

SUPPORTING INFORMATION

N-(3-aminoalkyl)proline derivatives with potent antiglycation activity

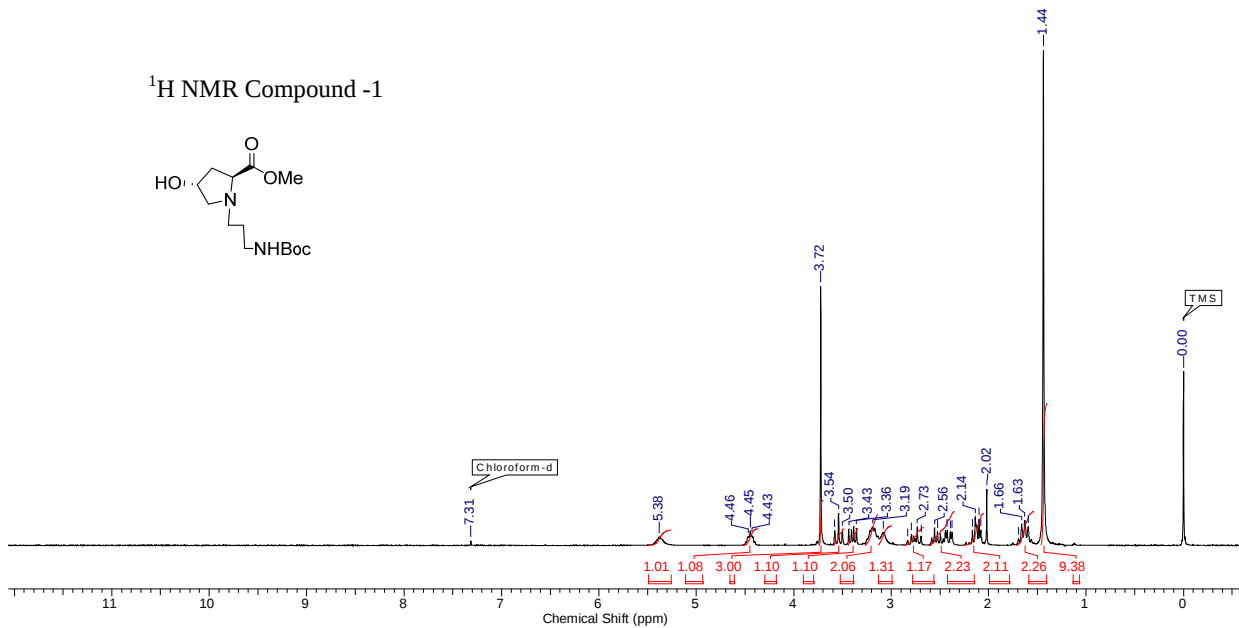
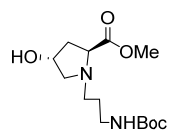
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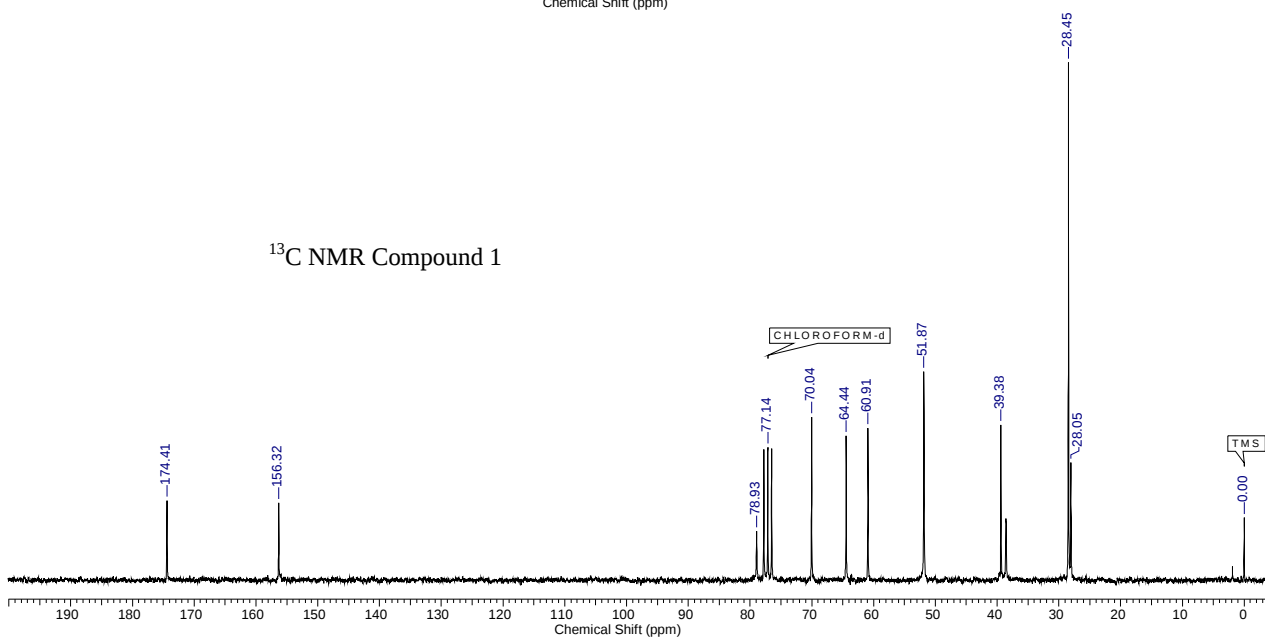
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¹H NMR Compound -1



¹³C NMR Compound 1



¹³C DEPT Compound 1

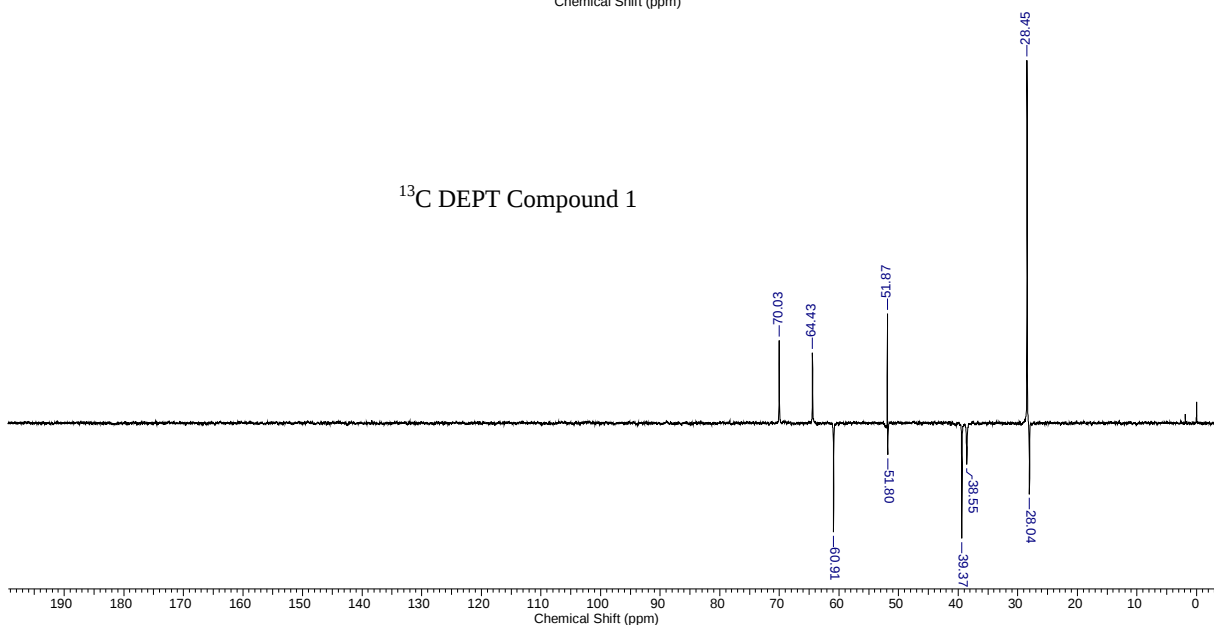


Fig. S1. ¹H NMR, ¹³C NMR, ¹³C DEPT NMR of compound 1.

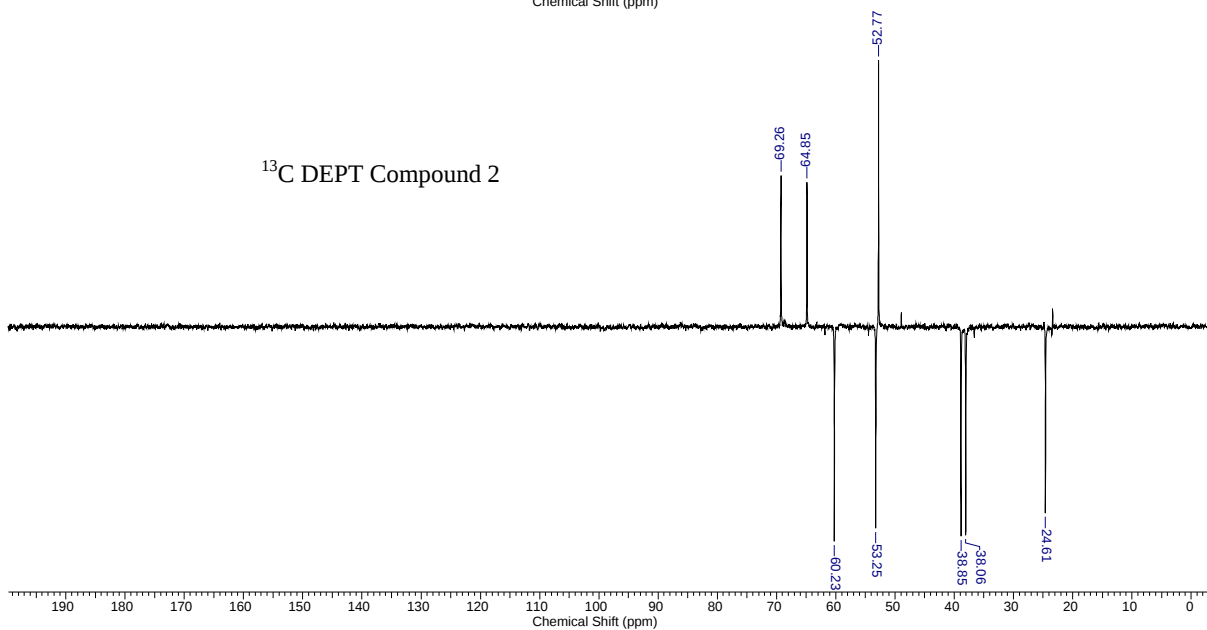
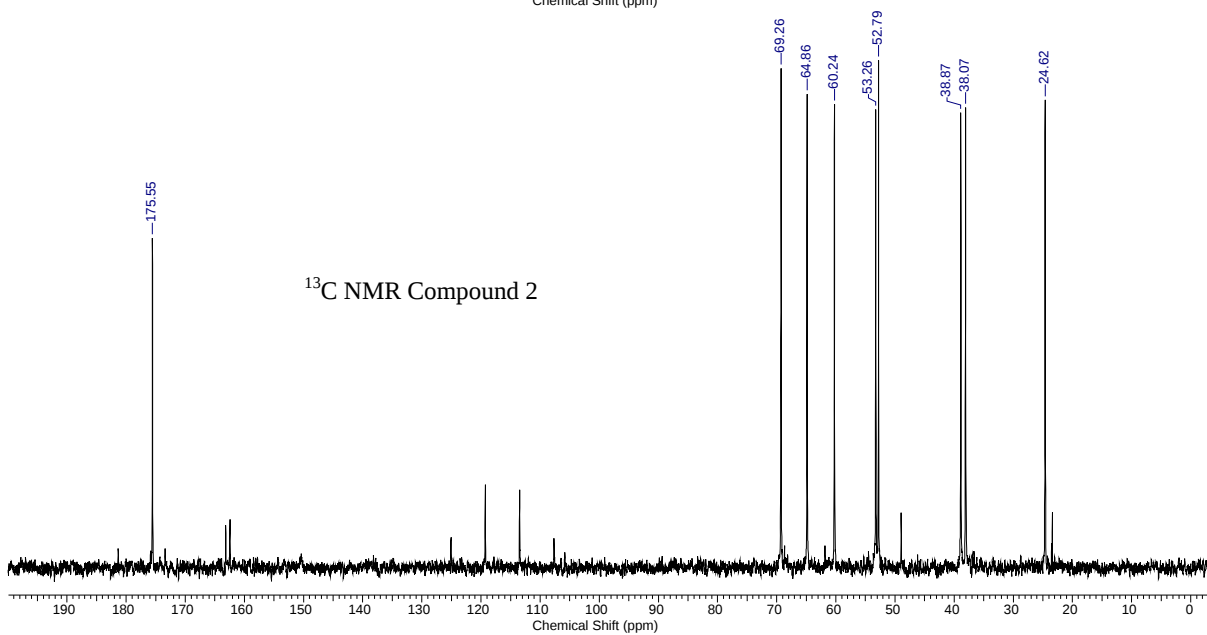
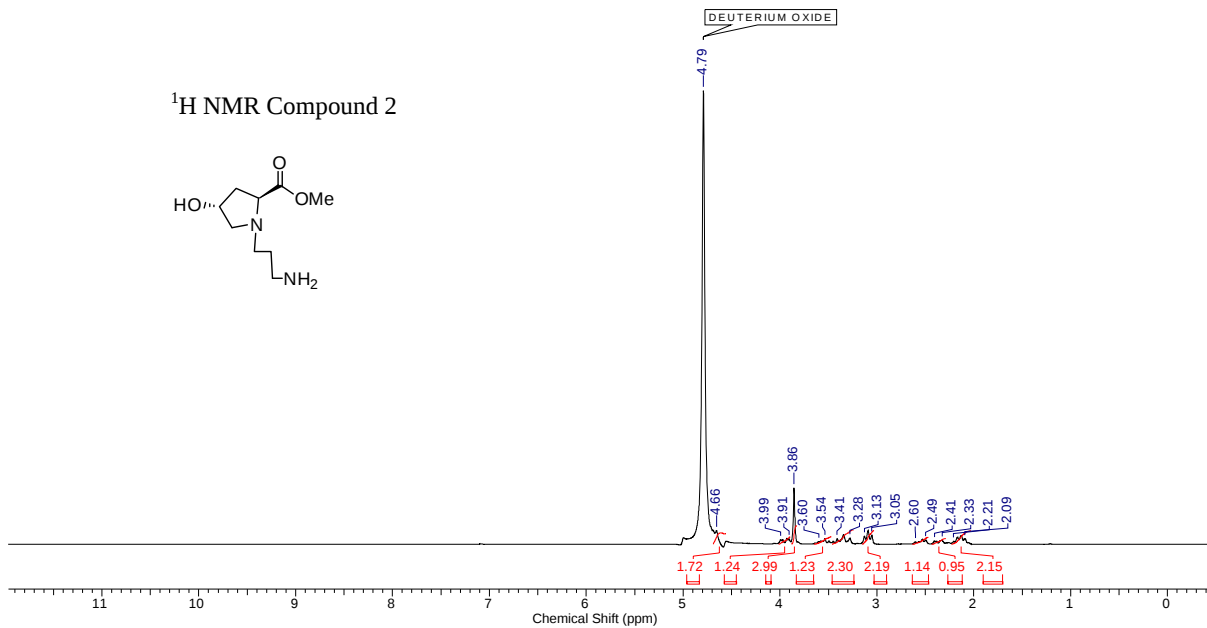


Fig. S2. ¹H NMR, ¹³C NMR, ¹³C DEPT NMR of compound 2.

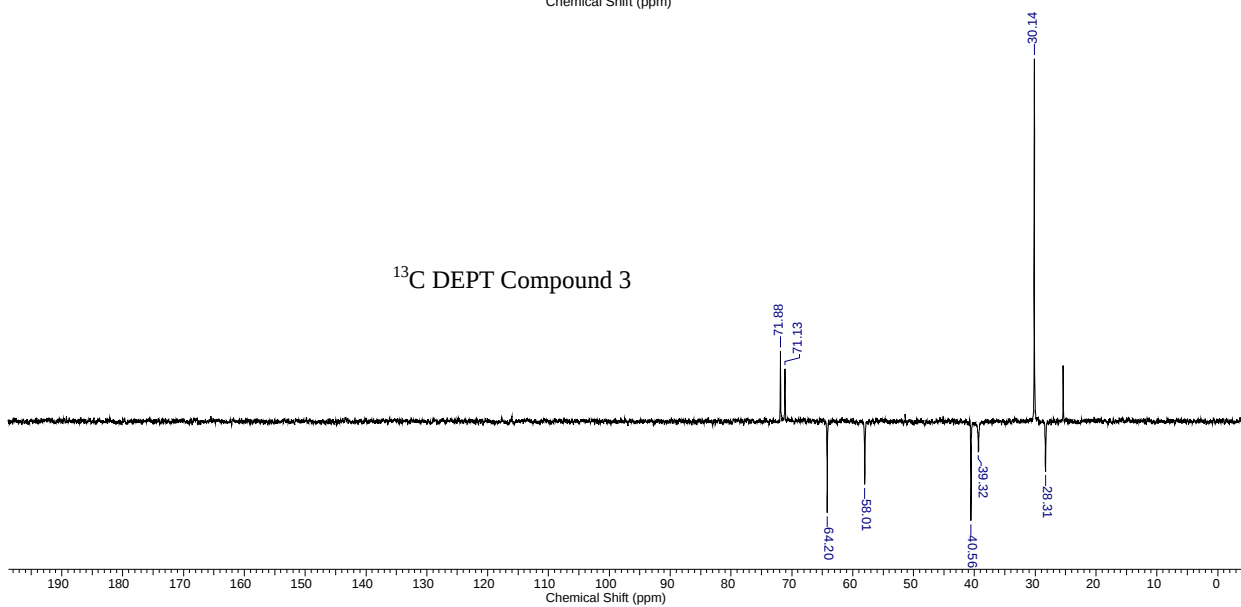
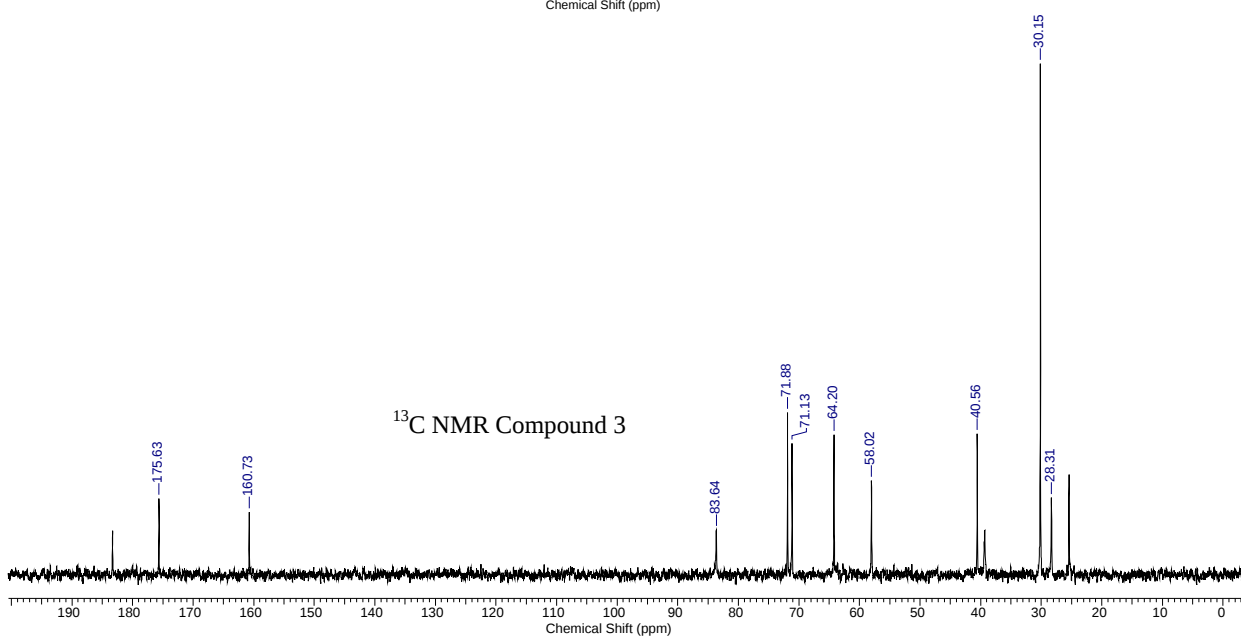
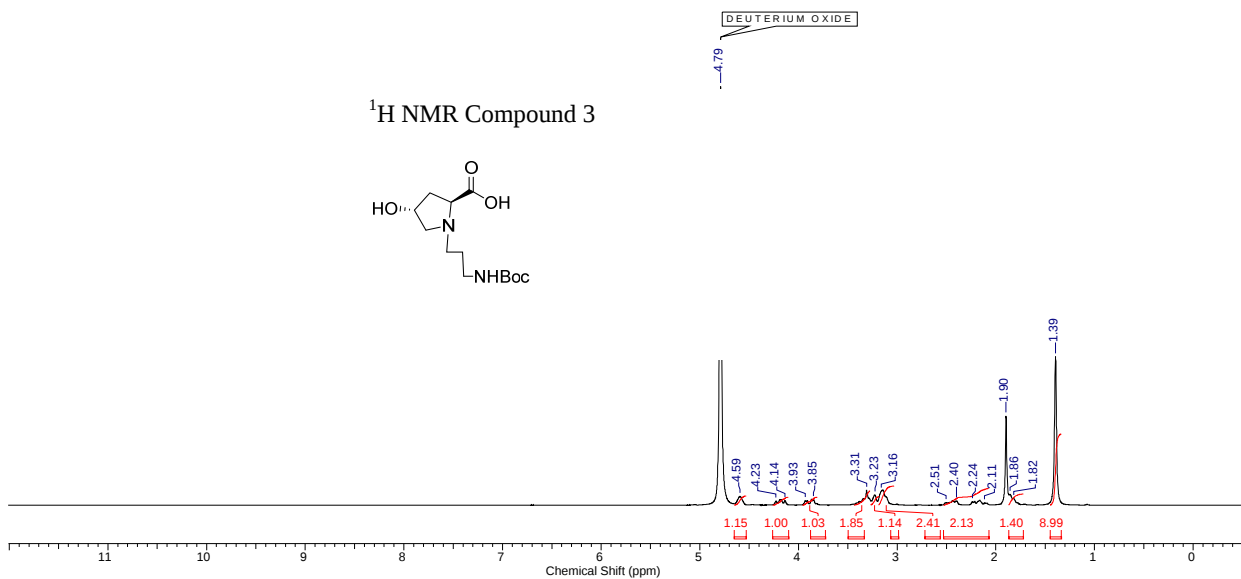


Fig. S3. ¹H NMR, ¹³C NMR, ¹³C DEPT NMR of compound 3.

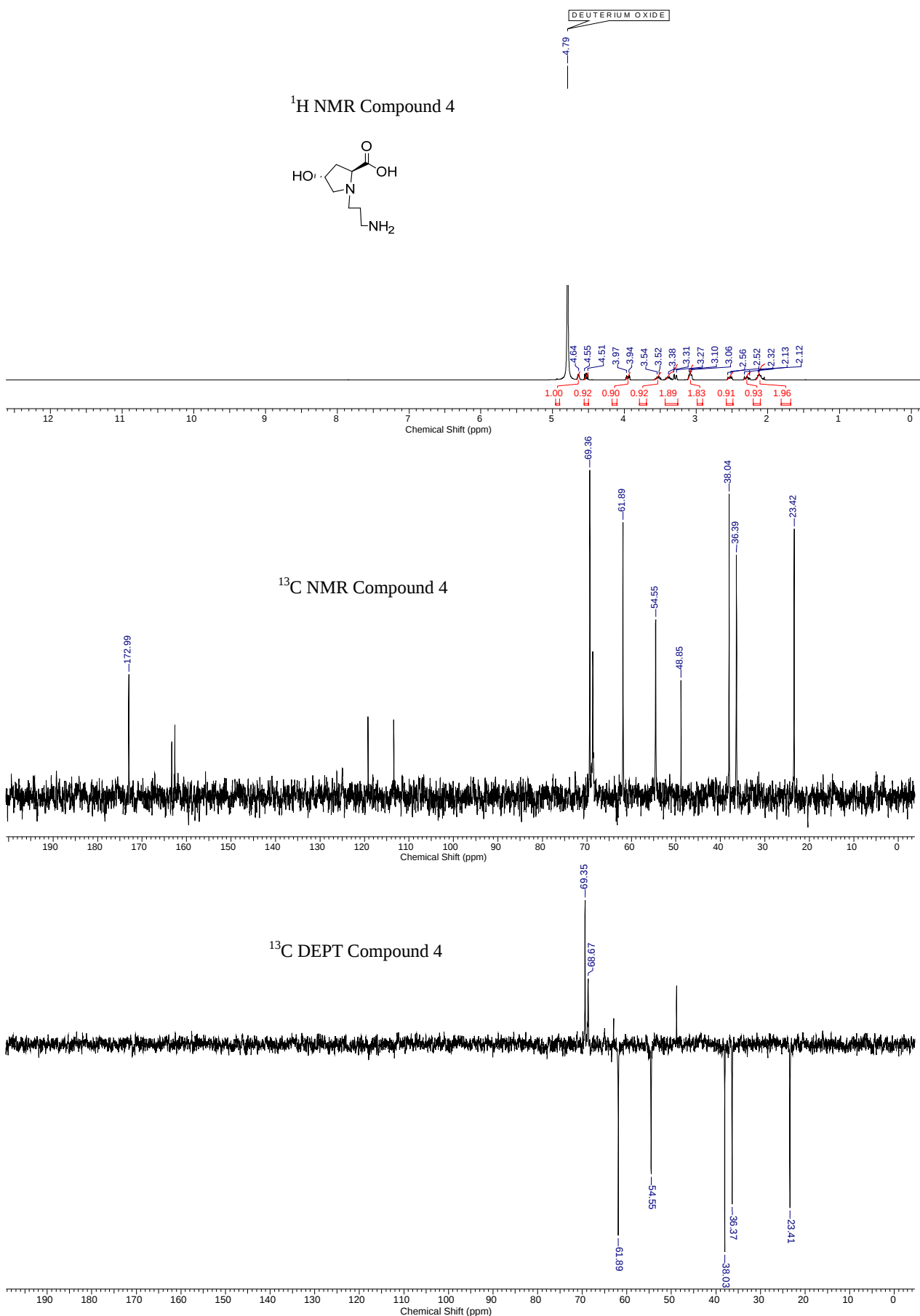
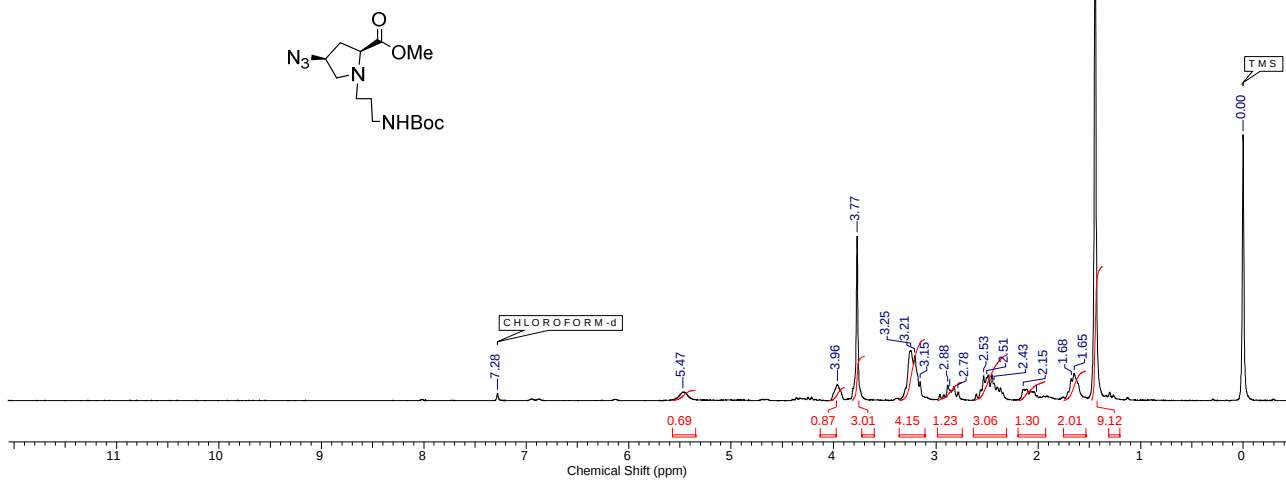
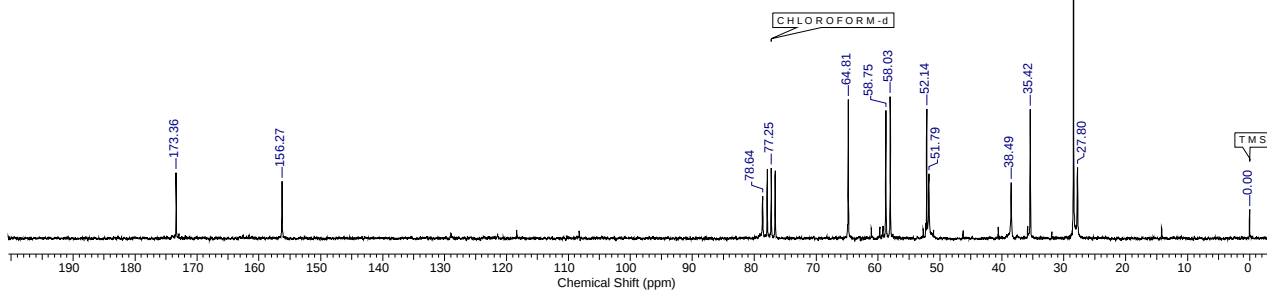


Fig. S4. ¹H NMR, ¹³C NMR, ¹³C DEPT NMR of compound 4.

¹H NMR Compound 5



¹³C NMR Compound 5



¹³C DEPT Compound 5

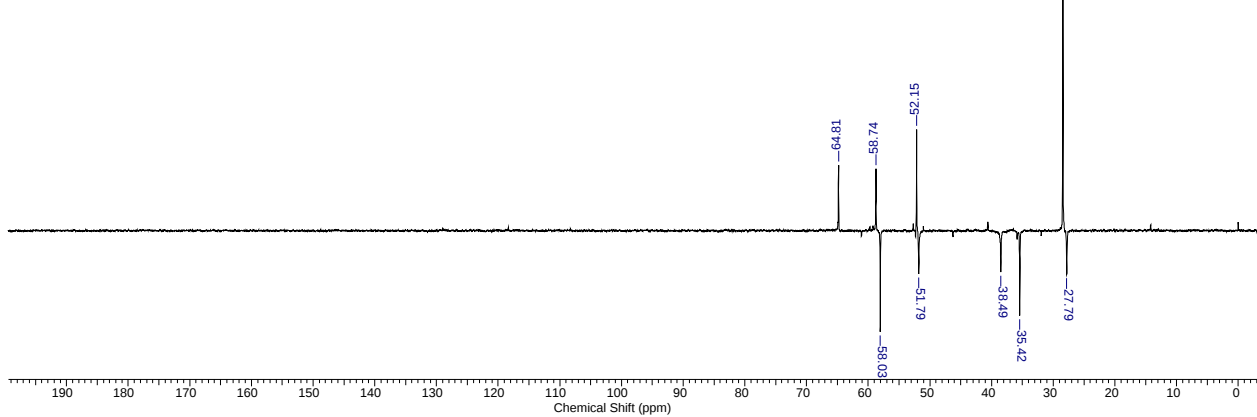


Fig. S5. ¹H NMR, ¹³C NMR, ¹³C DEPT NMR of compound 5.

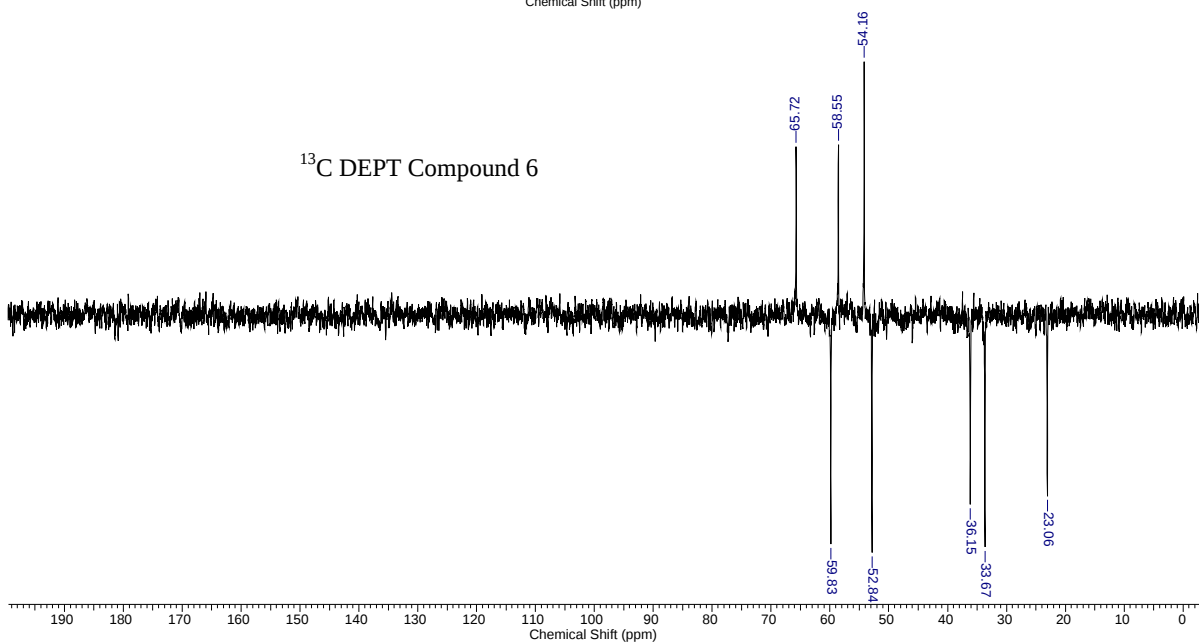
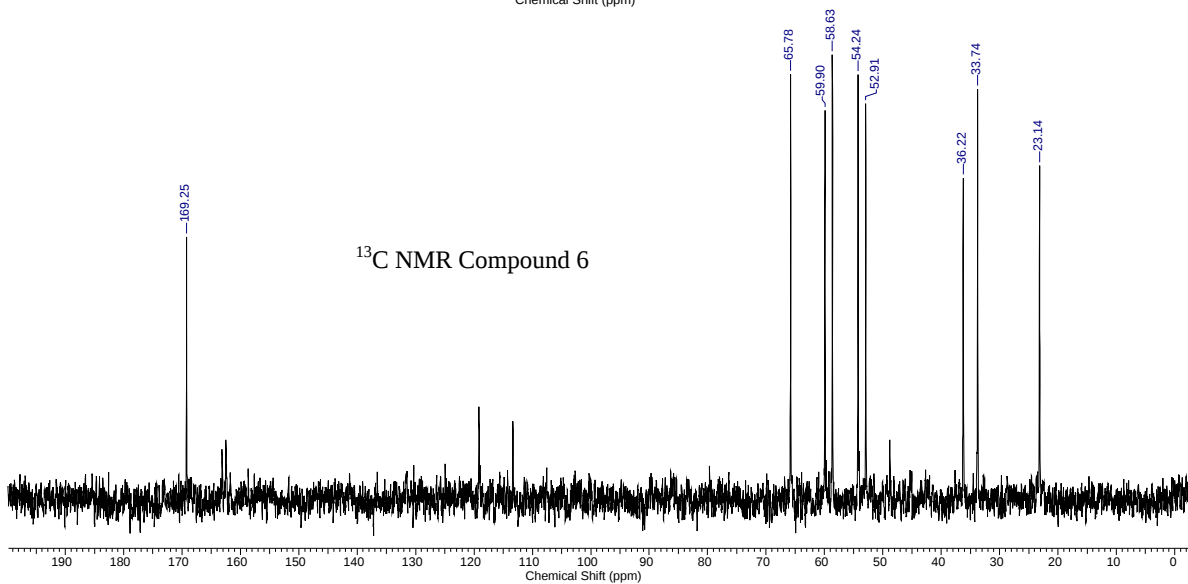
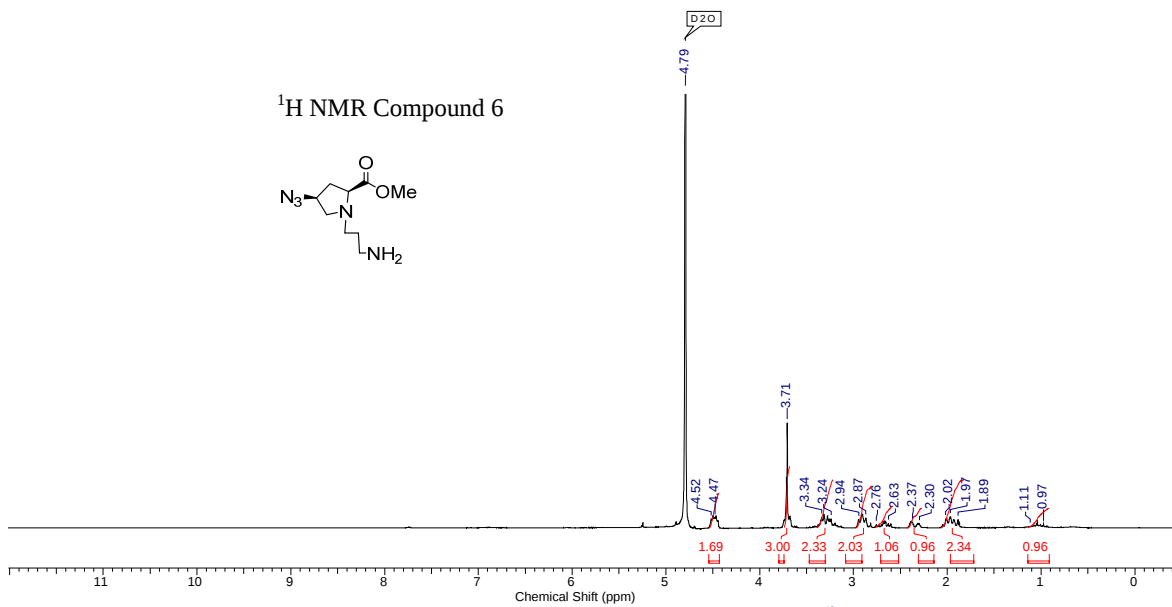


Fig. S6. ¹H NMR, ¹³C NMR, ¹³C DEPT NMR of compound 6.

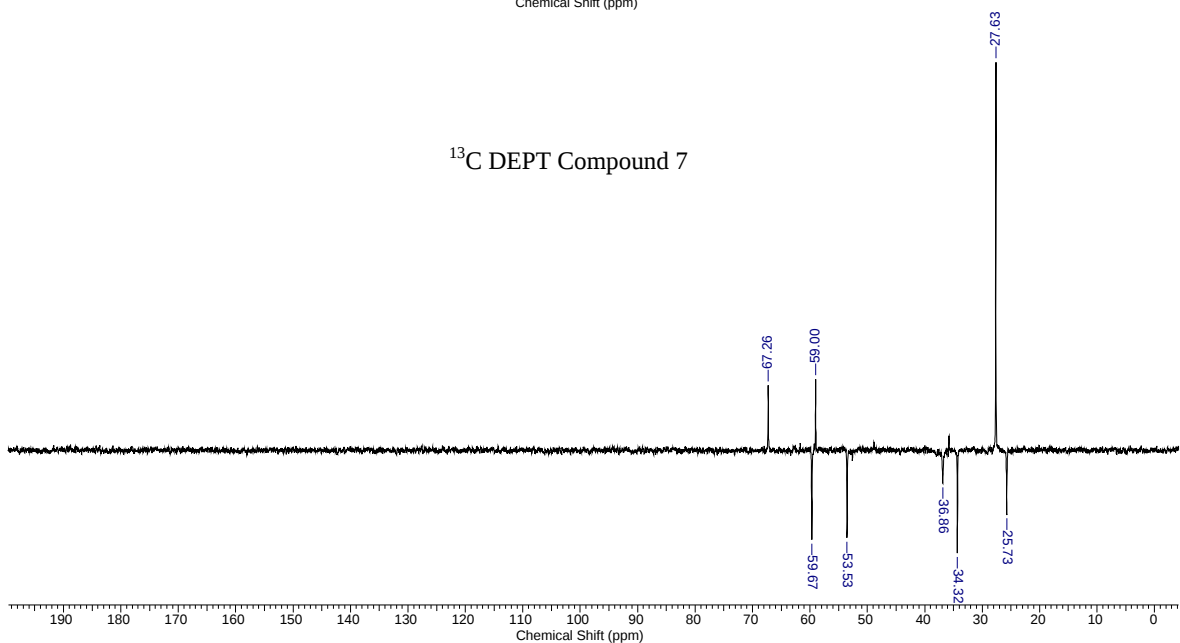
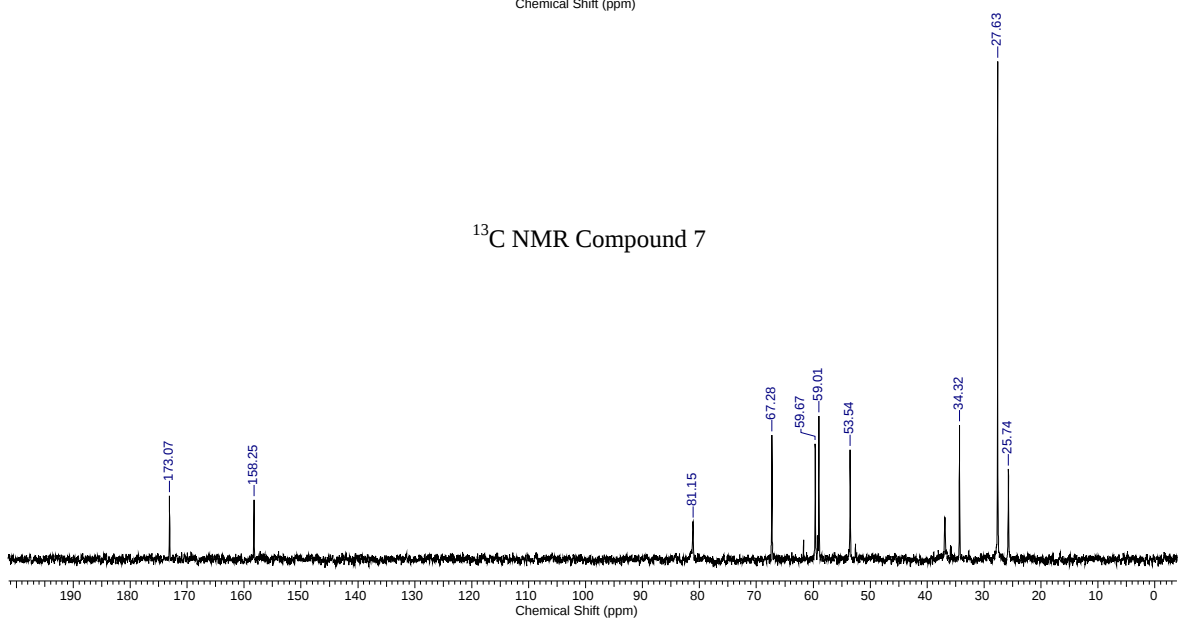
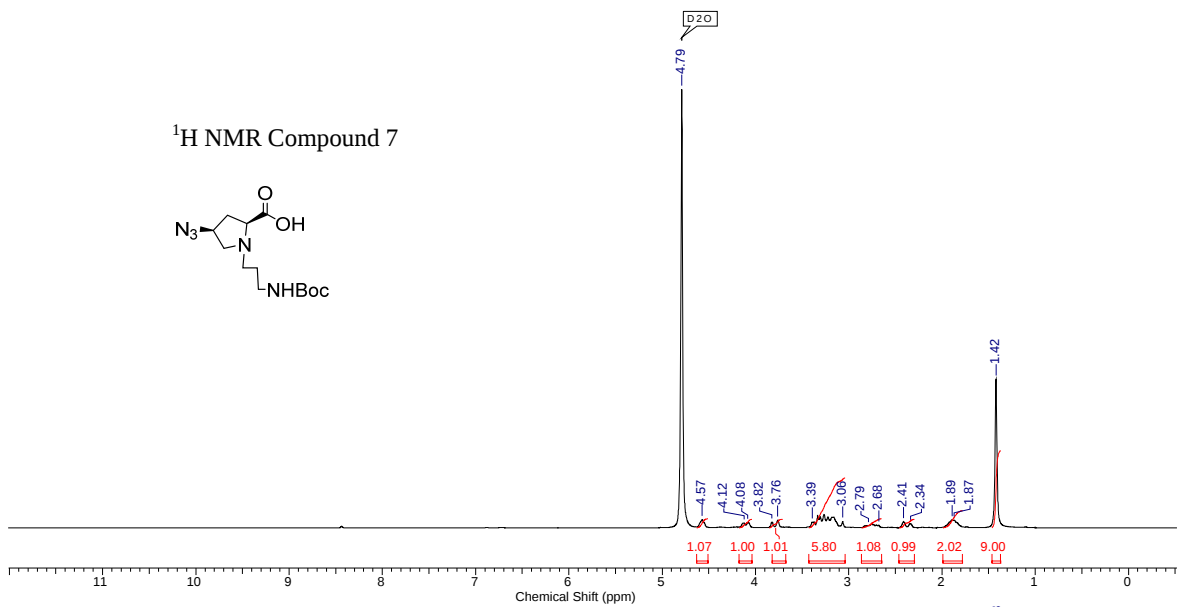


Fig. S7. ¹H NMR, ¹³C NMR, ¹³C DEPT NMR of compound 7.

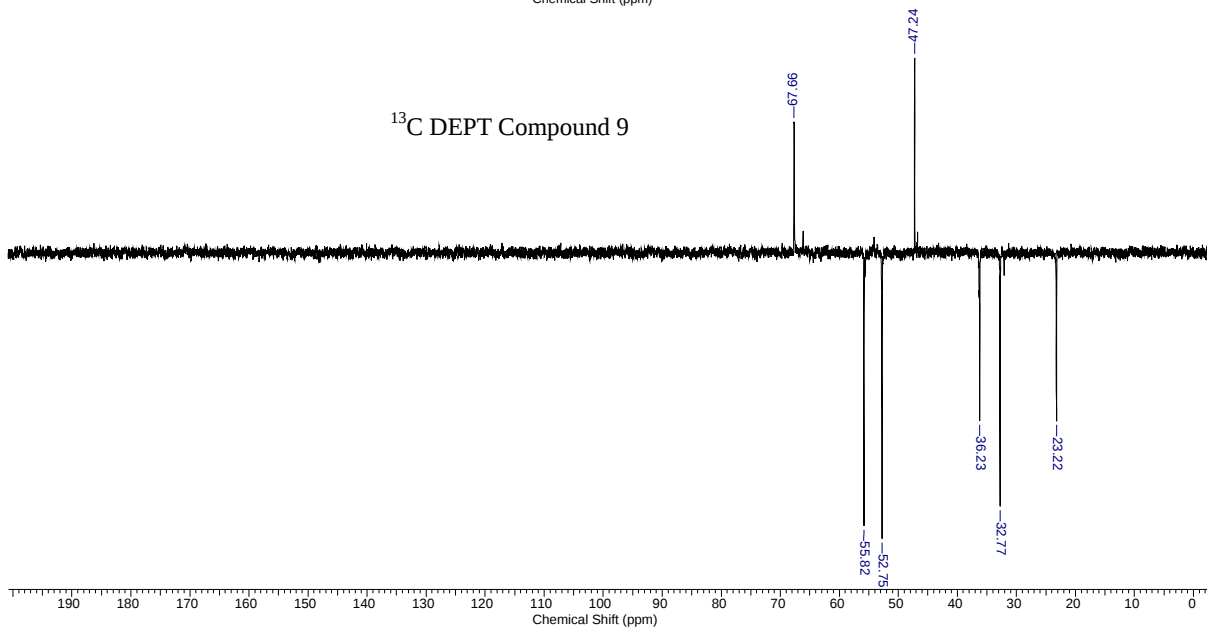
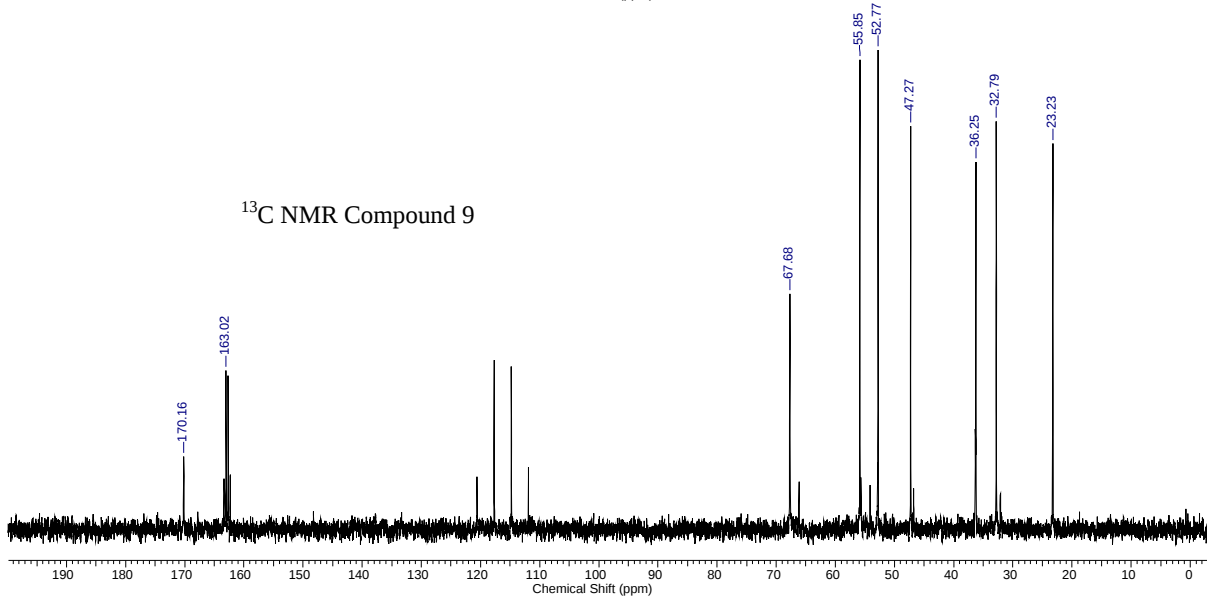
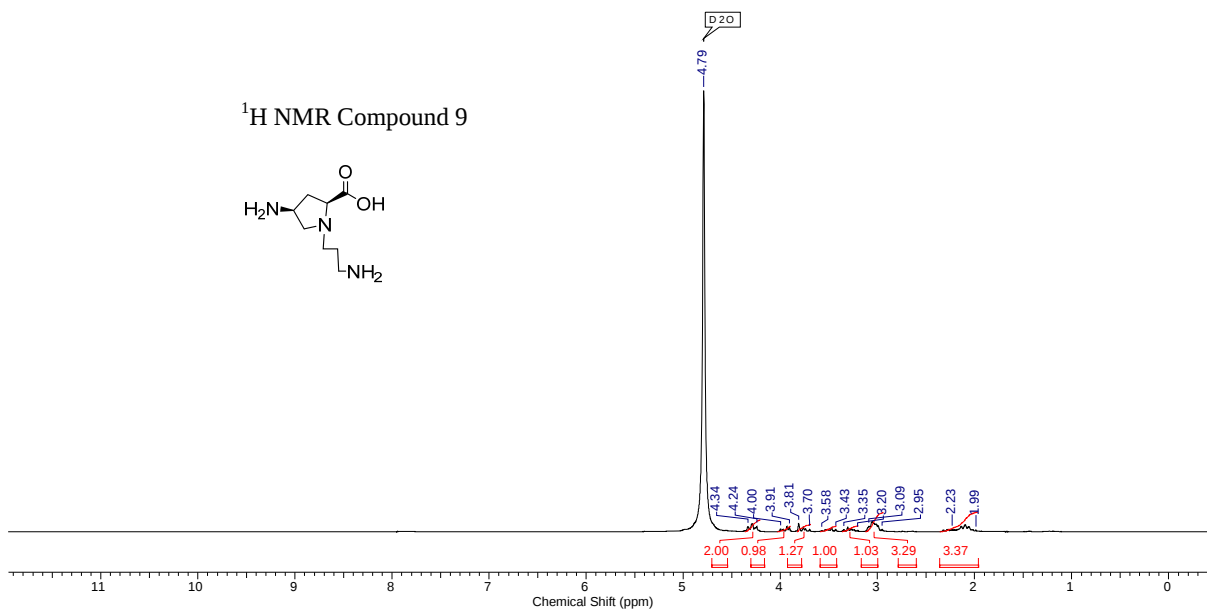
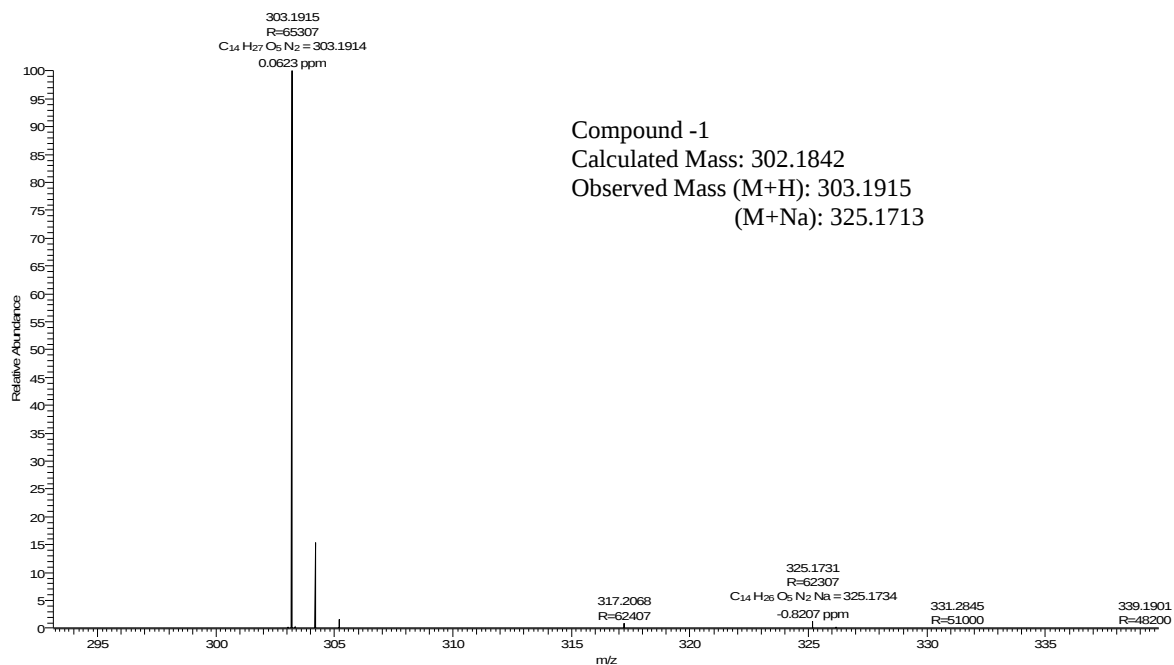


Fig. S9. ¹H NMR, ¹³C NMR, ¹³C DEPT NMR of compound 9

H-4 #78 RT: 0.35 AM: 1 NL: 3.90E9
T: FTMS + p ESI Full ms [86.00-1290.00]



G-H8 #496 RT: 2.21 AM: 1 NL: 6.16E9
T: FTMS + p ESI Full ms [100.00-1500.00]

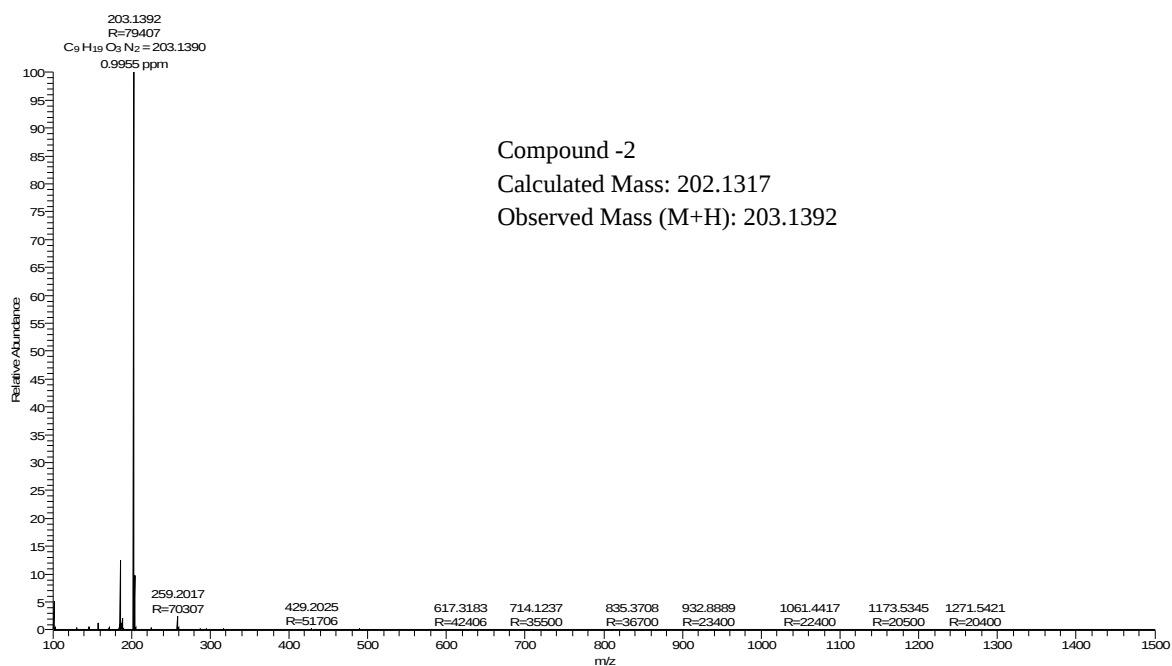
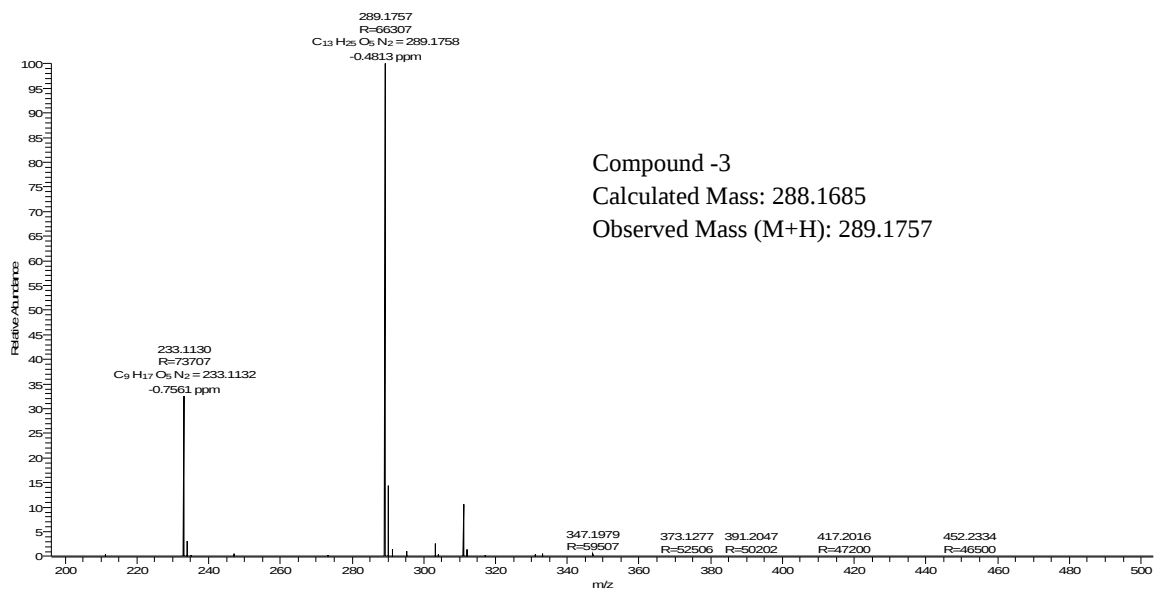


Fig. S10. HRMS spectra of compounds **1** and **2**.

H-6 #96 RT: 0.43 AM: 1 NL: 6.01E9
T: FTMS + p ES Full ms [85.40-1281.00]



G+H #483 RT: 2.15 AM: 1 NL: 1.66E8
T: FTMS + p ES Full ms [100.00-1500.00]

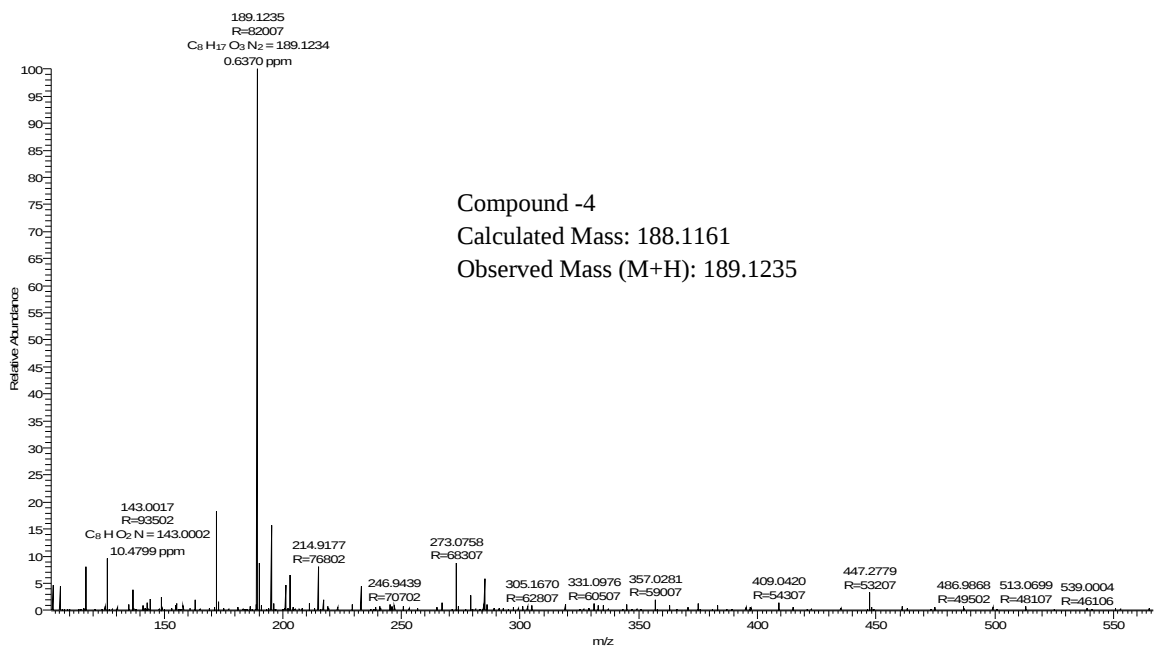
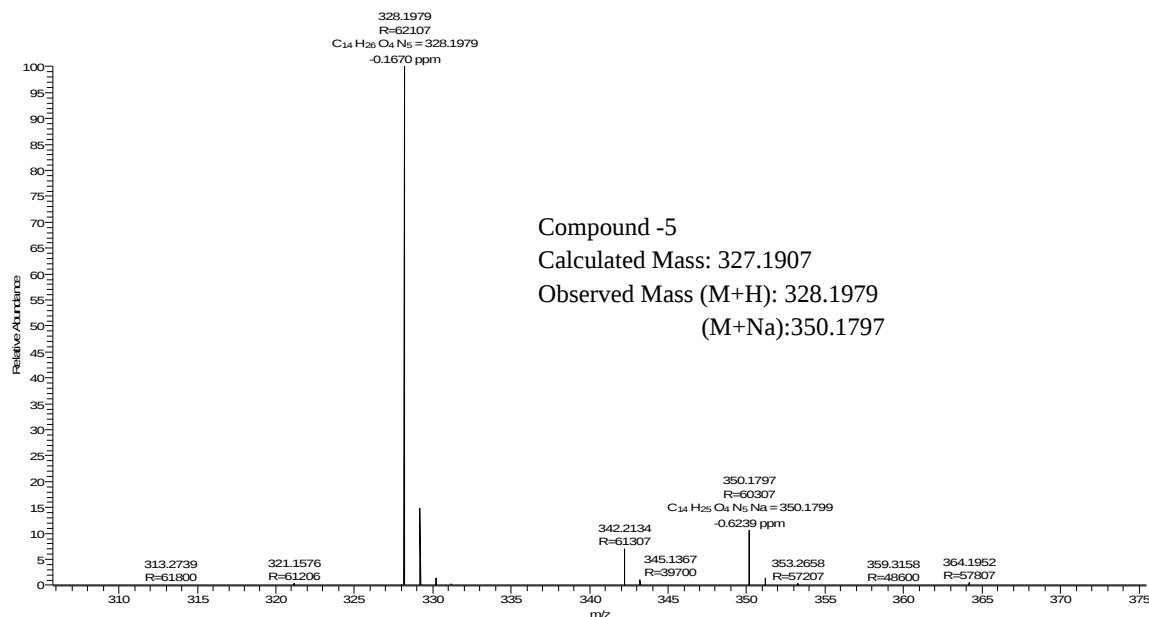


Fig. S11. HRMS spectra of compounds **3** and **4**.

H-5 #88 RT: 0.39 AM: 1 NL: 1.55E9
T: FTMS + p ESI Full ms [86.00-1290.00]



H-6 #96 RT: 0.43 AM: 1 NL: 6.01E9
T: FTMS + p ESI Full ms [85.40-1281.00]

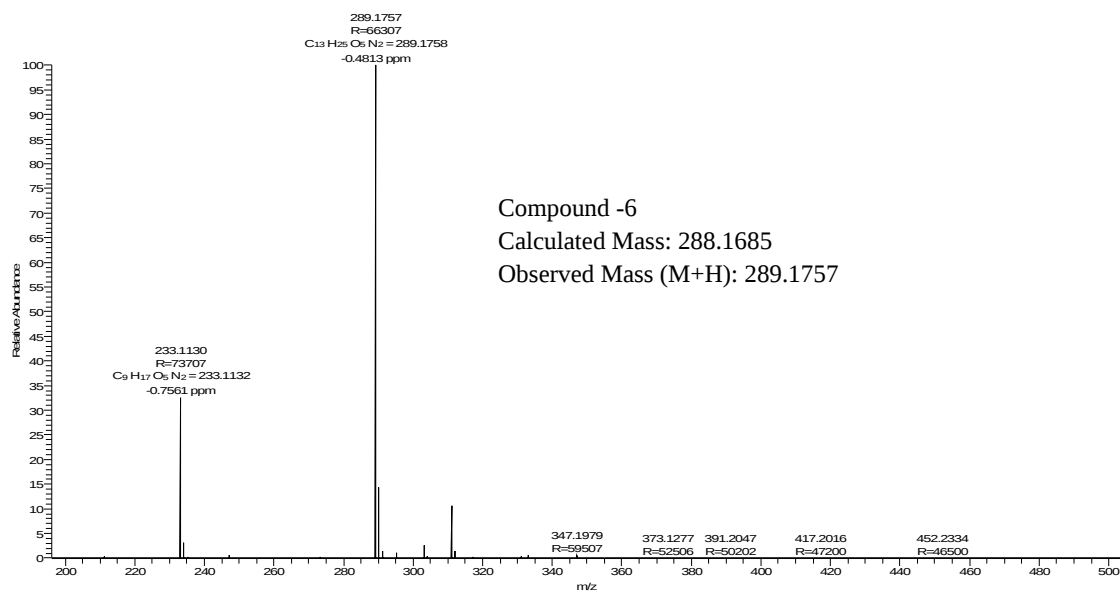
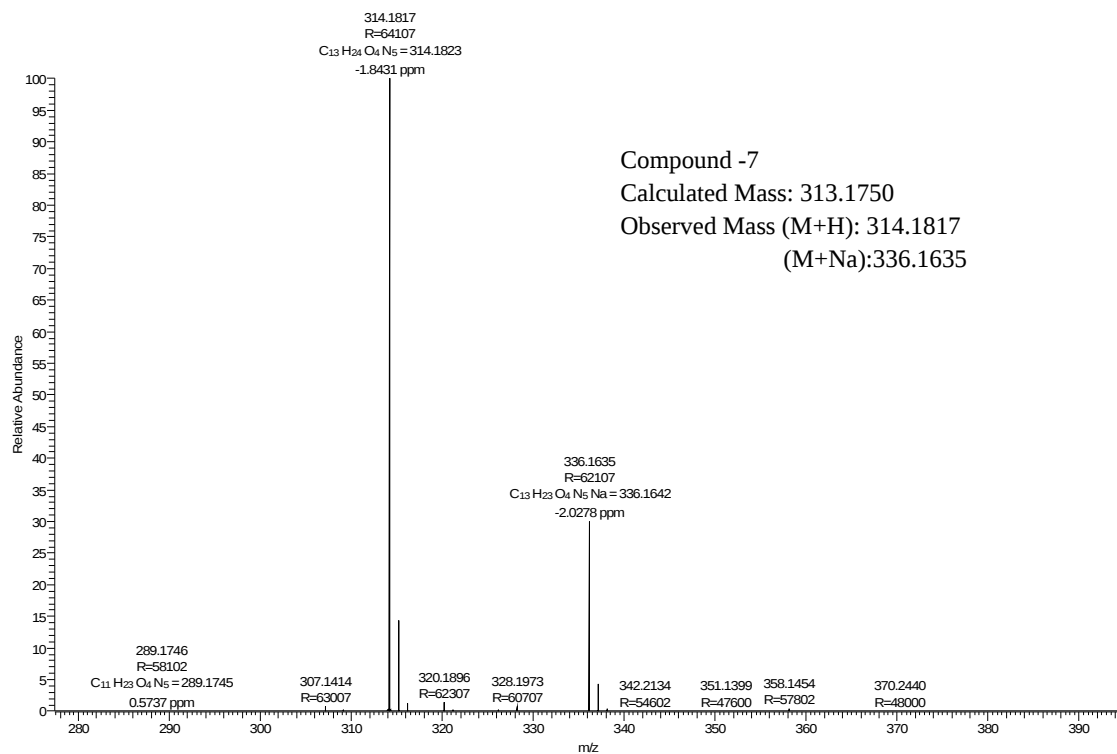


Fig. S12. HRMS spectra of compounds **5** and **6**.

H-10 #93 RT: 0.42 AM: 1 NL: 3.63E9
T: FTMS + p ESI Full ms [85.40-1281.00]



G-H11 #534 RT: 2.38 AM: 1 NL: 2.46E9
T: FTMS + p ESI Full ms [100.00-1500.00]

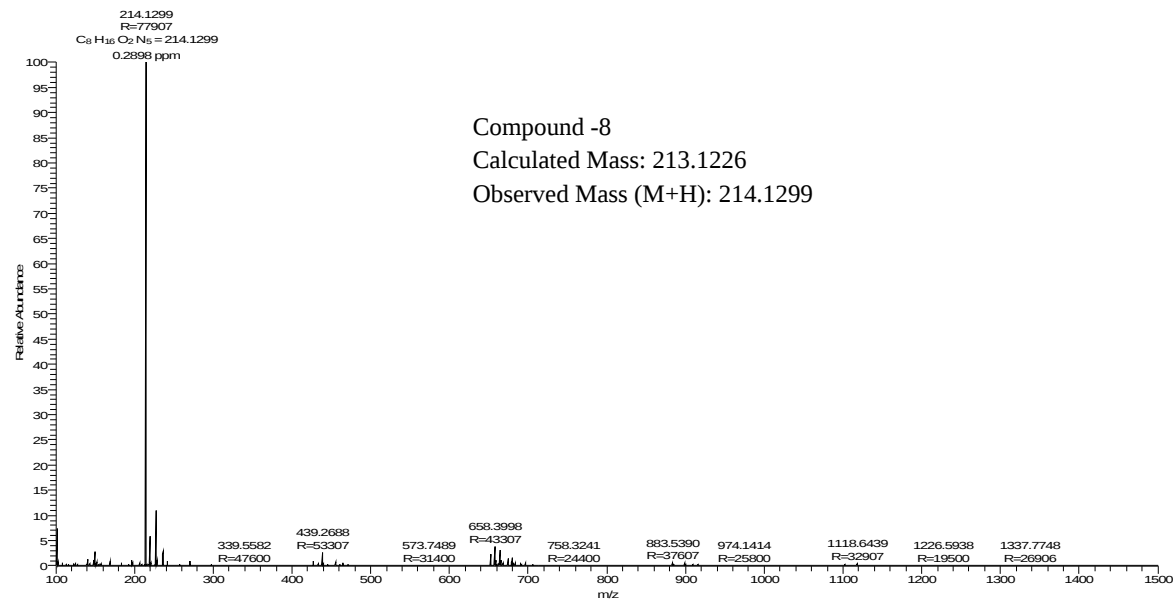


Fig. S13. HRMS spectra of compounds 7 and 8.

H-13_150326135800 #79 RT: 0.35 AV: 1 NL: 2.09E8
T: FTMS + p ESI Full ms [85.40-1281.00]

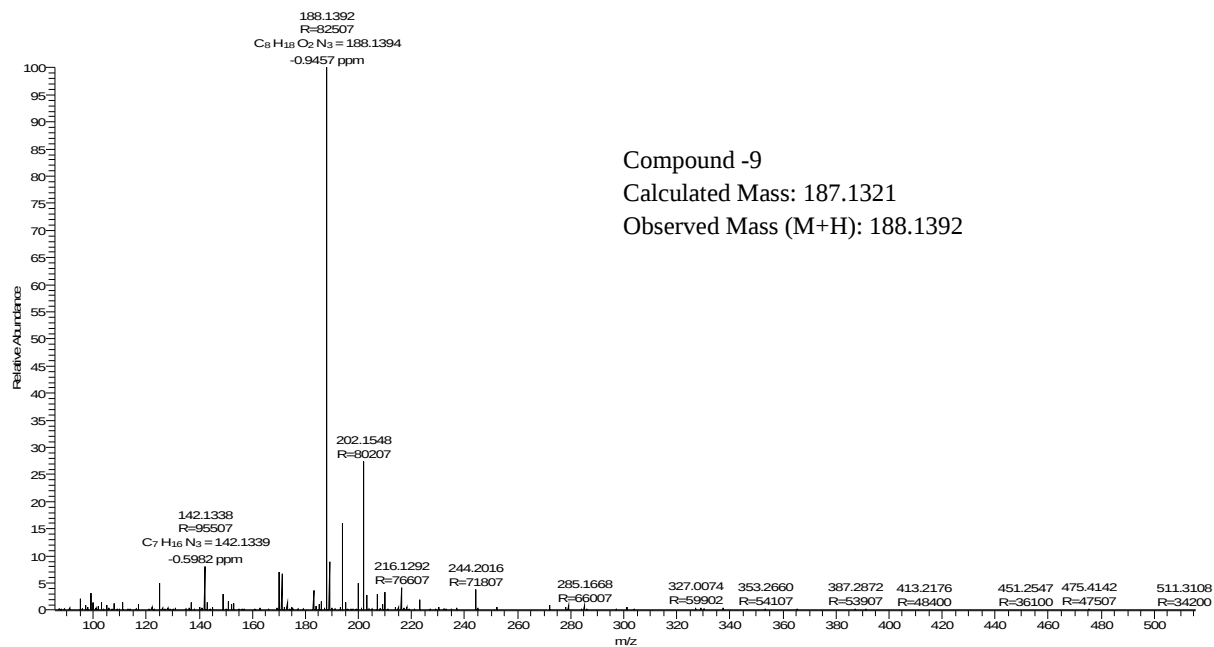
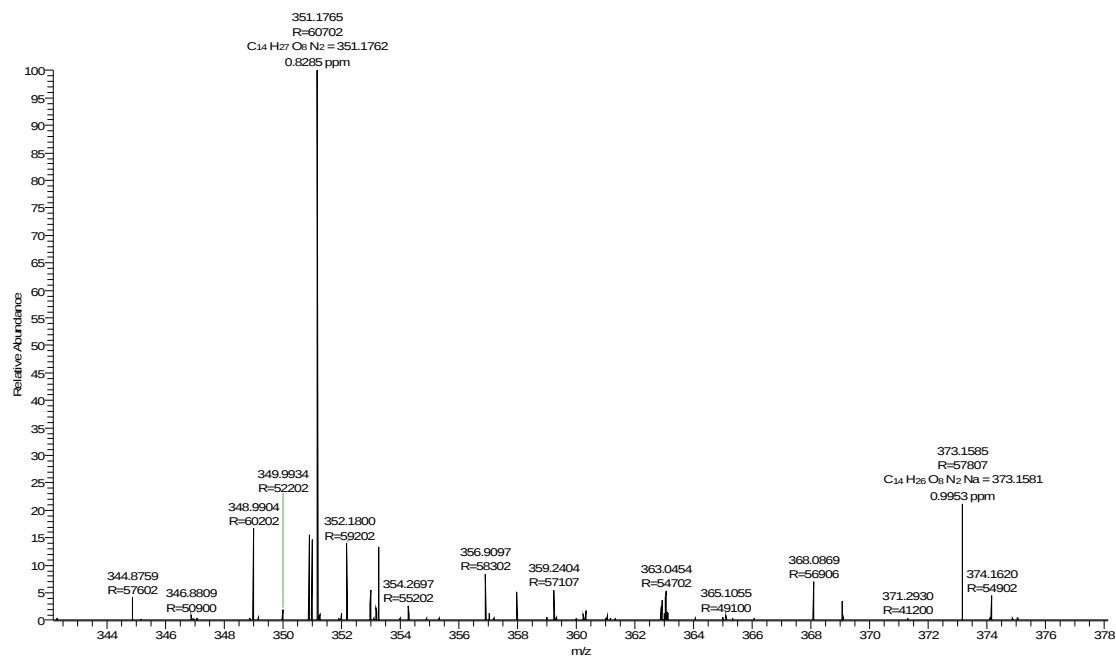


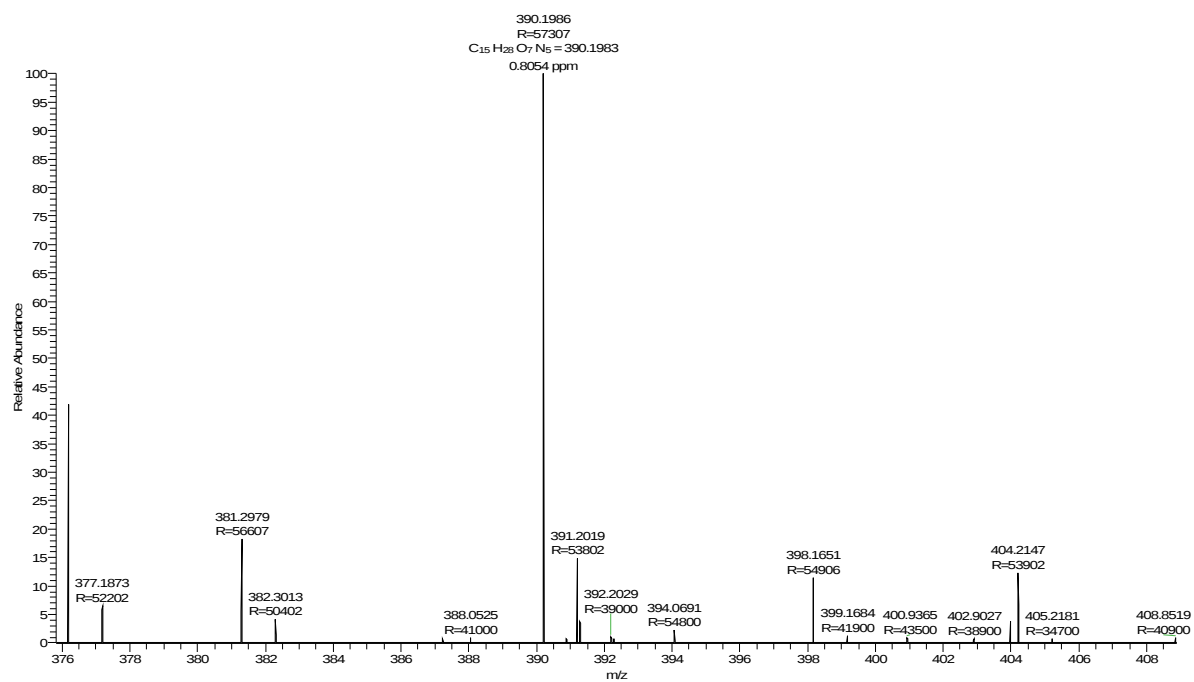
Fig. S14. HRMS spectrum of compound 9.

HARSHA-9 #80 RT: 0.36 AV: 1 NL: 8.67E5
T: FTMS + p ESI Full ms [86.00-1290.00]



Compound 4 – glucose adduct, m/z 351.1765

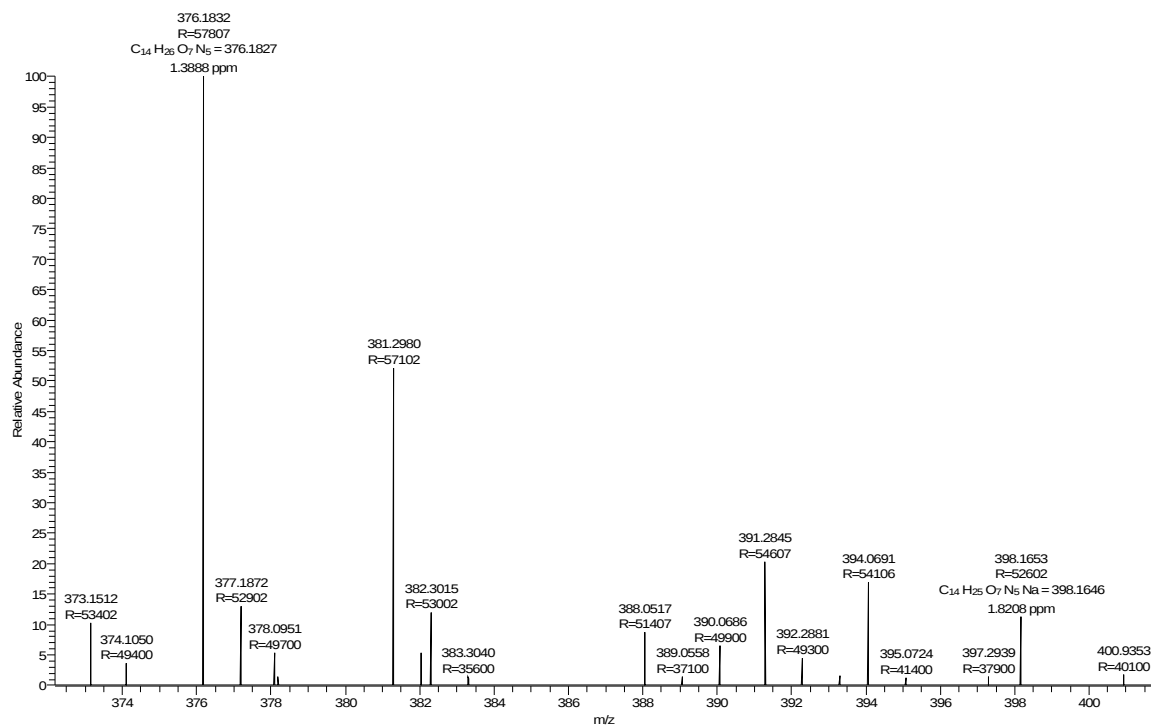
HARSHA-12 #77 RT: 0.34 AV: 1 NL: 6.72E5
T: FTMS + p ESI Full ms [86.00-1290.00]



Compound 6- glucose adduct, m/z 390.198

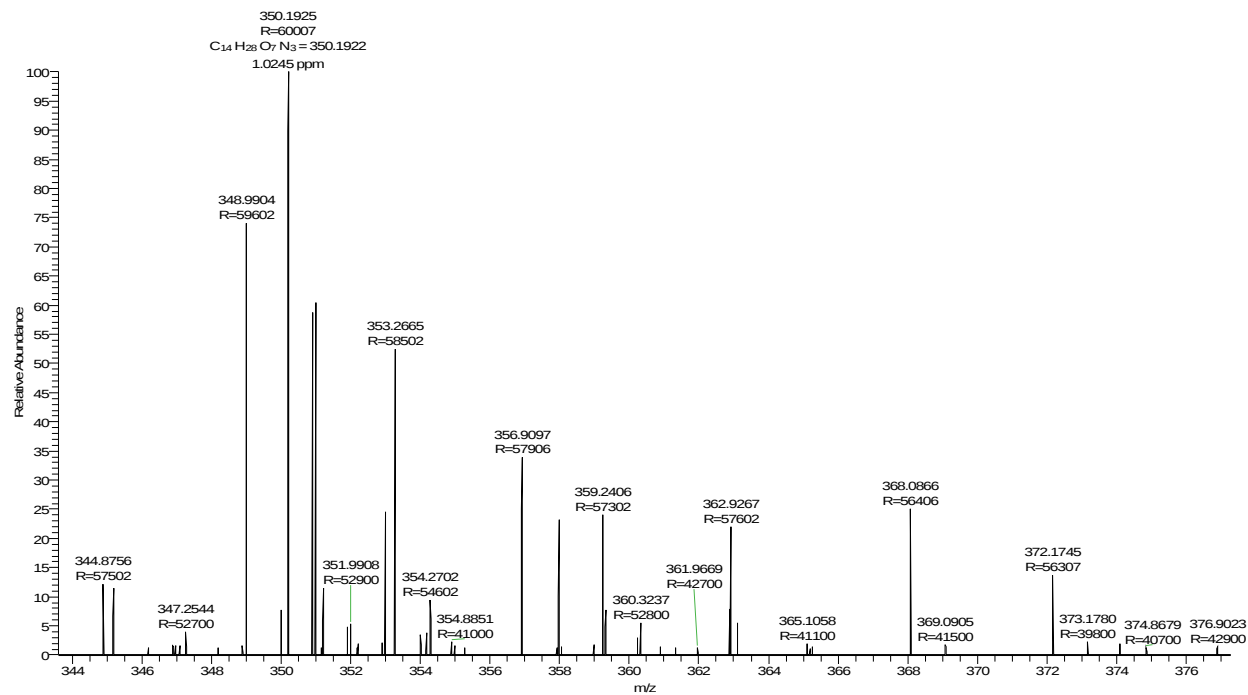
Fig. S15. LC-MS spectra of glucose adducts with compounds 4 and 6.

HARSHA-11 #78 RT: 0.35 AM: 1 NL: 2.50E6
T: FTMS + p ESI Full ms [86.00-1290.00]



Compound 8- glucose adduct, m/z 378.1832

HARSHA-13 #80 RT: 0.36 AM: 1 NL: 2.15E6
T: FTMS + p ESI Full ms [86.00-1290.00]



Compound 9- glucose adduct, m/z 350.1925

Fig. S15. LC-MS spectra of glucose adducts with compounds **8** and **9**.

List of AGE modified peptides for *in vitro* modified Bovine Serum Albumin. The analysis depicting the number of AGE modified peptides in glycated BSA, glycated BSA in presence of compounds **2, 4, 6, 8, 9** (20mM) and aminoguanidine (20mM) is given below.

Table 1. Glycated BSA

Sr. No.	Peptide sequence	XCorr	CS	Peptide MH+	ΔM [ppm]	RT [min]	MC	Modifications
1	ECCHGDLLECADDRADLAK*YICDNQDTISSK	6.07	+4	3834.64589	6.78	21.67	2	Amadori
2	RHPYFYAPELLYYANK*YNGVFQECCQAEDK	5.71	+4	3935.79409	6.61	25.61	2	Amadori
3	TCVADESHAGCEK*SLHTLFGDELCK	5.52	+3	3026.33255	4.90	19.54	1	Amadori
4	TVMENFVAFVDK*CCAADDKEACFAVEGPK	5.42	+4	3470.53994	3.99	26.74	2	Amadori
5	SHCIAEVEK*DAIPENLPPLTADFAEDKDVCK	4.85	+4	3673.74404	5.19	23.30	2	Amadori
6	NYQEAK*DAFLGSFLYEYSR	4.69	+3	2463.14811	5.27	26.54	1	Amadori
7	CCAADDKEACFAVEGPK*LVVSTQTALA	4.65	+3	3073.43186	5.02	22.94	2	Amadori
8	HLVDEPQNLIK*QNCDQFEK	4.28	+3	2517.20414	4.55	18.02	1	Amadori
9	QNCDQFEK*LGEYGFQNALIVR	4.23	+3	2691.28836	6.08	24.88	1	Amadori
10	LAK*EYEATLEECCA	4.10	+2	1976.89238	4.84	14.54	1	Amadori
11	HPYFYAPELLYYANK*YNGVFQECCQAEDK	4.01	+4	3779.68935	5.92	27.12	1	Amadori
12	RPCFSALTPDETYVPK*AFDEK	4.01	+3	2633.25656	4.75	21.20	1	Amadori
13	ATEEQLK*TVMENFVAFVDK	3.98	+2	2361.16435	4.75	32.28	1	Amadori
14	LVNELTEFAK*TCVADESHAGCEK	3.98	+3	2770.26926	5.25	21.29	1	Amadori
15	AFDEK*LFTFHADICTLPDTEK	3.81	+3	2660.26133	6.61	24.26	1	Amadori
16	LAK*EYEATLEECCA	3.68	+5	3512.52790	2.83	18.59	2	Amadori
17	VHK*ECCHGDLLECADDRADLAK	3.66	+3	2774.23001	4.34	14.63	2	Amadori
18	ADLAK*YICDNQDTISSK	3.59	+3	2103.98252	3.51	18.21	1	Amadori
19	K*FWGKYLEIAR	3.41	+2	1735.91374	4.79	21.12	2	Amadori
20	CCAADDK*EACFAVEGPK	3.41	+3	2089.85831	3.39	14.57	1	Amadori
21	K*VPQVSTPTLVEVSR	3.40	+3	1801.99857	4.40	18.40	1	Amadori
22	AEFVEVTK*LVTDLTK	3.26	+2	1855.00322	4.57	27.83	1	Amadori
23	EYEATLEECCA*DDPHACYSTVFDK	3.21	+3	3200.31406	3.83	18.30	1	Amadori
24	SLHTLFGDELCK*VASLR	3.18	+4	2108.08217	6.10	25.33	1	Amadori
25	VHK*ECCHGDLLECADDR	3.03	+3	2275.94767	4.36	12.30	1	Amadori
26	VTK*CTESLVNR	2.91	+3	1628.77274	6.66	11.20	1	Amadori
27	GLVLIAFSQYLQCPFDEHVK*LVNELTEFAK	2.87	+4	3798.95522	6.63	33.74	1	Amadori
28	K*QTALVELLK	2.65	+2	1304.77324	4.62	20.23	1	Amadori
29	FWGK*YLEIAR	2.51	+3	1607.81778	4.55	23.50	1	Amadori
30	LK*HLVDEPQNLIK	2.49	+2	1708.95476	3.93	16.43	1	Amadori
31	LKECCDKPLLEK*SHCIAEVEK	2.47	+5	2748.34547	7.31	14.22	2	Amadori
32	LCVLHEK*TPVSEK	2.44	+2	1701.87895	3.60	13.47	1	Amadori
33	LKECCDKPLLEK	2.33	+4	1694.84072	3.96	12.09	1	Amadori
34	FKDLGEEHF*GLVLIAFSQYLQCPFDEHVK	2.30	+5	3884.94733	6.90	30.14	2	Amadori

Static modification: Carbamidomethyl (57.02146 Da), Oxidation (15.995 Da), CS-Charge state, RT-Retention time, MC-Missed cleavage

Table 2. Aminoguanidine

Sr. No	Peptide sequence	XCorr	CS	Peptide MH+	ΔM [ppm]	RT [min]	MC	Modifications
1	TVMENFVAFVDK*CCAADDKEACFAVEGPK	5.53	+4	3470.54067	4.20	26.73	2	Amadori
2	ECCHGDLLECADDRADLAK*YICDNQDTISSK	5.52	+4	3834.64638	6.91	21.66	2	Amadori
3	RHPYFYAPELLYYANK*YNGVFQECCQAEDK	5.49	+4	3935.79531	6.92	25.75	2	Amadori
4	NYQEAK*DAFLGSFLYEYSR	4.76	+3	2463.14774	5.12	26.52	1	Amadori
5	SHCIAEVEK*DAIPENLPPLTADFAEDKDVCK	4.74	+4	3673.74355	5.06	23.26	2	Amadori
6	TCVADESHAGCEK*SLHTLFGDELCK	4.62	+3	3026.33127	4.47	19.55	1	Amadori
7	HPYFYAPELLYYANK*YNGVFQECCQAEDK	4.55	+4	3779.68349	4.37	27.06	1	Amadori
8	CCAADDKEACFAVEGPK*LVVSTQTALA	4.45	+3	3073.43113	4.79	22.91	2	Amadori
9	QNCDQFEK*LGEYGFQNALIVR	4.20	+3	2691.28525	4.92	25.13	1	Amadori
10	RPCFSALTPDETYVPK*AFDEK	4.08	+3	2633.25693	4.88	21.20	1	Amadori
11	LAK*EYEATLEECCAADDPHACYSTVFDK	4.05	+4	3512.52944	3.27	18.58	2	Amadori
12	HLVDEPQNLIK*QNCDQFEK	4.03	+3	2517.20121	3.38	18.29	1	Amadori
13	ATEEQLK*TVMENFVAFVDK	3.94	+3	2361.16294	4.15	31.98	1	Amadori
14	K*VPQVSTPTLVEVSR	3.42	+3	1801.99894	4.60	18.40	1	Amadori
15	VHK*ECCHGDLLECADDRADLAK	3.63	+3	2774.22837	3.75	14.62	2	Amadori
16	AFDEK*LFTFHADICTLPDTEK	3.80	+3	2660.26059	6.34	24.24	1	Amadori
17	ADLAK*YICDNQDTISSK	3.38	+3	2103.98160	3.08	18.21	1	Amadori
18	SLHTLFGDELCK*VASLR	3.22	+4	2108.08022	5.17	25.29	1	Amadori
19	LFTFHADICTLPDTEK*QIK	2.76	+3	2439.22300	4.80	22.18	1	Amadori
20	GLVLIAFSQYLQQCFDEHVK*LVNELTEFAK	2.73	+4	3798.96303	8.69	33.27	1	Amadori
21	K*QTALVELLK	2.71	+2	1304.77300	4.43	20.18	1	Amadori
22	LCVLHEK*TPVSEK	2.48	+2	1701.87822	3.17	13.48	1	Amadori
23	GACLLPK*IETMR	2.15	+2	1550.79863	4.43	20.01	1	Amadori
24	ALK*AWSVAR	1.95	+2	1163.64678	4.14	14.80	1	Amadori

Static modification: Carbamidomethyl (57.02146 Da), Oxidation (15.995 Da), CS-Charge state, RT-Retention time, MC-Missed cleavage

Table 3. Compound- 2

Sr. No	Peptide sequence	XCorr	CS	Peptide MH+	ΔM [ppm]	RT [min]	MC	Modifications
1	TCVADESHAGCEK*SLHTLFGDELCK	5.29	+3	3026.32962	3.93	19.32	1	Amadori
2	TVMENFVAFVDK*CCAADDKEACFAVEGPK	5.11	+4	3470.53481	2.52	26.53	2	Amadori
3	NYQEAK*DAFLGSFLYEYSR	4.84	+3	2463.14994	6.01	26.33	1	Amadori
4	SHCIAEVEK*DAIPENLPPLTADFAEDKDVCK	4.76	+4	3673.74038	4.20	22.97	2	Amadori
5	CCAADDKEACFAVEGPK*LVVSTQTALA	4.58	+3	3073.42710	3.47	22.69	2	Amadori
6	ATEEQLK*TVMENFVAFVDK	4.41	+3	2361.16312	4.23	31.72	1	Amadori
7	HPYFYAPELLYYANK*YNGVFQECCQAEDK	4.33	+4	3779.68667	5.21	26.88	1	Amadori
8	LAK*EYEATLEECCA	4.25	+2	1976.88994	3.61	14.39	1	Amadori
9	HLVDEPQNLIK*QNCDQFEK	4.17	+3	2517.19919	2.58	17.79	1	Amadori
10	QNCDQFEK*LGEYGFQNALIVR	4.12	+3	2691.28653	5.40	24.67	1	Amadori
11	VHK*ECCHGDLLECADDRADLAK	4.01	+3	2774.22745	3.42	14.49	2	Amadori
12	LVNELTEFAK*TCVADESHAGCEK	3.99	+3	2770.26743	4.59	21.06	1	Amadori
13	AFDEK*LFTFHADICTLPDTEK	3.98	+3	2660.25583	4.55	24.02	1	Amadori
14	EYEATLEECCA*DDPHACYSTVFDK	3.88	+4	3200.31020	2.63	18.02	1	Amadori
15	RPCFSALTPDETYVPK*AFDEK	3.59	+3	2633.25418	3.84	20.98	1	Amadori
16	ADLAK*YICDNQDTISSK	3.49	+3	2103.97995	2.29	17.98	1	Amadori
17	K*VPQVSTPTLVEVSR	3.45	+3	1801.99674	3.38	18.22	1	Amadori
18	LAK*EYEATLEECCA*DDPHACYSTVFDK	3.40	+4	3512.52871	3.06	18.33	2	Amadori
19	AEFVEVTK*LVTDLTK	3.40	+2	1855.00127	3.52	27.69	1	Amadori
20	K*FWGKYLYEIAR	3.32	+2	1735.91228	3.94	20.93	2	Amadori
21	CCAADDK*EACFAVEGPK	3.20	+3	2089.85318	0.94	14.42	1	Amadori
22	VHK*ECCHGDLLECADDR	3.11	+3	2275.94529	3.32	12.06	1	Amadori
23	SLHTLFGDELCK*VASLR	3.03	+4	2108.08071	5.40	25.10	1	Amadori
24	GLVLIAFSQYLQQCPFDEHVK*LVNELTEFAK	2.98	+4	3798.95064	5.42	33.07	1	Amadori
25	VTK*CCTESLVNR	2.92	+3	1628.76706	3.17	11.52	1	Amadori
26	FK*DLGEEHFKGLVLIAFSQYLQQCPFDEHVK	2.75	+5	3884.94245	5.64	29.88	2	Amadori
27	K*QTALVELLK	2.74	+2	1304.77117	3.03	20.05	1	Amadori
28	K*QTALVELLK	2.53	+3	1286.76175	3.93	20.07	1	FL-1H20
29	LFTFHADICTLPDTEK*QIK	2.48	+3	2439.22153	4.19	21.98	1	Amadori

Static modification: Carbamidomethyl (57.02146 Da), Oxidation (15.995 Da), CS-Charge state, RT-Retention time, MC-Missed cleavage

Table 4. Compound -4

Sr. No	Peptide sequence	XCorr	CS	Peptide MH+	ΔM [ppm]	RT [min]	MC	Modifications
1	RHPYFYAPELLYYANK*YNGVFQECCQAEDK	5.99	+5	3935.79176	6.01	25.44	2	Amadori
2	ECCHGDLLECADDRADLAK*YICDNQDTISSK	5.94	+4	3834.65029	7.92	21.53	2	Amadori
3	TVMENFVAFVDK*CCAADDKEACFAVEGPK	5.38	+4	3470.53725	3.22	26.63	2	Amadori
4	CCAADDKEACFAVEGPK*LVVSTQTALA	5.37	+3	3073.42600	3.12	22.75	2	Amadori
5	TCVADESHAGCEK*SLHTLFGDELCK	4.87	+2	3026.32842	3.53	19.40	1	Amadori
6	HPYFYAPELLYYANK*YNGVFQECCQAEDK	4.84	+4	3779.68349	4.37	26.96	1	Amadori
7	NYQEAQ*DAFLGSFLYEYSR	4.83	+3	2463.15122	6.53	26.42	1	Amadori
8	SHCIAEVEK*DAIPENLPLTADFAEDKDVCK	4.72	+4	3673.73916	3.86	23.12	2	Amadori
9	VHK*ECCHGDLLECADDRADLAK	4.36	+3	2774.22983	4.28	14.48	2	Amadori
10	ATEEQLK*TVMENFVAFVDK	4.30	+3	2361.16458	4.85	31.82	1	Amadori
11	QNCDQFEK*LGEYGFQNALIVR	4.26	+3	2691.28489	4.78	24.74	1	Amadori
12	HLVDEPQNLIK*QNCDQFEK	4.19	+3	2517.20102	3.31	17.83	1	Amadori
13	LAK*EYEATLEECCA	4.19	+2	1976.89055	3.91	14.39	1	Amadori
14	RPCFSALTPDETYVPK*AFDEK	4.09	+3	2633.25455	3.98	21.07	1	Amadori
15	LVNELTEFAK*TCVADESHAGCEK	4.03	+3	2770.26761	4.65	21.16	1	Amadori
16	EYEATLEECCA*DDPHACYSTVFDK	3.85	+4	3200.31167	3.08	18.09	1	Amadori
17	AFDEK*LFTFHADICTLPDTEK	3.80	+3	2660.25876	5.65	24.09	1	Amadori
18	VHK*ECCHGDLLECADDR	3.66	+3	2275.94675	3.96	12.05	1	Amadori
19	ADLAK*YICDNQDTISSK	3.51	+2	2103.98345	3.95	18.05	1	Amadori
20	K*FWGKLYLEIAR	3.44	+2	1735.91289	4.29	21.01	2	Amadori
21	LAK*EYEATLEECCA/DDPHACYSTVFDK	3.43	+4	3512.52993	3.41	18.42	2	Amadori
22	AEFVEVTK*LVTDLTK	3.38	+2	1855.00151	3.65	27.75	1	Amadori
23	K*VPQVSTPTLVEVSR	3.38	+3	1801.99692	3.48	18.32	1	Amadori
24	FKDLGEEHF*GLVLIAFSQYLQQCPFDEHVK	3.25	+5	3884.94459	6.19	29.96	2	Amadori
25	GLVLIAFSQYLQQCPFDEHVK*LVNELTEFAK	3.19	+4	3798.94800	4.73	33.29	1	Amadori
26	LK*HLVDEPQNLIK	3.01	+2	1708.95378	3.36	16.33	1	Amadori
27	SLHTLFGDELCK*VASLR	3.01	+4	2108.07802	4.13	25.13	1	Amadori
28	CCAADDK*EACFAVEGPK	3.00	+3	2089.85794	3.21	14.40	1	Amadori
29	VTK*CTESLVNR	2.90	+3	1628.77347	7.11	11.27	1	Amadori
30	LFTFHADICTLPDTEK*QIK	2.82	+3	2439.22007	3.59	22.03	1	Amadori
31	LK*PDPNTLCDEFK	2.72	+3	1738.82700	3.76	17.82	0	Amadori
32	LK*PDPNTLCDEFKADEK	2.52	+3	2182.02738	2.41	17.92	1	Amadori

Static modification: Carbamidomethyl (57.02146 Da), Oxidation (15.995 Da), CS-Charge state, RT-Retention time, MC-Missed cleavage

Table 5. Compound 6

Sr. No	Peptide sequence	XCorr	CS	Peptide MH+	ΔM [ppm]	RT [min]	MC	Modifications
1	ECCHGDLLECADDRADLAK*YICDNQDTISSK	6.19	+4	3834.64321	6.08	21.68	2	Amadori
2	RHPYFYAPELLYYANK*YNGVFQECCQAEDK	6.12	+4	3935.79165	5.99	25.57	2	Amadori
3	TVMENFVAFVDK*CCAADDKEACFAVEGPK	5.20	+4	3470.54213	4.63	26.75	2	Amadori
4	TCVADESHAGCEK*SLHTLFGDELCK	5.13	+2	3026.33330	5.14	19.56	1	Amadori
5	CCAADDKEACFAVEGPK*LVVSTQTALA	5.01	+3	3073.43003	4.43	22.87	2	Amadori
6	NYQEAQ*DAFLGSFLYEYSR	4.83	+3	2463.14719	4.90	26.80	1	Amadori
7	SHCIAVEK*DAIPENLPPLTADFAEDKDVCK	4.66	+4	3673.74160	4.53	23.50	2	Amadori
8	HPYFYAPELLYYANK*YNGVFQECCQAEDK	4.46	+4	3779.68984	6.05	27.02	1	Amadori
9	ATEEQLK*TVMENFVAFVDK	4.42	+3	2361.16971	7.02	31.97	1	Amadori
10	QNCDQFEK*LGEYGFQNALIVR	4.27	+3	2691.28965	6.55	24.89	1	Amadori
11	VHK*ECCHGDLLECADDRADLAK	4.23	+3	2774.23001	4.34	14.63	2	Amadori
12	HLVDEPQNLIK*QNCDQFEK	4.18	+3	2517.20285	4.04	18.00	1	Amadori
13	LAK*EYEATLEECCAQ	4.13	+2	1976.89214	4.72	14.53	1	Amadori
14	LVNELTEFAK*TCVADESHAGCEK	4.08	+3	2770.27201	6.24	21.57	1	Amadori
15	RPCFSALTPDETYVPK*AFDEK	4.00	+3	2633.25675	4.81	21.21	1	Amadori
16	DDPHACYSTVFDK*LK*HLVDEPQNLIK	3.88	+5	3406.65662	6.05	27.76	2	Amadori
17	AFDEK*LFTFHADICTLPDTEK	3.88	+3	2660.26023	6.20	24.25	1	Amadori
18	AEFVEVTK*LVTDLTK	3.51	+2	1855.00286	4.38	27.86	1	Amadori
19	LAKEYEATLEECCAQ*DDPHACYSTVFDK	3.42	+5	3512.52698	2.57	18.82	2	Amadori
20	ADLAK*YICDNQDTISSK	3.41	+2	2103.98638	5.35	18.21	1	Amadori
21	GLVLIAFSQYLQQCPFDEHVK*LVNELTEFAK	3.41	+3	3798.94809	4.75	33.20	1	Amadori
22	K*FWGKYLIEIAR	3.38	+2	1735.91448	5.21	21.12	2	Amadori
23	ATEEQLK*TVMENFVAFVDK	3.27	+3	2377.15885	4.54	26.45	1	Amadori
24	K*VPQVSTPTLVEVSR	3.26	+3	1801.99948	4.91	18.40	1	Amadori
25	VHK*ECCHGDLLECADDR	3.25	+2	2275.94390	2.71	12.28	1	Amadori
26	SLHTLFGDELCKVASLR	3.12	+4	2108.08095	5.52	25.29	1	Amadori
27	K*QTALVELLK	2.88	+2	1304.77422	5.37	20.18	1	Amadori
28	LKHLVDEPQNLIK*QNCDQFEK	1.48	+4	2758.38296	4.07	17.62	2	Amadori

Static modification: Carbamidomethyl (57.02146 Da), Oxidation (15.995 Da), CS-Charge state, RT-Retention time, MC-Missed cleavage

Table 6. Compound -8

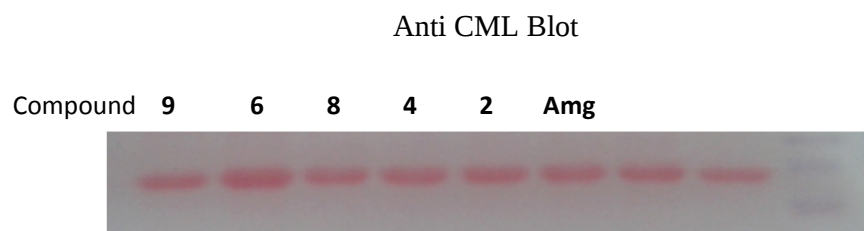
Sr. No	Peptide sequence	XCorr	CS	Peptide MH+	ΔM [ppm]	RT [min]	MC	Modifications
1	RHPYFYAPELLYYANK*YNGVFQECCQAEDK	6.46	+3	3935.78244	3.65	25.47	2	Amadori
2	CCAADDKEACFAVEGPK*LVVSTQTALA	5.70	+3	3073.42710	3.47	22.70	2	Amadori
3	ECCHGDLLECADDRADLAK*YICDNQDTISSK	5.64	+4	3834.64052	5.38	21.43	2	Amadori
4	TVMENFVAFVDK*CCAADDKEACFAVEGPK	5.42	+4	3470.53969	3.92	26.54	2	Amadori
5	TCVADESHAGCEK*SLHTLFGDELCK	5.19	+2	3026.32720	3.13	19.34	1	Amadori
6	HPYFYAPELLYYANK*YNGVFQECCQAEDK	4.95	+4	3779.68886	5.79	26.91	1	Amadori
7	NYQEA*DAFLGSFLYEYSR	4.91	+2	2463.14238	2.95	26.39	1	Amadori
8	SHCIAEVEK*DAIPENLPPLTADFAEDKDVCK	4.87	+4	3673.74257	4.79	22.88	2	Amadori
9	ATEEQLK*TVMENFVAFVDK	4.76	+2	2361.16240	3.92	31.82	1	Amadori
10	QNCDQFEK*LGEYGFQNALIVR	4.30	+3	2691.28800	5.94	24.70	1	Amadori
11	LVNELTEFAK*TCVADESHAGCEKSLHTLFGDELCK	4.30	+6	4333.02294	9.12	24.43	2	Amadori
12	LAK*EYEATLEECCA	4.28	+2	1976.88909	3.17	14.35	1	Amadori
13	LVNELTEFAK*TCVADESHAGCEK	4.24	+3	2770.26670	4.32	21.07	1	Amadori
14	RPCFSALTPDETYVPK*AFDEK	4.15	+3	2633.25473	4.05	20.99	1	Amadori
15	HLVDEPQNLIK*QNCDQFEK	4.08	+3	2517.20139	3.46	17.80	1	Amadori
16	EYEATLEECCA*DDPHACYSTVFDK	4.02	+4	3200.31167	3.08	18.05	1	Amadori
17	AFDEK*LFTFHADICTLPDTEK	3.99	+3	2660.25840	5.51	24.08	1	Amadori
18	RHPYFYAPELLYYANK*YNGVFQECCQAEDK	3.95	+5	3831.73414	3.50	26.66	2	Amadori
19	VHK*ECCHGDLLECADDRADLAK	3.82	+3	2774.22672	3.15	14.46	2	Amadori
20	VHK*ECCHGDLLECADDR	3.65	+2	2275.94463	3.03	12.05	1	Amadori
21	ADLAK*YICDNQDTISSK	3.63	+2	2103.98320	3.84	17.99	1	Amadori
22	K*FWGKYLYEIAR	3.39	+2	1735.91203	3.80	20.95	2	Amadori
23	AEFVEVTK*LVTDLTK	3.33	+2	1855.00176	3.79	27.67	1	Amadori
24	K*VPQVSTPTLVEVSR	3.29	+3	1801.99546	2.67	18.55	1	Amadori
25	FKDLGEEHF*GLVLIAFSQYLQQCPFDEHVK	3.28	+5	3884.94062	5.17	29.95	2	Amadori
26	SLHTLFGDELCK*VASLR	3.18	+4	2108.08144	5.75	25.11	1	Amadori
27	GLVLIAFSQYLQQCPFDEHVK*LVNELTEFAK	3.14	+3	3798.94297	3.40	33.05	1	Amadori
28	DDSPDLPK*LKPDPNTLCDEFKADEK	3.10	+5	3049.43159	3.94	20.62	2	Amadori
29	VT*CTESLVNR	2.91	+2	1628.76628	2.70	10.97	1	Amadori
30	DLGEEHF*GLVLIAFSQYLQQCPFDEHVK	2.90	+5	3609.76911	3.31	31.25	1	Amadori
31	LFTFHADICTLPDTEK*QIK	2.88	+3	2439.21988	3.52	22.02	1	Amadori

Static modification: Carbamidomethyl (57.02146 Da), Oxidation (15.995 Da), CS-Charge state, RT-Retention time, MC-Missed cleavage

Table 7. Compound- 9

Sr. No	Peptide sequence	XCorr	CS	Peptide MH+	ΔM [ppm]	RT [min]	MC	Modifications
1	ECCHGDLLECADDRADLAK*YICDNQDTISSK	5.84	+4	3834.65127	8.18	21.67	2	Amadori
2	RHPYFYAPELLYYANK*YNGVFQECCQAEDK	5.29	+4	3935.78847	5.18	25.66	2	Amadori
3	TVMENFVAFVDK*CCAADDKEACFAVEGPK	4.99	+4	3470.53774	3.36	26.74	2	Amadori
4	SHCIAEVEK*DAIPENLPPLTADFAEDKDVCK	4.97	+4	3673.74380	5.13	23.24	2	Amadori
5	TCVADESHAGCEK*SLHTLFGDELCK	4.96	+3	3026.33164	4.59	19.52	1	Amadori
6	HPYFYAPELLYYANK*YNGVFQECCQAEDK	4.90	+4	3779.68300	4.24	27.04	1	Amadori
7	NYQEAK*DAFLGSFLYEYSR	4.79	+3	2463.15250	7.05	26.53	1	Amadori
8	ATEEQLK*TVMENFVAFVDK	4.42	+2	2361.16313	4.23	32.03	1	Amadori
9	LAK*EYEATLEECCA	4.32	+2	1976.89018	3.73	14.52	1	Amadori
10	QNCDQFEK*LGEYGFQNALIVR	4.23	+3	2691.28763	5.80	24.87	1	Amadori
11	LVNELTEFAK*TCVADESHAGCEK	4.22	+3	2770.26926	5.25	21.32	1	Amadori
12	HLVDEPQNLIK*QNCDQFEK	4.17	+3	2517.20432	4.62	17.99	1	Amadori
13	CCAADDKEACFAVEGPK*LVVSTQTALA	4.16	+3	3073.43003	4.43	22.92	2	Amadori
14	RPCFSALTPDETYVPK*AFDEK	3.92	+3	2633.25418	3.84	21.20	1	Amadori
15	ADLAK*YICDNQDTISSK	3.84	+2	2103.98418	4.30	18.22	1	Amadori
16	VHK*ECCHGDLLECADDR	3.83	+2	2275.94634	3.78	12.24	1	Amadori
17	AFDEK*LFTFHADICTLPDTEK	3.79	+3	2660.25840	5.51	24.24	1	Amadori
18	VHK*ECCHGDLLECADDRADLAK	3.70	+3	2774.22745	3.42	14.60	2	Amadori
19	EYEATLEECCA*DDPHACYSTVFDK	3.56	+3	3200.31113	2.92	18.29	1	Amadori
20	AEFVEVTK*LVTDLT	3.29	+2	1855.00176	3.79	27.85	1	Amadori
21	K*FWGKYLIEIAR	3.27	+2	1735.91045	2.89	21.10	2	Amadori
22	VTK*CCTESLVNR	2.97	+2	1628.76836	3.97	11.14	1	Amadori
23	FKDLGEEHFK*GLVLIAFSQYLQQCPFDEHVK	2.97	+5	3884.94062	5.17	30.15	2	Amadori
24	SLHTLFGDELCK*VASLR	2.90	+4	2108.07998	5.06	25.82	1	Amadori
25	CCAADDK*EACFAVEGPK	2.79	+3	2089.85538	1.99	14.54	1	Amadori
26	K*QTALVELLK	2.67	+2	1304.77190	3.59	20.44	1	Amadori
27	K*VPQVSTPTLVEVSR	2.62	+3	1801.99820	4.19	18.62	1	Amadori

Static modification: Carbamidomethyl (57.02146 Da), Oxidation (15.995 Da), CS-Charge state,
RT-Retention time, MC-Missed cleavage



Anti CML Blot Lane (L-R) compound 9, 6, 8, 4, 2, aminoguanidine, glycated BSA, BSA , ladder



Anti AGE Blot Lane (L-R) compound 9, 6, 8, 4, 2, aminoguanidine, glycated BSA, BSA

Fig. S16. Ponceau Staining of Anti-AGE and Anti-CML Blots

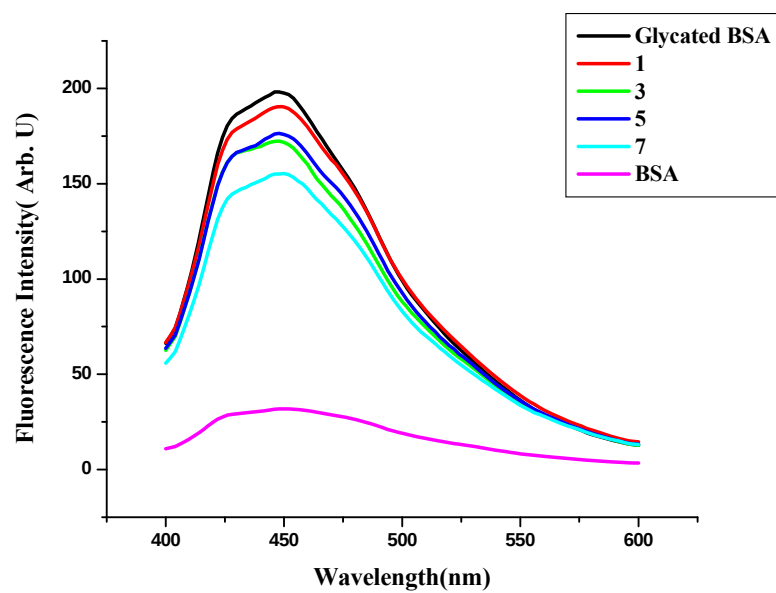


Fig. S17. AGE-fluorescence spectra of BSA, glycated BSA and glycated BSA treated with compounds **1**, **3**, **5** and **7**.