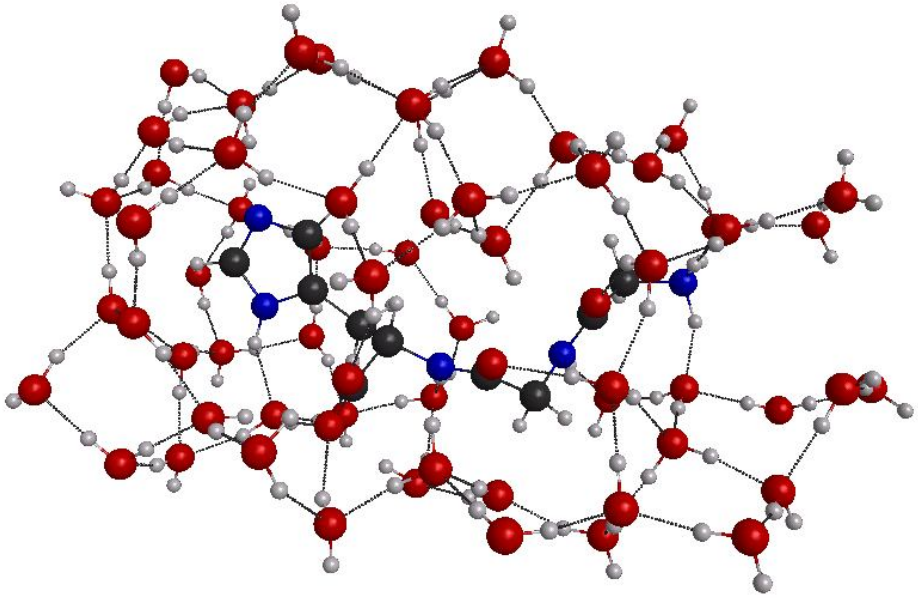
Electronic supplementary materials *Mendeleev Commun.*, 2011, **21**, 72−74

Spatial structures of tripeptides glycylglycyl-L-histidine and glycylglycyl-L-tyrosine based on residual dipolar couplings and quantum-chemical computations

Vladimir V. Klochkov, Anton V. Klochkov, Marat N. Shamsutdinov, Sergey V. Efimov, Alexander A. Krutikov, Edward M. Gilyazetdinov, Yulia I. Zyavkina and Valery G. Shtyrlin*



GlyGlyHis·60H_2O

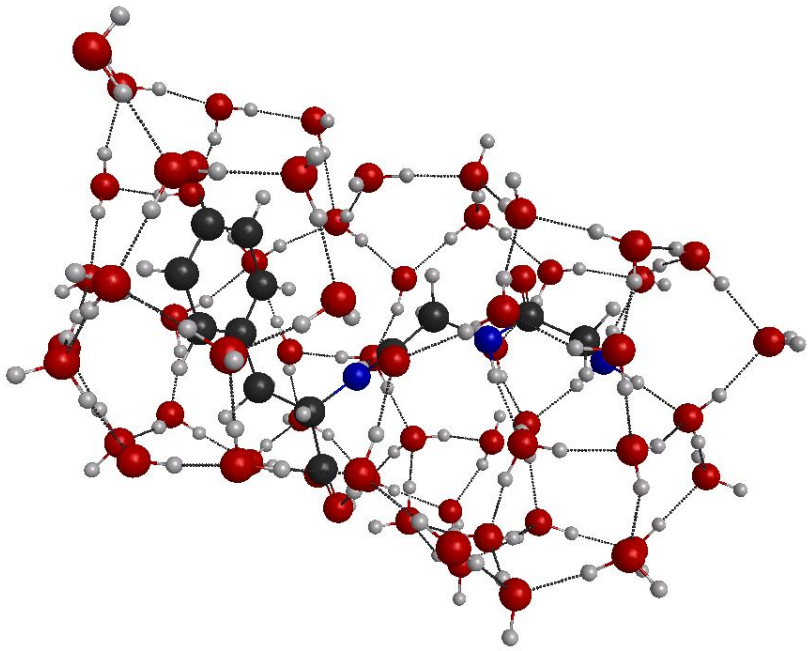


Figure 1S The optimized structures of tripeptides GlyGlyHis and GlyGlyTyr with hydrate shells included 60 (GlyGlyHis) or 56 (GlyGlyTyr) water molecules.

Table S1 The coordinates of the tripeptide GlyGlyHis conformation atoms in the pdb format.

Atom nr.	Atom	Part of tripeptide	x-Coordinate	y-Coordinate	z-Coordinate
1	C	1GLY	3.770	0.290	0.232
2	CA	1GLY	4.669	0.840	1.333
3	N	1GLY	6.084	0.445	1.071
4	O	1GLY	3.748	-0.926	0.004
5	1HA	1GLY	4.634	1.928	1.399
6	2HA	1GLY	4.372	0.403	2.286
7	1HN	1GLY	6.344	0.832	0.162
8	2HN	1GLY	6.209	-0.573	1.061
9	3HN	1GLY	6.658	0.851	1.823
10	C	2GLY	1.123	-0.198	-1.412
11	CA	2GLY	2.278	0.788	-1.657
12	N	2GLY	3.017	1.175	-0.448
13	O	2GLY	1.262	-1.419	-1.622
14	1HA	2GLY	1.881	1.704	-2.093
15	2HA	2GLY	2.943	0.334	-2.386
16	HN	2GLY	3.247	2.155	-0.359
17	C	3HIS	-1.990	-0.861	-1.805
18	CA	3HIS	-1.219	-0.364	-0.546
19	CB	3HIS	-1.994	0.652	0.321
20	CD2	3HIS	-3.207	-0.527	2.309
21	CE1	3HIS	-5.195	0.236	2.001
22	CG	3HIS	-3.164	0.193	1.134
23	N	3HIS	-0.007	0.364	-0.963
24	ND1	3HIS	-4.453	0.667	0.952
25	NE2	3HIS	-4.478	-0.491	2.848
26	O	3HIS	-2.628	0.009	-2.490
27	OXT	3HIS	-1.906	-2.078	-2.103
28	HA	3HIS	-0.928	-1.234	0.042
29	1HB	3HIS	-2.307	1.476	-0.315
30	2HB	3HIS	-1.258	1.063	1.019
31	HD2	3HIS	-2.392	-1.057	2.774
32	HE1	3HIS	-6.230	0.498	2.127
33	HN	3HIS	-0.054	1.375	-0.881
34	HD1	3HIS	-4.791	1.242	0.186

Table S2 The coordinates of the tripeptide GlyGlyTyr conformation atoms in the pdb format.

Atom nr.	Atom	Part of tripeptide	x-Coordinate	y-Coordinate	z-Coordinate
1	C	1GLY	3.720	-0.429	-0.310
2	CA	1GLY	4.749	0.173	0.636
3	N	1GLY	5.421	-0.861	1.483
4	O	1GLY	4.055	-1.230	-1.190
5	1HA	1GLY	5.512	0.648	0.031
6	2HA	1GLY	4.319	0.910	1.295
7	1HN	1GLY	5.944	-0.331	2.184
8	2HN	1GLY	6.062	-1.412	0.913
9	3HN	1GLY	4.713	-1.422	1.963
10	C	2GLY	0.066	0.161	-0.574
11	CA	2GLY	1.398	-0.411	-1.052
12	N	2GLY	2.456	-0.001	-0.137
13	O	2GLY	-0.105	1.406	-0.553
14	1HA	2GLY	1.598	-0.017	-2.054
15	2HA	2GLY	1.352	-1.498	-1.131
16	HN	2GLY	2.224	0.560	0.673
17	C	3TYR	-2.341	-0.815	1.729
18	CA	3TYR	-2.208	-0.487	0.212
19	CB	3TYR	-3.183	-1.325	-0.645
20	CD1	3TYR	-2.313	-1.492	-3.033
21	CD2	3TYR	-4.032	0.110	-2.545
22	CE1	3TYR	-2.270	-1.054	-4.359
23	CE2	3TYR	-4.004	0.554	-3.865
24	CG	3TYR	-3.179	-0.908	-2.098
25	CZ	3TYR	-3.098	-0.006	-4.775
26	N	3TYR	-0.828	-0.751	-0.208
27	OH	3TYR	-3.025	0.440	-6.068
28	O	3TYR	-2.301	0.151	2.546
29	OXT	3TYR	-2.447	-2.028	2.052
30	HA	3TYR	-2.402	0.574	0.056
31	1HB	3TYR	-4.183	-1.186	-0.226
32	2HB	3TYR	-2.932	-2.383	-0.533
33	HD1	3TYR	-1.666	-2.304	-2.721
34	HD2	3TYR	-4.737	0.557	-1.856
35	HE1	3TYR	-1.605	-1.522	-5.079
36	HE2	3TYR	-4.694	1.317	-4.198
37	HN	3TYR	-0.539	-1.725	-0.256
38	HH	3TYR	-3.290	1.378	-6.082