SUPPLEMENTARY DATA

Sculpting the β-peptide foldamer H12 helix via a designed side chain shape

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Materials and methods

Peptide synthesis. Peptide oligomers containing three (**1**), four (**2**), five (**3**) or six (**4**) *trans*-ABHC units were synthetized by a solid-phase technique, utilizing Fmoc chemistry. The peptide chains were elongated on a Tentagel R RAM resin (0.17 $mmolg^{-1}$), and the syntheses were carried out manually on a 0.3-mmol scale. Couplings were performed with the uronium reagent, HATU, without difficulty. The amino acid incorporation was monitored by means of the ninhydrin test and by the cleavage of aliquots from the resin. The peptide sequences were cleaved from the resign with 95 % TFA + 5 % H_2O at 25 °C for 3 h. The TFA was removed, and the resulting free peptides were solubilized in 10 % aqueous acetic acid, filtered, and lyophilized. The crude peptides were purified by reverse-phase HPLC, using a Phenomenex 10 μ column (10 mm x 250 mm). The solvent system used was as follows: 0.1% TFA in water (A), 0.1% TFA in MeCN (B); the gradient was 0%→50% B during 15 min, then 50%→80% during 60 min, at a flow rate of 4 $mLmin^{-1}$, with detection at 206 nm. The appropiate fractions were pooled and lyophilized. The peptides were characterized by MS, using a Finnigan MAT 95S double focusing mass spectrometer equipped with an electrospray ion source. The measured molecular weights were as follows: **1** m/z(M+H)=513.8, **2** m/z(M+H)=649.1, **3** m/z(M+H)=844.2, **4** m/z(M+H)=1009.8.

NMR experiments. NMR measurements were performed on a Bruker Avance III 600 MHz spectrometer with a triple resonance 2.5-mm capillary probe with z-gradient coil in 4 mM CD_3OH or DMSO-d_6 solution at 298.1 K. The ROESY measurements in CD_3OH were performed with the WATERGATE solvent suppression scheme. For the ROESY spinlock, a mixing time of 225 ms was used, the number of scans being 64. The TOCSY measurements were performed with homonuclear Hartman-Hahn transfer with the MLEV17 sequence, with a mixing time of 80 ms, the number of scans being 32. For all the 2D spectra, 2K time domain points and 512 increments were applied. The processing was carried out by using a cosine-bell window function, single zero filling, and automatic baseline correction. The DOSY (PFGSE) NMR measurements were performed by using the stimulated echo and longitudinal eddy current delay sequence. A time of 2.0 ms was used for the dephasing/refocusing gradient pulse length (δ), and 250 ms for the diffusion delay (Δ). The gradient strength was changed quadratically from 5 % to 95 % of the maximum value (10 A gradient amplifier); and the number of steps was 32. Each measurement was run with 256 scans and 2K time domain points. For the processing, an exponential window function and single zero filling were applied. During the diffusion measurements, the fluctuation of the temperature was less than 0.1 K. Prior to the NMR scans, all the samples were equilibrated for 30 min. DOSY spectra were processed and evaluated by using the exponential fit implemented in Topspin 2.0.

ECD experiments. Spectra were measured on a Jobin-Yvon Mark VI dichrograph at 25 °C in a 0.02-cm cell. Four spectra were accumulated for each sample. The baseline spectum recorded with only the solvent was subtracted from the raw data. The concentration of the sample solutions was 4 mM in CD_3OH. Molar ellipticity, [Θ], is given in deg cm^2 $dmol^{-1}$. The data were normalized for the number of chromophores.

Modeling. Molecular mechanical simulations were carried out in the Chemical Computing Group's Molecular Operating Environment (MOE). For the energy calculations, the MMFF94x force field was used, without cutoff for van der Waals and Coulomb interactions and the dielectric constant was set to 30. The conformational sampling was carried out by using the hybrid molecular dynamics (MD) – Monte Carlo (MC) simulation (as implemented in MOE) at 300 K with a random Monte Carlo sampling step after every 10 MD steps. The MD-MC was run for 4 ns with a step size of 2 fs, and the conformations were saved after every 1000 MD steps (2000 structures). The resulting structures were minimized to a gradient of 0.05 kcal/mol and the minimization was applied in a cascade manner, using the steepest-descent, conjugate gradient and truncated Newton algorithm. For the NMR restrained simulation, the distance restraints were applied as a flat-bottomed quadratic penalty term with a force constant of 10 kcal/$Å^2$ and ±20% of the experimental distances for lower and upper limits.
The cluster analysis was carried out on the basis of the root mean square deviation of heavy atoms (RMSD) from the lowest energy conformation and the relative conformational energies.
For the *ab initio* calculations**,** the molecular structure, stereochemistry and geometry of the ABHC oligomers were exclusively defined in terms of their z-matrix internal coordinate system. The optimizations were carried out in with the Gaussian03 program: first optimization by using the HF/3-21G level of theory, and then, single point calculation by using density-functional theory at the B3LYP/6-311G** level with a default set-up.

Supporting Table-01. NMR signal assignment for **4** in DMSO-d_6 (ppm)

i	**NH**	**H-1**	**H-2 (β)**	**H-3 (α)**	**H-4**	**H-4**	**H-5**	**C-6-Me(ax)**	**C-6-Me(eq)**	**H-7**	**H-7**
1	7.95	2.01	3.82	2.69	1.61	2.17	1.98	0.90	1.24	1.51	2.22
2	8.70	1.86	4.14	2.53	1.96	2.12	1.95	1.06	1.21	1.38	2.20
3	8.15	1.84	4.19	2.47	1.86	2.06	1.86	1.02	1.19	1.29	2.12
4	8.81	1.65	4.21	2.63	1.70	2.11	1.82	1.05	1.12	1.31	1.95
5	9.09	1.65	4.24	2.49	1.63	2.24	1.82	0.99	1.14	1.49	1.96
6	8.73	1.68	4.36	2.51	1.68	2.13	1.86	0.99	1.14	1.60	1.95
7	7.91, 6.67										

Supporting Table-02. NMR signal assignment of the backbone for **4** in CD_3OH (ppm)

i	**NH**	**H-2 (β)**	**H-3 (α)**
1	8.19	4.06	2.77
2	8.33	4.34	2.66
3	7.84	4.34	2.68
4	8.66	4.34	2.83
5	9.24	4.40	2.72
6	9.20	4.55	2.78
7	8.38, 6.41		

Supporting Table-03. ^3J (NH_i-$C^{\beta}H_i$) values in DMSO-d_6

i	**1**	**2**	**3**	**4**
2	7.40	7.48	7.25	7.03
3	8.07	8.71	8.50	8.55
4	-	8.88	9.45	9.07
5	-	-	9.25	9.50
6	-	-	-	9.25

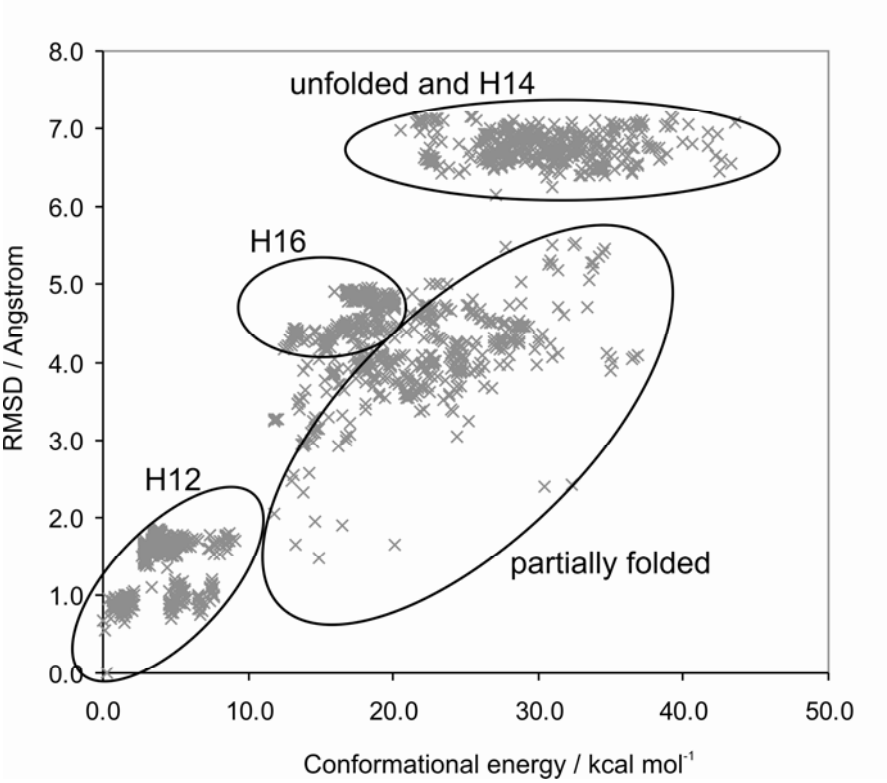
Supporting Table-04. ^3J (NH_i-$C^{\beta}H_i$) values in CD_3OH

i	**1**	**2**	**3**	**4**
2	7.20	7.98	7.73	6.83
3	7.90	8.38	8.07	7.82
4	-	8.26	9.06	8.68
5	-	-	9.10	9.23
6	-	-	-	9.04

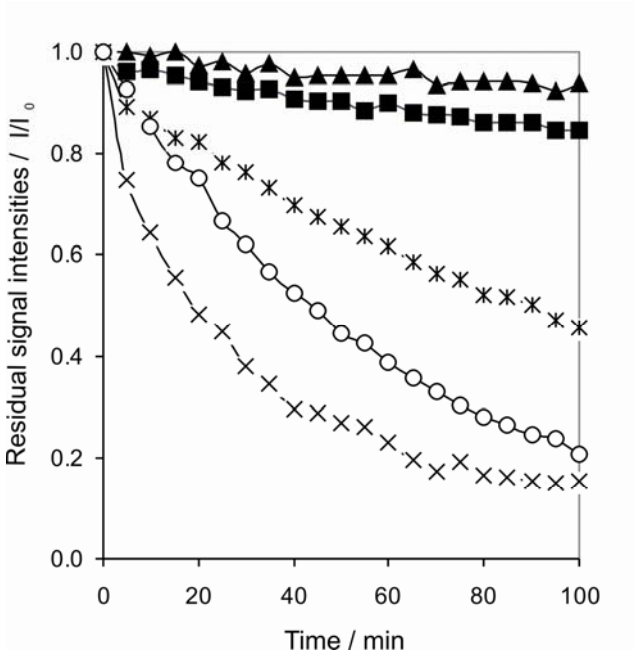
Supporting Table-05. NMR distances for **4** estimated from the ROESY spectrum in DMSO

Atom	Atom	Estimated distance[a]
NH5	CβH5	2.75
NH5	CαH4	2.13
NH5	CβH3	2.80
NH5	CαH5	2.58
NH5	CγH5	2.69
NH5	CH_2-bridge5	2.66
NH5	Me2	3.23
NH4	CβH4	2.72
NH4	CβH1	3.79
NH4	CβH2	2.91
NH4	CαH4	2.61
NH4	CαH3	2.08
NH4	CγH4	2.46
NH4	CH_2-bridge4	2.84
NH4	Me1	3.23
NH6	CβH6	2.75
NH6	CβH5	2.92
NH6	CβH4	[b]
NH6	CαH5	2.03
NH6	CγH6	2.50
NH6	Me3	3.37
NH2	CβH2	2.88
NH2	CαH1	2.12
NH2	CαH2	2.48
NH2	CγH2	2.28
NH2	CH_2-bridge2	2.63
NH3	CβH3	2.92
NH3	CαH2	2.04
NH3	CγH3	2.46
NH3	CH_2-bridge3	2.72
NH1	CβH1	2.54
NH1	CαH1	2.70
NH1	CγH1	2.65
NH1	CH_2-bridge1	3.53
NH7a	CβH6	4.13
NH7a	CβH5	3.02
NH7a	CαH6	2.47
NH7a	Me4	3.95
NH7b	CβH6	4.79
NH7b	CβH5	4.12
NH7b	CαH6	4.19
CβH1	CαH3	2.67
CβH2	CαH4	2.53

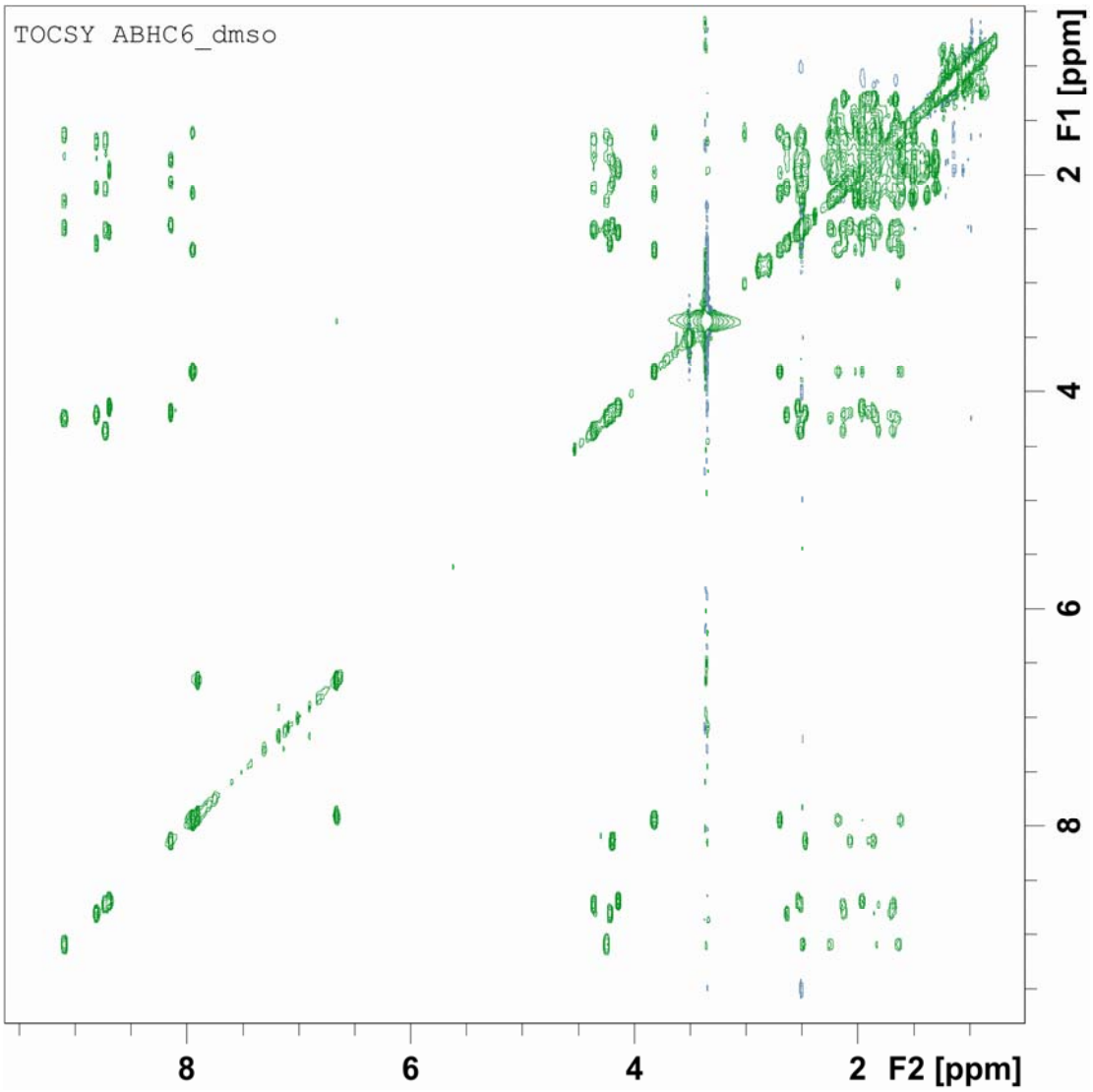
[a] Calculated by using the isolated spin-pair approximation and offset compensation
[b] Accurate integration was not possible due to overlap



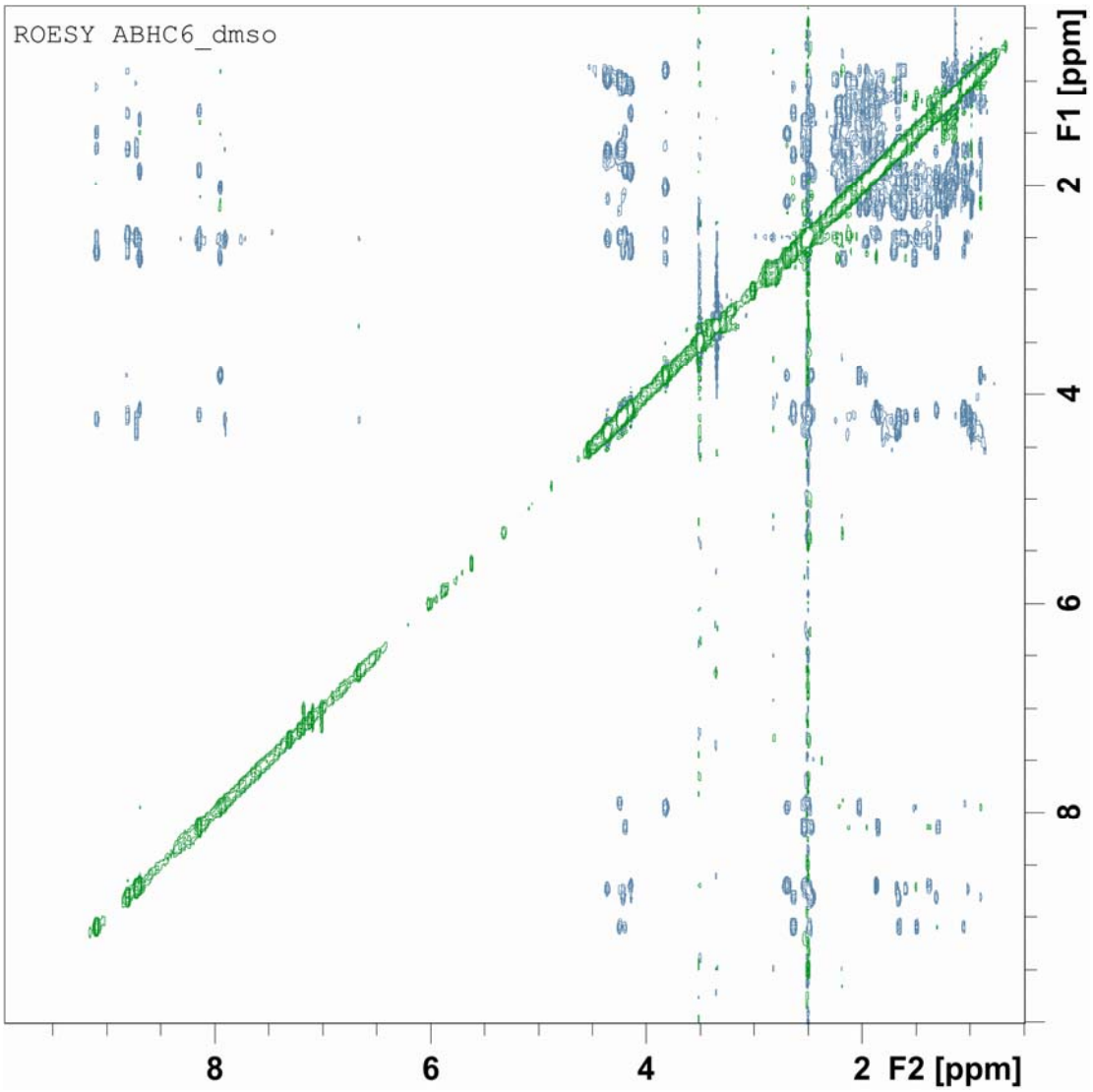
Supporting Figure-1 Cluster analysis of the unrestrained conformational sampling for **4** (2000 conformers) carried out by using MMFF94x force-field and the hybrid MD-MC algorithm. RMSD was calculated with the lowest energy H12 helix conformer as the reference structure. The conformational energies are referenced to the the lowest energy conformer.



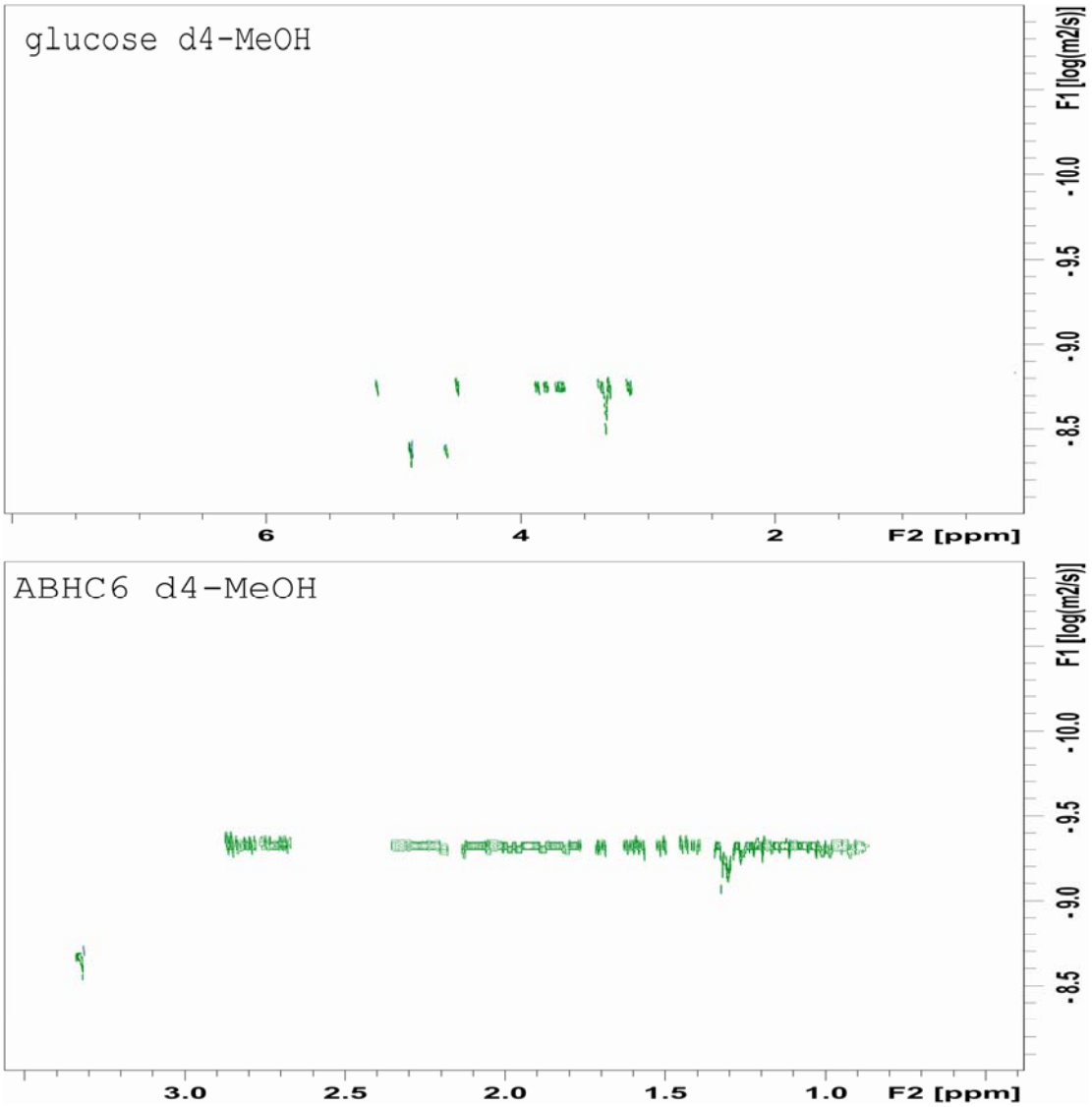
Supporting Figure-2 Time dependence of the NH/ND exchange for **4** in CD_3OD, * : NH_2; ○ : NH_3; ▲: NH_4; ■ : NH_5; x : NH_6.



Supporting Figure-03. TOCSY spectrum of **4** in DMSO-d_6.



Supporting Figure-04. ROESY spectrum of **4** in DMSO-d_6.



Supporting Figure-05. DOSY spectrum of glucose (top) and **4** (bottom) in CD_3OD.

Supporting Table-06 Aggregation numbers in CD_3OD, based on DOSY NMR measurements.

Compound	Calculated volume Å^3	Calculated radius Å	Diffusion constant x10^{-9} m^{2}s^{-1}	Measured radius Å	Aggregation number
glucose[a]	506.83	4.95	2.08	-[b]	1
3	2140.14	7.99	0.63	16.4	8.6
4	2513.36	8.43	0.51	20.3	13.9

a external reference, b not applicable

Computational data
(at the B3LYP/6-311G** level):

4: H8
B3LYP/6-311G**: -3177.796867 a. u.

C	9.2917	0.2515	0.9646
H	8.4925	0.6392	1.5802
N	9.8034	1.4115	0.19
H	10.6259	1.1787	-0.3447
H	9.9873	2.2134	0.7709
C	10.3297	-0.4178	1.8679
H	10.8794	0.314	2.4457
C	11.1304	-1.4798	1.0447
H	11.3169	-1.2689	0.0001
H	12.0575	-1.7583	1.5204
C	9.6673	-1.6059	2.6528
C	10.541	-2.0443	3.8388
H	10.1912	-2.9971	4.2231
H	10.477	-1.3136	4.6391
H	11.5825	-2.1544	3.5667
C	8.2186	-1.4715	3.1355
H	7.8962	-2.4106	3.5745
H	7.5203	-1.2259	2.3485
H	8.1535	-0.7068	3.9042
C	9.9567	-2.4616	1.3717
H	10.188	-3.5069	1.5188
C	8.8444	-2.2612	0.3368
H	7.8985	-2.6229	0.7083
H	9.076	-2.8368	-0.5534
C	8.7159	-0.7714	-0.0704
H	9.2794	-0.6172	-0.9812
C	7.2789	-0.3786	-0.3778
O	6.3259	-1.1348	-0.163
N	7.1421	0.8569	-0.8665
H	7.9744	1.4217	-0.8876
C	5.8682	1.463	-1.292
H	5.3243	0.7196	-1.8571
C	6.2682	2.6341	-2.1964
C	6.8334	3.7774	-1.2861
H	7.3231	3.4826	-0.3685
H	7.4646	4.4667	-1.8239
H	6.8743	2.2775	-3.0176
C	5.0706	3.5787	-2.5453
C	3.691	2.9858	-2.8407
H	2.9994	3.7848	-3.0903
H	3.2666	2.4498	-2.0103
H	3.7512	2.3224	-3.699
C	5.4516	4.5096	-3.7109
H	6.4321	4.9505	-3.592
H	4.7278	5.3141	-3.7886
H	5.4418	3.9558	-4.6447
C	5.3539	4.2529	-1.1595
H	5.1589	5.3128	-1.075
C	4.7044	3.4718	-0.014
H	5.0885	3.8626	0.9226
H	3.6362	3.6172	-0.0095
C	4.988	1.9344	-0.0647
H	5.5459	1.658	0.8202
C	3.6613	1.1538	0.0336
O	2.5736	1.7471	0.0989
N	3.7467	-0.1714	0.0613
H	4.6561	-0.61	0.0004
C	2.583	-1.0627	0.261
H	1.9569	-0.6201	1.0225
C	3.1741	-2.3872	0.7561
C	2.13	-3.5539	0.7778
C	2.6748	-4.7338	1.6033
H	3.7046	-4.9668	1.3688
H	2.0769	-5.6197	1.4156
H	2.6134	-4.5035	2.6627
C	0.6895	-3.2882	1.2218
H	0.6804	-2.9111	2.2409
H	0.1291	-4.2183	1.21
H	0.165	-2.5973	0.586
H	3.7539	-2.223	1.6535
C	3.8635	-3.0998	-0.4552
H	4.2826	-2.4678	-1.2218
H	4.607	-3.8157	-0.1452
C	2.465	-3.7196	-0.7437
H	2.4132	-4.7179	-1.1565
C	1.6832	-2.721	-1.6019
H	2.104	-2.7362	-2.602
H	0.6481	-3.0107	-1.6832
C	1.7375	-1.2523	-1.0633
H	2.2154	-0.6304	-1.8089
C	0.3038	-0.6959	-0.9325
O	-0.682	-1.3912	-1.2245
N	0.1809	0.5592	-0.516
H	1.0133	1.0831	-0.2799
C	-1.1117	1.2724	-0.445
H	-1.6837	1.0043	-1.3217
C	-1.936	0.8912	0.851
H	-1.3431	0.1476	1.3672
C	-2.2041	2.0814	1.8314
H	-3.2688	2.1615	1.9793
H	-1.7602	1.8421	2.7923
C	-1.616	3.4131	1.3565
H	-1.8119	4.2052	2.0665
C	-0.1465	3.1494	0.9151
H	0.4636	4.0367	0.8675
H	0.3914	2.381	1.4469
C	-0.7517	2.7618	-0.4755
C	-1.9671	3.692	-0.1447
C	-3.3608	3.3563	-0.6813
H	-4.0603	4.1326	-0.3855
H	-3.7505	2.425	-0.3104
H	-3.3415	3.3264	-1.7674
C	-1.6414	5.145	-0.536
H	-2.3656	5.8171	-0.0869
H	-1.6985	5.2592	-1.6145
H	-0.6544	5.4518	-0.217
H	-0.1808	2.9875	-1.3652
C	-3.2678	0.1857	0.5179
O	-4.3403	0.5829	0.9996

N	-3.2062	-0.8706	-0.2848
C	-4.3737	-1.7203	-0.6018
H	-4.9592	-1.8219	0.3006
H	-2.3113	-1.149	-0.6659
C	-5.277	-1.0963	-1.7415
H	-4.8164	-0.1503	-1.9942
C	-5.3817	-1.9617	-3.0413
H	-6.4249	-2.1569	-3.2296
H	-5.0045	-1.3776	-3.8746
C	-4.5828	-3.2666	-2.9781
H	-4.6713	-3.8272	-3.899
C	-3.1616	-2.9241	-2.4431
H	-2.7621	-1.9577	-2.705
H	-2.4203	-3.6785	-2.6511
C	-3.7855	-3.0739	-1.0151
H	-3.1648	-3.4664	-0.2219
C	-4.8494	-4.0377	-1.6405
C	-6.2642	-4.1002	-1.0604
H	-6.8428	-4.8486	-1.594
H	-6.802	-3.1723	-1.1396
H	-6.2232	-4.3983	-0.0163
C	-4.2923	-5.4718	-1.6996
H	-4.9146	-6.0806	-2.3478
H	-4.3043	-5.914	-0.7078
H	-3.2779	-5.5104	-2.0729
C	-6.6961	-0.7362	-1.2461
O	-7.7019	-1.1395	-1.8504
N	-6.7773	0.0391	-0.1686
H	-5.9286	0.3118	0.3082
C	-8.0523	0.5808	0.351
H	-8.7014	0.736	-0.4976
C	-8.7499	-0.4059	1.3678
H	-8.0949	-1.265	1.4355
C	-8.9666	0.1701	2.8041
H	-10.0205	0.1165	3.0271
H	-8.452	-0.4691	3.5146
C	-8.4357	1.5954	2.9787
H	-8.5874	1.9538	3.9883
C	-8.9082	2.5251	1.81
C	-10.3351	2.401	1.2689
H	-10.4044	2.8778	0.2947
H	-11.0212	2.914	1.9368
H	-10.6779	1.3842	1.1865
C	-8.6408	4.0075	2.1271
H	-7.6365	4.1813	2.4898
H	-9.3381	4.3529	2.8839
H	-8.7865	4.6088	1.2343
C	-7.7059	1.9213	1.0059
C	-7.0008	1.6419	2.3756
H	-6.4095	0.7441	2.4506
H	-6.4121	2.4798	2.7144
H	-7.2105	2.5672	0.2943
C	-10.0861	-0.9556	0.8284
O	-11.1176	-0.928	1.4931
N	-10.0424	-1.4818	-0.4048
H	-9.2279	-1.4415	-0.9969
H	-10.8934	-1.854	-0.7693

4: H12

B3LYP/6-311G**: -3177.817811 a. u.

C	-6.6381	-1.0047	0.0249
H	-6.2164	-0.7348	-0.9327
N	-7.4665	0.1563	0.4419
H	-7.9764	-0.0256	1.2924
H	-8.1001	0.4583	-0.2805
C	-7.42	-2.3135	-0.1248
H	-8.3369	-2.1628	-0.6799
C	-7.4907	-3.0384	1.26
H	-8.2654	-3.7879	1.2942
H	-7.5538	-2.4236	2.1474
C	-6.4636	-3.4592	-0.6113
C	-7.2584	-4.6649	-1.1384
H	-7.6873	-4.4338	-2.1086
H	-8.0637	-4.9512	-0.4751
H	-6.5996	-5.5193	-1.2552
C	-5.3541	-3.1332	-1.6167
H	-5.7893	-2.88	-2.5792
H	-4.7231	-4.0055	-1.756
H	-4.718	-2.3166	-1.305
C	-6.0869	-3.63	0.9011
H	-5.8484	-4.6279	1.2398
C	-5.0071	-2.6162	1.2969
H	-4.762	-2.7397	2.3463
H	-4.0974	-2.7877	0.743
C	-5.4992	-1.1629	1.0824
H	-5.9172	-0.8104	2.0173
C	-4.3591	-0.2101	0.7543
O	-3.1849	-0.5776	0.6385
N	-4.7258	1.0645	0.604
H	-5.7115	1.2675	0.6412
C	-3.7572	2.1464	0.3794
H	-2.9138	1.973	1.0278
C	-4.4448	3.4689	0.7341
C	-5.2215	3.9863	-0.5231
H	-5.9701	4.7214	-0.2746
H	-5.6532	3.2461	-1.1824
H	-4.9678	3.3872	1.6765
C	-3.4623	4.676	0.5578
C	-4.0122	5.9388	1.2427
H	-3.9226	5.8439	2.3201
H	-5.0515	6.1253	1.0063
H	-3.4358	6.804	0.9318
C	-1.9933	4.5078	0.9551
H	-1.5256	3.6355	0.5278
H	-1.9159	4.4388	2.0366
H	-1.4298	5.381	0.6398
C	-3.8627	4.6293	-0.9583
H	-3.8845	5.568	-1.4935
C	-3.0266	3.5753	-1.6924
H	-1.9787	3.8308	-1.6265
H	-3.2945	3.5579	-2.7435
C	-3.267	2.1423	-1.1047
H	-4.0479	1.6706	-1.6808
C	-1.9804	1.35	-1.248

O	-0.9855	1.618	-0.5653
N	-1.9605	0.4163	-2.2009
H	-2.7983	0.2068	-2.699
C	-0.7854	-0.424	-2.4936
H	0.0885	0.1912	-2.3603
C	-0.8996	-0.8891	-3.9489
C	0.3202	-1.7867	-4.349
C	1.7138	-1.4294	-3.8268
H	2.4151	-2.211	-4.1041
H	1.7585	-1.3092	-2.7566
H	2.0509	-0.5065	-4.2908
C	0.398	-1.9557	-5.8761
H	-0.5562	-2.2077	-6.3204
H	1.1018	-2.7446	-6.1203
H	0.7516	-1.0365	-6.3322
H	-1.14	-0.0588	-4.5986
C	-1.7927	-2.1766	-3.996
H	-2.5937	-2.2601	-3.2736
H	-2.1785	-2.3785	-4.9826
C	-0.4763	-2.9621	-3.6832
H	-0.3517	-3.9473	-4.11
C	-0.2521	-2.9637	-2.1667
H	0.7956	-3.1116	-1.9504
H	-0.8008	-3.7852	-1.7176
C	-0.7448	-1.6355	-1.5046
H	-1.7519	-1.7717	-1.1494
C	0.1566	-1.3213	-0.3206
O	1.374	-1.1635	-0.4843
N	-0.427	-1.2779	0.8714
H	-1.4294	-1.2345	0.9189
C	0.32	-1.0166	2.1094
H	1.3116	-1.4162	1.9761
C	0.3895	0.5294	2.3596
H	-0.4297	0.9557	1.8072
C	0.2528	0.9299	3.8617
H	1.2311	1.1196	4.2768
H	-0.3125	1.8556	3.9119
C	-0.4634	-0.1516	4.678
H	-0.7512	0.2071	5.6567
C	-1.5535	-0.8239	3.779
H	-2.056	-0.2053	3.0511
H	-2.286	-1.3729	4.3508
C	-0.3956	-1.7381	3.2557
C	0.3404	-1.4973	4.6171
C	1.8707	-1.4614	4.6438
H	2.2986	-0.7631	3.9427
H	2.2616	-2.4518	4.4259
H	2.2093	-1.1858	5.6387
C	-0.1449	-2.4905	5.6868
H	0.2633	-3.4766	5.4879
H	-1.2235	-2.5732	5.723
H	0.202	-2.1737	6.6654
H	-0.6184	-2.7592	2.9802
C	1.6961	1.0895	1.8107
O	2.7614	0.8803	2.409
N	1.5966	1.8194	0.7042
C	2.7185	2.5356	0.0794
H	3.5436	2.488	0.7708
H	0.7098	1.8568	0.2341
C	3.1068	1.8487	-1.2849
H	2.2789	1.2065	-1.5384
C	3.3701	2.8427	-2.453
H	4.4332	2.897	-2.6298
H	2.9075	2.4409	-3.3502
C	2.8023	4.2378	-2.1807
H	2.8436	4.868	-3.0589
C	1.4357	4.0814	-1.4378
H	0.8289	4.9737	-1.4757
H	0.8288	3.2236	-1.6878
C	2.2873	3.9919	-0.1281
H	1.8783	4.3965	0.787
C	3.3997	4.821	-0.8535
C	3.1239	6.3293	-0.7285
H	3.3481	6.6642	0.2797
H	2.0953	6.5857	-0.9479
H	3.7619	6.8771	-1.4151
C	4.8695	4.5636	-0.5104
H	5.5023	5.1709	-1.152
H	5.173	3.5361	-0.6335
H	5.06	4.8625	0.5172
C	4.3366	0.9683	-1.0606
O	5.4751	1.3848	-1.2709
N	4.0757	-0.2592	-0.5927
H	3.1258	-0.563	-0.4741
C	5.1444	-1.2059	-0.2633
H	6.0624	-0.742	-0.5827
C	5.1644	-1.4398	1.2899
H	4.1745	-1.2051	1.6449
C	5.5293	-2.8914	1.7058
H	6.5688	-2.9298	1.9952
H	4.9351	-3.1532	2.5768
C	5.2507	-3.8962	0.5825
H	5.305	-4.919	0.9316
C	6.0921	-3.5302	-0.6899
C	7.5193	-3.0009	-0.5171
H	8.1699	-3.8128	-0.2018
H	7.6045	-2.2079	0.2094
H	7.888	-2.6334	-1.4713
C	6.1174	-4.6893	-1.7008
H	6.5123	-4.3425	-2.6511
H	5.1356	-5.1099	-1.877
H	6.7638	-5.4821	-1.3362
C	4.9364	-2.5229	-1.018
C	3.9721	-3.4395	-0.1963
H	3.5434	-4.2293	-0.7954
H	3.1885	-2.9489	0.3601
H	4.7162	-2.3337	-2.059
C	6.147	-0.4472	1.8935
O	7.3541	-0.6747	1.9266
N	5.598	0.6907	2.3415
H	4.6049	0.8419	2.3538
H	6.21	1.3977	2.6889

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C	-4.978	1.5377	-1.1978
H	-5.4235	0.9028	-1.9471
N	-3.8602	2.2474	-1.8341
H	-3.1264	1.6767	-2.2181
H	-3.4747	2.9673	-1.253
C	-6.0073	2.5779	-0.7418
H	-6.14	3.3213	-1.513
C	-5.6548	3.0491	0.7118
H	-4.612	3.067	0.9901
H	-6.1108	3.9926	0.9701
C	-7.2902	1.9015	-0.1475
C	-8.4455	2.9118	-0.0336
H	-8.1399	3.8484	0.4149
H	-9.2444	2.4926	0.571
H	-8.8457	3.1255	-1.02
C	-7.8293	0.6184	-0.7853
H	-8.2567	0.8508	-1.7572
H	-8.6242	0.2117	-0.1645
H	-7.0797	-0.1441	-0.9236
C	-6.4818	1.8144	1.1932
H	-7.0427	1.893	2.1154
C	-5.5643	0.5856	1.1862
H	-6.1635	-0.3113	1.11
H	-5.0152	0.5351	2.1217
C	-4.5288	0.6342	0.008
H	-3.5941	1.0295	0.3769
C	-4.3207	-0.7886	-0.473
O	-5.2106	-1.3886	-1.0786
N	-3.1544	-1.3845	-0.1688
H	-2.4094	-0.8517	0.2363
C	-2.9325	-2.7762	-0.6043
H	-3.2198	-2.833	-1.6399
C	-3.7915	-3.7679	0.1913
C	-3.0082	-4.2202	1.4593
H	-2.3824	-3.4782	1.9301
H	-3.641	-4.6777	2.2043
H	-4.7994	-3.4022	0.2807
C	-3.5964	-5.2157	-0.3813
C	-3.4565	-5.4186	-1.8943
H	-3.2003	-6.4556	-2.0972
H	-2.711	-4.7889	-2.354
H	-4.4093	-5.2115	-2.3727
C	-4.6907	-6.1661	0.1345
H	-4.423	-7.1944	-0.0904
H	-5.6309	-5.9448	-0.3604
H	-4.8462	-6.0845	1.2026
C	-2.316	-5.2721	0.5246
H	-2.043	-6.2335	0.9389
C	-1.1361	-4.6046	-0.1974
H	-0.2398	-4.6802	0.4105
H	-0.9412	-5.1129	-1.1309
C	-1.4149	-3.097	-0.4703
H	-1.0233	-2.5239	0.3574
C	-0.7551	-2.6501	-1.7616
O	-1.1046	-3.1254	-2.8409
N	0.1736	-1.6866	-1.6721
H	0.4868	-1.3587	-0.7811
C	0.5863	-0.9535	-2.8821
H	-0.3204	-0.7072	-3.4065
C	1.4955	-1.7677	-3.8047
C	1.7928	-0.9258	-5.0957
C	2.3767	-1.8052	-6.2138
H	3.173	-2.4479	-5.8613
H	2.7728	-1.1811	-7.0097
H	1.5974	-2.4342	-6.6317
C	0.6818	-0.0557	-5.696
H	0.2027	0.5956	-4.9799
H	-0.086	-0.6932	-6.1229
H	1.0901	0.5591	-6.4937
H	1.1106	-2.7643	-3.933
C	2.9803	-1.5483	-3.3825
H	3.1727	-1.4405	-2.3251
H	3.6457	-2.2913	-3.7962
C	2.926	-0.2426	-4.2513
H	3.8188	0.065	-4.7802
C	2.3348	0.8975	-3.4093
H	3.1138	1.3829	-2.8325
H	1.8938	1.6437	-4.0577
C	1.2844	0.3319	-2.4047
H	1.8232	0.095	-1.4986
C	0.2481	1.3764	-2.028
O	-0.9015	1.3653	-2.4474
N	0.722	2.3062	-1.1684
H	1.6889	2.2645	-0.9085
C	-0.16	3.1274	-0.3436
H	-1.1619	2.8051	-0.5655
C	0.2242	2.8256	1.1237
H	1.3025	2.7329	1.1185
C	-0.1013	3.9752	2.1174
H	-1.101	3.8869	2.5209
H	0.5905	3.9312	2.954
C	0.0674	5.3296	1.3997
H	0.1462	6.149	2.1007
C	1.1575	5.1954	0.2788
H	1.5075	6.1581	-0.0596
H	2.0063	4.5548	0.4681
C	0.0059	4.6297	-0.622
C	-0.9929	5.4681	0.253
C	-2.409	4.9493	0.4936
H	-2.9912	5.0301	-0.4179
H	-2.8967	5.551	1.2548
H	-2.4386	3.9195	0.8154
C	-1.0982	6.9201	-0.2464
H	-0.1329	7.3709	-0.4327
H	-1.6173	7.5269	0.4892
H	-1.6666	6.9494	-1.1702
H	0.0294	4.8215	-1.6835
C	-0.2259	1.4366	1.5611
O	-0.9098	0.6864	0.8769
N	0.3139	1.0556	2.7513
C	0.5985	-0.345	3.0912
H	0.268	-0.9151	2.2424

H	0.7649	1.7515	3.3042
C	2.1371	-0.446	3.245
H	2.4616	0.4924	3.6756
C	2.6291	-1.5605	4.2203
H	2.8591	-2.4735	3.688
H	3.5446	-1.2259	4.6982
C	1.5583	-1.83	5.2876
H	1.9481	-2.412	6.1108
C	0.7941	-0.5017	5.6084
H	1.3613	0.4189	5.5975
H	0.2428	-0.561	6.5334
C	-0.0965	-0.831	4.3627
H	-1.1367	-0.544	4.3734
C	0.2514	-2.3482	4.5976
C	0.3945	-3.29	3.3986
H	-0.5804	-3.5088	2.9858
H	0.8321	-4.2281	3.7278
H	1.0091	-2.8954	2.6019
C	-0.7079	-2.9925	5.6114
H	-0.3235	-3.9591	5.9214
H	-1.6796	-3.1463	5.154
H	-0.8454	-2.3856	6.4967
C	2.8115	-0.5379	1.8837
O	2.2266	-0.8784	0.8632
N	4.1222	-0.2006	1.9177
H	4.5409	-0.0084	2.8025
C	4.9804	-0.0977	0.7342
H	4.3276	-0.2433	-0.107
C	5.5973	1.3271	0.7117
H	5.7146	1.6299	1.7463
C	7.0158	1.4062	0.0644
H	6.9509	1.6769	-0.9808
H	7.5865	2.1818	0.5663
C	7.7518	0.0673	0.2147
H	8.8071	0.1651	0.0033
C	6.9678	-1.06	-0.5393
C	6.3077	-0.7324	-1.88
H	7.0736	-0.5207	-2.6202
H	5.638	0.1149	-1.8418
H	5.7346	-1.5837	-2.2268
C	7.8321	-2.3192	-0.7234
H	8.3451	-2.6102	0.1835
H	8.5788	-2.1447	-1.4914
H	7.2101	-3.1499	-1.0398
C	6.0871	-1.1585	0.7565
C	7.3167	-0.609	1.5573
H	7.1263	0.038	2.403
H	7.9933	-1.3909	1.8622
H	5.6848	-2.1261	1.0157
C	4.6275	2.3312	0.1129
O	3.4923	2.0264	-0.2416
N	5.0836	3.5949	0.0255
H	4.49	4.295	-0.3679
H	6.001	3.8576	0.3066

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C	4.708111	-1.83134	0.431563
H	4.269658	-1.18565	-0.33673
N	4.134452	-3.1915	0.39853
H	4.335754	-3.63057	-0.49528
H	3.121555	-3.14392	0.473263
C	6.226496	-1.90741	0.205158
H	6.454138	-2.55912	-0.64519
C	6.954204	-2.16695	1.552631
H	6.454347	-2.81325	2.275571
H	7.97342	-2.52462	1.419479
C	6.872568	-0.47593	0.198484
C	8.293943	-0.4975	-0.38509
H	8.911995	-1.30399	0.012863
H	8.8058	0.446768	-0.17366
H	8.256289	-0.61538	-1.4728
C	6.11754	0.695513	-0.43517
H	6.640135	1.634733	-0.2242
H	5.089781	0.805031	-0.09096
H	6.089147	0.581906	-1.5242
C	6.87953	-0.62623	1.762107
H	7.68952	-0.13164	2.305907
C	5.51116	-0.25819	2.352503
H	5.268622	0.781731	2.119773
H	5.545136	-0.33458	3.444055
C	4.39574	-1.21947	1.824942
H	4.356257	-2.07603	2.503434
C	3.037845	-0.51949	1.861043
O	2.641367	0.194325	0.941819
N	2.324115	-0.72635	2.999848
H	2.763079	-1.29014	3.713351
C	1.089025	-0.02804	3.373599
H	0.85218	0.625393	2.535646
C	1.316788	0.792659	4.657827
C	1.087656	-0.11406	5.904344
H	1.367298	-1.17009	5.839821
H	1.530359	0.295759	6.809835
H	2.250292	1.356448	4.582499
C	0.027934	1.585971	5.076096
C	-0.85666	2.203987	3.992747
H	-1.79927	2.549644	4.43
H	-1.10011	1.527747	3.174043
H	-0.3647	3.080067	3.559771
C	0.345217	2.669587	6.118555
H	0.955908	2.308585	6.94815
H	-0.58276	3.067767	6.540556
H	0.878928	3.502913	5.651482
C	-0.41809	0.240443	5.748346
H	-1.03152	0.313028	6.650559
C	-1.06173	-0.69199	4.715503
H	-1.38729	-1.61776	5.199651
H	-1.95772	-0.22195	4.303883
C	-0.06266	-1.0619	3.565426
H	0.416807	-2.00348	3.84797

C	-0.85393	-1.29814	2.273504
O	-1.13848	-0.38682	1.506684
N	-1.26619	-2.58273	2.096554
H	-0.98618	-3.26008	2.790309
C	-2.23999	-3.03211	1.093359
H	-2.7876	-2.14578	0.778359
C	-3.19216	-4.04757	1.74917
C	-4.29619	-4.54082	0.750178
C	-5.43907	-5.25585	1.488963
H	-5.09585	-5.98843	2.222133
H	-6.07813	-5.78089	0.772345
H	-6.06392	-4.52772	2.01534
C	-4.9133	-3.55469	-0.24208
H	-4.18762	-2.97394	-0.81037
H	-5.56086	-2.84605	0.283367
H	-5.54181	-4.09474	-0.95852
H	-3.53043	-3.67349	2.719914
C	-2.56867	-5.47435	1.670183
H	-1.48099	-5.56992	1.740388
H	-3.01739	-6.17071	2.375635
C	-3.2024	-5.54897	0.252108
H	-3.54899	-6.52072	-0.11055
C	-2.26608	-4.88045	-0.76241
H	-1.51979	-5.60241	-1.10895
H	-2.83406	-4.56904	-1.64128
C	-1.51306	-3.65509	-0.14378
H	-0.55137	-4.01746	0.22939
C	-1.26331	-2.60809	-1.23583
O	-2.16654	-1.90789	-1.67033
N	0.011421	-2.57106	-1.70951
H	0.673084	-3.2179	-1.30831
C	0.452304	-1.82879	-2.89476
H	-0.44856	-1.418	-3.34958
C	1.407836	-0.66193	-2.48326
H	1.807622	-0.91437	-1.4996
C	2.625868	-0.47111	-3.45594
H	2.448418	0.37595	-4.12226
H	3.505271	-0.2194	-2.85583
C	2.906674	-1.72616	-4.28962
H	3.867862	-1.64932	-4.80646
C	2.632969	-2.9898	-3.4265
H	3.088558	-3.89253	-3.82989
H	2.87654	-2.92875	-2.36106
C	1.143404	-2.81802	-3.85289
C	1.659302	-2.11999	-5.15773
C	0.811803	-1.02209	-5.80189
H	1.379957	-0.52967	-6.59892
H	0.473754	-0.25433	-5.10729
H	-0.07805	-1.46096	-6.26574
C	2.020917	-3.15011	-6.24018
H	1.112256	-3.57872	-6.67463
H	2.631355	-3.97595	-5.86947
H	2.576486	-2.66629	-7.04973
H	0.525295	-3.71193	-3.97465
C	0.68583	0.685046	-2.37972
O	-0.09122	1.049624	-3.26402
N	1.042583	1.457607	-1.33051
C	0.795163	2.902665	-1.25995
H	0.219539	3.147167	-2.15188
H	1.648764	1.054118	-0.62308
C	-0.02601	3.27567	0.031879
H	0.094144	2.43378	0.716546
C	0.478175	4.569264	0.742777
H	-0.22786	5.377405	0.548094
H	0.470683	4.393711	1.823664
C	1.889941	4.9806	0.314024
H	2.275316	5.78503	0.948149
C	2.756961	3.70459	0.127668
H	2.570673	2.861898	0.796548
H	3.827184	3.906049	0.11805
C	2.148077	3.641203	-1.30311
H	2.759315	3.240809	-2.11732
C	1.971051	5.19776	-1.23801
C	0.800272	5.852003	-1.97342
H	-0.17575	5.441875	-1.71729
H	0.936902	5.755766	-3.05645
H	0.770325	6.923709	-1.74762
C	3.262997	5.922348	-1.64861
H	3.406722	5.858725	-2.73222
H	4.157711	5.517738	-1.17143
H	3.199098	6.983436	-1.3867
C	-1.52097	3.406819	-0.31018
O	-1.99777	4.482628	-0.65326
N	-2.25652	2.266226	-0.23704
H	-1.82412	1.41753	0.107805
C	-3.69369	2.254108	-0.52621
H	-3.94262	3.294047	-0.73271
C	-4.00793	1.369728	-1.78885
H	-3.22783	0.607238	-1.83857
C	-5.38305	0.645207	-1.70486
H	-6.11615	1.19166	-2.30032
H	-5.27198	-0.34499	-2.15768
C	-5.876	0.490649	-0.2611
H	-6.7279	-0.19473	-0.20393
C	-6.04008	1.886913	0.436501
C	-6.58539	3.067686	-0.3693
H	-6.45688	3.99935	0.19297
H	-7.66021	2.937661	-0.53935
H	-6.11593	3.196477	-1.34421
C	-6.83787	1.785797	1.746031
H	-7.9006	1.632317	1.531031
H	-6.74834	2.715126	2.318464
H	-6.50939	0.967122	2.390158
C	-4.49621	1.779978	0.698492
C	-4.65343	0.233699	0.664927
H	-3.82812	-0.34357	0.248192
H	-4.92234	-0.18367	1.635226
H	-4.1072	2.251941	1.605425
C	-3.93242	2.243174	-3.049
O	-4.89024	2.904296	-3.43321

N	-2.73949	2.258935	-3.6881
H	-2.65024	2.886305	-4.47227
H	-1.91826	1.747138	-3.38714

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