Supporting Information

Rational Design and Synthesis of Right-Handed D-Sulfono-γ-AApeptide Helical Foldamers as Potent Inhibitors of Protein-Protein Interactions

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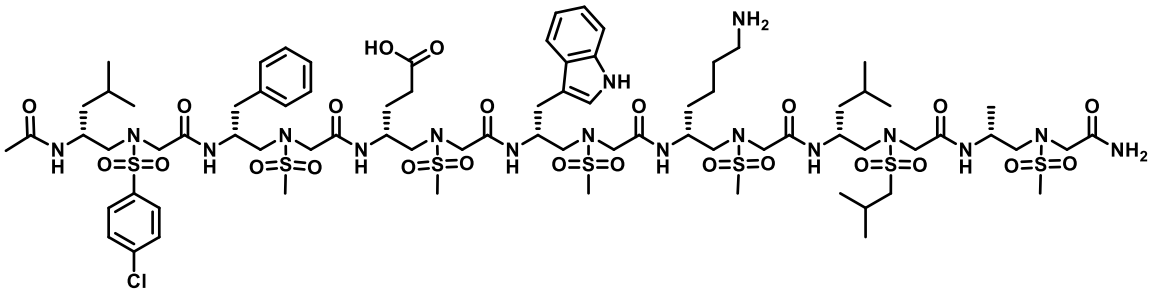
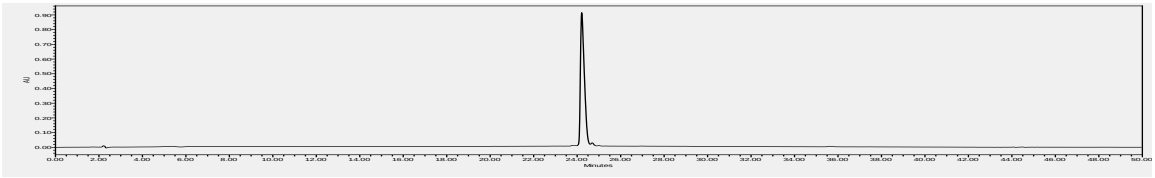
1. D-Sulfono-γ-AApeptides

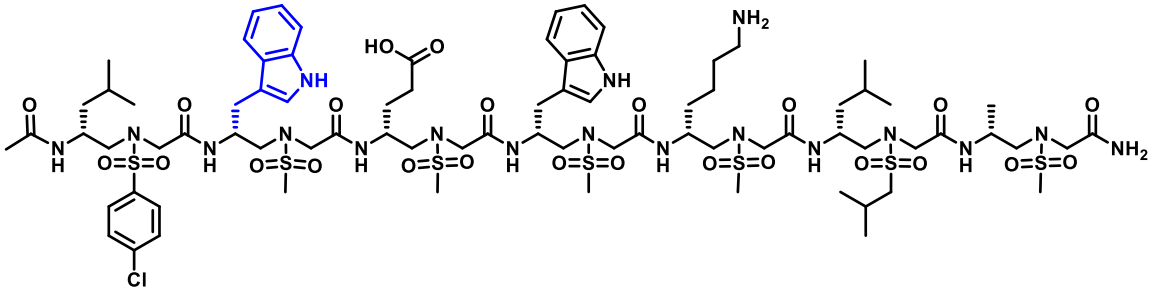
1.1 HPLC Trace



1

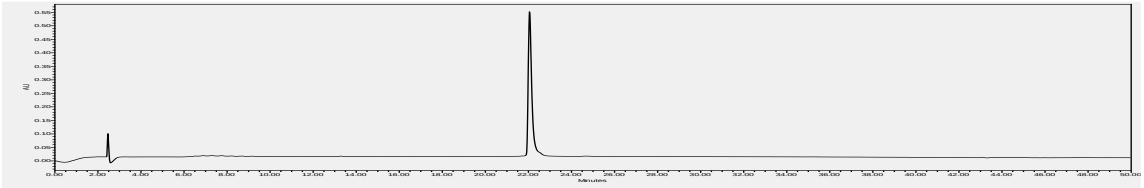
HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{77}H_{127}ClN_{17}O_{24}S_7$: 1932.6973, found: 967.8494 [M+2H]$^{2+}$, 989.8296 [M+2Na]$^{2+}$.

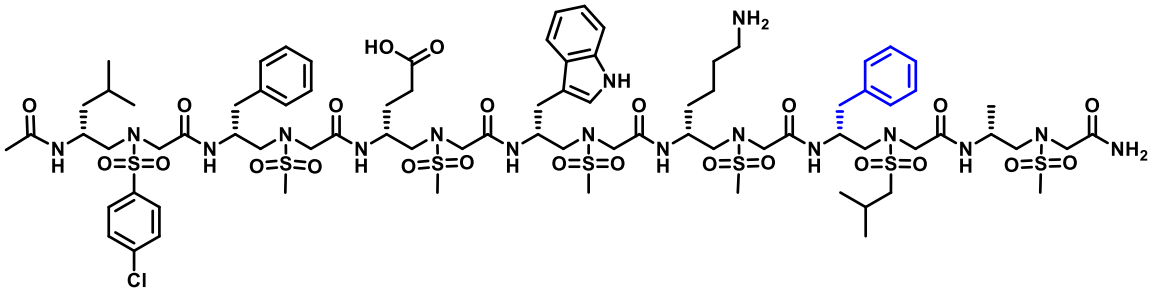




2

HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{79}H_{128}ClN_{18}O_{24}S_7$: 1971.7082, found: 987.3563 [M+2H]$^{2+}$, 1008.3370 [M+2Na]$^{2+}$.





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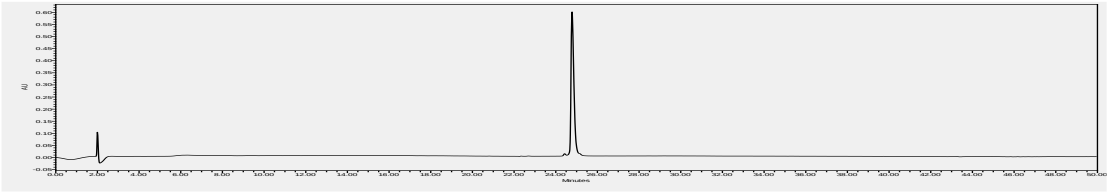
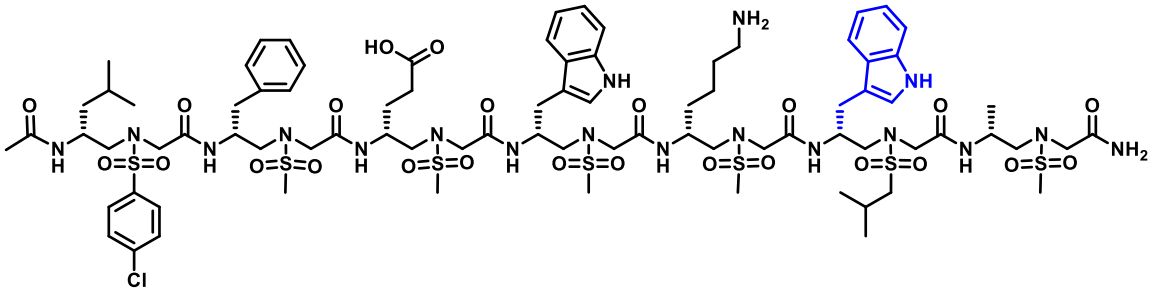
HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{80}H_{125}ClN_{17}O_{24}S_7$: 1966.6817, found: 984.8426 [M+2H]$^{2+}$, 1006.8241 [M+2Na]$^{2+}$, 1022.7915 [M+2K]$^{2+}$.





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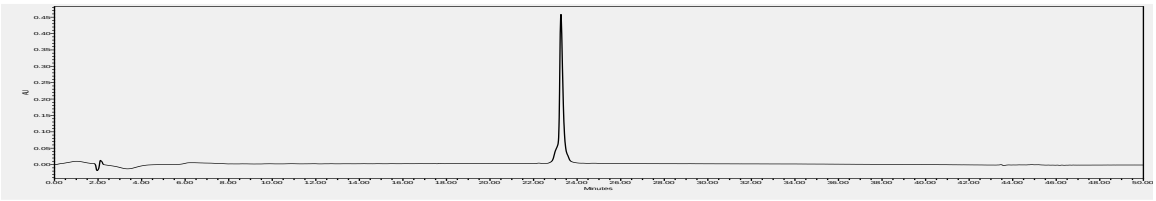
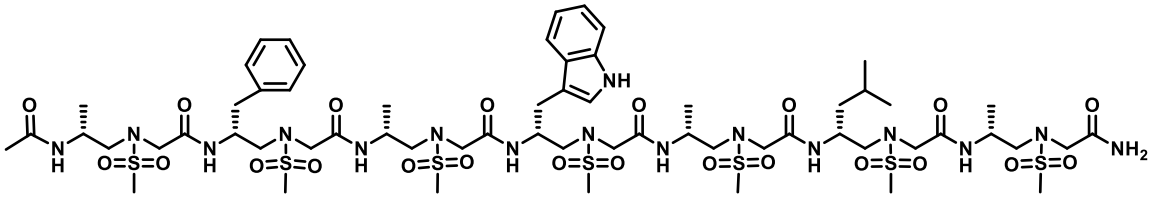
HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{82}H_{126}ClN_{18}O_{24}S_7$: 2005.6926, found: 1004.3481 [M+2H]$^{2+}$, 1026.3316 [M+2Na]$^{2+}$.





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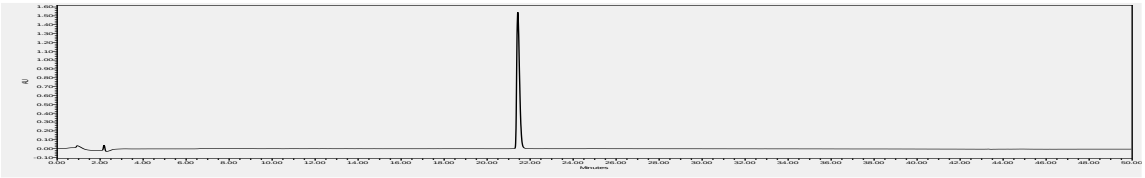
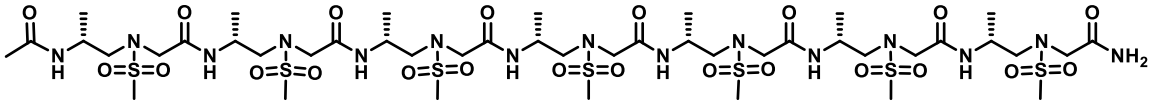
HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{61}H_{105}N_{16}O_{22}S_7$: 1637.5634, found: 819.2843 [M+2H]$^{2+}$.





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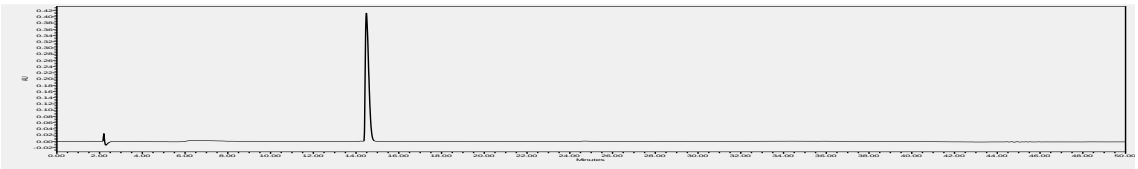
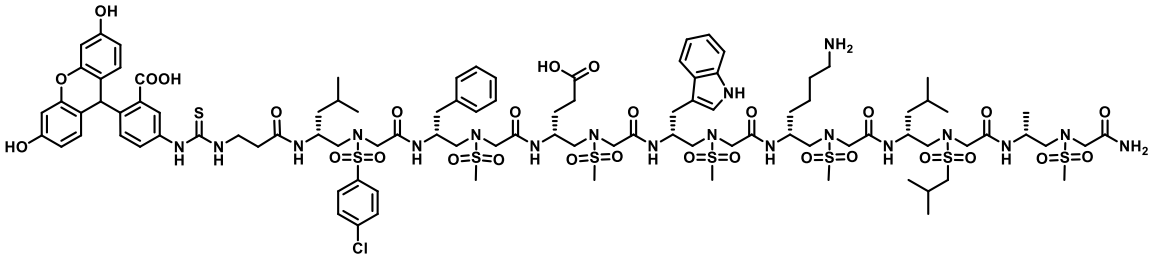
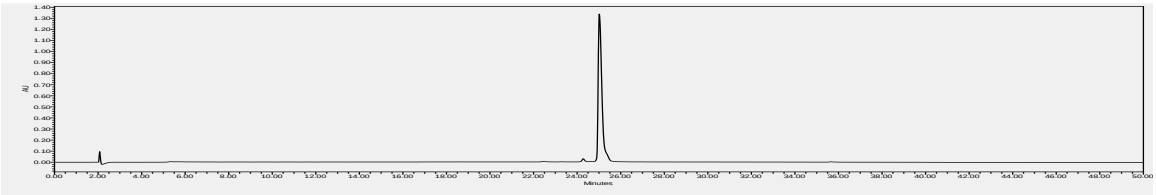
HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{44}H_{90}N_{15}O_{22}S_7$: 1404.4430, found: 702.7242 [M+2H]$^{2+}$, 724.7053 [M+2Na]$^{2+}$.

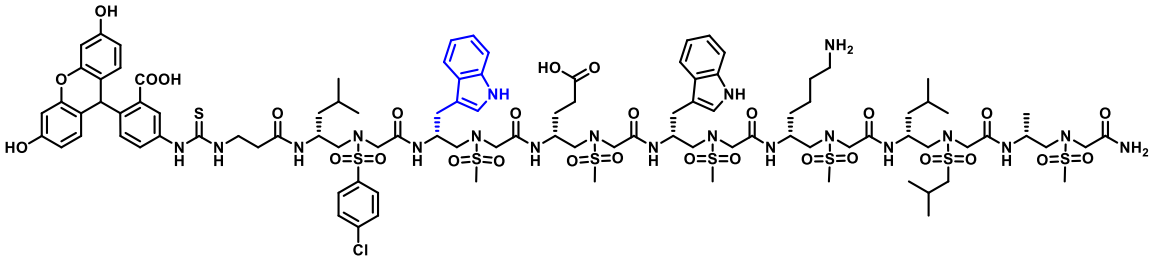




1-FITC

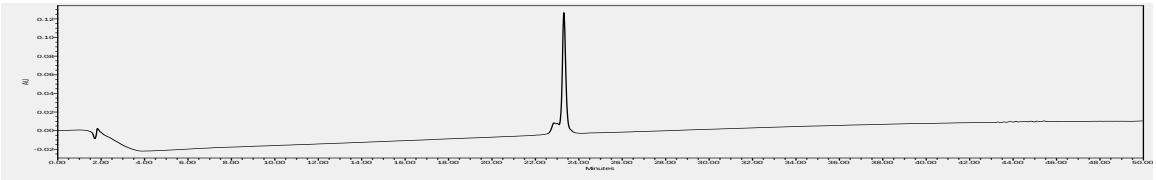
HRMS (ESI) ([M+H]$^+$) Calcd. for $C_{99}H_{143}ClN_{19}O_{29}S_8$: 2352.7753, found: 1176.8810 [M+2H]$^{2+}$.

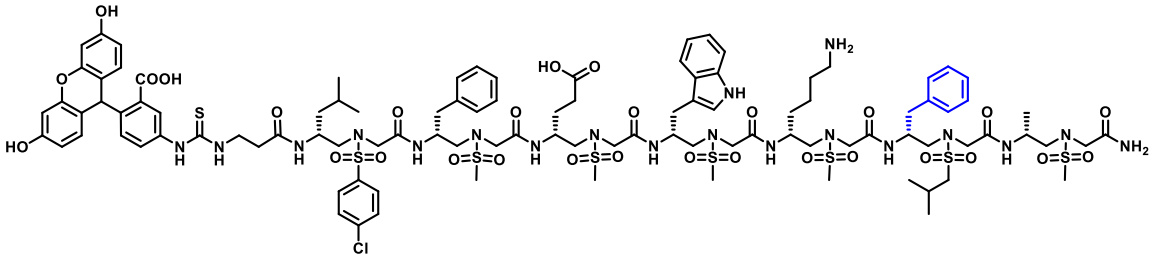




2-FITC

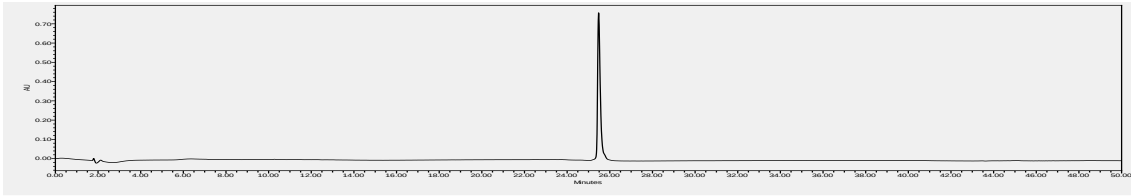
HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{101}H_{144}ClN_{20}O_{29}S_8$: 2391.7862, found: 1196.3865 $[M+2H]^{2+}$.

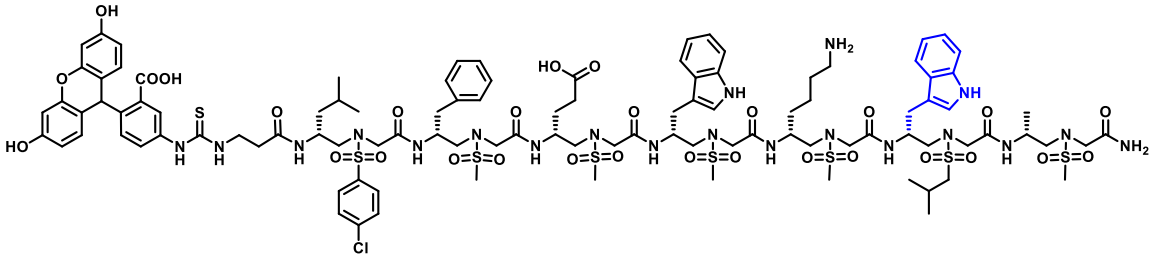




3-FITC

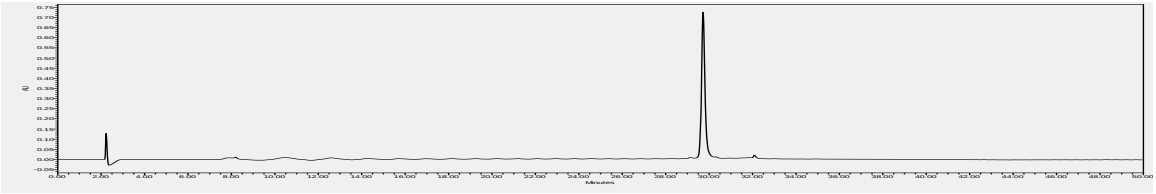
HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{102}H_{141}ClN_{19}O_{29}S_8$: 2386.7597, found: 1193.8731 $[M+2H]^{2+}$.

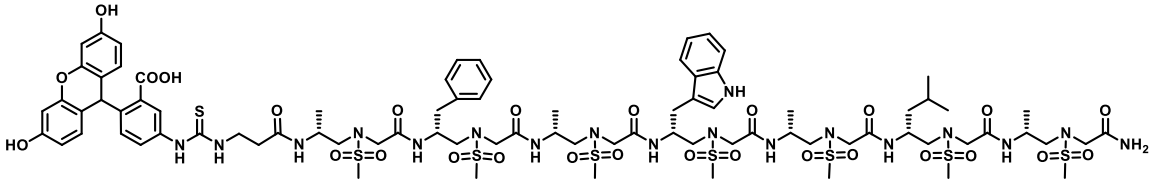




4-FITC

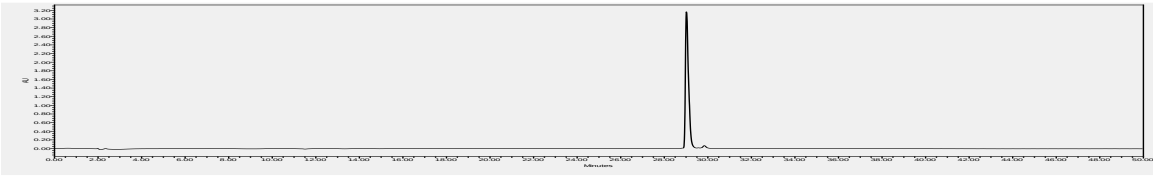
HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{104}H_{142}ClN_{20}O_{29}S_8$: 2425.7706, found: 809.2550 $[M+3H]^{3+}$.

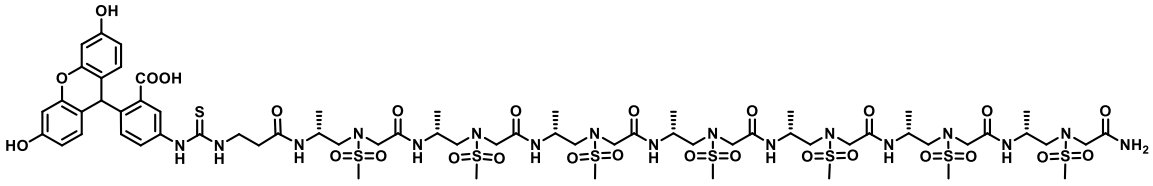




5-FITC

HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{83}H_{121}N_{18}O_{27}S_8$: 2057.6414, found: 1029.3132 $[M+2H]^{2+}$.





6-FITC

HRMS (ESI) ($[M+H]^+$) Calcd. for $C_{66}H_{106}N_{17}O_{27}S_8$: 1824.5210, found: 912.7547 $[M+2H]^{2+}$, 934.7352 $[M+2Na]^{2+}$.

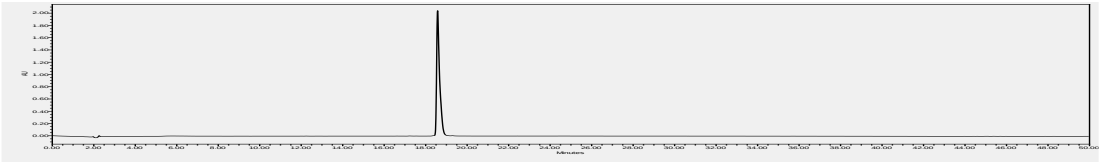


Figure S1. HPLC spectra of D-sulfono-γ-AApeptides

1.2 HPLC Purities and Retention Time of Pure Peptides.

Table S1. HPLC purities and retention time of D-sulfono-γ-AApeptides.[a]

Peptide Name	Purity trace after HPLC purification (%)	Retention Time (min)
1	99.56%	24.211
2	100.00%	22.054
3	98.86%	24.784
4	99.10%	23.255
5	100.00%	21.426
6	100.00%	14.484
1-FITC	98.71%	25.021
2-FITC	96.66%	23.312
3-FITC	100.00%	25.476
4-FITC	98.96%	29.723
5-FITC	99.10%	29.021
6-FITC	100.00%	18.391

[a] The gradient eluting method of 5% to 100% of solvent B (0.1% TFA in acetonitrile) in A (0.1% TFA in water) over 50 min was performed.

2. Fluorescence Polarization Assay

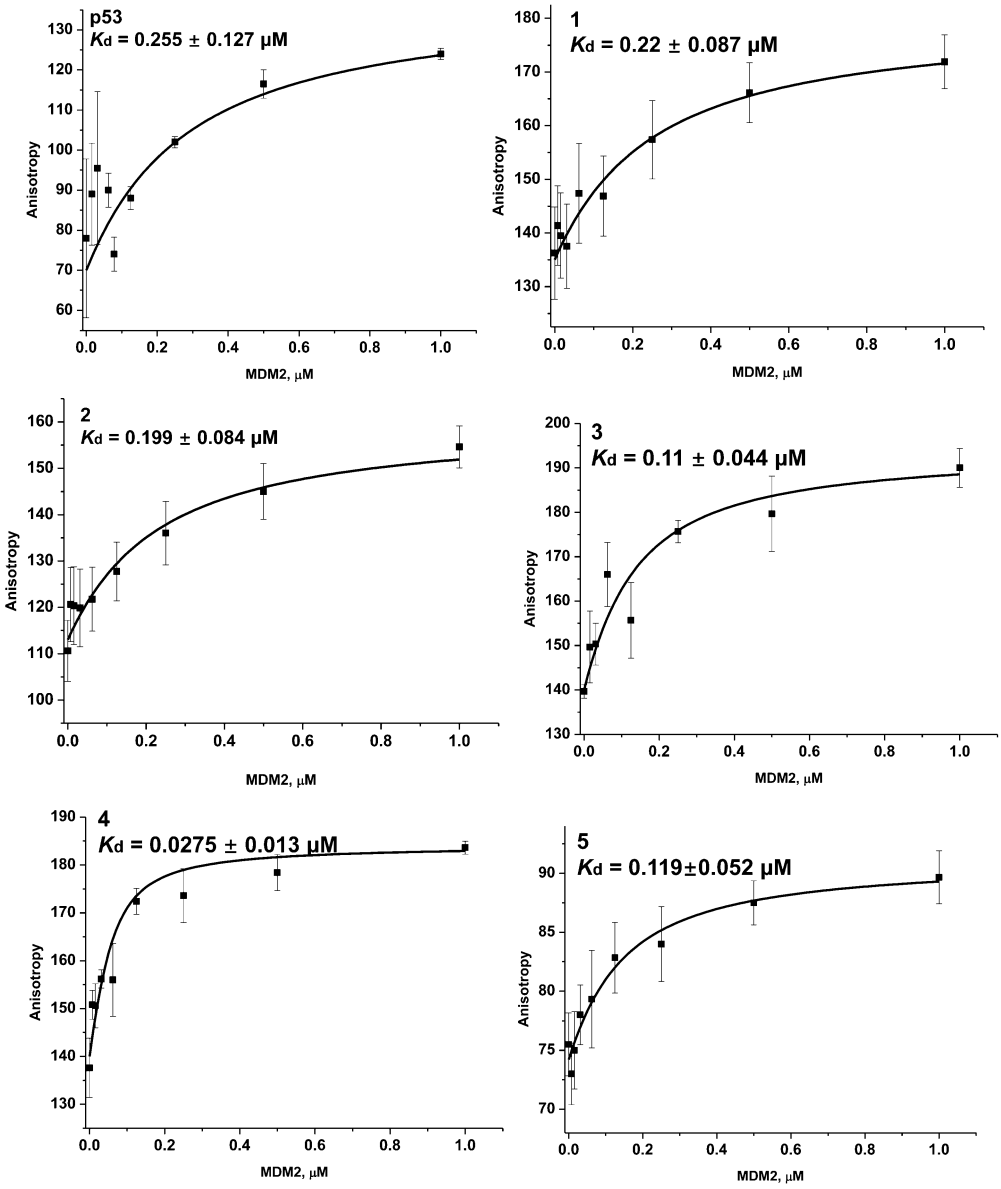


Figure S2. The K_d data of regular p53 and D-sulfono-γ-AApeptides **1-5**.

3. ^{15}N-^{1}H HSQC NMR of Lead Peptide 4 in Complex with MDM2

Methods

Protein Purification for NMR

^{15}N-labeled human MDM2 residues 17–125 was expressed and purified as described in [2].

NMR Data Collection and Analysis

Experiments for 200 µM $MDM2_{17-125}$ in the presence and absence of stochiometric equivalent of peptide **4** were carried out at 25 °C on a Varian VNMRS 800-MHz spectrometry with a triple resonance pulse field Z-axis gradient cold probe at 30 °C. ^{1}H-^{15}N heteronuclear single-quantum coherence spectroscopy experiments were performed on ^{15}N-labeled samples in 90% H_2O/ 10% D_2O. Buffer for peptide 4 and $MDM2_{17-125}$ experiments was 50 mM NaH_2PO_4, 50 mM NaCl, 1 mM EDTA, 2 mM DTT, 5% DMSO, and 0.02% NaN_3 at pH 6.8. Data were acquired in the ^{1}H and ^{15}N dimension using 9689.92-Hz (t_2) x 2430.26-Hz (t_1) sweep widths and 1024 (t_2) x 128 (t_1) complex data points. Bound spectra were collected in a molar equivalent of the peptide **4**.

Resonance assignments for apo $MDM2_{17-125}$ were previously made [2]. Bound chemical shifts were inferred based on the overlap of resonances in parallel titrations (Figure S3). Using this method, the bound resonances for 99 residues were assigned. For the nine unassignable residues, four were prolines which are not detected, two residues, S17 and Q18, were near the N-terminus, and the remaining three were D46, L81, and N106 were not assigned in apo $MDM2_{17-125}$ [2]. In addition, residue Y67 experienced line broadening during titration and the bound peak was not observed.

The combined average chemical shifts were calculated from the formula $\Delta ave = [((\Delta^{1}H^{N})^2 + (\Delta^{15}N/5)^2)/2)]^{1/2}$. All NMR spectra were processed with NMRFx and analyzed using NMRViewJ software [3, 4].

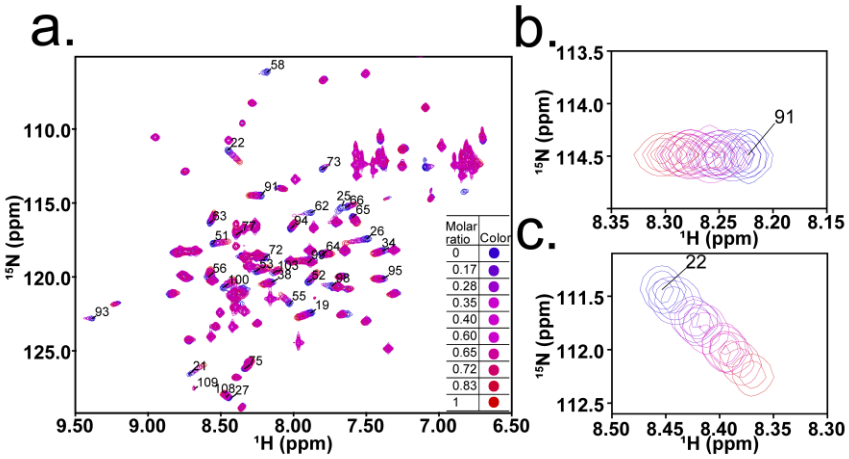


Figure S3. NMR titration results and resonance assignments of $MDM2_{17-125}$ interacting with **4**. **a.** Overlay of ^{1}H -^{15}N HSQC spectra for $MDM2_{17-125}$ before (blue) and after the addition of increasing concentrations of **4** (see legend for molar ratios of titration points).

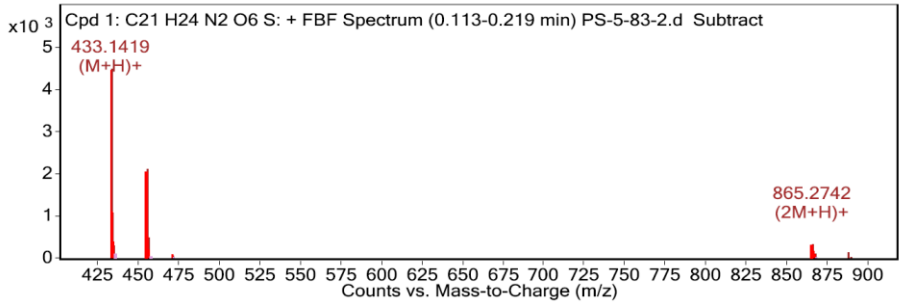
For clarity residue labels are shown for resonances with chemical shift changes greater than 0.032 ppm. **b.** Chemical shifts of F91 during the titration show clear overlap of free and bound resonances. **c.** Chemical shifts of S22 during the titration show clear overlap of free and bound resonances.

4. References

(1) Sang, P.; Zhang, M.; Shi, Y.; Li, C.; Abdulkadir, S.; Li, Q.; Ji, H.; Cai, J., *Proc. Natl. Acad. Sci. U. S. A.*, **2019**, 116, 10757-10762.
(2) Borcherds, W.; Theillet, F.-X.; Katzer, A.; Finzel, A.; Mishall, K. M.; Powell, A. T.; Wu, H.; Manieri, W.; Dieterich, C.; Selenko, P.; Loewer, A.; Daughdrill, G. W., *Nat. Chem. Biol.*, **2014**, 10 (12), 1000-1002
(3) Johnson, B.A., Using NMRView to visualize and analyze the NMR spectra of macromolecules, in *Protein NMR Techniques*. **2004**, Springer. p. 313-352.
(4) Johnson, B.A.; Blevins, R.A., *J. biomol. NMR*, **1994**, 4(5), 603-614.

5. HRMS Spectra of Building Blocks 1a-j and D-Sulfono-γ-AApeptides

HRMS spectra of 1a



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
433.1419	1	4511.36	C21H25N2O6S	(M+H)+
434.1447	1	1101.61	C21H25N2O6S	(M+H)+
435.1424	1	324.79	C21H25N2O6S	(M+H)+
455.1229	1	2135.01	C21H24N2NaO6S	(M+Na)+
456.1259	1	525.02	C21H24N2NaO6S	(M+Na)+
457.1226	1	52.91	C21H24N2NaO6S	(M+Na)+
471.0901	1	79.55	C21H24KN2O6S	(M+K)+
865.2742	1	359.58	C42H49N4O12S2	(2M+H)+
866.2785	1	129.05	C42H49N4O12S2	(2M+H)+
887.2566	1	164.59	C42H48N4NaO12S2	(2M+Na)+

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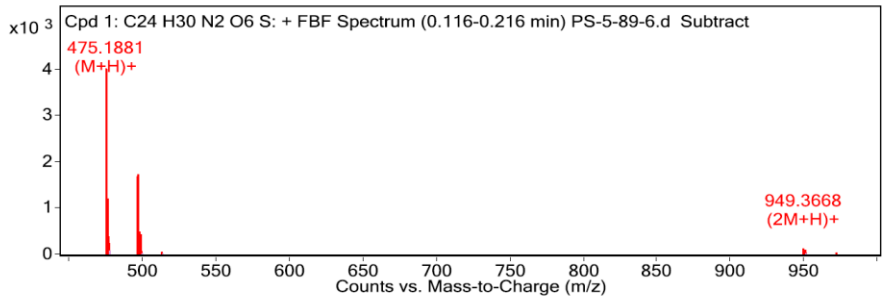
HRMS spectra of 1b



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
475.1881	1	4027.52	C24H31N2O6S	(M+H)+
476.1914	1	1223.82	C24H31N2O6S	(M+H)+
477.1893	1	273.12	C24H31N2O6S	(M+H)+
497.1702	1	1749.32	C24H30N2NaO6S	(M+Na)+
498.1718	1	450.11	C24H30N2NaO6S	(M+Na)+
499.1718	1	102.88	C24H30N2NaO6S	(M+Na)+
513.1378	1	54.12	C24H30KN2O6S	(M+K)+
949.3668	1	111.59	C48H61N4O12S2	(2M+H)+
950.368	1	82	C48H61N4O12S2	(2M+H)+
971.3451	1	81.86	C48H60N4NaO12S2	(2M+Na)+

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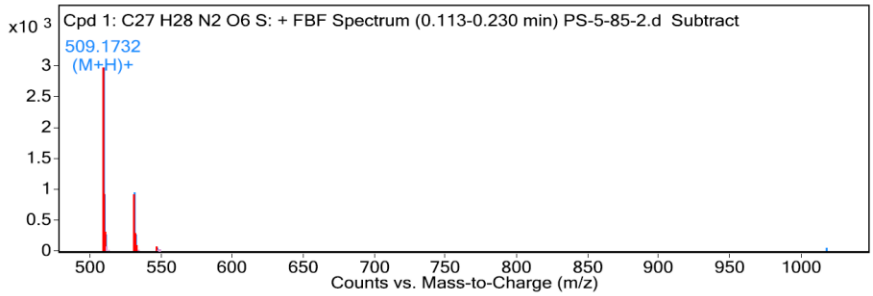
HRMS spectra of 1c



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
509.1732	1	2994.12	C27H29N2O6S	(M+H)+
510.1754	1	926.66	C27H29N2O6S	(M+H)+
511.1737	1	290.31	C27H29N2O6S	(M+H)+
531.1538	1	965.32	C27H28N2NaO6S	(M+Na)+
532.1577	1	291.12	C27H28N2NaO6S	(M+Na)+
533.1565	1	30.93	C27H28N2NaO6S	(M+Na)+
547.1198	1	67.87	C27H28KN2O6S	(M+K)+
1017.3375	1	79.76	C54H57N4O12S2	(2M+H)+

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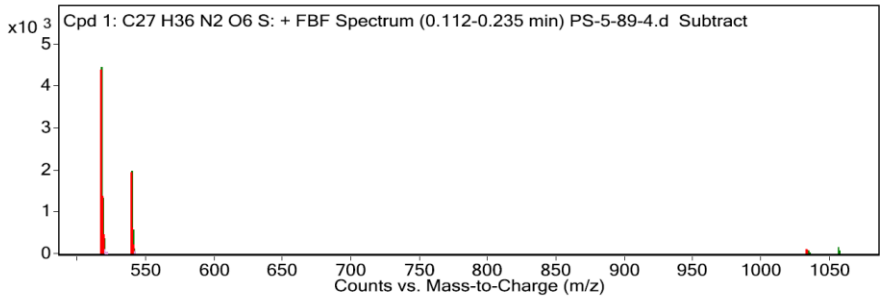
HRMS spectra of 1d



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
517.2355	1	4447.79	C27H37N2O6S	(M+H)+
518.2377	1	1358.69	C27H37N2O6S	(M+H)+
519.2376	1	410.22	C27H37N2O6S	(M+H)+
539.217	1	1988.83	C27H36N2NaO6S	(M+Na)+
540.2202	1	613.62	C27H36N2NaO6S	(M+Na)+
541.2178	1	153.67	C27H36N2NaO6S	(M+Na)+
1033.4607	1	118.26	C54H73N4O12S2	(2M+H)+
1034.4656	1	64.81	C54H73N4O12S2	(2M+H)+
1055.442	1	188.55	C54H72N4NaO12S2	(2M+Na)+
1056.4472	1	107.43	C54H72N4NaO12S2	(2M+Na)+

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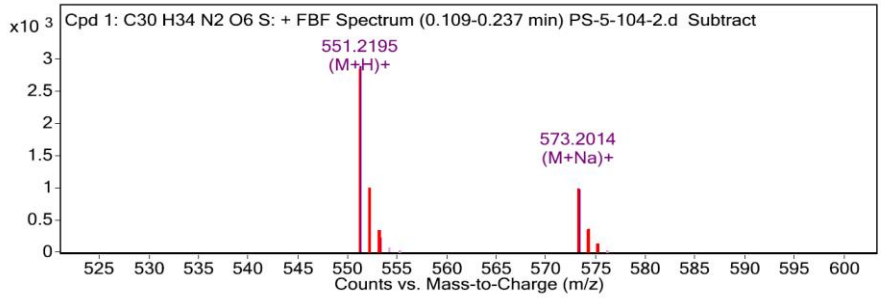
HRMS spectra of 1e



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
551.2195	1	2890.08	C30H35N2O6S	(M+H)+
552.2227	1	1020.49	C30H35N2O6S	(M+H)+
553.2221	1	244.34	C30H35N2O6S	(M+H)+
573.2014	1	1004.49	C30H34N2NaO6S	(M+Na)+
574.2041	1	372.53	C30H34N2NaO6S	(M+Na)+
575.2039	1	57.92	C30H34N2NaO6S	(M+Na)+

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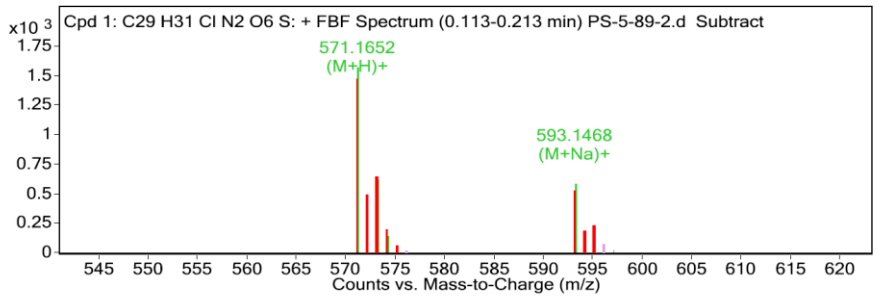
HRMS spectra of 1f

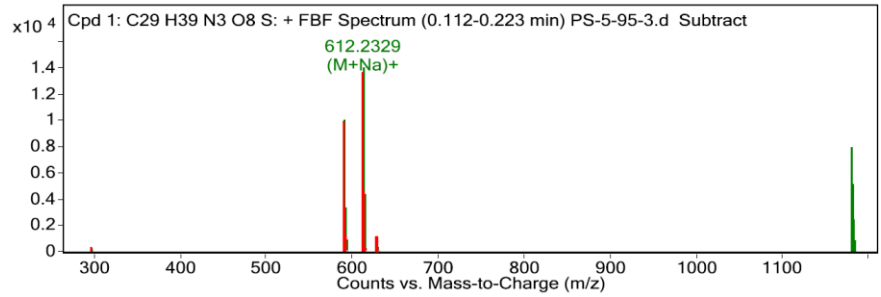


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
571.1652	1	1568.21	C29H32ClN2O6S	(M+H)+
572.1686	1	474.51	C29H32ClN2O6S	(M+H)+
573.1635	1	629.57	C29H32ClN2O6S	(M+H)+
574.1641	1	148.2	C29H32ClN2O6S	(M+H)+
575.1581	1	22.59	C29H32ClN2O6S	(M+H)+
593.1468	1	585.31	C29H31ClN2NaO6S	(M+Na)+
594.1481	1	163.69	C29H31ClN2NaO6S	(M+Na)+
595.1448	1	182.49	C29H31ClN2NaO6S	(M+Na)+

--- End Of Report ---

HRMS spectra of 1g

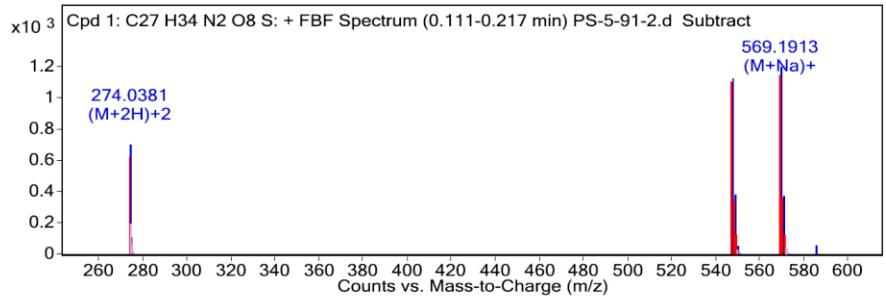


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
295.5567	2	326.82	C29H41N3O8S	(M+2H)+2
590.2509	1	10094.98	C29H40N3O8S	(M+H)+
591.254	1	3431.81	C29H40N3O8S	(M+H)+
612.2329	1	14097.46	C29H39N3NaO8S	(M+Na)+
613.2357	1	4482.54	C29H39N3NaO8S	(M+Na)+
614.235	1	1361.39	C29H39N3NaO8S	(M+Na)+
628.2025	1	1126.39	C29H39KN3O8S	(M+K)+
1179.495	1	8017.3	C58H79N6O16S2	(2M+H)+
1180.498	1	5193.55	C58H79N6O16S2	(2M+H)+
1181.4986	1	2517.77	C58H79N6O16S2	(2M+H)+

--- End Of Report ---

HRMS spectra of 1h

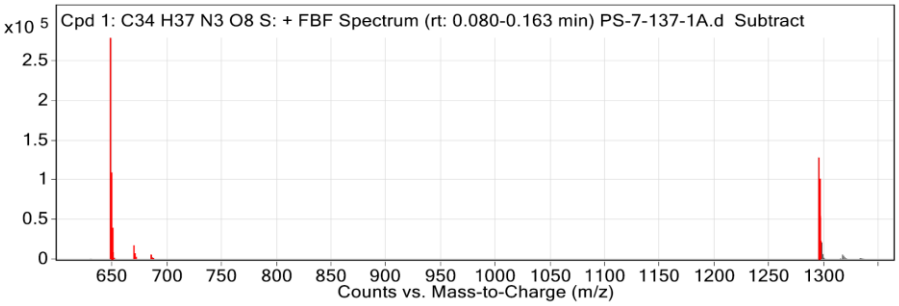


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
274.0381	2	705.22	C27H36N2O8S	(M+2H)+2
274.5394	2	114.17	C27H36N2O8S	(M+2H)+2
547.2094	1	1129.57	C27H35N2O8S	(M+H)+
548.2118	1	384	C27H35N2O8S	(M+H)+
549.2106	1	56.93	C27H35N2O8S	(M+H)+
569.1913	1	1202.22	C27H34N2NaO8S	(M+Na)+
570.195	1	381.85	C27H34N2NaO8S	(M+Na)+
571.1941	1	45.25	C27H34N2NaO8S	(M+Na)+
585.1541	1	65.99	C27H34KN2O8S	(M+K)+

--- End Of Report ---

HRMS spectra of 1i

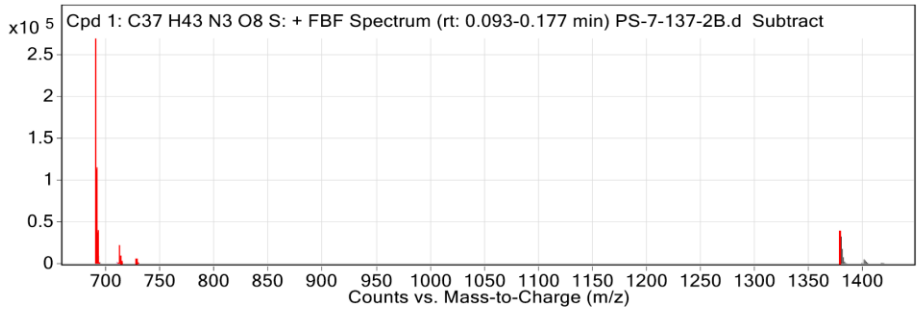


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
630.176	1	179.22	C34H37N3O8S	(M+H)+[-H2O]
648.236	1	278874.63	C34H37N3O8S	(M+H)+
649.2388	1	107343.41	C34H37N3O8S	(M+H)+
670.217	1	17149.75	C34H37N3O8S	(M+Na)+
686.1883	1	5279.58	C34H37N3O8S	(M+K)+
1295.4637	1	128047.95	C34H37N3O8S	(2M+H)+
1296.4672	1	100762.45	C34H37N3O8S	(2M+H)+
1315.4918	1	703.74	C34H37N3O8S	(2M+K)+[-H2O]
1317.4441	1	5706.52	C34H37N3O8S	(2M+Na)+
1333.4162	1	1215.78	C34H37N3O8S	(2M+K)+

--- End Of Report ---

HRMS spectra of 1j

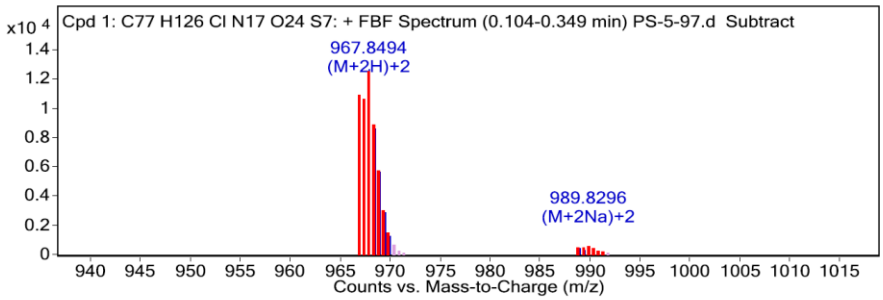


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
690.283	1	269786.13	C37H43N3O8S	(M+H)+
691.2856	1	112971.25	C37H43N3O8S	(M+H)+
692.2854	1	37546.63	C37H43N3O8S	(M+H)+
710.3115	1	1966.81	C37H43N3O8S	(M+K)+[-H2O]
712.2636	1	22394.12	C37H43N3O8S	(M+Na)+
728.2359	1	6018.28	C37H43N3O8S	(M+K)+
1379.5569	1	38415.02	C37H43N3O8S	(2M+H)+
1399.5766	1	806.01	C37H43N3O8S	(2M+K)+[-H2O]
1401.5359	1	5150.48	C37H43N3O8S	(2M+Na)+
1417.511	1	947.69	C37H43N3O8S	(2M+K)+

--- End Of Report ---

HRMS spectra of 1

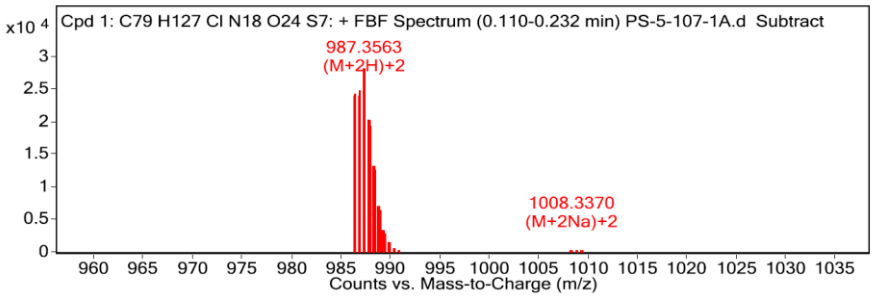


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
966.849	2	10970.96	C77H128ClN17O24S7	(M+2H)+2
967.3504	2	10581.76	C77H128ClN17O24S7	(M+2H)+2
967.8494	2	12732.34	C77H128ClN17O24S7	(M+2H)+2
968.3496	2	8657.85	C77H128ClN17O24S7	(M+2H)+2
968.849	2	5717.75	C77H128ClN17O24S7	(M+2H)+2
969.3486	2	2945.85	C77H128ClN17O24S7	(M+2H)+2
969.8485	2	1355.23	C77H128ClN17O24S7	(M+2H)+2
988.8291	2	502.26	C77H126ClN17Na2O24S7	(M+2Na)+2
989.3307	2	413.52	C77H126ClN17Na2O24S7	(M+2Na)+2
989.8296	2	561.39	C77H126ClN17Na2O24S7	(M+2Na)+2

--- End Of Report ---

HRMS spectra of 2

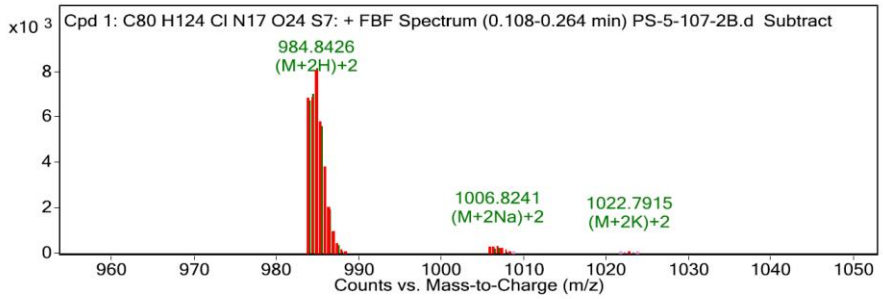


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
986.3557	2	24358.23	C79H129ClN18O24S7	(M+2H)+2
986.8571	2	24820.71	C79H129ClN18O24S7	(M+2H)+2
987.3563	2	28260.01	C79H129ClN18O24S7	(M+2H)+2
987.8564	2	19501.39	C79H129ClN18O24S7	(M+2H)+2
988.3555	2	12751.56	C79H129ClN18O24S7	(M+2H)+2
988.8556	2	6632.99	C79H129ClN18O24S7	(M+2H)+2
989.3553	2	3010.12	C79H129ClN18O24S7	(M+2H)+2
989.8553	2	1177.02	C79H129ClN18O24S7	(M+2H)+2
990.3543	2	481.65	C79H129ClN18O24S7	(M+2H)+2
1008.337	2	140.05	C79H127ClN18Na2O24S7	(M+2Na)+2

--- End Of Report ---

HRMS spectra of 3

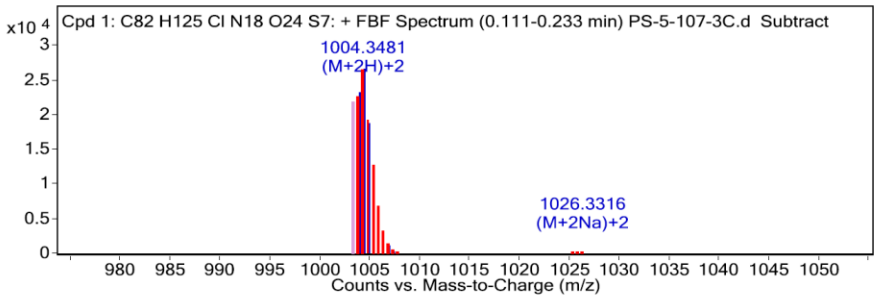


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
983.8422	2	6740.5	C80H126ClN17O24S7	(M+2H)+2
984.3435	2	7053.95	C80H126ClN17O24S7	(M+2H)+2
984.8426	2	8184.98	C80H126ClN17O24S7	(M+2H)+2
985.3428	2	5613.13	C80H126ClN17O24S7	(M+2H)+2
985.8425	2	3663.93	C80H126ClN17O24S7	(M+2H)+2
986.3428	2	1977.39	C80H126ClN17O24S7	(M+2H)+2
986.8415	2	949.15	C80H126ClN17O24S7	(M+2H)+2
987.3431	2	390.48	C80H126ClN17O24S7	(M+2H)+2
1005.8222	2	270.46	C80H124ClN17Na2O24S7	(M+2Na)+2
1022.7915	2	65.45	C80H124ClK2N17O24S7	(M+2K)+2

--- End Of Report ---

HRMS spectra of 4

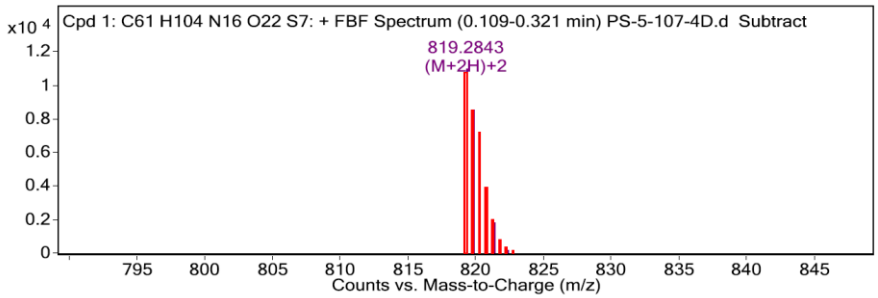


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
1003.8485	2	23340.62	C82H127ClN18O24S7	(M+2H)+2
1004.3481	2	26718.61	C82H127ClN18O24S7	(M+2H)+2
1004.8482	2	18850.31	C82H127ClN18O24S7	(M+2H)+2
1005.3475	2	12182.81	C82H127ClN18O24S7	(M+2H)+2
1005.8475	2	6510.62	C82H127ClN18O24S7	(M+2H)+2
1006.3471	2	2962.8	C82H127ClN18O24S7	(M+2H)+2
1006.8467	2	1308.35	C82H127ClN18O24S7	(M+2H)+2
1007.3467	2	481.44	C82H127ClN18O24S7	(M+2H)+2
1025.3265	2	117.69	C82H125ClN18Na2O24S7	(M+2Na)+2
1026.3316	2	145.25	C82H125ClN18Na2O24S7	(M+2Na)+2

--- End Of Report ---

HRMS spectra of 5

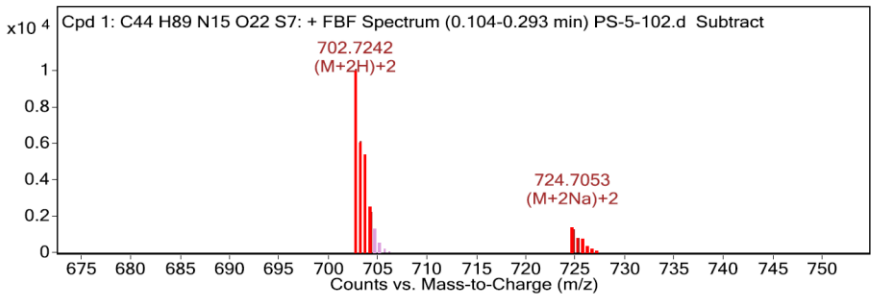


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
819.2843	2	11062.34	C61H106N16O22S7	(M+2H)+2
819.7855	2	8579.07	C61H106N16O22S7	(M+2H)+2
820.2846	2	6986.26	C61H106N16O22S7	(M+2H)+2
820.7845	2	3902.19	C61H106N16O22S7	(M+2H)+2
821.2841	2	1947.75	C61H106N16O22S7	(M+2H)+2
821.7839	2	760.61	C61H106N16O22S7	(M+2H)+2
822.2832	2	284.88	C61H106N16O22S7	(M+2H)+2
822.782	2	79.1	C61H106N16O22S7	(M+2H)+2

--- End Of Report ---

HRMS spectra of 6

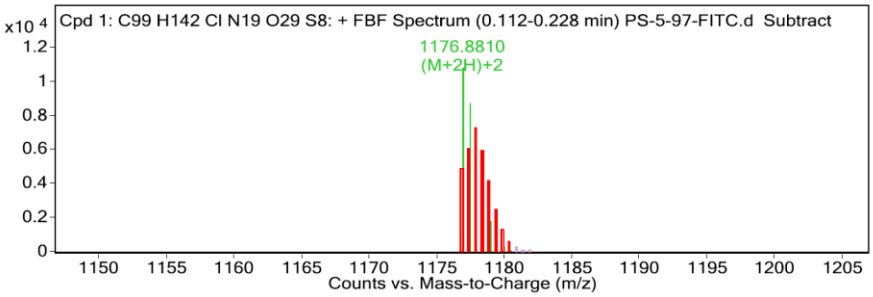


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
702.7242	2	10162.73	C44H91N15O22S7	(M+2H)+2
703.2252	2	6169.12	C44H91N15O22S7	(M+2H)+2
703.7242	2	5215.91	C44H91N15O22S7	(M+2H)+2
704.2244	2	2309.95	C44H91N15O22S7	(M+2H)+2
724.7053	2	1342.12	C44H89N15Na2O22S7	(M+2Na)+2
725.2065	2	849.6	C44H89N15Na2O22S7	(M+2Na)+2
725.7046	2	728.89	C44H89N15Na2O22S7	(M+2Na)+2
726.2048	2	294.39	C44H89N15Na2O22S7	(M+2Na)+2
726.7051	2	127.69	C44H89N15Na2O22S7	(M+2Na)+2
727.2028	2	29.15	C44H89N15Na2O22S7	(M+2Na)+2

--- End Of Report ---

HRMS spectra of 1-FITC

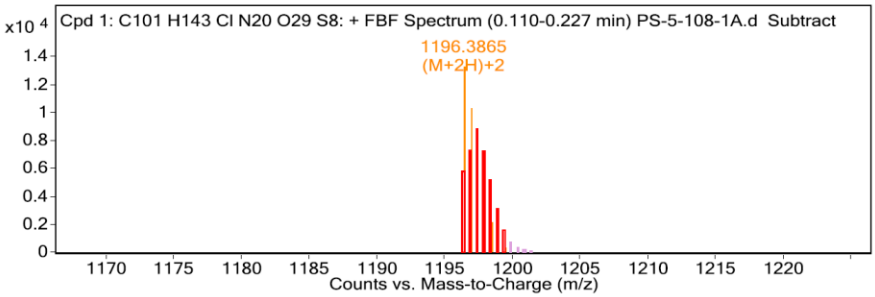


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
1176.881	2	10861.65	C99H144ClN19O29S8	(M+2H)+2
1177.3815	2	8735.57	C99H144ClN19O29S8	(M+2H)+2
1177.8808	2	6133.46	C99H144ClN19O29S8	(M+2H)+2
1178.3807	2	3570.78	C99H144ClN19O29S8	(M+2H)+2
1178.8809	2	1910.52	C99H144ClN19O29S8	(M+2H)+2
1179.3798	2	856.76	C99H144ClN19O29S8	(M+2H)+2
1179.8785	2	366.92	C99H144ClN19O29S8	(M+2H)+2
1180.3788	2	134.07	C99H144ClN19O29S8	(M+2H)+2

--- End Of Report ---

HRMS spectra of 2-FITC

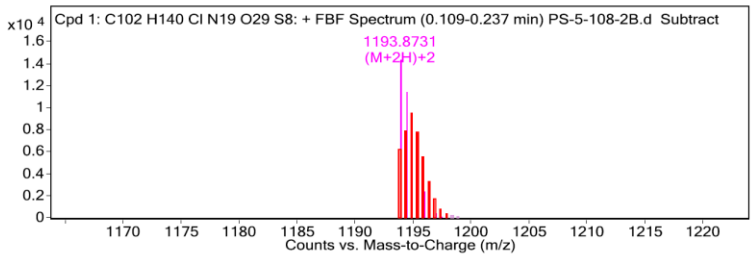


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
1196.3865	2	13316.92	C101H145ClN20O29S8	(M+2H)+2
1196.8869	2	10396.94	C101H145ClN20O29S8	(M+2H)+2
1197.387	2	7434.07	C101H145ClN20O29S8	(M+2H)+2
1197.8868	2	4156.46	C101H145ClN20O29S8	(M+2H)+2
1198.386	2	2234.87	C101H145ClN20O29S8	(M+2H)+2
1198.885	2	1041.17	C101H145ClN20O29S8	(M+2H)+2
1199.3857	2	432.68	C101H145ClN20O29S8	(M+2H)+2

--- End Of Report ---

HRMS spectra of 3-FITC

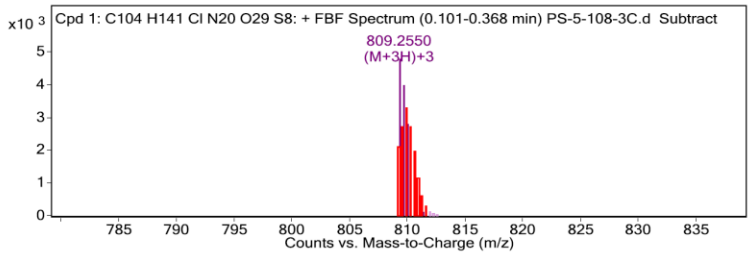


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
1193.8731	2	14409.95	C102H142ClN19O29S8	(M+2H)+2
1194.3732	2	11427.2	C102H142ClN19O29S8	(M+2H)+2
1194.8729	2	7915.61	C102H142ClN19O29S8	(M+2H)+2
1195.3725	2	4890.26	C102H142ClN19O29S8	(M+2H)+2
1195.8723	2	2459.77	C102H142ClN19O29S8	(M+2H)+2
1196.372	2	1077.29	C102H142ClN19O29S8	(M+2H)+2
1196.8731	2	524.97	C102H142ClN19O29S8	(M+2H)+2
1197.3721	2	153.16	C102H142ClN19O29S8	(M+2H)+2
1197.8741	2	27.78	C102H142ClN19O29S8	(M+2H)+2

--- End Of Report ---

HRMS spectra of 4-FITC

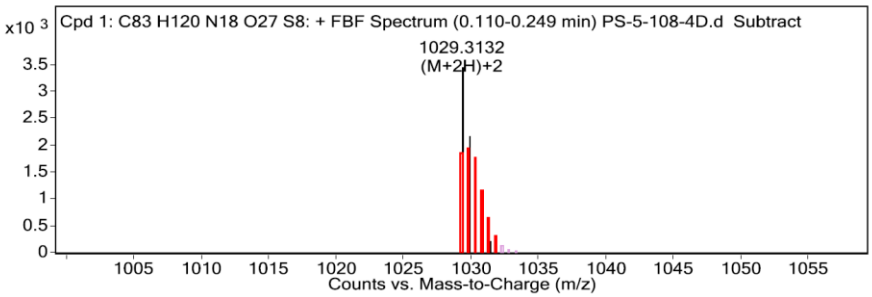


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
809.255	3	4817.22	C104H144ClN20O29S8	(M+3H)+3
809.5885	3	4011.91	C104H144ClN20O29S8	(M+3H)+3
809.9217	3	2813.06	C104H144ClN20O29S8	(M+3H)+3
810.2548	3	1670.02	C104H144ClN20O29S8	(M+3H)+3
810.5885	3	876.2	C104H144ClN20O29S8	(M+3H)+3
810.9207	3	422.02	C104H144ClN20O29S8	(M+3H)+3
811.2533	3	143.89	C104H144ClN20O29S8	(M+3H)+3
811.5848	3	54.35	C104H144ClN20O29S8	(M+3H)+3

--- End Of Report ---

HRMS spectra of 5-FITC

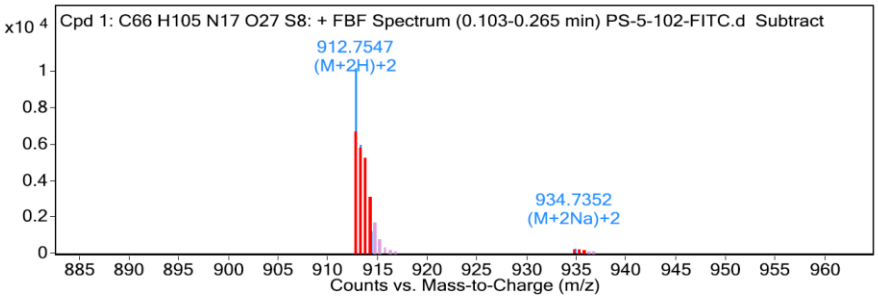


MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
1029.3132	2	3449.52	C83H122N18O27S8	(M+2H)+2
1029.8132	2	2189.28	C83H122N18O27S8	(M+2H)+2
1030.3134	2	1153.83	C83H122N18O27S8	(M+2H)+2
1030.8125	2	554.84	C83H122N18O27S8	(M+2H)+2
1031.3132	2	232.76	C83H122N18O27S8	(M+2H)+2
1031.809	2	74.75	C83H122N18O27S8	(M+2H)+2

--- End Of Report ---

HRMS spectra of 6-FITC

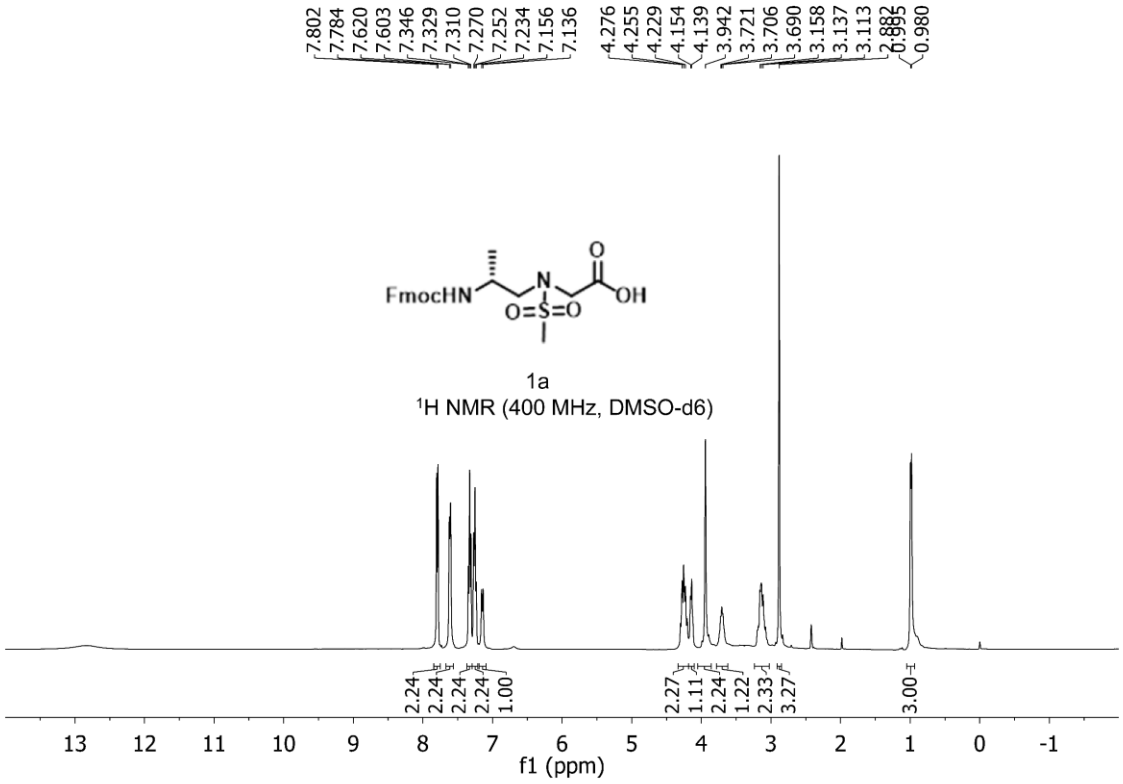


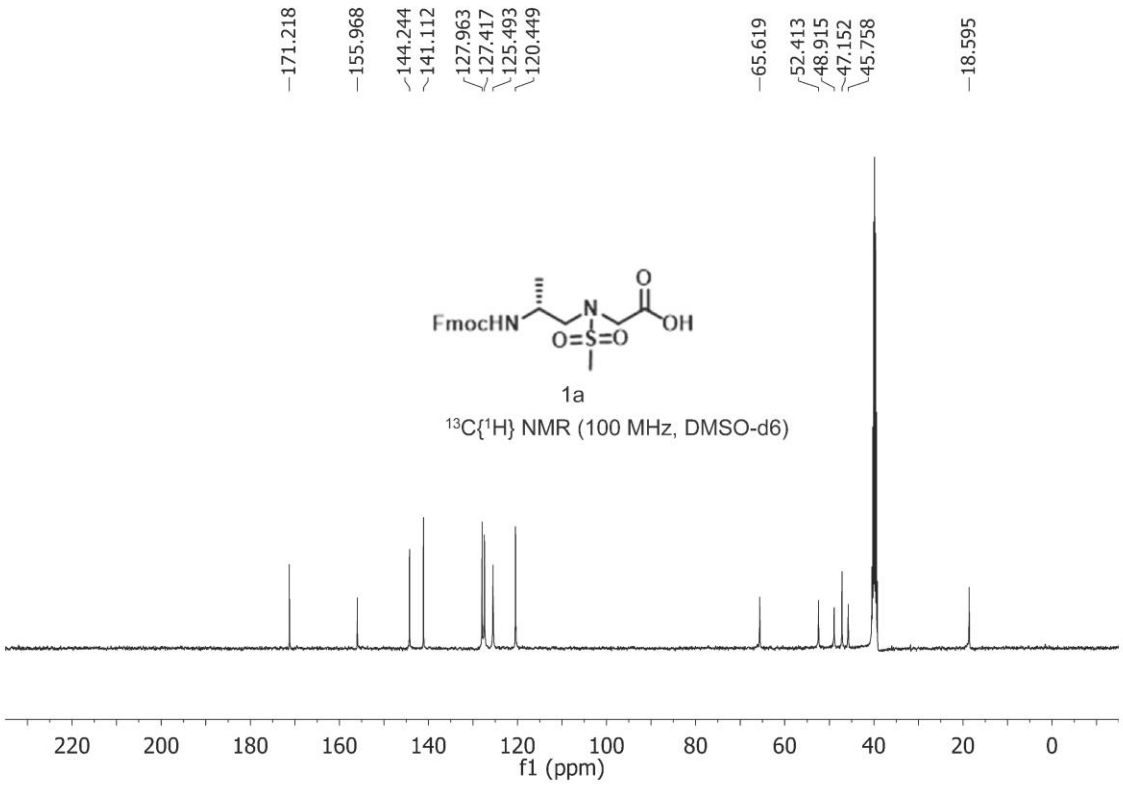
MS Spectrum Peak List

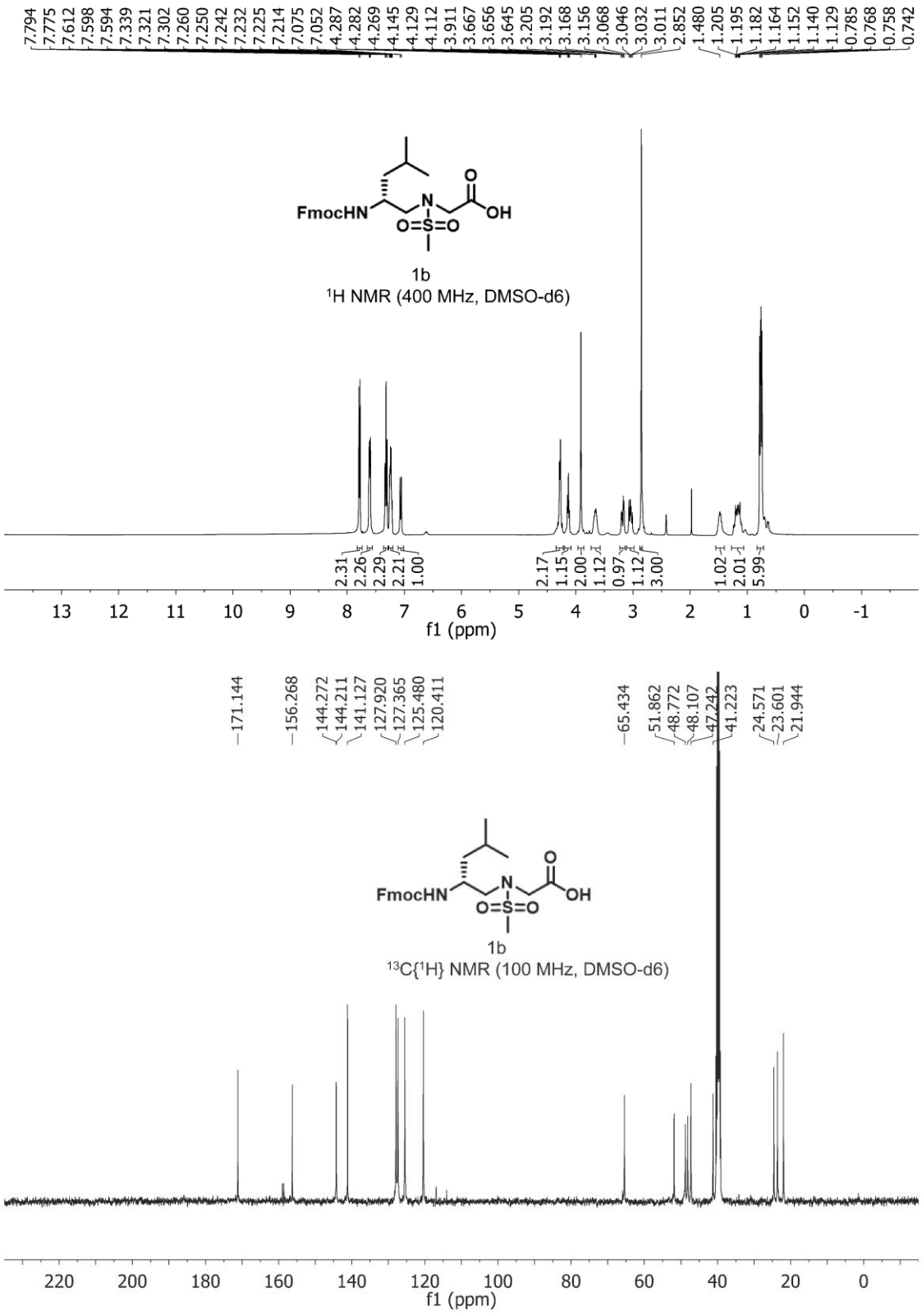
m/z	z	Abund	Formula	Ion
912.7547	2	10222.49	C66H107N17O27S8	(M+2H)+2
913.2544	2	5983.9	C66H107N17O27S8	(M+2H)+2
913.7537	2	3049.32	C66H107N17O27S8	(M+2H)+2
914.2537	2	1313.44	C66H107N17O27S8	(M+2H)+2
934.7352	2	278.5	C66H105N17Na2O27S8	(M+2Na)+2
935.2348	2	139.58	C66H105N17Na2O27S8	(M+2Na)+2
935.7305	2	51.55	C66H105N17Na2O27S8	(M+2Na)+2

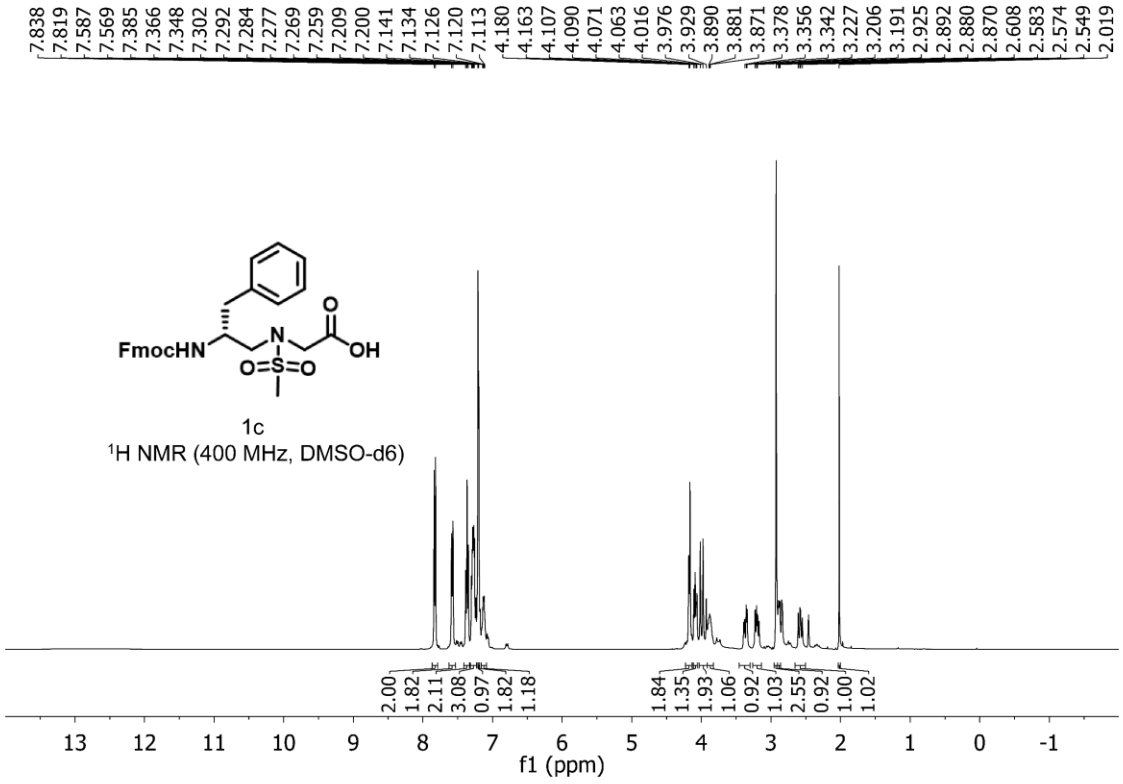
--- End Of Report ---

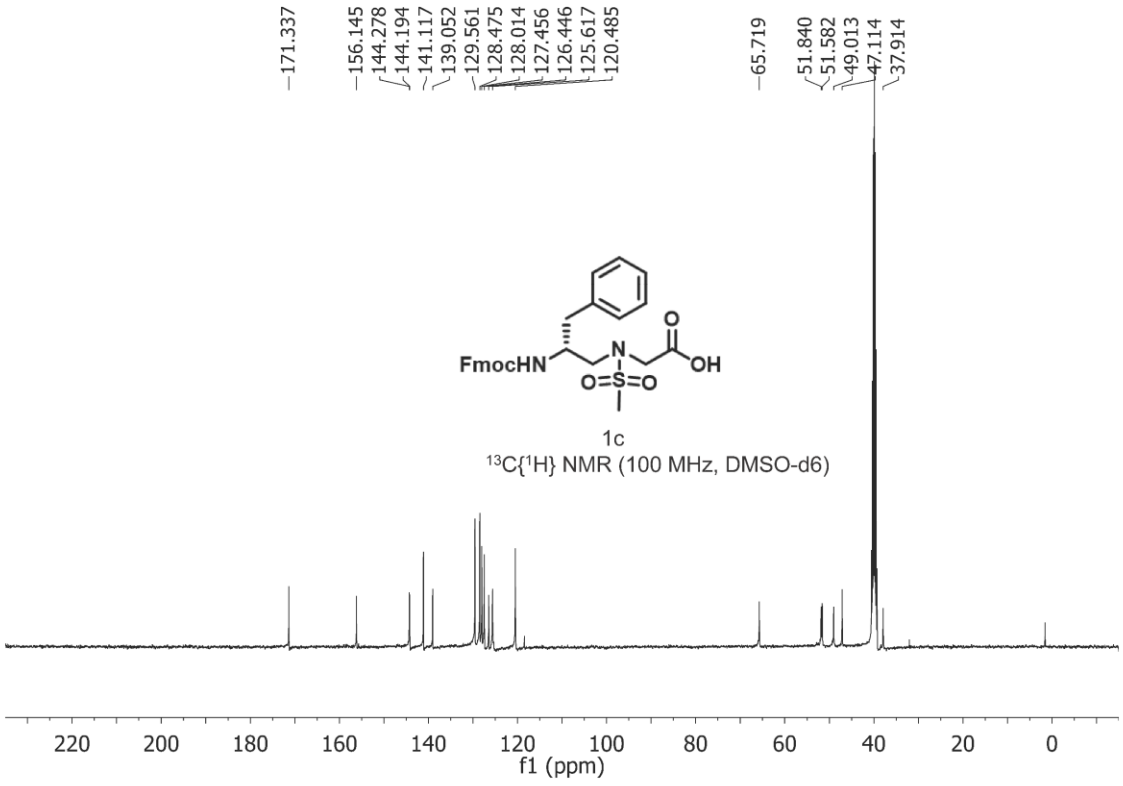
6. The ^{1}H and ^{13}C NMR Spectra of D-Sulfono-γ-AApeptide Building Blocks 1a-j

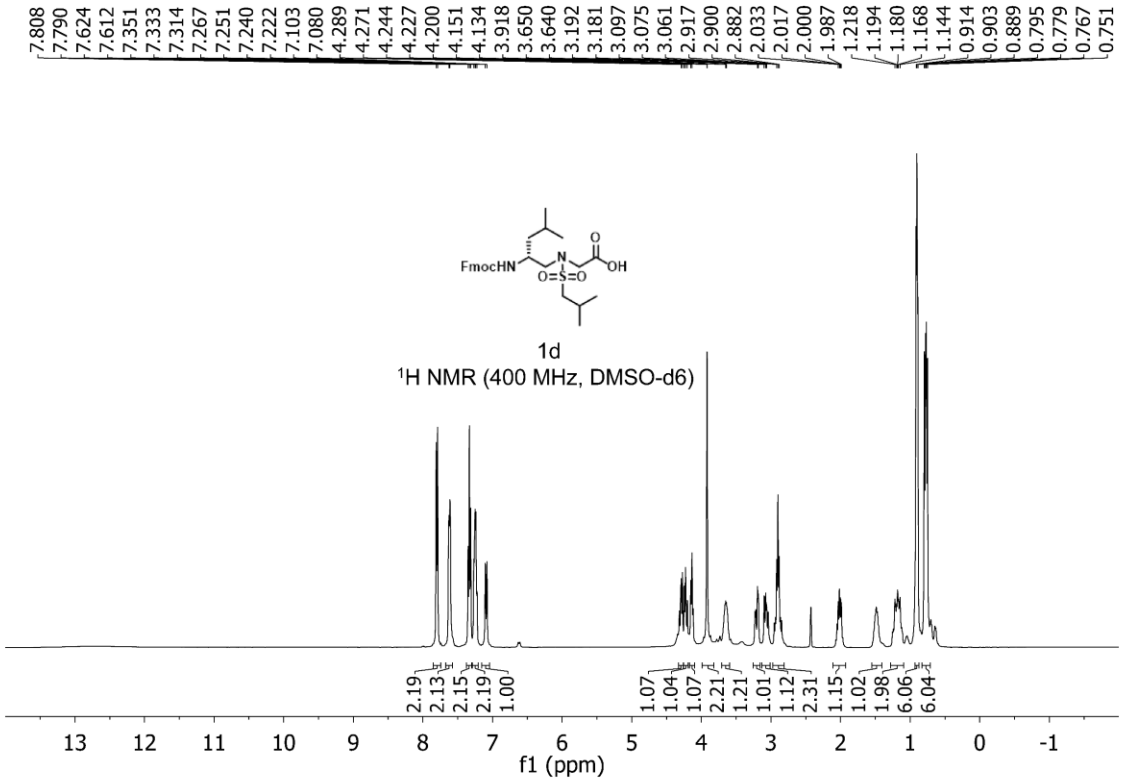


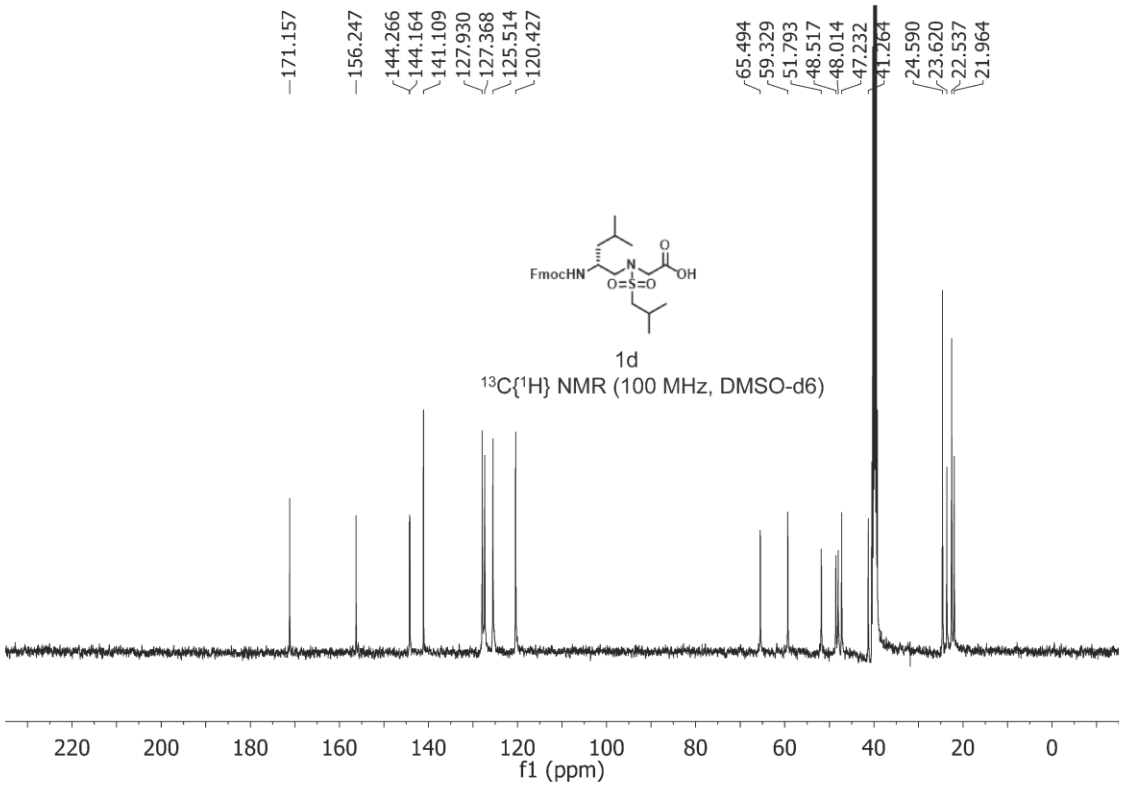


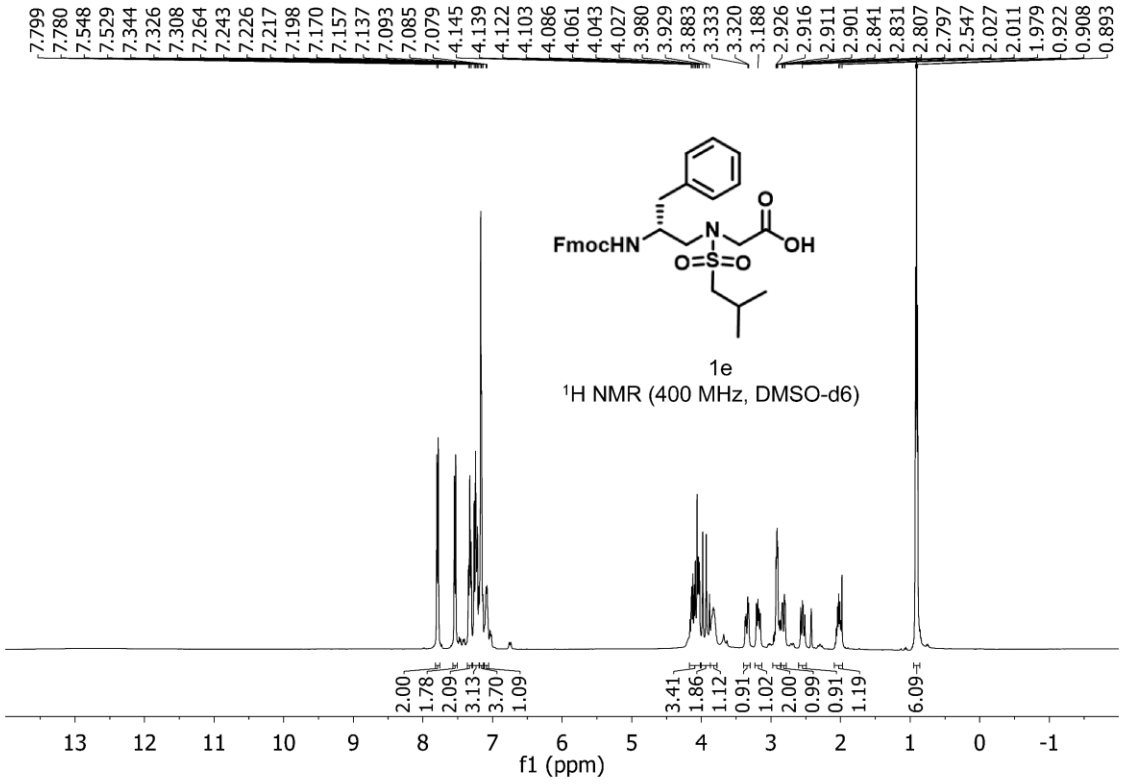

7.794
7.775
7.612
7.598
7.594
7.339
7.321
7.302
7.260
7.250
7.242
7.232
7.225
7.214
7.075
7.052
4.287
4.282
4.269
4.145
4.129
4.112
3.911
3.667
3.656
3.645
3.205
3.192
3.168
3.156
3.068
3.046
3.032
3.011
2.852
1.480
1.205
1.195
1.182
1.164
1.152
1.140
1.129
0.785
0.768
0.758
0.742
FmocHN
N
O=S=O
O
OH
1b
1H NMR (400 MHz, DMSO-d6)
2.31
2.26
2.29
2.21
1.00
2.17
1.15
2.00
1.12
0.97
1.12
3.00
1.02
2.01
5.99
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)
171.144
156.268
144.272
144.211
141.127
127.920
127.365
125.480
120.411
65.434
51.862
48.772
48.107
47.242
41.223
24.571
23.601
21.944
FmocHN
N
O=S=O
O
OH
1b
13C{1H} NMR (100 MHz, DMSO-d6)
220 200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

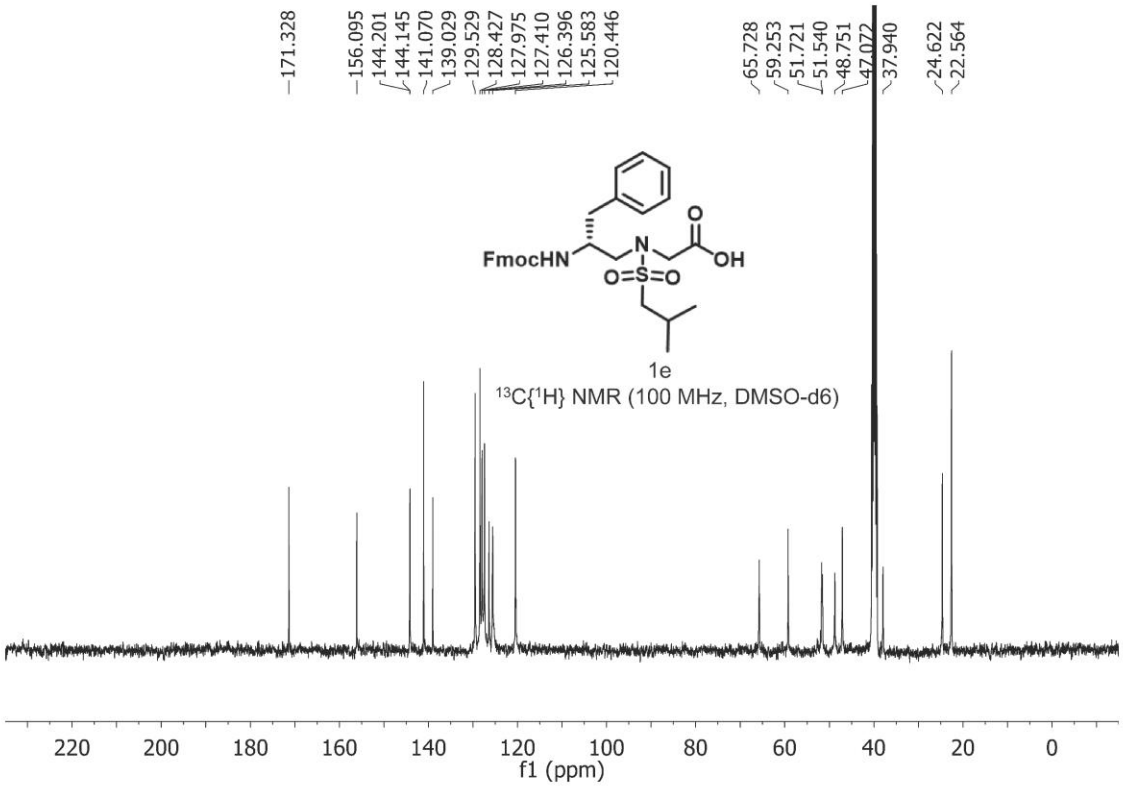

7.838
7.819
7.587
7.569
7.385
7.366
7.348
7.302
7.292
7.284
7.277
7.269
7.259
7.209
7.200
7.141
7.134
7.126
7.120
7.113
4.180
4.163
4.107
4.090
4.071
4.063
4.016
3.976
3.929
3.890
3.881
3.871
3.378
3.356
3.342
3.227
3.206
3.191
2.925
2.892
2.880
2.870
2.608
2.583
2.574
2.549
2.019
FmocHN
N
O
OH
O=S=O
1c
1H NMR (400 MHz, DMSO-d6)
2.00
1.82
2.11
3.08
0.97
1.82
1.18
1.84
1.35
1.93
1.06
0.92
1.03
2.55
0.92
1.00
1.02
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

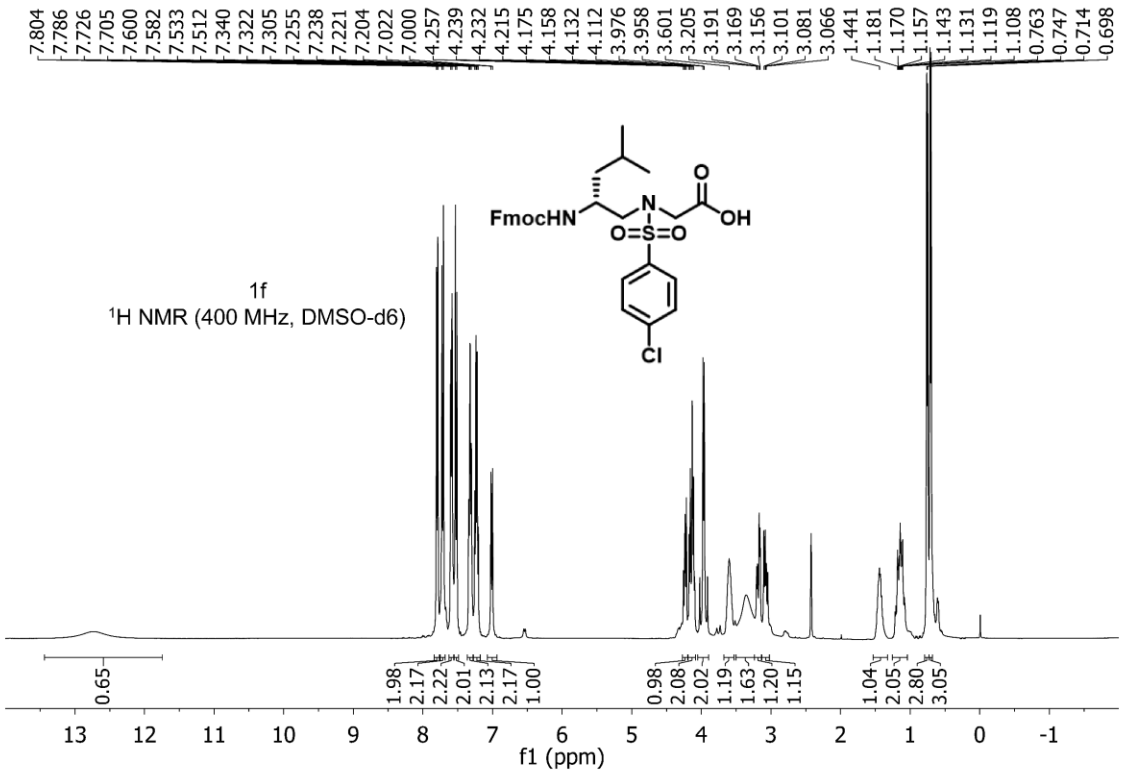

171.337
156.145
144.278
144.194
141.117
139.052
129.561
128.475
128.014
127.456
126.446
125.617
120.485
65.719
51.840
51.582
49.013
47.114
37.914
FmocHN
N
O
OH
O=S=O
1c
13C{1H} NMR (100 MHz, DMSO-d6)
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

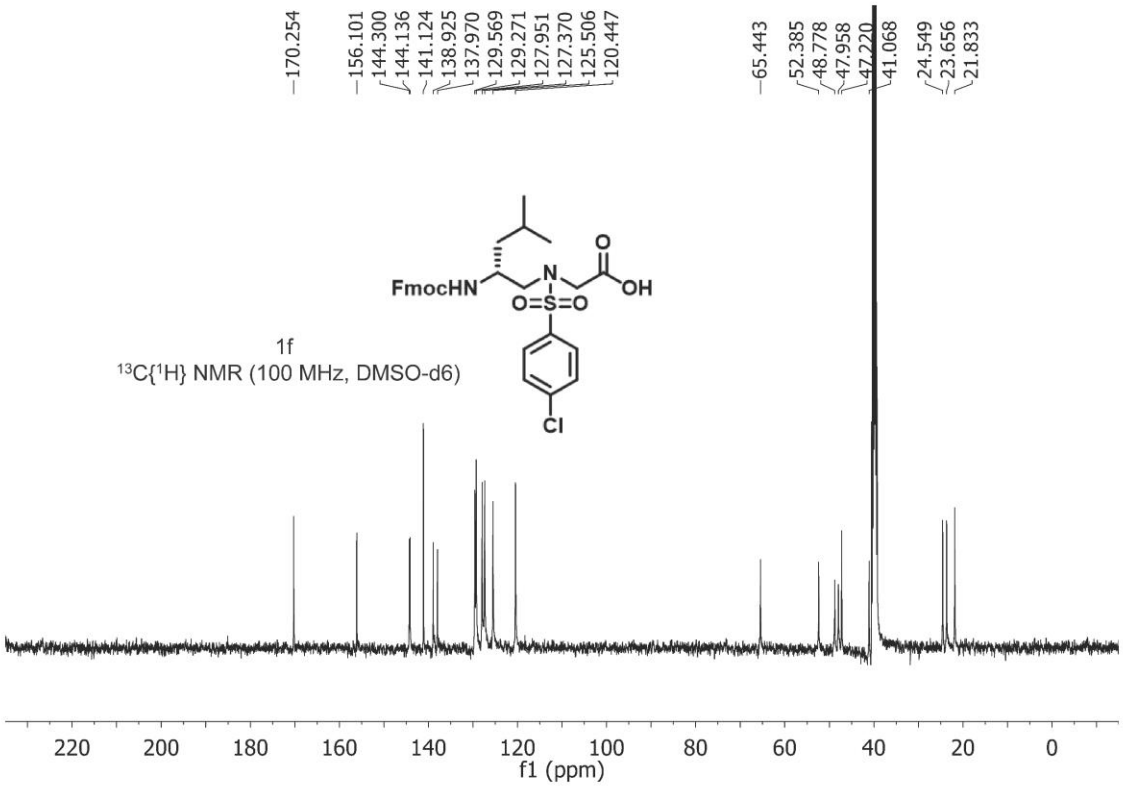

7.808
7.790
7.624
7.612
7.351
7.333
7.314
7.267
7.251
7.240
7.222
7.103
7.080
4.289
4.271
4.244
4.227
4.200
4.151
4.134
3.918
3.650
3.640
3.192
3.181
3.097
3.075
3.061
2.917
2.900
2.882
2.033
2.017
2.000
1.987
1.218
1.194
1.180
1.168
1.144
0.914
0.903
0.889
0.795
0.779
0.767
0.751
FmocHN
N
O=S=O
O
OH
1d
1H NMR (400 MHz, DMSO-d6)
2.19
2.13
2.15
2.19
1.00
1.07
1.04
1.07
2.21
1.21
1.01
1.12
2.31
1.15
1.02
1.98
6.06
6.04
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

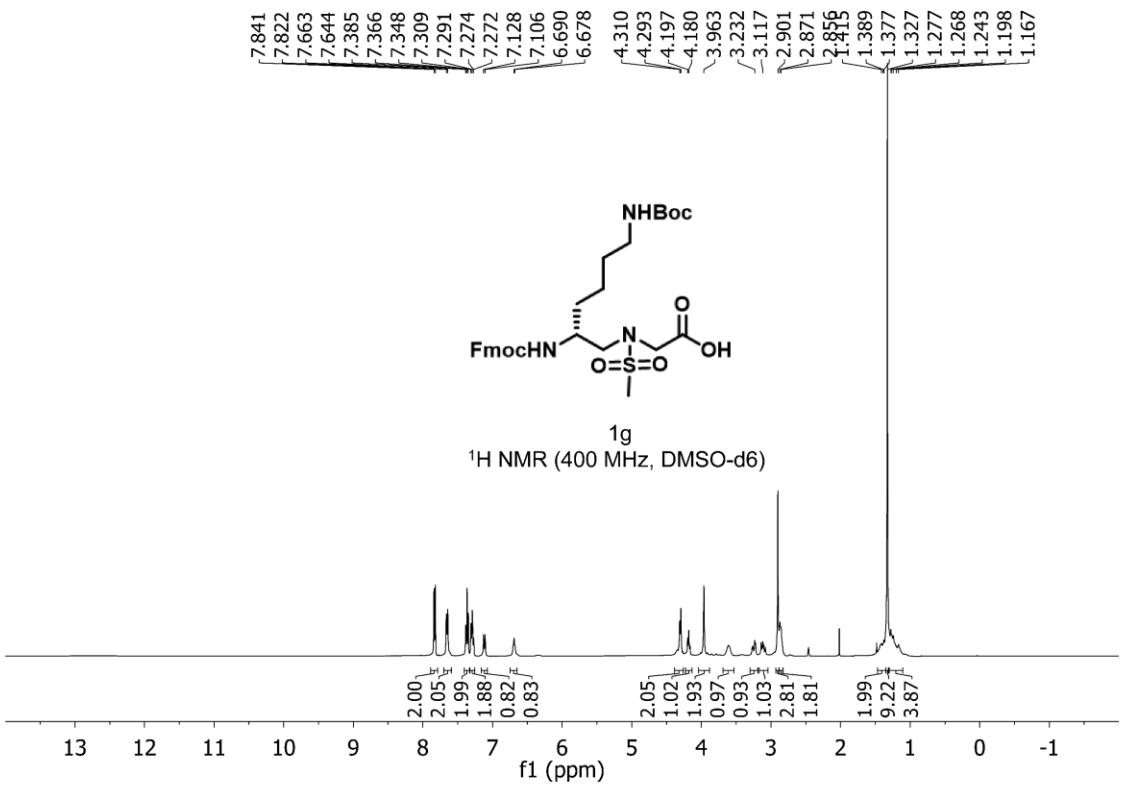

171.157
156.247
144.266
144.164
141.109
127.930
127.368
125.514
120.427
65.494
59.329
51.793
48.517
48.014
47.232
41.264
24.590
23.620
22.537
21.964
FmocHN
N
O=S=O
O
OH
1d
13C{1H} NMR (100 MHz, DMSO-d6)
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

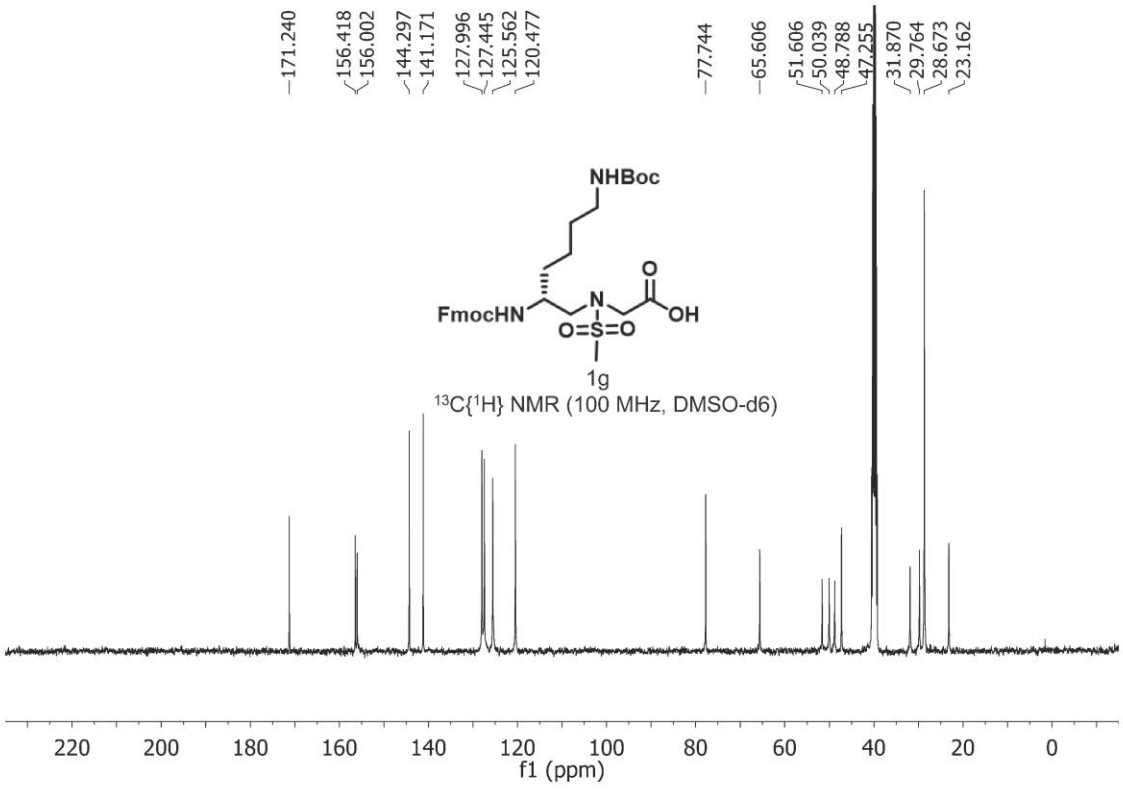

7.799
7.780
7.548
7.529
7.344
7.326
7.308
7.264
7.243
7.226
7.217
7.198
7.170
7.157
7.137
7.093
7.085
7.079
4.145
4.139
4.122
4.103
4.086
4.061
4.043
4.027
3.980
3.929
3.883
3.333
3.320
3.188
2.926
2.916
2.911
2.901
2.841
2.831
2.807
2.797
2.547
2.027
2.011
1.979
0.922
0.908
0.893
FmocHN
N
O
OH
O=S=O
1e
1H NMR (400 MHz, DMSO-d6)
2.00
1.78
2.09
3.13
3.70
1.09
3.41
1.86
1.12
0.91
1.02
2.00
0.99
0.91
1.19
6.09
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)

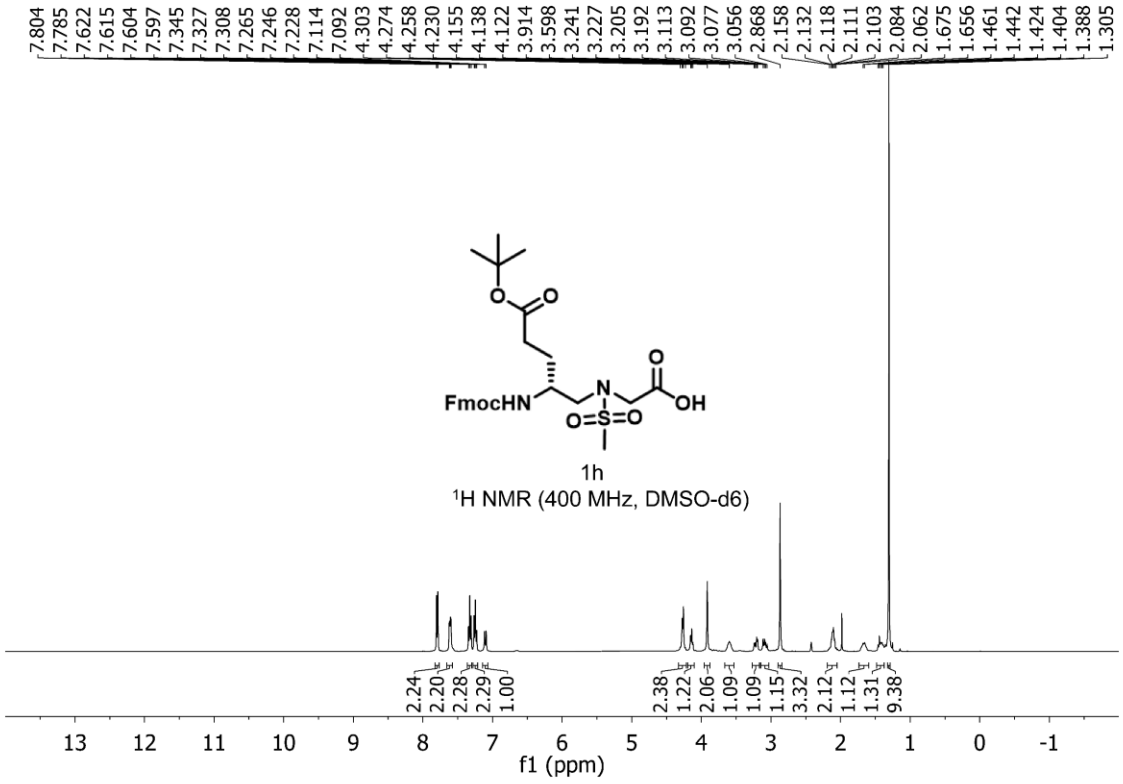

171.328
156.095
144.201
144.145
141.070
139.029
129.529
128.427
127.975
127.410
126.396
125.583
120.446
65.728
59.253
51.721
51.540
48.751
47.072
37.940
24.622
22.564
FmocHN
N
O
OH
O=S=O
1e
13C{1H} NMR (100 MHz, DMSO-d6)
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)

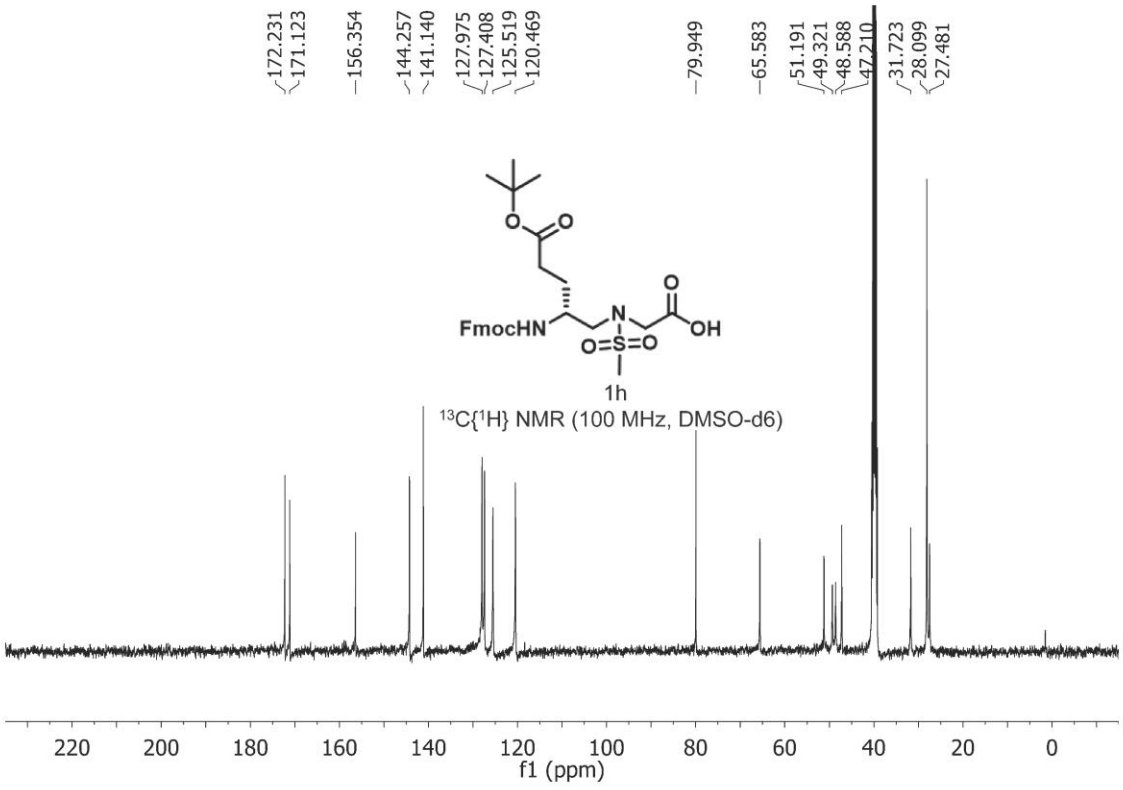

1f
1H NMR (400 MHz, DMSO-d6)
FmocHN
O=S=O
OH
Cl
f1 (ppm)

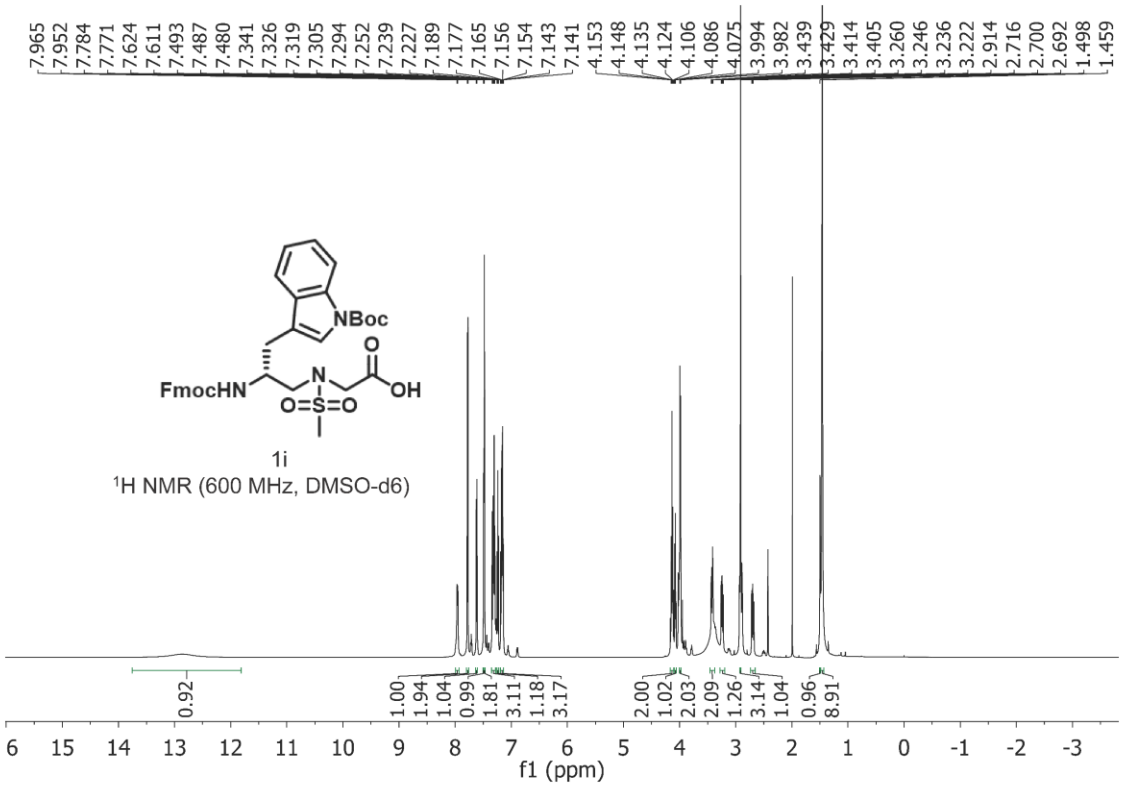

1f
13C{1H} NMR (100 MHz, DMSO-d6)
FmocHN
O=S=O
OH
Cl
f1 (ppm)

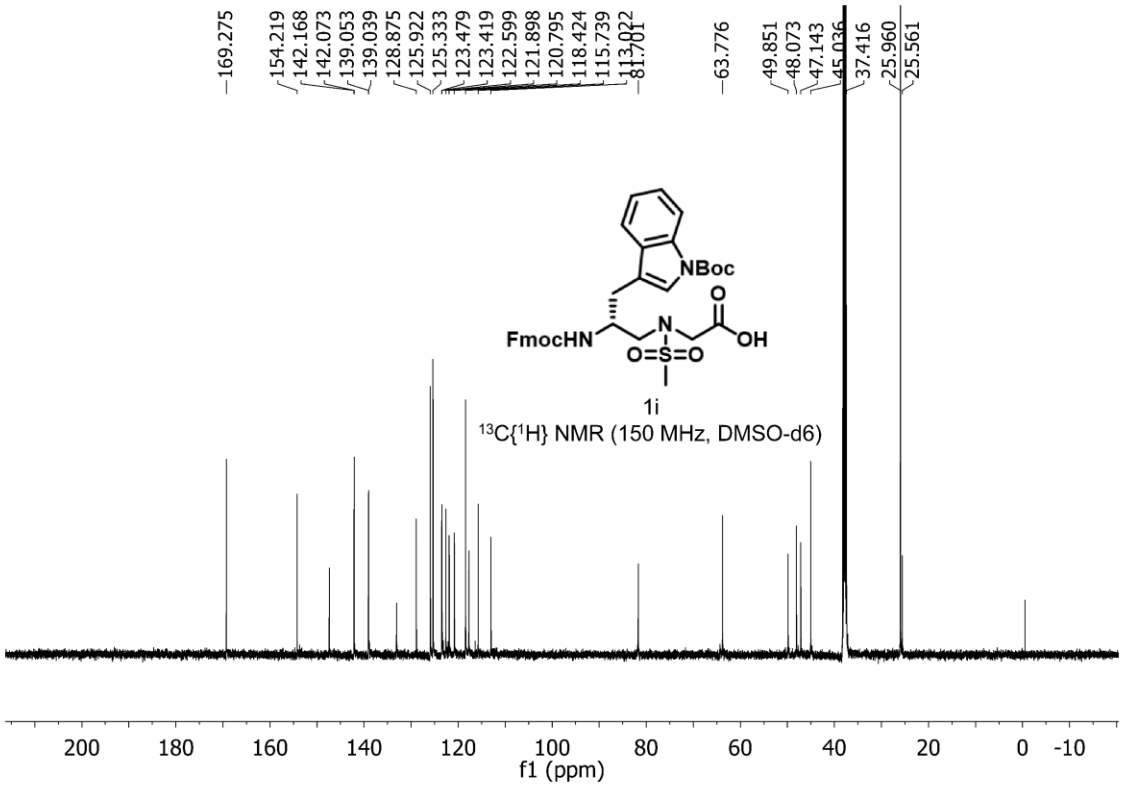

7.841
7.822
7.663
7.644
7.385
7.366
7.348
7.309
7.291
7.274
7.272
7.128
7.106
6.690
6.678
4.310
4.293
4.197
4.180
3.963
3.232
3.117
2.901
2.871
1.389
1.377
1.327
1.277
1.268
1.243
1.198
1.167
NHBoc
FmocHN
N
O
OH
O=S=O
1g
¹H NMR (400 MHz, DMSO-d6)
2.00
2.05
1.99
1.88
0.82
0.83
2.05
1.02
1.93
0.97
0.93
1.03
2.81
1.81
1.99
9.22
3.87
13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1
f1 (ppm)

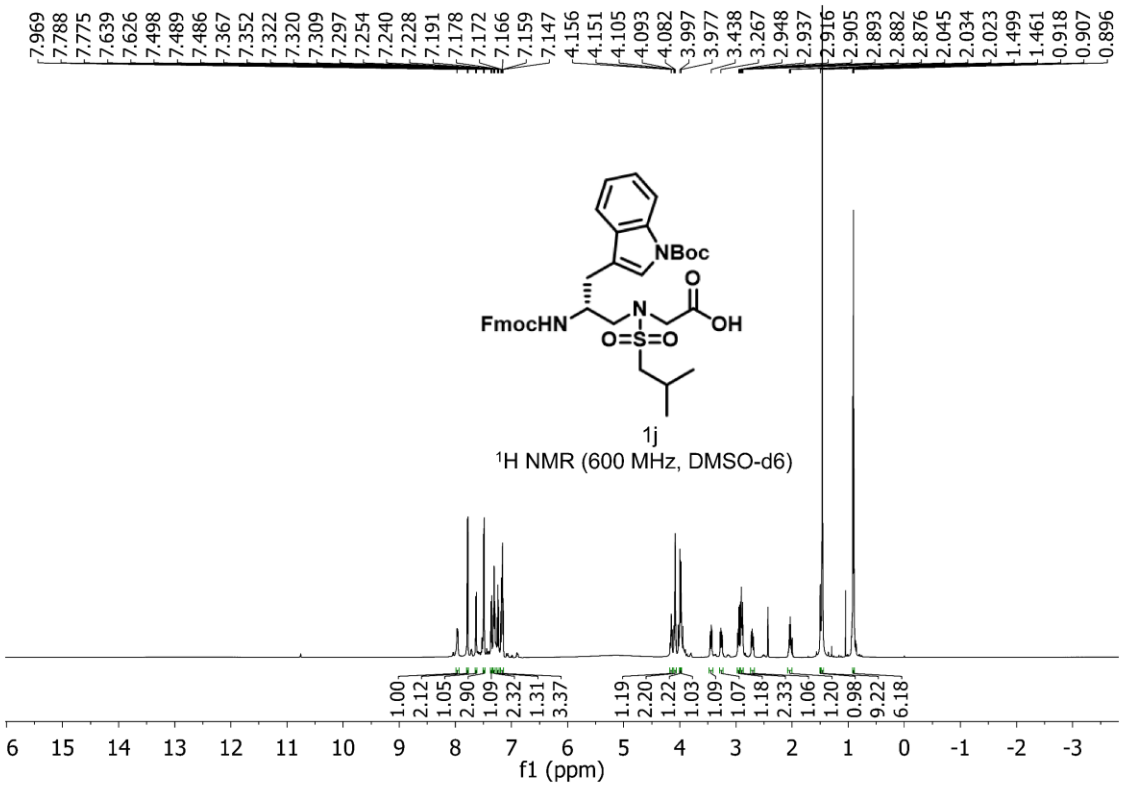

171.240
156.418
156.002
144.297
141.171
127.996
127.445
125.562
120.477
77.744
65.606
51.606
50.039
48.788
47.255
31.870
29.764
28.673
23.162
NHBoc
FmocHN
N
O
OH
O=S=O
1g
¹³C{¹H} NMR (100 MHz, DMSO-d6)
220 200 180 160 140 120 100 80 60 40 20 0
f1 (ppm)

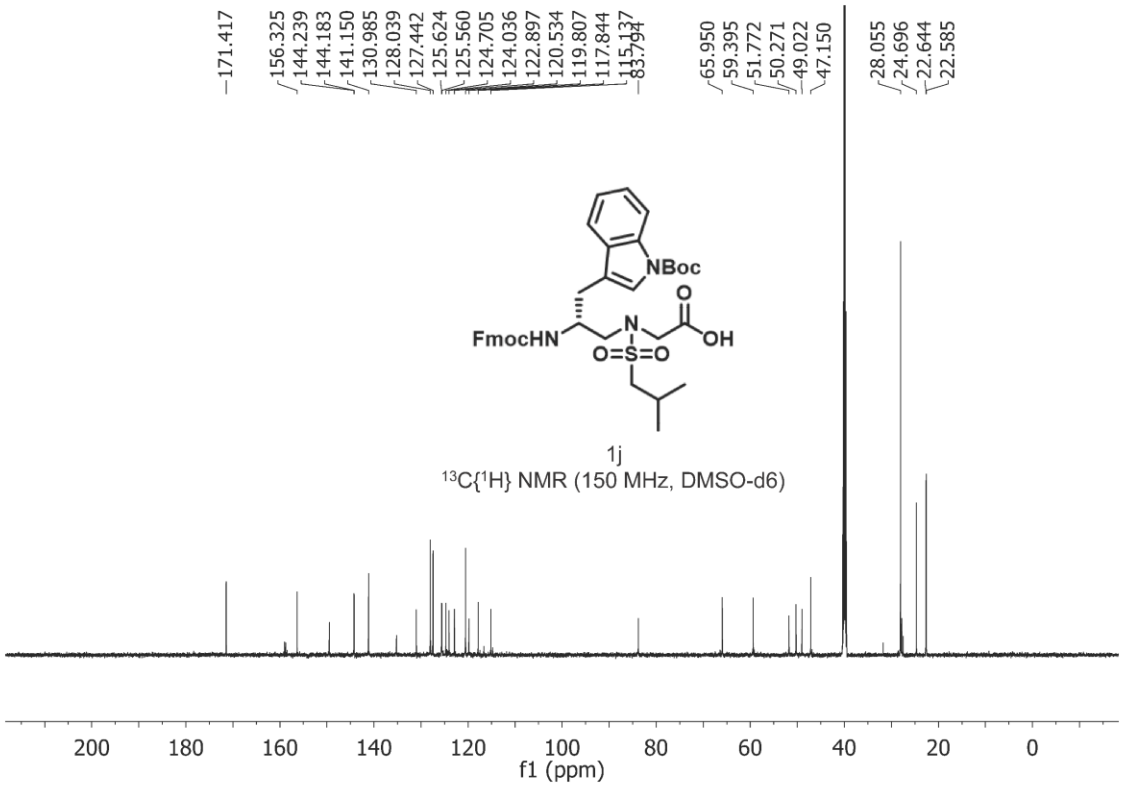

7.804
7.785
7.622
7.615
7.604
7.597
7.345
7.327
7.308
7.265
7.246
7.228
7.114
7.092
4.303
4.274
4.258
4.230
4.155
4.138
4.122
3.914
3.598
3.241
3.227
3.205
3.192
3.113
3.092
3.077
3.056
2.868
2.158
2.132
2.118
2.111
2.103
2.084
2.062
1.675
1.656
1.461
1.442
1.424
1.404
1.388
1.305
FmocHN
N
O=S=O
OH
1h
1H NMR (400 MHz, DMSO-d6)
2.24
2.20
2.28
2.29
1.00
2.38
1.22
2.06
1.09
1.09
1.15
3.32
2.12
1.12
1.31
9.38
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
f1 (ppm)


172.231
171.123
156.354
144.257
141.140
127.975
127.408
125.519
120.469
79.949
65.583
51.191
49.321
48.588
47.210
31.723
28.099
27.481
FmocHN
N
O=S=O
OH
1h
13C{1H} NMR (100 MHz, DMSO-d6)
220
200
180
160
140
120
100
80
60
40
20
0
f1 (ppm)


NBoc
FmocHN
N
O=S=O
OH
1i
¹H NMR (600 MHz, DMSO-d6)
f1 (ppm)


NBoc
FmocHN
N
O=S=O
OH
1i
¹³C{¹H} NMR (150 MHz, DMSO-d6)
f1 (ppm)


7.969
7.788
7.775
7.639
7.626
7.498
7.489
7.486
7.367
7.352
7.322
7.320
7.309
7.297
7.254
7.240
7.228
7.191
7.178
7.172
7.166
7.159
7.147
4.156
4.151
4.105
4.093
4.082
3.997
3.977
3.438
3.267
2.948
2.937
2.916
2.905
2.893
2.882
2.876
2.045
2.034
2.023
1.499
1.461
0.918
0.907
0.896
NBoc
FmocHN
N
O=S=O
O
OH
1j
1H NMR (600 MHz, DMSO-d6)
1.00
2.12
1.05
2.90
1.09
2.32
1.31
3.37
1.19
2.20
1.22
1.03
1.09
1.07
1.18
2.33
1.06
1.20
0.98
9.22
6.18
f1 (ppm)


171.417
156.325
144.239
144.183
141.150
130.985
128.039
127.442
125.624
125.560
124.705
124.036
122.897
120.534
119.807
117.844
115.137
83.794
65.950
59.395
51.772
50.271
49.022
47.150
28.055
24.696
22.644
22.585
NBoc
FmocHN
N
O=S=O
O
OH
1j
13C{1H} NMR (150 MHz, DMSO-d6)
f1 (ppm)