Benchmark of a functional-group database for distributed polarizability and dipole moment in biomolecules

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Electronic Support Information

1. Atomic coordinates

Table S1: glycine atomic coordinates. Values in atomic units.

	x	y	z
N1	0.6179	1.0431	-1.0771
H2	2.1675	1.4400	0.1020
H3	-0.0113	2.7439	-1.8765
H4	1.2699	-0.1247	-2.5247
C5	-1.4003	-0.1361	0.4857
H6	-0.5745	-1.7726	1.3814
H7	-2.9650	-0.5953	-0.7427
C8	-2.3924	1.6233	2.5625
O9	-1.7518	3.9117	2.6097
O10	-3.8172	0.7068	4.2292

Table S2: alanine atomic coordinates. Values in atomic units.

	x	y	z
N1	-0.8220	-0.2740	-0.0869
H2	-1.5741	-1.9464	-0.7578
H3	-1.4872	1.3134	-1.0110
H4	-1.1622	-0.1020	1.8822
C5	1.9842	-0.2967	-0.0416
H6	2.6683	-2.0900	-0.7408
C7	2.9801	1.9351	-1.6384
H8	2.3244	3.7738	-0.8636
H9	2.3981	1.7745	-3.6453
H10	5.0834	1.9445	-1.5704

C11	2.8138	-0.0661	2.7439
O12	1.1017	0.1247	4.4012
O13	5.1306	-0.1191	3.2088

Table S3: aspartic acid atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.1225	-0.2268	-0.1247
H2	-1.4853	-0.7143	1.7858
H3	-1.9011	-1.5609	-1.3209
H4	-1.7858	1.5817	-0.4554
C5	1.6989	-0.3024	-0.0926
H6	2.3092	-1.9086	-1.2038
C7	2.7987	2.2393	-1.0658
H8	2.9310	3.6717	0.4573
H9	1.6157	3.0255	-2.6154
C10	5.4065	1.8652	-2.2412
O11	5.8317	2.2242	-4.4654
O12	7.2320	1.0582	-0.5934
H13	6.5479	0.5046	1.0375
C14	2.4831	-0.7786	2.6834
O15	0.7616	-1.1074	4.2972
O16	4.7980	-0.7710	3.1766

Table S4: glutamic acid atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.5552	-0.7011	0.2438
H2	-1.8330	-0.7049	2.2318
H3	-2.3376	-2.3055	-0.5442
H4	-2.2526	0.9638	-0.5083
C5	1.2642	-0.7370	0.2041
H6	1.9048	-2.4604	-0.6860
C7	2.2488	1.6535	-1.1962
H8	2.0409	3.3373	0.0529
H9	1.0771	1.9804	-2.9177
C10	5.0323	1.4249	-2.0919
H11	5.2742	-0.2381	-3.3429
H12	6.2928	1.1905	-0.4271
C13	5.8770	3.7757	-3.5338
O14	4.5297	5.5104	-4.2160
O15	8.4093	3.7795	-4.0931
H16	8.7797	5.3177	-4.9643
C17	2.1184	-0.7786	2.9971

O18	0.4309	-0.6954	4.6884
O19	4.4371	-0.9392	3.4393

Table S5: histidine atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	0.4309	-1.7272	0.2532
H2	0.8447	-3.5829	0.7143
H3	0.2665	-1.4400	-1.6762
H4	-1.2264	-1.1697	1.2264
C5	2.2960	0.0586	1.3965
H6	3.9061	-0.9959	2.0806
C7	3.0992	2.0976	-0.5499
H8	4.6620	3.2390	0.2740
H9	1.4967	3.4166	-0.8976
N10	2.8705	1.4740	-5.3234
H11	1.5798	2.8062	-5.6937
C12	3.9703	0.9713	-3.0122
C13	4.1120	0.0605	-7.0619
H14	3.6869	0.0926	-9.0820
N15	5.9111	-1.3058	-6.0244
C16	5.8563	-0.7124	-3.4847
H17	7.2017	-1.5760	-2.2053
C18	1.0337	1.3568	3.6623
O19	-1.2567	0.8504	4.1026
O20	2.3489	2.8648	4.9227

Table S6: serine atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-0.9959	-0.2929	-0.1606
H2	-1.3190	-0.5291	1.8028
H3	-1.6932	-1.8349	-1.1395
H4	-1.7669	1.4041	-0.7427
C5	1.8330	-0.2268	-0.1436
H6	2.5549	-1.8746	-1.1130
C7	2.9158	2.2318	-1.3285
H8	2.4132	3.9080	-0.1606
H9	2.1543	2.5096	-3.2673
O10	5.5955	2.0674	-1.5193
H11	6.1586	1.5326	0.1682
C12	2.6985	-0.3761	2.6286
O13	1.0186	-0.5858	4.3086
O14	5.0267	-0.2419	3.0538

Table S7: threonine atomic coordinates. Values in atomic units.

	x	y	z
N1	-0.8787	-0.3364	-0.1323
H2	-1.4834	-2.1751	-0.3855
H3	-1.3776	0.8598	-1.6119
H4	-1.4740	0.3420	1.6460
C5	1.9464	-0.2098	0.1531
H6	2.7496	-1.9672	-0.4989
C7	3.0557	2.0333	-1.3323
H8	2.8384	3.8172	-0.2268
O9	1.8217	2.3470	-3.7114
H10	2.7477	3.6642	-4.5712
C11	5.8619	1.5855	-1.9294
H12	6.1170	-0.1568	-3.0708
H13	6.9655	1.3719	-0.1531
H14	6.6745	3.2050	-2.9877
C15	2.5247	0.0926	2.9858
O16	0.6803	0.4101	4.4692
O17	4.7848	0.0132	3.6812

Table S8: tyrosine atomic coordinates. Values in atomic units.

	x	y	z
N1	-1.9294	-0.5159	0.3912
H2	-2.4000	-0.2986	2.3300
H3	-2.5341	-2.2582	-0.2532
H4	-2.6418	0.9921	-0.6236
C5	0.8768	-0.3666	0.6217
H6	1.6743	-2.1581	0.0454
C7	1.8538	1.8746	-1.0261
H8	1.7442	3.6831	0.0378
H9	0.7351	2.0863	-2.7873
C10	4.5561	1.4419	-1.8217
C11	5.1079	0.2872	-4.1536
H12	3.5905	-0.3288	-5.3706
C13	7.6175	-0.0680	-4.9227
H14	8.0351	-0.9638	-6.7104
C15	9.5998	0.7313	-3.3732
O16	12.1150	0.3534	-4.1517
H17	13.1884	0.9430	-2.8157
C18	6.5706	2.2696	-0.3024
H19	6.1756	3.1521	1.4986

C20	9.0820	1.9030	-1.0601
H21	10.5957	2.5228	0.1568
C22	1.4286	-0.0132	3.4790
O23	-0.4403	0.1946	4.9549
O24	3.6812	0.0038	4.1952

Table S9: Ala-Ala atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	1.1924	2.7231	0.4838
H2	0.1417	3.1199	2.1014
H3	0.8390	4.0081	-0.9354
H4	3.0897	2.9631	1.1263
C5	0.9014	0.0132	-0.2910
H6	-1.0507	-0.3005	-0.8145
C7	2.6853	-0.5046	-2.5492
H8	4.6827	-0.0435	-2.0844
H9	2.1297	0.6501	-4.2122
H10	2.5889	-2.5247	-3.1180
C11	1.4419	-1.6819	1.9615
O12	-0.2986	-2.5114	3.2409
N13	3.8947	-1.9785	2.6003
H14	5.2761	-1.8500	1.3398
C15	4.7375	-0.8844	4.9624
H16	3.3939	-1.2718	6.4610
C17	7.3907	-1.8387	5.6805
H18	8.7702	-1.3776	4.1687
H19	7.3586	-3.9155	5.9640
H20	8.0276	-0.9241	7.4606
C21	4.7810	2.0069	4.4314
O22	5.9148	2.7666	2.4737
O23	3.2390	3.3694	5.6144

Table S10: Asp-Asp atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.5439	-0.1625	-1.2453
H2	-2.2034	-1.9389	-0.7238
H3	-2.0957	0.2627	-3.0784
H4	-2.3017	1.1527	0.0227
C5	1.2718	-0.0397	-0.9543
H6	2.0674	-1.7726	-1.7008
C7	2.2677	2.3111	-2.4472
H8	1.4022	4.0818	-1.7234

H9	1.8330	2.1354	-4.4919
C10	5.1268	2.6513	-2.2223
O11	6.1926	4.6279	-1.8066
O12	6.3551	0.3987	-2.4151
H13	7.9047	0.4989	-1.4135
C14	1.8425	0.0548	1.8576
O15	0.2116	0.8258	3.3165
N16	4.1158	-0.7521	2.6022
H17	5.4821	-1.3304	1.4135
C18	5.3026	-0.2665	4.9851
H19	4.6657	1.5345	5.7240
C20	4.8925	-2.4831	6.8578
H21	6.1775	-4.0837	6.4477
H22	2.9140	-3.1596	6.6575
C23	5.1797	-1.7045	9.6168
O24	3.5754	-2.0674	11.2212
O25	7.4436	-0.5707	10.1800
H26	8.4622	-0.2665	8.6606
C27	8.1391	-0.0340	4.2519
O28	8.7438	-0.2872	1.9502
O29	9.7000	0.3439	5.9923

Table S11: Glu-Glu atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.8576	0.6727	-0.1663
H2	-2.7288	-0.8239	0.7616
H3	-2.6947	0.9902	-1.9105
H4	-2.0239	2.2752	0.9789
C5	0.9184	0.1720	-0.4346
H6	1.1849	-1.7650	-1.0337
C7	2.0560	2.0050	-2.4472
H8	1.5534	3.9911	-1.9483
H9	1.1811	1.5647	-4.3105
C10	4.9738	1.9048	-2.7590
H11	5.6163	-0.0567	-3.1464
H12	5.9659	2.5644	-1.0280
C13	5.8770	3.5338	-4.9681
O14	6.2229	2.8251	-7.1243
O15	6.1605	6.0377	-4.3426
H16	6.8200	6.8918	-5.7920
C17	2.1373	0.4535	2.1278
O18	1.0526	1.7140	3.7473
N19	4.3142	-0.7540	2.5228

H20	5.3177	-1.6781	1.1962
C21	6.0339	-0.3439	4.5788
H22	5.8657	1.5609	5.2988
C23	5.7958	-2.3452	6.7085
H24	7.4002	-2.0560	8.0446
H25	6.0207	-4.2481	5.8430
C26	3.2749	-2.1921	8.1787
H27	1.6611	-2.4340	6.8635
H28	3.1010	-0.3175	9.1047
C29	3.0576	-4.2557	10.1762
O30	1.7952	-6.1700	10.0118
O31	4.4257	-3.7719	12.3305
H32	4.2084	-5.1760	13.4416
C33	8.6474	-0.5877	3.2862
O34	8.6927	-1.3814	1.0261
O35	10.5768	0.0246	4.5202

Table S12: His-His atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	0.8334	2.7363	-1.3247
H2	-0.5990	4.0365	-1.0337
H3	1.3682	2.6626	-3.2125
H4	2.4359	3.4242	-0.3099
C5	0.1606	0.1417	-0.3496
H6	-1.8406	-0.1153	-0.6803
C7	1.6516	-1.9974	-1.7707
H8	0.2305	-3.3429	-2.5398
H9	2.8951	-3.1369	-0.5310
N10	5.5067	0.1625	-3.6736
H11	6.3589	0.6841	-2.0201
C12	3.2522	-1.1149	-3.9590
C13	6.4288	0.5934	-6.0188
H14	8.2109	1.5741	-6.3684
N15	4.9265	-0.3231	-7.7800
C16	2.9480	-1.4343	-6.4931
H17	1.4608	-2.3811	-7.5343
C18	0.5216	0.1550	2.4907
O19	-1.1508	0.9638	3.8702
N20	2.8233	-0.4687	3.3807
H21	3.9817	-1.6554	2.5001
C22	4.3010	1.5193	4.5410
H23	3.1010	2.8743	5.4991
C24	6.3551	0.5235	6.3665

H25	7.4247	2.1600	7.1337
H26	7.7082	-0.6916	5.3139
N27	2.9215	-0.6784	9.5412
H28	1.5949	0.5027	8.8968
C29	5.3158	-0.9770	8.5529
C30	2.6494	-2.4264	11.3932
H31	0.9279	-2.6475	12.5062
N32	4.6903	-3.8286	11.6521
C33	6.3684	-2.9215	9.8644
H34	8.2184	-3.7757	9.6678
C35	5.5161	2.8100	2.2185
O36	7.1451	1.6100	0.9808
O37	4.4711	4.7923	1.4135

Table S13: Ser-Ser atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.4230	1.0299	-1.1452
H2	-2.6929	-0.0831	-0.1285
H3	-1.9256	1.1093	-3.0387
H4	-1.4626	2.8289	-0.3420
C5	1.1867	-0.0491	-0.7861
H6	1.2699	-1.8784	-1.6932
C7	3.2144	1.7556	-1.9407
H8	3.4525	3.4998	-0.7861
H9	2.6343	2.3376	-3.8758
O10	5.5955	0.5310	-2.1996
H11	6.6367	1.0904	-0.7370
C12	1.6365	-0.4157	2.0050
O13	-0.0529	0.1436	3.4941
N14	3.8853	-1.3209	2.7307
H15	5.1930	-1.8009	1.4608
C16	5.0305	-0.6161	5.1174
H17	3.6812	0.3042	6.3476
C18	6.2739	-2.8610	6.5252
H19	7.7932	-3.7020	5.3423
H20	4.8264	-4.3331	6.9051
O21	7.3114	-2.0352	8.8704
H22	8.1353	-0.4327	8.4150
C23	7.1262	1.3247	4.4635
O24	7.4739	1.9030	2.1713
O25	8.4112	2.1996	6.2607

Table S14: Thr-Thr atomic coordinates. Values in atomic units.

	x	y	z
N1	-1.2604	0.4989	-1.3323
H2	-2.1429	-1.1773	-1.8311
H3	-1.3701	1.8293	-2.7930
H4	-2.0485	1.2170	0.3326
C5	1.5307	0.1323	-0.8428
H6	2.0598	-1.7064	-1.5552
C7	3.1691	2.2034	-2.1070
H8	3.6887	3.7341	-0.7483
O9	1.8859	3.3694	-4.1706
H10	3.0632	4.5788	-4.8755
C11	5.5860	1.0261	-3.2031
H12	5.1401	-0.4403	-4.6355
H13	6.7577	0.1531	-1.6932
H14	6.7728	2.4944	-4.1215
C15	1.8973	0.1512	1.9710
O16	0.0737	0.5272	3.3618
N17	4.2235	-0.2457	2.8403
H18	5.8090	-0.4649	1.8085
C19	5.0342	-0.0094	5.4292
H20	4.0043	1.4834	6.3646
C21	4.9435	-2.4737	6.9221
H22	6.2890	-3.8702	6.0963
O23	2.4718	-3.5300	6.8370
H24	1.3568	-2.0957	6.8994
C25	5.5860	-2.0258	9.7151
H26	4.2821	-0.6198	10.5617
H27	7.5476	-1.3020	9.9022
H28	5.4405	-3.8210	10.7922
C29	7.7932	0.8579	5.0909
O30	8.8704	0.2835	3.0292
O31	8.7986	2.1524	6.8011

Table S15: Tyr-Tyr atomic coordinates. Values in atomic units.

	x	y	z
N1	-2.3697	0.6047	-2.1070
H2	-3.3429	-0.8636	-1.2340
H3	-2.9839	0.8428	-3.9533
H4	-2.6853	2.2488	-1.0564
C5	0.4157	0.1209	-2.0069
H6	0.7483	-1.8368	-2.5001
C7	1.7820	1.8463	-4.0100

H8	0.9751	3.7851	-3.9930
H9	1.5647	1.0620	-5.9451
C10	4.5637	2.1014	-3.4639
C11	6.1813	0.0510	-3.9382
H12	5.4953	-1.6119	-4.8982
C13	8.6209	0.0208	-2.9102
H14	9.7756	-1.6592	-3.0425
C15	9.4619	2.0560	-1.4551
O16	11.6218	1.7631	0.0548
H17	11.0322	0.7540	1.5061
C18	5.4934	4.2216	-2.1543
H19	4.2670	5.7939	-1.7310
C20	7.9368	4.1876	-1.1357
H21	8.5812	5.7089	0.0624
C22	1.2831	0.4176	0.7238
O23	0.0756	1.8293	2.1165
N24	3.2692	-0.9449	1.5004
H25	4.3010	-2.1448	0.4498
C26	4.5675	-0.6992	3.8720
H27	4.7546	1.2718	4.3861
C28	3.2825	-2.3074	5.9659
H29	3.4450	-4.3501	5.5123
H30	1.2472	-1.8066	6.0641
C31	4.4560	-1.8406	8.5227
C32	3.2201	-0.3288	10.3255
H33	1.4400	0.5480	9.8549
C34	4.2878	0.0586	12.7216
H35	3.3391	1.2321	14.0936
C36	6.5970	-1.0658	13.3339
O37	7.6761	-0.6576	15.7320
H38	9.2956	-1.4683	15.7301
C39	6.7596	-2.9839	9.1784
H40	7.7290	-4.1423	7.8008
C41	7.8405	-2.5889	11.5651
H42	9.6282	-3.4601	12.0092
C43	7.2036	-1.7537	3.1558
O44	7.2395	-3.7190	1.7971
O45	9.1614	-0.5707	3.8059

Table S16: Gly-Gly atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.0904	-0.3439	-0.8466
H2	-1.8463	0.1058	-2.6003

H3	-2.0050	0.6727	0.5820
H4	-1.3512	-2.2563	-0.4611
C5	1.6762	0.3005	-0.6746
H6	1.9615	2.1694	-1.4494
H7	2.7609	-1.1679	-1.5987
C8	2.4264	0.3931	2.0390
O9	0.7691	0.5839	3.6510
N10	4.8831	0.2381	2.5568
H11	6.3155	0.0397	1.3096
C12	6.0282	0.1701	5.0248
H13	5.2818	-1.3871	6.1133
H14	5.8941	2.0031	5.9130
C15	8.8194	-0.3685	4.4749
O16	9.4713	-0.5801	2.1826
O17	10.2990	-0.5707	6.3155

Table S17: Ala-Ala-Ala atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.8708	0.1890	-1.3474
H2	-2.7703	-0.7880	0.1191
H3	-2.4907	-0.4611	-3.0916
H4	-2.2941	2.0976	-1.1527
C5	0.9127	-0.1909	-1.0186
H6	1.3984	-2.0371	-1.7556
C7	2.3414	1.9067	-2.4699
H8	1.9559	3.8097	-1.6686
H9	1.8047	1.9200	-4.5013
H10	4.4182	1.5874	-2.3924
C11	1.5137	-0.2287	1.7801
O12	-0.2362	-0.5953	3.2598
N13	3.9155	0.1606	2.5039
H14	5.3252	0.4535	1.2737
C15	4.9303	-0.1814	5.0172
H16	4.4333	1.4286	6.1718
C17	4.1839	-2.7023	6.3060
H18	4.6714	-4.3388	5.0853
H19	2.1241	-2.7496	6.6972
H20	5.1797	-2.9253	8.1428
C21	7.7592	-0.1587	4.5996
O22	8.5869	-0.3231	2.4264
N23	9.2351	0.1663	6.6235
H24	8.6398	0.2305	8.4244
C25	11.9431	0.1304	6.6367

H26	12.6234	-1.4305	5.5104
C27	13.0637	2.6759	5.7618
H28	12.3494	4.2292	6.9750
H29	12.5270	3.0538	3.7719
H30	15.1575	2.6192	5.9092
C31	12.6820	-0.3874	9.4222
O32	10.9358	-0.3817	11.0568
O33	14.9685	-0.7994	9.9230

Table S18: Asp-Asp-Asp atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.7763	0.3326	0.0416
H2	-2.5700	-0.5877	1.5987
H3	-2.3886	-0.5027	-1.6233
H4	-2.3395	2.2223	0.1209
C5	1.0412	0.2570	0.2948
H6	1.5439	-1.6856	0.7086
C7	2.3395	1.1811	-2.1902
H8	1.8784	3.1899	-2.5851
H9	1.7310	0.0170	-3.8248
C10	5.2175	0.9808	-2.0371
O11	6.7123	2.5587	-2.7401
O12	5.9621	-1.1981	-0.8636
H13	7.7630	-1.1130	-0.4970
C14	1.7178	1.8255	2.5908
O15	0.3326	3.5678	3.2409
N16	3.7681	1.1074	3.8872
H17	4.9246	-0.2438	3.2352
C18	4.3294	1.7971	6.4591
H19	4.8906	3.7643	6.5139
C20	2.1203	1.2831	8.3620
H21	0.6406	2.7401	8.0729
H22	2.8119	1.4702	10.3330
C23	0.8504	-1.2888	7.9879
O24	-0.4157	-1.9426	6.1681
O25	1.1981	-2.9026	9.9853
H26	0.4460	-4.4975	9.5998
C27	6.6329	0.2041	7.0373
O28	6.5819	-2.0863	6.6462
N29	8.7286	1.4192	7.7460
H30	8.8194	3.2390	8.2808
C31	11.1834	0.3156	8.1050
H32	11.0247	-1.4778	9.0764

C33	12.7273	0.1512	5.6125
H34	14.6983	-0.4309	6.0452
H35	12.7745	2.0333	4.6922
C36	11.5689	-1.7272	3.7983
O37	10.2669	-1.2548	1.9464
O38	12.1358	-4.1952	4.3823
H39	11.2363	-5.2742	3.2560
C40	12.5572	2.1807	9.8870
O41	11.5198	4.2935	10.3066
O42	14.6492	1.5193	10.7998

Table S19: Glu-Glu-Glu atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-2.9650	0.3345	-1.2359
H2	-3.9949	-1.0582	-0.3080
H3	-3.5773	0.5140	-3.0916
H4	-3.2484	2.0277	-0.2589
C5	-0.1871	-0.2494	-1.1055
H6	0.0888	-2.2091	-1.6214
C7	1.2642	1.5288	-2.9555
H8	1.2302	3.5092	-2.2374
H9	0.2627	1.5212	-4.8131
C10	4.0402	0.7483	-3.5073
H11	4.1309	-1.2245	-4.2179
H12	5.2421	0.8901	-1.7934
C13	5.2534	2.4226	-5.5350
O14	5.6673	1.8217	-7.7082
O15	5.8015	4.7999	-4.6733
H16	6.6443	5.6994	-5.9999
C17	0.6709	0.1172	1.6025
O18	-0.7294	1.2245	3.0803
N19	2.9196	-0.8126	2.3017
H20	4.1139	-1.7178	1.1414
C21	4.0459	-0.4233	4.7508
H22	3.7001	1.4872	5.3933
C23	3.1275	-2.3981	6.7199
H24	3.5999	-4.3331	6.0415
H25	1.0280	-2.2488	6.7992
C26	4.1801	-2.0201	9.4278
H27	3.8021	-0.0624	10.0836
H28	6.2550	-2.3376	9.4921
C29	2.9536	-3.8135	11.3232
O30	1.3682	-3.2673	12.8974

O31	3.7587	-6.2739	11.0889
H32	2.9555	-7.2320	12.3890
C33	6.8370	-0.6954	4.2065
O34	7.5098	-1.7745	2.2544
N35	8.4603	0.3534	5.8279
H36	7.9973	1.1679	7.4795
C37	11.1626	0.1568	5.7315
H38	11.7050	-1.7348	5.1892
C39	12.3059	2.2015	3.9684
H40	11.9053	4.0969	4.7829
H41	11.2949	2.0674	2.1297
C42	15.1726	1.8784	3.4941
H43	15.5581	-0.0416	2.7477
H44	16.2101	2.1014	5.3082
C45	16.1779	3.8154	1.6214
O46	14.9553	5.2988	0.3534
O47	18.7725	3.7606	1.3852
H48	19.2223	5.0418	0.1984
C49	11.9657	0.5953	8.5151
O50	10.3122	1.4211	10.0344
O51	14.1975	0.0775	9.1463

Table S20: His-His-His atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-2.1486	1.2926	-0.9997
H2	-3.2976	0.2929	0.2476
H3	-2.9196	1.2453	-2.8044
H4	-2.0730	3.1540	-0.3534
C5	0.4894	0.2211	-0.9392
H6	0.3704	-1.7820	-1.3323
C7	2.1486	1.5515	-2.9669
H8	2.5001	3.5565	-2.4302
H9	1.1603	1.5685	-4.8226
N10	4.9719	-2.0088	-4.5883
H11	3.6434	-3.1577	-5.2837
C12	4.6620	0.3080	-3.4261
C13	7.4928	-2.3678	-4.8755
H14	8.3224	-4.0440	-5.7542
N15	8.8023	-0.4460	-4.0119
C16	7.0392	1.2434	-3.0954
H17	7.6477	3.0292	-2.2960
C18	1.5779	0.5329	1.6951
O19	0.4006	1.8141	3.2277

N20	3.7511	-0.6406	2.2809
H21	4.8112	-1.6063	1.0337
C22	4.9927	-0.5027	4.7243
H23	5.0456	1.4381	5.3668
C24	3.8550	-2.2658	6.7936
H25	5.3177	-3.4355	7.7498
H26	2.5058	-3.5961	5.8941
N27	0.7049	0.9638	8.4698
H28	0.1946	1.6384	6.7709
C29	2.5133	-0.8636	8.8723
C30	-0.0680	1.7839	10.7677
H31	-1.4834	3.2579	11.0417
N32	1.1168	0.6123	12.6120
C33	2.7533	-1.0507	11.4291
H34	3.9949	-2.2450	12.5383
C35	7.6836	-1.2642	4.2046
O36	8.2146	-2.2563	2.1694
N37	9.3825	-0.7956	6.0150
H38	8.9252	-0.2400	7.7611
C39	11.9771	-1.6119	5.9564
H40	12.2322	-3.1105	4.5920
C41	13.8347	0.6009	5.4840
H42	15.7887	-0.1701	5.4235
H43	13.7232	1.9426	7.0959
N44	12.8709	0.9354	0.7748
H45	12.4986	-0.8976	0.4819
C46	13.3434	2.0466	3.0803
C47	12.4854	2.8233	-0.9071
H48	12.0319	2.4737	-2.8894
N49	12.6479	5.0701	0.1587
C50	13.2016	4.5807	2.6702
H51	13.4435	6.1246	3.9911
C52	12.5346	-2.7155	8.5983
O53	10.8867	-2.4340	10.3028
O54	14.6170	-3.8135	8.9252

Table S21: Ser-Ser-Ser atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.9105	1.9351	-0.5631
H2	-2.8516	1.3814	1.0866
H3	-3.0614	1.6554	-2.1278
H4	-1.4608	3.8361	-0.3647
C5	0.4649	0.3647	-0.6973

H6	-0.0510	-1.5023	-1.3512
C7	2.4850	1.5515	-2.4907
H8	3.5262	3.1294	-1.5609
H9	1.5515	2.3149	-4.2141
O10	4.2046	-0.3534	-3.3108
H11	5.6087	0.4384	-4.1820
C12	1.4891	0.0926	1.9445
O13	0.1493	0.7502	3.7228
N14	3.8286	-0.8258	2.2393
H15	4.9038	-1.2642	0.7427
C16	5.0342	-1.2113	4.6733
H17	4.0686	-0.1398	6.1227
C18	5.2138	-4.0289	5.4764
H19	6.0698	-4.1744	7.3964
H20	6.4270	-5.0909	4.1234
O21	2.7666	-5.1627	5.5048
H22	2.9215	-6.7652	6.3551
C23	7.6836	-0.1984	4.4446
O24	8.6039	0.2457	2.3546
N25	8.9441	0.2494	6.5819
H26	8.3016	-0.0926	8.3394
C27	11.5557	1.0110	6.7898
H28	12.7311	-0.2041	5.6465
C29	12.0602	3.8361	6.1926
H30	14.0709	4.2991	6.6065
H31	10.8432	5.0361	7.4172
O32	11.5481	4.3804	3.5961
H33	10.4804	2.9971	3.0236
C34	12.2303	0.5310	9.5790
O35	10.4842	-0.2135	11.0341
O36	14.4734	0.8976	10.2688

Table S22: Thr-Thr-Thr atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.7499	0.6765	-1.1679
H2	-2.6872	-1.0375	-0.9978
H3	-2.0919	1.5004	-2.9329
H4	-2.3206	1.8935	0.2759
C5	1.0866	0.3609	-0.9694
H6	1.5760	-1.4645	-1.7423
C7	2.4888	2.4604	-2.4170
H8	2.5360	4.2557	-1.3096
O9	1.2434	2.9688	-4.7470

H10	2.2885	4.1706	-5.6484
C11	5.1930	1.6422	-3.0821
H12	5.1967	-0.1266	-4.2141
H13	6.3570	1.3398	-1.3625
H14	6.1586	3.1275	-4.2141
C15	1.7745	0.4403	1.7839
O16	0.3723	1.5515	3.2598
N17	3.8758	-0.7540	2.5511
H18	5.0758	-1.6516	1.3984
C19	4.6903	-0.8296	5.1741
H20	4.1668	0.8995	6.1265
C21	3.7530	-3.1426	6.6292
H22	4.6506	-4.9038	5.8941
O23	1.1017	-3.4299	6.3230
H24	0.3666	-1.9219	7.0222
C25	4.2613	-2.8988	9.4751
H26	3.4204	-1.1414	10.2499
H27	6.3230	-2.8781	9.8795
H28	3.4355	-4.5372	10.5012
C29	7.5211	-0.9222	4.9662
O30	8.5132	-1.9521	3.1313
N31	8.8855	0.2570	6.7293
H32	8.2014	1.1584	8.2562
C33	11.6143	0.3175	6.8521
H34	12.3758	-1.5458	6.5120
C35	12.8350	2.2885	5.1363
H36	12.1415	4.2103	5.6522
O37	12.2095	1.8085	2.5644
H38	11.1305	0.3288	2.6381
C39	15.7301	2.2053	5.3328
H40	16.4387	0.2910	4.8528
H41	16.3442	2.6664	7.2868
H42	16.5899	3.5943	4.0194
C43	12.1037	1.0072	9.6319
O44	10.5333	2.4718	10.6807
O45	13.9613	0.0321	10.7412

Table S23: Tyr-Tyr-Tyr atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-3.1313	-0.0510	-2.0806
H2	-4.0100	-1.7045	-1.4853
H3	-3.5905	0.3307	-3.9495
H4	-3.7643	1.4173	-0.9146

C5	-0.3250	-0.2268	-1.7234
H6	0.2986	-2.0655	-2.3697
C7	0.9600	1.9181	-3.2938
H8	0.3307	3.8135	-2.6324
H9	0.4630	1.7499	-5.3271
C10	3.8059	1.8198	-3.1256
C11	5.1760	0.0794	-4.5920
H12	4.2065	-1.1924	-5.8582
C13	7.8197	-0.0208	-4.4371
H14	8.8742	-1.3625	-5.5577
C15	9.1160	1.6157	-2.8195
O16	11.7692	1.4815	-2.6759
H17	12.3135	2.5455	-1.3096
C18	5.1344	3.4809	-1.5288
H19	4.1215	4.8415	-0.3931
C20	7.7762	3.3694	-1.3644
H21	8.7683	4.6393	-0.1096
C22	0.2305	-0.0302	1.0847
O23	-1.3266	1.0110	2.4529
N24	2.3811	-1.0318	1.9842
H25	3.6906	-1.8878	0.9146
C26	3.2390	-0.6954	4.5486
H27	2.8459	1.2245	5.1363
C28	1.9540	-2.5851	6.4345
H29	2.0976	-4.5391	5.6843
H30	-0.0718	-2.0995	6.6726
C31	3.2182	-2.4793	8.9819
C32	2.9858	-0.2948	10.4766
H33	1.6837	1.1792	9.9362
C34	4.6620	0.1247	12.4854
H35	4.6620	1.9086	13.4775
C36	6.5385	-1.6535	13.0240
O37	8.5737	-0.9845	14.5887
H38	9.8870	-0.4044	13.4000
C39	4.9832	-4.3445	9.6659
H40	5.2364	-5.9904	8.4886
C41	6.6594	-3.9155	11.6691
H42	8.1787	-5.2270	12.0376
C43	6.1076	-0.9260	4.4144
O44	7.0638	-2.2507	2.7609
N45	7.4814	0.4044	6.0830
H46	6.7463	1.5307	7.4115
C47	10.1724	0.2343	6.4270
H48	10.7412	-1.7272	6.4666
C49	11.5859	1.7612	4.3539

H50	11.1551	3.8059	4.5524
H51	10.9056	1.1036	2.4850
C52	14.4054	1.3908	4.4711
C53	15.6375	-0.1965	2.7325
H54	14.5396	-1.2170	1.3455
C55	18.2718	-0.4819	2.7987
H56	19.2072	-1.7140	1.4683
C57	19.6947	0.8201	4.6034
O58	22.3385	0.5159	4.6790
H59	22.9356	1.4362	6.1189
C60	15.8643	2.7118	6.2550
H61	14.9269	3.9287	7.6043
C62	18.4947	2.4170	6.3363
H63	19.5700	3.4261	7.7460
C64	10.5655	1.3833	9.0915
O65	9.6017	3.5243	9.5072
O66	11.7144	0.1247	10.7544

Table S24: Gly-Gly-Gly atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-1.6800	-0.4630	-1.2926
H2	-2.3848	-0.1644	-3.1029
H3	-2.6740	0.6387	0.0113
H4	-1.9426	-2.3433	-0.7729
C5	1.0847	0.2135	-1.0904
H6	1.3398	2.1014	-1.8293
H7	2.1770	-1.2170	-2.0598
C8	1.8746	0.2476	1.6252
O9	0.2513	0.0643	3.2654
N10	4.3426	0.4762	2.1562
H11	5.7221	0.5745	0.8579
C12	5.3479	0.4063	4.7054
H13	4.6072	-1.2094	5.7126
H14	5.0210	2.2072	5.6144
C15	8.1353	0.0510	4.4182
O16	9.0367	-0.1682	2.2866
N17	9.5204	0.0132	6.5271
H18	8.8609	0.1965	8.2997
C19	12.2284	-0.2891	6.6405
H20	13.1374	1.2812	5.7089
H21	12.7462	-2.1297	5.9281
C22	12.9276	-0.1890	9.4486
O23	11.1626	0.1115	11.0284

O24	15.2199	-0.4120	10.0307

Table S25: atomic coordinates of a cluster composed by glycine surrounded by fifty-eight water molecules. Values in atomic units.

	x	y	z
N1	0.6179	1.0431	-1.0771
H2	2.1675	1.4400	0.1020
H3	-0.0113	2.7439	-1.8765
H4	1.2699	-0.1247	-2.5247
C5	-1.4003	-0.1361	0.4857
H6	-0.5745	-1.7726	1.3814
H7	-2.9650	-0.5953	-0.7427
C8	-2.3924	1.6233	2.5625
O9	-1.7518	3.9117	2.6097
O10	-3.8172	0.7068	4.2292
O11	10.8943	3.2522	-1.2038
H12	11.1853	4.3501	0.2683
H13	9.2597	3.9231	-1.7631
O14	6.5668	4.4106	5.9999
H15	7.4380	2.9574	6.7671
H16	5.6238	3.5413	4.6582
O17	-7.6817	1.2302	-2.5606
H18	-8.0446	2.5814	-1.3493
H19	-7.5570	-0.2154	-1.3871
O20	-8.6342	4.6695	1.2831
H21	-9.1954	3.3448	2.4529
H22	-7.4795	5.5577	2.4226
O23	2.1713	6.3495	7.8839
H24	3.8267	5.6994	7.3567
H25	2.5417	7.0468	9.5204
O26	8.8874	-0.0699	6.9674
H27	9.0461	-1.8160	7.5154
H28	9.1217	-0.2494	5.1476
O29	-1.7140	-3.4790	5.9281
H30	-2.5814	-1.9086	5.4197
H31	-2.2790	-4.6223	4.5694
O32	12.5119	-4.5183	3.3826
H33	11.5519	-4.8660	4.9360
H34	14.2296	-4.7149	3.9514
O35	-8.7419	0.9808	4.9700
H36	-9.0234	-0.8258	5.2062
H37	-6.8937	0.9694	4.7168
O38	-5.0286	-4.4484	9.7340
H39	-5.3045	-2.8251	10.6014

H40	-3.5565	-4.0157	8.7003
O41	-8.6757	7.8669	-2.8251
H42	-10.3406	8.5680	-2.6740
H43	-8.6190	6.7331	-1.3606
O44	0.8050	-10.5787	5.9111
H45	0.6142	-12.2794	6.5233
H46	-0.7861	-9.8304	6.5441
O47	6.4837	4.8018	-3.2862
H48	5.3763	6.1756	-2.7250
H49	7.0921	5.4537	-4.9057
O50	6.0698	0.2797	-8.9479
H51	7.7346	0.5480	-8.2203
H52	5.8090	-1.5156	-8.6039
O53	-2.4340	3.6850	8.2090
H54	-2.5908	2.7099	6.6348
H55	-0.7918	4.5013	7.9898
O56	8.6474	6.2588	-7.8178
H57	9.9192	7.2906	-8.6115
H58	7.1148	6.8219	-8.6965
O59	-3.7379	-9.1878	7.8159
H60	-5.2629	-9.3598	6.7898
H61	-4.1895	-7.7328	8.8590
O62	5.7580	-4.8320	-7.5854
H63	4.5977	-5.5123	-6.3174
H64	5.0512	-5.6163	-9.1141
O65	-5.4953	0.5102	11.0379
H66	-7.0506	1.5004	10.8678
H67	-4.2859	1.6837	10.2782
O68	5.2875	-0.3572	-3.1124
H69	5.9016	1.3663	-3.3467
H70	6.8106	-1.3606	-3.3278
O71	9.3712	-0.6595	1.8217
H72	10.1535	0.5272	0.6331
H73	10.6845	-1.9483	1.9918
O74	2.7401	-6.8087	-11.2779
H75	1.2831	-6.2871	-10.2574
H76	1.9578	-7.5192	-12.7481
O77	-7.7422	-2.7930	0.5272
H78	-7.6043	-3.2125	2.3206
H79	-8.9800	-4.0308	-0.0397
O80	-10.4464	-2.4434	-5.2629
H81	-9.5450	-2.4755	-6.8692
H82	-9.6981	-0.9675	-4.4522
O83	3.3732	-3.1483	5.2667
H84	1.5874	-3.2050	5.7901

H85	4.0138	-4.6941	6.0509
O86	9.5526	-5.3120	7.6250
H87	9.8360	-5.9356	9.3126
H88	7.9973	-6.2248	7.1696
O89	-0.7200	-0.2891	-6.3986
H90	-2.3792	0.4857	-6.6783
H91	0.3817	0.9392	-7.2320
O92	4.5259	1.0696	2.5757
H93	6.1548	0.4365	1.9615
H94	4.0742	-0.2872	3.7643
O95	-2.9688	-6.3438	1.8330
H96	-4.4919	-7.0090	1.0318
H97	-1.6951	-7.5306	1.2227
O98	3.0009	8.4849	-2.0239
H99	1.6025	7.3907	-2.5662
H100	2.7023	8.4660	-0.1814
O101	9.5526	-3.3297	-4.4106
H102	8.4603	-4.0459	-5.7315
H103	10.2971	-1.8822	-5.2856
O104	10.4653	1.5269	-6.1907
H105	11.0889	2.0163	-4.5202
H106	10.0571	3.1823	-6.8994
O107	-5.3366	6.5441	4.8774
H108	-4.0421	5.7561	3.7908
H109	-4.7375	5.8808	6.4912
O110	2.8705	11.6804	-6.0150
H111	3.7530	13.1582	-5.4197
H112	2.9518	10.5900	-4.5013
O113	10.5655	6.1529	3.0519
H114	9.1047	5.6956	4.0894
H115	11.3289	7.4663	4.0440
O116	-5.2950	2.0371	-7.0052
H117	-5.1816	3.8909	-7.0241
H118	-6.1832	1.8009	-5.3838
O119	1.5741	7.5684	2.7798
H120	1.7934	7.5400	4.6053
H121	0.2891	6.2342	2.6135
O122	-4.7583	7.0695	-6.0887
H123	-6.1832	7.5362	-4.9851
H124	-4.1158	8.7400	-6.5933
O125	9.2956	-6.3929	-0.2608
H126	9.5847	-5.4065	-1.8122
H127	10.6883	-5.8109	0.8088
O128	4.2765	-5.2138	0.5858
H129	4.1347	-4.2632	2.1637

H130	6.1114	-5.3763	0.3968
O131	-0.7521	-5.2194	-7.8027
H132	-0.7540	-3.4128	-7.3699
H133	0.2249	-5.8808	-6.3703
O134	-7.3397	-1.9861	-9.4902
H135	-6.4742	-0.5235	-8.7419
H136	-7.6269	-1.4173	-11.1928
O137	-8.0294	-9.4297	4.8150
H138	-7.5816	-9.3409	3.0103
H139	-9.2408	-10.7847	4.8226
O140	-2.2677	11.4725	-7.1961
H141	-2.6777	13.2092	-7.5268
H142	-0.4668	11.5519	-6.8011
O143	4.2292	8.2581	-9.7208
H144	3.6944	9.5186	-8.4660
H145	3.5527	8.9630	-11.2590
O146	-0.3779	5.2364	-4.0969
H147	-2.0107	5.8770	-4.7111
H148	0.4309	4.7319	-5.6881
O149	2.2337	3.5905	-8.2562
H150	2.9234	5.1212	-9.0197
H151	3.6207	2.3886	-8.6020
O152	-9.6735	8.1636	7.1772
H153	-9.7907	9.9551	6.9466
H154	-8.1428	7.7346	6.2323
O155	-8.1939	-4.2443	5.5690
H156	-8.3583	-6.0736	5.3725
H157	-7.2792	-4.1820	7.1772
O158	-9.4864	3.4714	9.4883
H159	-9.4902	2.6154	7.8518
H160	-9.8209	5.2119	8.9743
O161	-11.2080	-6.0490	-1.7442
H162	-12.9994	-6.3306	-1.8538
H163	-10.9510	-4.8623	-3.1615
O164	5.2591	-7.9142	6.3363
H165	3.6585	-8.8345	6.5044
H166	6.0112	-8.8893	4.9379
O167	-7.1583	-8.8817	-0.2098
H168	-8.6398	-7.9482	-0.8258
H169	-6.6613	-9.7245	-1.7952
O170	-6.2626	-10.6581	-4.9284
H171	-6.1492	-9.2030	-6.0849
H172	-6.1133	-12.0413	-6.0887
O173	1.1527	-9.3560	0.7521
H174	2.4491	-8.0483	0.9127

H175	1.1338	-10.0552	2.4623
O176	7.1091	-10.3425	2.2280
H177	7.9860	-9.0612	1.2113
H178	6.9032	-11.6955	1.0356
O179	-5.6465	-6.8219	-8.2676
H180	-6.4307	-5.2251	-8.7513
H181	-3.8645	-6.3306	-8.2090
O182	2.3036	-6.7047	-3.9287
H183	1.6327	-8.1655	-3.0368
H184	3.0387	-5.7939	-2.4907

Table S26: H-Asp-Ala-Glu-Gly-Ser-OH (polypeptide 1) atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-11.3006	14.9175	2.5303
H2	-11.9676	14.7153	0.6916
H3	-10.8206	16.7902	2.8705
H4	-12.7557	14.3600	3.7473
C5	-9.1066	13.1733	2.9763
H6	-7.8424	13.3415	1.3738
C7	-7.7706	13.9707	5.4878
H8	-9.0480	13.7251	7.1356
H9	-7.1828	15.9852	5.4027
C10	-5.3819	12.4476	6.0377
O11	-4.7583	11.6161	8.0748
O12	-3.9779	12.0168	3.9098
H13	-2.5360	11.0133	4.3879
C14	-10.1138	10.4804	3.0387
O15	-12.3815	10.1346	3.3618
N16	-8.4754	8.5756	2.7118
H17	-6.6140	8.8307	2.4472
C18	-9.1274	5.9394	2.8743
H19	-10.3954	5.6371	4.4522
C20	-10.2744	4.9379	0.3874
H21	-8.9592	5.2421	-1.2208
H22	-12.0678	5.9470	-0.0283
H23	-10.7034	2.8856	0.5216
C24	-6.6537	4.6223	3.4506
O25	-4.6506	5.7826	3.2182
N26	-6.7331	2.2242	4.2746
H27	-8.3431	1.2567	4.4522
C28	-4.4919	0.7975	4.8982
H29	-3.0179	1.2208	3.5470
C30	-3.5773	1.3852	7.6307

H31	-5.1571	1.0016	8.9668
H32	-3.1842	3.4544	7.7063
C33	-1.1867	-0.0605	8.5038
H34	0.3704	0.2211	7.1262
H35	-1.5628	-2.1184	8.6738
C36	-0.2362	0.8749	11.0625
O37	1.6384	2.1467	11.4404
O38	-1.7480	0.1512	13.0467
H39	-1.0053	0.8050	14.5585
C40	-5.1816	-1.9634	4.5920
O41	-7.4002	-2.6343	4.7413
N42	-3.3089	-3.6094	4.0931
H43	-1.5080	-3.0519	4.0383
C44	-3.6566	-6.3306	3.9911
H45	-3.8380	-6.8899	2.0371
H46	-5.2232	-6.8937	5.1760
C47	-1.3228	-7.5343	5.0437
O48	0.3893	-6.2172	5.8978
N49	-1.2000	-10.0533	4.9662
H50	-2.5020	-11.1928	4.1876
C51	0.9581	-11.5462	5.7070
H52	2.6437	-10.8036	4.8264
C53	1.3096	-11.7862	8.6077
H54	-0.4101	-12.6479	9.4581
H55	1.5798	-9.8757	9.4335
O56	3.4639	-13.3056	9.1765
H57	3.3165	-14.6737	7.9274
C58	0.4649	-14.2145	4.6223
O59	-1.5666	-14.5887	3.4299
O60	2.1014	-15.8964	5.0361

Table S27: H-Thr-Gly-Pro-Tyr-Ser-OH (polypeptide 2) atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	24.0581	-7.1602	6.8692
H2	25.1900	-8.1712	5.6314
H3	23.7709	-8.1655	8.5510
H4	24.8820	-5.4065	7.2547
C5	21.4503	-6.6575	5.8033
H6	21.0138	-8.1296	4.4579
C7	19.4510	-6.6008	7.9312
H8	19.4113	-4.7224	8.8949
O9	20.0084	-8.4584	9.7963
H10	18.6440	-8.3942	11.0152

C11	16.8034	-7.2339	6.9202
H12	16.7808	-9.0971	5.9489
H13	16.1137	-5.7618	5.5955
H14	15.4145	-7.3151	8.4962
C15	21.5467	-4.1385	4.4862
O16	23.3362	-2.7250	4.9171
N17	19.6683	-3.4941	2.8799
H18	18.3152	-4.7130	2.3981
C19	19.1448	-0.8712	2.1940
H20	17.8806	-0.9392	0.5934
H21	20.8985	0.1096	1.8141
C22	17.7993	0.4932	4.3275
O23	17.7143	-0.5178	6.4251
N24	16.6806	2.7174	3.9590
C25	16.7864	4.1536	1.5836
H26	16.8412	2.9329	-0.1247
H27	18.4796	5.3989	1.6365
C28	14.6794	3.6510	5.6276
H29	15.4769	3.9080	7.4909
C30	13.8536	6.1511	4.3974
H31	15.0914	7.6969	5.1042
H32	11.8561	6.6537	4.7923
C33	14.3657	5.7410	1.5817
H34	12.7972	4.6128	0.7483
H35	14.5717	7.5362	0.5197
C36	12.5157	1.7669	5.9394
O37	11.9242	0.3779	4.1725
N38	11.3667	1.6441	8.1957
H39	11.7824	2.8025	9.6244
C40	9.4581	-0.2154	8.7702
H41	8.1863	-0.3704	7.1753
C42	10.7318	-2.8233	9.3504
H43	12.0791	-2.6229	10.9453
H44	11.7843	-3.4828	7.6591
C45	8.7721	-4.7659	9.9910
C46	7.0846	-5.5690	8.1069
H47	7.3680	-4.9851	6.1718
C48	4.8660	-6.8484	8.7759
H49	3.4317	-7.2206	7.3718
C50	4.3634	-7.3529	11.3176
O51	1.8689	-7.8632	12.0432
H52	1.1414	-6.1681	12.2492
C53	8.3545	-5.4726	12.5157
H54	9.5960	-4.7923	13.9840
C55	6.1303	-6.7425	13.1827

H56	5.6560	-7.0222	15.1480
C57	7.9217	0.8447	10.9736
O58	8.8798	2.4472	12.3626
N59	5.5274	0.0359	11.3081
H60	4.7073	-1.3323	10.2914
C61	3.9344	0.7937	13.4019
H62	4.9945	0.6179	15.1386
C63	2.8535	3.5111	13.1468
H64	1.6743	3.6377	11.4121
H65	4.4390	4.8755	12.9786
O66	1.3701	4.1574	15.3049
H67	0.4705	2.5681	15.6602
C68	1.6630	-1.0469	13.5663
O69	1.3606	-2.6910	11.8694
O70	0.1663	-0.7710	15.3994

Table S28: H-His-Ala-Glu-Pro-Tyr-OH (polypeptide 3) atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-3.2201	3.1369	-1.6497
H2	-4.6072	2.3036	-0.5310
H3	-3.7965	3.1596	-3.5262
H4	-2.9725	4.9851	-0.9959
C5	-0.7446	1.7782	-1.3152
H6	-1.0809	-0.2343	-1.4456
C7	1.1830	2.5927	-3.4015
H8	1.1395	4.6846	-3.6113
H9	0.6557	1.7612	-5.2553
N10	4.9945	-0.3893	-3.1729
H11	4.2179	-1.9445	-3.9117
C12	3.9042	1.9578	-2.8289
C13	7.4531	-0.1757	-2.4737
H14	8.7986	-1.7404	-2.5303
N15	8.0068	2.1335	-1.7385
C16	5.7958	3.4865	-1.9823
H17	5.7656	5.4783	-1.5042
C18	0.2835	2.2941	1.3020
O19	-0.4592	4.1706	2.4377
N20	1.9502	0.6557	2.2903
H21	2.6022	-0.8731	1.3833
C22	3.2843	1.0545	4.6260
H23	3.9533	2.9877	4.7168
C24	1.6686	0.3742	6.9580
H25	0.9997	-1.6119	6.8503

H26	-0.0094	1.6308	7.0562
H27	2.7666	0.6161	8.7324
C28	5.5596	-0.6690	4.4409
O29	5.5293	-2.4548	2.9499
N30	7.5797	-0.1512	5.8846
H31	7.6269	1.2831	7.1073
C32	9.8852	-1.6082	5.7788
H33	9.4335	-3.5395	5.2988
C34	11.6993	-0.4705	3.7738
H35	11.9884	1.5685	4.2122
H36	10.6996	-0.5650	1.9219
C37	14.2996	-1.7820	3.5300
H38	14.0463	-3.8343	3.1880
H39	15.4315	-1.5269	5.2780
C40	15.8227	-0.7370	1.3152
O41	16.2649	-1.8274	-0.6595
O42	16.7108	1.6705	1.7083
H43	17.6047	2.1694	0.2230
C44	11.0492	-1.5099	8.4055
O45	10.8130	0.4687	9.6093
N46	12.2341	-3.4790	9.4278
C47	12.0262	-6.0944	8.5321
H48	12.7953	-6.2833	6.5876
H49	10.0061	-6.6802	8.5812
C50	13.5531	-3.3014	11.8391
H51	12.6271	-1.9823	13.0958
C52	13.4870	-6.0396	12.8180
H53	11.6577	-6.3589	13.8026
H54	15.0498	-6.4761	14.1465
C55	13.5720	-7.6534	10.4143
H56	15.5619	-7.7838	9.7396
H57	12.8105	-9.5828	10.7015
C58	16.2479	-2.4056	11.4158
O59	17.3401	-2.8913	9.4203
N60	17.3193	-1.0469	13.2621
H61	16.5049	-0.6274	14.9137
C62	19.8761	-0.1380	13.2224
H63	21.0950	-1.4929	12.2964
C64	19.9971	2.5096	11.9506
H65	19.0069	3.9231	13.1468
H66	19.0125	2.4075	10.0987
C67	22.6767	3.3807	11.5198
C68	23.7331	3.3429	9.0801
H69	22.6276	2.6248	7.5230
C70	26.2029	4.2084	8.6644

H71	27.0099	4.1593	6.7936
C72	27.6372	5.1230	10.6864
O73	30.1260	5.9715	10.2744
H74	30.8195	6.3740	11.8977
C75	24.1280	4.3388	13.5248
H76	23.3306	4.3634	15.4069
C77	26.6036	5.1892	13.1204
H78	27.6902	5.8808	14.7002
C79	20.5961	-0.0151	16.0551
O80	19.0295	1.0016	17.5423
O81	22.6578	-0.9675	16.7562

Table S29: H-Thr-Asp-His-Pro-Ala-OH (polypeptide 4) atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-0.5783	4.0913	-2.1600
H2	-2.4264	3.4979	-2.4151
H3	0.1436	4.8812	-3.8286
H4	-0.4762	5.3952	-0.6784
C5	1.1830	1.9219	-1.5345
H6	0.2192	0.1814	-1.9974
C7	3.6925	2.0976	-3.0236
H8	5.1930	3.0632	-1.9011
O9	3.4053	3.4998	-5.3045
H10	5.0777	3.5867	-6.0471
C11	4.5788	-0.5556	-3.8002
H12	3.1521	-1.5118	-5.0078
H13	4.9738	-1.7574	-2.1278
H14	6.3684	-0.4233	-4.8963
C15	1.6800	1.9918	1.2718
O16	0.7672	3.7095	2.5341
N17	3.1124	0.1795	2.3225
H18	3.8985	-1.2453	1.3530
C19	3.9174	0.2268	4.9265
H20	4.2878	2.1637	5.4802
C21	1.9426	-1.0450	6.7066
H22	1.6271	-3.0387	6.1397
H23	0.1209	-0.0170	6.5422
C24	2.6985	-1.0223	9.4883
O25	2.3659	-2.7231	10.9906
O26	3.8834	1.1716	10.2177
H27	4.3369	1.0016	11.9657
C28	6.4175	-1.1679	4.8793
O29	6.8087	-2.7855	3.2598

N30	8.1693	-0.5027	6.5876
H31	7.7970	0.7181	7.9841
C32	10.7223	-1.4702	6.5914
H33	10.7091	-3.3921	5.9016
C34	12.5251	0.2343	5.0229
H35	14.4810	-0.5310	5.0267
H36	12.6007	2.1467	5.8941
N37	12.0224	-1.1697	0.4422
H38	12.8445	-2.8592	0.6255
C39	11.6388	0.5688	2.3414
C40	11.0247	-0.1795	-1.6970
H41	11.0662	-1.1508	-3.5149
N42	10.0363	2.0749	-1.3096
C43	10.4559	2.5644	1.2283
H44	9.8625	4.3426	2.0504
C45	11.5746	-1.4192	9.3220
O46	10.4785	0.0246	10.7866
N47	13.4416	-2.8913	10.1100
C48	14.3959	-5.1174	8.7589
H49	15.1254	-4.5901	6.8597
H50	12.8520	-6.5328	8.5888
C51	14.7002	-2.5058	12.5232
H52	13.3906	-1.8708	13.9556
C53	15.8454	-5.1249	13.0561
H54	14.3638	-6.3457	13.9103
H55	17.4913	-5.0569	14.3544
C56	16.5275	-6.1435	10.4294
H57	18.3587	-5.3064	9.8171
H58	16.6693	-8.2316	10.3822
C59	16.7505	-0.5197	12.2095
O60	17.4837	0.0605	10.0760
N61	17.6293	0.5707	14.3147
H62	17.1417	0.0850	16.0778
C63	19.6513	2.3697	14.4281
H64	21.1668	1.7839	13.1903
C65	18.7253	5.0645	13.8044
H66	17.1889	5.6144	15.1216
H67	18.0015	5.1344	11.8391
H68	20.3089	6.4270	14.0048
C69	20.6528	2.2639	17.1776
O70	19.4264	0.9638	18.7650
O71	22.6427	3.4582	17.6973

Table S30: H-Tyr-Ser-Glu-Asp-His-OH (polypeptide 5) atomic coordinates. Values in atomic units.

	x	y	z
N1	-3.3977	2.5587	-1.5609
H2	-4.4106	0.8863	-1.3814
H3	-3.8154	3.4261	-3.2711
H4	-3.9174	3.7398	-0.0643
C5	-0.6142	2.0768	-1.3058
H6	-0.1417	0.4157	-2.4037
C7	0.8353	4.4427	-2.3074
H8	0.3987	6.1416	-1.1490
H9	0.2910	4.8623	-4.2935
C10	3.6604	4.0516	-2.3111
C11	4.7791	2.4226	-4.0875
H12	3.6321	1.4438	-5.4613
C13	7.4039	2.0711	-4.1177
H14	8.2694	0.8239	-5.4859
C15	8.9327	3.3505	-2.3867
O16	11.5670	2.9952	-2.4604
H17	12.3116	3.9703	-1.0960
C18	5.2194	5.3385	-0.5839
H19	4.4031	6.6140	0.7842
C20	7.8461	4.9832	-0.6142
H21	9.0291	5.9810	0.7181
C22	-0.0435	1.5212	1.4551
O23	-1.5628	2.2091	3.0651
N24	2.0749	0.2570	2.0541
H25	3.3580	-0.3326	0.7861
C26	2.9347	-0.0869	4.6336
H27	2.7798	1.6819	5.6465
C28	1.5666	-2.2280	6.1019
H29	1.9294	-4.0931	5.1967
H30	-0.5027	-1.8538	6.0339
O31	2.3414	-2.2715	8.6871
H32	1.3965	-3.5735	9.5431
C33	5.7032	-0.7105	4.3483
O34	6.4893	-1.4740	2.2998
N35	7.2433	-0.3383	6.3268
H36	6.5630	0.1493	8.0238
C37	9.9343	-0.7823	6.2153
H38	10.2707	-2.5662	5.2742
C39	11.3081	1.3946	4.7905
H40	10.8376	3.2163	5.7296
H41	10.4691	1.4532	2.8592

C42	14.2126	1.1376	4.5353
H43	14.6983	-0.7351	3.7247
H44	15.1480	1.3360	6.4043
C45	15.2973	3.1672	2.7949
O46	14.1087	4.7753	1.6516
O47	17.8693	3.0047	2.5568
H48	18.4513	4.3955	1.5590
C49	10.8546	-1.0412	8.9119
O50	9.6282	-0.1474	10.6675
N51	13.0202	-2.3017	9.3220
H52	14.0369	-3.0387	7.9161
C53	14.1257	-2.6003	11.7957
H54	13.7364	-0.9316	12.9182
C55	13.0580	-5.0134	13.1279
H56	13.3131	-6.6745	11.8750
H57	11.0077	-4.7489	13.4737
C58	14.3185	-5.6371	15.6469
O59	15.0101	-7.7233	16.2970
O60	14.6983	-3.5395	17.1058
H61	16.3102	-3.7360	17.9940
C62	16.9697	-2.7042	11.3894
O63	17.8598	-3.5376	9.4052
N64	18.4078	-1.8028	13.2697
H65	17.6444	-1.2132	14.8929
C66	21.0875	-2.2091	13.5815
H67	21.7224	-3.7398	12.3872
C68	22.7013	0.2098	13.1619
H69	24.7044	-0.2589	13.5928
H70	22.0796	1.6819	14.5244
N71	21.7337	0.0888	8.4282
H72	20.8172	-1.5779	8.4622
C73	22.6332	1.3228	10.5352
C74	21.9435	1.7026	6.4572
H75	21.3388	1.2302	4.5448
N76	22.9073	3.8947	7.1469
C77	23.3419	3.6566	9.7170
H78	24.1375	5.2156	10.7752
C79	21.4616	-3.0557	16.3594
O80	19.5813	-3.0236	17.8371
O81	23.6461	-3.7095	17.0208

Table S31: H-Ala-Thr-Ser-Gly-His-OH (polypeptide 6) atomic coordinates. Values in atomic units.

	x	**y**	**z**

N1	-2.9801	1.3247	-2.0050
H2	-4.1102	1.2094	-0.3912
H3	-3.9703	0.7030	-3.5810
H4	-2.4604	3.2050	-2.2412
C5	-0.6557	-0.2305	-1.5685
H6	-1.1849	-2.2053	-1.6648
C7	1.3115	0.4044	-3.6358
H8	1.9389	2.4056	-3.5224
H9	0.5291	0.0643	-5.5558
H10	3.0160	-0.8126	-3.4469
C11	0.3477	0.2343	1.0734
O12	-0.9260	1.4778	2.5644
N13	2.5851	-0.7672	1.7348
H14	3.7001	-1.7404	0.5537
C15	3.6132	-0.5877	4.2802
H16	3.1710	1.2416	5.0739
C17	2.7552	-2.7193	6.0490
H18	3.6717	-4.5448	5.5274
O19	0.1077	-3.1199	5.8487
H20	-0.6709	-1.5156	6.2096
C21	3.2995	-2.1070	8.8326
H22	2.4377	-0.2797	9.3900
H23	5.3593	-2.0277	9.2162
H24	2.4963	-3.6094	10.0647
C25	6.4307	-0.7597	3.8909
O26	7.2660	-1.7971	1.9899
N27	7.9614	0.2986	5.6125
H28	7.3246	1.1433	7.1791
C29	10.6940	0.1209	5.5104
H30	11.2306	-1.7990	5.0569
C31	11.9393	1.9993	3.6264
H32	11.5878	3.9835	4.2330
H33	11.0417	1.7197	1.7442
O34	14.5906	1.5439	3.3845
H35	15.2520	2.7212	2.1618
C36	11.5406	0.6727	8.1806
O37	10.0174	1.5250	9.7170
N38	13.9367	0.1436	8.8212
H39	15.1651	-0.4857	7.5249
C40	14.9118	0.4687	11.3629
H41	13.7837	-0.6368	12.6593
H42	14.9666	2.4642	11.7938
C43	17.5574	-0.5253	11.4744
O44	18.4362	-1.7499	9.7019
N45	18.8859	0.0113	13.5588

H46	18.1319	0.8069	15.0989
C47	21.3539	-0.9751	14.1805
H48	21.6827	-2.7477	13.2186
C49	23.5668	0.9241	13.7704
H50	25.3129	0.0661	14.5698
H51	23.1548	2.6683	14.8646
N52	23.1057	0.5990	8.9630
H53	21.6600	-0.6425	8.9913
C54	24.1658	1.6724	11.0832
C55	24.1148	1.7763	6.9315
H56	23.5876	1.3247	4.9889
N57	25.7494	3.5338	7.5910
C58	25.7834	3.4695	10.2083
H59	26.9947	4.7451	11.2533
C60	21.2500	-1.5269	17.0453
O61	19.4510	-0.5877	18.3058
O62	22.9904	-2.8440	17.9883

Table S32: H-Glu-Pro-Asp-Tyr-Thr-OH (polypeptide 7) atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	0.5612	4.4975	-2.9177
H2	-1.1452	5.1495	-3.6302
H3	2.0371	4.9549	-4.1328
H4	0.9335	5.3328	-1.1546
C5	0.5480	1.6932	-2.4377
H6	-1.3738	1.0318	-2.6645
C7	2.3508	0.4516	-4.4295
H8	2.3489	1.5571	-6.2210
H9	1.5250	-1.4192	-4.9454
C10	5.1023	-0.0586	-3.5602
H11	5.1533	-1.6006	-2.1354
H12	5.9772	1.6460	-2.7061
C13	6.7822	-0.9279	-5.7448
O14	7.4380	-3.0784	-6.1945
O15	7.4701	1.0299	-7.2981
H16	8.5548	0.3458	-8.5794
C17	1.3039	1.3701	0.3288
O18	1.9294	3.3202	1.4419
N19	1.2094	-0.8107	1.5949
C20	0.2797	-3.2106	0.5575
H21	0.7408	-3.4771	-1.4702
H22	-1.8009	-3.3127	0.8523
C23	2.3622	-1.1603	4.0950

H24	1.4532	0.1266	5.3952
C25	1.8330	-3.9476	4.7281
H26	-0.0170	-4.0818	5.7259
H27	3.3014	-4.8339	5.9356
C28	1.6044	-5.2270	2.1448
H29	3.5300	-5.5785	1.3701
H30	0.5480	-7.0336	2.2223
C31	5.1703	-0.5140	4.1914
O32	6.4534	-0.6104	2.2601
N33	6.1511	0.1909	6.4213
H34	5.1325	0.2494	8.0087
C35	8.7797	0.8353	6.7407
H36	9.9173	-0.4913	5.6730
C37	9.2691	3.6150	5.8789
H38	8.1315	4.9360	7.0430
H39	8.6512	3.8116	3.8834
C40	12.0205	4.4673	6.0037
O41	12.7443	6.5857	6.5044
O42	13.7308	2.5814	5.4783
H43	15.3937	3.2730	5.6881
C44	9.3409	0.4271	9.5280
O45	7.6232	0.4573	11.0908
N46	11.7522	-0.0057	10.1837
H47	13.1412	-0.0057	8.9006
C48	12.5931	-0.3704	12.7500
H49	11.6785	1.0261	13.9292
C50	11.9620	-3.0992	13.7137
H51	12.8539	-4.5316	12.4665
H52	9.8852	-3.3939	13.6930
C53	12.8747	-3.4431	16.3764
C54	11.7957	-1.9880	18.3190
H55	10.1327	-0.8674	17.9411
C56	13.0486	-1.7310	20.6377
H57	12.3701	-0.4082	22.0361
C58	15.3540	-2.9574	21.0194
O59	16.9490	-2.1354	22.9696
H60	18.1225	-0.9789	22.1136
C61	15.0706	-4.8528	16.8677
H62	15.9663	-5.9111	15.3691
C63	16.3272	-4.5826	19.1807
H64	18.1773	-5.4084	19.4453
C65	15.4183	0.2646	12.7330
O66	16.5597	0.4214	10.7091
N67	16.5880	0.7634	14.9345
H68	15.7206	0.6727	16.6088

C69	19.2941	1.1565	15.2161
H70	20.3032	-0.1531	14.0199
C71	20.1653	3.8494	14.6794
H72	19.1184	5.1949	15.9172
O73	19.6909	4.4730	12.1075
H74	18.5647	3.1483	11.5273
C75	23.0244	4.1461	15.1008
H76	24.0770	2.7684	13.9216
H77	23.5139	3.8097	17.1134
H78	23.6348	6.0849	14.5830
C79	19.9272	0.4781	17.9751
O80	18.7442	1.5874	19.7212
O81	21.5448	-1.2151	18.3814

Table S33: MAGE-1 fragment (polypeptide 8) atomic coordinates. Values in atomic units.

	x	**y**	**z**
N1	-25.1674	10.7280	13.9235
H2	-25.3809	12.6442	13.5474
H3	-26.8454	9.7737	13.5645
H4	-23.7387	10.0458	12.7424
C5	-24.3094	10.3330	16.6012
H6	-25.4962	11.4593	17.8277
C7	-24.6023	7.4814	17.3193
H8	-23.8389	6.2966	15.7490
H9	-26.6603	7.0581	17.4875
C10	-23.2436	6.5876	19.7665
H11	-23.8502	7.7252	21.4238
H12	-21.1574	6.7482	19.5776
C13	-23.7803	3.8078	20.3637
O14	-22.2969	2.0711	20.1672
O15	-26.2181	3.4034	21.1366
H16	-26.3900	1.6422	21.5221
C17	-21.6336	11.3081	16.9112
O18	-20.3221	11.5689	15.0214
N19	-20.7927	11.9091	19.2317
H20	-21.8074	11.6766	20.8078
C21	-18.2264	12.6725	19.7457
H22	-16.9584	11.8883	18.3436
C23	-17.9732	15.5732	19.8629
H24	-19.2506	16.3820	21.3218
H25	-18.4891	16.4066	18.0053
H26	-16.0022	16.1477	20.3032
C27	-17.5688	11.4952	22.2704

O28	-19.2544	10.6543	23.6310
N29	-15.1197	11.3346	22.9224
H30	-13.7383	12.0205	21.8339
C31	-14.2826	10.2196	25.2675
H32	-15.7452	10.4710	26.6735
C33	-13.7024	7.3680	24.8272
H34	-12.0829	7.1469	23.5120
H35	-15.3805	6.4761	23.9353
C36	-13.0864	5.9904	27.2687
O37	-11.1645	6.2550	28.5084
O38	-14.9534	4.3785	28.0624
H39	-14.4111	3.5338	29.5667
C40	-11.9261	11.7087	26.0215
O41	-10.4483	12.2927	24.3246
N42	-11.4480	12.4212	28.3912
C43	-13.1865	12.0924	30.5247
H44	-13.8007	10.0949	30.7307
H45	-14.8551	13.3434	30.2432
C46	-9.2030	13.8857	29.0810
H47	-8.8666	15.3408	27.6883
C48	-9.9248	14.9610	31.6888
H49	-11.0152	16.7373	31.4054
H50	-8.2751	15.3880	32.9096
C51	-11.6691	12.9522	32.8245
H52	-10.5182	11.3516	33.5559
H53	-12.8766	13.7024	34.3647
C54	-6.7973	12.3116	29.2473
O55	-4.8453	13.3377	29.9805
N56	-6.8125	9.8549	28.5745
H57	-8.3998	9.0329	27.9887
C58	-4.5637	8.2676	28.7749
H59	-3.5130	8.8439	30.4303
C60	-5.0947	5.4481	29.0829
H61	-5.9148	4.6279	27.3217
O62	-6.8503	5.0399	31.0709
H63	-8.4716	5.5860	30.4114
C64	-2.6664	4.0176	29.7953
H65	-1.8482	4.8018	31.5622
H66	-1.2264	4.1404	28.2741
H67	-3.0992	1.9899	30.1203
C68	-2.8705	8.6285	26.4958
O69	-3.0935	7.3284	24.5834
N70	-1.1130	10.4710	26.6546
H71	-1.1679	11.6180	28.1531
C72	0.9108	10.8451	24.8178

H73	2.0995	12.3456	25.5245
H74	0.0340	11.2949	23.0282
C75	2.5946	8.5718	24.4172
O76	3.1048	7.1110	26.1444
N77	3.5773	8.2505	22.1022
H78	3.2352	9.4392	20.6812
C79	5.1949	6.1359	21.5013
H80	6.4326	5.7637	23.0868
C81	3.6358	3.7209	20.8871
H82	2.1297	4.2462	19.5190
H83	2.6796	3.0746	22.6427
N84	7.0090	0.2627	21.0024
H85	7.6439	0.5707	22.7542
C86	5.1117	1.5571	19.7684
C87	7.8820	-1.5137	19.3754
H88	9.4486	-2.7836	19.8138
N89	6.6537	-1.4721	17.2116
C90	4.9095	0.4535	17.4535
H91	3.6472	0.8976	15.9039
C92	6.8748	6.8597	19.3054
O93	6.1907	8.4490	17.7596
N94	9.1387	5.7240	19.1675
H95	9.6754	4.3917	20.3958
C96	10.9245	6.0263	17.1228
H97	9.9456	5.8789	15.3370
C98	12.5157	8.5038	17.2551
H99	13.7459	8.5208	18.9615
H100	11.1702	10.1119	17.4195
O101	14.0048	8.9138	15.0347
H102	15.6394	8.0219	15.2388
C103	12.6631	3.7889	17.4119
O104	12.5705	2.4774	19.3357
N105	14.2712	3.3505	15.5109
H106	14.2580	4.4711	14.0029
C107	16.6598	2.0825	15.8529
H108	16.5956	0.8371	17.4743
C109	17.3552	0.6142	13.4057
H110	17.7615	1.9672	11.8505
H111	15.7112	-0.5631	12.8426
C112	19.6210	-1.0828	13.7553
C113	22.0777	-0.0775	13.7685
H114	22.3290	1.9464	13.6155
C115	24.1885	-1.6535	14.0463
H116	26.0518	-0.8296	14.0898
C117	23.8559	-4.2670	14.2769

O118	25.9686	-5.8600	14.5622
H119	27.4218	-4.7867	14.6983
C120	19.3168	-3.7152	13.9689
H121	17.4403	-4.5146	13.9424
C122	21.4238	-5.3007	14.2315
H123	21.1801	-7.3189	14.4111
C124	18.5647	4.2519	16.3990
O125	18.3152	6.2833	15.1632
O126	20.2144	3.9306	18.0771

2. Molecular dipole moments

Table S34: aminoacids molecular dipole moments obtained using the database. Values in atomic units.

	μ_x	μ_y	μ_z	$\lvert\mu\rvert$
Gly	3.01	-0.96	-4.19	5.25
Ala	-3.41	-0.08	-3.39	4.81
Asp	-5.15	0.26	-1.44	5.35
Glu	-3.50	-0.34	-3.24	4.78
His	-1.21	-1.99	-3.52	4.22
Ser	-4.28	-0.57	-2.24	4.86
Thr	-2.47	-0.04	-3.58	4.35
Tyr	-4.95	-0.83	-2.16	5.47

Table S35: aminoacids molecular dipole moments obtained by quantum calculations (M06-HF /aug-cc-pVDZ). Values in atomic units.

	μ_x	μ_y	μ_z	$\lvert\mu\rvert$
Gly	2.78	-1.42	-3.85	4.96
Ala	-2.56	-0.14	-3.36	4.23
Asp	-3.81	0.16	-1.34	4.04
Glu	-2.22	-0.38	-2.92	3.68
His	-0.46	-1.43	-3.27	3.60
Ser	-3.15	-0.09	-2.53	4.04
Thr	-1.59	-0.02	-3.32	3.69
Tyr	-2.10	-0.13	-2.72	3.44

Table S36: dipeptides molecular dipole moments obtained using the database. Values in atomic units.

	μ_x	μ_y	μ_z	$\lvert\mu\rvert$
Ala-Ala	-0.32	0.60	-3.22	3.29
Asp-Asp	-7.48	-1.31	-7.15	10.43
Glu-Glu	-8.05	0.63	-3.10	8.65
His-His	-2.47	1.17	-1.63	3.18

Ser-Ser	-6.59	-0.20	-5.23	8.42
Thr-Thr	-5.82	-0.07	-5.43	7.96
Tyr-Tyr	-9.51	0.61	-6.81	11.71
Gly-Gly	-7.99	0.30	-5.37	9.63

Table S37: dipeptides molecular dipole moments obtained by quantum calculations (M06-HF /aug-cc-pVDZ). Values in atomic units.

	μ_x	μ_y	μ_z	$\lvert\mu\rvert$
Ala-Ala	-0.81	-0.31	-2.86	2.99
Asp-Asp	-6.16	-0.87	-6.48	8.98
Glu-Glu	-7.06	1.20	-2.55	7.60
His-His	-2.24	0.39	-1.28	2.61
Ser-Ser	-5.83	-0.34	-4.73	7.52
Thr-Thr	-5.00	0.12	-5.24	7.25
Tyr-Tyr	-6.75	0.37	-4.07	7.89
Gly-Gly	-7.41	0.13	-4.67	8.77

Table S38: tripeptides molecular dipole moments obtained using the database. Values in atomic units.

	μ_x	μ_y	μ_z	$\lvert\mu\rvert$
Ala-Ala-Ala	-10.27	0.68	-8.34	13.25
Asp-Asp-Asp	-10.42	-1.48	-6.50	12.36
Glu-Glu-Glu	-11.03	-0.77	-7.83	13.55
His-His-His	-12.20	1.10	-9.47	15.48
Ser-Ser-Ser	-9.45	0.49	-6.16	11.29
Thr-Thr-Thr	-9.37	0.14	-7.99	12.32
Tyr-Tyr-Tyr	-14.52	-1.39	-9.32	17.31
Gly-Gly-Gly	-11.46	-0.11	-9.16	14.67

Table S39: tripeptides molecular dipole moments obtained by quantum calculations (M06-HF /aug-cc-pVDZ). Values in atomic units.

	μ_x	μ_y	μ_z	$\lvert\mu\rvert$
Ala-Ala-Ala	-10.49	0.98	-9.10	13.92
Asp-Asp-Asp	-9.40	-2.29	-6.50	11.66
Glu-Glu-Glu	-9.98	-0.72	-7.66	12.61
His-His-His	-11.47	1.00	-9.88	15.18
Ser-Ser-Ser	-10.30	-0.06	-8.46	13.33
Thr-Thr-Thr	-9.24	-0.17	-8.09	12.28
Tyr-Tyr-Tyr	-9.00	-0.18	-9.22	12.89
Gly-Gly-Gly	-11.08	0.00	-9.33	14.48

Table S40: polypeptides molecular dipole moments obtained using the database. Values in atomic units.

	μ_x	μ_y	μ_z	$\|\mu\|$
1	-10.11	21.40	-3.86	23.99
2	16.11	-2.78	-6.52	17.60
3	-20.22	-0.84	-12.60	23.84
4	-12.91	-1.23	-14.99	19.82
5	-19.71	3.81	-14.38	24.70
6	-18.61	2.32	-13.48	23.10
7	-16.88	1.52	-17.07	24.05
8	-36.40	6.90	0.86	37.06

Table S41: polypeptides molecular dipole moments obtained by quantum calculations (M06-HF /aug-cc-pVDZ). Values in atomic units.

	μ_x	μ_y	μ_z	$\|\mu\|$
1	-9.75	23.26	-3.33	25.44
2	16.20	-3.39	-7.33	18.11
3	-20.57	0.33	-13.76	24.75
4	-14.24	-1.43	-15.37	21.00
5	-18.58	3.67	-13.78	23.42
6	-20.19	1.99	-15.52	25.54
7	-16.71	0.79	-17.40	24.14
8	-40.88	7.24	0.79	41.53

3. Molecular polarizabilities

Table S42: aminoacids molecular polarizabilities obtained using the database. Values in atomic units.

	α_{xx}	α_{yy}	α_{zz}	α_{xy}	α_{xz}	α_{yz}	α_{iso}	α_{11}	α_{22}	α_{33}	$\Delta\alpha$
Gly	43.7	42.0	47.7	4.0	-11.8	0.4	44.5	32.5	42.8	58.0	22.2
Ala	66.0	45.6	57.5	3.2	4.1	-3.1	56.4	44.1	57.3	67.8	20.6
Asp	86.4	59.0	78.9	1.8	3.7	-7.8	74.7	56.0	80.3	88.0	28.9
Glu	102.6	78.2	82.4	0.8	2.2	-10.6	87.8	69.4	91.1	102.9	29.4
His	91.1	99.5	112.2	-3.5	-3.8	15.1	100.9	89.0	90.8	123.0	33.2
Ser	74.7	50.2	60.2	3.1	4.4	-2.3	61.7	49.1	59.9	76.2	23.6
Thr	83.7	59.2	76.6	4.4	4.0	-1.4	73.2	58.2	75.3	86.0	24.2
Tyr	166.7	94.6	125.7	6.1	-5.5	11.0	129.0	90.4	128.9	167.7	66.9

Table S43: aminoacids molecular polarizabilities obtained by quantum calculations (M06-HF /aug-cc-pVDZ). Values in atomic units.

	α_{xx}	α_{yy}	α_{zz}	α_{xy}	α_{xz}	α_{yz}	α_{iso}	α_{11}	α_{22}	α_{33}	$\Delta\alpha$
Gly	42.4	45.6	46.2	3.1	-9.0	0.3	44.8	34.6	45.8	53.9	16.8
Ala	61.8	46.5	59.2	1.1	1.7	-2.1	55.9	46.1	58.8	62.6	15.0
Asp	81.7	58.3	77.3	3.0	-4.3	-8.9	72.4	54.7	76.1	86.4	28.0

Glu	97.0	76.5	84.3	4.4	-6.5	-10.8	86.0	69.0	86.2	102.7	29.2
His	94.1	86.3	120.4	-4.1	-8.2	9.9	100.3	83.3	91.9	125.6	38.7
Ser	68.5	50.3	61.0	3.0	0.1	-4.5	59.9	48.3	62.5	69.0	18.4
Thr	79.9	60.5	76.5	2.2	-1.7	-4.0	72.3	59.4	76.2	81.3	19.9
Tyr	164.7	90.4	128.5	2.7	-13.0	11.1	127.8	86.9	127.7	168.9	71.0

Table S44: dipeptides molecular polarizabilities obtained using the database. Values in atomic units.

	α_{xx}	α_{yy}	α_{zz}	α_{xy}	α_{xz}	α_{yz}	α_{iso}	α_{11}	α_{22}	α_{33}	$\Delta\alpha$
Ala-Ala	107.4	104.0	101.7	-13.1	2.2	-5.4	104.3	91.7	101.0	120.3	25.3
Asp-Asp	164.8	116.2	142.1	6.0	14.4	-3.9	141.0	114.1	136.9	172.0	50.5
Glu-Glu	181.1	148.0	172.1	0.4	4.8	-9.2	167.1	144.8	172.8	183.5	34.6
His-His	196.6	171.2	212.5	-2.6	-6.8	-24.2	193.4	159.3	196.4	224.6	56.7
Ser-Ser	126.5	99.9	118.6	-2.0	18.6	-5.2	115.0	97.9	104.9	142.1	41.2
Thr-Thr	156.3	112.1	145.2	4.8	12.4	-4.1	137.9	110.7	138.6	164.4	46.5
Tyr-Tyr	283.2	208.1	257.2	-18.8	45.0	11.8	249.5	193.3	237.6	317.7	109.2
Gly-Gly	102.0	54.8	84.7	-3.4	16.1	1.1	80.5	54.4	75.4	111.7	50.2

Table S45: dipeptides molecular polarizabilities obtained by quantum calculations (M06-HF /aug-cc-pVDZ). Values in atomic units.

	α_{xx}	α_{yy}	α_{zz}	α_{xy}	α_{xz}	α_{yz}	α_{iso}	α_{11}	α_{22}	α_{33}	$\Delta\alpha$
Ala-Ala	102.9	95.0	103.4	-2.2	6.0	-2.5	100.5	94.3	97.2	109.9	14.3
Asp-Asp	150.5	111.0	154.6	3.5	10.8	-10.4	138.7	107.8	144.1	164.2	49.5
Glu-Glu	170.0	142.8	185.0	3.3	0.7	-18.9	165.9	135.3	170.3	192.2	49.7
His-His	185.8	158.0	228.7	0.9	-9.2	-14.1	190.8	155.2	184.0	233.2	68.3
Ser-Ser	119.2	93.3	123.7	-1.0	16.0	-8.0	112.1	91.0	106.7	138.6	42.0
Thr-Thr	143.7	112.2	155.2	2.7	10.8	-9.2	137.0	109.6	138.9	162.6	46.0
Tyr-Tyr	259.5	198.9	272.3	-17.4	32.7	4.7	243.6	191.8	239.1	299.8	93.7
Gly-Gly	101.2	56.9	83.2	-3.2	13.8	0.2	80.4	56.7	75.9	108.8	45.7

Table S46*:* tripeptides molecular polarizabilities obtained using the database. Values in atomic units.

	α_{xx}	α_{yy}	α_{zz}	α_{xy}	α_{xz}	α_{yz}	α_{iso}	α_{11}	α_{22}	α_{33}	$\Delta\alpha$
Ala-Ala-Ala	181.1	118.2	157.5	9.6	23.9	-8.7	152.3	112.9	147.8	196.1	72.4
Asp-Asp-Asp	237.9	185.0	198.9	7.4	33.4	5.6	207.3	179.4	184.1	258.3	76.6
Glu-Glu-Glu	280.6	203.4	255.0	3.8	10.9	-15.8	246.4	198.5	255.9	284.7	76.1
His-His-His	307.1	254.5	296.0	-28.7	17.6	-4.1	285.9	241.6	286.7	329.3	75.9
Ser-Ser-Ser	193.6	142.2	168.9	2.8	22.6	-8.5	168.2	137.8	159.8	207.1	61.3
Thr-Thr-Thr	229.1	168.0	210.8	0.1	19.4	0.6	202.6	167.9	198.6	241.4	63.9
Tyr-Tyr-Tyr	445.9	309.6	354.8	2.0	47.5	39.8	370.1	283.0	359.0	468.1	161.2
Gly-Gly-Gly	149.5	75.7	124.3	-0.8	26.8	2.9	116.5	75.4	107.6	166.5	80.0

Table S47: tripeptides molecular polarizabilities obtained by quantum calculations (M06-HF /aug-cc-pVDZ). Values in atomic units.

	α_{xx}	α_{yy}	α_{zz}	α_{xy}	α_{xz}	α_{yz}	α_{iso}	α_{11}	α_{22}	α_{33}	$\Delta\alpha$
Ala-Ala-Ala	185.1	118.2	161.1	6.4	27.8	-8.4	154.8	114.3	146.7	203.4	78.1
Asp-Asp-Asp	229.3	178.7	204.0	-0.2	27.1	1.0	204.0	178.6	186.8	246.6	64.3
Glu-Glu-Glu	275.7	199.5	264.5	12.3	-1.7	-21.3	246.6	191.6	268.1	280.0	83.1
His-His-His	307.2	237.9	313.0	-20.2	3.9	-0.7	286.0	232.4	308.9	316.8	80.7
Ser-Ser-Ser	186.3	139.9	170.3	6.1	22.8	-8.5	165.5	134.4	159.7	202.5	59.6
Thr-Thr-Thr	235.6	164.9	213.2	3.3	21.5	-9.3	204.6	162.3	202.6	248.7	74.9
Tyr-Tyr-Tyr	448.4	278.0	367.6	-2.0	45.4	21.0	364.7	272.5	352.5	469.1	171.2
Gly-Gly-Gly	147.7	79.2	124.3	-0.8	25.8	0.8	117.1	79.2	107.8	164.4	75.1

Table S48: polypeptides molecular polarizabilities obtained using the database. Values in atomic units.

	α_{xx}	α_{yy}	α_{zz}	α_{xy}	α_{xz}	α_{yz}	α_{iso}	α_{11}	α_{22}	α_{33}	$\Delta\alpha$
1	281.8	345.6	246.2	-43.2	29.3	0.4	291.2	225.2	279.7	368.8	125.6
2	378.6	336.5	336.1	13.6	-33.0	-24.7	350.4	307.8	338.2	405.1	86.2
3	466.4	368.1	413.8	8.9	39.1	-0.2	416.1	366.9	393.7	487.7	109.9
4	341.6	326.4	373.8	-19.6	52.2	-9.0	347.3	298.7	326.8	416.4	106.5
5	480.7	354.6	425.5	-13.1	56.7	-23.8	420.3	347.2	394.0	519.7	154.4
6	346.0	233.8	328.8	-2.1	36.4	-6.4	302.9	233.4	300.2	375.0	122.7
7	411.9	371.2	437.0	0.8	55.7	-2.8	406.7	366.2	372.3	481.6	112.5
8	687.6	622.8	598.7	-32.7	-3.8	13.0	636.4	591.7	615.5	701.9	100.4

Table S49: polypeptides molecular polarizabilities obtained by quantum calculations (M06-HF /aug-cc-pVDZ). Values in atomic units.

	α_{xx}	α_{yy}	α_{zz}	α_{xy}	α_{xz}	α_{yz}	α_{iso}	α_{11}	α_{22}	α_{33}	$\Delta\alpha$
1	277.9	350.1	244.7	-42.8	32.9	-1.5	290.9	220.4	280.3	372.0	132.2
2	374.6	339.9	320.1	8.3	-48.0	-23.1	344.8	287.1	339.5	407.9	104.9
3	492.3	353.1	410.1	16.4	41.9	-3.8	418.5	349.7	394.8	511.1	144.3
4	351.4	305.2	389.9	-12.7	58.6	-9.7	348.8	300.8	311.5	434.2	128.3
5	493.5	337.7	433.2	-1.8	61.0	-43.3	421.5	318.3	411.6	534.6	187.9
6	354.0	230.3	329.4	7.1	40.3	-10.8	304.6	228.0	301.8	383.9	135.1
7	410.8	351.7	446.9	11.6	60.0	-15.0	403.1	339.2	378.5	491.7	137.1
8	740.1	612.7	563.1	-50.3	-18.3	17.8	638.6	557.3	598.2	760.3	185.9

4. Molecular Dynamics

Table S50: glycine molecular polarizabilities (au) and dipole moments (au) obtained after molecular dynamics.

Time(ps)	μ_x	μ_y	μ_z	α_{xx}	α_{yy}	α_{zz}	α_{xy}	α_{xz}	α_{yz}
0	-5.40	-1.94	-2.55	48.5	50.6	35.7	2.3	4.7	1.9

20	3.76	-2.83	4.42	44.5	42.9	47.2	0.4	3.7	-6.9
40	3.39	1.66	5.21	42.2	45.8	46.1	-2.6	8.1	2.2
60	-3.87	-5.25	2.15	48.4	43.5	43.3	0.3	3.5	-6.4
80	-1.89	-5.24	0.51	40.1	48.6	46.6	0.3	-4.6	2.8
100	1.32	-5.40	-3.27	53.6	39.6	44.6	-1.3	5.7	5.3
120	5.63	-2.64	0.17	51.1	37.4	47.9	-4.9	-4.1	-4.0
140	-5.95	0.23	2.90	49.8	32.3	54.6	-1.9	-3.1	0.7
160	-2.50	-5.19	0.52	46.3	49.5	37.4	-2.3	0.9	-6.2
180	3.78	-4.70	0.94	49.2	47.6	36.6	0.0	1.7	-0.2
200	4.47	-4.14	1.05	40.8	44.4	49.6	-3.8	-5.9	-6.8
220	-3.03	-5.25	2.36	41.2	46.2	47.6	0.4	-8.5	1.6
240	-1.68	5.25	2.75	36.4	49.5	49.1	-4.6	3.1	1.0
260	-2.09	4.04	4.01	44.9	39.1	49.5	-6.0	3.0	3.7
280	3.15	5.06	0.01	36.6	46.5	51.5	7.0	-0.4	-2.2
300	-2.08	5.98	-0.09	34.5	48.9	53.3	-2.8	-2.7	1.6
320	0.80	5.91	-2.92	46.2	46.2	41.2	-2.9	-4.4	-5.3
340	-5.24	1.65	-1.97	44.7	45.3	44.2	-5.7	1.5	5.1
360	-2.36	-0.80	-5.95	41.7	43.0	48.7	6.5	3.7	-3.3
380	-1.90	-5.79	-1.43	37.7	48.0	50.5	3.1	5.0	-4.8
400	-5.40	-1.94	-2.55	48.5	50.6	35.7	2.3	4.7	1.9