Supplementary information

Conformational preferences of aza-proline residues and their impact on the relative stability of polyproline structures

Hae Sook Park[a] and Young Kee Kang*[b]

[a] *Department of Nursing, Cheju Halla University, Cheju 63092, Republic of Korea*
[b] *Department of Chemistry, Chungbuk National University, Cheongju, Chungbuk 28644, Republic of Korea*

E-mail: ykkang@chungbuk.ac.kr

Table S1 Torsion angles, relative thermodynamic properties, and populations of local minima for Ac-Pro-OMe in water[a]

Conf.	Torsion angles[b]								ΔE_0[c]	ΔE_w[d]	ΔH_w[e]	ΔG_w[f]	w[g]
	ω'	ϕ	ψ	χ^0	χ^1	χ^2	χ^3	χ^4					
tFd	176	-63	158	-13	31	-38	30	-11	0.00	0.00	0.00	0.00	35.6
tAd	176	-62	-23	-13	31	-38	30	-10	0.98	0.68	0.61	0.14	28.0
tFu	180	-53	143	9	-30	40	-34	16	0.83	0.19	0.15	0.62	12.5
cFd	-6	-74	169	-21	35	-37	25	-2	1.22	0.72	0.70	0.65	11.8
tAu	178	-52	-36	6	-28	39	-35	18	1.28	0.53	0.62	0.87	8.2
cAd	-8	-70	-13	-21	35	-37	25	-3	1.53	1.43	1.39	1.54	2.7
cAu	-8	-52	-33	2	-24	38	-36	22	1.89	1.82	1.96	2.38	0.6
cFu	-7	-57	162	1	-24	38	-36	22	2.04	1.54	1.74	2.43	0.6
ts1	116	-99	80	16	11	-34	44	-38	18.36	22.69	21.87	23.78	
ts2	115	-101	43	13	-35	42	-35	13	19.59	23.42	22.29	23.78	
ts3	-62	-110	76	5	21	-38	41	-29	22.13	22.26	21.30	22.34	
ts4	-58	-85	-91	26	-42	42	-27	1	24.03	23.29	22.43	23.65	

[a] Calculated at the M06-2X/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in water at 25 °C: taken from ref. 52 except for ts1 and ts2. [b] Torsion angles are defined in Fig. 1c. [c] Relative energies calculated at the M06-2X/def2-TZVP level of theory in the gas phase. [d] Relative energies in water calculated by the sum of ΔE_0 and the solvation free energy ($\Delta\Delta G_s$) at the SMD M06-2Z/6-31G(d) level of theory in water. [e] ΔH_w are relative enthalpies in water calculated by the sum of ΔE_w and thermal-enthalpic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [f] ΔG_w are relative Gibbs free energies in water calculated by the sum of ΔH_w and entropic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [g] Populations in water calculated from ΔG_w values at 25 °C.

Table S2 Torsion angles, relative thermodynamic properties, and populations of local minima for Ac-α-azPro-OMe in water[a]

Conf.	Torsion angles[b]								ΔE_0[c]	ΔE_w[d]	ΔH_w[e]	ΔG_w[f]	w[g]
	ω'	ϕ	ψ	χ^0	χ^1	χ^2	χ^3	χ^4					
cFd	10	-93	-164	-24	38	-37	23	0	0.66	0.08	0.00	0.00	16.6
cBd	11	-99	22	-26	38	-36	21	2	0.00	0.36	0.27	0.11	13.9
tBd	-171	-88	22	-22	37	-37	25	-2	4.43	0.16	0.10	0.13	13.3
tB*u	171	88	-22	22	-37	37	-25	2	4.43	0.16	0.10	0.13	13.3
tFe	-171	-80	-171	-17	-8	28	-38	34	6.12	0.12	0.11	0.36	9.0
tFd	-173	-81	-169	-19	35	-38	27	-6	6.08	0.00	0.03	0.38	8.7
tF*u	173	81	169	19	-35	38	-27	6	6.08	0.00	0.03	0.38	8.7
tB*e	170	86	-16	20	4	-25	37	-36	4.49	0.34	0.42	0.72	4.9
tBe	-170	-86	16	-20	-4	25	-37	36	4.49	0.34	0.42	0.72	4.9
cFe	16	-95	-167	-22	-3	25	-38	37	0.89	0.74	0.68	0.73	4.8
cBe	18	-102	18	-25	1	22	-36	38	0.31	1.06	1.16	1.63	1.1
cB*e	-18	102	-18	25	-1	-22	36	-38	0.30	1.06	1.16	1.63	1.1
ts1	116	-116	23	-15	34	-39	31	-10	15.25	17.66	16.59	18.11	
ts1	116	-116	23	-15	34	-39	31	-10	15.25	17.66	16.59	18.11	
ts2	115	-108	13	-22	3	16	-29	31	13.93	15.93	14.83	15.31	
ts3	-74	-98	14	-17	-2	19	-29	28	18.96	15.76	14.85	15.91	

[a] Calculated at the M06-2X/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in water at 25 °C. [b] Torsion angles are defined in Fig. 1c. [c] Relative energies calculated at the M06-2X/def2-TZVP level of theory in the gas phase. [d] Relative energies in water calculated by the sum of ΔE_0 and the solvation free energy ($\Delta\Delta G_s$) at the SMD M06-2Z/6-31G(d) level of theory in water. [e] ΔH_w are relative enthalpies in water calculated by the sum of ΔE_w and thermal-enthalpic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [f] ΔG_w are relative Gibbs free energies in water calculated by the sum of ΔH_w and entropic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [g] Populations in water calculated from ΔG_w values at 25 °C.

Table S3 Torsion angles, relative thermodynamic properties, and populations of local minima for Ac-β-azPro-OMe in water[a]

Conf.	Torsion angles[b]								ΔE_0[c]	ΔE_w[d]	ΔH_w[e]	ΔG_w[f]	w[g]
	ω'	ϕ	ψ	χ^0	χ^1	χ^2	χ^3	χ^4					
tFd	173	-56	149	-8	26	-35	29	-13	0.00	0.00	0.00	0.00	42.6
tAd	175	-54	-37	-7	25	-34	28	-13	1.66	0.64	0.45	0.25	28.1
cFd	-5	-70	160	-18	32	-34	23	-3	1.50	1.03	1.01	0.37	22.6
cAd	-7	-63	-25	-17	31	-34	24	-4	2.51	1.70	1.67	1.50	3.4
tFu	179	-53	142	7	-30	42	-36	18	2.90	2.45	2.12	1.88	1.8
cFu	-1	-55	138	10	-30	39	-32	13	2.07	2.30	2.26	2.31	0.9
tAu	177	-52	-36	3	-27	41	-37	21	2.37	2.62	2.37	2.61	0.5
cAu	-10	-50	-33	1	-25	39	-37	23	2.94	4.26	3.89	3.43	0.1
ts1	120	-107	-92	7	18	-36	40	-28	17.52	21.55	20.36	21.07	
ts2	120	-107	77	12	-33	40	-32	12	16.16	20.65	19.48	20.41	
ts3	-58	-114	75	2	22	-37	38	-24	22.51	20.10	19.09	20.47	
ts4	-60	-87	-98	25	-40	39	-23	-1	22.10	21.31	20.31	21.36	

[a] Calculated at the M06-2X/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in water at 25 °C. [b] Torsion angles are defined in Fig. 1c. [c] Relative energies calculated at the M06-2X/def2-TZVP level of theory in the gas phase. [d] Relative energies in water calculated by the sum of ΔE_0 and the solvation free energy ($\Delta\Delta G_s$) at the SMD M06-2Z/6-31G(d) level of theory in water. [e] ΔH_w are relative enthalpies in water calculated by the sum of ΔE_w and thermal-enthalpic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [f] ΔG_w are relative Gibbs free energies in water calculated by the sum of ΔH_w and entropic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [g] Populations in water calculated from ΔG_w values at 25 °C.

Table S4 Torsion angles, relative thermodynamic properties, and populations of local minima for Ac-γ-azPro-OMe in water[a]

Conf.	Torsion angles[b]								ΔE_0[c]	ΔE_w[d]	ΔH_w[e]	ΔG_w[f]	w[g]
	ω'	ϕ	ψ	χ^0	χ^1	χ^2	χ^3	χ^4					
tFd	173	-56	149	-7	28	-38	33	-16	0.00	0.00	0.00	0.00	38.8
tFu	178	-53	144	5	-26	38	-35	18	1.83	0.64	0.63	0.37	20.9
cFd	-2	-70	160	-12	30	-38	30	-11	1.01	0.69	0.71	0.40	19.8
tAd	174	-52	-37	-6	27	-38	34	-17	1.53	0.71	0.73	0.81	9.8
cAd	-6	-61	-31	-13	31	-38	29	-9	1.66	1.51	1.52	1.32	4.2
tAu	177	-51	-37	3	-25	38	-35	20	2.32	0.94	1.04	1.39	3.7
cFu	-6	-58	165	2	-24	37	-36	21	2.53	1.70	1.73	1.65	2.4
cAu	-9	-51	-33	1	-23	37	-36	22	2.39	1.97	2.22	2.90	0.3
ts1	120	-94	17	22	3	-28	42	-40	19.03	22.19	21.28	22.16	
ts2	120	-119	21	-2	-22	36	-39	26	18.54	21.52	20.50	21.55	
ts3	-61	-109	66	6	23	-43	47	-32	26.84	24.71	23.64	24.77	
ts4	-61	-97	46	17	-35	40	-30	8	24.19	21.41	20.37	21.50	

[a] Calculated at the M06-2X/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in water at 25 °C. [b] Torsion angles are defined in Fig. 1c. [c] Relative energies calculated at the M06-2X/def2-TZVP level of theory in the gas phase. [d] Relative energies in water calculated by the sum of ΔE_0 and the solvation free energy ($\Delta\Delta G_s$) at the SMD M06-2Z/6-31G(d) level of theory in water. [e] ΔH_w are relative enthalpies in water calculated by the sum of ΔE_w and thermal-enthalpic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [f] ΔG_w are relative Gibbs free energies in water calculated by the sum of ΔH_w and entropic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [g] Populations in water calculated from ΔG_w values at 25 °C.

Table S5 Torsion angles, relative thermodynamic properties, and populations of local minima for Ac-δ-azPro-OMe in water[a]

Conf.	Torsion angles[b]								ΔE_0[c]	ΔE_w[d]	ΔH_w[e]	ΔG_w[f]	w[g]
	ω'	ϕ	ψ	χ^0	χ^1	χ^2	χ^3	χ^4					
tAd	172	-47	-40	-1	22	-36	35	-22	0.77	0.53	0.47	0.00	43.5
tFu	-177	-63	150	0	-23	37	-37	23	0.00	0.15	0.19	0.16	33.2
tFd	171	-50	148	-3	24	-37	35	-20	0.03	0.00	0.00	0.59	16.1
tAu	-179	-60	-33	-2	-21	37	-37	25	0.74	0.49	0.58	1.23	5.5
cFu	-5	-64	165	-8	-16	33	-38	29	6.02	1.52	1.75	2.38	0.8
cAu	-5	-57	-31	-2	-21	36	-37	25	5.88	1.88	2.03	2.65	0.5
cFd	-7	-63	162	-10	31	-41	35	-16	5.03	2.65	2.76	3.13	0.2
cAd	-7	-57	-29	-7	26	-37	33	-16	6.56	2.24	2.39	3.35	0.2
ts1	124	-152	101	-28	16	0	-18	29	14.43	19.30	18.33	19.83	
ts2	120	-112	78	8	-28	39	-35	17	15.73	19.79	18.75	20.37	
ts3	-50	-147	100	-26	19	-6	-10	22	18.62	19.63	18.92	20.35	

[a] Calculated at the M06-2X/def2-TZVP//SMD M06-2X/6-31+G(d) level of theory in water at 25 °C. [b] Torsion angles are defined in Fig. 1c. [c] Relative energies calculated at the M06-2X/def2-TZVP level of theory in the gas phase. [d] Relative energies in water calculated by the sum of ΔE_0 and the solvation free energy ($\Delta\Delta G_s$) at the SMD M06-2Z/6-31G(d) level of theory in water. [e] ΔH_w are relative enthalpies in water calculated by the sum of ΔE_w and thermal-enthalpic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [f] ΔG_w are relative Gibbs free energies in water calculated by the sum of ΔH_w and entropic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [g] Populations in water calculated from ΔG_w values at 25 °C.

Table S6 Torsion angles, relative thermodynamic properties, and populations of local minima for Ac-α-azPro-NHMe in water[a]

Conf.	Torsion angles[b]								ΔE_0[c]	ΔE_w[d]	ΔH_w[e]	ΔG_w[f]	w[g]
	ω'	ϕ	ψ	χ^0	χ^1	χ^2	χ^3	χ^4					
cDd	13	-109	18	-28	40	-37	21	4	0.00	0.00	0.00	0.00	17.6
tBd	-170	-90	33	-22	38	-39	25	-3	2.01	0.14	0.95	0.06	16.0
tB*u	170	90	-33	22	-38	39	-25	3	2.01	0.14	0.95	0.06	16.0
cFd	2	-87	-173	-28	39	-36	20	5	4.77	0.60	1.40	0.28	11.0
tF*u	176	80	172	24	-38	38	-23	0	9.99	0.89	1.67	0.31	10.4
tFd	-176	-80	-172	-24	38	-38	23	0	9.99	0.89	1.67	0.31	10.4
tBe	-168	-92	16	-19	-6	27	-38	36	4.89	0.55	1.42	0.47	8.0
tB*e	168	92	-16	19	6	-27	38	-36	4.89	0.55	1.42	0.47	8.0
cFe	13	-96	-168	-22	-3	26	-38	37	5.13	1.72	2.50	1.15	2.5
ts1	118	-129	17	-28	12	9	-25	33	13.74	15.51	15.10	14.57	
ts3	-73	-109	17	-7	29	-39	35	-19	15.48	16.28	15.89	15.89	
ts4	-69	-110	16	-15	-4	21	-30	28	14.87	15.05	15.00	14.86	

[a] Calculated at the M06-2X/def2-TZVP//PCM M06-2X/6-31+G(d) level of theory in water at 25 °C. [b] Torsion angles are defined in Fig. 1c. [c] Relative energies calculated at the M06-2X/def2-TZVP level of theory in the gas phase. [d] Relative energies in water calculated by the sum of ΔE_0 and the solvation free energy ($\Delta\Delta G_s$) at the SMD M06-2Z/6-31G(d) level of theory in water. [e] ΔH_w are relative enthalpies in water calculated by the sum of ΔE_w and thermal-enthalpic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [f] ΔG_w are relative Gibbs free energies in water calculated by the sum of ΔH_w and entropic contributions at the SMD M06-2Z/6-31G(d) level of theory in water. [g] Populations in water calculated from ΔG_w values at 25 °C.

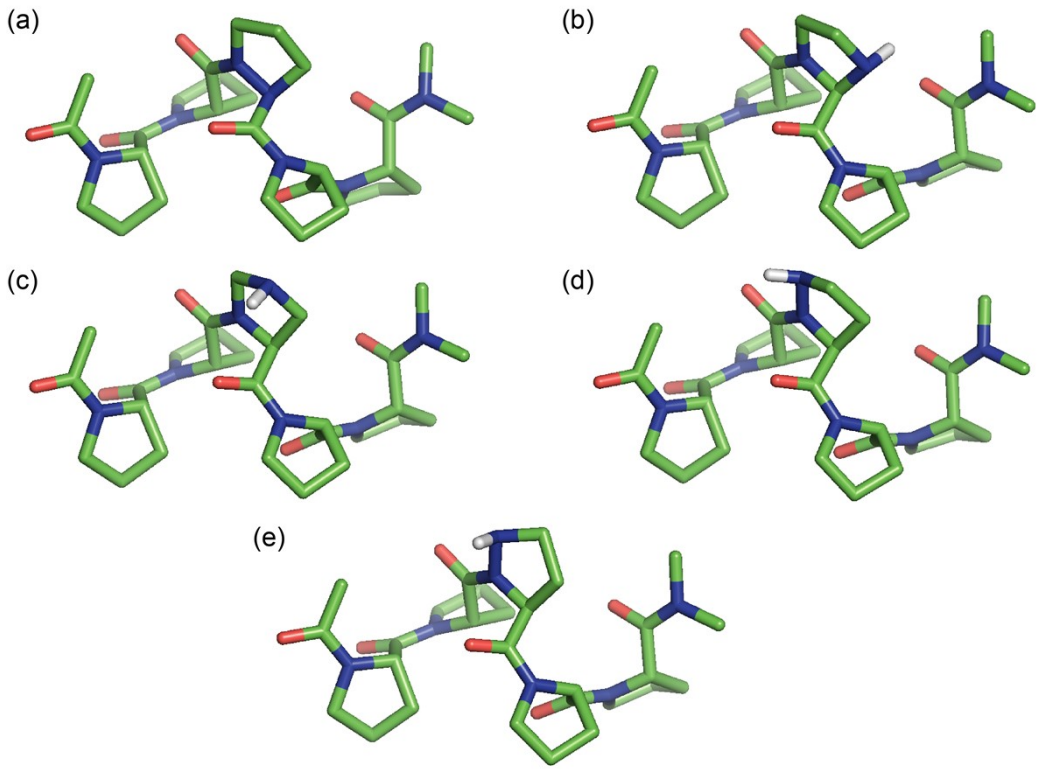

Fig. S1 PPI structures of the polyproline model peptide Ac-Pro_2-**azPro**-Pro_2-NMe_2 (PMP1) optimized at the SMD M06-2X/6-31+G(d) level of theory in water: (a) α-azPro(d), (b) β-azPro(d), (c) γ-azPro(d), (d) δ-azPro(d), and (e) δ-azPro(u).

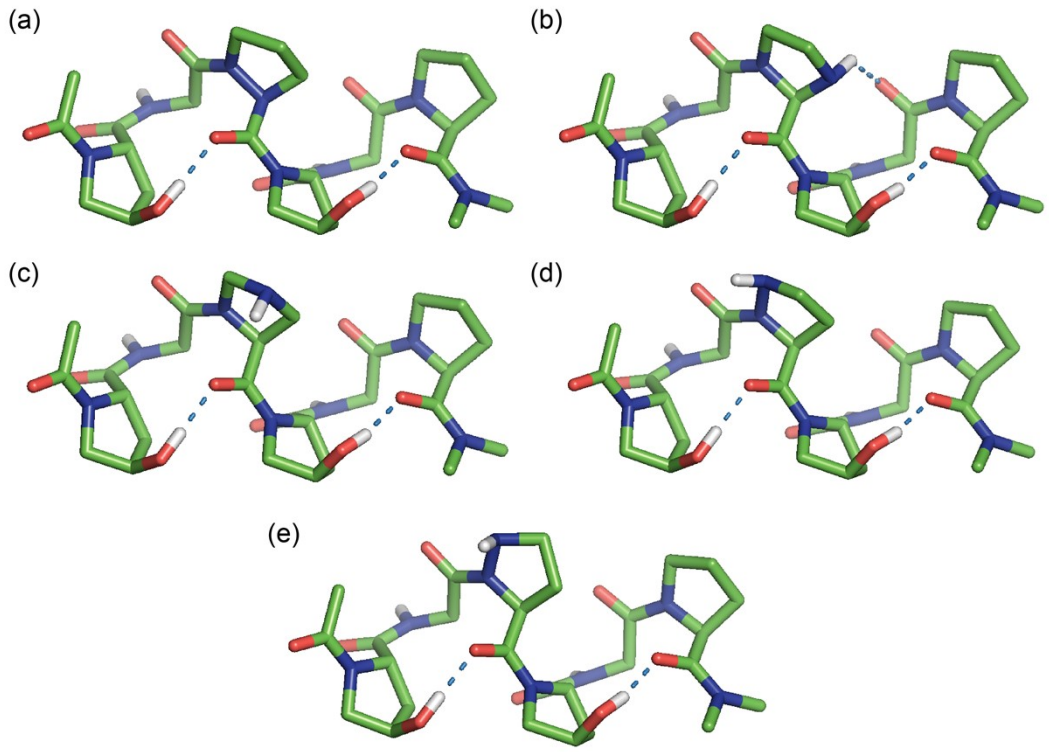

Fig. S2 PPI structures of the collagen model peptide Ac-Hyp-Gly-**azPro**-Hyp-Gly-Pro-NMe_2 (CMP1) optimized at the SMD M06-2X/6-31+G(d) level of theory in water: (a) α-azPro(d), (b) β-azPro(d), (c) γ-azPro(d), (d) δ-azPro(d), and (e) δ-azPro(u). H-bonds are represented by dotted lines.

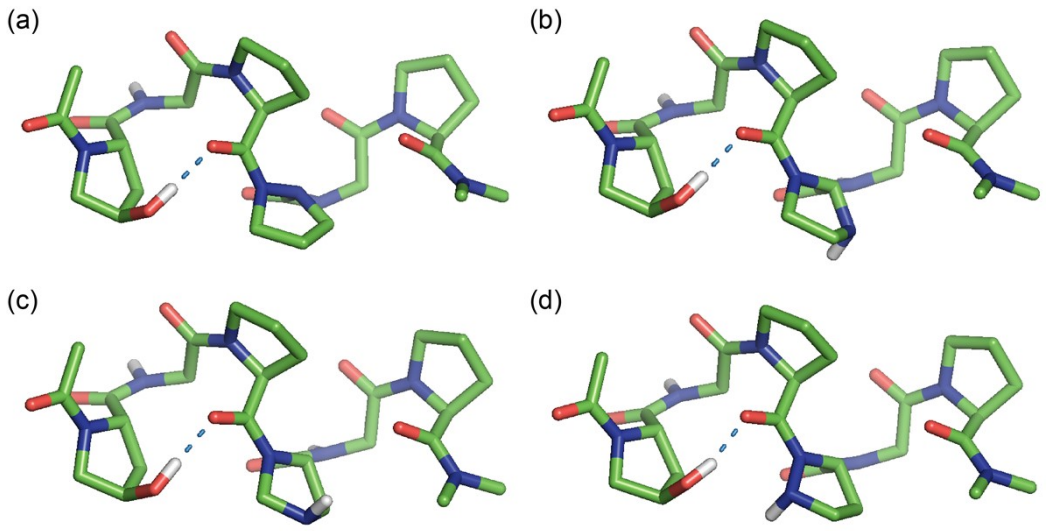

Fig. S3 PPI structures of the collagen model peptide Ac-Hyp-Gly-Pro-**azPro**-Gly-Pro-NMe_2 (CMP2) optimized at the SMD M06-2X/6-31+G(d) level of theory in water: (a) α-azPro(u), (b) β-azPro(u), (c) γ-azPro(u), and (d) δ-azPro(u). H-bonds are represented by dotted lines.

Cartesian Coordinates of PPI and PPII structures of the polyproline model peptide Ac-Pro_2-X-Pro_2-NMe_2 optimized at the SMD M06-2X/6-31+G(d) level of theory in water**:**

(1) Ac-Pro_5-NMe_2

(1a) PPI structure

C	-5.117237	-1.506317	-1.032793
C	-5.654063	-0.12104	-0.779901
O	-6.832535	0.182849	-1.049772
N	-4.809114	0.789313	-0.266401
C	-3.447973	0.515051	0.175033
C	-2.8787	1.935088	0.360066
C	-4.084968	2.719012	0.885737
C	-5.263762	2.139664	0.100015
C	-3.44857	-0.264229	1.497555
O	-4.461648	-0.306702	2.213925
N	-2.298764	-0.850145	1.863255
C	-1.096443	-0.948095	1.039812
C	-0.046043	-1.442018	2.050848
C	-0.857832	-2.36093	2.970083
C	-2.210101	-1.655605	3.093223
C	-1.291172	-1.96244	-0.095181
O	-2.166635	-2.839692	-0.027538
N	-0.459531	-1.872139	-1.141422
C	0.581595	-0.864902	-1.321223
C	1.440496	-1.480717	-2.442627
C	0.405201	-2.200434	-3.313783
C	-0.595458	-2.766108	-2.303542
C	-0.01804	0.472447	-1.771804
O	-1.139814	0.527896	-2.301257
N	0.744854	1.562495	-1.611592
C	2.061558	1.600216	-0.9832
C	2.611844	2.962376	-1.453223
C	1.357163	3.838804	-1.512356
C	0.280006	2.892035	-2.041447
C	1.947452	1.567259	0.548569
O	0.885728	1.871979	1.115308
N	3.05982	1.269459	1.234342
C	4.304386	0.765815	0.657564
C	5.282776	0.878258	1.841125
C	4.394764	0.558953	3.0478
C	3.059984	1.223661	2.706628
C	4.135848	-0.700456	0.220173
O	3.160077	-1.352992	0.626217
N	5.070506	-1.221059	-0.59489
C	6.317541	-0.562486	-0.970553
C	5.010412	-2.629311	-0.969413
H	-5.904054	-2.112582	-1.482679
H	-4.79506	-1.974301	-0.096376
H	-4.253906	-1.474464	-1.706256
H	-2.902101	-0.035548	-0.595952
H	-2.011892	1.969455	1.02447
H	-2.576594	2.308607	-0.623672
H	-4.217302	2.53322	1.956384
H	-3.981983	3.795521	0.734771
H	-6.183101	2.079698	0.688972
H	-5.475189	2.711025	-0.8103
H	-0.829352	0.032928	0.636368
H	0.797405	-1.9426	1.570445
H	0.330336	-0.575203	2.60427
H	-0.985458	-3.34338	2.505153
H	-0.382519	-2.501744	3.942879
H	-3.053784	-2.349277	3.143724
H	-2.253787	-0.992833	3.963823
H	1.1589	-0.744181	-0.400568
H	2.016366	-0.728739	-2.988676
H	2.136826	-2.196516	-1.991892
H	-0.090687	-1.484864	-3.976471
H	0.851731	-2.98506	-3.927774
H	-1.627716	-2.750803	-2.664788
H	-0.348283	-3.790882	-2.006854
H	2.678511	0.775128	-1.347744
H	3.383835	3.353166	-0.786266
H	3.042759	2.835499	-2.45114
H	1.09195	4.188479	-0.509767
H	1.486065	4.709568	-2.158251
H	-0.711303	3.093381	-1.627886
H	0.211968	2.913518	-3.134753
H	4.607108	1.388974	-0.185618
H	6.137426	0.204429	1.744188
H	5.652541	1.907246	1.891711
H	4.262775	-0.523802	3.140052
H	4.809536	0.935359	3.984931
H	2.194853	0.659696	3.064655
H	2.993316	2.244019	3.09929
H	5.800053	-3.187241	-0.453701
H	4.041926	-3.046823	-0.703134
H	5.165154	-2.719688	-2.048233
H	6.494125	-0.730094	-2.036523
H	6.285667	0.509743	-0.791513
H	7.153191	-0.991527	-0.406509

(1b) PPII structure

C	8.865315	0.555652	-1.305186
C	7.840808	-0.021373	-0.366503
O	7.709052	-1.252021	-0.213779
N	7.062701	0.844369	0.305614
C	5.957776	0.352495	1.118928
C	5.372153	1.643217	1.721667
C	5.618142	2.680904	0.622467
C	6.988423	2.297254	0.061736
C	4.926194	-0.354174	0.238835
O	4.823773	-0.097126	-0.972379
N	4.119933	-1.240131	0.841677
C	3.00819	-1.819377	0.096409
C	2.357135	-2.770973	1.117915
C	2.633009	-2.086845	2.459816
C	4.039025	-1.510686	2.290912
C	2.032394	-0.722697	-0.328752
O	1.952806	0.351155	0.290935
N	1.248494	-0.985576	-1.384389
C	0.190458	-0.045043	-1.736026
C	-0.472366	-0.700164	-2.96245
C	-0.27202	-2.197805	-2.711223
C	1.123204	-2.276168	-2.091297
C	-0.806202	0.091667	-0.585422
O	-0.996605	-0.830945	0.224757
N	-1.478853	1.249414	-0.512669
C	-2.568094	1.390791	0.446497
C	-3.034218	2.842614	0.231262
C	-2.781088	3.068757	-1.261848
C	-1.469908	2.326428	-1.524937
C	-3.693864	0.410536	0.115809
O	-3.847663	-0.033243	-1.034594
N	-4.523169	0.08663	1.11699
C	-5.724356	-0.692441	0.837578
C	-6.316635	-0.926225	2.238606
C	-5.916051	0.341917	2.997849
C	-4.506793	0.63996	2.485412
C	-6.682326	0.118559	-0.047183
O	-6.551883	1.350261	-0.149326
N	-7.660692	-0.546914	-0.68885
C	-8.041031	-1.931129	-0.423296
C	-8.648877	0.22802	-1.43157
H	9.591015	-0.217834	-1.55886
H	9.377504	1.416555	-0.86741
H	8.366743	0.889521	-2.222588
H	6.328526	-0.337681	1.880802
H	4.31563	1.541354	1.983776
H	5.934355	1.895456	2.626271
H	4.854739	2.590093	-0.15664
H	5.604712	3.705256	1.000736
H	7.080321	2.512544	-1.005381
H	7.798619	2.807014	0.594116
H	3.381003	-2.344387	-0.786884
H	1.290909	-2.919434	0.926246
H	2.859709	-3.7417	1.065829
H	1.914337	-1.277695	2.623583
H	2.575666	-2.776822	3.304286
H	4.185524	-0.595831	2.868372
H	4.80891	-2.236205	2.575261
H	0.621441	0.932412	-1.965689
H	-1.523975	-0.417843	-3.063945
H	0.062604	-0.384819	-3.863693
H	-1.016668	-2.565921	-1.99878
H	-0.343122	-2.791298	-3.625143
H	1.22604	-3.113888	-1.3986
H	1.901108	-2.353233	-2.858744
H	-2.201189	1.211125	1.45982
H	-4.0797	2.989466	0.515064
H	-2.410255	3.506674	0.837363
H	-3.588152	2.622052	-1.850878
H	-2.708275	4.126812	-1.521727
H	-1.422774	1.913916	-2.535078
H	-0.601265	2.974719	-1.367696
H	-5.44324	-1.619739	0.335192
H	-7.397334	-1.087728	2.215579
H	-5.843215	-1.808665	2.680675
H	-6.588829	1.164985	2.735891
H	-5.936086	0.210192	4.081543
H	-4.286409	1.709581	2.475345
H	-3.743389	0.126808	3.0803
H	-9.392698	0.663595	-0.754281
H	-8.159464	1.027879	-1.987221
H	-9.152576	-0.439513	-2.13279
H	-8.227321	-2.436072	-1.374556
H	-7.260286	-2.473307	0.10538
H	-8.958318	-1.95962	0.175601

(2) Ac-Pro_2-α-azPro(d)-Pro_2-NMe_2

(2a) PPI structure

C	5.021901	-0.982218	1.428511
C	5.54026	0.237036	0.710377
O	6.703724	0.652723	0.877512
N	4.693089	0.880268	-0.11047
C	3.34312	0.440666	-0.435416
C	2.745348	1.685905	-1.119111
C	3.948104	2.289112	-1.851992
C	5.12139	2.044227	-0.900912
C	3.362052	-0.756991	-1.393459
O	4.367734	-1.025355	-2.070667

N	2.226642	-1.463603	-1.498937
C	1.04121	-1.28668	-0.66264
C	-0.009094	-2.147643	-1.38577
C	0.817863	-3.307376	-1.952124
C	2.146133	-2.661255	-2.352939
C	1.286309	-1.846616	0.74009
O	2.145046	-2.714002	0.955348
N	0.514243	-1.391146	1.736211
N	-0.480034	-0.411292	1.560917
C	-1.49583	-0.798248	2.579686
C	-0.647532	-1.256621	3.769639
C	0.550197	-1.938441	3.102659
C	0.057916	0.909535	1.719156
O	1.234443	1.101002	2.034483
N	-0.814993	1.905505	1.473737
C	-2.054789	1.768796	0.71114
C	-2.63409	3.195743	0.776934
C	-1.385685	4.079367	0.71919
C	-0.343345	3.304323	1.527718
C	-1.758103	1.375648	-0.741798
O	-0.627451	1.540359	-1.22661
N	-2.787866	0.931558	-1.475027
C	-4.125353	0.621691	-0.972958
C	-4.940173	0.46682	-2.273071
C	-3.920399	-0.123045	-3.251138
C	-2.624907	0.605513	-2.901365
C	-4.115892	-0.693386	-0.180873
O	-3.161557	-1.478758	-0.290007
N	-5.166903	-0.957535	0.619576
C	-6.438691	-0.240138	0.57451
C	-5.224952	-2.277163	1.242043
H	1.504284	-1.701779	3.581634
H	0.439776	-3.024715	3.045241
H	-2.142961	0.042833	2.821831
H	-2.092216	-1.61271	2.160742
H	-0.32168	-0.386274	4.34675
H	-1.19472	-1.933102	4.428284
H	0.741987	-0.237742	-0.626664
H	-0.807877	-2.473083	-0.71633
H	-0.449718	-1.552399	-2.191993
H	3.009225	-3.306993	-2.169064
H	2.158947	-2.357598	-3.404853
H	0.984986	-4.062861	-1.178909
H	0.328501	-3.790905	-2.799976
H	-2.731817	1.048494	1.172139
H	0.660007	3.377049	1.100476
H	-0.300595	3.629486	2.571926
H	-3.342084	3.39963	-0.029569
H	-3.152696	3.314669	1.733272
H	-1.050766	4.189442	-0.316649
H	-1.560447	5.075425	1.130741
H	2.798635	0.192613	0.479139
H	1.912873	1.443647	-1.782891
H	2.379682	2.36366	-0.339457
H	6.055971	1.821858	-1.423146
H	5.296775	2.893867	-0.231945
H	4.11408	1.762798	-2.797396
H	3.81381	3.350565	-2.070449
H	5.802385	-1.363676	2.087594
H	4.743356	-1.764431	0.714084
H	4.133166	-0.737853	2.021001
H	-1.73078	-0.004007	-3.05096
H	-2.508407	1.534397	-3.471226
H	-4.497454	1.440445	-0.354101
H	-3.80639	-1.197339	-3.073488
H	-4.204705	0.026787	-4.29461
H	-5.823221	-0.163477	-2.141629
H	-5.265874	1.458646	-2.602136
H	-6.82603	-0.14088	1.591016
H	-6.327835	0.756627	0.152557
H	-7.165599	-0.799736	-0.0254
H	-5.471167	-3.046838	0.501353
H	-4.267022	-2.520418	1.703261
H	-5.998927	-2.259528	2.010777

(2b) PPII structure

C	8.805839	0.676808	-1.685465
C	7.805945	-0.116336	-0.888595
O	7.529374	-1.299772	-1.168936
N	7.212829	0.504824	0.144445
C	6.163703	-0.164159	0.903253
C	5.817163	0.862318	1.998641
C	6.090919	2.207083	1.318601
C	7.33733	1.935451	0.476125
C	4.953036	-0.442659	0.015164
O	4.708143	0.247314	-0.988528
N	4.150092	-1.449663	0.390394
C	2.900338	-1.671707	-0.326768
C	2.305379	-2.905135	0.376408
C	2.814733	-2.767951	1.813981
C	4.23424	-2.224392	1.644581
C	1.987844	-0.455875	-0.167194
O	2.044115	0.277583	0.830095
N	1.097999	-0.272995	-1.154417
N	0.151077	0.764766	-1.036599
C	-0.409368	0.88094	-2.408734
C	-0.432414	-0.561171	-2.913362
C	0.84424	-1.153247	-2.315567
C	-0.832095	0.452229	-0.041838

O	-0.948445	-0.677304	0.446367
N	-1.589085	1.491721	0.339547
C	-2.785334	1.230368	1.134825
C	-3.373286	2.637482	1.365758
C	-2.905085	3.421469	0.137605
C	-1.490635	2.899315	-0.096029
C	-3.759344	0.353527	0.344827
O	-3.720243	0.296761	-0.895198
N	-4.668678	-0.325413	1.057558
C	-5.739691	-1.038916	0.369282
C	-6.492517	-1.726222	1.522457
C	-6.321746	-0.740824	2.682144
C	-4.890086	-0.231748	2.514583
C	-6.639903	-0.045401	-0.377564
O	-6.623097	1.162481	-0.08503
N	-7.443763	-0.526293	-1.342952
C	-7.724503	-1.941022	-1.567177
C	-8.365932	0.404379	-1.988521
H	0.715523	-2.189467	-1.993765
H	1.68811	-1.087728	-3.007943
H	-1.399541	1.334231	-2.373763
H	0.262253	1.510419	-2.997773
H	-1.313889	-1.076304	-2.519823
H	-0.441625	-0.621418	-4.002844
H	3.103967	-1.853138	-1.384456
H	1.214778	-2.935106	0.30467
H	2.710733	-3.806638	-0.093405
H	4.536335	-1.58772	2.478805
H	4.965836	-3.0318	1.532487
H	2.20262	-2.046162	2.363501
H	2.803974	-3.715578	2.356436
H	-2.519762	0.733206	2.071251
H	-1.174158	2.986891	-1.134275
H	-0.759353	3.420023	0.532363
H	-4.460986	2.61879	1.471657
H	-2.942105	3.05703	2.279915
H	-3.535304	3.182982	-0.725985
H	-2.921794	4.501924	0.294832
H	6.538702	-1.103904	1.316027
H	4.787231	0.761708	2.352149
H	6.493358	0.713707	2.846333
H	7.372392	2.539067	-0.433399
H	8.255816	2.106047	1.048989
H	5.252019	2.478931	0.670294
H	6.249907	3.015049	2.035914
H	9.390585	-0.003813	-2.30516
H	9.471572	1.253622	-1.037615
H	8.274273	1.382042	-2.334818
H	-4.769428	0.795032	2.866043
H	-4.171322	-0.871552	3.038086
H	-5.304997	-1.750531	-0.334693
H	-7.027271	0.089347	2.575789
H	-6.47679	-1.204046	3.658659
H	-7.539807	-1.923482	1.280195
H	-6.001869	-2.67871	1.746855
H	-7.72989	-2.136617	-2.642349
H	-6.975416	-2.580313	-1.105011
H	-8.708164	-2.196217	-1.156783
H	-9.201563	0.656905	-1.326063
H	-7.842682	1.320349	-2.266032
H	-8.756961	-0.069822	-2.889826

(3) Ac-Pro_2-β-azPro(d)-Pro_2-NMe_2

(3a) PPI structure

C	4.9791	1.266727	-1.469582
C	5.558138	-0.047564	-1.012502
O	6.706882	-0.405592	-1.338801
N	4.785482	-0.8336	-0.243569
C	3.457244	-0.48686	0.244373
C	2.922608	-1.847641	0.730571
C	4.178687	-2.528323	1.284291
C	5.283044	-2.100776	0.314311
C	3.531482	0.518491	1.400013
O	4.581336	0.690103	2.039769
N	2.396003	1.158097	1.716632
C	1.15783	1.108225	0.947293
C	0.145909	1.741453	1.919083
C	0.977091	2.816228	2.627004
C	2.356688	2.170069	2.785608
C	1.288061	1.944124	-0.332845
O	2.146017	2.83441	-0.431902
N	0.410212	1.692455	-1.311877
C	-0.610997	0.64339	-1.318865
N	-1.499643	0.992558	-2.420684
C	-0.615197	1.646566	-3.405179
C	0.430239	2.41454	-2.587586
C	0.021951	-0.733508	-1.59525
O	1.143494	-0.831032	-2.115632
N	-0.726938	-1.799769	-1.290347
C	-2.043815	-1.75788	-0.658073
C	-2.563477	-3.193381	-0.872357
C	-1.287099	-4.037176	-0.82002
C	-0.255673	-3.171867	-1.541527
C	-1.93142	-1.43177	0.838175
O	-0.873897	-1.626915	1.459223
N	-3.037486	-0.975514	1.440679
C	-4.295979	-0.647955	0.773942
C	-5.271061	-0.520442	1.958492

C	-4.391604	0.070732	3.064311
C	-3.045327	-0.629252	2.871584
C	-4.172774	0.682822	0.009332
O	-3.222903	1.446622	0.249299
N	-5.118128	0.966735	-0.904385
C	-6.343744	0.201041	-1.109617
C	-5.10246	2.252683	-1.593247
H	-1.170616	0.641378	-0.381472
H	1.429048	2.377622	-3.031192
H	0.149393	3.459974	-2.424092
H	-2.153847	1.685917	-2.053323
H	-0.13225	0.877321	-4.013258
H	-1.198719	2.294061	-4.059288
H	0.890015	0.073566	0.714299
H	-0.737269	2.134626	1.407553
H	-0.171146	0.968582	2.626428
H	3.178771	2.879594	2.656293
H	2.474454	1.676387	3.755778
H	1.047464	3.71071	2.001108
H	0.550349	3.104736	3.589717
H	-2.676006	-1.024749	-1.163719
H	0.758367	-3.296845	-1.154568
H	-0.242594	-3.357968	-2.621292
H	-3.305793	-3.483425	-0.125029
H	-3.024376	-3.252125	-1.86322
H	-0.982268	-4.197498	0.218949
H	-1.410676	-5.011004	-1.297914
H	2.8473	-0.090279	-0.571147
H	2.118891	-1.754095	1.46519
H	2.538332	-2.392127	-0.138337
H	6.247102	-1.942473	0.805484
H	5.423752	-2.824488	-0.495896
H	4.395045	-2.155442	2.290429
H	4.076904	-3.614271	1.335844
H	5.700822	1.761945	-2.119971
H	4.766225	1.914203	-0.611805
H	4.04166	1.115556	-2.016002
H	-2.1916	0.01112	3.107102
H	-2.967026	-1.546797	3.464953
H	-4.580697	-1.457183	0.099688
H	-4.277955	1.149534	2.91814
H	-4.801514	-0.099532	4.061776
H	-6.140581	0.096934	1.720322
H	-5.617677	-1.52179	2.233143
H	-6.528983	0.11859	-2.183868
H	-6.273453	-0.802445	-0.696685
H	-7.191721	0.717974	-0.647036
H	-5.886751	2.904789	-1.192166
H	-4.136748	2.737122	-1.4648
H	-5.292251	2.088618	-2.65733

(3b) PPII structure

C	-9.024529	0.477098	0.954106
C	-7.887048	-0.138849	0.185072
O	-7.682306	-1.369187	0.183738
N	-7.088908	0.693378	-0.504254
C	-5.913574	0.180232	-1.195583
C	-5.346337	1.431804	-1.893619
C	-5.734757	2.567742	-0.94212
C	-7.126213	2.165917	-0.451303
C	-4.903402	-0.383867	-0.196435
O	-4.86298	0.009832	0.981276
N	-4.038535	-1.295855	-0.664794
C	-2.945119	-1.753891	0.184685
C	-2.233408	-2.800361	-0.694028
C	-2.462505	-2.276214	-2.114306
C	-3.887783	-1.725151	-2.069977
C	-2.006516	-0.593617	0.511826
O	-1.913959	0.401653	-0.225184
N	-1.257679	-0.715319	1.616903
C	-0.189413	0.254294	1.878815
N	0.441792	-0.190784	3.113474
C	0.261123	-1.654134	3.111772
C	-1.112045	-1.900455	2.476208
C	0.82972	0.215331	0.730629
O	1.019544	-0.826398	0.081489
N	1.512188	1.339294	0.487311
C	2.566784	1.335535	-0.521562
C	3.031727	2.804154	-0.549591
C	2.784676	3.276436	0.885874
C	1.472766	2.592069	1.268407
C	3.707716	0.409882	-0.099252
O	3.925241	0.151414	1.096406
N	4.477619	-0.076997	-1.082118
C	5.678138	-0.837836	-0.755483
C	6.16949	-1.31014	-2.135087
C	5.75967	-0.158472	-3.057486
C	4.396786	0.274107	-2.514186
C	6.71	0.074171	-0.077136
O	6.605653	1.309704	-0.158604
N	7.725734	-0.505908	0.587977
C	8.06921	-1.922761	0.508809
C	8.773097	0.361851	1.118377
H	-0.601904	1.25792	1.989286
H	-1.134959	-2.823388	1.893334
H	-1.909271	-1.923885	3.22588
H	-0.106619	0.194442	3.882553
H	1.046714	-2.111375	2.505857
H	0.329133	-2.042778	4.127622

H	-3.338338	-2.180646	1.110829
H	-1.17486	-2.905056	-0.441906
H	-2.723286	-3.768834	-0.554104
H	-4.029773	-0.885896	-2.753802
H	-4.62703	-2.499774	-2.300957
H	-1.757411	-1.46883	-2.335896
H	-2.350404	-3.053	-2.873444
H	-6.20552	-0.598336	-1.904427
H	-4.268189	1.362234	-2.061406
H	-5.843135	1.550883	-2.861509
H	-7.329716	2.509103	0.565389
H	-7.912157	2.543295	-1.114988
H	-5.038056	2.606869	-0.098841
H	-5.740828	3.543596	-1.432077
H	-9.715409	-0.309449	1.258903
H	-9.5534	1.226073	0.358323
H	-8.632284	0.973723	1.848813
H	1.40675	2.381995	2.336948
H	0.604614	3.188211	0.966825
H	2.160122	1.006778	-1.481059
H	3.590242	2.929597	1.540696
H	2.714442	4.363056	0.966567
H	4.075385	2.90206	-0.859727
H	2.404402	3.360013	-1.253189
H	4.218477	1.343645	-2.646544
H	3.579397	-0.28227	-2.985338
H	5.412547	-1.663889	-0.093637
H	6.474503	0.665835	-2.969233
H	5.702714	-0.455847	-4.106477
H	7.243422	-1.511232	-2.15217
H	5.639258	-2.229418	-2.403223
H	8.373723	-2.268505	1.499387
H	7.225198	-2.525401	0.180159
H	8.902759	-2.070843	-0.187102
H	9.413601	0.74046	0.313605
H	8.330559	1.207039	1.646487
H	9.380042	-0.218206	1.814577

(4) Ac-Pro_2-γ-azPro(d)-Pro_2-NMe_2

(4a) PPI structure

C	-4.995259	-1.254935	-1.451672
C	-5.570258	0.061613	-0.995776
O	-6.71882	0.421725	-1.320376
N	-4.794185	0.847366	-0.230018
C	-3.466117	0.498008	0.256046
C	-2.926141	1.858445	0.737646
C	-4.179222	2.543393	1.293128
C	-5.287669	2.116255	0.327523
C	-3.541689	-0.503803	1.415308
O	-4.592034	-0.672936	2.054852
N	-2.406118	-1.141772	1.734306
C	-1.171124	-1.095643	0.960108
C	-0.155725	-1.72737	1.929144
C	-0.985286	-2.799576	2.643214
C	-2.365024	-2.153425	2.8036
C	-1.3082	-1.93707	-0.314362
O	-2.1624	-2.832456	-0.406014
N	-0.442469	-1.68737	-1.303757
C	0.583345	-0.659381	-1.330635
C	1.430786	-1.145897	-2.532661
N	0.465088	-1.762248	-3.447538
C	-0.46646	-2.450972	-2.570862
C	-0.021275	0.720613	-1.61105
O	-1.140566	0.830942	-2.136795
N	0.737105	1.784611	-1.315139
C	2.056687	1.738898	-0.689901
C	2.58092	3.171824	-0.913938
C	1.308442	4.020346	-0.849931
C	0.267522	3.15834	-1.561719
C	1.949381	1.423878	0.809886
O	0.890473	1.613798	1.429781
N	3.060795	0.987075	1.416071
C	4.320587	0.662574	0.751855
C	5.303167	0.585991	1.934548
C	4.441938	0.002405	3.05948
C	3.071721	0.651667	2.849475
C	4.217954	-0.697278	0.039735
O	3.307839	-1.484133	0.347931
N	5.139736	-0.98585	-0.897728
C	6.346203	-0.203924	-1.151885
C	5.158579	-2.310994	-1.506816
H	1.172235	-0.66508	-0.409998
H	-1.472446	-2.469992	-2.993147
H	-0.136445	-3.474353	-2.36917
H	1.986749	-0.347137	-3.024978
H	2.13378	-1.903637	-2.174968
H	-0.045631	-1.007986	-3.908132
H	-0.901702	-0.063648	0.718634
H	0.724612	-2.122831	1.414458
H	0.166528	-0.953379	2.63301
H	-3.187018	-2.863341	2.675572
H	-2.481733	-1.659635	3.7738
H	-1.057167	-3.696283	2.020699
H	-0.55585	-3.084878	3.605684
H	2.689732	1.003818	-1.194116
H	-0.742351	3.285689	-1.16448
H	0.244125	3.345958	-2.640976
H	3.332456	3.460939	-0.175557

H	3.031012	3.225689	-1.910053
H	1.014247	4.182001	0.191915
H	1.431249	4.993641	-1.329059
H	-2.859444	0.097045	-0.559978
H	-2.12157	1.76426	1.471182
H	-2.54129	2.399706	-0.133181
H	-6.250254	1.960259	0.822368
H	-5.429976	2.838949	-0.483264
H	-4.393349	2.17297	2.300677
H	-4.074838	3.629183	1.342326
H	-5.719946	-1.749958	-2.098891
H	-4.781288	-1.901098	-0.593195
H	-4.059144	-1.106917	-2.001252
H	2.240184	-0.018928	3.082457
H	2.953436	1.569865	3.434861
H	4.586685	1.454902	0.05112
H	4.363795	-1.083462	2.949308
H	4.847224	0.218166	4.050049
H	6.184534	-0.018662	1.706503
H	5.629013	1.601294	2.181572
H	6.50865	-0.149574	-2.231572
H	6.267626	0.80908	-0.76461
H	7.212759	-0.692682	-0.692593
H	5.935716	-2.929339	-1.042759
H	4.192729	-2.796294	-1.383512
H	5.380069	-2.206438	-2.572089

(4b) PPII structure

C	-8.961246	0.625831	1.139054
C	-7.871041	-0.099214	0.397527
O	-7.662397	-1.318251	0.560603
N	-7.121722	0.620911	-0.453774
C	-5.985918	0.007242	-1.129176
C	-5.462482	1.142481	-2.02913
C	-5.792541	2.403751	-1.225075
C	-7.152297	2.08733	-0.600734
C	-4.923493	-0.412991	-0.114556
O	-4.816637	0.152474	0.986523
N	-4.090356	-1.397581	-0.483923
C	-2.951347	-1.724395	0.365417
C	-2.289728	-2.901909	-0.37293
C	-2.589371	-2.603899	-1.844889
C	-4.005844	-2.026631	-1.818086
C	-2.004221	-0.527369	0.45317
O	-1.945094	0.322844	-0.449306
N	-1.227559	-0.45334	1.543753
C	-0.179185	0.550275	1.632772
C	0.467915	0.191413	2.99085
N	0.275017	-1.256549	3.131053
C	-1.056512	-1.483454	2.599166
C	0.832028	0.368562	0.504847
O	1.034863	-0.750267	0.003842
N	1.512956	1.455519	0.114653
C	2.623998	1.303824	-0.81993
C	3.116498	2.749437	-1.012914
C	2.832076	3.398464	0.345228
C	1.502657	2.77767	0.776181
C	3.719743	0.435713	-0.200715
O	3.872816	0.372228	1.030925
N	4.515406	-0.226705	-1.050865
C	5.677323	-0.948847	-0.546218
C	6.213444	-1.65367	-1.804595
C	5.880562	-0.661695	-2.923113
C	4.512366	-0.107058	-2.522944
C	6.706251	0.038314	0.02209
O	6.652735	1.243445	-0.277605
N	7.664834	-0.444949	0.833125
C	7.955134	-1.862737	1.025908
C	8.718068	0.471584	1.259502
H	-0.604786	1.555932	1.620029
H	-1.146146	-2.491717	2.195453
H	-1.809877	-1.327477	3.376188
H	1.526942	0.448963	3.04062
H	-0.065015	0.71094	3.79126
H	0.934875	-1.71181	2.498162
H	-3.296633	-1.997536	1.365931
H	-1.220237	-2.978463	-0.158585
H	-2.776547	-3.830452	-0.059095
H	-4.169222	-1.290998	-2.608537
H	-4.763476	-2.813068	-1.9034
H	-1.887696	-1.857296	-2.229291
H	-2.52686	-3.493705	-2.474843
H	2.269041	0.852222	-1.749117
H	1.428263	2.672617	1.860958
H	0.648282	3.361853	0.41839
H	4.171263	2.792548	-1.297161
H	2.522937	3.222582	-1.801283
H	3.617222	3.134201	1.060201
H	2.770108	4.487114	0.286659
H	-6.314675	-0.86386	-1.701322
H	-4.396281	1.041119	-2.249572
H	-6.017696	1.128477	-2.972196
H	-7.290415	2.567649	0.370467
H	-7.977242	2.378592	-1.260345
H	-5.046227	2.553934	-0.438631
H	-5.826169	3.301952	-1.84527
H	-9.638851	-0.105288	1.581244
H	-9.518897	1.297119	0.48005
H	-8.51763	1.229647	1.939034

H	4.37931	0.93278	-2.83105
H	3.696212	-0.707092	-2.93949
H	5.357545	-1.64755	0.228662
H	6.619206	0.145875	-2.942845
H	5.855448	-1.129874	-3.909263
H	7.280419	-1.880315	-1.736942
H	5.667217	-2.592044	-1.943277
H	8.177423	-2.038716	2.081108
H	7.11207	-2.490637	0.746003
H	8.827021	-2.154485	0.429633
H	9.407378	0.686535	0.434942
H	8.283692	1.407217	1.613487
H	9.271371	0.00347	2.074768

(5) Ac-Pro_2-δ-azPro(d)-Pro_2-NMe_2

(5a) PPI structure

C	-4.942321	-1.135307	-1.413321
C	-5.476424	0.178542	-0.902734
O	-6.612666	0.588802	-1.210811
N	-4.675178	0.904694	-0.104968
C	-3.352855	0.495283	0.347809
C	-2.767565	1.811114	0.895261
C	-3.99646	2.515656	1.481056
C	-5.123958	2.164401	0.507111
C	-3.43625	-0.556908	1.45803
O	-4.46772	-0.705462	2.133241
N	-2.324747	-1.267059	1.69541
C	-1.102835	-1.221234	0.898994
C	-0.083428	-1.918781	1.817542
C	-0.928694	-2.983433	2.525074
C	-2.277694	-2.294811	2.747859
C	-1.292983	-2.005281	-0.406191
O	-2.163171	-2.885507	-0.519304
N	-0.456808	-1.706992	-1.402292
C	0.559789	-0.666834	-1.43085
C	1.41821	-1.108453	-2.631542
C	0.373414	-1.7276	-3.550447
N	-0.521327	-2.45155	-2.623301
C	-0.071216	0.70941	-1.685072
O	-1.20391	0.81103	-2.180971
N	0.686831	1.776501	-1.40268
C	1.999234	1.741048	-0.762504
C	2.531805	3.163619	-1.024741
C	1.263982	4.020108	-0.972409
C	0.212246	3.147554	-1.656266
C	1.865636	1.467775	0.744205
O	0.784497	1.634564	1.330522
N	2.977099	1.095919	1.392134
C	4.243464	0.730718	0.763989
C	5.203552	0.701567	1.966725
C	4.321682	0.155589	3.094481
C	2.950793	0.784762	2.831544
C	4.130987	-0.661996	0.118622
O	3.17778	-1.400584	0.416286
N	5.087607	-1.03322	-0.751815
C	6.328	-0.30156	-0.98988
C	5.091941	-2.400243	-1.262025
H	-5.691003	-1.593676	-2.060176
H	-4.723113	-1.812499	-0.580347
H	-4.01484	-0.988504	-1.978431
H	-2.767595	0.120287	-0.495165
H	-1.974619	1.646125	1.628757
H	-2.354354	2.37884	0.054704
H	-4.218566	2.114044	2.474665
H	-3.855064	3.594575	1.571975
H	-6.087831	2.018283	1.002496
H	-5.249287	2.923967	-0.272052
H	-0.811948	-0.186347	0.697538
H	0.763795	-2.329579	1.262156
H	0.293538	-1.181392	2.534043
H	-1.05406	-3.855898	1.876968
H	-0.481804	-3.315089	3.464454
H	-3.127808	-2.974771	2.644374
H	-2.339941	-1.809417	3.72774
H	1.139235	-0.682335	-0.504401
H	1.95352	-0.2807	-3.100548
H	2.140935	-1.857559	-2.294059
H	-0.165595	-0.948886	-4.100404
H	0.803708	-2.433819	-4.261031
H	-1.489117	-2.378962	-2.94582
H	2.634054	0.986142	-1.23472
H	3.290706	3.468215	-0.30043
H	2.973642	3.188366	-2.025815
H	0.979363	4.208522	0.06767
H	1.387931	4.981218	-1.47519
H	-0.791097	3.281097	-1.245403
H	0.171094	3.320193	-2.737397
H	4.530495	1.482237	0.026517
H	6.091665	0.092694	1.781416
H	5.52067	1.726875	2.181845
H	4.254749	-0.934522	3.025211
H	4.704437	0.412959	4.084043
H	2.120857	0.107639	3.051434
H	2.802179	1.710228	3.397593
H	5.707262	-3.044139	-0.622819
H	4.077309	-2.793096	-1.297212
H	5.512898	-2.394891	-2.269911
H	6.529592	-0.290552	-2.064114

H	6.268306	0.726105	-0.639278
H	7.16055	-0.801016	-0.48193

(5b) PPII structure

C	9.089672	0.25613	0.536793
C	7.850374	-0.009993	-0.274098
O	7.58226	0.646295	-1.300275
N	7.033953	-0.9886	0.151776
C	5.763337	-1.226429	-0.520911
C	5.1778	-2.423263	0.252161
C	5.725436	-2.226623	1.669273
C	7.142374	-1.699423	1.438611
C	4.857117	-0.002638	-0.397111
O	4.97598	0.801634	0.542994
N	3.909119	0.137522	-1.334001
C	2.91903	1.200103	-1.21626
C	2.12971	1.086607	-2.531837
C	2.171723	-0.415683	-2.8262
C	3.583861	-0.826817	-2.404372
C	2.000889	0.92625	-0.025755
O	1.919923	-0.19007	0.506371
N	1.248785	1.951265	0.411651
C	0.09087	1.725591	1.281718
C	-0.639061	3.081162	1.22032
C	-0.182095	3.624731	-0.136549
N	1.228969	3.217773	-0.242372
C	-0.802186	0.631481	0.695531
O	-0.882894	0.453869	-0.53066
N	-1.523529	-0.089024	1.564454
C	-2.510956	-1.035395	1.058408
C	-3.054085	-1.687911	2.342291
C	-2.970184	-0.554806	3.36962
C	-1.670515	0.169863	3.011651
C	-3.62346	-0.294972	0.316305
O	-3.8916	0.890935	0.573032
N	-4.310148	-0.999236	-0.594031
C	-5.509753	-0.430895	-1.200779
C	-5.905855	-1.498234	-2.235936
C	-5.473673	-2.804466	-1.564061
C	-4.156075	-2.440143	-0.879263
C	-6.599469	-0.249756	-0.133673
O	-6.517597	-0.84669	0.953909
N	-7.637193	0.556592	-0.418218
C	-7.932821	1.112432	-1.735723
C	-8.720815	0.643751	0.555917
H	9.773321	0.870559	-0.050033
H	9.585518	-0.672094	0.833699
H	8.817774	0.79967	1.44896
H	5.933784	-1.454426	-1.576032
H	4.085294	-2.447806	0.213173
H	5.563437	-3.349074	-0.186106
H	5.130457	-1.478559	2.202517
H	5.722809	-3.149833	2.252563
H	7.470449	-1.018542	2.227283
H	7.86843	-2.515556	1.354017
H	3.409962	2.166184	-1.097082
H	1.115879	1.483372	-2.439226
H	2.656788	1.64895	-3.308926
H	1.430856	-0.938991	-2.212165
H	1.97746	-0.647826	-3.875293
H	3.625543	-1.853178	-2.032341
H	4.296943	-0.719441	-3.228876
H	0.417093	1.46175	2.289496
H	-1.723917	2.970726	1.29919
H	-0.285934	3.72644	2.029778
H	-0.743295	3.167043	-0.955747
H	-0.249825	4.710527	-0.215821
H	1.771834	3.845892	0.355104
H	-2.030889	-1.754337	0.390771
H	-4.067702	-2.077106	2.214427
H	-2.395229	-2.515851	2.622265
H	-3.821298	0.123285	3.25303
H	-2.958735	-0.919969	4.398591
H	-1.727091	1.242899	3.209515
H	-0.81361	-0.247323	3.55093
H	-5.262993	0.530362	-1.65514
H	-6.970795	-1.474922	-2.479584
H	-5.336454	-1.326449	-3.15497
H	-6.212994	-3.102534	-0.813525
H	-5.350603	-3.625097	-2.273731
H	-3.994865	-3.007834	0.039958
H	-3.299827	-2.594074	-1.544899
H	-9.323726	-0.271269	0.553992
H	-8.316283	0.801734	1.556557
H	-9.355355	1.489892	0.288895
H	-8.194915	2.168008	-1.628187
H	-7.081483	1.036697	-2.408615
H	-8.781208	0.582367	-2.182622

(6) Ac-Pro_2-δ-azPro(u)-Pro_2-NMe_2

(6a) PPI structure

C	-5.112632	-1.540014	-1.084214
C	-5.67233	-0.162632	-0.836703
O	-6.856505	0.120135	-1.103775
N	-4.840295	0.763929	-0.330662
C	-3.478239	0.507586	0.117843
C	-2.928264	1.934446	0.306691

C	-4.147156	2.701639	0.828609
C	-5.316611	2.105524	0.040675
C	-3.477887	-0.271203	1.440505
O	-4.493134	-0.321708	2.152838
N	-2.3253	-0.849219	1.809978
C	-1.119757	-0.936105	0.991509
C	-0.066211	-1.412122	2.009116
C	-0.868755	-2.335644	2.932151
C	-2.233663	-1.652112	3.041703
C	-1.29279	-1.977946	-0.123551
O	-2.131056	-2.880352	-0.023991
N	-0.466091	-1.848219	-1.177871
C	0.574392	-0.825367	-1.349899
C	1.463591	-1.417827	-2.470673
C	1.014578	-2.878972	-2.518956
N	-0.415904	-2.848906	-2.181119
C	-0.028644	0.508223	-1.792057
O	-1.139322	0.553535	-2.343635
N	0.725509	1.600571	-1.614569
C	2.034264	1.643642	-0.96643
C	2.574487	3.020079	-1.407044
C	1.310229	3.88186	-1.476189
C	0.254701	2.930323	-2.038703
C	1.903366	1.586939	0.562503
O	0.835953	1.886525	1.121286
N	3.006753	1.274102	1.256393
C	4.269352	0.80378	0.688333
C	5.223692	0.879303	1.895827
C	4.311464	0.533295	3.075973
C	2.992046	1.221086	2.728247
C	4.128887	-0.643911	0.186768
O	3.152758	-1.327458	0.538785
N	5.086491	-1.120842	-0.626428
C	6.342145	-0.447907	-0.942059
C	5.010966	-2.504099	-1.082635
H	1.144523	-0.721658	-0.422446
H	-0.921668	-2.467692	-2.986643
H	1.248976	-0.924581	-3.424381
H	2.526107	-1.302984	-2.244277
H	1.148326	-3.340948	-3.497626
H	1.53491	-3.473054	-1.762155
H	-0.865232	0.044957	0.581959
H	0.78532	-1.905212	1.534419
H	0.296759	-0.537257	2.558118
H	-3.065808	-2.360107	3.085387
H	-2.296845	-0.988732	3.910554
H	-0.977212	-3.324663	2.47701
H	-0.396133	-2.458496	3.908643
H	2.664723	0.832145	-1.338167
H	-0.747012	3.115285	-1.643386
H	0.210163	2.963801	-3.132857
H	3.328501	3.41077	-0.7197
H	3.02584	2.913936	-2.398197
H	1.022466	4.213608	-0.473826
H	1.440173	4.763649	-2.106721
H	-2.921409	-0.036634	-0.649815
H	-2.064616	1.978885	0.974919
H	-2.626956	2.313494	-0.675141
H	-6.23427	2.02791	0.630277
H	-5.538488	2.676414	-0.867328
H	-4.279442	2.515007	1.89907
H	-4.058748	3.779359	0.677171
H	-5.887832	-2.160169	-1.53532
H	-4.788018	-2.0005	-0.144824
H	-4.247211	-1.496693	-1.754014
H	2.114568	0.670454	3.075627
H	2.940052	2.240491	3.126252
H	4.584365	1.462071	-0.12391
H	4.166504	-0.550308	3.132683
H	4.712096	0.878214	4.031235
H	6.075554	0.202054	1.798834
H	5.599388	1.903768	1.98175
H	6.493732	-0.462206	-2.024919
H	6.349285	0.585762	-0.604536
H	7.173848	-0.977562	-0.464721
H	5.600801	-3.158122	-0.430031
H	3.975137	-2.841586	-1.088971
H	5.415749	-2.559382	-2.096145

(6b) PPII structure

C	-9.004118	-0.163141	-1.207524
C	-7.896658	0.076131	-0.217309
O	-7.734951	1.181945	0.336324
N	-7.080998	-0.956484	0.054086
C	-5.932417	-0.775006	0.933039
C	-5.320139	-2.187834	1.001083
C	-5.654759	-2.77924	-0.370987
C	-7.05886	-2.247177	-0.657736
C	-4.941437	0.217403	0.326489
O	-4.871054	0.396966	-0.900876
N	-4.131689	0.857949	1.182621
C	-3.050155	1.6905	0.670273
C	-2.432147	2.283935	1.947941
C	-2.632533	1.166369	2.975284
C	-4.013528	0.605541	2.633278
C	-2.039402	0.825236	-0.078526
O	-1.973888	-0.405517	0.068269
N	-1.179192	1.466286	-0.880609
C	-0.100227	0.773548	-1.584908

C	0.561896	1.909569	-2.395704
C	-0.495618	3.019016	-2.346598
N	-1.13455	2.87469	-1.028486
C	0.871935	0.166193	-0.579357
O	1.041532	0.691646	0.53342
N	1.541852	-0.927384	-0.963553
C	2.615104	-1.446282	-0.122873
C	3.071387	-2.703417	-0.884167
C	2.850294	-2.32114	-2.350605
C	1.557357	-1.503014	-2.325522
C	3.74914	-0.424458	-0.031024
O	3.917686	0.432823	-0.91447
N	4.564049	-0.521242	1.028085
C	5.768937	0.299142	1.090607
C	6.347792	-0.044856	2.474032
C	5.941618	-1.509411	2.663157
C	4.537152	-1.574225	2.062808
C	6.733477	-0.101724	-0.034739
O	6.614833	-1.204532	-0.59581
N	7.702156	0.766919	-0.378056
C	8.07516	1.943014	0.403221
C	8.694664	0.333382	-1.35631
H	-0.53118	0.001173	-2.227312
H	-0.47086	3.214435	-0.324094
H	1.477445	2.243295	-1.896077
H	0.807163	1.594263	-3.411152
H	-0.075358	4.021148	-2.437508
H	-1.256729	2.87408	-3.117615
H	-3.437222	2.456681	-0.003131
H	-1.383116	2.563091	1.816488
H	-2.997986	3.177189	2.23011
H	-4.093913	-0.461474	2.852889
H	-4.808503	1.137804	3.166416
H	-1.870134	0.391946	2.840313
H	-2.583439	1.524008	4.005799
H	2.23381	-1.673452	0.87526
H	1.551812	-0.713027	-3.080145
H	0.676795	-2.137803	-2.46821
H	4.108408	-2.9702	-0.664692
H	2.427155	-3.540578	-0.598286
H	3.68035	-1.703337	-2.707195
H	2.764266	-3.192002	-3.003705
H	-6.262075	-0.415091	1.910631
H	-4.247242	-2.166935	1.209677
H	-5.819552	-2.74913	1.796926
H	-7.246243	-2.101243	-1.723724
H	-7.830554	-2.91031	-0.250773
H	-4.951938	-2.406369	-1.12275
H	-5.622069	-3.870811	-0.378306
H	-9.724789	0.652573	-1.141058
H	-9.506337	-1.117735	-1.027605
H	-8.588138	-0.188797	-2.221367
H	4.317977	-2.550341	1.624435
H	3.769003	-1.339953	2.807745
H	5.493014	1.350764	0.997662
H	6.616803	-2.162006	2.100421
H	5.9518	-1.820492	3.709651
H	7.428394	0.110235	2.526078
H	5.868227	0.590191	3.225663
H	8.283268	2.77087	-0.278947
H	7.279664	2.247354	1.079767
H	8.977396	1.734528	0.989359
H	9.405781	-0.369887	-0.907792
H	8.203808	-0.147017	-2.203183
H	9.236894	1.212251	-1.708069

Cartesian Coordinates of PPI and PPII structures of the collagen model peptide Ac-Hyp-Gly-X-Hyp-Gly-Pro-NMe_2 optimized at the SMD M06-2X/6-31+G(d) level of theory in water**:**

(1) Ac-(Hyp-Gly-Pro)$_2$-NMe_2

(1a) PPI structure

C	-6.065224	-1.256514	-1.259909
C	-6.369646	0.195705	-0.999194
O	-7.334267	0.767616	-1.539639
N	-5.540928	0.866274	-0.174919
C	-4.37948	0.288055	0.499185
C	-3.695823	1.516011	1.151477
C	-4.146773	2.687255	0.283249
O	-3.386789	2.796382	-0.916969
C	-5.5962	2.325424	-0.026163
C	-4.760117	-0.727265	1.577473
O	-5.891193	-0.755667	2.075752
N	-3.776391	-1.540177	2.008373
C	-2.462098	-1.655927	1.414568
C	-2.491587	-2.355883	0.056186
O	-3.428769	-3.103564	-0.258693
N	-1.449255	-2.142	-0.758155
C	-0.332623	-1.237456	-0.501286
C	0.674715	-1.648749	-1.595389
C	-0.228701	-2.017044	-2.775336
C	-1.413083	-2.721759	-2.112027
C	-0.752232	0.224974	-0.700451
O	-1.762349	0.503781	-1.370631
N	0.047649	1.17412	-0.196067
C	1.234978	0.942048	0.631434
C	1.872754	2.347913	0.728213
C	1.407488	3.028288	-0.55377
O	2.114053	2.553008	-1.696187
C	-0.044897	2.57499	-0.636996
C	0.88198	0.417834	2.022265
O	-0.256521	0.536397	2.486618
N	1.892088	-0.11897	2.733818
C	3.226806	-0.387354	2.24129
C	3.274932	-1.544273	1.240328
O	2.34501	-2.359908	1.162014
N	4.384942	-1.655561	0.497395
C	5.477359	-0.68681	0.445309
C	6.559777	-1.458215	-0.331739
C	5.739864	-2.27736	-1.33279
C	4.503711	-2.699321	-0.535901
C	5.049373	0.581536	-0.311777
O	3.981467	0.591096	-0.957742
N	5.854867	1.646936	-0.269835
C	7.116768	1.732991	0.461001
C	5.450531	2.848469	-0.998073
H	-6.125897	-1.848641	-0.341654
H	-3.715683	-0.168632	-0.242987
H	-4.076156	1.657788	2.168797
H	-2.607176	1.415853	1.196899
H	-4.078414	3.64116	0.812012
H	-6.25959	2.611374	0.798613
H	-5.950987	2.786218	-0.949545
H	-2.821686	2.004975	-1.042483
H	-4.049632	-2.229945	2.701685
H	-1.989187	-0.673302	1.35226
H	-1.838609	-2.252333	2.087904
H	0.07729	-1.407226	0.497505
H	1.398221	-0.860622	-1.823658
H	1.218578	-2.528785	-1.239657
H	-0.567112	-1.114419	-3.292977
H	0.274441	-2.661393	-3.499018
H	-2.36448	-2.539091	-2.619046
H	-1.261072	-3.80409	-2.04007
H	-5.05331	-1.365861	-1.66527
H	-6.787204	-1.643311	-1.979593
H	-0.682299	3.159521	0.036267
H	-0.44603	2.621667	-1.651132
H	1.919054	0.2562	0.119932
H	1.491524	4.117339	-0.500415
H	1.465043	2.888055	1.589194
H	2.960092	2.306147	0.820114
H	2.843988	1.956933	-1.42265
H	1.640005	-0.488879	3.645292
H	3.664383	0.52083	1.821431
H	3.847741	-0.661768	3.099092
H	3.593457	-2.731689	-1.140322
H	4.635404	-3.673558	-0.05351
H	5.798984	-0.432415	1.457144
H	5.445694	-1.649857	-2.180331
H	6.290162	-3.138208	-1.717711
H	7.284847	-0.795201	-0.809457
H	7.090176	-2.114045	0.36569
H	7.074097	2.575121	1.157484
H	7.320748	0.826292	1.025877
H	7.937338	1.897402	-0.243558
H	5.151762	2.59183	-2.017019
H	4.617427	3.347939	-0.492985
H	6.302799	3.527769	-1.035662

(1b) PPII structure

C	-10.479837	-0.880728	0.333836
C	-9.128877	-0.992466	-0.318832
O	-8.660899	-2.084068	-0.696512
N	-8.437963	0.146495	-0.494577
C	-7.108136	0.13186	-1.09519
C	-6.644093	1.594858	-0.957588
C	-7.95013	2.387625	-0.941707
O	-8.506073	2.50294	-2.24984
C	-8.878363	1.498817	-0.128074
C	-6.154189	-0.78246	-0.340914
O	-6.182542	-0.883851	0.890785
N	-5.237865	-1.418699	-1.092509
C	-4.092563	-2.024185	-0.457354
C	-3.205506	-0.977917	0.214297
O	-3.313085	0.231634	-0.0421
N	-2.305928	-1.441515	1.093044
C	-1.332481	-0.532066	1.683361
C	-0.577932	-1.432951	2.677533
C	-0.597885	-2.798073	1.983687
C	-1.988965	-2.860715	1.34925
C	-0.377229	-0.007315	0.612112
O	-0.212139	-0.606473	-0.462196
N	0.320244	1.100543	0.908915
C	1.430607	1.509413	0.04879
C	2.123497	2.626372	0.856919
C	1.029143	3.140233	1.79142
O	0.118462	3.998322	1.108569
C	0.27102	1.874193	2.158204
C	2.398255	0.354054	-0.172126
O	2.64851	-0.461031	0.723938
N	2.99963	0.313727	-1.37193
C	4.128735	-0.558482	-1.582026
C	5.321831	-0.163044	-0.715658
O	5.38317	0.93911	-0.148086
N	6.298413	-1.074044	-0.615613
C	7.541101	-0.747296	0.074799
C	8.301511	-2.085448	0.055979
C	7.852831	-2.719315	-1.263824
C	6.373268	-2.345098	-1.360666
C	8.303936	0.340365	-0.693278
O	8.035884	0.574578	-1.884203
N	9.268312	1.013366	-0.040048
C	10.064802	1.975191	-0.796285
C	9.820478	0.633886	1.25722
H	-11.173059	-0.353312	-0.330507
H	-7.172035	-0.177445	-2.144394
H	-6.131518	1.733879	0.000881
H	-5.974004	1.895971	-1.766145
H	-7.833398	3.376758	-0.489579
H	-8.739197	1.675283	0.944289
H	-9.926875	1.658129	-0.388668
H	-7.877069	2.99142	-2.805726
H	-5.184435	-1.197029	-2.080629
H	-4.422373	-2.763482	0.277399
H	-3.50483	-2.547539	-1.216686
H	-1.845069	0.297144	2.173868
H	0.43238	-1.069867	2.884039
H	-1.137612	-1.466135	3.617321
H	0.170897	-2.832805	1.204868
H	-0.428452	-3.625459	2.67572
H	-1.998937	-3.434437	0.419561
H	-2.72761	-3.285808	2.037182
H	-10.418489	-0.317131	1.269857
H	-10.864782	-1.88146	0.531076
H	0.781319	1.341862	2.968736
H	-0.757272	2.092489	2.453208
H	1.052336	1.873194	-0.911938
H	1.434742	3.640869	2.675502
H	2.938102	2.206475	1.45732
H	2.528377	3.410078	0.212766
H	0.608181	4.775454	0.793235
H	2.833387	1.06978	-2.027426
H	3.844257	-1.593284	-1.371842
H	4.425353	-0.501326	-2.632975
H	6.043203	-2.209705	-2.393381
H	5.73387	-3.092919	-0.878956
H	7.311013	-0.403623	1.084683
H	8.403714	-2.277034	-2.100087
H	8.001373	-3.800834	-1.285069
H	9.384517	-1.952801	0.1204
H	7.974295	-2.689937	0.907884
H	9.943167	1.532173	1.867571
H	9.17006	-0.057299	1.788452
H	10.800425	0.162168	1.124092
H	10.788389	1.465539	-1.442738
H	9.416922	2.60062	-1.411509
H	10.603556	2.607138	-0.088783

(2) Ac-Hyp-Gly-α-azPro(d)-Hyp-Gly-Pro-NMe_2

(2a) PPI structure

C	-6.148663	-1.319112	-1.159351
C	-6.455329	0.126978	-0.868508
O	-7.462517	0.686794	-1.340349
N	-5.58392	0.806386	-0.09784
C	-4.385758	0.240233	0.517836
C	-3.713424	1.465811	1.182714

C	-4.211458	2.646653	0.354792
O	-3.486955	2.795248	-0.863351
C	-5.660892	2.262612	0.07502
C	-4.704309	-0.815791	1.575752
O	-5.810736	-0.86761	2.125867
N	-3.699477	-1.642849	1.920341
C	-2.387063	-1.679923	1.309244
C	-2.411112	-2.296596	-0.086149
O	-3.307884	-3.069643	-0.447806
N	-1.412939	-1.967584	-0.917403
N	-0.370011	-1.084248	-0.568213
C	0.744199	-1.551987	-1.445516
C	0.038902	-1.893664	-2.758893
C	-1.284236	-2.499617	-2.285398
C	-0.745372	0.278153	-0.809465
O	-1.800666	0.575944	-1.382971
N	0.122584	1.191746	-0.355631
C	1.250717	0.964263	0.549587
C	1.855152	2.380753	0.707109
C	1.455614	3.081288	-0.587385
O	2.250394	2.661784	-1.6921
C	0.022355	2.597686	-0.773277
C	0.809548	0.428047	1.907436
O	-0.347566	0.571533	2.313929
N	1.773732	-0.121988	2.671538
C	3.128527	-0.409587	2.249252
C	3.204027	-1.579407	1.266028
O	2.286962	-2.410549	1.198447
N	4.314928	-1.683121	0.522853
C	5.427305	-0.734424	0.502722
C	6.511577	-1.518631	-0.260423
C	5.697153	-2.320898	-1.279235
C	4.447176	-2.734844	-0.50119
C	5.051323	0.55453	-0.245643
O	4.010729	0.597914	-0.933112
N	5.873536	1.603839	-0.148363
C	7.122569	1.643223	0.608331
C	5.523608	2.826615	-0.869345
H	-2.142182	-2.194432	-2.890244
H	-1.253157	-3.591524	-2.234072
H	1.508245	-0.781011	-1.547626
H	1.178481	-2.435496	-0.976255
H	-0.138644	-0.981785	-3.336911
H	0.618998	-2.590269	-3.366432
H	-1.941315	-0.685181	1.299618
H	-1.738261	-2.299164	1.936018
H	-3.926684	-2.348358	2.614503
H	-3.736071	-0.17425	-0.260115
H	-4.069777	1.574033	2.212819
H	-2.622954	1.388395	1.19566
H	-6.309148	2.525687	0.919111
H	-6.04599	2.730701	-0.832701
H	-4.148753	3.589436	0.904047
H	-6.20224	-1.927307	-0.251065
H	-5.141295	-1.422604	-1.57606
H	-6.878425	-1.69419	-1.877472
H	-2.876243	2.040609	-0.996435
H	1.986793	0.29948	0.09157
H	-0.669514	3.150773	-0.127078
H	-0.315773	2.659935	-1.809475
H	1.387577	2.897656	1.551685
H	2.936165	2.354293	0.864164
H	1.507236	4.170041	-0.503128
H	1.468053	-0.489033	3.567654
H	2.926339	2.012525	-1.40124
H	3.598207	0.489029	1.842736
H	3.702644	-0.684298	3.13918
H	5.73208	-0.501275	1.524757
H	3.546516	-2.768779	-1.119772
H	4.569556	-3.706855	-0.01155
H	7.254409	-0.863741	-0.721845
H	7.020689	-2.186195	0.441725
H	5.420811	-1.683933	-2.125803
H	6.243163	-3.18502	-1.662984
H	7.086588	2.470734	1.322368
H	7.295679	0.719885	1.156013
H	7.959447	1.803537	-0.077913
H	5.25359	2.59384	-1.901989
H	4.686393	3.338159	-0.383962
H	6.392845	3.48516	-0.867167

(2b) PPII structure

C	-10.43083	-0.917076	0.711011
C	-9.113845	-1.093041	0.004473
O	-8.602244	-2.213799	-0.180589
N	-8.504562	0.020893	-0.436681
C	-7.203894	-0.042998	-1.095528
C	-6.808683	1.439462	-1.242422
C	-8.151292	2.16731	-1.290962
O	-8.77535	2.024858	-2.565265
C	-8.992242	1.398243	-0.283913
C	-6.172711	-0.771727	-0.246786
O	-6.144604	-0.664492	0.984442
N	-5.257944	-1.48054	-0.930748
C	-4.084551	-1.988471	-0.265859
C	-3.19385	-0.859273	0.245978
O	-3.351364	0.319227	-0.094
N	-2.216559	-1.257459	1.074947
N	-1.29966	-0.310906	1.564518

C	-0.701622	-0.987123	2.741822
C	-0.59196	-2.443842	2.288475
C	-1.862118	-2.641595	1.456373
C	-0.368521	0.085869	0.55993
O	-0.327925	-0.434697	-0.560321
N	0.432635	1.102526	0.916607
C	1.486681	1.5297	0.003424
C	2.189525	2.652657	0.788126
C	1.068426	3.22118	1.658734
O	0.168497	4.018655	0.893822
C	0.314515	1.973253	2.095158
C	2.44795	0.391276	-0.308377
O	2.678006	-0.515869	0.499108
N	3.06031	0.469395	-1.501555
C	4.190523	-0.37813	-1.79586
C	5.353341	-0.120858	-0.840238
O	5.404609	0.896704	-0.131938
N	6.304443	-1.063279	-0.806566
C	7.486012	-0.879526	0.025343
C	8.20509	-2.233785	-0.103603
C	7.873327	-2.663438	-1.535856
C	6.42247	-2.214853	-1.723551
C	8.353872	0.258815	-0.525656
O	8.192507	0.664897	-1.689546
N	9.299614	0.77587	0.278151
C	10.212835	1.76297	-0.289484
C	9.705756	0.216635	1.564002
H	-1.693355	-3.252826	0.566071
H	-2.675924	-3.072487	2.045731
H	0.259835	-0.539121	2.988099
H	-1.386924	-0.869701	3.584787
H	0.297722	-2.56604	1.662744
H	-0.536899	-3.139903	3.12696
H	-4.375283	-2.636393	0.566268
H	-3.5134	-2.593648	-0.975256
H	-5.274296	-1.453976	-1.943943
H	-7.299289	-0.534137	-2.070453
H	-6.25512	1.767327	-0.355298
H	-6.196717	1.62058	-2.129138
H	-8.809425	1.766681	0.731658
H	-10.059166	1.46718	-0.507573
H	-8.065225	3.225091	-1.025703
H	-11.184896	-0.544211	0.009549
H	-10.343093	-0.191132	1.525292
H	-10.754535	-1.879013	1.109058
H	-8.206736	2.443759	-3.231813
H	1.051436	1.908928	-0.927961
H	0.800196	1.530429	2.970646
H	-0.734049	2.174197	2.324566
H	2.96992	2.232188	1.432824
H	2.635914	3.399747	0.127975
H	1.447124	3.785746	2.515828
H	2.897466	1.287336	-2.078285
H	0.655855	4.782972	0.54518
H	3.895152	-1.429946	-1.742416
H	4.519247	-0.176659	-2.819007
H	7.174526	-0.658173	1.04751
H	6.207776	-1.915111	-2.752304
H	5.716067	-2.998682	-1.429888
H	9.279815	-2.15673	0.080519
H	7.775914	-2.933307	0.620524
H	8.520363	-2.138152	-2.245525
H	7.989664	-3.737739	-1.69282
H	10.947002	1.283588	-0.947066
H	9.65723	2.508272	-0.859942
H	10.737662	2.258146	0.528628
H	9.820822	1.030511	2.284274
H	8.971208	-0.484099	1.954229
H	10.666201	-0.300673	1.460537

(3) Ac-Hyp-Gly-β-azPro(d)-Hyp-Gly-Pro-NMe_2

(3a) PPI structure

C	-6.048487	-1.285818	-1.304149
C	-6.363409	0.167325	-1.06075
O	-7.324659	0.729273	-1.617312
N	-5.547747	0.849783	-0.233399
C	-4.395875	0.282329	0.465731
C	-3.72768	1.519305	1.117202
C	-4.171983	2.681224	0.232718
O	-3.396113	2.784433	-0.957735
C	-5.614752	2.309042	-0.094174
C	-4.792823	-0.725239	1.544771
O	-5.930079	-0.74837	2.028651
N	-3.818299	-1.54229	1.988495
C	-2.488037	-1.650092	1.431429
C	-2.465324	-2.36949	0.082564
O	-3.378632	-3.134972	-0.255171
N	-1.388266	-2.160094	-0.686892
C	-0.300581	-1.212961	-0.425828
N	0.71813	-1.523545	-1.415526
C	-0.031893	-2.023689	-2.581171
C	-1.248841	-2.765948	-2.015871
C	-0.756161	0.240231	-0.661995
O	-1.760372	0.48375	-1.352373
N	0.028237	1.201326	-0.16294
C	1.221713	0.973794	0.657567
C	1.841678	2.384366	0.770976
C	1.378939	3.069088	-0.510285

O	2.10653	2.61821	-1.648951	H	7.268221	-0.783759	-0.852213
C	-0.068114	2.599257	-0.612772	H	7.07228	-2.128231	0.293065
C	0.880389	0.420921	2.03942	H	5.430678	-1.608852	-2.244293
O	-0.247981	0.551261	2.525741	H	6.276344	-3.106197	-1.813796
N	1.88649	-0.169471	2.711558	H	7.074966	2.526632	1.220845
C	3.211665	-0.43358	2.192527	H	7.311023	0.780868	1.037194
C	3.24321	-1.558077	1.153753	H	7.937815	1.885364	-0.197949
O	2.298986	-2.353789	1.038327	H	5.166999	2.647035	-1.95987
N	4.360043	-1.665915	0.421717	H	4.628729	3.364726	-0.418856
C	5.459439	-0.702526	0.402502	H	6.318627	3.548307	-0.946674
C	6.542512	-1.457087	-0.390157				
C	5.724994	-2.254455	-1.410494	(3b) PPII structure			
C	4.488368	-2.694461	-0.625394				
C	5.041595	0.592009	-0.315027	C	-10.427223	-0.566389	0.190544
O	3.974277	0.631162	-0.960395	C	-9.073901	-0.689683	-0.455177
N	5.853636	1.650279	-0.236138	O	-8.626629	-1.779398	-0.861774
C	7.114366	1.705545	0.499459	N	-8.3576	0.439433	-0.590088
C	5.461664	2.873978	-0.932749	C	-7.01943	0.417234	-1.170674
H	0.099847	-1.357646	0.578882	C	-6.520122	1.858172	-0.95749
H	-2.156403	-2.604431	-2.603844	C	-7.806037	2.683761	-0.944889
H	-1.073137	-3.841748	-1.916812	O	-8.322225	2.861586	-2.26241
H	1.300788	-2.26522	-1.024605	C	-8.779066	1.789638	-0.191596
H	-0.353195	-1.174254	-3.189662	C	-6.111132	-0.568435	-0.450134
H	0.608511	-2.662891	-3.188824	O	-6.175527	-0.748006	0.771673
H	-2.021331	-0.663491	1.372743	N	-5.200005	-1.181545	-1.221819
H	-1.877701	-2.23339	2.128108	C	-4.152414	-1.975539	-0.632034
H	-4.098554	-2.220703	2.690066	C	-3.214139	-1.139882	0.23076
H	-3.718349	-0.181136	-0.259505	O	-3.217019	0.100029	0.209805
H	-4.123304	1.668154	2.127618	N	-2.378704	-1.83165	1.018436
H	-2.639325	1.425124	1.179669	C	-1.331932	-1.136611	1.771575
H	-6.291288	2.595153	0.719867	N	-0.621818	-2.183816	2.492964
H	-5.959838	2.762324	-1.024879	C	-0.734305	-3.36996	1.622832
H	-4.115403	3.639849	0.754235	C	-2.118035	-3.277807	0.967551
H	-6.122618	-1.869985	-0.381739	C	-0.364561	-0.445994	0.801433
H	-5.029698	-1.394533	-1.692013	O	-0.168627	-0.907807	-0.333524
H	-6.757478	-1.681627	-2.031811	N	0.300764	0.626555	1.249308
H	-2.832357	1.990921	-1.072933	C	1.349661	1.221108	0.422565
H	1.903564	0.301135	0.126234	C	1.976562	2.277761	1.348671
H	-0.721015	3.180125	0.048524	C	0.826185	2.662333	2.275915
H	-0.45453	2.637869	-1.633074	O	-0.113512	3.507327	1.616448
H	1.420929	2.912756	1.633005	C	0.134211	1.332071	2.532405
H	2.929144	2.353773	0.871534	C	2.390629	0.19012	0.012701
H	1.446386	4.158626	-0.446263	O	2.72923	-0.732961	0.762525
H	1.645886	-0.554992	3.619703	N	2.955324	0.388973	-1.189503
H	2.828097	2.011098	-1.377635	C	4.118967	-0.364933	-1.583567
H	3.650817	0.484447	1.796011	C	5.328616	-0.05171	-0.706323
H	3.841309	-0.739248	3.033306	O	5.339175	0.90668	0.081968
H	5.77749	-0.480423	1.423113	N	6.376723	-0.872612	-0.849233
H	3.582322	-2.726061	-1.235753	C	7.624443	-0.609722	-0.140959
H	4.62411	-3.673577	-0.153919	C	8.475241	-1.847566	-0.480648

C	8.004877	-2.210994	-1.89182
C	6.498644	-1.954941	-1.844053
C	8.274348	0.676997	-0.667473
O	7.926671	1.153796	-1.761152
N	9.2314	1.254077	0.08223
C	9.933501	2.40429	-0.479045
C	9.883088	0.628858	1.229923
H	-1.77204	-0.420834	2.464786
H	-2.110072	-3.641741	-0.062564
H	-2.878215	-3.819706	1.53879
H	-1.156717	-2.369083	3.341894
H	0.04922	-3.33388	0.862834
H	-0.610314	-4.279075	2.210892
H	-4.582379	-2.782245	-0.029589
H	-3.570824	-2.43433	-1.436383
H	-5.144738	-0.9427	-2.205285
H	-7.074765	0.162514	-2.235113
H	-6.02964	1.943617	0.018841
H	-5.820821	2.174938	-1.734694
H	-8.671628	1.927419	0.889984
H	-9.815132	1.981444	-0.479188
H	-7.67759	3.652291	-0.453043
H	-11.098041	0.01332	-0.452605
H	-10.354724	-0.048537	1.152098
H	-10.844796	-1.562328	0.339432
H	-7.666796	3.354786	-2.782288
H	0.908865	1.678356	-0.470193
H	0.631563	0.791275	3.343456
H	-0.920836	1.473618	2.773713
H	2.781017	1.827929	1.941365
H	2.376452	3.129207	0.793153
H	1.170211	3.124639	3.205674
H	2.695311	1.209197	-1.725658
H	0.336023	4.332185	1.370095
H	3.902244	-1.436829	-1.543848
H	4.360966	-0.112463	-2.619387
H	7.419657	-0.517318	0.927409
H	6.095917	-1.642189	-2.810317
H	5.94927	-2.837614	-1.498388
H	9.548319	-1.648736	-0.424606
H	8.233232	-2.648116	0.22564
H	8.471946	-1.546572	-2.625959
H	8.234539	-3.243476	-2.16259
H	10.63913	2.092927	-1.257711
H	9.220193	3.110049	-0.906014
H	10.483758	2.895873	0.324558
H	10.025185	1.380494	2.01017
H	9.288365	-0.183274	1.642122
H	10.863719	0.236033	0.938025

(4) Ac-Hyp-Gly-γ-azPro(d)-Hyp-Gly-Pro-NMe_2

(4a) PPI structure

C	-6.056632	-1.237791	-1.29679
C	-6.352192	0.217224	-1.040832
O	-7.307471	0.796012	-1.590456
N	-5.524847	0.882119	-0.211006
C	-4.380603	0.293615	0.482959
C	-3.69039	1.516918	1.138137
C	-4.127096	2.692225	0.267383
O	-3.359263	2.797178	-0.928087
C	-5.576087	2.339833	-0.053643
C	-4.794602	-0.709293	1.56028
O	-5.932346	-0.710582	2.043755
N	-3.83508	-1.544062	2.003595
C	-2.508767	-1.676886	1.44061
C	-2.512996	-2.365066	0.077106
O	-3.43883	-3.113415	-0.267076
N	-1.455006	-2.143505	-0.713429
C	-0.3361	-1.248621	-0.463781
C	0.618339	-1.681285	-1.607039
N	-0.272077	-2.027206	-2.717317
C	-1.379255	-2.715403	-2.077532
C	-0.743913	0.215126	-0.663785
O	-1.743117	0.492239	-1.352021
N	0.052203	1.16211	-0.152723
C	1.246144	0.924171	0.663631
C	1.872258	2.333134	0.786316
C	1.394914	3.036511	-0.478957
O	2.104564	2.597285	-1.633798
C	-0.052525	2.56929	-0.569888
C	0.905795	0.366684	2.04436
O	-0.230795	0.466375	2.517679
N	1.924493	-0.179281	2.735986
C	3.253673	-0.433211	2.221412
C	3.291657	-1.563908	1.190195
O	2.357902	-2.373099	1.093749
N	4.398399	-1.660467	0.440874
C	5.488471	-0.688847	0.402541
C	6.569498	-1.443758	-0.392393
C	5.747725	-2.248853	-1.403499
C	4.515712	-2.686961	-0.609142
C	5.05287	0.592796	-0.327465
O	3.978478	0.613918	-0.962684
N	5.858293	1.657504	-0.273081
C	7.122542	1.733632	0.454682
C	5.448517	2.871611	-0.976097
H	-6.125652	-1.827416	-0.377454
H	-3.712556	-0.177272	-0.246093

H	-4.074919	1.662324	2.153325
H	-2.602842	1.40764	1.190071
H	-4.056006	3.645106	0.797654
H	-6.243648	2.62313	0.768836
H	-5.922635	2.808004	-0.976415
H	-2.797396	2.002992	-1.048956
H	-4.12759	-2.218762	2.703682
H	-2.014191	-0.703515	1.39664
H	-1.912968	-2.291534	2.122483
H	0.107721	-1.434022	0.51663
H	1.335306	-0.907944	-1.889699
H	1.160332	-2.573248	-1.282916
H	-0.632975	-1.15742	-3.110926
H	-2.315818	-2.55346	-2.613706
H	-1.183628	-3.788995	-2.002886
H	-5.043582	-1.354862	-1.697166
H	-6.77774	-1.621519	-2.018963
H	-0.696864	3.133572	0.114131
H	-0.45308	2.631169	-1.583384
H	1.932171	0.256828	0.130608
H	1.466284	4.124913	-0.401392
H	1.465278	2.851359	1.66097
H	2.960638	2.299723	0.87036
H	2.833273	1.991848	-1.378368
H	1.680767	-0.57744	3.637838
H	3.685066	0.486307	1.820198
H	3.884872	-0.728308	3.064704
H	3.603137	-2.712541	-1.210791
H	4.651878	-3.667689	-0.141302
H	5.813171	-0.452403	1.417827
H	5.448338	-1.60876	-2.23971
H	6.298721	-3.101746	-1.804797
H	7.290448	-0.770964	-0.862566
H	7.104995	-2.109566	0.291578
H	7.079376	2.562767	1.166637
H	7.331209	0.817219	1.001979
H	7.940088	1.913334	-0.249608
H	5.137055	2.632374	-1.995393
H	4.622575	3.36424	-0.452628
H	6.30203	3.549454	-1.012413

(4b) PPII structure

C	-10.472858	-0.768843	0.449863
C	-9.136744	-0.91648	-0.226362
O	-8.696551	-2.023765	-0.591987
N	-8.42712	0.204609	-0.437279
C	-7.124385	0.14973	-1.091967
C	-6.649404	1.615217	-1.061527
C	-7.952971	2.41218	-1.030509
O	-8.575615	2.442202	-2.312932
C	-8.840582	1.577742	-0.11938
C	-6.148145	-0.737265	-0.333592
O	-6.151151	-0.813642	0.900339
N	-5.244129	-1.384383	-1.089753
C	-4.104348	-2.010317	-0.466788
C	-3.197541	-0.986465	0.212388
O	-3.266863	0.224903	-0.041918
N	-2.319811	-1.479082	1.098139
C	-1.307245	-0.62792	1.697001
C	-0.568518	-1.636607	2.605484
N	-0.680476	-2.922945	1.907992
C	-2.024382	-2.910627	1.358447
C	-0.355877	-0.089045	0.632444
O	-0.193347	-0.684249	-0.44489
N	0.347896	1.009313	0.943435
C	1.441089	1.446412	0.075431
C	2.141261	2.541086	0.905421
C	1.041681	3.05382	1.833481
O	0.138329	3.915925	1.145906
C	0.275724	1.788907	2.18939
C	2.413054	0.308892	-0.209558
O	2.679582	-0.551276	0.637671
N	3.006271	0.343603	-1.414291
C	4.155857	-0.486591	-1.680254
C	5.324059	-0.14642	-0.757868
O	5.356992	0.911274	-0.110414
N	6.305999	-1.057011	-0.687887
C	7.522727	-0.752467	0.056843
C	8.312378	-2.068551	-0.03685
C	7.94176	-2.592237	-1.427559
C	6.461895	-2.227148	-1.577064
C	8.28116	0.399656	-0.61679
O	8.043172	0.698673	-1.799869
N	9.21205	1.05171	0.102246
C	10.021987	2.055288	-0.581162
C	9.727858	0.612361	1.39563
H	-11.182175	-0.28751	-0.232482
H	-7.236022	-0.215995	-2.118895
H	-6.089933	1.81013	-0.139789
H	-6.019177	1.864447	-1.918277
H	-7.815677	3.427847	-0.648231
H	-8.641572	1.809353	0.932707
H	-9.900508	1.731308	-0.332024
H	-7.980753	2.897267	-2.930731
H	-5.219111	-1.199562	-2.086394
H	-4.44101	-2.754163	0.260928
H	-3.526746	-2.53118	-1.235655
H	-1.76915	0.182059	2.263087
H	0.476569	-1.374614	2.777766

H	-1.086514	-1.695388	3.566179
H	-0.028151	-2.902749	1.122559
H	-2.072895	-3.502325	0.443866
H	-2.740072	-3.297513	2.088994
H	-10.396366	-0.149799	1.348411
H	-10.848191	-1.757446	0.715647
H	0.765692	1.256128	3.011739
H	-0.757704	2.012701	2.460722
H	1.042005	1.842176	-0.864234
H	1.441171	3.550294	2.722615
H	2.941838	2.100361	1.509813
H	2.564551	3.327809	0.276865
H	0.632563	4.692002	0.834745
H	2.822638	1.133941	-2.022352
H	3.890466	-1.542003	-1.571083
H	4.467561	-0.326446	-2.716201
H	6.201261	-1.96938	-2.606583
H	5.809368	-3.039504	-1.24072
H	7.259128	-0.487505	1.081627
H	8.531992	-2.077595	-2.192051
H	8.106275	-3.666635	-1.531791
H	9.387878	-1.923636	0.094069
H	7.955834	-2.749604	0.742402
H	9.816248	1.478233	2.056417
H	9.071095	-0.115013	1.86707
H	10.718551	0.161408	1.270606
H	10.750955	1.581674	-1.248621
H	9.385806	2.721284	-1.16541
H	10.554197	2.638241	0.171694

(5) Ac-Hyp-Gly-δ-azPro(d)-Hyp-Gly-Pro-NMe_2

(5a) PPI structure

C	-6.040478	-1.247431	-1.285521
C	-6.346747	0.202579	-1.014418
O	-7.308462	0.778838	-1.555419
N	-5.522095	0.866536	-0.180927
C	-4.366916	0.281986	0.498679
C	-3.68312	1.505407	1.159793
C	-4.134222	2.684364	0.301183
O	-3.372969	2.807409	-0.896542
C	-5.581865	2.323287	-0.015893
C	-4.763004	-0.73642	1.568235
O	-5.897211	-0.755507	2.059552
N	-3.792856	-1.566341	1.998188
C	-2.470488	-1.692106	1.423965
C	-2.493118	-2.36755	0.05381
O	-3.422377	-3.114443	-0.292911
N	-1.454602	-2.114947	-0.745192
C	-0.332507	-1.218128	-0.505568
C	0.645162	-1.638688	-1.620987
C	-0.30906	-2.034833	-2.738635
N	-1.382012	-2.756331	-2.024529
C	-0.751302	0.24443	-0.700127
O	-1.756987	0.521055	-1.376411
N	0.047704	1.187479	-0.186972
C	1.236325	0.944342	0.636421
C	1.876687	2.347783	0.746879
C	1.412147	3.04095	-0.52856
O	2.116007	2.572691	-1.675461
C	-0.041724	2.59272	-0.614857
C	0.882963	0.405055	2.021515
O	-0.25641	0.516843	2.485109
N	1.893022	-0.138079	2.727951
C	3.225441	-0.405958	2.229316
C	3.267527	-1.554684	1.218546
O	2.332758	-2.363904	1.131987
N	4.378239	-1.666195	0.476899
C	5.473261	-0.699986	0.432197
C	6.553877	-1.467906	-0.350848
C	5.73222	-2.280004	-1.356242
C	4.496202	-2.70523	-0.561072
C	5.048584	0.576248	-0.313407
O	3.979757	0.595797	-0.957892
N	5.857873	1.638293	-0.262356
C	7.119354	1.714368	0.470364
C	5.457482	2.848048	-0.978735
H	-6.101195	-1.846402	-0.371622
H	-3.699751	-0.175253	-0.23988
H	-4.062379	1.639493	2.17855
H	-2.59452	1.404743	1.203623
H	-4.068513	3.633093	0.839495
H	-6.248413	2.598614	0.810013
H	-5.934669	2.793637	-0.935203
H	-2.812721	2.014779	-1.033805
H	-4.079413	-2.255135	2.686986
H	-1.97991	-0.716518	1.386121
H	-1.870652	-2.312445	2.096829
H	0.090189	-1.401683	0.484509
H	1.333776	-0.838922	-1.904713
H	1.220588	-2.5014	-1.276323
H	-0.694141	-1.148788	-3.25442
H	0.151166	-2.703401	-3.466635
H	-2.282484	-2.583115	-2.476768
H	-5.027978	-1.353089	-1.690716
H	-6.761427	-1.629898	-2.008545
H	-0.67708	3.171448	0.065165
H	-0.443631	2.650107	-1.628129
H	1.917914	0.26369	0.114071

H	1.499294	4.129222	-0.465949
H	1.470884	2.880084	1.613587
H	2.964033	2.30289	0.837189
H	2.846089	1.974271	-1.407533
H	1.639318	-0.523527	3.632577
H	3.663638	0.504758	1.815829
H	3.848372	-0.688806	3.082929
H	3.58592	-2.734846	-1.165497
H	4.627812	-3.681426	-0.082612
H	5.795527	-0.454878	1.446135
H	5.438104	-1.647216	-2.199883
H	6.281171	-3.139182	-1.746797
H	7.279197	-0.802766	-0.825198
H	7.084271	-2.128761	0.341826
H	7.077147	2.548817	1.176103
H	7.321842	0.801159	1.025223
H	7.940598	1.885372	-0.231796
H	5.157308	2.602044	-1.999855
H	4.626594	3.34577	-0.468281
H	6.312288	3.524491	-1.01032

(5b) PPII structure

C	-10.398592	-0.36512	-0.465202
C	-8.967332	-0.580813	-0.876221
O	-8.536571	-1.698683	-1.218791
N	-8.158109	0.491888	-0.869628
C	-6.753317	0.370793	-1.243788
C	-6.192487	1.775017	-0.953658
C	-7.402611	2.686913	-1.146693
O	-7.697038	2.87315	-2.529851
C	-8.540826	1.874225	-0.547509
C	-6.025231	-0.669731	-0.405629
O	-6.276683	-0.843924	0.791867
N	-5.050034	-1.340974	-1.043952
C	-4.085383	-2.109235	-0.296624
C	-3.193759	-1.206269	0.550191
O	-3.256983	0.029095	0.500849
N	-2.33393	-1.826238	1.374113
C	-1.253142	-1.108322	2.050677
C	-0.412784	-2.258068	2.642003
C	-0.737228	-3.408989	1.686628
N	-2.166153	-3.241268	1.370948
C	-0.414809	-0.325567	1.040235
O	-0.340828	-0.672718	-0.147836
N	0.296735	0.70837	1.514929
C	1.303275	1.344699	0.66465
C	2.070812	2.262674	1.636692
C	1.070048	2.525091	2.75968
O	0.089064	3.483512	2.371523
C	0.359804	1.188555	2.904397
C	2.257216	0.314994	0.072941
O	2.610184	-0.684615	0.709068
N	2.734444	0.597329	-1.150445
C	3.84441	-0.154857	-1.682592
C	5.109938	0.032821	-0.849086
O	5.213738	0.937793	-0.006453
N	6.098735	-0.839456	-1.083119
C	7.381988	-0.692146	-0.406964
C	8.148687	-1.94908	-0.856354
C	7.612835	-2.19416	-2.269961
C	6.126754	-1.849458	-2.156962
C	8.08235	0.592539	-0.869854
O	7.74293	1.146511	-1.929187
N	9.064525	1.090099	-0.095349
C	9.794648	2.255093	-0.58602
C	9.715122	0.365456	0.993111
H	-10.921123	0.217155	-1.232106
H	-6.666092	0.11424	-2.306034
H	-5.859492	1.836626	0.088517
H	-5.357285	2.033462	-1.608887
H	-7.283824	3.653629	-0.648953
H	-8.595197	2.022238	0.536381
H	-9.50168	2.133399	-0.997969
H	-6.933453	3.304105	-2.947649
H	-4.819681	-1.069394	-1.9936
H	-4.596283	-2.832591	0.342938
H	-3.457656	-2.669006	-0.993386
H	-1.658899	-0.4484	2.818686
H	0.652473	-2.016223	2.680992
H	-0.764748	-2.486018	3.651857
H	-0.158917	-3.329522	0.762342
H	-0.581359	-4.395631	2.124467
H	-2.699072	-3.586637	2.17329
H	-10.459802	0.187791	0.476891
H	-10.886997	-1.333801	-0.356722
H	0.945253	0.50278	3.527302
H	-0.637219	1.312111	3.330278
H	0.816003	1.912055	-0.134975
H	1.554746	2.830245	3.691695
H	2.937466	1.73279	2.047052
H	2.413698	3.180545	1.154024
H	0.537871	4.327921	2.202255
H	2.493262	1.484324	-1.578663
H	3.587148	-1.216859	-1.730519
H	4.040255	0.186122	-2.702942
H	5.721345	-1.439704	-3.085122
H	5.530698	-2.719879	-1.861928
H	7.216239	-0.660786	0.671258
H	8.098462	-1.516932	-2.97965

H	7.768518	-3.220428	-2.60862
H	9.232673	-1.813986	-0.824863
H	7.883185	-2.779365	-0.194221
H	9.875796	1.049811	1.829695
H	9.112871	-0.470338	1.342568
H	10.68626	-0.01815	0.660305
H	10.500097	1.973975	-1.376376
H	9.097998	2.996748	-0.977774
H	10.348174	2.690015	0.247657

(6) Ac-Hyp-Gly-δ-azPro(u)-Hyp-Gly-Pro-NMe_2

(6a) PPI structure

C	-5.94757	-1.418709	-1.227787
C	-6.322381	0.027538	-1.03017
O	-7.321693	0.524301	-1.581754
N	-5.520775	0.776505	-0.247796
C	-4.335292	0.28276	0.449733
C	-3.725202	1.564753	1.068936
C	-4.227007	2.682866	0.158534
O	-3.456949	2.799725	-1.033781
C	-5.651804	2.235407	-0.155263
C	-4.669895	-0.722895	1.551745
O	-5.793003	-0.779225	2.064793
N	-3.656596	-1.50059	1.978479
C	-2.342556	-1.568657	1.378158
C	-2.335996	-2.36857	0.074371
O	-3.18626	-3.237091	-0.141476
N	-1.346526	-2.067847	-0.787496
C	-0.273363	-1.089396	-0.565646
C	0.747085	-1.438421	-1.67363
C	0.351724	-2.868325	-2.034514
N	-1.115506	-2.883554	-1.926915
C	-0.75002	0.34688	-0.762906
O	-1.739918	0.589743	-1.474112
N	0.006491	1.311771	-0.224805
C	1.177816	1.088833	0.630645
C	1.804239	2.497093	0.739646
C	1.366362	3.170174	-0.556013
O	2.104025	2.696609	-1.679277
C	-0.083548	2.710946	-0.67083
C	0.79829	0.563117	2.012894
O	-0.333114	0.732783	2.478592
N	1.779548	-0.036754	2.713871
C	3.104532	-0.350204	2.222072
C	3.11733	-1.516405	1.229925
O	2.169631	-2.313271	1.167993
N	4.217874	-1.656621	0.477811
C	5.343006	-0.723216	0.427736
C	6.397638	-1.522624	-0.36081
C	5.54761	-2.323817	-1.350368
C	4.324774	-2.729662	-0.527575
C	4.961762	0.572037	-0.308912
O	3.893433	0.63667	-0.950725
N	5.809903	1.603524	-0.254469
C	7.069346	1.63602	0.485043
C	5.446209	2.834021	-0.954788
H	0.168744	-1.253266	0.420425
H	-1.493088	-2.368289	-2.727618
H	0.601185	-0.781815	-2.538204
H	1.774778	-1.334739	-1.319247
H	0.645119	-3.158994	-3.043747
H	0.760751	-3.583735	-1.315036
H	-1.939266	-0.562935	1.252919
H	-1.673846	-2.079846	2.078727
H	-3.896732	-2.190409	2.684153
H	-3.64207	-0.158184	-0.274639
H	-4.124577	1.71847	2.077115
H	-2.633421	1.524229	1.12795
H	-6.341124	2.516705	0.649566
H	-6.017286	2.64245	-1.099567
H	-4.216573	3.654532	0.658442
H	-6.031772	-1.980588	-0.292059
H	-4.91482	-1.504835	-1.582555
H	-6.622341	-1.856642	-1.963915
H	-2.868531	2.023452	-1.147091
H	1.877999	0.411657	0.131746
H	-0.737716	3.293594	-0.012371
H	-0.462988	2.752785	-1.693482
H	1.372667	3.037434	1.58867
H	2.889492	2.457048	0.860783
H	1.444165	4.259616	-0.506497
H	1.513884	-0.397887	3.62506
H	2.801955	2.068796	-1.393707
H	3.569995	0.541587	1.796829
H	3.716902	-0.638849	3.08157
H	5.678441	-0.492786	1.440961
H	3.406797	-2.790073	-1.11775
H	4.470669	-3.689864	-0.020858
H	7.133666	-0.877088	-0.845566
H	6.919398	-2.19121	0.331123
H	5.244058	-1.687141	-2.188108
H	6.076516	-3.191009	-1.750718
H	7.037812	2.447698	1.217712
H	7.257383	0.701698	1.008817
H	7.894581	1.817087	-0.209621
H	5.144417	2.611058	-1.980721
H	4.626737	3.347036	-0.441045
H	6.319417	3.487008	-0.972585

(6b) PPII structure

C	-10.431036	-0.491993	0.546058
C	-9.121539	-0.652197	-0.177648
O	-8.731574	-1.753268	-0.611336
N	-8.378805	0.454469	-0.349881
C	-7.073937	0.393117	-1.002249
C	-6.507101	1.808215	-0.78666
C	-7.755048	2.684039	-0.688558
O	-8.330721	2.916847	-1.972115
C	-8.723758	1.812259	0.095984
C	-6.163874	-0.640682	-0.354393
O	-6.131642	-0.803646	0.871097
N	-5.359844	-1.31443	-1.194222
C	-4.270436	-2.109881	-0.683132
C	-3.214371	-1.241266	-0.009695
O	-3.231495	-0.002201	-0.055695
N	-2.233867	-1.889917	0.629465
C	-1.178848	-1.189865	1.360874
C	-0.392481	-2.346801	2.012141
C	-1.399244	-3.500941	1.956198
N	-2.131825	-3.301792	0.693139
C	-0.290825	-0.402852	0.408628
O	-0.064785	-0.821764	-0.738271
N	0.297191	0.701658	0.886211
C	1.355364	1.354577	0.116467
C	1.92522	2.390533	1.103848
C	0.745623	2.692706	2.025314
O	-0.206578	3.540866	1.388038
C	0.088524	1.332785	2.201167
C	2.43696	0.360466	-0.281127
O	2.771149	-0.571219	0.460778
N	3.047314	0.598756	-1.452663
C	4.237207	-0.138502	-1.802156
C	5.373457	0.13256	-0.81902
O	5.381603	1.13893	-0.092636
N	6.351499	-0.781477	-0.783317
C	7.51063	-0.582569	0.077243
C	8.264046	-1.917881	-0.056998
C	7.971248	-2.332325	-1.501727
C	6.511913	-1.922711	-1.705981
C	8.362322	0.586266	-0.433325
O	8.211039	1.018244	-1.589124
N	9.287213	1.101557	0.396313
C	10.19756	2.107304	-0.143149
C	9.682045	0.521026	1.676631
H	-1.639119	-0.541891	2.109564
H	-1.507843	-3.57524	-0.072397
H	0.48904	-2.591008	1.410006
H	-0.074976	-2.096845	3.025731
H	-0.930796	-4.485642	1.950659
H	-2.111408	-3.442513	2.783538
H	-4.641051	-2.847189	0.032707
H	-3.81351	-2.653751	-1.512898
H	-5.365691	-1.069145	-2.177863
H	-7.195793	0.166812	-2.067517
H	-5.964375	1.852011	0.164223
H	-5.836937	2.114317	-1.593412
H	-8.557341	1.924101	1.173004
H	-9.764252	2.050652	-0.135533
H	-7.560893	3.633765	-0.181512
H	-11.117009	0.119154	-0.05024
H	-10.285885	0.00792	1.508747
H	-10.87291	-1.475854	0.705355
H	-7.677222	3.384643	-2.517267
H	0.938493	1.831966	-0.77681
H	0.582683	0.760501	2.993259
H	-0.975081	1.432955	2.426134
H	2.734385	1.942838	1.691639
H	2.304984	3.280042	0.596038
H	1.057896	3.118901	2.98312
H	2.793765	1.422053	-1.98684
H	0.2217	4.390969	1.195594
H	4.014771	-1.208649	-1.830108
H	4.556922	0.164653	-2.802827
H	7.171253	-0.386763	1.095887
H	6.302375	-1.622656	-2.735643
H	5.823454	-2.726872	-1.424281
H	9.332544	-1.820334	0.150692
H	7.835965	-2.637748	0.647583
H	8.614089	-1.774004	-2.189812
H	8.122086	-3.399615	-1.675781
H	10.922207	1.651228	-0.827078
H	9.638875	2.876515	-0.678113
H	10.732836	2.569578	0.68726
H	9.796337	1.324056	2.408881
H	8.939535	-0.179336	2.052422
H	10.640061	-0.000975	1.574281

Cartesian Coordinates of PPI and PPII structures of the collagen model peptide Ac-Hyp-Gly-Pro-X-Gly-Pro-NMe_2 optimized at the SMD M06-2X/6-31+G(d) level of theory in water**:**

(1) Ac-Hyp-Gly-Pro-α-azPro(u)-Gly-Pro-NMe_2

(1a) PPI structure

C	-6.0056	-1.636869	-1.187314
C	-6.431243	-0.219522	-0.902947
O	-7.50563	0.237667	-1.336011
N	-5.594186	0.55153	-0.183602
C	-4.35305	0.099333	0.439885
C	-3.804331	1.383518	1.109249
C	-4.415489	2.508307	0.278739
O	-3.720722	2.707339	-0.949395
C	-5.82265	1.986237	0.010344
C	-4.590318	-0.980755	1.492942
O	-5.686223	-1.104261	2.05263
N	-3.5347	-1.75099	1.812262
C	-2.212781	-1.660492	1.230605
C	-2.123631	-2.282815	-0.164336
O	-2.958505	-3.111266	-0.554849
N	-1.074204	-1.917029	-0.915211
C	-0.115958	-0.871207	-0.574081
C	0.998729	-1.082692	-1.612944
C	0.227718	-1.5473	-2.854011
C	-0.904511	-2.412606	-2.292166
C	-0.740163	0.516397	-0.759886
O	-1.779908	0.683129	-1.4157
N	-0.098615	1.546395	-0.188009
N	1.092287	1.381074	0.528232
C	1.984933	2.521085	0.154081
C	1.102087	3.456899	-0.693027
C	-0.3247	2.967399	-0.438169
C	0.892515	1.061434	1.879422
O	-0.228094	0.857636	2.346864
N	2.028969	0.974652	2.634504
C	3.288601	0.504198	2.089171
C	3.189606	-0.915562	1.527453
O	2.163131	-1.595543	1.682892
N	4.282479	-1.394402	0.92037
C	5.474057	-0.613416	0.600168
C	6.483296	-1.70556	0.199576
C	5.601246	-2.753652	-0.486017
C	4.312443	-2.745935	0.338147
C	5.192961	0.331582	-0.578866
O	4.191717	0.151779	-1.292407
N	6.056973	1.335259	-0.808838
C	7.364039	1.471898	-0.172193
C	5.851852	2.145826	-2.006236
H	-6.063865	-2.251301	-0.282879
H	-3.662899	-0.258089	-0.331016
H	-4.174606	1.455758	2.137481
H	-2.711007	1.418633	1.128954
H	-4.434242	3.457499	0.820229
H	-6.485001	2.167889	0.865455
H	-6.264596	2.422898	-0.887174
H	-3.032508	2.020912	-1.074289
H	-3.701651	-2.464408	2.515269
H	-1.874657	-0.622314	1.229073
H	-1.520767	-2.204723	1.881388
H	0.25546	-1.001999	0.443325
H	1.585227	-0.175759	-1.778728
H	1.668379	-1.867796	-1.246381
H	-0.187746	-0.682706	-3.381332
H	0.856427	-2.103918	-3.551747
H	-1.841767	-2.301453	-2.844462
H	-0.64193	-3.475126	-2.265195
H	-4.975346	-1.671099	-1.554675
H	-6.675535	-2.056708	-1.938573
H	-0.771519	3.422387	0.45311
H	-0.988405	3.09175	-1.29286
H	1.343564	3.343016	-1.752405
H	1.236964	4.501776	-0.409554
H	2.332659	3.007017	1.067564
H	2.840757	2.150075	-0.413749
H	1.814521	0.585241	3.548717
H	3.672544	1.194315	1.336596
H	4.018692	0.499857	2.904499
H	3.417003	-2.917173	-0.265078
H	4.332063	-3.486308	1.145317
H	5.802998	-0.05214	1.476875
H	5.389175	-2.449917	-1.515904
H	6.066069	-3.741346	-0.508243
H	7.278541	-1.324372	-0.445641
H	6.935725	-2.112191	1.109485
H	7.534782	2.525074	0.062711
H	7.423659	0.899488	0.750939
H	8.152513	1.130308	-0.852021
H	6.13498	1.590811	-2.907659
H	4.805649	2.445336	-2.085075
H	6.472595	3.039186	-1.928039

(1b) PPII structure

C	-10.471627	-0.996187	0.777714
C	-9.167256	-0.971623	0.027264
O	-8.668403	-1.997875	-0.473112
N	-8.550637	0.217346	-0.085137
C	-7.269338	0.343206	-0.772473
C	-6.872025	1.805526	-0.502015
C	-8.217177	2.517699	-0.370134
O	-8.827612	2.713162	-1.644156
C	-9.065311	1.510152	0.391395
C	-6.218496	-0.605246	-0.215364
O	-6.143362	-0.877414	0.988199
N	-5.342612	-1.075035	-1.119627
C	-4.15227	-1.771355	-0.699221
C	-3.213535	-0.87636	0.10417
O	-3.371972	0.351189	0.174192
N	-2.20662	-1.506871	0.728698
C	-1.155707	-0.745489	1.386917
C	-0.353775	-1.840324	2.106905
C	-0.413161	-2.999072	1.107163
C	-1.838602	-2.926908	0.549565
C	-0.305898	-0.027447	0.327625
O	-0.465518	-0.222974	-0.881718
N	0.672147	0.765205	0.807695
N	1.491083	1.472311	-0.084768
C	1.881197	2.757887	0.561303
C	1.093973	2.766376	1.874837
C	0.894415	1.279757	2.15986
C	2.457192	0.695518	-0.723713
O	2.494499	-0.53423	-0.631759
N	3.290498	1.391587	-1.545905
C	4.490952	0.725981	-1.996568
C	5.413148	0.352474	-0.840013
O	5.255024	0.827857	0.295989
N	6.396474	-0.50994	-1.125825
C	7.404644	-0.837727	-0.125872
C	8.216419	-1.947538	-0.817247
C	8.162775	-1.54518	-2.294313
C	6.744224	-1.00091	-2.473146
C	8.270064	0.395812	0.167226
O	8.278514	1.357736	-0.620993
N	9.016362	0.394406	1.284647
C	9.890749	1.5359	1.529959
C	9.238328	-0.760222	2.148374
H	-11.239095	-0.448264	0.220708
H	-7.394804	0.156281	-1.845287
H	-6.333025	1.875921	0.449596
H	-6.248508	2.221136	-1.297064
H	-8.138933	3.469234	0.163813
H	-8.915044	1.616763	1.471073
H	-10.127514	1.622483	0.162743
H	-8.255219	3.296773	-2.168497
H	-5.40066	-0.740034	-2.074745
H	-4.41962	-2.652413	-0.107809
H	-3.622418	-2.119013	-1.590469
H	-1.595155	-0.015152	2.069907
H	0.665372	-1.531275	2.350159
H	-0.871975	-2.100041	3.035348
H	0.314506	-2.83638	0.304719
H	-0.207431	-3.967949	1.566334
H	-1.886908	-3.209585	-0.505034
H	-2.526949	-3.560849	1.117798
H	-10.365642	-0.520954	1.757921
H	-10.791185	-2.030949	0.903464
H	1.798997	0.820783	2.575119
H	0.044718	1.067656	2.806458
H	0.121467	3.24659	1.738982
H	1.641224	3.276316	2.668895
H	2.958214	2.750813	0.753569
H	1.631005	3.60001	-0.085503
H	3.355453	2.395626	-1.414545
H	4.228549	-0.166279	-2.569983
H	5.028212	1.402963	-2.667036
H	6.696965	-0.190801	-3.205393
H	6.043449	-1.788054	-2.771277
H	6.911204	-1.177225	0.78696
H	8.894323	-0.75626	-2.495171
H	8.364216	-2.38113	-2.967238
H	9.236228	-2.025528	-0.432493
H	7.710962	-2.905224	-0.657214
H	9.051649	-0.476479	3.187635
H	8.584525	-1.590547	1.892198
H	10.278079	-1.09247	2.054255
H	10.778924	1.495052	0.889322
H	9.357012	2.468078	1.340692
H	10.205186	1.509511	2.574332

(2) Ac-Hyp-Gly-Pro-β-azPro(u)-Gly-Pro-NMe_2

(2a) PPI structure

C	-5.869053	-1.657368	-1.169757
C	-6.312732	-0.230027	-0.979164
O	-7.360087	0.202404	-1.495412
N	-5.520035	0.577225	-0.248148
C	-4.29318	0.164291	0.429327
C	-3.750063	1.490113	1.018822
C	-4.334188	2.559764	0.099679
O	-3.608067	2.682563	-1.119572
C	-5.73805	2.026285	-0.168012
C	-4.547267	-0.838319	1.554142

O	-5.660847	-0.957917	2.077538	H	-0.750385	-3.672391	-1.987072
N	-3.477782	-1.528945	1.99359	H	-4.836985	-1.696417	-1.533371
C	-2.163591	-1.524235	1.387301	H	-6.529134	-2.133114	-1.895715
C	-2.121754	-2.284459	0.061355	H	-1.018703	3.300365	0.110319
O	-2.967691	-3.149289	-0.208643	H	-0.696148	2.944287	-1.614205
N	-1.116744	-1.988531	-0.774655	H	1.943706	0.776225	0.047217
C	-0.107743	-0.951908	-0.569389	H	1.687955	3.317247	-1.33383
C	0.922747	-1.269205	-1.672465	H	1.062017	4.563053	-0.225931
C	0.057143	-1.809879	-2.814721	H	1.266518	3.163364	1.546002
C	-1.027033	-2.619036	-2.102742	H	1.710709	0.006402	3.589907
C	-0.691079	0.449458	-0.784629	H	3.588285	0.944612	1.51548
O	-1.720422	0.610115	-1.464505	H	3.959353	0.074408	2.992268
N	-0.011639	1.47883	-0.265278	H	3.657792	-2.895045	-0.606827
C	1.200512	1.391437	0.565812	H	4.708688	-3.600126	0.637802
N	1.682238	2.76875	0.69959	H	5.841503	-0.070485	1.426417
C	1.086765	3.494151	-0.437252	H	5.490333	-2.051958	-1.860144
C	-0.298442	2.877138	-0.600021	H	6.358956	-3.39567	-1.099145
C	0.894962	0.851694	1.971043	H	7.316222	-0.895195	-0.723893
O	-0.246858	0.916529	2.433851	H	7.160751	-1.934359	0.707525
N	1.942693	0.406483	2.684499	H	7.200187	2.81192	0.163714
C	3.257732	0.12188	2.154174	H	7.33315	1.11749	0.6491
C	3.303873	-1.215912	1.413404	H	7.908486	1.621752	-0.953736
O	2.344283	-1.999352	1.453436	H	5.292432	1.969712	-2.763866
N	4.449735	-1.513999	0.783465	H	4.424704	2.936258	-1.54904
C	5.515875	-0.55489	0.502501	H	6.137776	3.270318	-1.891596
C	6.609059	-1.452468	-0.105639				
C	5.79775	-2.48048	-0.90069	(2b) PPII structure			
C	4.570637	-2.740087	-0.025636				
C	5.030916	0.494501	-0.514366	C	-10.422302	-0.697764	0.177634
O	3.939376	0.342718	-1.091998	C	-9.061828	-0.789419	-0.458356
N	5.812662	1.555381	-0.758827	O	-8.587239	-1.869404	-0.859955
C	7.138559	1.780158	-0.191504	N	-8.371938	0.355792	-0.593724
C	5.387203	2.484665	-1.803249	C	-7.033302	0.362769	-1.172513
H	-5.917691	-2.214621	-0.22866	C	-6.575692	1.821272	-0.981358
H	-3.588915	-0.24549	-0.302474	C	-7.885444	2.608108	-0.983345
H	-4.143134	1.636999	2.030507	O	-8.407842	2.74425	-2.303349
H	-2.657074	1.516732	1.061784	C	-8.829555	1.698605	-0.211837
H	-4.364483	3.541623	0.579203	C	-6.092398	-0.582362	-0.439067
H	-6.420598	2.27714	0.652616	O	-6.172525	-0.778031	0.778938
H	-6.152796	2.397828	-1.106634	N	-5.132026	-1.138932	-1.196284
H	-2.928327	1.979069	-1.191124	C	-4.035039	-1.844968	-0.58351
H	-3.662945	-2.204846	2.728498	C	-3.176596	-0.927937	0.284003
H	-1.806782	-0.498393	1.274786	O	-3.286108	0.306672	0.244518
H	-1.470115	-2.012833	2.079181	N	-2.295843	-1.542196	1.088064
H	0.338033	-1.048429	0.424355	C	-1.335057	-0.757573	1.853222
H	1.515703	-0.396222	-1.954866	C	-0.578838	-1.828893	2.660398
H	1.601172	-2.042066	-1.296335	C	-0.580599	-3.031746	1.712899
H	-0.394165	-0.981966	-3.369956	C	-1.966794	-2.981513	1.069124
H	0.630105	-2.421703	-3.514317	C	-0.381693	-0.021475	0.912995
H	-1.998879	-2.567579	-2.601081	O	-0.239637	-0.354592	-0.272973

N	0.332396	0.985411	1.441562
C	1.413303	1.582076	0.668727
N	2.120293	2.418238	1.645409
C	1.124064	2.752846	2.678122
C	0.375463	1.441775	2.837158
C	2.371773	0.505351	0.148395
O	2.645682	-0.497992	0.815514
N	2.924154	0.76102	-1.045947
C	4.004824	-0.052951	-1.544311
C	5.265358	0.094231	-0.696878
O	5.389986	0.999346	0.14244
N	6.228638	-0.809074	-0.920442
C	7.513973	-0.691319	-0.24221
C	8.2485	-1.971485	-0.679894
C	7.706474	-2.215187	-2.091351
C	6.229448	-1.83409	-1.980457
C	8.251031	0.567973	-0.717103
O	7.926696	1.12117	-1.78165
N	9.254815	1.038024	0.04712
C	10.036466	2.157466	-0.468652
C	9.881768	0.306656	1.144845
H	-11.111295	-0.170968	-0.491764
H	-7.080634	0.090726	-2.23296
H	-6.090815	1.935706	-0.005196
H	-5.883592	2.145712	-1.761911
H	-7.786408	3.589338	-0.510235
H	-8.719744	1.854609	0.867007
H	-9.871782	1.857456	-0.497004
H	-7.76621	3.242905	-2.835164
H	-5.059155	-0.870304	-2.171134
H	-4.41214	-2.676971	0.019372
H	-3.40886	-2.264444	-1.375634
H	-1.857215	-0.040697	2.491161
H	0.426852	-1.50921	2.944799
H	-1.145057	-2.05039	3.570293
H	0.192305	-2.906118	0.947456
H	-0.405983	-3.977987	2.228951
H	-1.965064	-3.36599	0.046705
H	-2.705559	-3.537464	1.656382
H	-10.380948	-0.14308	1.119937
H	-10.800176	-1.704323	0.358371
H	0.937472	0.733507	3.455887
H	-0.627908	1.575069	3.24301
H	1.002823	2.154708	-0.173428
H	0.43503	3.541114	2.34873
H	1.614787	3.066874	3.600175
H	2.435046	3.265878	1.177327
H	2.714058	1.638979	-1.507329
H	3.698017	-1.10274	-1.574601
H	4.230248	0.2573	-2.568268
H	5.830235	-1.428821	-2.913227
H	5.614918	-2.686644	-1.671257
H	7.347881	-0.645863	0.835319
H	8.208272	-1.55493	-2.805896
H	7.838038	-3.24729	-2.422416
H	9.335487	-1.862018	-0.651455
H	7.963835	-2.788853	-0.009711
H	10.056547	0.994346	1.976017
H	9.258995	-0.511177	1.500051
H	10.844453	-0.101727	0.816854
H	10.732413	1.823515	-1.246952
H	9.376142	2.919469	-0.883161
H	10.605324	2.588795	0.356643

(3) Ac-Hyp-Gly-Pro-γ-azPro(u)-Gly-Pro-NMe_2

(3a) PPI structure

C	-5.857161	-1.432433	-1.276746
C	-6.243572	0.0084	-1.066159
O	-7.232989	0.507865	-1.632962
N	-5.462128	0.751546	-0.257802
C	-4.281869	0.260126	0.451588
C	-3.672465	1.546218	1.06533
C	-4.169739	2.658793	0.146205
O	-3.395649	2.764577	-1.044732
C	-5.593915	2.210812	-0.168329
C	-4.620513	-0.73592	1.561117
O	-5.757882	-0.823256	2.036357
N	-3.592257	-1.458307	2.049416
C	-2.273302	-1.540953	1.459127
C	-2.272449	-2.318903	0.143245
O	-3.164668	-3.140195	-0.113475
N	-1.256056	-2.088227	-0.698911
C	-0.183603	-1.116698	-0.502347
C	0.834734	-1.532236	-1.583492
C	-0.056911	-2.019364	-2.729755
C	-1.197997	-2.745055	-2.016138
C	-0.669451	0.316417	-0.756305
O	-1.692105	0.532612	-1.431458
N	0.090491	1.308584	-0.279402
C	1.276991	1.170779	0.555155
C	1.834432	2.62772	0.558663
N	1.241844	3.285319	-0.605523
C	-0.094199	2.724417	-0.661315
C	0.938915	0.739307	1.979144
O	-0.202215	0.862944	2.435962
N	1.967617	0.293721	2.72451
C	3.289432	-0.012155	2.221717
C	3.321591	-1.301839	1.399309

O	2.402108	-2.130399	1.480613	H	5.553534	2.500563	-2.560814
N	4.405759	-1.506967	0.640763	H	4.198407	2.893705	-1.476879
C	5.469457	-0.534068	0.393814	H	5.773849	3.690086	-1.253967
C	6.539728	-1.390368	-0.310184				
C	5.705217	-2.389036	-1.117192	(3b) PPII structure			
C	4.534908	-2.715016	-0.191348				
C	4.969538	0.59771	-0.521779	C	10.458761	0.655808	0.249649
O	3.909472	0.464351	-1.156698	C	9.107163	0.713235	-0.408583
N	5.70823	1.71738	-0.601482	O	8.626978	1.773969	-0.852346
C	7.058907	1.875385	-0.07053	N	8.429476	-0.442951	-0.509757
C	5.279745	2.757567	-1.531062	C	7.097985	-0.487979	-1.102402
H	-5.913501	-2.000196	-0.342922	C	6.64708	-1.937041	-0.840526
H	-3.584471	-0.188182	-0.264538	C	7.959978	-2.717327	-0.799375
H	-4.07542	1.706796	2.070995	O	8.482328	-2.923724	-2.110306
H	-2.580886	1.505775	1.129041	C	8.901956	-1.765973	-0.07734
H	-4.158518	3.634419	0.638265	C	6.147367	0.491022	-0.428395
H	-6.284222	2.494038	0.634933	O	6.19499	0.720798	0.785805
H	-5.958239	2.615051	-1.11415	N	5.221612	1.038546	-1.232293
H	-2.817425	1.979966	-1.153706	C	4.133287	1.808973	-0.685546
H	-3.841077	-2.147543	2.752718	C	3.210032	0.961219	0.184684
H	-1.852682	-0.54088	1.337051	O	3.275931	-0.27716	0.204468
H	-1.618843	-2.063654	2.163746	N	2.324305	1.64105	0.926734
H	0.241913	-1.216635	0.499739	C	1.332104	0.925415	1.717568
H	1.504414	-0.716773	-1.86693	C	0.598565	2.057634	2.460193
H	1.436289	-2.355913	-1.186114	C	0.662322	3.218883	1.463992
H	-0.446576	-1.166676	-3.294103	C	2.057808	3.090649	0.851451
H	0.475456	-2.676424	-3.420322	C	0.371151	0.162794	0.806222
H	-2.160734	-2.640187	-2.523663	O	0.230105	0.456061	-0.39
H	-0.989426	-3.811857	-1.882189	N	-0.350285	-0.818801	1.372081
H	-4.830484	-1.500954	-1.653124	C	-1.443667	-1.449103	0.639625
H	-6.540058	-1.874544	-2.002784	C	-2.138177	-2.26928	1.738794
H	-0.744711	3.216931	0.068805	N	-1.045601	-2.519202	2.691892
H	-0.528332	2.794806	-1.657894	C	-0.378096	-1.222043	2.779863
H	1.995794	0.491012	0.087715	C	-2.403953	-0.412346	0.070642
H	1.745168	2.955631	-1.431767	O	-2.671873	0.627325	0.683377
H	1.506871	3.143915	1.466165	N	-2.973086	-0.732098	-1.102109
H	2.923608	2.648559	0.511482	C	-4.08992	0.031435	-1.600913
H	1.72844	-0.031546	3.656634	C	-5.317151	-0.106339	-0.703024
H	3.683331	0.835898	1.656481	O	-5.378697	-0.956884	0.198409
H	3.953929	-0.146852	3.080405	N	-6.317612	0.750654	-0.946854
H	3.601614	-2.901252	-0.728419	C	-7.576865	0.633472	-0.221307
H	4.743775	-3.576145	0.452769	C	-8.364962	1.859483	-0.714935
H	5.830627	-0.12715	1.340424	C	-7.895448	2.008883	-2.165192
H	5.337691	-1.916077	-2.033624	C	-6.40582	1.665369	-2.102239
H	6.269966	-3.281777	-1.392859	C	-8.281159	-0.677482	-0.596568
H	7.213144	-0.793541	-0.929208	O	-7.958653	-1.289873	-1.629019
H	7.130988	-1.905849	0.45327	N	-9.250401	-1.131027	0.218972
H	7.137727	2.85109	0.415224	C	-9.988479	-2.320645	-0.195752
H	7.299213	1.107105	0.660937	C	-9.870946	-0.355001	1.288837
H	7.788085	1.828313	-0.887056	H	11.152617	0.076039	-0.368581

H	7.155824	-0.270529	-2.175057
H	6.158276	-2.004553	0.138058
H	5.959852	-2.3039	-1.606408
H	7.864966	-3.672088	-0.273956
H	8.806035	-1.877873	1.008222
H	9.942833	-1.928384	-0.365994
H	7.845906	-3.461299	-2.609402
H	5.18257	0.752918	-2.204081
H	4.523169	2.647508	-0.099739
H	3.553262	2.223289	-1.514741
H	1.828768	0.231039	2.399112
H	-0.42304	1.783665	2.736254
H	1.154063	2.298598	3.371657
H	-0.099321	3.091176	0.688074
H	0.514209	4.191372	1.937723
H	2.093397	3.438137	-0.183488
H	2.80725	3.63608	1.435293
H	10.394571	0.16939	1.228059
H	10.842995	1.669241	0.367
H	-0.945456	-0.488463	3.371168
H	0.627461	-1.324529	3.18805
H	-1.050257	-2.087955	-0.157651
H	-1.442838	-2.743931	3.603506
H	-2.94468	-1.672903	2.187466
H	-2.552566	-3.200109	1.35192
H	-2.785318	-1.64358	-1.504759
H	-3.813433	1.086441	-1.689281
H	-4.33954	-0.331765	-2.601465
H	-6.053705	1.174178	-3.012646
H	-5.793161	2.554826	-1.920958
H	-7.377204	0.659135	0.851321
H	-8.417329	1.290239	-2.805172
H	-8.0649	3.01162	-2.562646
H	-9.446347	1.729756	-0.626812
H	-8.070219	2.729985	-0.12047
H	-10.016012	-1.000974	2.158097
H	-9.254556	0.490128	1.587568
H	-10.847252	0.021061	0.96253
H	-10.681216	-2.088331	-1.012623
H	-9.29673	-3.096514	-0.525905
H	-10.556182	-2.68769	0.660471

(4) Ac-Hyp-Gly-Pro-δ-azPro(u)-Gly-Pro-NMe_2

(4a) PPI structure

C	-6.087086	-1.466443	-1.036448
C	-6.397113	0.000611	-0.886743
O	-7.420744	0.503805	-1.386299
N	-5.51163	0.759494	-0.212864
C	-4.291512	0.264657	0.42237
C	-3.609657	1.55961	0.926962
C	-4.135391	2.632392	-0.021636
O	-3.490999	2.596739	-1.291749
C	-5.594797	2.224581	-0.185197
C	-4.579095	-0.671056	1.596512
O	-5.674323	-0.671126	2.170187
N	-3.561317	-1.450059	2.009045
C	-2.256165	-1.537924	1.391011
C	-2.263343	-2.319609	0.076964
O	-3.177377	-3.10933	-0.1987
N	-1.213743	-2.132618	-0.737192
C	-0.149745	-1.151531	-0.540759
C	0.88016	-1.563768	-1.610952
C	0.002147	-2.063477	-2.762283
C	-1.149976	-2.782776	-2.058155
C	-0.667304	0.266817	-0.816392
O	-1.680825	0.448263	-1.507036
N	0.044573	1.275944	-0.291121
C	1.25516	1.161801	0.531816
C	1.825495	2.600846	0.514144
C	1.075932	3.243145	-0.653913
N	-0.254351	2.616469	-0.644316
C	0.918662	0.737058	1.960866
O	-0.224816	0.857227	2.412419
N	1.94561	0.294811	2.709613
C	3.276018	0.012472	2.218235
C	3.341956	-1.275169	1.393285
O	2.417831	-2.101197	1.423245
N	4.463027	-1.479615	0.688845
C	5.514873	-0.488933	0.470525
C	6.621632	-1.330799	-0.191827
C	5.829335	-2.330439	-1.039909
C	4.611365	-2.662892	-0.176289
C	5.017498	0.614729	-0.48093
O	3.966255	0.45173	-1.123774
N	5.749267	1.735783	-0.592289
C	7.084857	1.923841	-0.033277
C	5.331387	2.726975	-1.579972
H	-6.086739	-1.975128	-0.067514
H	-3.662085	-0.23484	-0.322606
H	-3.948226	1.788023	1.943277
H	-2.518838	1.48924	0.934145
H	-4.041021	3.636642	0.401109
H	-6.199875	2.570002	0.661181
H	-6.029817	2.595414	-1.114804
H	-2.747258	1.956925	-1.290339
H	-3.769309	-2.076006	2.780919
H	-1.835401	-0.539459	1.258817
H	-1.588222	-2.05773	2.085138

H	0.267536	-1.234613	0.466326
H	1.544424	-0.742573	-1.892861
H	1.485722	-2.378938	-1.203079
H	-0.37927	-1.217631	-3.341871
H	0.543493	-2.727744	-3.438671
H	-2.107101	-2.666886	-2.573608
H	-0.952881	-3.851896	-1.927444
H	-5.100861	-1.604635	-1.49171
H	-6.84686	-1.91995	-1.67352
H	-0.792774	3.006459	0.136671
H	1.955039	0.46508	0.061067
H	1.560239	3.007301	-1.605936
H	0.969397	4.324066	-0.55723
H	1.581247	3.115826	1.448571
H	2.909193	2.599707	0.379723
H	1.707401	-0.016831	3.646443
H	3.65743	0.866073	1.652852
H	3.936559	-0.107217	3.081856
H	3.701137	-2.813193	-0.762461
H	4.772945	-3.549012	0.44641
H	5.83557	-0.062272	1.423177
H	5.50931	-1.858011	-1.974032
H	6.409712	-3.221368	-1.287248
H	7.315642	-0.725884	-0.779563
H	7.184977	-1.84553	0.592703
H	7.154381	2.930971	0.384107
H	7.294237	1.209061	0.759447
H	7.841002	1.814917	-0.818662
H	5.569196	2.390936	-2.595531
H	4.256726	2.903741	-1.509149
H	5.862194	3.658287	-1.378536

(4b) PPII structure

C	-10.453993	-0.638471	0.399617
C	-9.147415	-0.673861	-0.346137
O	-8.695431	-1.721753	-0.846532
N	-8.477922	0.485902	-0.460156
C	-7.160552	0.53706	-1.085403
C	-6.686302	1.976316	-0.800662
C	-7.986742	2.761922	-0.636812
O	-8.593692	3.034484	-1.897937
C	-8.886083	1.781588	0.098975
C	-6.204678	-0.464288	-0.450978
O	-6.23174	-0.715157	0.759857
N	-5.299647	-1.006694	-1.281129
C	-4.21192	-1.799701	-0.765378
C	-3.263443	-0.977861	0.103179
O	-3.306431	0.261434	0.134672
N	-2.382748	-1.680834	0.829102
C	-1.362057	-0.993417	1.610833
C	-0.643934	-2.148548	2.331462
C	-0.744577	-3.297467	1.324385
C	-2.146003	-3.134666	0.734023
C	-0.403865	-0.24634	0.687574
O	-0.29453	-0.509137	-0.520051
N	0.364669	0.694447	1.254743
C	1.415975	1.392678	0.515406
C	2.013568	2.339016	1.57948
C	0.944943	2.32924	2.679166
N	0.380186	0.97039	2.646199
C	2.453048	0.397461	0.013008
O	2.73599	-0.620507	0.656369
N	3.0546	0.715449	-1.142965
C	4.198186	-0.032532	-1.603784
C	5.398351	0.122129	-0.673116
O	5.427515	0.974413	0.22816
N	6.413832	-0.724613	-0.890625
C	7.655165	-0.592861	-0.137528
C	8.464844	-1.813922	-0.608682
C	8.032528	-1.969144	-2.06999
C	6.539288	-1.637562	-2.044317
C	8.356232	0.722585	-0.503832
O	8.044121	1.332124	-1.541092
N	9.311553	1.181991	0.324837
C	10.051829	2.372684	-0.082819
C	9.92176	0.407362	1.401449
H	-11.184115	-0.028495	-0.142926
H	-7.244161	0.342481	-2.160312
H	-6.129239	2.007752	0.142402
H	-6.052392	2.369296	-1.598834
H	-7.84767	3.689297	-0.073477
H	-8.695458	1.818304	1.177479
H	-9.943648	1.977145	-0.090969
H	-7.988245	3.593939	-2.41109
H	-5.275078	-0.705709	-2.248747
H	-4.60354	-2.642529	-0.187175
H	-3.650605	-2.207423	-1.610645
H	-1.817379	-0.285519	2.304994
H	0.387159	-1.900597	2.597457
H	-1.192953	-2.387091	3.247655
H	0.008201	-3.175234	0.538844
H	-0.608243	-4.278023	1.784801
H	-2.204262	-3.469691	-0.304027
H	-2.897284	-3.671962	1.323057
H	-10.322135	-0.198059	1.392999
H	-10.836361	-1.654758	0.496879
H	1.078089	0.338189	3.052968
H	0.973902	1.938688	-0.323154
H	0.14571	3.042453	2.461614

H	1.346423	2.52731	3.673564	H	9.542783	-1.676499	-0.494037
H	2.951341	1.927707	1.966882	H	8.161414	-2.68545	-0.020078
H	2.203746	3.332493	1.171047	H	10.060707	1.055359	2.270153
H	2.839265	1.604345	-1.580564	H	9.300624	-0.435364	1.697265
H	3.9406	-1.092058	-1.698116	H	10.900087	0.028575	1.084254
H	4.471643	0.332468	-2.597453	H	10.753092	2.140853	-0.892531
H	6.205241	-1.148954	-2.962894	H	9.36231	3.147336	-0.420431
H	5.930283	-2.532729	-1.879519	H	10.6103	2.740981	0.778879
H	7.432574	-0.615482	0.930779				
H	8.565016	-1.247875	-2.698205				
H	8.21926	-2.971343	-2.461108				