Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for "Is a Cross-β-Sheet Structure of Low Molecular Weight Peptides Necessary for the Formation of Fibrils and Peptide Hydrogels?"

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Table S1: List of backbone dihedral angles (in degrees) of the GAG monomer and indicated oligomers with parallel-oriented peptides obtained from the geometry optimization described in the main text. The conformation of the central residue is listed in the last (right) column.

A: GAG monomer

Solvent	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
Implicit water	-174	-159	162	-178	β
H_2O+ethanol	152	-58	139	-66	pPII

B: GAG dimer with parallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	167	-76	172	-77	pPII
2	-161	-163	157	166	β

C: GAG trimer with parallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-169	-159	152	161	β
2	164	-83	176	-81	pPII
3	-148	-79	86	-66	γ_{inv}

D: GAG tetramer with parallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-167	-144	143	178	β
2	-159	-139	145	-163	β
3	-160	-140	143	-158	β
4	-168	-146	1141	-179	β

E: GAG pentamer with antiparallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-147	-78	86	-68	γ_{inv}
2	165	-89	173	-93	pPII
3	156	-126	159	-150	β
4	-166	-153	155	-115	β
5	166	-90	80	-109	γ_{inv}

F: GAG hexamer with parallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-147	-78	84	-68	γ_{inv}
2	166	-85	170	-87	pPII
3	159	-131	159	-162	β
4	-165	-152	155	-113	β
5	154	-87	89	-116	γ_{inv}
6	-152	-152	161	-78	β

G: GAG heptamer with parallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-149	-153	161	112	β
2	-153	-88	88	-115	γ_{inv}
3	-166	-152	154	-116	β
4	167	-79	152	-163	pPII
5	-147	-129	162	-78	β
6	163	-100	128	-63	pPII-β
7	165	-53	150	-53	pPII

Table S2: List of backbone dihedral angles (in degrees) of the GAG monomer and indicated oligomers of antiparallel-oriented peptides obtained from the geometry optimization described in the main text. The conformation of the central residue is listed in the last (right) column.

A: GAG monomer

Solvent	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
Implicit water	-174	-159	162	-178	β
H_2O+ethanol	152	-58	139	-66	pPII

B: GAG dimer with antiparallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-167	-147	144	-176	β
2	-157	-147	144	-161	β

C: GAG trimer with antiparallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-167	-147	144	-176	β
2	-157	147	144	-161	β
3	-162	-152	159	-176	β

D: GAG tetramer with antiparallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-147	-79	85	-68	γ_{inv}
2	167	-83	171	-87	pPII
3	158	-130	168	-166	β
4	-170	-154	153	-109	β

E: GAG pentamer with antiparallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-167	145	145	-176	β
2	-162	-143	141	-167	β
3	-161	-142	138	-162	β
4	178	-156	146	-159	β
5	157	-151	162	125	β

F: GAG hexamer with antiparallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-171	-148	143	-178	β
2	-155	-141	149	146	β
3	178	-152	149	-155	β
4	-161	-135	138	-149	β
5	-161	136	138	-149	β
6	-168	-145	143	-177	β

G: GAG heptamer with antiparallel-oriented peptides in explicit water

Peptide	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-163	-150	157	-179	β
2	-158	-146	141	-160	β
3	-164	-141	140	-173	β
4	-161	-140	134	-162	β
5	166	-153	146	-162	β
6	-158	-143	147	-156	β
7	168	-146	143	-179	β

Table S3: List of dihedral angles (in degrees) of the GAG backbone obtained from the geometry optimization of a GAG octamer in implicit ethanol. The conformation of the central residue is listed in the last (right) column.

A: GAG octamer with parallel-oriented peptides

Peptide #	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-172	-101	138	-71	β_p
2	-162	-121	144	-58	β_p
3	-148	-127	166	-95	β_{ext} /β_T
4	-150	-86	85	-109	γ_{inv}
5	-168	-152	155	-115	β_{ext}
6	162	-108	157	-156	pPII
7	-158	-109	158	-87	β_{ext}
8	-157	-63	164	-77	pPII

B: GAG octamer with antiparallel-oriented peptides

Peptide #	Ψ_1	Φ_2	Ψ_2	Φ_3	Conformation
1	-158	-119	157	121	β
2	-164	-157	166	168	β
3	-155	-151	141	-163	β
4	-160	-141	141	-169	β
5	-158	-142	139	-166	β
6	178	-150	146	-164	β
7	-154	-136	142	150	β
8	-165	-140	140	-178	β

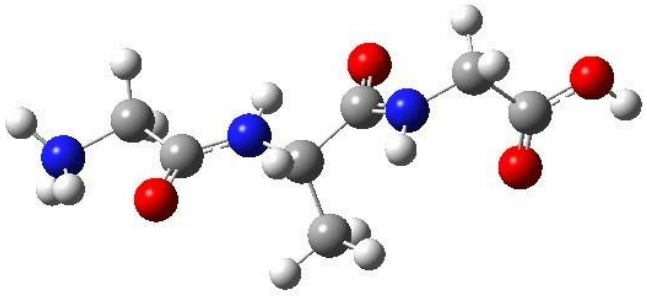

Figure S1: Structure of cationic GAG in implicit water as obtained from the DFT-based geometry optimization described in the main manuscript.

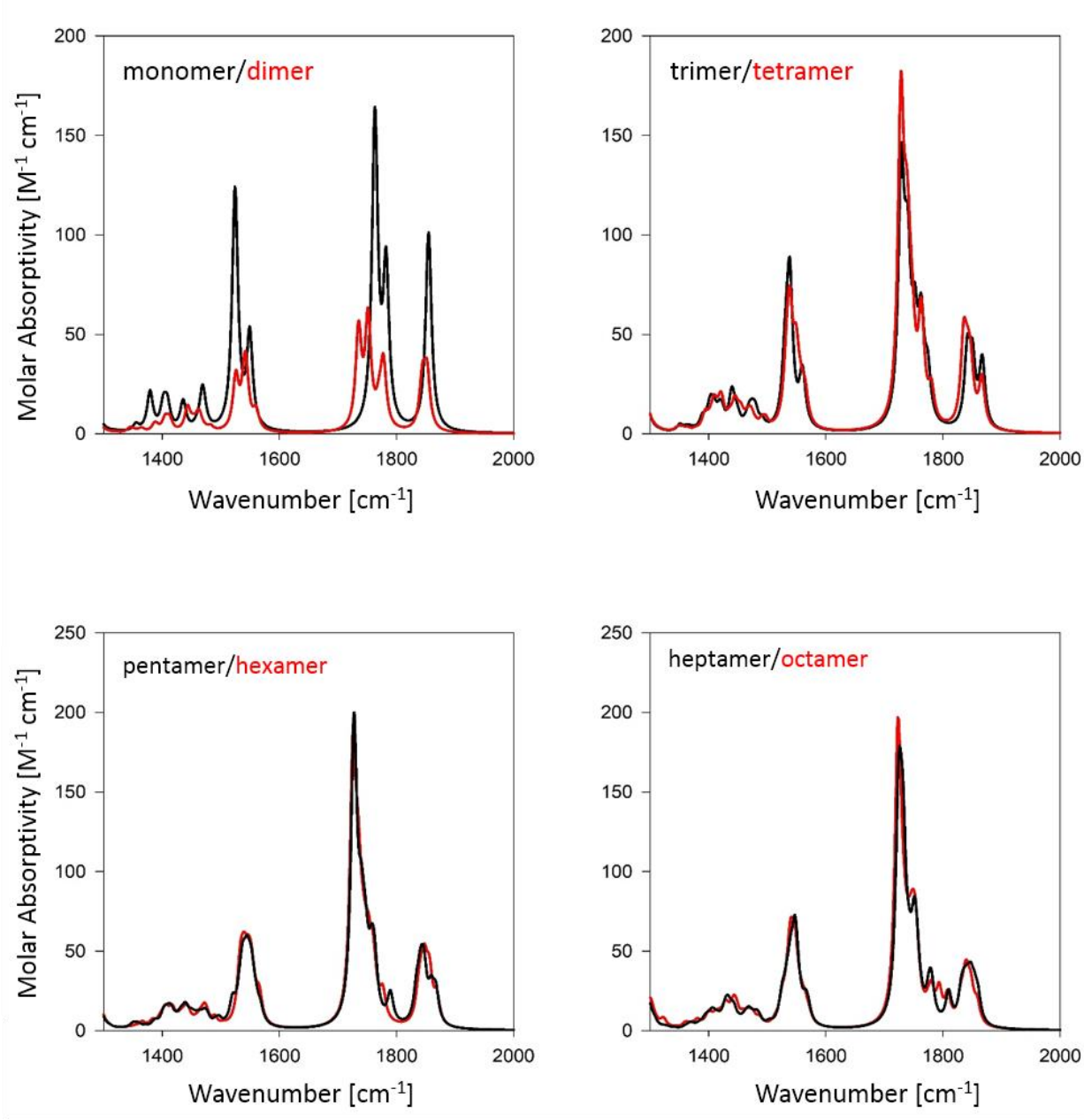

Figure S2: IR-spectra of GAG oligomers with a parallel orientation calculated for the optimized geometry as described in the text. For comparison, we added the calculated spectra of a GAG monomer in implicit water (black). Color code: black for oligomers containing an odd number of peptides, red for oligomers containing an even number of peptides.

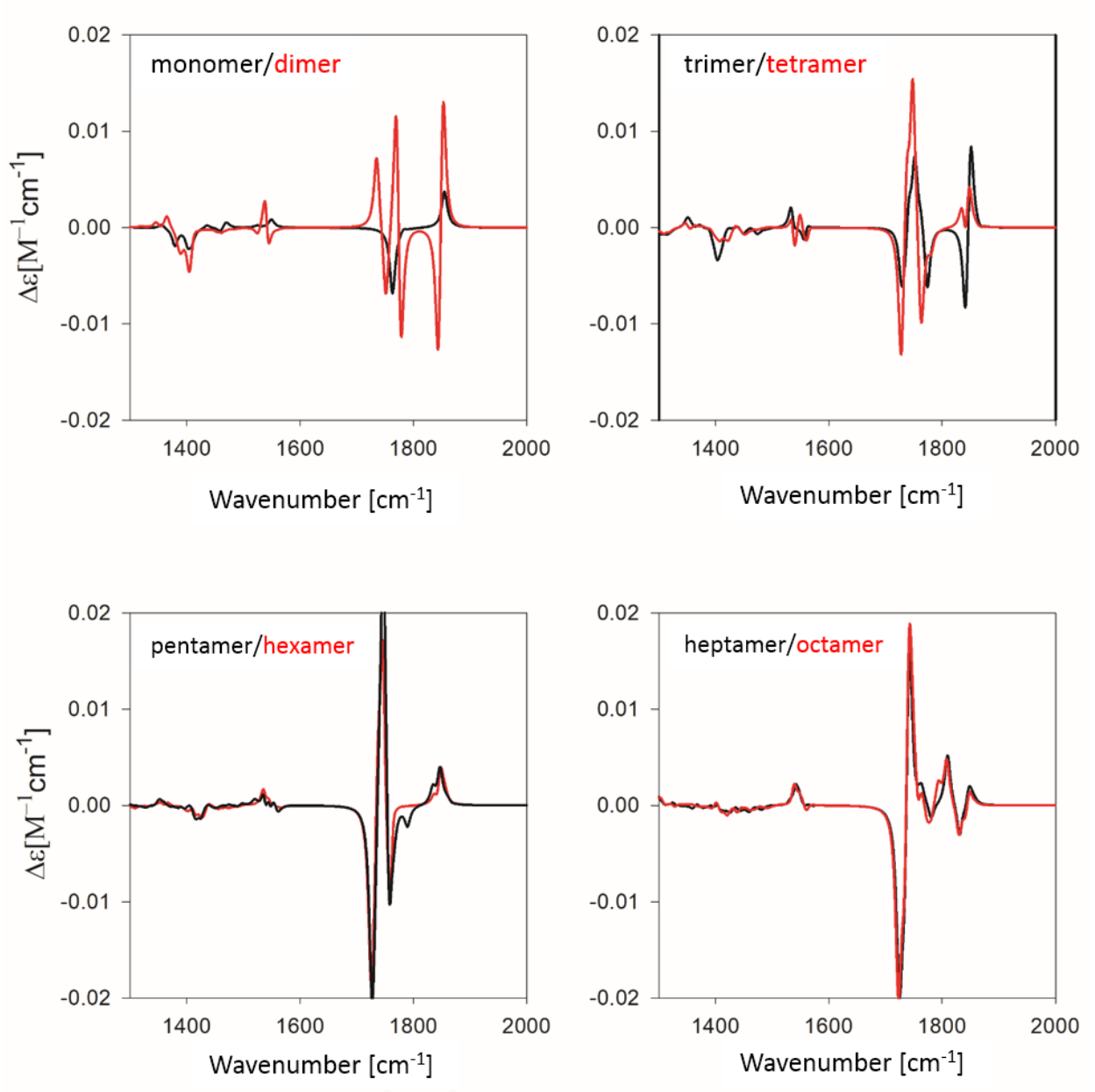

Figure S3: VCD-spectra of GAG oligomers with a parallel orientation calculated for the optimized geometry as described in the text. For comparison, we added the calculated spectra of a GAG monomer in implicit water (black). Color code: black for oligomers containing an odd number of peptides, red for oligomers containing an even number of peptides.

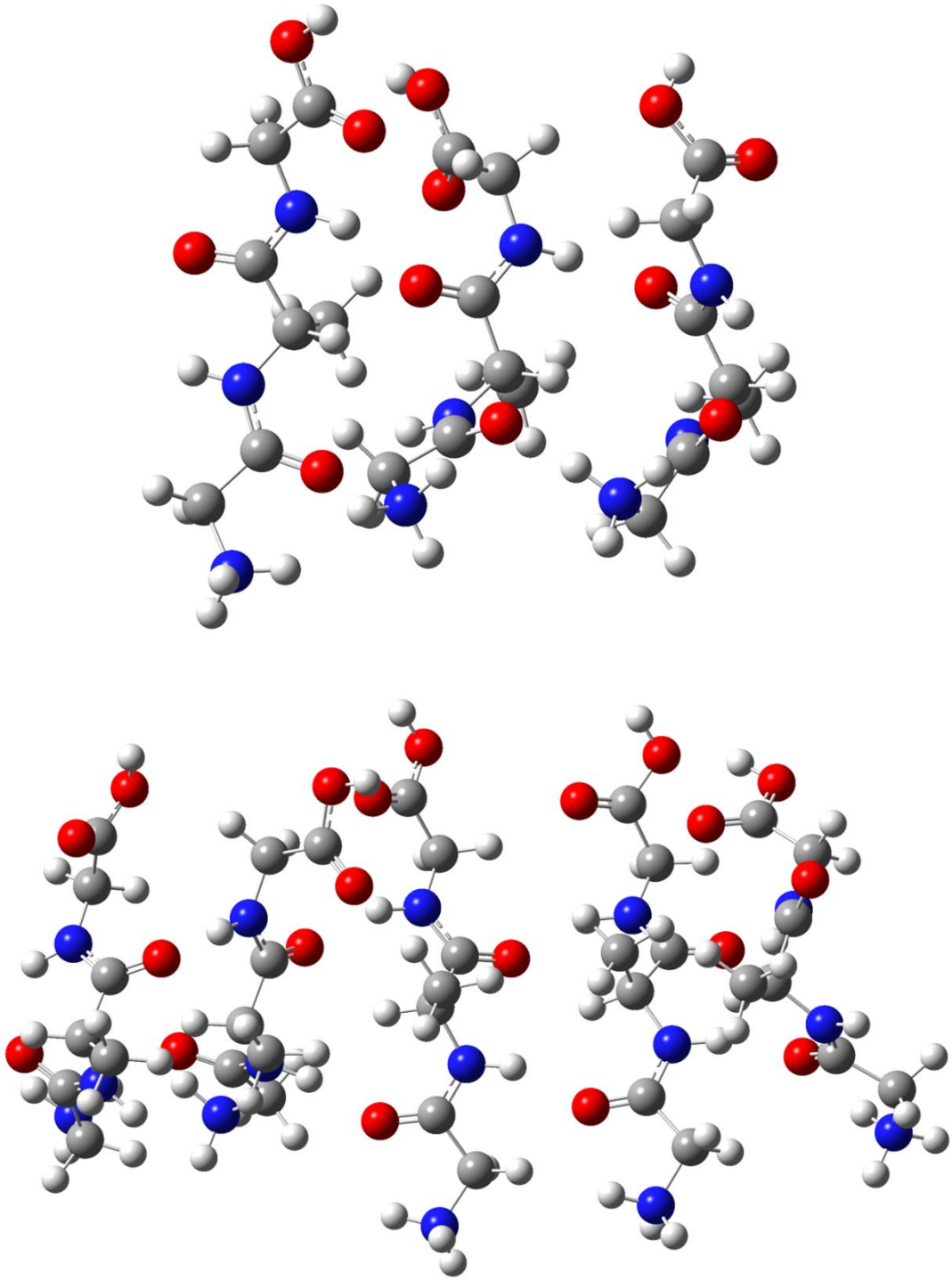

Figure S4: Structure of the trimer (upper part) and pentamer (lower part) of the geometry-optimized parallel oriented GAG.

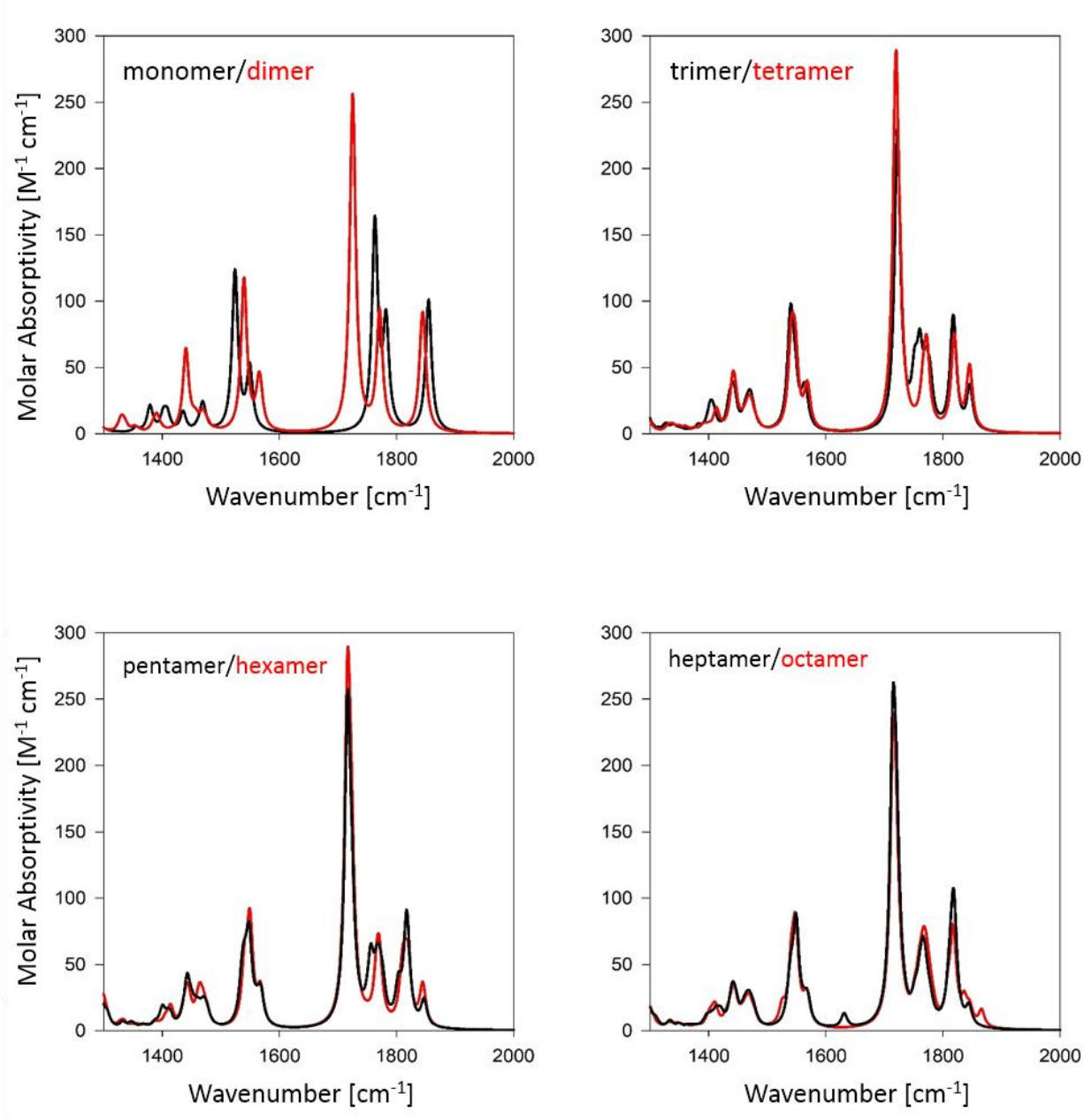

Figure S5: IR-spectra of GAG oligomers with an antiparallel orientation calculated for the optimized geometry as described in the text. For comparison, we added the calculated spectra of a GAG monomer in implicit water (black). Color code: black for oligomers containing an odd number of peptides, red for oligomers containing an even number of peptides.

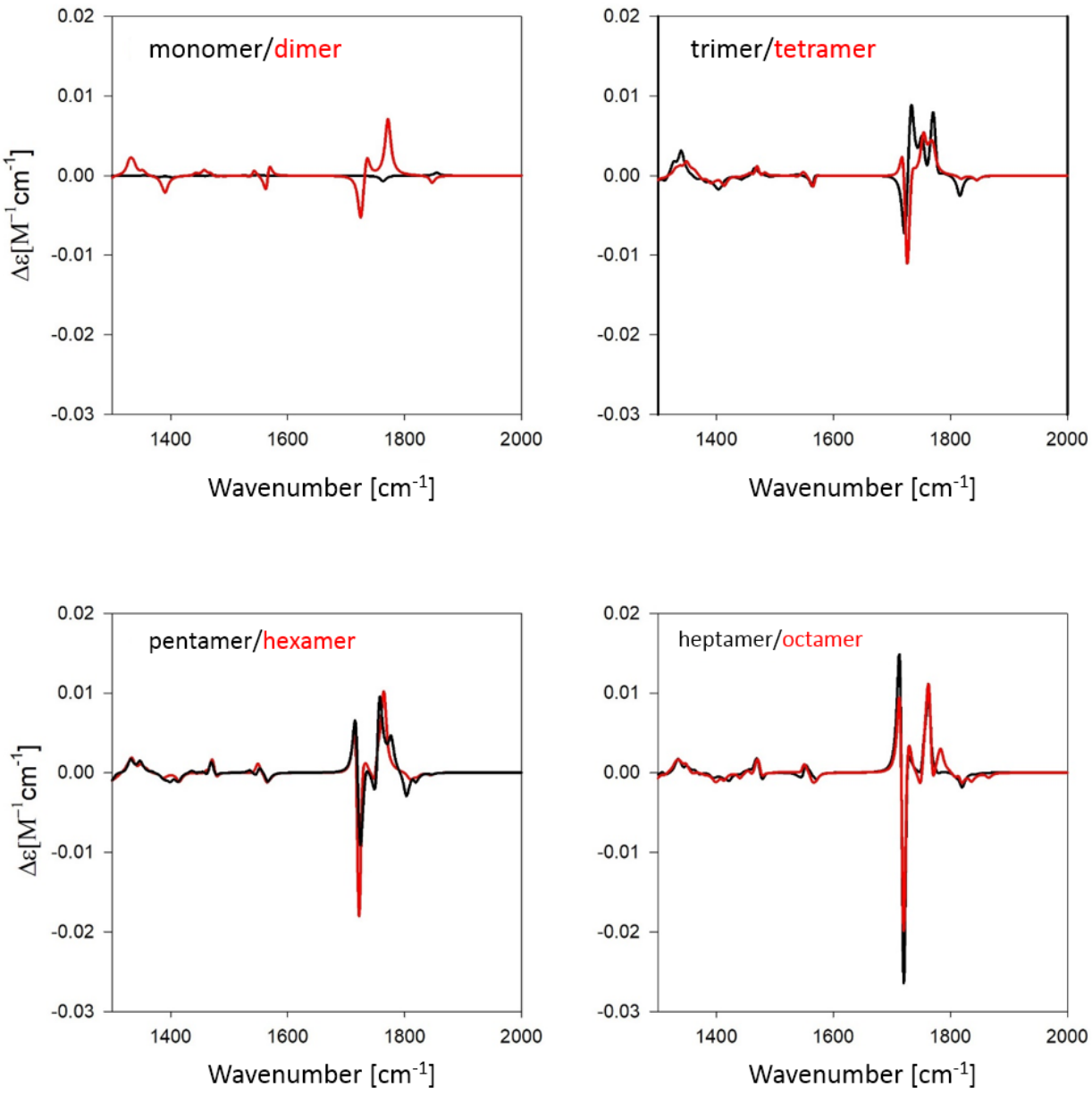

Figure S6: VCD-spectra of GAG oligomers with an antiparallel orientation calculated for the optimized geometry as described in the text. For comparison, we added the calculated spectra of a GAG monomer in implicit water (black). Color code: black for oligomers containing an odd number of peptides, red for oligomers containing an even number of peptides.

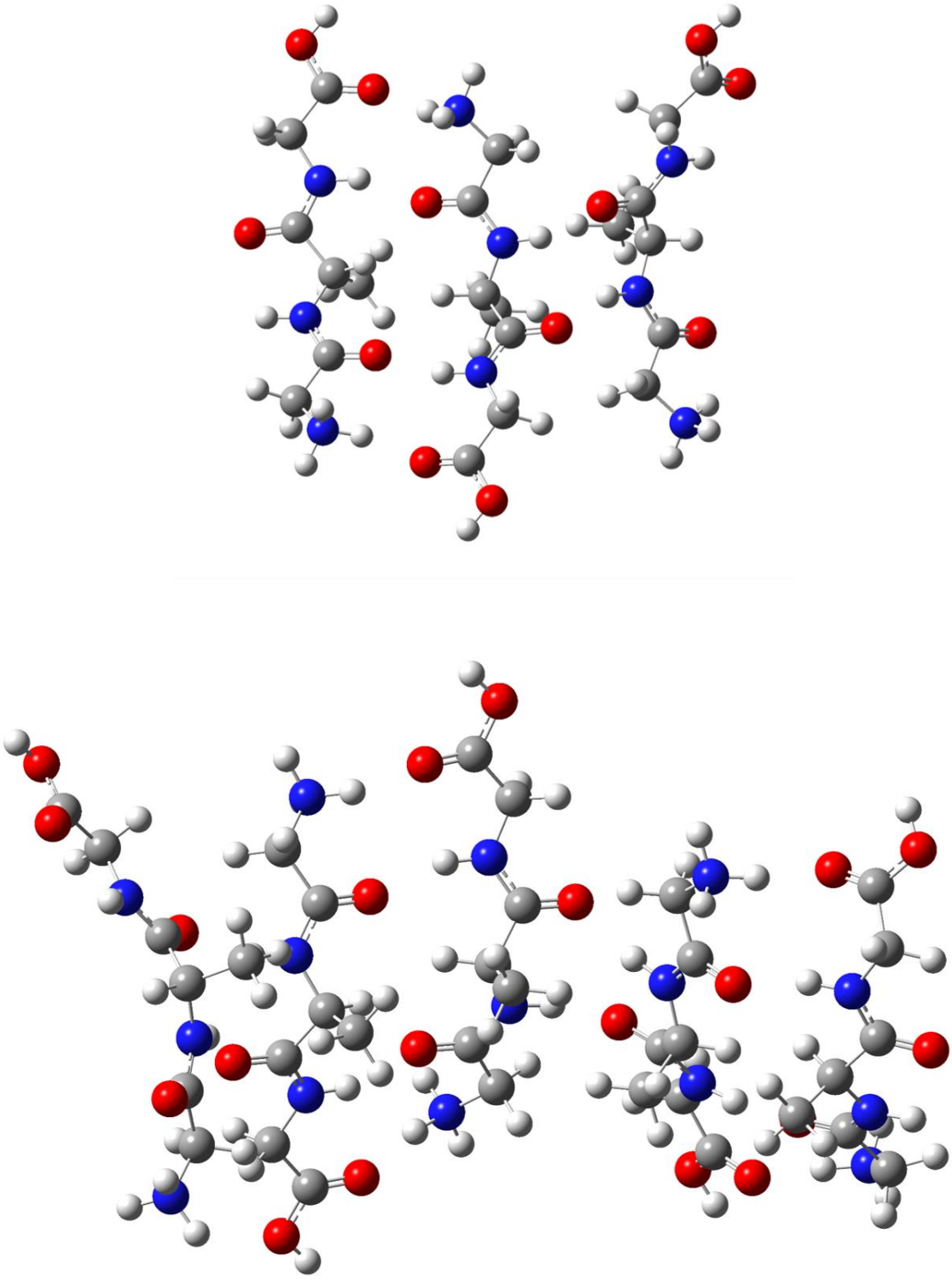

Figure S7: Structure of the trimer (lower part) and pentamer (upper part) of the geometry-optimized antiparallel oriented GAG.

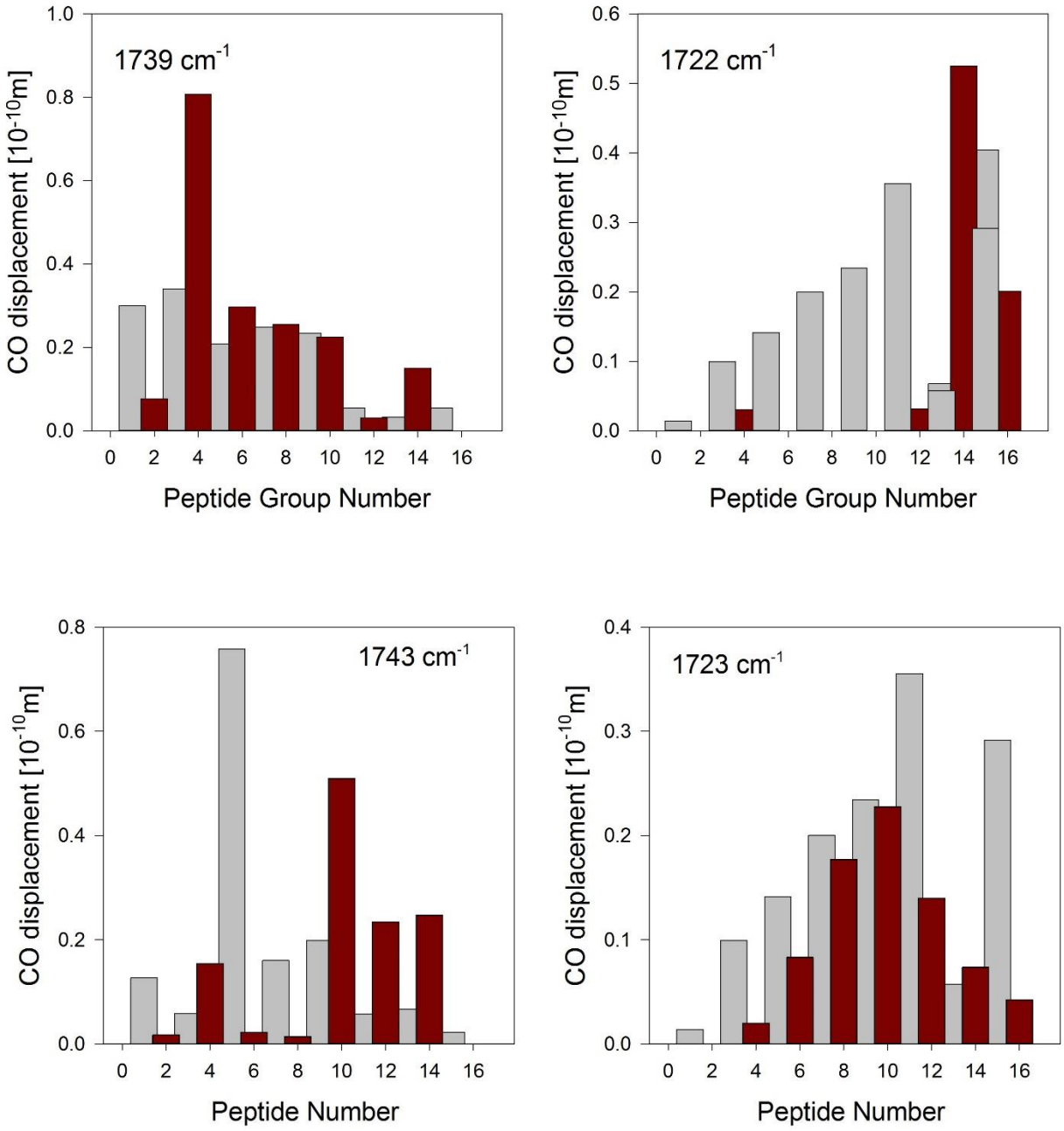

Figure S8: Representation of amide I' eigenvectors and delocalization of a GAG octamer with a parallel peptide orientation characterized by the displacements of the carbonyl groups for the indicated excitonic vibrations. Peptide groups (CO groups) were counted from the N-terminal of one out peptide group to the C-terminal of the peptide at the other end of the octamer. Displacements displayed with the same color belong to adjacent CO groups in different strands (i.e. grey for 1, 3, 5, …, 17, and dark red for 2, 4, 6,…, 18).

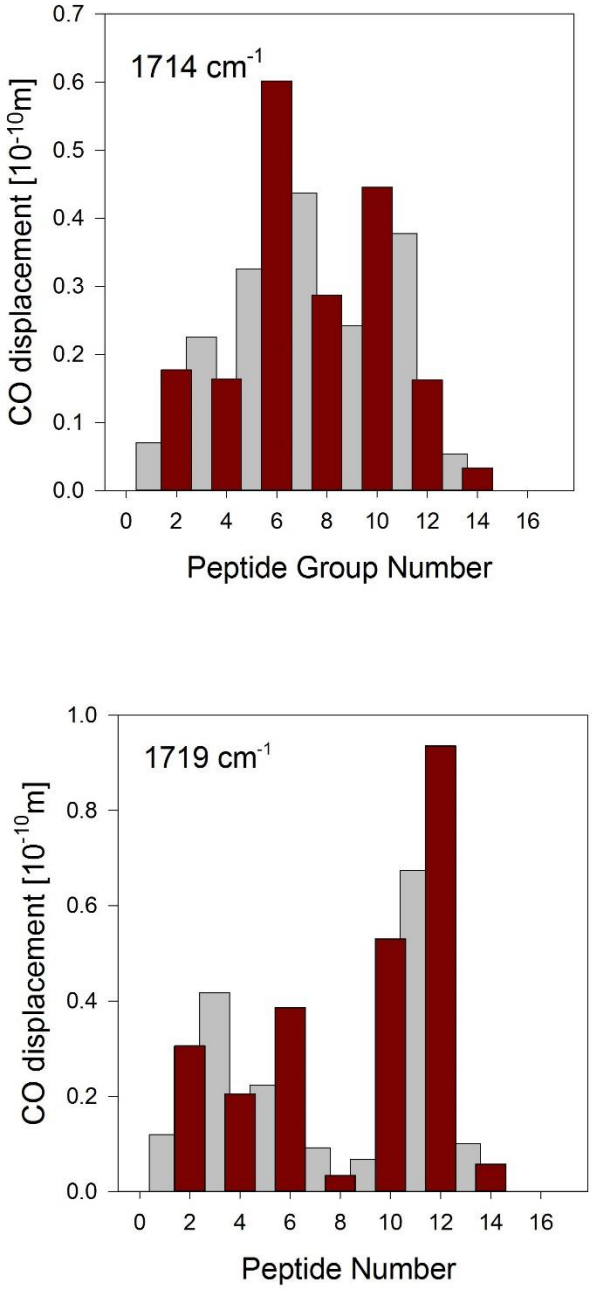

Figure S9: Representation of amide I' eigenvectors and delocalization of a GAG octamer with an antiparallel peptide orientation characterized by the displacement of the carbonyl groups for the indicated excitonic vibrations. Peptide groups (CO groups) were counted from the N-terminal of one out peptide group to the N-terminal of the peptide at the other end of the octamer. Displacements displayed with the same color belong to adjacent CO groups in different strands (i.e. grey for 1, 3, 5, ..., 17, and dark red for 2, 4, 6, …, 18).

Table S4: Cartesian coordinates (in Å) for all optimized geometries of the GAG oligomers arranged in the parallel configuration.

A: GAG monomer

C	1.060667	-4.530296	-5.790432
C	1.820130	-3.328465	-5.220334
O	1.447034	-2.841339	-4.152682
H	1.729157	-5.367014	-6.016201
H	0.525911	-4.243633	-6.702498
N	2.841196	-2.883606	-5.948615
C	3.627662	-1.721960	-5.581357
C	4.309350	-1.245088	-6.864360
O	4.417856	-1.980610	-7.838767
H(Iso=2)	3.091536	-3.310951	-6.838426
H	2.948090	-0.940837	-5.208058
C	4.674341	-2.050635	-4.510404
H	4.171513	-2.423394	-3.608262
H	5.254383	-1.156417	-4.243252
H	5.367998	-2.819380	-4.880635
N	4.787784	0.018032	-6.831117
C	5.683785	0.492913	-7.849106
C	7.106921	0.008164	-7.627504
O	7.459870	-0.723643	-6.735253
O	7.925886	0.498134	-8.561933
H(Iso=2)	4.741089	0.533867	-5.961331
H	5.349957	0.132661	-8.832103
H	5.677786	1.590077	-7.877942
N	0.084908	-4.917859	-4.745461
H(Iso=2)	0.324509	-5.796579	-4.278267
H(Iso=2)	0.142776	-4.146616	-4.040993
H(Iso=2)	8.817257	0.155621	-8.382335
H(Iso=2)	0.874625	-4.995282	-5.091172

B: GAG dimer

C	0.057919	-0.109397	-3.671911
C	1.127617	0.541611	-2.793038
O	1.035250	1.740944	-2.538738
H	-0.295101	-1.066955	-3.278395
H	0.461312	-0.263524	-4.679389
N	2.105285	-0.262696	-2.363673
C	3.264207	0.278333	-1.686144
C	4.201376	0.944582	-2.709559
O	3.997758	0.863577	-3.919311
H(Iso=2)	2.126803	-1.222436	-2.720612
H	2.913685	1.064319	-1.000582
C	3.974982	-0.818621	-0.894839
H	4.811991	-0.407604	-0.316305
H	4.374472	-1.592179	-1.565145
H	3.269533	-1.284178	-0.193778
N	5.241474	1.628704	-2.198576
C	6.249363	2.197985	-3.052604

C	7.230191	1.158980	-3.564146
O	7.137538	-0.033485	-3.393483
O	8.217984	1.733931	-4.253119
H(Iso=2)	5.400437	1.625688	-1.199300
H	5.783096	2.654805	-3.937577
H	6.798067	2.980593	-2.514275
H(Iso=2)	8.801551	1.027370	-4.576435
C	1.060533	-4.437057	-5.346577
C	1.933734	-3.303995	-4.814300
O	1.669131	-2.826655	-3.700321
H	1.620441	-5.378480	-5.307895
H	0.729176	-4.261460	-6.374860
N	2.944824	-2.927101	-5.582346
C	3.925992	-1.944591	-5.158600
C	4.639977	-1.456883	-6.416236
O	4.716112	-2.167939	-7.416639
H(Iso=2)	3.124531	-3.363723	-6.485054
H	3.413138	-1.100441	-4.682241
C	4.948824	-2.546233	-4.189476
H	4.430612	-2.984083	-3.324422
H	5.641641	-1.768247	-3.839849
H	5.522570	-3.341785	-4.687917
N	5.214772	-0.247530	-6.306859
C	6.030393	0.281772	-7.367329
C	6.259001	1.758927	-7.173206
O	5.788157	2.422679	-6.278848
O	7.054677	2.250050	-8.121734
H(Iso=2)	5.008466	0.340223	-5.494108
H	7.014172	-0.213685	-7.417725
H	5.552771	0.126560	-8.347526
N	-1.053021	0.867573	-3.743462
H(Iso=2)	-1.817011	0.644038	-3.099155
H(Iso=2)	-0.633124	1.770781	-3.433852
N	-0.108213	-4.537598	-4.442940
H(Iso=2)	0.166810	-4.054388	-3.565367
H(Iso=2)	-0.933170	-4.054097	-4.810775
H(Iso=2)	7.166214	3.200086	-7.950707
H(Iso=2)	-1.450044	0.968466	-4.680565
H(Iso=2)	-0.376203	-5.503547	-4.237837

C: GAG trimer

C	0.283437	0.157713	1.932039
C	1.309179	1.256249	2.180032
O	0.928012	2.423761	2.229841
H	-0.174221	-0.118342	2.889908
H	0.696978	-0.739946	1.460856
N	2.583643	0.869047	2.337775
C	3.641926	1.813115	2.697493
C	4.054674	2.592106	1.437441
O	4.989568	2.223432	0.720812
H(Iso=2)	2.814388	-0.117656	2.297175
H	3.215777	2.523259	3.421692
C	4.818616	1.076951	3.311804

H	4.492665	0.532682	4.208342
H	5.596499	1.795223	3.600959
H	5.256279	0.368960	2.593898
N	3.314620	3.679612	1.171482
C	3.545607	4.479927	-0.001838
C	4.891479	5.182120	0.047073
O	5.535581	5.396938	1.041601
O	5.263579	5.567043	-1.181310
H(Iso=2)	2.474537	3.826752	1.722976
H	3.475323	3.885883	-0.923789
H	2.770928	5.256011	-0.057565
H(Iso=2)	6.106175	6.044667	-1.098788
C	0.106622	-1.574698	-2.783483
C	0.937411	-0.632075	-1.924025
O	0.399656	0.376220	-1.443090
H	0.321399	-2.629523	-2.592700
H	0.314014	-1.358270	-3.839015
N	2.219310	-0.955118	-1.783491
C	3.196758	-0.018366	-1.260679
C	3.681170	0.884739	-2.410454
O	3.296666	0.695635	-3.565538
H(Iso=2)	2.546795	-1.793831	-2.275666
H	2.686143	0.621181	-0.527339
C	4.349134	-0.757936	-0.583611
H	5.003056	-0.043718	-0.067587
H	4.947837	-1.320474	-1.313718
H	3.949481	-1.462448	0.158875
N	4.528774	1.871273	-2.080793
C	5.123792	2.691275	-3.103232
C	6.320478	2.018986	-3.747168
O	6.820139	0.981933	-3.381361
O	6.768266	2.730012	-4.787315
H(Iso=2)	4.835075	1.982039	-1.110130
H	4.393785	2.912874	-3.894590
H	5.449147	3.646810	-2.668517
H(Iso=2)	7.552164	2.275283	-5.138632
C	2.452386	-5.233495	-4.854735
C	2.893369	-3.846483	-4.399734
O	2.574180	-3.462890	-3.264301
H	3.312620	-5.912530	-4.826595
H	2.031186	-5.232552	-5.864611
N	3.630995	-3.155378	-5.257464
C	4.236380	-1.882333	-4.909545
C	4.542541	-1.148337	-6.211857
O	4.817373	-1.767078	-7.237277
H(Iso=2)	3.877919	-3.533619	-6.169687
H	3.517134	-1.300231	-4.322727
C	5.530608	-2.076680	-4.113563
H	5.325074	-2.664598	-3.207371
H	5.949515	-1.103935	-3.821369
H	6.271528	-2.617997	-4.720303
N	4.553115	0.193862	-6.114163
C	4.931535	1.014169	-7.234400
C	4.441595	2.427757	-7.048112
O	3.756785	2.810915	-6.127650
O	4.856157	3.213051	-8.040779

H(Iso=2)	4.159503	0.638922	-5.279388
H	6.024251	1.043749	-7.375805
H	4.507715	0.616468	-8.170143
N	-0.753436	0.741836	1.055540
H(Iso=2)	-0.888709	1.725173	1.335150
H(Iso=2)	-0.429424	0.723698	0.065213
N	-1.321310	-1.289221	-2.520890
H(Iso=2)	-1.671505	-1.787280	-1.695605
H(Iso=2)	-1.414967	-0.279926	-2.326331
N	1.441474	-5.711606	-3.885295
H(Iso=2)	1.624034	-5.216687	-2.993828
H(Iso=2)	0.485618	-5.474300	-4.169568
H(Iso=2)	4.509577	4.105650	-7.875161
H(Iso=2)	1.478658	-6.723080	-3.733304
H(Iso=2)	-1.924400	-1.535622	-3.310768
H(Iso=2)	-1.647383	0.248187	1.115442

D: GAG tetramer

C	-0.551924	1.359169	0.729674
C	0.730404	1.881114	1.363583
O	0.840943	3.087858	1.571884
H	-1.299313	1.206105	1.517779
H	-0.423567	0.426105	0.170609
N	1.669470	0.972580	1.662353
C	2.905217	1.332666	2.358799
C	3.867773	1.963940	1.338610
O	4.723921	1.296671	0.751945
H(Iso=2)	1.502632	-0.005217	1.452282
H	2.646107	2.091140	3.111673
C	3.511179	0.111481	3.025403
H	2.800385	-0.312618	3.747439
H	4.426993	0.395286	3.559892
H	3.774286	-0.651722	2.280036
N	3.682518	3.275759	1.119579
C	4.448913	3.994239	0.135967
C	5.913450	4.103363	0.522961
O	6.361065	3.950779	1.630402
O	6.656022	4.426428	-0.544637
H(Iso=2)	2.860142	3.711044	1.528448
H	4.366989	3.537103	-0.860597
H	4.051111	5.014609	0.055409
H(Iso=2)	7.576984	4.518684	-0.247566
C	-0.322917	0.188126	-3.991988
C	0.640415	0.632698	-2.899007
O	0.510915	1.756229	-2.390796
H	-0.661311	-0.845384	-3.870770
H	0.183297	0.278097	-4.961526
N	1.599844	-0.236487	-2.597384
C	2.762895	0.124717	-1.811233
C	3.807840	0.787337	-2.730239
O	3.660979	0.795922	-3.952619
H(Iso=2)	1.612158	-1.118226	-3.122263
H	2.449374	0.868468	-1.065106

C	3.331719	-1.107115	-1.108953
H	4.143460	-0.813878	-0.431811
H	3.720824	-1.833048	-1.837605
H	2.543902	-1.594930	-0.517826
N	4.855026	1.344311	-2.103697
C	5.963018	1.910506	-2.825617
C	7.019761	0.878233	-3.160215
O	6.871639	-0.319590	-3.089489
O	8.150144	1.461922	-3.562279
H(Iso=2)	4.920843	1.278939	-1.083825
H	5.618094	2.326525	-3.783126
H	6.415335	2.722634	-2.241596
H(Iso=2)	8.775142	0.757577	-3.801640
C	0.669632	-4.372331	-5.672405
C	1.513335	-3.204684	-5.178570
O	1.086371	-2.537289	-4.225901
H	1.272440	-5.209724	-6.036059
H	0.021986	-4.017361	-6.483748
N	2.637099	-2.976992	-5.849514
C	3.522140	-1.874116	-5.523434
C	3.868464	-1.089190	-6.789246
O	3.633324	-1.536986	-7.915849
H(Iso=2)	2.942800	-3.686755	-6.519808
H	2.972350	-1.193779	-4.863365
C	4.781399	-2.358313	-4.800928
H	4.491591	-2.965099	-3.930933
H	5.379298	-1.509047	-4.445477
H	5.403805	-2.978280	-5.462787
N	4.473706	0.085944	-6.581473
C	4.906694	0.902135	-7.686335
C	5.826126	1.991541	-7.198665
O	6.123387	2.186122	-6.042455
O	6.272157	2.731906	-8.212261
H(Iso=2)	4.494552	0.482901	-5.637335
H	5.446831	0.300263	-8.433786
H	4.061297	1.378345	-8.212007
N	-1.024005	2.420607	-0.183944
H(Iso=2)	-0.820540	3.330602	0.256914
H(Iso=2)	-0.497033	2.364023	-1.080717
N	-1.483669	1.106949	-3.990408
H(Iso=2)	-2.179205	0.852423	-3.280992
H(Iso=2)	-1.153981	2.056046	-3.759187
N	-0.190214	-4.798149	-4.544739
H(Iso=2)	0.285293	-5.465037	-3.928261
H(Iso=2)	-0.398151	-3.957296	-3.980267
H(Iso=2)	6.849914	3.420513	-7.843107
C	3.440770	-7.629389	-8.488257
C	3.637567	-6.135310	-8.262516
O	3.188807	-5.612877	-7.234133
H	4.389478	-8.150603	-8.312186
H	3.088809	-7.859586	-9.499215
N	4.334103	-5.496734	-9.196271
C	4.695467	-4.100489	-9.059857
C	4.873300	-3.515537	-10.456037
O	5.236932	-4.213890	-11.397677
H(Iso=2)	4.676879	-5.974239	-10.026588

H	3.878360	-3.577335	-8.551946
C	5.991390	-3.919939	-8.262234
H	5.881365	-4.368165	-7.264545
H	6.217503	-2.850470	-8.149971
H	6.832034	-4.408397	-8.776604
N	4.640402	-2.188478	-10.520750
C	5.019698	-1.398616	-11.656703
C	6.187899	-0.487497	-11.336137
O	6.702591	-0.372346	-10.247211
O	6.576052	0.194988	-12.413588
H(Iso=2)	4.348190	-1.715932	-9.662303
H	5.301832	-2.069328	-12.479206
H	4.186484	-0.773282	-12.012239
N	2.453954	-8.109840	-7.495796
H(Iso=2)	2.565639	-7.547752	-6.637266
H(Iso=2)	1.487672	-7.977756	-7.812989
H(Iso=2)	7.309512	0.774901	-12.148584
H(Iso=2)	2.572992	-9.101550	-7.270361
H(Iso=2)	-1.066270	-5.228804	-4.852591
H(Iso=2)	-1.961944	1.131020	-4.895556
H(Iso=2)	-2.025045	2.358750	-0.384911

E: GAG pentamer

C	0.250014	1.056037	1.278478
C	1.707667	1.307387	1.702271
O	2.039168	2.428893	2.117777
H	-0.367259	0.897609	2.170221
H	0.127475	0.214349	0.590083
N	2.538471	0.247928	1.594700
C	3.950612	0.301219	2.018982
C	4.763640	0.990863	0.889632
O	5.342285	0.338455	0.000292
H(Iso=2)	2.187824	-0.628902	1.223834
H	3.990137	0.929096	2.919320
C	4.465088	-1.106154	2.317373
H	3.848762	-1.569080	3.098767
H	5.504003	-1.050943	2.665668
H	4.437091	-1.722246	1.409081
N	4.751479	2.340842	0.940350
C	5.409188	3.163515	-0.057620
C	6.937813	3.032000	-0.001625
O	7.583938	2.547095	0.906918
O	7.477629	3.570664	-1.126130
H(Iso=2)	4.165777	2.786294	1.640778
H	5.060603	2.916500	-1.069602
H	5.150410	4.212720	0.132441
H(Iso=2)	8.448813	3.495272	-1.053914
C	-0.653647	1.027995	-3.664139
C	0.560857	1.116600	-2.724688
O	0.742857	2.147721	-2.037564
H	-1.129662	0.043947	-3.663444
H	-0.333416	1.272605	-4.683440
N	1.373349	0.054408	-2.754682

C	2.724069	0.084913	-2.199014
C	3.673731	0.793745	-3.211676
O	3.273297	1.119346	-4.342961
H(Iso=2)	1.137581	-0.703878	-3.408109
H	2.701913	0.681343	-1.278819
C	3.190552	-1.346711	-1.883477
H	4.173936	-1.319929	-1.403147
H	3.256673	-1.945106	-2.801495
H	2.473986	-1.826841	-1.204058
N	4.923445	1.016598	-2.753111
C	5.988552	1.548706	-3.583776
C	6.976449	0.460403	-4.012635
O	6.777240	-0.741740	-3.959724
O	8.116126	1.026601	-4.473308
H(Iso=2)	5.163212	0.731607	-1.794942
H	5.554473	1.980476	-4.495319
H	6.529657	2.339629	-3.048404
H(Iso=2)	8.696013	0.305313	-4.785204
C	-0.386346	-3.762188	-5.936887
C	0.587479	-2.651887	-5.508798
O	0.245347	-1.876680	-4.590562
H	0.115741	-4.657512	-6.311790
H	-1.065263	-3.370576	-6.703263
N	1.725217	-2.599616	-6.213683
C	2.741730	-1.568491	-6.021333
C	2.952202	-0.761998	-7.322849
O	2.735603	-1.259938	-8.442252
H(Iso=2)	1.936502	-3.368665	-6.854945
H	2.381487	-0.887640	-5.244213
C	4.083802	-2.191562	-5.586213
H	3.935500	-2.808616	-4.690204
H	4.810892	-1.403299	-5.359682
H	4.488073	-2.827109	-6.384622
N	3.434428	0.480305	-7.111399
C	3.950494	1.331992	-8.163045
C	5.429262	1.647665	-7.932180
O	6.133440	1.153621	-7.066329
O	5.855353	2.566342	-8.829628
H(Iso=2)	3.557417	0.790693	-6.143081
H	3.854718	0.817216	-9.127642
H	3.390397	2.277282	-8.224713
N	-0.234868	2.303129	0.593240
H(Iso=2)	0.103174	3.122059	1.120553
H(Iso=2)	0.142103	2.350713	-0.383342
N	-1.654033	2.066794	-3.236835
H(Iso=2)	-2.215527	1.745799	-2.440009
H(Iso=2)	-1.143369	2.910301	-2.929831
N	-1.223708	-4.129500	-4.740165
H(Iso=2)	-0.715436	-4.754229	-4.104184
H(Iso=2)	-1.444884	-3.266612	-4.217892
H(Iso=2)	6.803597	2.725674	-8.658112
C	2.203253	-7.457211	-8.523457
C	2.464713	-5.940602	-8.455461
O	2.140500	-5.307846	-7.429084
H	3.119231	-8.002035	-8.269282
H	1.844436	-7.787790	-9.501579

N	3.084993	-5.426336	-9.526313
C	3.535886	-4.035812	-9.553560
C	3.581363	-3.530603	-11.002495
O	3.752280	-4.299435	-11.966307
H(Iso=2)	3.308053	-6.035412	-10.319878
H	2.824315	-3.435353	-8.978175
C	4.944100	-3.873105	-8.932114
H	4.970900	-4.366600	-7.951949
H	5.164613	-2.805545	-8.808285
H	5.711369	-4.306123	-9.586228
N	3.493296	-2.182620	-11.097902
C	3.888207	-1.451361	-12.285854
C	5.060736	-0.520773	-11.972525
O	5.341603	-0.076940	-10.876299
O	5.733791	-0.189336	-13.115617
H(Iso=2)	3.344137	-1.646630	-10.238730
H	4.153069	-2.161062	-13.076525
H	3.063874	-0.823344	-12.662317
N	1.174175	-7.803122	-7.482155
H(Iso=2)	1.369085	-7.258787	-6.627911
H(Iso=2)	0.227877	-7.554509	-7.791172
H(Iso=2)	6.436089	0.446833	-12.874770
C	4.391283	-9.938583	-11.864131
C	4.632392	-8.570593	-11.203910
O	3.749880	-7.692138	-11.282920
H	4.775399	-10.776656	-11.275227
H	4.846282	-9.950447	-12.861506
N	5.824613	-8.426435	-10.604449
C	6.320455	-7.141617	-10.074795
C	7.079897	-6.405613	-11.219757
O	8.308093	-6.461020	-11.336938
H(Iso=2)	6.488264	-9.194933	-10.640316
H	5.435969	-6.560187	-9.792817
C	7.207527	-7.376833	-8.854178
H	6.653108	-7.935307	-8.089001
H	7.519505	-6.410004	-8.438790
H	8.109055	-7.933364	-9.142657
N	6.246596	-5.777181	-12.093523
C	6.722714	-4.995941	-13.215387
C	6.656713	-3.492767	-12.924858
O	6.709677	-2.992123	-11.811279
O	6.537220	-2.788951	-14.072533
H(Iso=2)	5.258144	-5.662208	-11.870519
H	7.770808	-5.264660	-13.409782
H	6.134584	-5.218973	-14.114946
N	2.907819	-10.113049	-12.040681
H(Iso=2)	2.457952	-10.423052	-11.172021
H(Iso=2)	2.495450	-9.199195	-12.289837
H(Iso=2)	6.480436	-1.833332	-13.839290
H(Iso=2)	2.689649	-10.796463	-12.773203
H(Iso=2)	1.184593	-8.803496	-7.257855
H(Iso=2)	-2.094940	-4.595320	-5.013653
H(Iso=2)	-2.295707	2.314408	-3.997077
H(Iso=2)	-1.257865	2.335066	0.549219

F: GAG hexamer

C	0.511057	1.125534	1.444584
C	1.934403	1.635158	1.725883
O	2.113352	2.837023	1.982323
H	-0.023117	0.987858	2.391673
H	0.476742	0.199810	0.862602
N	2.909905	0.703064	1.676876
C	4.321069	1.011412	1.981442
C	4.955188	1.666752	0.722387
O	5.620839	1.009677	-0.100126
H(Iso=2)	2.673597	-0.255306	1.442174
H	4.317321	1.746808	2.797610
C	5.061838	-0.257645	2.400353
H	4.573702	-0.701803	3.277369
H	6.098990	-0.007638	2.655918
H	5.075736	-0.983435	1.576427
N	4.691017	2.985521	0.592641
C	5.151067	3.766729	-0.540673
C	6.678347	3.918053	-0.556880
O	7.429664	3.708891	0.375888
O	7.076834	4.354886	-1.780667
H(Iso=2)	4.046789	3.407028	1.257124
H	4.820606	3.326853	-1.491125
H	4.710759	4.769451	-0.470151
H(Iso=2)	8.046292	4.471173	-1.751231
C	-0.603769	0.462562	-3.371559
C	0.643456	0.810269	-2.539669
O	0.725217	1.928265	-1.979881
H	-0.948503	-0.563666	-3.221157
H	-0.374202	0.612778	-4.432397
N	1.588713	-0.135700	-2.521748
C	2.955738	0.124867	-2.076304
C	3.744605	0.814830	-3.230006
O	3.242683	0.953766	-4.358572
H(Iso=2)	1.409169	-0.994015	-3.057492
H	2.908844	0.815634	-1.225634
C	3.626904	-1.191268	-1.642762
H	4.612860	-0.979273	-1.215632
H	3.745426	-1.868335	-2.499068
H	3.009372	-1.687854	-0.882472
N	4.981791	1.235155	-2.890998
C	5.935463	1.746047	-3.858321
C	6.913065	0.659951	-4.318145
O	6.727223	-0.542578	-4.232717
O	8.021099	1.224491	-4.851816
H(Iso=2)	5.307744	1.104158	-1.925563
H	5.397480	2.097375	-4.749163
H	6.488245	2.590018	-3.427775
H(Iso=2)	8.586060	0.501068	-5.185646
C	-0.378236	-4.105589	-5.407716
C	0.654126	-3.020828	-5.061542
O	0.539597	-2.405234	-3.980244
H	0.043977	-4.929271	-5.988632
H	-1.210671	-3.651000	-5.956783

N	1.578276	-2.797415	-6.003892
C	2.595972	-1.753863	-5.885684
C	2.759468	-1.032313	-7.238534
O	2.482586	-1.596387	-8.314690
H(Iso=2)	1.654723	-3.449258	-6.784383
H	2.243618	-1.028587	-5.145861
C	3.948613	-2.341526	-5.431455
H	3.807300	-2.899016	-4.495843
H	4.676059	-1.538450	-5.262965
H	4.340655	-3.028289	-6.192989
N	3.255876	0.216192	-7.128004
C	3.618283	1.040381	-8.263584
C	5.050108	1.556887	-8.136760
O	5.836028	1.264113	-7.250656
O	5.326901	2.406039	-9.152789
H(Iso=2)	3.428017	0.588631	-6.189433
H	3.545773	0.445338	-9.181707
H	2.940288	1.902334	-8.365287
N	-0.195154	2.198142	0.664689
H(Iso=2)	0.019072	3.112673	1.088681
H(Iso=2)	0.140349	2.203138	-0.328096
N	-1.702419	1.421840	-3.003127
H(Iso=2)	-2.224319	1.105597	-2.178890
H(Iso=2)	-1.274315	2.332605	-2.766871
N	-0.934449	-4.644221	-4.116282
H(Iso=2)	-0.303621	-5.334380	-3.693574
H(Iso=2)	-1.028006	-3.860786	-3.449422
H(Iso=2)	6.251094	2.702185	-9.043749
C	1.799133	-7.767981	-8.494254
C	2.139875	-6.269808	-8.381941
O	1.799673	-5.634608	-7.364257
H	2.645022	-8.364826	-8.134279
H	1.541559	-8.077453	-9.510814
N	2.841910	-5.772420	-9.411225
C	3.361547	-4.406952	-9.386642
C	3.504643	-3.877045	-10.818544
O	3.729826	-4.632517	-11.783035
H(Iso=2)	3.063414	-6.375023	-10.210536
H	2.653531	-3.783020	-8.832673
C	4.742289	-4.327536	-8.693114
H	4.677410	-4.787287	-7.698353
H	5.037867	-3.275748	-8.591062
H	5.508065	-4.839338	-9.289999
N	3.439214	-2.527585	-10.898005
C	3.956396	-1.780898	-12.027862
C	5.179190	-0.963471	-11.604441
O	5.434672	-0.609391	-10.470268
O	5.935302	-0.624216	-12.691678
H(Iso=2)	3.228887	-2.005372	-10.042110
H	4.209875	-2.473911	-12.837096
H	3.205225	-1.073516	-12.414484
N	0.635529	-8.046750	-7.582777
H(Iso=2)	0.758927	-7.502467	-6.714975
H(Iso=2)	-0.251843	-7.752399	-8.004911
H(Iso=2)	6.670151	-0.059507	-12.379983
C	3.672760	-10.342468	-11.650023

C	4.144338	-8.982391	-11.115428
O	3.399462	-7.990426	-11.235517
H	3.066439	-10.847844	-10.888914
H	4.492949	-10.996801	-11.958893
N	5.342306	-8.979280	-10.504647
C	5.956194	-7.769003	-9.930798
C	6.788411	-7.092462	-11.054697
O	7.985729	-7.382448	-11.225478
H(Iso=2)	5.910301	-9.820199	-10.522641
H	5.135033	-7.107439	-9.632604
C	6.813931	-8.128130	-8.718115
H	6.199311	-8.639559	-7.966407
H	7.230246	-7.211895	-8.280175
H	7.646847	-8.775540	-9.021962
N	6.070551	-6.255317	-11.836094
C	6.606191	-5.472943	-12.933398
C	6.638101	-3.980398	-12.588400
O	6.707738	-3.525416	-11.457313
O	6.591101	-3.236658	-13.714413
H(Iso=2)	5.098082	-6.042172	-11.602577
H	7.631928	-5.795519	-13.152395
H	6.001140	-5.626271	-13.836326
N	2.804397	-10.081968	-12.844709
H(Iso=2)	2.078200	-9.398527	-12.594569
H(Iso=2)	3.385226	-9.656032	-13.609582
H(Iso=2)	6.596906	-2.286402	-13.453510
C	4.567831	-9.054697	-16.781663
C	5.269170	-8.855419	-15.428774
O	4.583981	-8.689946	-14.393254
H	4.232623	-10.094891	-16.865694
H	5.185909	-8.791355	-17.644282
N	6.602040	-8.884061	-15.455953
C	7.434700	-8.768902	-14.256256
C	8.780982	-8.150353	-14.692295
O	9.217905	-8.309125	-15.841191
H(Iso=2)	7.110217	-8.957424	-16.336784
H	6.909706	-8.120585	-13.547129
C	7.687946	-10.144397	-13.603390
H	6.729097	-10.632837	-13.390035
H	8.240984	-10.004864	-12.665873
H	8.273799	-10.783044	-14.277994
N	9.425822	-7.476126	-13.708320
C	10.803450	-7.061469	-13.866496
C	11.784910	-8.223539	-13.652785
O	11.479096	-9.374626	-13.396444
O	13.058486	-7.781534	-13.796067
H(Iso=2)	9.006687	-7.447101	-12.771160
H	10.959915	-6.662926	-14.878114
H	11.030932	-6.263638	-13.148208
H(Iso=2)	13.651597	-8.545000	-13.657050
N	3.335326	-8.185732	-16.803557
H(Iso=2)	2.880814	-8.213260	-15.878964
H(Iso=2)	3.566649	-7.206323	-17.005024
H(Iso=2)	2.663631	-8.501592	-17.511121
H(Iso=2)	2.356796	-10.940126	-13.179506
H(Iso=2)	0.563148	-9.042627	-7.351568

H(Iso=2)	-1.847990	-5.089968	-4.250462
H(Iso=2)	-2.369765	1.548902	-3.770569
H(Iso=2)	-1.209915	2.057790	0.667881

G: GAG heptamer

C	0.540296	-1.009161	1.640521
C	1.355373	0.230495	1.983275
O	0.759448	1.259561	2.308899
H	0.515234	-1.676086	2.511652
H	0.938720	-1.560005	0.782651
N	2.682507	0.092234	1.946155
C	3.607598	1.129074	2.381574
C	4.146979	1.878668	1.166022
O	4.681462	1.260536	0.238546
H(Iso=2)	3.078967	-0.794372	1.652905
H	3.058603	1.812837	3.039418
C	4.778060	0.506659	3.137368
H	4.406179	-0.042109	4.013000
H	5.449943	1.304292	3.476662
H	5.333381	-0.181686	2.483688
N	4.051897	3.215903	1.184106
C	4.744049	4.018014	0.210615
C	6.250617	3.852159	0.323337
O	6.847441	3.593483	1.348413
O	6.858954	4.052525	-0.838577
H(Iso=2)	3.612101	3.712769	1.959333
H	4.422445	3.794188	-0.815257
H	4.510218	5.073175	0.410136
H(Iso=2)	7.819437	3.980523	-0.700003
C	-1.240120	-0.147780	-3.017171
C	-0.017149	0.209712	-2.184258
O	-0.188557	0.659350	-1.035839
H	-1.575297	-1.151953	-2.729219
H	-1.054139	-0.120581	-4.094343
N	1.155096	-0.006990	-2.755594
C	2.428769	0.253188	-2.108118
C	3.277382	1.089838	-3.070991
O	3.000253	1.122007	-4.272179
H(Iso=2)	1.171500	-0.346675	-3.722757
H	2.224366	0.823683	-1.192951
C	3.160803	-1.044878	-1.752240
H	4.054830	-0.815512	-1.157840
H	3.464873	-1.589629	-2.657472
H	2.501899	-1.699033	-1.165441
N	4.323061	1.727466	-2.528008
C	5.318060	2.361074	-3.353375
C	6.296683	1.360019	-3.933683
O	6.115331	0.164916	-3.974183
O	7.387577	1.962954	-4.403946
H(Iso=2)	4.533107	1.577945	-1.534321
H	4.843838	2.862394	-4.209252
H	5.865879	3.110095	-2.769273
H(Iso=2)	7.948584	1.281982	-4.810727

C	0.216380	-3.782650	-5.989507
C	1.135224	-2.632595	-5.593173
O	0.642733	-1.570993	-5.194104
H	0.561449	-4.750067	-5.611183
H	0.154753	-3.830493	-7.083738
N	2.434548	-2.872854	-5.751050
C	3.436180	-1.829947	-5.642971
C	3.484721	-1.019819	-6.944000
O	3.209809	-1.545701	-8.026561
H(Iso=2)	2.711494	-3.783332	-6.133185
H	3.150458	-1.149458	-4.832242
C	4.799385	-2.448776	-5.347812
H	4.748299	-3.030004	-4.415980
H	5.550499	-1.659850	-5.225657
H	5.105919	-3.120388	-6.161765
N	3.887940	0.248794	-6.827086
C	4.024810	1.088206	-7.989848
C	4.853475	2.303091	-7.661699
O	5.256354	2.593985	-6.558979
O	5.076207	3.040303	-8.749100
H(Iso=2)	3.906125	0.688392	-5.902466
H	4.496120	0.534269	-8.815602
H	3.048438	1.440597	-8.366319
N	-0.831850	-0.564083	1.330912
H(Iso=2)	-1.102602	0.169120	2.000493
H(Iso=2)	-0.845254	-0.132947	0.382071
N	-2.319611	0.807568	-2.672859
H(Iso=2)	-2.275243	1.013525	-1.664261
H(Iso=2)	-2.218157	1.700463	-3.167741
N	-1.133466	-3.490345	-5.459450
H(Iso=2)	-1.226758	-3.754739	-4.473374
H(Iso=2)	-1.284058	-2.471967	-5.509836
H(Iso=2)	5.595178	3.816042	-8.478503
C	2.636394	-7.699530	-7.800102
C	2.948402	-6.205893	-7.807759
O	2.810088	-5.569975	-6.754065
H	3.577124	-8.260183	-7.742168
H	2.081137	-8.026064	-8.684591
N	3.389631	-5.709179	-8.958303
C	3.829275	-4.331749	-9.078434
C	3.617022	-3.868230	-10.512975
O	3.659077	-4.665902	-11.454757
H(Iso=2)	3.459738	-6.324947	-9.774010
H	3.231696	-3.711402	-8.400379
C	5.317585	-4.159569	-8.740114
H	5.549981	-4.664918	-7.792312
H	5.550320	-3.090257	-8.642858
H	5.954705	-4.568892	-9.537528
N	3.463708	-2.541959	-10.645751
C	3.622309	-1.870119	-11.907219
C	4.792749	-0.909668	-11.849317
O	5.219231	-0.395042	-10.846950
O	5.284111	-0.643815	-13.074514
H(Iso=2)	3.440197	-1.973096	-9.794376
H	3.760323	-2.613118	-12.700802
H	2.729213	-1.276970	-12.163900

N	1.856996	-7.976992	-6.573080
H(Iso=2)	2.145601	-7.279303	-5.865661
H(Iso=2)	0.849235	-7.858390	-6.717201
H(Iso=2)	5.979250	0.030384	-12.975668
C	4.026114	-10.314825	-10.966081
C	4.543998	-8.909976	-10.700892
O	3.748059	-7.967226	-10.737760
H	3.698481	-10.757565	-10.016669
H	4.767023	-10.976291	-11.427369
N	5.841419	-8.796622	-10.402928
C	6.470033	-7.516993	-10.081100
C	6.947221	-6.878807	-11.395609
O	8.072658	-7.114241	-11.838988
H(Iso=2)	6.430209	-9.622413	-10.425162
H	5.692148	-6.884806	-9.636509
C	7.609887	-7.706841	-9.097443
H	7.238457	-8.184955	-8.181537
H	8.040032	-6.730573	-8.836949
H	8.405535	-8.323096	-9.538397
N	6.026854	-6.122117	-12.014822
C	6.254295	-5.389001	-13.231156
C	6.248015	-3.892868	-12.984651
O	6.469948	-3.366987	-11.917482
O	5.963491	-3.226109	-14.101490
H(Iso=2)	5.120620	-5.952111	-11.574920
H	7.230034	-5.660211	-13.656568
H	5.487228	-5.629271	-13.979848
N	2.862325	-10.190902	-11.865450
H(Iso=2)	2.242916	-9.447436	-11.517915
H(Iso=2)	3.180380	-9.897352	-12.815913
H(Iso=2)	5.934770	-2.270478	-13.889337
C	3.662670	-9.788619	-16.344250
C	4.552096	-9.352832	-15.187299
O	4.031577	-9.106178	-14.087932
H	3.518500	-10.874264	-16.286161
H	4.063857	-9.530351	-17.328616
N	5.849517	-9.276119	-15.436175
C	6.833688	-8.854775	-14.455972
C	7.993102	-8.252860	-15.257605
O	8.137998	-8.526105	-16.445344
H(Iso=2)	6.219558	-9.398432	-16.378384
H	6.366047	-8.096695	-13.812835
C	7.339586	-10.017895	-13.598456
H	6.492460	-10.517691	-13.110767
H	8.026691	-9.643771	-12.827513
H	7.868676	-10.753762	-14.220332
N	8.820822	-7.452385	-14.560031
C	10.078979	-7.038568	-15.114812
C	11.147075	-8.106358	-14.951608
O	10.971005	-9.195423	-14.462026
O	12.320235	-7.682508	-15.429530
H(Iso=2)	8.663911	-7.336626	-13.553764
H	9.965931	-6.830138	-16.187843
H	10.420956	-6.115175	-14.629394
H(Iso=2)	12.964531	-8.399500	-15.308290
N	2.343075	-9.139183	-16.161027

H(Iso=2)	2.144428	-9.085227	-15.150440
H(Iso=2)	2.331255	-8.178358	-16.520898
C	0.493107	3.542710	0.141432
C	0.349997	4.579943	1.253536
O	0.121764	5.748238	0.949763
H	0.004195	2.588566	0.351779
H	1.562554	3.358685	-0.019626
N	0.511622	4.106045	2.494901
C	0.744575	4.979437	3.627969
C	2.248493	5.296359	3.668655
O	2.904164	5.332534	2.623243
H(Iso=2)	0.717179	3.109440	2.595728
H	0.244708	5.934479	3.405426
C	0.168514	4.376289	4.903366
H	-0.893685	4.146494	4.748396
H	0.230150	5.085443	5.740579
H	0.692132	3.449651	5.181779
N	2.833222	5.535459	4.852858
C	4.257798	5.778515	4.890647
C	5.002407	4.653521	4.181704
O	4.672470	3.488695	4.247083
O	6.042680	5.096769	3.493119
H(Iso=2)	2.319103	5.441284	5.717772
H	4.511064	6.733716	4.411935
H	4.583609	5.814670	5.937573
H(Iso=2)	6.396791	4.362092	2.940134
N	-0.073495	4.161121	-1.077387
H(Iso=2)	-0.052373	5.186156	-0.899518
H(Iso=2)	0.448595	3.939934	-1.928563
H(Iso=2)	1.584777	-9.652703	-16.620113
H(Iso=2)	2.330565	-11.062062	-11.937044
H(Iso=2)	2.011874	-8.920934	-6.208596
H(Iso=2)	-1.873504	-3.967805	-5.981741
H(Iso=2)	-3.250243	0.439065	-2.891577
H(Iso=2)	-1.051515	3.897328	-1.228150
H(Iso=2)	-1.511966	-1.327120	1.369436

H: GAG octamer

C	0.757951	-1.185175	1.849006
C	1.601968	0.032999	2.199691
O	1.031812	1.056037	2.585695
H	0.752461	-1.875686	2.701920
H	1.116815	-1.718457	0.962972
N	2.924597	-0.116249	2.100229
C	3.879207	0.896479	2.528165
C	4.367087	1.686945	1.316478
O	4.841899	1.101138	0.337407
H(Iso=2)	3.298718	-0.994867	1.758071
H	3.370962	1.561057	3.236834
C	5.078685	0.237069	3.202652
H	4.745433	-0.335149	4.078891
H	5.778032	1.015222	3.531263
H	5.589857	-0.436958	2.499777

N	4.292258	3.023791	1.395914
C	4.947328	3.864175	0.429137
C	6.455678	3.685089	0.469707
O	7.092194	3.374867	1.455768
O	7.016056	3.936324	-0.706291
H(Iso=2)	3.900991	3.489238	2.214986
H	4.578718	3.689192	-0.590290
H	4.729790	4.910388	0.686182
H(Iso=2)	7.980936	3.853323	-0.611825
C	-1.259506	-0.108697	-2.718520
C	0.006067	0.196474	-1.929228
O	-0.107622	0.594622	-0.754321
H	-1.563422	-1.140815	-2.504177
H	-1.134772	0.015287	-3.797653
N	1.148479	-0.007271	-2.561334
C	2.452181	0.215513	-1.959737
C	3.258227	1.106457	-2.909724
O	2.929939	1.207971	-4.093747
H(Iso=2)	1.116014	-0.292971	-3.545997
H	2.291111	0.733977	-1.005816
C	3.196445	-1.099736	-1.706338
H	4.117002	-0.900990	-1.142187
H	3.459674	-1.599789	-2.649543
H	2.562931	-1.780710	-1.122440
N	4.324852	1.716801	-2.374458
C	5.296670	2.375132	-3.208146
C	6.220848	1.382813	-3.884433
O	6.001686	0.196957	-3.977479
O	7.306887	1.979652	-4.372386
H(Iso=2)	4.584013	1.500796	-1.404853
H	4.798053	2.934205	-4.012910
H	5.889185	3.077332	-2.609595
H(Iso=2)	7.829409	1.306494	-4.838997
C	-0.048999	-3.440525	-6.092678
C	0.926424	-2.375938	-5.604864
O	0.488089	-1.336331	-5.098767
H	0.256289	-4.454289	-5.815567
H	-0.122564	-3.379141	-7.185587
N	2.212002	-2.653293	-5.813770
C	3.251023	-1.650733	-5.667437
C	3.287659	-0.764198	-6.918320
O	2.982255	-1.221210	-8.023719
H(Iso=2)	2.437058	-3.537419	-6.281588
H	3.006050	-1.015429	-4.808146
C	4.606085	-2.318604	-5.452217
H	4.562109	-2.973109	-4.569841
H	5.373514	-1.554472	-5.282096
H	4.885944	-2.925776	-6.324462
N	3.713823	0.489410	-6.737898
C	3.836138	1.389557	-7.856251
C	4.677433	2.581558	-7.480892
O	5.108896	2.808441	-6.374031
O	4.876421	3.378122	-8.530335
H(Iso=2)	3.761182	0.874601	-5.790261
H	4.290276	0.877705	-8.718191
H	2.855341	1.765328	-8.196721

N	-0.617457	-0.712280	1.601704
H(Iso=2)	-0.856850	-0.001302	2.306176
H(Iso=2)	-0.659082	-0.246616	0.669820
N	-2.324859	0.797592	-2.227372
H(Iso=2)	-2.176210	0.961877	-1.219692
H(Iso=2)	-2.297189	1.712143	-2.691558
N	-1.380316	-3.142163	-5.520993
H(Iso=2)	-1.477004	-3.490255	-4.561646
H(Iso=2)	-1.493062	-2.118665	-5.479534
H(Iso=2)	5.405935	4.135541	-8.229903
C	2.031968	-7.334010	-8.221842
C	2.434481	-5.865182	-8.127877
O	2.353655	-5.299058	-7.029603
H	2.934884	-7.955771	-8.191297
H	1.469341	-7.568721	-9.131006
N	2.886262	-5.313618	-9.249646
C	3.401939	-3.957435	-9.278263
C	3.203878	-3.380204	-10.673087
O	3.179523	-4.108620	-11.669437
H(Iso=2)	2.902638	-5.867880	-10.111468
H	2.845673	-3.354631	-8.551232
C	4.899181	-3.893624	-8.943629
H	5.106160	-4.463477	-8.027132
H	5.195201	-2.846951	-8.789000
H	5.505704	-4.293466	-9.768794
N	3.137115	-2.040195	-10.709545
C	3.317071	-1.294191	-11.925506
C	4.545425	-0.412311	-11.829265
O	5.012075	0.018974	-10.805599
O	5.040537	-0.107949	-13.044122
H(Iso=2)	3.158650	-1.531902	-9.820681
H	3.394799	-1.988547	-12.769678
H	2.459255	-0.630408	-12.122734
N	1.221282	-7.649592	-7.024901
H(Iso=2)	1.572644	-7.067524	-6.247079
H(Iso=2)	0.231968	-7.412310	-7.151927
H(Iso=2)	5.778142	0.514325	-12.916393
C	3.261022	-9.641308	-11.982661
C	3.837634	-8.372289	-11.372551
O	3.100522	-7.386424	-11.266788
H	2.766049	-10.223944	-11.195600
H	4.007364	-10.268273	-12.480790
N	5.112649	-8.410883	-10.978701
C	5.825225	-7.232569	-10.484732
C	6.361694	-6.481086	-11.715850
O	7.502531	-6.689149	-12.134504
H(Iso=2)	5.656807	-9.249922	-11.150061
H	5.089780	-6.602305	-9.970992
C	6.931376	-7.628898	-9.526489
H	6.510382	-8.187921	-8.680433
H	7.426893	-6.727480	-9.142180
H	7.686609	-8.244269	-10.034513
N	5.467526	-5.673495	-12.306398
C	5.721608	-4.884443	-13.481029
C	5.802080	-3.406441	-13.153062
O	6.063077	-2.953589	-12.061432

O	5.546368	-2.662881	-14.227831
H(Iso=2)	4.557112	-5.513839	-11.872883
H	6.672513	-5.185067	-13.939711
H	4.932239	-5.044335	-14.227610
N	2.251264	-9.208706	-12.970999
H(Iso=2)	1.716520	-8.426008	-12.568983
H(Iso=2)	2.725004	-8.855252	-13.834072
H(Iso=2)	5.574119	-1.720926	-13.961151
C	3.706641	-9.646493	-16.998964
C	4.463043	-8.939614	-15.880964
O	3.818331	-8.278201	-15.048997
H	3.357907	-10.618882	-16.628413
H	4.308068	-9.796121	-17.900114
N	5.777857	-9.099642	-15.884326
C	6.652524	-8.513447	-14.886917
C	7.690874	-7.638538	-15.595498
O	7.916231	-7.768225	-16.802240
H(Iso=2)	6.196166	-9.674936	-16.623023
H	6.021868	-7.892462	-14.236915
C	7.360266	-9.591043	-14.059474
H	6.621958	-10.298058	-13.657697
H	7.903296	-9.128135	-13.224831
H	8.076512	-10.151056	-14.677211
N	8.357181	-6.777791	-14.813361
C	9.494845	-6.066220	-15.331536
C	10.619150	-7.018156	-15.713684
O	10.709668	-8.155877	-15.310492
O	11.472571	-6.445028	-16.549657
H(Iso=2)	8.152985	-6.745785	-13.808217
H	9.224860	-5.472817	-16.216282
H	9.863124	-5.371474	-14.564975
H(Iso=2)	12.091584	-7.131543	-16.908207
N	2.516198	-8.824893	-17.323885
H(Iso=2)	2.167965	-8.392717	-16.454756
H(Iso=2)	2.740414	-8.059584	-17.969030
C	0.782447	3.384370	0.467978
C	0.662487	4.401916	1.600671
O	0.444348	5.578058	1.320514
H	0.266453	2.439960	0.656885
H	1.847681	3.175452	0.308880
N	0.832698	3.902971	2.831154
C	1.098306	4.752976	3.975399
C	2.607182	5.046842	3.992481
O	3.237291	5.114535	2.932972
H(Iso=2)	1.027924	2.902086	2.910123
H	0.609564	5.719187	3.777746
C	0.535422	4.138048	5.250713
H	-0.533533	3.930068	5.112440
H	0.626903	4.831837	6.098085
H	1.046856	3.197298	5.503289
N	3.226006	5.228022	5.169604
C	4.655309	5.446197	5.176985
C	5.359807	4.339797	4.400629
O	5.014170	3.177934	4.431141
O	6.384081	4.794643	3.695721
H(Iso=2)	2.733354	5.106997	6.043712

H	4.911689	6.416343	4.731215
H	5.011480	5.432065	6.214397
H(Iso=2)	6.709139	4.077382	3.103738
N	0.238939	4.042763	-0.739990
H(Iso=2)	0.261561	5.061690	-0.524882
H(Iso=2)	0.776495	3.848519	-1.588056
H(Iso=2)	1.762300	-9.375219	-17.745660
H(Iso=2)	1.604873	-9.958929	-13.227962
H(Iso=2)	1.273122	-8.637499	-6.761308
H(Iso=2)	-2.142838	-3.541910	-6.075364
H	-3.264082	0.412125	-2.363077
H(Iso=2)	-0.736125	3.787324	-0.918620
H(Iso=2)	-1.305309	-1.468632	1.635964
C	6.779059	-12.952582	-19.339835
C	7.250592	-11.772208	-18.495434
O	6.419744	-11.142225	-17.830941
H	7.026312	-13.886921	-18.821188
H	7.228096	-12.967293	-20.338042
N	8.560145	-11.545982	-18.519178
C	9.226341	-10.523798	-17.725704
C	10.159107	-9.768743	-18.668880
O	10.920877	-10.372073	-19.420025
H(Iso=2)	9.157415	-12.103692	-19.123171
H	8.457070	-9.843887	-17.345031
C	10.023325	-11.140438	-16.578075
H	9.356819	-11.731720	-15.934009
H	10.488565	-10.342116	-15.984105
H	10.809180	-11.801336	-16.972304
N	10.109908	-8.424199	-18.607903
C	10.951361	-7.655455	-19.488394
C	12.425714	-7.922074	-19.235512
O	12.932597	-8.033857	-18.133325
O	13.128998	-7.971591	-20.355045
H(Iso=2)	9.409843	-7.972051	-18.017633
H	10.735005	-7.865140	-20.545216
H	10.776387	-6.587533	-19.302154
H(Iso=2)	14.065656	-8.080036	-20.115724
N	5.307123	-12.858934	-19.456994
H(Iso=2)	4.953025	-12.419909	-18.592188
H(Iso=2)	5.016156	-12.258633	-20.235827
H(Iso=2)	4.858841	-13.771059	-19.582355

Table S5: List of final optimized geometries of the GAG oligomers arranged in the antiparallel configuration.

A: GAG dimer

C	0.830834	0.305701	2.894301
C	1.907180	1.350865	3.203907
O	2.186063	1.582031	4.380947
H	1.304599	-0.617691	2.542015
H	0.116640	0.642370	2.137407
N	2.479944	1.923095	2.144112
C	3.551050	2.892930	2.287368
C	3.429682	3.905570	1.154928
O	3.118522	3.558085	0.009111
H(Iso=2)	2.156064	1.653421	1.205816
H	3.417735	3.391805	3.256819
C	4.933948	2.233716	2.237238
H	5.015878	1.488305	3.040067
H	5.723707	2.986533	2.371361
H	5.084698	1.732230	1.270194
N	3.731051	5.171018	1.456901
C	3.751123	6.213076	0.461772
C	4.053284	7.526954	1.140873
O	4.250615	7.647461	2.327757
O	4.076162	8.529901	0.268643
H(Iso=2)	3.946494	5.451090	2.409632
H	4.516442	6.025923	-0.308119
H	2.783938	6.291866	-0.057839
N	0.149874	0.038449	4.182396
H(Iso=2)	0.797613	0.414682	4.908355
H(Iso=2)	-0.738599	0.540110	4.268202
H(Iso=2)	4.274323	9.346267	0.757539
H(Iso=2)	-0.030492	-0.953710	4.352774
C	5.171462	2.949347	-2.211832
C	4.752227	1.476001	-2.182926
O	5.329278	0.681571	-2.926142
H	5.785468	3.174051	-1.331940
H	4.319692	3.635483	-2.227402
N	3.785099	1.168976	-1.317504
C	3.319909	-0.194953	-1.142369
C	1.823882	-0.154361	-0.851622
O	1.329643	0.716773	-0.125777
H(Iso=2)	3.370143	1.926541	-0.758925
H	3.507362	-0.729183	-2.083557
C	4.045506	-0.907452	0.004480
H	5.125159	-0.927971	-0.197615
H	3.685357	-1.941289	0.104592
H	3.872720	-0.380839	0.954344
N	1.093771	-1.139933	-1.380192
C	-0.313920	-1.287703	-1.109652
C	-0.830135	-2.479491	-1.879376
O	-0.143854	-3.174726	-2.592053
O	-2.129769	-2.666583	-1.672191
H(Iso=2)	1.507148	-1.831485	-1.999363
H	-0.507193	-1.445747	-0.036954

H	-0.879563	-0.392325	-1.410414
N	6.001231	3.104738	-3.429228
H(Iso=2)	6.271435	2.132544	-3.693059
H(Iso=2)	5.479823	3.505638	-4.214094
H(Iso=2)	-2.405753	-3.442741	-2.188114
H(Iso=2)	6.838410	3.674075	-3.284528

B: GAG trimer

C	1.419054	-0.093519	2.716460
C	2.366377	1.051037	3.087817
O	2.740929	1.153666	4.256370
H	1.979955	-0.881982	2.201331
H	0.595109	0.227863	2.072705
N	2.731318	1.848536	2.082910
C	3.674120	2.934912	2.279761
C	3.293828	4.073325	1.340566
O	2.883811	3.855229	0.193785
H(Iso=2)	2.345676	1.668091	1.146149
H	3.584435	3.263092	3.324222
C	5.118683	2.503175	2.003654
H	5.389403	1.673454	2.670828
H	5.810808	3.338320	2.181792
H	5.228764	2.170426	0.961557
N	3.480617	5.309660	1.809688
C	3.268763	6.483976	1.001684
C	3.641369	7.701369	1.813717
O	4.036779	7.658336	2.955632
O	3.477998	8.820569	1.115536
H(Iso=2)	3.799780	5.470757	2.761037
H	3.882273	6.462659	0.087568
H	2.218641	6.575637	0.683283
N	0.913479	-0.627615	4.002291
H(Iso=2)	1.579267	-0.267596	4.719768
H(Iso=2)	-0.018481	-0.273682	4.237518
H(Iso=2)	3.728194	9.567299	1.685269
H(Iso=2)	0.880991	-1.649062	4.036031
C	4.861964	3.851250	-2.217583
C	4.617624	2.360991	-2.409006
O	5.213296	1.757750	-3.303613
H	5.652201	3.990971	-1.468556
H	3.967549	4.386157	-1.882195
N	3.767237	1.801382	-1.545799
C	3.508431	0.371444	-1.542950
C	2.058149	0.135968	-1.137604
O	1.519329	0.806378	-0.246958
H(Iso=2)	3.303419	2.403392	-0.853032
H	3.665072	-0.007397	-2.560154
C	4.428487	-0.376499	-0.571774
H	5.478666	-0.190680	-0.835115
H	4.236701	-1.457896	-0.623912
H	4.259084	-0.037911	0.460667
N	1.438126	-0.875370	-1.754887
C	0.110229	-1.277926	-1.370021

C	-0.194877	-2.669844	-1.858957
O	0.492279	-3.308881	-2.630612
O	-1.328991	-3.123316	-1.350089
H(Iso=2)	1.899375	-1.362621	-2.526678
H	-0.000471	-1.252052	-0.276850
H	-0.662883	-0.605277	-1.779214
N	5.340584	4.418840	-3.497091
H(Iso=2)	6.123445	3.862281	-3.901943
H(Iso=2)	4.597840	4.438473	-4.202972
H(Iso=2)	-1.496689	-4.007097	-1.720063
H(Iso=2)	5.670469	5.380928	-3.379437
C	2.926332	-3.581734	-5.553677
C	3.587138	-2.387437	-4.883328
O	3.019574	-1.823519	-3.945142
H	3.351334	-4.506151	-5.142865
H	3.058520	-3.584179	-6.640850
N	4.785759	-2.034360	-5.344383
C	5.533047	-0.950309	-4.738373
C	6.432330	-0.343719	-5.810980
O	6.779400	-0.979628	-6.802722
H(Iso=2)	5.206765	-2.481677	-6.154555
H	4.820773	-0.188214	-4.401406
C	6.362362	-1.420506	-3.539838
H	5.704265	-1.891894	-2.796743
H	6.862317	-0.562729	-3.069496
H	7.121277	-2.151589	-3.854921
N	6.834691	0.912680	-5.546558
C	7.745257	1.604816	-6.416609
C	8.095397	2.952805	-5.844627
O	7.585998	3.448980	-4.858596
O	9.037183	3.554746	-6.552699
H(Iso=2)	6.442917	1.410293	-4.745481
H	8.676385	1.036636	-6.565878
H	7.316452	1.768753	-7.420152
N	1.482463	-3.557144	-5.236114
H(Iso=2)	1.313445	-3.388116	-4.220792
H(Iso=2)	0.997241	-2.808451	-5.741051
H(Iso=2)	9.206817	4.425494	-6.154279
H(Iso=2)	1.026764	-4.438640	-5.489527

C: GAG tetramer

C	2.414527	-0.445224	2.752329
C	3.418337	0.689388	2.979429
O	4.051701	0.715933	4.035169
H	2.838781	-1.179168	2.057431
H	1.460886	-0.092370	2.348998
N	3.533119	1.567013	1.981718
C	4.464285	2.679132	2.046493
C	3.819756	3.877814	1.361260
O	3.152291	3.743791	0.327934
H(Iso=2)	2.935255	1.445322	1.153539
H	4.640768	2.896171	3.108577
C	5.796574	2.360687	1.359159

H	6.244448	1.467725	1.816086
H	6.495372	3.202037	1.469373
H	5.640082	2.172444	0.286927
N	4.062871	5.073395	1.902882
C	3.603574	6.299026	1.299904
C	4.016787	7.454381	2.179592
O	4.631652	7.331505	3.213559
O	3.621123	8.617528	1.672633
H(Iso=2)	4.586734	5.166965	2.768697
H	4.034669	6.443946	0.296679
H	2.508793	6.307764	1.184978
N	2.229612	-1.085224	4.075191
H(Iso=2)	3.038363	-0.753240	4.644961
H(Iso=2)	1.371691	-0.781692	4.544674
H(Iso=2)	3.912039	9.321156	2.276844
H(Iso=2)	2.223392	-2.106996	4.038300
C	4.262897	4.110351	-2.548878
C	4.035363	2.630175	-2.818495
O	4.296638	2.164456	-3.930327
H	5.243015	4.243884	-2.072963
H	3.498464	4.538832	-1.891808
N	3.576744	1.923662	-1.784119
C	3.393763	0.485862	-1.865262
C	2.124399	0.102685	-1.115786
O	1.799491	0.658355	-0.058376
H(Iso=2)	3.335564	2.424313	-0.918489
H	3.276723	0.220194	-2.921651
C	4.581125	-0.284351	-1.277703
H	5.508245	0.019709	-1.782722
H	4.436984	-1.364423	-1.423871
H	4.684952	-0.086172	-0.200827
N	1.427934	-0.908633	-1.645810
C	0.276389	-1.451998	-0.974781
C	-0.087794	-2.798514	-1.541636
O	0.432661	-3.313507	-2.511107
O	-1.063962	-3.366673	-0.853430
H(Iso=2)	1.713540	-1.305864	-2.544214
H	0.468837	-1.564303	0.102057
H	-0.606959	-0.798220	-1.068664
N	4.280449	4.829519	-3.840803
H(Iso=2)	4.937962	4.390405	-4.519877
H(Iso=2)	3.355794	4.835005	-4.282857
H(Iso=2)	-1.276455	-4.218538	-1.271961
H(Iso=2)	4.563513	5.805982	-3.719841
C	2.409339	-3.360456	-5.719934
C	3.065271	-2.091289	-5.194918
O	2.594629	-1.523112	-4.206489
H	2.935773	-4.232997	-5.312617
H	2.429216	-3.423031	-6.813358
N	4.153203	-1.697065	-5.858865
C	4.940543	-0.556572	-5.427060
C	5.384675	0.232946	-6.652004
O	5.747911	-0.331844	-7.692288
H(Iso=2)	4.423507	-2.215782	-6.705354
H	4.299878	0.079367	-4.806444
C	6.171067	-0.977233	-4.616888

H	5.857691	-1.566509	-3.744020
H	6.714664	-0.088036	-4.266821
H	6.850476	-1.589636	-5.227392
N	5.409865	1.561713	-6.501676
C	5.923664	2.421999	-7.534876
C	6.345586	3.751664	-6.966431
O	6.112085	4.135596	-5.837437
O	6.999391	4.476313	-7.859190
H(Iso=2)	5.072174	1.977734	-5.630514
H	6.783585	1.953418	-8.033467
H	5.174721	2.621381	-8.320336
N	1.012493	-3.405090	-5.236490
H(Iso=2)	0.954862	-3.264397	-4.205720
H(Iso=2)	0.439668	-2.672997	-5.667809
H(Iso=2)	7.216808	5.334212	-7.455585
H(Iso=2)	0.571430	-4.303085	-5.454453
C	8.726935	-0.940000	-8.220756
C	8.452742	-2.436363	-8.041390
O	9.396146	-3.224613	-8.105057
H	8.676356	-0.435206	-7.249203
H	8.019102	-0.460150	-8.902910
N	7.181078	-2.764976	-7.805675
C	6.781488	-4.143200	-7.578914
C	5.385073	-4.332194	-8.158850
O	4.512146	-3.464641	-8.029343
H(Iso=2)	6.475365	-2.016239	-7.788981
H	7.499890	-4.784840	-8.106448
C	6.771175	-4.506408	-6.090066
H	7.768773	-4.336589	-5.662260
H	6.506454	-5.564735	-5.955324
H	6.041610	-3.888908	-5.546422
N	5.148601	-5.498642	-8.763275
C	3.849379	-5.853450	-9.276464
C	3.940299	-7.217932	-9.916795
O	4.952961	-7.876795	-9.966434
O	2.768685	-7.600036	-10.414849
H(Iso=2)	5.886090	-6.185900	-8.890728
H	3.091472	-5.884266	-8.478013
H	3.498833	-5.126999	-10.025638
N	10.110034	-0.842082	-8.742308
H(Iso=2)	10.534878	-1.776038	-8.555947
H(Iso=2)	10.138983	-0.683834	-9.753291
H(Iso=2)	2.884771	-8.479975	-10.811130
H(Iso=2)	10.665871	-0.110181	-8.293781

D: GAG pentamer

C	3.595495	-0.870348	2.669091
C	4.326607	0.463195	2.849572
O	5.095233	0.592377	3.802905
H	4.071750	-1.443978	1.865731
H	2.535428	-0.745570	2.430488
N	4.079114	1.388515	1.920966
C	4.742139	2.680158	1.939497

C	3.763745	3.727056	1.420775
O	2.997544	3.485087	0.479828
H(Iso=2)	3.403427	1.167017	1.177057
H	5.008871	2.896862	2.982673
C	6.008414	2.691828	1.075614
H	6.707140	1.924007	1.434989
H	6.502210	3.672358	1.132468
H	5.760831	2.482944	0.024687
N	3.822350	4.927554	2.002268
C	3.040570	6.047135	1.541506
C	3.405326	7.260902	2.362300
O	4.214804	7.252626	3.260600
O	2.724657	8.333899	1.972470
H(Iso=2)	4.442240	5.104865	2.787804
H	3.232108	6.262404	0.478845
H	1.960492	5.858824	1.643256
N	3.768355	-1.598315	3.947239
H(Iso=2)	4.568108	-1.123770	4.418794
H(Iso=2)	2.953499	-1.512213	4.561129
H(Iso=2)	2.996150	9.079917	2.533259
H(Iso=2)	3.969739	-2.593867	3.828877
C	3.671083	4.194252	-2.486863
C	3.721010	2.708076	-2.810899
O	3.960604	2.342233	-3.964251
H	4.624215	4.502742	-2.038906
H	2.865833	4.441890	-1.787222
N	3.512759	1.889485	-1.778728
C	3.616231	0.448057	-1.920805
C	2.553326	-0.213047	-1.053286
O	2.296293	0.196507	0.086569
H(Iso=2)	3.281071	2.301120	-0.864536
H	3.424786	0.199040	-2.970560
C	5.000047	-0.070866	-1.516975
H	5.771883	0.415238	-2.129732
H	5.058422	-1.157680	-1.672854
H	5.204467	0.144348	-0.458089
N	1.967173	-1.292947	-1.580953
C	1.037394	-2.080848	-0.814764
C	0.756712	-3.391662	-1.500566
O	1.129271	-3.691370	-2.617793
O	0.034501	-4.194025	-0.736785
H(Iso=2)	2.169356	-1.560549	-2.547376
H	1.431408	-2.284197	0.191727
H	0.072537	-1.564684	-0.675236
N	3.491545	4.946278	-3.747174
H(Iso=2)	4.207191	4.685531	-4.458373
H(Iso=2)	2.576064	4.762354	-4.169861
H(Iso=2)	-0.141917	-5.011017	-1.234224
H(Iso=2)	3.555867	5.955849	-3.589767
C	2.483026	-3.089594	-6.034177
C	3.146724	-1.860079	-5.430211
O	2.768514	-1.440006	-4.333771
H	3.095333	-3.977269	-5.829016
H	2.350318	-2.999408	-7.117465
N	4.127769	-1.324744	-6.156907
C	4.906040	-0.196595	-5.676599

C	5.194952	0.733968	-6.848120
O	5.560585	0.297953	-7.947870
H(Iso=2)	4.336682	-1.733882	-7.078440
H	4.302606	0.337909	-4.934825
C	6.226196	-0.641786	-5.040920
H	6.024443	-1.329411	-4.208018
H	6.776250	0.228993	-4.655878
H	6.856086	-1.160640	-5.778086
N	5.085527	2.041929	-6.591062
C	5.440136	3.026131	-7.580062
C	5.637098	4.377514	-6.944860
O	5.377163	4.652826	-5.790183
O	6.125038	5.252894	-7.807769
H(Iso=2)	4.738752	2.354389	-5.680911
H	6.363832	2.738290	-8.102715
H	4.662474	3.134361	-8.355428
N	1.169541	-3.279794	-5.381737
H(Iso=2)	1.257661	-3.316395	-4.344003
H(Iso=2)	0.526011	-2.512680	-5.599902
H(Iso=2)	6.202917	6.112282	-7.358968
H(Iso=2)	0.723570	-4.148399	-5.689662
C	8.520599	-0.183047	-8.650421
C	8.298802	-1.687008	-8.570082
O	9.264448	-2.453654	-8.629301
H	8.125900	0.324057	-7.763215
H	8.030265	0.240478	-9.534545
N	7.029948	-2.075172	-8.434975
C	6.671588	-3.482291	-8.363265
C	5.225268	-3.637201	-8.815606
O	4.365366	-2.789742	-8.539083
H(Iso=2)	6.303196	-1.354257	-8.327731
H	7.319351	-4.043033	-9.047880
C	6.828172	-4.055333	-6.950112
H	7.861874	-3.910598	-6.607950
H	6.606156	-5.131984	-6.954262
H	6.145298	-3.554615	-6.248100
N	4.939563	-4.766404	-9.470939
C	3.586510	-5.089737	-9.842113
C	3.438612	-6.566303	-10.102608
O	4.357549	-7.354426	-10.207709
O	2.167347	-6.912129	-10.222973
H(Iso=2)	5.690402	-5.414375	-9.721098
H	2.886763	-4.792542	-9.049097
H	3.269022	-4.560203	-10.756755
N	9.972884	0.071221	-8.747476
H(Iso=2)	10.469822	-0.322110	-7.941505
H(Iso=2)	10.393769	-0.366751	-9.597557
H(Iso=2)	2.128668	-7.862450	-10.426413
H(Iso=2)	10.171760	1.075177	-8.777674
C	7.956288	-8.058829	-11.370684
C	8.267393	-6.796809	-10.580690
O	7.350100	-6.179603	-10.034567
H	8.060548	-8.927091	-10.707935
H	8.609244	-8.195498	-12.239090
N	9.549869	-6.451113	-10.491814
C	9.974303	-5.292366	-9.731163

C	11.250849	-4.762926	-10.382437
O	11.929893	-5.464118	-11.125877
H(Iso=2)	10.276923	-6.934195	-11.013814
H	9.199824	-4.519965	-9.814612
C	10.190395	-5.617318	-8.250943
H	9.258948	-6.012716	-7.821855
H	10.465108	-4.707014	-7.701803
H	10.984693	-6.368629	-8.130079
N	11.556624	-3.494157	-10.037065
C	12.697826	-2.813720	-10.583425
C	12.315348	-1.504668	-11.232477
O	11.294140	-0.882397	-11.002901
O	13.243097	-1.076872	-12.072267
H(Iso=2)	10.875605	-2.964806	-9.491397
H	13.446992	-2.578463	-9.808317
H	13.183314	-3.465738	-11.319595
N	6.550233	-7.993842	-11.824542
H(Iso=2)	5.909987	-7.680443	-11.062654
H(Iso=2)	6.432545	-7.329311	-12.596167
H(Iso=2)	12.969621	-0.206653	-12.410882
H(Iso=2)	6.220375	-8.904231	-12.157514

E: GAG hexamer

C	3.684647	-1.033003	2.628957
C	4.500154	0.250955	2.808921
O	5.306945	0.313953	3.737267
H	4.082376	-1.607590	1.784944
H	2.623095	-0.838634	2.451218
N	4.275464	1.210385	1.910101
C	5.004538	2.465848	1.941103
C	4.064096	3.574204	1.483448
O	3.265229	3.400939	0.554322
H(Iso=2)	3.564874	1.045289	1.184337
H	5.312891	2.640444	2.980616
C	6.244497	2.437900	1.040805
H	6.920717	1.637220	1.370113
H	6.779416	3.396645	1.096435
H	5.959502	2.253159	-0.004968
N	4.187596	4.749635	2.104480
C	3.436498	5.912912	1.704512
C	3.860375	7.080688	2.562526
O	4.688665	7.009846	3.440672
O	3.208751	8.190381	2.230081
H(Iso=2)	4.829902	4.874035	2.882246
H	3.612078	6.162504	0.646606
H	2.352958	5.757044	1.823141
N	3.879891	-1.808415	3.875641
H(Iso=2)	4.709440	-1.369772	4.332232
H(Iso=2)	3.089145	-1.725066	4.520571
H(Iso=2)	3.518322	8.904579	2.812227
H(Iso=2)	4.052211	-2.803562	3.716181
C	3.940108	4.150078	-2.399177
C	3.875728	2.672748	-2.758012

O	4.071714	2.319102	-3.923587
H	4.905323	4.369805	-1.925910
H	3.142893	4.447373	-1.709605
N	3.628076	1.841526	-1.745587
C	3.641528	0.403105	-1.940046
C	2.586799	-0.236187	-1.048238
O	2.374420	0.162024	0.104414
H(Iso=2)	3.442813	2.239962	-0.814705
H	3.388160	0.203210	-2.987039
C	5.011802	-0.209449	-1.630325
H	5.779252	0.261503	-2.260286
H	4.998188	-1.289021	-1.838153
H	5.279415	-0.056647	-0.574471
N	1.956996	-1.291219	-1.577326
C	1.032740	-2.075560	-0.801337
C	0.754146	-3.392642	-1.476095
O	1.127782	-3.700842	-2.590733
O	0.032853	-4.189847	-0.706313
H(Iso=2)	2.137922	-1.552513	-2.549574
H	1.432842	-2.269843	0.204379
H	0.066365	-1.562332	-0.661358
N	3.850272	4.940697	-3.645491
H(Iso=2)	4.539821	4.622210	-4.359919
H(Iso=2)	2.924611	4.859870	-4.078051
H(Iso=2)	-0.142086	-5.011209	-1.197060
H(Iso=2)	4.017376	5.935306	-3.468790
C	2.498674	-3.125952	-5.999487
C	3.156669	-1.882734	-5.417876
O	2.765493	-1.434529	-4.337216
H	3.111720	-4.008031	-5.773407
H	2.374244	-3.056489	-7.085270
N	4.147043	-1.371890	-6.149848
C	4.923248	-0.224469	-5.714985
C	5.089333	0.727691	-6.895192
O	5.382838	0.310121	-8.022882
H(Iso=2)	4.347656	-1.799822	-7.063694
H	4.361513	0.279832	-4.920696
C	6.303104	-0.631616	-5.190495
H	6.191555	-1.336567	-4.355178
H	6.849901	0.254262	-4.836276
H	6.893967	-1.115938	-5.981770
N	4.948490	2.028013	-6.612741
C	5.190608	3.048309	-7.598401
C	5.694152	4.314263	-6.952477
O	5.647426	4.557860	-5.762234
O	6.180954	5.158653	-7.846749
H(Iso=2)	4.669577	2.309547	-5.670091
H	5.921818	2.694679	-8.337120
H	4.275874	3.310658	-8.157892
N	1.180591	-3.306439	-5.354014
H(Iso=2)	1.260655	-3.340554	-4.315697
H(Iso=2)	0.542493	-2.536829	-5.579352
H(Iso=2)	6.445291	5.972905	-7.384720
H(Iso=2)	0.732358	-4.173957	-5.661899
C	8.201825	0.038874	-9.191270
C	8.106267	-1.477519	-9.095227

O	9.095765	-2.170993	-9.352387
H	7.968375	0.513965	-8.232496
H	7.508281	0.427993	-9.945473
N	6.919549	-1.960124	-8.727706
C	6.690700	-3.390652	-8.625330
C	5.214892	-3.671302	-8.872951
O	4.333085	-2.878504	-8.516572
H(Iso=2)	6.168529	-1.296933	-8.492756
H	7.279359	-3.890273	-9.403523
C	7.098454	-3.957156	-7.260489
H	8.151038	-3.713699	-7.061158
H	6.985822	-5.050497	-7.261913
H	6.474015	-3.537520	-6.457706
N	4.941086	-4.849012	-9.443592
C	3.584082	-5.296449	-9.617898
C	3.528320	-6.791559	-9.793915
O	4.490735	-7.513952	-9.961769
O	2.283537	-7.237733	-9.756787
H(Iso=2)	5.707642	-5.451613	-9.753039
H	2.970815	-5.017128	-8.749871
H	3.105668	-4.840489	-10.501423
N	9.581740	0.394784	-9.582037
H(Iso=2)	10.258377	0.058236	-8.889033
H(Iso=2)	9.856800	-0.035386	-10.492258
H(Iso=2)	2.300001	-8.198571	-9.906609
H(Iso=2)	9.695025	1.408753	-9.662597
C	8.051718	-8.121737	-11.206585
C	8.335274	-6.729630	-10.662580
O	7.420567	-6.066140	-10.168360
H	8.209983	-8.852194	-10.402582
H	8.699281	-8.387005	-12.048878
N	9.607825	-6.338604	-10.734851
C	10.053972	-5.076776	-10.175485
C	11.092816	-4.468317	-11.110578
O	11.864936	-5.174215	-11.771366
H(Iso=2)	10.278963	-6.945120	-11.223376
H	9.191054	-4.404022	-10.120506
C	10.641026	-5.240785	-8.769942
H	9.888353	-5.689632	-8.106787
H	10.924388	-4.260136	-8.363372
H	11.527932	-5.891283	-8.787448
N	11.134726	-3.130151	-11.124191
C	12.102902	-2.416900	-11.914984
C	11.536386	-1.118664	-12.429881
O	10.532669	-0.577737	-12.004654
O	12.277677	-0.608484	-13.397480
H(Iso=2)	10.460205	-2.605399	-10.562307
H	13.011514	-2.170562	-11.338049
H	12.421101	-3.041245	-12.759645
N	6.632568	-8.195033	-11.615991
H(Iso=2)	5.993431	-7.823174	-10.881004
H(Iso=2)	6.454771	-7.649416	-12.465173
H(Iso=2)	11.895174	0.248053	-13.655768
H(Iso=2)	6.351780	-9.159718	-11.814062
C	14.719407	-5.502088	-10.644166
C	14.424848	-6.978220	-10.352891

O	15.288529	-7.655672	-9.794360
H	14.131746	-4.861868	-9.977084
H	14.493661	-5.228345	-11.679109
N	13.221449	-7.413104	-10.727769
C	12.792110	-8.779004	-10.484093
C	11.857119	-9.187348	-11.615657
O	11.031790	-8.392731	-12.083094
H(Iso=2)	12.585728	-6.756444	-11.198870
H	13.689322	-9.412880	-10.483788
C	12.060455	-8.927590	-9.145202
H	12.710760	-8.584359	-8.329116
H	11.798790	-9.980432	-8.968153
H	11.136486	-8.330330	-9.142707
N	11.941658	-10.453920	-12.029076
C	11.046139	-11.001492	-13.016574
C	11.388513	-12.456811	-13.225922
O	12.281336	-13.032251	-12.648177
O	10.586491	-13.020597	-14.123488
H(Iso=2)	12.640998	-11.088580	-11.653616
H	9.994882	-10.923280	-12.698034
H	11.131570	-10.473622	-13.979128
N	16.160048	-5.316241	-10.352328
H(Iso=2)	16.445678	-6.198255	-9.869948
H(Iso=2)	16.728607	-5.214061	-11.197149
H(Iso=2)	10.851937	-13.950819	-14.218396
H(Iso=2)	16.352589	-4.515047	-9.746851

F: GAG heptamer

C	4.465057	-0.954879	2.536354
C	5.033713	0.446320	2.716124
O	5.871911	0.653760	3.595720
H	5.042665	-1.479711	1.764444
H	3.411806	-0.948475	2.237024
N	4.580551	1.363633	1.858777
C	5.100556	2.721383	1.843065
C	3.969713	3.672832	1.470538
O	3.161362	3.392259	0.575145
H(Iso=2)	3.857931	1.083755	1.181071
H	5.458920	2.960748	2.851434
C	6.246099	2.886966	0.838467
H	7.050707	2.176308	1.071398
H	6.650586	3.908175	0.890136
H	5.895293	2.699689	-0.186557
N	3.948737	4.838905	2.123723
C	3.001228	5.867514	1.780981
C	3.457018	7.210766	2.288932
O	4.392220	7.394932	3.042149
O	2.697162	8.187931	1.821835
H	4.603139	5.005090	2.892075
H(Iso=2)	2.868188	5.923280	0.691563
H	2.003621	5.673583	2.210648
N	4.624911	-1.695892	3.806469
H(Iso=2)	5.587813	-1.603193	4.193931

H(Iso=2)	3.981284	-1.355959	4.527927
H(Iso=2)	3.009014	9.025427	2.205751
H(Iso=2)	4.435753	-2.694431	3.682331
C	3.437412	4.186431	-2.452055
C	3.609901	2.713790	-2.795393
O	3.755682	2.374845	-3.972682
H	4.382965	4.592924	-2.070271
H	2.662002	4.346214	-1.695145
N	3.600990	1.878592	-1.755711
C	3.825333	0.454268	-1.928429
C	2.899584	-0.310124	-0.992051
O	2.721681	0.047690	0.180375
H(Iso=2)	3.430629	2.265549	-0.816485
H	3.572349	0.199943	-2.963523
C	5.278526	0.059407	-1.647748
H	5.951313	0.624017	-2.308281
H	5.420844	-1.015040	-1.832717
H	5.549139	0.274477	-0.603772
N	2.342237	-1.413581	-1.500545
C	1.532413	-2.278636	-0.682690
C	1.159803	-3.527247	-1.437179
O	1.402805	-3.735768	-2.609115
O	0.520642	-4.388251	-0.663247
H(Iso=2)	2.469929	-1.639245	-2.490182
H	2.062627	-2.569848	0.236731
H	0.599091	-1.786358	-0.362766
N	3.091520	4.918151	-3.689406
H(Iso=2)	3.788735	4.742268	-4.444019
H(Iso=2)	2.177909	4.631819	-4.054899
H(Iso=2)	0.284156	-5.164107	-1.199907
H(Iso=2)	3.054648	5.927857	-3.525071
C	2.589708	-3.009965	-6.056027
C	3.256804	-1.786018	-5.444489
O	2.925221	-1.412427	-4.316746
H	3.225988	-3.890537	-5.900195
H	2.414359	-2.893006	-7.130633
N	4.187294	-1.204147	-6.201496
C	4.961717	-0.067927	-5.731128
C	5.131000	0.911621	-6.886094
O	5.507561	0.531276	-8.003108
H(Iso=2)	4.353738	-1.577642	-7.146842
H	4.394004	0.416181	-4.928680
C	6.338931	-0.490782	-5.213706
H	6.223817	-1.209652	-4.390811
H	6.892581	0.384639	-4.844237
H	6.923966	-0.964877	-6.015153
N	4.900484	2.197856	-6.603005
C	5.125120	3.224284	-7.587478
C	5.219360	4.579495	-6.937275
O	4.954401	4.817047	-5.775188
O	5.618421	5.503742	-7.794671
H(Iso=2)	4.541200	2.461645	-5.682123
H	6.050853	3.028029	-8.146926
H	4.312658	3.270290	-8.332757
N	1.307039	-3.241197	-5.357677
H(Iso=2)	1.438033	-3.300201	-4.325859

H(Iso=2)	0.641902	-2.481399	-5.532199
H(Iso=2)	5.628530	6.361383	-7.335827
H(Iso=2)	0.864845	-4.110466	-5.668893
C	8.419820	0.096543	-9.021039
C	8.218380	-1.409004	-8.943194
O	9.175777	-2.169756	-9.112235
H	7.910006	0.619764	-8.205056
H	8.026283	0.478746	-9.971346
N	6.968751	-1.807099	-8.699293
C	6.628847	-3.219000	-8.649690
C	5.159356	-3.383146	-9.011290
O	4.305112	-2.562579	-8.648491
H(Iso=2)	6.252696	-1.095872	-8.497267
H	7.237295	-3.746899	-9.393235
C	6.886318	-3.833180	-7.268601
H	7.939318	-3.685024	-6.992970
H	6.676905	-4.912067	-7.291679
H	6.248246	-3.363857	-6.505443
N	4.849839	-4.493749	-9.686968
C	3.480826	-4.829268	-9.979686
C	3.353707	-6.284447	-10.346407
O	4.284604	-7.040290	-10.543294
O	2.086941	-6.651702	-10.442424
H(Iso=2)	5.594396	-5.117277	-10.008725
H	2.835634	-4.623634	-9.113879
H	3.078248	-4.237918	-10.819462
N	9.867889	0.387595	-8.969396
H(Iso=2)	10.285390	0.065391	-8.090306
H(Iso=2)	10.387821	-0.083303	-9.740988
H(Iso=2)	2.060169	-7.586114	-10.710929
H(Iso=2)	10.043578	1.393991	-9.041307
C	7.848288	-7.799851	-11.556894
C	8.196296	-6.507377	-10.832799
O	7.293378	-5.765839	-10.437670
H	7.828889	-8.623301	-10.831346
H	8.567004	-8.048256	-12.344943
N	9.498012	-6.281388	-10.653772
C	9.974578	-5.133076	-9.905327
C	11.249909	-4.616477	-10.558685
O	12.070526	-5.385004	-11.076432
H(Iso=2)	10.172116	-6.938734	-11.067918
H	9.207936	-4.352169	-9.952663
C	10.248154	-5.470696	-8.435923
H	9.333800	-5.864298	-7.970556
H	10.557717	-4.566069	-7.893949
H	11.041397	-6.227854	-8.350396
N	11.439735	-3.294072	-10.486981
C	12.647680	-2.689564	-10.984891
C	12.424727	-1.241924	-11.334150
O	11.437376	-0.595267	-11.041761
O	13.452634	-0.736574	-11.994004
H(Iso=2)	10.723781	-2.704652	-10.055056
H	13.466437	-2.728327	-10.245432
H	13.001029	-3.226793	-11.875306
N	6.492922	-7.665594	-12.132914
H(Iso=2)	5.799633	-7.343678	-11.424270

H(Iso=2)	6.473868	-6.981583	-12.895825
H(Iso=2)	13.276891	0.205647	-12.159648
H(Iso=2)	6.159942	-8.555345	-12.514668
C	14.571417	-6.243039	-9.490426
C	14.016726	-7.669363	-9.404179
O	14.652899	-8.514290	-8.773312
H	13.999740	-5.583445	-8.827711
H	14.535932	-5.832717	-10.503660
N	12.852390	-7.874976	-10.020762
C	12.186774	-9.165185	-9.991784
C	11.468775	-9.357480	-11.322385
O	10.884689	-8.419979	-11.879947
H(Iso=2)	12.423124	-7.090698	-10.529019
H	12.961505	-9.933523	-9.864440
C	11.171470	-9.269400	-8.848148
H	11.678277	-9.105006	-7.887424
H	10.709221	-10.266677	-8.836501
H	10.379207	-8.515603	-8.966589
N	11.460808	-10.597717	-11.816526
C	10.727883	-10.949077	-13.006713
C	10.907197	-12.425987	-13.264307
O	11.565627	-13.160305	-12.564715
O	10.250392	-12.813105	-14.353056
H(Iso=2)	11.964445	-11.352589	-11.359262
H	9.653234	-10.733867	-12.898518
H	11.083394	-10.386173	-13.883572
N	15.966848	-6.328893	-9.000209
H(Iso=2)	16.019622	-7.254065	-8.519182
H(Iso=2)	16.654100	-6.330735	-9.759274
H(Iso=2)	10.399029	-13.766695	-14.468343
H(Iso=2)	16.219582	-5.582370	-8.348649
C	6.751620	6.365698	5.824931
C	6.687399	5.007478	5.144532
O	5.842314	4.801331	4.270898
H	7.547364	6.965605	5.365914
H	6.941508	6.290240	6.901164
N	7.593929	4.109933	5.528623
C	7.669534	2.801546	4.909291
C	8.183321	1.816743	5.954587
O	8.868047	2.180879	6.906730
H(Iso=2)	8.238146	4.289600	6.294437
H	6.658082	2.504732	4.608986
C	8.576834	2.799164	3.675845
H	8.220485	3.543905	2.950718
H	8.558617	1.809694	3.198521
H	9.612939	3.043369	3.953222
N	7.860290	0.533484	5.710540
C	8.323746	-0.527189	6.562468
C	7.838256	-1.858208	6.053320
O	7.071814	-2.014483	5.123016
O	8.346745	-2.862862	6.748419
H(Iso=2)	7.212850	0.310695	4.953099
H	9.423183	-0.555367	6.618437
H	7.963015	-0.412067	7.598676
N	5.465282	7.061036	5.605212
H(Iso=2)	5.182104	7.041069	4.601705

H(Iso=2)	4.703366	6.621715	6.132217
H(Iso=2)	7.984984	-3.692133	6.392010
H(Iso=2)	5.513219	8.040151	5.901629

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C	4.303038	-0.474319	2.779879
C	5.011979	0.870152	2.877190
O	5.899607	1.023946	3.718803
H	4.825781	-1.105573	2.049889
H	3.255651	-0.382075	2.475610
N	4.616527	1.799380	2.005021
C	5.248683	3.108125	1.944019
C	4.217814	4.122074	1.462137
O	3.428146	3.850509	0.547392
H(Iso=2)	3.867815	1.560822	1.340229
H	5.577548	3.377315	2.955826
C	6.448763	3.124642	0.990691
H	7.180885	2.367404	1.301694
H	6.933004	4.111583	1.007888
H	6.129486	2.907316	-0.039013
N	4.267691	5.327098	2.037663
C	3.425083	6.402048	1.580745
C	3.924326	7.730098	2.088006
O	4.798187	7.879540	2.918681
O	3.279733	8.737172	1.521684
H(Iso=2)	4.872818	5.483643	2.847415
H	3.392480	6.429925	0.482456
H	2.382600	6.286675	1.923291
N	4.386303	-1.137575	4.100329
H(Iso=2)	5.351724	-1.110075	4.485663
H(Iso=2)	3.782054	-0.679923	4.790317
H(Iso=2)	3.612540	9.566091	1.906574
H(Iso=2)	4.096672	-2.118361	4.048067
C	3.853656	4.416002	-2.499843
C	3.939072	2.916469	-2.744964
O	4.108554	2.494346	-3.891667
H	4.826780	4.790687	-2.156360
H	3.099011	4.670712	-1.748562
N	3.831486	2.152115	-1.657358
C	3.952471	0.706996	-1.729359
C	2.931274	0.078591	-0.789507
O	2.704422	0.548814	0.333696
H(Iso=2)	3.651130	2.609472	-0.752528
H	3.725910	0.402150	-2.756997
C	5.358291	0.226002	-1.356291
H	6.098006	0.688792	-2.024388
H	5.424850	-0.866608	-1.460171
H	5.603081	0.497316	-0.319068
N	2.346413	-1.038505	-1.234317
C	1.450354	-1.790697	-0.395047
C	1.125847	-3.122409	-1.017806
O	1.462395	-3.476644	-2.130239
O	0.411370	-3.877537	-0.200413

H(Iso=2)	2.522166	-1.360050	-2.189571
H	1.891759	-1.966314	0.597307
H	0.498693	-1.259906	-0.225416
N	3.534191	5.082666	-3.780820
H(Iso=2)	4.210874	4.818971	-4.528480
H(Iso=2)	2.600871	4.826014	-4.117623
H(Iso=2)	0.207622	-4.712351	-0.655965
H(Iso=2)	3.554005	6.101739	-3.684510
C	2.714593	-3.038701	-5.628269
C	3.389247	-1.778808	-5.106420
O	3.084616	-1.337529	-3.995679
H	3.351519	-3.907614	-5.416970
H	2.533359	-2.992926	-6.707090
N	4.300727	-1.243194	-5.918826
C	5.079037	-0.079301	-5.533546
C	5.272304	0.805425	-6.758637
O	5.571588	0.330804	-7.862203
H(Iso=2)	4.446557	-1.672693	-6.842505
H	4.507792	0.473832	-4.779632
C	6.446436	-0.464463	-4.961416
H	6.313377	-1.116397	-4.086992
H	6.994370	0.436762	-4.650144
H	7.045538	-0.999905	-5.712324
N	5.155171	2.120797	-6.547547
C	5.426343	3.068587	-7.596756
C	5.579752	4.456953	-7.034219
O	5.343374	4.775951	-5.885562
O	5.999317	5.310141	-7.953130
H(Iso=2)	4.848496	2.464923	-5.634335
H	6.344111	2.799486	-8.139729
H	4.617562	3.101081	-8.346452
N	1.435702	-3.221543	-4.908932
H(Iso=2)	1.568339	-3.199240	-3.875523
H(Iso=2)	0.764319	-2.482381	-5.139697
H(Iso=2)	6.049692	6.193541	-7.549213
H(Iso=2)	0.997650	-4.114894	-5.149986
C	8.372663	-0.140546	-9.061901
C	8.202096	-1.642200	-8.877798
O	9.151940	-2.399963	-9.100468
H	8.143338	0.404020	-8.139250
H	7.711884	0.232583	-9.852714
N	6.994500	-2.037110	-8.475257
C	6.686455	-3.442036	-8.275719
C	5.204615	-3.661204	-8.548224
O	4.357740	-2.805204	-8.258420
H(Iso=2)	6.287274	-1.319746	-8.264502
H	7.270157	-4.028395	-8.994635
C	7.022613	-3.920572	-6.858469
H	8.083050	-3.725956	-6.647184
H	6.841151	-5.001319	-6.774118
H	6.406377	-3.398498	-6.111192
N	4.880943	-4.853338	-9.059493
C	3.505673	-5.237264	-9.242592
C	3.372705	-6.734738	-9.332551
O	4.298538	-7.514001	-9.445639
O	2.106825	-7.114125	-9.285997

H(Iso=2)	5.621136	-5.508769	-9.322605
H	2.888851	-4.875981	-8.408426
H	3.072351	-4.809744	-10.162991
N	9.773440	0.127032	-9.447015
H(Iso=2)	10.423748	-0.204444	-8.727014
H(Iso=2)	10.038006	-0.361473	-10.330828
H(Iso=2)	2.075214	-8.081467	-9.382603
H(Iso=2)	9.936774	1.129080	-9.577563
C	7.791237	-8.311116	-10.739422
C	8.172595	-6.936997	-10.207445
O	7.308478	-6.208848	-9.713327
H	7.909669	-9.047040	-9.933615
H	8.411070	-8.622556	-11.586770
N	9.468735	-6.634586	-10.291376
C	10.005992	-5.395354	-9.758973
C	11.066321	-4.874143	-10.721899
O	11.821226	-5.645120	-11.328305
H(Iso=2)	10.092156	-7.292817	-10.777029
H	9.189764	-4.667342	-9.697341
C	10.615640	-5.575273	-8.365203
H	9.855224	-5.969936	-7.676950
H	10.966531	-4.606948	-7.981366
H	11.464551	-6.274145	-8.395579
N	11.148288	-3.542104	-10.823684
C	12.145392	-2.912270	-11.649478
C	11.636187	-1.615995	-12.225146
O	10.665681	-1.004280	-11.819206
O	12.389595	-1.193926	-13.225110
H(Iso=2)	10.490346	-2.960571	-10.299112
H	13.065562	-2.678458	-11.085755
H	12.433807	-3.588940	-12.463772
N	6.366566	-8.293646	-11.135138
H(Iso=2)	5.756690	-7.891677	-10.390889
H(Iso=2)	6.214241	-7.730578	-11.977963
H(Iso=2)	12.046943	-0.333599	-13.523506
H(Iso=2)	6.025725	-9.237216	-11.340178
C	14.665554	-6.215508	-10.248742
C	14.261465	-7.664857	-9.964210
O	15.095754	-8.427337	-9.476273
H	14.276462	-5.567207	-9.454944
H	14.296911	-5.848191	-11.211197
N	12.997837	-7.975561	-10.258193
C	12.448000	-9.294672	-10.001101
C	11.503122	-9.642846	-11.144887
O	10.732471	-8.798729	-11.618904
H(Iso=2)	12.410901	-7.258721	-10.704881
H	13.287439	-10.002071	-9.973298
C	11.683865	-9.352568	-8.674035
H	12.355550	-9.077747	-7.849303
H	11.301672	-10.367804	-8.496050
H	10.833852	-8.654806	-8.688083
N	11.519689	-10.909964	-11.564483
C	10.608238	-11.402059	-12.566277
C	10.853860	-12.879164	-12.758688
O	11.697273	-13.508334	-12.162859
O	10.028695	-13.395306	-13.663801

H(Iso=2)	12.175127	-11.585540	-11.181532
H	9.559187	-11.248514	-12.269293
H	10.748198	-10.889166	-13.530625
N	16.145757	-6.195092	-10.198571
H(Iso=2)	16.407761	-7.066815	-9.689842
H(Iso=2)	16.572300	-6.235036	-11.128786
H(Iso=2)	10.231249	-14.342262	-13.747393
H(Iso=2)	16.527929	-5.380210	-9.712833
C	6.684199	6.803446	6.031151
C	6.603157	5.434128	5.375227
O	5.866103	5.265464	4.401003
H	7.585845	7.321944	5.682333
H	6.709616	6.745891	7.124442
N	7.379147	4.485393	5.894630
C	7.441248	3.170647	5.288348
C	7.908326	2.173075	6.341801
O	8.442836	2.521651	7.391417
H(Iso=2)	7.934676	4.661766	6.731648
H	6.428651	2.890853	4.969478
C	8.364802	3.138983	4.064349
H	8.082943	3.942206	3.369805
H	8.254236	2.178425	3.544204
H	9.417769	3.254279	4.355525
N	7.712456	0.887776	5.995086
C	8.259153	-0.188138	6.771794
C	7.648951	-1.494663	6.345783
O	6.788622	-1.631958	5.506135
O	8.169604	-2.539076	6.999238
H(Iso=2)	7.187777	0.672101	5.147305
H	9.354579	-0.250744	6.653226
H	8.066311	-0.045009	7.846548
N	5.505174	7.591096	5.612367
H(Iso=2)	5.352021	7.537593	4.582216
H(Iso=2)	4.646014	7.245251	6.051552
H(Iso=2)	7.724192	-3.344781	6.680727
H(Iso=2)	5.601967	8.577385	5.869064
C	11.459082	-2.683550	7.155763
C	11.931392	-1.336517	7.702218
O	12.035686	-1.198923	8.917545
H	12.337024	-3.297927	6.920408
H	10.826900	-2.609314	6.264960
N	12.227797	-0.405398	6.787231
C	12.743760	0.903645	7.137633
C	11.768028	1.970267	6.628191
O	11.034956	1.758313	5.669648
H(Iso=2)	12.022345	-0.576537	5.808537
H	12.790049	0.936107	8.234007
C	14.137301	1.127630	6.544659
H	14.829857	0.359403	6.914409
H	14.521511	2.116182	6.831228
H	14.100762	1.074131	5.446147
N	11.854218	3.151230	7.280264
C	10.981610	4.263055	7.017825
C	10.243993	4.662187	8.274972
O	10.515033	4.283807	9.385775
O	9.267569	5.551156	8.016552

H(Iso=2)	12.391284	3.191942	8.139064
H	11.537733	5.144376	6.658575
H	10.264780	3.977802	6.241454
N	10.703342	-3.325303	8.252426
H(Iso=2)	11.091222	-2.943555	9.134852
H(Iso=2)	9.707505	-3.067279	8.202329
H(Iso=2)	8.871097	5.802032	8.868701
H(Iso=2)	10.771896	-4.345742	8.252658