Supporting Information

For

Chemoselective Protection of Glutathione in the Preparation of Bioconjugates: The Case of Trypanothione Disulphide[†]

[†]*Article dedicated to the memory of Professor Paul Cordopatis*

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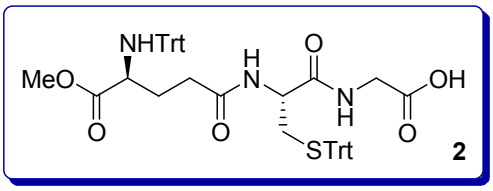
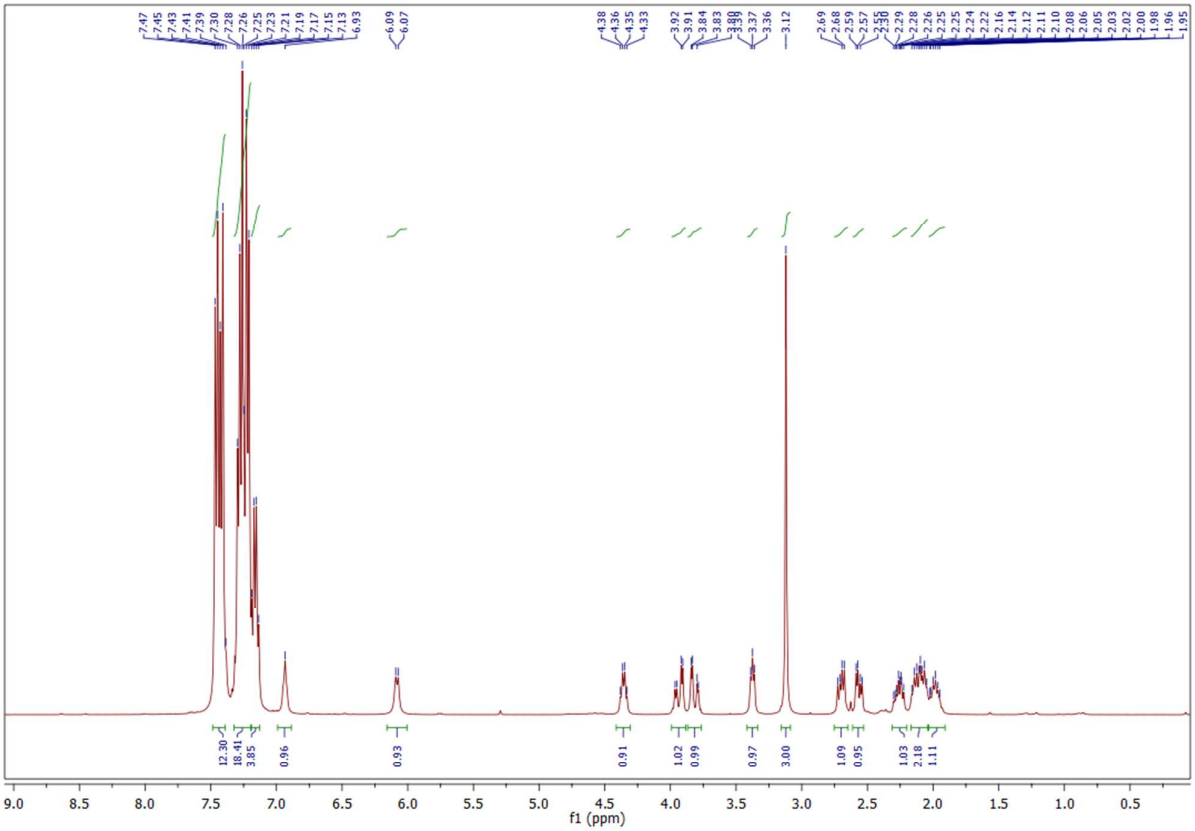
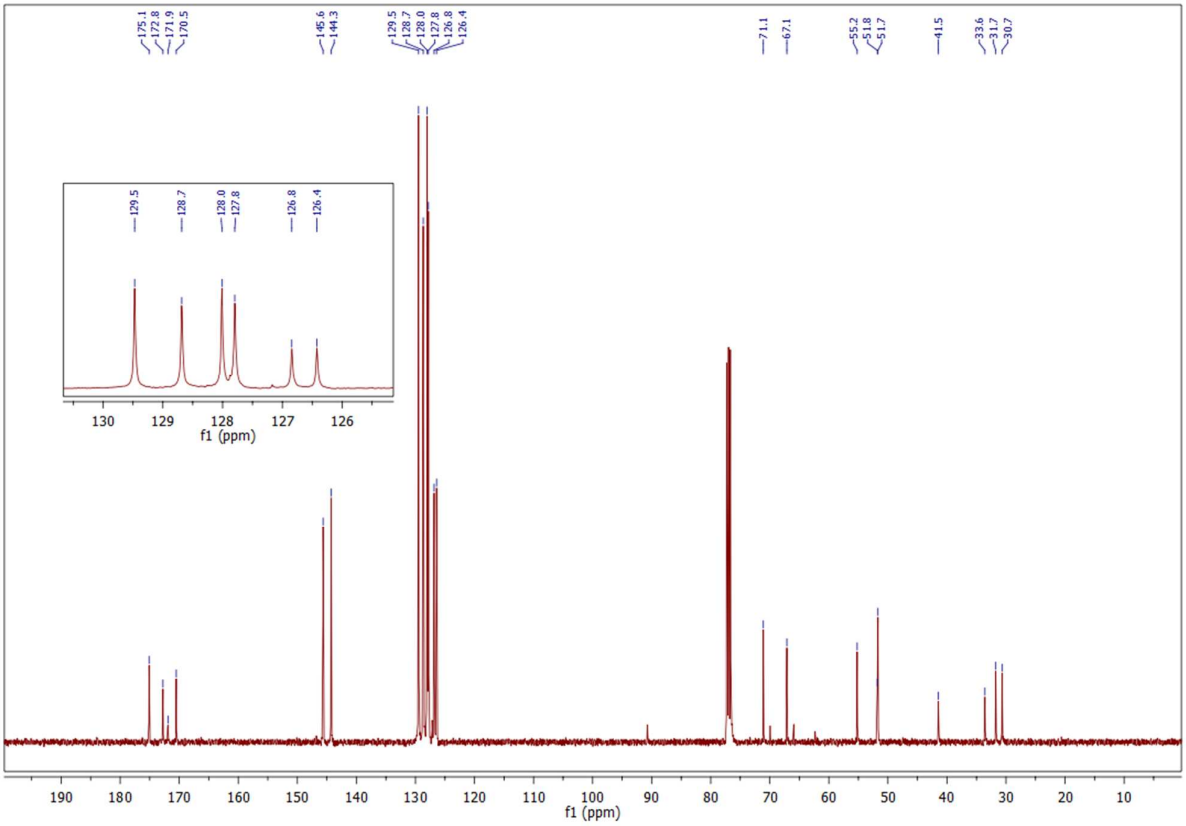
^{1}H (400 MHz) NMR spectra ($CDCl_3$) for compound 2



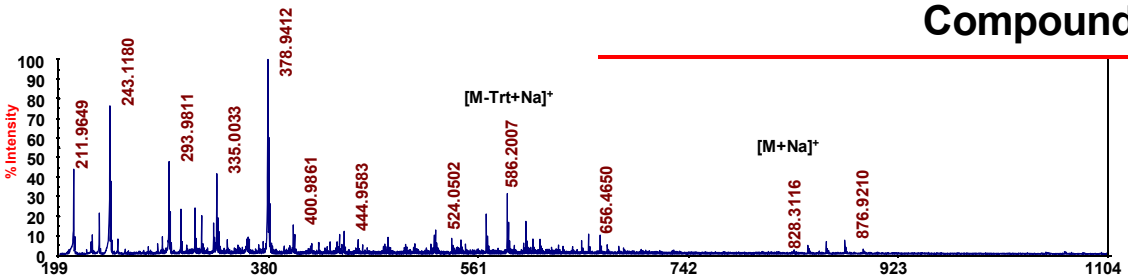


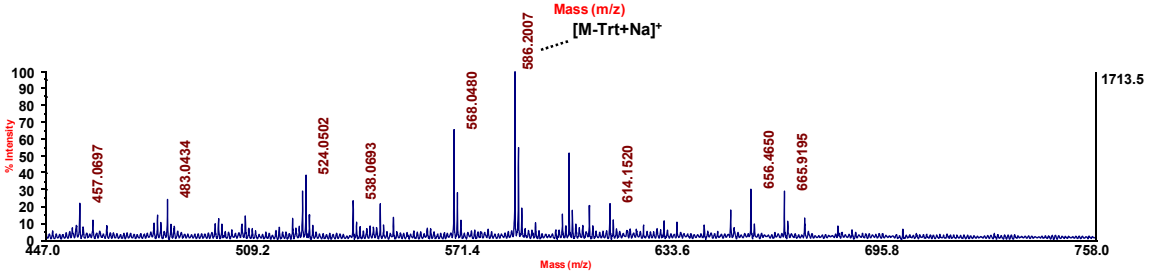
^{13}C (100 MHz) NMR spectra ($CDCl_3$) for compound 2

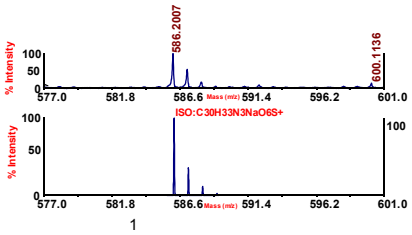


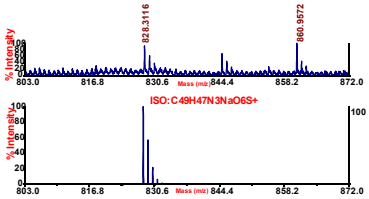
MALDI MS and MS/MS spectra for compound 2

Compound 2



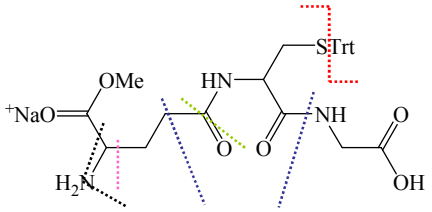


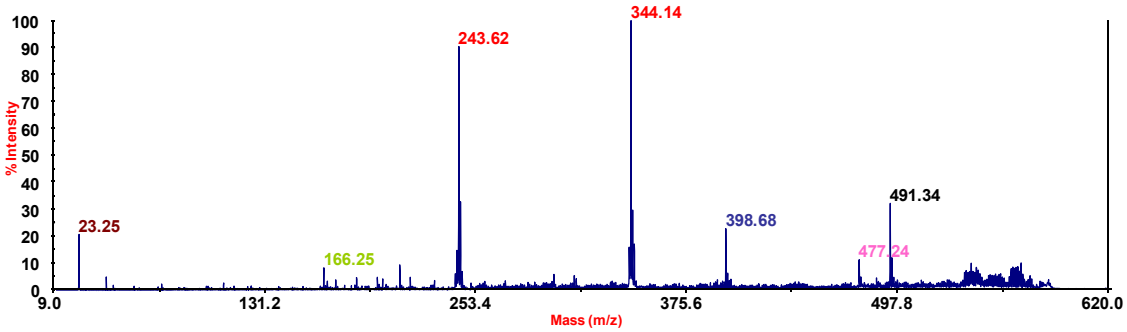




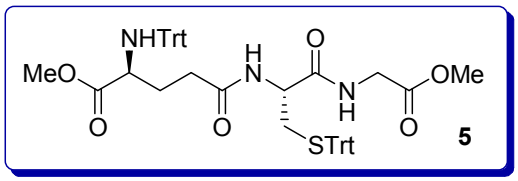
Index	Input m/z	Calc. Mass	Error (mDa)	Error (ppm)	DBE	Formula	
1	828.31160	828.30778	3.8203	4.6122	27.50	C49 H47 N3 O6 Na S	(<3%)
2	586.20070	586.19823	2.4709	4.2151	15.50	C30 H33 N3 O6 Na S	

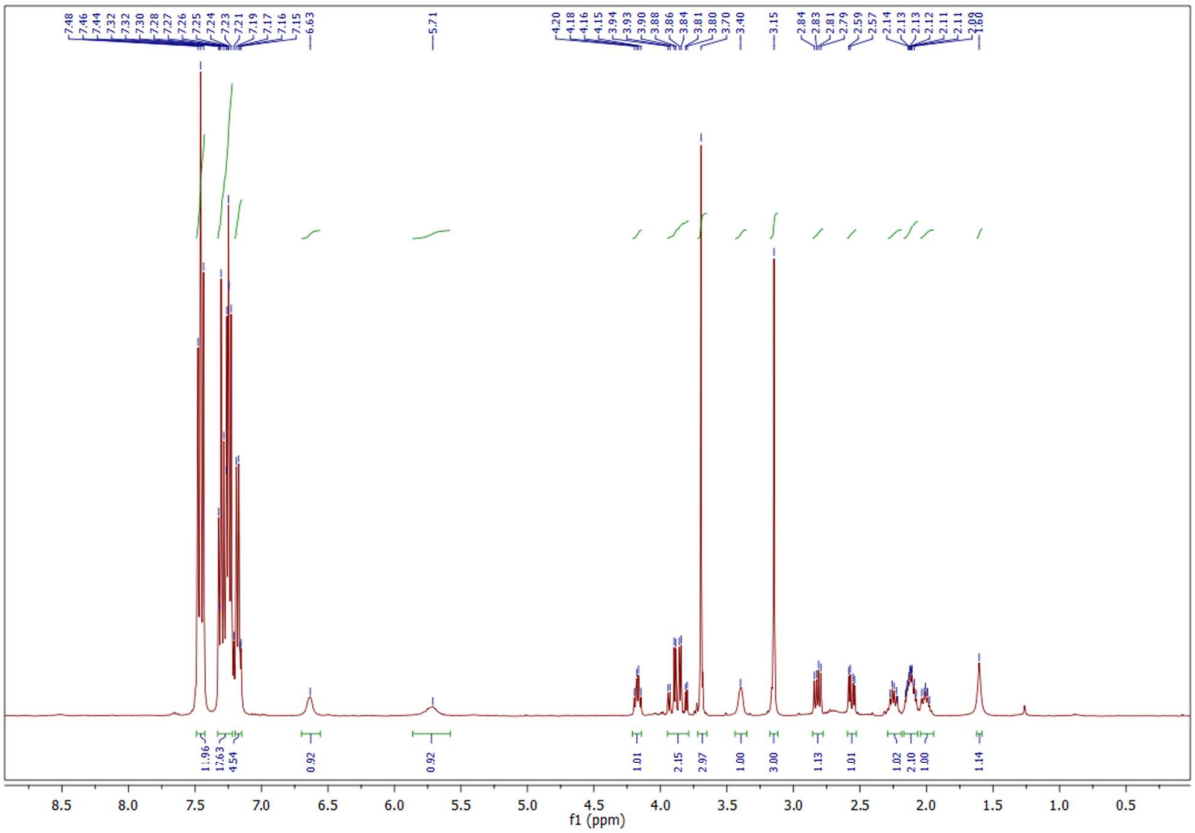
MS/MS m/z 586.20



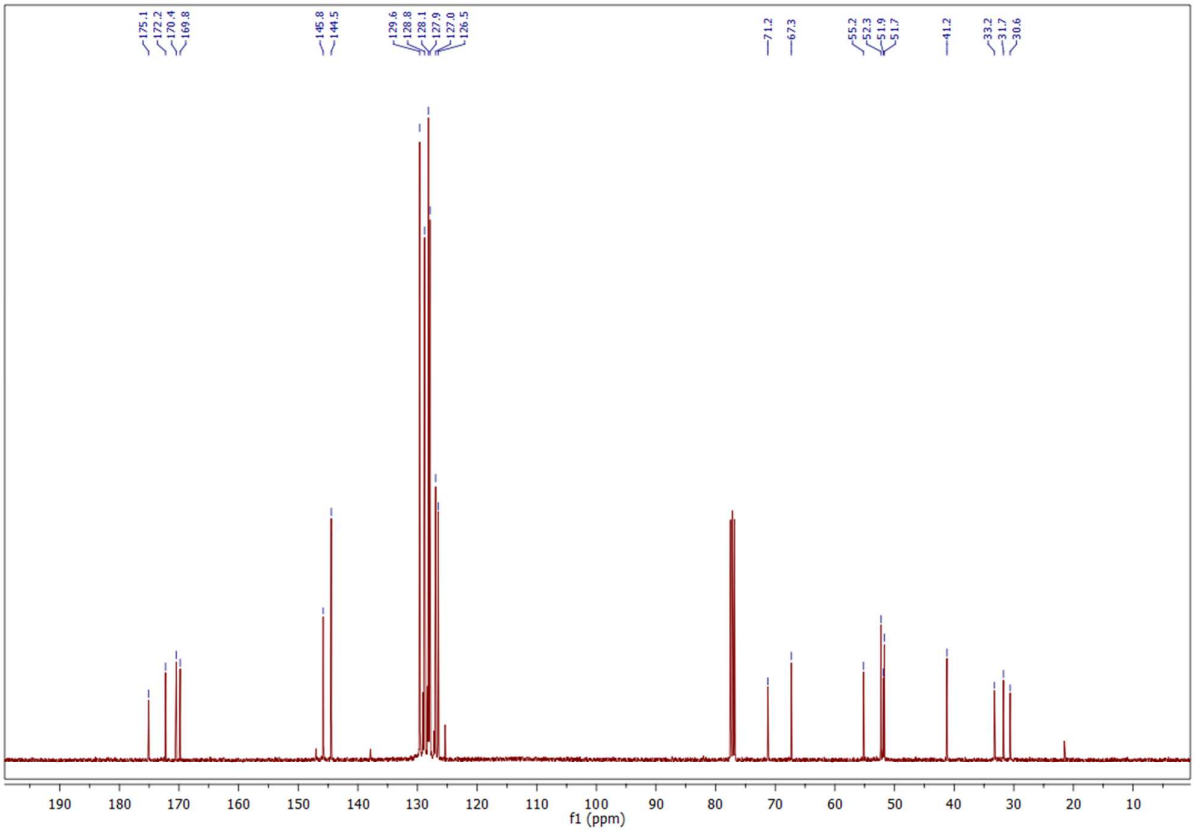


^{1}H (400 MHz) NMR spectra ($CDCl_3$) for compound 5

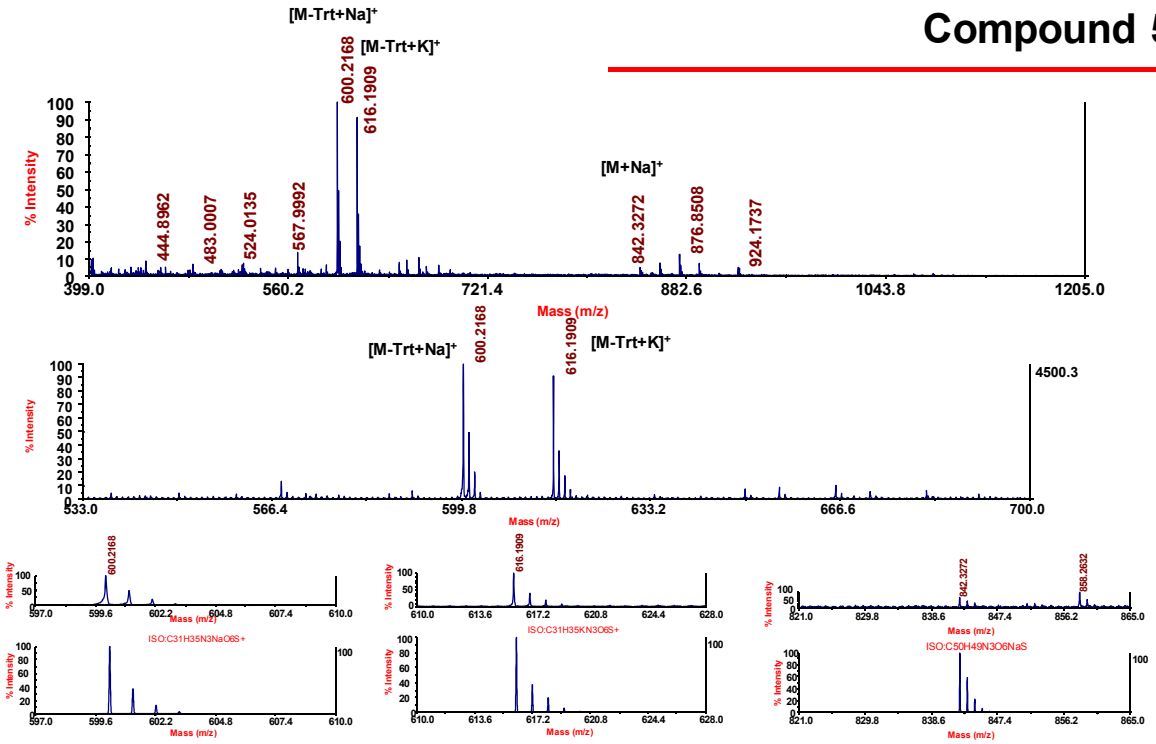




^{13}C (100 MHz) NMR spectra ($CDCl_3$) for compound 5

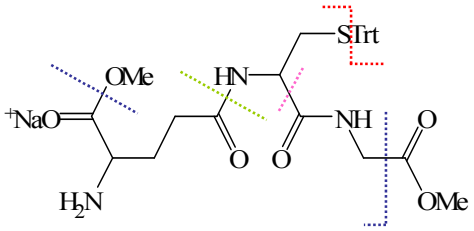


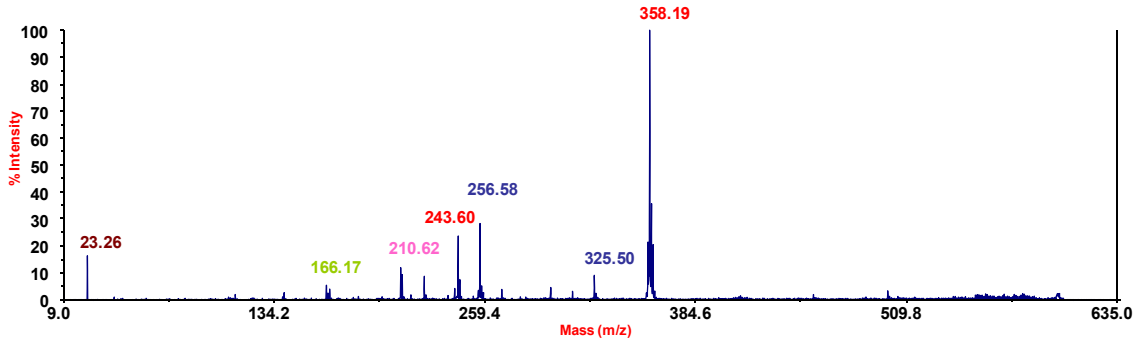
MALDI MS and MS/MS spectra for compound 5



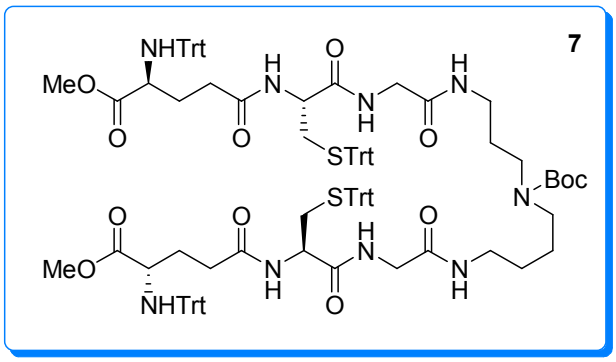
Index	Input m/z	Calc. Mass	Error (mDa)	Error (ppm)	DBE	Formula	
1	842.32720	842.32343	3.7703	4.4760	27.50	C50 H49 N3 O6 Na S	(<3%)
2	600.21680	600.21388	2.9208	4.8663	15.50	C31 H35 N3 O6 Na S	
3	616.19090	616.18782	3.0826	5.0027	15.50	C31 H35 N3 O6 S K	

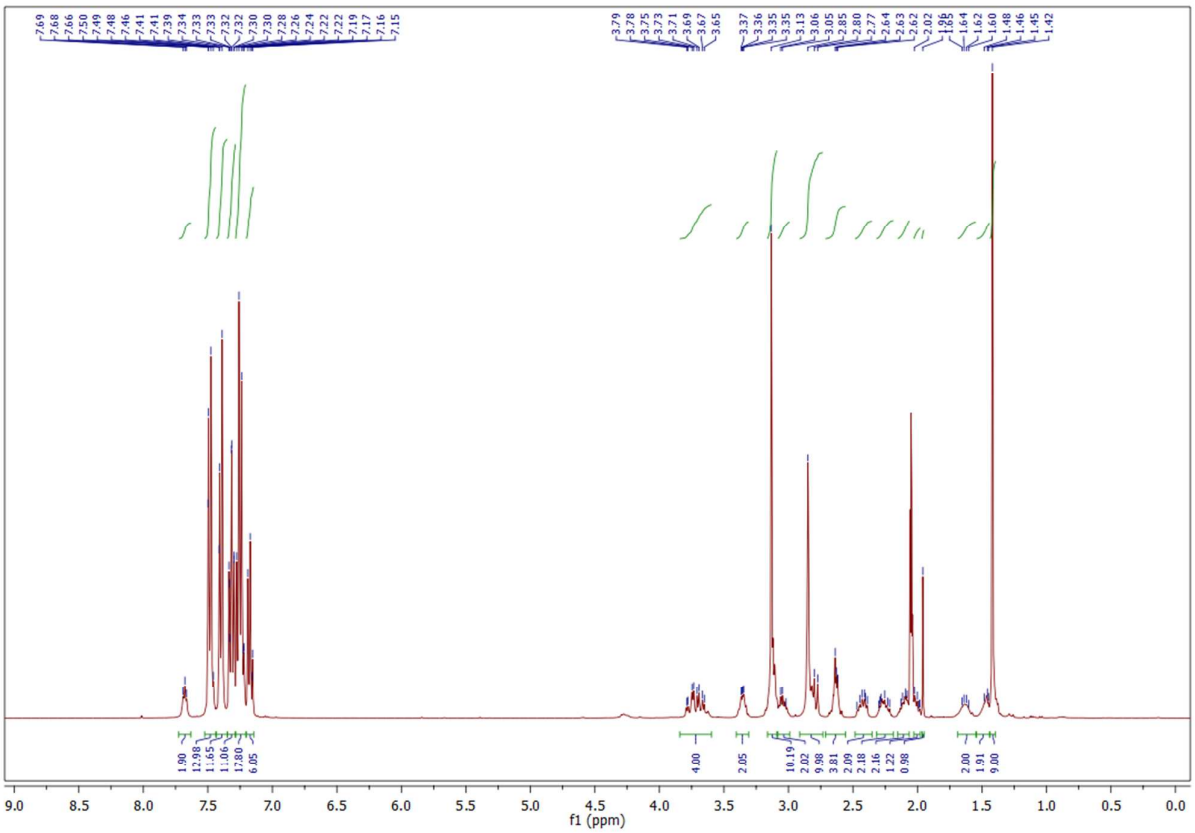
MS/MS m/z 600.22



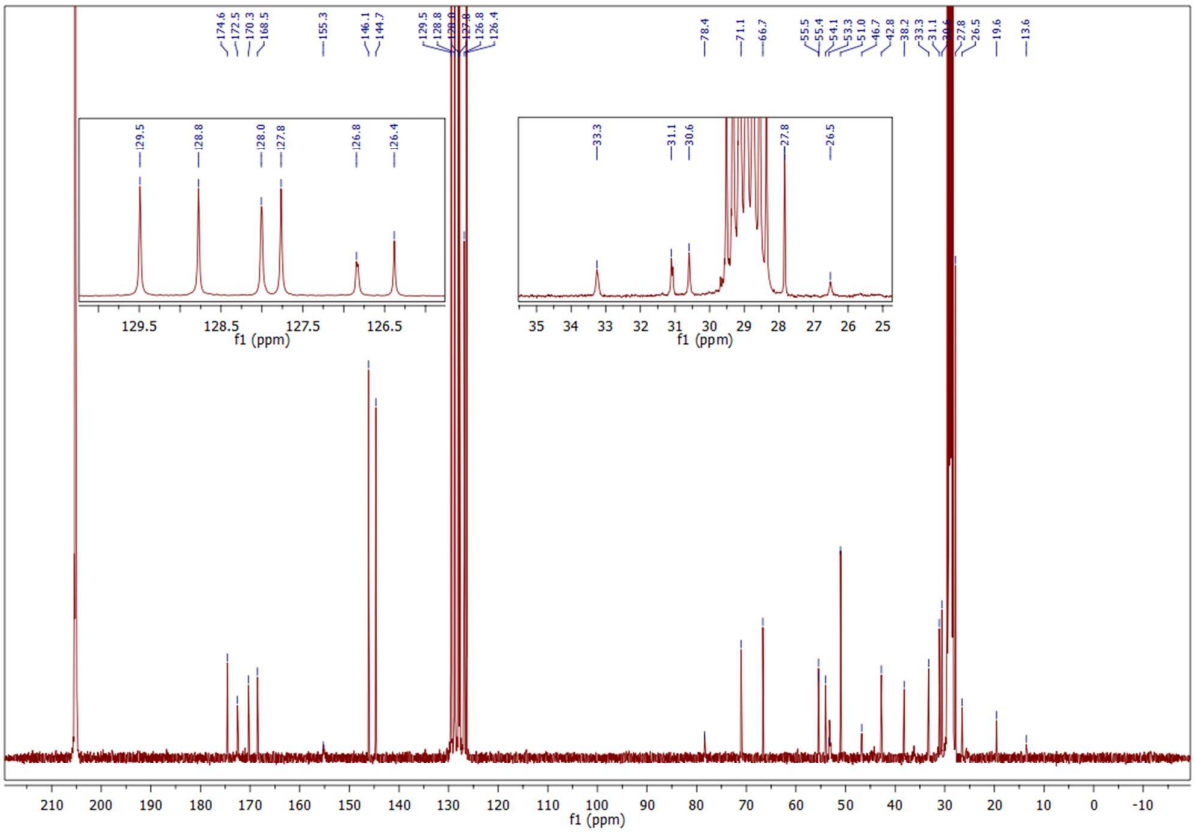


^{1}H NMR spectrum (400 MHz) NMR spectra ($(CD_3)_2CO$) for compound 7

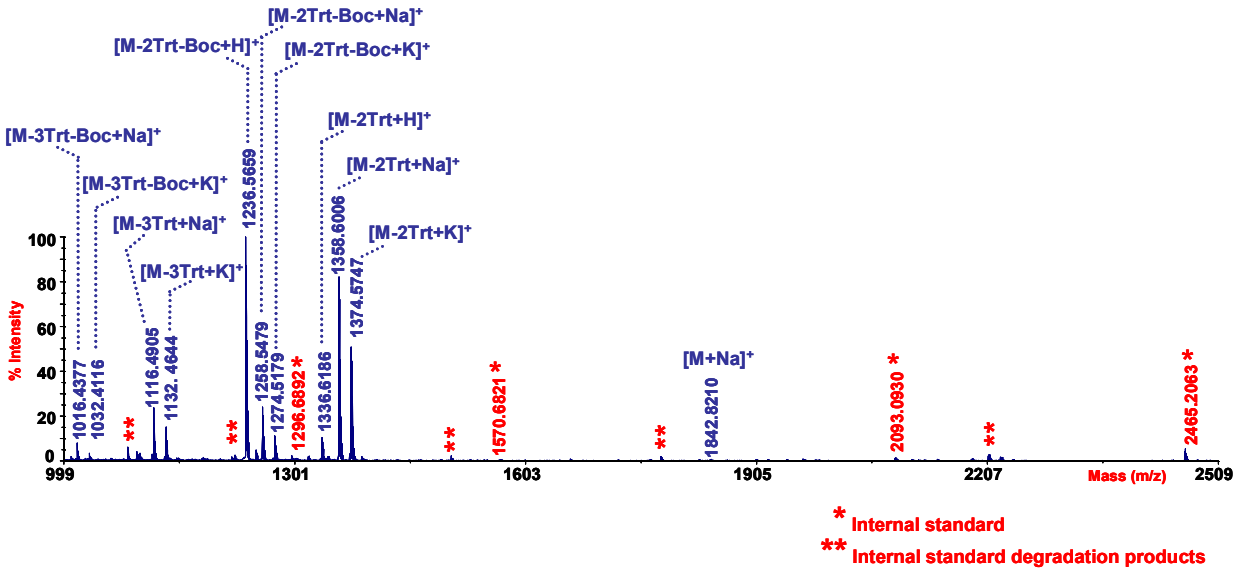




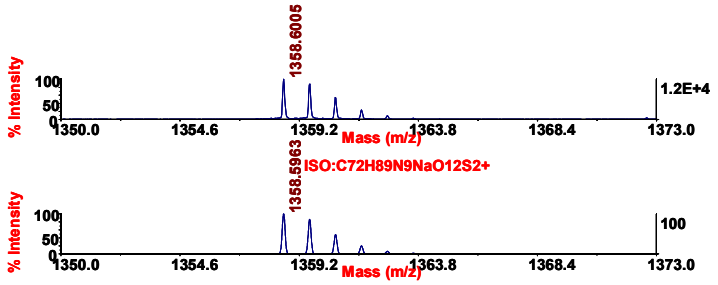
^{13}C NMR spectrum (100 MHz) spectra ($(CD_3)_2CO$) for compound 7

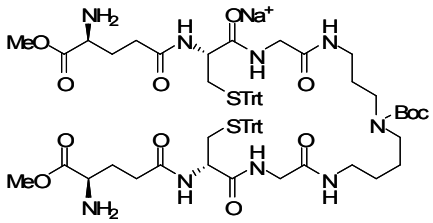


MALDI MS and MS/MS spectra for compound 7

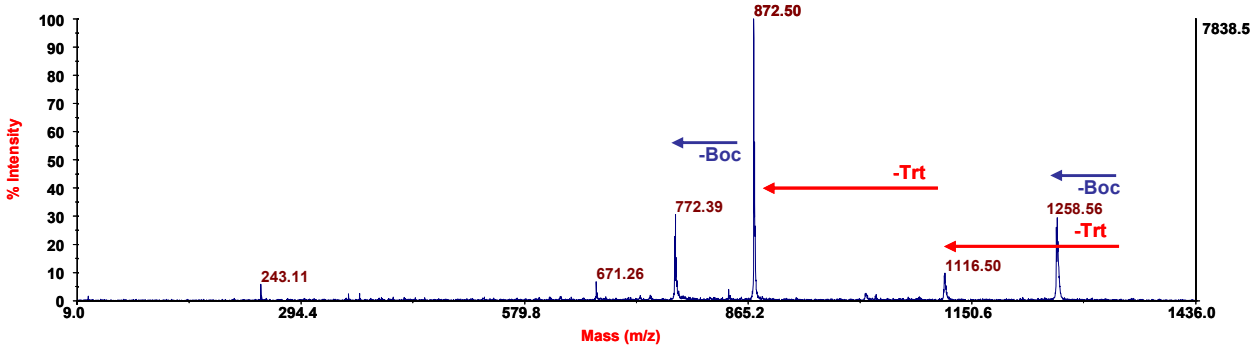


SAMPLE 7					
Exact Mass	**Exp Mass**	**Error (ppm)**	**DBE**		**Chemical Formula**
1842.8155	1842.8210	3.0	56.5	$[M+Na]^+$ **<3%**	$C_{110}H_{117}N_9O_{12}S_2Na^+$
1374.5704	1374.5747	3.1	32.5	$[M-2Trt+K]^+$	$C_{72}H_{89}N_9O_{12}S_2K^+$
1358.5964	1358.6005	3.1	32.5	$[M-2Trt+Na]^+$	$C_{72}H_{89}N_9O_{12}S_2Na^+$
1336.6145	1336.6186	3.1	32.5	$[M-2Trt+H]^+$	$C_{72}H_{90}N_9O_{12}S_2^+$
1274.5179	1274.5217	3.0	31.5	$[M-2Trt-Boc+K]^+$	$C_{67}H_{81}N_9O_{10}S_2K^+$
1258.5440	1258.5479	3.1	31.5	$[M-2Trt-Boc+Na]^+$	$C_{67}H_{81}N_9O_{10}S_2Na^+$
1236.5621	1236.5659	3.1	31.5	$[M-2Trt-Boc+H]^+$	$C_{67}H_{82}N_9O_{10}S_2^+$
1132.4608	1132.4644	3.2	20.5	$[M-3Trt+K]^+$	$C_{53}H_{75}N_9O_{12}S_2K^+$
1116.4869	1116.4905	3.2	20.5	$[M-3Trt+Na]^+$	$C_{53}H_{75}N_9O_{12}S_2Na^+$
1032.4084	1032.4116	3.1	19.5	$[M-3Trt-Boc+K]^+$	$C_{48}H_{67}N_9O_{10}S_2K^+$
1016.4345	1016.4377	3.1	19.5	$[M-3Trt-Boc+Na]^+$	$C_{48}H_{67}N_9O_{10}S_2Na^+$

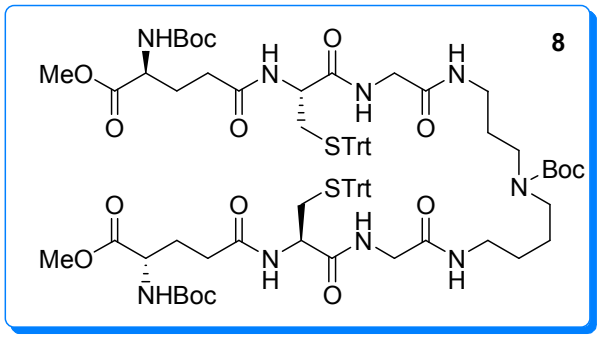


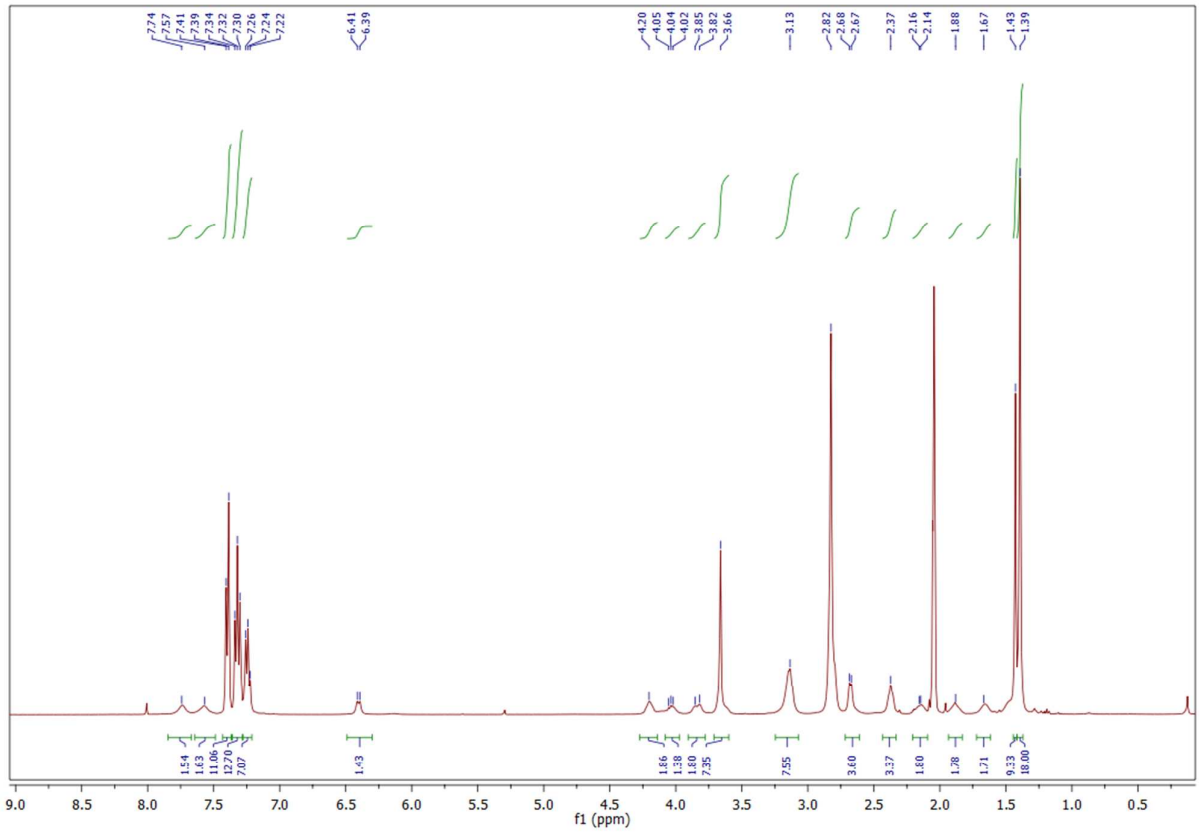


MS/MS m/z 1358.60

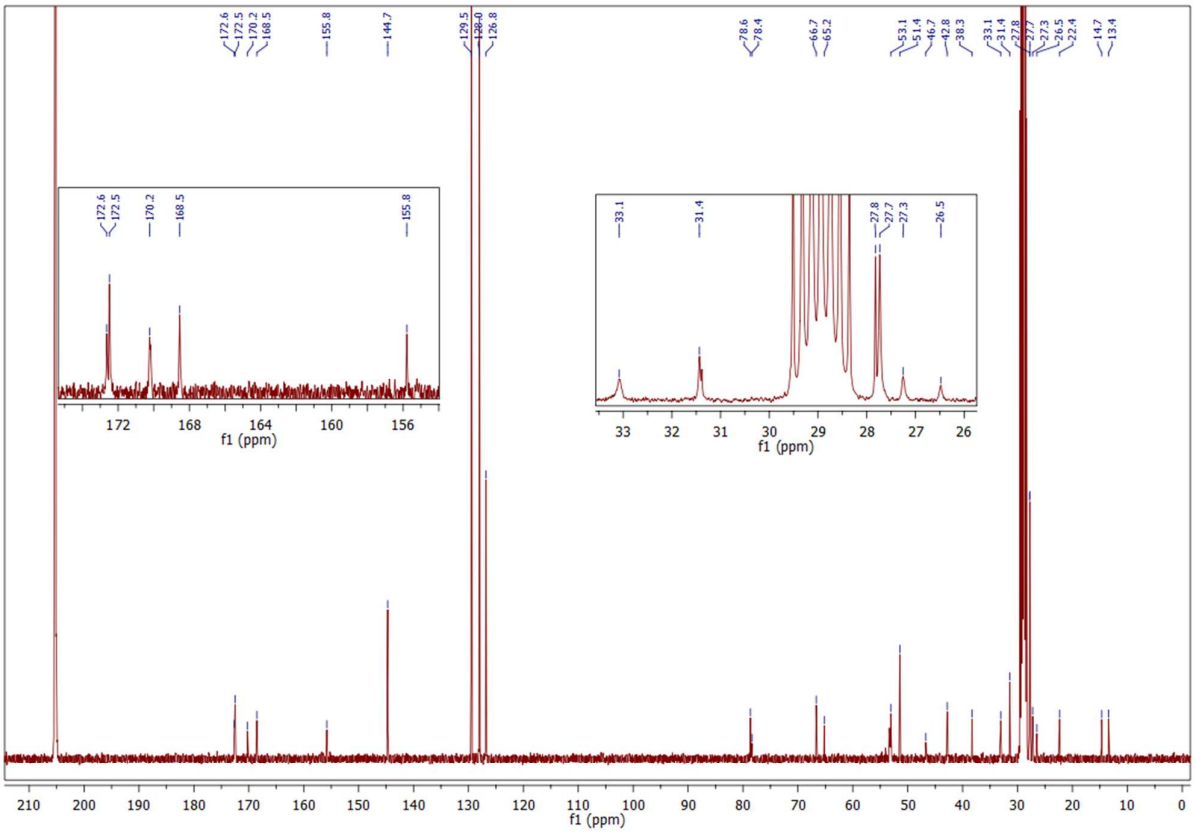


^{1}H NMR (400 MHz) spectra ($(CD_3)_2CO$) for compound 8

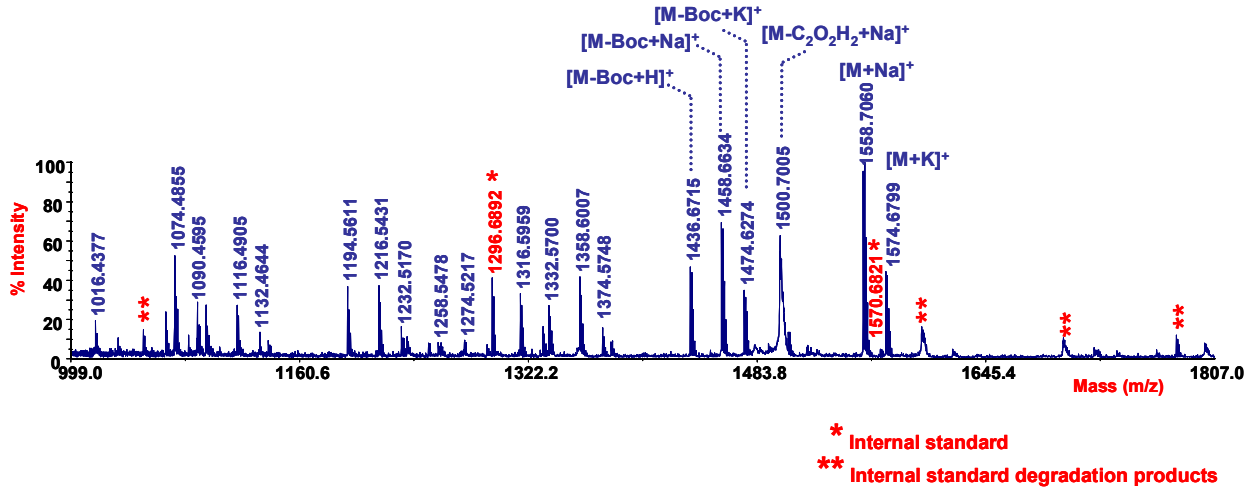




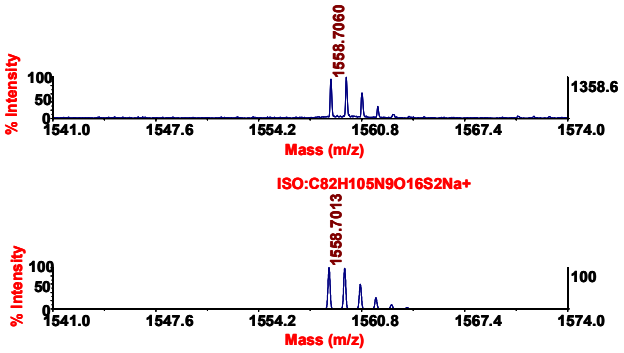
^{13}C NMR (100 MHz) spectra $(CD_3)_2CO$) for compound 8

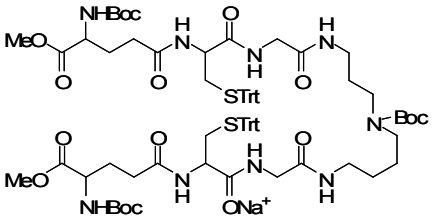


MALDI MS and MS/MS spectra for compound 8

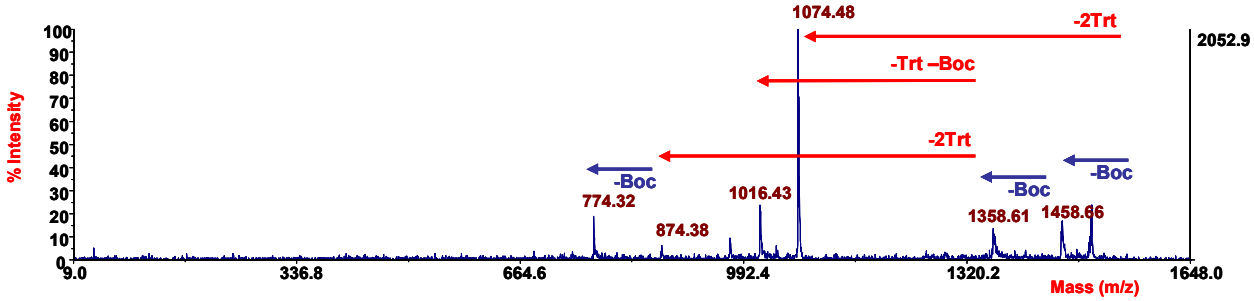


SAMPLE 8					
Exact Mass	**Exp Mass**	**Error (ppm)**	**DBE**		**Chemical Formula**
1574.6752	1574.6799	3.0	34.5	$[M+K]^+$	$C_{82}H_{105}N_9O_{16}S_2K^+$
1558.7013	1558.7060	3.0	34.5	$[M+Na]^+$	$C_{82}H_{105}N_9O_{16}S_2Na^+$
1500.6958	1500.7005	3.1	33.5	$[M-C_2O_2H_2+Na]^+$	$C_{80}H_{103}N_9O_{14}S_2Na^+$
1474.6228	1474.6274	3.1	33.5	$[M-Boc+K]^+$	$C_{77}H_{97}N_9O_{14}S_2K^+$
1458.6589	1458.6634	3.1	33.5	$[M-Boc+Na]^+$	$C_{77}H_{97}N_9O_{14}S_2Na^+$
1436.6669	1436.6715	3.2	33.5	$[M-Boc+H]^+$	$C_{77}H_{98}N_9O_{14}S_2^+$
1374.5704	1374.5748	3.2	32.5	$[M-2Boc+K]^+$	$C_{72}H_{89}N_9O_{12}S_2K^+$
1358.5964	1358.6007	3.2	32.5	$[M-2Boc+Na]^+$	$C_{72}H_{89}N_9O_{12}S_2Na^+$
1332.5657	1332.5700	3.2	22.5	$[M-Trt+K]^+$	$C_{63}H_{91}N_9O_{16}S_2K^+$
1316.5917	1316.5959	3.2	22.5	$[M-Trt+Na]^+$	$C_{63}H_{91}N_9O_{16}S_2Na^+$
1274.5179	1274.5217	3.0	31.5	$[M-3Boc+K]^+$	$C_{67}H_{81}N_9O_{10}S_2K^+$
1258.5440	1258.5478	3.0	31.5	$[M-3Boc+Na]^+$	$C_{67}H_{81}N_9O_{10}S_2Na^+$
1232.5132	1232.5170	3.1	21.5	$[M-Boc-Trt+K]^+$	$C_{58}H_{83}N_9O_{14}S_2K^+$
1216.5393	1216.5431	3.1	21.5	$[M-Boc-Trt+Na]^+$	$C_{58}H_{83}N_9O_{14}S_2Na^+$
1194.5574	1194.5611	3.1	21.5	$[M-Boc-Trt+H]^+$	$C_{58}H_{84}N_9O_{14}S_2^+$
1132.4608	1132.4644	3.2	20.5	$[M-2Boc-Trt+K]^+$	$C_{53}H_{75}N_9O_{12}S_2K^+$
1116.4869	1116.4905	3.2	20.5	$[M-2Boc-Trt+Na]^+$	$C_{53}H_{75}N_9O_{12}S_2Na^+$
1090.4561	1090.4595	3.1	10.5	$[M-2Trt+K]^+$	$C_{44}H_{77}N_9O_{16}S_2K^+$
1074.4822	1074.4895	3.1	10.5	$[M-2Trt+Na]^+$	$C_{44}H_{77}N_9O_{16}S_2Na^+$
1016.4345	1016.4377	3.1	19.5	$[M-3Boc-Trt+Na]^+$	$C_{48}H_{67}N_9O_{10}S_2Na+$

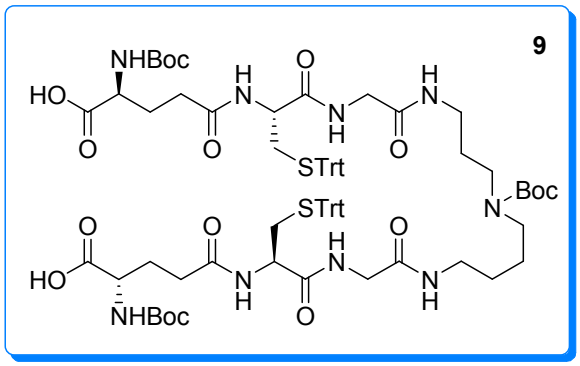


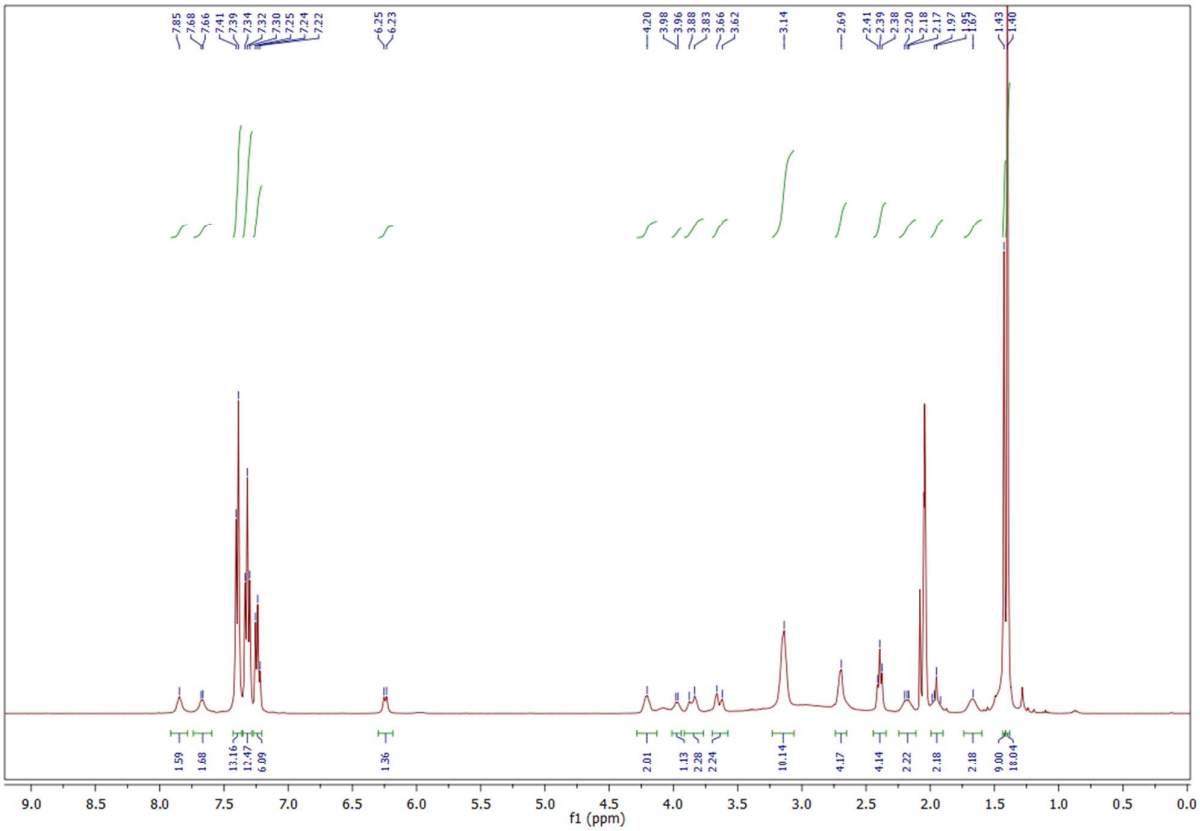


MS/MS m/z 1558.71

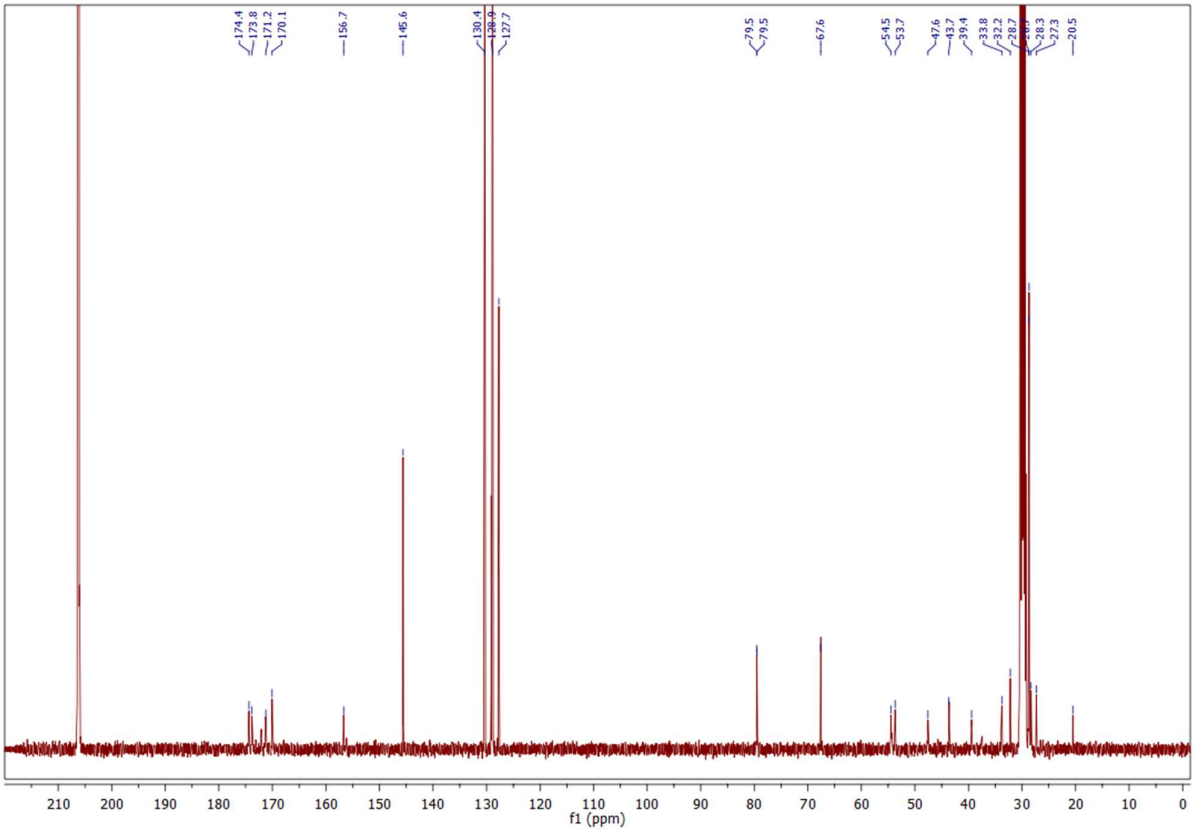


^{1}H NMR (400 MHz) spectra ($(CD_3)_2CO$) for compound 9

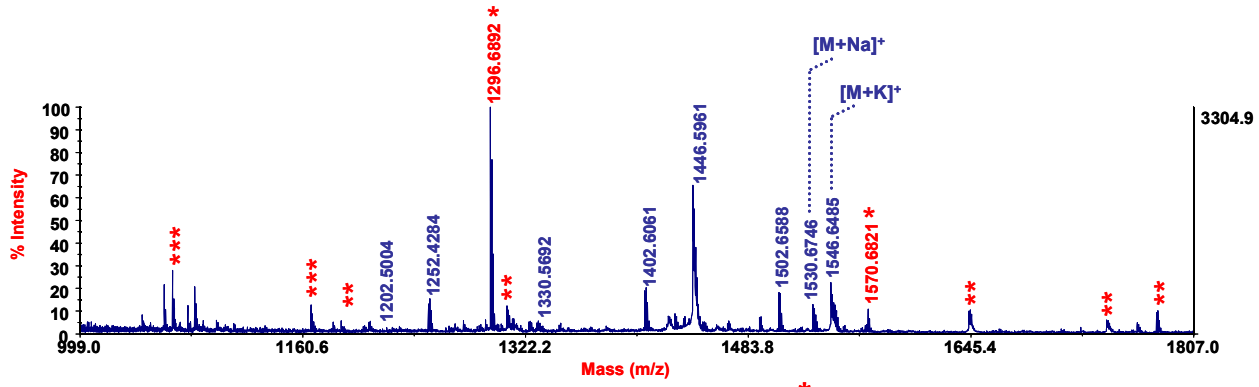




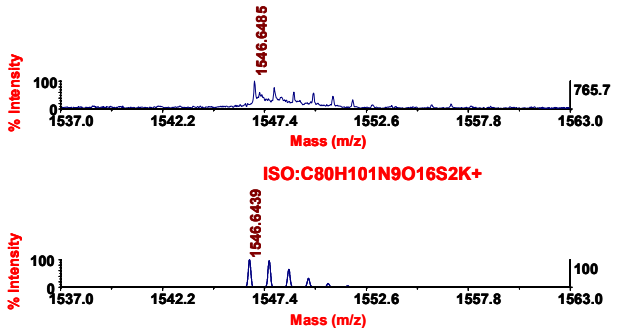
^{13}C NMR (100 MHz) spectra $(CD_3)_2CO$) for compound 9

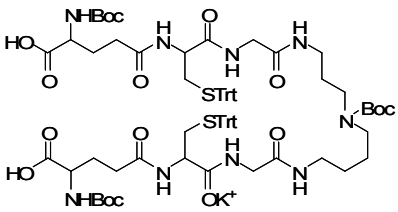


MALDI MS and MS/MS spectra for compound 9

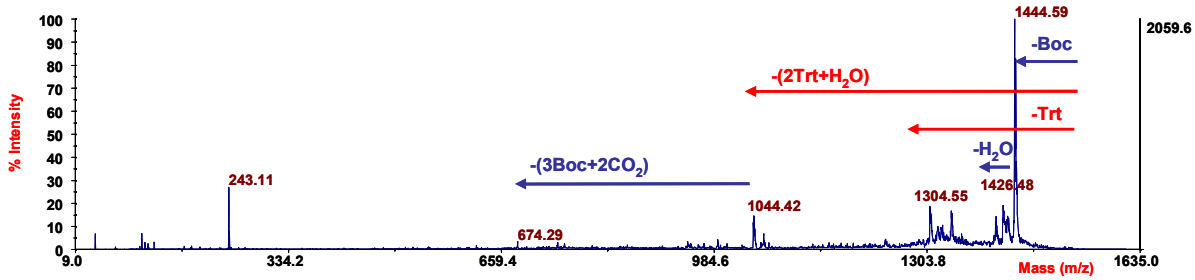


SAMPLE 9					
Exact Mass	**Exp Mass**	**Error (ppm)**	**DBE**		**Chemical Formula**
1546.6439	1546.6485	3.0	34.5	$[M+K]^+$	$C_{80}H_{101}N_9O_{16}S_2K^+$
1530.6700	1530.6746	3.0	34.5	$[M+Na]^+$	$C_{80}H_{101}N_9O_{16}S_2Na^+$
1502.6541	1502.6588	3.1	33.5	$[M-CO_2+K]^+$	$C_{79}H_{101}N_9O_{14}S_2K^+$
1446.5915	1446.5961	3.2	33.5	$[M-Boc+K]^+$	$C_{75}H_{93}N_9O_{14}S_2K^+$
1402.6017	1402.6062	3.2	32.5	$[M-Boc-CO_2+K]^+$	$C_{74}H_{93}N_9O_{12}S_2K^+$
1330.5651	1330.5692	3.1	32.5	$[M-2Boc+Na]^+$	$C_{70}H_{85}N_9O_{12}S_2Na^+$
1252.4946	1252.4984	3.0	31.5	$[M-3Boc+2Na]^+$	$C_{65}H_{76}N_9O_{10}S_2Na_2^+$
1202.4968	1202.5004	3.0	30.5	$[M-3Boc-CO_2+K]^+$	$C_{64}H_{77}N_9O_8S_2K^+$
1088.4556	1088.4590	3.1	20.5	$[M-2Boc-1Trt+Na]^+$	$C_{51}H_{71}N_9O_{12}S_2Na^+$

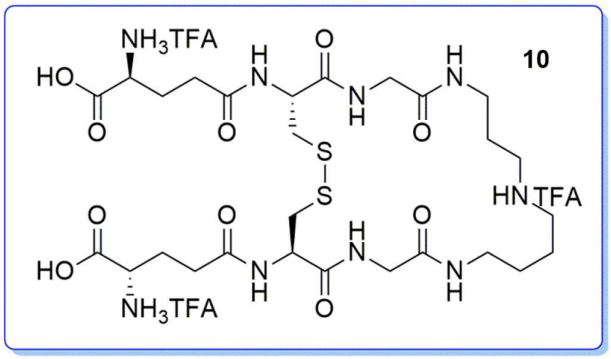


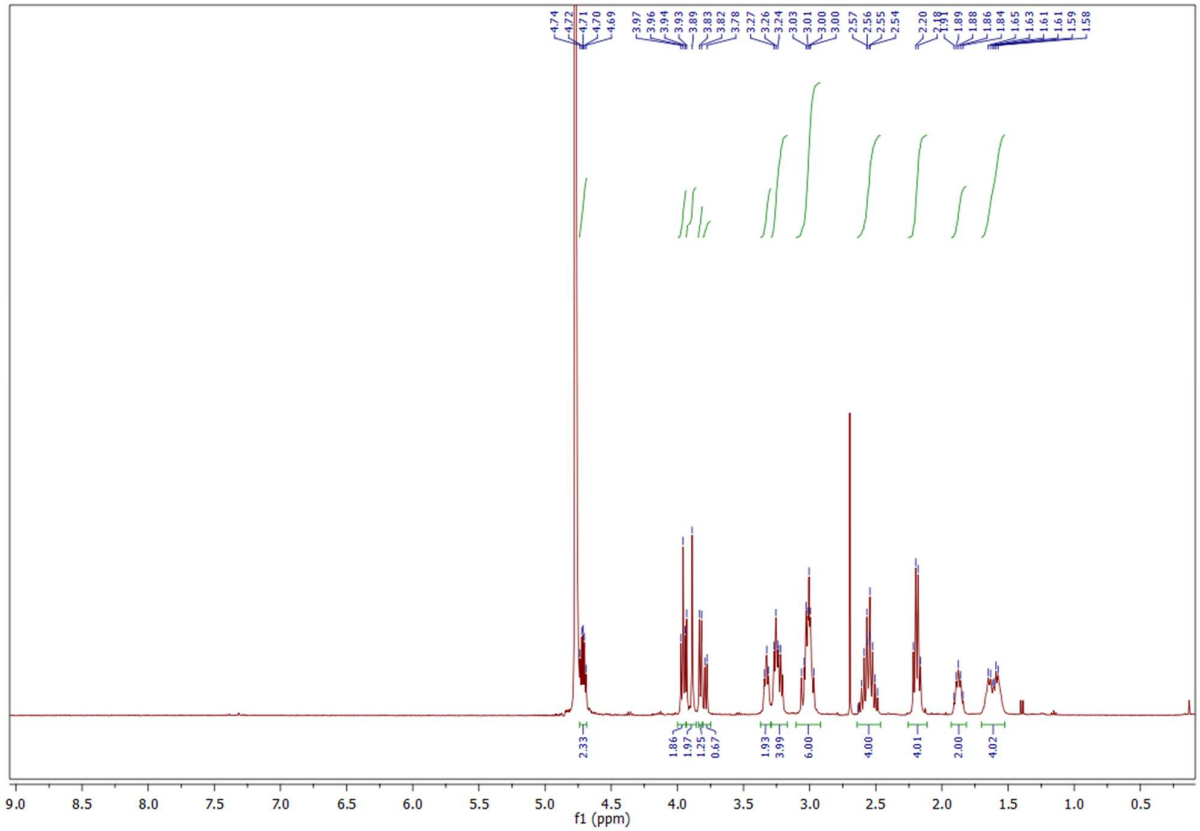


MS/MS m/z 1546.65

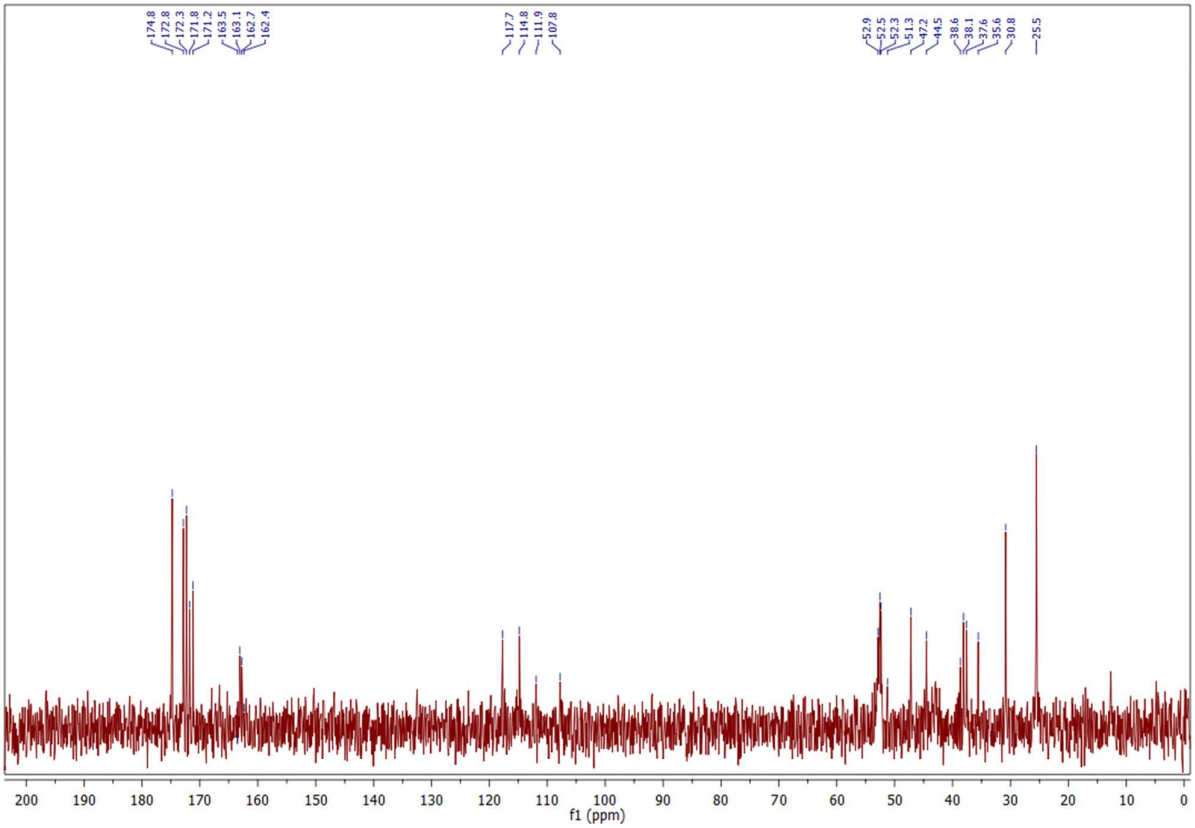


^{1}H NMR spectrum (400 MHz, D_2O) for compound 10

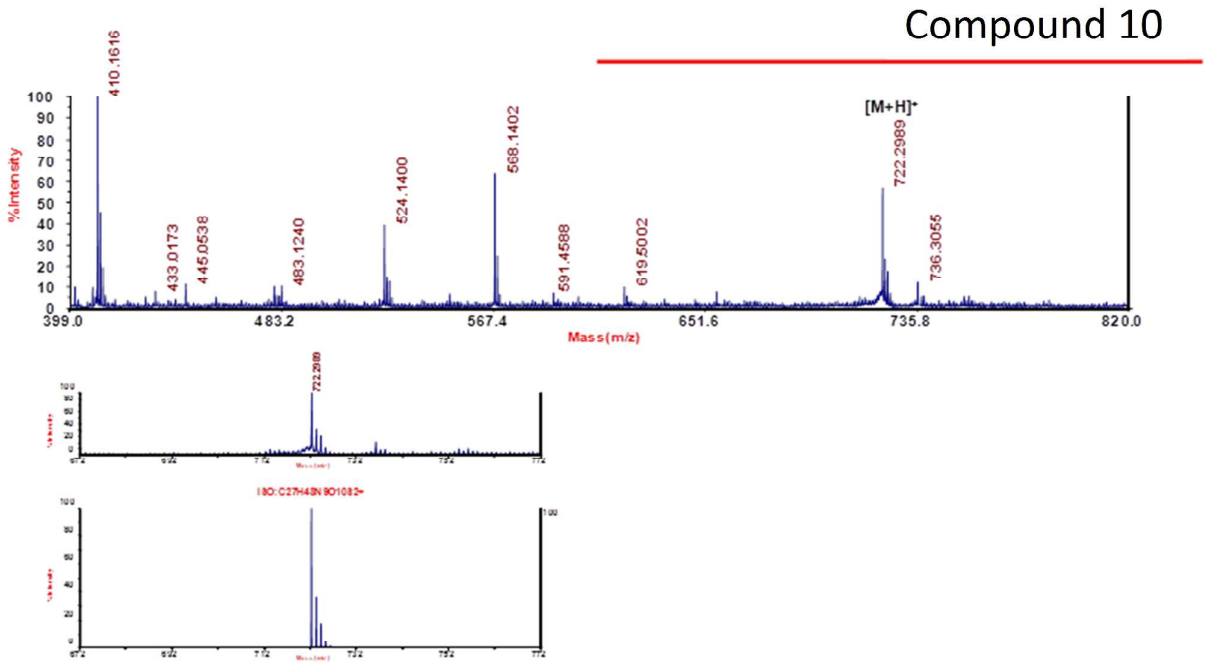




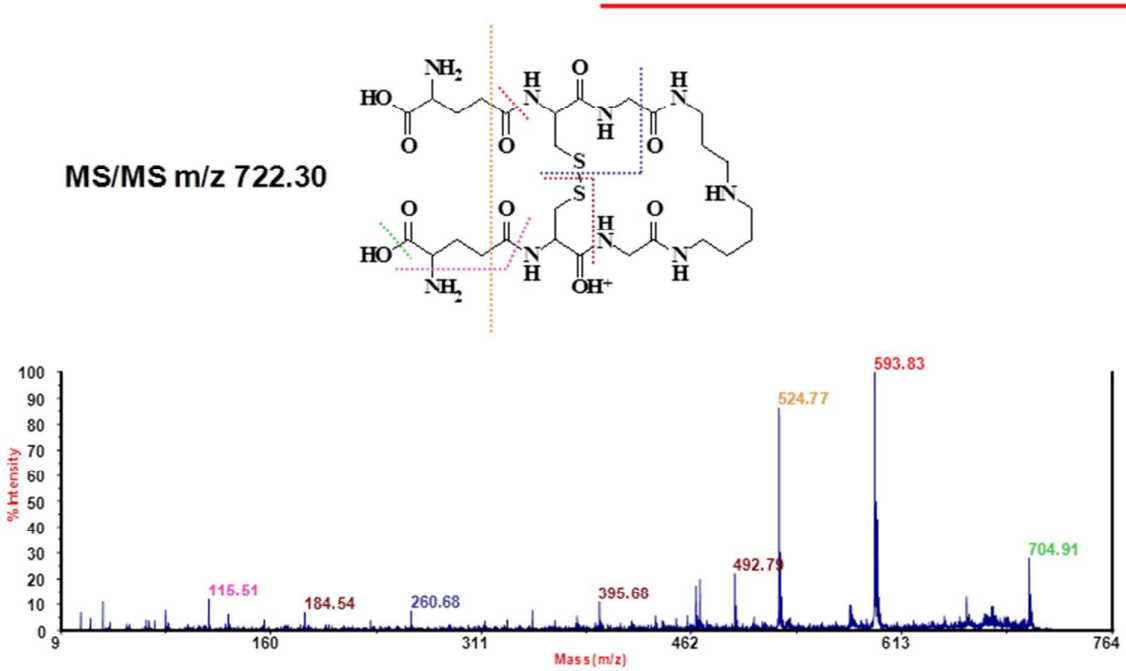
^{13}C NMR (100 MHz) spectra (D_2O) for compound 10

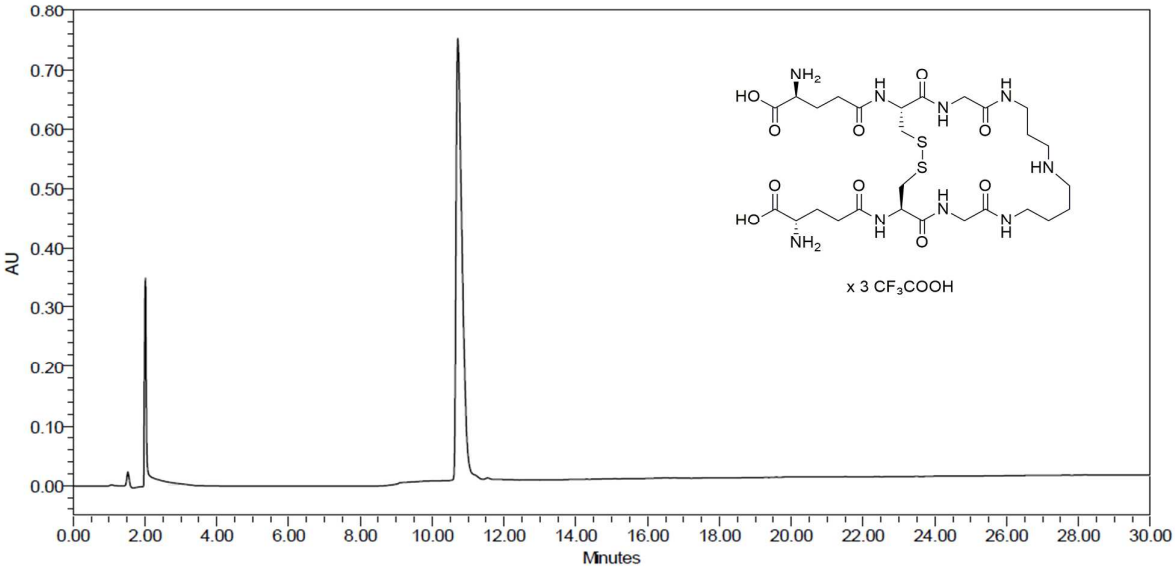


MALDI MS and MS/MS spectra for compound 10



Index	Input m/z	Calc. Mass	Error (mDa)	Error (ppm)	DBE	Formula
1	722.29890	722.29601	2.8906	4.0019	8.50	C27 H48 N9 O10 S2



Analytical HPLC profile for compound 10

Purified TS_2 HPLC chromatogram