Hydroxyethylene Isosteres Introduced in Type II Collagen Fragments Substantially Alter the Structure and Dynamics of Class II MHC A^q/Glycopeptide Complexes

Cecilia Lindgren,[a] Ida E. Andersson,[a,b] Lotta Berg,[a] Doreen Dobritzsch,[c] Changrong Ge,[b] Sabrina Haag,[b] Urszula Uciechowska,[a] Rikard Holmdahl,[b] Jan Kihlberg*[c] and Anna Linusson*[a]

[a] Department of Chemistry, Umeå University, SE-901 87 Umeå, Sweden. E-mail: anna.linusson@umu.se, phone: +46-90-7866890

[b] Medical Inflammation Research, Department of Medical Biochemistry and Biophysics, Karolinska Institute, SE-171 77 Stockholm, Sweden.

[c] Department of Chemistry - BMC, Uppsala University, Box 576, SE-751 23 Uppsala, Sweden. E-mail: jan.kihlberg@kemi.uu.se, phone: +46-18-4713801

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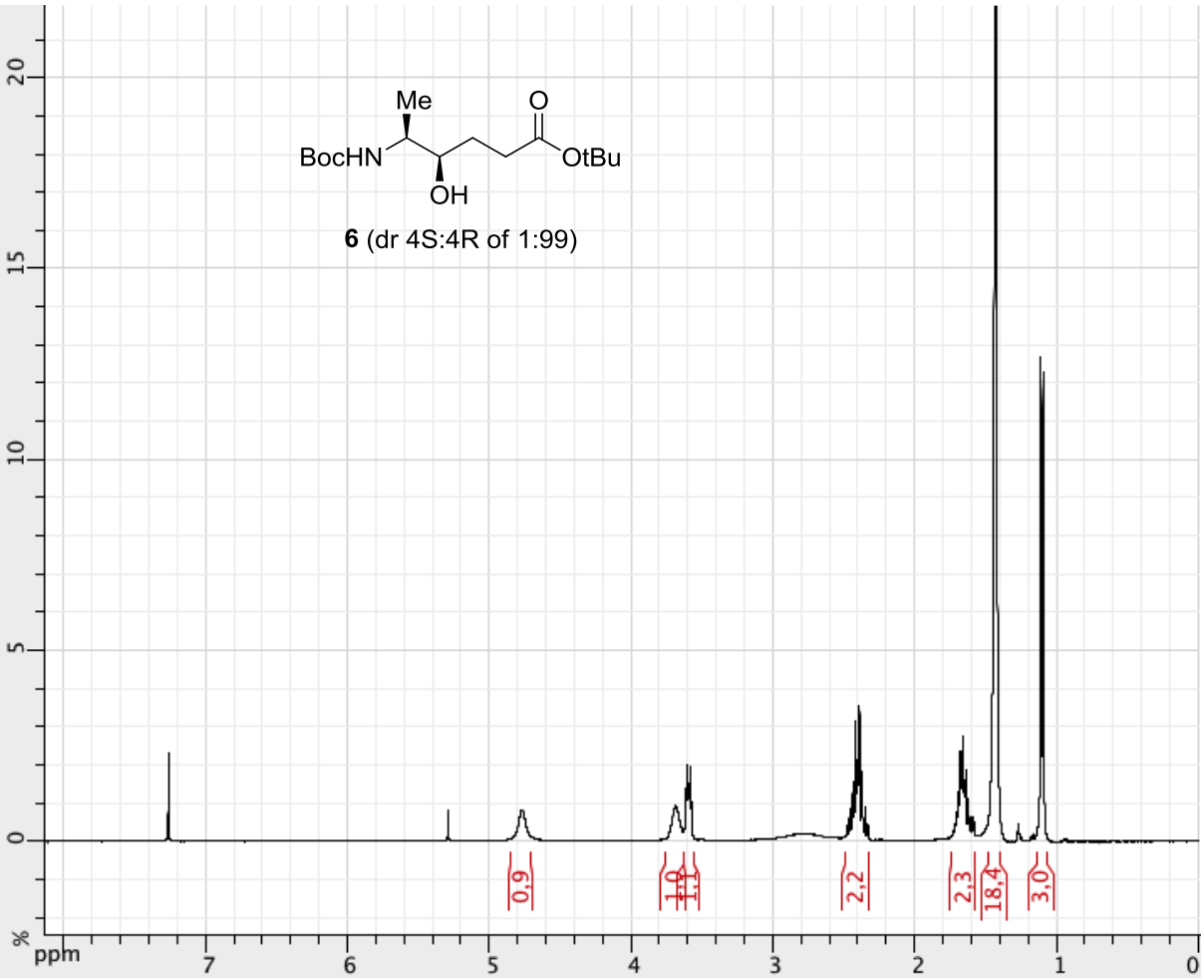
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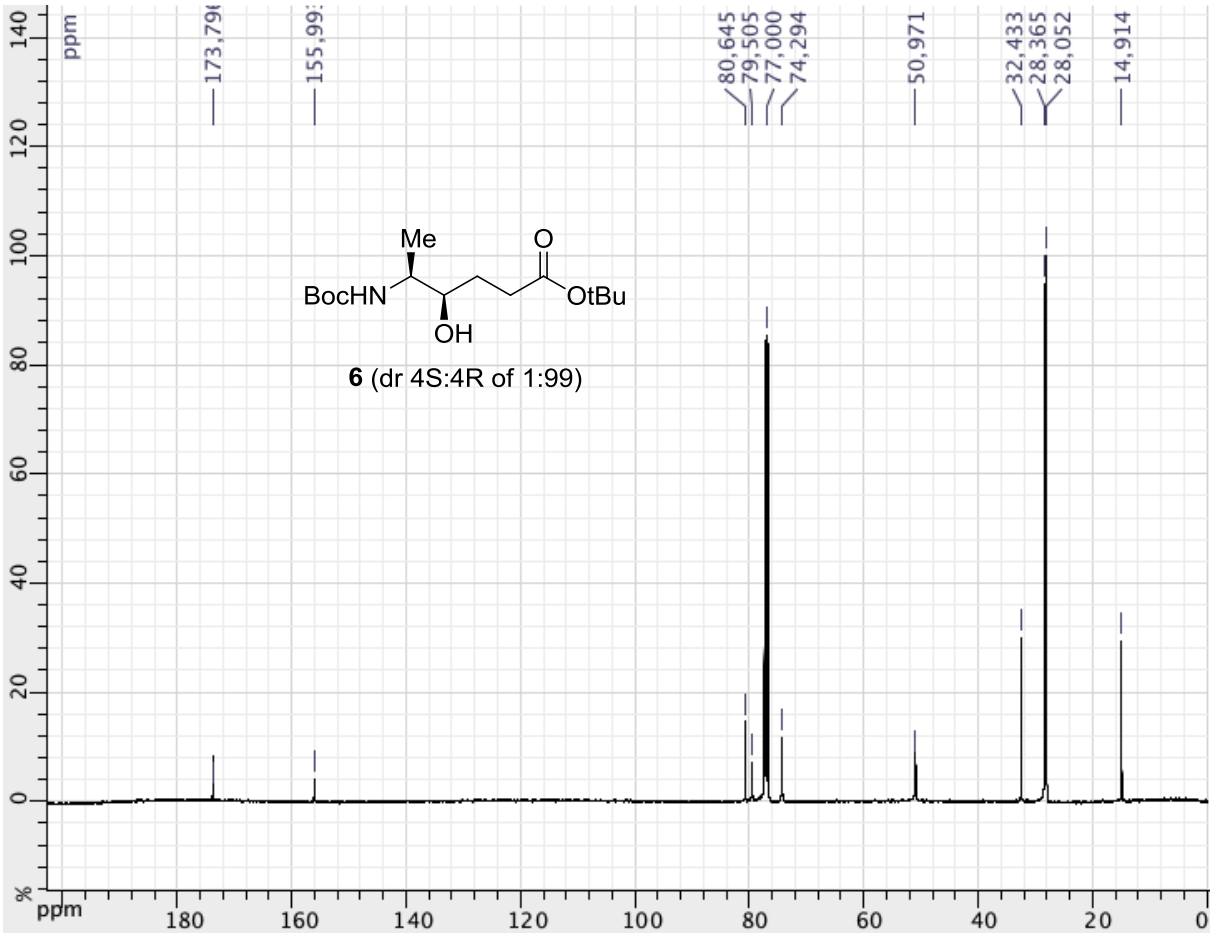
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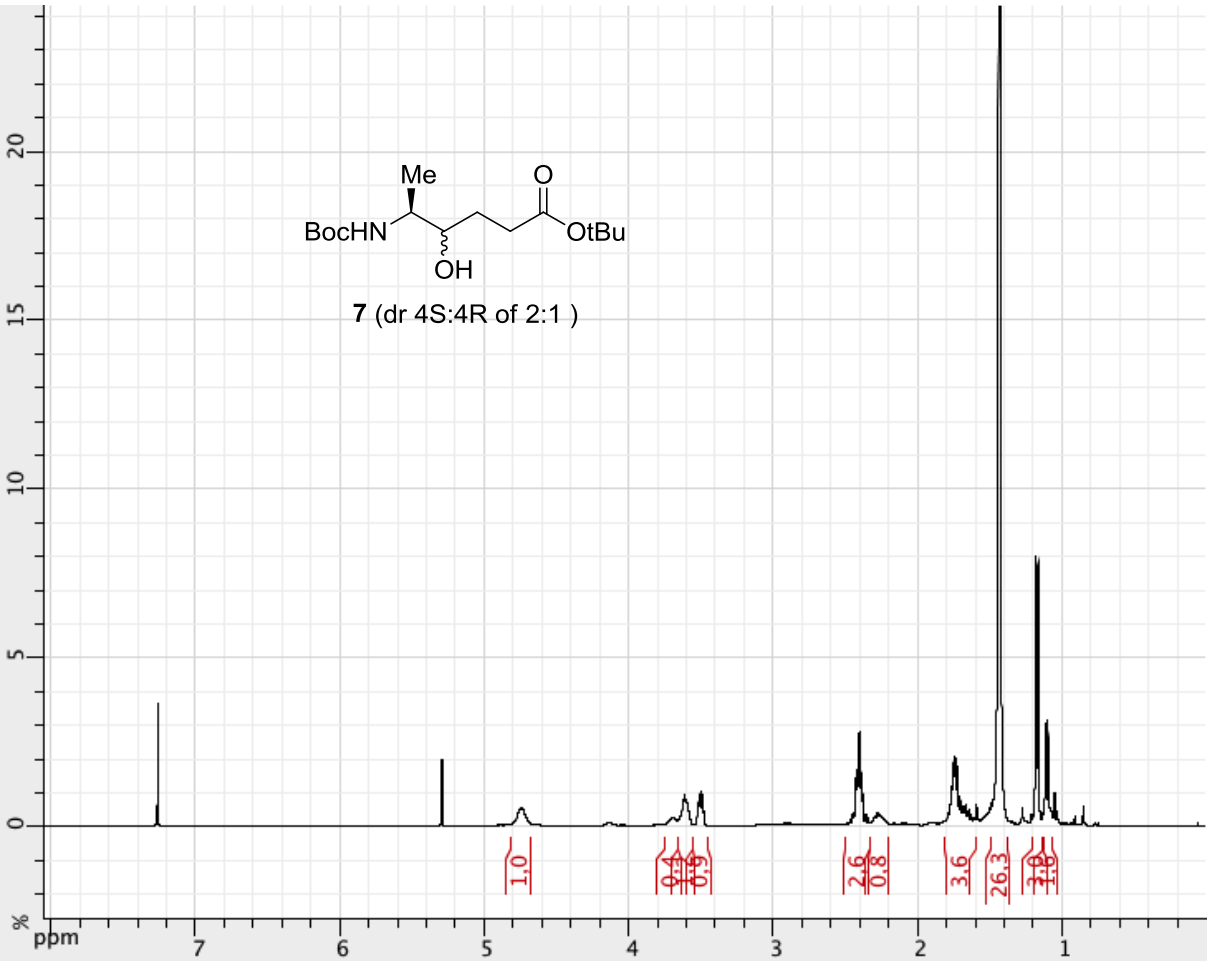
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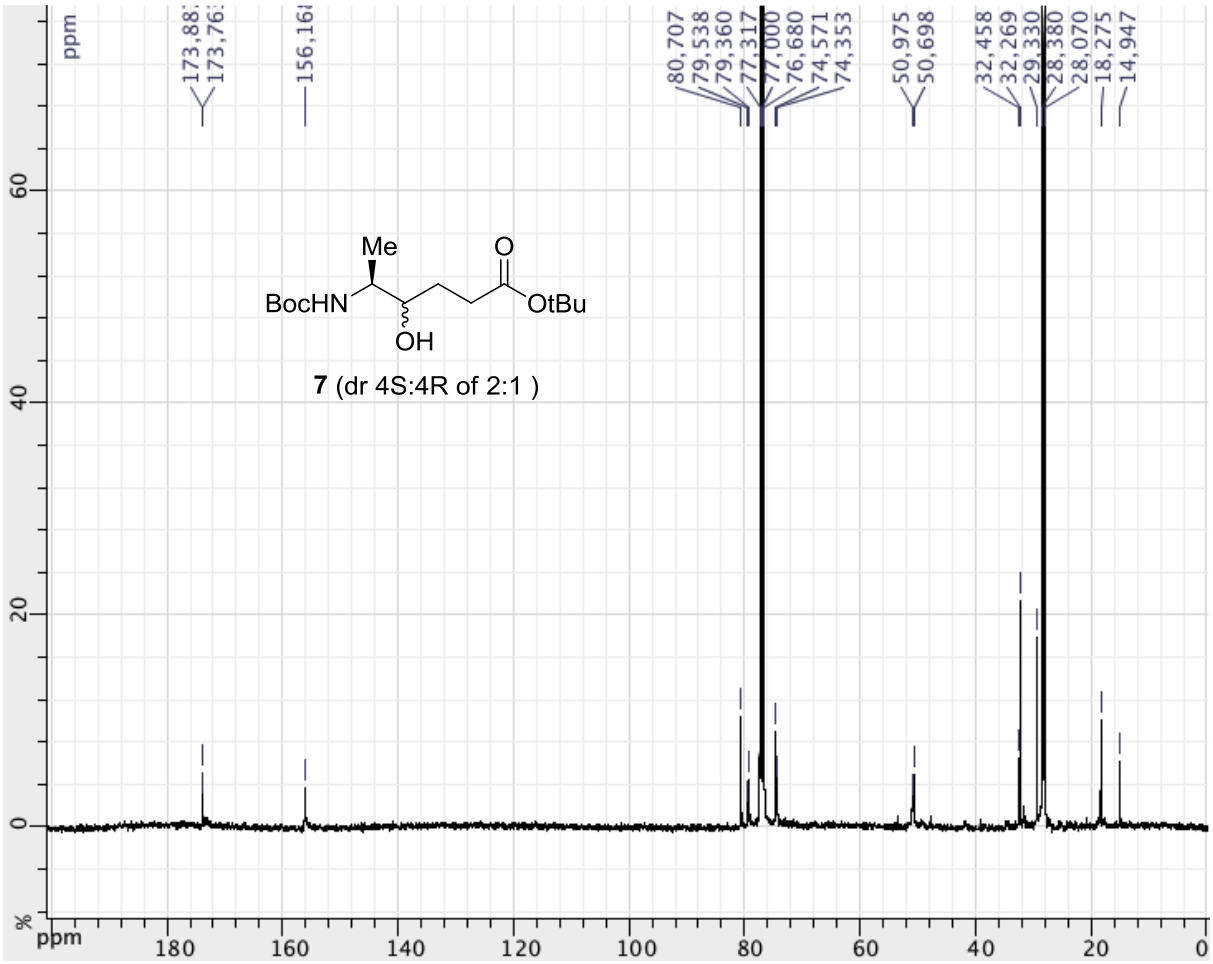
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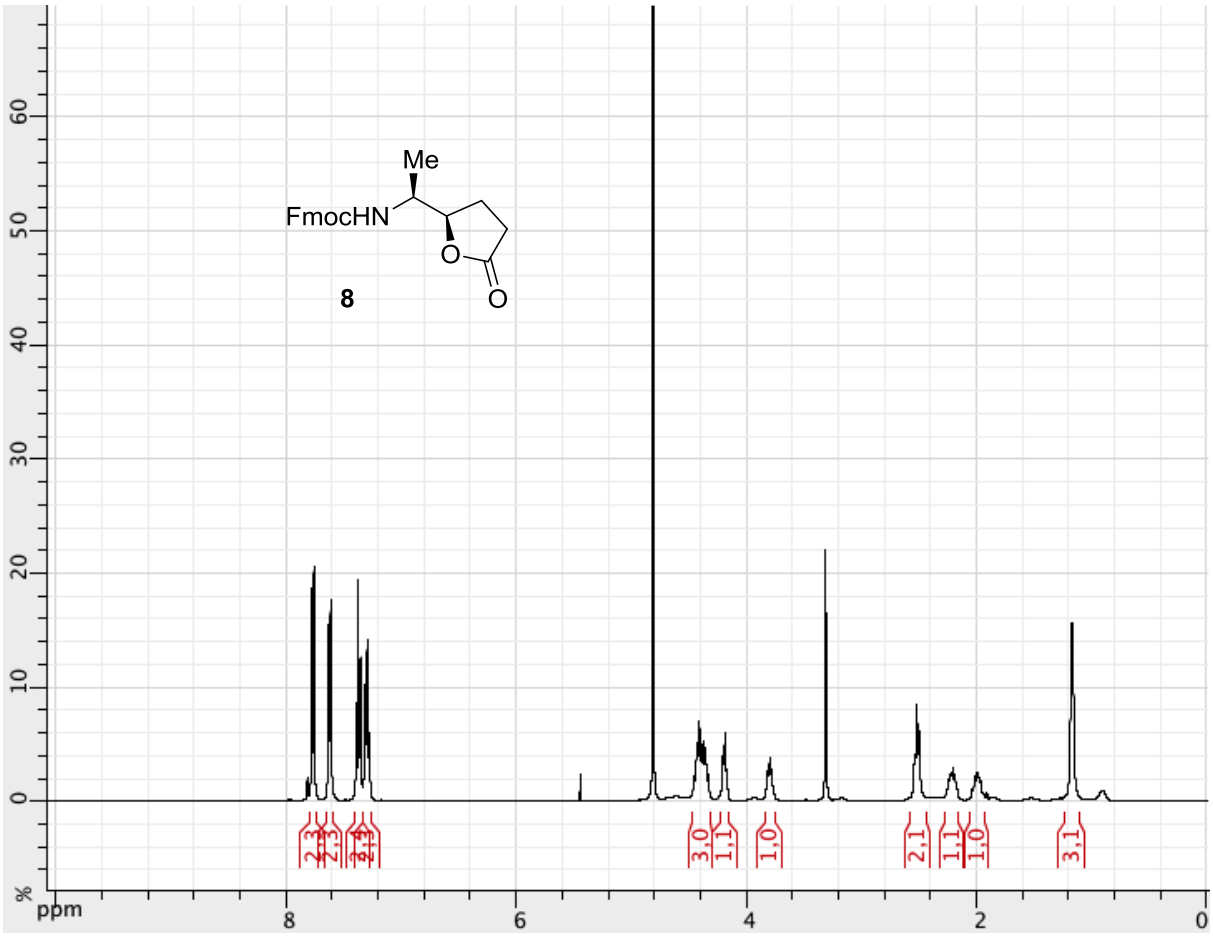
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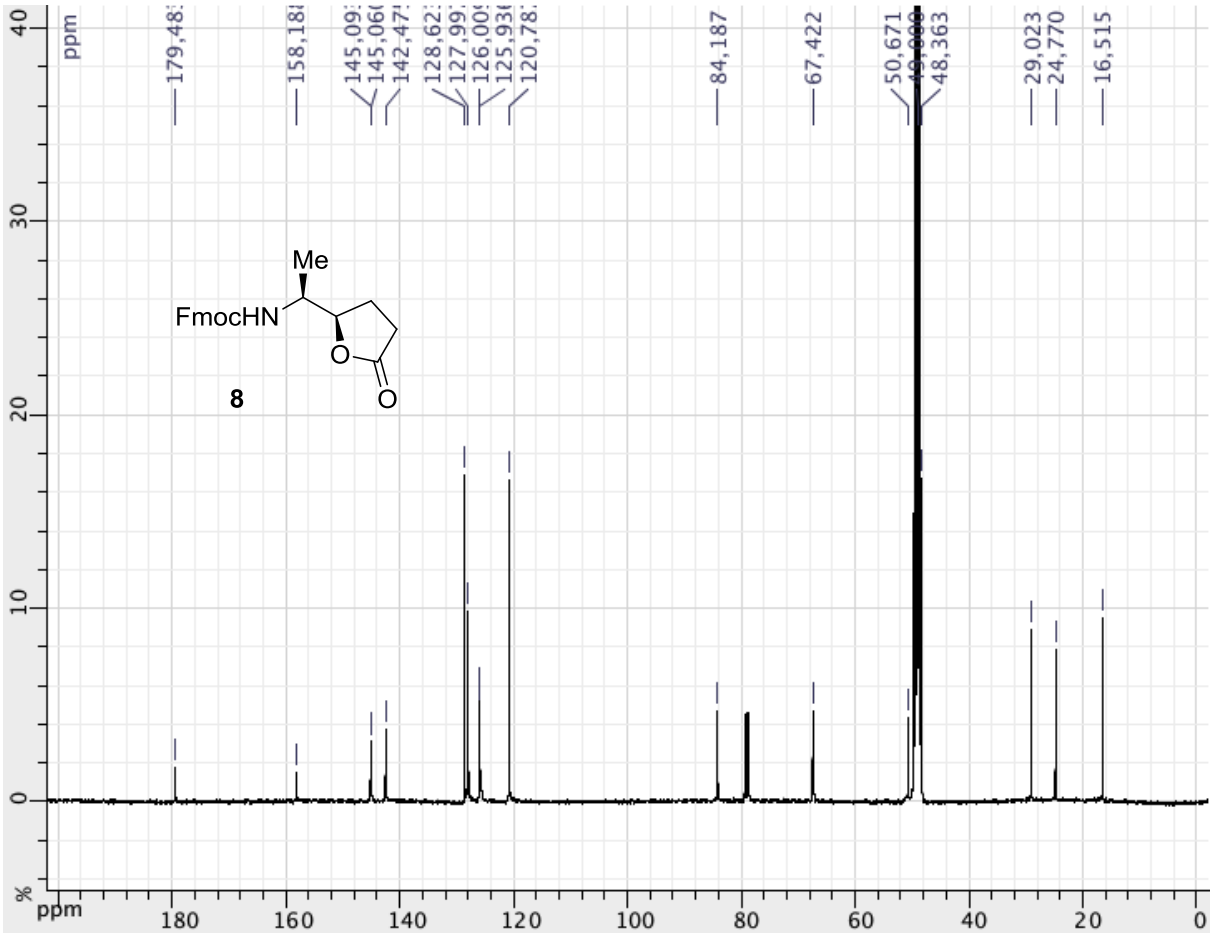
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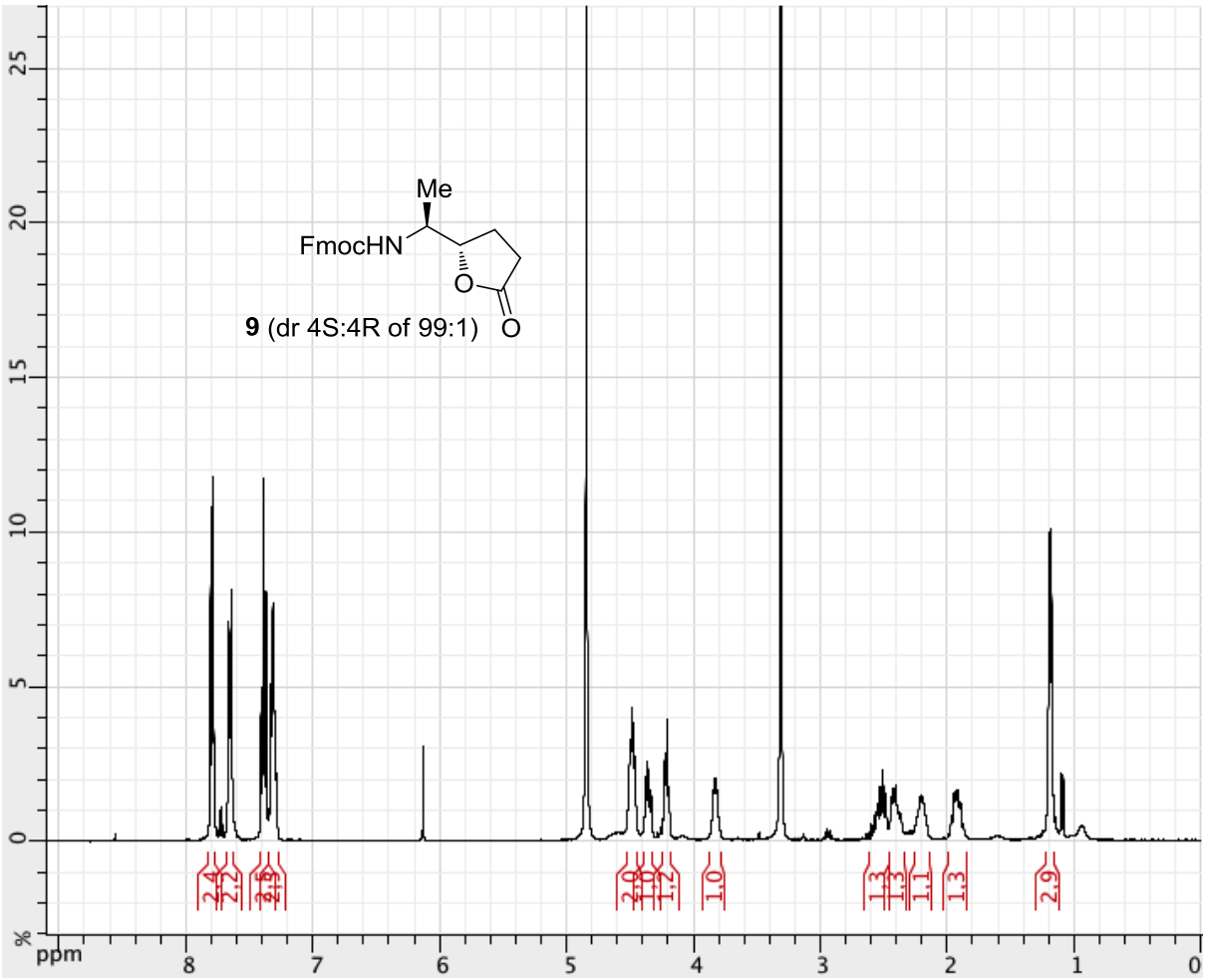
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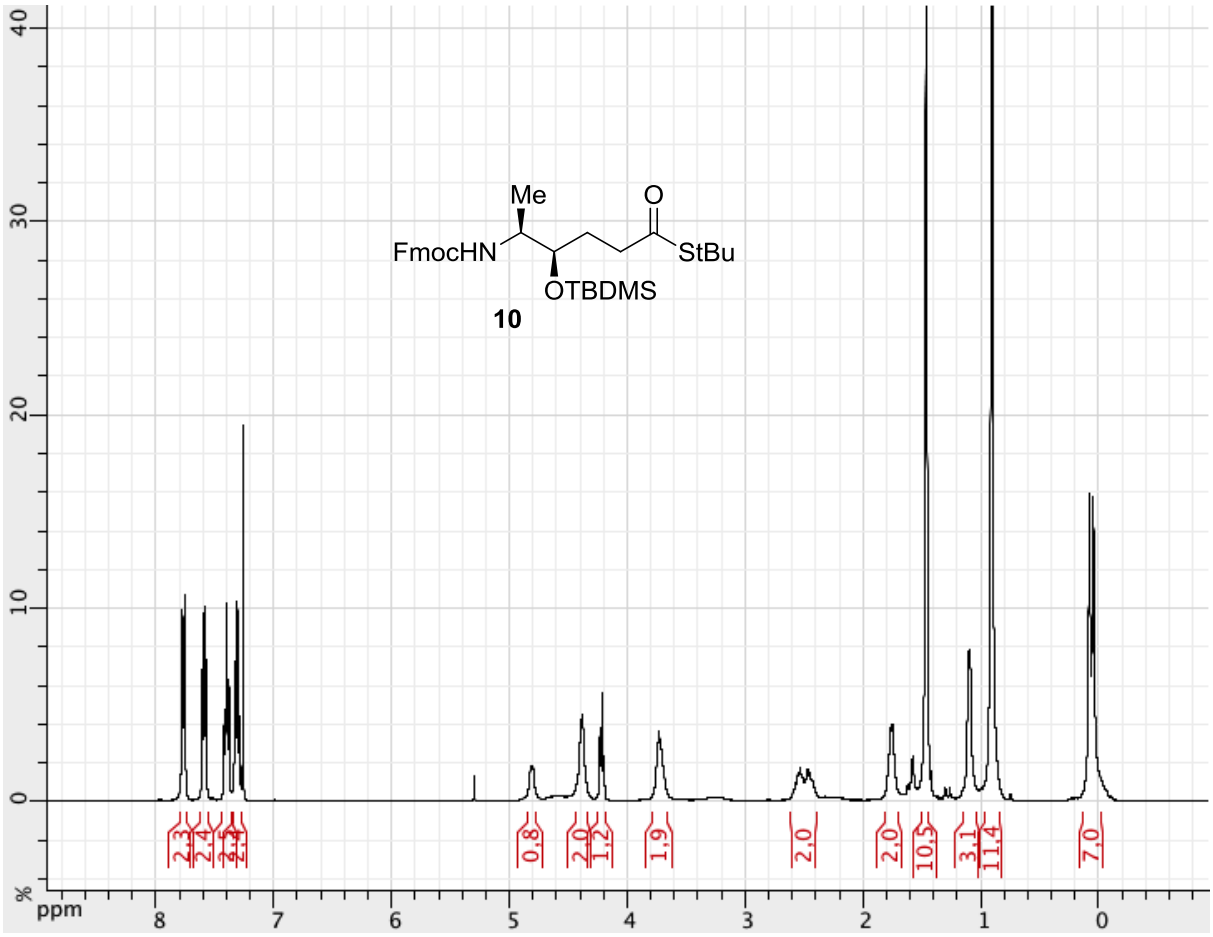
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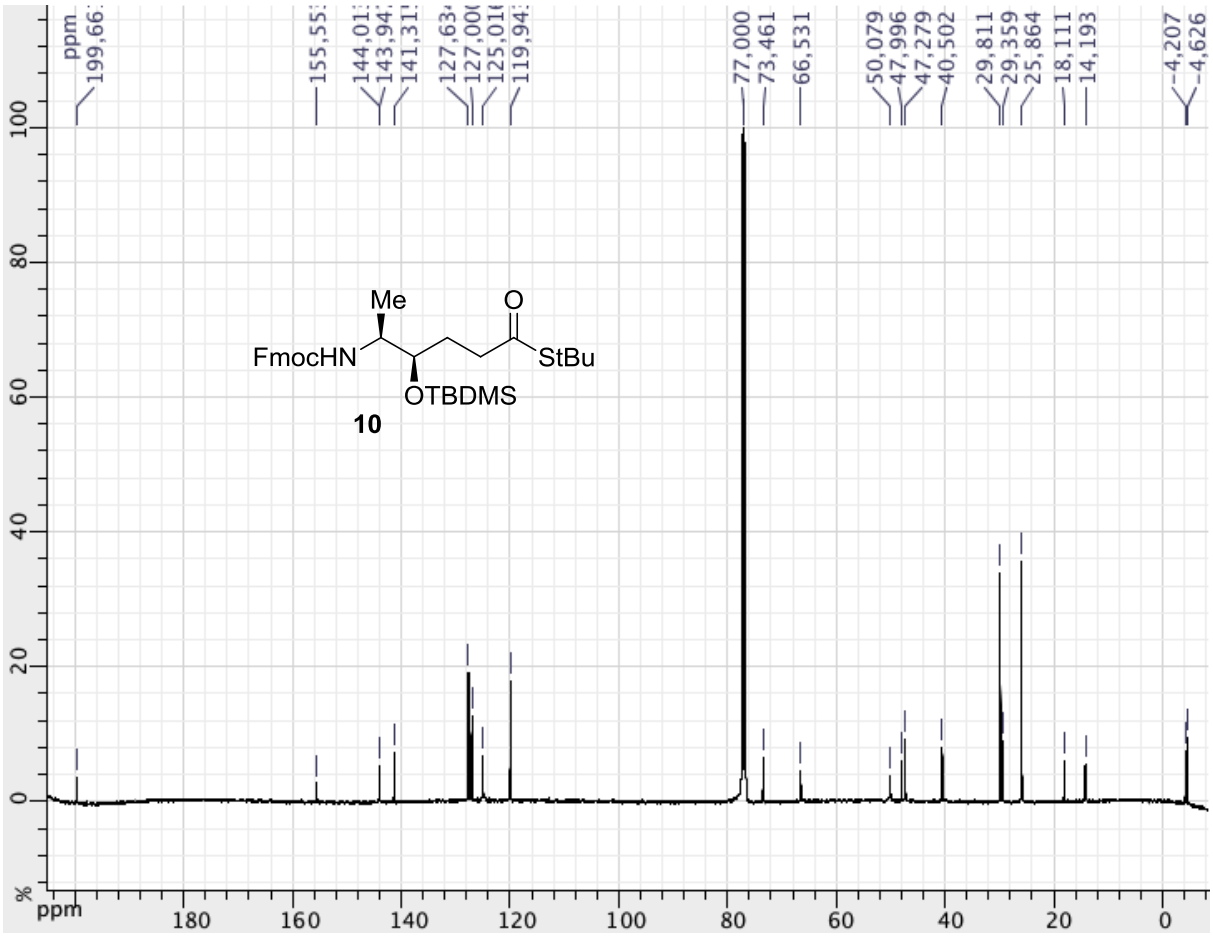
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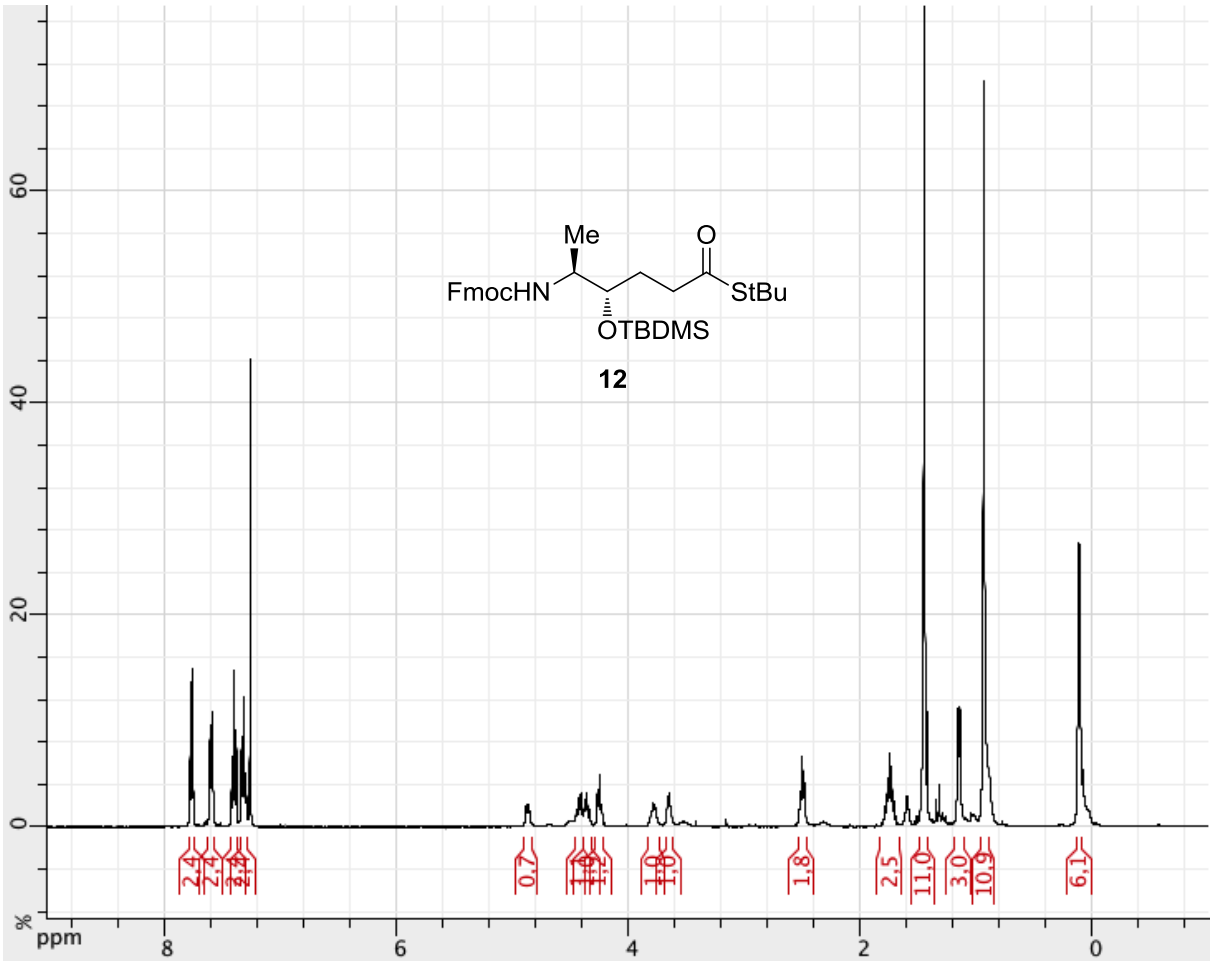
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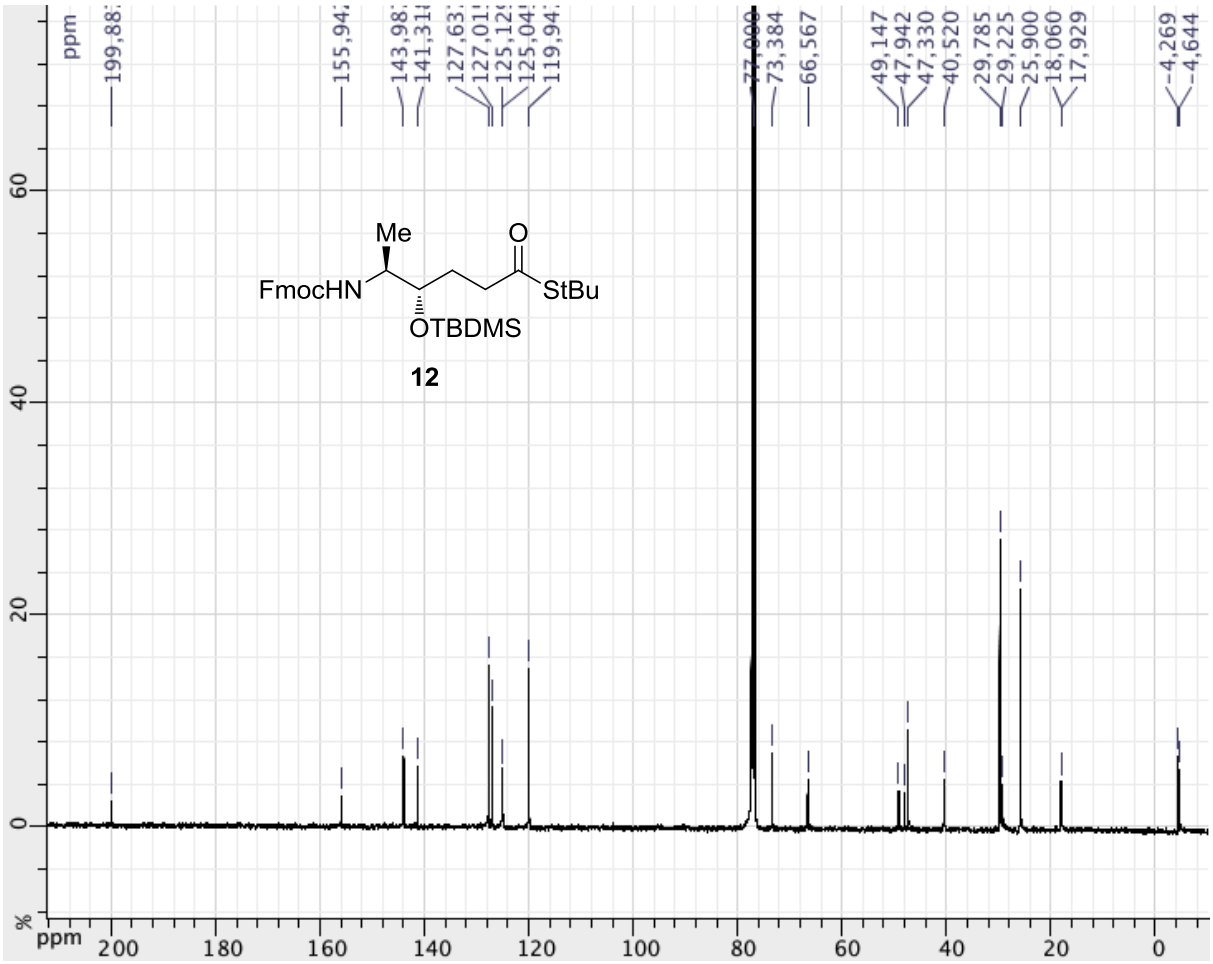
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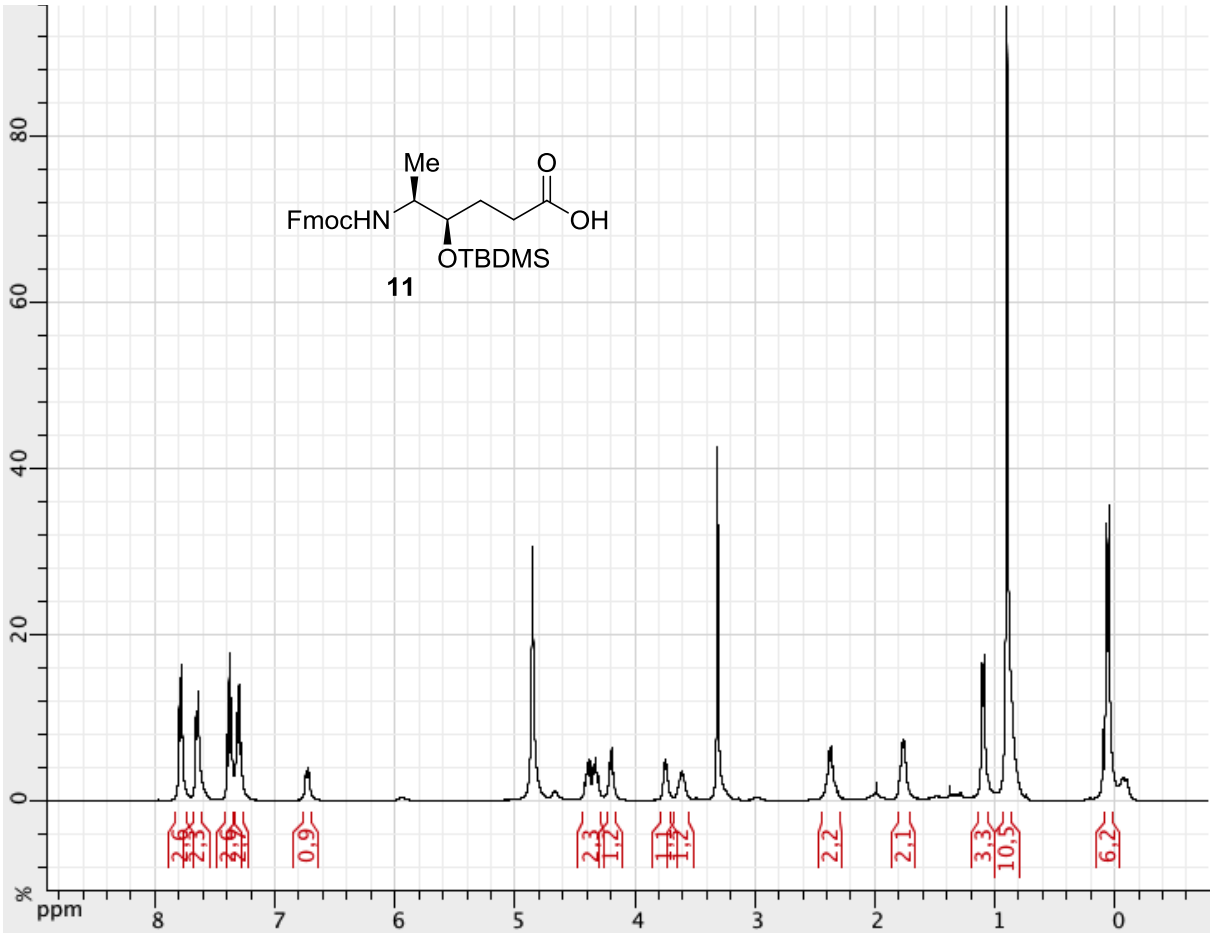
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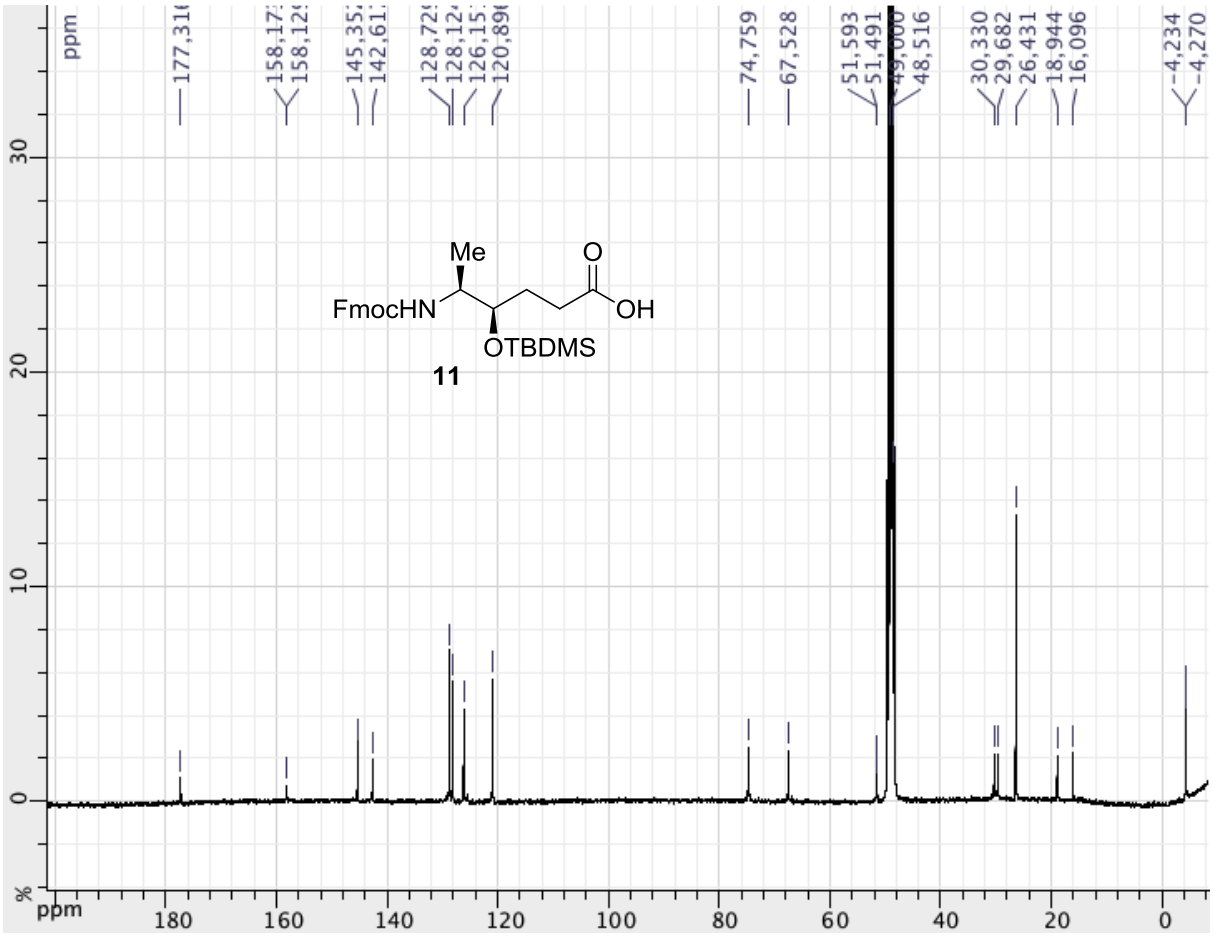
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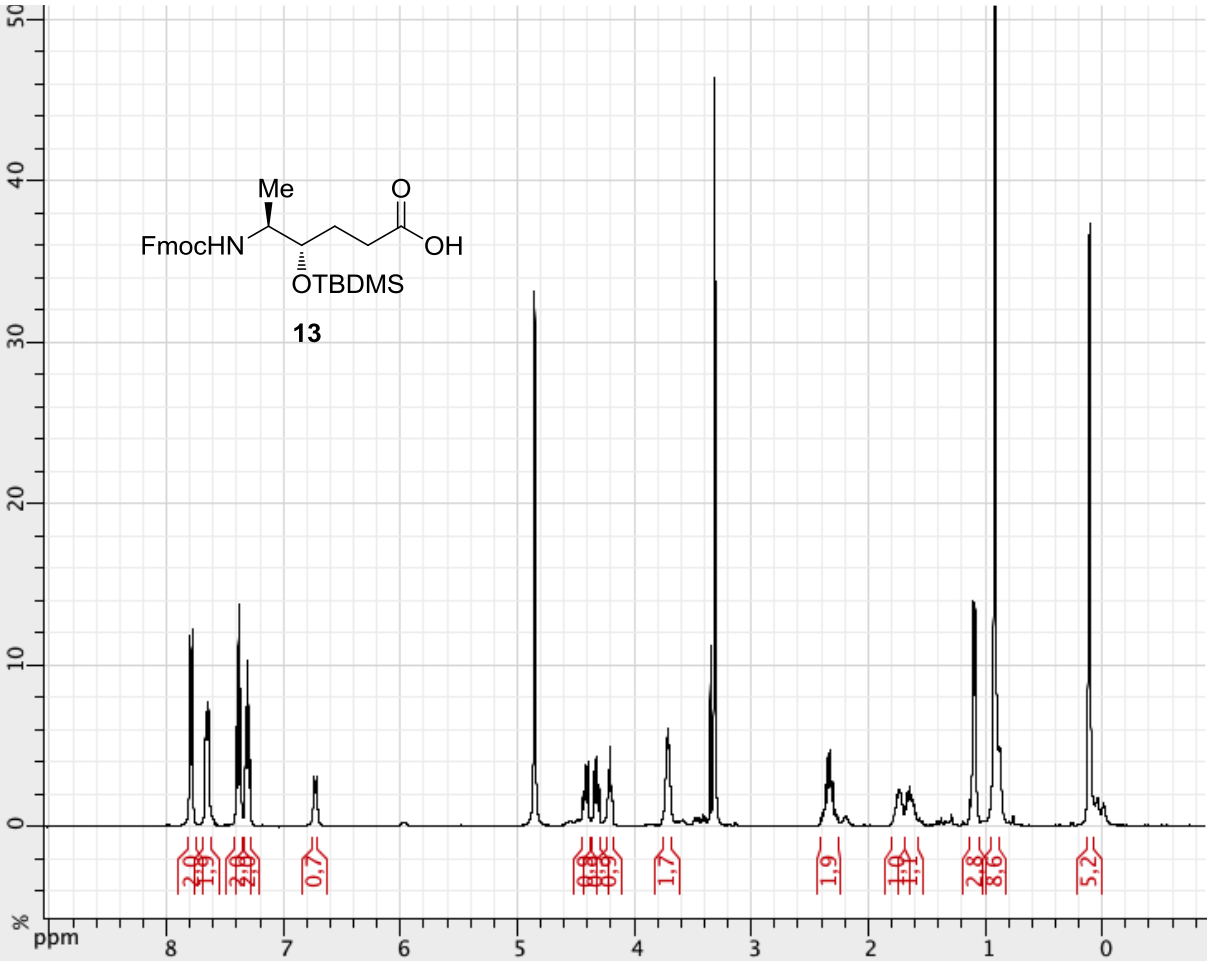
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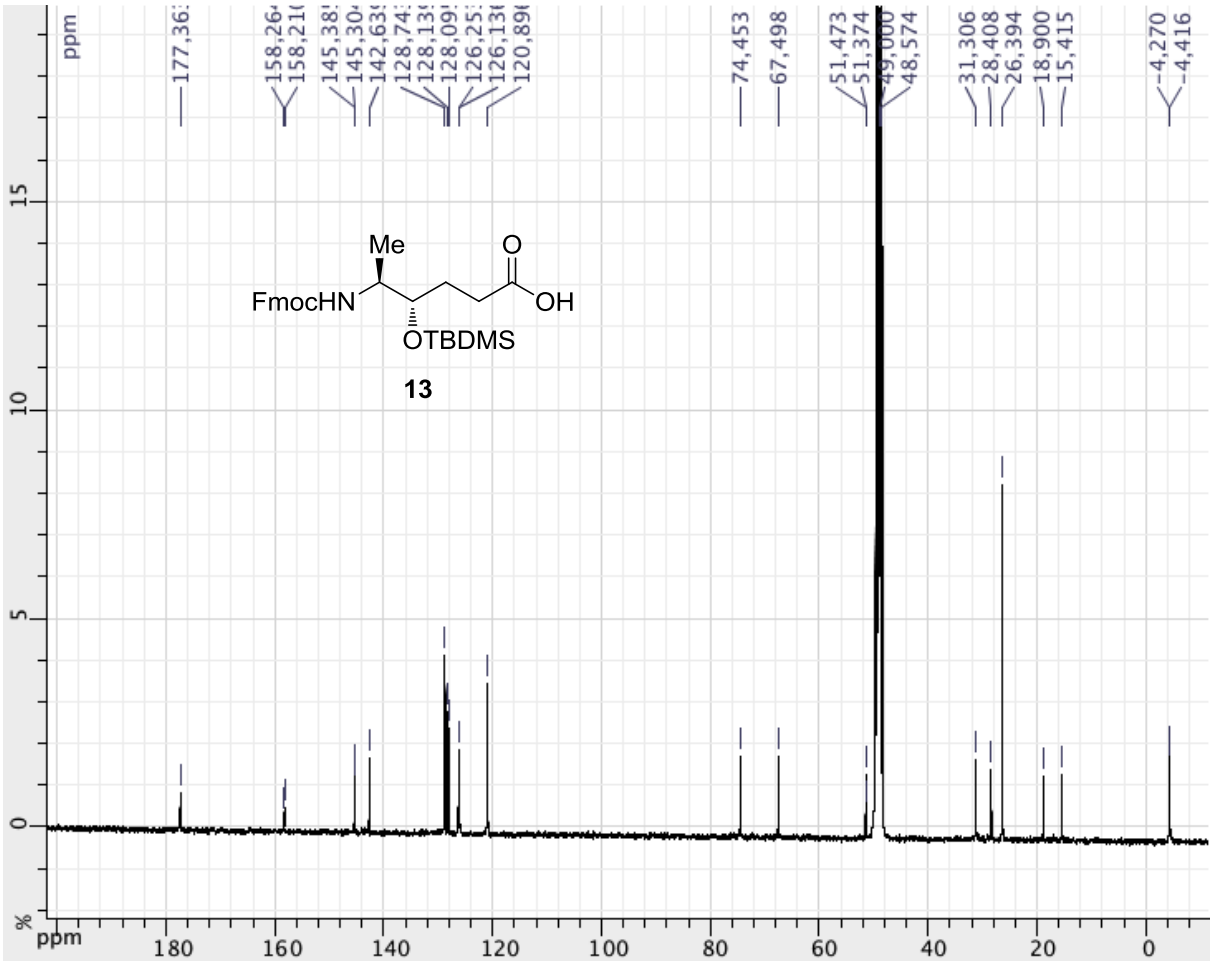
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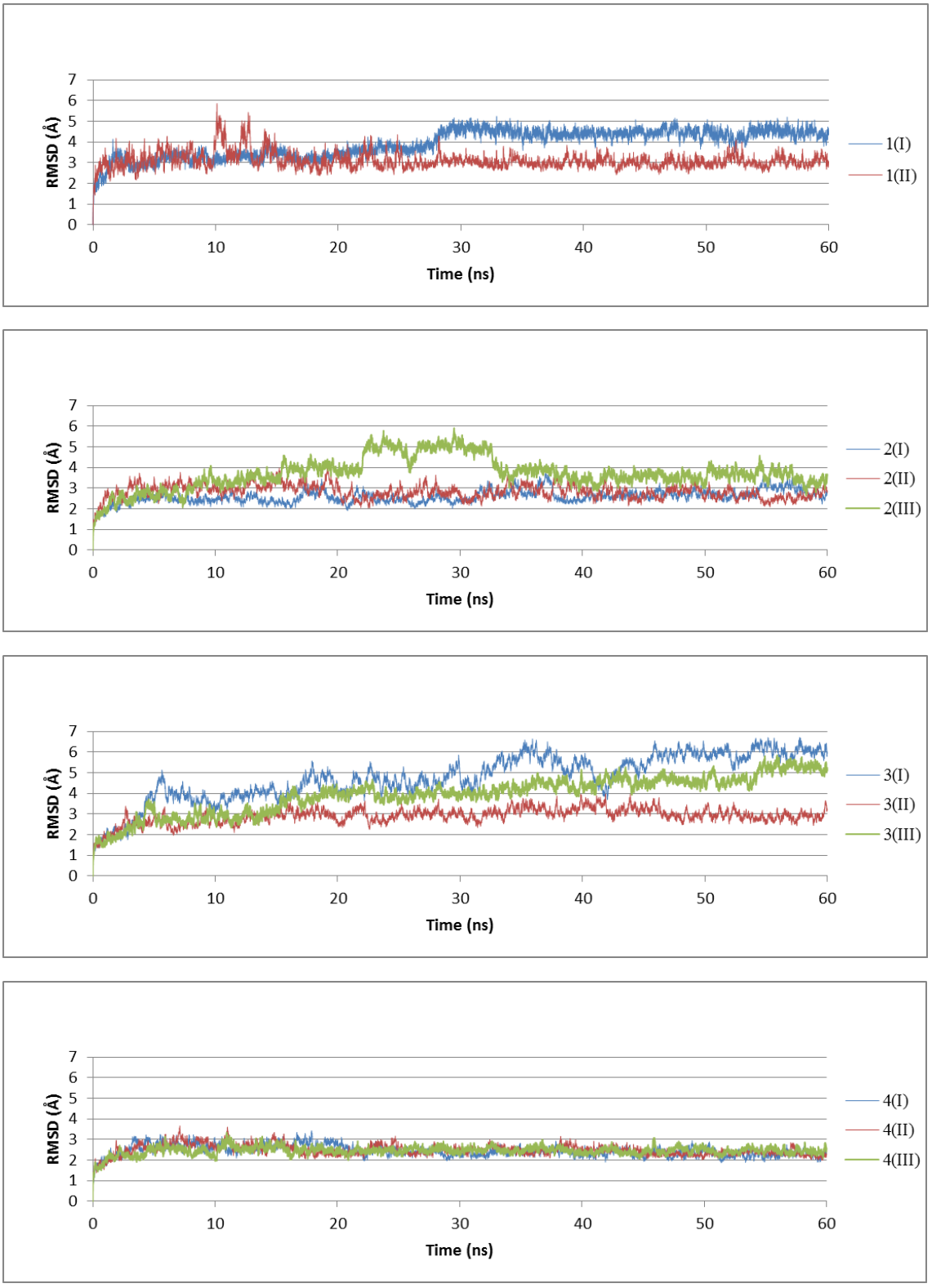


Figure S17. Backbone RMSD (N, CA, C, O) of A^q vs simulation time for A^q in complex with glycopeptide **1-4**.

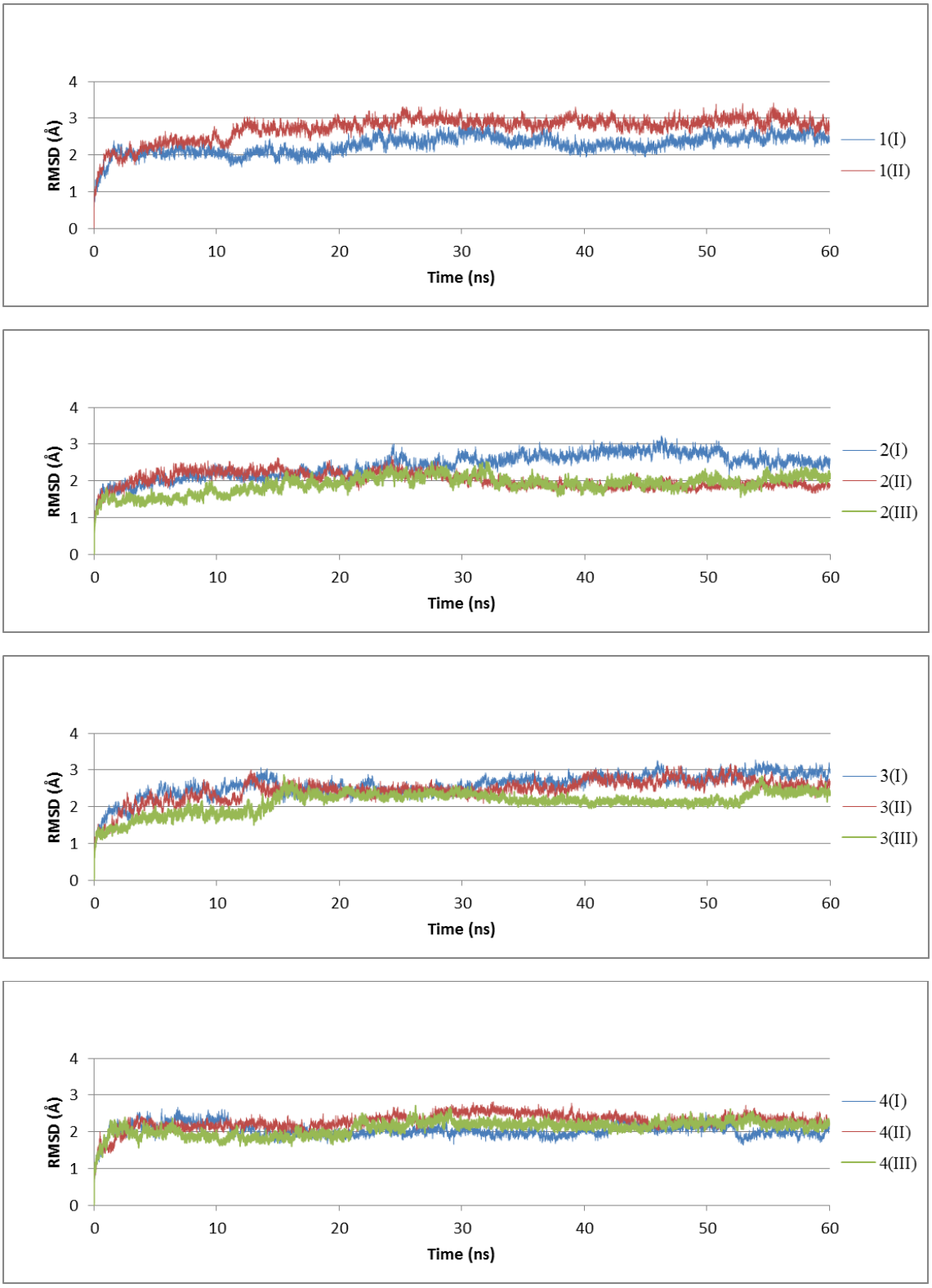


Figure S18. Backbone RMSD (N, CA, C, O) of the binding groove (αAla^{3}-Asn^{85}, βGlu^{4}-Gln^{97}) of A^{q} in complex with glycopeptide **1-4** vs simulation time.

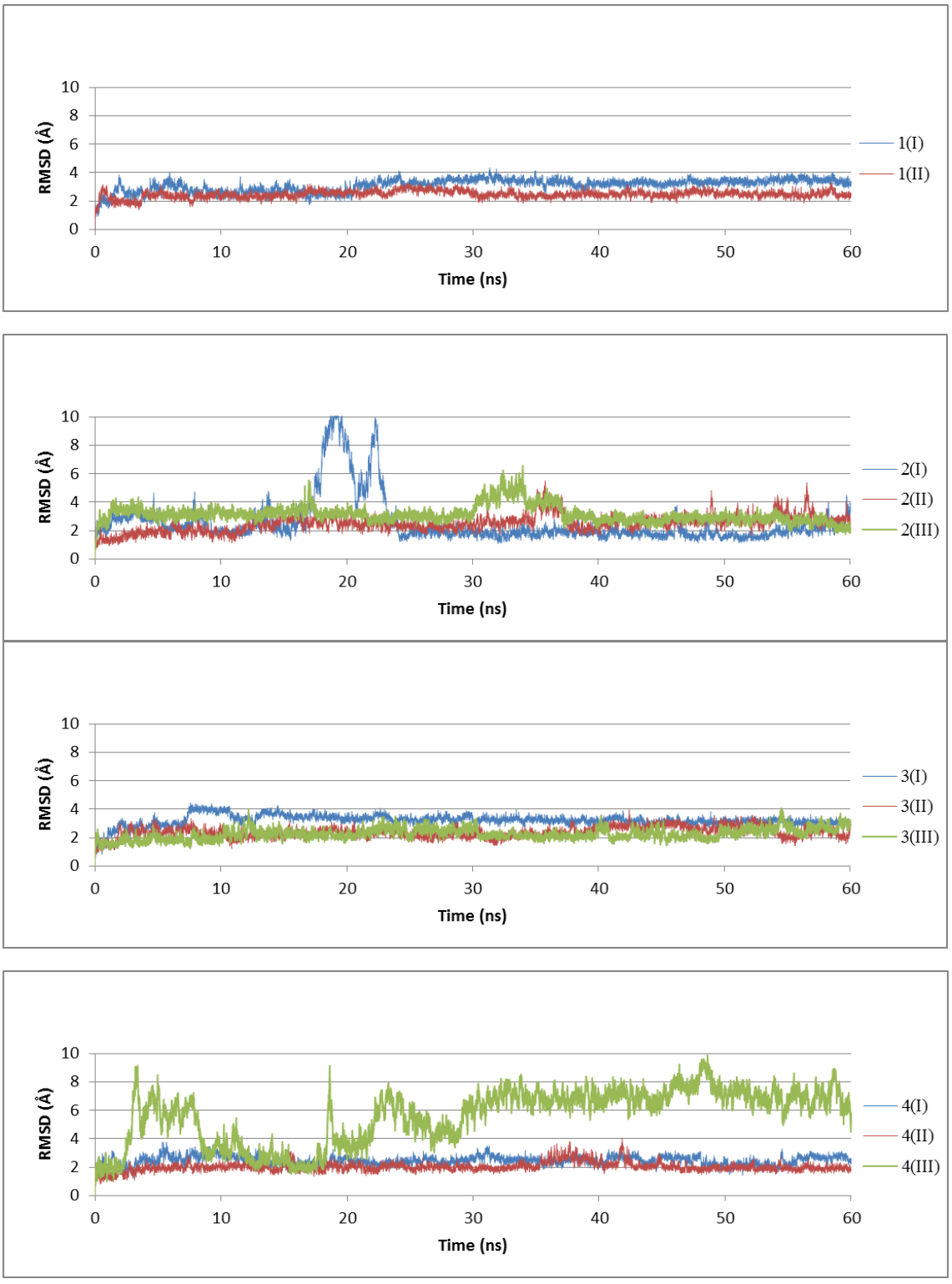


Figure S19. Backbone RMSD (N, CA, C, O) of glycopeptide **1-4** of A^q in complex with **1-4** vs simulation time.

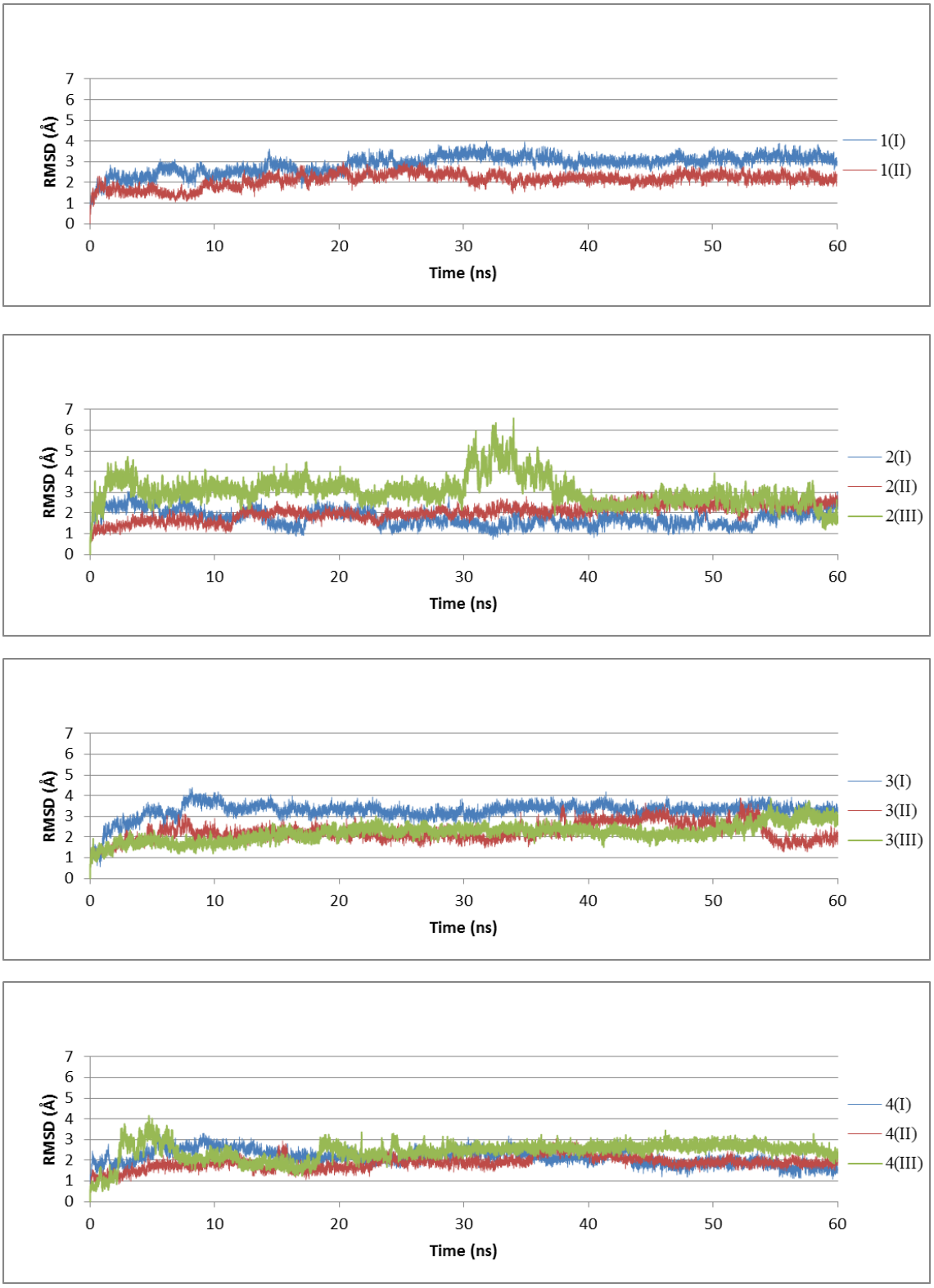


Figure S20. Backbone RMSD (N, CA, C, O) of Ile^{260}-Glu^{266} of glycopeptide **1-4** of A^q in complex with **1-4** vs simulation time.

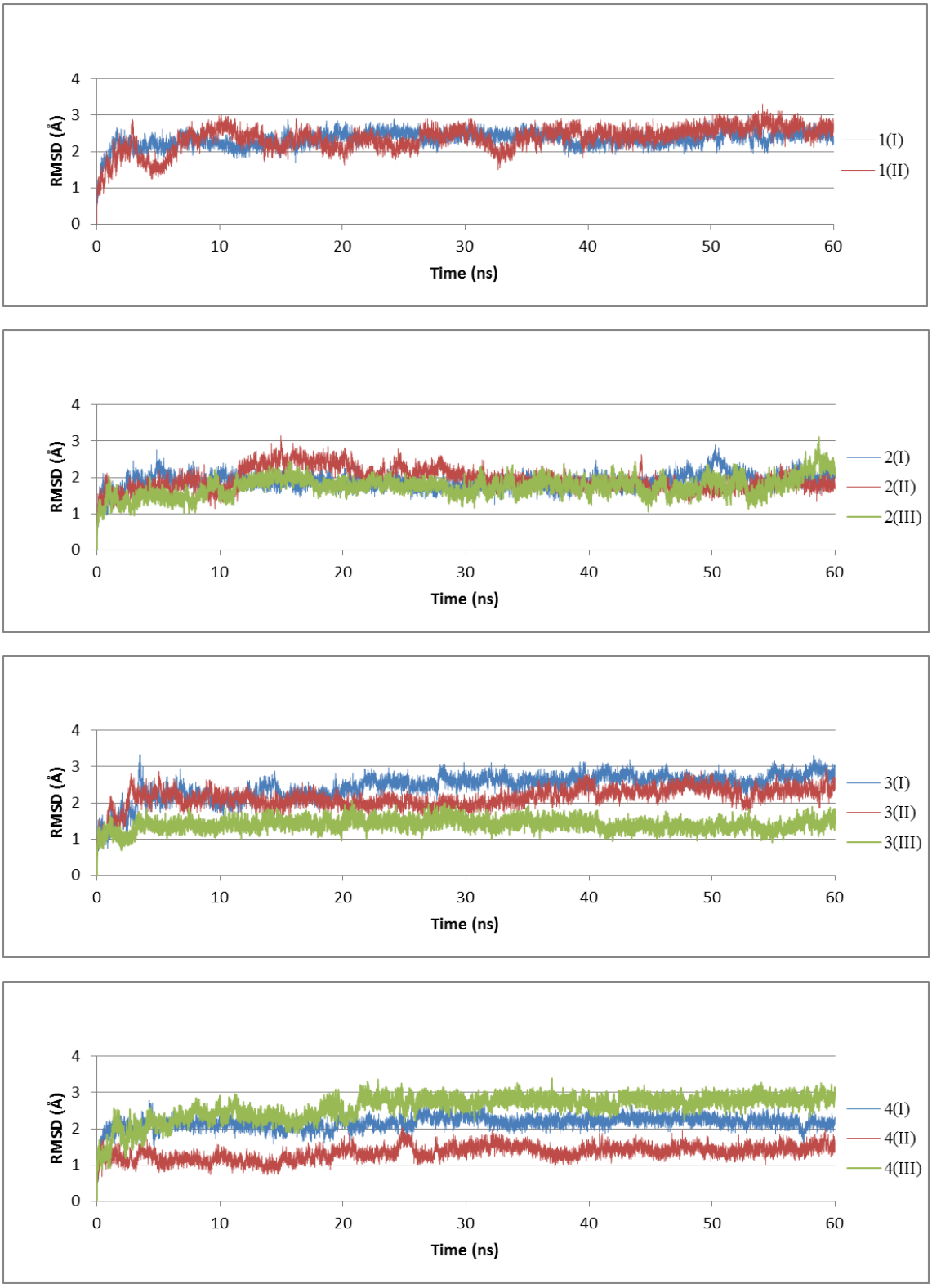


Figure S21. Backbone RMSD (N, CA, C, O) of the α_1-helix (αAsp^{56}-Asn^{79}) of A^q in complex with glycopeptide **1-4** vs simulation time.

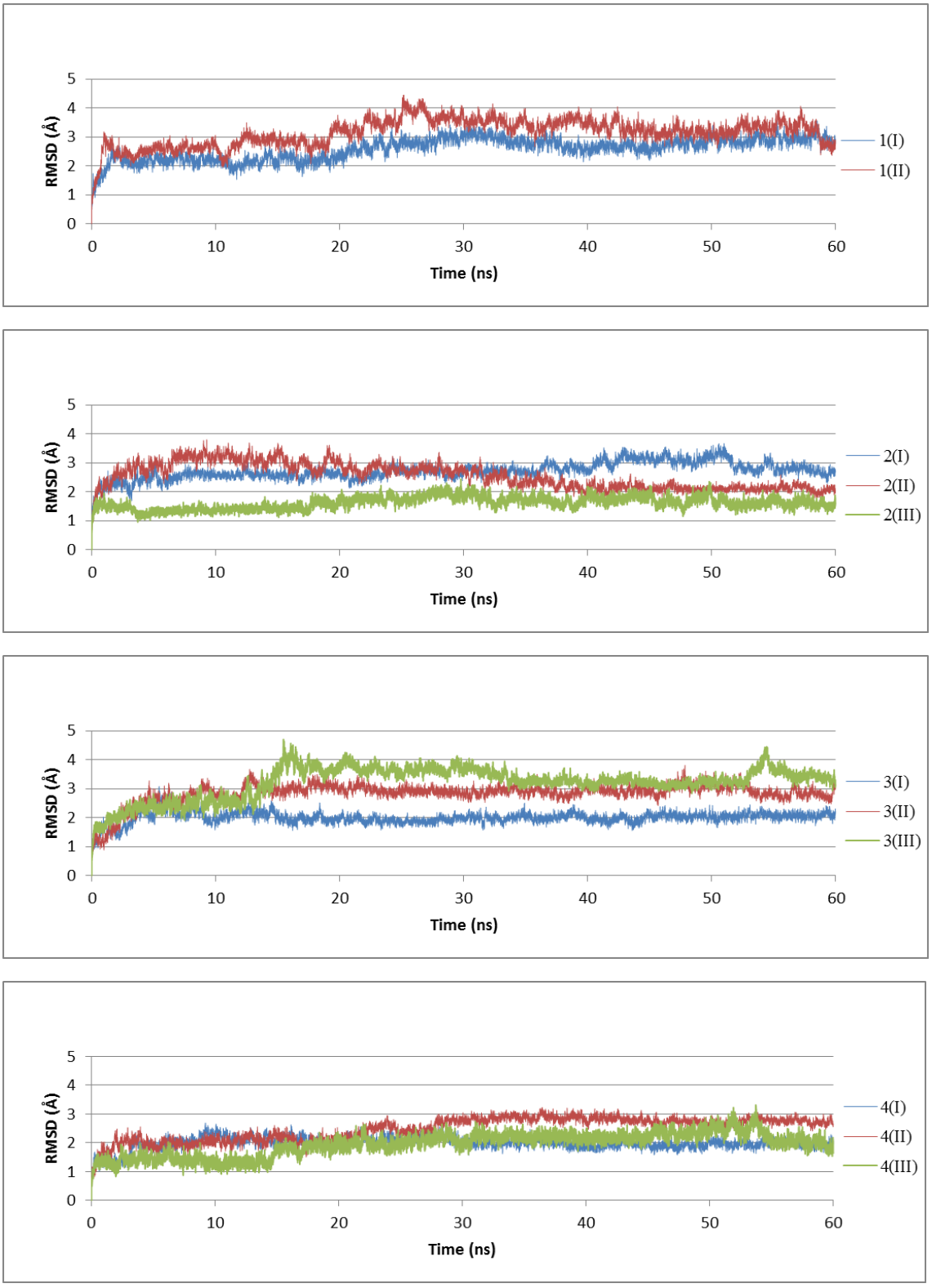
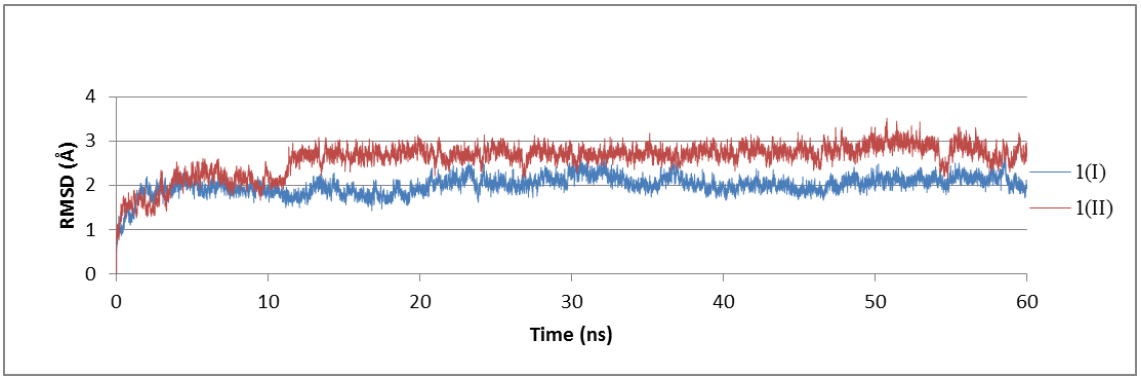
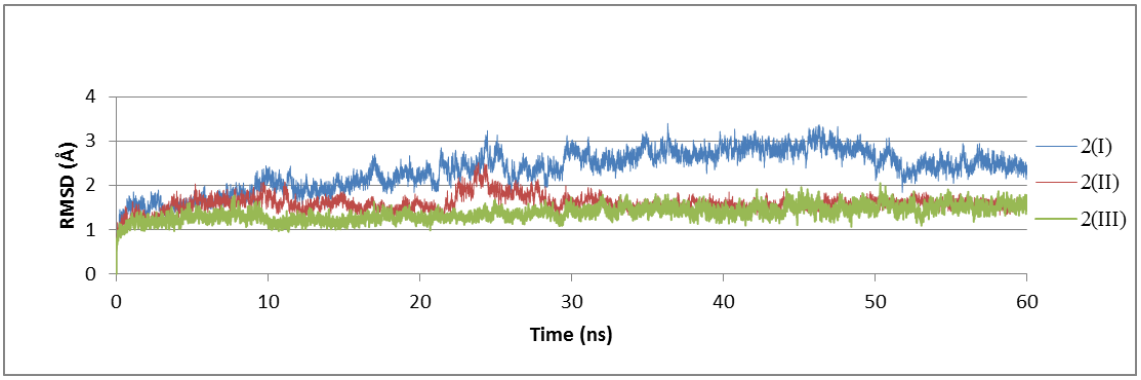
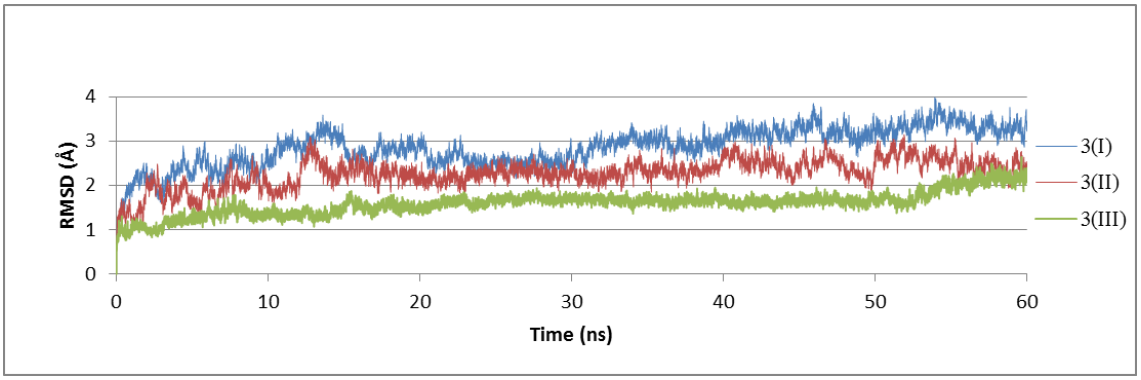


Figure S22. Backbone RMSD (N, CA, C, O) of the β_1-helix (βGlu^{52}-Arg^{94}) of A^q in complex with glycopeptide **1-4** vs simulation time.







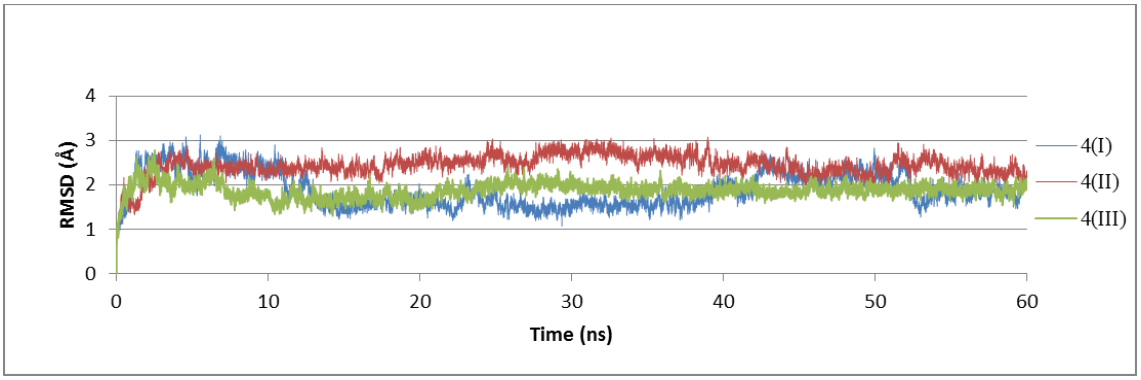


Figure S23. Backbone RMSD of the β-sheet of the $\alpha_1\beta_1$-domain (αAla^3-Leu^{46}, βPhe^7-Ser^{42}) of A^q in complex with glycopeptide **1-4** vs simulations time.

Table S24. The number of frames occupying each cluster in every MD simulation. Clustering against the minimal epitope of the glycopeptide (Ile^{260}-Gln^{267}) over the last 20 ns has been performed in VMD with the clustering plugin. The frames were superposed against the binding groove (αAla^{3}-Asn^{85}, βGlu^{4}-Gln^{97}) of A^{q} at 40 ns. Frames from each cluster have been compared to aid the visual comparison.

Cluster	1(I)	1(II)	2(I)	2(II)	2(III)	3(I)	3(II)	3(III)	4(I)	4(II)	4(III)
C1	2552	2445	758	1519	269	2888	1121	410	3111	1509	5011
C2	1293	1331	233	1243	235	1967	692	251	1274	1006	612
C3	728	1028	232	703	188	478	388	233	407	937	416
C4	543	886	217	579	149	443	306	170	382	637	403
C5	483	498	205	501	135	398	306	157	303	520	318
C6	317	326	170	483	125	351	292	154	278	377	261
C7	235	300	145	255	121	347	225	138	264	374	212
C8	210	284	142	251	118	257	167	131	259	310	199
C9	200	267	136	238	112	184	160	124	253	232	173
C10	163	212	133	218	101	167	153	122	200	225	145
C11	159	182	125	199	95	165	152	116	196	223	142
C12	158	153	110	183	88	154	151	107	163	194	110
C13	135	152	103	160	77	150	146	106	149	184	106
C14	129	148	103	139	67	133	114	105	145	175	87
C15	124	103	88	134	63	86	105	103	141	173	82
C16	99	101	86	130	60	78	103	95	108	159	81
C17	93	97	86	111	57	70	101	94	94	121	77
C18	88	63	86	107	57	66	97	91	90	97	70
C19	84	61	80	102	56	61	97	88	75	95	62
C20	83	61	76	91	56	56	96	83	73	92	56
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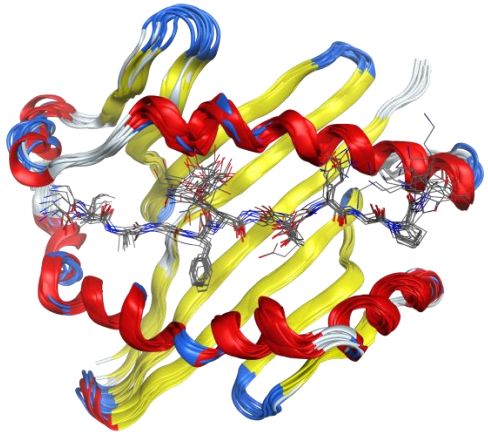
1(I)



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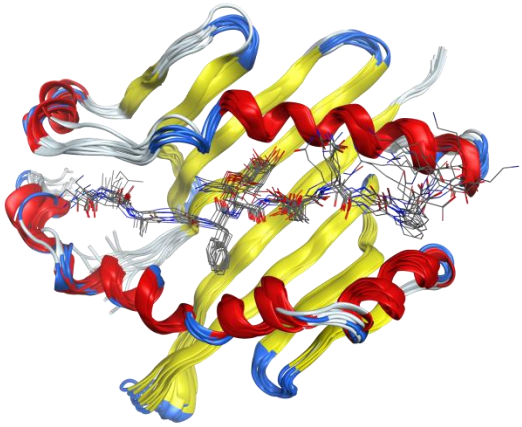

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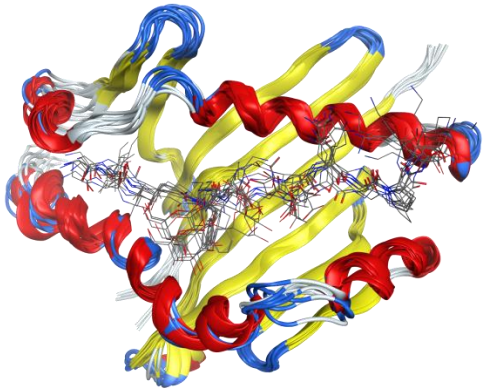

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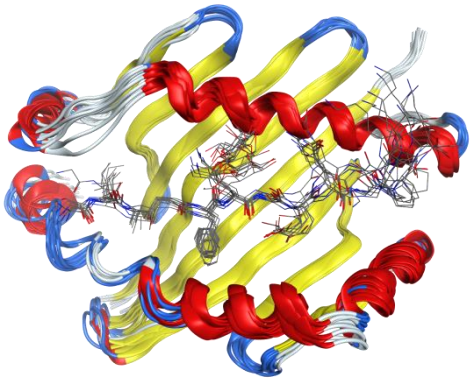

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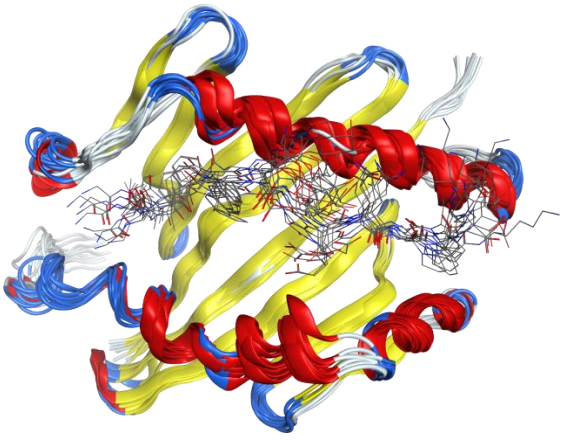

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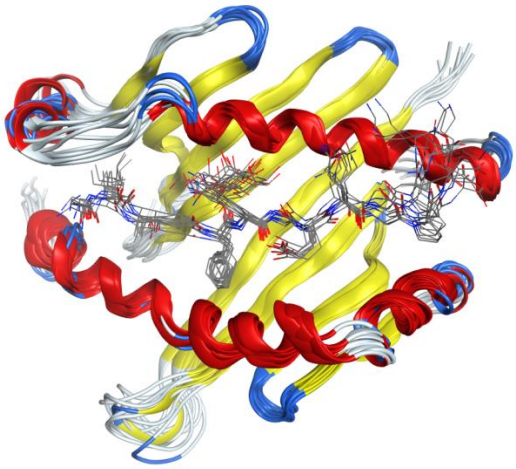

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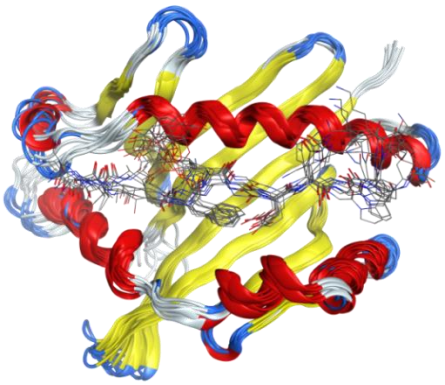

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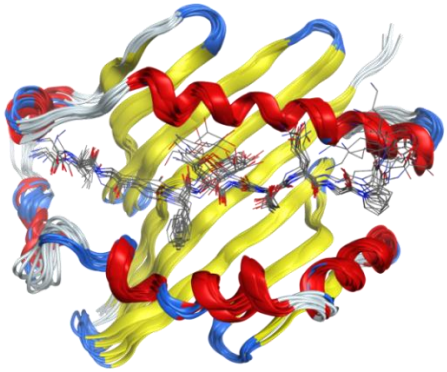

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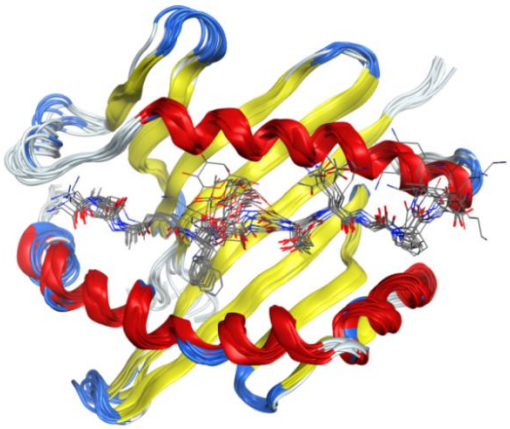
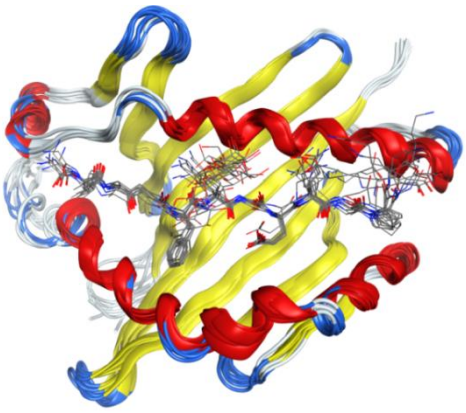


4(II)



4(III)

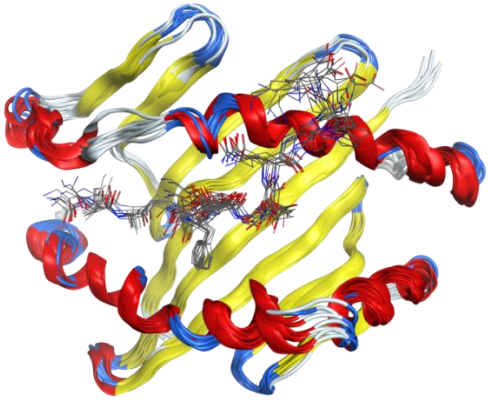
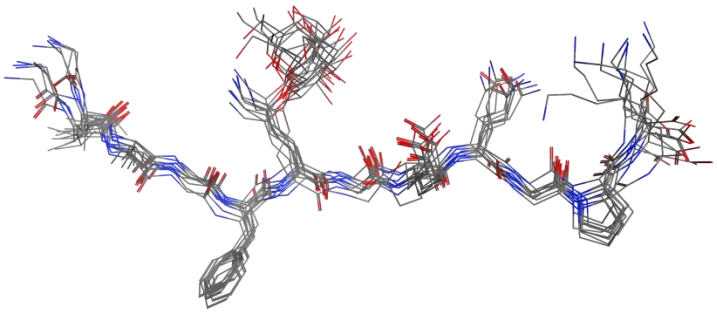
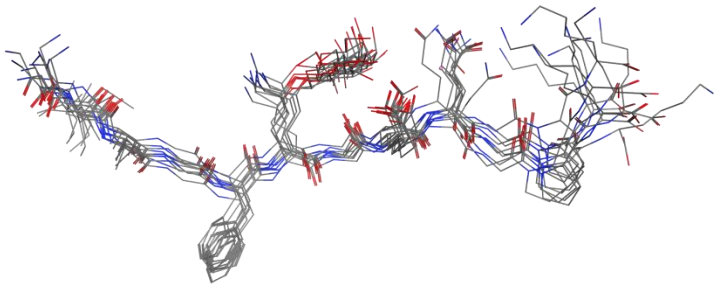


Figure S26. Superposition of one frame from each of the top 10 clusters displaying a complex between A^q and glycopeptide **1-4**. Superposed against the binding groove (αAla^3-Asn^{85}, $\beta Glu4$-Gln^{97}). Only the secondary structure is displayed for the protein, the glycopeptide is displayed with carbons in grey, oxygen in red and nitrogen in blue.

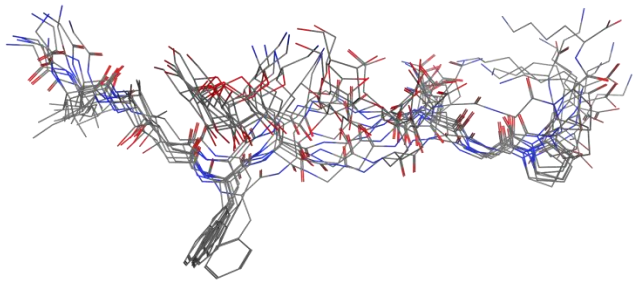
1(I)



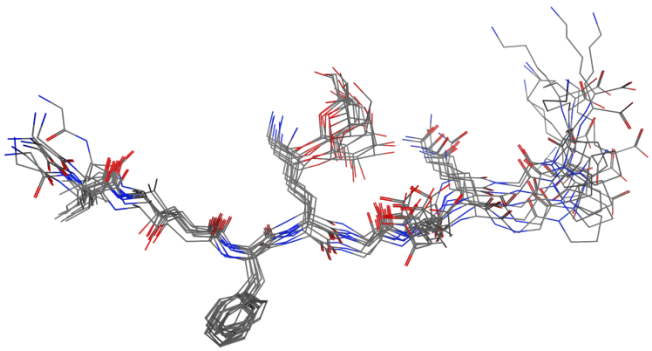
1(II)



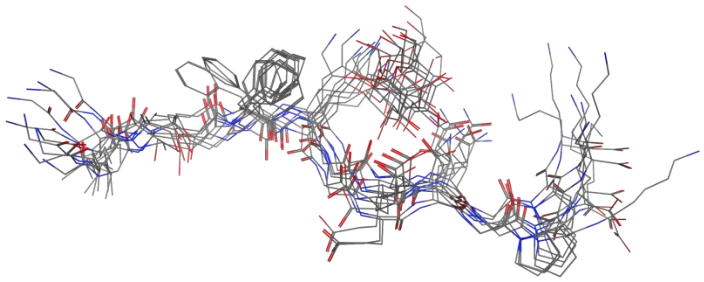
2(I)



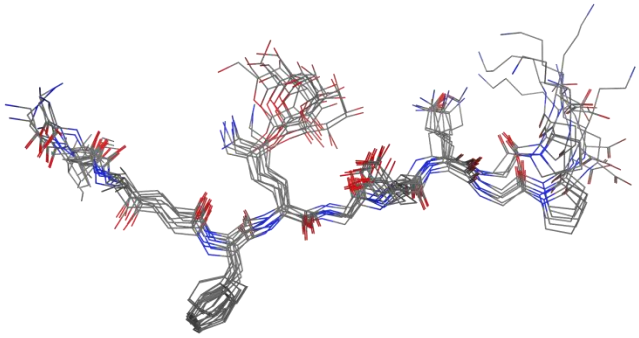
2(II)



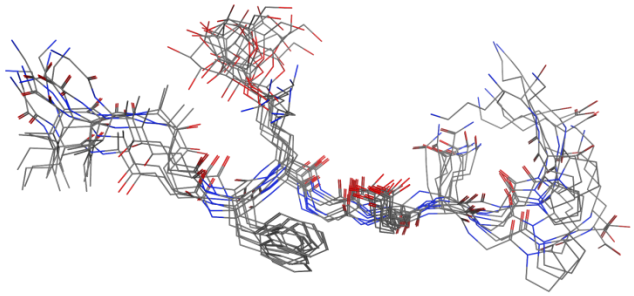
2(III)



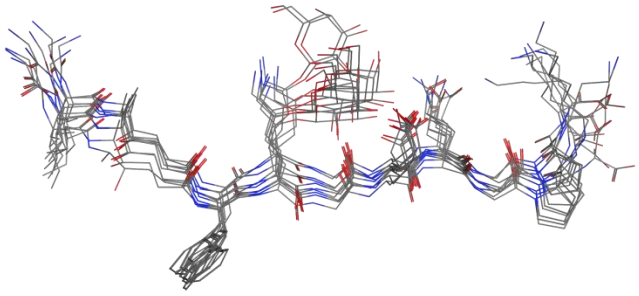
3(I)



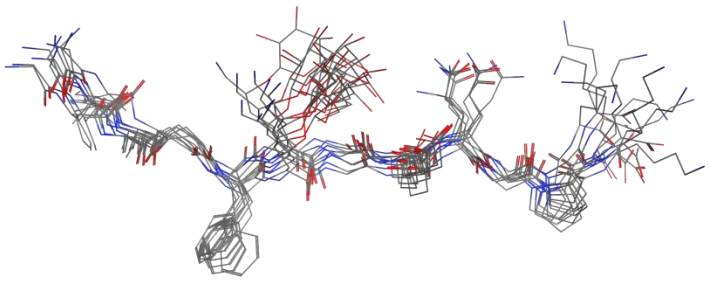
3(II)



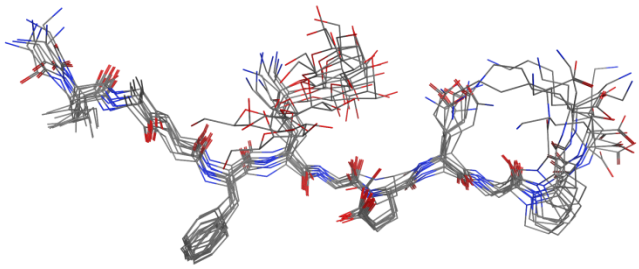
3(III)



4(I)



4(II)



4(III)

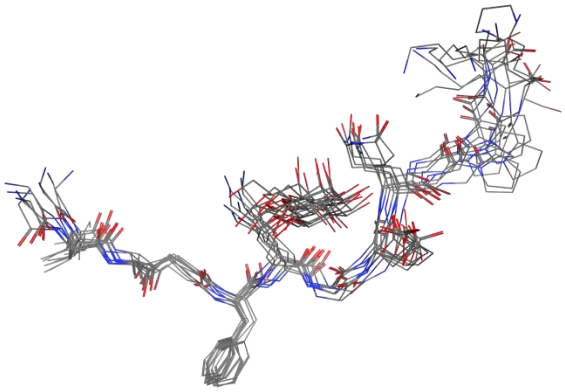
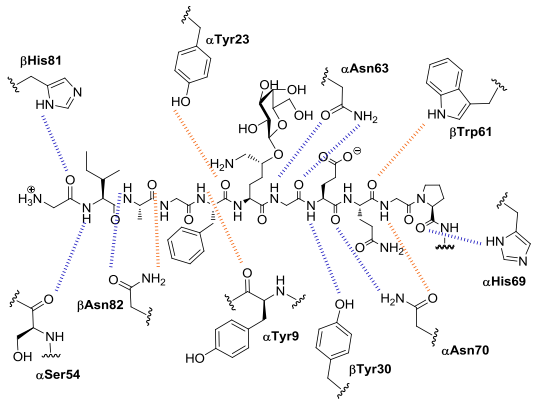
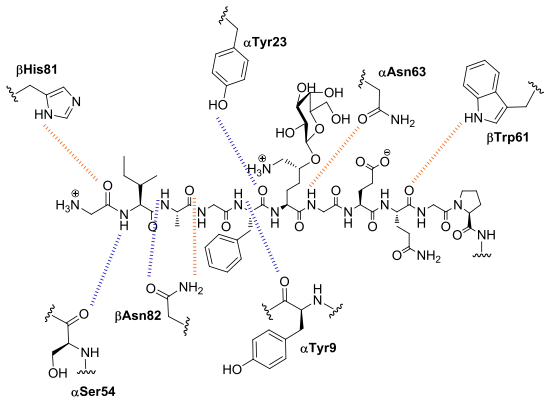


Figure S29. Superposition of one frame from each of the top 10 clusters displaying glycopeptide **1**-**4**. Superposed against the binding groove (αAla^{3}-Asn^{85}, βGlu^{4}-Gln^{97}). The glycopeptide is displayed with carbons in grey, oxygen in red and nitrogen in blue.

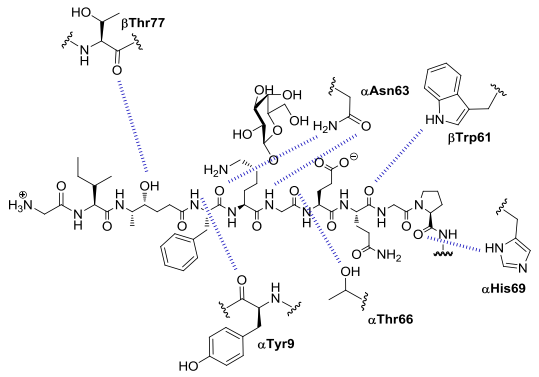
1(I)



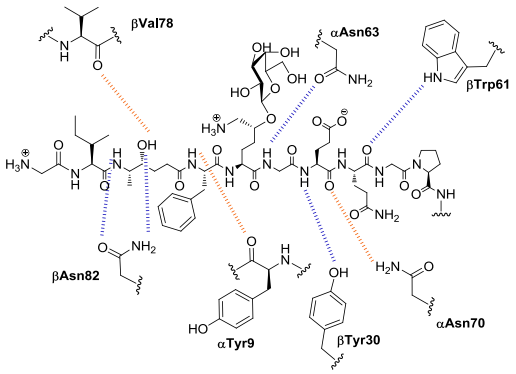
1(I)



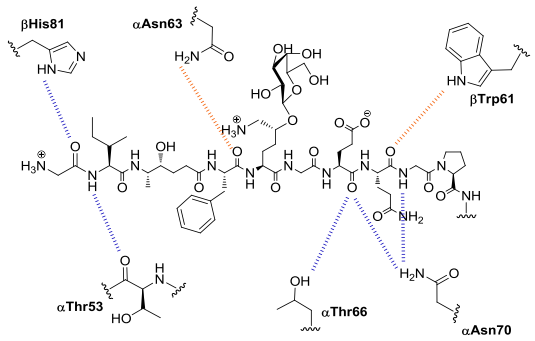
2(I)



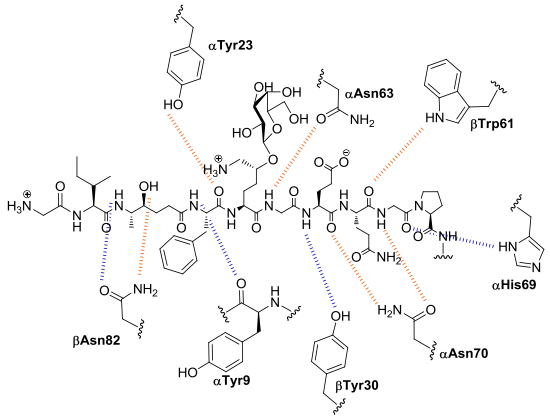
2(II)



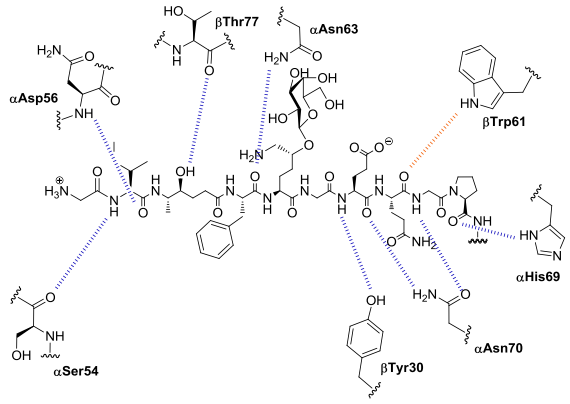
2(III)



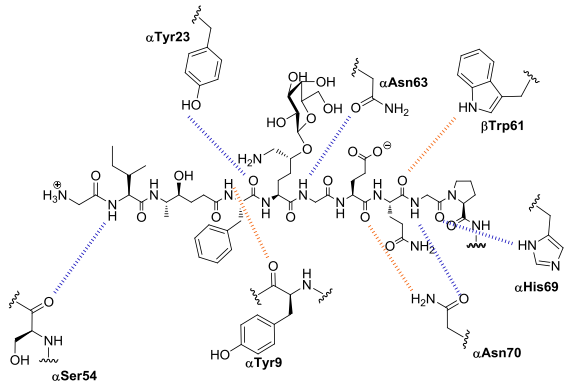
3(I)



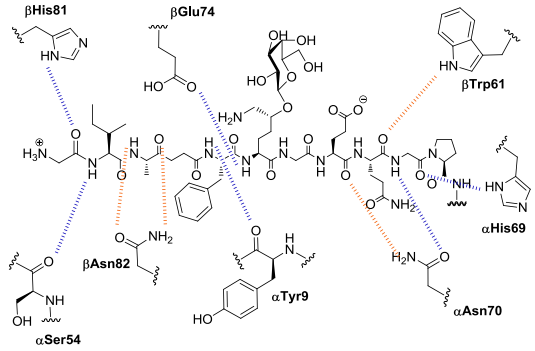
3(II)



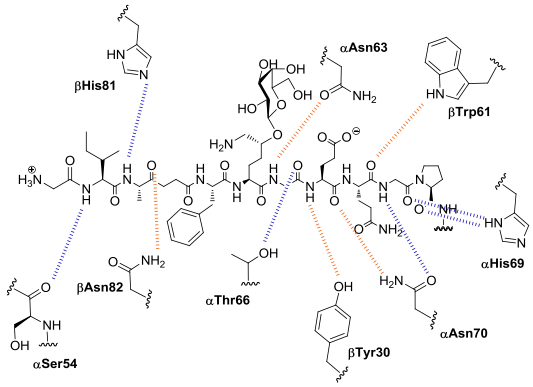
3(III)



4(I)



4(II)



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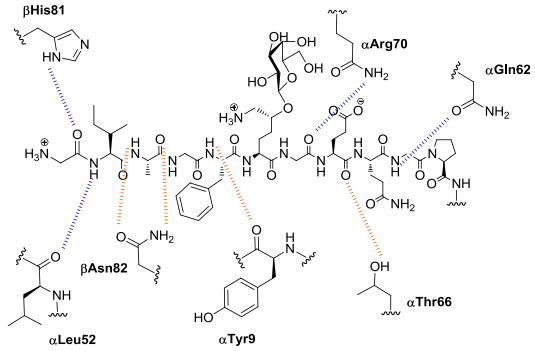

Figure S31. Visualization of hydrogen bonds formed between A^q and the glycipeptides **1**-**4**. Orange indicates a strong hydrogen bond with an occupancy > 40 %, blue indicates a weak hydrogen bond with an occupancy < 40 %. Only hydrogen bonds with an occupancy > 10 % are reported.