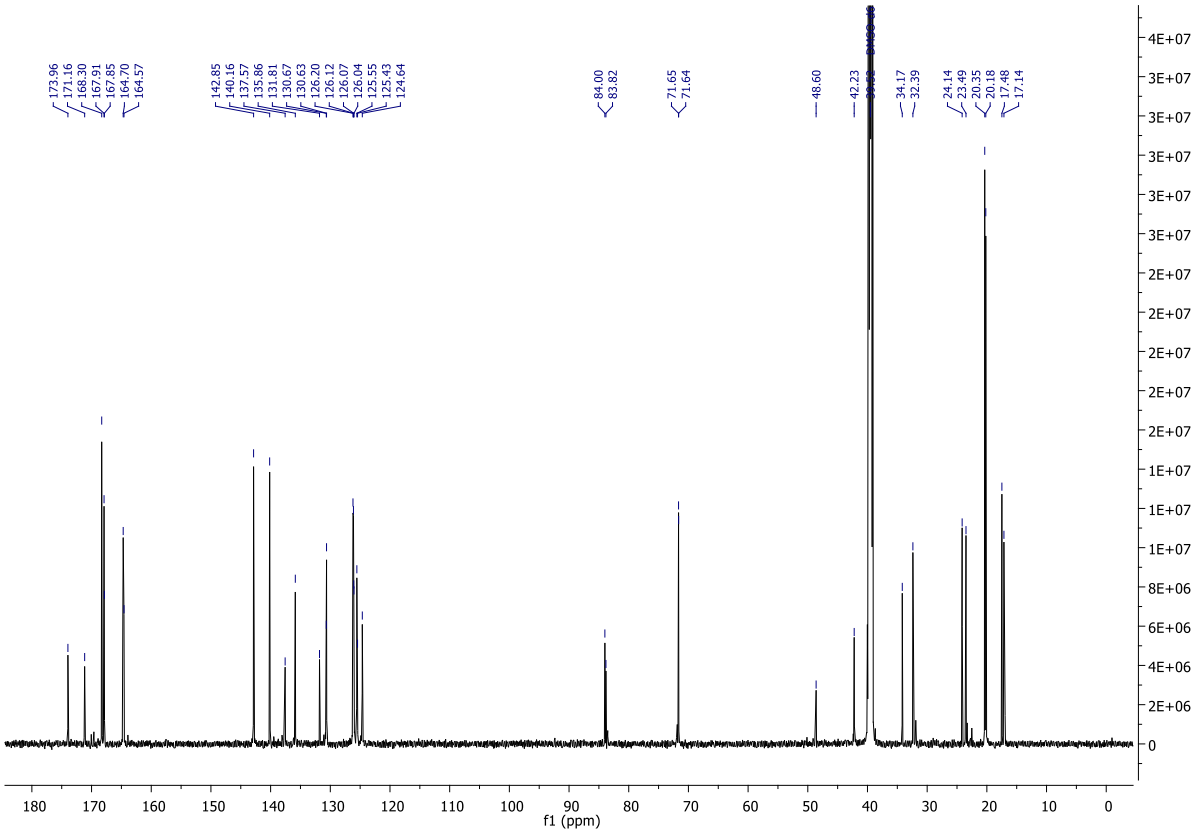
8.50
8.31
8.05
7.23
6.89
6.66
6.62
3.90
3.37
3.24
3.05
3.04
3.04
2.50
2.50
DMSO-d6
3.00
1.00
3.00
3.00
3.00
3.00
2.00
6.00
12.00
1.00
18.00
f1 (ppm)


170.34
169.94
164.47
164.40
150.02
149.99
146.36
118.55
117.59
117.56
117.28
115.03
81.10
72.86
57.34
57.07
52.46
39.52
DMSO-d6
38.91
38.01
27.87
f1 (ppm)

Compound 3


9.54
8.95
8.78
7.53
7.44
7.38
7.35
7.31
7.23
7.21
4.39
4.34
2.81
2.51
2.50
DMSO-d6
2.29
2.28
2.17
2.16
1.81
f1 (ppm)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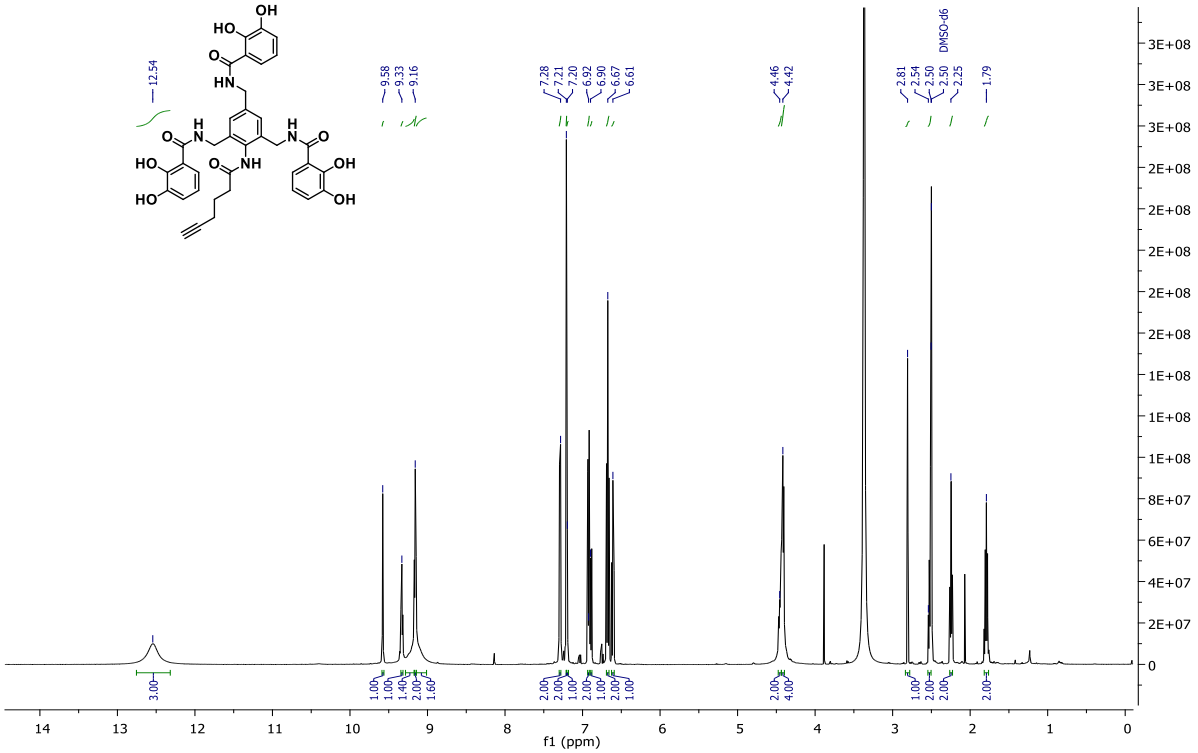
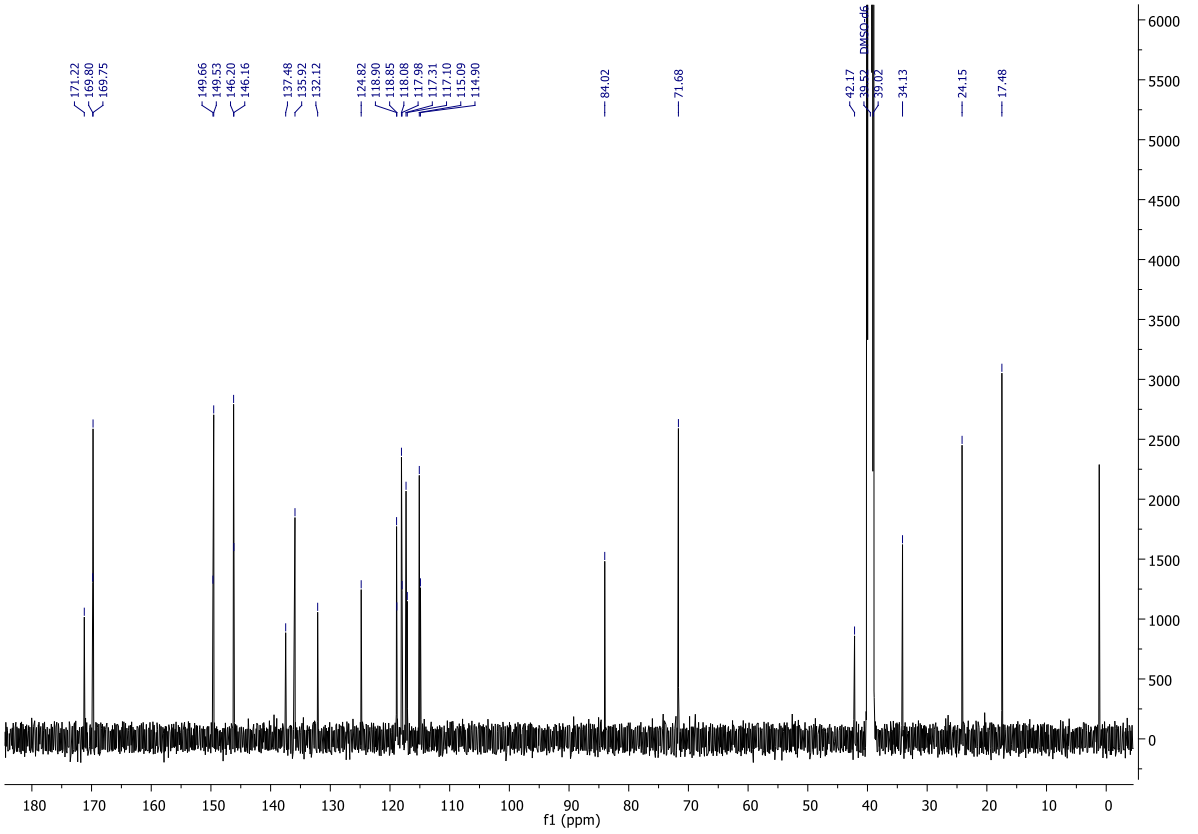
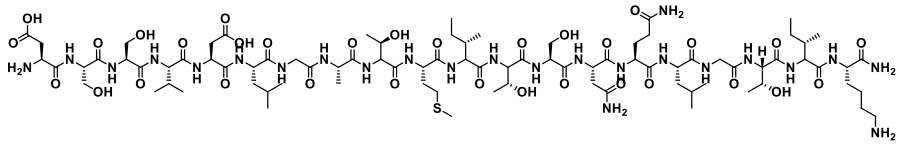
168.30
167.91
167.85
164.70
164.57
142.85
140.16
137.57
135.86
131.81
130.67
130.63
126.20
126.12
126.07
126.04
125.55
125.43
124.64
84.00
83.82
71.65
71.64
48.60
42.23
34.17
32.39
24.14
23.49
20.35
20.18
17.48
17.14
f1 (ppm)

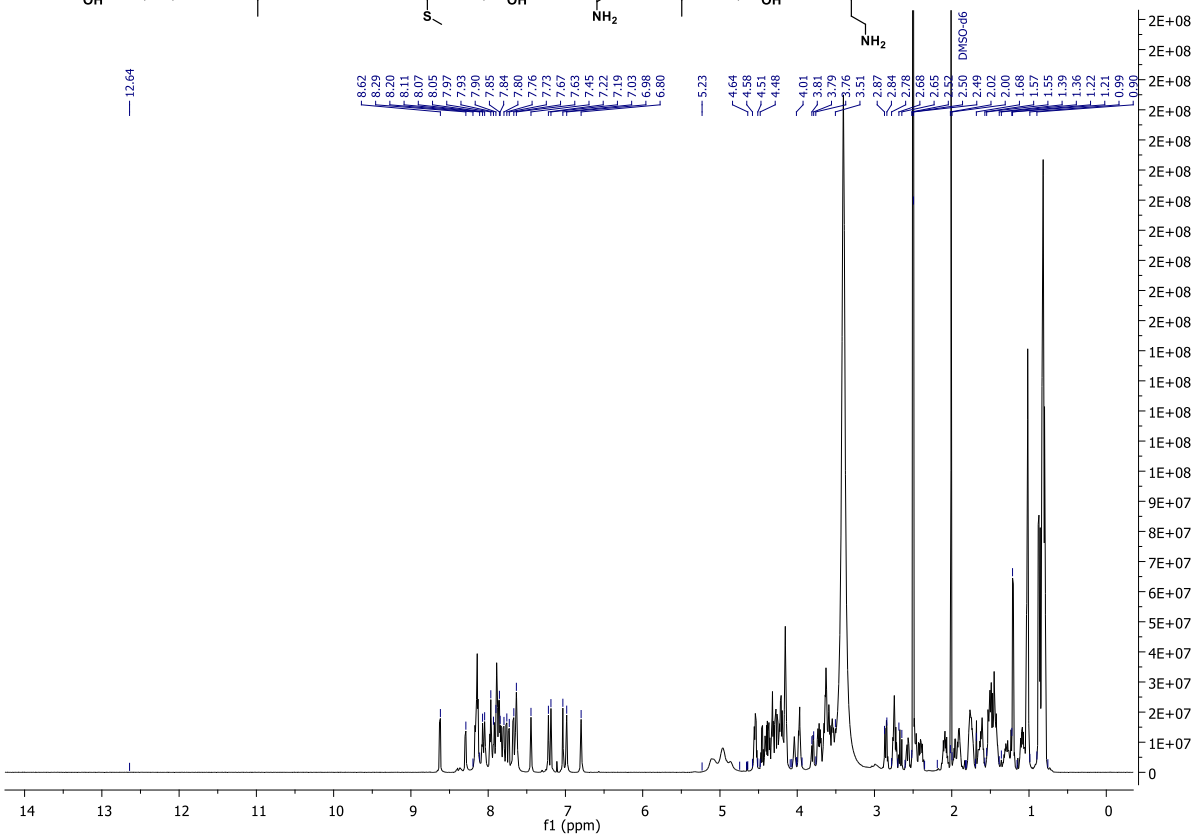
Compound 4

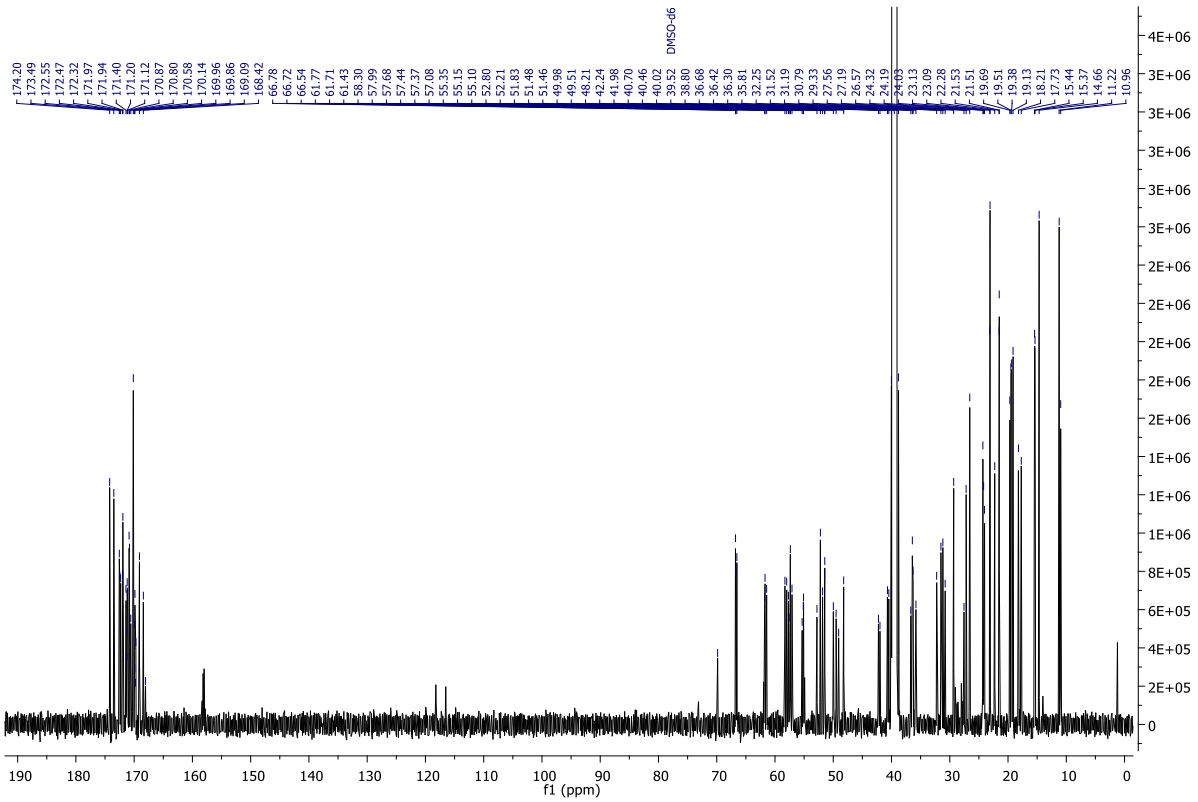

12.54
9.58
9.33
9.16
7.28
7.21
7.20
6.92
6.90
6.67
6.61
4.46
4.42
2.81
2.54
2.50
2.50
2.25
DMSO-d6
1.79
f1 (ppm)

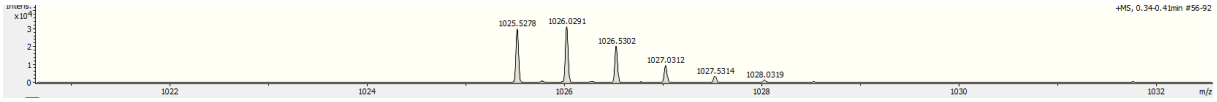

171.22
169.80
169.75
149.66
149.53
146.20
146.16
137.48
135.92
132.12
124.82
118.90
118.85
118.08
117.98
117.31
117.10
115.09
114.90
84.02
71.68
42.17
39.52
DMSO-d6
39.02
34.13
24.15
17.48
f1 (ppm)

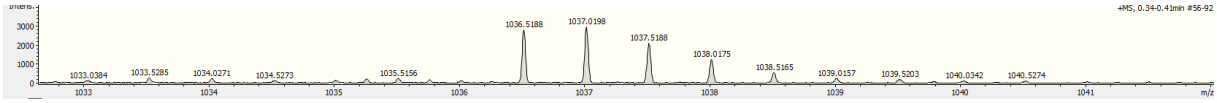
Compound 5 (*FpvA* 121-139 peptide)

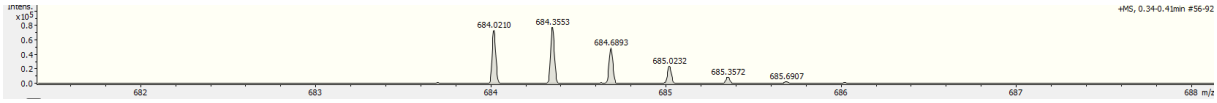




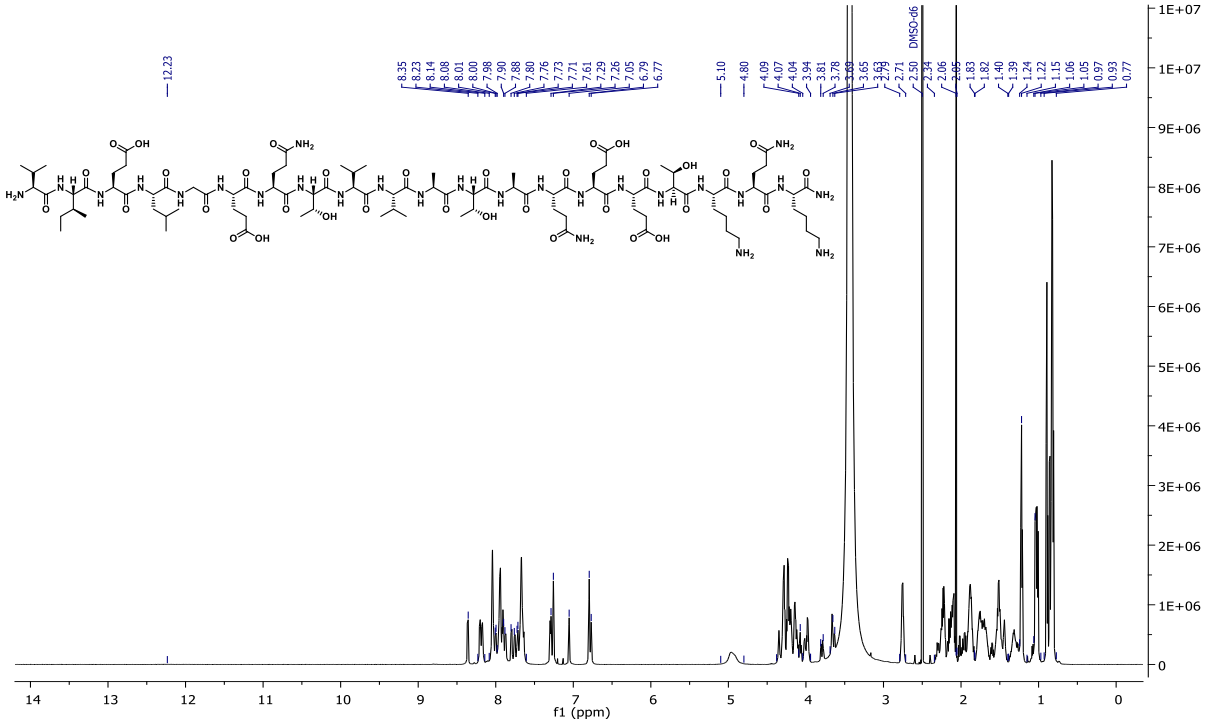


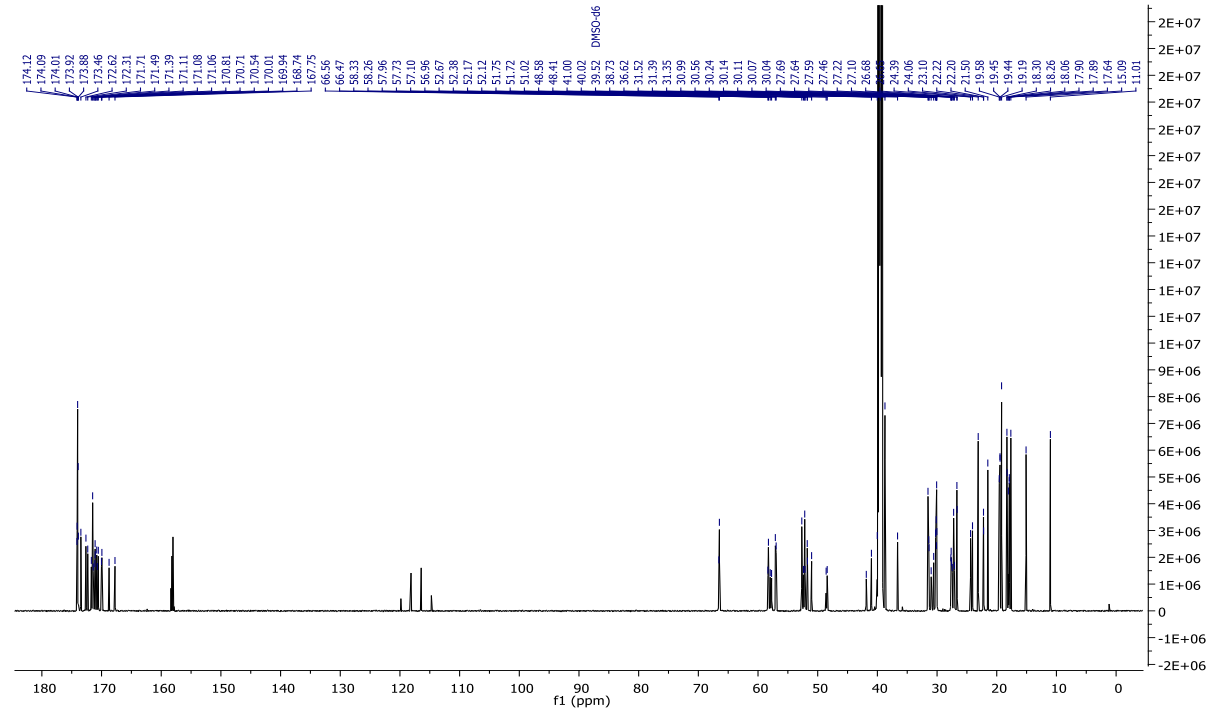

+MS, 0.34-0.41min #56-92
1025.5278
1026.0291
1026.5302
1027.0312
1027.5314
1028.0319
1022
1024
1026
1028
1030
1032
m/z

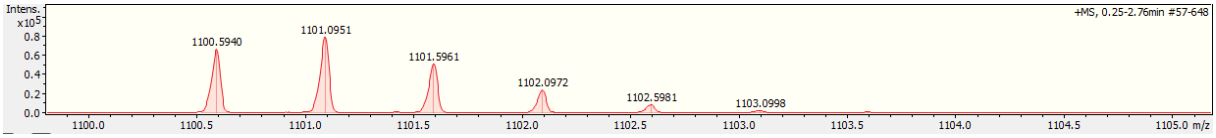

+MS, 0.34-0.41min #56-92
1033.0384
1033.5285
1034.0271
1034.5273
1035.5156
1036.5188
1037.0198
1037.5188
1038.0175
1038.5165
1039.0157
1039.5203
1040.0342
1040.5274
1033
1034
1035
1036
1037
1038
1039
1040
1041
m/z


+MS, 0.34-0.41min #56-92
684.0210
684.3553
684.6893
685.0232
685.3572
685.6907
682
683
684
685
686
687
688
m/z

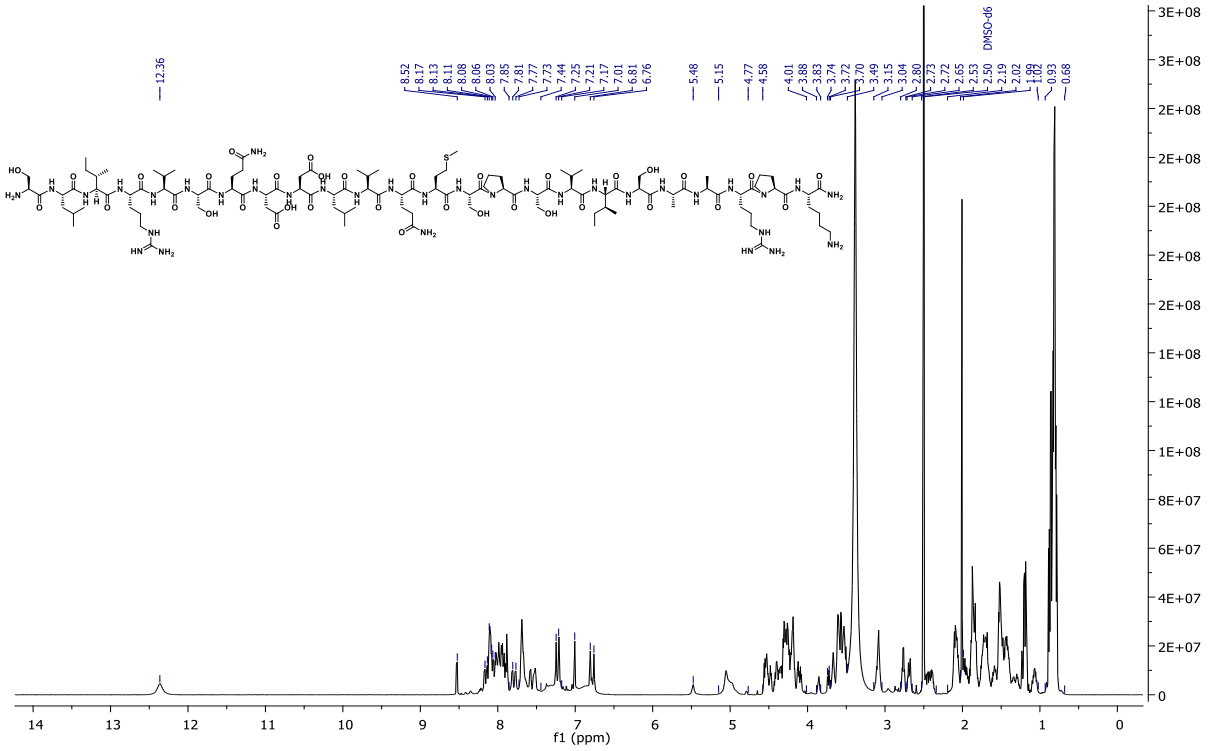
Compound 6 (*PfeA* 33-51 peptide)

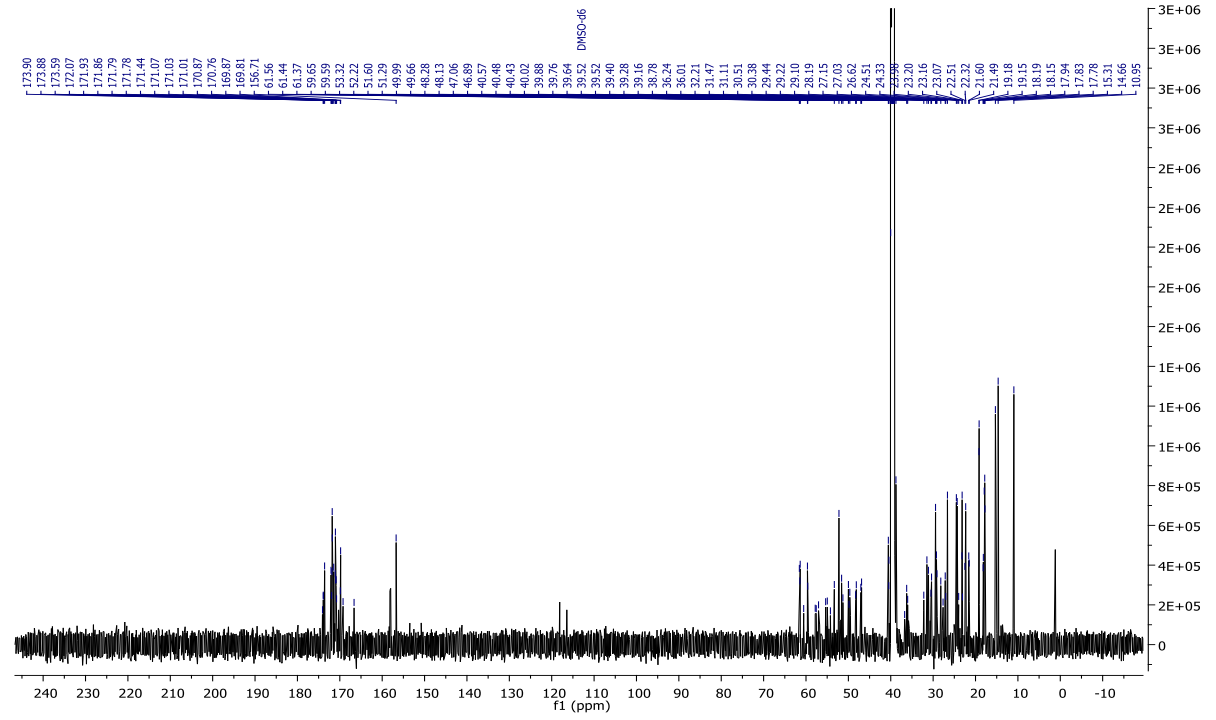


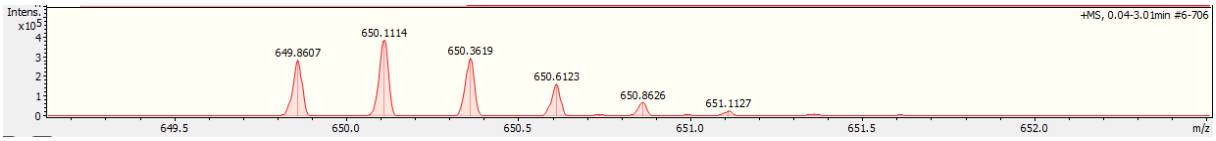




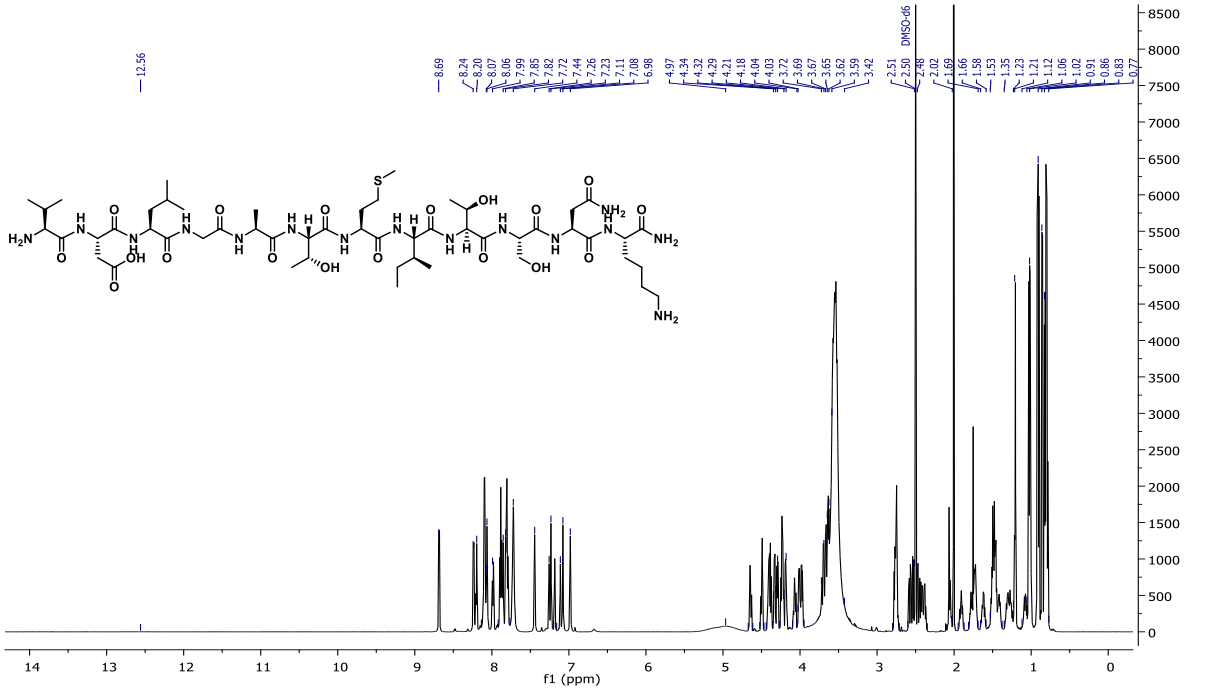
Compound 7 (*HasR* 122-144 peptide)

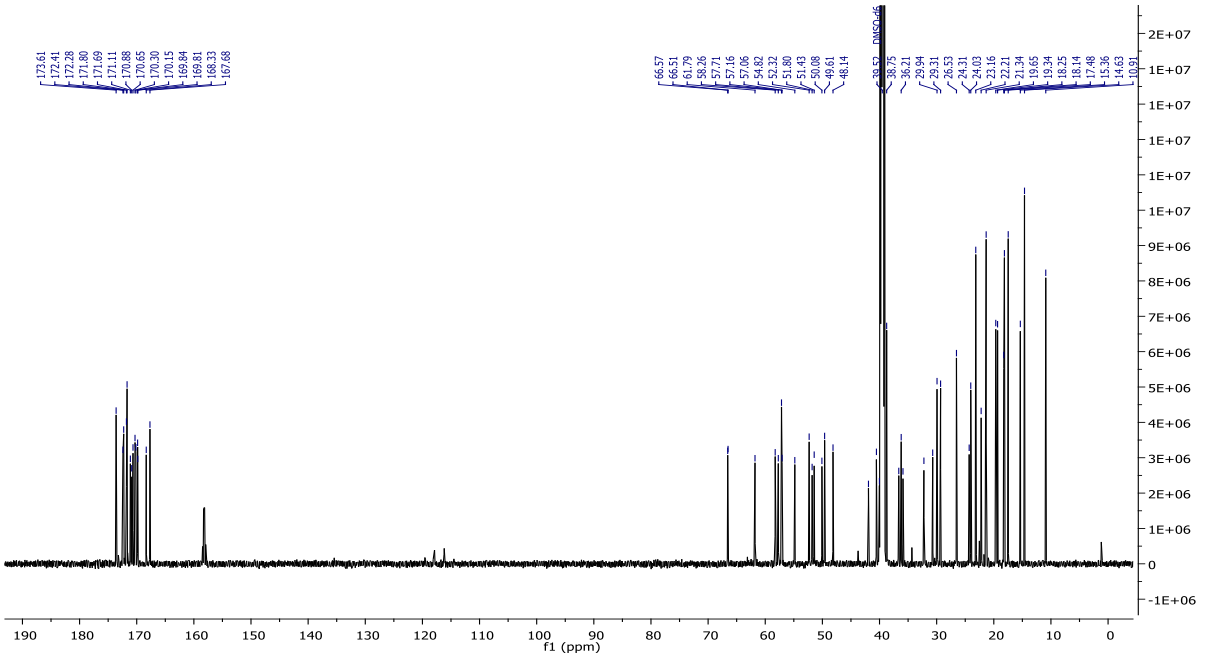


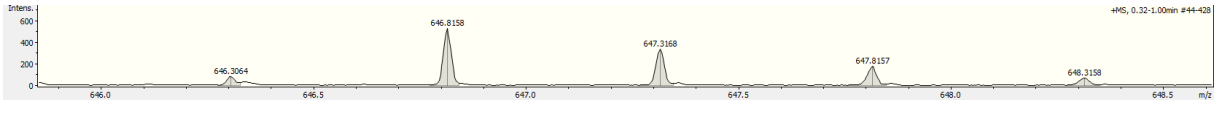


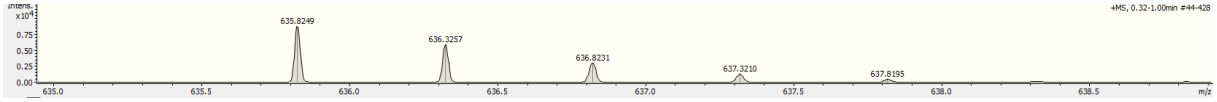


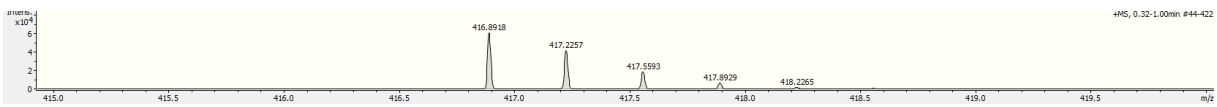
Compound 8 (*FpvA* 124-134 peptide)



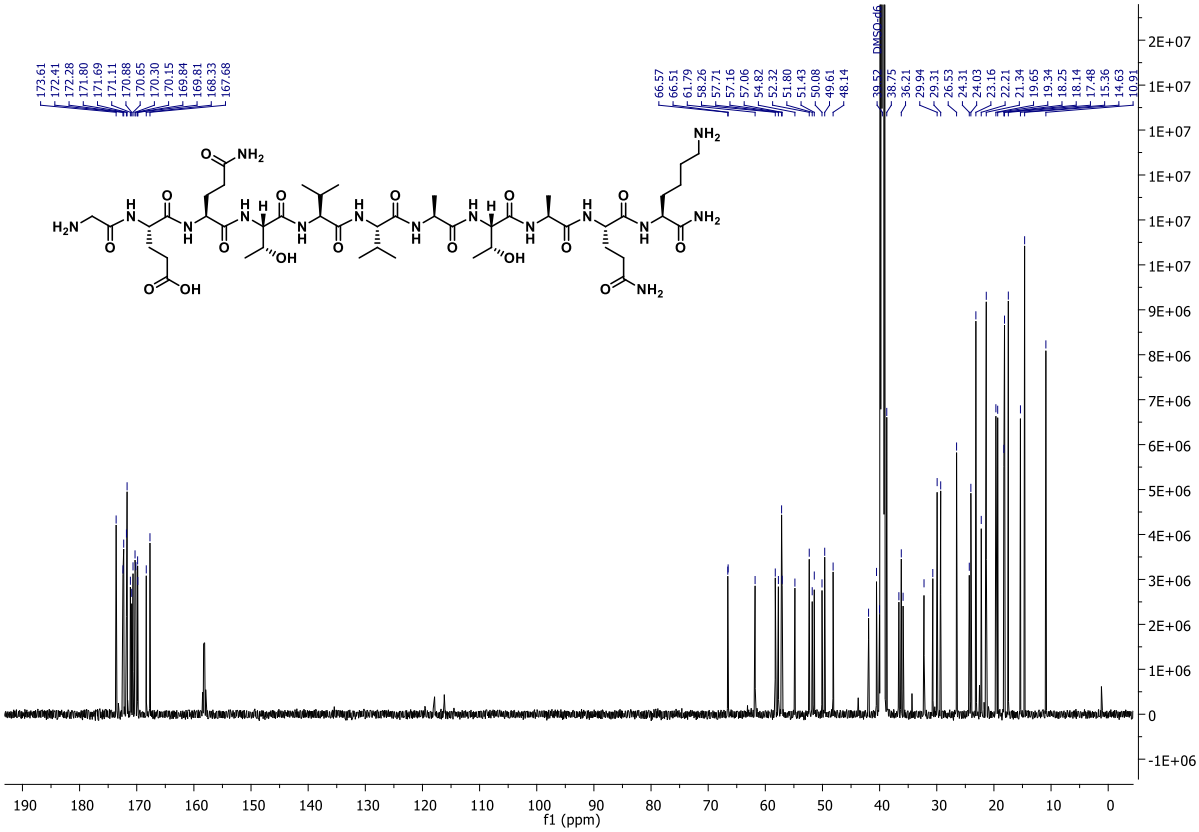


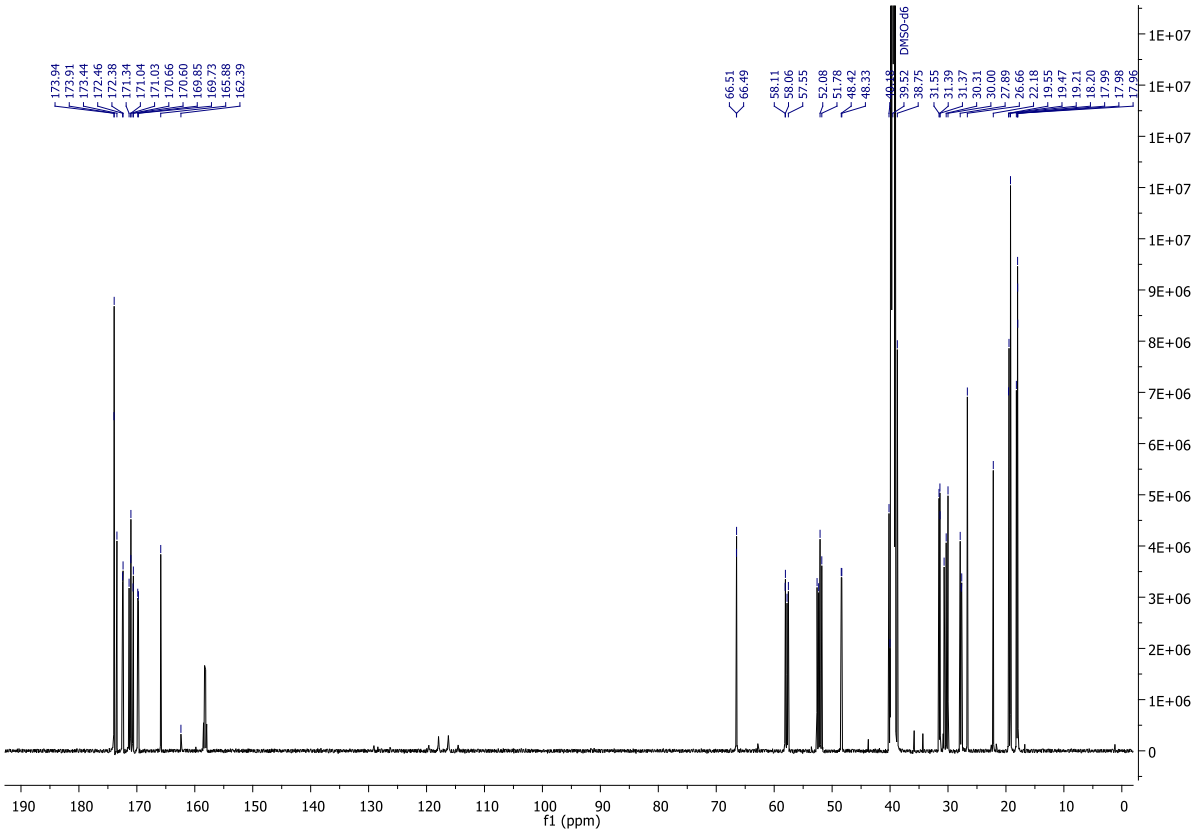


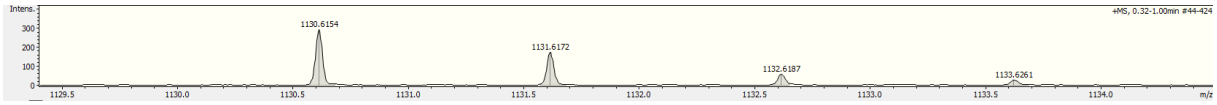


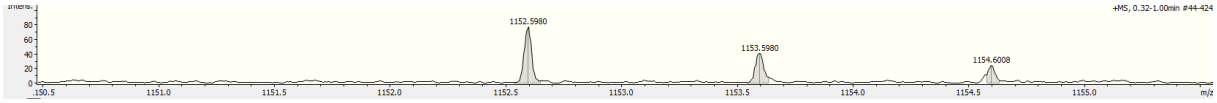


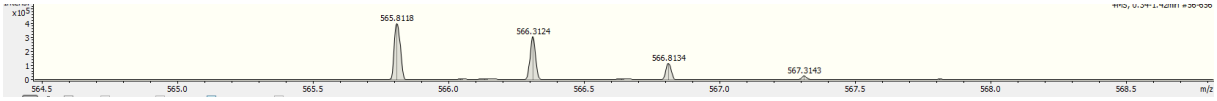
Compound 9 (*PfeA* 37-46 peptide)

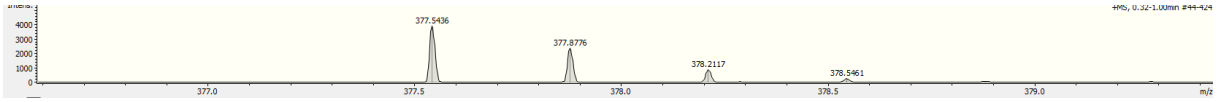




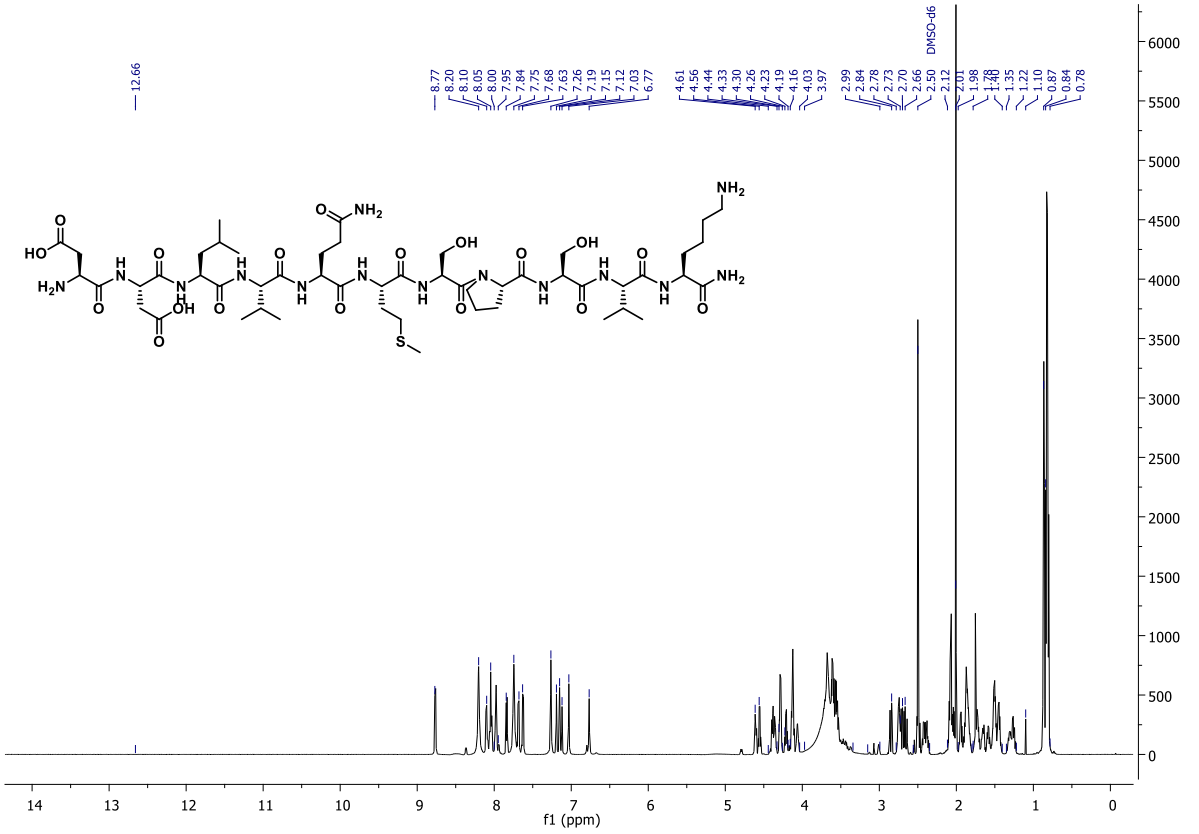

Intens.
+MS, 0.32-1.00min #44-424
1130.6154
1131.6172
1132.6187
1133.6261
m/z

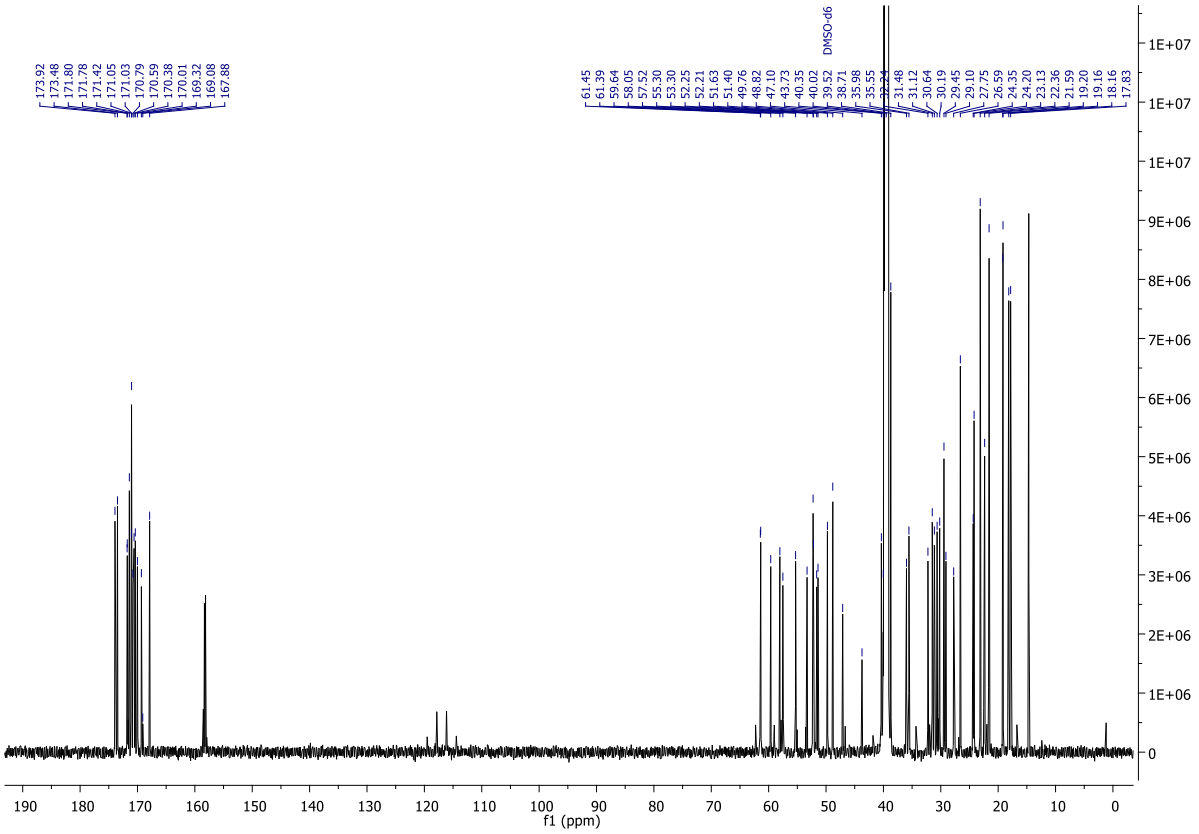

+MS, 0.32-1.00min #44-424
1152.5980
1153.5980
1154.6008
m/z

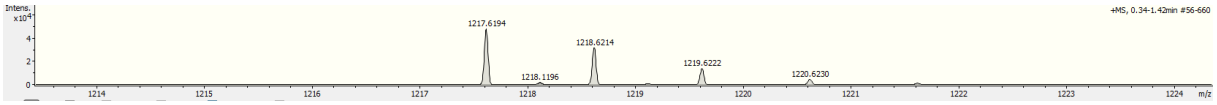

x10^5
565.8118
566.3124
566.8134
567.3143
m/z

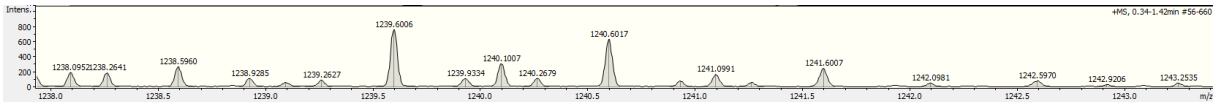

+MS, 0.32-1.00min #44-424
377.5436
377.8776
378.2117
378.5461
m/z

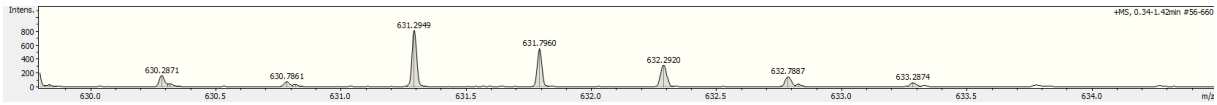
Compound 10 (*HasR* 129-138 peptide)

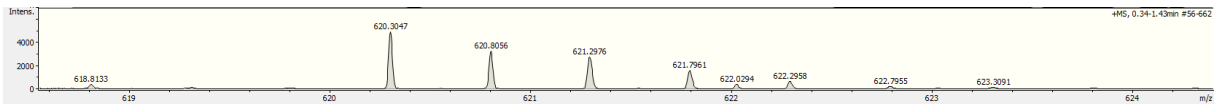


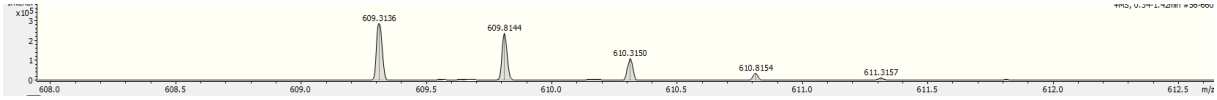



Intens.
x10^4
+MS, 0.34-1.42min #56-660
1217.6194
1218.6214
1218.1196
1219.6222
1220.6230
m/z

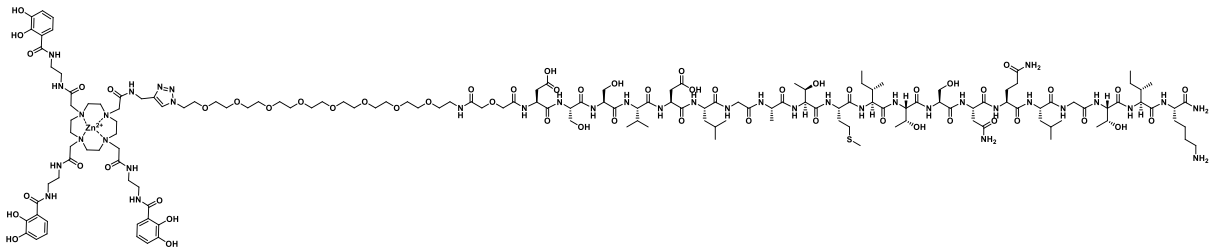

Intens.
+MS, 0.34-1.42min #56-660
1239.6006
1240.6017
1238.0952
1238.2641
1238.5960
1238.9285
1239.2627
1239.9334
1240.1007
1240.2679
1241.0991
1241.6007
1242.0981
1242.5970
1242.9206
1243.2535
m/z

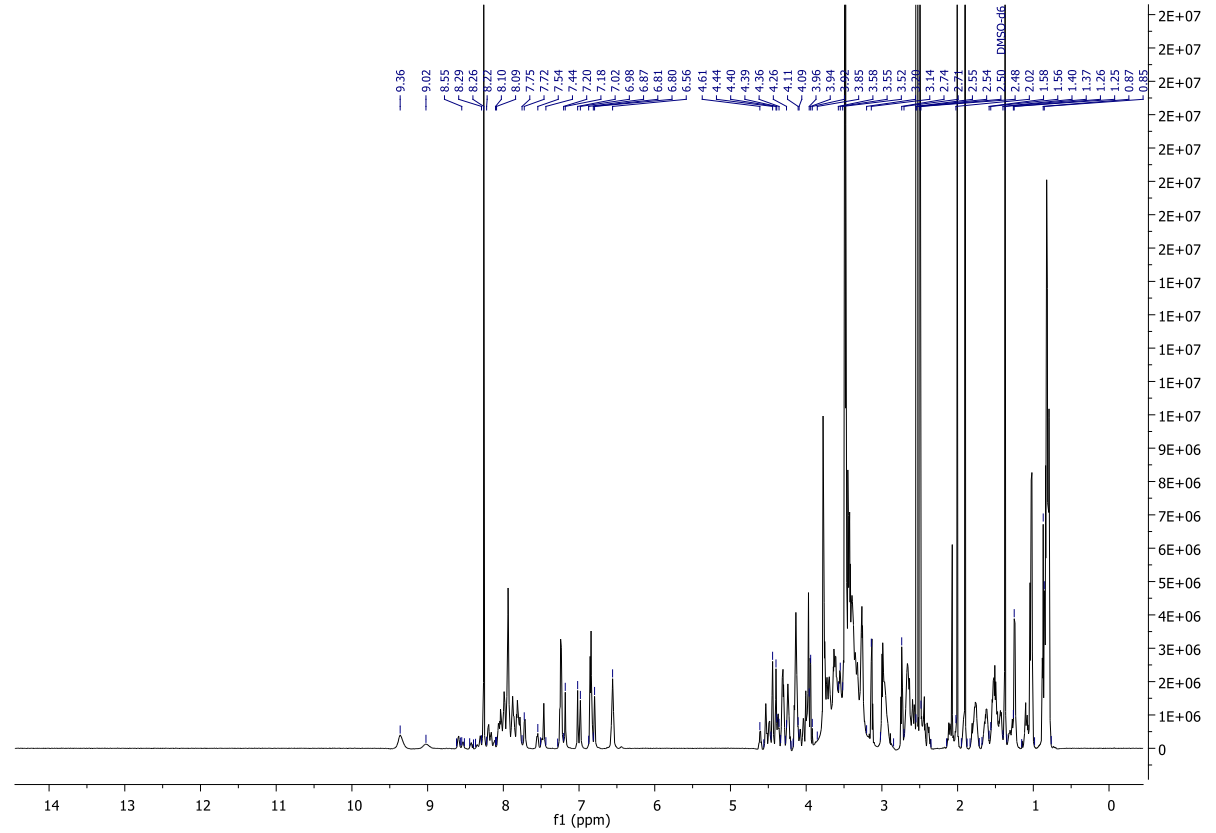

Intens.
+MS, 0.34-1.42min #56-660
631.2949
631.7960
630.2871
630.7861
632.2920
632.7887
633.2874
m/z

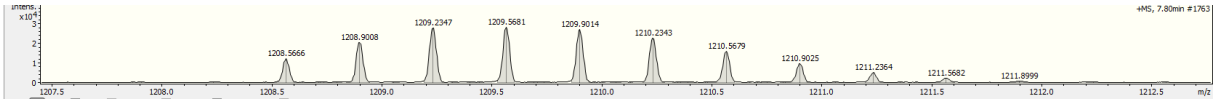

Intens.
+MS, 0.34-1.43min #56-662
620.3047
620.8056
621.2976
621.7961
618.8133
622.0294
622.2958
622.7955
623.3091
m/z

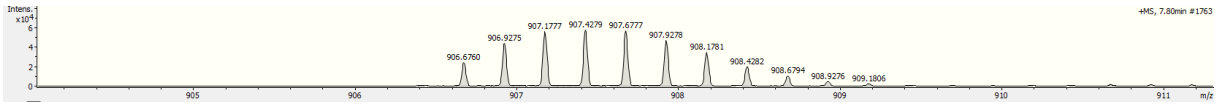

x10^3
609.3136
609.8144
610.3150
610.8154
611.3157
m/z

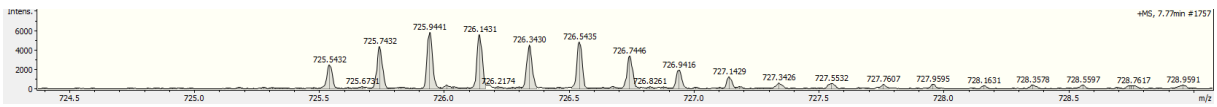
Compound 11 (*FpvA* 121-139 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)



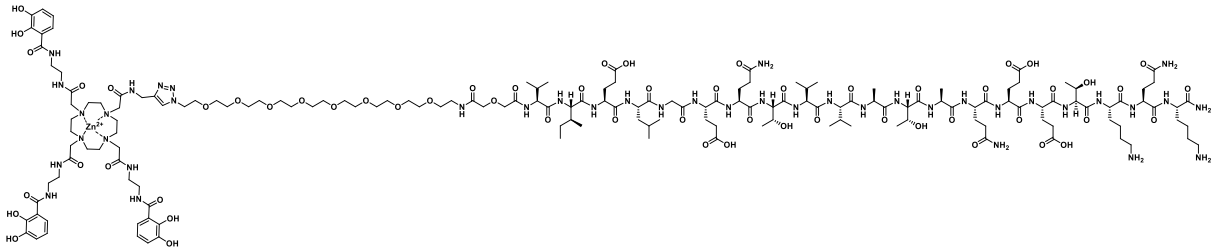


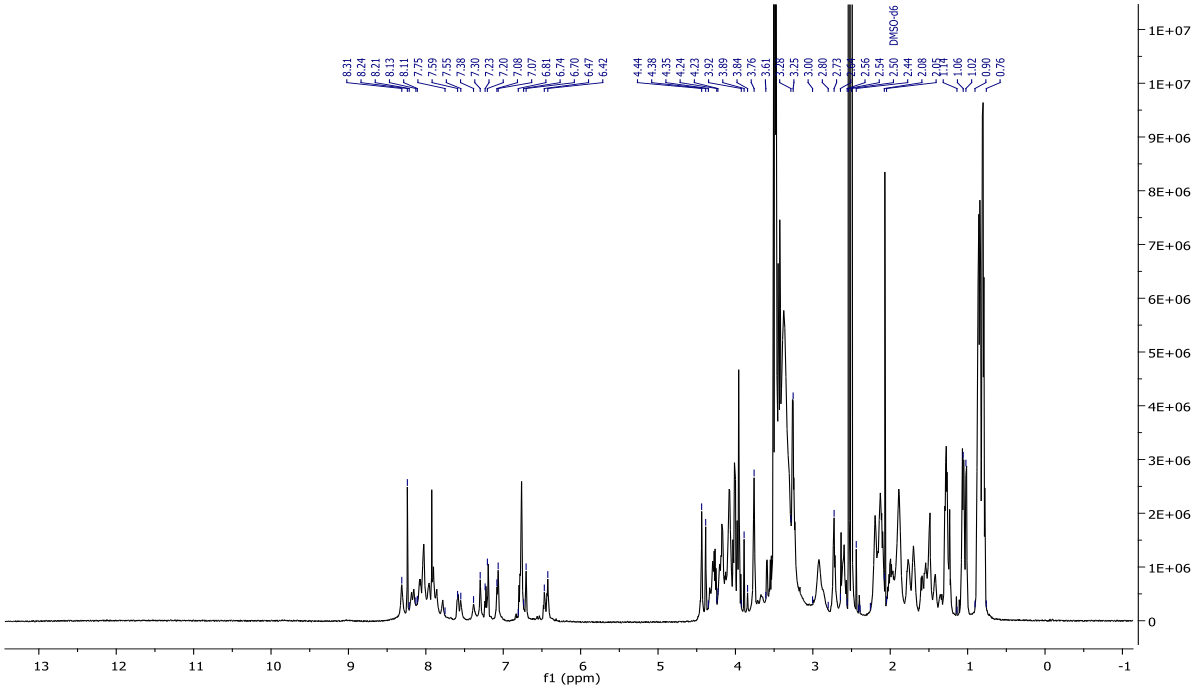


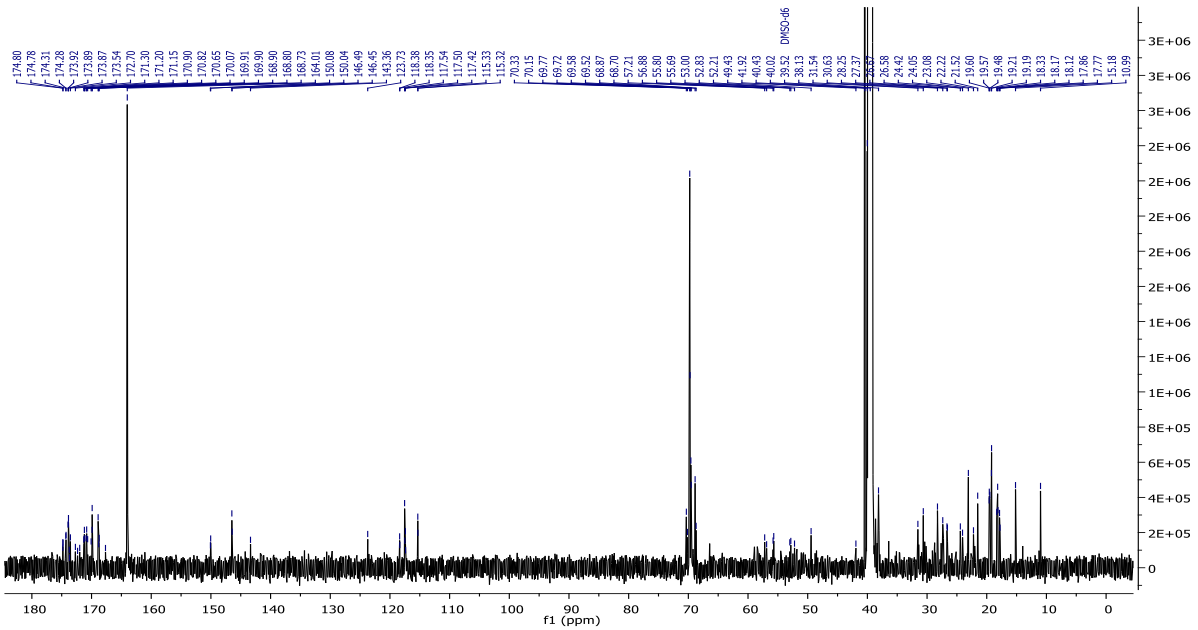


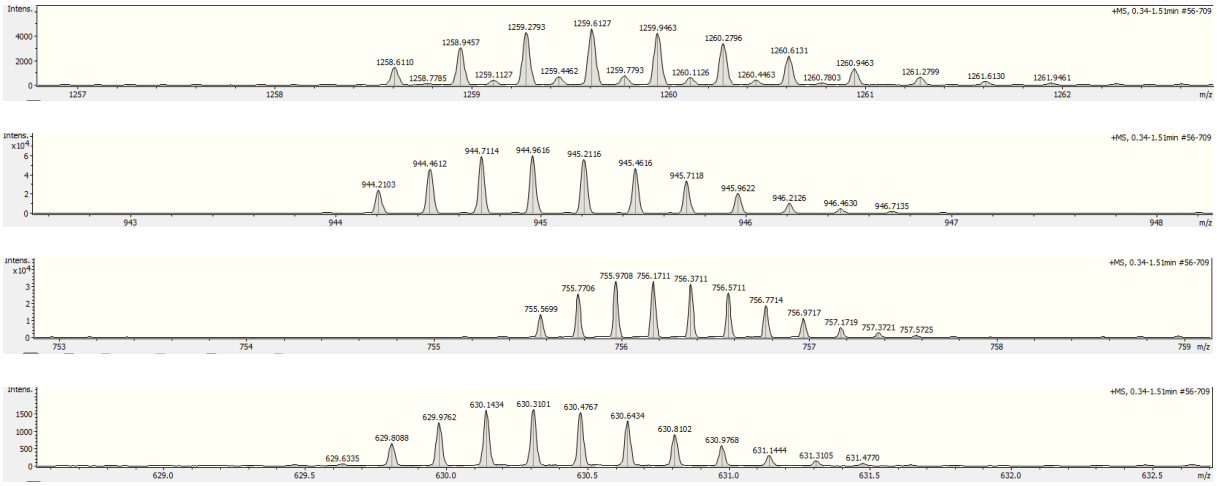


Compound 12 (*PfeA* 33-51 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)







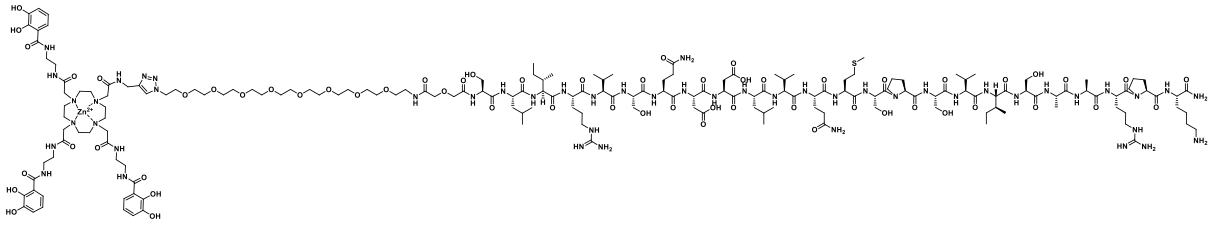

+MS, 0.34-1.51min #56-709
Intens.
4000
2000
0
1258.6110
1258.9457
1258.7785
1259.1127
1259.2793
1259.4462
1259.6127
1259.7793
1259.9463
1260.1126
1260.2796
1260.4463
1260.6131
1260.7803
1260.9463
1261.2799
1261.6130
1261.9461
1257
1258
1259
1260
1261
1262
m/z

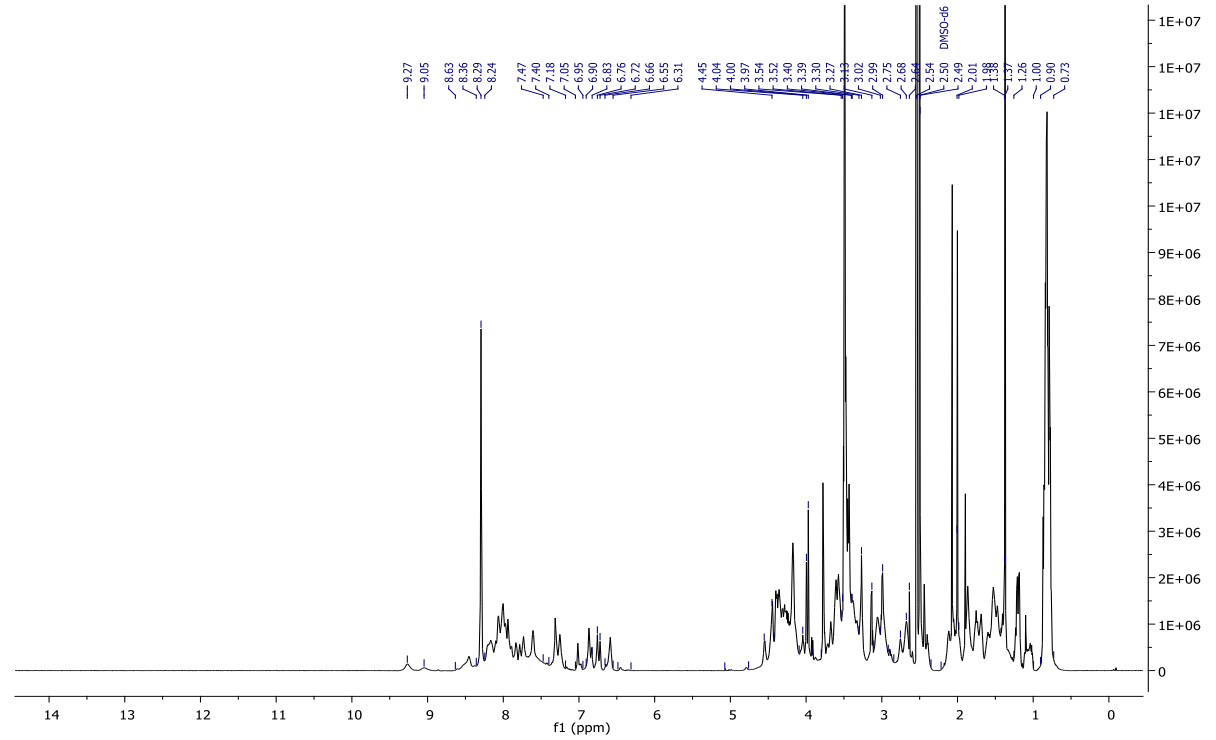
+MS, 0.34-1.51min #56-709
Intens.
x10^4
6
4
2
0
944.2103
944.4612
944.7114
944.9616
945.2116
945.4616
945.7118
945.9622
946.2126
946.4630
946.7135
943
944
945
946
947
948
m/z

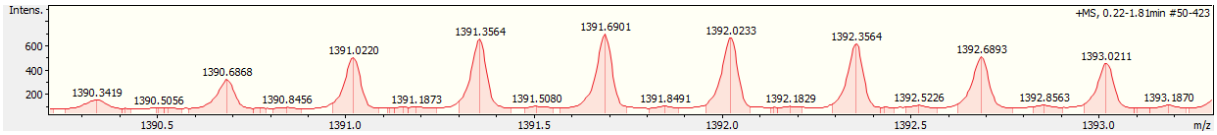
+MS, 0.34-1.51min #56-709
Intens.
x10^4
3
2
1
0
755.5699
755.7706
755.9708
756.1711
756.3711
756.5711
756.7714
756.9717
757.1719
757.3721
757.5725
753
754
755
756
757
758
759
m/z

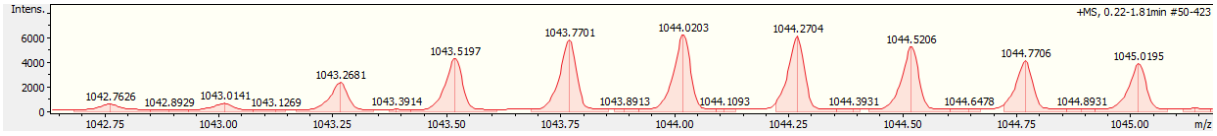
+MS, 0.34-1.51min #56-709
Intens.
1500
1000
500
0
629.6335
629.8088
629.9762
630.1434
630.3101
630.4767
630.6434
630.8102
630.9768
631.1444
631.3105
631.4770
629.0
629.5
630.0
630.5
631.0
631.5
632.0
632.5
m/z

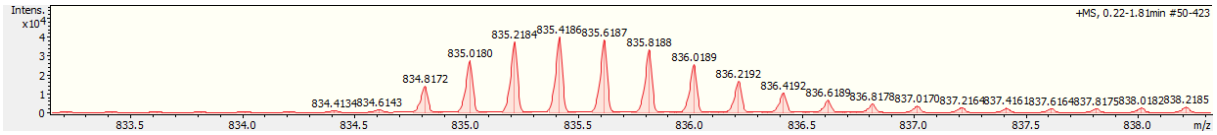
Compound 13 (*HasR* 122-144 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)

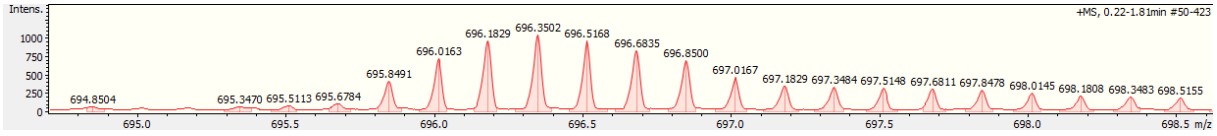




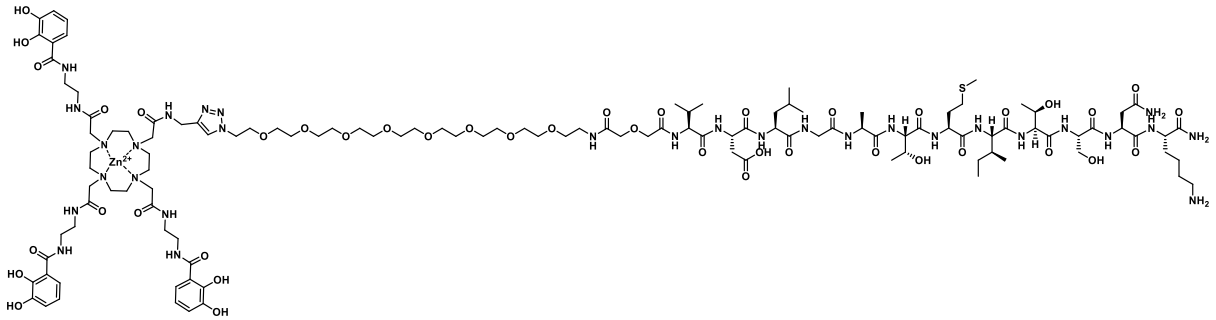


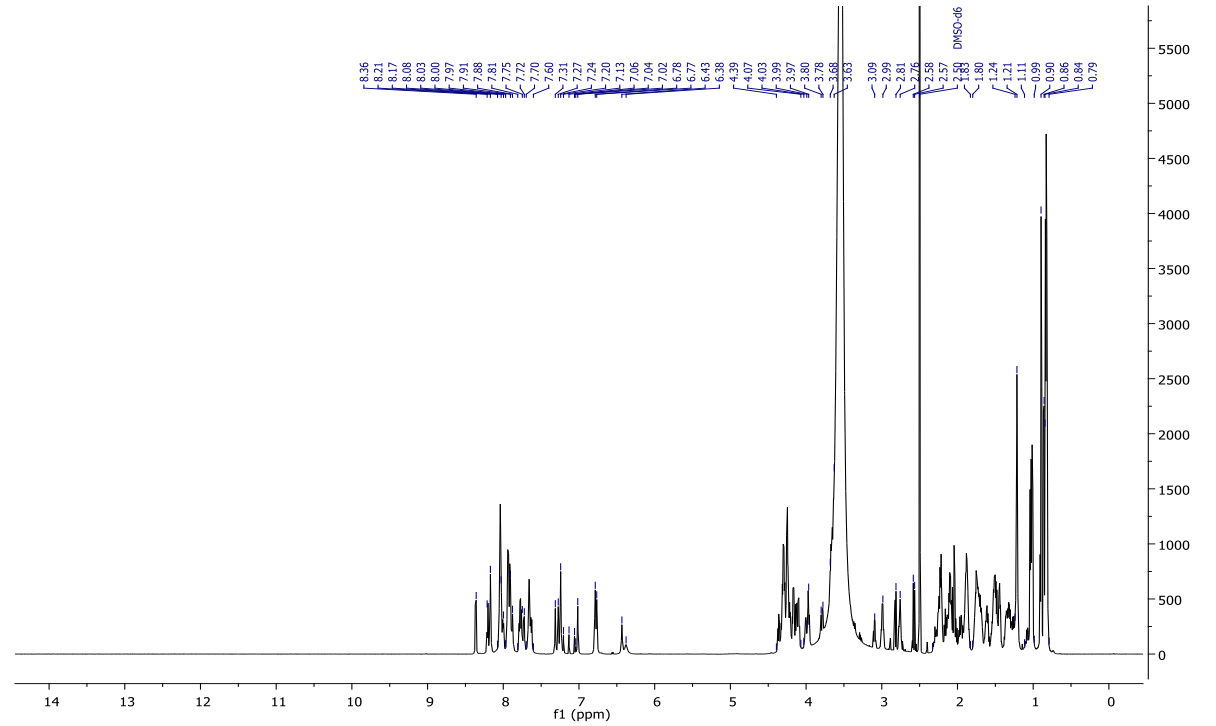


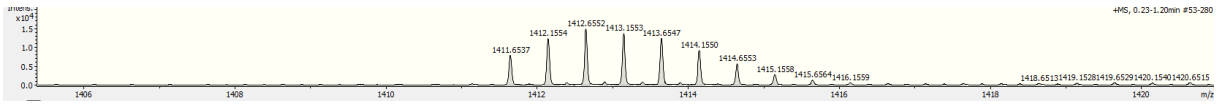


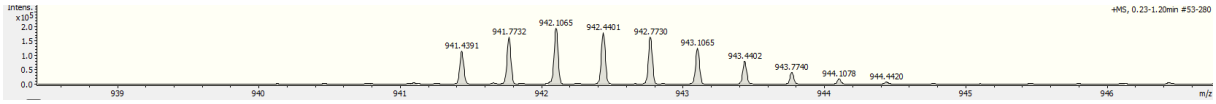


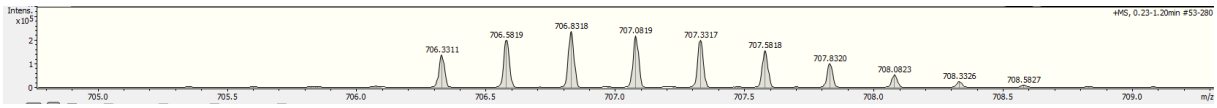
Compound 17 (*FpvA* 124-134 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)

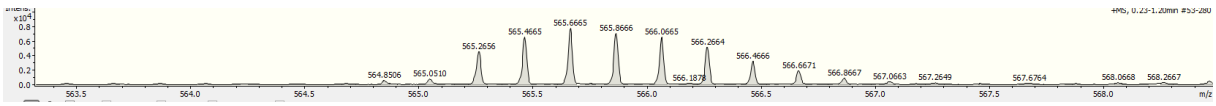




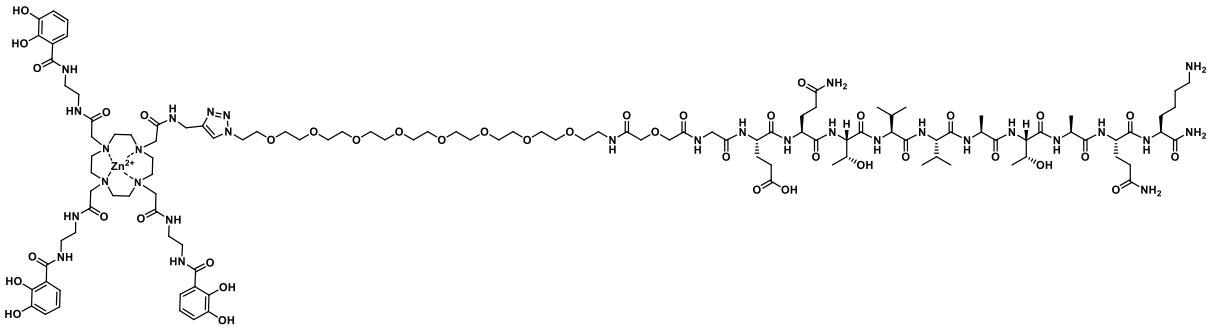


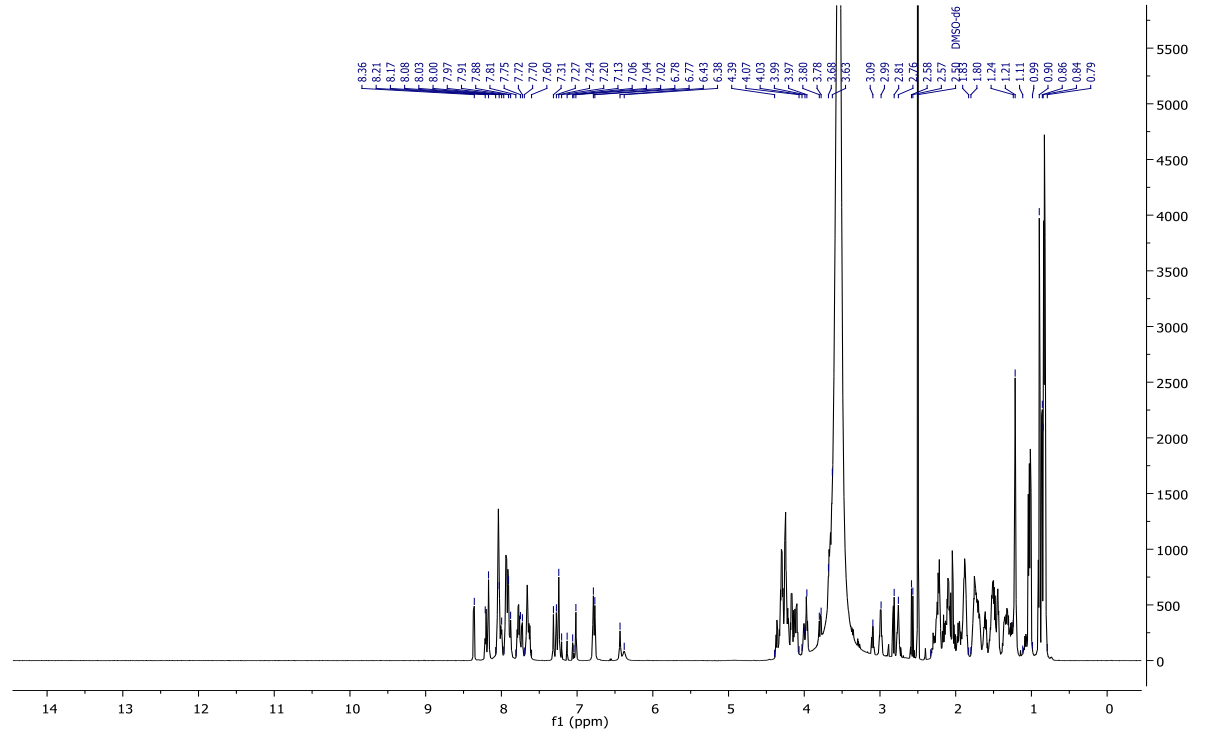


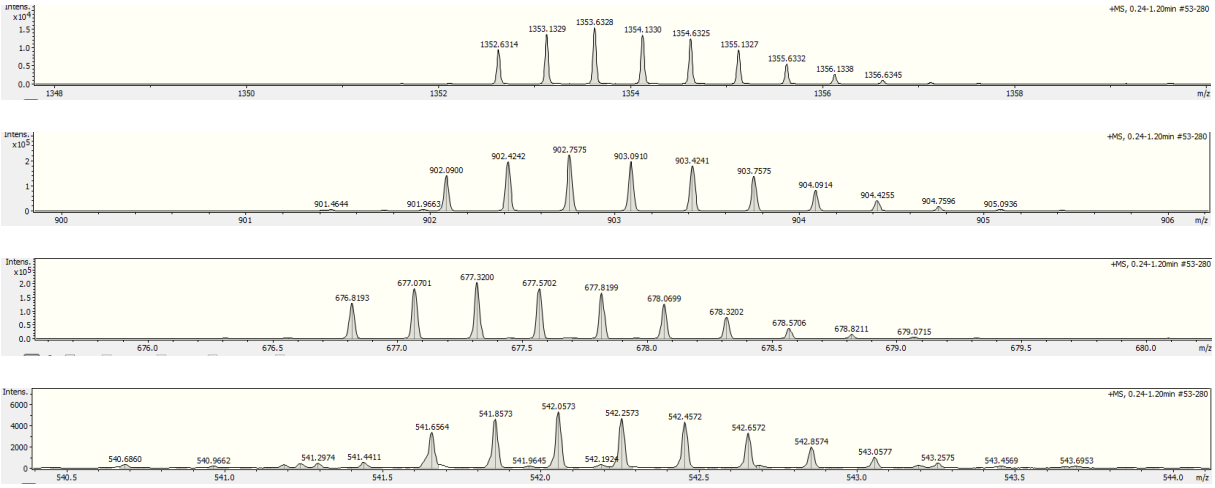




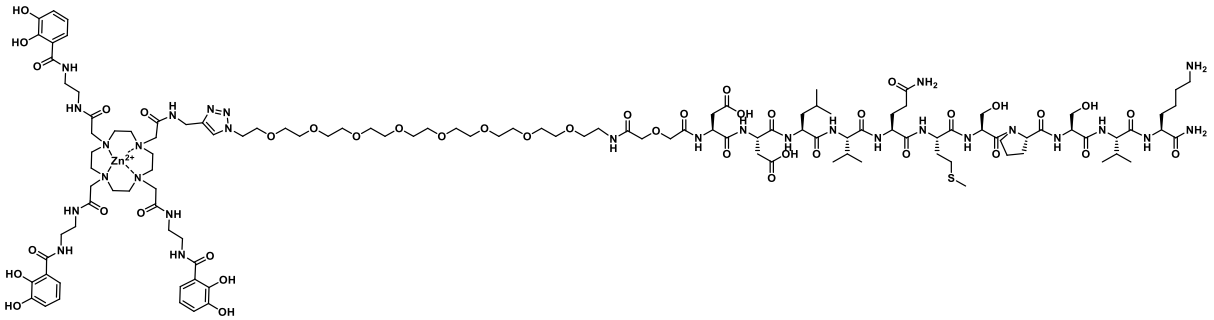
Compound 18 (*PfeA* 37-46 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)

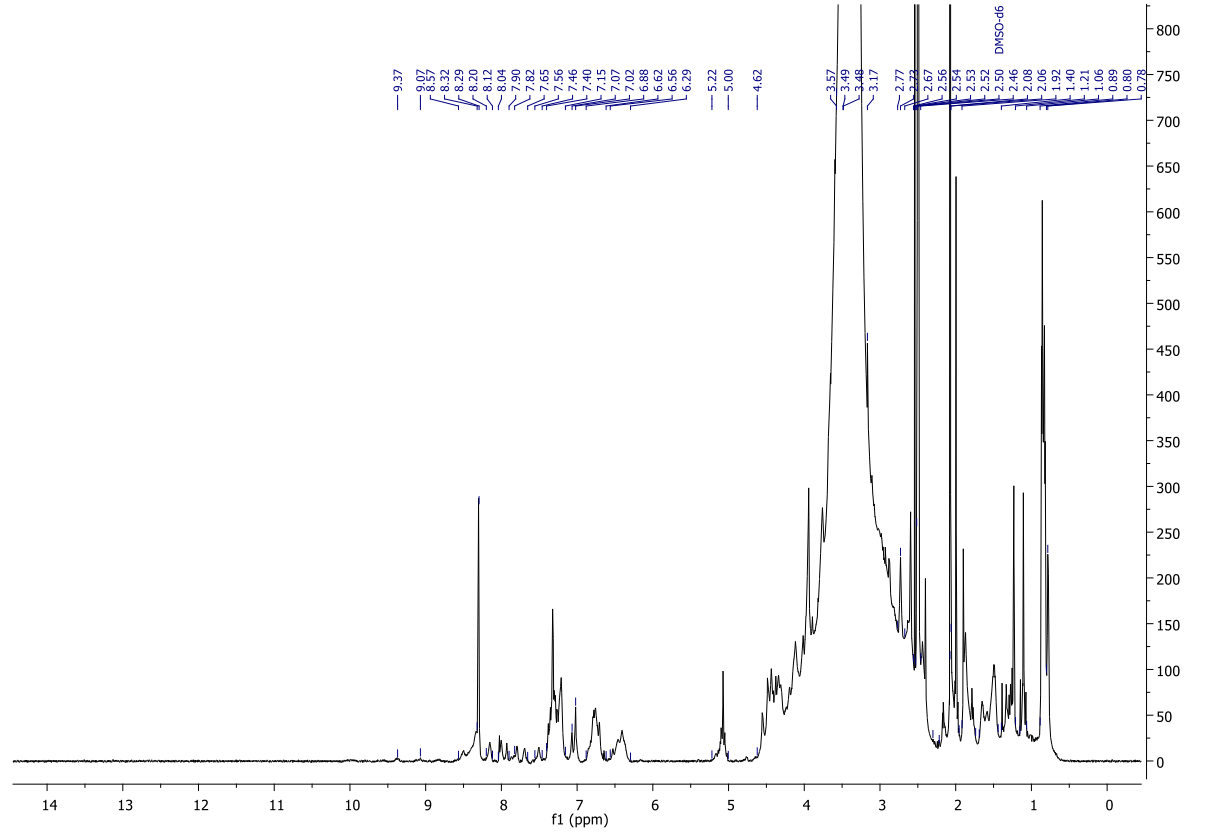


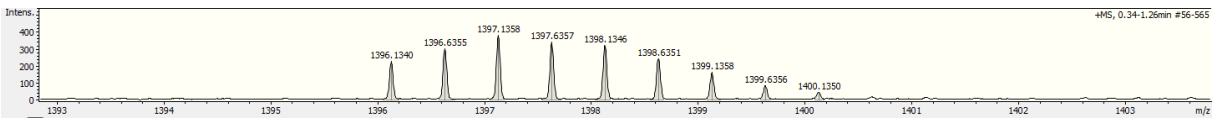


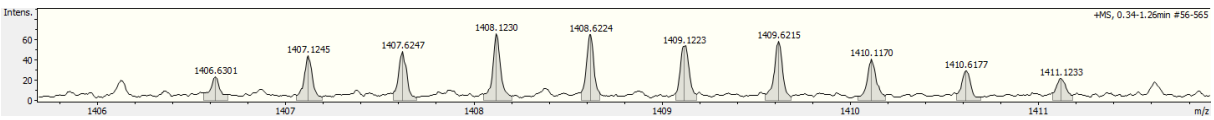


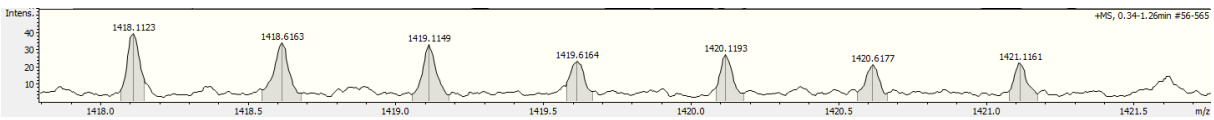
Compound 19 (*HasR* 129-138 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM)

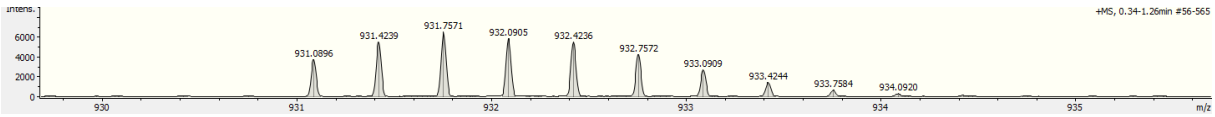




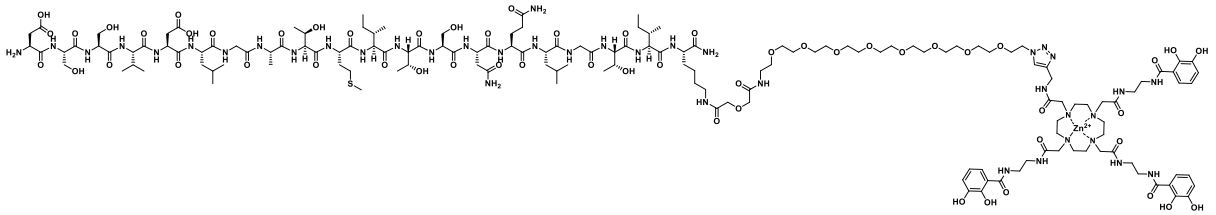


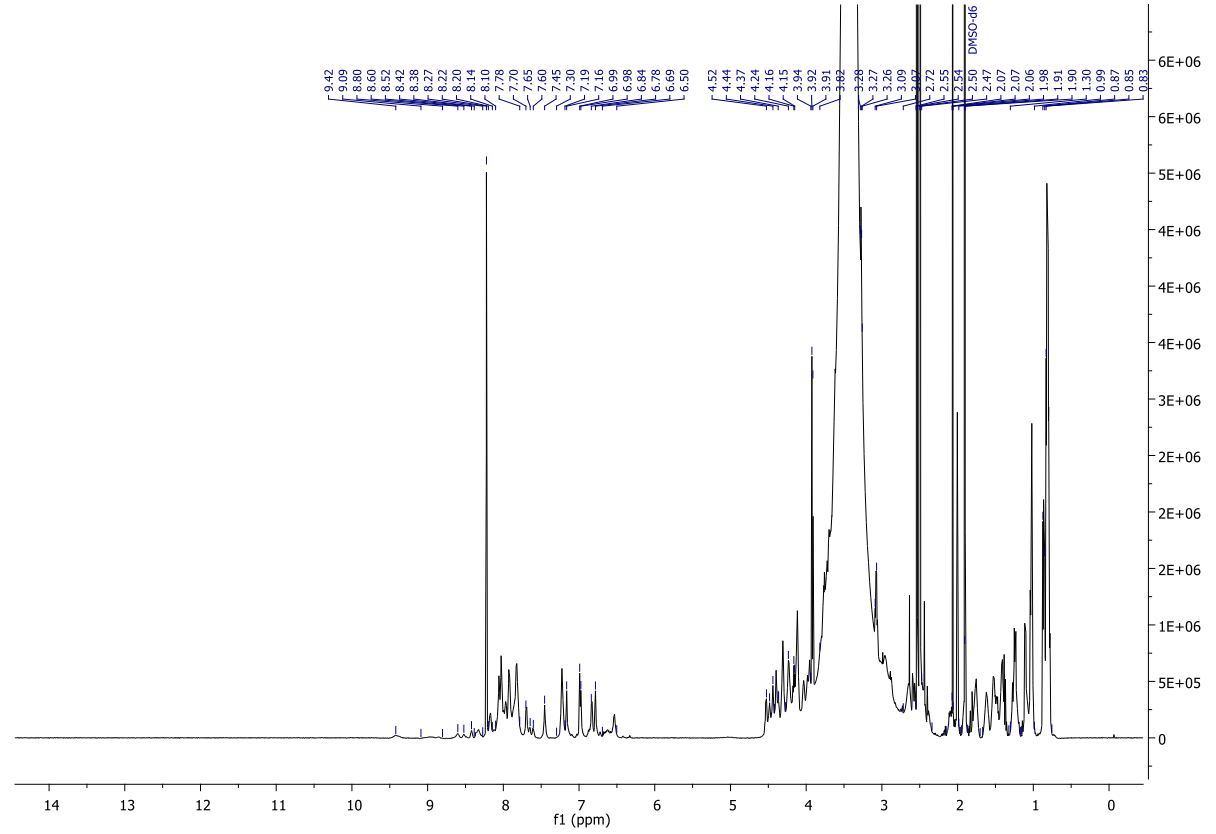


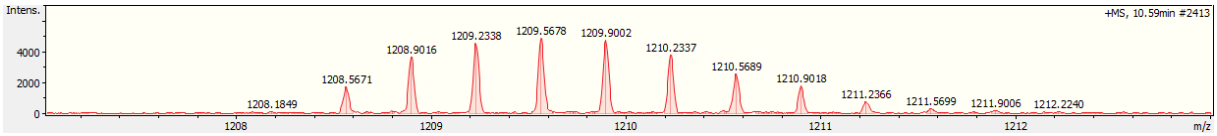


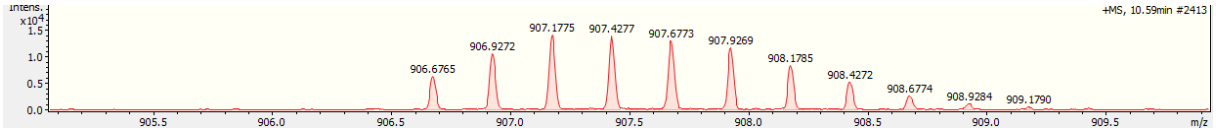


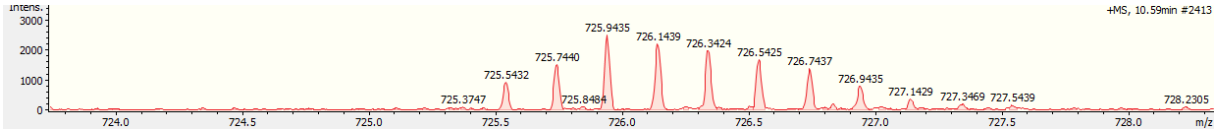
Compound 14 (*FpvA* 121-139 *C*-term $(PEG)_7$-Zn^{2+}-DOTAM)



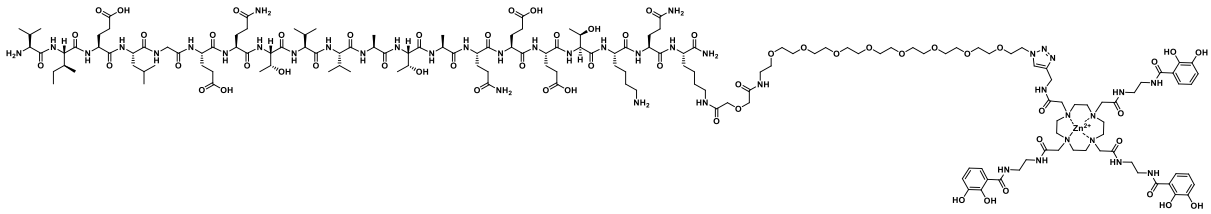


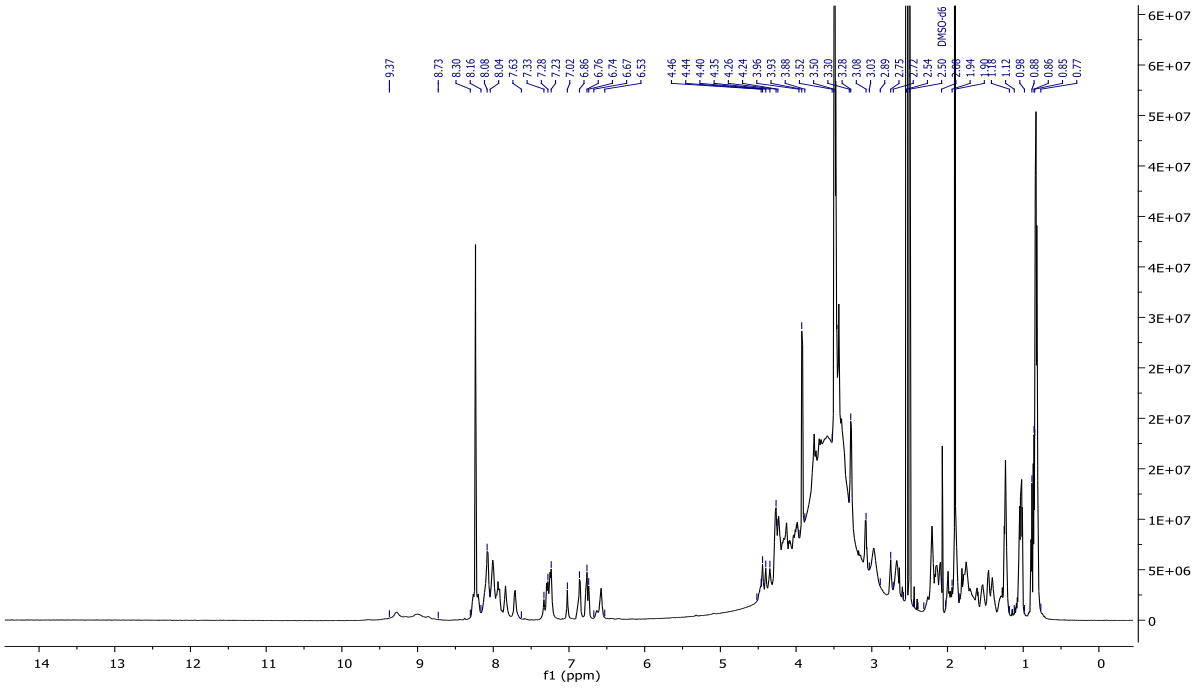


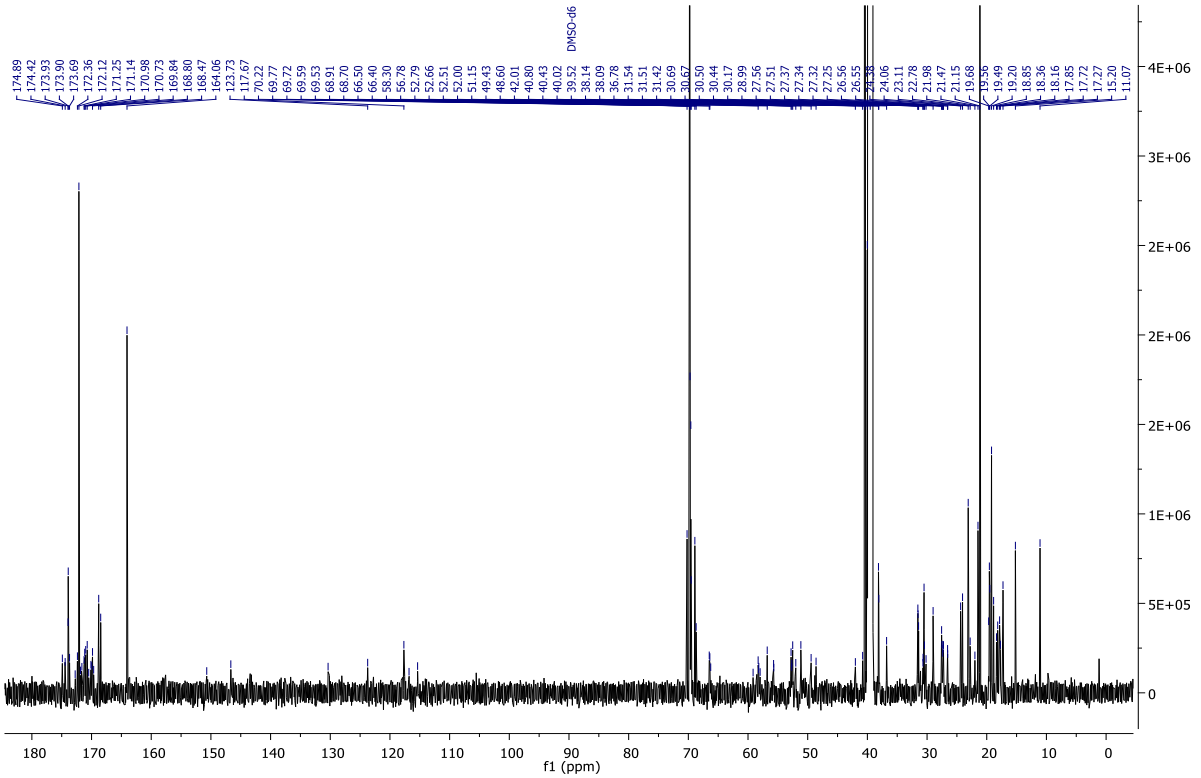


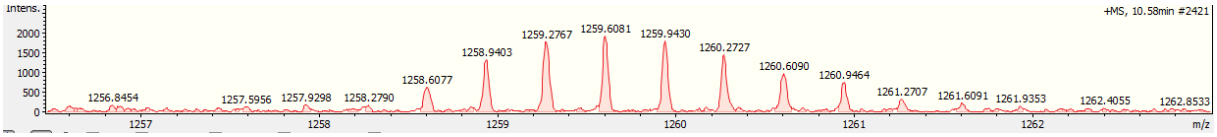


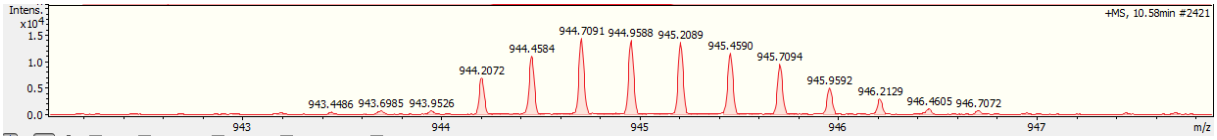
Compound 15 (*PfeA* 33-51 *C*-term $(PEG)_7$-Zn^{2+}-DOTAM)

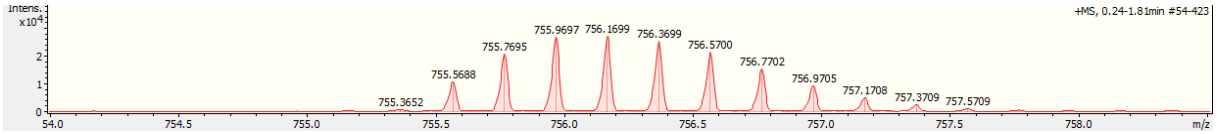


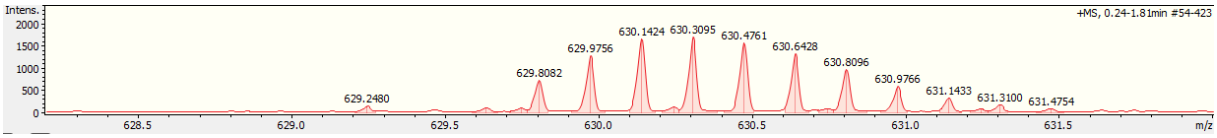




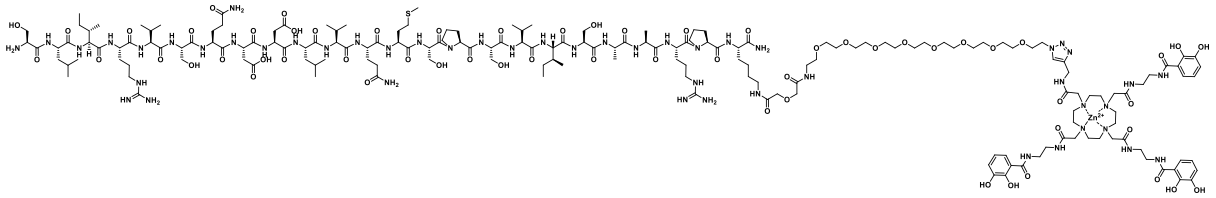

Intens.
+MS, 10.58min #2421
1256.8454
1257.5956
1257.9298
1258.2790
1258.6077
1258.9403
1259.2767
1259.6081
1259.9430
1260.2727
1260.6090
1260.9464
1261.2707
1261.6091
1261.9353
1262.4055
1262.8533
m/z

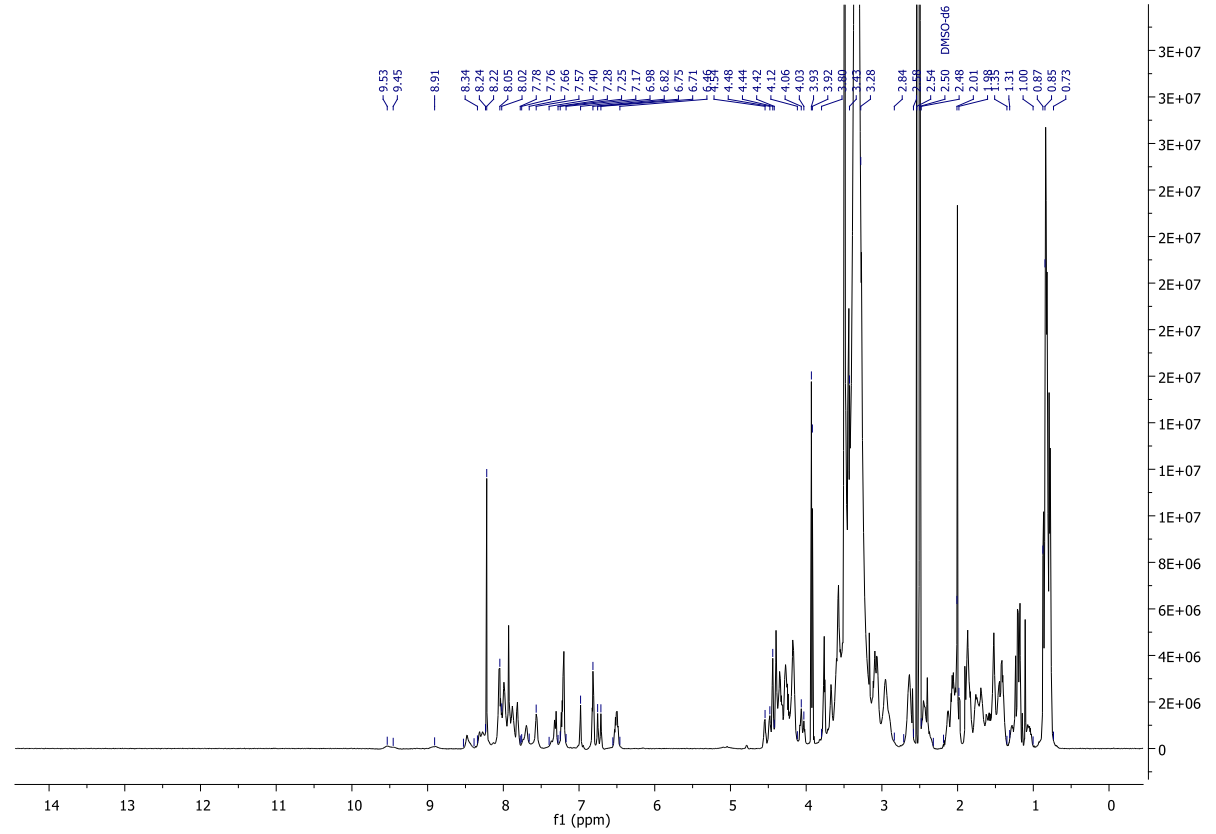

Intens.
+MS, 10.58min #2421
943.4486
943.6985
943.9526
944.2072
944.4584
944.7091
944.9588
945.2089
945.4590
945.7094
945.9592
946.2129
946.4605
946.7072
m/z

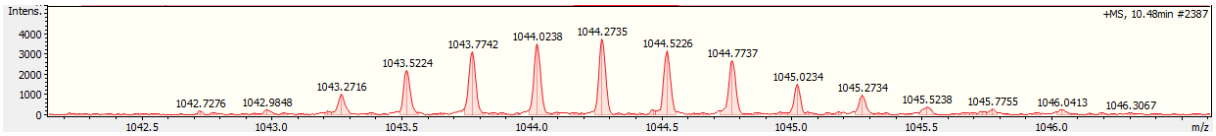

Intens.
+MS, 0.24-1.81min #54-423
755.3652
755.5688
755.7695
755.9697
756.1699
756.3699
756.5700
756.7702
756.9705
757.1708
757.3709
757.5709
m/z

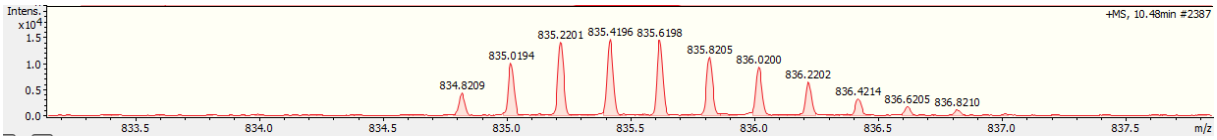

Intens.
+MS, 0.24-1.81min #54-423
629.2480
629.8082
629.9756
630.1424
630.3095
630.4761
630.6428
630.8096
630.9766
631.1433
631.3100
631.4754
m/z

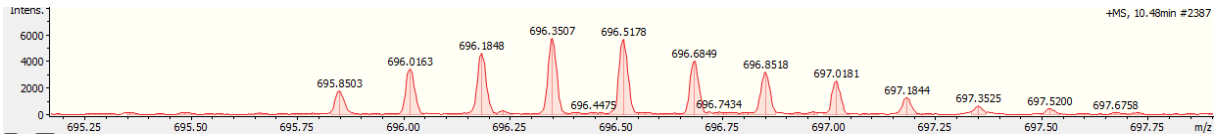
Compound 16 (*HasR* 122-144 *C*-term $(PEG)_7$-Zn^{2+}-DOTAM)



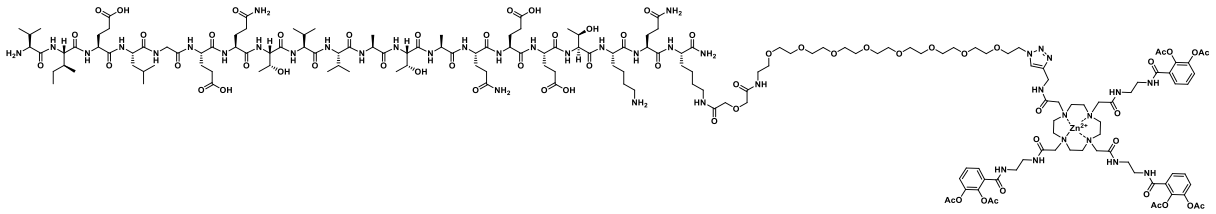


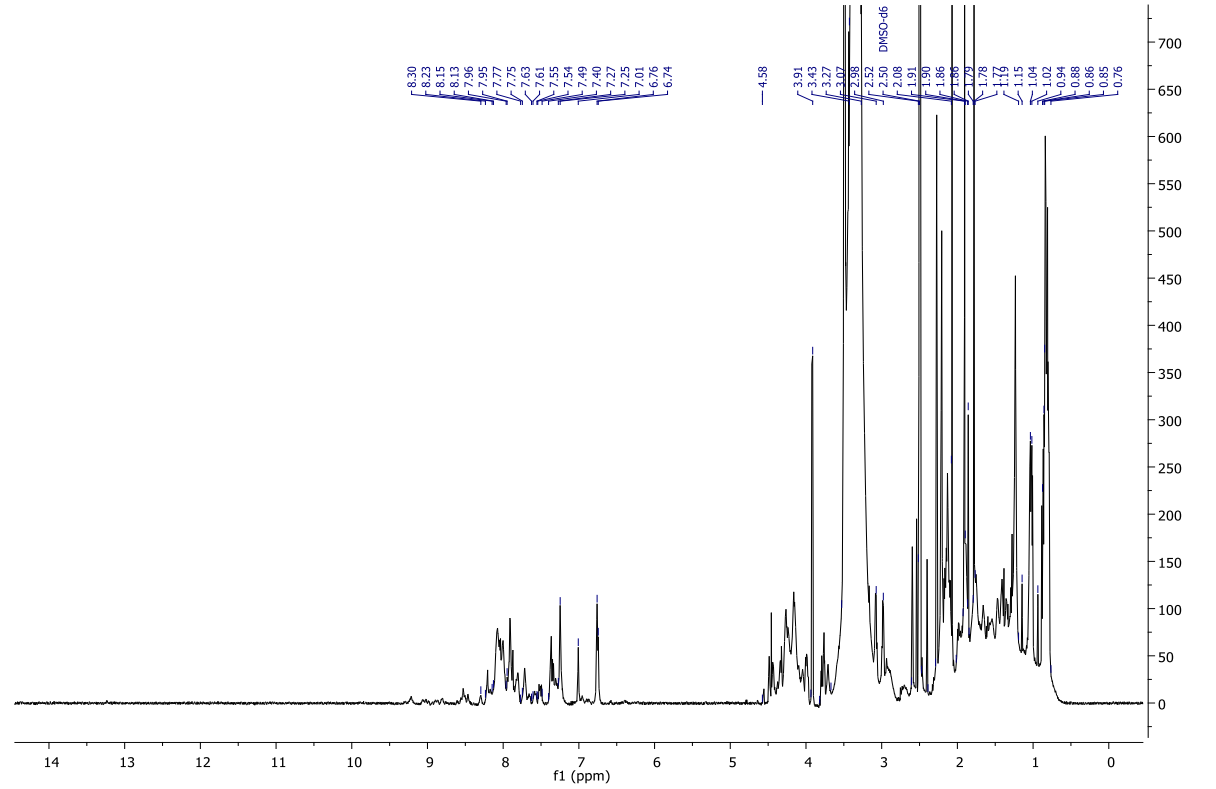


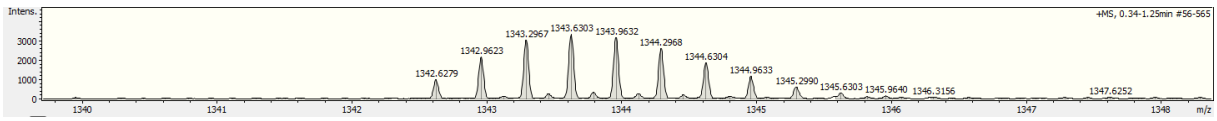


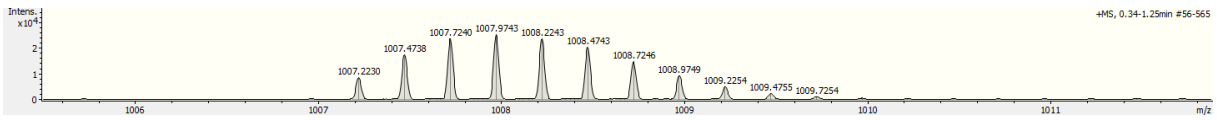


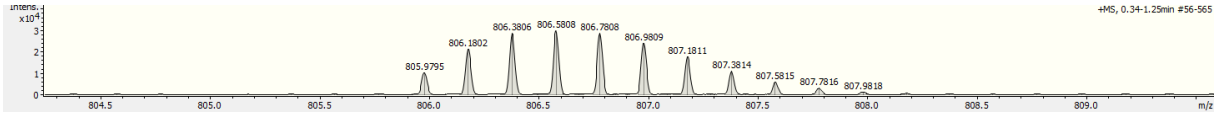
Compound 20 (*PfeA* 33-51 *C*-term $(PEG)_7$-Zn^{2+}-DOTAM)

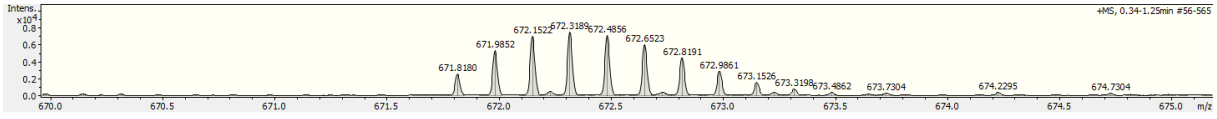


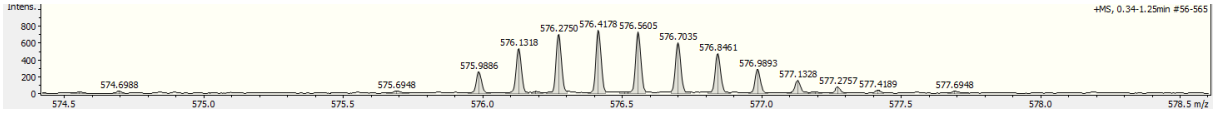




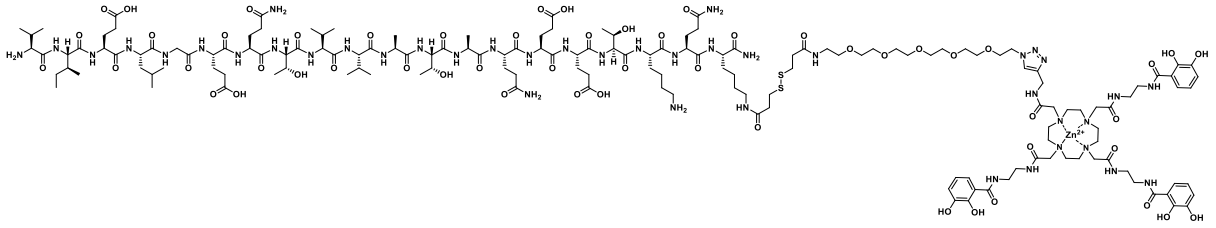


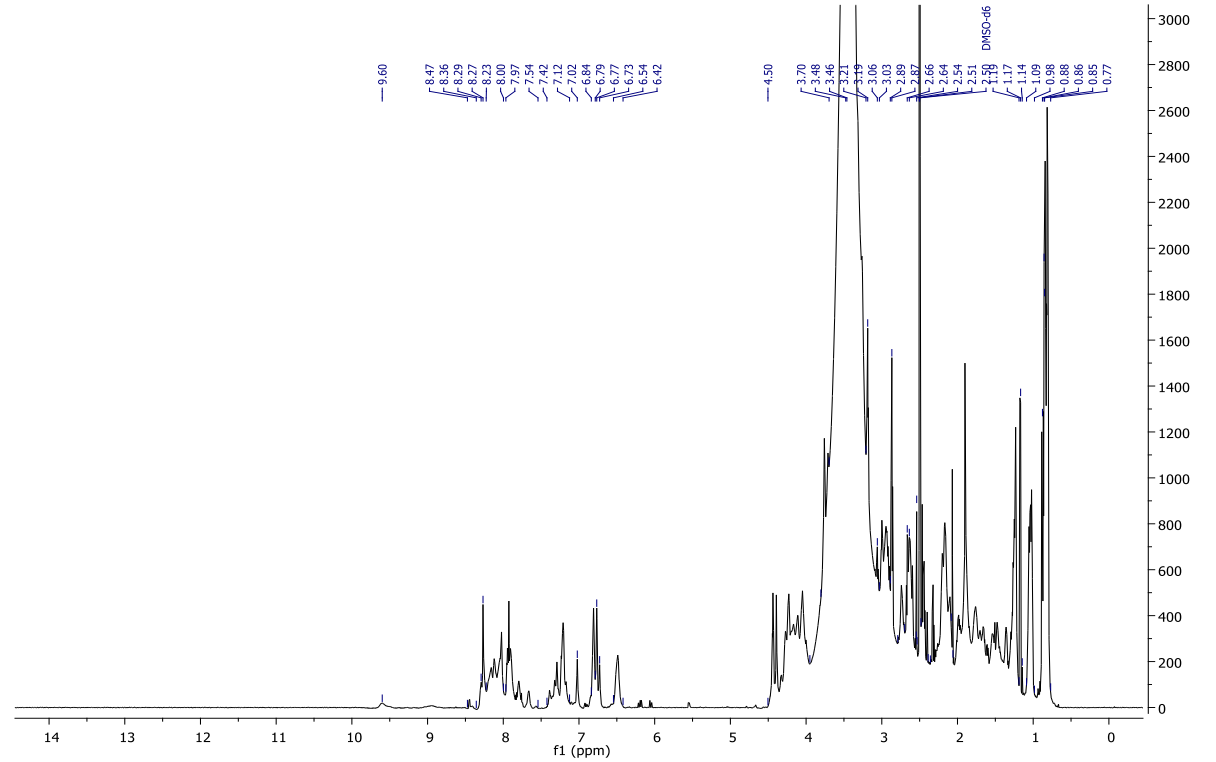


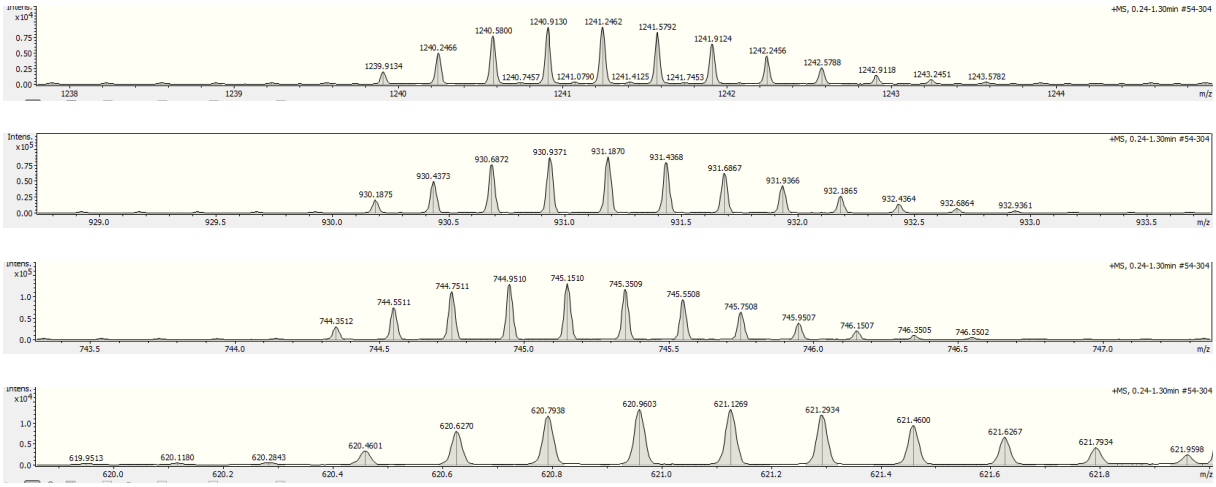




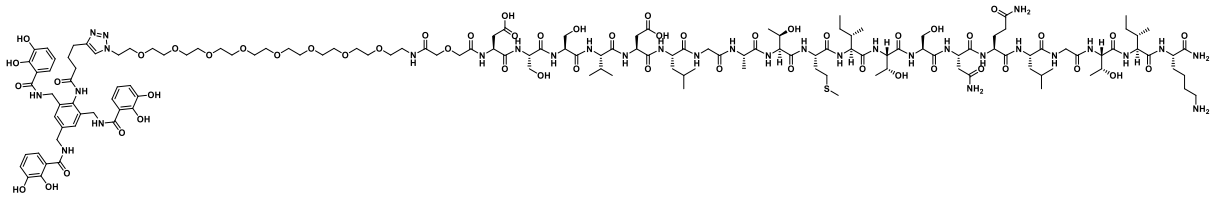
Compound 21 (*PfeA* 33-51 *C*-term disulfide-$(PEG)_5$-Zn^{2+}-DOTAM)

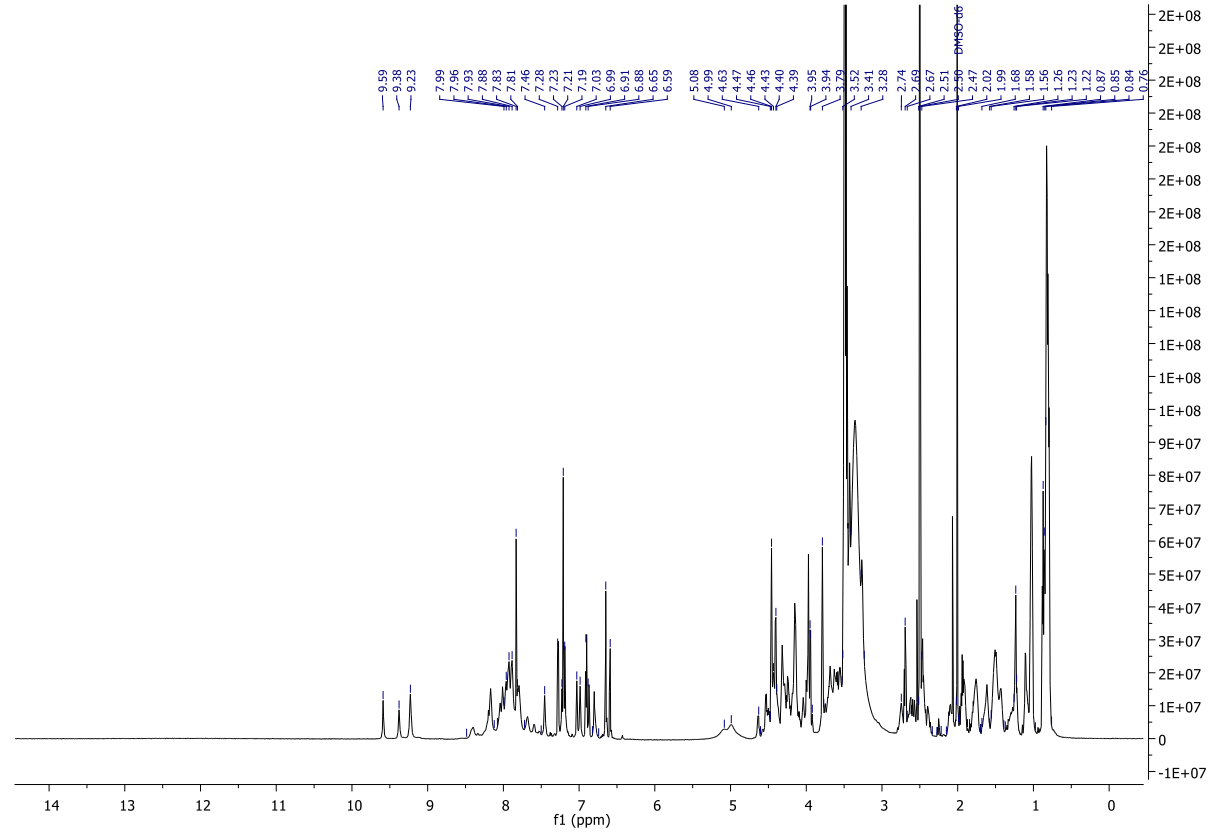


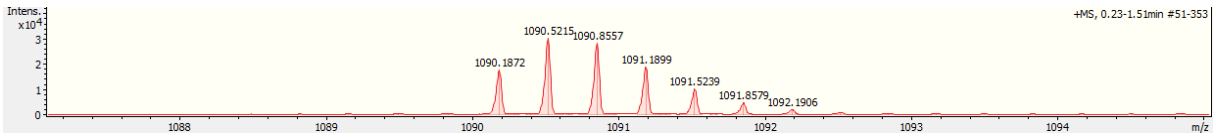


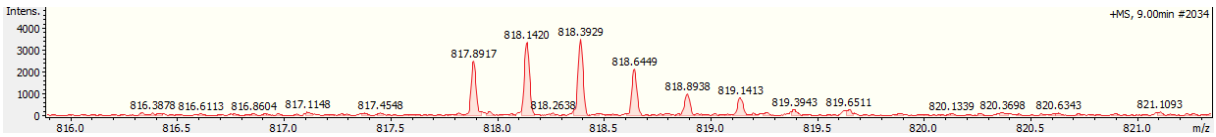


Compound 22 (*FpvA* 121-139 *N*-term-$(PEG)_7$-MECAM)

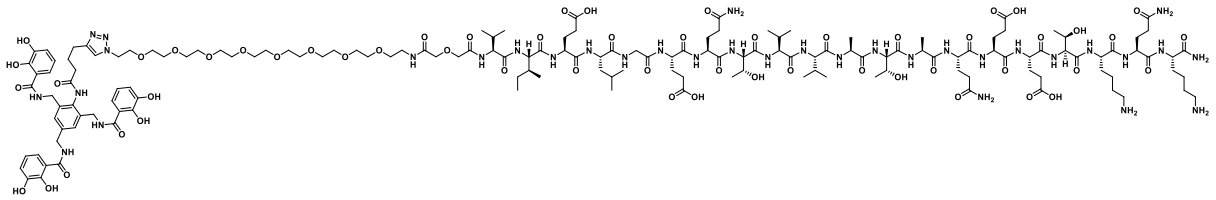


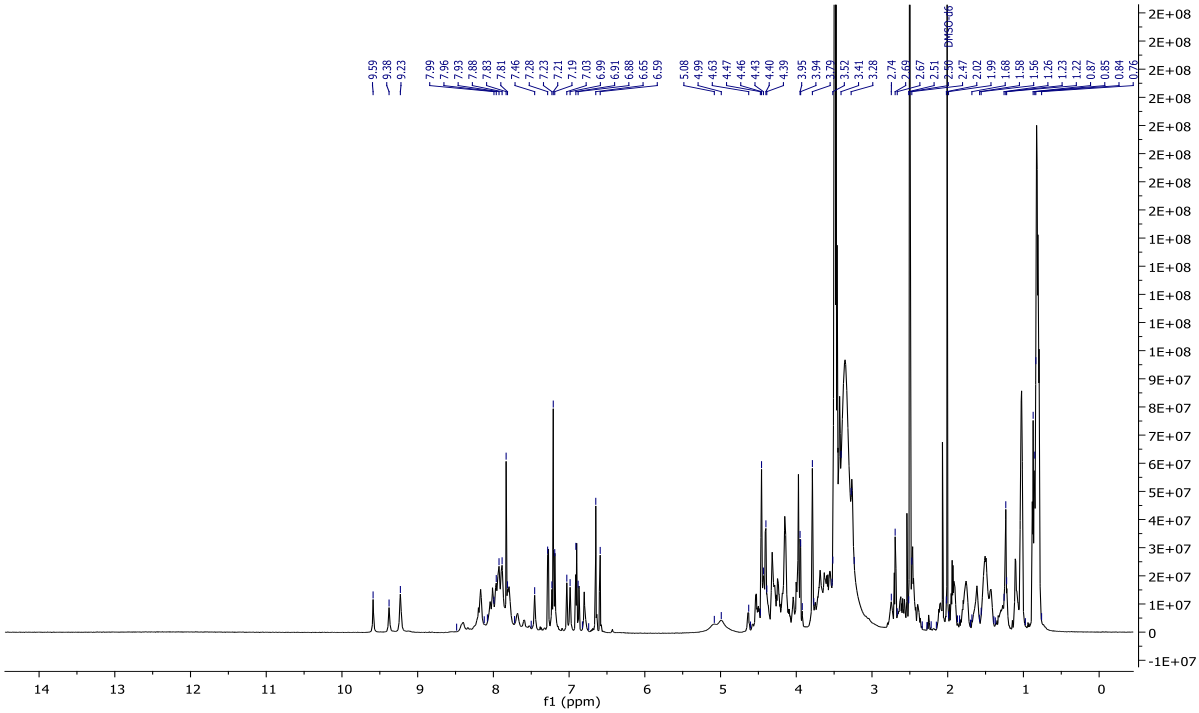


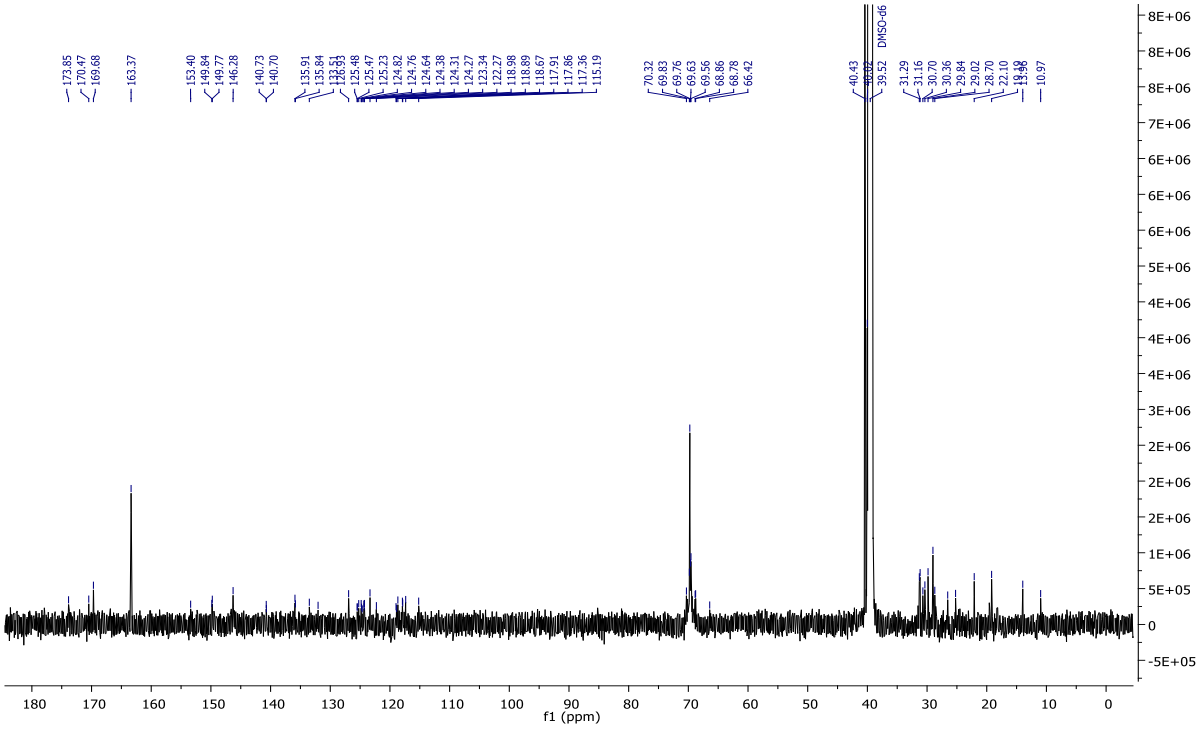


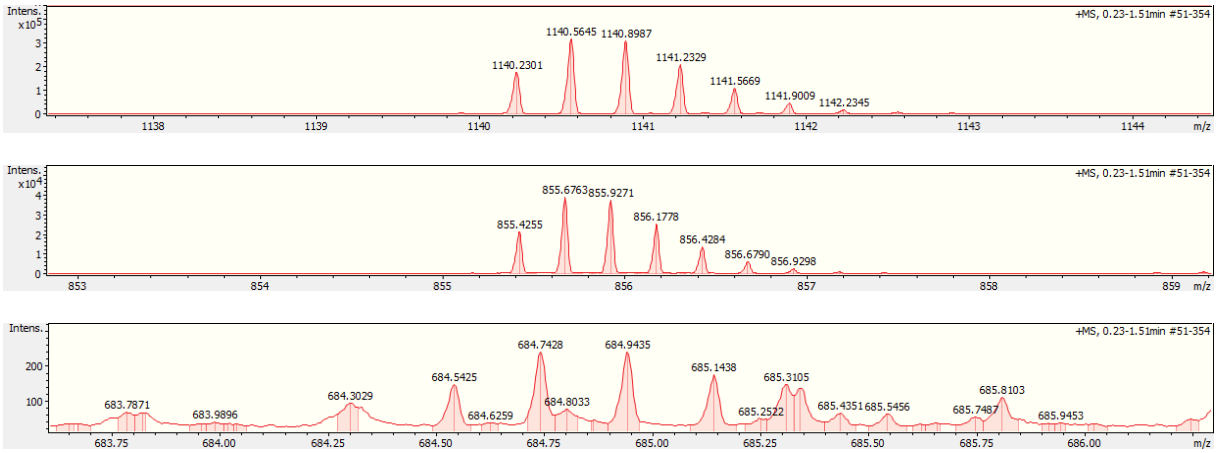


Compound 23 (*PfeA* 33-51 *N*-term $(PEG)_7$-MECAM)





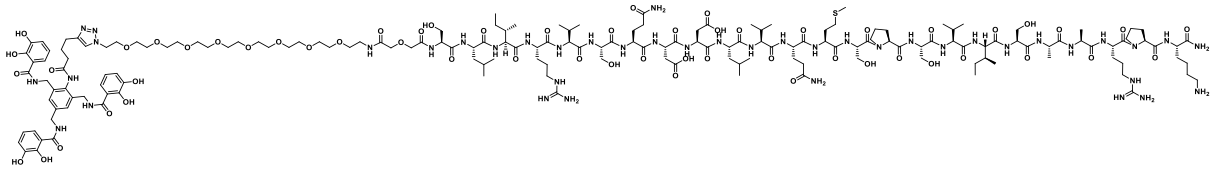


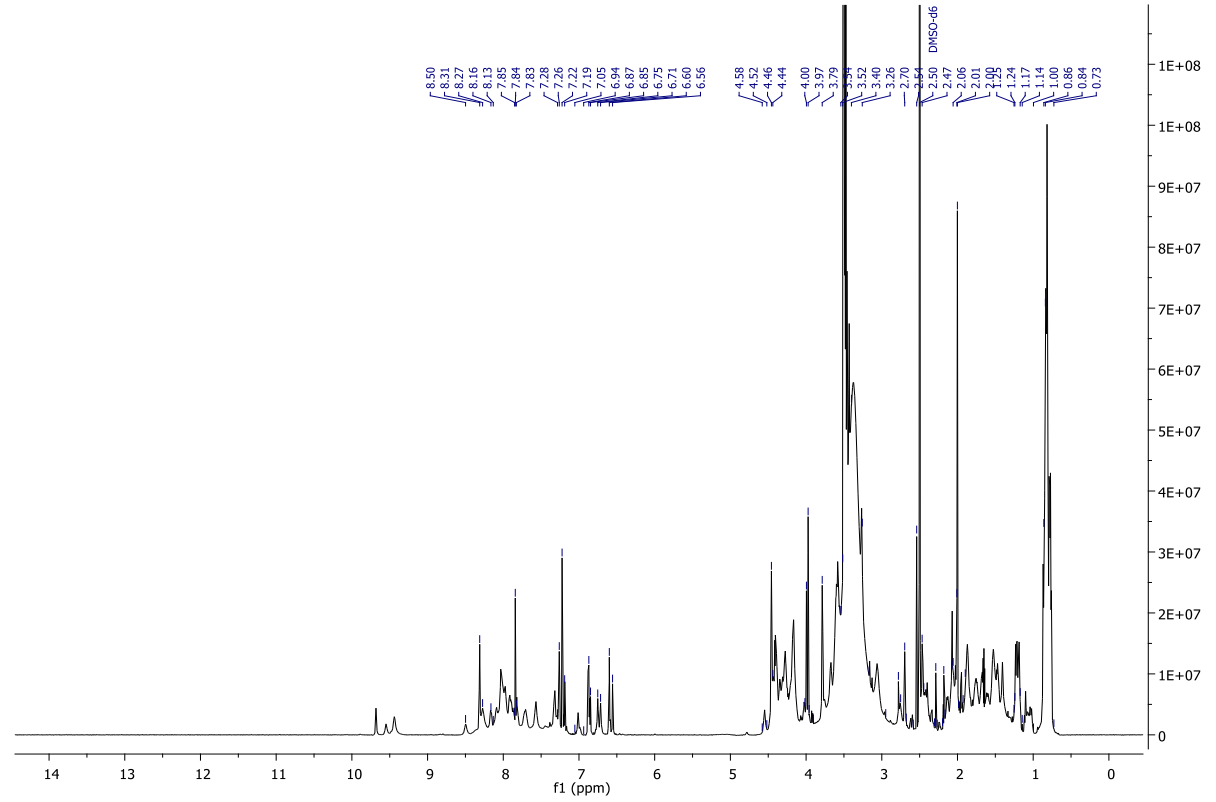

Intens.
x10^5
+MS, 0.23-1.51min #51-354
1140.5645
1140.8987
1140.2301
1141.2329
1141.5669
1141.9009
1142.2345
1138
1139
1140
1141
1142
1143
1144
m/z

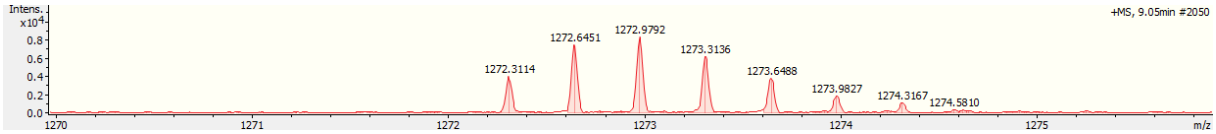
Intens.
x10^4
+MS, 0.23-1.51min #51-354
855.6763
855.9271
855.4255
856.1778
856.4284
856.6790
856.9298
853
854
855
856
857
858
859
m/z

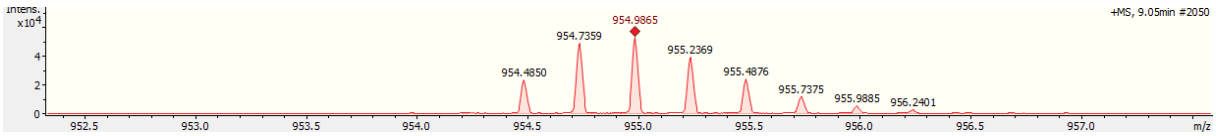
Intens.
+MS, 0.23-1.51min #51-354
684.7428
684.9435
684.5425
685.1438
685.3105
685.8103
683.7871
684.3029
683.9896
684.6259
684.8033
685.2522
685.4351
685.5456
685.7487
685.9453
683.75
684.00
684.25
684.50
684.75
685.00
685.25
685.50
685.75
686.00
m/z

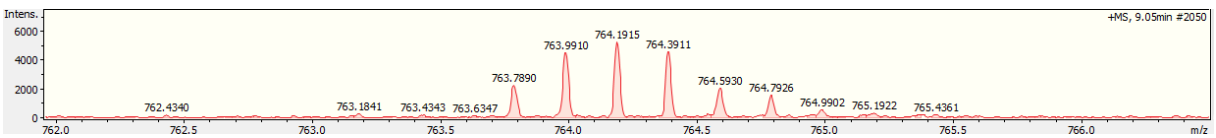
Compound 24 (*HasR* 122-144 *N*-term $(PEG)_7$-MECAM)

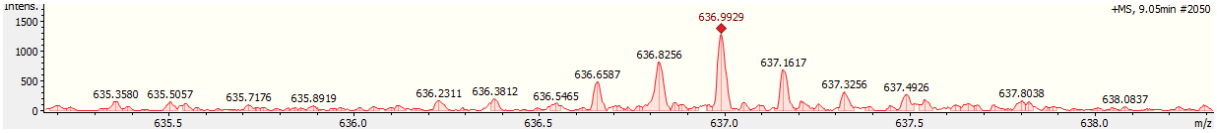




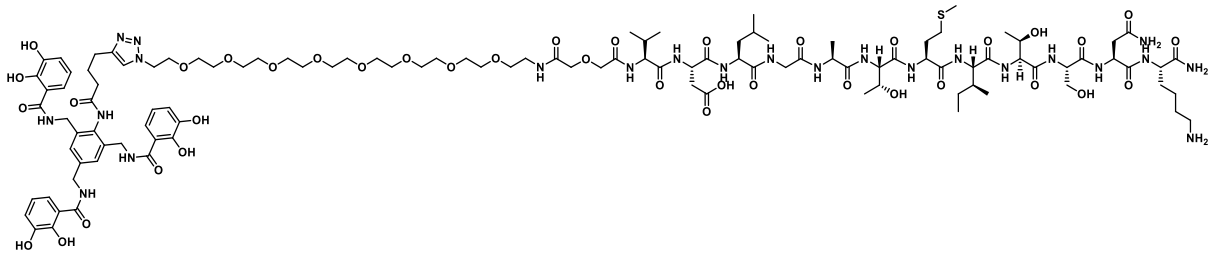


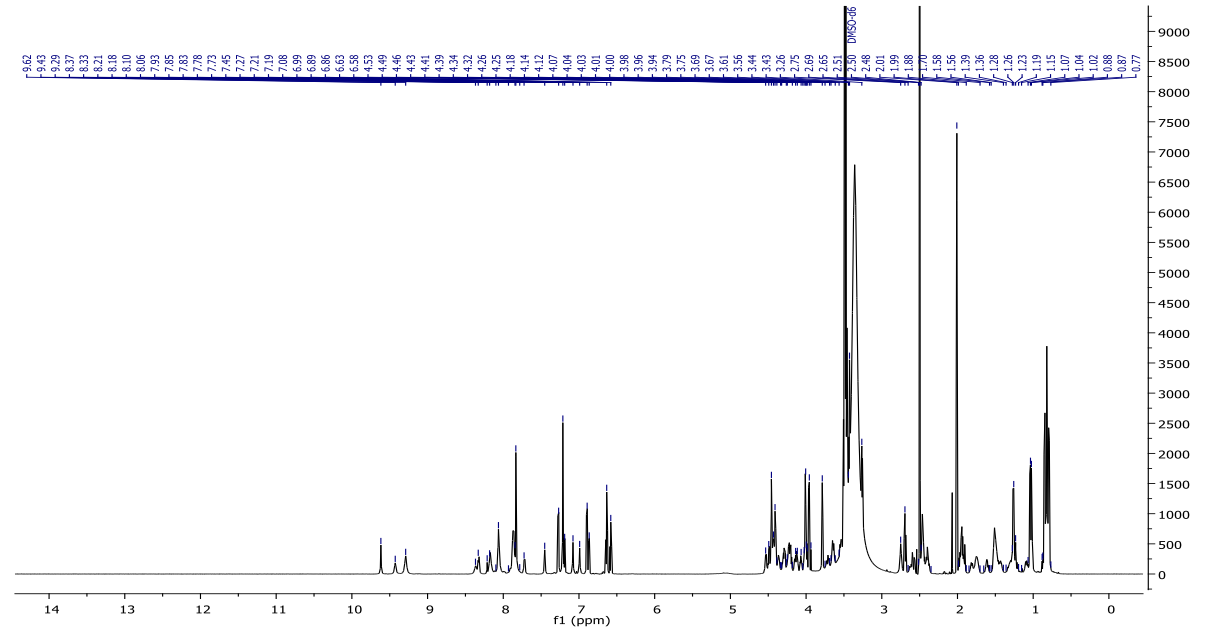


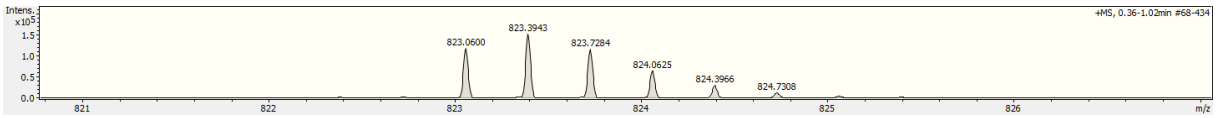


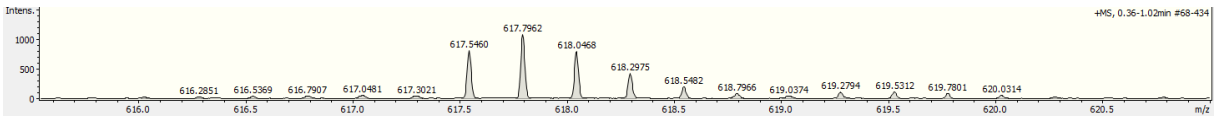


Compound 25 (*FpvA* 124-134 *N*-term $(PEG)_7$-MECAM)

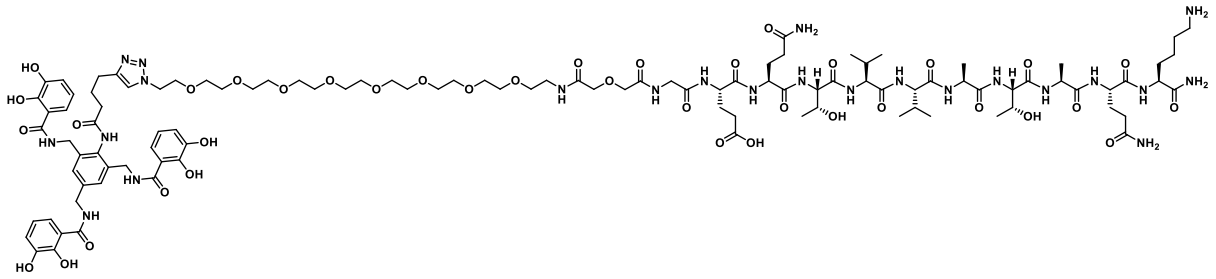


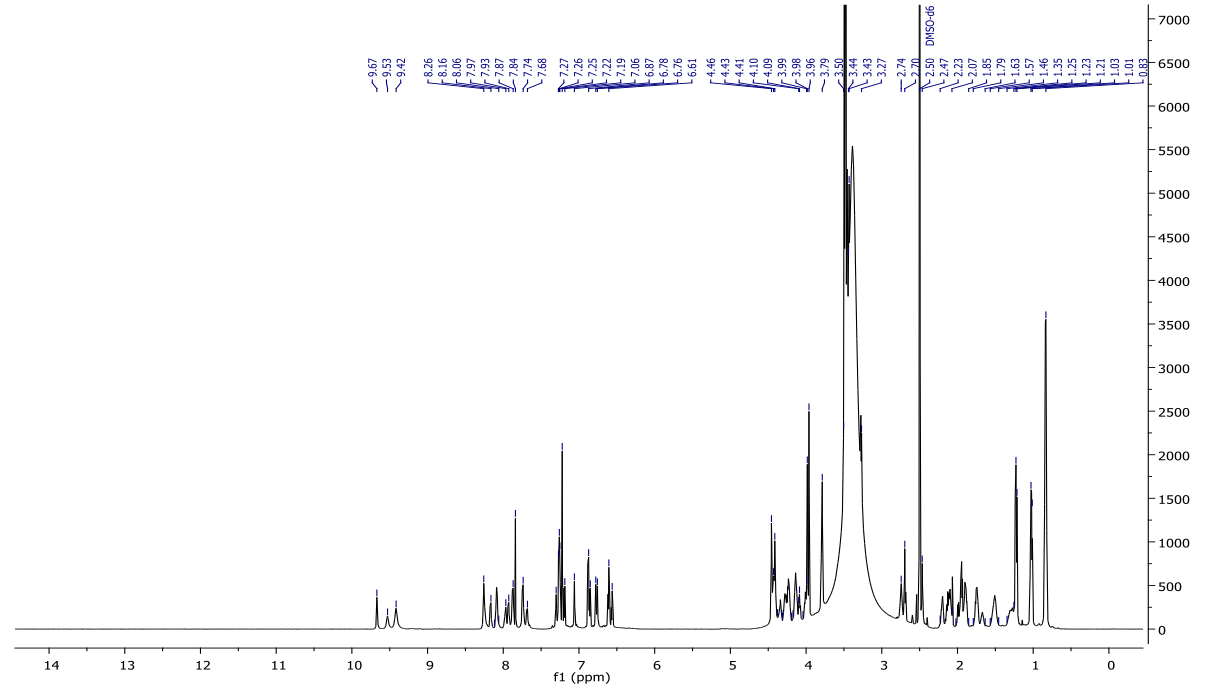


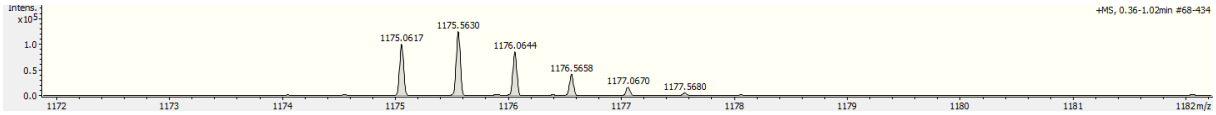


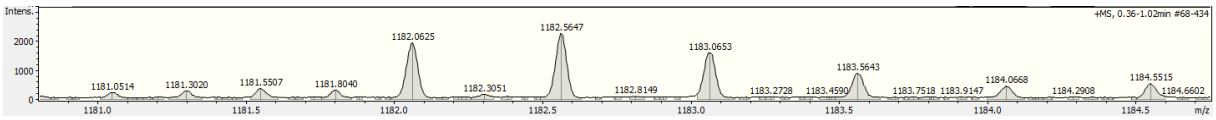


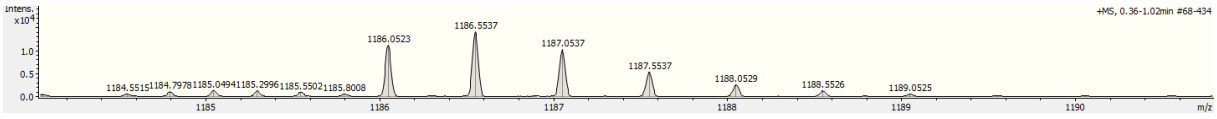
Compound 26 (*PfeA* 37-46 *N*-term $(PEG)_7$-MECAM)

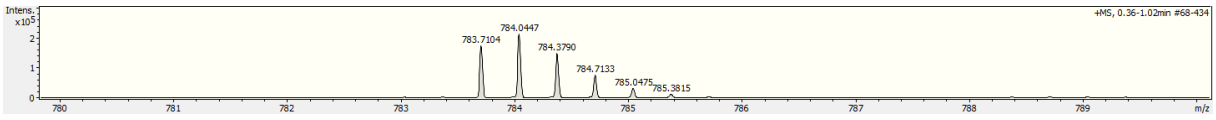




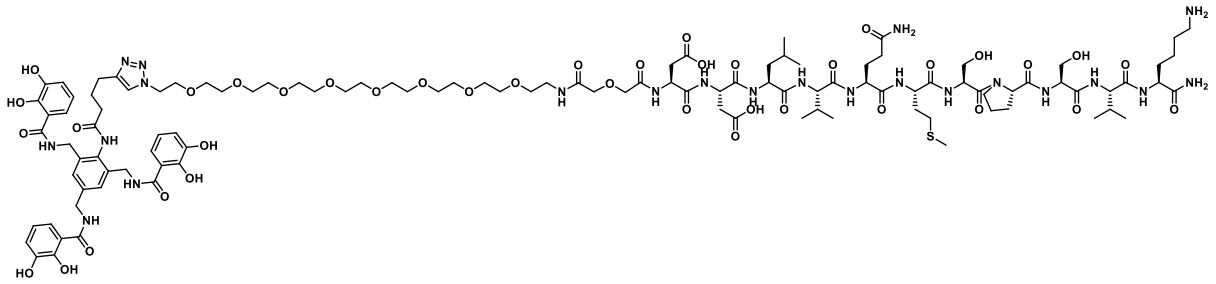


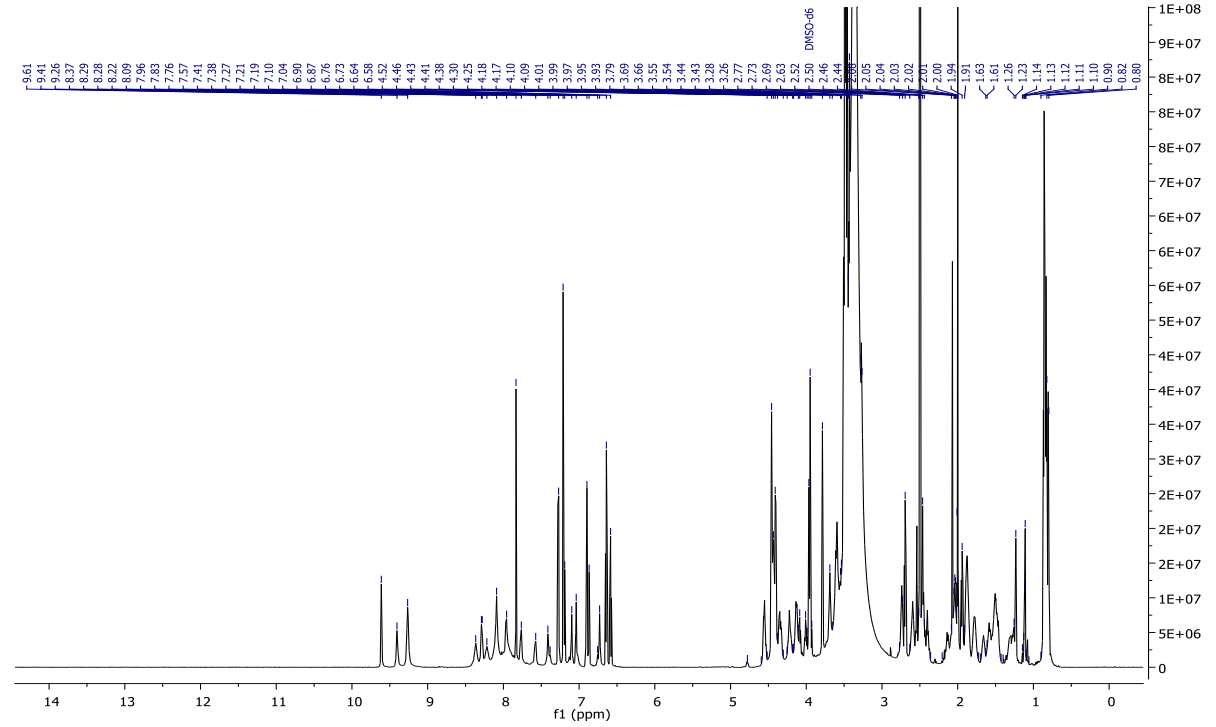


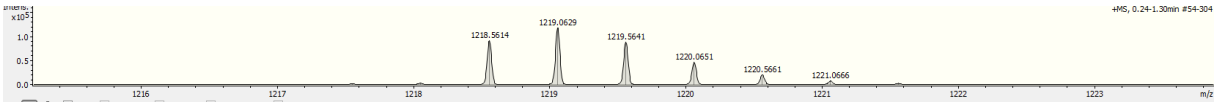


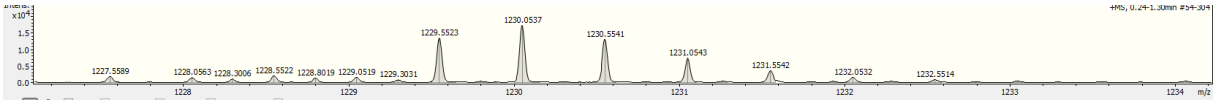


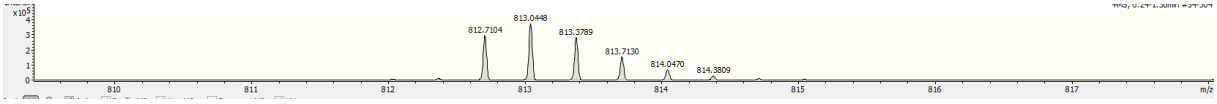
Compound 27 (*HasR* 129-138 *N*-term $(PEG)_7$-MECAM)

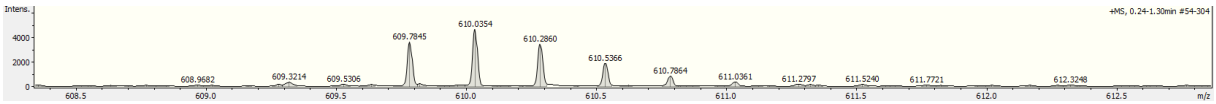




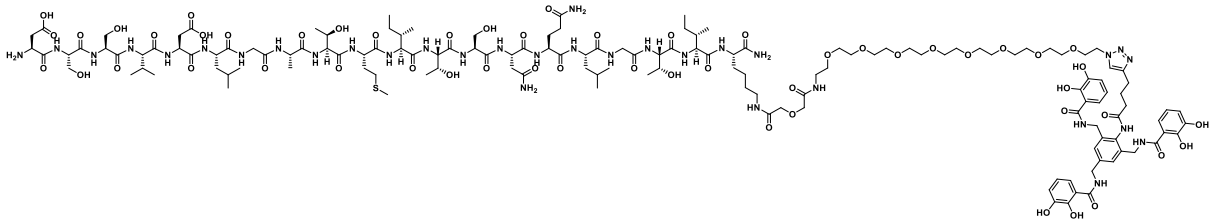


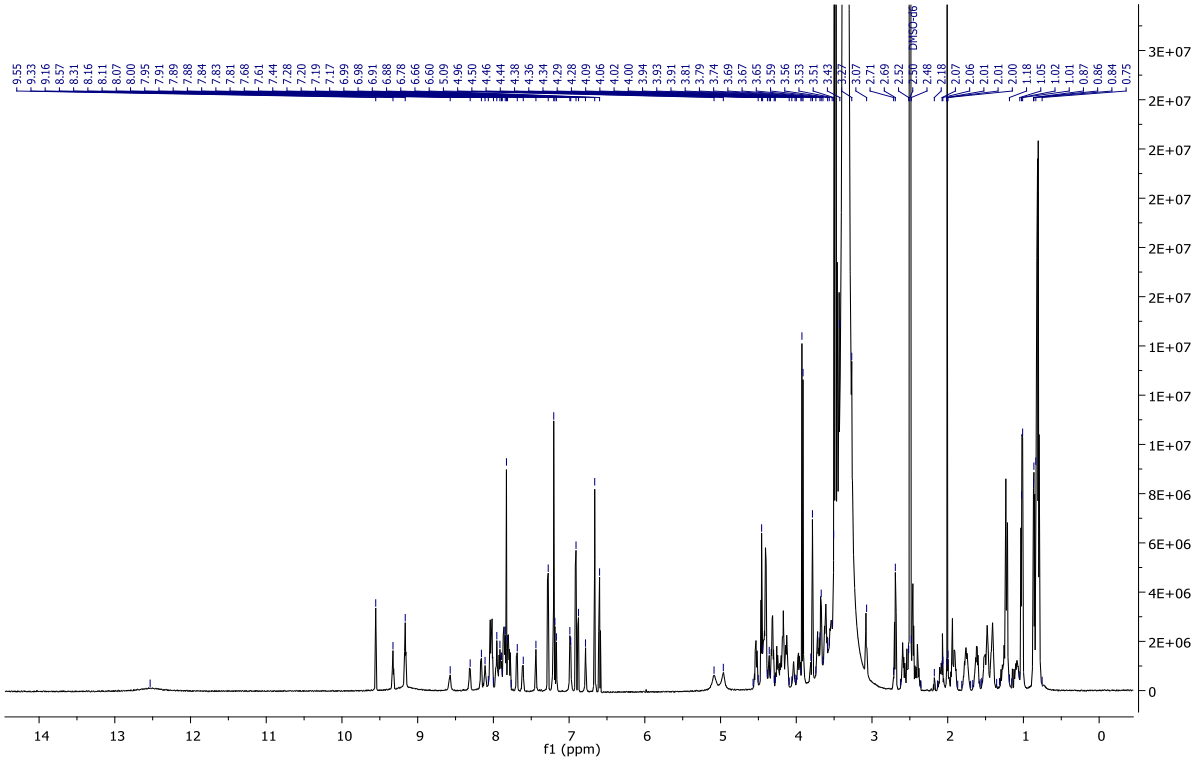


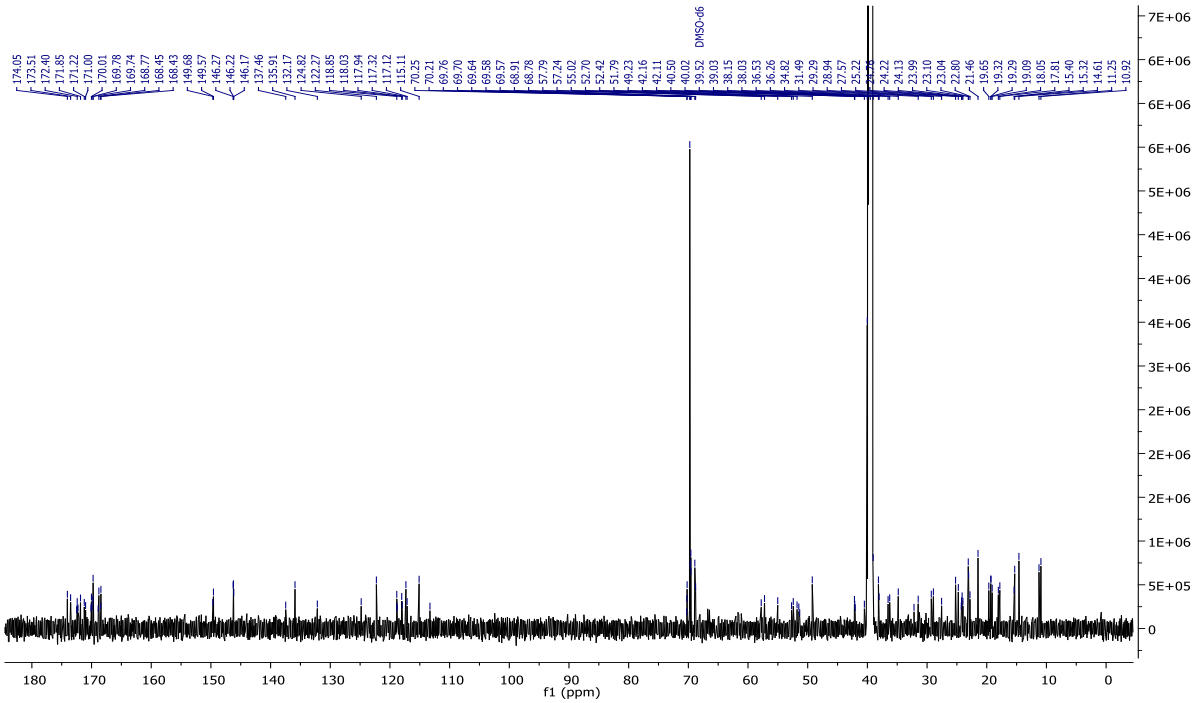


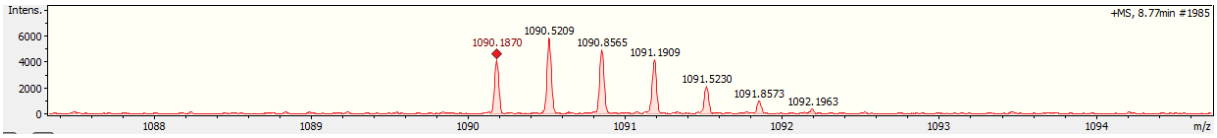


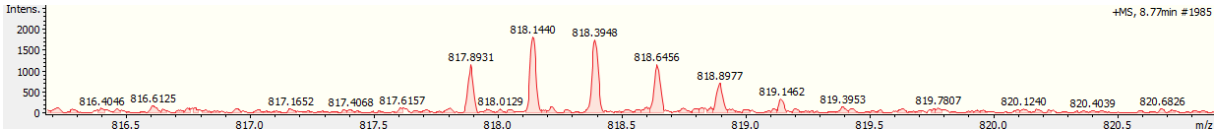
Compound 28 (*FpvA* 121-139 *C*-term $(PEG)_7$-MECAM)



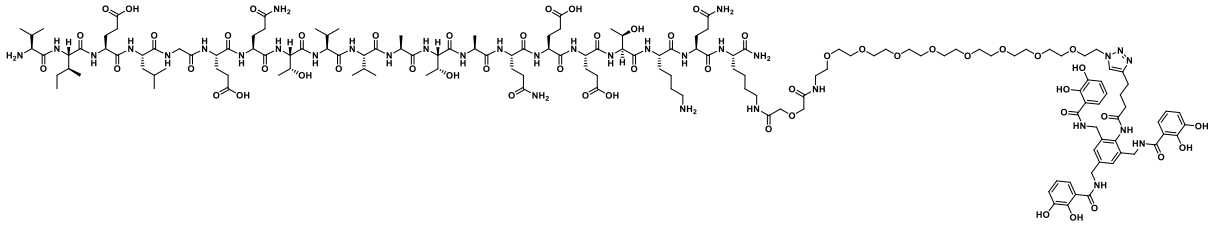


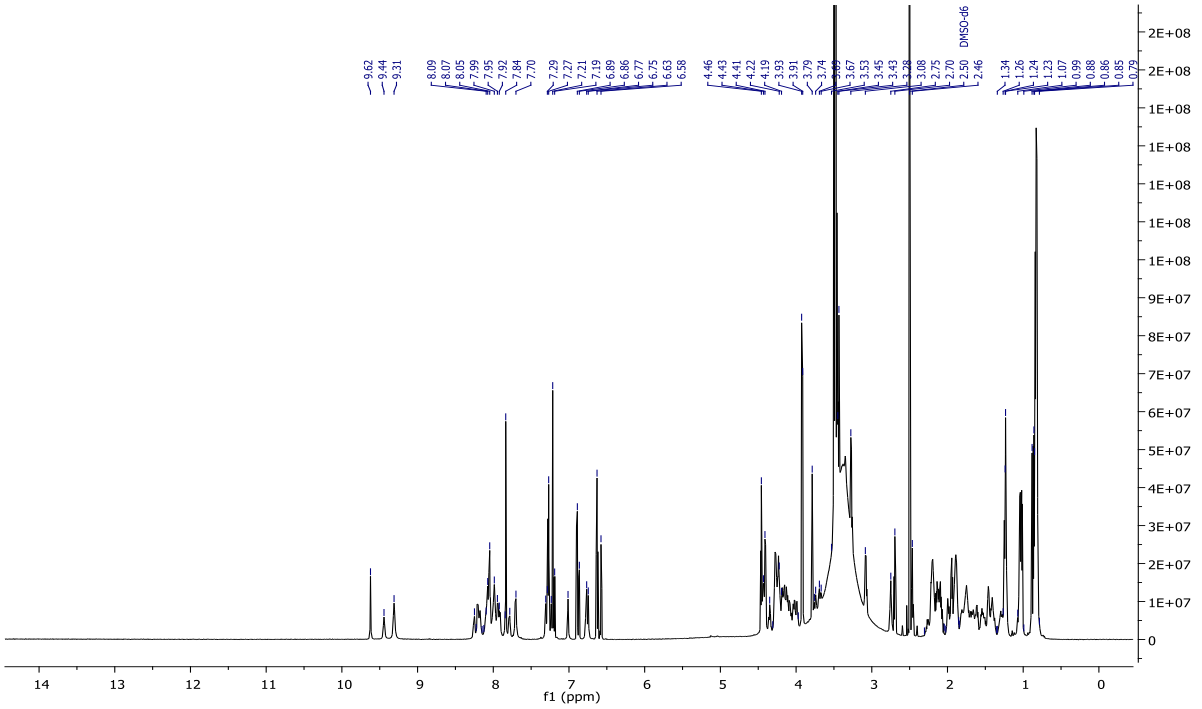


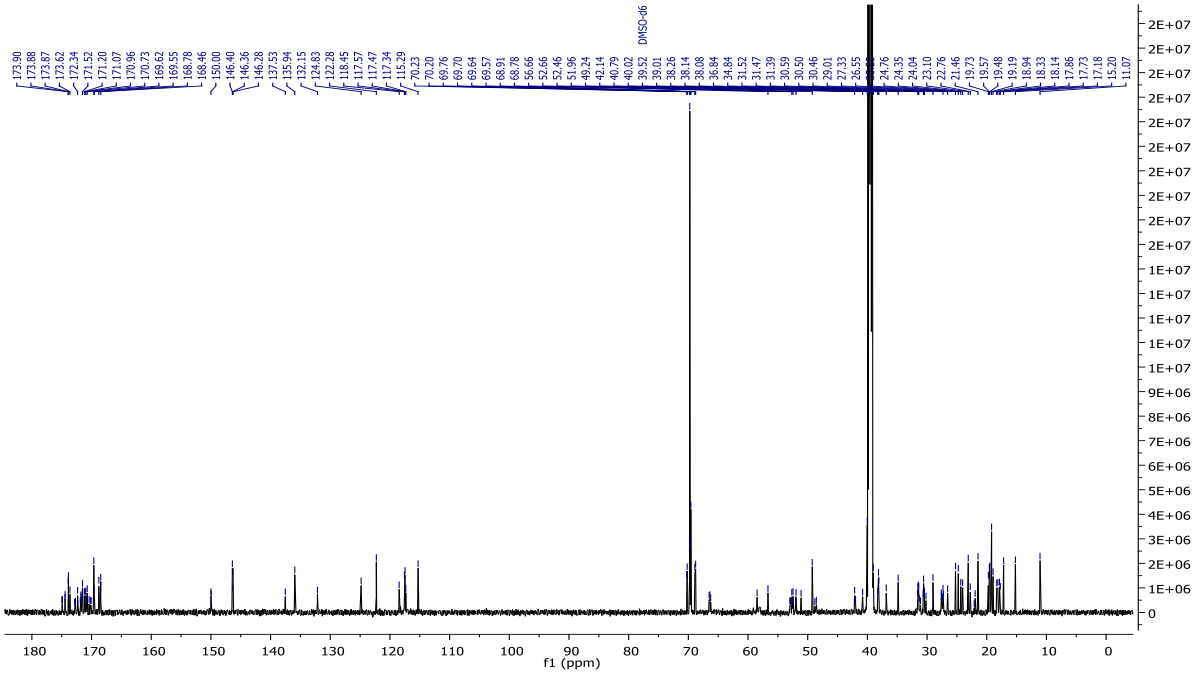

Intens.
+MS, 8.77min #1985
6000
4000
2000
0
1090.1870
1090.5209
1090.8565
1091.1909
1091.5230
1091.8573
1092.1963
1088
1089
1090
1091
1092
1093
1094
m/z

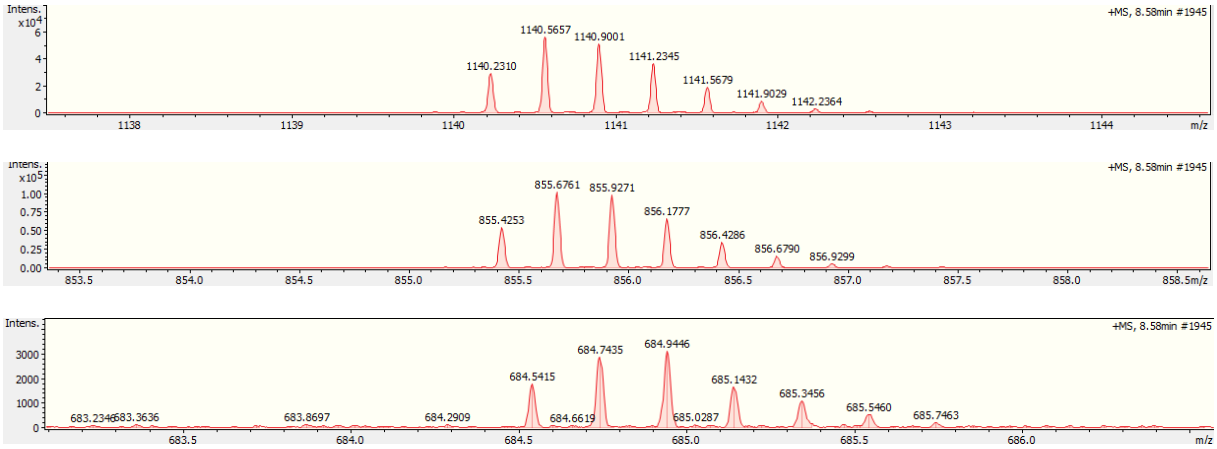

Intens.
+MS, 8.77min #1985
2000
1500
1000
500
0
816.4046
816.6125
817.1652
817.4068
817.6157
817.8931
818.0129
818.1440
818.3948
818.6456
818.8977
819.1462
819.3953
819.7807
820.1240
820.4039
820.6826
816.5
817.0
817.5
818.0
818.5
819.0
819.5
820.0
820.5
m/z

Compound 29 (*PfeA* 33-51 *C*-term $(PEG)_7$-MECAM)





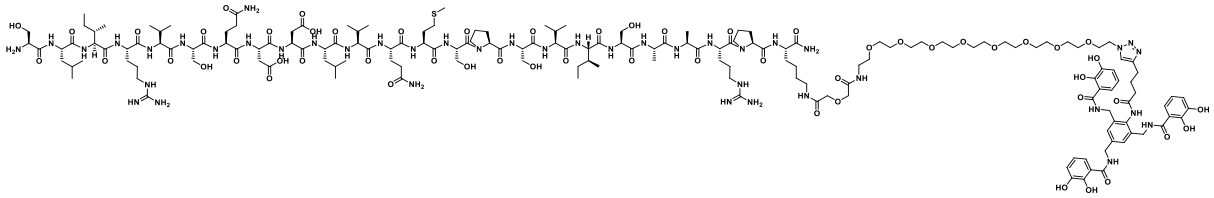


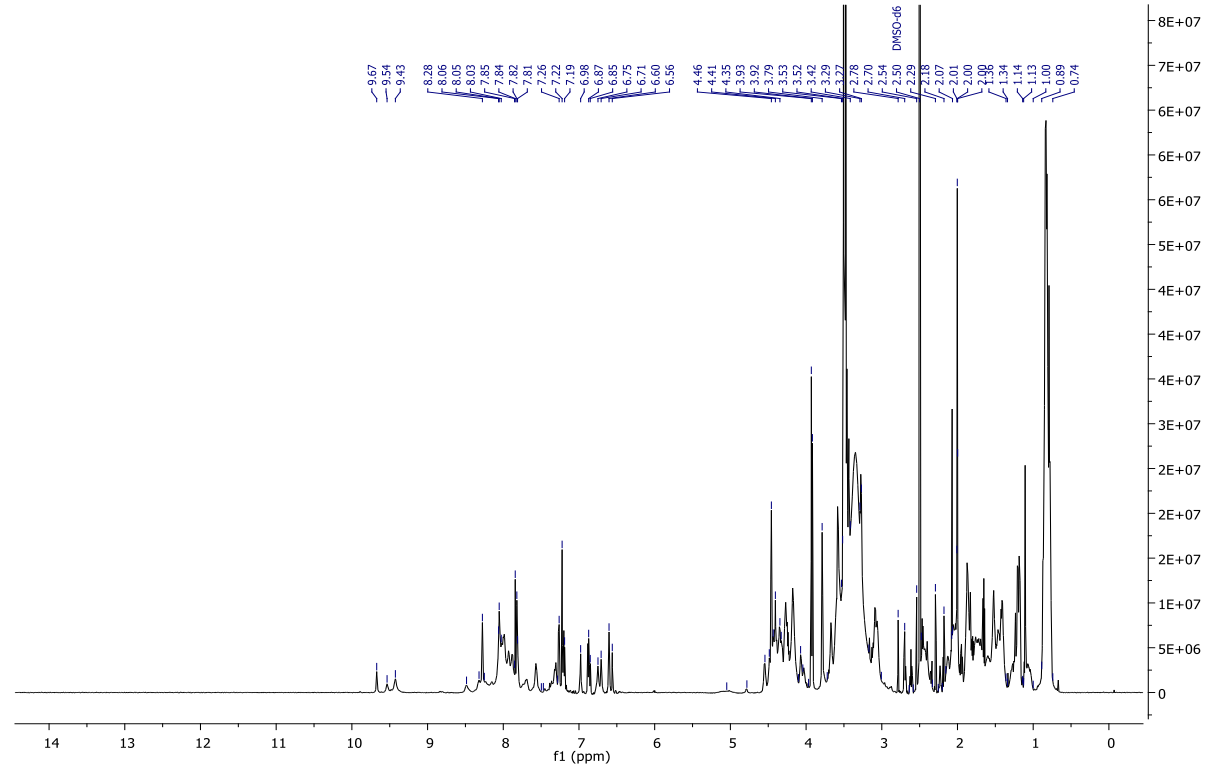

Intens.
x10^4
6
4
2
0
+MS, 8.58min #1945
1140.5657
1140.9001
1140.2310
1141.2345
1141.5679
1141.9029
1142.2364
1138
1139
1140
1141
1142
1143
1144
m/z

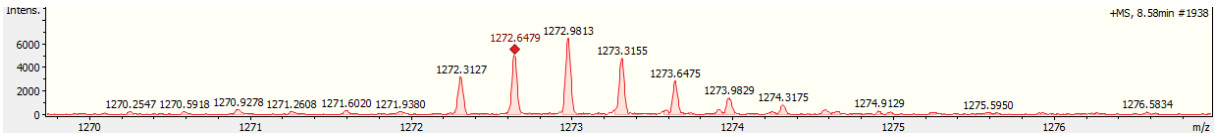
Intens.
x10^5
1.00
0.75
0.50
0.25
0.00
+MS, 8.58min #1945
855.6761
855.9271
855.4253
856.1777
856.4286
856.6790
856.9299
853.5
854.0
854.5
855.0
855.5
856.0
856.5
857.0
857.5
858.0
858.5m/z

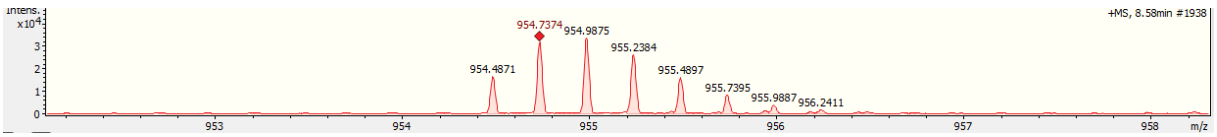
Intens.
3000
2000
1000
0
+MS, 8.58min #1945
684.7435
684.9446
684.5415
685.1432
685.3456
685.5460
685.7463
683.2346
683.3636
683.8697
684.2909
684.6619
685.0287
683.5
684.0
684.5
685.0
685.5
686.0
m/z

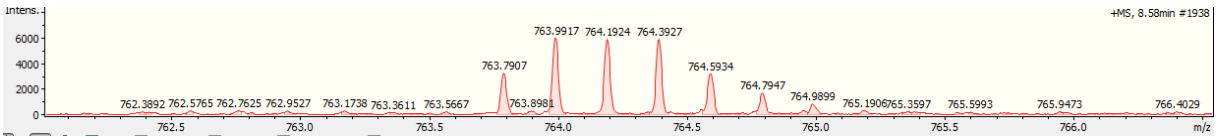
Compound 30 (*HasR* 122-144 *C*-term $(PEG)_7$-MECAM)



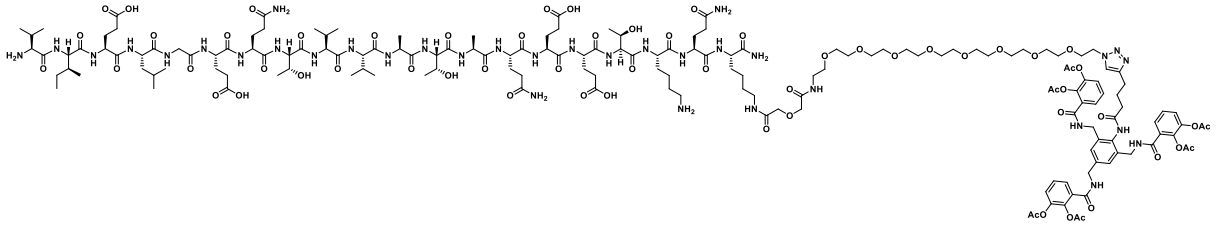


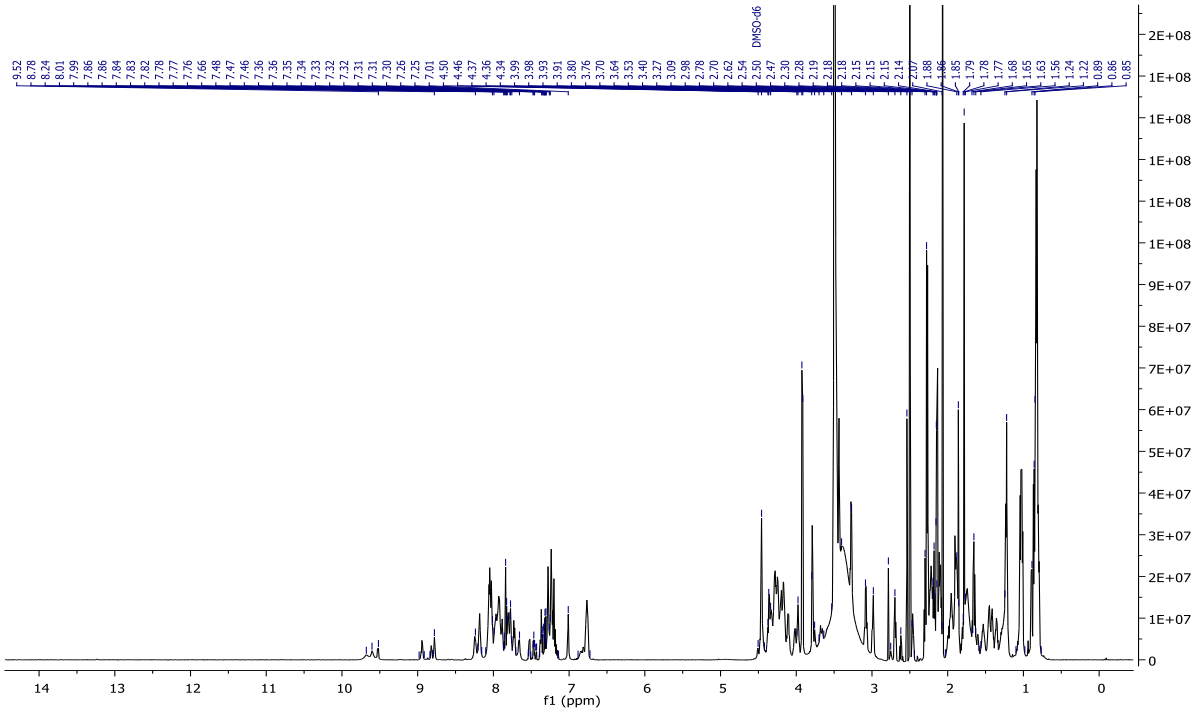


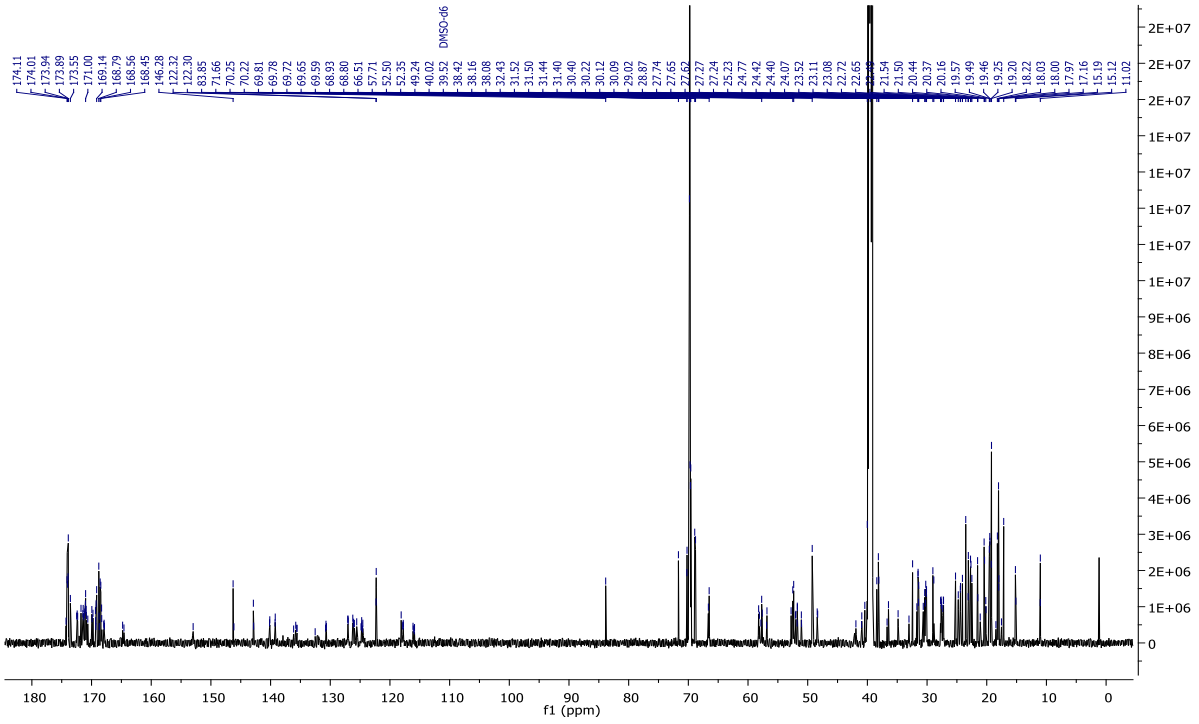


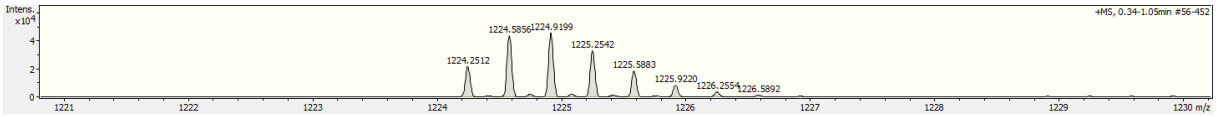


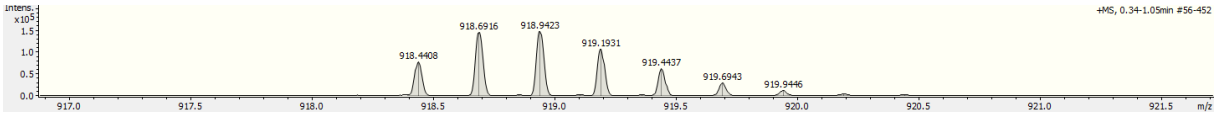
Compound 31 (*PfeA* 33-51 *C*-term $(PEG)_7$-MECAM-OAc)

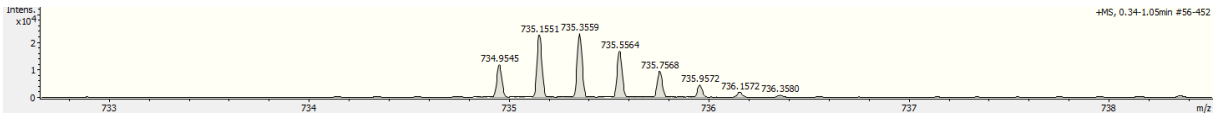


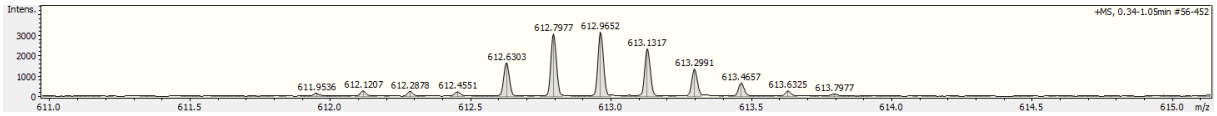




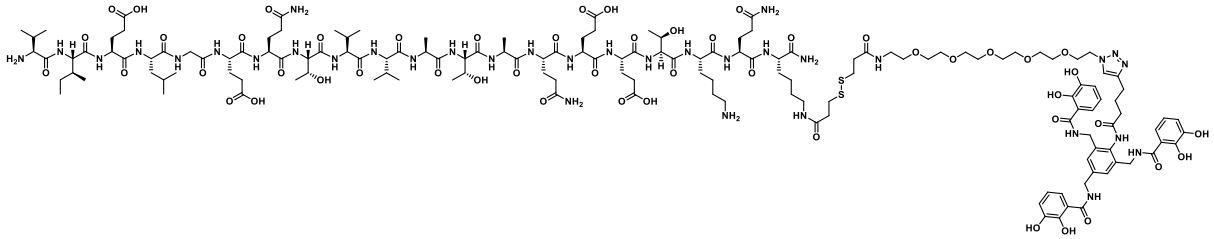

Intens.
x10^4
+MS, 0.34-1.05min #56-452
1224.5856
1224.9199
1224.2512
1225.2542
1225.5883
1225.9220
1226.2554
1226.5892
1221
1222
1223
1224
1225
1226
1227
1228
1229
1230 m/z

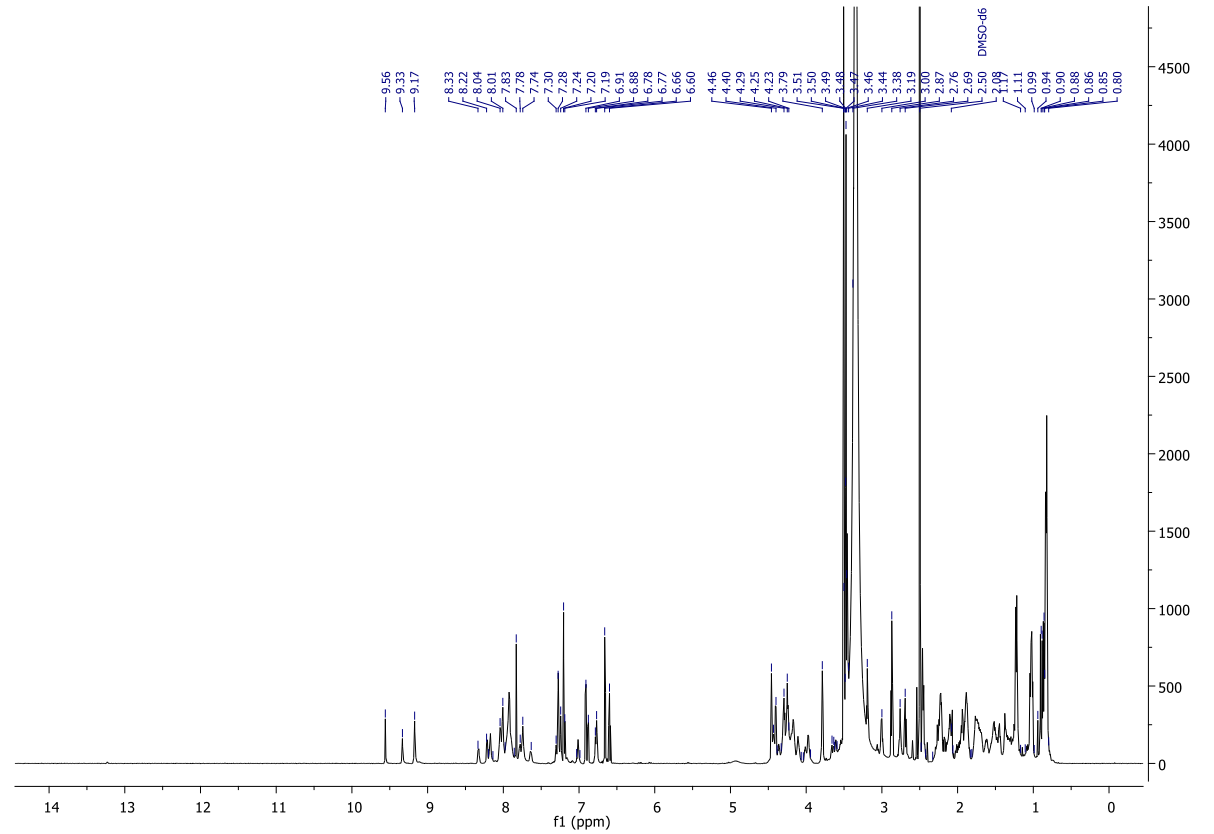

Intens.
x10^5
+MS, 0.34-1.05min #56-452
918.6916
918.9423
918.4408
919.1931
919.4437
919.6943
919.9446
917.0
917.5
918.0
918.5
919.0
919.5
920.0
920.5
921.0
921.5
m/z

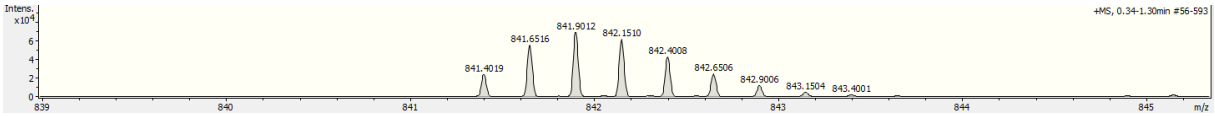

Intens.
x10^4
+MS, 0.34-1.05min #56-452
735.1551
735.3559
735.5564
734.9545
735.7568
735.9572
736.1572
736.3580
733
734
735
736
737
738
m/z

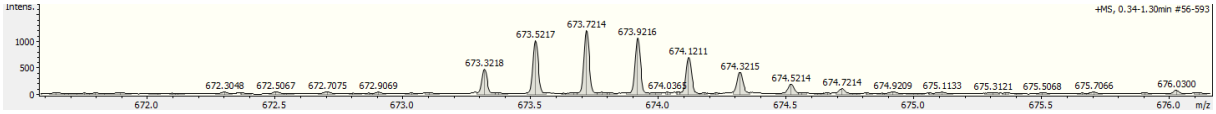

Intens.
+MS, 0.34-1.05min #56-452
612.7977
612.9652
613.1317
612.6303
613.2991
613.4657
611.9536
612.1207
612.2878
612.4551
613.6325
613.7977
611.0
611.5
612.0
612.5
613.0
613.5
614.0
614.5
615.0
m/z

Compound 32 (*PfeA* 33-51 *C*-term disulfide-$(PEG)_5$-MECAM)

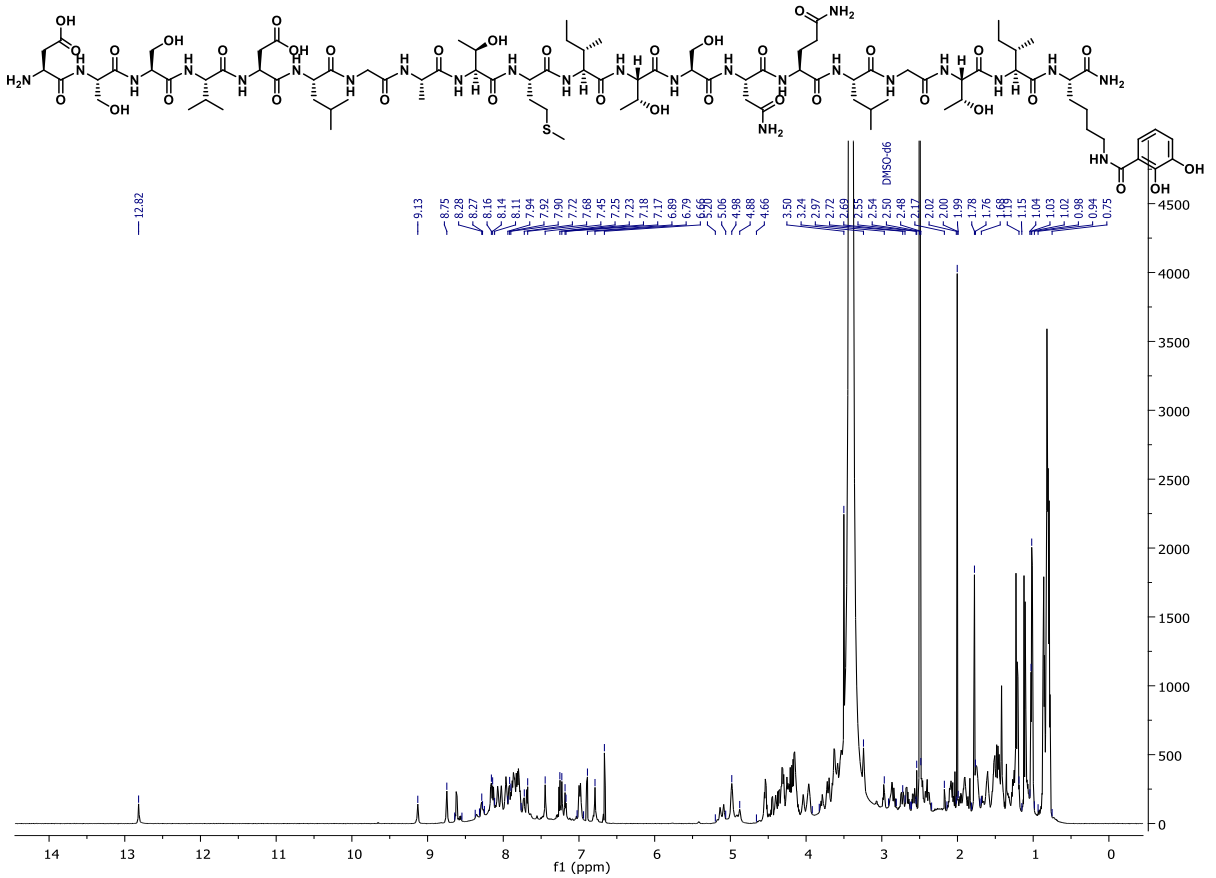


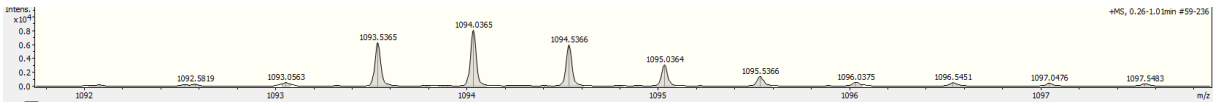


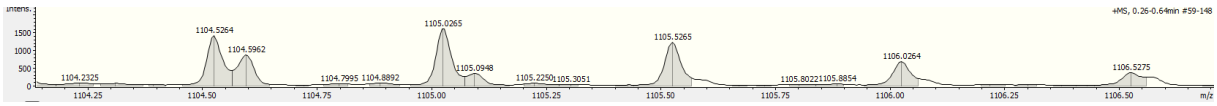


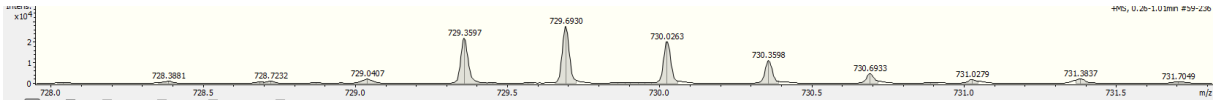


Compound C33 (*FpvA* 121-139 *C*-term 2,3-dihydroxybenzamide)

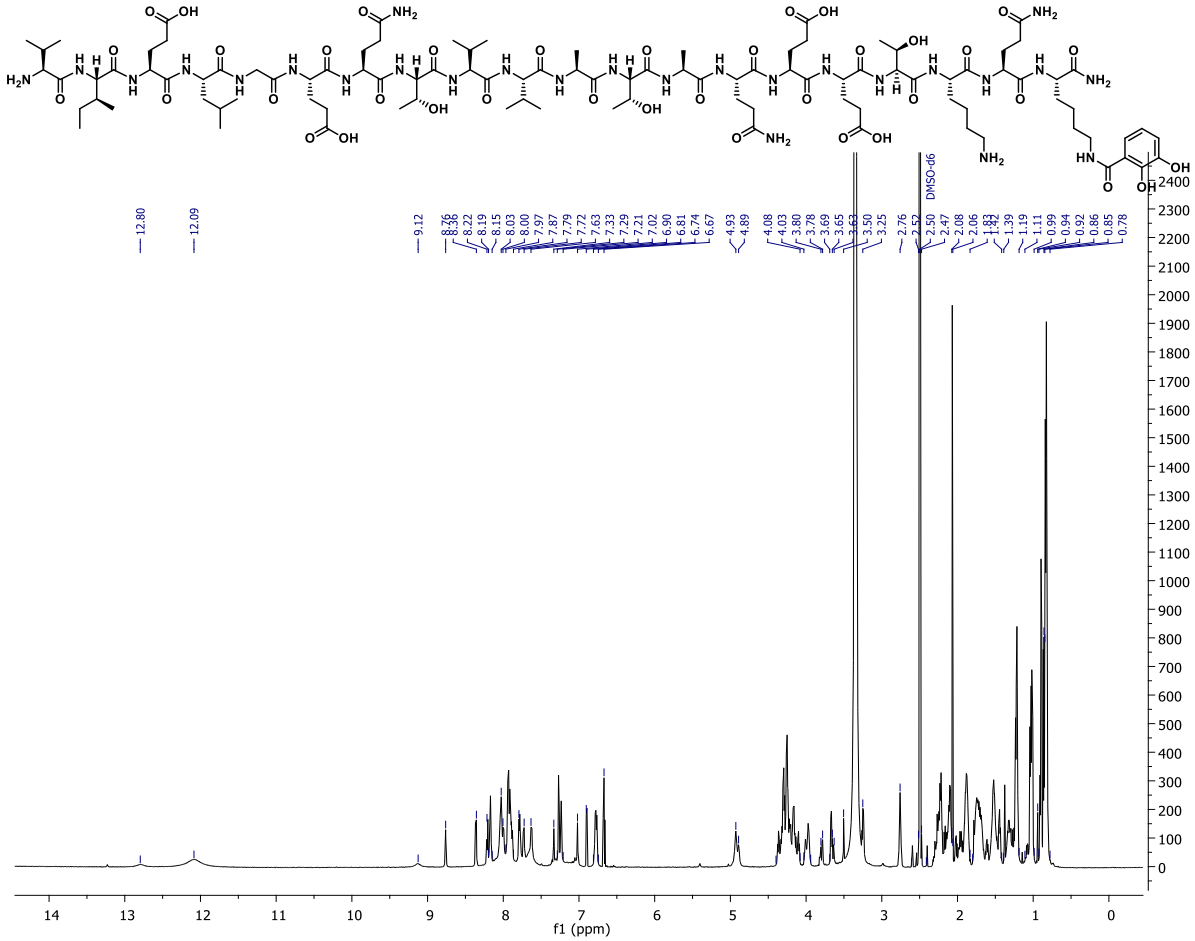


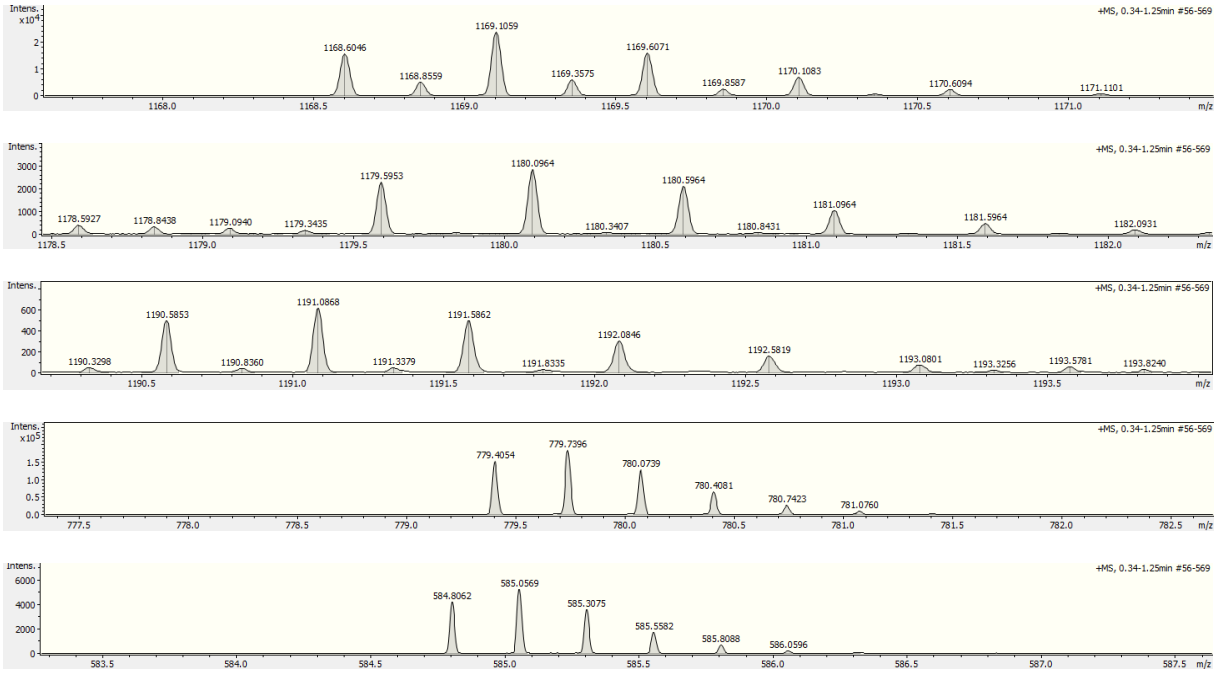




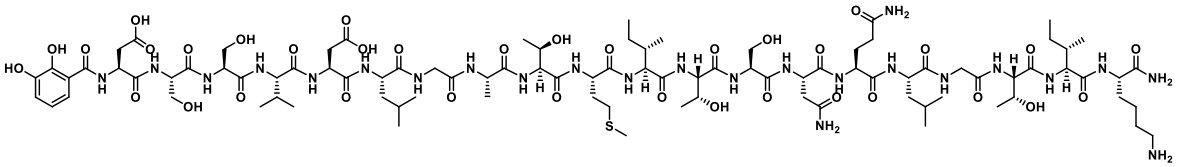


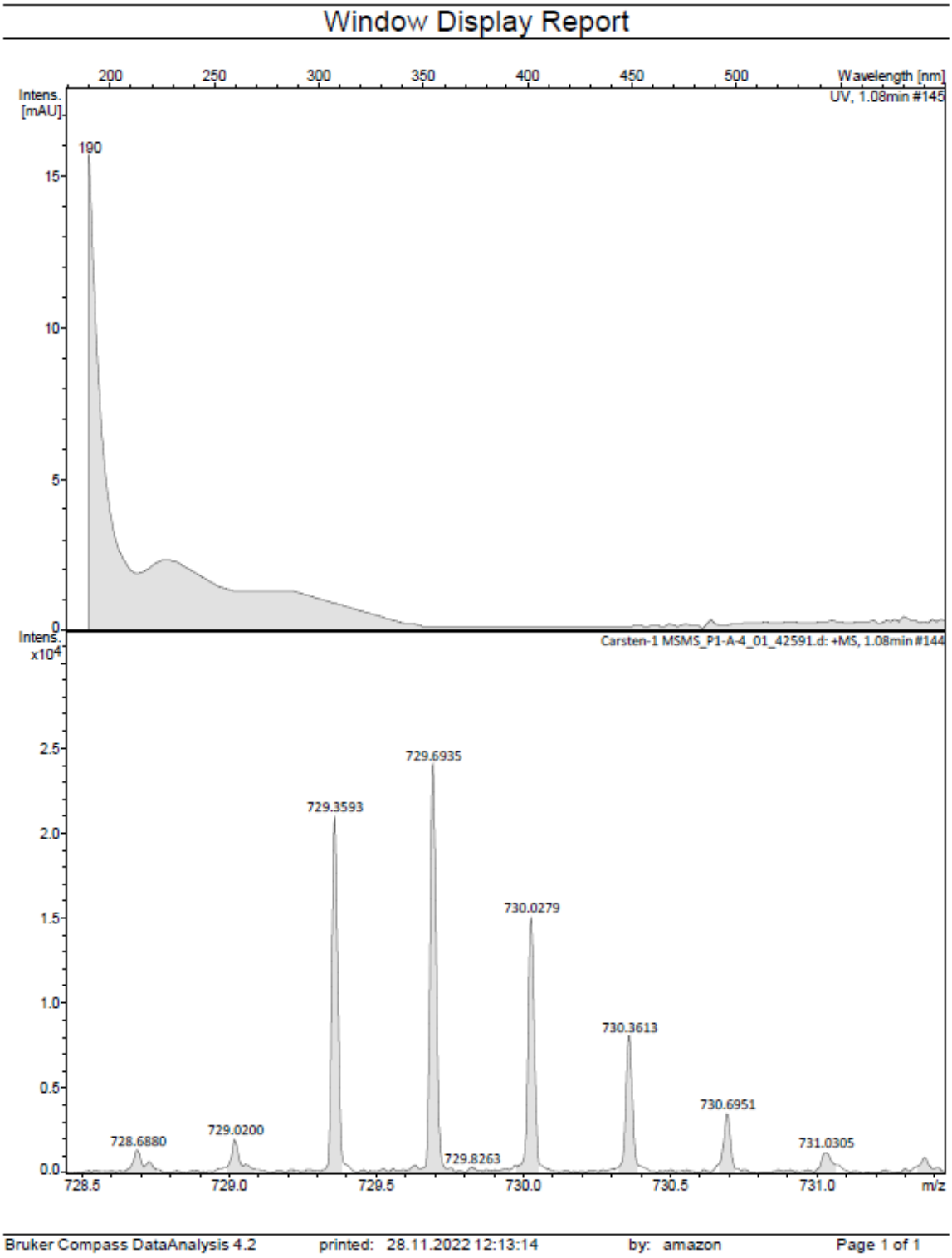
Compound C34 (*PfeA* 33-51 *C*-term 2,3-dihydroxybenzamide)



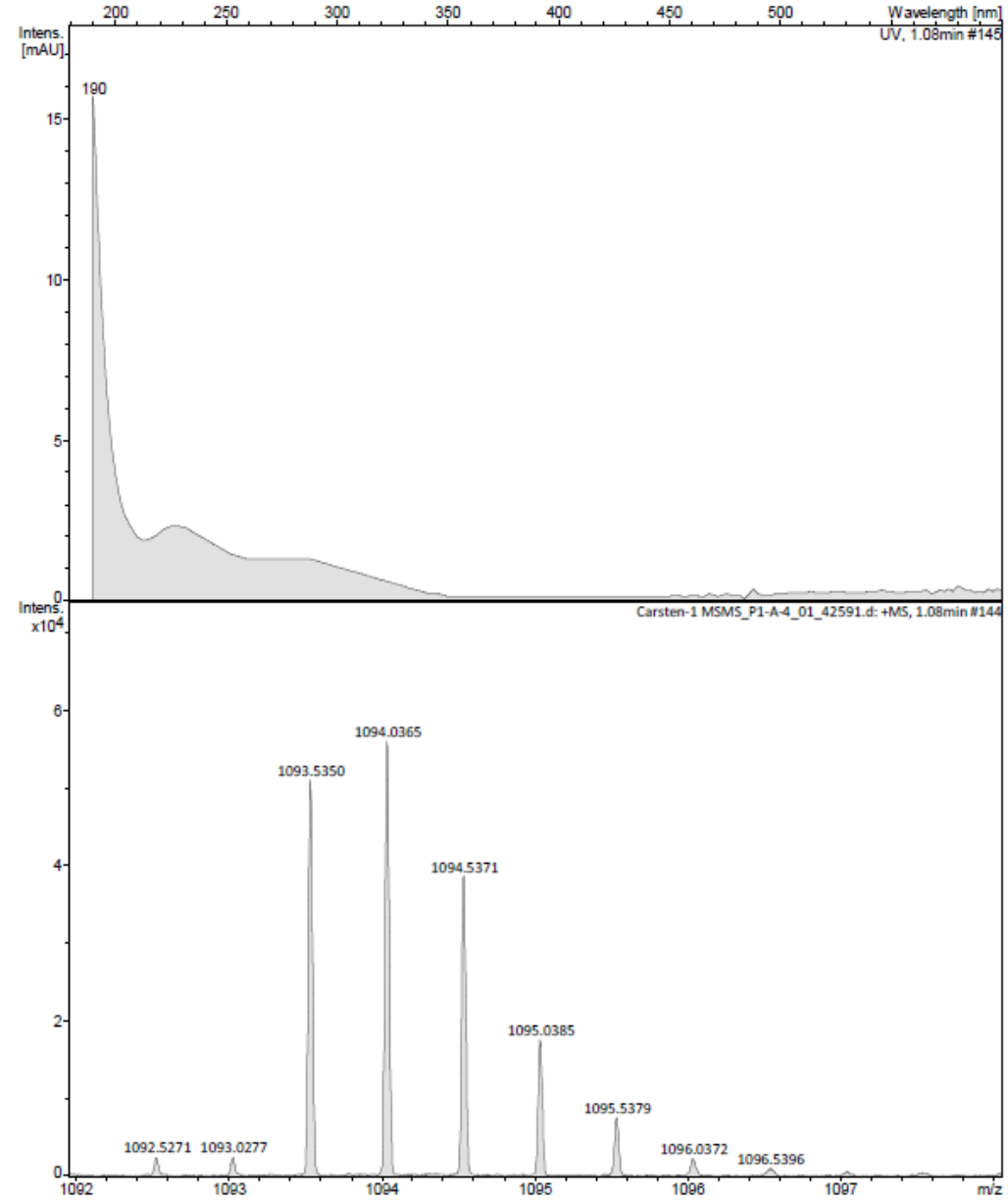


Compound N33$_L$ (*FpvA* 121-139 *N*-term 2,3-dihydroxybenzamide)

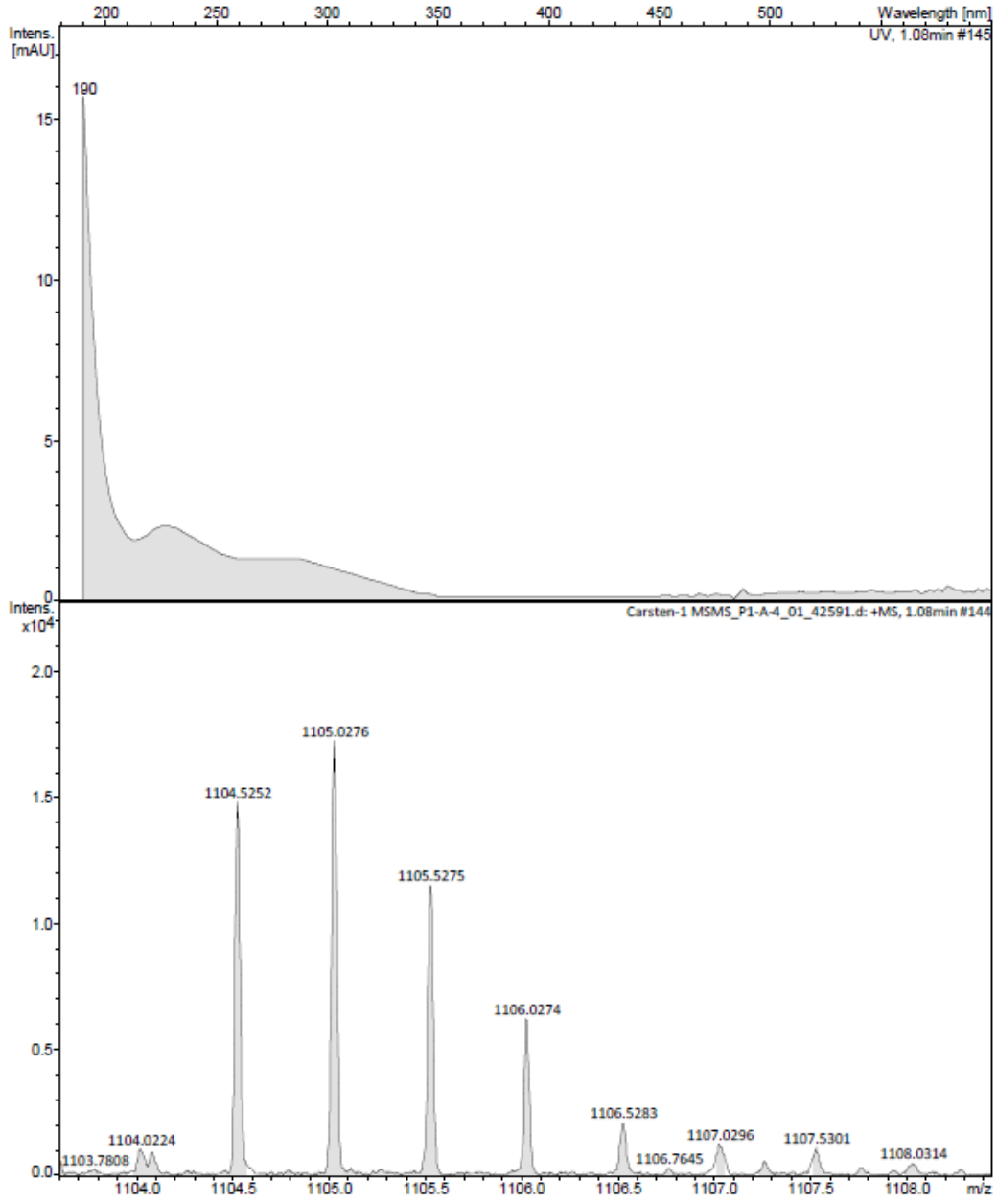


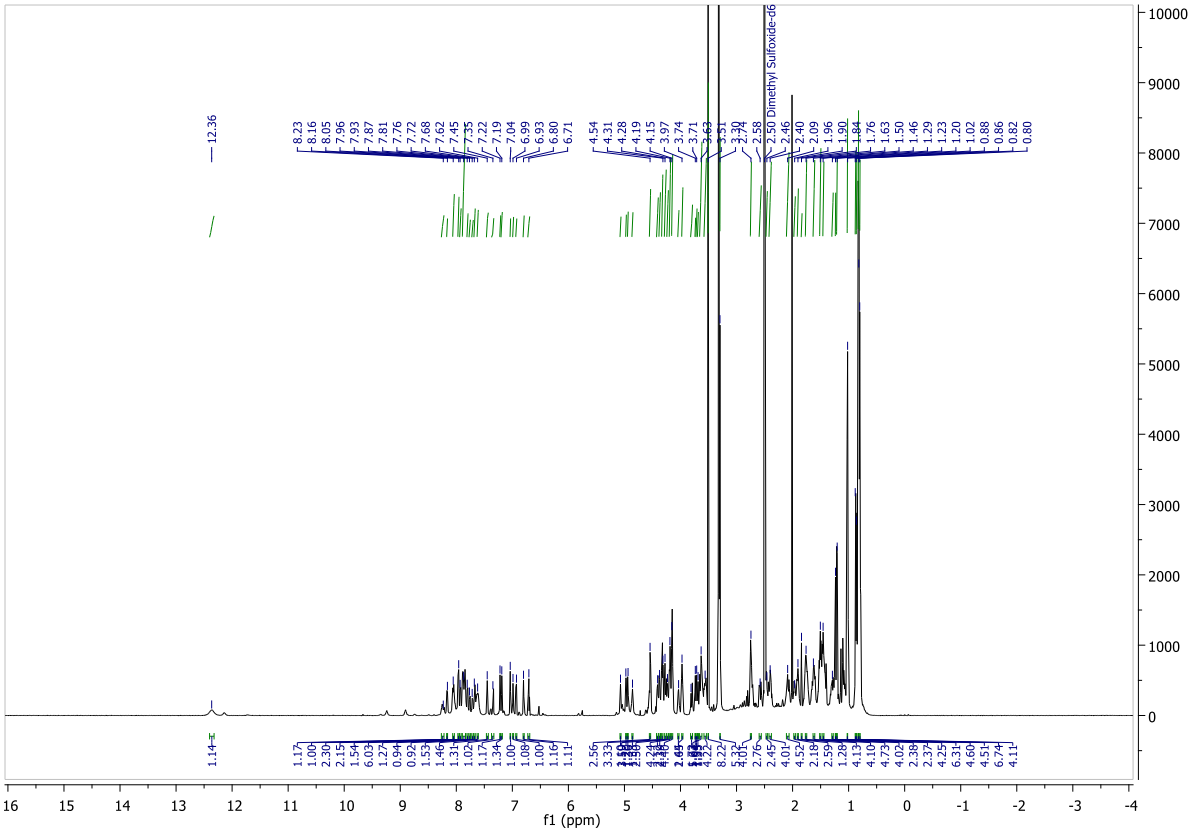


Window Display Report

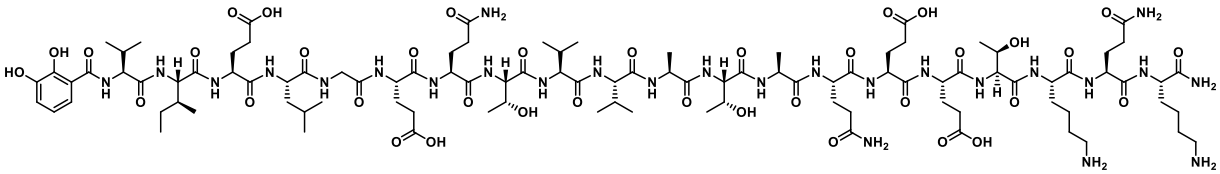


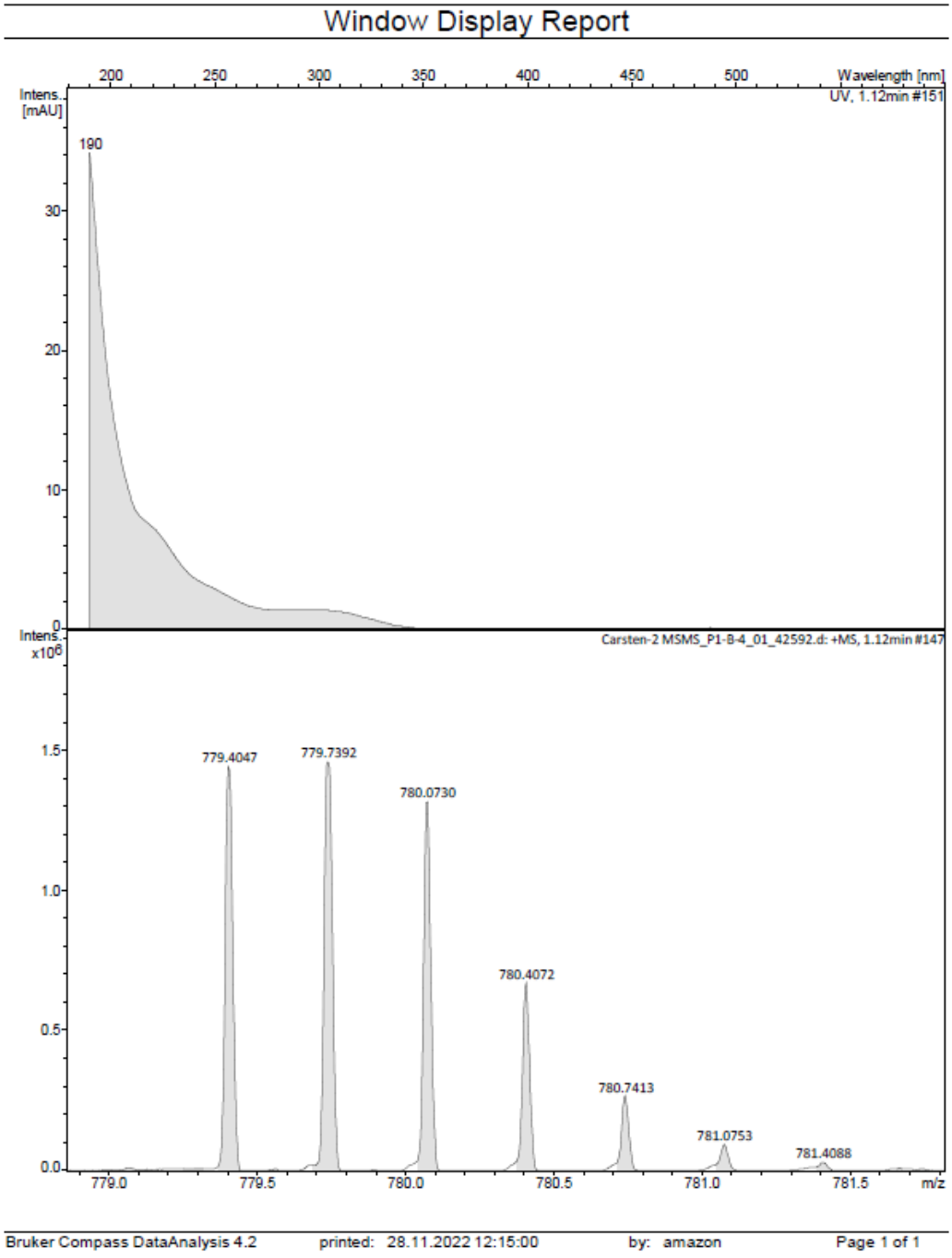
Window Display Report



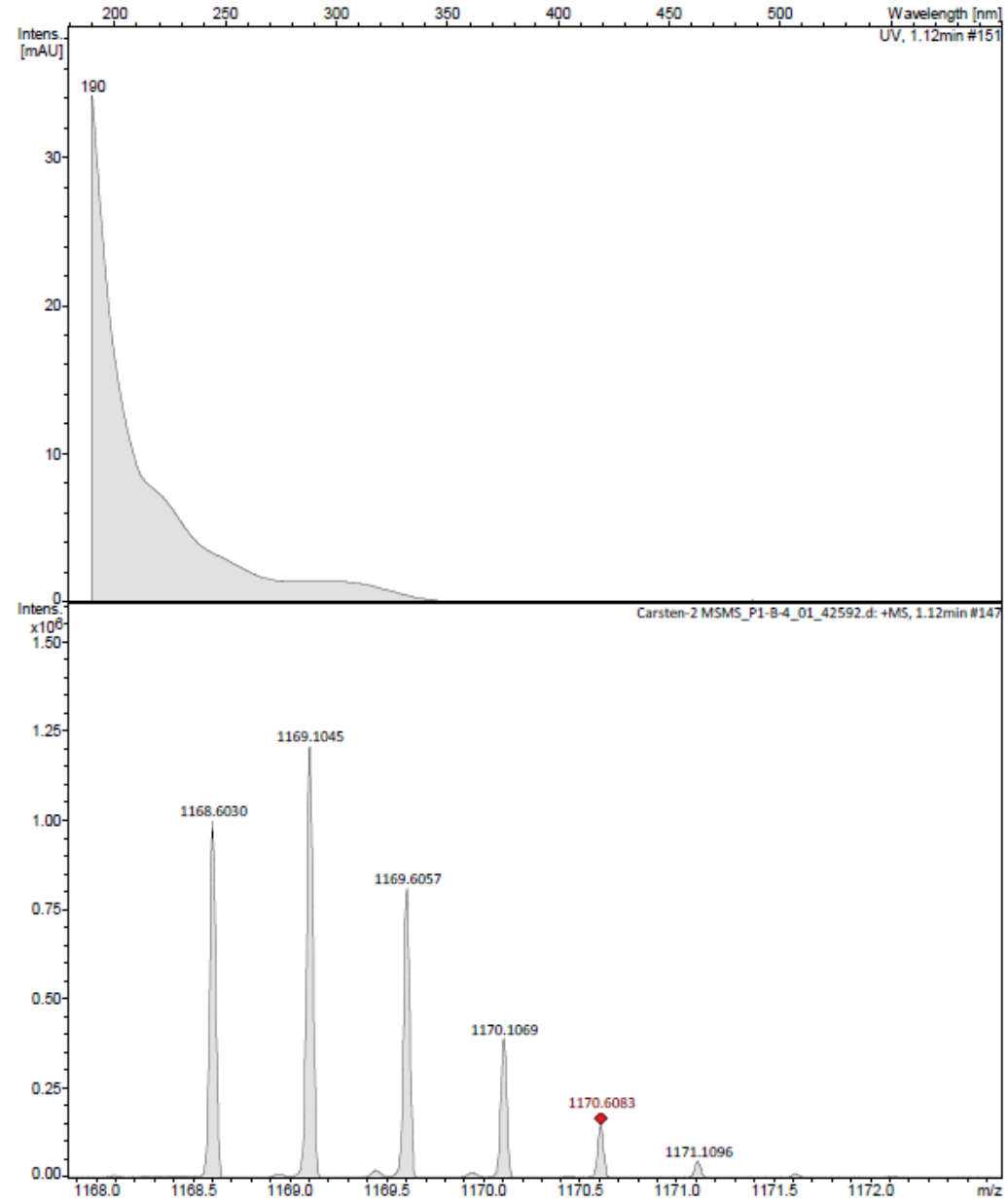

12.36
8.23
8.16
8.05
7.96
7.93
7.87
7.81
7.76
7.72
7.68
7.62
7.45
7.35
7.22
7.19
7.04
6.99
6.93
6.80
6.71
4.54
4.31
4.28
4.19
4.15
3.97
3.74
3.71
3.63
3.51
3.30
2.58
2.50 Dimethyl Sulfoxide-d6
2.46
2.40
2.09
1.96
1.90
1.84
1.76
1.63
1.50
1.46
1.29
1.23
1.20
1.02
0.88
0.86
0.82
0.80
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
16
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

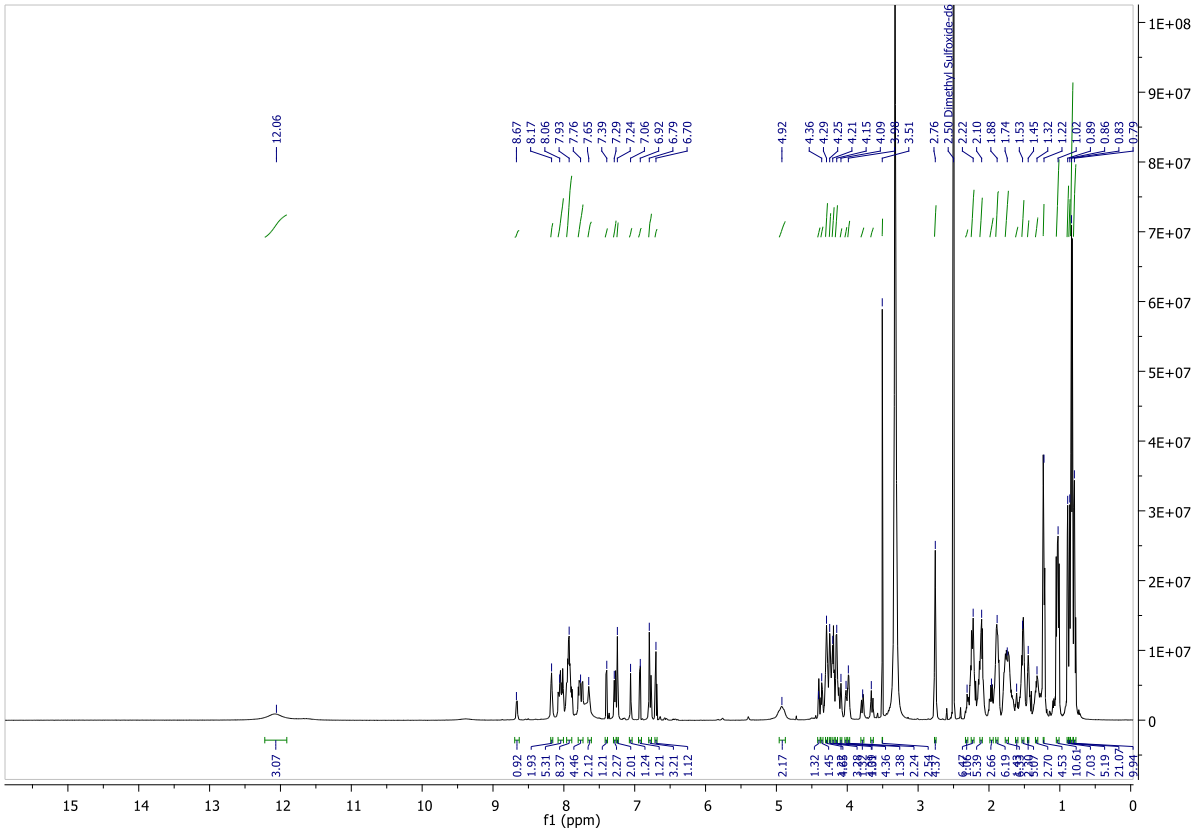
Compound N34$_L$ (*PfeA* 33-51 *N*-term 2,3-dihydroxybenzamide)



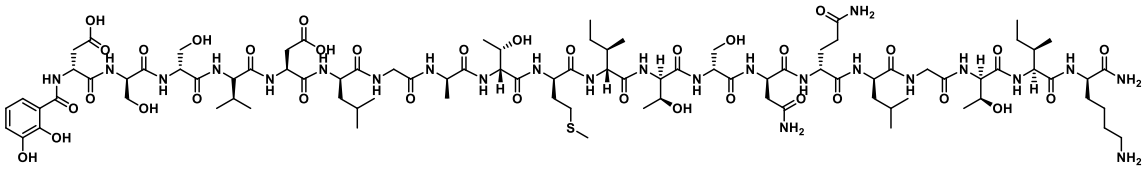


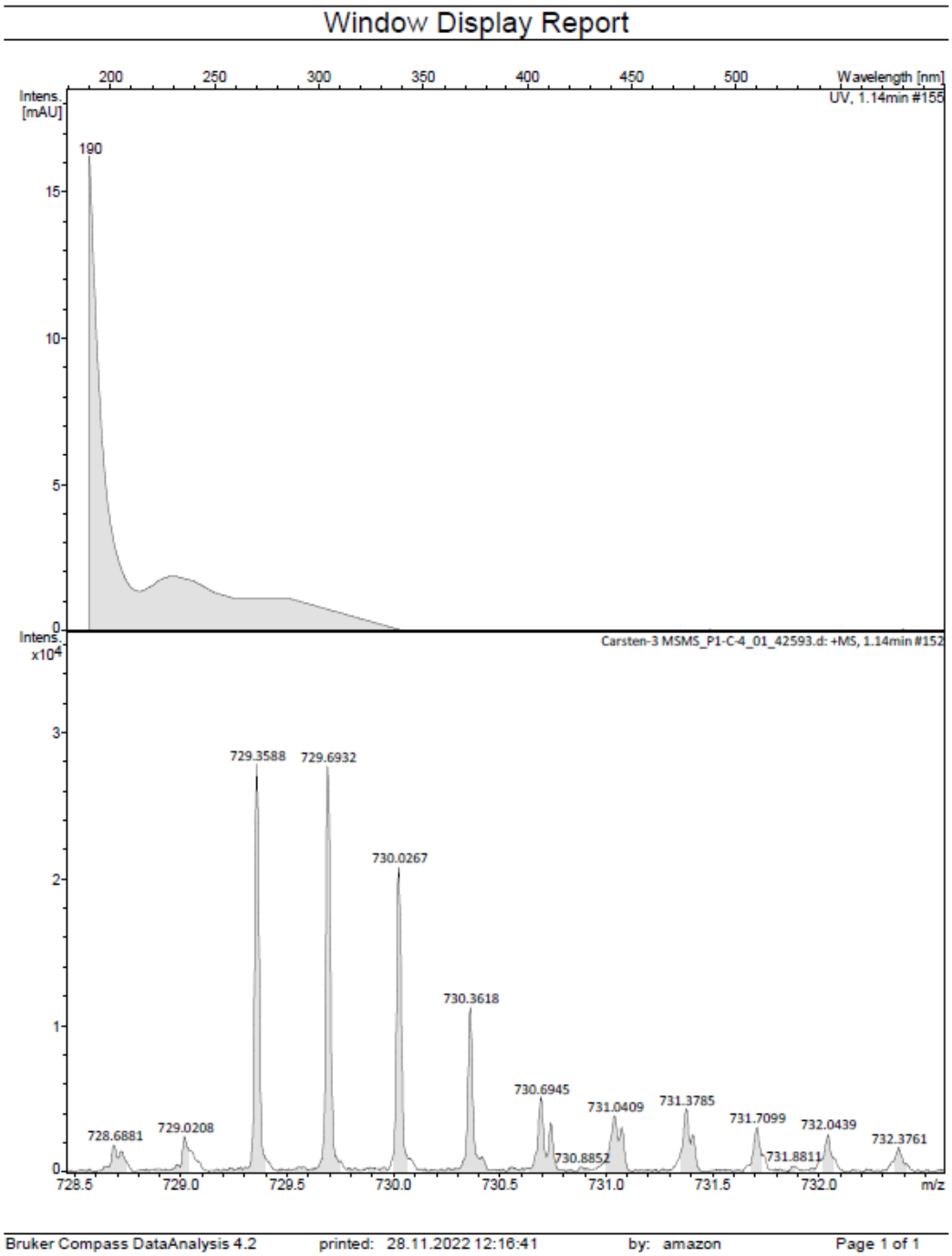
Window Display Report



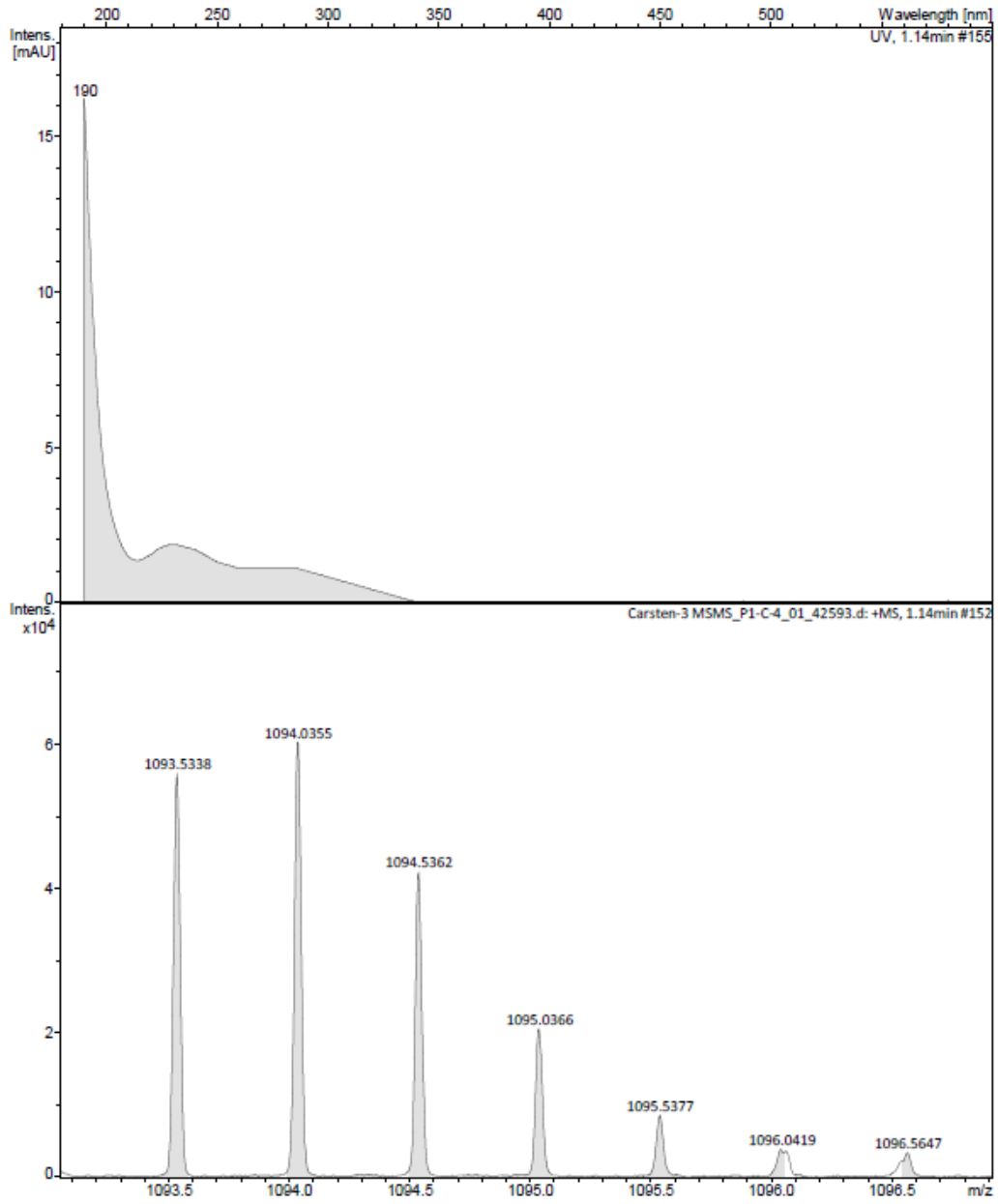

12.06
8.67
8.17
8.06
7.93
7.76
7.65
7.39
7.29
7.24
7.06
6.92
6.79
6.70
4.92
4.36
4.29
4.25
4.21
4.15
4.09
3.88
3.51
2.76
2.50 Dimethyl Sulfoxide-d6
2.22
2.10
1.88
1.74
1.53
1.45
1.32
1.22
1.02
0.89
0.86
0.83
0.79
3.07
0.92
1.93
5.31
8.37
4.46
2.12
1.21
2.27
2.01
1.24
1.21
3.21
1.12
2.17
1.32
1.38
2.24
6.19
2.66
5.39
2.70
4.53
10.61
7.03
5.19
21.07
9.94
1E+08
9E+07
8E+07
7E+07
6E+07
5E+07
4E+07
3E+07
2E+07
1E+07
0
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

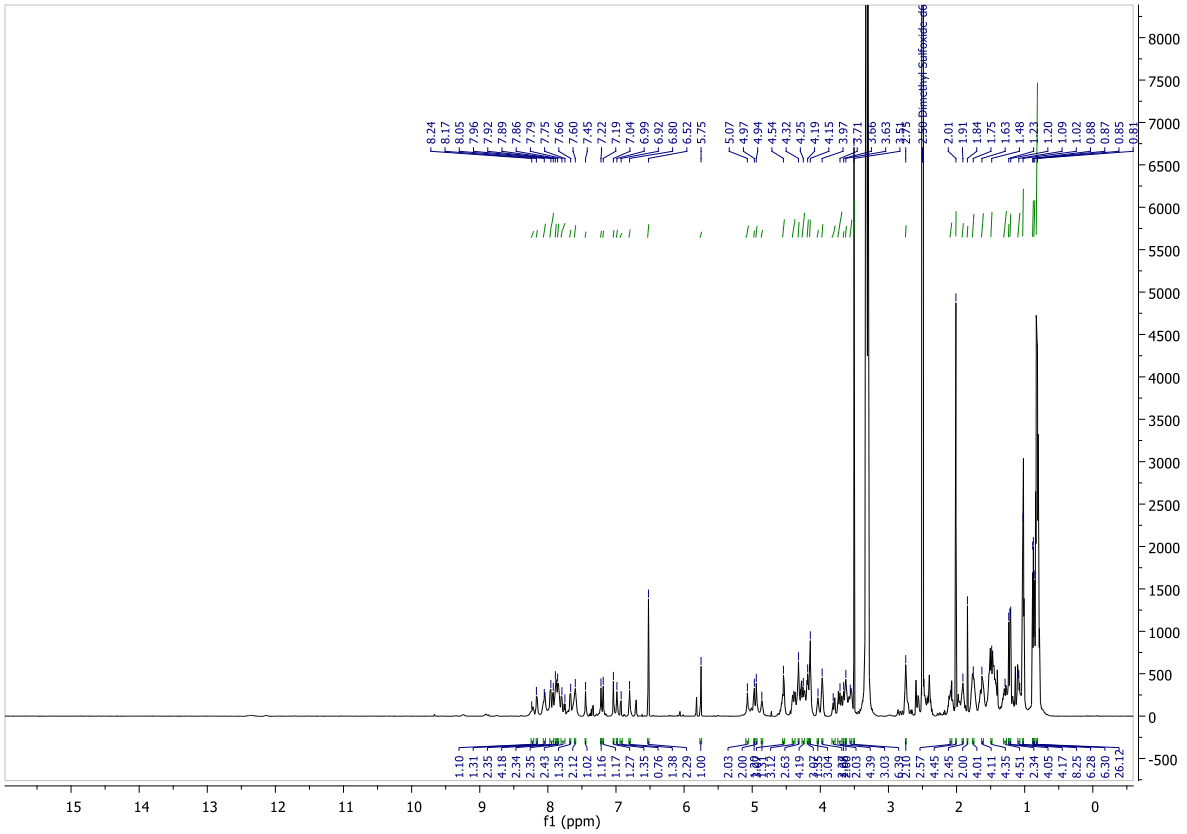
Compound N33$_D$ (D-aa *FpvA* 121-139 *C*-term 2,3-dihydroxybenzamide)



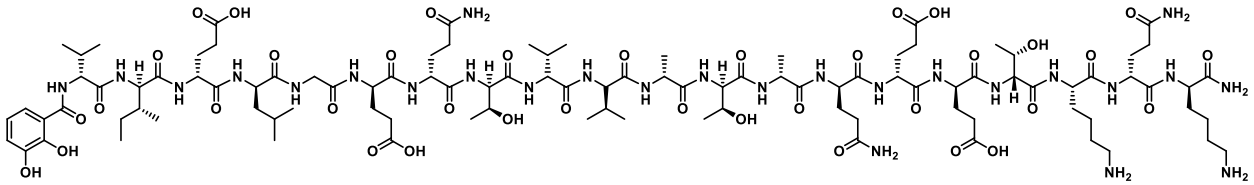


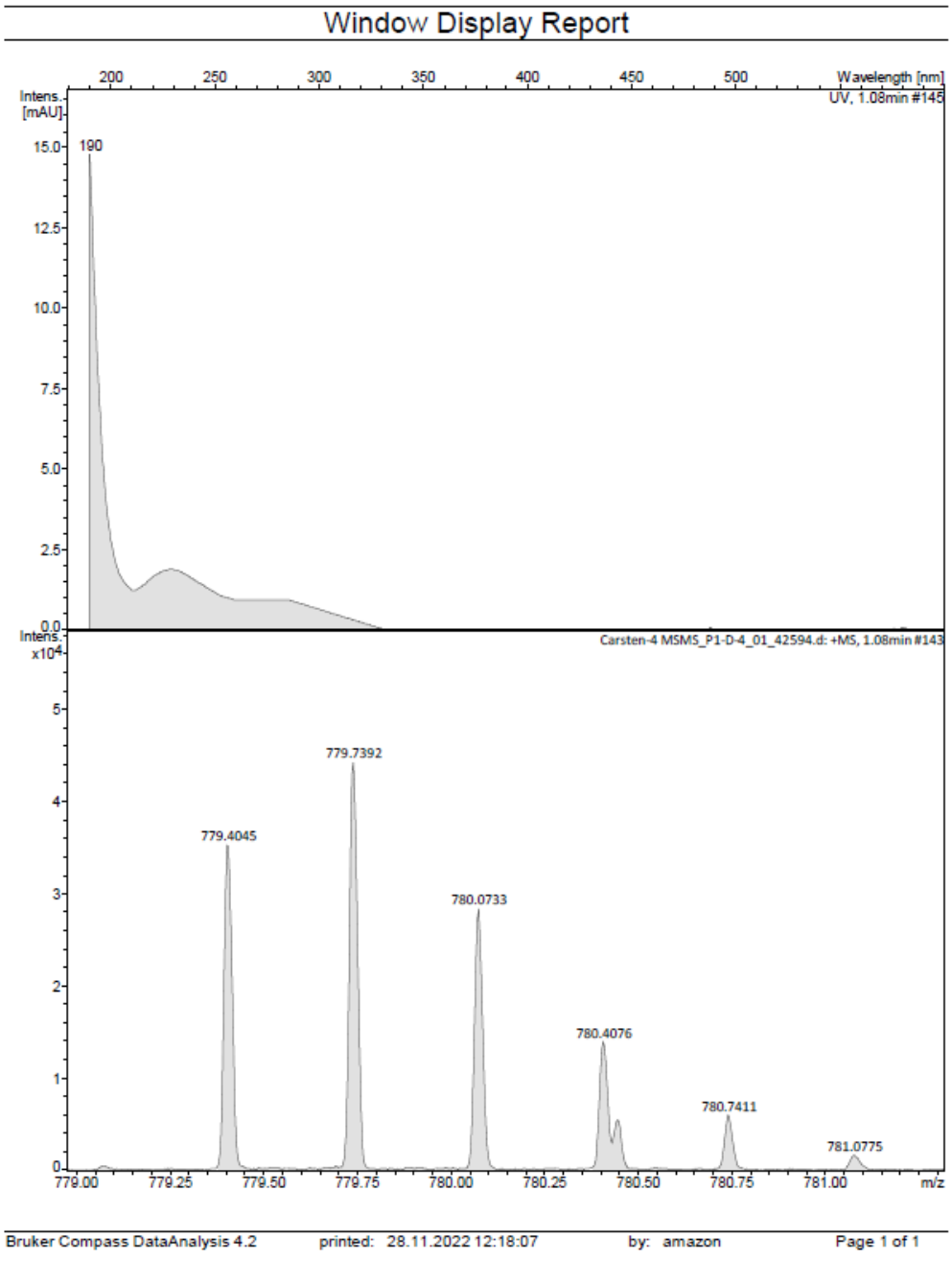
Window Display Report



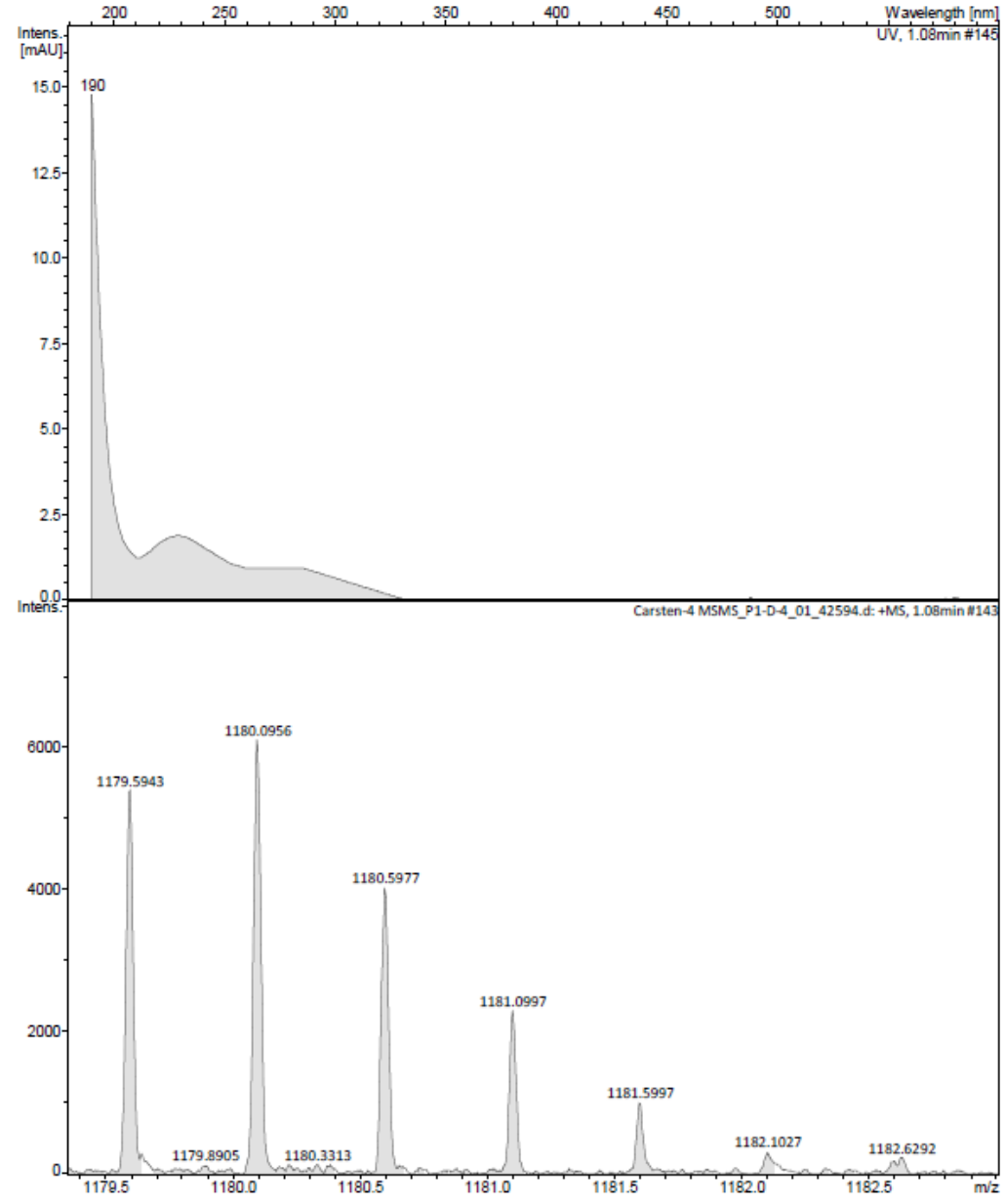

f1 (ppm)

Compound N34$_D$ (D-aa *PfeA* 33-51 *N*-term 2,3-dihydroxybenzamide)





Window Display Report



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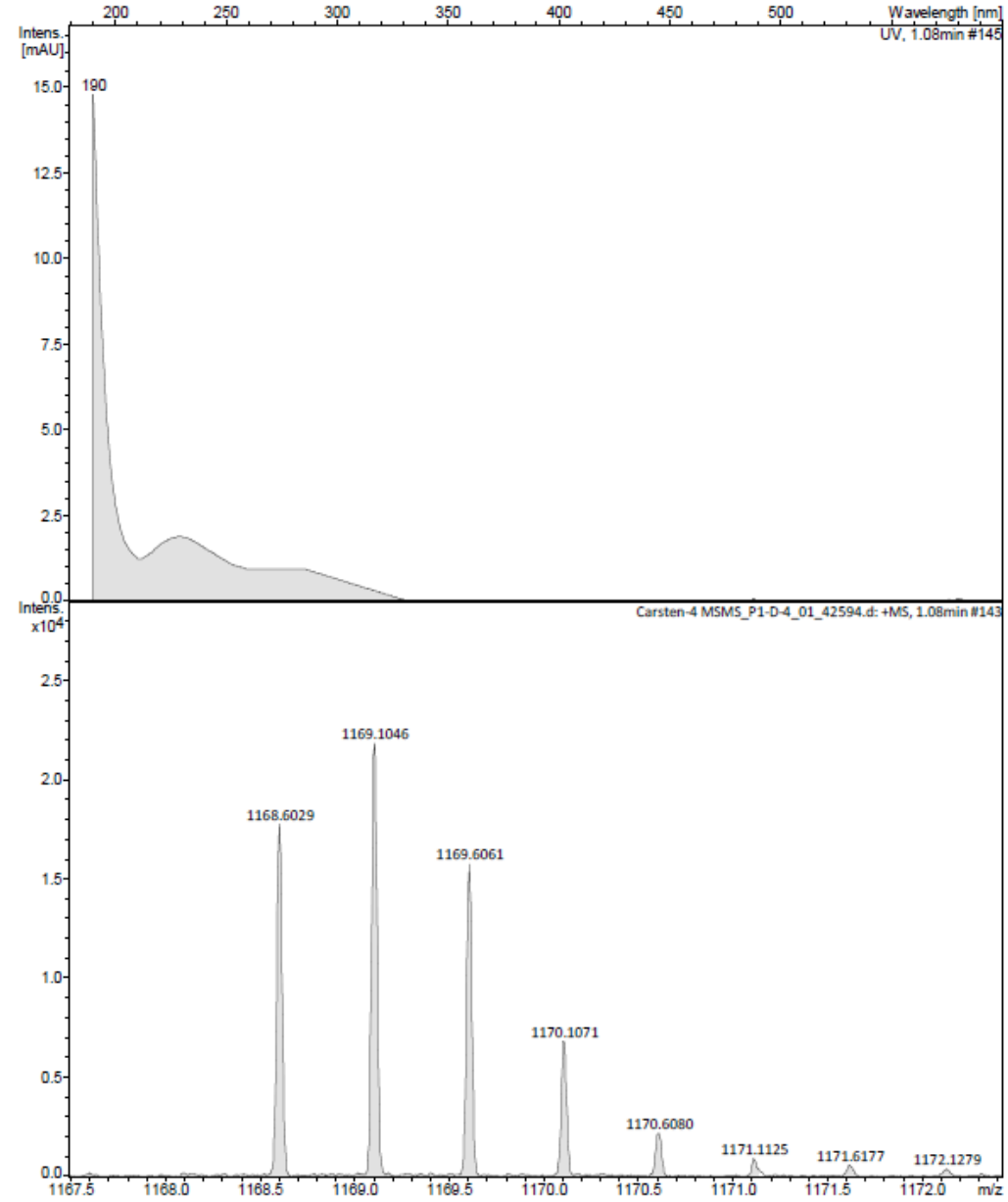
Window Display Report



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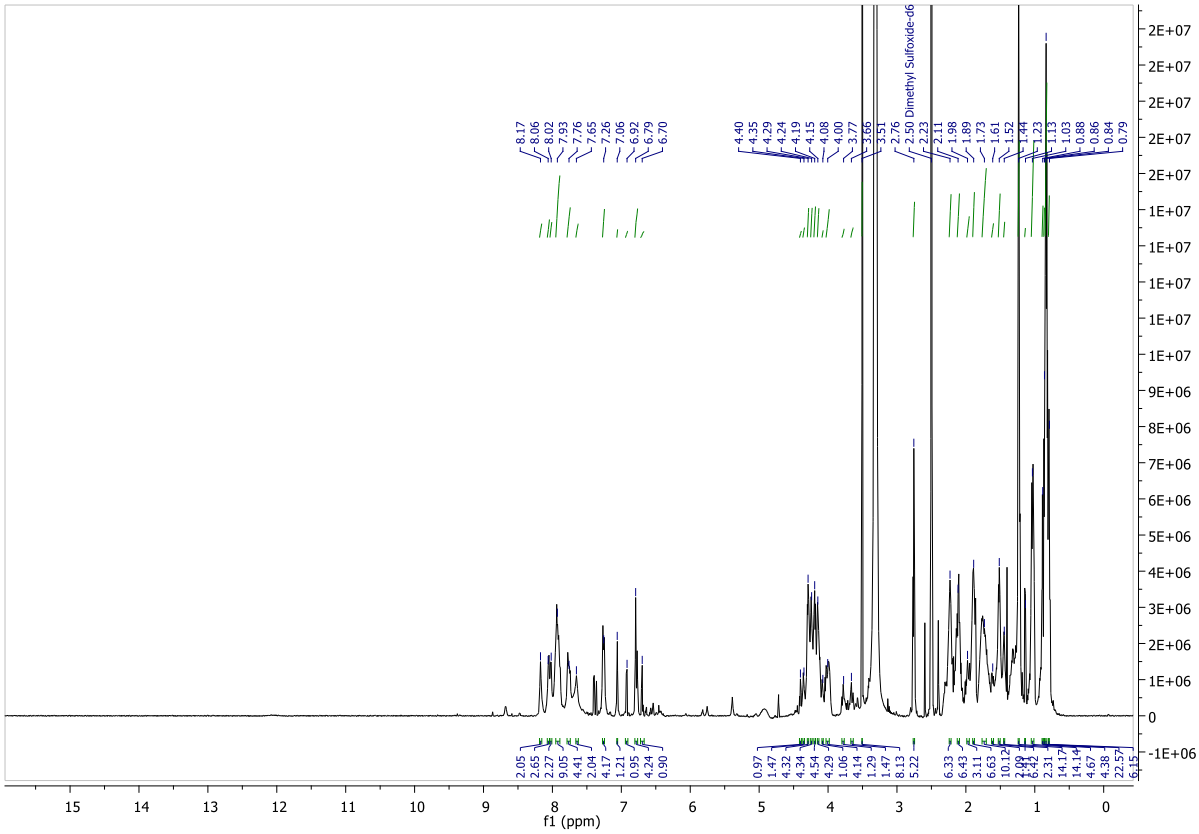
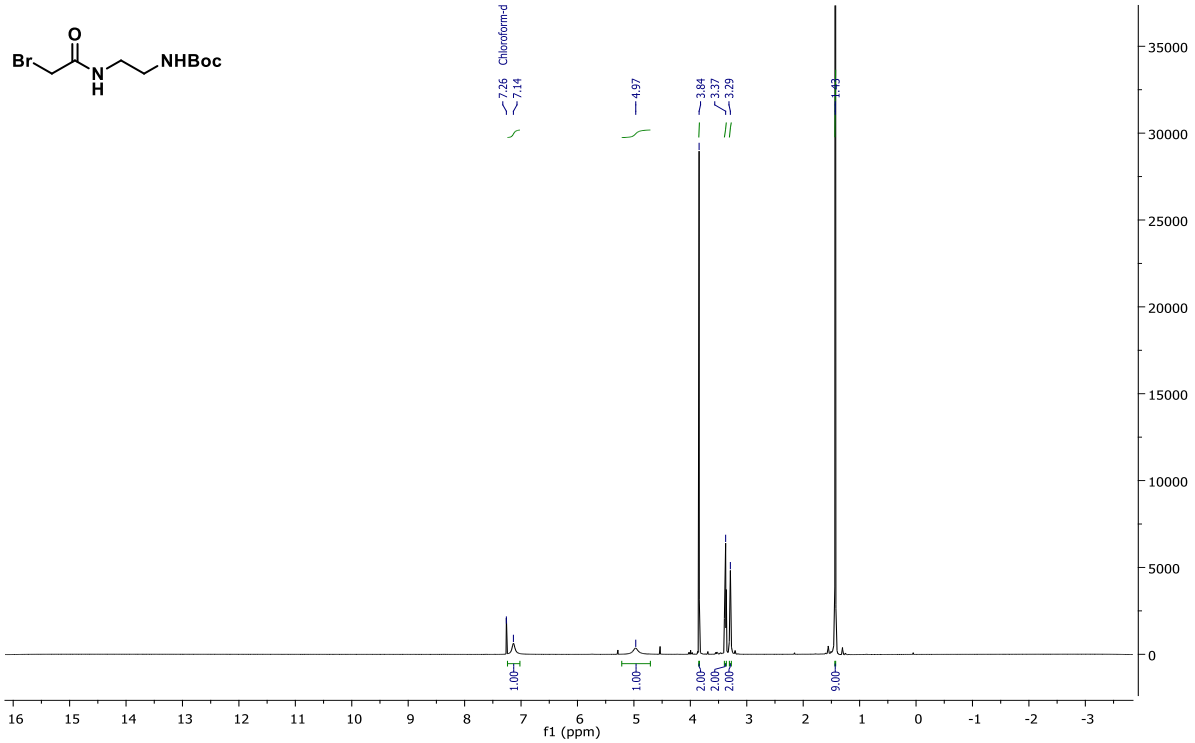
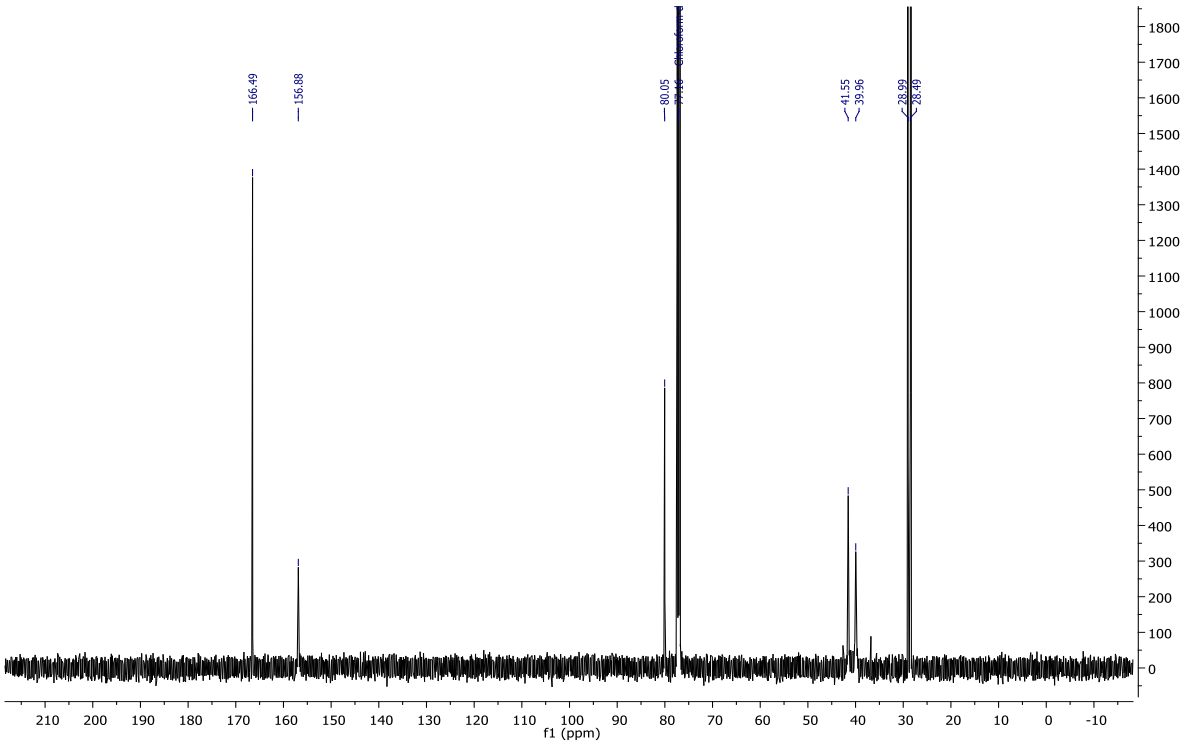
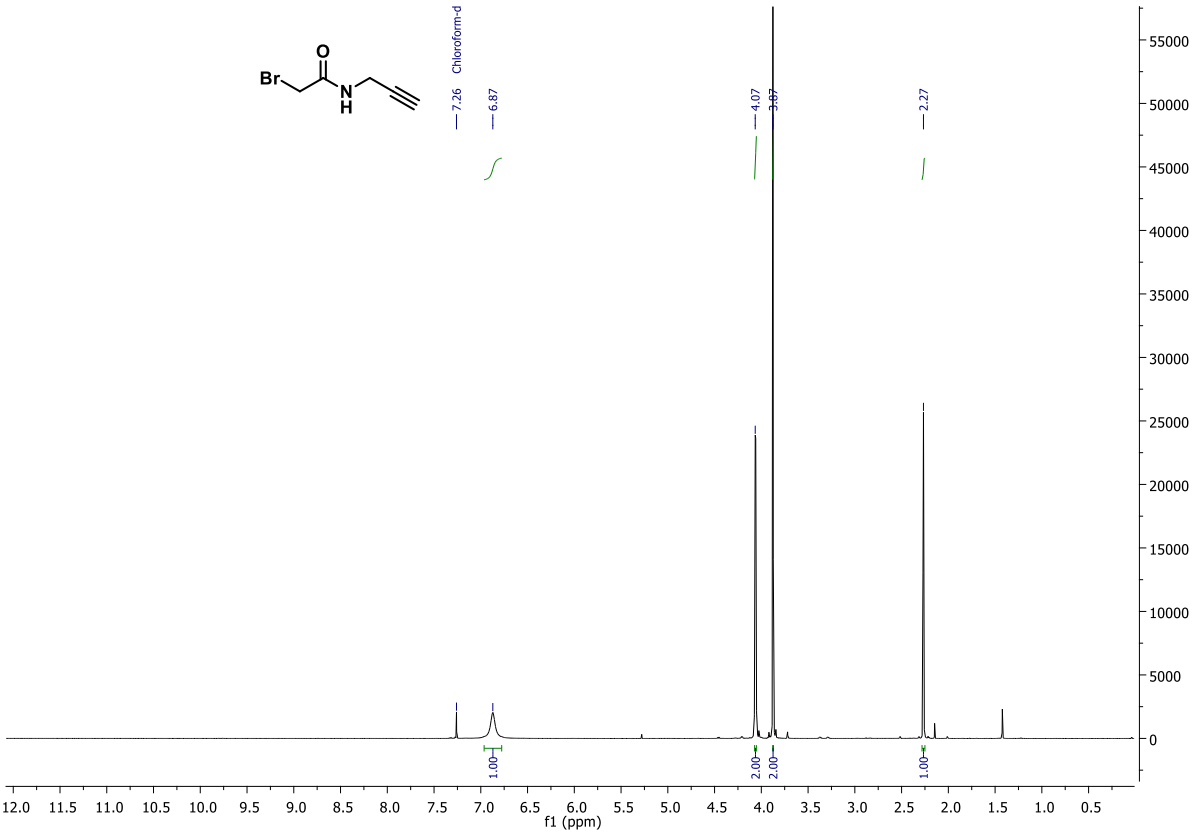

8.17
8.06
8.02
7.93
7.76
7.65
7.26
7.06
6.92
6.79
6.70
4.40
4.35
4.29
4.24
4.19
4.15
4.08
4.00
3.77
3.66
3.51
2.76
2.50 Dimethyl Sulfoxide-d6
2.23
2.11
1.98
1.89
1.73
1.61
1.52
1.44
1.23
1.13
1.03
0.88
0.86
0.84
0.79
2.05
2.65
2.27
9.05
4.41
2.04
4.17
1.21
0.95
4.24
0.90
0.97
1.47
4.32
4.34
4.54
4.29
1.06
4.14
1.29
1.47
8.13
5.22
6.33
6.43
3.11
6.63
10.12
2.08
6.42
2.31
14.17
14.14
4.67
4.38
22.57
6.15
2E+07
2E+07
2E+07
2E+07
2E+07
1E+07
1E+07
1E+07
1E+07
1E+07
1E+07
9E+06
8E+06
7E+06
6E+06
5E+06
4E+06
3E+06
2E+06
1E+06
0
-1E+06
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
f1 (ppm)

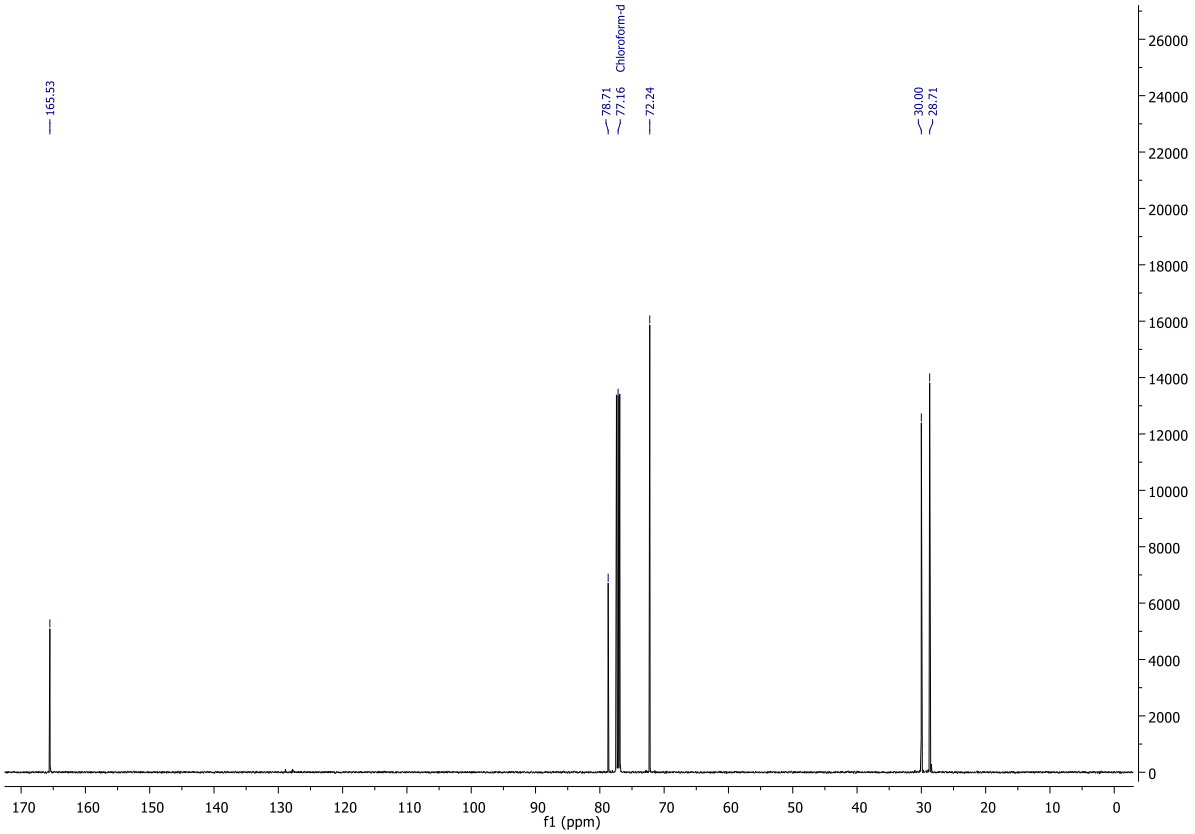
Compound 36


Br
O
N
H
NHBoc
Chloroform-d
7.26
7.14
4.97
3.84
3.37
3.29
1.43
1.00
1.00
2.00
2.00
2.00
9.00
f1 (ppm)

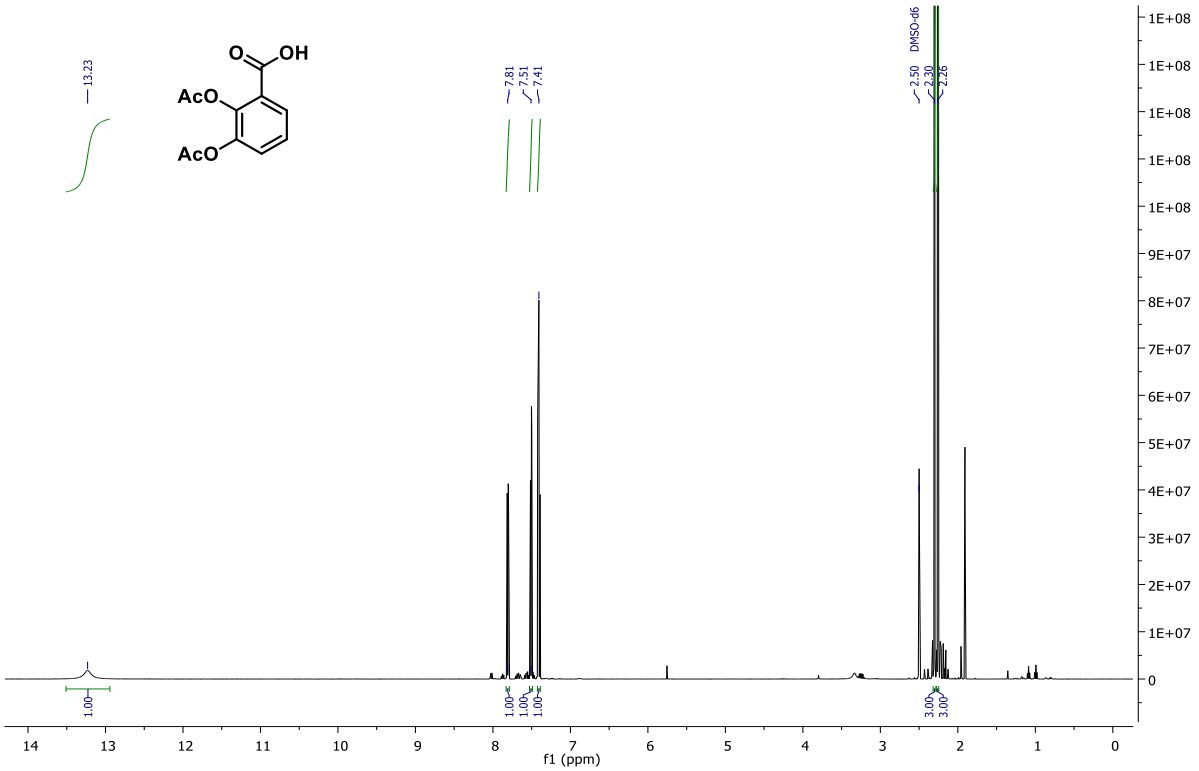

166.49
156.88
80.05
41.55
39.96
28.99
28.49
f1 (ppm)

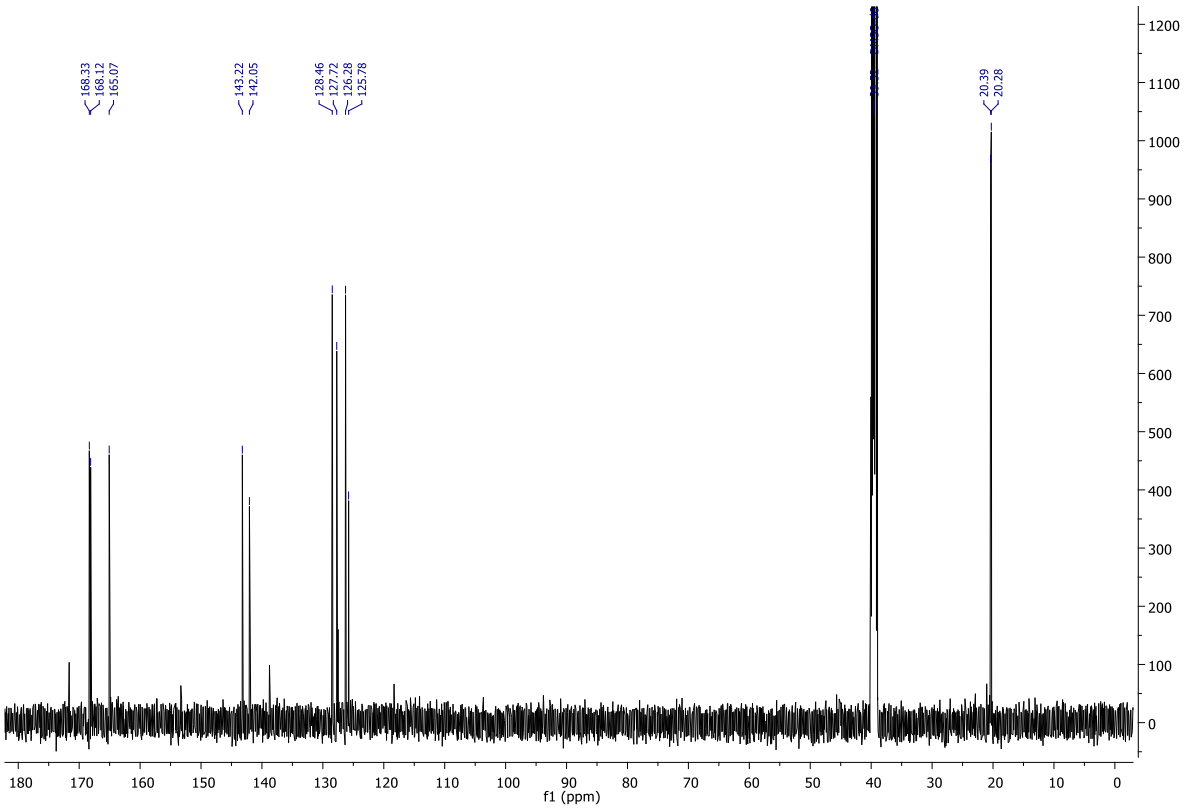
Compound 38


Br
O
N
H
Chloroform-d
7.26
6.87
4.07
3.87
2.27
1.00
2.00
2.00
1.00
f1 (ppm)

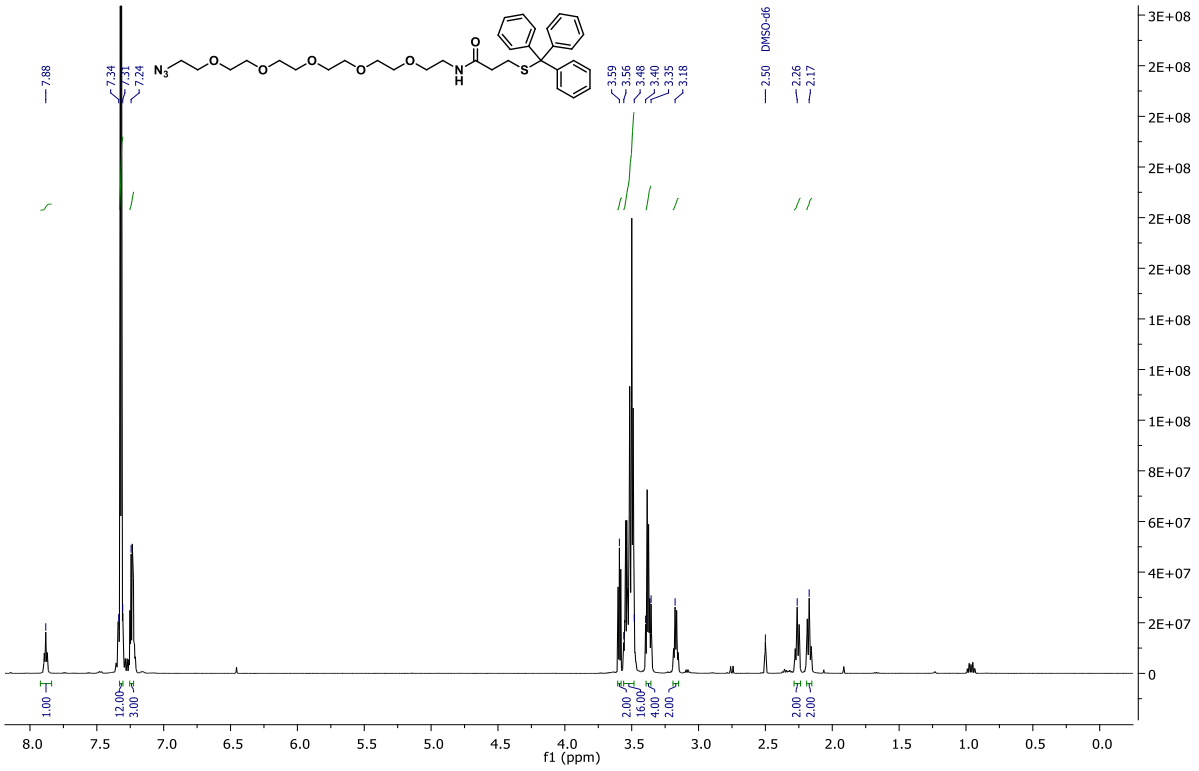

165.53
Chloroform-d
78.71
77.16
72.24
30.00
28.71
f1 (ppm)

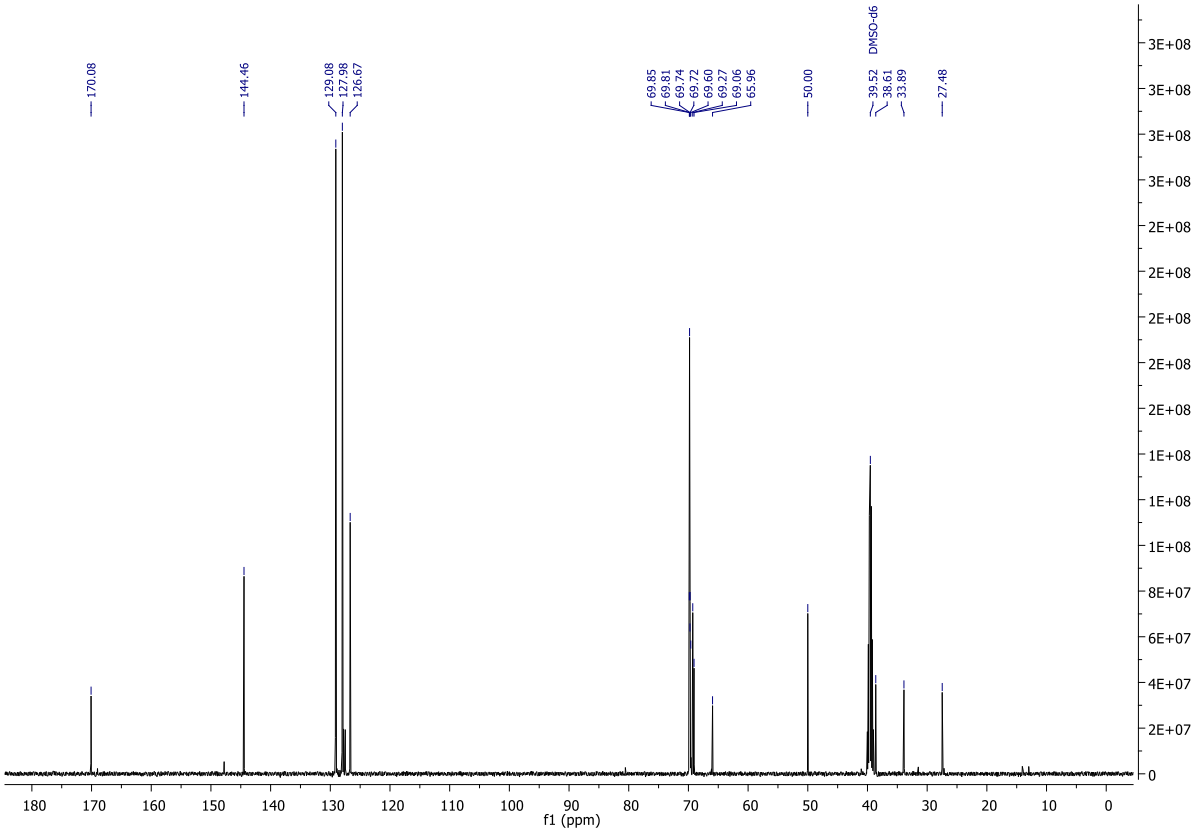
Compound 40


13.23
7.81
7.51
7.41
2.50
DMSO-d6
2.30
2.26
O
OH
AcO
AcO
1.00
1.00
1.00
1.00
3.00
3.00
f1 (ppm)

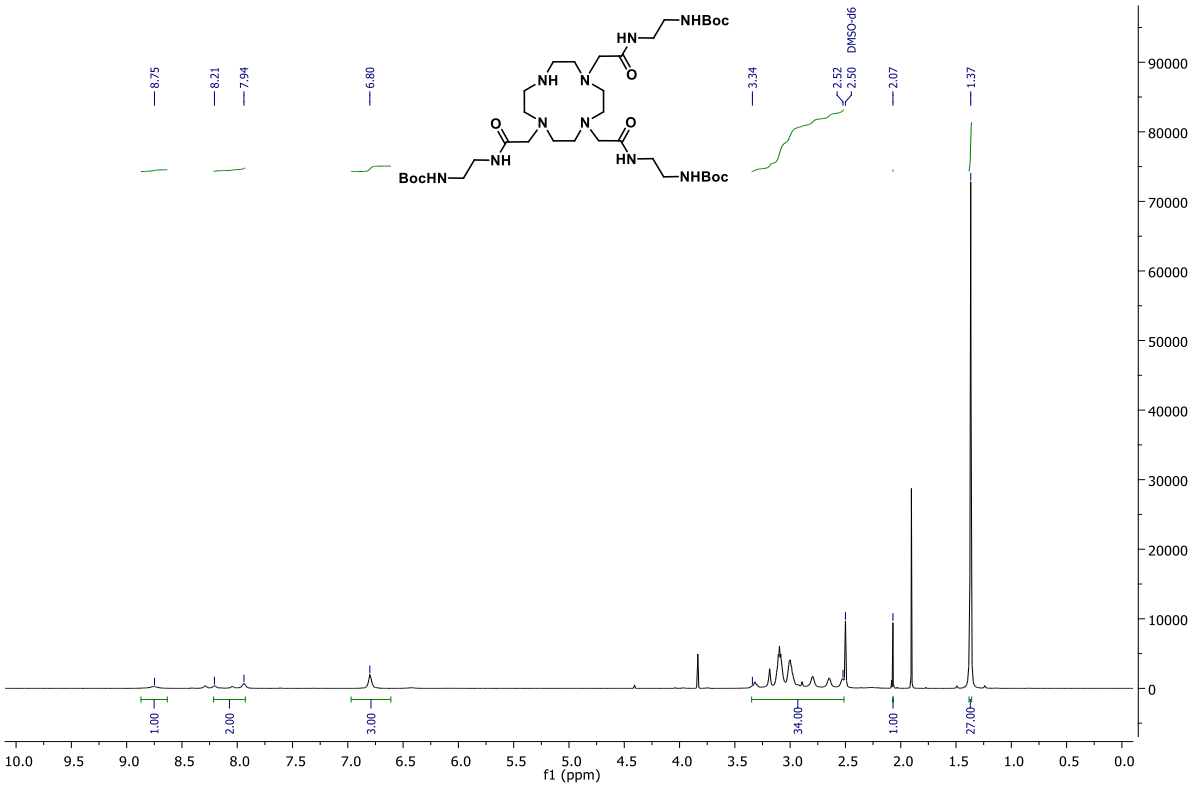

168.33
168.12
165.07
143.22
142.05
128.46
127.72
126.28
125.78
20.39
20.28
f1 (ppm)

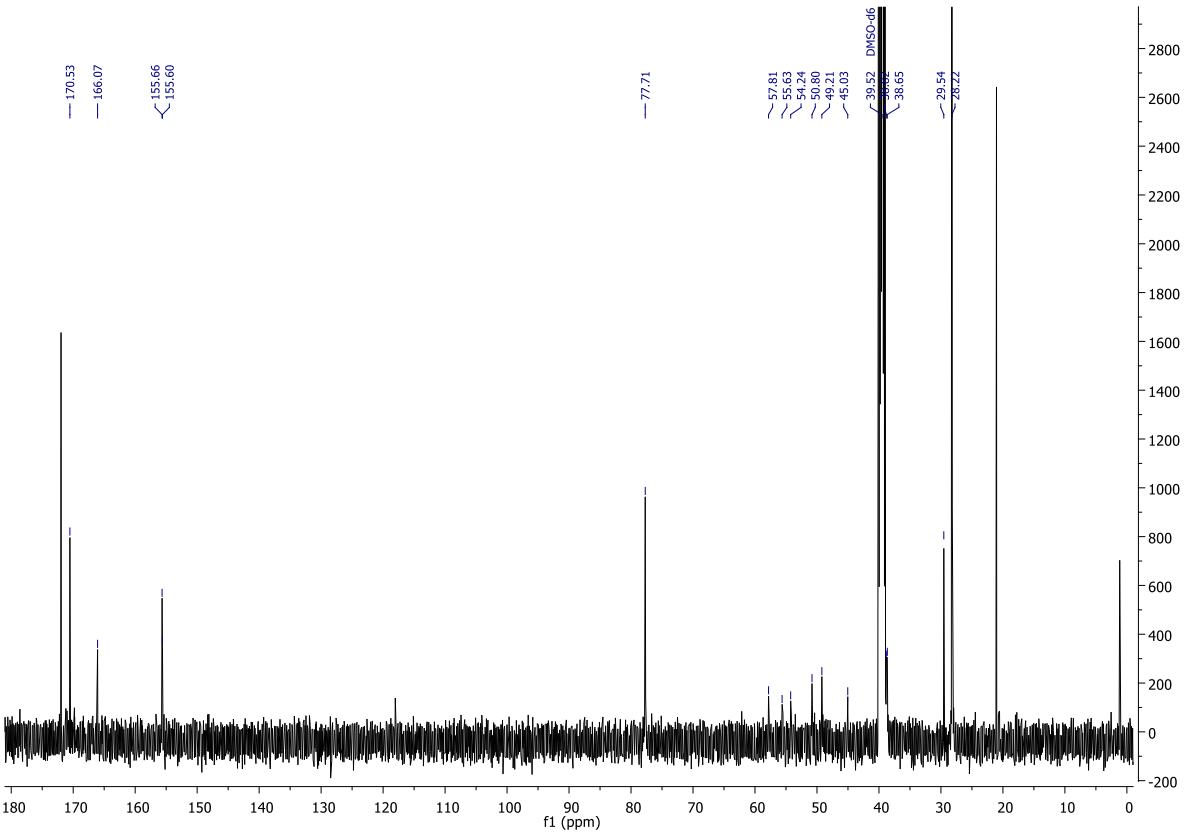
Compound 42


7.88
7.34
7.31
7.24
3.59
3.56
3.48
3.40
3.35
3.18
DMSO-d6
2.50
2.26
2.17
1.00
12.00
3.00
2.00
16.00
4.00
2.00
2.00
2.00
f1 (ppm)

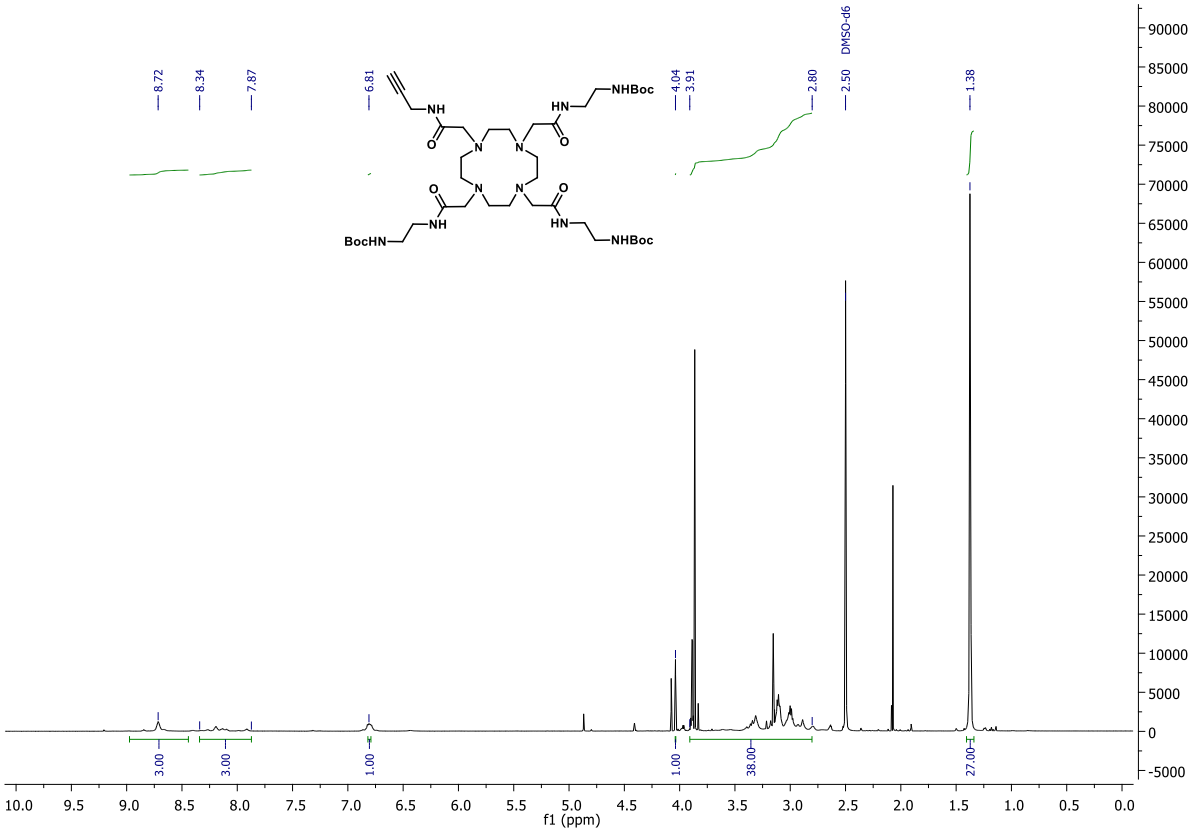

170.08
144.46
129.08
127.98
126.67
69.85
69.81
69.74
69.72
69.60
69.27
69.06
65.96
50.00
DMSO-d6
39.52
38.61
33.89
27.48
f1 (ppm)

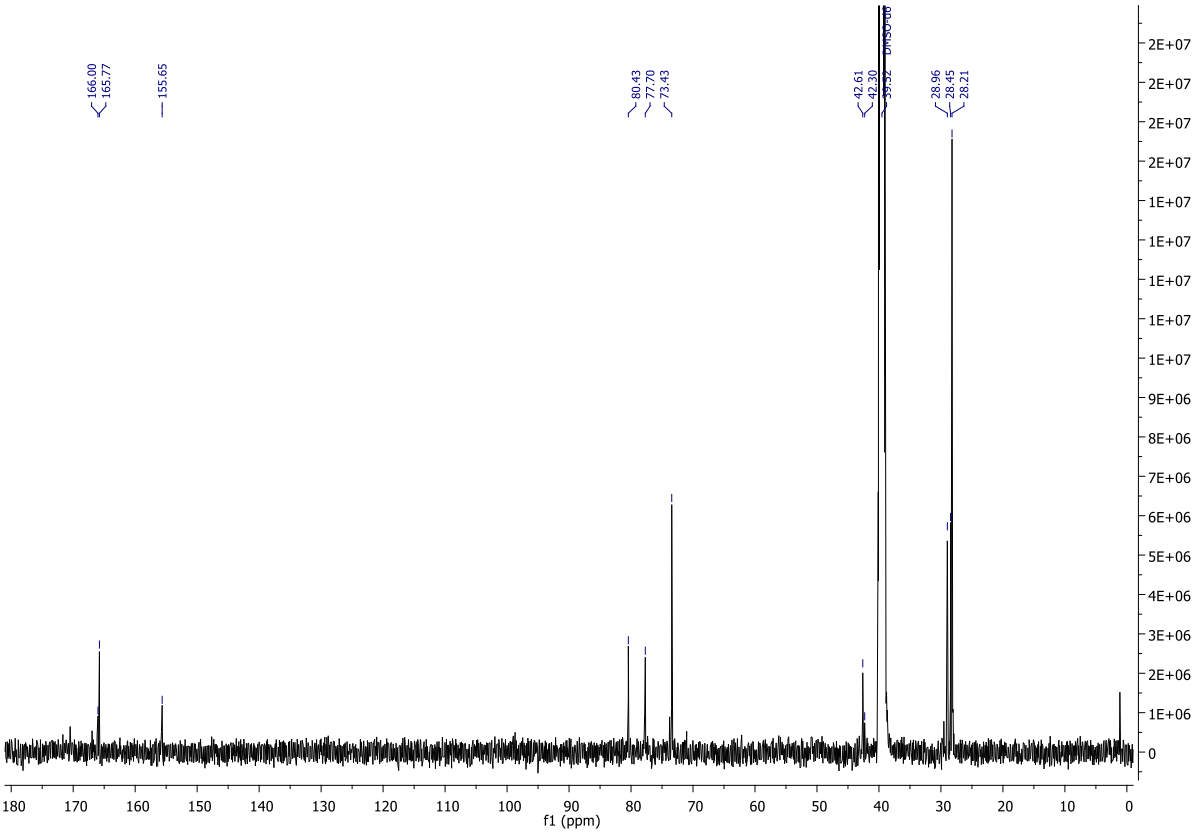
Compound 44


NHBoc
HN
NH
N
O
BocHN
8.75
8.21
7.94
6.80
3.34
2.52
2.50
DMSO-d6
2.07
1.37
1.00
2.00
3.00
34.00
1.00
27.00
f1 (ppm)

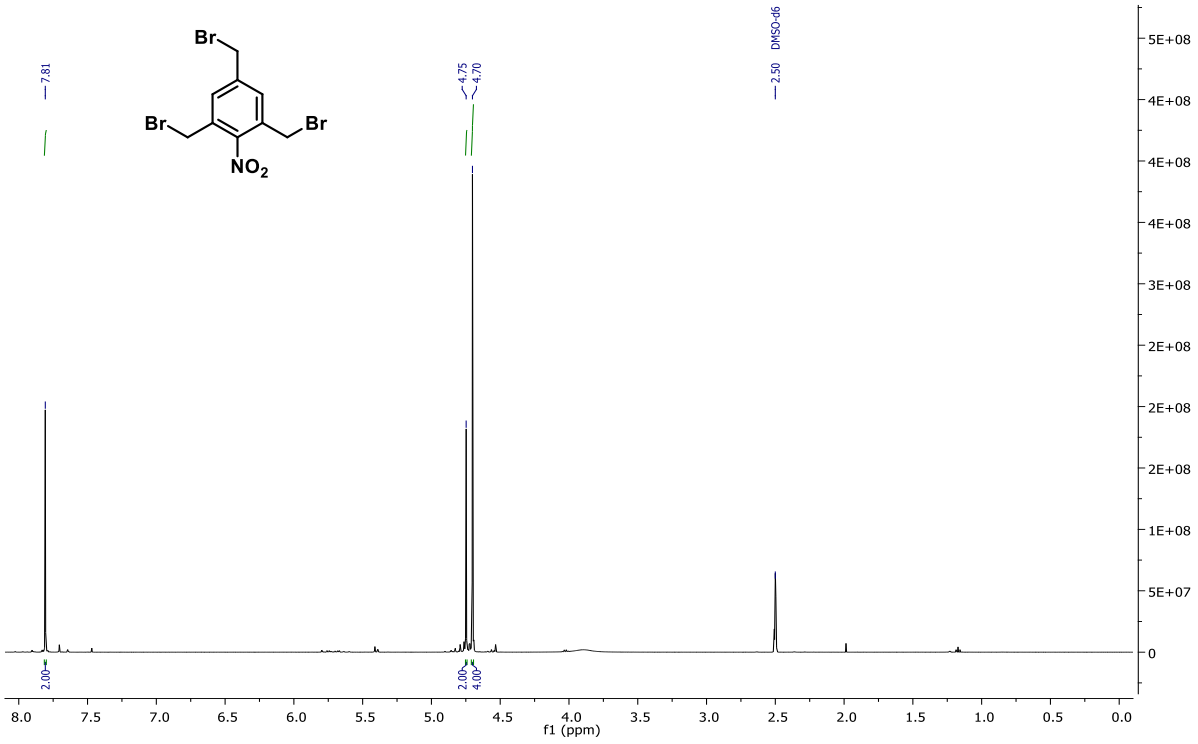

170.53
166.07
155.66
155.60
77.71
57.81
55.63
54.24
50.80
49.21
45.03
DMSO-d6
39.52
38.65
29.54
28.22
f1 (ppm)

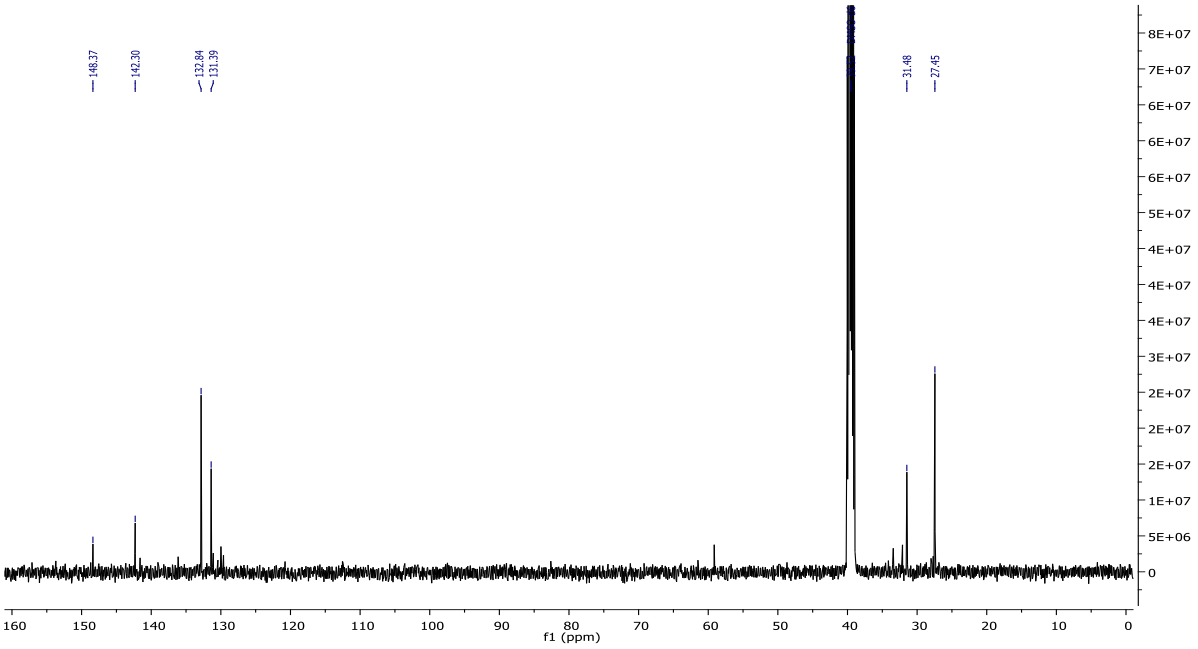
Compound 45


8.72
8.34
7.87
6.81
4.04
3.91
2.80
2.50
DMSO-d6
1.38
NHBoc
HN
NH
BocHN
3.00
3.00
1.00
1.00
38.00
27.00
f1 (ppm)

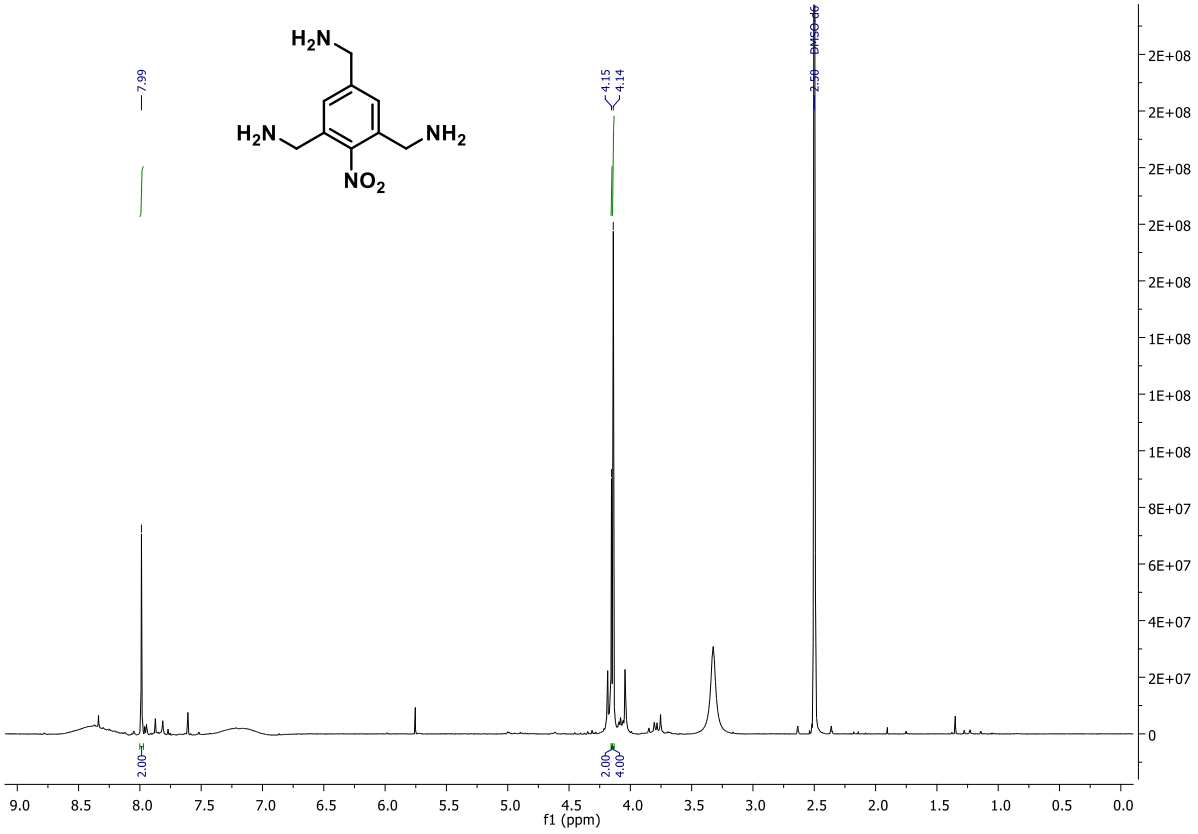

166.00
165.77
155.65
80.43
77.70
73.43
42.61
42.30
39.92
DMSO-d6
28.96
28.45
28.21
f1 (ppm)

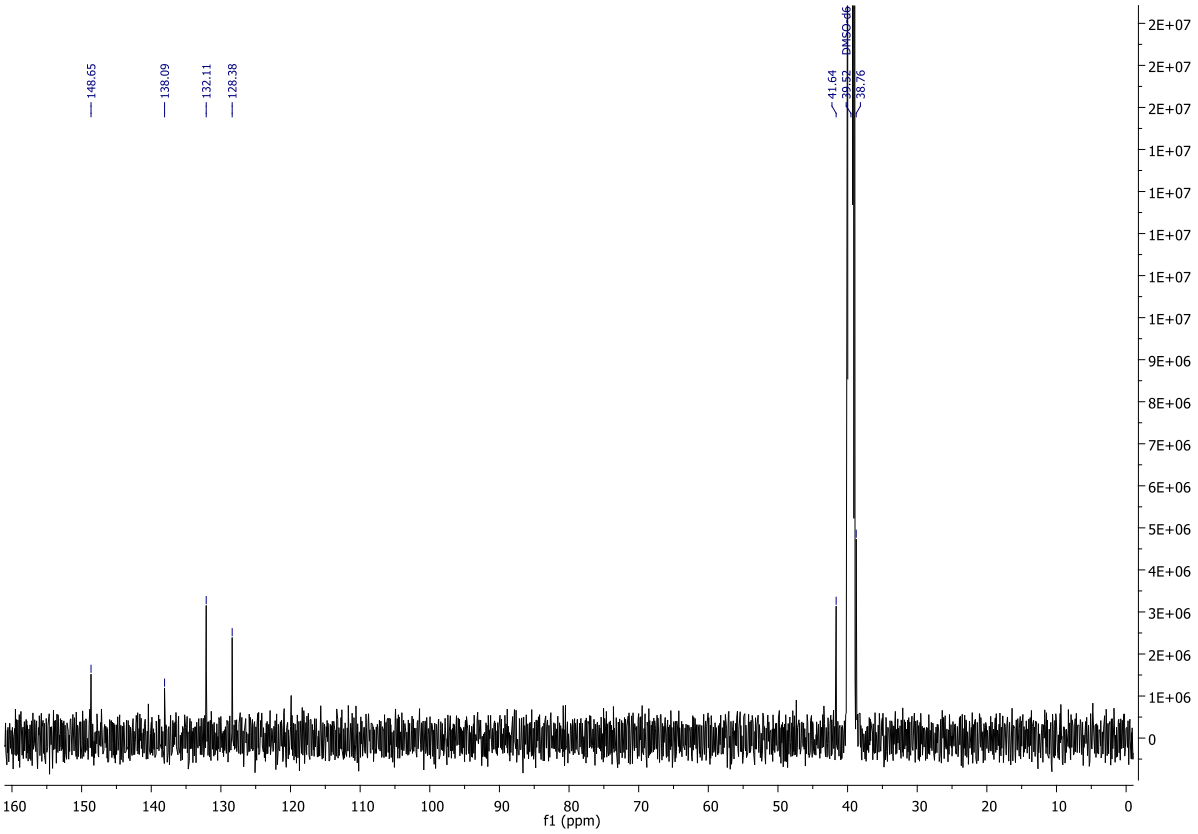
Compound 48


Br
Br
Br
NO2
7.81
4.75
4.70
2.50
DMSO-d6
2.00
2.00
4.00
f1 (ppm)

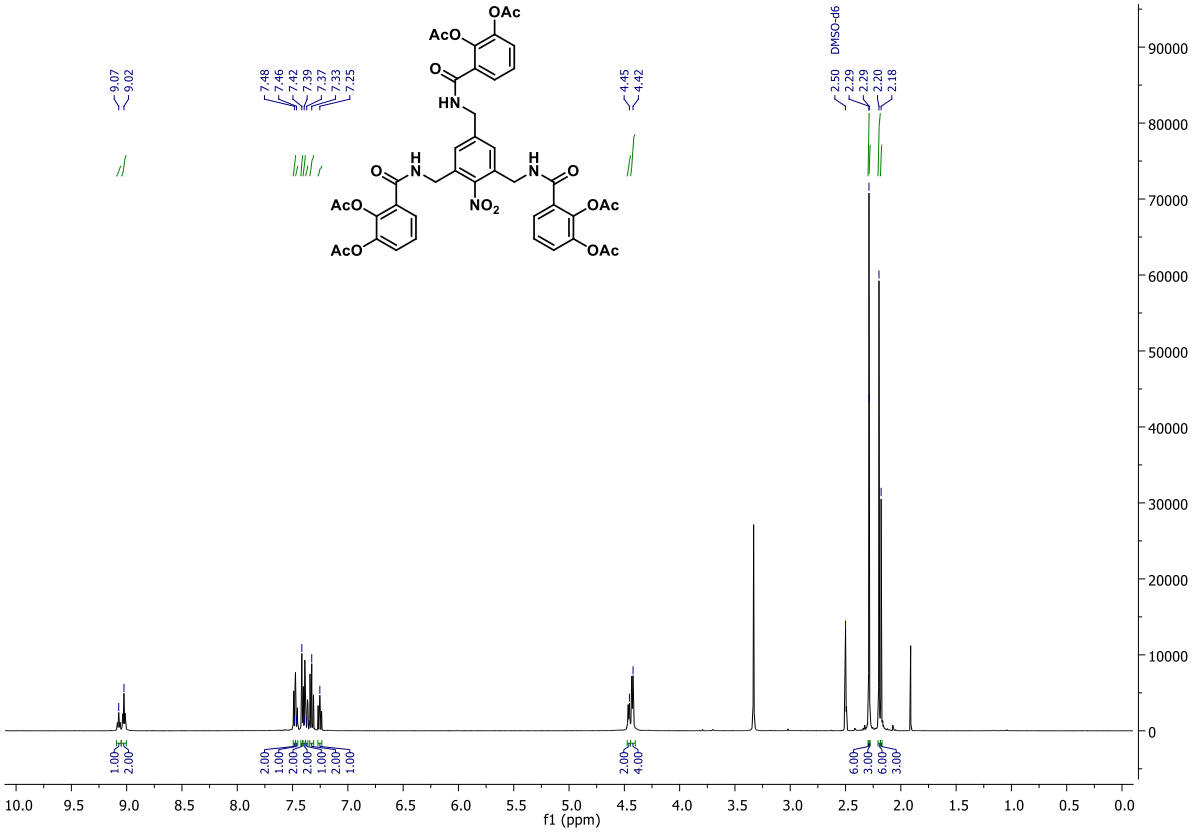

148.37
142.30
132.84
131.39
31.48
27.45
f1 (ppm)

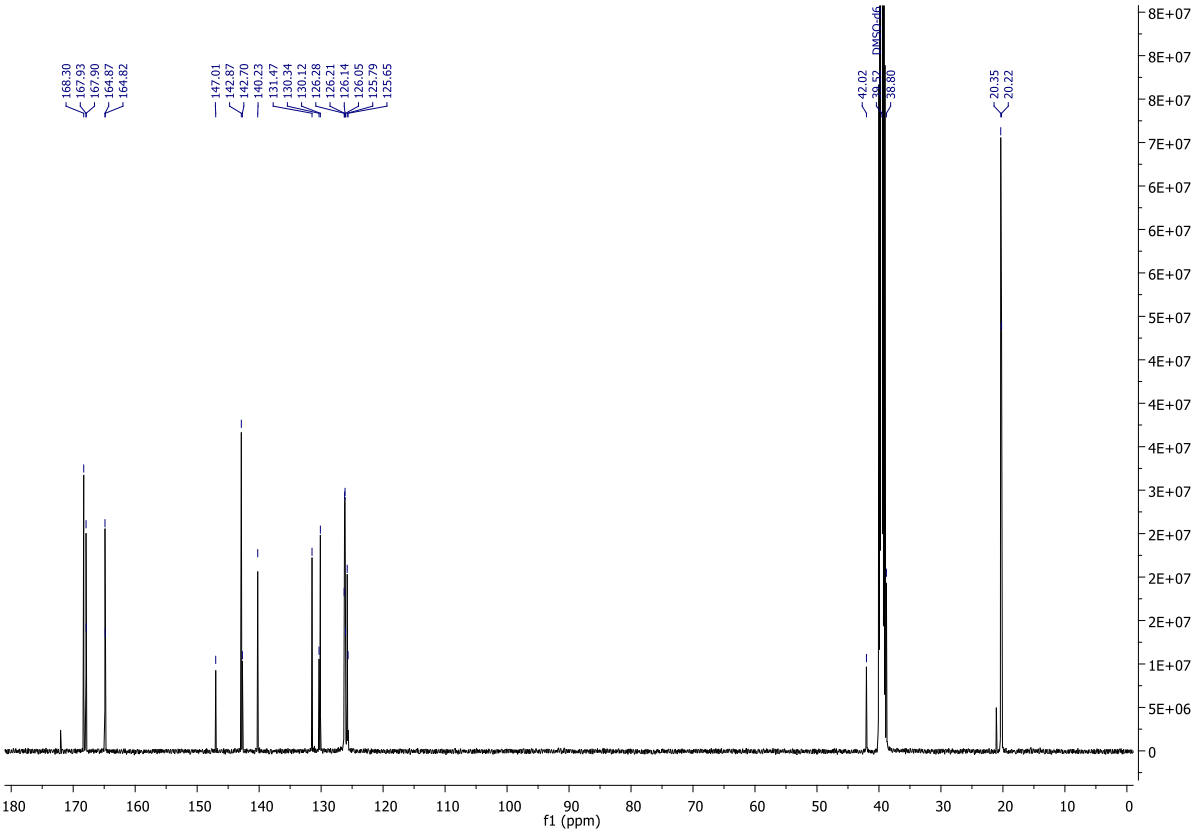
Compound 49


H2N
NH2
H2N
NO2
7.99
4.15
4.14
2.50 DMSO-d6
2.00
2.00
4.00
f1 (ppm)

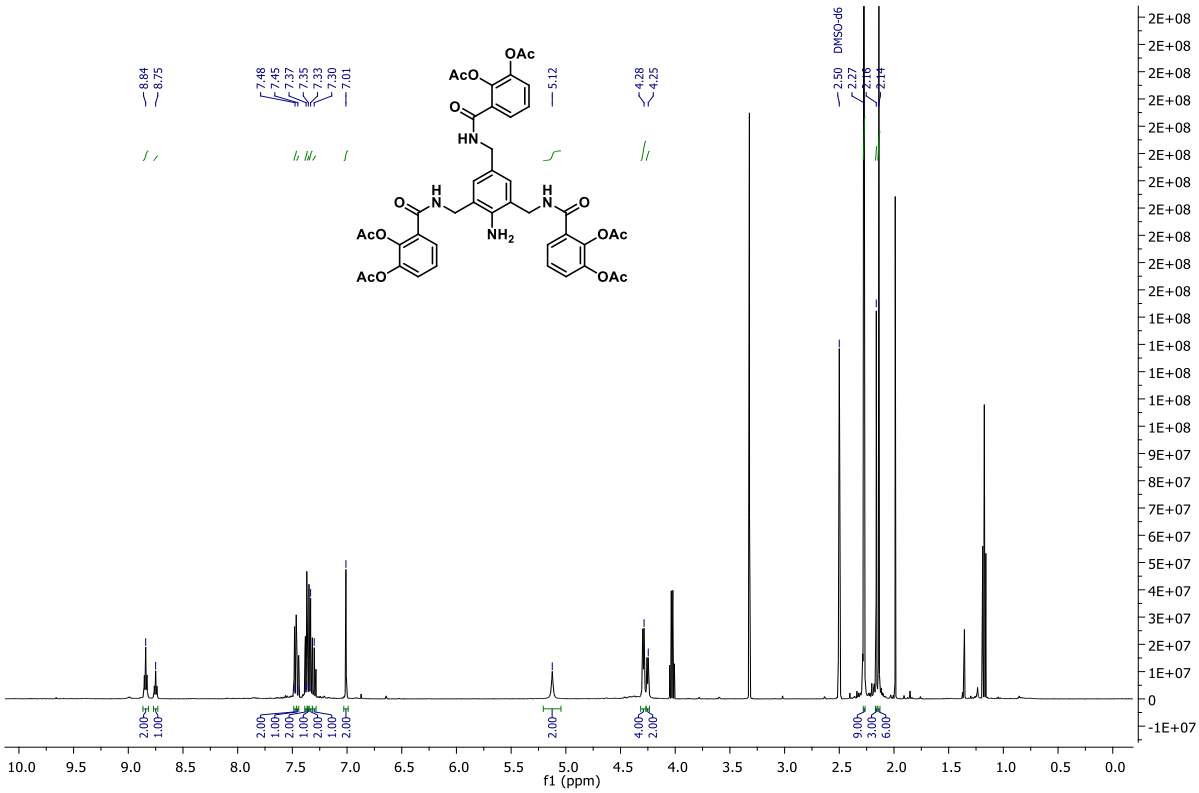

148.65
138.09
132.11
128.38
41.64
39.52 DMSO-d6
38.76
f1 (ppm)

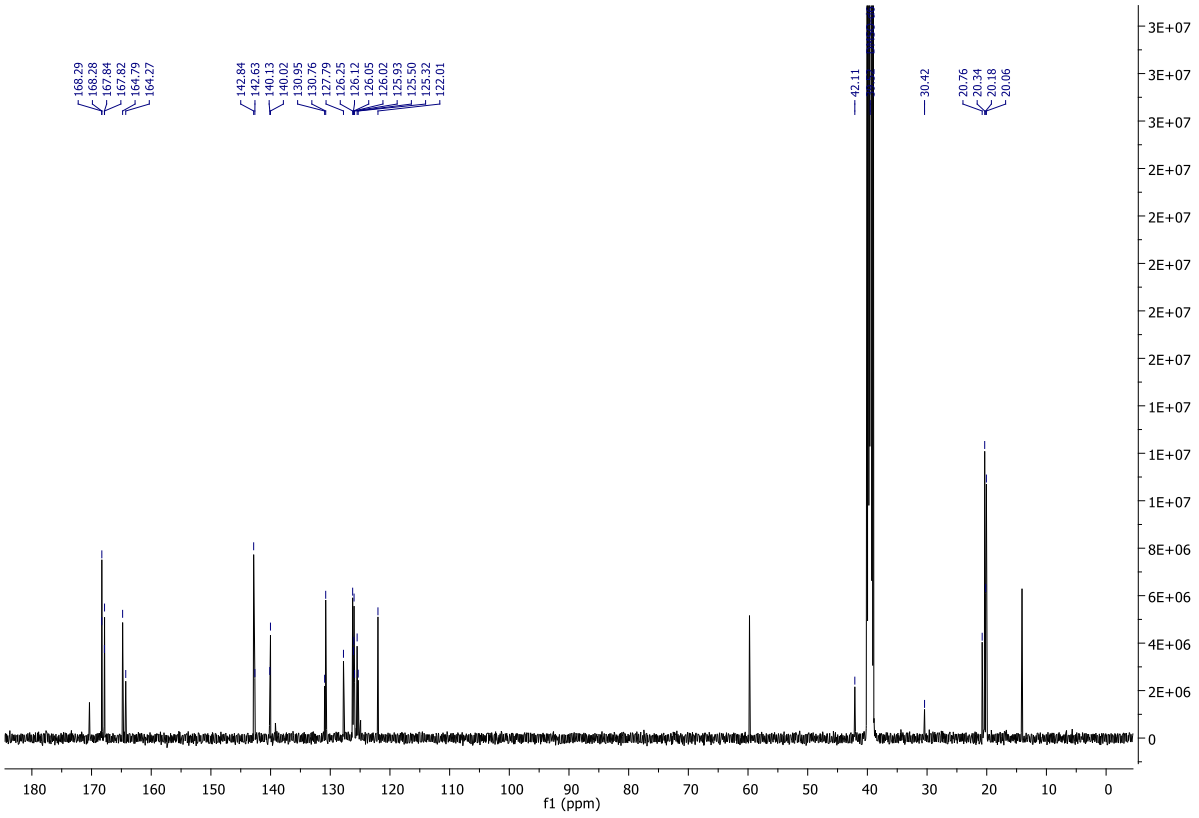
Compound 50


OAc
AcO
O
HN
H
N
O
NO2
AcO
AcO
OAc
OAc
9.07
9.02
7.48
7.46
7.42
7.39
7.37
7.33
7.25
4.45
4.42
DMSO-d6
2.50
2.29
2.29
2.20
2.18
f1 (ppm)

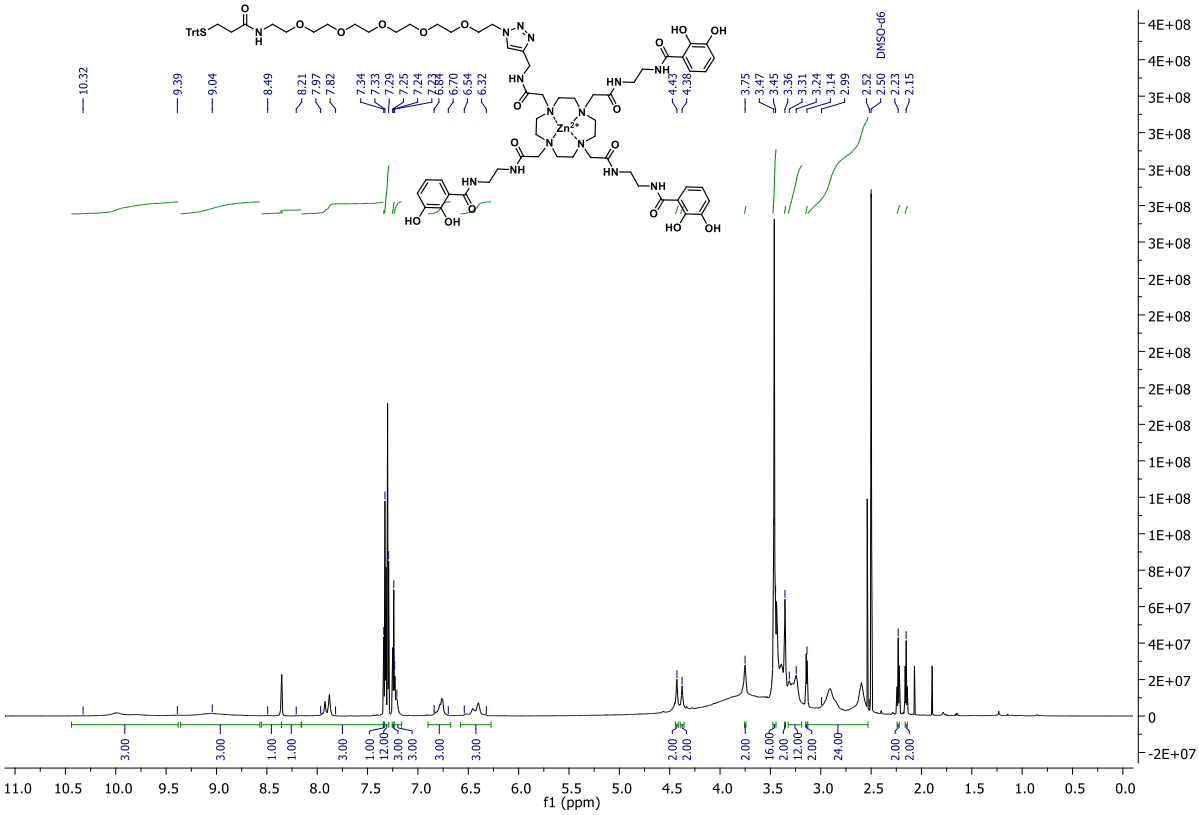

168.30
167.93
167.90
164.87
164.82
147.01
142.87
142.70
140.23
131.47
130.34
130.12
126.28
126.21
126.14
126.05
125.79
125.65
DMSO-d6
42.02
39.52
38.80
20.35
20.22
f1 (ppm)

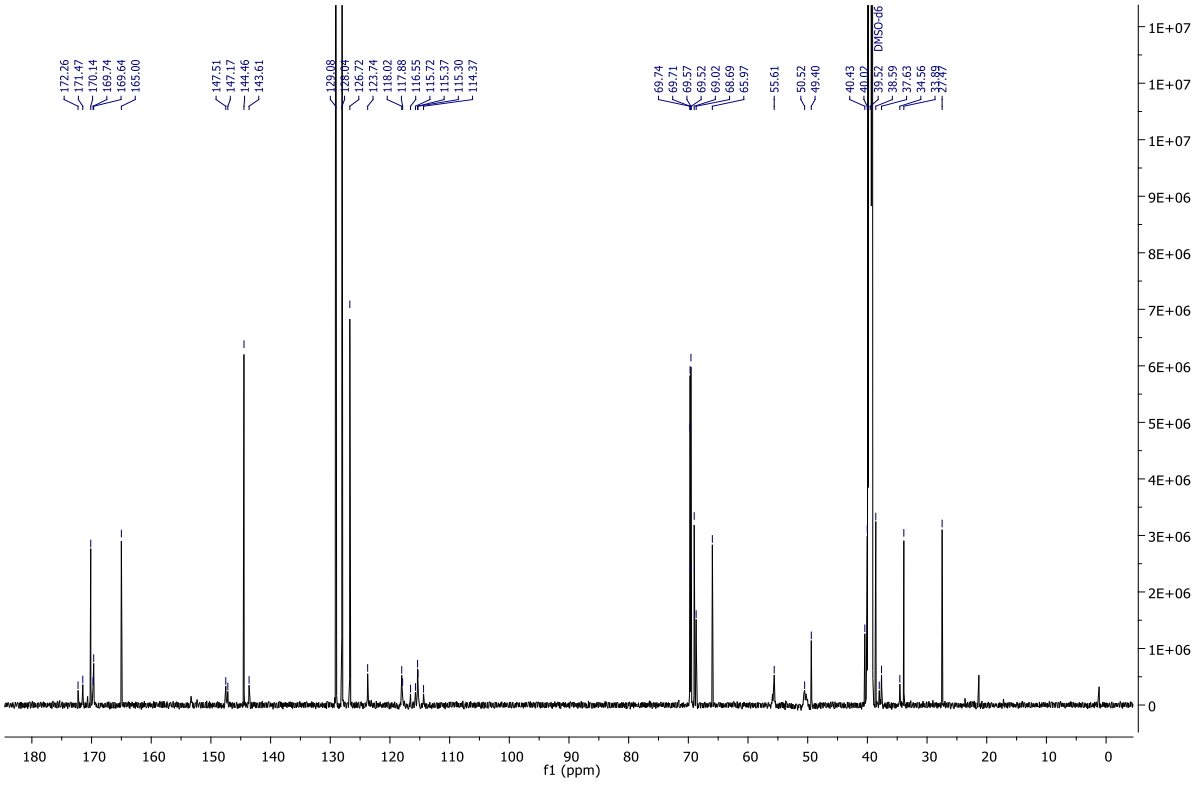
Compound 51


8.84
8.75
7.48
7.45
7.37
7.35
7.33
7.30
7.01
5.12
4.28
4.25
2.50
DMSO-d6
2.27
2.16
2.14
OAc
AcO
HN
NH2
f1 (ppm)

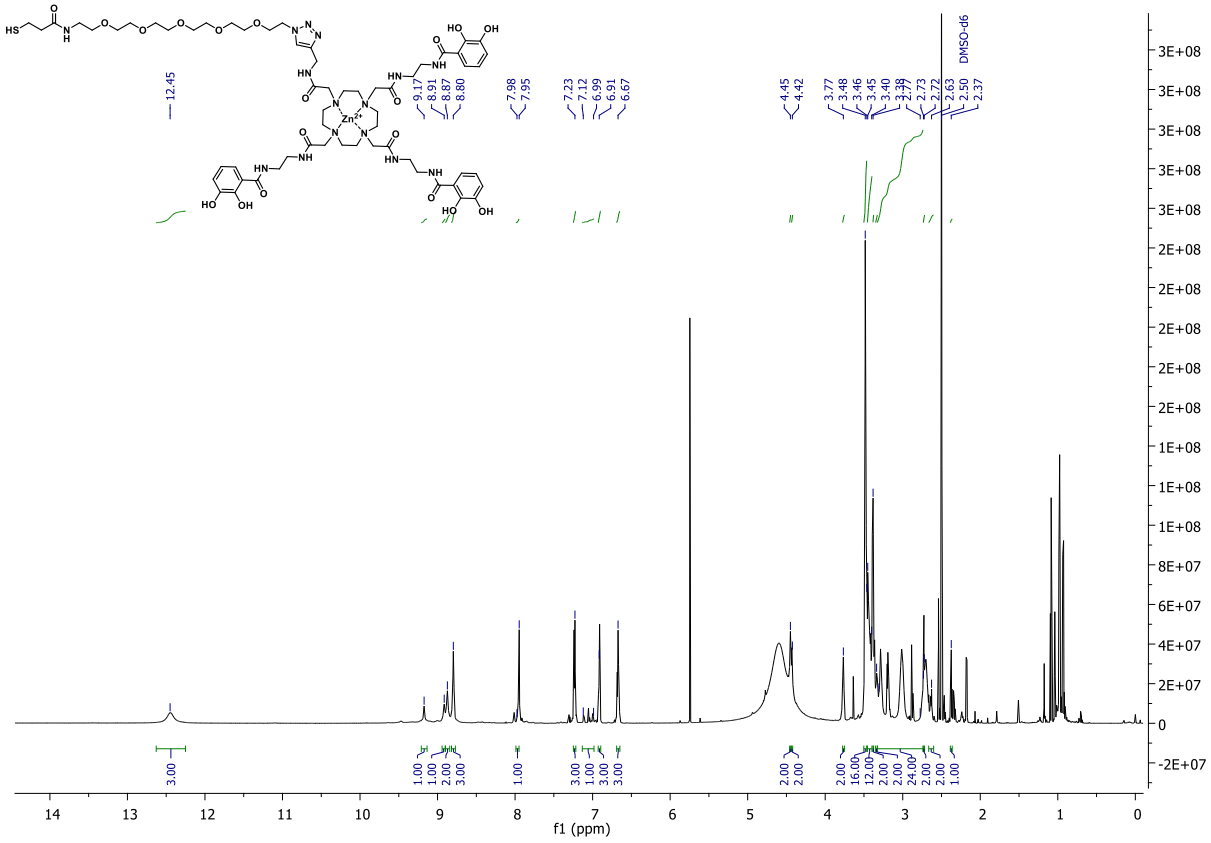

168.29
168.28
167.84
167.82
164.79
164.27
142.84
142.63
140.13
140.02
130.95
130.76
127.79
126.25
126.12
126.05
126.02
125.93
125.50
125.32
122.01
42.11
30.42
20.76
20.34
20.18
20.06
f1 (ppm)

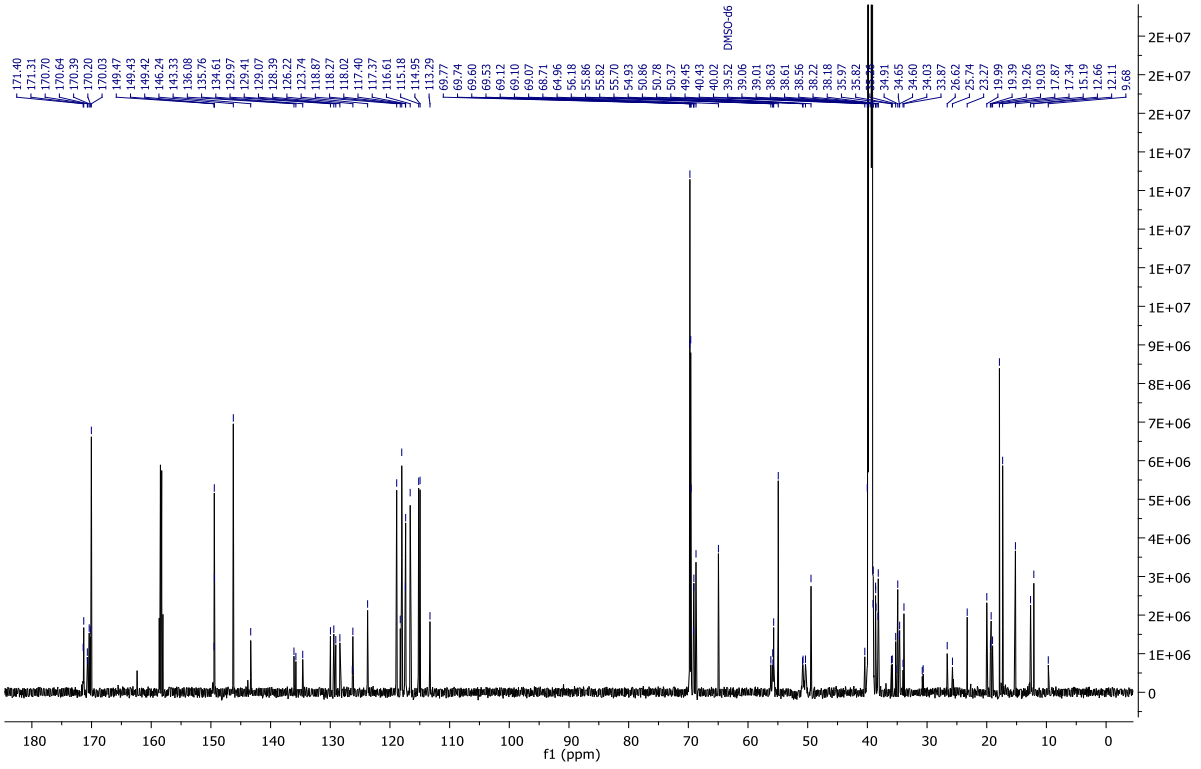
Compound 52a



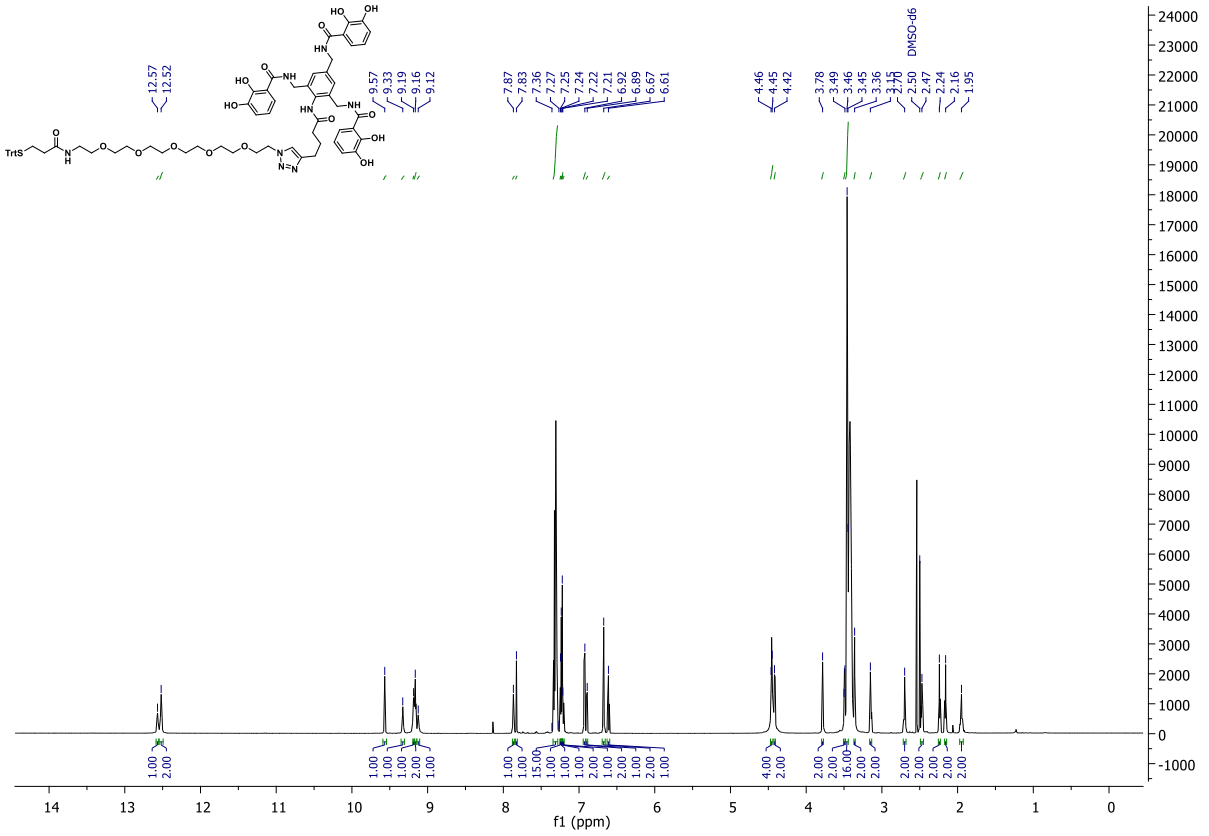


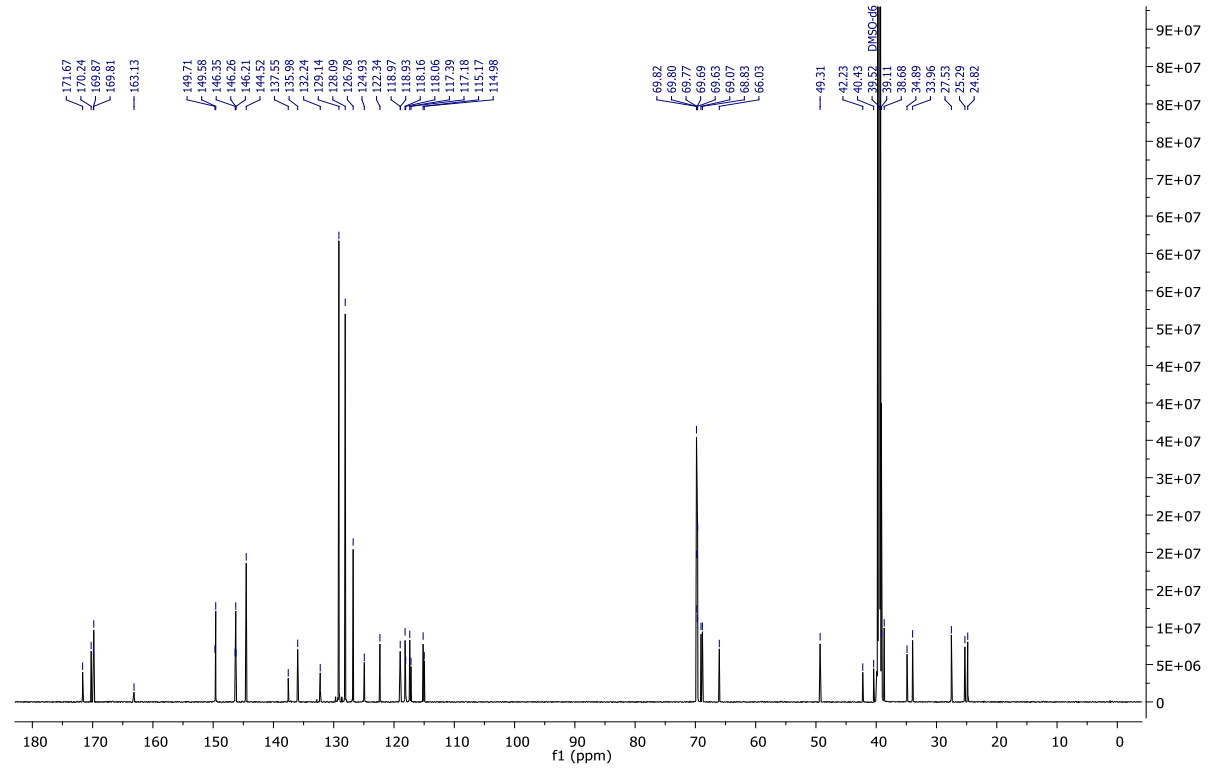
Compound 52


12.45
9.17
8.91
8.87
8.80
7.98
7.95
7.23
7.12
6.99
6.91
6.67
4.45
4.42
3.77
3.48
3.46
3.45
3.40
2.77
2.73
2.72
2.63
2.50
2.37
DMSO-d6
f1 (ppm)

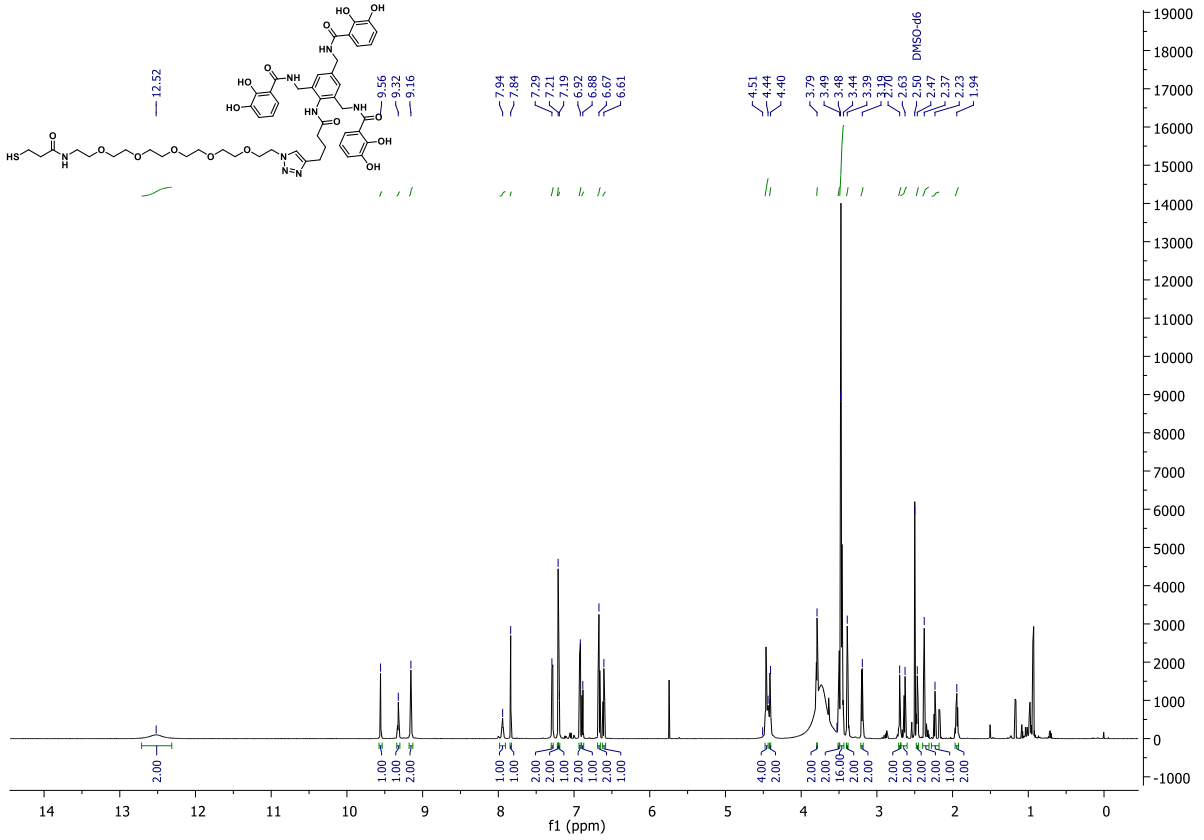

DMSO-d6
f1 (ppm)

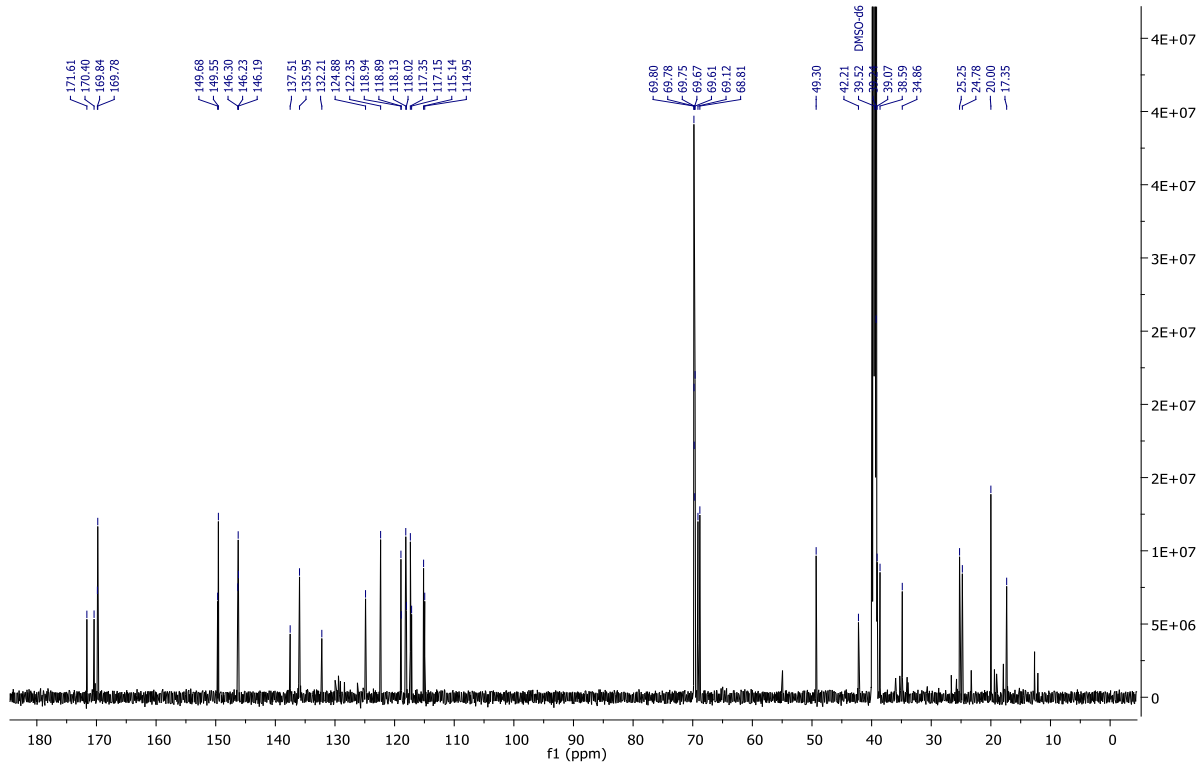
Compound 53a



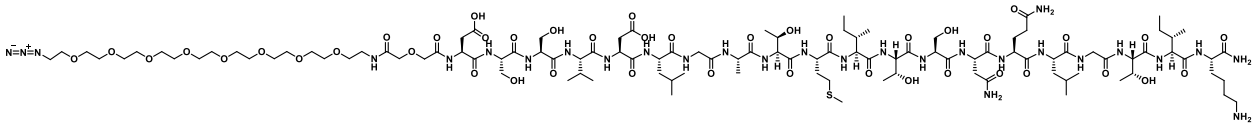


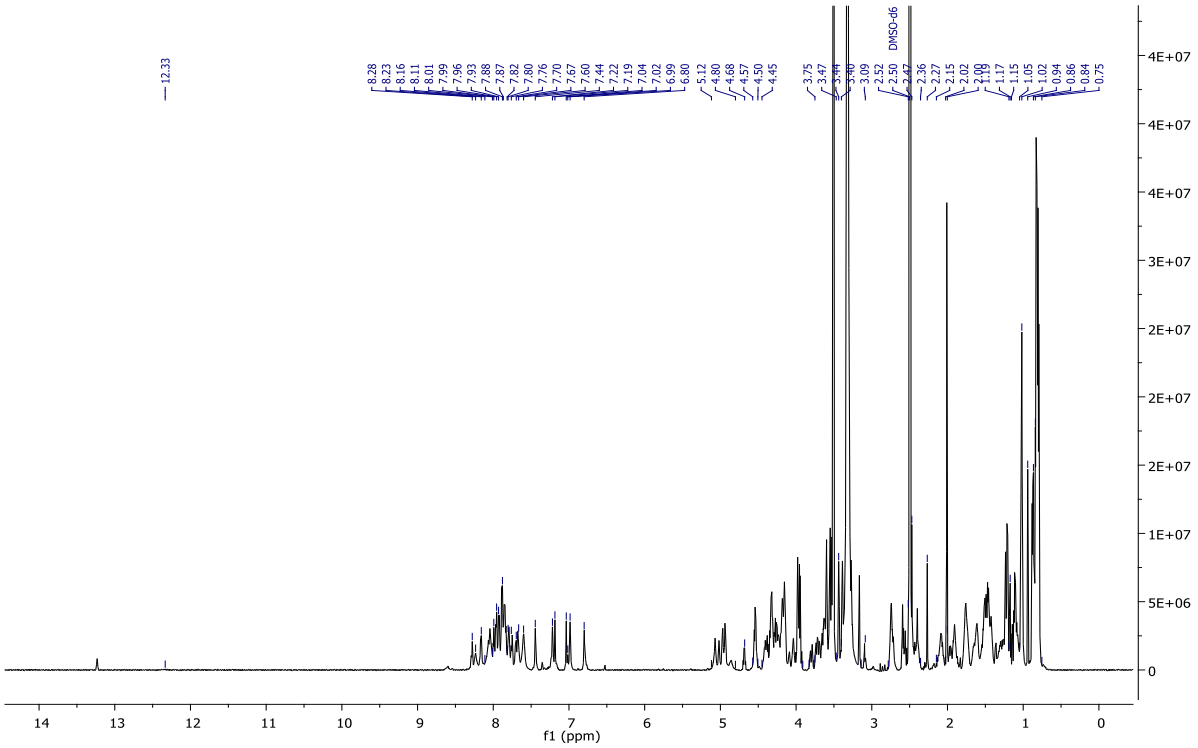
Compound 53

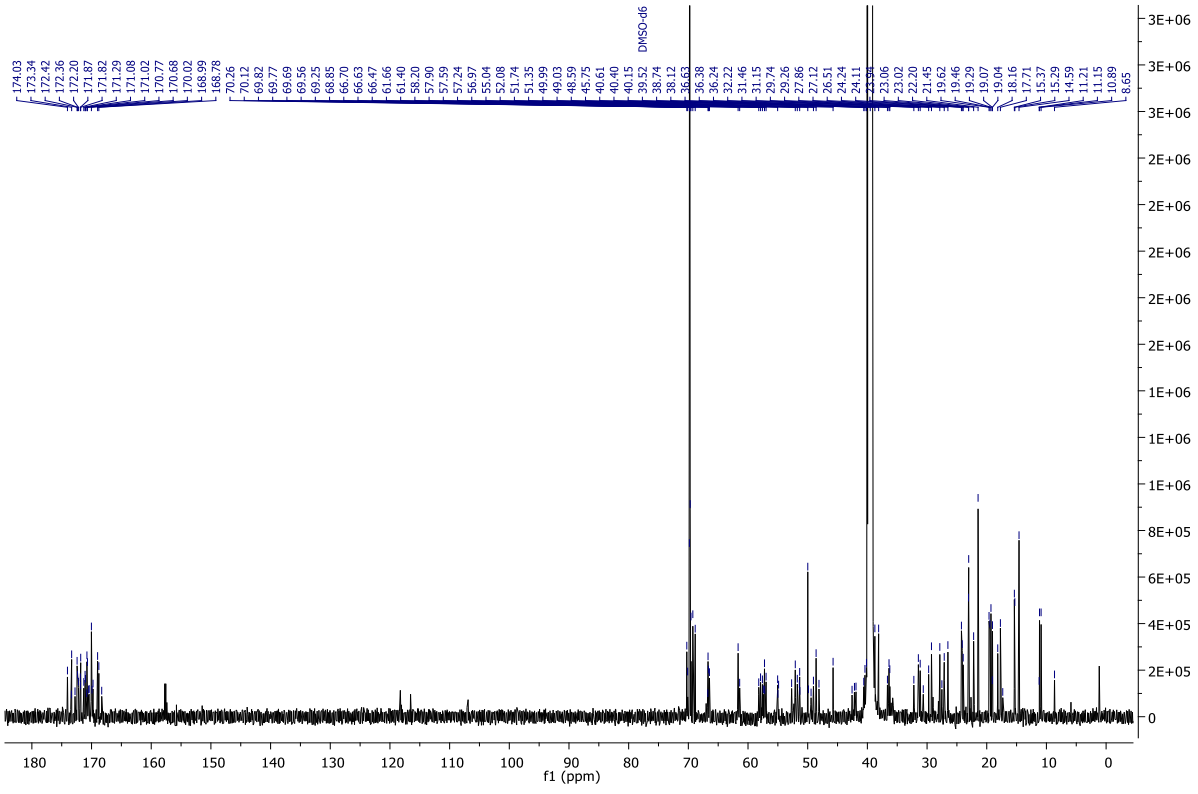

12.52
9.56
9.32
9.16
7.94
7.84
7.29
7.21
7.19
6.92
6.88
6.67
6.61
4.51
4.44
4.40
3.79
3.49
3.48
3.44
3.39
3.18
2.70
2.63
2.50
DMSO-d6
2.47
2.37
2.23
1.94
f1 (ppm)

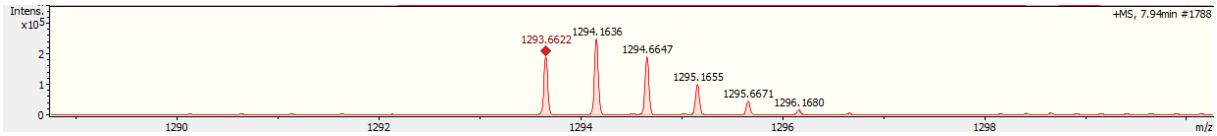

171.61
170.40
169.84
169.78
149.68
149.55
146.30
146.23
146.19
137.51
135.95
132.21
124.88
122.35
118.94
118.89
118.13
118.02
117.35
117.15
115.14
114.95
69.80
69.78
69.75
69.67
69.61
69.12
68.81
49.30
42.21
39.52
DMSO-d6
39.07
38.59
34.86
25.25
24.78
20.00
17.35
f1 (ppm)

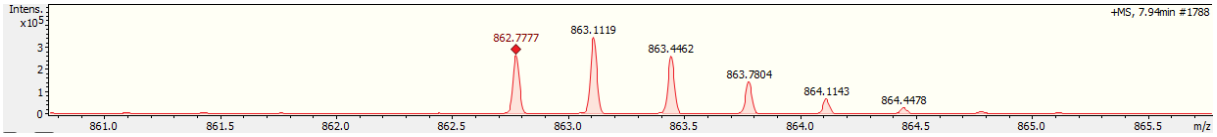
Compound 61 (*FpvA* 121-139 *N*-term Carbonyl-$(PEG)_7$-azide peptide)



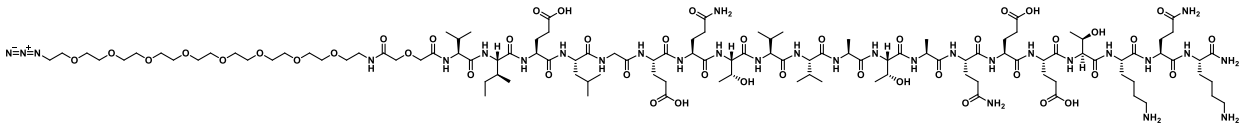


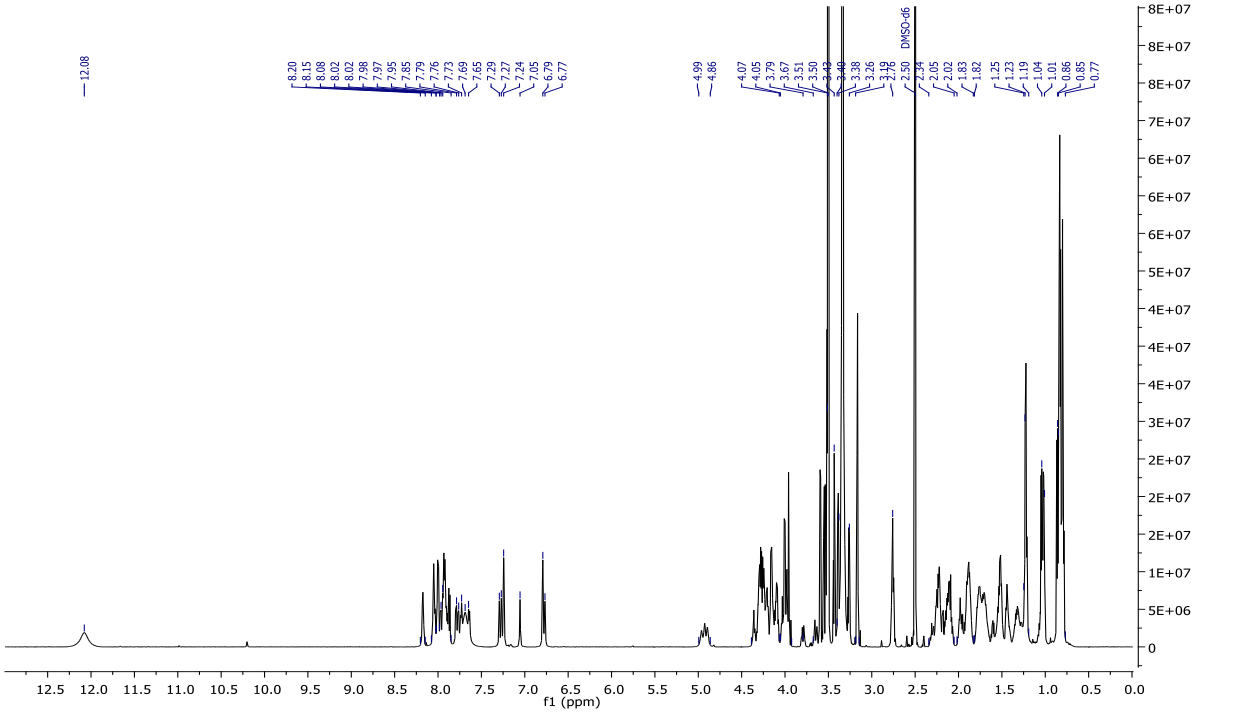


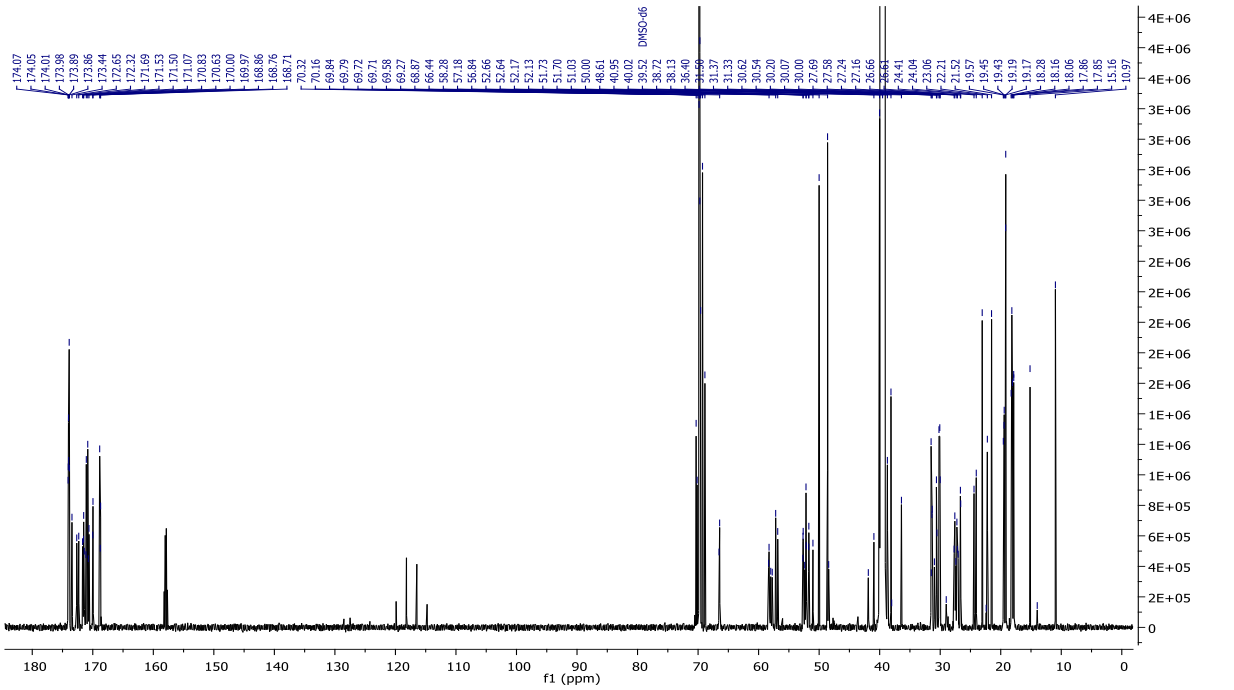

Intens.
x10^5
+MS, 7.94min #1788
1293.6622
1294.1636
1294.6647
1295.1655
1295.6671
1296.1680
1290
1292
1294
1296
1298
m/z


Intens.
x10^5
+MS, 7.94min #1788
862.7777
863.1119
863.4462
863.7804
864.1143
864.4478
861.0
861.5
862.0
862.5
863.0
863.5
864.0
864.5
865.0
865.5
m/z

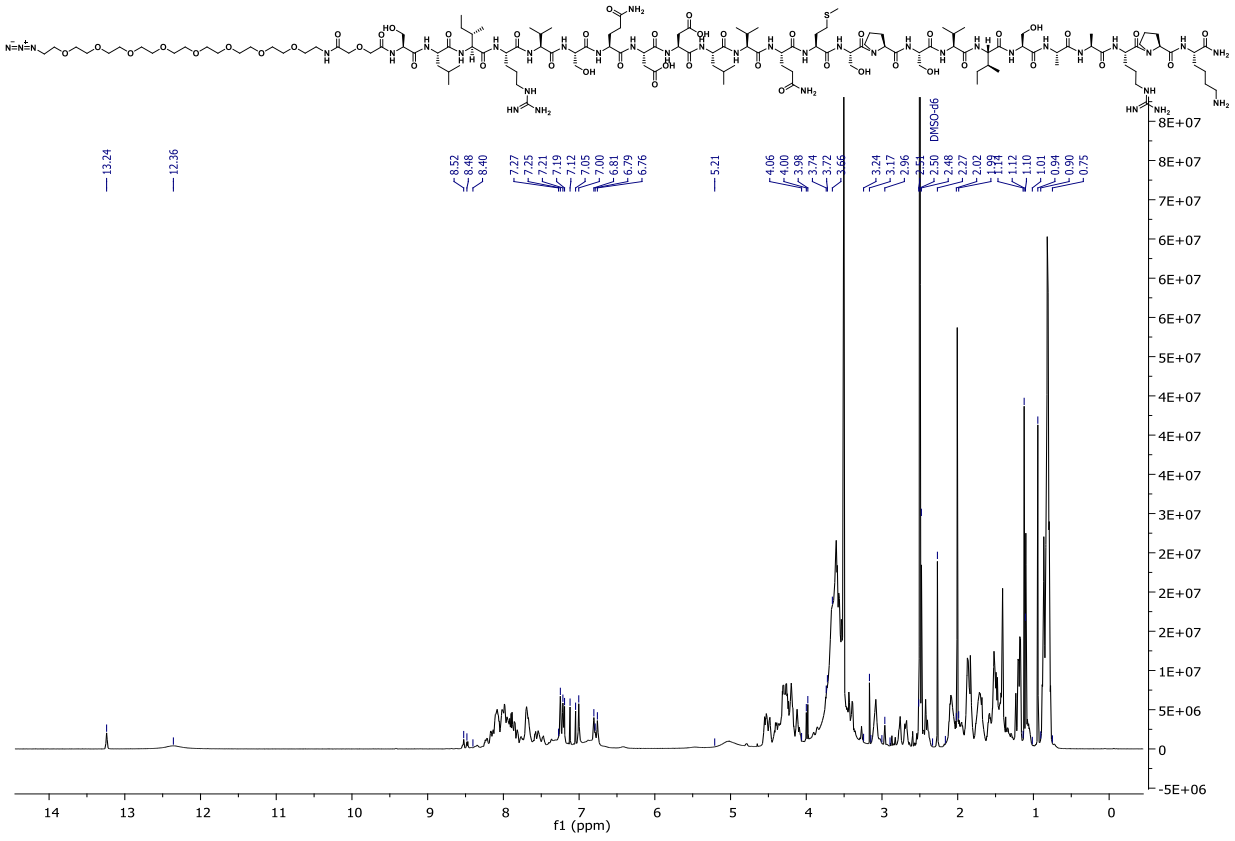
Compound 62 (*PfeA* 33-51 *N*-term Carbonyl-$(PEG)_7$-azide peptide)

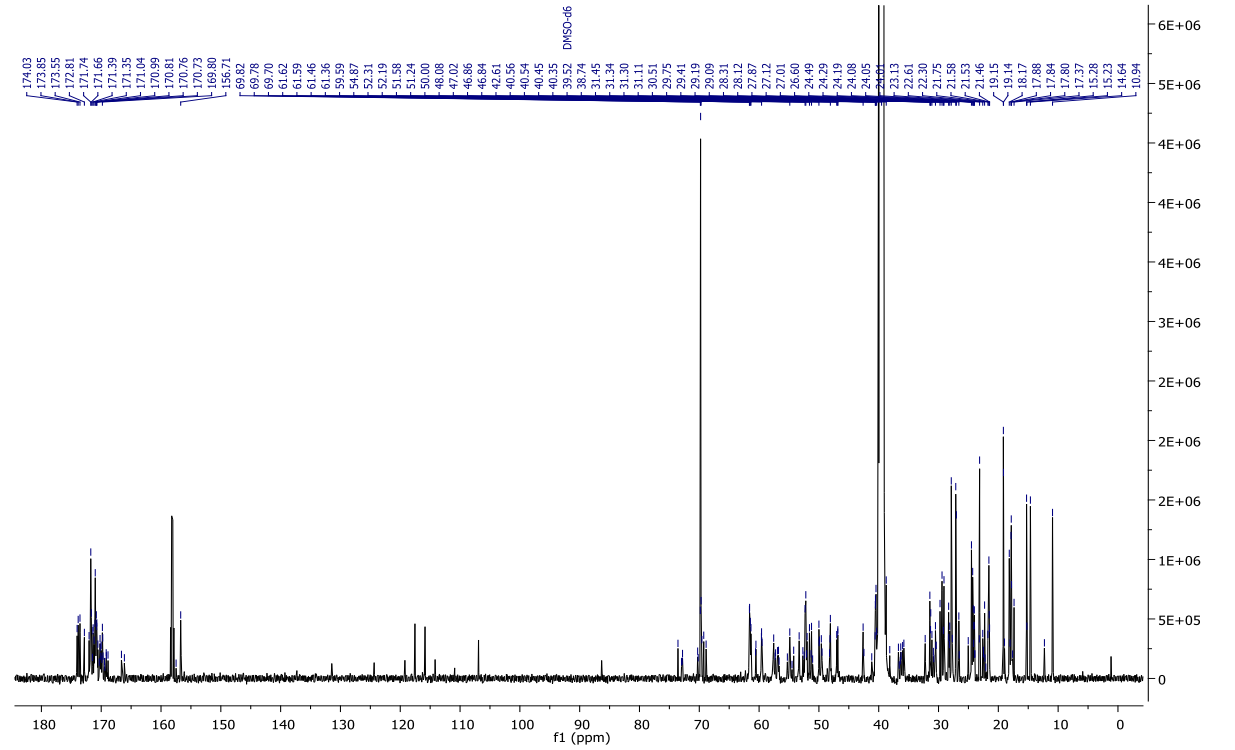


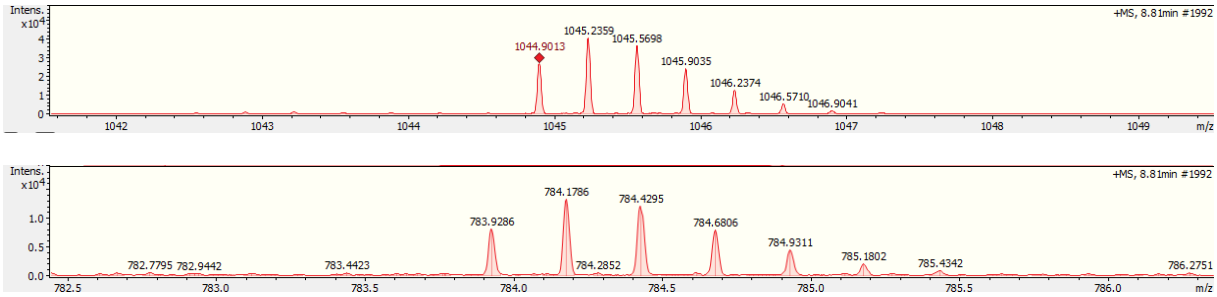




Compound 63 (*HasR* 122-144 *N*-term Carbonyl-$(PEG)_7$-azide peptide)

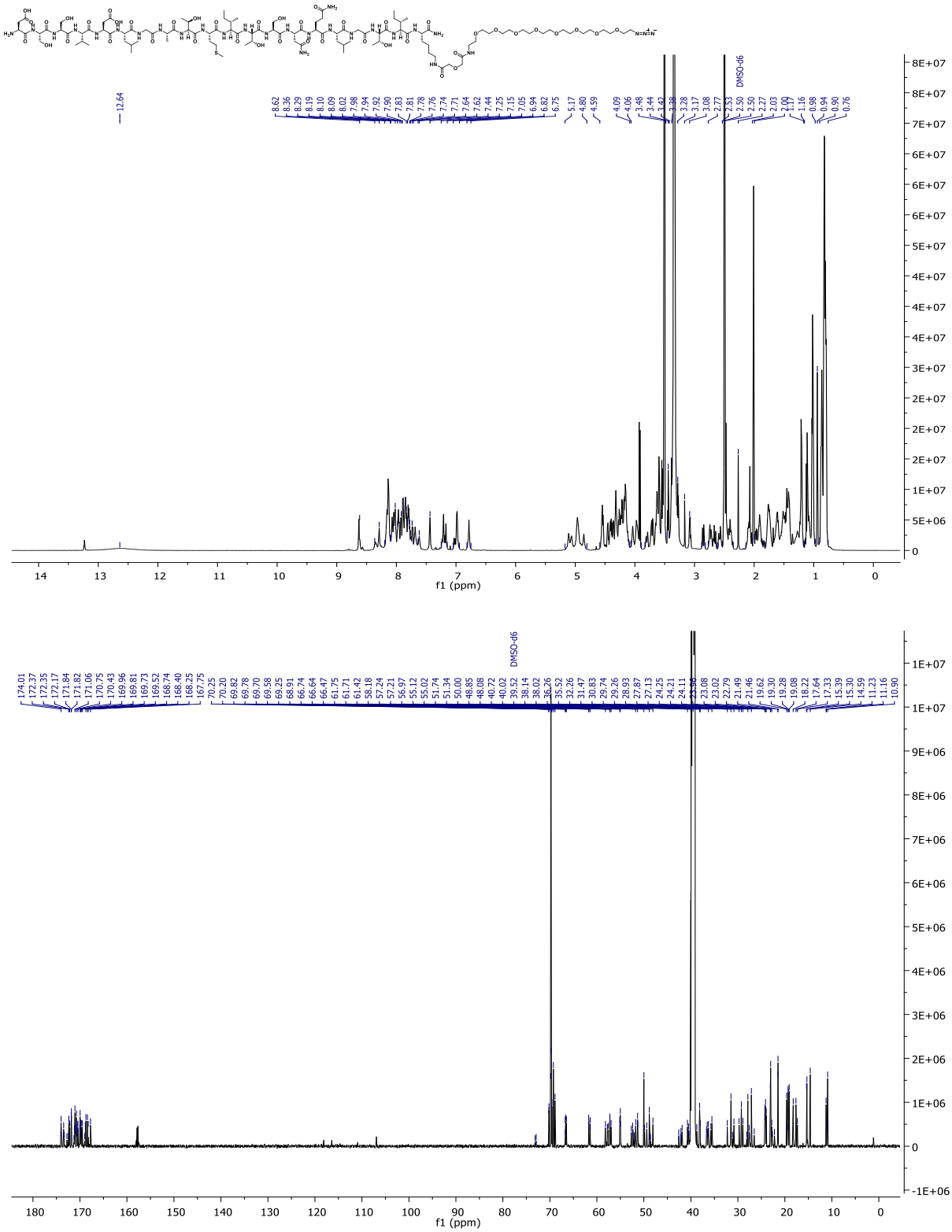


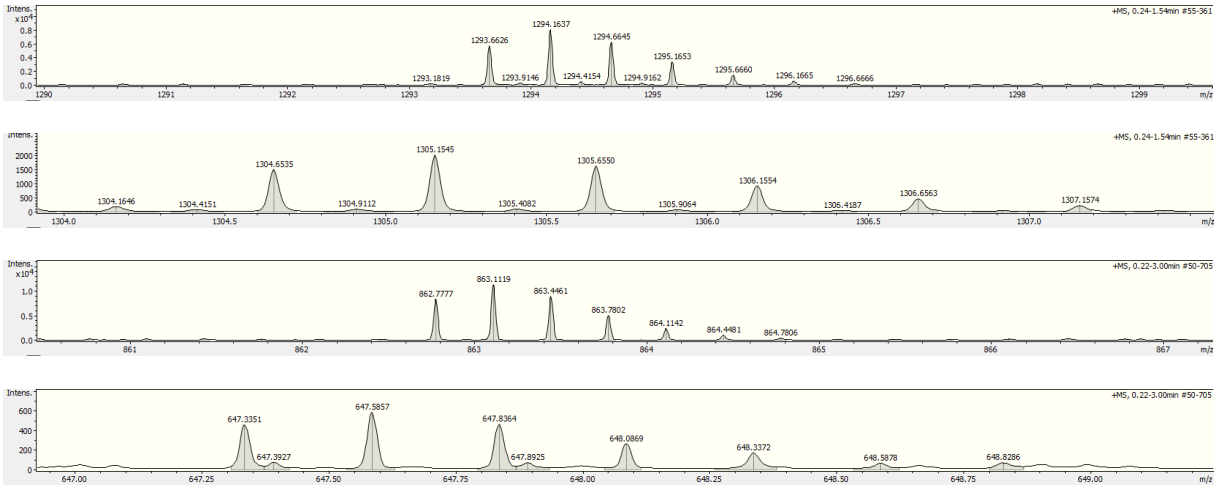



Intens.
x10^4
+MS, 8.81min #1992
1044.9013
1045.2359
1045.5698
1045.9035
1046.2374
1046.5710
1046.9041
1042
1043
1044
1045
1046
1047
1048
1049
m/z

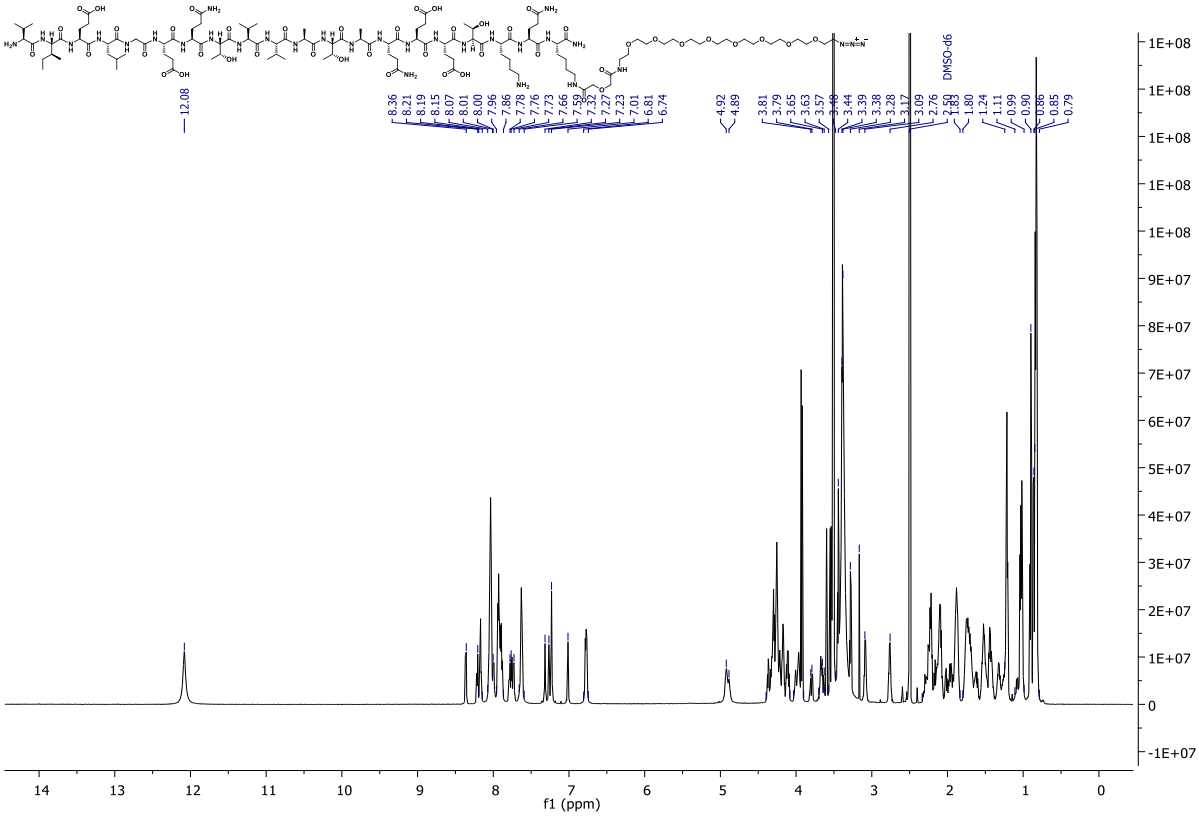
Intens.
x10^4
+MS, 8.81min #1992
782.7795
782.9442
783.4423
783.9286
784.1786
784.2852
784.4295
784.6806
784.9311
785.1802
785.4342
786.2751
782.5
783.0
783.5
784.0
784.5
785.0
785.5
786.0
m/z

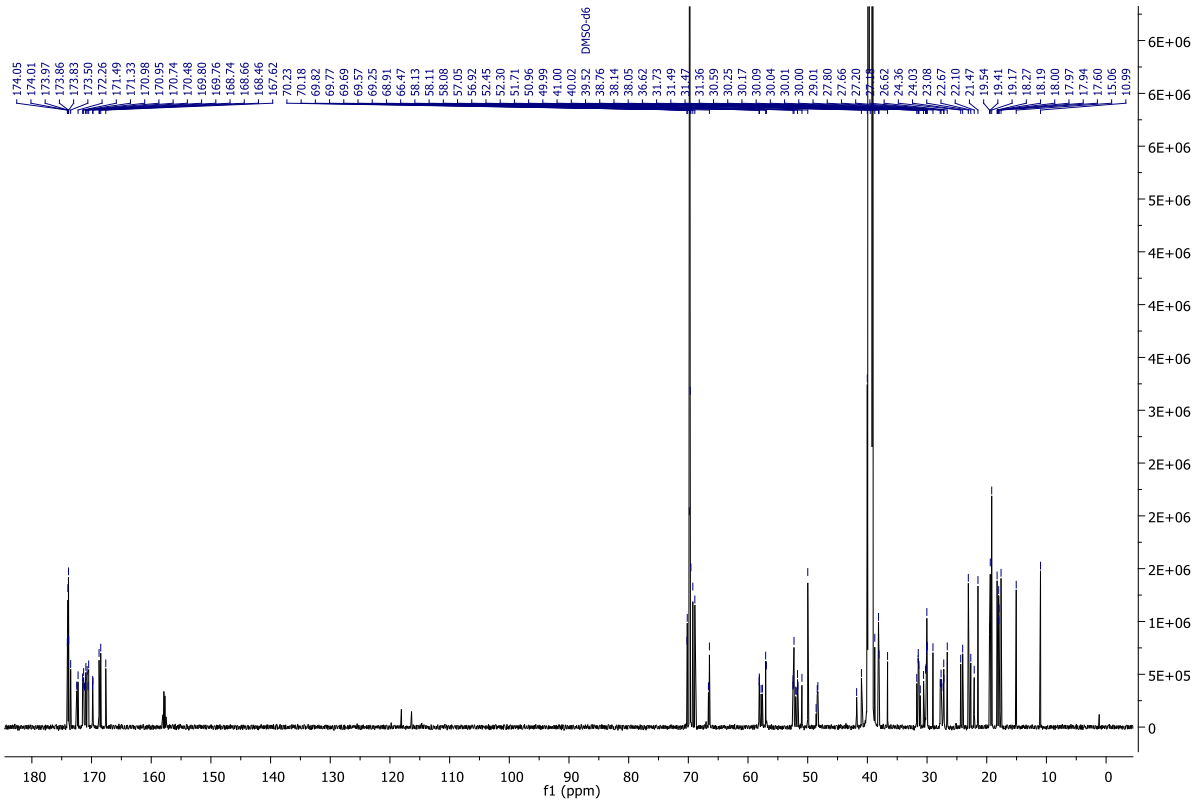
Compound 64 (*FpvA* 121-139 *C*-term Carbonyl-$(PEG)_7$-azide peptide)

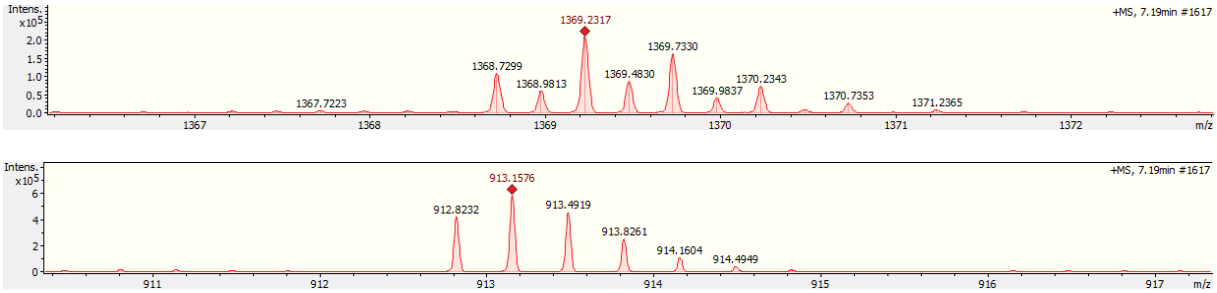



+MS, 0.24-1.54min #55-361
1294.1637
1293.6626
1294.6645
1295.1653
1295.6660
1293.1819
1293.9146
1294.4154
1294.9162
1296.1665
1296.6666
+MS, 0.24-1.54min #55-361
1304.6535
1305.1545
1305.6550
1306.1554
1304.1646
1304.4151
1304.9112
1305.4082
1305.9064
1306.4187
1306.6563
1307.1574
+MS, 0.22-3.00min #50-705
862.7777
863.1119
863.4461
863.7802
864.1142
864.4481
864.7806
+MS, 0.22-3.00min #50-705
647.3351
647.5857
647.8364
648.0869
647.3927
647.8925
648.3372
648.5878
648.8286

Compound 65 (*PfeA* 33-51 *C*-term Carbonyl-$(PEG)_7$-azide peptide)

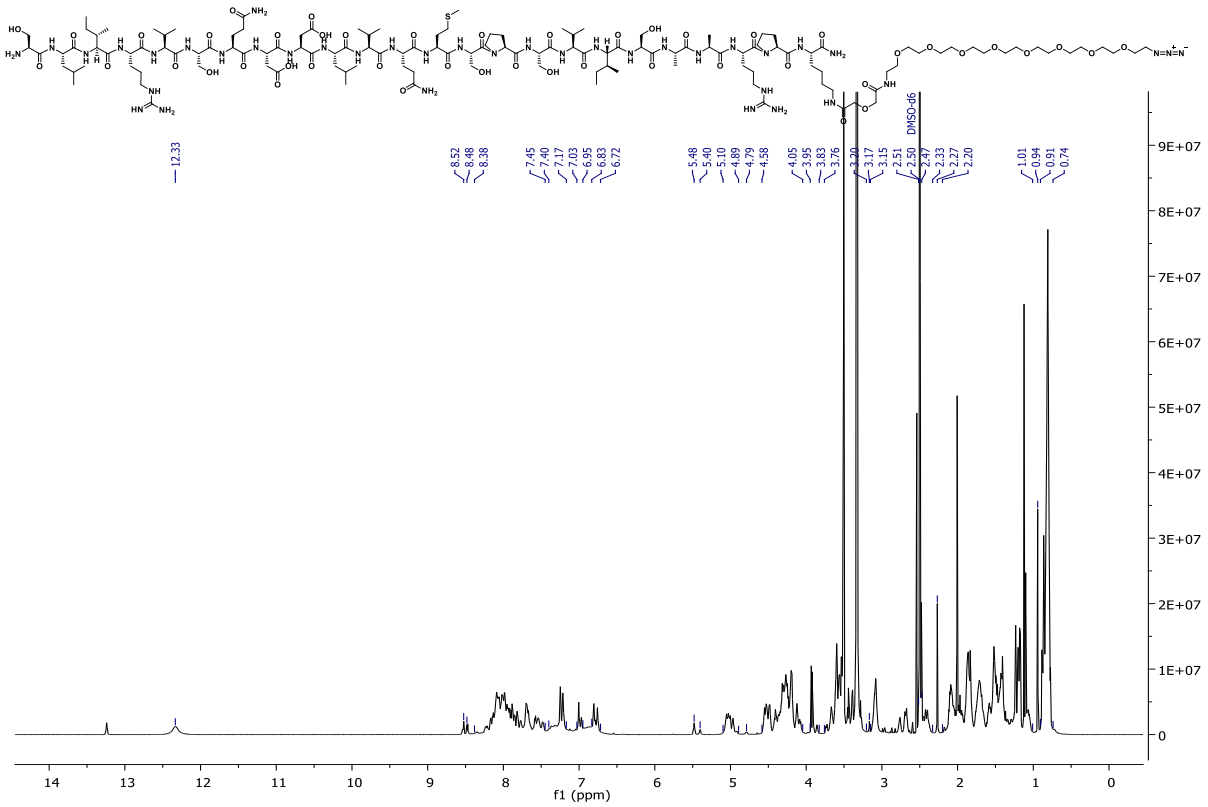


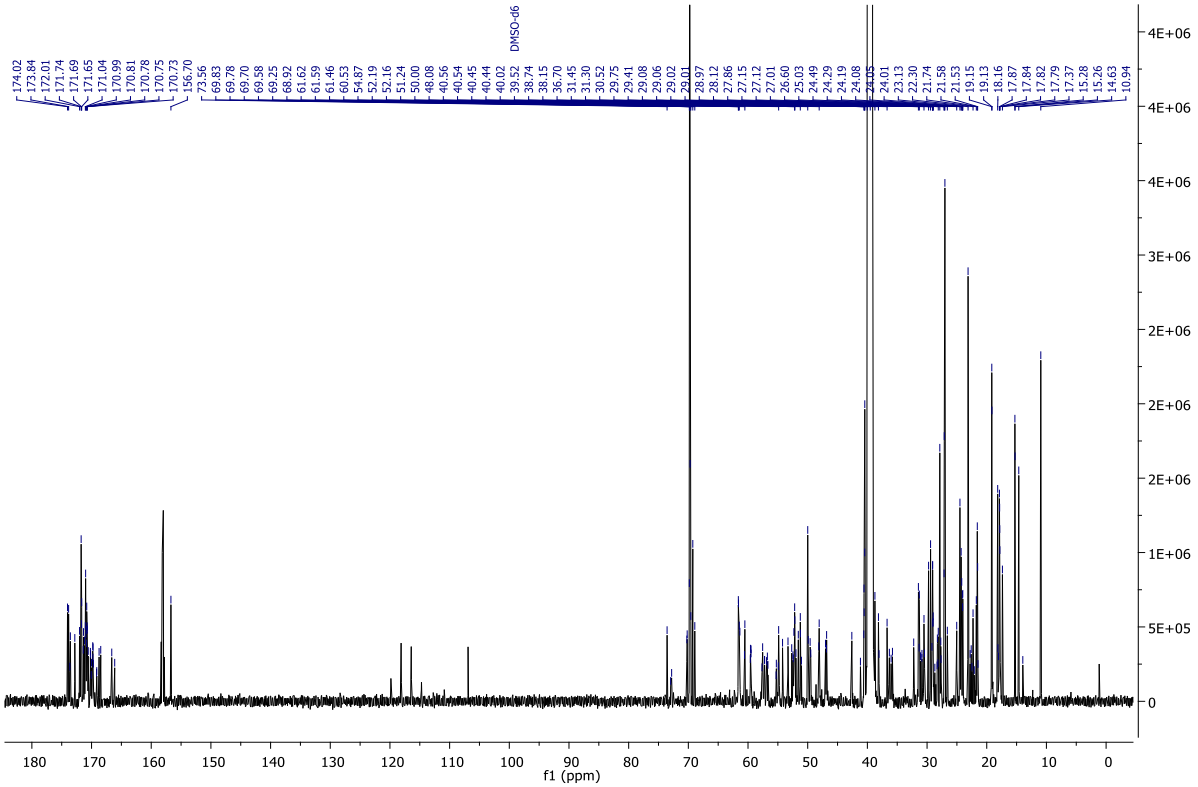


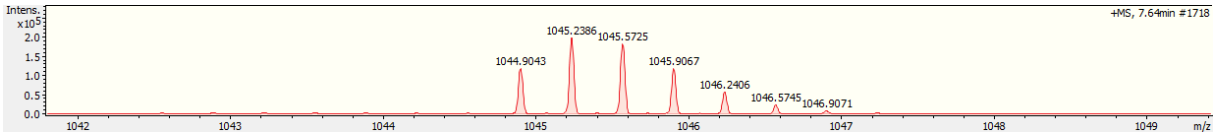

Intens.
x10^5
2.0
1.5
1.0
0.5
0.0
+MS, 7.19min #1617
1369.2317
1369.7330
1368.7299
1369.4830
1368.9813
1370.2343
1369.9837
1370.7353
1367.7223
1371.2365
1367
1368
1369
1370
1371
1372
m/z

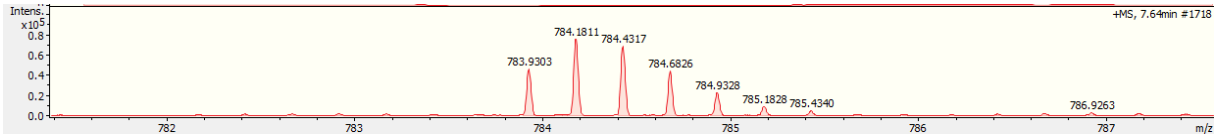
Intens.
x10^5
6
4
2
0
+MS, 7.19min #1617
913.1576
912.8232
913.4919
913.8261
914.1604
914.4949
911
912
913
914
915
916
917
m/z

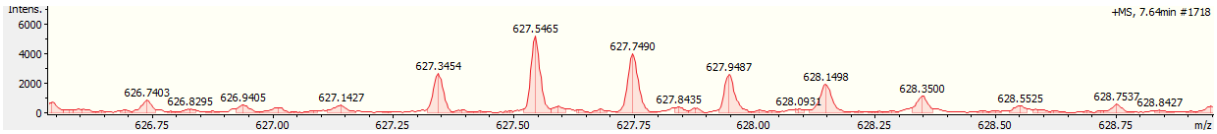
Compound 66 (HasR 122-144 *C*-term Carbonyl-$(PEG)_7$-azide peptide)



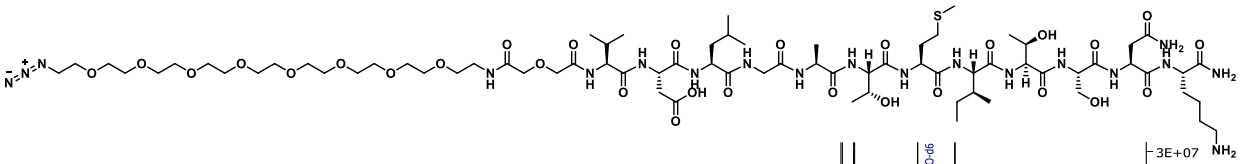


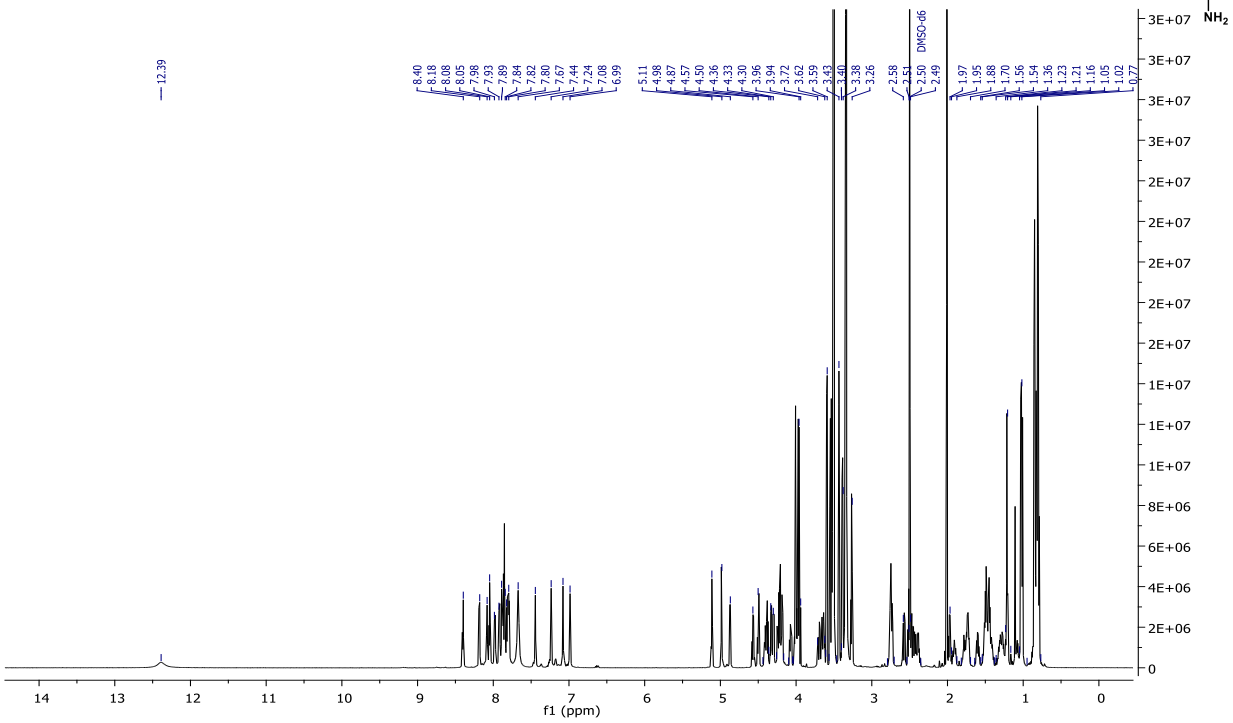

Intens.
x10^5
2.0
1.5
1.0
0.5
0.0
+MS, 7.64min #1718
1045.2386
1045.5725
1044.9043
1045.9067
1046.2406
1046.5745
1046.9071
1042
1043
1044
1045
1046
1047
1048
1049
m/z

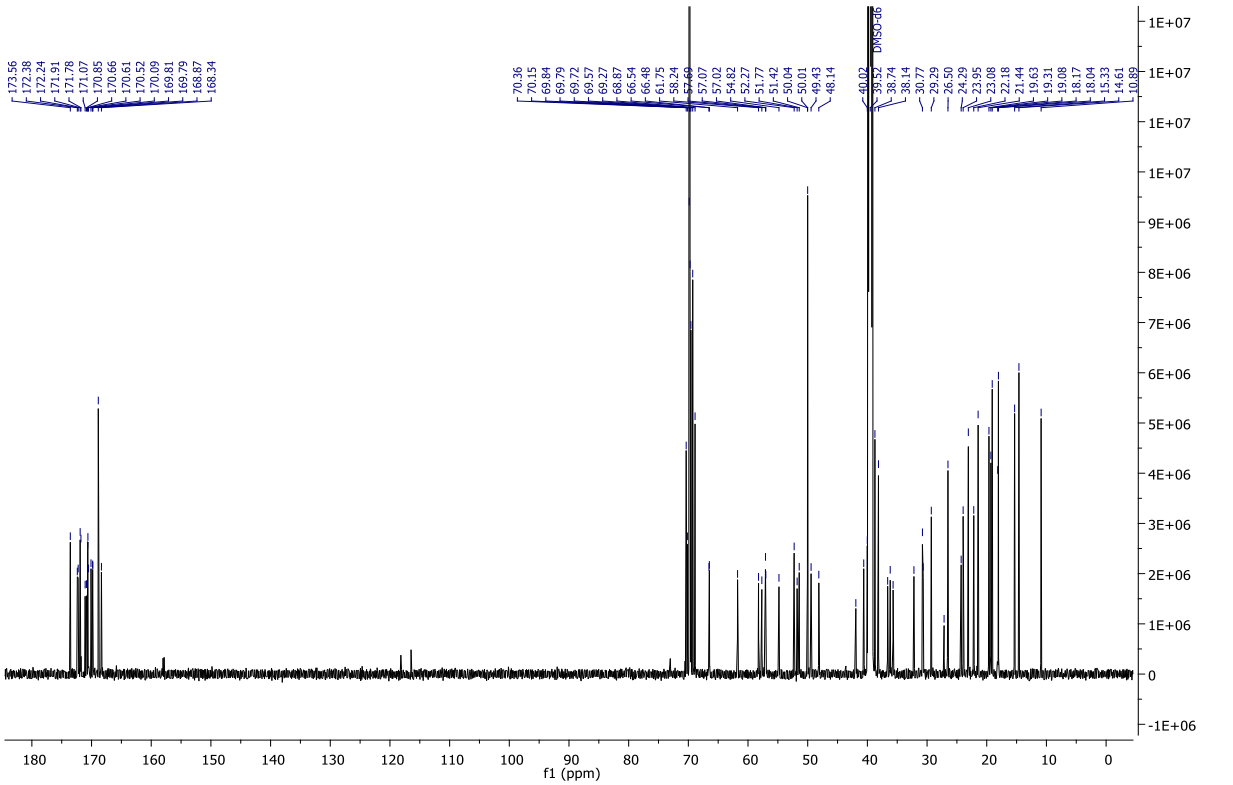

Intens.
x10^5
0.8
0.6
0.4
0.2
0.0
+MS, 7.64min #1718
784.1811
784.4317
783.9303
784.6826
784.9328
785.1828
785.4340
786.9263
782
783
784
785
786
787
m/z

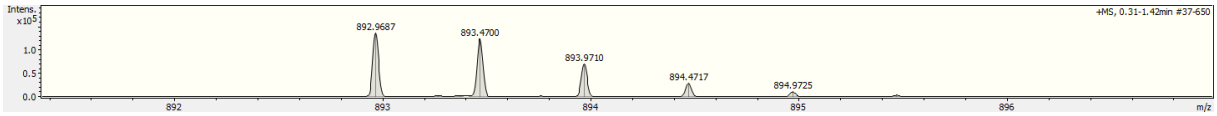

Intens.
6000
4000
2000
0
+MS, 7.64min #1718
627.5465
627.7490
627.3454
627.9487
628.1498
626.7403
626.8295
626.9405
627.1427
627.8435
628.0931
628.3500
628.5525
628.7537
628.8427
626.75
627.00
627.25
627.50
627.75
628.00
628.25
628.50
628.75
m/z

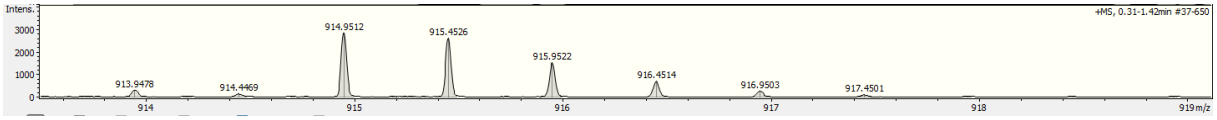
Compound 67 (*FpvA* 124-134 *N*-term Carbonyl-$(PEG)_7$-azide peptide)

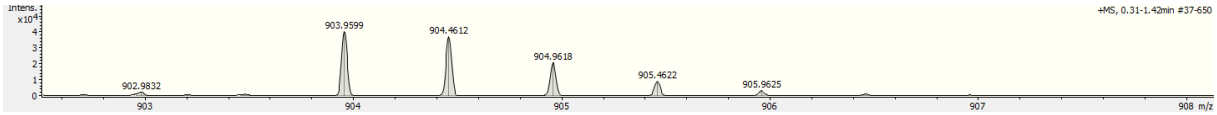


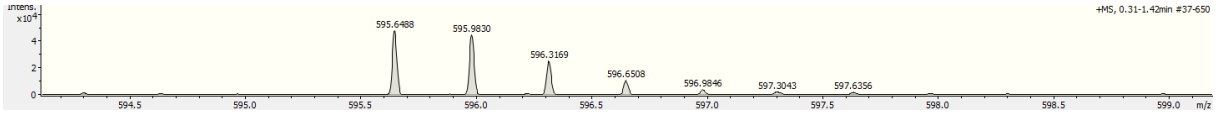




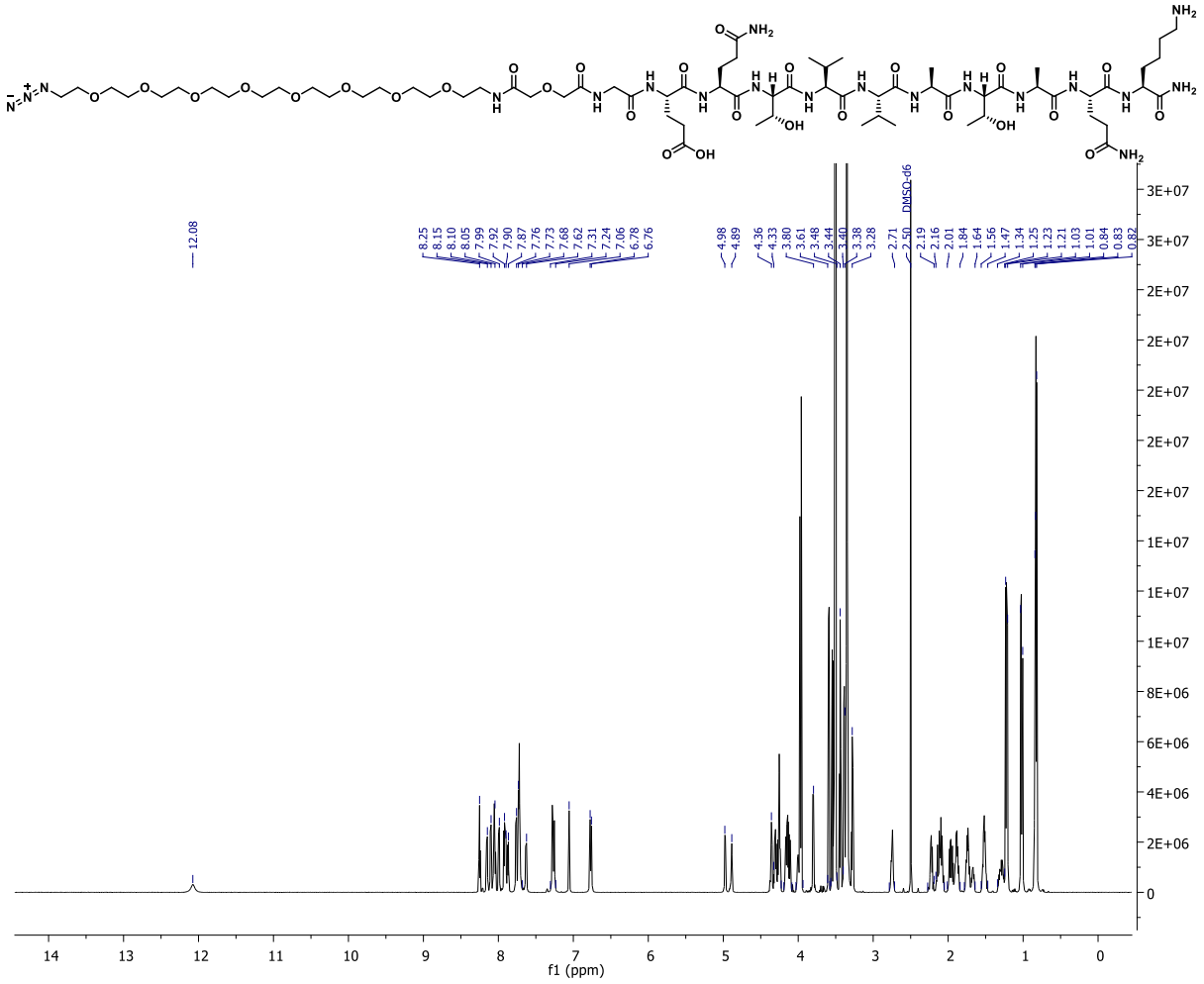

Intens.
x10^5
1.0
0.5
0.0
892.9687
893.4700
893.9710
894.4717
894.9725
892
893
894
895
896
m/z
+MS, 0.31-1.42min #37-650

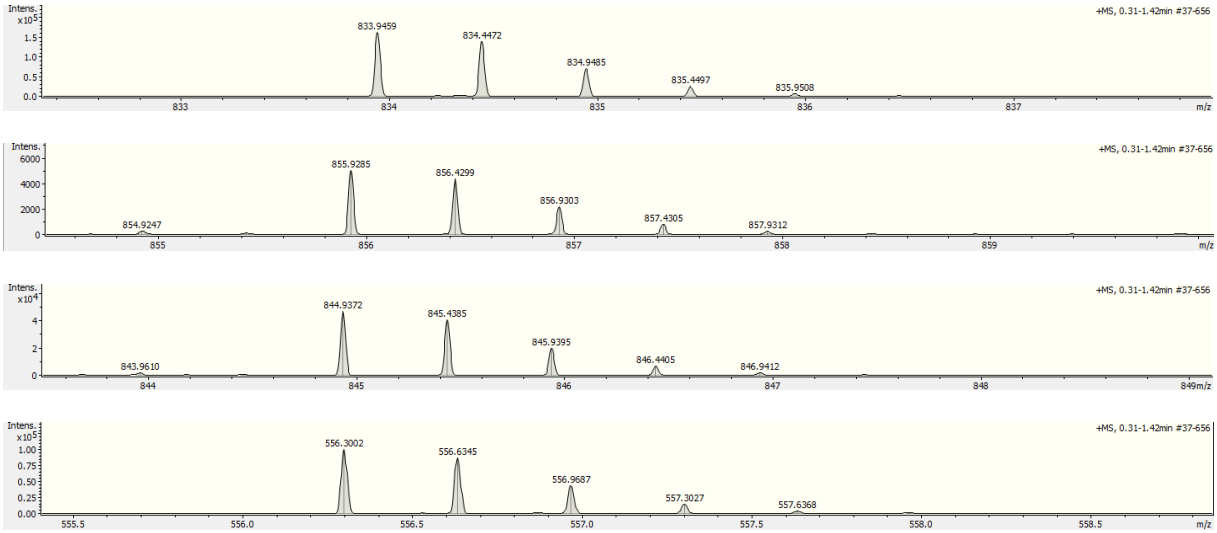

Intens.
3000
2000
1000
0
913.9478
914.4469
914.9512
915.4526
915.9522
916.4514
916.9503
917.4501
914
915
916
917
918
919
m/z
+MS, 0.31-1.42min #37-650


Intens.
x10^4
4
3
2
1
0
902.9832
903.9599
904.4612
904.9618
905.4622
905.9625
903
904
905
906
907
908
m/z
+MS, 0.31-1.42min #37-650

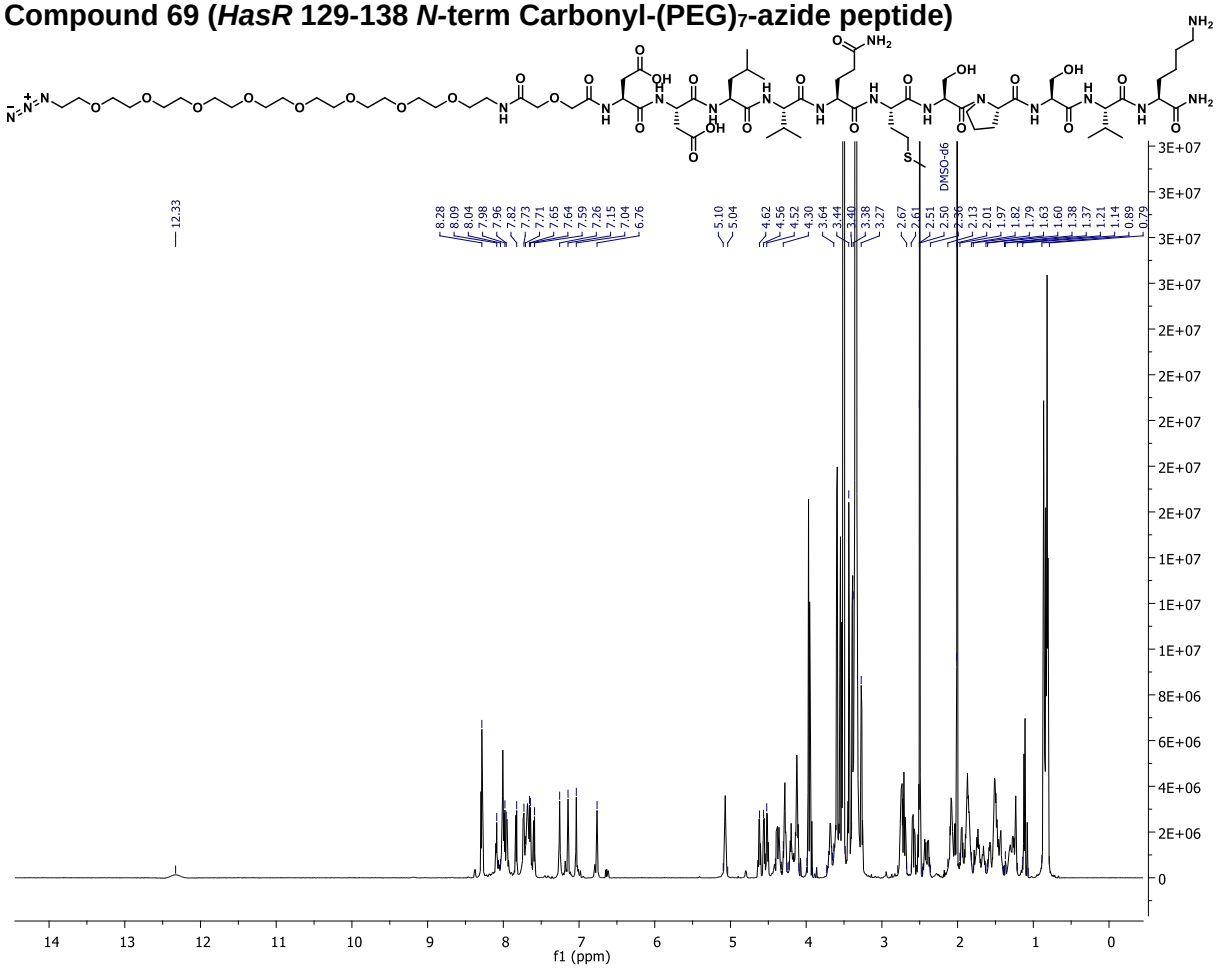

Intens.
x10^4
4
2
0
595.6488
595.9830
596.3169
596.6508
596.9846
597.3043
597.6356
594.5
595.0
595.5
596.0
596.5
597.0
597.5
598.0
598.5
599.0
m/z
+MS, 0.31-1.42min #37-650

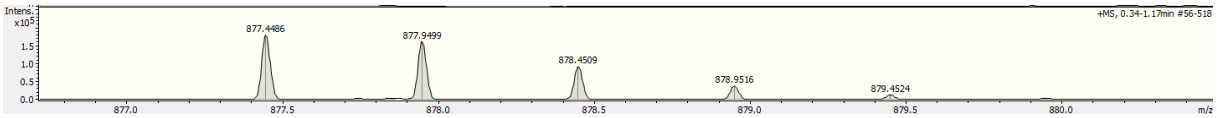
Compound 68 (*PfeA* 37-46 *N*-term Carbonyl-$(PEG)_7$-azide peptide)

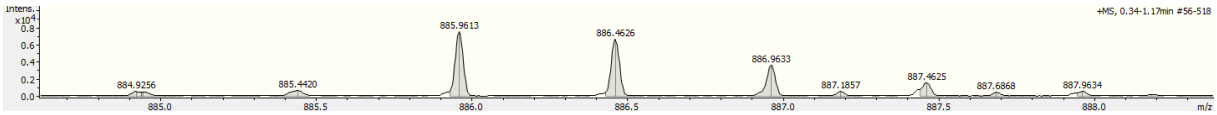


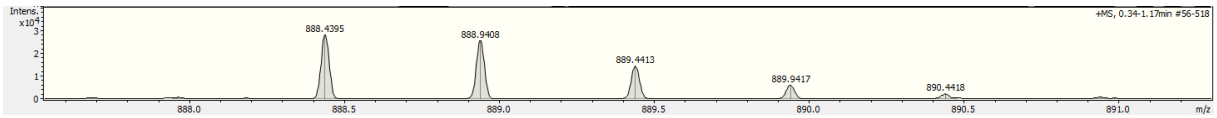


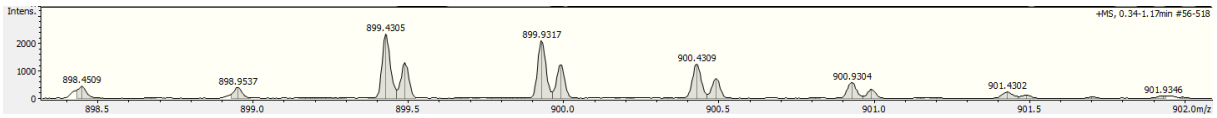
Compound 69 (*HasR* 129-138 *N*-term Carbonyl-$(PEG)_7$-azide peptide)

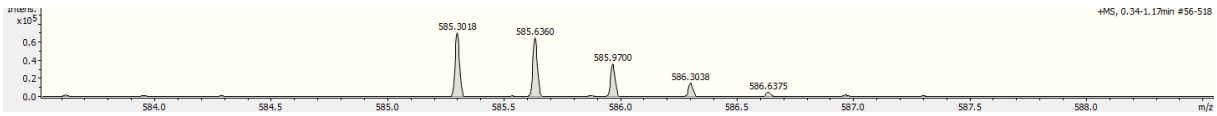




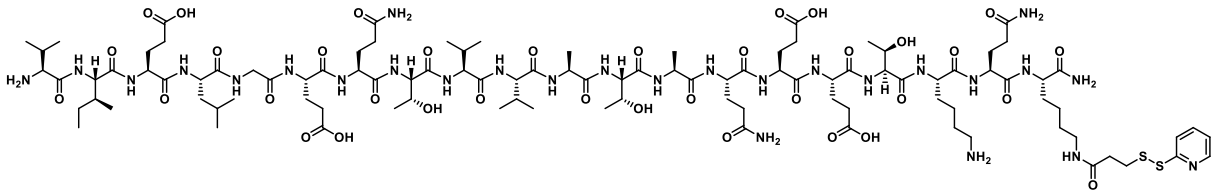


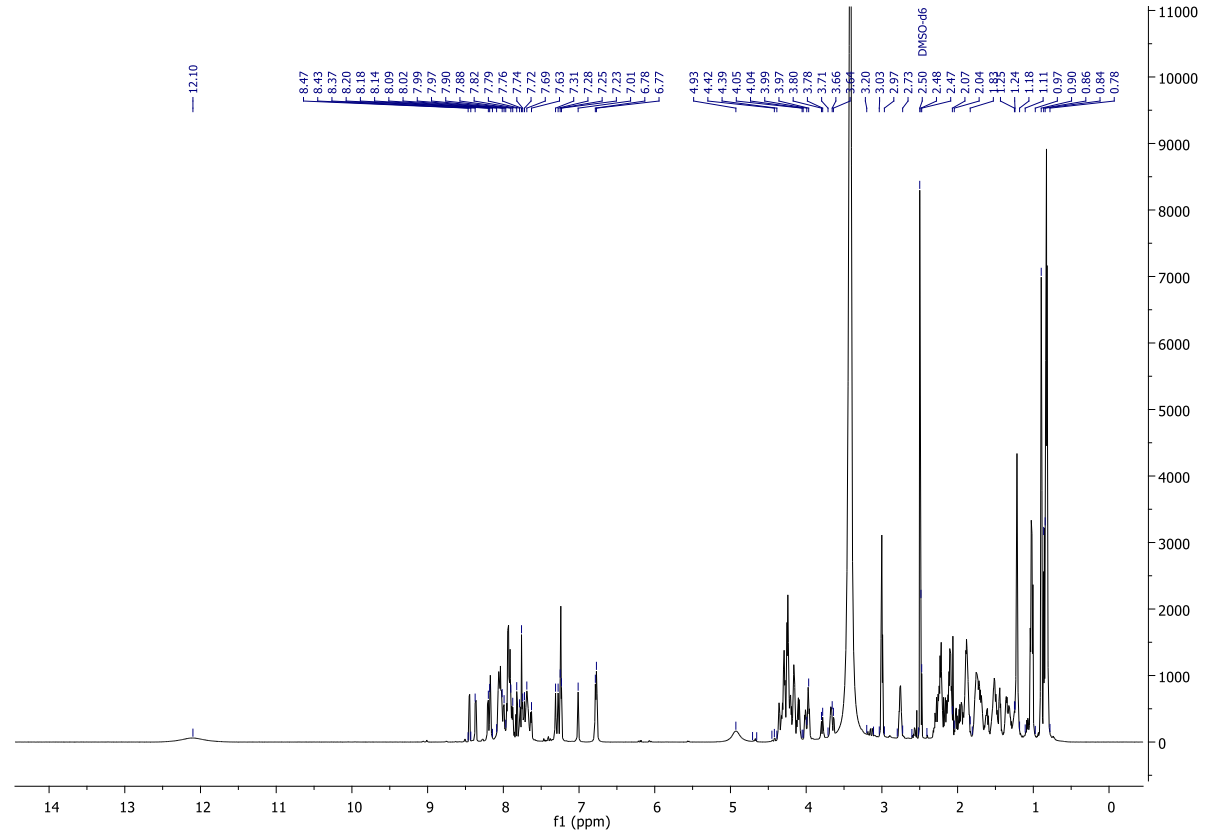


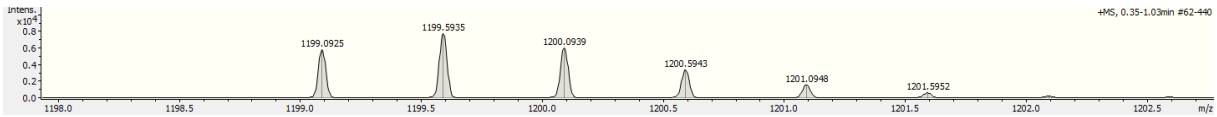


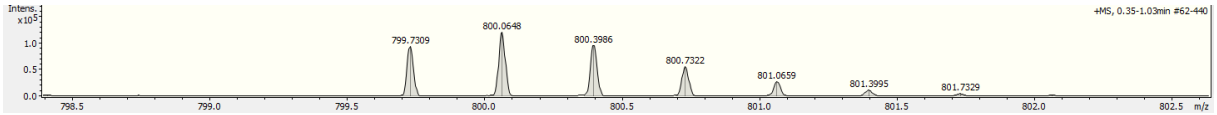


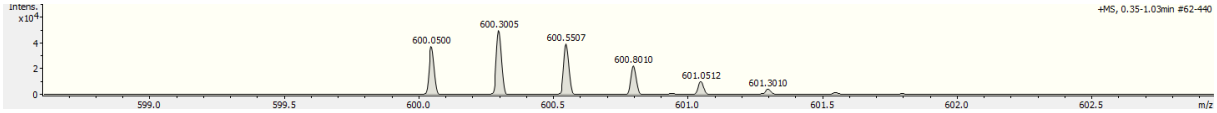
Compound 70 (*PfeA* 33-51 *C*-term 3-(Pyridin-2-yldisulfanyl)propanamide peptide)

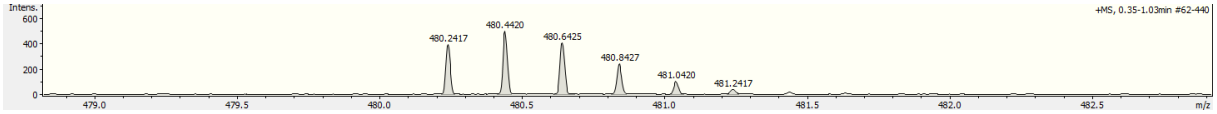






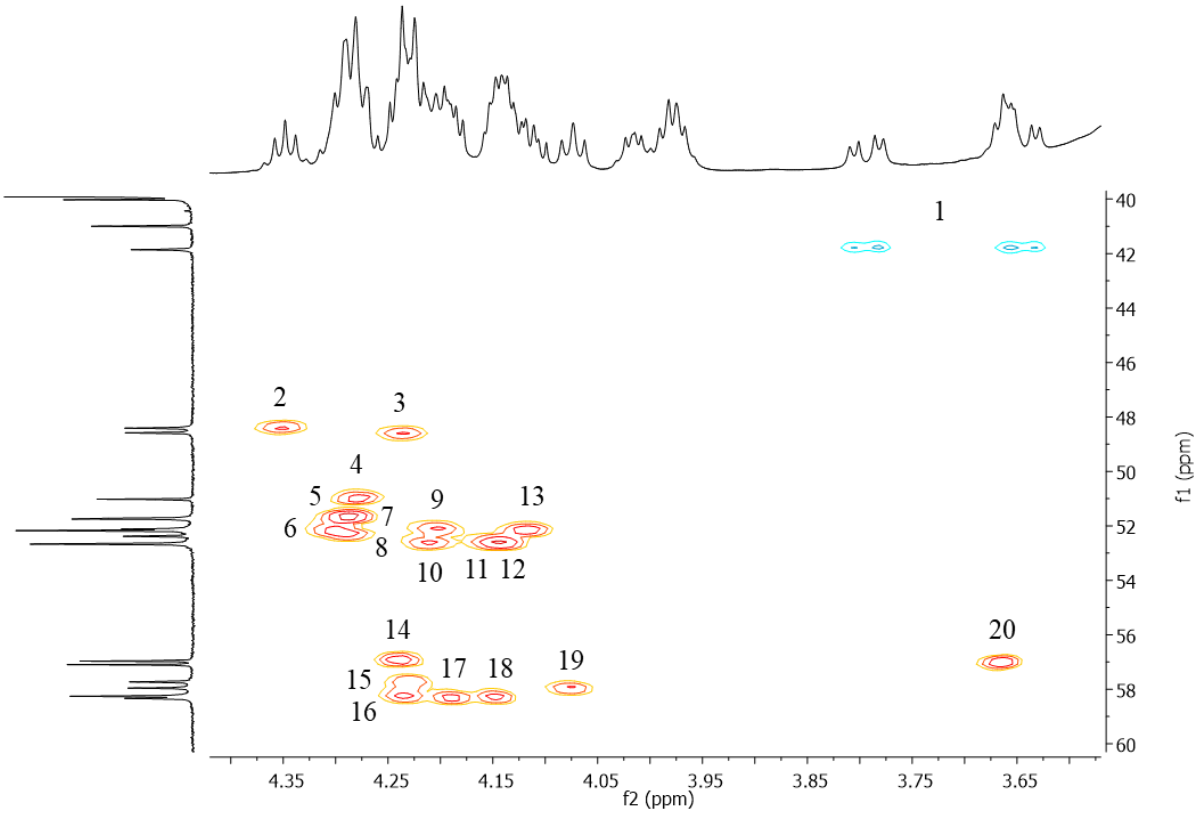


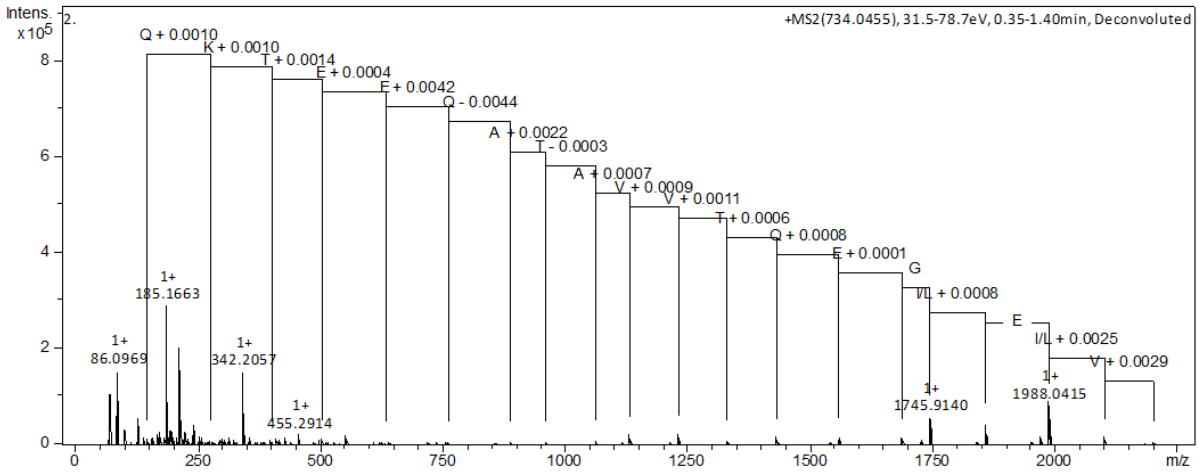




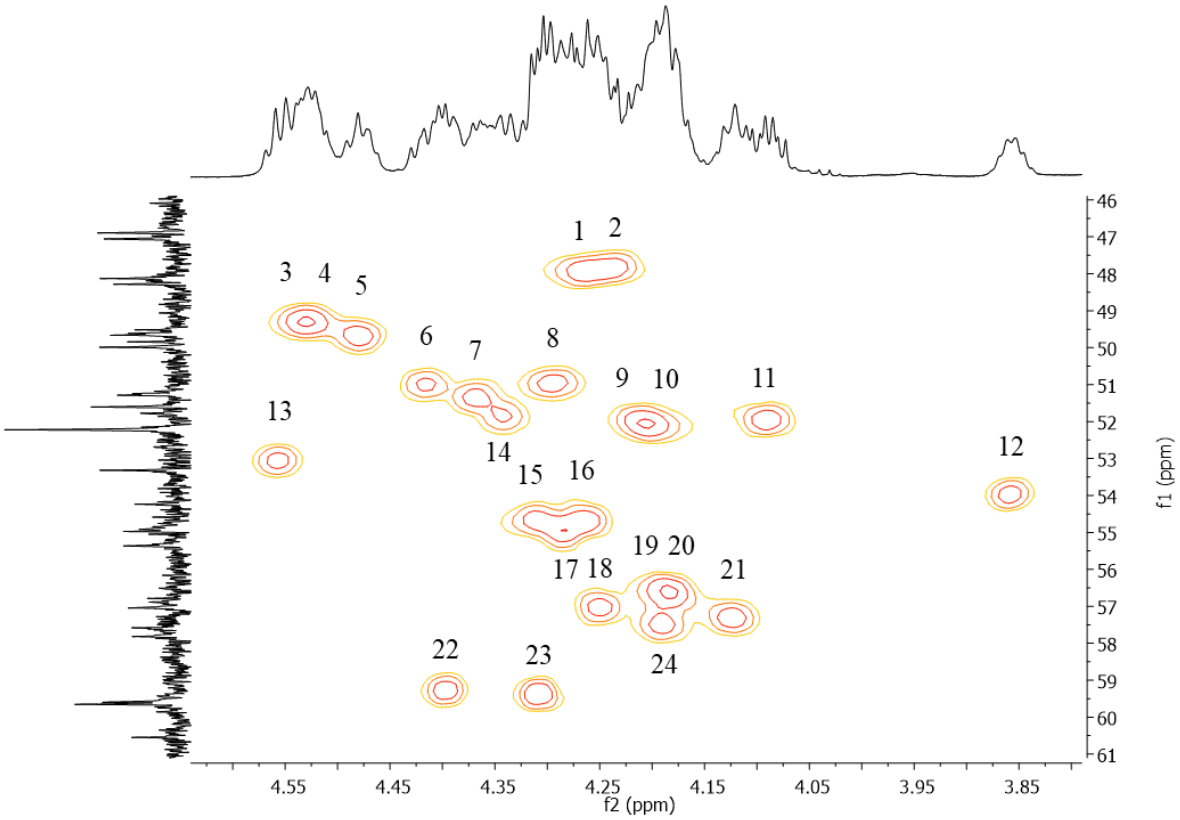
2D-NMR data and MS/MS spectra

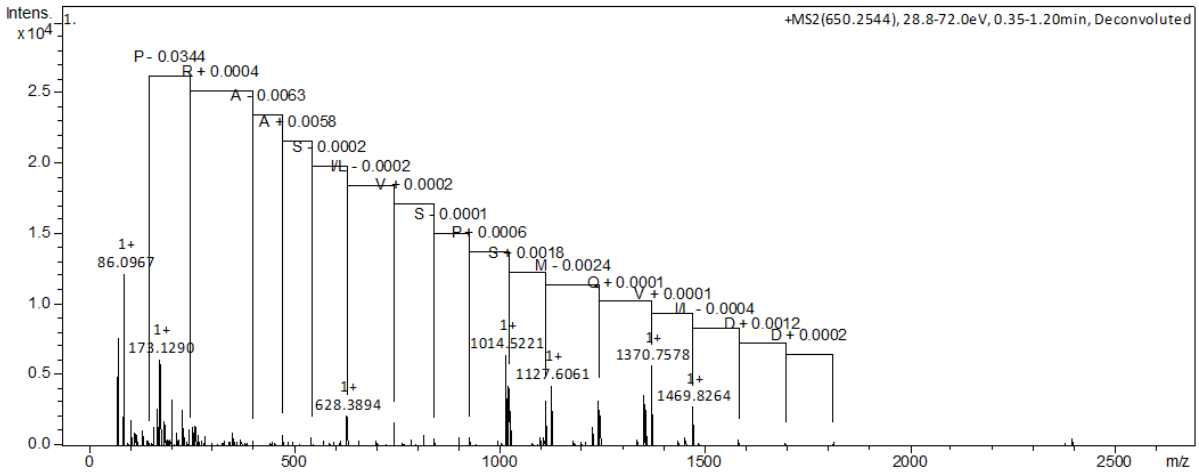
PfeA 33-51 peptide 6



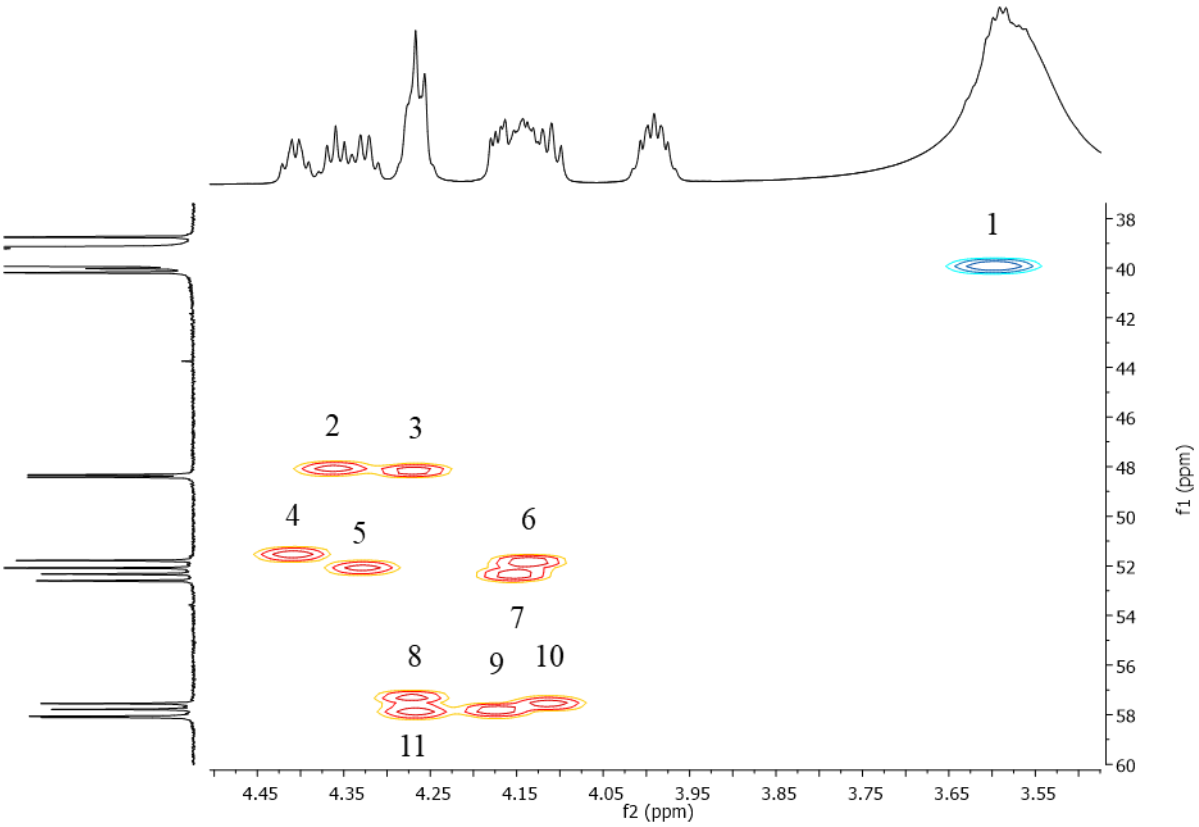


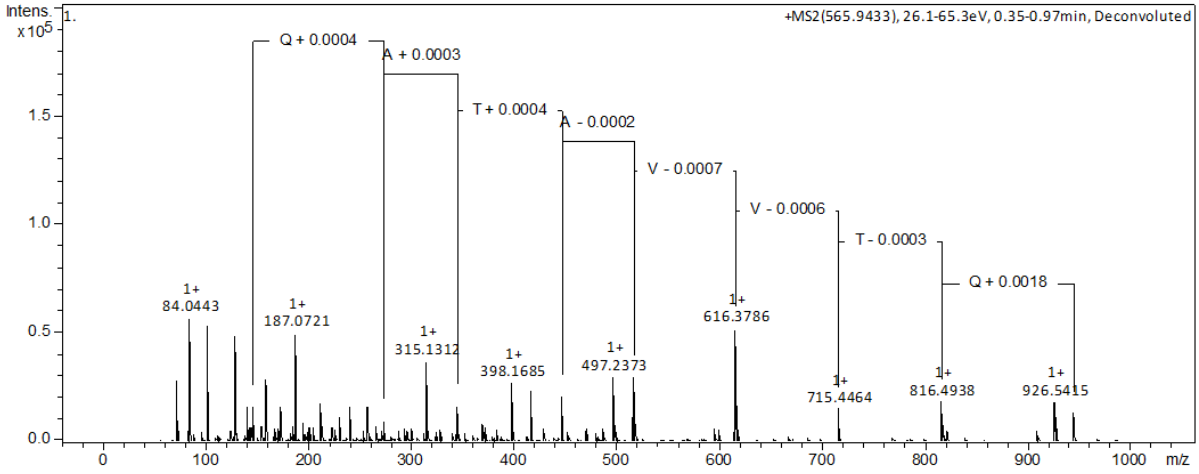
***HasR* 122-144 peptide 7**



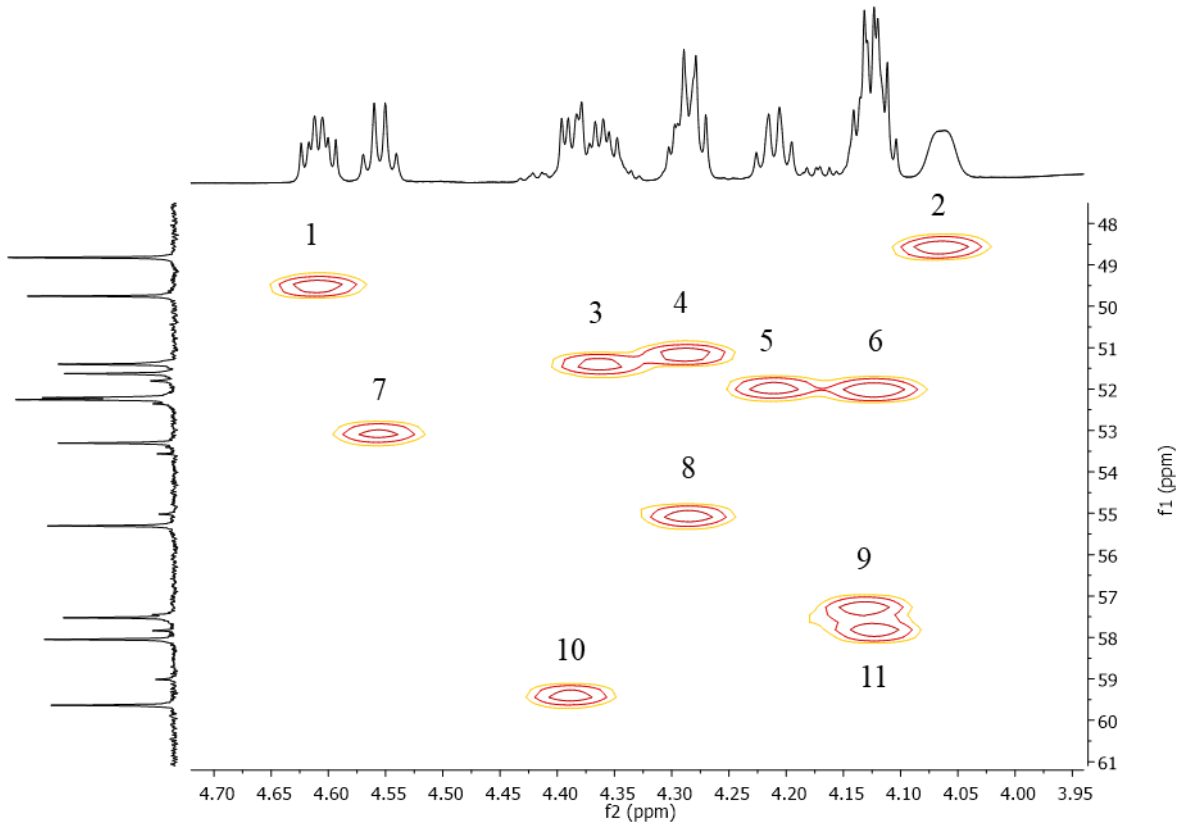


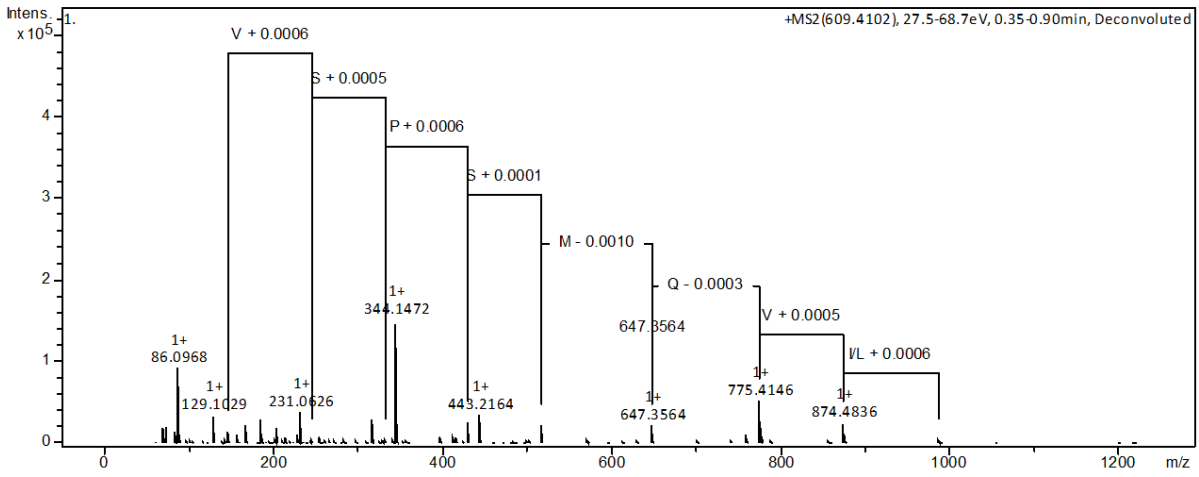
PfeA 37-46 peptide 9



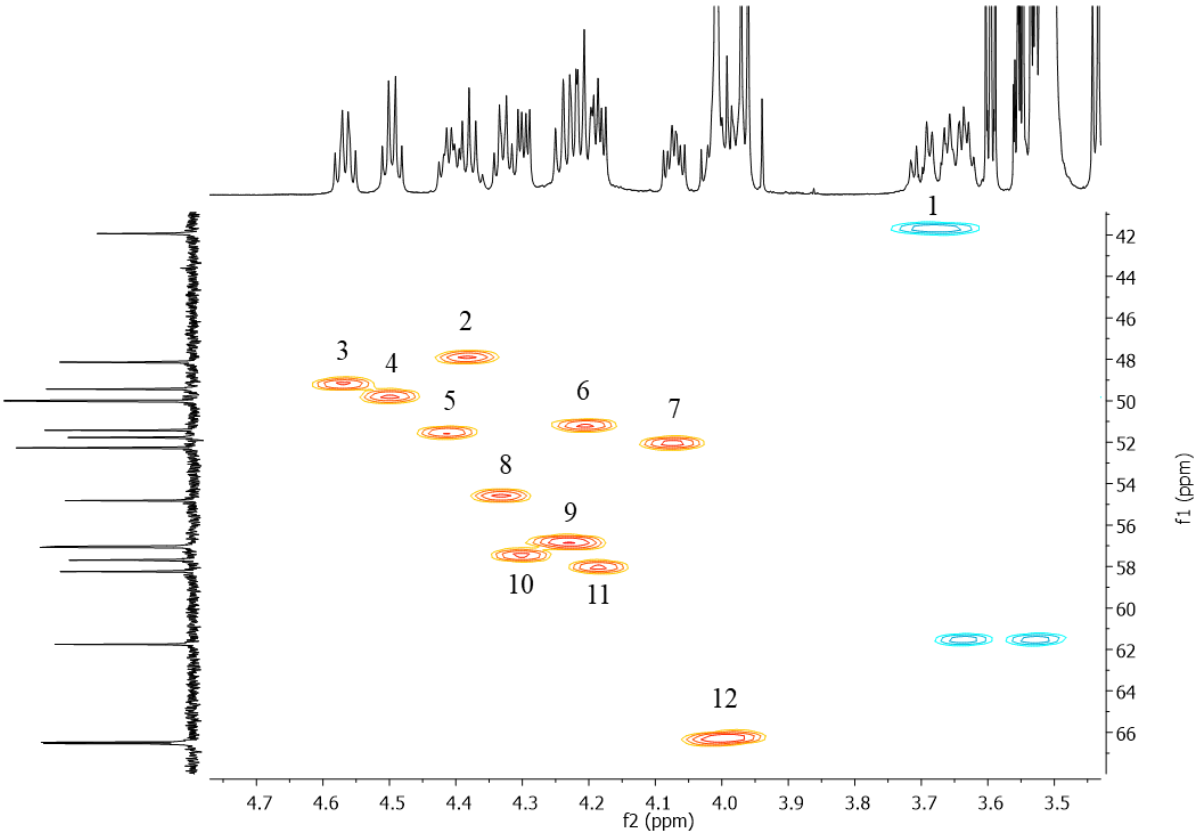


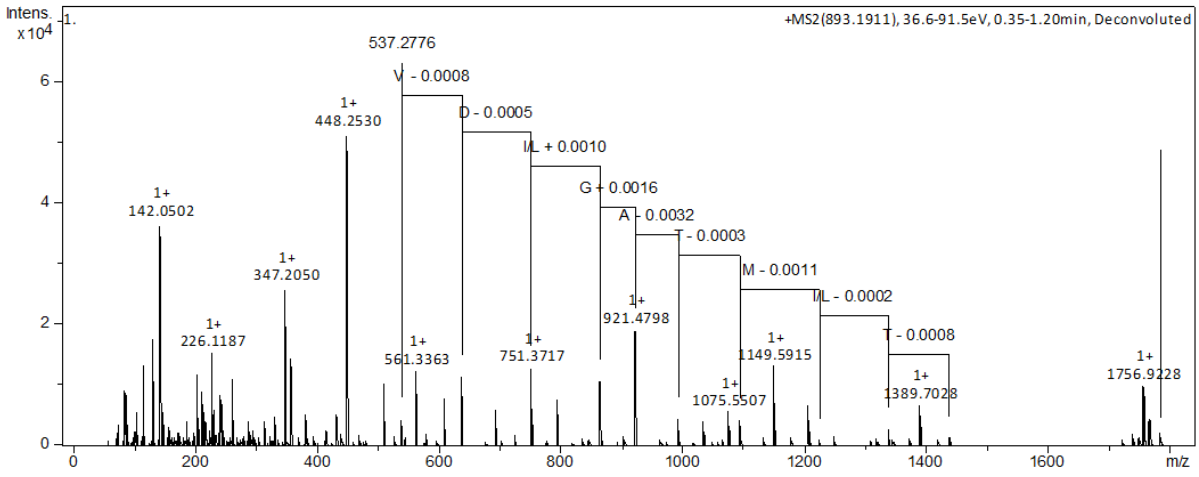
***HasR* 129-138 peptide 10**



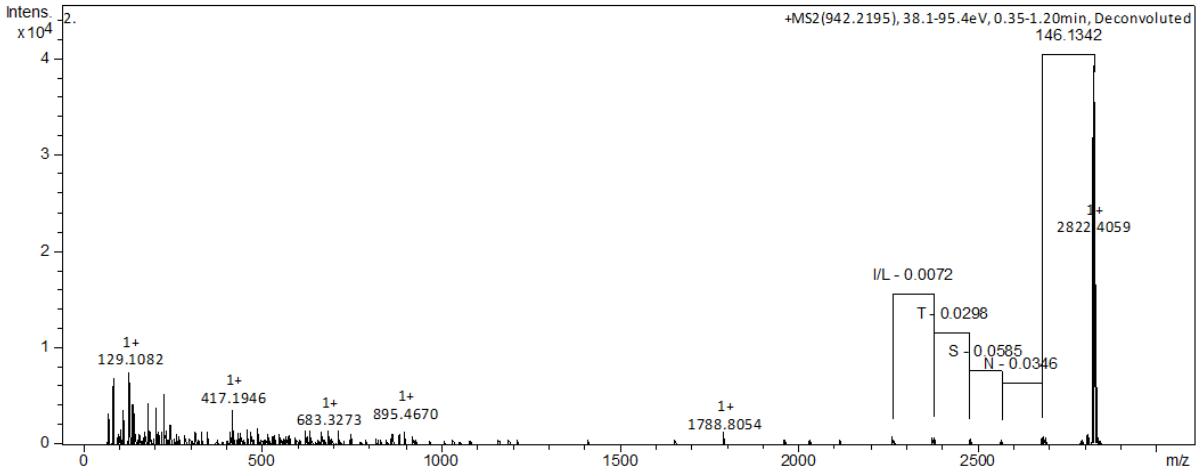


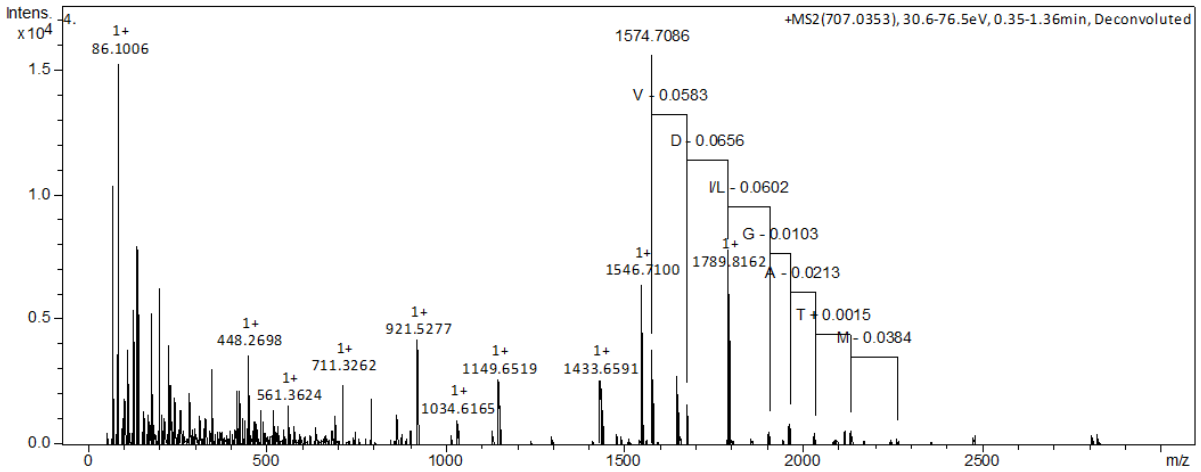
***FpvA* 124-134 *N*-term Carbonyl-$(PEG)_7$-azide peptide 61**



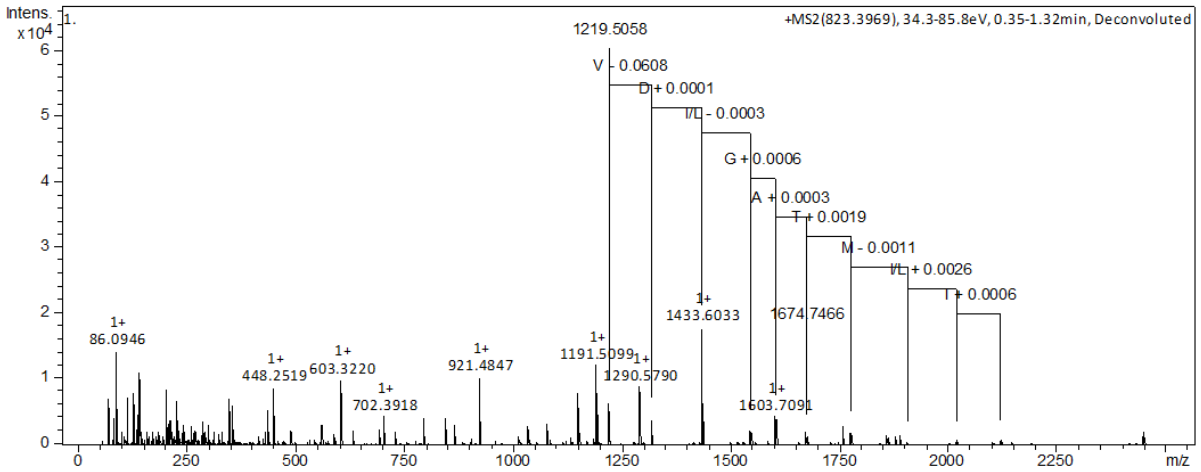


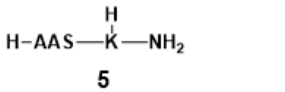
FpvA 124-134 *N*-term $(PEG)_7$-Zn^{2+}-DOTAM 14





FpvA 124-134 *N*-term $(PEG)_7$-MECAM-OH 25

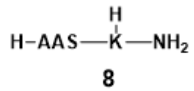




5

AAS: DSSVDLG*A*T*MITSNQLGTI

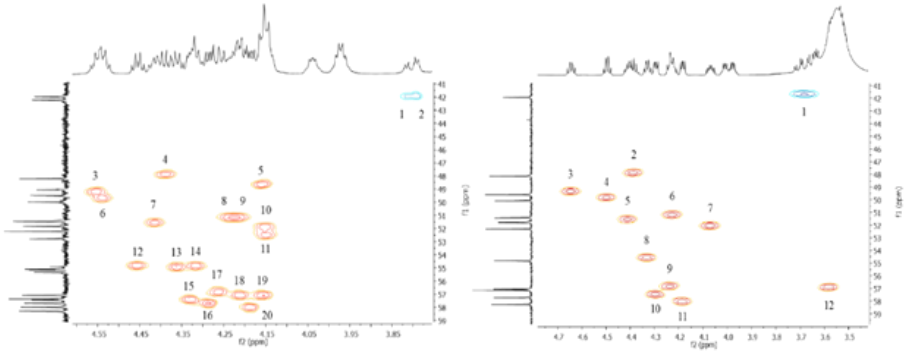
Chemical Formula: $C_{85}H_{148}N_{24}O_{32}S$
Exact Mass: 2049,04122
Molecular Weight: 2050,31500

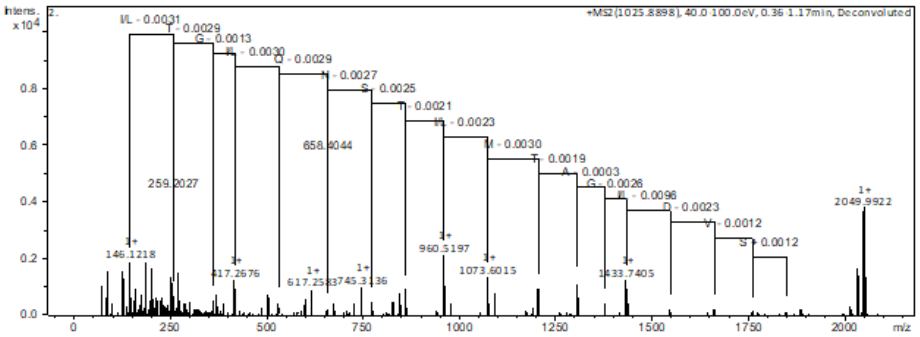


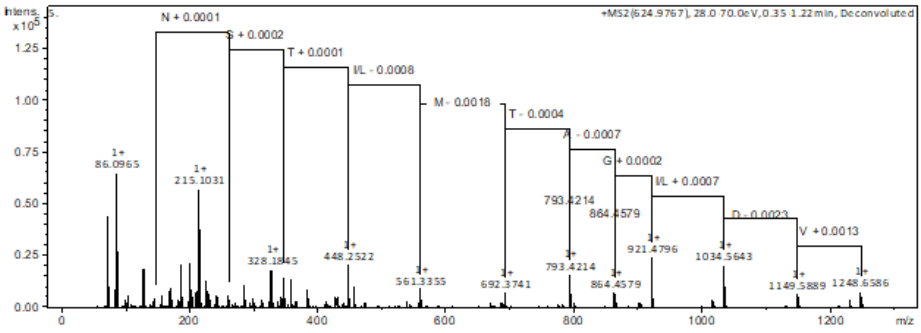
8

AAS: VDLG*A*T*MITSN

Chemical Formula: $C_{52}H_{93}N_{15}O_{18}S$
Exact Mass: 1247,65437
Molecular Weight: 1248,46300

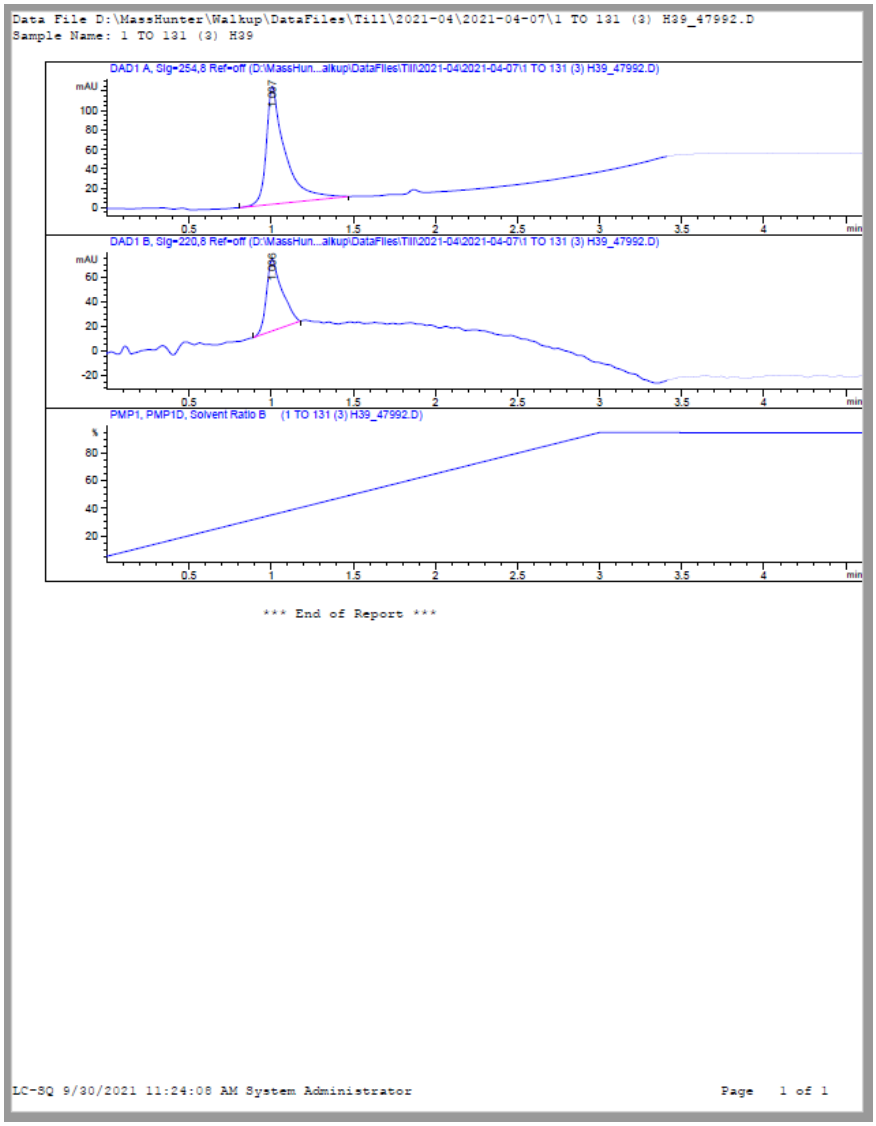




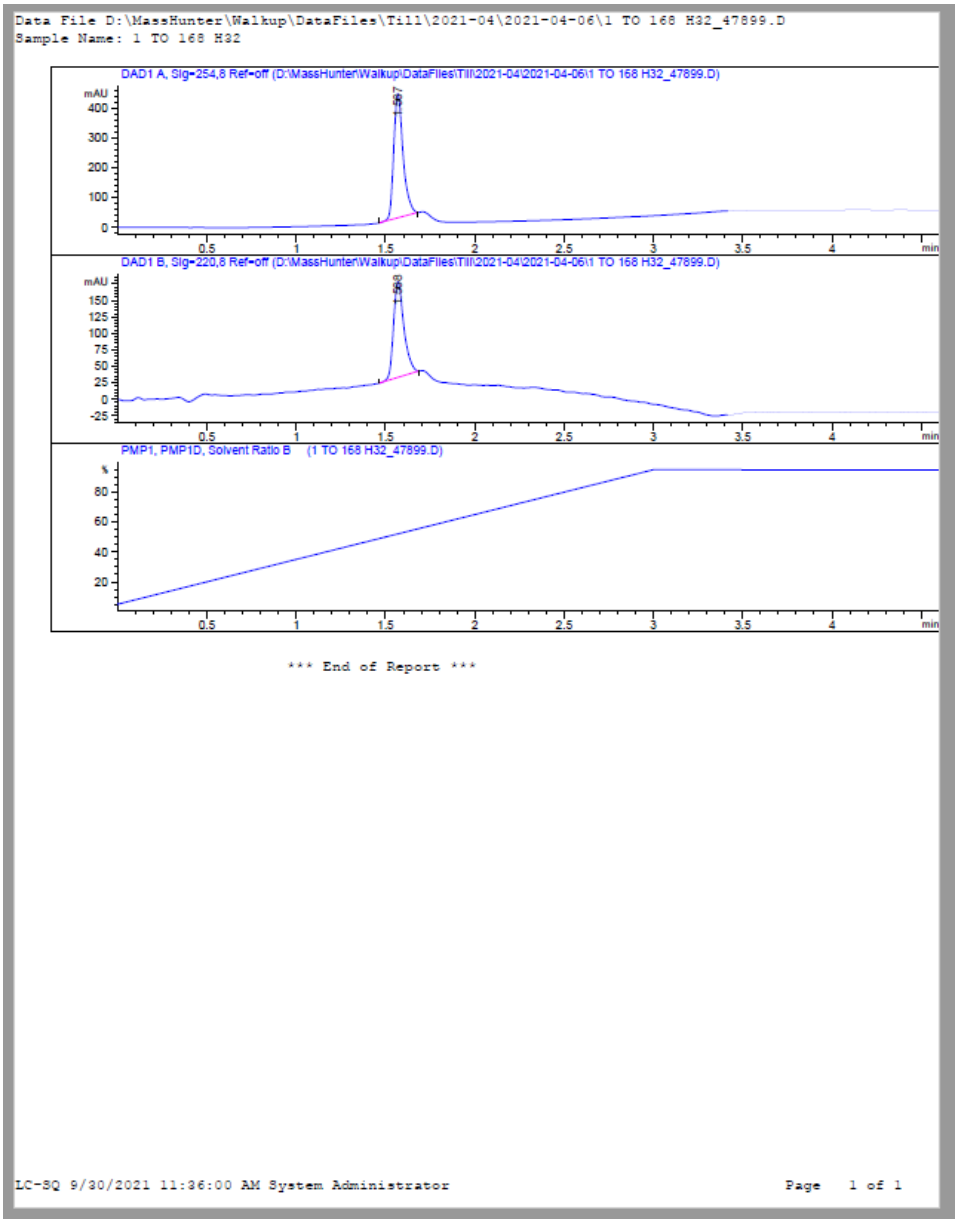


LC traces

Compound 2



Compound 4

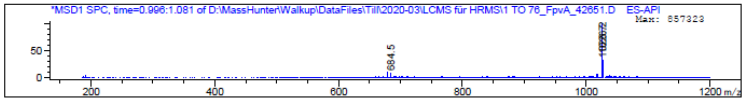

Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-06\1 TO 168 H32_47899.D
Sample Name: 1 TO 168 H32
DAD1 A, Sig=254,8 Ref=off (D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-06\1 TO 168 H32_47899.D)
mAU
1.567
DAD1 B, Sig=220,8 Ref=off (D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-06\1 TO 168 H32_47899.D)
mAU
1.563
PMP1, PMP1D, Solvent Ratio B (1 TO 168 H32_47899.D)
%
min
*** End of Report ***
LC-SQ 9/30/2021 11:36:00 AM System Administrator
Page 1 of 1

Compound 5

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS für HRMS\1 TO 76_FpvA_42651.D
Sample Name: 1 TO 76_FpvA

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 1000 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.025	30441984	1026.70 I
		1026.20 I
		1025.75 I

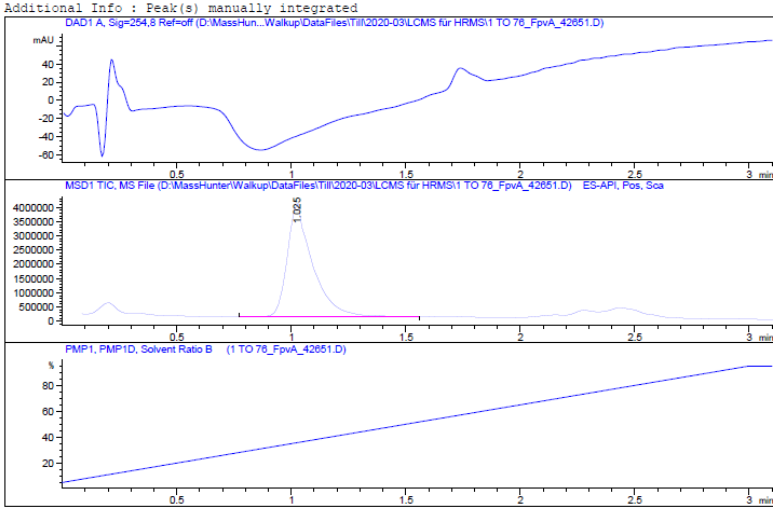


*** End of Report ***

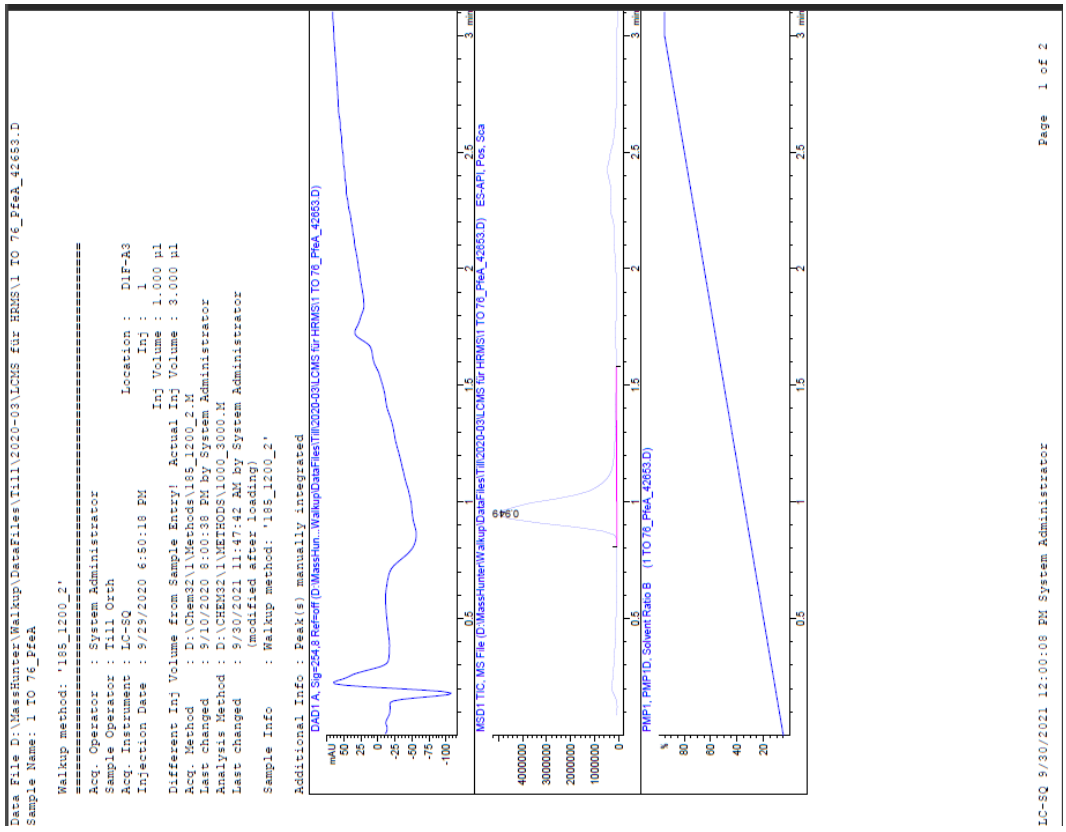
Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS für HRMS\1 TO 76_FpvA_42651.D
Sample Name: 1 TO 76_FpvA

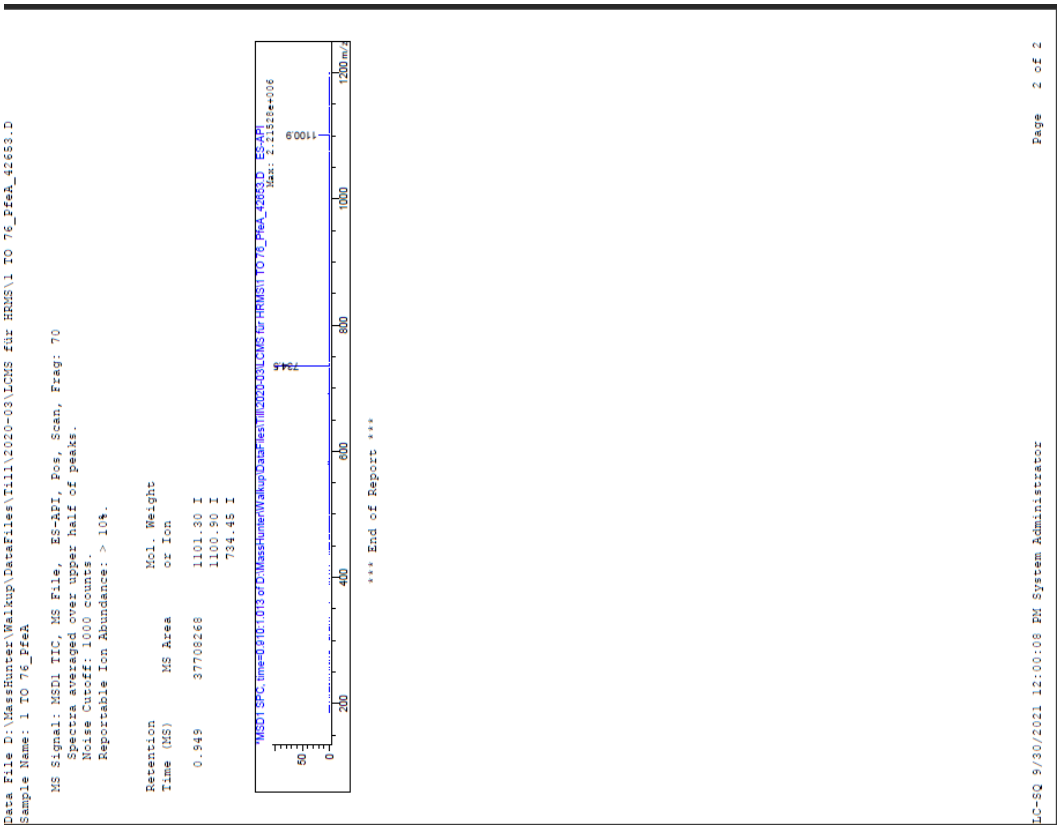
Walkup method: '185_1200_2'
==========
Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-A2
Injection Date : 9/29/2020 6:26:17 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 3.000 µl
Acq. Method : D:\Chem32\1\Methods\185_1200_2.M
Last changed : 9/10/2020 8:00:38 PM by System Administrator
Analysis Method : D:\CHEM32\1\METHODS\1000_3000.M
Last changed : 9/30/2021 11:47:42 AM by System Administrator
(modified after loading)
Sample Info : Walkup method: '185_1200_2'

Additional Info : Peak(s) manually integrated



Compound 6


Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS für HRMS\1 TO 76_PfeA_42653.D
Sample Name: 1 TO 76_PfeA
Walkup method: '185_1200_2'
Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ
Location : DiF-A3
Injection Date : 9/29/2020 6:80:18 PM
Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 3.000 µl
Acq. Method : D:\Chem32\1\Methods\185_1200_2.M
Last changed : 9/10/2020 8:00:38 PM by System Administrator
Analysis Method : D:\CHEM32\1\METHODS\1000_3000.M
Last changed : 9/30/2021 11:47:42 AM by System Administrator
(modified after loading)
Sample Info : Walkup method: '185_1200_2'
Additional Info : Peak(s) manually integrated
DAD1 A, Sig=254,8 Ref=off (D:\MassHun..\Walkup\DataFiles\Till\2020-03\LCMS für HRMS\1 TO 76_PfeA_42653.D)
MSD1 TIC, MS File (D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS für HRMS\1 TO 76_PfeA_42653.D) ES-API, Pos, Sca
PMP1, PMP1D, Solvent Ratio B (1 TO 76_PfeA_42653.D)
LC-SQ 9/30/2021 12:00:08 PM System Administrator
Page 1 of 2

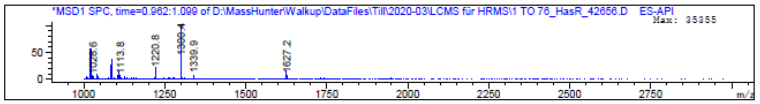

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS für HRMS\1 TO 76_PfeA_42653.D
Sample Name: 1 TO 76_PfeA
MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 1000 counts.
Reportable Ion Abundance: > 10%.
Retention Time (MS) Mol. Weight or Ion MS Area
0.949 1101.30 I 37708268
1100.90 I
734.45 I
"MSD1 SPC, time=0.870:1.013 of D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS für HRMS\1 TO 76_PfeA_42653.D ES-API
Max: 2.21928e+006
734.5
1100.9
*** End of Report ***
LC-SQ 9/30/2021 12:00:08 PM System Administrator
Page 2 of 2

Compound 7

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS für HRMS\1 TO 76_HasR_42656.D
Sample Name: 1 TO 76_HasR

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 1000 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.020	6071139	1626.20 I
		1625.20 I
		1300.40 I
		1299.90 I
		1299.40 I
		1298.95 I
		1221.85 I
		1221.30 I
		1220.85 I
		1106.70 I
		1086.70 I
		1086.20 I
		1085.75 I
		1085.25 I
		1022.70 I
		1022.20 I
		1021.70 I
		1021.20 I



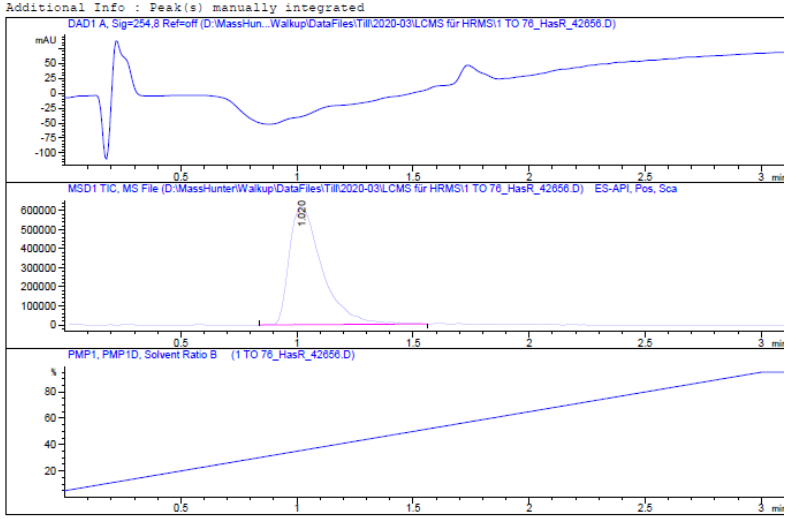
*** End of Report ***

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS für HRMS\1 TO 76_HasR_42656.D
Sample Name: 1 TO 76_HasR

Walkup method: '1000_3000_positive'

Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-A4
Injection Date : 9/29/2020 7:04:52 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 5.000 µl
Acq. Method : D:\Chem32\1\Methods\1000_3000.M
Last changed : 12/2/2019 9:06:09 AM by System Administrator
Analysis Method : D:\CHEM32\1\METHODS\1000_3000.M
Last changed : 9/30/2021 11:47:42 AM by System Administrator
(modified after loading)
Sample Info : Walkup method: '1000_3000_positive'

Additional Info : Peak(s) manually integrated



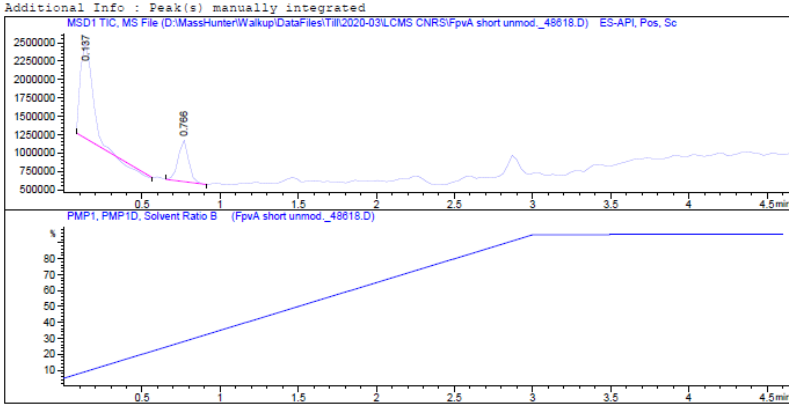
Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS CNRS\FpvA short unmod._48618.D
Sample Name: FpvA short unmod.

Walkup method: '0100-3000-new'

Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-A6
Injection Date : 4/19/2021 12:17:37 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 0.500 µl
Acq. Method : D:\Chem32\1\Methods\100-3000-new.M
Last changed : 3/25/2021 7:12:45 PM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 5/20/2022 8:22:22 PM by System Administrator
(modified after loading)
Method Info : Water Rinse 95%

Sample Info : Walkup method: '0100-3000-new'

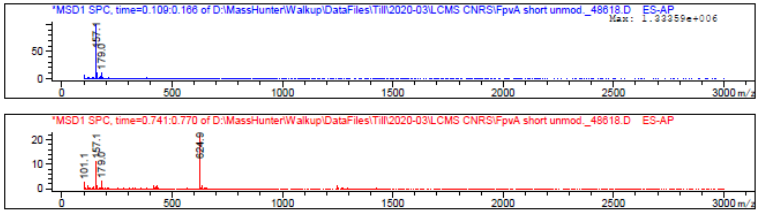
Additional Info : Peak(s) manually integrated



Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS CNRS\FpvA short unmod._48618.D
Sample Name: FpvA short unmod.

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
0.137	6478773	179.00 I
		157.10 I
0.766	2615125	624.90 I
		179.00 I
		157.10 I
		101.10 I



*** End of Report ***

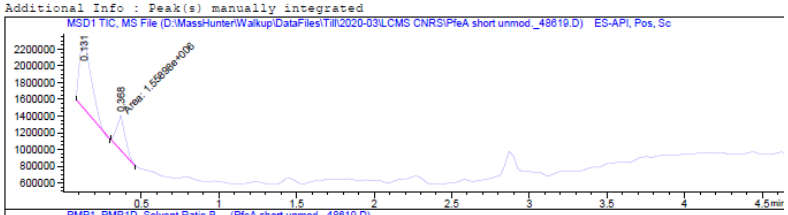
Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS CNRS\PfeA short unmod._48619.D
Sample Name: PfeA short unmod.

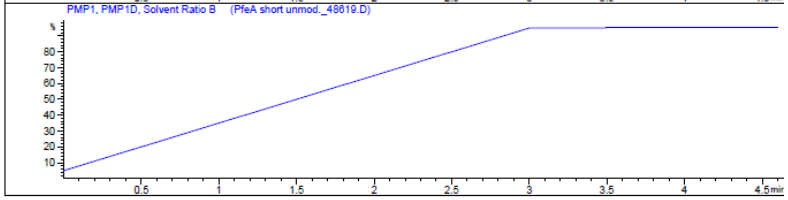
Walkup method: '0100-3000-new'

Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-A7
Injection Date : 4/19/2021 12:23:46 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 0.500 µl
Acq. Method : D:\Chem32\1\Methods\100-3000-new.M
Last changed : 3/25/2021 7:12:45 PM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 5/20/2022 8:22:22 PM by System Administrator
(modified after loading)
Method Info : Water Rinse 95%

Sample Info : Walkup method: '0100-3000-new'

Additional Info : Peak(s) manually integrated

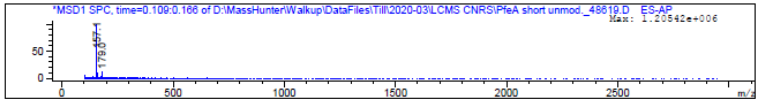


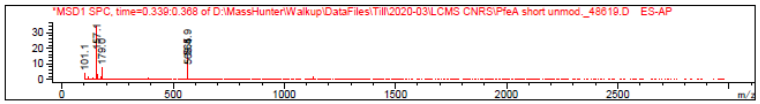


Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS CNRS\PfeA short unmod._48619.D
Sample Name: PfeA short unmod.

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion	
0.131	4157878	179.00	I
		157.05	I
0.368	1558976	566.40	I
		565.90	I
		179.00	I
		157.10	I
		101.05	I



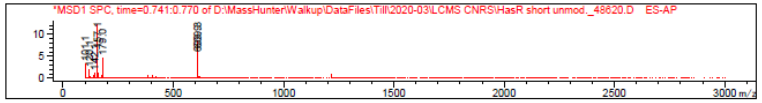


*** End of Report ***

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS CNRS\HasR short unmod._48620.D
Sample Name: HasR short unmod.

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
0.125	1497478	179.00 I
		159.00 I
		157.10 I
0.743	1530958	609.90 I
		609.30 I
		179.00 I
		157.10 I
		142.10 I
		120.10 I
		101.10 I



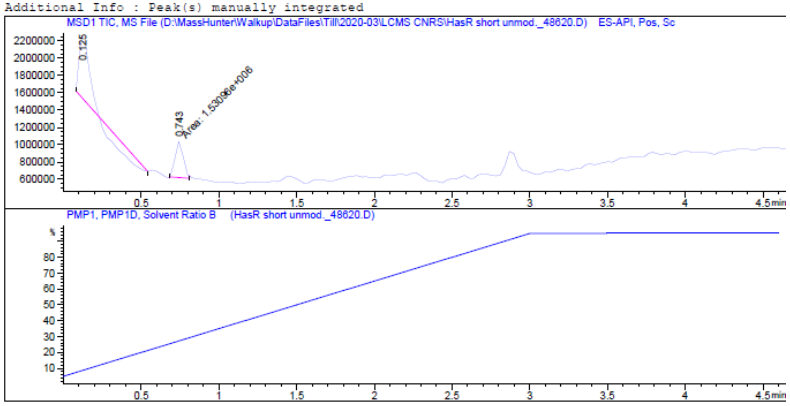
*** End of Report ***

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\LCMS CNRS\HasR short unmod._48620.D
Sample Name: HasR short unmod.

Walkup method: '0100-3000-new'
==========
Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-A8
Injection Date : 4/19/2021 12:29:56 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 0.500 µl
Acq. Method : D:\Chem32\1\Methods\100-3000-new.M
Last changed : 3/25/2021 7:12:45 PM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 5/20/2022 8:22:22 PM by System Administrator
(modified after loading)
Method Info : Water Rinse 95%

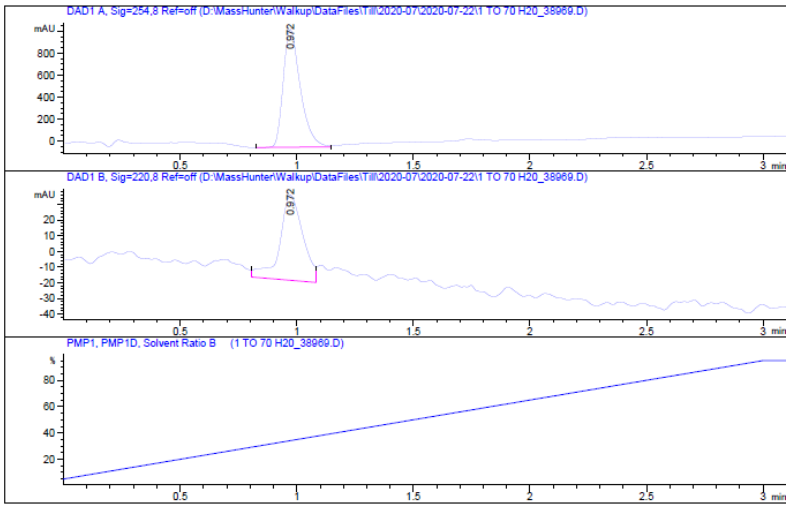
Sample Info : Walkup method: '0100-3000-new'

Additional Info : Peak(s) manually integrated



Compound 11

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-07\2020-07-22\1 TO 70 H20_38969.D
Sample Name: 1 TO 70 H20



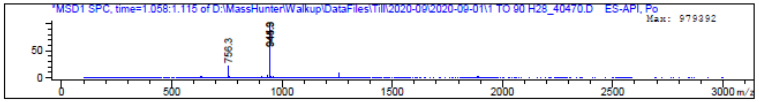
*** End of Report ***

LC-SQ 5/21/2022 2:41:16 PM System Administrator Page 1 of 1

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-09\2020-09-01\1 TO 90 H28_40470.D
Sample Name: 1 TO 90 H28

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.076	25337692	945.30 I
		944.90 I
		756.35 I



*** End of Report ***

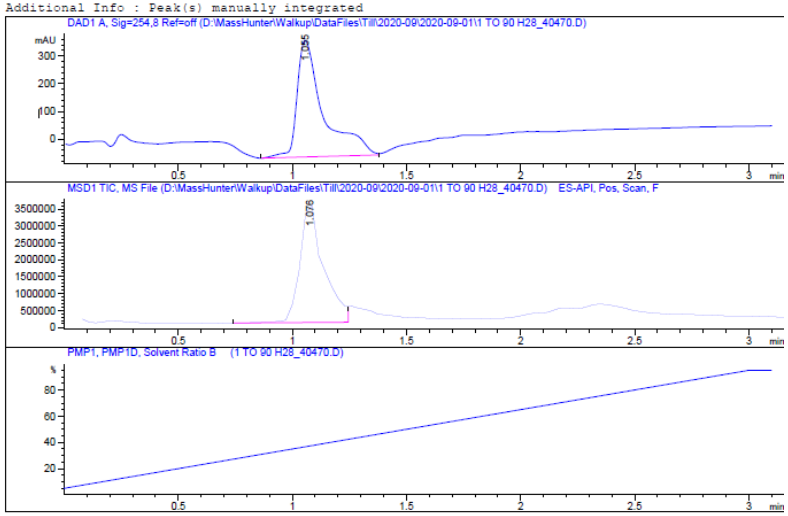
Data File D:\MassHunter\Walkup\DataFiles\Till\2020-09\2020-09-01\1 TO 90 H28_40470.D
Sample Name: 1 TO 90 H28

Walkup method: 'full_range_positive'

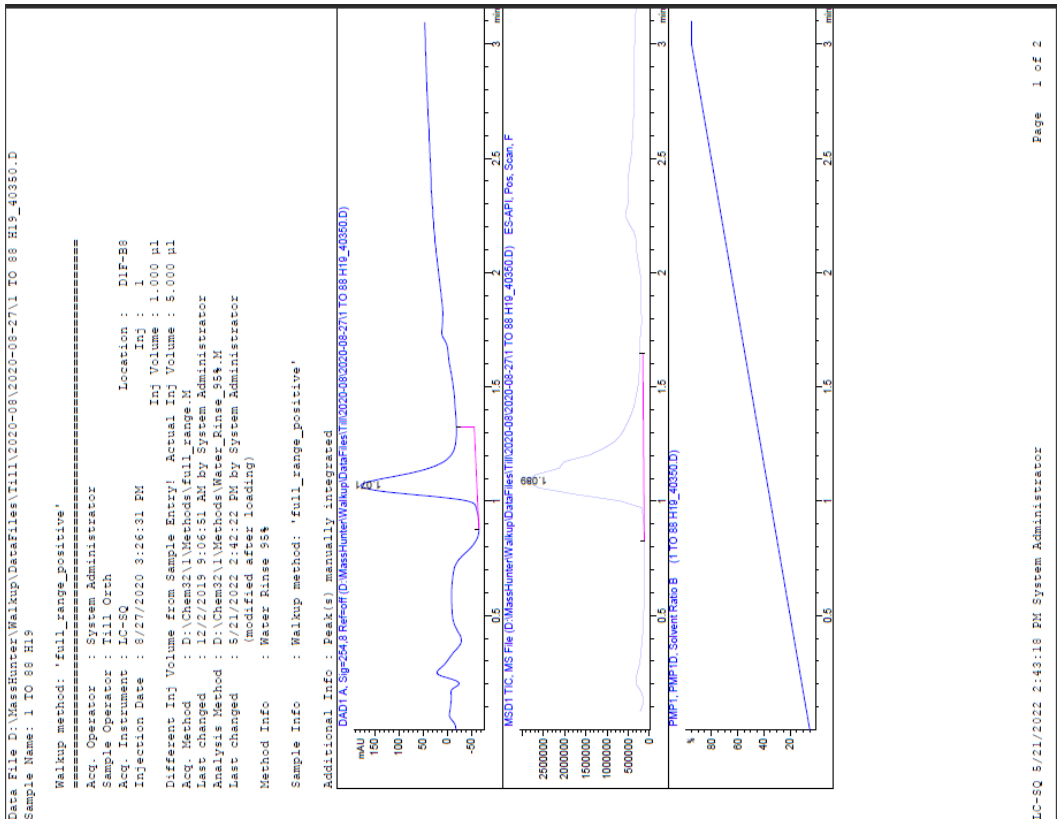
Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-F9
Injection Date : 9/1/2020 12:36:05 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 5.000 µl
Acq. Method : D:\Chem32\1\Methods\full_range.M
Last changed : 12/2/2019 9:06:51 AM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 5/21/2022 2:42:22 PM by System Administrator
(modified after loading)
Method Info : Water Rinse 95%

Sample Info : Walkup method: 'full_range_positive'

Additional Info : Peak(s) manually integrated



Compound 13



Data File D:\MassHunter\Walkup\DataFiles\Till\2020-08\2020-08-27\1 TO 88 H19_40350.D
Sample Name: 1 TO 88 H19

Walkup method: 'full_range_positive'

Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : DIF-B8
Injection Date : 8/27/2020 3:26:31 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 5.000 µl
Acq. Method : D:\Chem32\1\Methods\full_range.M
Last changed : 12/2/2019 9:06:51 AM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 5/21/2022 2:42:22 PM by System Administrator
(modified after loading)
Method Info : Water Rinse 95%
Sample Info : Walkup method: 'full_range_positive'
Additional Info : Peak(s) manually integrated

DAD1 A, Sig=254,8 Ref=off (D:\MassHunter\Walkup\DataFiles\Till\2020-08\2020-08-27\1 TO 88 H19_40350.D)
mAU
1.089
MSD1 TIC, MS File (D:\MassHunter\Walkup\DataFiles\Till\2020-08\2020-08-27\1 TO 88 H19_40350.D) ES-API, Pos, Scan, F
1.089
PMP1, PMPID, Solvent Ratio B (1 TO 88 H19_40350.D)
%
min

LC-SQ 5/21/2022 2:43:18 PM System Administrator Page 1 of 2

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-08\2020-08-27\1 TO 88 H19_40350.D
Sample Name: 1 TO 88 H19

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion	
1.089	33915692	1044.30	I
		835.60	I
		696.50	I

"MSD1 SPC, time=1.029:1.173 of D:\MassHunter\Walkup\DataFiles\Till\2020-08\2020-08-27\1 TO 88 H19_40350.D ES-API, Po..." Max: 558869
1044.3
835.5
696.5
m/z

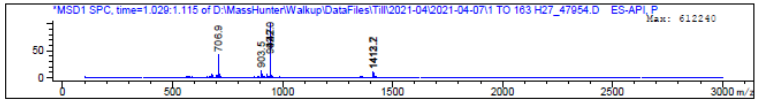
*** End of Report ***

LC-SQ 5/21/2022 2:43:18 PM System Administrator Page 2 of 2

Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-07\1 TO 163 H27_47954.D
Sample Name: 1 TO 163 H27

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.055	76162104	1413.15 I
		1412.70 I
		942.65 I
		942.05 I
		903.55 I
		706.90 I



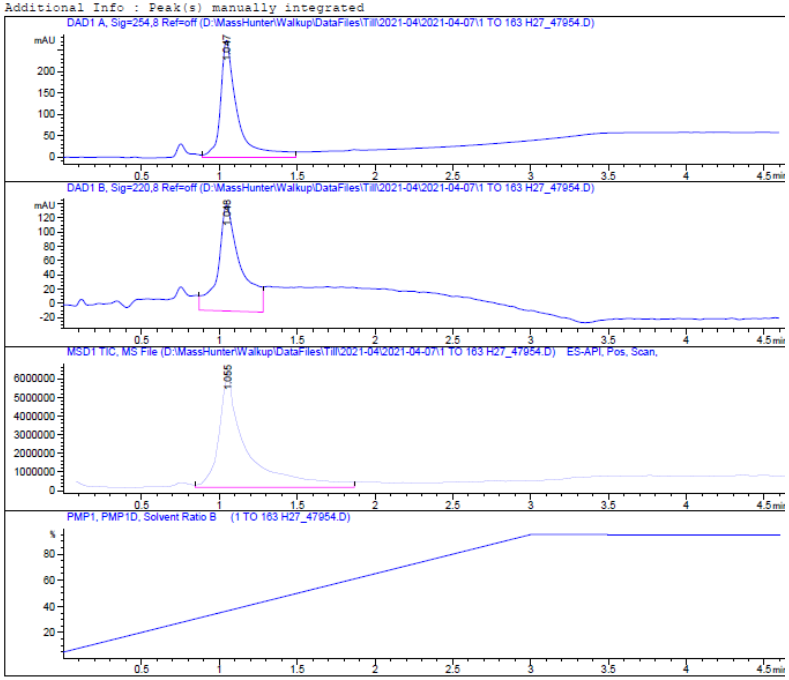
*** End of Report ***

Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-07\1 TO 163 H27_47954.D
Sample Name: 1 TO 163 H27

Walkup method: '0100-3000-new'
==========
Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-A7
Injection Date : 4/7/2021 1:46:44 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 1.800 µl
Acq. Method : D:\Chem32\1\Methods\100-3000-new.M
Last changed : 3/25/2021 7:12:45 PM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

Sample Info : Walkup method: '0100-3000-new'

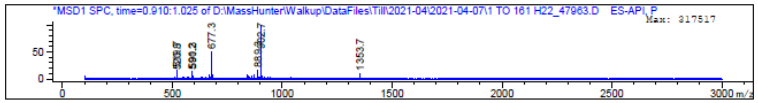
Additional Info : Peak(s) manually integrated



Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-07\1 TO 161 H22_47963.D
Sample Name: 1 TO 161 H22

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
0.943	45362920	1353.70 I
		902.70 I
		889.35 I
		677.35 I
		591.15 I
		590.25 I
		520.75 I
		519.70 I



*** End of Report ***

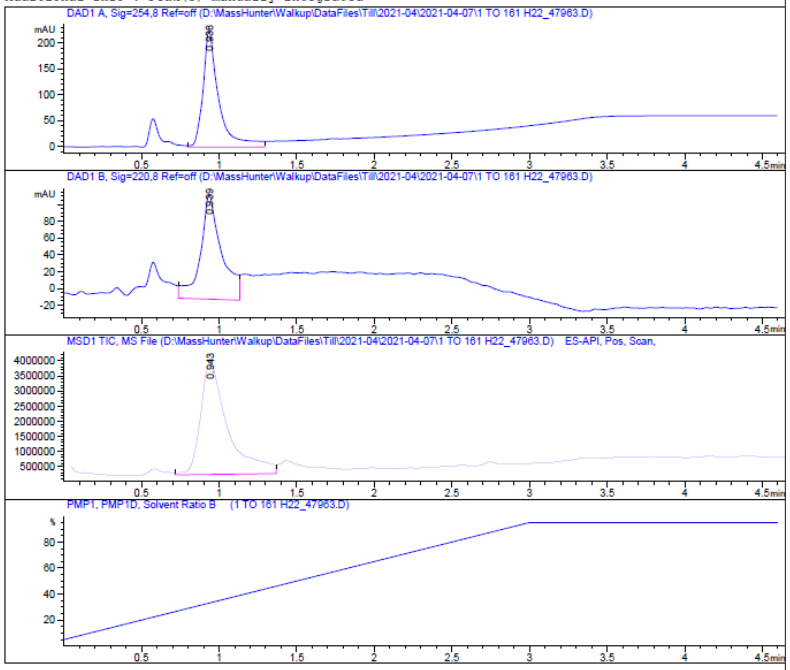
Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-07\1 TO 161 H22_47963.D
Sample Name: 1 TO 161 H22

Walkup method: '0100-3000-new'
==========
Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-B7
Injection Date : 4/7/2021 3:02:14 PM Inj : 1
Inj Volume : 1.000 µl

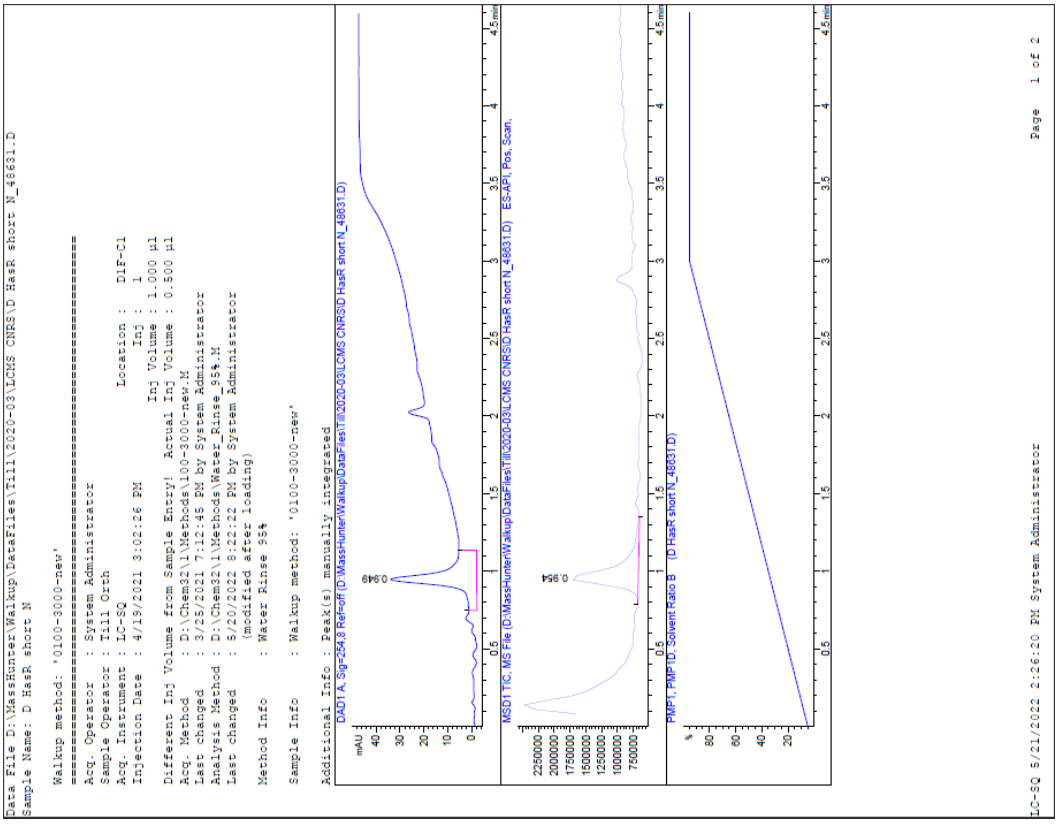
Acq. Method : D:\Chem32\1\Methods\100-3000-new.M
Last changed : 3/25/2021 7:12:45 PM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

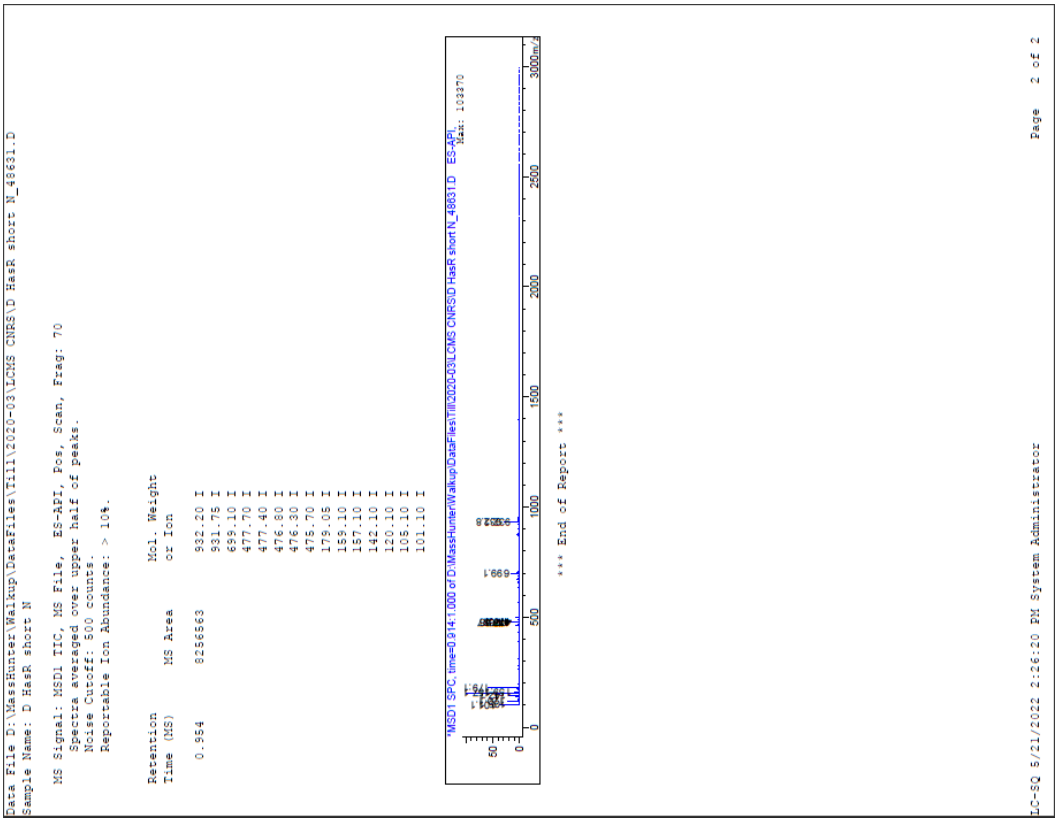
Sample Info : Walkup method: '0100-3000-new'

Additional Info : Peak(s) manually integrated



Compound 16

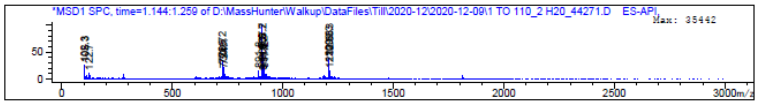




Data File D:\MassHunter\Walkup\DataFiles\Till\2020-12\2020-12-09\1 TO 110_2 H20_44271.D
Sample Name: 1 TO 110_2 H20

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.199	9690410	1210.85 I
		1210.25 I
		1209.80 I
		1209.30 I
		917.20 I
		913.15 I
		911.60 I
		911.10 I
		908.15 I
		907.70 I
		907.25 I
		891.80 I
		734.10 I
		730.85 I
		726.65 I
		726.15 I
		122.70 I
		105.25 I
		102.25 I



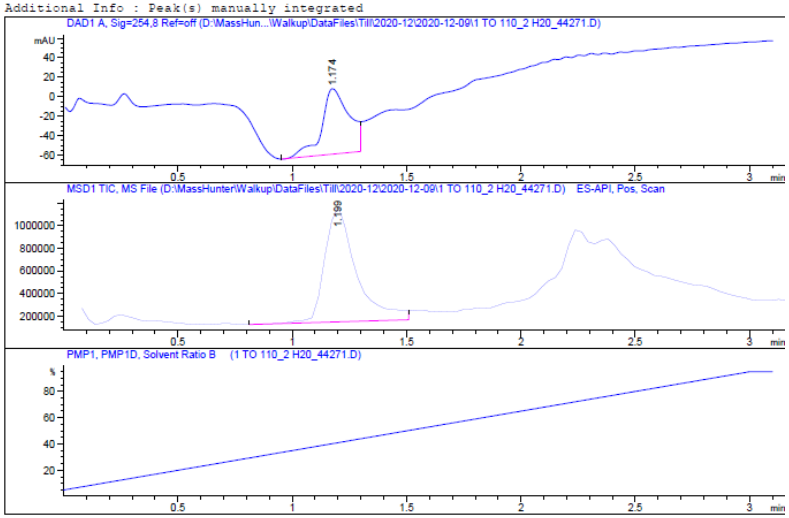
*** End of Report ***

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-12\2020-12-09\1 TO 110_2 H20_44271.D
Sample Name: 1 TO 110_2 H20

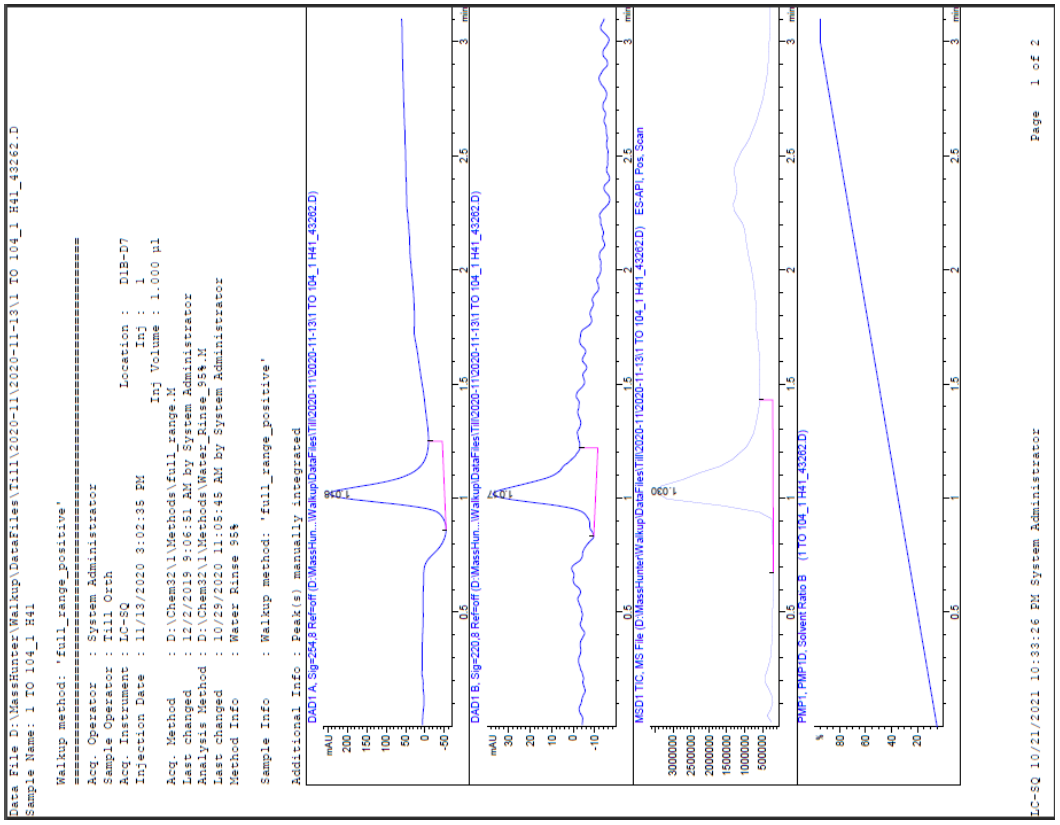
Walkup method: 'full_range_positive'
==========
Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-D8
Injection Date : 12/9/2020 6:36:31 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 0.500 µl
Acq. Method : D:\Chem32\1\Methods\full_range.M
Last changed : 12/2/2019 9:06:51 AM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

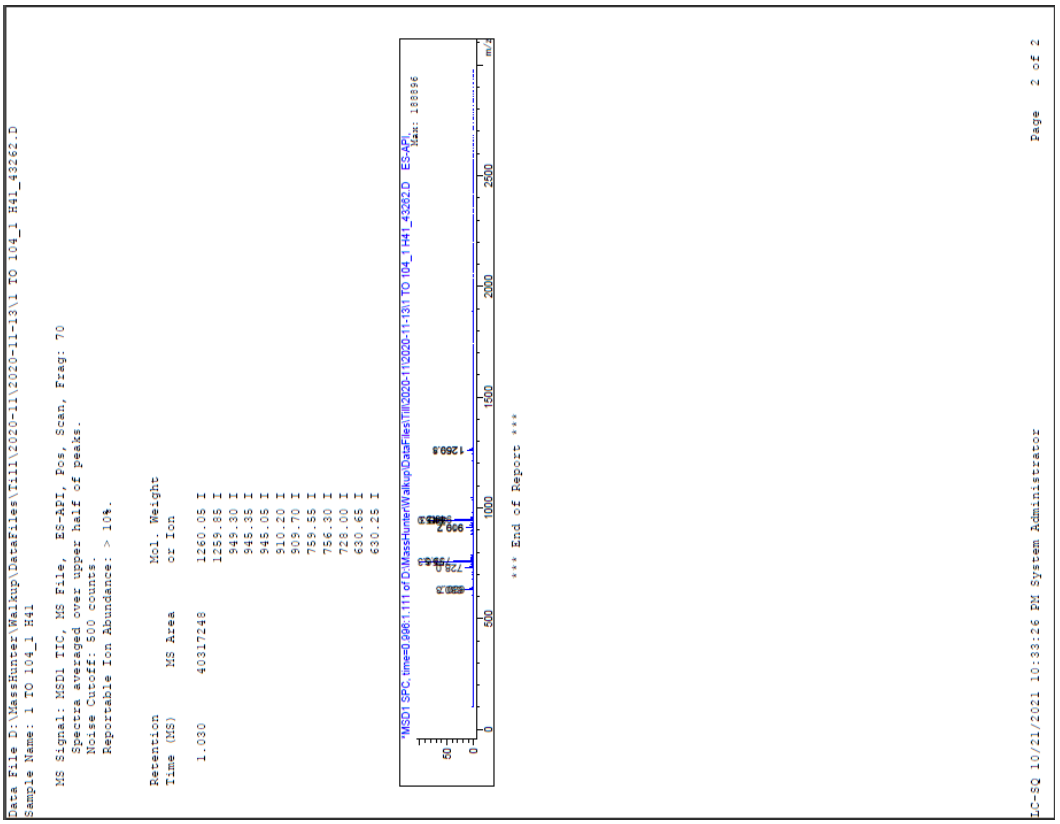
Sample Info : Walkup method: 'full_range_positive'

Additional Info : Peak(s) manually integrated



Compound 18

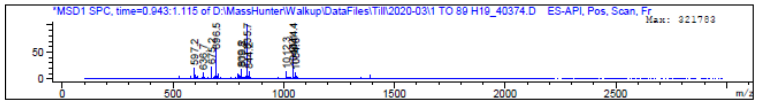




Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\1 TO 89 H19_40374.D
Sample Name: 1 TO 89 H19

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.000	71713992	1054.60 I
		1044.45 I
		1044.10 I
		1012.30 I
		844.15 I
		835.70 I
		810.15 I
		809.80 I
		696.55 I
		675.20 I
		636.65 I
		597.20 I



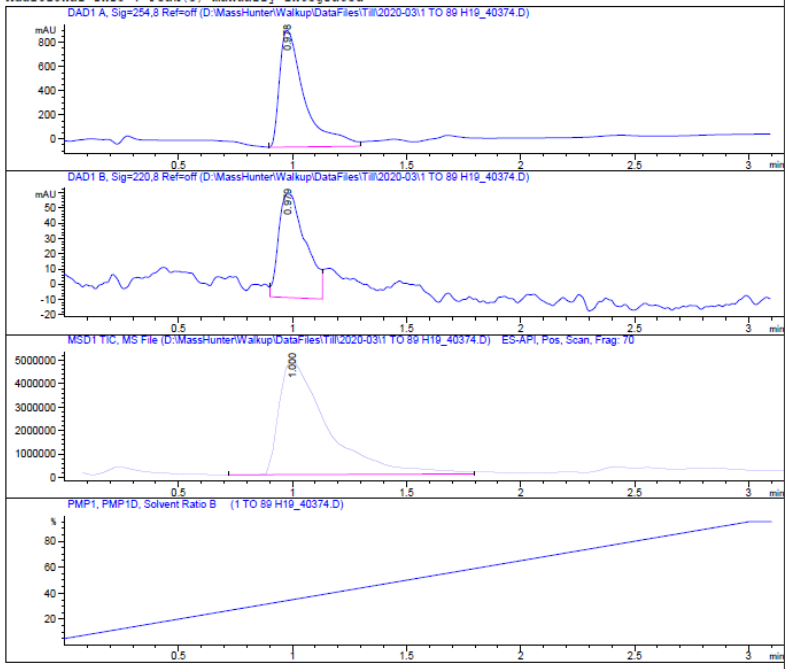
*** End of Report ***

Data File D:\MassHunter\Walkup\DataFiles\Till\2020-03\1 TO 89 H19_40374.D
Sample Name: 1 TO 89 H19

Walkup method: 'full_range_positive'
==========
Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-E4
Injection Date : 8/27/2020 6:02:50 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 10.000 µl
Acq. Method : D:\Chem32\1\Methods\full_range.M
Last changed : 12/2/2019 9:06:51 AM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

Sample Info : Walkup method: 'full_range_positive'

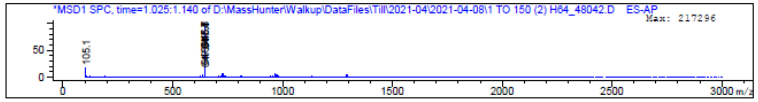
Additional Info : Peak(s) manually integrated



Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-08\1 TO 150 (2) H64_48042.D
Sample Name: 1 TO 150 (2) H64

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.056	18851602	647.70 I
		647.40 I
		646.65 I
		646.40 I
		645.80 I
		105.10 I

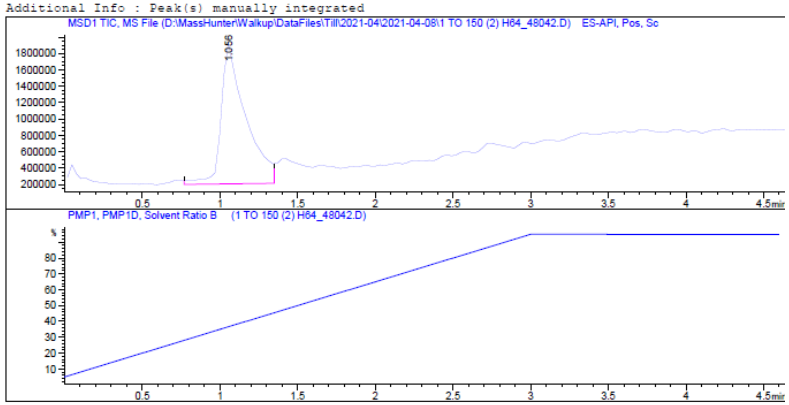


*** End of Report ***

Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-08\1 TO 150 (2) H64_48042.D
Sample Name: 1 TO 150 (2) H64

Walkup method: '0100-3000-new'

Acq. Operator	: System Administrator		
Sample Operator	: Till Orth		
Acq. Instrument	: LC-SQ	Location	: D1F-D1
Injection Date	: 4/8/2021 3:43:23 PM	Inj	: 1
		Inj Volume	: 1.000 µl
Acq. Method	: D:\Chem32\1\Methods\100-3000-new.M		
Last changed	: 3/25/2021 7:12:45 PM by System Administrator		
Analysis Method	: D:\Chem32\1\Methods\Water_Rinse_95%.M		
Last changed	: 5/20/2022 8:22:22 PM by System Administrator (modified after loading)		
Method Info	: Water Rinse 95%		
Sample Info	: Walkup method: '0100-3000-new'		
Additional Info	: Peak(s) manually integrated		

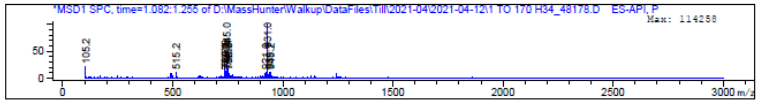


Compound 20

Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-12\1 TO 170 H34_48178.D
Sample Name: 1 TO 170 H34

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.148	38609968	945.15 I
		939.65 I
		930.95 I
		921.05 I
		752.60 I
		751.35 I
		749.40 I
		745.00 I
		739.90 I
		738.95 I
		737.75 I
		515.15 I
		105.15 I



*** End of Report ***

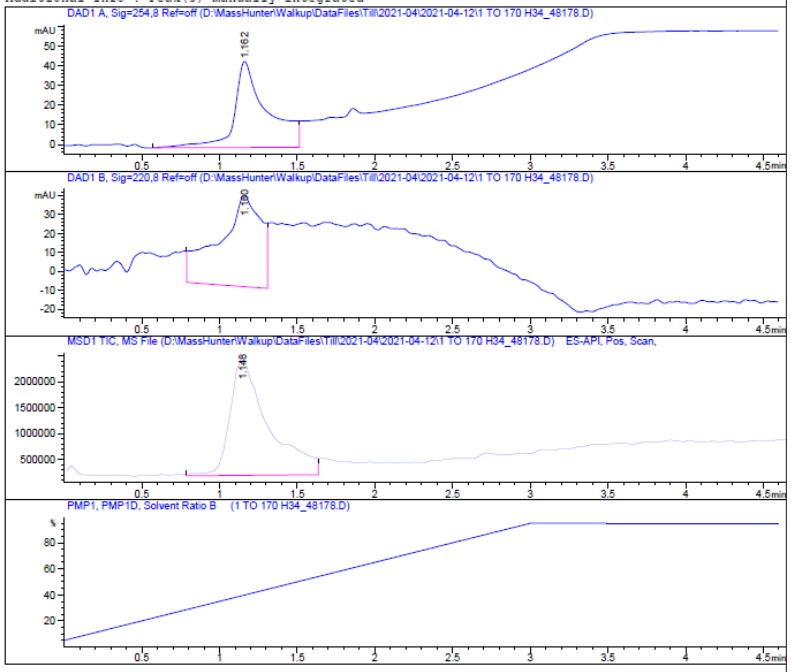
Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-12\1 TO 170 H34_48178.D
Sample Name: 1 TO 170 H34

Walkup method: '0100-3000-new'

Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1B-B9
Injection Date : 4/12/2021 5:23:16 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 1.200 µl
Acq. Method : D:\Chem32\1\Methods\100-3000-new.M
Last changed : 3/25/2021 7:12:45 PM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

Sample Info : Walkup method: '0100-3000-new'

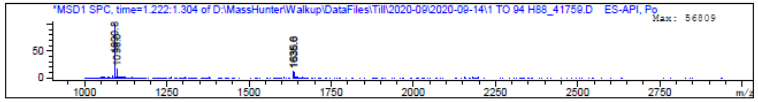
Additional Info : Peak(s) manually integrated



Data File D:\MassHunter\Walkup\DataFiles\Till\2020-09\2020-09-14\1 TO 94 H88_41759.D
Sample Name: 1 TO 94 H88

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.255	1065877	1636.00 I
		1635.60 I
		1098.00 I
		1090.75 I



*** End of Report ***

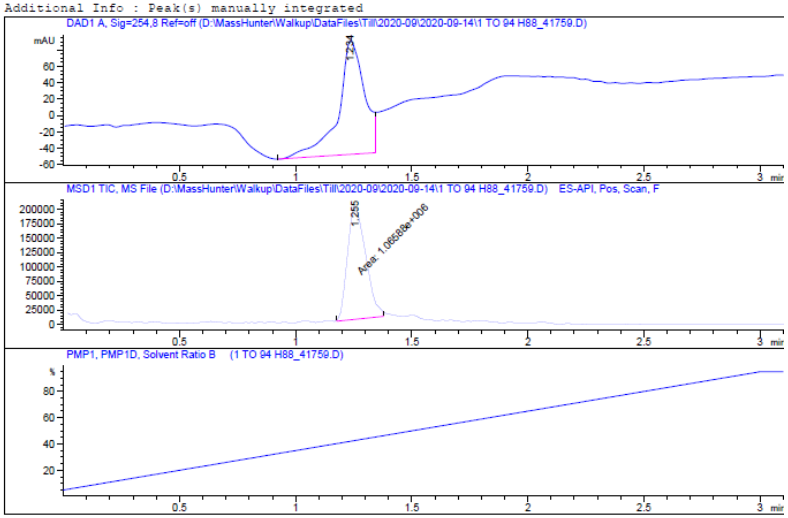
Data File D:\MassHunter\Walkup\DataFiles\Till\2020-09\2020-09-14\1 TO 94 H88_41759.D
Sample Name: 1 TO 94 H88

Walkup method: '1000_3000_positive'

Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1B-A4
Injection Date : 9/14/2020 11:22:41 AM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 0.500 µl
Acq. Method : D:\Chem32\1\Methods\1000_3000.M
Last changed : 12/2/2019 9:06:09 AM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

Sample Info : Walkup method: '1000_3000_positive'

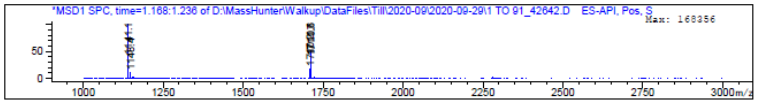
Additional Info : Peak(s) manually integrated



Data File D:\MassHunter\Walkup\DataFiles\Till\2020-09\2020-09-29\1 TO 91_42642.D
Sample Name: 1 TO 91

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.200	4229497	1711.65 I
		1711.10 I
		1710.60 I
		1710.20 I
		1148.40 I
		1141.10 I



*** End of Report ***

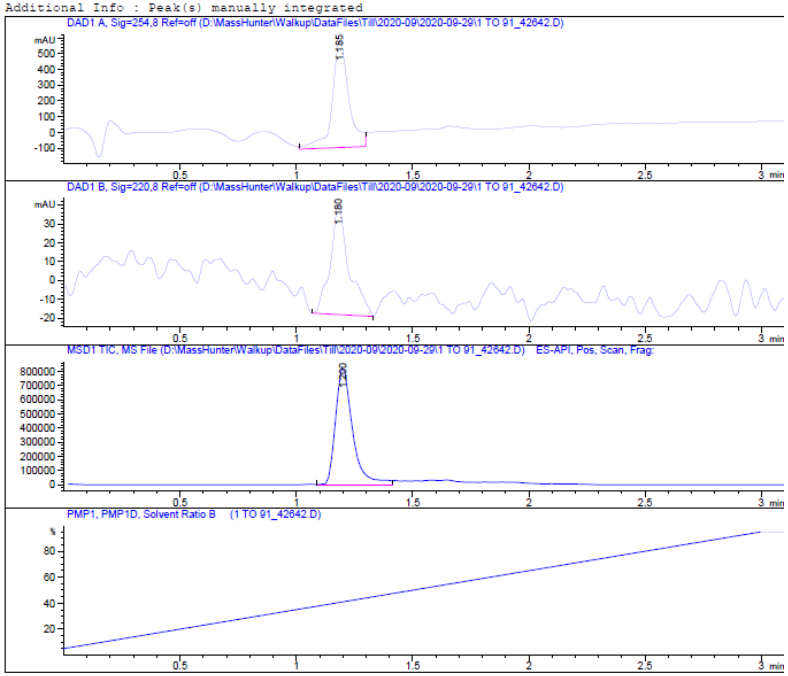
Data File D:\MassHunter\Walkup\DataFiles\Till\2020-09\2020-09-29\1 TO 91_42642.D
Sample Name: 1 TO 91

Walkup method: '1000_3000_positive'

Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1B-E1
Injection Date : 9/29/2020 5:43:22 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 3.000 µl
Acq. Method : D:\Chem32\1\Methods\1000_3000.M
Last changed : 12/2/2019 9:06:09 AM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

Sample Info : Walkup method: '1000_3000_positive'

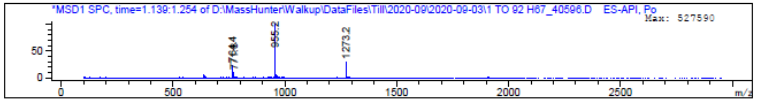
Additional Info : Peak(s) manually integrated



Data File D:\MassHunter\Walkup\DataFiles\Till\2020-09\2020-09-03\1 TO 92 H67_40596.D
Sample Name: 1 TO 92 H67

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.179	23932568	1273.20 I
		955.15 I
		771.85 I
		764.40 I



*** End of Report ***

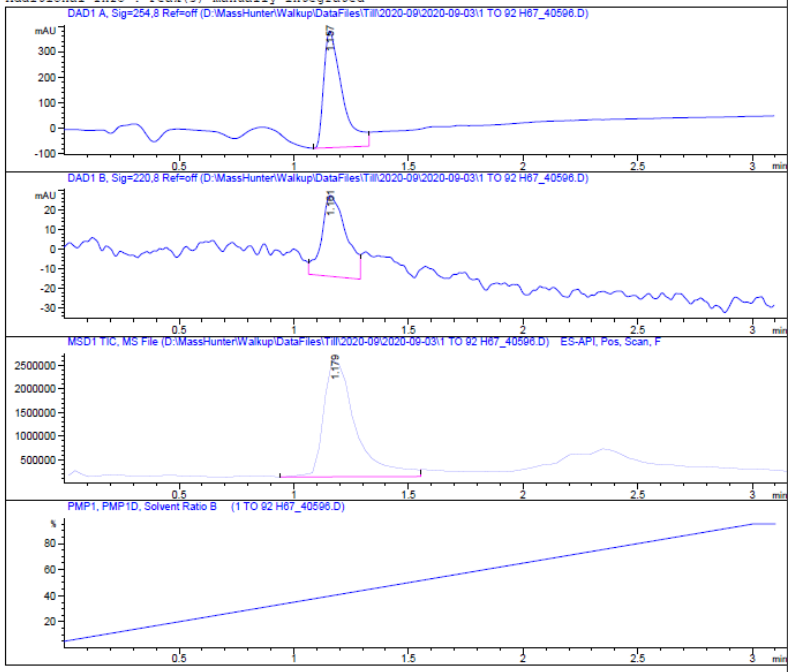
Data File D:\MassHunter\Walkup\DataFiles\Till\2020-09\2020-09-03\1 TO 92 H67_40596.D
Sample Name: 1 TO 92 H67

Walkup method: 'full_range_positive'

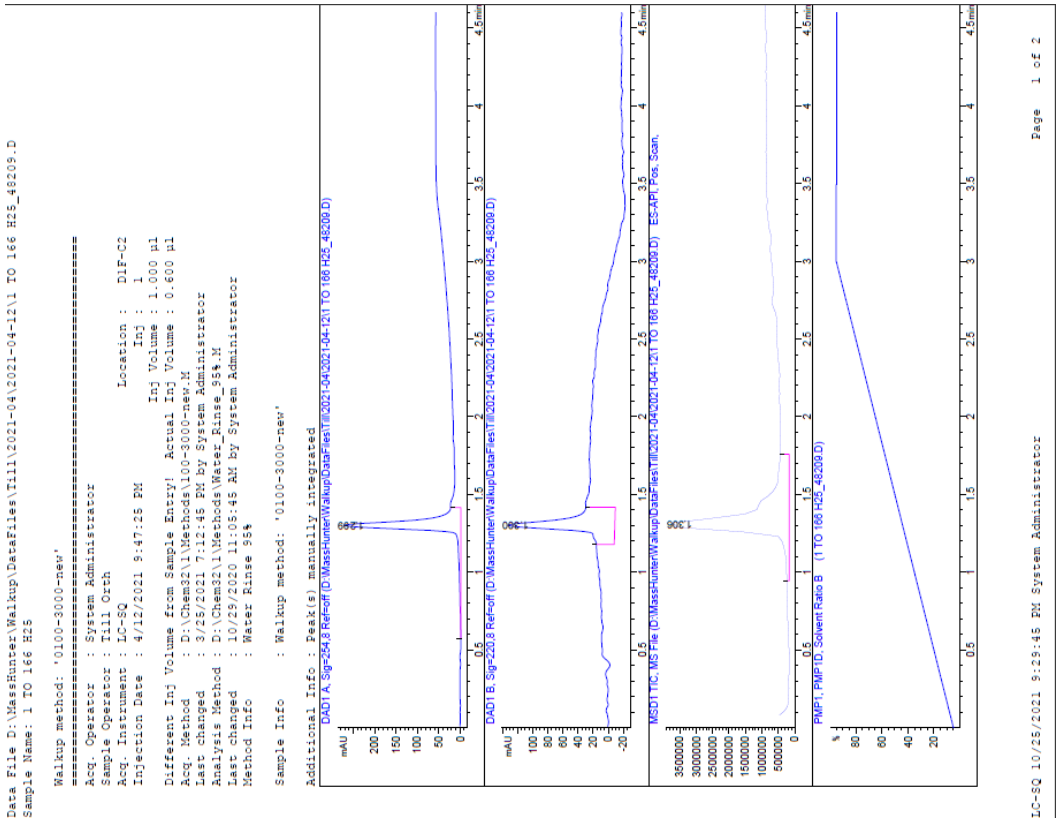
Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1B-C4
Injection Date : 9/3/2020 2:54:51 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 3.000 µl
Acq. Method : D:\Chem32\1\Methods\full_range.M
Last changed : 12/2/2019 9:06:51 AM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

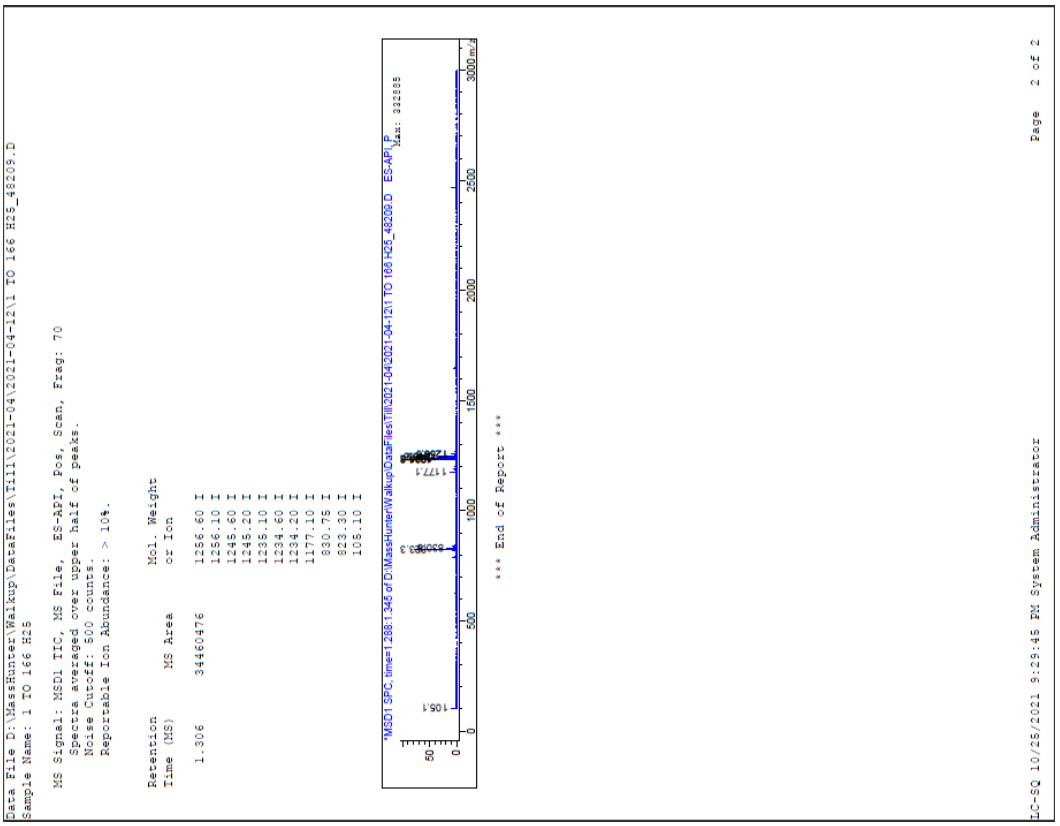
Sample Info : Walkup method: 'full_range_positive'

Additional Info : Peak(s) manually integrated



Compound 25

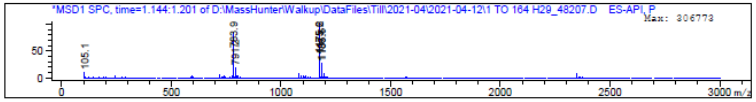




Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-12\1 TO 164 H29_48207.D
Sample Name: 1 TO 164 H29

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.156	20625412	1186.60 I
		1186.10 I
		1175.60 I
		1175.20 I
		791.20 I
		783.90 I
		105.10 I



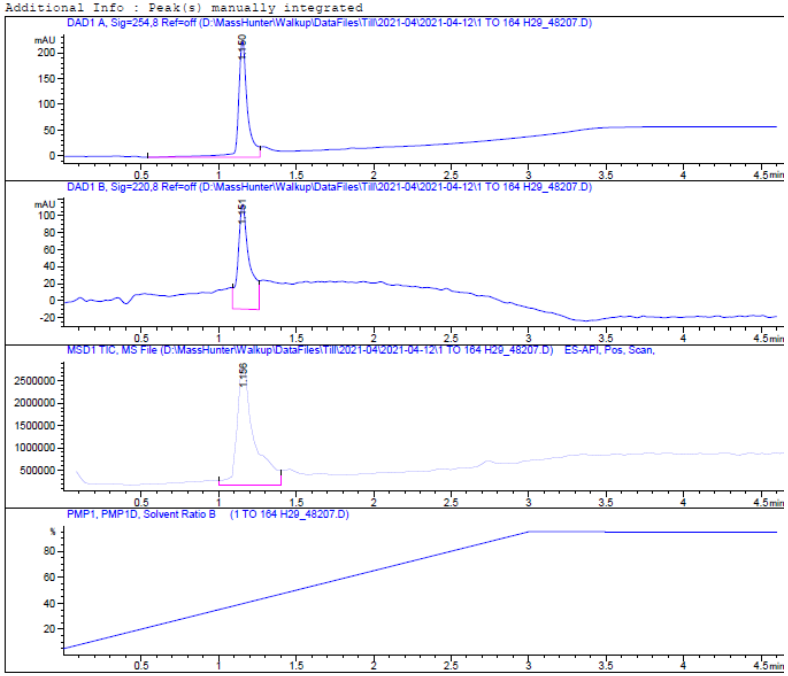
*** End of Report ***

Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-12\1 TO 164 H29_48207.D
Sample Name: 1 TO 164 H29

Walkup method: '0100-3000-new'
==========
Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-B9
Injection Date : 4/12/2021 9:34:56 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 0.600 µl
Acq. Method : D:\Chem32\1\Methods\100-3000-new.M
Last changed : 3/25/2021 7:12:45 PM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

Sample Info : Walkup method: '0100-3000-new'

Additional Info : Peak(s) manually integrated

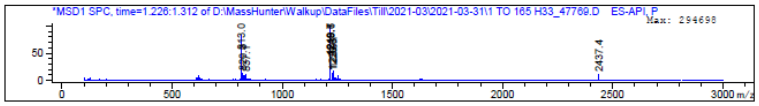


Compound 27

Data File D:\MassHunter\Walkup\DataFiles\Till\2021-03\2021-03-31\1 TO 165 H33_47769.D
Sample Name: 1 TO 165 H33

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.263	38051636	2437.40 I
		1230.60 I
		1230.10 I
		1229.60 I
		1219.55 I
		1219.10 I
		1218.70 I
		837.10 I
		820.25 I
		813.00 I



*** End of Report ***

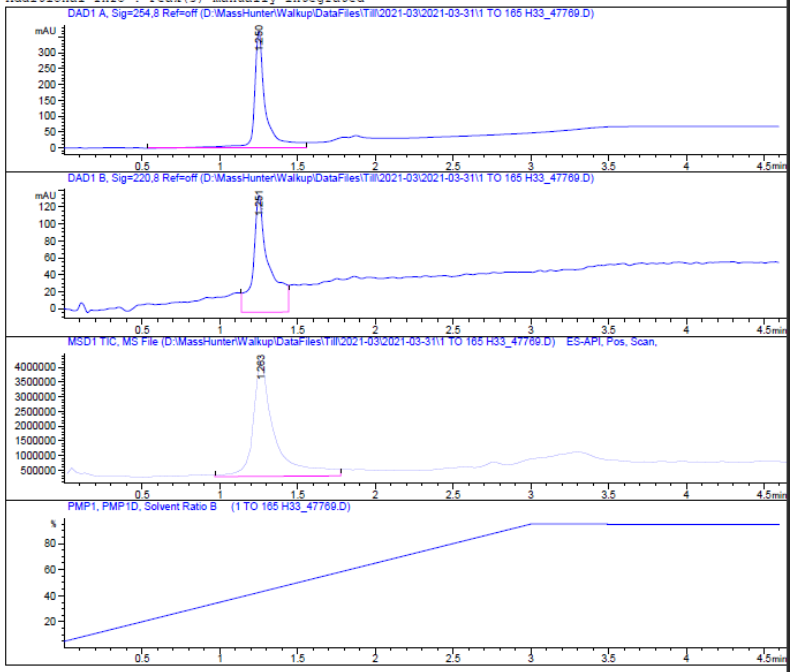
Data File D:\MassHunter\Walkup\DataFiles\Till\2021-03\2021-03-31\1 TO 165 H33_47769.D
Sample Name: 1 TO 165 H33

Walkup method: '0100-3000-new'

Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1F-D6
Injection Date : 3/31/2021 7:44:42 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 3.000 µl
Acq. Method : D:\Chem32\1\Methods\100-3000-new.M
Last changed : 3/25/2021 7:12:45 PM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

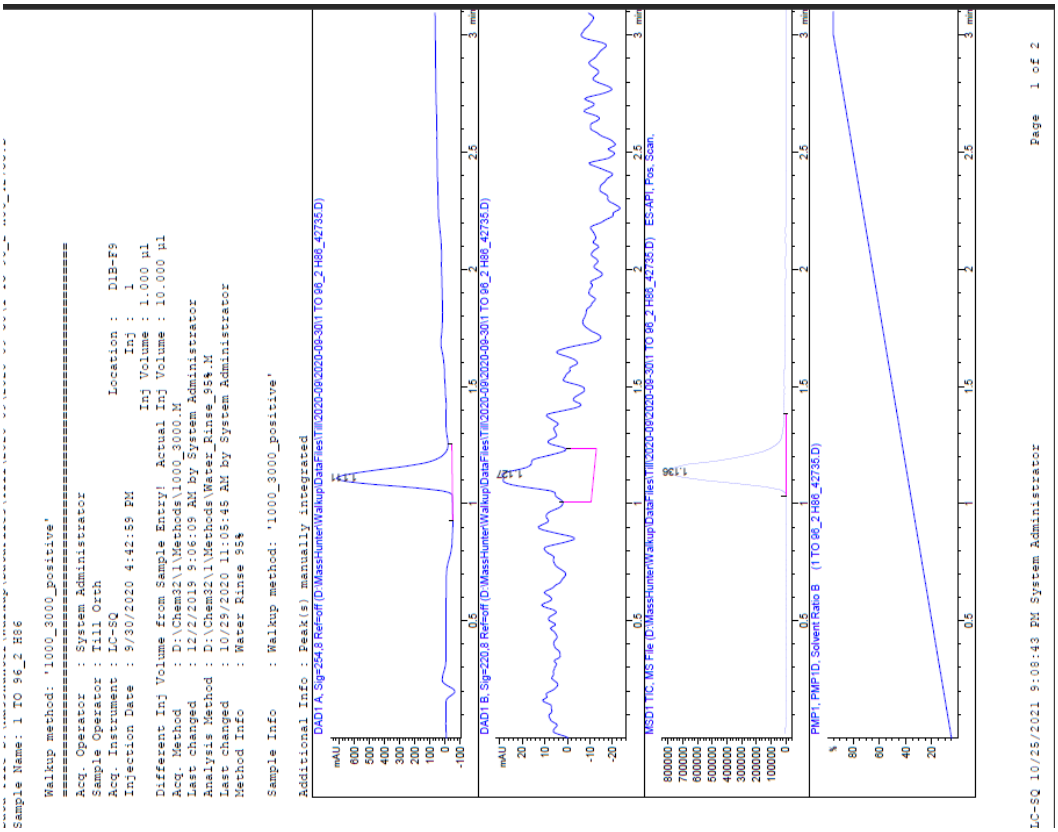
Sample Info : Walkup method: '0100-3000-new'

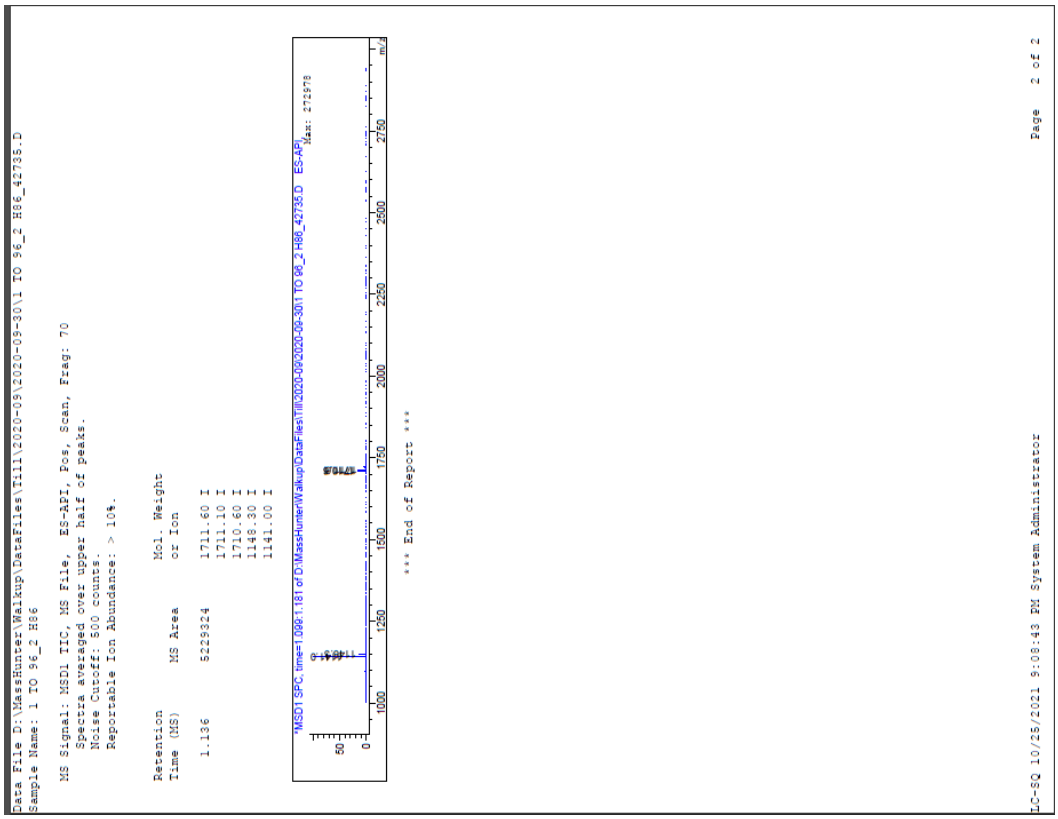
Additional Info : Peak(s) manually integrated



Compound 28

Compound 29





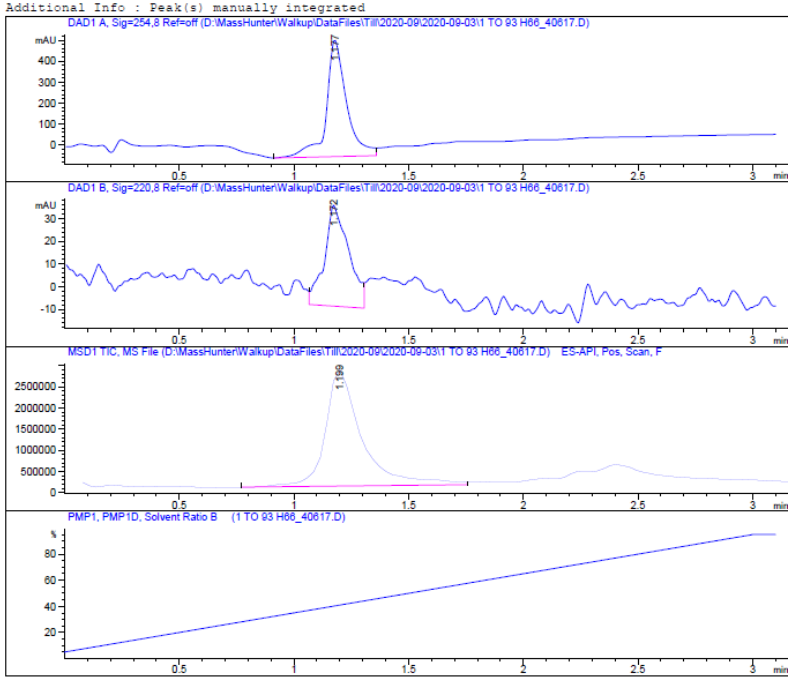
Data File D:\MassHunter\Walkup\DataFiles\Till\2020-09\2020-09-03\1 TO 93 H66_40617.D
Sample Name: 1 TO 93 H66

Walkup method: 'full_range_positive'

Acq. Operator : System Administrator
Sample Operator : Till Orth
Acq. Instrument : LC-SQ Location : D1B-E4
Injection Date : 9/3/2020 4:54:18 PM Inj : 1
Inj Volume : 1.000 µl
Different Inj Volume from Sample Entry! Actual Inj Volume : 6.000 µl
Acq. Method : D:\Chem32\1\Methods\full_range.M
Last changed : 12/2/2019 9:06:51 AM by System Administrator
Analysis Method : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed : 10/29/2020 11:05:45 AM by System Administrator
Method Info : Water Rinse 95%

Sample Info : Walkup method: 'full_range_positive'

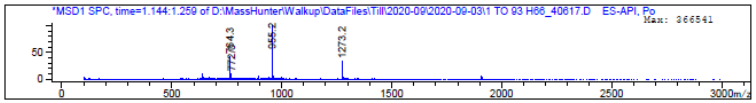
Additional Info : Peak(s) manually integrated



Data File D:\MassHunter\Walkup\DataFiles\Till\2020-09\2020-09-03\1 TO 93 H66_40617.D
Sample Name: 1 TO 93 H66

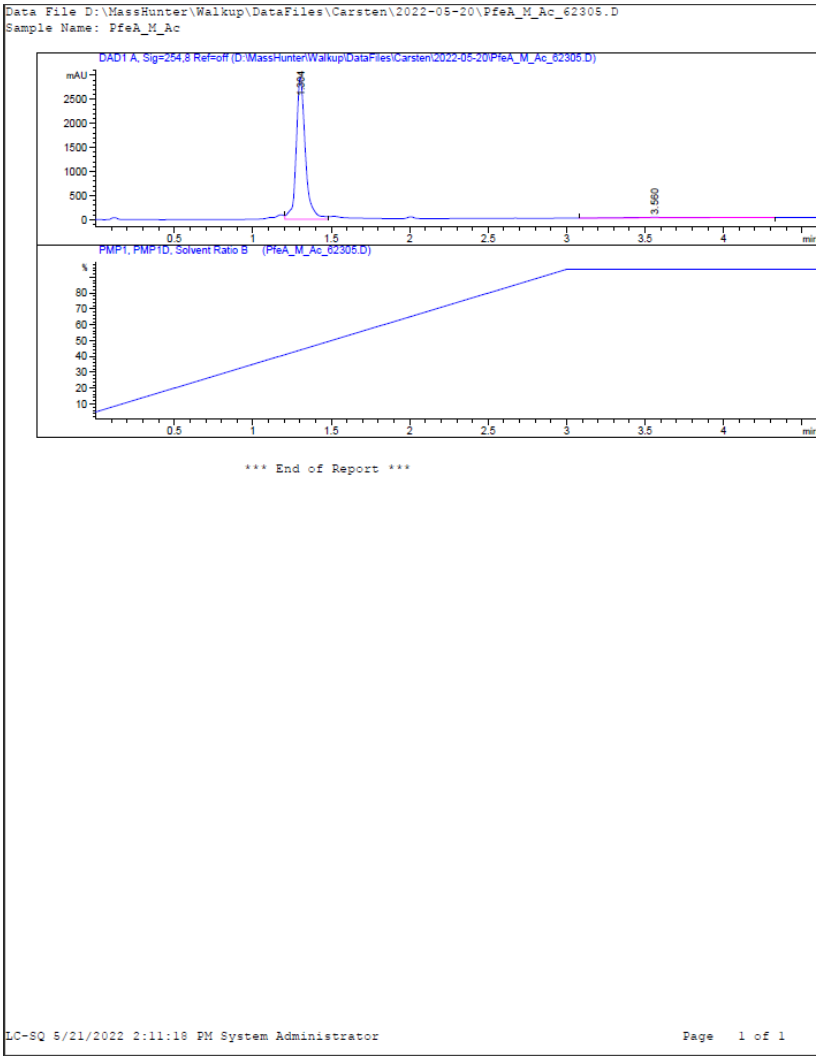
MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

Retention Time (MS)	MS Area	Mol. Weight or Ion
1.199	30348488	1273.15 I
		955.15 I
		771.95 I
		764.30 I

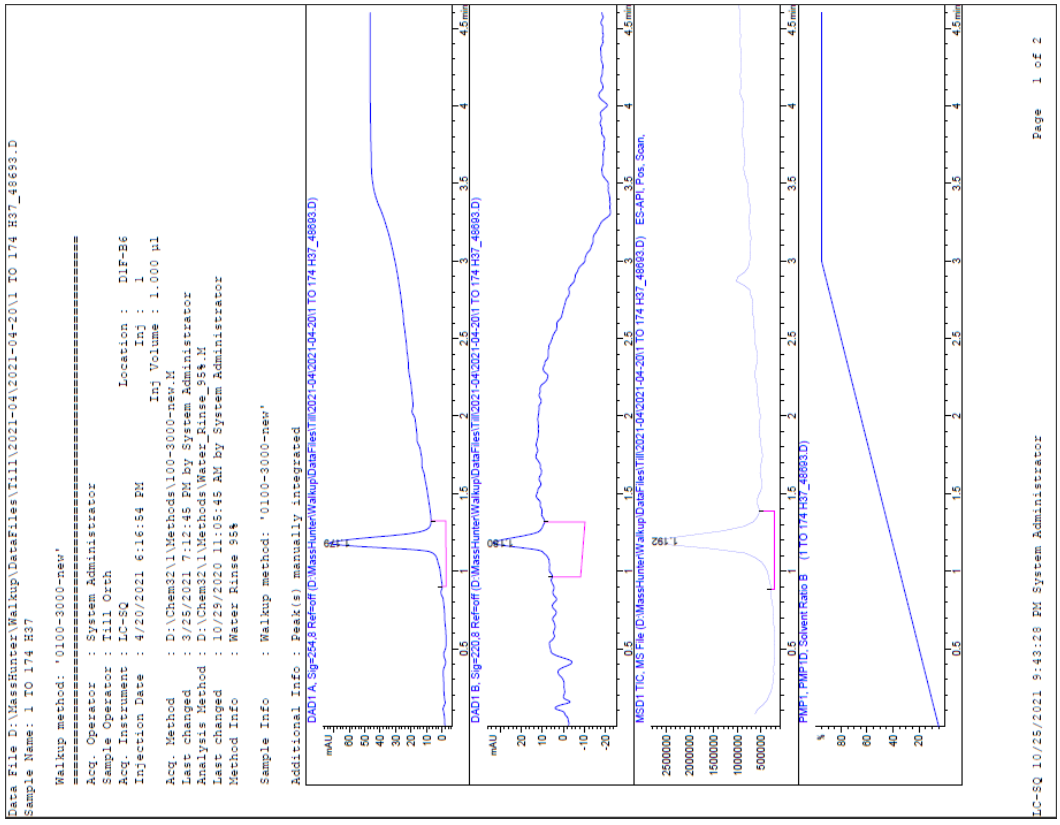


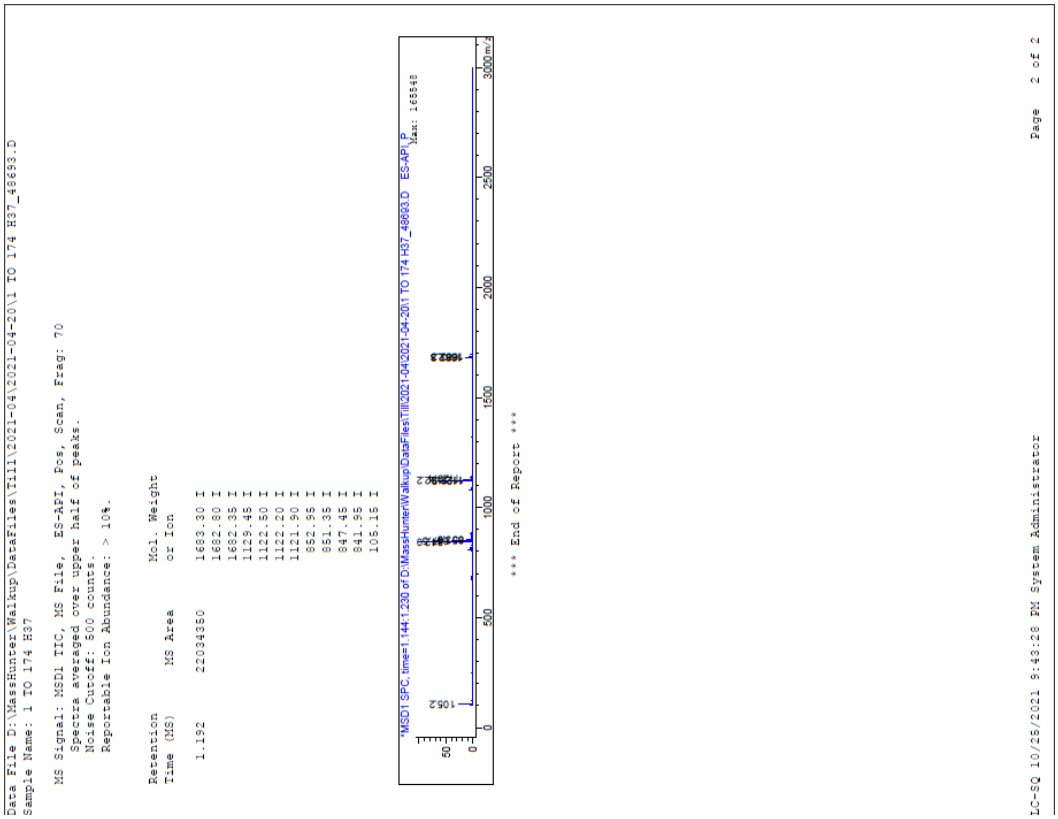
*** End of Report ***

Compound 31


Data File D:\MassHunter\Walkup\DataFiles\Carsten\2022-05-20\PfeA_M_Ac_62305.D
Sample Name: PfeA_M_Ac
DAD1 A, Sig=254,8 Ref=off (D:\MassHunter\Walkup\DataFiles\Carsten\2022-05-20\PfeA_M_Ac_62305.D)
mAU
3.564
3.560
min
PMP1, PMP1D, Solvent Ratio B (PfeA_M_Ac_62305.D)
%
*** End of Report ***
LC-SQ 5/21/2022 2:11:18 PM System Administrator
Page 1 of 1

Compound 32





Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-22\1 TO 175 H22_48803.D
Sample Name: 1 TO 175 H22

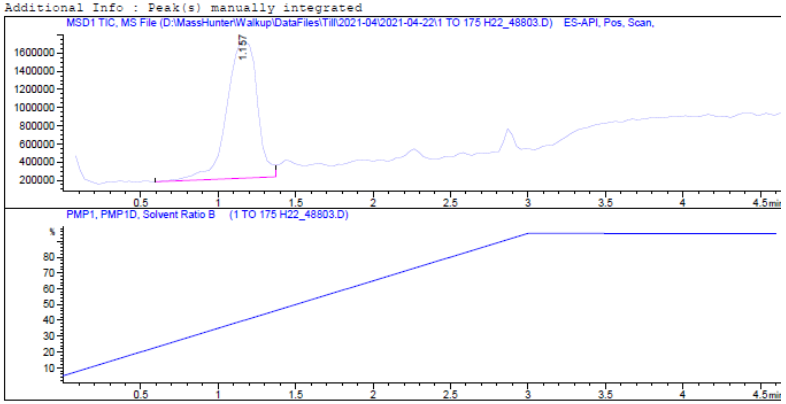
Walkup method: '0100-3000-new'

```
Acq. Operator    : System Administrator
Sample Operator  : Till Orth
Acq. Instrument  : LC-SQ                          Location :   D1B-D2
Injection Date   : 4/22/2021 8:23:36 PM             Inj :   1
                                                 Inj Volume : 1.000 µl

Acq. Method      : D:\Chem32\1\Methods\100-3000-new.M
Last changed     : 3/25/2021 7:12:45 PM by System Administrator
Analysis Method  : D:\Chem32\1\Methods\Water_Rinse_95%.M
Last changed     : 5/21/2022 2:42:22 PM by System Administrator
                   (modified after loading)
Method Info      : Water Rinse 95%

Sample Info      : Walkup method: '0100-3000-new'

Additional Info  : Peak(s) manually integrated
```

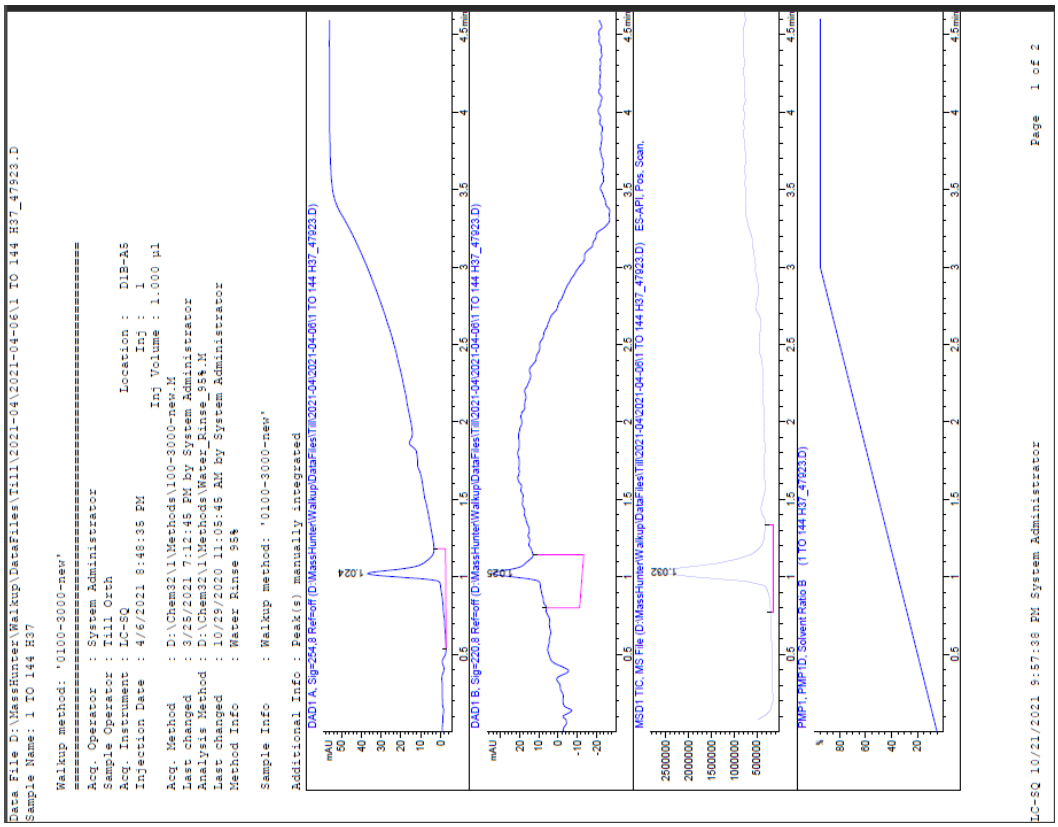


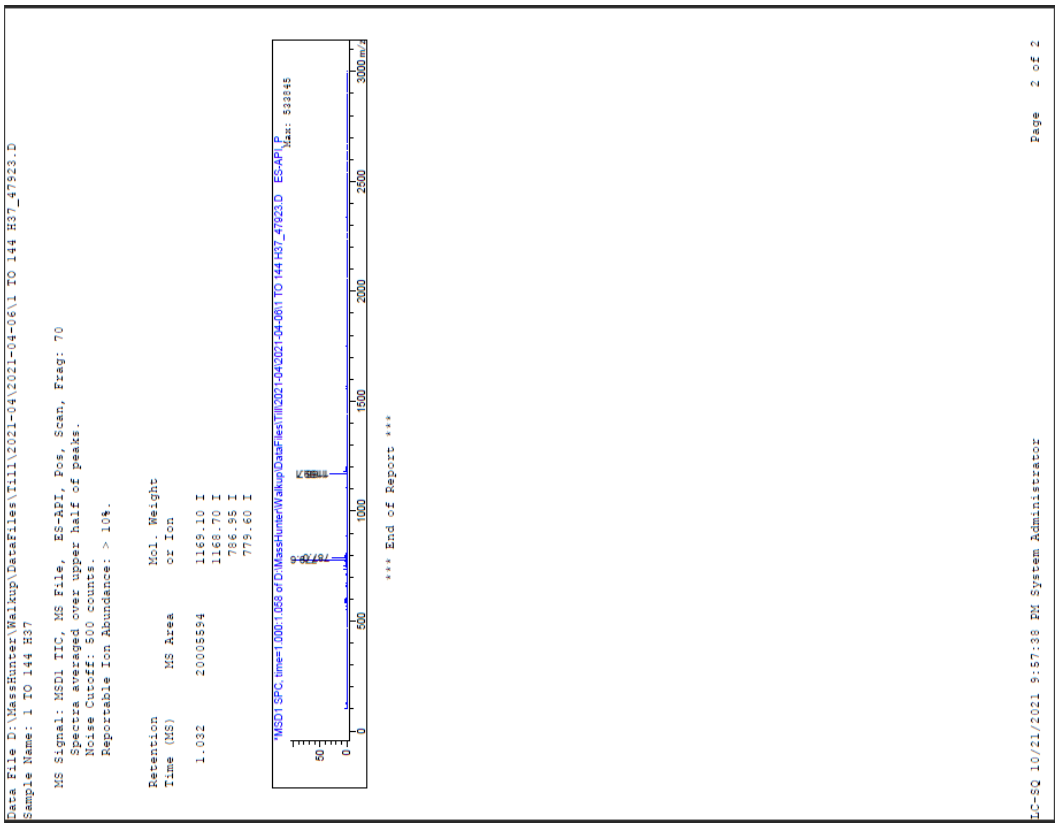
Data File D:\MassHunter\Walkup\DataFiles\Till\2021-04\2021-04-22\1 TO 175 H22_48803.D
Sample Name: 1 TO 175 H22

MS Signal: MSD1 TIC, MS File, ES-API, Pos, Scan, Frag: 70
Spectra averaged over upper half of peaks.
Noise Cutoff: 500 counts.
Reportable Ion Abundance: > 10%.

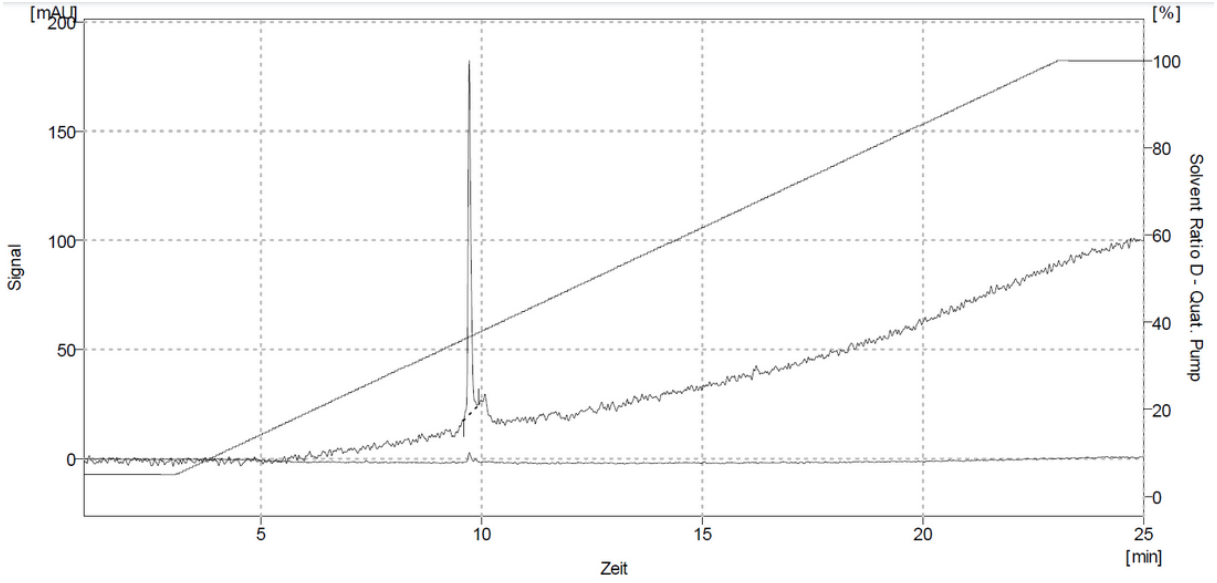
Retention Time (MS)	MS Area	Mol. Weight or Ion
1.157	20598022	1151.70 I
		1150.60 I
		1150.10 I
		1149.65 I
		1122.10 I
		1121.60 I
		1115.55 I
		1113.95 I
		1105.55 I
		1105.05 I
		1104.65 I
		1103.20 I
		1096.70 I
		1094.15 I
		1093.65 I
		1086.05 I
		1075.15 I
		1074.65 I
		859.40 I
		858.40 I
		778.50 I
		774.20 I
		767.80 I
		766.90 I
		755.80 I
		754.15 I
		748.65 I
		748.30 I
		743.05 I
		742.00 I
		737.45 I
		736.80 I
		735.65 I
		729.55 I
		724.30 I
		717.30 I
		716.95 I
		710.75 I
		698.10 I
		282.25 I
		207.10 I
		130.20 I
		122.70 I
		105.10 I
		102.15 I
		101.10 I

Compound C34

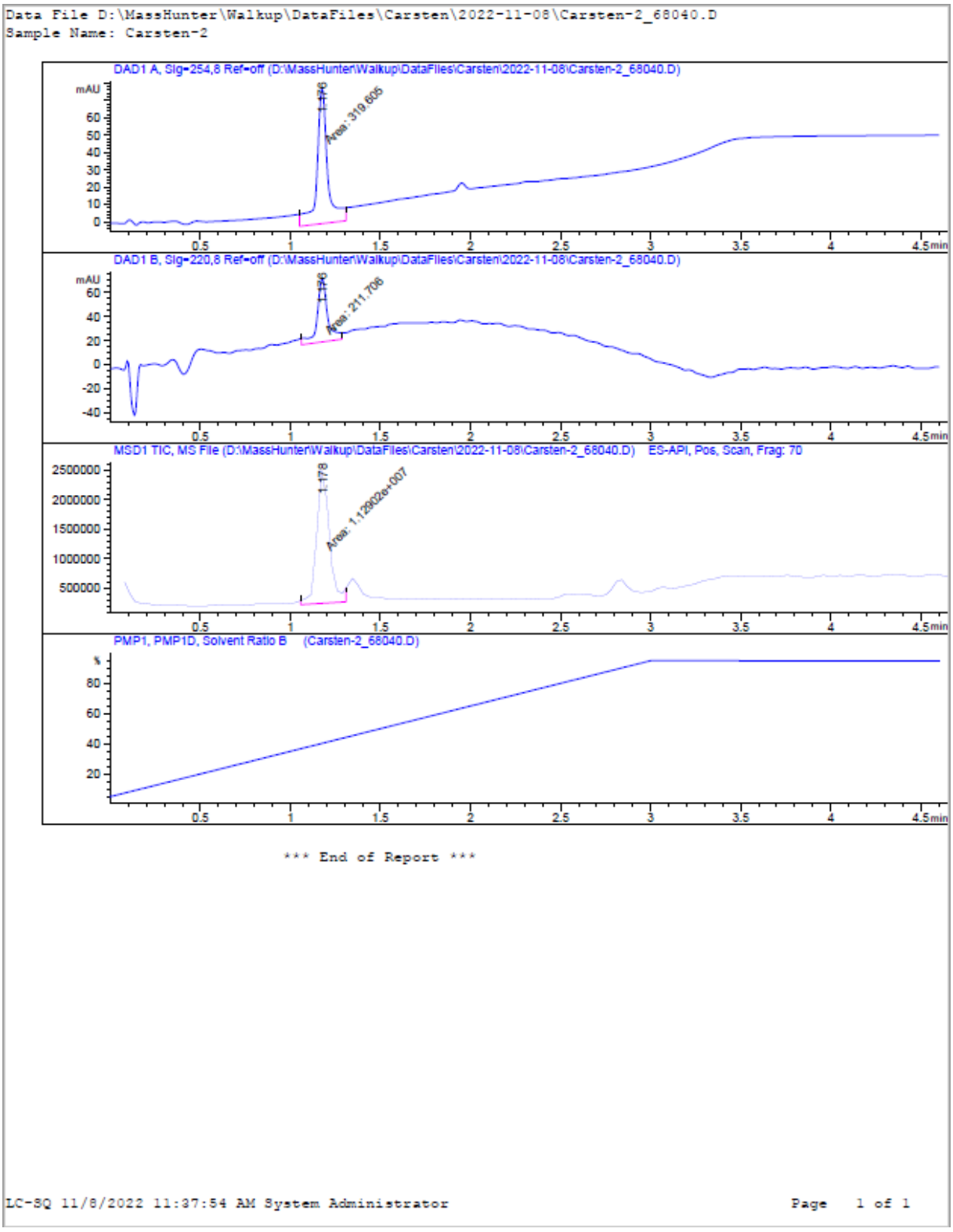




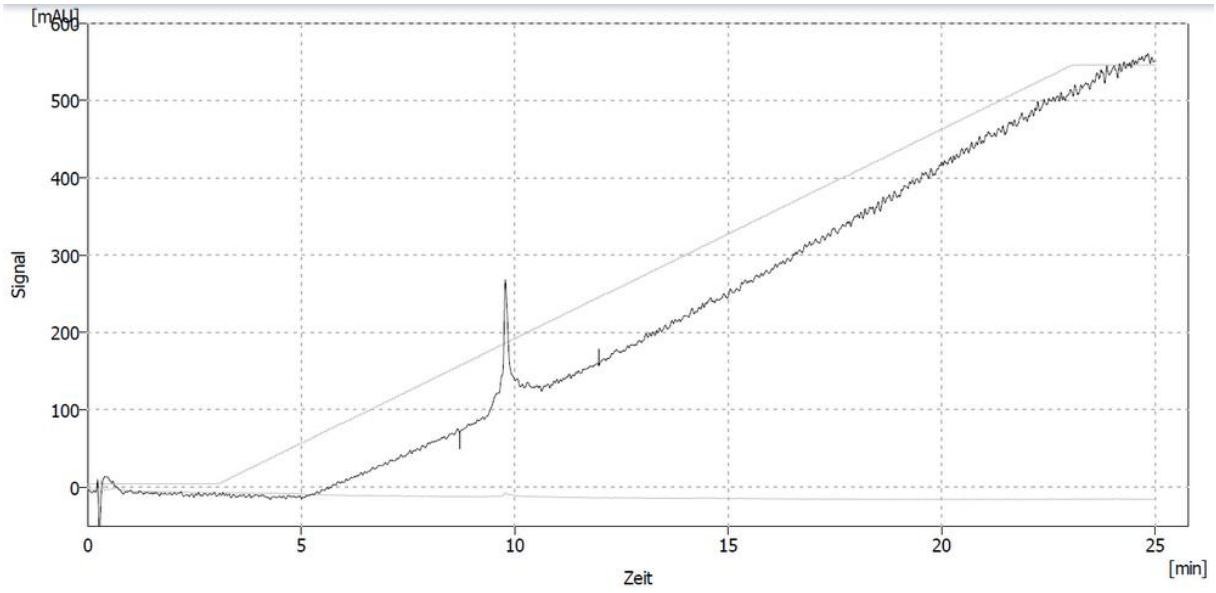
Compound N33$_L$



Compound N34$_L$

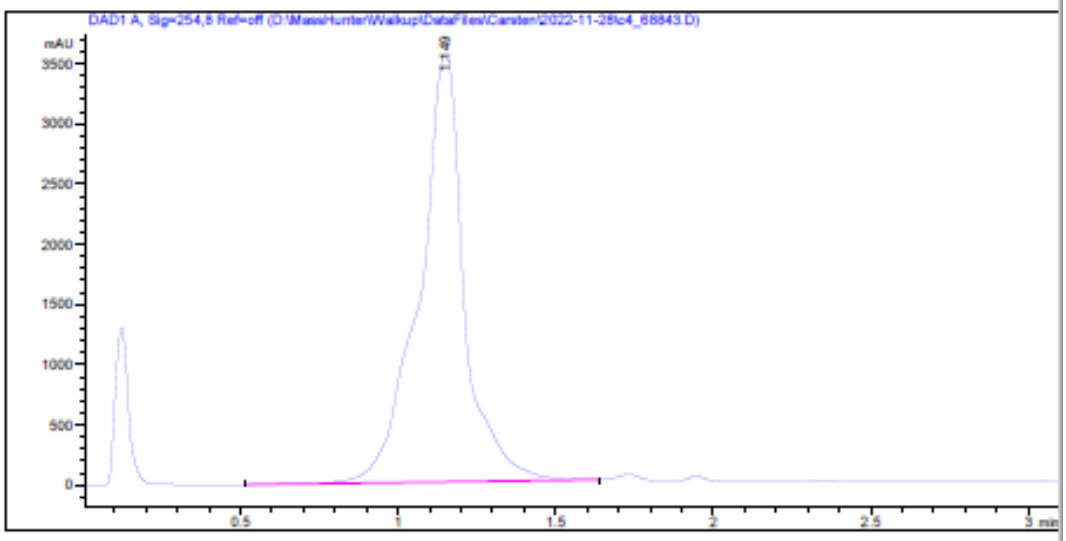


Compound N34$_D$



Compound N34$_D$

Data File D:\MassHunter\Walkup\DataFiles\Carsten\2022-11-28\c4_68843.D
Sample Name: c4



*** End of Report ***

LC-SQ 11/28/2022 12:12:42 PM System Administrator Page 1 of 1

Supplementary References

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3. Peukert, C.; Langer, L. N. B.; Wegener, S. M.; Tutov, A.; Bankstahl, J. P.; Karge, B.; Bengel, F. M.; Ross, T. L.; Brönstrup, M., Optimization of artificial siderophores as ^{68}Ga-complexed PET tracers for in vivo imaging of bacterial infections. *J. Med. Chem.* **2021,** *64* (16), 12359-12378.

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