

A refined cluster-in-molecule local correlation approach for predicting the relative energies of large systems

Wei Li ^a, Yang Guo ^a and Shuhua Li*^a

^a School of Chemistry and Chemical Engineering, Key Laboratory of Mesoscopic Chemistry of Ministry of Education, Institute of Theoretical and Computational Chemistry, Nanjing University, Nanjing, 210093, P. R. China. E-mail: shuhua@nju.edu.cn

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7. α-helix acetyl(ala)₁₄NH₂
8. α-helix acetyl(ala)₁₈NH₂
9. α-helix acetyl(ala)₂₄NH₂
10. α-helix acetyl(ala)₃₀NH₂
11. β-strand acetyl(ala)₁₀NH₂
12. β-strand acetyl(ala)₁₄NH₂
13. β-strand acetyl(ala)₁₈NH₂
14. β-strand acetyl(ala)₂₄NH₂
15. β-strand acetyl(ala)₃₀NH₂

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1. Ic-(H₂O)₉₆
2. Ih-(H₂O)₉₆

D. Foldamer W

1. Foldamer W
2. Monomer in Foldamer W

A. Alanine peptides

1. 3₁₀-helix acetyl(ala)₁₀NH₂

H 25.708174 12.393408 -3.699258
C 25.992149 11.907181 -4.632387
H 27.048864 11.635901 -4.603076
H 25.833582 12.622883 -5.443457
C 25.086858 10.720920 -4.856389
O 23.893525 10.743793 -4.584492
N 25.665821 9.600284 -5.383000
H 26.612036 9.664606 -5.731696
C 24.824737 8.528705 -5.898938
H 24.086461 8.940668 -6.595591
C 25.676648 7.471574 -6.595223
H 26.405205 7.044610 -5.899792
H 25.031040 6.670829 -6.958549
H 26.207088 7.902665 -7.448265
C 23.989111 7.864142 -4.807168
O 22.952886 7.279569 -5.100465
N 24.465275 7.916450 -3.544149
H 25.314248 8.432353 -3.361883
C 23.722095 7.316210 -2.451000
H 23.536881 6.262607 -2.682515
C 24.497362 7.440230 -1.144086
H 24.676879 8.492501 -0.902059
H 23.913189 6.996086 -0.337188
H 25.456012 6.920384 -1.212475
C 22.325938 7.923440 -2.280932
O 21.465274 7.289543 -1.675636
N 22.109354 9.150857 -2.792187
H 22.826329 9.629733 -3.330678
C 20.787469 9.745444 -2.710086
H 20.470813 9.780660 -1.663057
C 20.802964 11.146807 -3.312830
H 21.116044 11.108084 -4.359860
H 19.801194 11.574736 -3.254173

H 21.499994 11.788689 -2.769346
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N 20.131874 8.045247 -4.366834
H 21.119239 7.937006 -4.581761
C 19.176500 7.178630 -5.029318
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H 20.678952 5.752213 -5.651391
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H 17.529339 7.641549 -2.076209
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2. 3₁₀-helix acetyl(ala)₁₄NH₂

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C 25.36138620 10.87176673 -4.45883067
O 24.18385092 10.87199166 -4.12290405
N 25.86831593 9.87207195 -5.24030658
H 26.79992824 9.97852236 -5.61680069
C 24.96219334 8.95828504 -5.92194657

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H 23.71440215	6.11347618	-3.18368154	H 16.72634844	9.30124480	-0.47301772
C 24.78082704	6.91391118	-1.48107654	C 14.64255440	7.01967692	-2.01488420
H 25.01137650	7.88640995	-1.03464105	O 13.51071967	7.05802895	-1.53246713
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O 21.73351329	6.97624358	-1.88061462	H 13.01032096	6.90842992	-4.16693678
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N 6.61294709 2.46803272 0.10268738
H 7.29428388 3.20252319 -0.07833613
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H 5.82002215 4.88137962 0.97862598
H 4.89702882 4.27682864 2.37829860
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H 2.35260474 0.67547561 0.77354443
H 1.80330309 -0.56956992 1.86296471

3. 3₁₀-helix acetyl(ala)₁₈NH₂

H 26.25005585 12.27451799 -2.55652612
C 26.45883131 12.10590774 -3.61274597
H 27.50256017 11.81520197 -3.74365256
H 26.28573944 13.04695507 -4.14177803
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O 24.31850922 11.03423460 -3.79293679
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O 16.62147939	4.59812976	-1.67058382	H 7.79182416	5.59998913	-2.49303376
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H 13.50204535	5.98641865	-6.13033445	N 6.95944460	2.19652243	-0.11134596
H 14.76870140	7.21175852	-5.87232304	H 7.67018961	2.92285387	-0.18635472
C 13.23310026	5.09975096	-3.61458910	C 5.94386389	2.32319257	0.91465216
O 12.05717490	4.88834221	-3.91308124	H 5.88265333	1.39252599	1.48818079

[illegible]

O	23.189118	8.518264	-5.636640	H	16.561821	6.096375	0.051044
N	25.016629	8.113218	-4.368299	C	16.885923	8.233349	-0.125062
H	25.951939	8.407121	-4.125121	H	17.000589	8.981915	-0.913635
C	24.386626	7.013828	-3.660307	H	16.029961	8.493563	0.499484
H	24.007784	6.291601	-4.390435	H	17.792529	8.240121	0.483896
C	25.379067	6.340657	-2.718891	C	15.327928	6.822989	-1.474376
H	25.756734	7.056356	-1.981867	O	14.281311	6.671035	-0.843287
H	24.875681	5.532329	-2.187229	N	15.350502	6.994666	-2.810031
H	26.220812	5.924507	-3.277420	H	16.232127	7.070030	-3.314710
C	23.145519	7.448715	-2.874390	C	14.119491	6.921519	-3.571768
O	22.321491	6.601166	-2.537812	H	13.405679	7.656628	-3.186402
N	23.019980	8.754781	-2.571742	C	14.401626	7.171365	-5.050605
H	23.695906	9.437519	-2.905058	H	15.112109	6.432910	-5.431075
C	21.827119	9.231177	-1.895626	H	13.469347	7.101795	-5.613244
H	21.700876	8.687782	-0.953866	H	14.835753	8.163682	-5.191206
C	21.932773	10.731656	-1.639290	C	13.411138	5.575242	-3.406549
H	22.057240	11.271183	-2.582284	O	12.201652	5.485802	-3.621954
H	21.023930	11.078171	-1.145265	N	14.164109	4.518008	-3.047226
H	22.793436	10.950678	-1.003604	H	15.153162	4.628089	-2.829590
C	20.551934	8.933318	-2.688133	C	13.543028	3.229000	-2.819784
O	19.468380	8.886349	-2.108670	H	13.000842	2.918543	-3.718963
N	20.675187	8.753321	-4.018262	C	14.601087	2.193943	-2.448017
H	21.588021	8.772447	-4.466217	H	15.138818	2.506894	-1.549176
C	19.513842	8.421490	-4.820173	H	14.118480	1.232302	-2.266357
H	18.746703	9.191752	-4.691171	H	15.327455	2.086851	-3.256568
C	19.909987	8.299788	-6.288744	C	12.474259	3.283261	-1.727230
H	20.681118	7.534046	-6.410913	O	11.583788	2.432117	-1.693990
H	19.034155	8.025683	-6.878505	N	12.567342	4.266763	-0.812558
H	20.308623	9.248199	-6.655578	H	13.285448	4.986511	-0.883152
C	18.837794	7.126819	-4.362905	C	11.546918	4.400712	0.208128
O	17.658477	6.920015	-4.646852	H	11.480169	3.473121	0.785926
N	19.583508	6.241870	-3.673761	C	11.871705	5.580996	1.119824
H	20.544521	6.454098	-3.415934	H	11.930537	6.504463	0.537744
C	18.977802	5.028246	-3.161134	H	11.093329	5.679746	1.878188
H	18.536376	4.461103	-3.986993	H	12.836111	5.427695	1.609014
C	20.023990	4.190445	-2.431591	C	10.149993	4.583735	-0.389222
H	20.459751	4.762123	-1.607572	O	9.153659	4.272180	0.264823
H	19.555415	3.287921	-2.036305	N	10.069052	5.118584	-1.622490
H	20.829104	3.909184	-3.114064	H	10.909124	5.317285	-2.164301
C	17.803880	5.313521	-2.222096	C	8.778751	5.269890	-2.264642
O	16.938133	4.455826	-2.047574	H	8.124790	5.881210	-1.634522
N	17.782311	6.505017	-1.594167	C	8.951231	5.910717	-3.639466
H	18.486057	7.215142	-1.789915	H	9.604220	5.296024	-4.264393
C	16.667286	6.851239	-0.734727	H	7.975689	6.009589	-4.118283

H	9.407656	6.898191	-3.541584	H	2.893001	0.370137	0.512247
C	8.038137	3.939397	-2.410020	C	1.271166	-0.618547	1.483972
O	6.811576	3.928787	-2.527283	H	1.166726	-1.707296	1.535931
N	8.777607	2.814025	-2.431534	C	1.875881	-0.075443	2.776021
H	9.785083	2.841656	-2.278128	H	1.976255	1.011588	2.718933
C	8.126017	1.522642	-2.515049	H	1.231484	-0.338173	3.616422
H	7.485487	1.493406	-3.402424	H	2.870296	-0.498028	2.935126
C	9.168594	0.409434	-2.570420	C	-0.161830	-0.103727	1.334538
H	9.808037	0.443042	-1.684569	O	-1.076847	-0.645439	1.957522
H	8.663533	-0.556696	-2.618857	N	-0.362718	0.955571	0.528845
H	9.803922	0.529749	-3.450778	H	0.401990	1.361778	-0.009919
C	7.169878	1.273580	-1.346969	C	-1.706871	1.445321	0.300064
O	6.257599	0.453412	-1.463490	H	-2.169483	1.713910	1.255550
N	7.384577	1.962662	-0.210549	C	-1.672478	2.649907	-0.636936
H	8.121012	2.665148	-0.154125	H	-1.205501	2.377123	-1.587003
C	6.472558	1.823641	0.906899	H	-2.691106	2.997171	-0.817832
H	6.418618	0.773006	1.210311	H	-1.087109	3.458298	-0.193326
C	6.934762	2.695693	2.071393	C	-2.626767	0.370450	-0.282208
H	6.995224	3.741768	1.759934	O	-3.847391	0.461584	-0.140616
H	6.227637	2.601025	2.897082	N	-2.050173	-0.638639	-0.962289
H	7.926748	2.385366	2.406685	H	-1.035708	-0.715838	-1.028538
C	5.034843	2.190757	0.532722	C	-2.864105	-1.716922	-1.486576
O	4.093234	1.746941	1.192055	H	-3.622513	-1.310980	-2.163802
N	4.861983	3.023296	-0.510843	C	-1.982936	-2.729671	-2.213127
H	5.657236	3.341458	-1.063053	H	-1.230974	-3.134719	-1.530783
C	3.527833	3.370228	-0.954965	H	-2.603648	-3.542164	-2.594472
H	2.966863	3.809694	-0.123340	H	-1.461280	-2.250411	-3.044427
C	3.601743	4.346266	-2.126266	C	-3.664589	-2.429269	-0.394018
H	4.159670	3.902325	-2.954824	O	-4.692700	-3.041994	-0.684991
H	2.591155	4.591162	-2.456937	N	-3.178829	-2.380006	0.861382
H	4.116960	5.260838	-1.824821	H	-2.355976	-1.821302	1.084406
C	2.709284	2.143489	-1.361622	C	-3.914067	-2.992927	1.949196
O	1.478212	2.203187	-1.371720	H	-4.083120	-4.051489	1.726072
N	3.382935	1.033530	-1.716511	C	-3.141427	-2.837862	3.256283
H	4.400771	0.997308	-1.667754	H	-2.969976	-1.780079	3.471964
C	2.659616	-0.179792	-2.039674	H	-3.712637	-3.288319	4.069605
H	1.963220	0.013875	-2.862152	H	-2.168627	-3.328983	3.181136
C	3.638293	-1.288884	-2.415639	C	-5.318867	-2.408438	2.111830
H	4.329691	-1.480454	-1.590766	O	-6.192405	-3.059529	2.686433
H	3.082676	-2.200140	-2.643032	N	-5.536543	-1.171235	1.626558
H	4.226926	-0.995948	-3.287676	H	-4.810127	-0.671615	1.115268
C	1.768910	-0.650450	-0.887384	C	-6.862524	-0.591332	1.690624
O	0.797310	-1.372956	-1.116237	H	-7.206073	-0.575638	2.730096
N	2.108540	-0.262440	0.356538	C	-6.846747	0.819890	1.109582

H	-6.498054	0.799108	0.073808
H	-7.854551	1.236697	1.147065
H	-6.169032	1.457616	1.681448
C	-7.906782	-1.435321	0.956324
O	-9.098874	-1.322593	1.243744
N	-7.467323	-2.266327	-0.008305
H	-6.471845	-2.368908	-0.200941
C	-8.400095	-3.138275	-0.692773
H	-9.194854	-2.540194	-1.150625
C	-7.668515	-3.958471	-1.751672
H	-6.868081	-4.542788	-1.290123
H	-8.375891	-4.631533	-2.238853
H	-7.219296	-3.300164	-2.498605
C	-9.135038	-4.080263	0.264395
O	-10.212334	-4.572401	-0.070154
N	-8.542458	-4.356194	1.442497
H	-7.672095	-3.900694	1.713661
C	-9.214449	-5.199658	2.410802
H	-9.466264	-6.158742	1.946101
C	-8.321667	-5.414198	3.629402
H	-8.073738	-4.454841	4.091481
H	-8.846024	-6.040328	4.353062
H	-7.388341	-5.900218	3.336271
C	-10.562609	-4.628630	2.858537
O	-11.405740	-5.371193	3.359268
N	-10.761497	-3.305065	2.700532
H	-10.062522	-2.717571	2.249620
C	-12.045388	-2.724191	3.038690
H	-12.291949	-2.963995	4.077980
C	-12.005525	-1.213422	2.829389
H	-11.752473	-0.982750	1.790982
H	-12.983651	-0.791415	3.066245
H	-11.247487	-0.759083	3.471650
C	-13.198267	-3.321776	2.225264
O	-14.349069	-3.242096	2.649828
N	-12.892661	-3.889640	1.042047
H	-11.925077	-3.982783	0.739444
C	-13.932315	-4.516120	0.247940
H	-14.756761	-3.807551	0.119799
C	-13.371157	-4.935282	-1.107010
H	-12.536887	-5.629342	-0.971433
H	-14.159148	-5.425216	-1.680782
H	-13.003753	-4.065396	-1.656998
C	-14.574856	-5.735930	0.927508

O	-15.629662	-6.176320	0.495157
N	-13.886443	-6.283022	1.956822
H	-13.017157	-5.863489	2.274370
C	-14.406411	-7.396857	2.718980
H	-15.136544	-7.906246	2.081936
C	-13.280871	-8.349410	3.112820
H	-12.494917	-7.799874	3.640376
H	-13.678216	-9.123903	3.769510
H	-12.844381	-8.806408	2.221662
C	-15.185711	-6.974430	3.976345
O	-15.593866	-7.825520	4.754064
N	-15.386564	-5.651234	4.147574
H	-15.049908	-4.938477	3.510922
H	-15.918665	-5.376710	4.957148

5. 3₁₀-helix acetyl(ala)₃₀NH₂

H	27.010370	11.838804	-2.241573
C	27.083827	11.950102	-3.323132
H	28.084425	11.672032	-3.658541
H	26.910972	13.002529	-3.563958
C	25.998227	11.126644	-3.970802
O	24.879091	11.015333	-3.486440
N	26.321630	10.499870	-5.141384
H	27.200553	10.729610	-5.583991
C	25.266334	9.944061	-5.977650
H	24.495140	10.702262	-6.152749
C	25.839406	9.456034	-7.304922
H	26.600424	8.688189	-7.137929
H	25.037777	9.026723	-7.907516
H	26.285095	10.284566	-7.861375
C	24.523020	8.798087	-5.295096
O	23.375438	8.526389	-5.630077
N	25.193815	8.093881	-4.357760
H	26.131105	8.376339	-4.108770
C	24.550517	6.995080	-3.661028
H	24.168894	6.281288	-4.397946
C	25.532374	6.306518	-2.719580
H	25.913313	7.013904	-1.976231
H	25.019396	5.499360	-2.195355
H	26.372789	5.886303	-3.277057
C	23.309768	7.435669	-2.877830
O	22.475219	6.593729	-2.553040
N	23.196287	8.740097	-2.563752

H	23.880715	9.418941	-2.887691	H	15.278604	6.553107	-5.469109
C	22.005705	9.222281	-1.887785	H	13.644469	7.243465	-5.649479
H	21.869293	8.669607	-0.952807	H	15.021342	8.284049	-5.209956
C	22.126507	10.718439	-1.613795	C	13.558291	5.692813	-3.460772
H	22.262402	11.267358	-2.549746	O	12.346788	5.622348	-3.672140
H	21.218732	11.069331	-1.120903	N	14.298994	4.619899	-3.122811
H	22.985774	10.920463	-0.970627	H	15.289348	4.713955	-2.903634
C	20.730748	8.946767	-2.688647	C	13.662048	3.335523	-2.914500
O	19.644121	8.907071	-2.114232	H	13.113698	3.046247	-3.816943
N	20.857630	8.776932	-4.019699	C	14.708032	2.281532	-2.562103
H	21.772673	8.788724	-4.463375	H	15.253857	2.575016	-1.661620
C	19.696378	8.462257	-4.828670	H	14.214104	1.323524	-2.392043
H	18.936380	9.239258	-4.697867	H	15.429245	2.176657	-3.375570
C	20.097566	8.346035	-6.296347	C	12.597152	3.386238	-1.818370
H	20.862870	7.574694	-6.419960	O	11.692324	2.549641	-1.798770
H	19.221947	8.082790	-6.891370	N	12.708346	4.349570	-0.884651
H	20.505583	9.293262	-6.655821	H	13.434089	5.062804	-0.945181
C	19.005375	7.171686	-4.382651	C	11.692038	4.476547	0.140991
O	17.824282	6.980209	-4.670367	H	11.616885	3.540060	0.703171
N	19.739541	6.272925	-3.699164	C	12.030361	5.638308	1.071323
H	20.702663	6.471704	-3.438026	H	12.096328	6.570804	0.504693
C	19.118394	5.062516	-3.197280	H	11.255231	5.731725	1.833749
H	18.675221	4.504981	-4.028718	H	12.994609	5.467879	1.555160
C	20.151944	4.209486	-2.467415	C	10.296602	4.683751	-0.450925
H	20.589642	4.771766	-1.637967	O	9.297525	4.357925	0.192107
H	19.671987	3.309626	-2.079740	N	10.218064	5.258958	-1.665982
H	20.957446	3.923556	-3.147479	H	11.058434	5.461462	-2.206045
C	17.943023	5.355001	-2.262383	C	8.926399	5.439230	-2.298399
O	17.064506	4.507815	-2.100629	H	8.281550	6.042842	-1.651781
N	17.934970	6.540183	-1.622219	C	9.100700	6.108907	-3.659263
H	18.647654	7.243630	-1.809680	H	9.747189	5.502849	-4.299160
C	16.821257	6.892391	-0.763608	H	8.125036	6.226877	-4.133598
H	16.703673	6.132112	0.015136	H	9.565142	7.090379	-3.540812
C	17.054679	8.266332	-0.140963	C	8.172385	4.119897	-2.471110
H	17.181026	9.020431	-0.922427	O	6.943288	4.118944	-2.559115
H	16.200029	8.531397	0.483363	N	8.904470	2.992585	-2.555949
H	17.959348	8.256686	0.470823	H	9.913579	3.007097	-2.412104
C	15.484745	6.887808	-1.508496	C	8.242908	1.709706	-2.679444
O	14.433717	6.738832	-0.883782	H	7.587129	1.719631	-3.556036
N	15.514206	7.077946	-2.841392	C	9.277629	0.593495	-2.796371
H	16.398509	7.148140	-3.342247	H	9.933733	0.591612	-1.922322
C	14.284818	7.031477	-3.607713	H	8.766595	-0.367713	-2.872030
H	13.579736	7.771466	-3.215710	H	9.896394	0.744177	-3.683863
C	14.575313	7.295235	-5.082544	C	7.307119	1.420291	-1.505005

O	6.379401	0.619733	-1.638302	H	-1.703654	1.580953	1.714314
N	7.556787	2.049760	-0.341664	C	-1.322360	2.842048	-0.008155
H	8.297138	2.746554	-0.268437	H	-0.928049	2.744807	-1.022689
C	6.667148	1.861531	0.786165	H	-2.341815	3.229403	-0.046576
H	6.615009	0.798166	1.041668	H	-0.688610	3.546755	0.534864
C	7.153752	2.678180	1.980561	C	-2.313709	0.550180	0.000338
H	7.209550	3.737622	1.717505	O	-3.517604	0.631186	0.252843
H	6.463649	2.545175	2.815427	N	-1.821216	-0.327273	-0.894674
H	8.151756	2.351828	2.281109	H	-0.817089	-0.416012	-1.048112
C	5.225518	2.250054	0.454584	C	-2.707680	-1.276378	-1.536885
O	4.289658	1.759030	1.088928	H	-3.508365	-0.739444	-2.055637
N	5.038882	3.158100	-0.521659	C	-1.924060	-2.147899	-2.514845
H	5.824397	3.506767	-1.069909	H	-1.117692	-2.670909	-1.994432
C	3.695832	3.532353	-0.915156	H	-2.597750	-2.875284	-2.970887
H	3.157582	3.937107	-0.051709	H	-1.476334	-1.530000	-3.296287
C	3.749008	4.557268	-2.045113	C	-3.434853	-2.165913	-0.527055
H	4.283690	4.145346	-2.904890	O	-4.504734	-2.698299	-0.829036
H	2.733164	4.824497	-2.340982	N	-2.845016	-2.355020	0.668269
H	4.278155	5.454783	-1.717381	H	-1.990652	-1.857162	0.915900
C	2.864414	2.327524	-1.357317	C	-3.509139	-3.141413	1.687596
O	1.635133	2.360286	-1.274351	H	-3.715089	-4.145295	1.302023
N	3.524159	1.268334	-1.863280	C	-2.641242	-3.213229	2.941425
H	4.543229	1.229894	-1.857842	H	-2.431587	-2.207274	3.314131
C	2.785499	0.086792	-2.261711	H	-3.161340	-3.786959	3.710351
H	2.040648	0.356408	-3.017465	H	-1.687214	-3.694021	2.714504
C	3.743544	-0.971944	-2.801871	C	-4.885034	-2.580648	2.050836
H	4.488331	-1.229992	-2.044622	O	-5.743450	-3.319544	2.537512
H	3.180106	-1.864723	-3.078453	N	-5.094920	-1.267285	1.843943
H	4.270876	-0.592276	-3.679851	H	-4.391482	-0.687069	1.387647
C	1.969092	-0.502473	-1.110568	C	-6.395760	-0.691030	2.117963
O	0.962474	-1.173947	-1.344795	H	-6.662802	-0.866965	3.165111
N	2.419245	-0.285809	0.139847	C	-6.380385	0.803908	1.810093
H	3.208968	0.334969	0.313541	H	-6.102720	0.972089	0.766394
C	1.673789	-0.793467	1.273572	H	-7.370202	1.223801	1.996946
H	1.546949	-1.876240	1.172326	H	-5.647151	1.312134	2.440189
C	2.398559	-0.455794	2.573780	C	-7.510672	-1.367684	1.318887
H	2.535557	0.625034	2.661260	O	-8.672396	-1.334577	1.729725
H	1.813653	-0.820229	3.420021	N	-7.172637	-1.960749	0.158611
H	3.385074	-0.924526	2.588962	H	-6.197955	-2.030505	-0.133061
C	0.247786	-0.243942	1.324443	C	-8.180105	-2.662142	-0.611257
O	-0.634627	-0.866957	1.918153	H	-8.996340	-1.976177	-0.860061
N	0.019072	0.939843	0.724943	C	-7.559815	-3.243256	-1.879209
H	0.748696	1.405387	0.186821	H	-6.744056	-3.924457	-1.623972
C	-1.322115	1.486075	0.692490	H	-8.323565	-3.782643	-2.441933

H	-7.149993	-2.443691	-2.500268	H	-14.610245	-5.142039	3.636927
C	-8.850173	-3.780346	0.189326	C	-16.429119	-5.492523	4.694920
O	-9.982313	-4.162336	-0.112413	H	-16.548124	-6.244676	5.481489
N	-8.143911	-4.333644	1.193157	C	-16.201819	-4.111249	5.303382
H	-7.237601	-3.955780	1.468061	H	-16.068795	-3.367000	4.513884
C	-8.743701	-5.364314	2.016298	H	-17.061774	-3.841237	5.918428
H	-9.062725	-6.199922	1.385065	H	-15.300823	-4.113032	5.920821
C	-7.746532	-5.837990	3.070683	C	-17.764192	-5.508875	3.947213
H	-7.422161	-4.997358	3.689421	O	-18.817019	-5.634796	4.573828
H	-8.216936	-6.595531	3.699832	N	-17.729268	-5.355254	2.609828
H	-6.862946	-6.264751	2.590931	H	-16.842998	-5.303724	2.109615
C	-10.025872	-4.888840	2.702307	C	-18.955579	-5.420733	1.840669
O	-10.878612	-5.705755	3.054537	H	-19.664092	-4.675609	2.216692
N	-10.155310	-3.566741	2.923863	C	-18.660429	-5.183506	0.362432
H	-9.467766	-2.903956	2.567176	H	-17.950942	-5.928929	-0.006024
C	-11.368535	-3.049734	3.523764	H	-19.589469	-5.251821	-0.205855
H	-11.530971	-3.526827	4.495621	H	-18.217767	-4.195413	0.217697
C	-11.270800	-1.534189	3.678426	C	-19.682127	-6.757596	2.008275
H	-11.100849	-1.065322	2.705811	O	-20.888234	-6.833645	1.775469
H	-12.197354	-1.153427	4.111364	N	-18.945390	-7.820205	2.387226
H	-10.433207	-1.273632	4.329236	H	-17.958482	-7.718980	2.618362
C	-12.614645	-3.400138	2.709319	C	-19.585441	-9.100277	2.615342
O	-13.718472	-3.440931	3.255514	H	-20.130301	-9.402729	1.715096
N	-12.450267	-3.623312	1.391541	C	-18.541974	-10.148991	2.988474
H	-11.520677	-3.644864	0.973670	H	-18.001155	-9.841806	3.887637
C	-13.586414	-3.998241	0.575104	H	-19.039480	-11.102703	3.171974
H	-14.367054	-3.235438	0.662261	H	-17.815634	-10.267475	2.181252
C	-13.156898	-4.163996	-0.879967	C	-20.656417	-9.034903	3.706798
H	-12.373876	-4.922313	-0.959739	O	-21.542228	-9.887128	3.751230
H	-14.018322	-4.463838	-1.478998	N	-20.561498	-8.039728	4.611474
H	-12.757278	-3.223639	-1.265988	H	-19.845939	-7.319663	4.530659
C	-14.254626	-5.285376	1.061359	C	-21.580657	-7.897966	5.631912
O	-15.430829	-5.515157	0.775064	H	-21.669581	-8.835120	6.190932
N	-13.504366	-6.143542	1.777819	C	-21.226529	-6.744161	6.565435
H	-12.550386	-5.908867	2.049379	H	-21.140261	-5.812826	5.999061
C	-14.103634	-7.349499	2.312827	H	-22.007604	-6.637499	7.320044
H	-14.532099	-7.940661	1.496938	H	-20.268844	-6.930942	7.056979
C	-13.058131	-8.159762	3.074359	C	-22.977650	-7.668663	5.045423
H	-12.638187	-7.564425	3.889239	O	-23.972641	-7.936467	5.715504
H	-13.522507	-9.059168	3.482218	N	-23.048379	-7.136456	3.809198
H	-12.240310	-8.444532	2.408669	H	-22.206572	-6.980362	3.258357
C	-15.289508	-7.051374	3.232794	C	-24.337458	-6.932621	3.176851
O	-16.160324	-7.903636	3.410607	H	-24.986602	-6.382516	3.865599
N	-15.311031	-5.852114	3.846552	C	-24.162430	-6.158213	1.874416

H	-23.494225	-6.700492	1.199544	C	21.564011	3.891440	1.584504
H	-25.137260	-6.038034	1.399762	H	21.881972	4.916486	1.798078
H	-23.725731	-5.175266	2.067665	H	20.945269	3.546001	2.414286
C	-25.098465	-8.236907	2.890850	H	22.444502	3.247690	1.517474
O	-26.284254	-8.186296	2.598403	C	19.467711	4.654731	0.444185
N	-24.375278	-9.379699	2.942003	O	18.435498	4.116304	0.824938
H	-23.392279	-9.356480	3.197856	N	19.562096	5.983308	0.212473
C	-24.982583	-10.678870	2.755050	H	20.358234	6.347525	-0.297691
H	-25.927456	-10.512410	2.227648	C	18.363293	6.803531	0.280491
C	-24.066800	-11.589726	1.942426	H	17.869561	6.616809	1.237946
H	-23.085572	-11.655823	2.422976	C	18.722008	8.278335	0.130162
H	-24.504963	-12.586703	1.887247	H	19.240841	8.449861	-0.817480
H	-23.932868	-11.186382	0.936033	H	17.811564	8.880101	0.148135
C	-25.363966	-11.373579	4.073250	H	19.366719	8.596414	0.952983
O	-25.765678	-12.528640	4.060071	C	17.342843	6.386946	-0.781616
N	-25.244735	-10.639300	5.199134	O	16.143972	6.362501	-0.526127
H	-24.892120	-9.689642	5.222658	N	17.831547	6.083303	-2.002727
H	-25.512627	-11.086466	6.060508	H	18.831158	6.086820	-2.173844

6. α -helix acetyl(ala)₁₀NH₂

H	22.741553	8.768635	-1.361250	C	16.208774	4.329116	-2.588166
C	23.024065	8.237092	-2.270318	O	15.024664	4.142680	-2.847273
H	24.087177	7.993406	-2.241980	N	16.967667	3.423303	-1.940257
H	22.834133	8.903107	-3.116126	H	17.950878	3.605646	-1.770488
C	22.144895	7.021576	-2.415772	C	16.369177	2.188262	-1.468859
O	20.941203	7.047566	-2.170960	H	15.868614	1.683335	-2.301208
N	22.741895	5.870502	-2.831637	C	17.443589	1.297846	-0.853154
H	23.692916	5.907388	-3.171391	H	17.910164	1.808820	-0.005110
C	21.910661	4.742100	-3.227551	H	16.996525	0.365348	-0.503627
H	21.202900	5.055772	-4.003487	H	18.211053	1.065045	-1.596817
C	22.776288	3.591106	-3.730371	C	15.258594	2.473103	-0.451902
H	23.470993	3.258419	-2.953732	O	14.212096	1.832654	-0.464473
H	22.138451	2.750653	-4.008488	N	15.521357	3.431255	0.456918
H	23.346827	3.894013	-4.612154	H	16.407598	3.925202	0.438137
C	21.030065	4.267055	-2.074132	C	14.512043	3.797560	1.433302
O	19.908784	3.826650	-2.295678	H	14.201420	2.908167	1.991131
N	21.553230	4.307280	-0.828992	C	15.070106	4.865970	2.368115
H	22.483904	4.673654	-0.686535	H	15.344046	5.755390	1.792308
C	20.755952	3.837062	0.293108	H	14.316436	5.139270	3.109137
H	20.421713	2.814873	0.090123	H	15.956889	4.489131	2.885550

C	13.238382	4.300461	0.742694
O	12.126577	3.982121	1.147500
N	13.425836	5.130044	-0.305408
H	14.362316	5.373883	-0.610936
C	12.275275	5.629470	-1.033517
H	11.596049	6.140964	-0.343582
C	12.738812	6.566116	-2.144706
H	13.397383	6.027324	-2.832849
H	11.874702	6.942281	-2.696089
H	13.284871	7.413321	-1.719890
C	11.449200	4.474146	-1.610873
O	10.224386	4.483296	-1.573408
N	12.153778	3.473111	-2.181902
H	13.168713	3.493887	-2.177679
C	11.455419	2.320008	-2.716839
H	10.711344	2.649445	-3.448616
C	12.460808	1.361293	-3.347476
H	13.175989	1.027185	-2.589486
H	11.937979	0.493540	-3.754836
H	13.004987	1.861287	-4.153748
C	10.644153	1.595443	-1.633490
O	9.552603	1.096144	-1.887700
N	11.232247	1.510720	-0.424068
H	12.138016	1.941791	-0.269932
C	10.569301	0.852180	0.683157
H	10.228394	-0.136456	0.358760
C	11.531644	0.731531	1.860623
H	11.841770	1.731883	2.178442
H	11.024977	0.231520	2.687598
H	12.417616	0.158202	1.573490
C	9.291031	1.568713	1.145209
O	8.476671	0.969037	1.831253
N	9.175800	2.862685	0.775967
H	9.926078	3.306920	0.259643
C	8.016118	3.662404	1.096080
H	7.554022	3.222990	1.986484
C	8.428846	5.107659	1.358321
H	8.940758	5.504758	0.475549
H	7.539174	5.707517	1.552400
H	9.110745	5.156566	2.210558
C	6.927788	3.634307	0.009712
O	5.930263	4.331850	0.133075
N	7.137269	2.806989	-1.033841
H	7.992509	2.282625	-1.171894

H 6.433064 2.799155 -1.753129

7. α -helix acetyl(ala)₁₄NH₂

H	22.65512271	8.71618725	-1.2072337800
C	22.93166717	8.23359411	-2.1450218600
H	23.99365472	7.98382076	-2.1339494200
H	22.74240603	8.94548951	-2.9527855500
C	22.04700826	7.03148058	-2.3519035200
O	20.84564294	7.04658333	-2.0911660100
N	22.63458320	5.90541554	-2.8412781200
H	23.58205967	5.95916070	-3.1888520400
C	21.79666278	4.80149075	-3.2881445400
H	21.07846231	5.15858339	-4.0349278100
C	22.65311499	3.68007220	-3.8679456100
H	23.35987838	3.30366252	-3.1228360200
H	22.01006981	2.85670482	-4.1829638000
H	23.20974104	4.03170024	-4.7404219500
C	20.93211043	4.26266714	-2.1510081700
O	19.80542082	3.83957720	-2.3802694000
N	21.47416168	4.22756186	-0.9140324200
H	22.41173716	4.57376766	-0.7660178000
C	20.69241903	3.69550153	0.1914745700
H	20.34651344	2.68982823	-0.0665069500
C	21.52274304	3.66627462	1.4697603400
H	21.85261094	4.67398169	1.7396191200
H	20.91614366	3.27453694	2.2878827000
H	22.39659823	3.02168363	1.3475130200
C	19.41569583	4.51419565	0.4130414400
O	18.38287728	3.96477889	0.7783715800
N	19.52188902	5.85246461	0.2601131600
H	20.31442815	6.23526832	-0.2420808700
C	18.33587292	6.68200232	0.3989525200
H	17.85559370	6.44437356	1.3519672000
C	18.71079678	8.15919910	0.3321137000
H	19.21876386	8.38235644	-0.6105777900
H	17.80856582	8.76985417	0.4002311800
H	19.37065935	8.41908364	1.1631525900
C	17.29460331	6.34015444	-0.6691316600
O	16.09977725	6.29517511	-0.3935026800
N	17.76093377	6.11903181	-1.9153963500
H	18.75662930	6.15472775	-2.1066569200
C	16.83433147	5.72053488	-2.9610164100
H	16.04183347	6.47028946	-3.0486687300

C 17.57619111	5.55234179	-4.2826904600	C 10.57385437	1.71773765	-1.7686756500
H 18.35237432	4.78810408	-4.1806772000	O 9.44600783	1.30438637	-2.0292316600
H 16.87635540	5.24590674	-5.0623518400	N 11.18543692	1.48027137	-0.5941737400
H 18.03735418	6.49809418	-4.5802668700	H 12.12518900	1.82876699	-0.4231218500
C 16.11474312	4.42211229	-2.5787217300	C 10.48065762	0.76909260	0.4542451200
O 14.91750525	4.27274924	-2.8055056600	H 10.12168025	-0.19091141	0.0688562400
N 16.87762203	3.46338748	-2.0198366600	C 11.40619244	0.57143175	1.6506699900
H 17.87023141	3.61766018	-1.8737135500	H 11.73551293	1.54478014	2.0266899600
C 16.27601846	2.20774799	-1.6109865900	H 10.87777449	0.03949860	2.4443221100
H 15.75849675	1.75362193	-2.4622664600	H 12.28386657	-0.00980496	1.3551835700
C 17.35300789	1.27683558	-1.0624120000	C 9.21460168	1.52420929	
H 17.83368578	1.73732121	-0.1937195200	0.8731771500		
H 16.90554948	0.32801767	-0.7605726800	O 8.16862129	0.92278099	
H 18.10844986	1.08289980	-1.8288556800	1.1068402300		
C 15.18646458	2.44479796	-0.5608060300	N 9.33461548	2.85839041	
O 14.12412710	1.82911202	-0.6022772600	0.9957671700		
N 15.48041552	3.33146806	0.4073659400	H 10.22428271	3.31257040	0.8067632100
H 16.38169368	3.80015710	0.4199578100	C 8.17583482	3.65712638	
C 14.49716279	3.64047175	1.4280378400	1.3467222900		
H 14.18772287	2.71975962	1.9336653800	H 7.74409106	3.28540401	
C 15.08447208	4.64092418	2.4190705800	2.2819321600		
H 15.35978111	5.56139586	1.8953095000	C 8.58283068	5.12197689	
H 14.34871205	4.87387681	3.1911196600	1.4725632400		
H 15.97524207	4.22062479	2.8937070900	H 8.98579921	5.47689000	
C 13.21817571	4.19950519	0.7975372900	0.5190942400		
O 12.11036395	3.85784016	1.2054473600	H 7.71322842	5.72491585	
N 13.38796116	5.09835906	-0.1892197400	1.7416363700		
H 14.32243411	5.36065711	-0.4904698200	H 9.34832982	5.23563752	
C 12.23163793	5.66204232	-0.8588924500	2.2451613100		
H 11.56307724	6.11523037	-0.1197559100	C 7.06302468	3.49723743	
C 12.68633573	6.68917290	-1.8912519000	0.3040310100		
H 13.33314443	6.20880911	-2.6317521800	O 5.88632576	3.39656140	
H 11.81804006	7.11647030	-2.3965379100	0.6359507100		
H 13.24215525	7.49309327	-1.4012735000	N 7.45969151	3.50489695	-0.9852556700
C 11.39909255	4.56307891	-1.5256634300	H 8.44287338	3.59701016	-1.2249775100
O 10.17105306	4.58724370	-1.4865279700	C 6.47516371	3.31781812	-2.0320368300
N 12.09029750	3.60777675	-2.1735616000	H 5.68831738	4.07343525	-1.9370246200
H 13.10654782	3.63094946	-2.1888338900	C 7.15409386	3.39810134	-3.3957770700
C 11.38394479	2.50823252	-2.8014691400	H 7.91773881	2.61850028	-3.4767187900
H 10.64198734	2.90140393	-3.5041769300	H 6.41368321	3.26021899	-4.1865226300
C 12.38116233	1.59581171	-3.5089729600	H 7.63132236	4.37418622	-3.5210131500
H 13.09784931	1.19896095	-2.7836293600	C 5.74984810	1.97718721	-1.8671549800
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N 13.32037077	5.00133628	-0.08343358	C 7.09806861	3.51391585	-3.28809659
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C 12.15320994	5.59350946	-0.70711369	H 6.35444569	3.42628574	-4.08279169
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C 11.31799863	4.52777982	-1.42169467	C 5.85448570	-0.37624916	-1.46678178
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C 11.28290532	2.54480899	-2.80360104	H 6.48100737	-2.41368002	-1.13459209
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H	4.00412918	-0.71116358	2.22004873	H	-0.62532358	1.80391254	3.42777299
C	4.99744585	1.00936938	3.10635371	C	-3.18312419	0.83444617	1.31473886
H	5.28036794	2.02313491	2.80761704	O	-4.26812122	1.14182757	1.78764808
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H	5.89756854	0.46380030	3.40208682	H	-1.98525404	0.53749728	-0.32302301
C	3.02097509	1.02235180	1.55363041	C	-3.95821554	0.88141726	-1.00808002
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C	1.99242921	2.85039760	0.34775186	H	-4.13647144	1.55935916	-3.04100985
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O	-0.13256998	1.98550659	-0.39276813				
N	1.71818337	1.16626785	-1.40228965	9. α -helix acetyl(ala) ₂₄ NH ₂			
H	2.73173615	1.17710250	-1.48165228	H	22.491303	8.530916	-0.781200
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H	-0.34423021	-2.96839114	0.03140192	H	21.584712	3.282496	-4.654068
C	1.05199463	-2.63622206	1.66703507	H	22.765980	4.528524	-5.080967
H	1.45200131	-1.78500423	2.22649229	C	20.631966	4.350307	-2.368017
H	0.52894208	-3.30600182	2.35310543	O	19.486328	3.980084	-2.596712
H	1.88303130	-3.17557827	1.20367049	N	21.240496	4.109805	-1.186120
C	-1.11723160	-1.44376587	1.24912932	H	22.191643	4.417182	-1.038293
O	-2.17024491	-2.04658554	1.43883024	C	20.514323	3.404756	-0.141027
N	-0.91923935	-0.16691081	1.62831021	H	20.137306	2.459620	-0.543526
H	-0.02389994	0.28047087	1.45245094	C	21.415057	3.154986	1.062989
C	-1.98239845	0.60024372	2.24463622	H	21.779454	4.100223	1.476322
H	-2.39359296	0.03492196	3.08761988				

H	20.849444	2.637886	1.839688	N	13.227800	4.925048	0.053211
H	22.267946	2.531809	0.783567	H	14.156321	5.214054	-0.243497
C	19.264409	4.183457	0.284942	C	12.058096	5.593430	-0.484072
O	18.239233	3.588578	0.598774	H	11.423732	5.939572	0.338695
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C	18.614987	7.796364	0.847934	C	11.188082	4.608953	-1.270764
H	19.071196	8.170398	-0.073189	O	9.961069	4.629887	-1.174173
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C	17.125423	6.176557	-0.367400	C	11.100190	2.759252	-2.826604
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N	17.528012	6.156526	-1.654130	C	12.059466	1.949774	-3.694223
H	18.513851	6.214212	-1.888405	H	12.803580	1.458561	-3.060373
C	16.543211	5.943770	-2.699913	H	11.506502	1.193051	-4.254207
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C	17.206430	6.001003	-4.071897	C	10.321861	1.837956	-1.882523
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H	16.457156	5.843329	-4.849792	N	10.971220	1.430558	-0.779707
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C	15.826810	4.603098	-2.502447	C	10.292799	0.590172	0.187751
O	14.619020	4.498707	-2.704407	H	9.908397	-0.306905	-0.309382
N	16.596125	3.564554	-2.128161	C	11.253335	0.224121	1.315327
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C	15.994853	2.264308	-1.899803	H	10.747425	-0.415162	2.041582
H	15.427681	1.962757	-2.786451	H	12.116753	-0.311265	0.911605
C	17.078166	1.241672	-1.571268	C	9.054492	1.297448	0.745673
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C	14.960296	2.337807	-0.773260	C	8.065217	3.352918	1.542876
O	13.888899	1.740501	-0.860375	H	7.655180	2.859615	2.430581
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C	14.362746	3.226627	1.396198	H	7.644952	5.353541	2.233145
H	14.049803	2.243107	1.761751	H	9.282824	4.776012	2.617491
C	15.002133	4.047158	2.512335	C	6.923293	3.347873	0.522498
H	15.287123	5.032507	2.131625	O	5.753293	3.205993	0.879966
H	14.293717	4.171956	3.333433	N	7.275096	3.535681	-0.760282
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C	13.075762	3.896663	0.905281	C	6.264996	3.505329	-1.799414
O	11.974604	3.517612	1.302015	H	5.484325	4.240844	-1.578012

C	6.914554	3.782970	-3.152247	C	0.051057	-0.624041	-1.468079
H	7.672201	3.021495	-3.359553	O	-1.115949	-0.911910	-1.735773
H	6.158217	3.764457	-3.939576	N	0.753618	-1.246824	-0.507329
H	7.393483	4.765606	-3.141811	H	1.722966	-0.989032	-0.329506
C	5.545621	2.153823	-1.816866	C	0.118841	-2.260588	0.310853
O	4.324969	2.086059	-1.967824	H	-0.297142	-3.045595	-0.329824
N	6.324897	1.067476	-1.690448	C	1.135686	-2.833506	1.294291
H	7.333543	1.166985	-1.588274	H	1.518069	-2.033772	1.935640
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H	5.126439	-0.406146	-2.565754	H	1.971879	-3.279780	0.749695
C	6.823472	-1.307150	-1.542558	C	-1.083271	-1.678351	1.060182
H	7.393145	-1.139686	-0.623637	O	-2.133151	-2.312705	1.168839
H	6.379835	-2.304576	-1.516857	N	-0.905651	-0.464376	1.607080
H	7.502223	-1.240800	-2.396840	H	-0.013605	0.018192	1.511690
C	4.738502	-0.374060	-0.499472	C	-2.000547	0.179632	2.304789
O	3.658243	-0.948647	-0.640832	H	-2.370262	-0.478744	3.098152
N	5.138653	0.151239	0.669879	C	-1.530239	1.516294	2.871082
H	6.050392	0.598520	0.746906	H	-1.186053	2.159853	2.055933
C	4.259928	0.112326	1.821443	H	-2.351516	2.006791	3.397546
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C	4.968454	0.724609	3.026473	C	-3.197237	0.383679	1.370805
H	5.236150	1.762432	2.807221	O	-4.347372	0.184525	1.761310
H	4.311998	0.696117	3.898503	N	-2.913970	0.817365	0.130896
H	5.880401	0.164172	3.248126	H	-1.949433	0.989815	-0.146840
C	2.954289	0.857956	1.531291	C	-3.983109	1.000537	-0.830073
O	1.869572	0.408233	1.903523	H	-4.737256	1.680269	-0.419203
N	3.074738	2.029066	0.884457	C	-3.407626	1.540394	-2.136274
H	3.992713	2.372554	0.606830	H	-2.671857	0.834272	-2.532451
C	1.891047	2.790018	0.538048	H	-4.207489	1.678103	-2.866692
H	1.300215	2.985296	1.439267	H	-2.915890	2.500723	-1.959774
C	2.302134	4.092255	-0.142927	C	-4.726929	-0.316199	-1.076234
H	2.871640	3.869141	-1.050010	O	-5.952081	-0.342297	-1.188827
H	1.414789	4.671460	-0.406134	N	-3.959055	-1.413055	-1.194724
H	2.928191	4.684189	0.529730	H	-2.947151	-1.343763	-1.108829
C	0.972763	1.973392	-0.375343	C	-4.575961	-2.709468	-1.390194
O	-0.248981	1.978304	-0.220615	H	-5.232857	-2.676117	-2.265917
N	1.580432	1.289407	-1.359114	C	-3.491917	-3.770880	-1.554310
H	2.593074	1.328001	-1.462163	H	-2.865005	-3.796573	-0.658140
C	0.797568	0.459012	-2.251852	H	-3.950685	-4.750439	-1.703738
H	0.013499	1.060552	-2.724073	H	-2.864253	-3.533623	-2.417456
C	1.712791	-0.170945	-3.298110	C	-5.498527	-3.060816	-0.218217
H	2.471614	-0.783970	-2.802565	O	-6.587606	-3.600170	-0.410375
H	1.128076	-0.796146	-3.975997	N	-5.032162	-2.774370	1.009298
H	2.213007	0.611001	-3.875436	H	-4.116420	-2.345692	1.125039

C	-5.860162	-3.027177	2.172627	H	-12.530209	-1.570862	4.437540
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C	-5.087822	-2.661145	3.436691	C	-13.542224	-2.541386	2.179799
H	-4.819307	-1.600728	3.410103	O	-14.494427	-2.149966	2.842898
H	-5.704279	-2.856172	4.316689	N	-13.524328	-2.560796	0.833107
H	-4.172369	-3.255528	3.502639	H	-12.719437	-2.845654	0.286970
C	-7.170439	-2.234743	2.097146	H	-14.344498	-2.216308	0.362347
O	-8.240616	-2.735210	2.431520	10. α -helix acetyl(ala) ₃₀ NH ₂			
N	-7.061178	-0.959170	1.675233	H	22.323121	8.511481	-0.711965
H	-6.156757	-0.575237	1.412404	C	22.488455	8.283093	-1.765258
C	-8.255768	-0.151253	1.538514	H	23.541501	8.053330	-1.933652
H	-8.793136	-0.122005	2.492495	H	22.221873	9.172206	-2.342635
C	-7.874927	1.252988	1.078913	C	21.568652	7.160472	-2.169747
H	-7.366153	1.200356	0.111626	O	20.398125	7.103436	-1.795964
H	-8.772586	1.867654	0.982786	N	22.086257	6.191389	-2.972495
H	-7.201738	1.715743	1.806049	H	22.997780	6.332396	-3.385948
C	-9.240060	-0.793464	0.554599	C	21.190830	5.221716	-3.587114
O	-10.445308	-0.828921	0.783653	H	20.408498	5.743523	-4.149741
N	-8.700533	-1.287769	-0.579242	C	21.966064	4.280685	-4.504338
H	-7.696017	-1.245455	-0.733019	H	22.740520	3.744086	-3.948805
C	-9.551624	-1.955190	-1.543554	H	21.281001	3.550590	-4.938252
H	-10.361902	-1.285151	-1.848564	H	22.434729	4.836611	-5.320287
C	-8.715089	-2.392168	-2.742937	C	20.433415	4.416869	-2.534483
H	-7.931711	-3.080385	-2.410968	O	19.283759	4.050996	-2.749433
H	-9.351294	-2.894381	-3.475000	N	21.089334	4.090822	-1.399728
H	-8.245567	-1.523081	-3.212342	H	22.043627	4.394580	-1.265375
C	-10.261022	-3.167445	-0.925199	C	20.408062	3.300144	-0.385907
O	-11.423113	-3.440692	-1.215385	H	20.019611	2.386371	-0.846074
N	-9.511957	-3.917189	-0.094479	C	21.356173	2.964685	0.759666
H	-8.549798	-3.653139	0.100929	H	21.734826	3.877848	1.228605
C	-10.062862	-5.089839	0.552006	H	20.822388	2.388004	1.516796
H	-10.524894	-5.735048	-0.202970	H	22.198670	2.368362	0.401331
C	-8.955380	-5.833235	1.293576	C	19.173443	4.035308	0.148401
H	-8.525207	-5.173623	2.053584	O	18.159549	3.414474	0.447207
H	-9.377083	-6.716738	1.776139	N	19.300177	5.367631	0.334411
H	-8.166477	-6.135223	0.598972	H	20.058086	5.861889	-0.121732
C	-11.199894	-4.769986	1.533487	C	18.150277	6.139015	0.777778
O	-11.970502	-5.654553	1.879374	H	17.745726	5.672065	1.679826
N	-11.243901	-3.500335	1.990754	C	18.554833	7.585028	1.046969
H	-10.530020	-2.837090	1.708972	H	18.985766	8.034171	0.147417
C	-12.275733	-3.043004	2.891435	H	17.678118	8.162996	1.344793
H	-12.600049	-3.900506	3.489947	H	19.289927	7.626984	1.854015
C	-11.732825	-1.932662	3.787038				
H	-11.373422	-1.107452	3.163751				

C	17.016852	6.075790	-0.248250	C	10.897512	2.929073	-2.794540
O	15.847818	5.956670	0.107899	H	10.118825	3.487759	-3.324440
N	17.373431	6.177597	-1.544413	C	11.820609	2.211267	-3.774806
H	18.349590	6.278651	-1.804105	H	12.570601	1.636613	-3.223249
C	16.355688	6.057839	-2.573341	H	11.239227	1.535195	-4.404851
H	15.578276	6.810256	-2.407269	H	12.329037	2.940006	-4.411576
C	16.982720	6.217462	-3.954463	C	10.142211	1.916497	-1.929607
H	17.740401	5.444304	-4.111870	O	8.981544	1.600083	-2.192747
H	16.213240	6.122400	-4.722799	N	10.827280	1.385300	-0.903880
H	17.447101	7.203005	-4.046751	H	11.790848	1.664126	-0.730551
C	15.635439	4.709583	-2.462775	C	10.179513	0.446050	-0.009678
O	14.418225	4.630924	-2.613064	H	9.771672	-0.391222	-0.586060
N	16.411709	3.636152	-2.228129	C	11.180962	-0.040745	1.033853
H	17.418629	3.739210	-2.143897	H	11.557751	0.810858	1.608103
C	15.809485	2.322735	-2.098974	H	10.699329	-0.748684	1.711245
H	15.210129	2.103218	-2.988646	H	12.021858	-0.536032	0.541471
C	16.899025	1.273594	-1.898434	C	8.967591	1.092383	0.667092
H	17.469059	1.499566	-0.992180	O	7.914828	0.469631	0.812781
H	16.448519	0.284311	-1.799047	N	9.136062	2.349424	1.109427
H	17.576741	1.267974	-2.756212	H	10.028438	2.823961	0.984389
C	14.817901	2.295222	-0.933059	C	8.029094	3.051049	1.728922
O	13.736526	1.718405	-1.035696	H	7.645985	2.464643	2.570867
N	15.212058	2.906190	0.197557	C	8.488022	4.432867	2.185889
H	16.121803	3.356582	0.249880	H	8.846382	5.005674	1.325470
C	14.317849	2.954889	1.338950	H	7.657353	4.964897	2.653890
H	14.022040	1.938041	1.617253	H	9.300581	4.335274	2.910489
C	15.005889	3.663756	2.501603	C	6.851654	3.169534	0.756996
H	15.270187	4.684621	2.210046	O	5.692670	3.002656	1.140086
H	14.337713	3.698982	3.364097	N	7.160902	3.492320	-0.509393
H	15.915788	3.126261	2.781181	H	8.130966	3.645489	-0.779066
C	13.011266	3.664849	0.970220	C	6.114041	3.595575	-1.505992
O	11.925421	3.237391	1.360706	H	5.349871	4.302449	-1.165444
N	13.132039	4.781645	0.232356	C	6.715081	4.034139	-2.838208
H	14.049339	5.104379	-0.064825	H	7.456478	3.300114	-3.167880
C	11.945841	5.496922	-0.196610	H	5.929473	4.118148	-3.591766
H	11.338359	5.757494	0.676245	H	7.204528	5.004803	-2.724475
C	12.350496	6.746640	-0.973247	C	5.381479	2.260334	-1.660160
H	12.933253	6.463235	-1.854585	O	4.156777	2.219168	-1.789785
H	11.459322	7.291395	-1.290860	N	6.151719	1.160928	-1.672076
H	12.957719	7.399164	-0.340559	H	7.163377	1.241321	-1.585683
C	11.049108	4.598122	-1.052679	C	5.540588	-0.148786	-1.775072
O	9.825714	4.608418	-0.913437	H	4.905890	-0.190624	-2.666604
N	11.670110	3.834439	-1.966860	C	6.627584	-1.218716	-1.823442
H	12.682655	3.864825	-2.063619	H	7.229320	-1.176229	-0.910654

H	6.173537	-2.207732	-1.911960	N	-0.993906	-0.629762	1.659387
H	7.279778	-1.047765	-2.683872	H	-0.094914	-0.154247	1.592095
C	4.592333	-0.394335	-0.598266	C	-2.066146	-0.034752	2.431991
O	3.495776	-0.930863	-0.765563	H	-2.434759	-0.756687	3.168518
N	5.040093	-0.017625	0.610225	C	-1.565642	1.236136	3.112591
H	5.962487	0.403487	0.709026	H	-1.230805	1.952353	2.356607
C	4.192336	-0.174159	1.775645	H	-2.368120	1.681635	3.704121
H	3.882167	-1.220470	1.869150	H	-0.725902	0.999790	3.771256
C	4.943065	0.291397	3.020115	C	-3.273102	0.272084	1.539968
H	5.222782	1.343311	2.908859	O	-4.421987	0.057082	1.931420
H	4.310091	0.176455	3.902424	N	-3.001179	0.806592	0.338865
H	5.850769	-0.302970	3.152877	H	-2.037557	0.997769	0.067350
C	2.890641	0.614552	1.606141	C	-4.077670	1.090617	-0.588900
O	1.807426	0.138357	1.951046	H	-4.816259	1.742730	-0.110337
N	3.012170	1.848861	1.092527	C	-3.509816	1.736651	-1.849912
H	3.930555	2.212514	0.842317	H	-2.798068	1.054409	-2.323810
C	1.830104	2.653194	0.855863	H	-4.317832	1.961438	-2.549181
H	1.261758	2.755839	1.786538	H	-2.992127	2.664583	-1.593104
C	2.239037	4.017195	0.307146	C	-4.844077	-0.187960	-0.940739
H	2.781627	3.886546	-0.633743	O	-6.073428	-0.186849	-1.029298
H	1.351762	4.629065	0.131856	N	-4.098205	-1.280632	-1.169615
H	2.888996	4.527865	1.022395	H	-3.082345	-1.231448	-1.108903
C	0.879733	1.946974	-0.115490	C	-4.738040	-2.547074	-1.463018
O	-0.338595	1.951525	0.071957	H	-5.407335	-2.433665	-2.322599
N	1.449648	1.359738	-1.179498	C	-3.674327	-3.608657	-1.729891
H	2.459369	1.400177	-1.310498	H	-3.033962	-3.715472	-0.849416
C	0.631632	0.635856	-2.131314	H	-4.151252	-4.566021	-1.949922
H	-0.157342	1.292137	-2.514080	H	-3.057225	-3.312959	-2.582254
C	1.507080	0.110037	-3.265178	C	-5.643676	-2.976324	-0.305395
H	2.270751	-0.559675	-2.859301	O	-6.749466	-3.477926	-0.515058
H	0.894190	-0.433737	-3.986928	N	-5.147277	-2.799624	0.929644
H	2.000947	0.942922	-3.772198	H	-4.218997	-2.399808	1.057811
C	-0.107497	-0.515257	-1.443863	C	-5.950292	-3.141893	2.086129
O	-1.282018	-0.768753	-1.718556	H	-6.269054	-4.187616	2.018398
N	0.603857	-1.233701	-0.560774	C	-5.148287	-2.892848	3.360285
H	1.580169	-1.005655	-0.378901	H	-4.866263	-1.837482	3.417446
C	-0.032139	-2.310477	0.170890	H	-5.747190	-3.156567	4.234357
H	-0.480433	-3.019070	-0.533476	H	-4.239744	-3.500650	3.353805
C	0.992127	-3.001102	1.066529	C	-7.248340	-2.329266	2.099965
H	1.407861	-2.279868	1.776026	O	-8.322116	-2.848505	2.408954
H	0.515572	-3.816259	1.614912	N	-7.131854	-1.028682	1.785330
H	1.804584	-3.407827	0.458809	H	-6.219787	-0.634189	1.559651
C	-1.204102	-1.781621	1.002573	C	-8.312223	-0.190157	1.732350
O	-2.264557	-2.405652	1.074143	H	-8.844404	-0.240737	2.688397

C	-7.908285	1.244538	1.404012	C	-15.110938	-2.656627	-0.231396
H	-7.405633	1.273842	0.432698	O	-16.340182	-2.627765	-0.275332
H	-8.793956	1.882485	1.373323	N	-14.387041	-3.698585	-0.674690
H	-7.222566	1.622406	2.166898	H	-13.370264	-3.671126	-0.634301
C	-9.306452	-0.720702	0.695361	C	-15.056887	-4.888057	-1.163649
O	-10.515956	-0.745476	0.928634	H	-15.755087	-4.614661	-1.962055
N	-8.783413	-1.123480	-0.474273	C	-14.016883	-5.889240	-1.657690
H	-7.779229	-1.066474	-0.637804	H	-13.348514	-6.161085	-0.835047
C	-9.649062	-1.675210	-1.497123	H	-14.513492	-6.787242	-2.031059
H	-10.441617	-0.958031	-1.737245	H	-13.423318	-5.447060	-2.462475
C	-8.825541	-2.019750	-2.735193	C	-15.929005	-5.513130	-0.068611
H	-8.058333	-2.754726	-2.473872	O	-17.050764	-5.948909	-0.311985
H	-9.474926	-2.433165	-3.509667	N	-15.372380	-5.573509	1.157685
H	-8.337161	-1.121087	-3.120945	H	-14.434901	-5.212780	1.319142
C	-10.379602	-2.917074	-0.977939	C	-16.140810	-6.107543	2.263792
O	-11.565417	-3.115846	-1.245832	H	-16.468586	-7.126294	2.030597
N	-9.643428	-3.773652	-0.251481	C	-15.294089	-6.077799	3.533032
H	-8.660127	-3.580325	-0.070037	H	-15.005274	-5.046973	3.759656
C	-10.259862	-4.957957	0.311188	H	-15.864276	-6.486035	4.370365
H	-10.739313	-5.537483	-0.485037	H	-14.388042	-6.674213	3.393499
C	-9.205750	-5.788394	1.038005	C	-17.436623	-5.312830	2.460459
H	-8.757403	-5.194265	1.839834	O	-18.505462	-5.871421	2.689621
H	-9.665168	-6.683319	1.462850	N	-17.316655	-3.970747	2.392152
H	-8.419907	-6.087910	0.339537	H	-16.413904	-3.544213	2.197763
C	-11.397176	-4.579091	1.264571	C	-18.493587	-3.136926	2.531855
O	-12.452004	-5.213975	1.275633	H	-18.991843	-3.356629	3.481720
N	-11.157112	-3.547992	2.092153	C	-18.088896	-1.667719	2.448129
H	-10.262034	-3.062851	2.062415	H	-17.617106	-1.473330	1.480081
C	-12.191358	-3.093926	2.999836	H	-18.972223	-1.034009	2.553992
H	-12.534804	-3.931238	3.616910	H	-17.376686	-1.426196	3.242152
C	-11.649911	-1.958864	3.864014	C	-19.544124	-3.454787	1.459381
H	-11.331372	-1.130318	3.224447	O	-20.743855	-3.446996	1.724165
H	-12.425567	-1.610479	4.549147	N	-19.061832	-3.692661	0.225270
H	-10.790931	-2.306922	4.443884	H	-18.058863	-3.673663	0.060909
C	-13.431703	-2.633892	2.227578	C	-19.948508	-4.011436	-0.874899
O	-14.564506	-2.894645	2.631856	H	-20.734603	-3.251587	-0.938389
N	-13.200645	-1.908577	1.119691	C	-19.147820	-4.071281	-2.172605
H	-12.246565	-1.700443	0.831141	H	-18.381013	-4.847385	-2.086768
C	-14.312967	-1.463793	0.304750	H	-19.818604	-4.312394	-2.999097
H	-15.022230	-0.904314	0.924143	H	-18.659564	-3.111495	-2.363518
C	-13.794083	-0.609053	-0.847798	C	-20.705782	-5.334378	-0.685978
H	-13.103342	-1.197471	-1.459150	O	-21.717203	-5.555071	-1.337573
H	-14.629651	-0.274720	-1.466299	N	-20.155950	-6.205964	0.186476
H	-13.264780	0.264540	-0.458004	H	-19.279009	-5.976379	0.641608

C	-20.766262	-7.476785	0.497282
H	-21.358753	-7.779855	-0.372092
C	-19.689377	-8.512977	0.807241
H	-19.084167	-8.164498	1.650498
H	-20.163011	-9.459018	1.072800
H	-19.036091	-8.647051	-0.058294
C	-21.759864	-7.418304	1.668380
O	-22.339081	-8.437282	2.023358
N	-21.939516	-6.215126	2.246812
H	-21.419364	-5.384938	1.987147
H	-22.570468	-6.177284	3.030020

11. β -strand acetyl(ala)₁₀NH₂

H	-30.148066	-47.321737	0.851572
C	-29.809382	-46.995210	-0.133853
H	-30.506299	-46.253334	-0.527472
H	-29.802477	-47.870010	-0.786222
C	-28.389579	-46.480132	-0.007639
O	-27.469121	-47.199686	0.351521
N	-28.207352	-45.171864	-0.314570
H	-28.969857	-44.552041	-0.554757
C	-26.911198	-44.550740	-0.179729
H	-26.475545	-44.849007	0.782346
C	-25.958269	-44.970882	-1.305672
H	-26.362295	-44.655319	-2.271309
H	-24.967936	-44.525980	-1.176637
H	-25.862006	-46.057408	-1.289917
C	-27.138069	-43.039025	-0.193532
O	-28.213328	-42.549731	-0.522230
N	-26.069528	-42.292107	0.148628
H	-25.170565	-42.698169	0.381943
C	-26.105113	-40.848540	0.083202
H	-26.569789	-40.550287	-0.864795
C	-26.904126	-40.244059	1.243466
H	-26.434622	-40.506520	2.195113
H	-26.954363	-39.154819	1.165021
H	-27.918202	-40.645873	1.217571
C	-24.650402	-40.374923	0.113182
O	-23.733377	-41.138294	0.395221
N	-24.461267	-39.070082	-0.158958
H	-25.225591	-38.435017	-0.359224
C	-23.151318	-38.462768	-0.076382
H	-22.672537	-38.783484	0.857061

C	-22.261692	-38.862685	-1.259134
H	-22.711147	-38.521044	-2.195198
H	-21.263837	-38.425705	-1.168775
H	-22.169093	-39.949595	-1.277648
C	-23.375555	-36.949358	-0.044486
O	-24.470488	-36.458769	-0.297522
N	-22.288869	-36.211325	0.247569
H	-21.378151	-36.620771	0.424133
C	-22.324226	-34.765596	0.218284
H	-22.841514	-34.444950	-0.694259
C	-23.051128	-34.186762	1.437240
H	-22.527748	-34.473016	2.353211
H	-23.098976	-33.095903	1.386701
H	-24.067677	-34.582407	1.462819
C	-20.866863	-34.299365	0.176060
O	-19.941992	-35.074796	0.392997
N	-20.685982	-32.991202	-0.079950
H	-21.456510	-32.350744	-0.235574
C	-19.370748	-32.389024	-0.063649
H	-18.841121	-32.722505	0.837159
C	-18.550657	-32.774510	-1.300173
H	-19.053247	-32.422105	-2.204673
H	-17.549629	-32.337099	-1.261562
H	-18.458456	-33.861006	-1.337445
C	-19.589906	-30.875667	-0.001029
O	-20.694727	-30.381421	-0.198253
N	-18.490182	-30.142972	0.250626
H	-17.573494	-30.555570	0.383899
C	-18.524981	-28.696687	0.242860
H	-19.078407	-28.363254	-0.643427
C	-19.201172	-28.134682	1.498294
H	-18.640727	-28.432818	2.388162
H	-19.250866	-27.043318	1.464272
H	-20.215867	-28.531046	1.560216
C	-17.070026	-28.230862	0.147525
O	-16.138183	-29.009946	0.315755
N	-16.899083	-26.919405	-0.097681
H	-17.675429	-26.277501	-0.213912
C	-15.584415	-26.316287	-0.128856
H	-15.017503	-26.659517	0.745150
C	-14.816596	-26.685403	-1.403208
H	-15.358805	-26.325318	-2.281439
H	-13.816324	-26.244503	-1.402929
H	-14.722219	-27.771076	-1.456479

C -15.802741 -24.804195 -0.039413
O -16.914527 -24.309410 -0.190644
N -14.695878 -24.072081 0.181109
H -13.774022 -24.484049 0.274168
C -14.736031 -22.625960 0.192839
H -15.322119 -22.283969 -0.668873
C -15.369839 -22.083063 1.478484
H -14.777236 -22.389203 2.344438
H -15.426815 -20.991678 1.460353
H -16.379592 -22.486012 1.570682
C -13.287942 -22.151935 0.050089
O -12.346521 -22.928218 0.168192
N -13.132250 -20.835211 -0.179869
H -13.915662 -20.195400 -0.249423
C -11.821870 -20.226241 -0.249650
H -11.219859 -20.586163 0.593738
C -11.103482 -20.564542 -1.560889
H -11.681461 -20.189271 -2.409442
H -10.105260 -20.120040 -1.592021
H -11.007128 -21.648440 -1.640391
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C -10.978836 -16.540800 0.111342
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H -11.621051 -14.940051 1.450562
H -12.543188 -16.450847 1.579740
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O -8.596891 -16.811108 -0.083467
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H -10.214937 -14.100559 -0.360508
H -8.494585 -14.337233 -0.428231

12. β -strand acetyl(ala)₁₄NH₂

H -30.004392 -47.338419 1.201950
C -29.628276 -46.960690 0.250075
H -30.333309 -46.235896 -0.160726
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C -28.242682 -46.389360 0.475792

O -27.366814 -47.019738 1.049796
N -28.032826 -45.141867 -0.013160
H -28.763998 -44.586536 -0.437823
C -26.762930 -44.479208 0.165694
H -26.432802 -44.627436 1.201533
C -25.690576 -45.035502 -0.779301
H -25.992048 -44.876340 -1.818089
H -24.724622 -44.550301 -0.615315
H -25.584600 -46.105168 -0.592332
C -26.995851 -42.990888 -0.092814
O -28.023013 -42.580201 -0.621864
N -25.984915 -42.177673 0.271681
H -25.122247 -42.525325 0.674819
C -26.016087 -40.759514 -0.006794
H -26.344223 -40.610604 -1.043111
C -26.971537 -40.013668 0.931733
H -26.639014 -40.124927 1.967067
H -27.014074 -38.948593 0.689086
H -27.970443 -40.439145 0.824915
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N -24.361938 -38.992346 -0.264119
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H -22.716722 -38.551147 0.922833
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H -22.378011 -38.666449 -2.119737
H -21.068739 -38.403616 -0.947722
H -21.936323 -39.953212 -0.968572
C -23.308057 -36.851974 -0.275604
O -24.358214 -36.417801 -0.736352
N -22.275886 -36.063642 0.076029
H -21.397146 -36.432855 0.422217
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H -22.679418 -34.430145 -1.142607
C -23.211515 -33.928591 0.887206
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H -23.257924 -32.853058 0.698010
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H -19.450637 -26.796991 0.859285
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H -15.047244 -26.273147 -2.279487
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H -14.546679 -27.684322 -1.312467
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H -9.891779 -20.078615 -1.185644

H -10.808127 -21.594994 -1.301005
C -11.984446 -18.597427 -0.028472
O -13.081612 -18.100690 -0.259646
N -10.890431 -17.867186 0.252446
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H -12.642590 -16.242822 1.512404
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O -8.537186 -16.743403 0.370228
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H -7.073728 -15.517086 -1.369427
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O -9.284781 -12.042420 -0.162746
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H -6.152566 -12.223716 0.352950
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H -7.680728 -10.024279 -0.623074
C -7.757353 -9.811973 1.522333
H -7.177718 -10.115503 2.397934
H -7.810392 -8.720513 1.497798
H -8.769699 -10.210976 1.602788
C -5.656040 -9.895079 0.123136
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N -5.492528 -8.580044 -0.110455
H -6.272569 -7.937741 -0.193766
C -4.179110 -7.976166 -0.166779
H -3.589230 -8.333467 0.686218
C -3.445276 -8.324364 -1.466836
H -4.010718 -7.951379 -2.324785
H -2.444977 -7.883940 -1.487293
H -3.352266 -9.409046 -1.539253
C -4.394003 -6.466421 -0.045351
O -5.508923 -5.967273 -0.150657
N -3.280241 -5.736260 0.151795

H	-2.354026	-6.146780	0.191961	C	-23.16327452	-38.17557147	-0.11997415
C	-3.327016	-4.291812	0.184340	H	-23.36727274	-38.12864099	0.95686582
H	-3.951714	-3.943402	-0.647933	C	-21.84757983	-38.92865670	-0.34723481
C	-3.911904	-3.771022	1.502274	H	-21.61775234	-38.96412791	-1.41524205
H	-3.281660	-4.080922	2.339507	H	-21.01807589	-38.44449769	0.17476398
H	-3.983191	-2.680254	1.503545	H	-21.95605344	-39.94541427	0.03336265
H	-4.912560	-4.186838	1.628960	C	-23.09332206	-36.75772266	-0.68956401
C	-1.889778	-3.805834	-0.014855	O	-23.73847068	-36.42994990	-1.67901938
O	-0.943890	-4.573650	0.023922	N	-22.25928981	-35.91550731	-0.04794171
N	-1.753945	-2.471812	-0.200306	H	-21.70587378	-36.19826681	0.75241983
H	-2.545476	-1.856725	-0.284983	C	-22.03993596	-34.56667201	-0.52137105
H	-0.825470	-2.101419	-0.328982	H	-21.88315802	-34.59722825	-1.60658100

13. β -strand acetyl(ala)₁₈NH₂

H	-30.64489885	-47.13734357	-0.67833296	C	-20.77107918	-34.06013228	0.16645575
C	-30.23355584	-46.29510721	-1.23156891	O	-20.26355105	-34.66276658	1.10542015
H	-31.01031198	-45.53998410	-1.37949068	N	-20.27776055	-32.90051560	-0.31149953
H	-29.89762308	-46.63203250	-2.21580664	H	-20.72362746	-32.38444157	-1.06113638
C	-29.07382010	-45.71891546	-0.44291247	C	-19.14344933	-32.25109773	0.30783368
O	-28.71574708	-46.16519132	0.63615320	H	-19.28460054	-32.26101949	1.39576170
N	-28.44966529	-44.66294868	-1.02832955	C	-17.82674693	-32.95879383	-0.03129993
H	-28.78074331	-44.23730511	-1.88476403	H	-17.65787256	-32.93570792	-1.11094861
C	-27.36750577	-43.97982714	-0.36075375	H	-16.97932423	-32.48100569	0.46727467
H	-27.64160780	-43.82985160	0.69146725	H	-17.89082442	-33.99564986	0.30236347
C	-26.06353844	-44.78537068	-0.41940304	C	-19.14171920	-30.80564520	-0.19378589
H	-25.75932697	-44.92672436	-1.45993786	O	-19.86494023	-30.44536892	-1.11571972
H	-25.25549820	-44.28138363	0.11786574	N	-18.28018807	-29.97580415	0.42636690
H	-26.23848825	-45.75885262	0.04113657	H	-17.65116921	-30.28584297	1.15789168
C	-27.20680158	-42.62090741	-1.04256651	C	-18.12124432	-28.60333088	-0.00119199
O	-27.77491885	-42.35341969	-2.09556580	H	-18.05372714	-28.58321566	-1.09582937
N	-26.38192585	-41.75500770	-0.41862374	C	-19.30037824	-27.72969608	0.44293145
H	-25.88494322	-41.99349098	0.43147356	H	-19.36746829	-27.72045504	1.53391162
C	-26.07110487	-40.46382093	-0.98944521	H	-19.18883431	-26.70149308	0.08894754
H	-25.83824638	-40.59609856	-2.05347505	H	-20.22057221	-28.14403539	0.02815782
C	-27.24340499	-39.48489498	-0.85334228	C	-16.80673994	-28.10415614	0.60114264
H	-27.46760028	-39.31599630	0.20309112	O	-16.20534677	-28.74582622	1.45499425
H	-27.01681680	-38.52373445	-1.32234298	N	-16.38093188	-26.90923561	0.14671087
H	-28.11738359	-39.91657344	-1.34326382	H	-16.91107069	-26.35779299	-0.51818013
C	-24.83268997	-39.94487412	-0.25541458	C	-15.20720390	-26.26645501	0.69536657
O	-24.40176088	-40.49787931	0.74991015	H	-15.24350673	-26.34335242	1.78922684
N	-24.27661259	-38.83053257	-0.77140005	C	-13.91453326	-26.91756829	0.19117591
H	-24.65871241	-38.35056527	-1.57788913	H	-13.84567521	-26.81997786	-0.89533365

H	-13.03293882	-26.45443209	0.64210738	N	-6.86954382	-11.76244168	0.80476262
H	-13.92852059	-27.97537204	0.45844474	H	-6.04295627	-12.07177960	1.30305295
C	-15.28810294	-24.79438252	0.28568414	C	-6.90109164	-10.36244172	0.44303313
O	-16.12239838	-24.39749351	-0.52042205	H	-7.16937866	-10.28134249	-0.61736685
N	-14.37441418	-23.97999486	0.84863500	C	-7.92191802	-9.58151449	1.27870270
H	-13.66065293	-24.31133035	1.48691712	H	-7.65338719	-9.63217234	2.33711365
C	-14.30594987	-22.57844002	0.49775996	H	-7.96101271	-8.53187922	0.97577677
H	-14.38162852	-22.48770673	-0.59258506	H	-8.90768951	-10.02611569	1.13396551
C	-15.43931585	-21.77526826	1.14674694	C	-5.48778771	-9.82112975	0.65860352
H	-15.36501688	-21.83959686	2.23544500	O	-4.64445181	-10.45527985	1.28235939
H	-15.39902497	-20.72300984	0.85317426	N	-5.25576555	-8.59768312	0.14516465
H	-16.39446439	-22.19258161	0.82412288	H	-5.96526847	-8.06904959	-0.34913841
C	-12.93916927	-22.07356756	0.96202787	C	-3.99556045	-7.91818590	0.34781377
O	-12.22979446	-22.73530098	1.71126477	H	-3.71109735	-8.01216042	1.40303522
N	-12.59636087	-20.85135307	0.51164204	C	-2.88313385	-8.50793025	-0.52655421
H	-13.21033838	-20.29511806	-0.07240855	H	-3.14252889	-8.39772489	-1.58270783
C	-11.37884429	-20.19607801	0.93582674	H	-1.92862665	-8.00717663	-0.34457524
H	-11.28722972	-20.29029119	2.02522395	H	-2.77484560	-9.56750365	-0.28976519
C	-10.14117171	-20.81279803	0.27441279	C	-4.23719149	-6.44678964	0.00849046
H	-10.20126968	-20.69673945	-0.81081325	O	-5.25035355	-6.08190318	-0.57747542
H	-9.22221673	-20.33834634	0.62846538	N	-3.25407767	-5.59945314	0.36796822
H	-10.10449861	-21.87460693	0.52264257	H	-2.40130134	-5.90949707	0.81964731
C	-11.53296430	-18.71972156	0.56324159	C	-3.31008322	-4.19588478	0.02428287
O	-12.46270411	-18.32871405	-0.13389818	H	-3.61790539	-4.10397805	-1.02456882
N	-10.57393809	-17.89557910	1.02721952	C	-4.30506769	-3.43251258	0.90593993
H	-9.78824593	-18.21968774	1.57902867	H	-3.99954772	-3.49548134	1.95356390
C	-10.56976525	-16.48945137	0.68790524	H	-4.36120276	-2.37917129	0.61889407
H	-10.77512777	-16.38862510	-0.38467098	H	-5.29269429	-3.88126303	0.78956023
C	-11.62925729	-15.71098631	1.47675111	C	-1.89256072	-3.64811329	0.19166890
H	-11.41980809	-15.77902453	2.54747451	O	-1.01731138	-4.29106676	0.76004188
H	-11.64257985	-14.65697254	1.18712754	N	-1.69048966	-2.41064979	-0.30056256
H	-12.60931383	-16.14456550	1.27184089	H	-2.42590969	-1.87028174	-0.74138086
C	-9.16765954	-15.96542506	0.99797743	C	-0.42414392	-1.73216284	-0.13799110
O	-8.37862710	-16.60802024	1.68134071	H	-0.08781530	-1.85993167	0.89824957
N	-8.88679902	-14.74676612	0.49816863	C	0.64593332	-2.28925112	-1.08408123
H	-9.55757761	-14.21168491	-0.04135441	H	0.33565908	-2.14646944	-2.12244582
C	-7.64043194	-14.07386274	0.78986215	H	1.60737282	-1.79165552	-0.93252031
H	-7.44036575	-14.15262901	1.86574472	H	0.76806101	-3.35540964	-0.88684339
C	-6.46790024	-14.68712221	0.01606878	C	-0.68568911	-0.25130084	-0.41485351
H	-6.64098039	-14.59228658	-1.05903751	O	-1.73250672	0.13126066	-0.92586004
H	-5.52552309	-14.19244232	0.26538748	N	0.31795975	0.58448338	-0.08749721
H	-6.39016480	-15.74352440	0.27773609	H	1.19553399	0.26089046	
C	-7.84453405	-12.60514308	0.41343428		0.30315467		
O	-8.82441506	-12.23739424	-0.22518196	C	0.24588993	1.99885995	-0.37972005

H	-0.12733135	2.12682435	-1.40313675
C	-0.68758245	2.73400835	0.58882379
H	-0.31631252	2.63356412	
	1.61196826		
H	-0.75597557	3.79688708	
	0.34255704		
H	-1.68304769	2.29252035	
	0.51998803		
C	1.67422266	2.53613528	-0.28300775
O	2.57767567	1.87206309	
	0.21218242		
N	1.85473961	3.78652389	-0.74965182
H	1.09674167	4.34627216	-1.12278498
C	3.13357861	4.45247641	-0.64046839
H	3.53199849	4.28332521	
	0.36733983		
C	4.13961335	3.92578805	-1.67056569
H	3.76595445	4.10515927	-2.68200724
H	5.11141240	4.41447962	-1.56247953
H	4.26800050	2.85294588	-1.51805502
C	2.86617921	5.94396454	-0.84139639
O	1.79054564	6.35408638	-1.26281585
N	3.89600442	6.76211769	-0.54944857
H	4.80091432	6.42019559	-0.24661065
C	3.80558053	8.18605124	-0.77612593
H	3.35682923	8.35451913	-1.76319707
C	2.94612337	8.87673274	
	0.28925327		
H	3.39406770	8.73864371	
	1.27642833		
H	2.85252245	9.94831538	
	0.09440066		
H	1.95038501	8.43084751	
	0.27773556		
C	5.23816470	8.72177500	-0.76470434
O	6.17683042	8.03352649	-0.40264684
N	5.37202214	10.01265970	-1.15044944
H	4.59854847	10.55199591	-1.50077519
H	6.29597714	10.41484575	-1.15303405

14. β -strand acetyl(ala)₂₄NH₂

H	-29.629030	-47.719286	0.019294
C	-29.625385	-46.647506	0.217305
H	-30.042830	-46.480303	1.214834
H	-30.253696	-46.131420	-0.512696
C	-28.190849	-46.158476	0.190596
O	-27.246660	-46.874499	0.487975
N	-28.026056	-44.856838	-0.159696
H	-28.804095	-44.236171	-0.341631
C	-26.720403	-44.241750	-0.126131
H	-26.211588	-44.546012	0.797627
C	-25.862001	-44.666811	-1.324414
H	-26.340704	-44.351299	-2.255446
H	-24.861560	-44.228068	-1.275436
H	-25.771069	-45.754004	-1.314447
C	-26.936584	-42.728405	-0.116811
O	-28.029892	-42.229333	-0.360009
N	-25.839502	-41.989130	0.146865
H	-24.933318	-42.403460	0.331492
C	-25.877858	-40.543788	0.119618
H	-26.399289	-40.222654	-0.790641
C	-26.604998	-39.969858	1.341807
H	-26.078334	-40.256660	2.255867
H	-26.658918	-38.878947	1.294400
H	-27.618942	-40.371810	1.367326
C	-24.424606	-40.065747	0.078106
O	-23.492646	-40.828995	0.303055
N	-24.250517	-38.754876	-0.184264
H	-25.025143	-38.124226	-0.354779
C	-22.935947	-38.149494	-0.171444
H	-22.407968	-38.475188	0.733333
C	-22.112579	-38.548342	-1.402094
H	-22.613782	-38.206858	-2.311537
H	-21.111471	-38.110563	-1.366246
H	-22.020697	-39.635151	-1.425859
C	-23.148654	-36.635275	-0.124855
O	-24.245705	-36.134176	-0.343409
N	-22.048638	-35.901341	0.138209
H	-21.139055	-36.317140	0.302219
C	-22.088663	-34.454789	0.133522
H	-22.627874	-34.122118	-0.761884
C	-22.792637	-33.899941	1.377549
H	-22.248047	-34.199086	2.276923
H	-22.847033	-32.808588	1.346188
H	-23.806028	-34.302185	1.417555

C	-20.637351	-33.974050	0.072111	C	-11.620910	-19.847937	-0.136206
O	-19.700875	-34.735881	0.284080	H	-11.093900	-20.171103	0.769994
N	-20.470529	-32.662455	-0.190644	C	-10.795547	-20.246818	-1.365441
H	-21.248715	-32.035392	-0.358907	H	-11.296229	-19.906521	-2.275640
C	-19.157821	-32.053271	-0.200667	H	-9.795310	-19.807300	-1.328697
H	-18.611687	-32.381417	0.692157	H	-10.701760	-21.333437	-1.388698
C	-18.357813	-32.443260	-1.449350	C	-11.836576	-18.333180	-0.093738
H	-18.879902	-32.101265	-2.346812	O	-12.935393	-17.836691	-0.314517
H	-17.358925	-31.999321	-1.432403	N	-10.737519	-17.596859	0.164879
H	-18.260272	-33.529500	-1.479407	H	-9.827893	-18.011507	0.331959
C	-19.375699	-30.539803	-0.145432	C	-10.774709	-16.149714	0.152259
O	-20.475995	-30.043482	-0.360883	H	-11.299177	-15.819476	-0.752868
N	-18.277787	-29.803231	0.117418	C	-11.494999	-15.586081	1.382791
H	-17.367536	-30.216887	0.284308	H	-10.964491	-15.881116	2.291831
C	-18.322350	-28.356419	0.123833	H	-11.545867	-14.494846	1.344148
H	-18.856189	-28.017736	-0.772546	H	-12.510118	-15.984731	1.410406
C	-19.035376	-27.813397	1.367843	C	-9.320190	-15.674133	0.108301
H	-18.495827	-28.119054	2.268071	O	-8.389538	-16.442326	0.324191
H	-19.090791	-26.721943	1.344916	N	-9.144355	-14.362081	-0.144045
H	-20.048495	-28.216976	1.398267	H	-9.918105	-13.728986	-0.309792
C	-16.871607	-27.871554	0.077108	C	-7.828749	-13.758175	-0.135975
O	-15.935719	-28.632891	0.291921	H	-7.297947	-14.082425	0.767672
N	-16.704875	-26.558367	-0.176578	C	-7.009707	-14.158457	-1.368918
H	-17.482757	-25.931143	-0.345763	H	-7.513926	-13.817559	-2.276901
C	-15.393041	-25.946713	-0.171287	H	-6.008731	-13.720182	-1.336632
H	-14.856478	-26.273055	0.728057	H	-6.917393	-15.245191	-1.392387
C	-14.578092	-26.335745	-1.410641	C	-8.041339	-12.243022	-0.092326
H	-15.089867	-25.993513	-2.313952	O	-9.140316	-11.744483	-0.307904
H	-13.579816	-25.891101	-1.381604	N	-6.940278	-11.508648	0.162161
H	-14.479272	-27.421838	-1.440159	H	-6.030478	-11.924468	0.325615
C	-15.613661	-24.433149	-0.120056	C	-6.976535	-10.061456	0.153349
O	-16.712973	-23.939053	-0.344181	H	-7.506485	-9.728611	-0.747611
N	-14.518272	-23.695064	0.149432	C	-7.688404	-9.501062	1.390218
H	-13.608083	-24.107943	0.318812	H	-7.151633	-9.799202	2.294598
C	-14.560264	-22.248022	0.145929	H	-7.738751	-8.409684	1.355232
H	-15.085757	-21.913726	-0.757066	H	-8.703501	-9.899340	1.423664
C	-15.282151	-21.695686	1.380543	C	-5.522205	-9.586465	0.103194
H	-14.750306	-21.996619	2.286890	O	-4.591132	-10.354945	0.317055
H	-15.335584	-20.604286	1.350246	N	-5.347293	-8.274302	-0.151274
H	-16.296205	-22.097345	1.405531	H	-6.121474	-7.640986	-0.316052
C	-13.107616	-21.767012	0.107929	C	-4.031696	-7.670441	-0.146557
O	-12.175740	-22.530524	0.332621	H	-3.496438	-8.000176	0.752393
N	-12.934770	-20.455439	-0.150578	C	-3.219671	-8.063528	-1.386392
H	-13.709521	-19.825190	-0.323494	H	-3.729382	-7.717318	-2.289331

H	-2.218588	-7.625251	-1.357375	N	4.434652	6.755412	0.195072
H	-3.127645	-9.150168	-1.416792	H	5.345435	6.342259	0.359755
C	-4.243683	-6.155638	-0.093826	C	4.394213	8.201915	0.180848
O	-5.341842	-5.655429	-0.308719	H	3.857361	8.529126	-0.717980
N	-3.142755	-5.423152	0.168113	C	3.688736	8.766041	1.419726
H	-2.233520	-5.840142	0.332751	H	4.231713	8.473208	2.322139
C	-3.178436	-3.975950	0.165041	H	3.635545	9.857191	1.380042
H	-3.709591	-3.639876	-0.733925	H	2.674775	8.365415	1.461205
C	-3.888575	-3.419680	1.404791	C	5.846154	8.680257	0.119442
H	-3.350907	-3.721233	2.307510	O	6.781008	7.918791	0.340321
H	-3.938383	-2.328131	1.373637	N	6.014681	9.989070	-0.152746
H	-4.903837	-3.817596	1.437977	H	5.237213	10.616572	-0.323334
C	-1.724343	-3.500819	0.114929	C	7.326467	10.599596	-0.151289
O	-0.793113	-4.267948	0.329250	H	7.861461	10.282005	0.752189
N	-1.549567	-2.189496	-0.142520	C	8.144903	10.199052	-1.384560
H	-2.323921	-1.557109	-0.309228	H	7.636525	10.532606	-2.292955
C	-0.234629	-1.584499	-0.135408	H	9.143306	10.643538	-1.356441
H	0.298484	-1.912567	0.765391	H	8.243734	9.112764	-1.403146
C	0.581634	-1.978309	-1.372320	C	7.104271	12.112647	-0.112952
H	0.074619	-1.633885	-2.277437	O	6.004042	12.604821	-0.334747
H	1.582204	-1.538977	-1.340660	N	8.198965	12.853954	0.145796
H	0.674991	-3.064893	-1.400952	H	9.110897	12.444607	0.313046
C	-0.448559	-0.070043	-0.084545	C	8.152879	14.299927	0.124589
O	-1.546665	0.428988	-0.304045	H	7.617484	14.620867	-0.777343
N	0.650710	0.663424	0.180618	C	7.441153	14.867546	1.358388
H	1.560129	0.247393	0.346486	H	7.981559	14.580824	2.264236
C	0.613571	2.110377	0.177263	H	7.384193	15.958322	1.313477
H	0.084328	2.446275	-0.722920	H	6.428398	14.463763	1.397833
C	-0.099533	2.666020	1.415673	C	9.602791	14.783016	0.064209
H	0.436595	2.364652	2.319373	O	10.540714	14.026449	0.288789
H	-0.149909	3.757541	1.384654	N	9.766554	16.091137	-0.213363
H	-1.114661	2.267575	1.447004	H	8.986909	16.716173	-0.382658
C	2.067320	2.586242	0.130900	C	11.076222	16.705207	-0.210901
O	2.998658	1.819461	0.350875	H	11.615281	16.379569	0.687171
N	2.240818	3.897817	-0.126079	C	11.890545	16.318932	-1.451396
H	1.465831	4.529712	-0.292400	H	11.377176	16.659564	-2.354366
C	3.554384	4.505009	-0.113739	H	12.888060	16.765561	-1.423648
H	4.085035	4.179019	0.789359	H	11.991997	15.233035	-1.480730
C	4.375896	4.112302	-1.347453	C	10.850404	18.216696	-0.156213
H	3.872040	4.456784	-2.254294	O	9.749918	18.709273	-0.373535
H	5.375969	4.552389	-1.311778	N	11.942968	18.955834	0.115256
H	4.470194	3.025840	-1.376241	H	12.856877	18.545732	0.269117
C	3.336861	6.018796	-0.065591	C	11.897683	20.401587	0.109653
O	2.237665	6.515306	-0.283491	H	11.358001	20.732432	-0.786134

C	11.192450	20.955921	1.352944	H	-24.675812	-44.064828	-1.093731
H	11.737447	20.659819	2.253058	H	-25.578363	-45.593921	-1.152264
H	11.134815	22.047045	1.320648	C	-26.837576	-42.533535	-0.153020
H	10.179868	20.551597	1.393819	O	-27.913456	-42.046924	-0.483327
C	13.348358	20.882675	0.043522	N	-25.760023	-41.781579	0.152150
O	14.286900	20.116612	0.231790	H	-24.862552	-42.185894	0.392845
N	13.511792	22.197786	-0.199039	C	-25.796820	-40.339031	0.062694
H	12.731582	22.832041	-0.326712	H	-26.268914	-40.057118	-0.886683
C	14.823724	22.806532	-0.201981	C	-26.589261	-39.717250	1.218993
H	15.379007	22.449339	0.673975	H	-26.112920	-39.963966	2.171508
C	15.611511	22.458691	-1.470435	H	-26.643166	-38.629411	1.124102
H	15.082214	22.831109	-2.351362	H	-27.602437	-40.121839	1.205926
H	16.611722	22.899356	-1.448706	C	-24.343204	-39.860736	0.075377
H	15.707088	21.373881	-1.537949	O	-23.421441	-40.616725	0.360888
C	14.604573	24.315244	-0.088528	N	-24.157528	-38.557037	-0.212735
O	13.498212	24.818579	-0.245488	H	-24.923954	-37.929073	-0.424441
N	15.708873	25.044180	0.166433	C	-22.844396	-37.952017	-0.154936
H	16.630855	24.632261	0.254683	H	-22.354648	-38.265194	0.775373
C	15.657953	26.487686	0.209177	C	-21.971917	-38.369647	-1.344692
H	15.069965	26.841688	-0.647097	H	-22.433786	-38.039700	-2.278859
C	15.013702	26.996940	1.504104	H	-20.971787	-37.934004	-1.273692
H	15.606651	26.680176	2.365863	H	-21.882231	-39.456871	-1.349414
H	14.942322	28.087787	1.511445	C	-23.057278	-36.437519	-0.138095
H	14.008669	26.579708	1.583075	O	-24.145273	-35.938303	-0.401793
C	17.100722	26.979746	0.080771	N	-21.965750	-35.701899	0.153127
O	18.047328	26.216521	0.164546	H	-21.061903	-36.116846	0.347800
N	17.239379	28.315540	-0.093335	C	-22.000834	-34.256024	0.122859
H	16.449808	28.924931	-0.224223	H	-22.511282	-33.936581	-0.794039
H	18.171199	28.689875	-0.178919	C	-22.740365	-33.678047	1.335186
15. β -strand acetyl(ala) ₃₀ NH ₂				H	-22.225366	-33.964098	2.255956
H	-29.535491	-47.526105	-0.045220	H	-22.790180	-32.587183	1.284495
C	-29.543029	-46.445450	0.091317	H	-23.756104	-34.076146	1.350252
H	-30.046702	-46.220507	1.035532	C	-20.546265	-33.782528	0.095082
H	-30.100998	-45.971740	-0.718804	O	-19.618456	-34.546672	0.335498
C	-28.109795	-45.957516	0.161358	N	-20.366815	-32.474392	-0.174470
O	-27.191745	-46.664681	0.547819	H	-21.137908	-31.842868	-0.357412
N	-27.918243	-44.664914	-0.209329	C	-19.051578	-31.872100	-0.152679
H	-28.680654	-44.050132	-0.463914	H	-18.531201	-32.197264	0.756626
C	-26.619426	-44.045575	-0.094020	C	-18.219847	-32.274151	-1.376548
H	-26.184457	-44.315229	0.876927	H	-18.713480	-31.932763	-2.290183
C	-25.669104	-44.507951	-1.205882	H	-17.218188	-31.838288	-1.333739
H	-26.072931	-44.225342	-2.181683	H	-18.130013	-33.361207	-1.398368
				C	-19.263729	-30.357755	-0.110739
				O	-20.358892	-29.857126	-0.340422

N	-18.165585	-29.625219	0.160250	C	-11.341102	-15.458056	1.407946
H	-17.258084	-30.041755	0.334106	H	-10.796505	-15.761578	2.305833
C	-18.202378	-28.178806	0.152102	H	-11.394071	-14.366547	1.381272
H	-18.732176	-27.846538	-0.749032	H	-12.355064	-15.858941	1.446660
C	-18.915699	-27.619027	1.388461	C	-9.186064	-15.529396	0.101994
H	-18.380239	-27.917698	2.293455	O	-8.251183	-16.294168	0.311282
H	-18.966278	-26.527594	1.354060	N	-9.017393	-14.217870	-0.155586
H	-19.930829	-28.017587	1.420343	H	-9.794447	-13.588074	-0.318966
C	-16.748923	-27.704028	0.102129	C	-7.704168	-13.610623	-0.160482
O	-15.817118	-28.469702	0.321605	H	-7.160817	-13.940610	0.733399
N	-16.575402	-26.393829	-0.159908	C	-6.900667	-13.998409	-1.407533
H	-17.350008	-25.762826	-0.329906	H	-7.418919	-13.652790	-2.305804
C	-15.260878	-25.789368	-0.156875	H	-5.901115	-13.556232	-1.385750
H	-14.724809	-26.118101	0.741890	H	-6.804651	-15.084673	-1.440468
C	-14.449079	-26.182814	-1.396771	C	-7.921930	-12.097648	-0.102339
H	-14.959593	-25.838468	-2.299956	O	-9.022219	-11.600177	-0.313551
H	-13.448417	-25.743471	-1.368831	N	-6.823180	-11.363319	0.159517
H	-14.355927	-27.269439	-1.425754	H	-5.912476	-11.778047	0.320835
C	-15.475494	-24.275679	-0.104282	C	-6.864324	-9.916980	0.162760
O	-16.573890	-23.776356	-0.321130	H	-7.403517	-9.579252	-0.730713
N	-14.376285	-23.542535	0.159794	C	-7.566682	-9.368261	1.410257
H	-13.466796	-23.958333	0.325001	H	-7.021414	-9.672213	2.307589
C	-14.415533	-22.096090	0.159524	H	-7.619845	-8.276746	1.384265
H	-14.952150	-21.759904	-0.736080	H	-8.580551	-9.769338	1.449431
C	-15.120666	-21.543814	1.403914	C	-5.412498	-9.438535	0.102867
H	-14.578112	-21.846313	2.303389	O	-4.477445	-10.203281	0.311448
H	-15.172787	-20.452305	1.375379	N	-5.244139	-8.126987	-0.154459
H	-16.135002	-21.943885	1.441234	H	-6.021326	-7.497174	-0.317174
C	-12.963135	-21.618971	0.102241	C	-3.931018	-7.519621	-0.159629
O	-12.029118	-22.384143	0.313944	H	-3.387272	-7.849877	0.733912
N	-12.793093	-20.307770	-0.156471	C	-3.127938	-7.906730	-1.407155
H	-13.569496	-19.677653	-0.321653	H	-3.646576	-7.560784	-2.305074
C	-11.479466	-19.701331	-0.159765	H	-2.128453	-7.464395	-1.385543
H	-10.937761	-20.030934	0.735264	H	-3.031747	-8.992963	-1.440621
C	-10.674208	-20.090778	-1.405166	C	-4.149082	-6.006773	-0.100749
H	-11.190733	-19.745582	-2.304598	O	-5.249468	-5.509377	-0.311593
H	-9.674340	-19.649364	-1.382154	N	-3.050423	-5.272502	0.161353
H	-10.578992	-21.177145	-1.436964	H	-2.139638	-5.687194	0.322316
C	-11.696262	-18.188118	-0.103208	C	-3.091619	-3.826219	0.164868
O	-12.796069	-17.690123	-0.315808	H	-3.631139	-3.488336	-0.728345
N	-10.597317	-17.454073	0.158973	C	-3.793447	-3.277666	1.412729
H	-9.686924	-17.869085	0.321264	H	-3.247827	-3.581763	2.309796
C	-10.638003	-16.007681	0.161254	H	-3.846576	-2.186146	1.386907
H	-11.176588	-15.670418	-0.732761	H	-4.807317	-3.678711	1.452258

C	-1.639816	-3.347966	0.104482	C	7.386278	10.748405	-0.155953
O	-0.704759	-4.112716	0.313021	H	7.929515	10.417648	0.737711
N	-1.471494	-2.036561	-0.153261	C	8.190064	10.361940	-1.403206
H	-2.248683	-1.406707	-0.315819	H	7.671982	10.708337	-2.301272
C	-0.158410	-1.429256	-0.158473	H	9.189562	10.804217	-1.380735
H	0.385439	-1.759679	0.734942	H	8.286222	9.275711	-1.437122
C	0.644546	-1.816062	-1.406166	C	7.167879	12.260885	-0.096333
H	0.125803	-1.469944	-2.303957	O	6.067950	12.758592	-0.308954
H	1.644014	-1.373685	-1.384553	N	8.265949	12.994639	0.168760
H	0.740782	-2.902285	-1.439873	H	9.176574	12.579804	0.330226
C	-0.376619	0.083480	-0.099246	C	8.225020	14.440685	0.171081
O	-1.476951	0.580908	-0.310308	H	7.685472	14.777938	-0.722348
N	0.721908	0.817627	0.163448	C	7.523527	14.990592	1.418527
H	1.632685	0.402919	0.324416	H	8.069072	14.687057	2.315830
C	0.680755	2.263844	0.166800	H	7.470744	16.082115	1.391735
H	0.141150	2.601653	-0.726389	H	6.509515	14.589914	1.458437
C	-0.020844	2.812637	1.414679	C	9.676815	14.917879	0.110056
H	0.524866	2.508616	2.311716	O	10.611644	14.153409	0.320783
H	-0.073881	3.904159	1.388700	N	9.845505	16.228373	-0.151066
H	-1.034746	2.411687	1.454397	H	9.068538	16.858357	-0.314130
C	2.132554	2.741799	0.106153	C	11.158516	16.835218	-0.154468
O	3.067552	1.977096	0.315160	H	11.701305	16.504058	0.739321
N	2.300952	4.052965	-0.152435	C	11.962874	16.449116	-1.401459
H	1.523815	4.682859	-0.315084	H	11.445272	16.795821	-2.299683
C	3.614003	4.660167	-0.157238	H	12.962418	16.891265	-1.378343
H	4.157617	4.329592	0.736263	H	12.058926	15.362880	-1.435636
C	4.417290	4.273554	-1.404773	C	10.940092	18.347536	-0.094300
H	3.898807	4.619817	-2.302658	O	9.840433	18.845539	-0.307689
H	5.416765	4.715901	-1.382799	N	12.037934	19.080939	0.172395
H	4.513506	3.187331	-1.438609	H	12.948489	18.665940	0.333815
C	3.395677	6.172783	-0.097800	C	11.997167	20.526879	0.174486
O	2.295507	6.670313	-0.309519	H	11.457556	20.864043	-0.718939
N	4.493991	6.906764	0.165947	C	11.295833	21.077106	1.421882
H	5.404713	6.492015	0.327108	H	11.841339	20.773625	2.319227
C	4.452926	8.352902	0.168844	H	11.243147	22.168635	1.394928
H	3.913348	8.690466	-0.724451	H	10.281770	20.676550	1.461864
C	3.751384	8.902193	1.416534	C	13.448945	21.003642	0.113154
H	4.297031	8.598394	2.313685	O	14.383753	20.239149	0.323943
H	3.698463	9.993715	1.390187	N	13.617764	22.313951	-0.148527
H	2.737433	8.501367	1.456351	H	12.840842	22.944199	-0.310716
C	5.904725	8.830505	0.108021	C	14.930789	22.920499	-0.150939
O	6.839643	8.065908	0.317827	H	15.473448	22.587859	0.742378
N	6.073251	10.141358	-0.151743	C	15.735191	22.536084	-1.398417
H	5.296196	10.771279	-0.314656	H	15.217745	22.884107	-2.296220

H	16.734845	22.977958	-1.374588	N	23.349261	37.335299	0.177874
H	15.831016	21.449863	-1.434075	H	24.265506	36.921686	0.307606
C	14.712457	24.432572	-0.088299	C	23.306993	38.780835	0.182237
O	13.612987	24.931221	-0.301164	H	22.738593	39.117272	-0.693390
N	15.810248	25.165248	0.180316	C	22.643563	39.328716	1.450965
H	16.720937	24.749887	0.340029	H	23.216198	39.025273	2.331260
C	15.769586	26.611056	0.183829	H	22.587738	40.420149	1.427212
H	15.229044	26.949085	-0.708718	H	21.631935	38.925822	1.521106
C	15.069490	27.160166	1.432405	C	24.755259	39.258755	0.071046
H	15.615741	26.855798	2.328997	O	25.697677	38.492903	0.237583
H	15.016740	28.251727	1.406585	N	24.913079	40.570970	-0.187112
H	14.055449	26.759596	1.472892	H	24.129984	41.203566	-0.304103
C	17.221231	27.087574	0.121120	C	26.225112	41.177157	-0.238117
O	18.156409	26.322753	0.329052	H	26.806083	40.831383	0.625592
N	17.389631	28.398214	-0.138966	C	26.973563	40.810928	-1.525082
H	16.612352	29.029010	-0.297187	H	26.415882	41.168920	-2.394469
C	18.702563	29.004639	-0.141544	H	27.973039	41.253575	-1.541578
H	19.246704	28.669104	0.749793	H	27.069122	39.725369	-1.578979
C	19.504906	28.624120	-1.391543	C	26.010175	42.687173	-0.140388
H	18.986055	28.974902	-2.287459	O	24.901572	43.189897	-0.285680
H	20.504733	29.065639	-1.368087	N	27.119871	43.417024	0.085372
H	19.600483	27.537983	-1.430674	H	28.042846	43.004429	0.159618
C	18.484093	30.516277	-0.073243	C	27.072696	44.861029	0.105651
O	17.383854	31.015624	-0.280444	H	26.475401	45.203479	-0.748927
N	19.582517	31.248374	0.194265	C	26.444098	45.390740	1.399942
H	20.494434	30.833082	0.346870	H	27.046484	45.086704	2.259607
C	19.540705	32.693983	0.200728	H	26.372108	46.481512	1.391560
H	18.993173	33.032878	-0.687208	H	25.440072	44.974868	1.496265
C	18.848972	33.240141	1.455218	C	28.514907	45.347239	-0.049079
H	19.401645	32.934670	2.347481	O	29.460598	44.581972	0.026965
H	18.794759	34.331696	1.431869	N	28.654752	46.680174	-0.241319
H	17.835653	32.838365	1.501957	H	27.865122	47.293930	-0.349087
C	20.991157	33.171971	0.127230	H	29.586458	47.052492	-0.335973
O	21.929090	32.407944	0.325102	B. Water clusters			
N	21.155570	34.483312	-0.131947	1. (H ₂ O) ₅₀ -I			
H	20.375832	35.113743	-0.279083	O	0.053353	-2.057217	20.154209
C	22.467597	35.091092	-0.145918	H	0.999937	-1.954009	20.251986
H	23.020852	34.754693	0.739504	H	-0.151558	-2.859126	20.635026
C	23.258180	34.713501	-1.404309	O	2.765616	-1.963342	20.076669
H	22.730154	35.064794	-2.294661	H	3.037438	-1.486456	19.292497
H	24.257952	35.155627	-1.390478	H	3.207646	-2.809600	20.008190
H	23.354457	33.627519	-1.445883	O	3.864704	-4.486794	19.857894
C	22.247774	36.602174	-0.072091				
O	21.143144	37.100025	-0.259612				

H	3.120643	-4.857996	20.332040	O	-1.102690	-7.161746	17.200331
H	4.622120	-4.680864	20.410062	H	-1.446894	-6.587922	17.884788
O	1.623252	-5.512437	20.978529	H	-0.825844	-6.565800	16.504316
H	1.346034	-5.727619	20.087979	O	-2.626761	-3.144495	17.997072
H	0.842992	-5.140133	21.389404	H	-1.709001	-3.082350	17.732332
O	-0.927825	-4.351126	21.305514	H	-3.100223	-2.628408	17.344599
H	-1.252655	-4.878958	20.576054	O	0.073440	-3.202017	17.684393
H	-1.716265	-3.987145	21.708147	H	0.316833	-4.098695	17.914525
O	-2.107812	-5.557945	19.138482	H	0.151416	-2.714241	18.504288
H	-2.936239	-6.013735	19.287467	O	0.973041	-5.716022	18.352942
H	-2.359027	-4.733423	18.722203	H	1.796816	-5.680786	17.866746
O	-4.597288	-6.611648	19.135278	H	0.484873	-6.432022	17.946409
H	-4.828957	-7.527714	18.982358	O	3.346397	-5.122255	17.184782
H	-4.684236	-6.195716	18.277564	H	3.102346	-4.263636	16.839172
O	-5.259589	-9.024488	17.925103	H	3.694165	-4.939596	18.057666
H	-6.016301	-8.608855	17.511743	O	3.360733	-0.698033	17.703039
H	-5.568011	-9.897612	18.167515	H	2.557211	-0.188455	17.598562
O	-7.285064	-7.643392	16.800777	H	4.065690	-0.066867	17.558479
H	-7.680947	-7.078189	17.464143	O	1.040996	0.570632	17.244689
H	-7.271821	-7.108784	16.006894	H	0.691738	0.154870	16.456405
O	-8.094731	-5.829988	18.680440	H	0.334248	1.139995	17.548937
H	-8.105589	-5.808436	19.637336	O	-1.161971	2.202034	17.778636
H	-7.561970	-5.075409	18.429426	H	-1.938924	1.782115	18.147749
O	-5.457713	-4.393769	20.570753	H	-1.112564	3.048350	18.223093
H	-4.728047	-4.007992	21.055518	O	-3.396136	1.032288	18.760302
H	-5.140864	-5.257814	20.307571	H	-3.198817	0.221515	19.229285
O	-3.356650	-3.120211	21.872149	H	-4.270041	0.892088	18.395795
H	-3.145558	-2.426653	21.247129	O	-5.431966	-6.563155	12.616829
H	-3.621786	-2.655467	22.665843	H	-5.077370	-5.905876	12.018098
O	-2.610086	-1.317137	19.988219	H	-4.690403	-7.136735	12.810019
H	-1.665283	-1.292268	20.139750	O	-3.330337	-8.202173	13.392606
H	-2.721183	-1.936046	19.266525	H	-3.394373	-8.178650	14.347373
O	-6.710355	-1.662888	16.542616	H	-3.356574	-9.133518	13.173194
H	-6.696623	-2.388289	17.166985	O	-3.666340	-3.866221	14.619503
H	-7.005085	-2.058023	15.722107	H	-2.743979	-3.635383	14.509067
O	-6.294998	-3.860509	18.057595	H	-4.106052	-3.462330	13.871333
H	-5.978791	-3.903494	18.960035	O	-1.122291	-3.011873	14.585431
H	-5.659511	-4.371234	17.556049	H	-0.756773	-2.195025	14.925118
O	-4.602106	-5.545715	16.536526	H	-0.634702	-3.699724	15.038588
H	-4.220882	-6.400422	16.335585	O	-0.161589	-5.490265	15.299457
H	-4.180806	-4.944607	15.922191	H	0.767459	-5.676054	15.163125
O	-3.468776	-7.971109	16.106155	H	-0.589805	-5.813441	14.506727
H	-2.616811	-7.839851	16.522278	O	2.433996	-6.099415	14.723326
H	-3.968386	-8.486337	16.739529	H	2.945607	-5.966035	15.521259

O	2.750216	1.202649	10.295407
H	2.917617	1.847526	9.608135
H	3.458768	0.565539	10.204425
O	3.026541	2.825951	8.150146
H	2.161186	3.195800	7.975203
H	3.260620	2.370107	7.341663
O	3.768746	1.314630	5.950732
H	4.226969	0.678888	6.500365
H	4.447826	1.669320	5.376905
O	4.836324	-0.595754	7.539860
H	5.007578	-0.605736	8.481563
H	4.022923	-1.090080	7.438604
O	4.540226	-0.860309	10.310928
H	3.939512	-1.603498	10.255740
H	4.782011	-0.815341	11.235996
O	2.758306	-2.943853	10.396904
H	3.222802	-3.620716	10.889177
H	2.079715	-2.633956	10.996663
O	4.313244	-4.833447	11.642358
H	3.932768	-5.711761	11.636501
H	5.143368	-4.928391	11.175332
O	3.159647	-7.319893	11.416625
H	2.511248	-7.461855	12.106304
H	3.547280	-8.182784	11.270364
O	1.308944	-7.688541	13.348923
H	1.687197	-7.290960	14.133197
H	0.384020	-7.443794	13.378037
O	2.390466	-6.231313	15.382592
H	3.247710	-6.023616	15.754382
H	2.042181	-5.387003	15.096109

O	4.101891	-3.285808	13.915662	H	-0.479609	4.543570	13.447195
H	4.369198	-2.409880	13.637222	O	0.582341	1.847486	14.533600
H	4.281430	-3.843478	13.158692	H	1.220572	1.365586	14.007610
O	4.712449	-0.736073	13.062142	H	0.275517	1.211963	15.180286
H	3.861042	-0.299675	13.092090	O	-3.000343	-7.081442	11.249680
H	5.280586	-0.191423	13.606943	H	-3.381597	-7.929348	11.021790
O	2.288065	0.459109	12.900235	H	-2.469645	-6.844713	10.489055
H	2.436679	0.957701	12.096772	O	-1.495996	-6.086790	9.246415
H	1.738719	-0.276082	12.628306	H	-1.577153	-5.207923	9.616872
O	-0.588589	-2.656879	15.562836	H	-0.573965	-6.313847	9.366987
H	0.220886	-3.052577	15.239718	O	-1.758479	-3.759317	10.676261
H	-1.224523	-3.372269	15.556711	H	-1.763570	-2.850811	10.374891
O	1.513045	-3.863711	14.367918	H	-2.672807	-3.946877	10.888529
H	2.411005	-3.564784	14.224594	O	-1.794696	-1.101319	9.957704
H	1.197938	-4.103454	13.496446	H	-2.054453	-0.240835	10.286832
O	0.422151	-4.707993	11.983786	H	-0.968861	-0.943930	9.500039
H	0.749336	-5.266460	11.278593	O	-0.737592	-2.950048	7.711652
H	-0.287796	-4.206452	11.582957	H	-1.048893	-2.191504	7.217755
O	1.144316	-6.273316	9.859287	H	-1.359527	-3.646118	7.499717
H	1.469194	-5.654732	9.205039	O	-0.388673	-2.066272	4.421639
H	1.932156	-6.693113	10.204703	H	0.340975	-1.450230	4.487508
O	1.660159	-4.158878	8.227271	H	-1.086084	-1.668900	4.943123
H	2.003762	-3.673214	8.977137	O	-0.216225	1.091240	7.101256
H	0.791472	-3.785851	8.077379	H	0.126014	0.670209	7.889824
O	0.831902	-1.519286	11.746308	H	-0.075975	2.026594	7.248483
H	0.657317	-1.101832	10.902813	O	-2.642701	1.415866	10.511883
H	-0.027029	-1.585830	12.163493	H	-2.829803	1.713476	11.402194
O	0.800540	-0.331728	9.208628	H	-3.501224	1.359091	10.092423
H	1.326042	-0.869526	8.616300	O	-3.110058	2.406008	12.998322
H	1.421530	0.296924	9.576598	H	-2.937608	1.726318	13.649870
O	2.335767	-1.636613	7.369457	H	-2.343567	2.977876	13.039448
H	1.984016	-1.299191	6.545655	O	-2.627966	0.320979	14.660521
H	2.139713	-2.573283	7.348366	H	-2.244203	-0.312367	14.054030
O	1.468174	-0.113395	5.286709	H	-2.007211	0.363260	15.387919
H	0.834551	0.380516	5.807100	O	-0.465400	-0.010891	16.365455
H	2.274121	0.400368	5.338974	H	-0.457509	-0.948815	16.174488
O	0.417959	3.664009	7.815815	H	-0.335256	0.042345	17.312272
H	0.082309	3.570737	8.707371	O	-2.379623	-4.738484	15.068334
H	0.111892	4.525763	7.533086	H	-1.958741	-5.366683	14.481429
O	-0.618259	3.241519	10.267943	H	-2.777291	-5.277830	15.751853
H	-1.335100	2.607401	10.251639	O	-1.208965	-6.440594	13.275427
H	-0.518777	3.467542	11.192740	H	-0.647692	-5.822766	12.806926
O	-0.680075	3.709795	13.021913	H	-1.844426	-6.731194	12.621230
H	-0.222705	3.055146	13.549625	O	-4.519543	-3.886422	8.568336

H	-3.934523	-4.269362	7.914622	O	-0.873887	5.394496	8.016319
H	-4.453605	-2.942217	8.425638	H	-1.156625	4.496699	7.842386
O	-2.486638	-4.898542	6.979339	H	-0.478317	5.357077	8.887156
H	-1.978225	-4.966224	6.171151	O	-0.171781	4.479026	10.588104
H	-2.090547	-5.542282	7.566658	H	-0.151813	3.567557	10.296459
O	-0.906343	-4.744447	4.759229	H	0.230994	4.462088	11.456274
H	-0.659798	-3.824982	4.659069	O	-0.183537	1.771655	10.092283
H	-0.977350	-5.072879	3.862946	H	0.647364	1.376616	10.356441
O	-1.973158	-0.893313	6.361976	H	-0.815197	1.457010	10.738994
H	-1.555656	-0.066399	6.603093	O	1.904378	0.262517	10.992897
H	-2.767835	-0.925197	6.894616	H	2.543543	-0.281467	10.532698
O	-3.929211	-1.193469	8.290733	H	1.178972	-0.331254	11.186430
H	-3.183190	-1.237708	8.888838	O	3.025929	-1.951825	9.669503
H	-4.494400	-0.515867	8.661744	H	2.657709	-2.604055	10.265525
O	-5.191379	0.932502	9.562610	H	3.866347	-2.321475	9.398784
H	-5.415466	0.930294	10.493208	O	1.623864	-3.523557	11.453802
H	-5.861950	1.481049	9.155591	H	2.034934	-3.293352	12.287024
O	-5.533093	1.190514	12.230788	H	0.894598	-2.909486	11.368233
H	-5.547510	0.472963	12.864148	O	2.523954	-2.507370	13.802982
H	-4.863840	1.789444	12.561873	H	3.214592	-2.156150	14.365028
O	-5.127015	-0.751155	14.127878	H	1.782257	-1.917305	13.936931
H	-4.348570	-0.338778	14.502313	O	1.702482	1.460184	13.486363
H	-4.832208	-1.621564	13.860090	H	1.373717	2.353293	13.383880
O	-1.472928	-1.655161	13.211657	H	1.994233	1.209784	12.609771
H	-2.282164	-2.143700	13.060991	O	0.569837	3.963184	13.212140
H	-1.123181	-2.015590	14.026519	H	-0.336513	3.710707	13.388259
O	-3.817577	-3.075462	13.376377	H	0.780169	4.596600	13.898271
H	-4.128921	-3.607972	12.644441	O	-2.022098	3.236260	13.495782
H	-3.444654	-3.707225	13.991224	H	-2.413597	3.876194	12.901269
O	-4.285715	-4.614508	11.176703	H	-2.063409	2.407969	13.017807
H	-4.523852	-4.422413	10.269717	O	-1.712005	-1.455484	15.472928
H	-4.038211	-5.539126	11.169163	H	-0.909966	-1.214960	15.009124

3. (H₂O)₅₀-III

O	-2.785159	4.762536	11.349882	O	0.353949	-0.848657	13.844585
H	-3.266475	5.423446	10.852121	H	0.770175	0.012555	13.808504
H	-1.892698	4.806386	11.006627	H	0.003231	-0.982778	12.964107
O	-4.206847	6.368875	9.682024	O	-0.215379	-1.524906	11.126018
H	-5.116057	6.069941	9.667555	H	-0.008780	-1.564972	10.192239
H	-3.930653	6.341618	8.765942	H	-1.139971	-1.767134	11.177852
O	-3.302632	6.143584	7.083864	O	0.466443	-1.786587	8.524743
H	-2.414959	5.965208	7.394431	H	0.202180	-0.971907	8.097315
H	-3.221404	6.950572	6.575529	H	1.418991	-1.723045	8.594366
				O	-0.744464	0.528936	7.744698
				H	-0.563865	0.986570	8.565787

H	-1.657303	0.251083	7.820569	H	-5.089685	2.759750	9.121593
O	-2.175468	1.065708	11.855091	H	-6.229798	3.722510	8.866386
H	-2.800567	1.432510	11.229839	O	-6.397179	1.269202	11.676148
H	-2.667964	0.387060	12.316738	H	-6.504429	1.219111	12.626001
O	-3.538928	2.540602	9.979862	H	-7.197874	0.880992	11.323424
H	-2.966883	2.628826	9.217488	O	-6.954032	1.336391	14.345598
H	-3.398108	3.344582	10.479881	H	-6.326902	0.811560	14.843084
O	-2.034512	2.963460	7.722937	H	-6.738597	2.242168	14.567833
H	-2.752866	3.080682	7.101280	O	-5.137123	-0.289345	15.502696
H	-1.580709	2.177079	7.419786	H	-4.598264	-0.430611	14.724296
O	-4.285643	3.627144	6.361027	H	-4.521228	0.016094	16.168739
H	-4.902124	3.459382	7.073797	O	-2.932704	0.533302	16.951714
H	-4.039630	4.546008	6.467789	H	-2.431251	-0.157291	16.518289
O	-6.721982	5.250128	9.685625	H	-2.692753	0.460404	17.875479
H	-6.634725	4.865228	10.557675	O	-2.069293	-4.072541	14.612086
H	-7.569517	5.694659	9.703213	H	-1.544568	-4.312502	13.848335
O	-6.387980	3.978576	12.017389	H	-2.053546	-4.851344	15.168368
H	-6.386085	3.038175	11.838857	O	-0.649292	-4.825828	12.405797
H	-6.207426	4.045204	12.955043	H	-1.057152	-5.230736	11.640334
O	-5.996190	3.871126	14.781024	H	0.227824	-4.582378	12.109768
H	-5.148755	3.575276	15.113531	O	-5.650477	-3.781157	8.842126
H	-6.273485	4.547641	15.398815	H	-5.049869	-3.461982	8.168606
O	-3.619670	2.953662	15.696719	H	-6.273792	-3.065449	8.966523
H	-3.008421	3.054154	14.966988	O	-3.784018	-2.623586	7.195682
H	-3.331991	2.157111	16.142791	H	-3.716144	-2.378301	6.272936
O	-1.892216	-5.796586	10.104940	H	-2.945806	-3.040370	7.395496
H	-1.770412	-6.611161	9.617227	O	-3.733736	-1.489853	4.713925
H	-1.708862	-5.105878	9.468122	H	-4.023163	-0.607187	4.944933
O	-1.603778	-3.579976	8.550569	H	-4.194388	-1.687752	3.898531
H	-2.049850	-3.101168	9.249136	O	-6.818292	0.660399	7.262458
H	-0.800711	-3.083178	8.394018	H	-6.631275	1.423133	7.809718
O	-2.784415	-2.354797	10.686203	H	-6.913300	-0.062477	7.882665
H	-3.426043	-1.648435	10.611368	O	-6.906251	-1.331315	9.180144
H	-3.304515	-3.130036	10.897702	H	-6.095079	-1.077711	9.620506
O	-4.651041	-0.405004	10.361373	H	-7.600305	-1.061369	9.781518
H	-5.127793	0.283547	10.824879	O	-8.641815	-0.192582	10.975757
H	-4.291352	0.030595	9.588643	H	-8.650137	-0.517364	11.876135
O	-3.400931	-0.039031	7.912615	H	-9.557391	0.012275	10.786057
H	-3.822539	0.403638	7.176053	O	-8.537377	-0.822170	13.591466
H	-3.546103	-0.970671	7.747678	H	-8.013809	-1.525407	13.975611
O	-4.643128	0.938818	5.687344	H	-8.169588	-0.019609	13.961411
H	-4.545486	1.890323	5.650780	O	-6.691358	-2.476896	14.790811
H	-5.491972	0.800650	6.107588	H	-6.225690	-1.773237	15.242753
O	-5.813141	2.933678	8.519437	H	-6.014970	-2.924496	14.282494

O	-3.413194	-0.789409	13.468077	O	6.499750	3.918170	18.200610
H	-3.806522	-1.629345	13.231365	H	5.903580	4.454140	18.723640
H	-2.779120	-1.005531	14.151798	H	5.924760	3.394900	17.642220
O	-4.447118	-3.349628	13.415240	O	0.076360	0.836490	15.013190
H	-4.513818	-3.875506	12.618223	H	0.615940	0.266630	15.561230
H	-3.676525	-3.694367	13.866432	H	-0.456840	0.234940	14.493500
O	-4.245816	-4.617621	11.009664	O	4.865030	5.599820	13.410400
H	-4.810210	-4.438811	10.257522	H	5.377000	4.991230	12.877720
H	-3.571792	-5.205980	10.669431	H	4.318280	5.037270	13.958890

C. Ice-like water clusters

1. Ic-(H₂O)₉₆

O	1.684530	2.208330	7.061710	H	5.414650	1.840030	16.023830
H	2.216250	2.823060	7.567300	O	3.284250	4.028970	15.020660
H	1.137080	2.764240	6.507190	H	2.756190	3.436440	14.485590
O	3.252150	0.691540	11.844650	H	3.825740	3.449810	15.556960
H	3.765980	1.275140	11.286410	O	1.735940	8.645150	7.038950
H	2.732710	1.279650	12.392870	H	1.145620	8.104660	7.563950
O	6.365450	3.911260	11.828650	H	1.154650	9.178210	6.496560
H	6.934560	4.449550	11.278540	O	3.245220	7.081420	11.747670
H	6.967370	3.367810	12.337160	H	3.802330	6.579080	12.342250
O	0.103450	0.708910	8.732610	H	2.701370	7.618060	12.324290
H	0.653300	1.227610	8.145360	O	6.390270	10.225940	11.899730
H	-0.448690	0.189570	8.148090	H	5.859380	9.704370	11.297760
O	4.831960	5.492980	6.956430	H	6.951110	10.752700	11.330320
H	4.288530	4.948070	7.525640	O	0.072340	7.065970	8.554050
H	5.352350	6.024690	7.558700	H	0.619270	6.532580	9.130770
O	1.668110	5.493910	10.150080	H	-0.442700	7.611390	9.148610
H	2.211960	6.033820	10.723630	O	4.861450	11.919430	7.085750
H	1.152640	4.952540	10.747950	H	5.390370	11.320540	6.558660
O	4.756640	2.344830	10.240890	H	4.301970	11.346940	7.610610
H	5.322390	2.885930	10.791690	O	1.663720	11.953220	10.207160
H	5.362250	1.822330	9.715080	H	2.196940	11.367850	9.669320
O	3.248760	3.911350	8.551390	H	1.133760	11.366820	10.747080
H	2.703140	4.456270	9.118490	O	4.824560	8.719390	10.203560
H	3.766220	3.379050	9.155660	H	4.277460	8.140220	10.734110
O	1.756360	2.362010	13.446420	H	5.353460	8.126930	9.669230
H	1.156850	1.838770	13.978430	O	3.234600	10.322460	8.630990
H	1.184350	2.891990	12.891290	H	2.723130	9.722500	8.088140
O	3.364330	0.742020	18.148000	H	3.782560	9.751230	9.169200
H	2.797620	1.283640	18.697300	O	1.652150	8.651710	13.352340
H	2.759630	0.221430	17.619260	H	1.102740	8.115190	13.923780

H	2.197580	9.160380	13.952350	H	9.115280	3.350980	8.138630
O	3.186700	7.105970	18.232210	H	10.154990	4.451240	8.120450
H	3.758990	6.538900	18.749090	O	8.051230	2.325370	13.316770
H	3.785480	7.634240	17.704350	H	7.504610	1.810490	13.910360
O	6.452810	10.314230	18.186270	H	8.578270	2.877700	13.894180
H	5.906180	9.727240	17.663880	O	9.630350	0.751980	18.095350
H	6.979850	9.729820	18.731190	H	9.111310	1.293930	18.689590
O	0.059240	7.081130	14.968680	H	10.160410	0.202590	18.672800
H	0.596370	6.541560	15.548850	O	12.779590	3.891970	18.088970
H	-0.481500	7.604580	15.560160	H	12.270510	4.436760	18.689210
O	4.827610	11.815280	13.531430	H	13.312820	3.339190	18.660230
H	5.360840	11.278860	12.944780	O	6.456780	0.811900	14.981680
H	4.292400	12.351400	12.946300	H	5.920850	0.224820	14.448430
O	1.673770	11.745690	16.623250	H	6.983010	0.227310	15.527190
H	2.226720	12.324520	17.148070	O	11.223150	5.588390	13.383070
H	1.138250	12.338500	16.095950	H	11.771070	5.009150	12.853450
O	4.860990	8.649910	16.691950	H	10.683400	4.995910	13.906400
H	4.306950	9.151170	16.093590	O	8.117690	5.485210	16.615120
H	5.401730	8.105840	16.119390	H	7.545180	4.947340	17.162080
O	3.245120	10.135190	15.034540	H	7.518930	6.028070	16.102240
H	3.789460	10.733040	14.522180	O	11.197830	2.323110	16.474050
H	2.705310	10.708680	15.578570	H	10.662890	1.785630	17.058160
O	8.110200	2.314870	7.079480	H	11.729900	2.859590	17.061700
H	7.540860	2.862970	6.539400	O	9.623580	3.935230	14.903310
H	7.508590	1.810290	7.626940	H	9.106780	4.460010	15.514670
O	9.644380	0.658600	11.817900	H	10.163000	3.376660	15.463010
H	10.198660	1.241830	11.299380	O	8.010490	8.663370	7.158950
H	9.097680	1.247110	12.338490	H	7.462500	9.205640	6.591580
O	12.820400	3.973980	11.827420	H	8.524230	8.127060	6.555060
H	12.276840	3.387970	11.300760	O	9.574370	7.103610	11.781200
H	13.367630	3.388240	12.350570	H	10.154530	6.576020	12.330120
O	6.448510	0.823090	8.688190	H	10.165920	7.630650	11.244050
H	5.905870	0.241460	8.155750	O	12.805300	10.319850	11.761660
H	6.993670	0.233010	9.208630	H	12.265040	10.842410	12.354350
O	11.113350	5.497390	7.026250	H	13.354760	9.791590	12.340690
H	11.684640	4.940490	6.497350	O	6.352830	7.046350	8.646690
H	11.712600	6.004060	7.574360	H	6.929660	6.505090	9.185720
O	7.972280	5.479890	10.230710	H	6.947450	7.594340	8.134460
H	8.571480	4.939600	9.715660	O	11.180750	11.847000	6.995440
H	8.544660	6.033540	10.761840	H	10.658950	11.307850	7.589820
O	11.239750	2.318920	10.309170	H	11.712330	12.395050	7.572770
H	10.693180	2.855390	9.734960	O	8.008640	11.755230	10.286900
H	11.769890	1.791390	9.711750	H	8.554100	12.334100	10.819470
O	9.646690	3.899870	8.715310	H	7.474450	12.348070	9.758300

O	11.259740	8.633610	10.217640	H	17.021570	5.942940	6.499020
H	11.787790	9.226950	10.751830	O	14.469840	5.467840	10.209230
H	10.715800	9.211930	9.682940	H	13.891150	4.948890	10.767840
O	9.668630	10.262910	8.670550	H	13.876830	5.984110	9.663290
H	9.085310	9.709550	8.151160	O	17.572650	2.293310	10.323130
H	9.081450	10.775610	9.226060	H	18.120810	1.753500	9.753600
O	8.024980	8.647830	13.467700	H	17.032150	2.805030	9.721260
H	7.463180	9.175700	12.900280	O	15.991120	3.791630	8.641920
H	8.549860	8.122260	12.863940	H	16.538830	4.360640	8.101110
O	9.632040	7.090810	18.259990	H	15.476080	4.393930	9.178780
H	9.116240	6.532570	17.678130	O	14.410220	2.312960	13.326560
H	10.161880	7.627320	17.670360	H	13.886230	1.775540	13.920580
O	12.748550	10.259080	18.156750	H	14.952910	2.849710	13.904160
H	13.327590	9.740020	18.714910	O	16.009720	0.734730	18.154230
H	13.341080	10.785100	17.619670	H	15.420270	1.264490	18.691020
O	6.453820	7.078340	15.095860	H	15.427740	0.181650	17.633040
H	5.915360	6.560250	14.497620	O	19.151710	3.908470	18.269290
H	7.002670	7.613380	14.522500	H	19.670850	4.467610	17.691270
O	11.244420	11.845810	13.442450	H	18.601700	3.395860	17.676870
H	10.659840	11.312710	13.981250	O	12.871700	0.740930	14.975160
H	10.657270	12.371380	12.899060	H	12.280170	1.282810	15.497380
O	8.010960	11.932350	16.590160	H	12.291610	0.181560	14.458600
H	7.479840	11.344760	17.127650	O	17.555090	5.510590	13.325140
H	8.544670	11.348170	16.051520	H	18.081390	6.041290	13.923140
O	11.145610	8.665430	16.584100	H	17.016060	4.965920	13.898750
H	11.721800	9.210060	17.120390	O	14.359730	5.492710	16.503060
H	11.740610	8.155140	16.034710	H	13.815560	4.940700	17.064670
O	9.584610	10.305970	15.017810	H	14.872260	6.023740	17.112610
H	9.053010	9.717680	14.481560	O	17.545490	2.422030	16.607860
H	10.118840	9.722490	15.556700	H	18.087760	1.852690	16.061940
O	14.387630	2.299380	6.986030	H	17.017680	1.819880	17.132340
H	13.841410	1.776820	7.573250	O	15.974010	3.921310	14.924180
H	14.937770	2.820810	7.570580	H	15.423060	4.462920	15.489300
O	15.980140	0.631200	11.820130	H	16.512150	3.412150	15.530320
H	16.534180	1.213920	11.300790	O	14.394250	8.552700	7.059310
H	15.435510	1.220210	12.342330	H	13.845970	9.140210	6.539270
O	19.213790	3.912380	11.825760	H	14.925320	9.136630	7.600820
H	18.629600	3.356670	11.309880	O	15.953580	7.146210	11.806340
H	18.626230	4.464160	12.342050	H	15.441730	6.555220	11.254080
O	12.794450	0.781820	8.636740	H	16.504490	6.566370	12.332200
H	12.266740	0.193730	8.096450	O	19.155130	10.319860	11.795130
H	13.340190	0.198350	9.163970	H	19.691210	9.735580	12.331290
O	17.570050	5.376510	7.041760	H	18.627280	9.732420	11.254270
H	18.099700	5.981460	7.561130	O	12.790760	6.968650	8.634300

H	7.580191	12.519884	0.610836	H	0.844011	12.166334	4.277568
O	11.254482	0.027500	0.027500	H	0.027509	11.694927	5.610910
H	10.437971	0.498902	0.360843	O	2.272896	12.991302	3.694217
H	11.254472	-0.915319	0.360843	H	2.272905	12.991296	2.694203
O	9.009085	1.323880	0.944179	H	3.089407	12.519889	4.027545
H	8.192574	0.852467	0.610851	O	6.763689	0.027500	4.610896
H	9.009076	1.323875	1.944193	H	5.947178	0.498913	4.277568
O	9.009085	3.916640	0.027500	H	6.763680	0.027505	5.610910
H	8.192574	4.388043	0.360843	O	4.518293	1.323880	3.694217
H	9.009076	2.973820	0.360843	H	4.518283	1.323875	2.694203
O	11.254482	5.213021	0.944179	H	3.701782	0.852467	4.027545
H	12.070983	4.741603	0.610836	O	4.518293	3.916640	4.610896
H	10.437980	4.741603	0.610836	H	3.701782	4.388043	4.277553
O	11.254482	7.805781	0.027500	H	4.518283	2.973820	4.277553
H	11.254482	6.862956	0.360828	O	6.763689	5.213021	3.694217
H	11.254482	7.805770	-0.972513	H	6.763680	5.213015	2.694203
O	9.009085	9.102161	0.944179	H	5.947178	4.741608	4.027545
H	9.825596	8.630759	0.610836	O	6.763689	7.805781	4.610896
H	9.009095	10.044981	0.610836	H	6.763689	6.862956	4.277568
O	9.009085	11.694922	0.027500	H	6.763689	7.805770	5.610910
H	9.825596	12.166334	0.360828	O	4.518293	9.102161	3.694217
H	9.009095	11.694927	-0.972513	H	5.334803	8.630759	4.027560
O	11.254482	12.991302	0.944179	H	4.518302	10.044981	4.027560
H	12.070993	12.519889	0.610851	O	4.518293	11.694922	4.610896
H	11.254491	12.991296	1.944193	H	5.334803	12.166334	4.277568
O	2.272896	0.027500	4.610896	H	4.518302	11.694927	5.610910
H	2.272896	-0.915325	4.277568	O	6.763689	12.991302	3.694217
H	2.272896	0.027489	5.610910	H	6.763689	12.991312	2.694203
O	0.027500	1.323880	3.694217	H	6.763689	13.934127	4.027545
H	0.844001	0.852462	4.027560	O	11.254482	0.027500	4.610896
H	-0.789001	0.852462	4.027560	H	10.437971	0.498902	4.277553
O	0.027500	3.916640	4.610896	H	11.254472	-0.915319	4.277553
H	0.027491	2.973820	4.277553	O	9.009085	1.323880	3.694217
H	-0.789010	4.388043	4.277553	H	8.192574	0.852478	4.027560
O	2.272896	5.213021	3.694217	H	9.009076	2.266700	4.027560
H	1.456385	4.741619	4.027560	O	9.009085	3.916640	4.610896
H	2.272887	6.155841	4.027560	H	8.192584	4.388059	4.277553
O	2.272896	7.805781	4.610896	H	9.825587	4.388059	4.277553
H	3.089407	8.277194	4.277568	O	11.254482	5.213021	3.694217
H	2.272905	7.805786	5.610910	H	11.254482	5.213031	2.694203
O	0.027500	9.102161	3.694217	H	11.254482	6.155846	4.027545
H	0.844011	8.630759	4.027560	O	11.254482	7.805781	4.610896
H	0.027509	10.044981	4.027560	H	12.070983	8.277199	4.277553
O	0.027500	11.694922	4.610896	H	10.437980	8.277199	4.277553

O	9.009085	9.102161	3.694217	H	6.763698	5.213015	9.277627
H	9.009076	9.102156	2.694203	O	6.763689	7.805781	7.360934
H	8.192574	8.630748	4.027545	H	6.763680	6.862961	7.694277
O	9.009085	11.694922	4.610896	H	5.947178	8.277183	7.694277
H	8.192574	12.166324	4.277553	O	4.518293	9.102161	8.277613
H	9.009076	10.752101	4.277553	H	4.518293	10.044987	7.944285
O	11.254482	12.991302	3.694217	H	4.518293	9.102172	9.277627
H	12.070983	12.519884	4.027560	O	4.518293	11.694922	7.360934
H	10.437980	12.519884	4.027560	H	3.701791	12.166340	7.694277
O	2.272896	0.027500	7.360934	H	5.334794	12.166340	7.694277
H	1.456395	0.498918	7.694277	O	6.763689	12.991302	8.277613
H	3.089398	0.498918	7.694277	H	7.580200	12.519889	7.944285
O	0.027500	1.323880	8.277613	H	6.763698	12.991296	9.277627
H	0.027491	2.266700	7.944270	O	11.254482	0.027500	7.360934
H	-0.789010	0.852478	7.944270	H	11.254482	0.027489	6.360920
O	0.027500	3.916640	7.360934	H	11.254482	-0.915325	7.694262
H	0.027509	3.916646	6.360920	O	9.009085	1.323880	8.277613
H	0.844011	4.388053	7.694262	H	9.825596	0.852478	7.944270
O	2.272896	5.213021	8.277613	H	9.009095	2.266700	7.944270
H	2.272905	6.155841	7.944270	O	9.009085	3.916640	7.360934
H	3.089407	4.741619	7.944270	H	9.009095	3.916646	6.360920
O	2.272896	7.805781	7.360934	H	9.825596	4.388053	7.694262
H	1.456395	8.277199	7.694277	O	11.254482	5.213021	8.277613
H	3.089398	8.277199	7.694277	H	12.070993	4.741619	7.944270
O	0.027500	9.102161	8.277613	H	11.254491	6.155841	7.944270
H	0.027491	10.044981	7.944270	O	11.254482	7.805781	7.360934
H	-0.789010	8.630759	7.944270	H	11.254472	7.805786	6.360920
O	0.027500	11.694922	7.360934	H	10.437971	8.277194	7.694262
H	0.844001	12.166340	7.694277	O	9.009085	9.102161	8.277613
H	-0.789001	12.166340	7.694277	H	8.192574	8.630748	7.944285
O	2.272896	12.991302	8.277613	H	9.009076	9.102156	9.277627
H	2.272896	13.934127	7.944285	O	9.009085	11.694922	7.360934
H	2.272896	12.991312	9.277627	H	9.009085	11.694911	6.360920
O	6.763689	0.027500	7.360934	H	9.009085	10.752096	7.694262
H	6.763698	-0.915319	7.694277	O	11.254482	12.991302	8.277613
H	7.580200	0.498902	7.694277	H	10.437971	12.519889	7.944285
O	4.518293	1.323880	8.277613	H	11.254472	12.991296	9.277627
H	5.334803	0.852478	7.944270	O	2.272896	0.027500	11.944330
H	4.518302	2.266700	7.944270	H	1.456395	0.498918	11.610987
O	4.518293	3.916640	7.360934	H	3.089398	0.498918	11.610987
H	4.518302	3.916646	6.360920	O	0.027500	1.323880	11.027651
H	5.334803	4.388053	7.694262	H	0.027491	1.323875	10.027637
O	6.763689	5.213021	8.277613	H	-0.789010	0.852467	11.360978
H	7.580200	4.741608	7.944285	O	0.027500	3.916640	11.944330

H	0.027509	2.973820	11.610987	O	9.009085	1.323880	11.027651
H	0.844011	4.388043	11.610987	H	9.009085	1.323891	10.027637
O	2.272896	5.213021	11.027651	H	9.009085	2.266706	11.360978
H	2.272896	5.213031	10.027637	O	9.009085	3.916640	11.944330
H	2.272896	6.155846	11.360978	H	9.009095	3.916646	12.944343
O	2.272896	7.805781	11.944330	H	9.825596	4.388053	11.611002
H	2.272905	7.805786	12.944343	O	11.254482	5.213021	11.027651
H	3.089407	8.277194	11.611002	H	11.254491	5.213015	10.027637
O	0.027500	9.102161	11.027651	H	12.070993	4.741608	11.360978
H	0.027509	9.102156	10.027637	O	11.254482	7.805781	11.944330
H	0.844011	8.630748	11.360978	H	12.070993	8.277183	11.610987
O	0.027500	11.694922	11.944330	H	11.254491	6.862961	11.610987
H	0.027509	10.752101	11.610987	O	9.009085	9.102161	11.027651
H	0.844011	12.166324	11.610987	H	8.192584	8.630743	11.360993
O	2.272896	12.991302	11.027651	H	9.825587	8.630743	11.360993
H	2.272905	13.934122	11.360993	O	9.009085	11.694922	11.944330
H	3.089407	12.519900	11.360993	H	9.009095	10.752101	11.610987
O	6.763689	0.027500	11.944330	H	9.825596	12.166324	11.610987
H	6.763698	0.027505	12.944343	O	11.254482	12.991302	11.027651
H	7.580200	0.498913	11.611002	H	12.070993	12.519900	11.360993
O	4.518293	1.323880	11.027651	H	11.254491	13.934122	11.360993
H	4.518302	1.323875	10.027637				
H	5.334803	0.852467	11.360978	D. Foldamer W			
O	4.518293	3.916640	11.944330	1. Foldamer W			
H	3.701782	4.388043	11.610987				
H	4.518283	2.973820	11.610987	O	-1.218133	-2.969088	-4.435723
O	6.763689	5.213021	11.027651	O	2.568927	-3.268627	0.423169
H	5.947187	4.741603	11.360993	O	3.635666	-2.016179	-1.131129
H	7.580191	4.741603	11.360993	O	0.108811	0.361751	1.138418
O	6.763689	7.805781	11.944330	O	0.676649	5.089705	0.804552
H	6.763689	7.805770	12.944343	O	6.510186	-3.037965	0.145497
H	6.763689	6.862956	11.611002	O	7.449544	-1.098502	-0.597296
O	4.518293	9.102161	11.027651	O	3.632168	-0.546006	2.160179
H	5.334803	8.630759	11.360993	O	2.788882	3.979525	3.513564
H	4.518302	10.044981	11.360993	O	-1.707012	-1.064027	5.279114
O	4.518293	11.694922	11.944330	O	0.024257	-6.394315	-0.320044
H	4.518302	11.694927	12.944343	O	2.643415	-1.928651	-5.030842
H	5.334803	12.166334	11.611002	O	-0.328927	-0.007117	-1.822093
O	6.763689	12.991302	11.027651	O	-0.851586	4.706997	-2.370586
H	6.763698	13.934122	11.360993	O	-2.064239	3.860154	-0.652929
H	7.580200	12.519900	11.360993	O	-4.570569	4.695171	-2.447431
O	11.254482	0.027500	11.944330	O	-3.902624	4.571536	-4.627600
H	11.254472	0.027505	12.944343	O	-3.320818	0.618645	-2.020772
H	10.437971	0.498913	11.611002	O	-4.416317	-4.747894	1.540683

O	-4.377615	2.532533	4.911686	C	4.709809	-5.009286	2.149712
N	1.776096	-1.239901	-0.012062	H	5.434447	-4.253403	1.877995
H	1.034829	-1.498925	0.655631	C	3.437557	-4.383975	0.096505
N	1.102745	0.894079	0.454006	H	4.381358	-3.990339	-0.260740
N	0.258406	2.857770	1.168373	H	2.961217	-4.941645	-0.706758
H	-0.332174	2.194314	1.664566	C	2.743261	-2.165278	-0.310491
N	-1.771596	3.429366	2.711928	C	1.976801	0.100390	-0.213883
N	-3.391177	1.407426	3.159058	C	2.976197	0.683515	-0.986631
H	-2.691539	1.529101	2.438571	H	3.642612	0.030912	-1.517499
N	5.727352	-1.128936	0.921106	C	3.079373	2.061952	-1.039045
H	4.978438	-1.674731	1.339529	H	3.859449	2.510420	-1.635392
N	4.419786	0.454339	1.843426	C	2.197600	2.869610	-0.342089
N	2.931405	1.756155	2.933674	H	2.229053	3.944742	-0.346569
H	2.483261	0.848613	3.052658	C	1.208741	2.253024	0.401738
N	0.664971	1.221074	4.062456	C	0.071288	4.188072	1.370034
N	-0.437515	-1.139383	3.349691	C	-0.986872	4.451361	2.385238
H	0.051559	-0.543830	2.667422	C	-1.119125	5.720390	2.932897
N	-0.272566	-2.702517	1.681140	H	-0.449287	6.500608	2.604318
N	-0.061209	-4.105322	-0.102232	C	-2.120539	5.927143	3.870406
H	0.166857	-3.257753	-0.603916	H	-2.261025	6.901364	4.318059
N	1.005404	-3.781958	-2.499434	C	-2.944871	4.868348	4.217931
N	1.206162	-1.265446	-3.372943	H	-3.747504	4.954179	4.933496
H	0.597423	-1.575096	-2.621667	C	-2.730463	3.639591	3.606198
N	0.321853	0.705178	-2.713551	C	-3.594663	2.475626	3.969729
N	-0.788455	2.472233	-1.833040	C	-3.941413	0.133325	3.239838
H	-1.191481	1.711905	-1.285329	C	-8.849614	5.678604	-3.468299
N	-3.619446	2.844692	-3.131320	H	-9.489814	5.631661	-4.339301
H	-3.851920	2.481603	-2.211335	C	-2.259997	-0.338330	-3.851751
N	-2.854476	0.727787	-3.242271	C	-2.975423	1.916867	-3.902322
N	-2.349490	-1.477695	-3.106147	C	-2.446638	2.085764	-5.169958
H	-2.779005	-1.332429	-2.195638	H	-2.562213	3.047515	-5.638218
N	-2.854961	-3.386552	-1.327324	C	-1.798053	1.014382	-5.764028
N	-3.612090	-2.631474	1.114240	H	-1.363910	1.130865	-6.746281
H	-3.101443	-2.096736	0.423481	C	-1.704180	-0.206481	-5.114671
N	-3.582549	-0.649725	2.221963	H	-1.226721	-1.071760	-5.538345
C	3.609856	-5.219473	1.320413	C	-1.886986	-2.705028	-3.437800
C	2.679193	-6.202881	1.650191	C	-2.331124	-3.766760	-2.492456
H	1.824445	-6.376113	1.010142	C	-3.285703	-4.342575	-0.504687
C	2.848725	-6.963565	2.799653	C	-3.238171	-5.696696	-0.816562
H	2.123942	-7.727736	3.048330	H	-3.622957	-6.400572	-0.095632
C	3.946788	-6.749326	3.624716	C	-2.687277	-6.077485	-2.029311
H	4.079061	-7.347110	4.516989	H	-2.604600	-7.122412	-2.292112
C	4.879000	-5.771110	3.298333	C	-2.213748	-5.094444	-2.884319
H	5.738173	-5.605937	3.935351	H	-1.745147	-5.310243	-3.831669

C	6.649405	-4.277130	-1.937803	H	1.020619	-7.127672	-2.426593
C	6.742050	-5.612524	-2.316593	C	1.876734	-5.934999	-4.032454
H	7.306456	-6.303425	-1.702374	H	2.219951	-6.769455	-4.627674
C	6.116588	-6.059827	-3.474422	C	2.109951	-4.632756	-4.444502
H	6.198288	-7.099067	-3.764591	H	2.636033	-4.390571	-5.353715
C	5.379586	-5.171566	-4.246380	C	1.650162	-3.590562	-3.649621
H	4.886811	-5.517788	-5.145335	C	1.893558	-2.192237	-4.096727
C	5.262622	-3.839391	-3.860787	C	1.179637	0.084182	-3.572942
H	4.666262	-3.150588	-4.444226	C	1.896498	0.818691	-4.504061
C	5.901249	-3.392436	-2.713337	H	2.561964	0.283835	-5.158346
H	5.795649	-2.363831	-2.405099	C	1.704629	2.189810	-4.548452
C	7.376664	-3.797511	-0.721920	H	2.250737	2.780490	-5.269995
H	7.728858	-4.634186	-0.123671	C	0.818845	2.819627	-3.687630
H	8.214276	-3.155695	-0.983927	H	0.635041	3.878289	-3.701100
C	6.638809	-1.697320	0.081143	C	0.125286	2.051137	-2.766210
C	5.555892	0.212644	1.129779	C	-1.201264	3.768131	-1.684290
C	6.382380	1.255741	0.744141	C	-2.514232	5.199065	-0.396625
H	7.258321	1.017374	0.166792	H	-2.743792	5.669782	-1.347343
C	6.042007	2.546560	1.120767	H	-1.691962	5.752466	0.054211
H	6.678755	3.370766	0.833076	C	-3.711133	5.166406	0.498835
C	4.900937	2.793302	1.868948	C	-4.165237	6.370611	1.034012
H	4.599995	3.773553	2.194560	H	-3.634630	7.287518	0.806366
C	4.094546	1.723993	2.223749	C	-9.398378	5.594309	-2.194103
C	2.358084	2.836021	3.547302	H	-10.467588	5.482415	-2.072313
C	1.127394	2.450228	4.292002	C	-8.573347	5.654297	-1.075491
C	0.531506	3.340374	5.174689	H	-8.998054	5.587675	-0.082553
H	0.956985	4.325001	5.294085	C	-7.202309	5.800679	-1.229321
C	-0.591019	2.911284	5.871696	H	-6.557382	5.842147	-0.362631
H	-1.087961	3.567922	6.571581	C	-6.648364	5.886879	-2.505045
C	-1.073526	1.630898	5.650354	C	-7.475986	5.821375	-3.622228
H	-1.944216	1.238699	6.152524	H	-7.036592	5.877498	-4.610117
C	-0.419594	0.826775	4.719579	C	-4.387282	3.989999	0.804249
C	-0.924039	-0.560990	4.477525	H	-4.027073	3.052398	0.408550
C	-0.699251	-2.432149	2.921343	C	-5.498341	4.019368	1.639644
C	-1.333454	-3.380984	3.728773	H	-6.005557	3.096309	1.884413
H	-1.695773	-3.085368	4.696009	C	-5.946238	5.221675	2.172518
C	-1.488176	-4.656719	3.219962	H	-6.806472	5.239298	2.827457
H	-1.980187	-5.413070	3.815045	C	-5.277438	6.401532	1.864393
C	-1.046233	-4.970378	1.945365	H	-5.617753	7.343819	2.273311
H	-1.150745	-5.944873	1.503562	C	-4.023828	4.091628	-3.519290
C	-0.469151	-3.938832	1.213368	C	-5.168324	5.992378	-2.664258
C	0.197893	-5.256445	-0.756421	H	-4.882680	6.334759	-3.653534
C	0.816389	-5.037202	-2.098241	H	-4.732550	6.635748	-1.902663
C	1.218797	-6.147381	-2.831939	C	-3.839766	-3.934169	0.824523

C	-4.020262	-1.908681	2.231759	C	19.309015	5.241119	13.066309
C	-4.815205	-2.448493	3.239614	H	19.113938	5.560335	12.052769
H	-5.115385	-3.480098	3.186771	C	18.931948	6.049921	14.128015
C	-5.179944	-1.597129	4.271355	H	18.422054	6.987342	13.947164
H	-5.799682	-1.970043	5.075457	C	18.824074	6.585917	16.553111
C	-4.757923	-0.278012	4.290279	H	19.510589	7.429118	16.633195
H	-5.012727	0.415948	5.071679	H	17.824343	6.989392	16.409044

2. Monomer in Foldamer W

O	18.857157	5.848537	17.780625	C	18.763572	6.617524	18.881565
O	18.612252	7.823334	18.870953	C	18.836298	6.265524	21.286432
O	19.317149	4.045021	21.704292	C	18.594571	7.548732	21.748865
O	19.202586	5.049473	26.370344	H	18.424266	8.317328	21.015807
O	19.926686	-1.647897	24.384910	C	18.581297	7.776896	23.116292
O	18.325982	-0.761499	16.645533	H	18.394692	8.771357	23.492656
O	15.850196	5.803349	16.640917	C	18.801523	6.739930	24.009589
O	16.417596	3.723905	20.903594	H	18.806982	6.863947	25.077730
O	15.405757	6.569814	24.594967	C	19.044626	5.474373	23.505367
O	16.279025	4.552417	25.161679	C	19.310401	4.150634	25.542557
N	18.872686	5.827737	19.988384	C	19.555435	2.727611	25.920053
H	18.998007	4.819443	19.930308	C	19.872955	2.411471	27.233450
N	19.074628	5.244636	22.158175	H	19.863807	3.197926	27.971158
N	19.264431	4.319087	24.197051	C	20.164397	1.090308	27.535062
H	19.379710	3.510503	23.588364	H	20.423018	0.803615	28.544296
N	19.490810	1.821457	24.942332	C	20.110649	0.141964	26.526029
N	19.285662	0.043697	22.957808	H	20.333782	-0.899766	26.684884
H	19.105508	1.039146	22.934156	C	19.748347	0.551553	25.247820
N	18.765720	0.162927	20.740410	C	19.663616	-0.470997	24.156398
N	18.199882	0.512100	18.559372	C	19.176346	-0.620550	21.736207
H	17.922348	1.424031	18.900855	C	19.483164	-1.972118	21.585125
N	17.118114	2.535528	17.156083	H	19.786957	-2.547885	22.440012
N	16.155371	4.569981	18.550107	C	19.378477	-2.497374	20.308057
H	16.472795	3.678439	18.924208	H	19.613095	-3.539499	20.140319
N	15.945087	4.935255	20.764225	C	18.974672	-1.708781	19.243152
N	15.929235	4.981984	23.017289	H	18.884118	-2.075858	18.236709
H	16.353756	4.079248	22.814336	C	18.665182	-0.378327	19.527545
C	19.200127	5.663734	15.438845	C	18.050190	0.283483	17.228771
C	19.829433	4.444123	15.676802	C	17.519664	1.461742	16.472841
H	20.000634	4.134878	16.699162	C	17.469461	1.375410	15.086012
C	20.188999	3.624684	14.612868	H	17.794876	0.459171	14.618945
H	20.654332	2.665998	14.805695	C	16.999842	2.464080	14.370643
C	19.938358	4.024196	13.305420	H	16.956561	2.440023	13.292180
H	20.225855	3.388473	12.478254	C	16.590456	3.589586	15.064762
				H	16.231298	4.479649	14.575111
				C	16.657605	3.571956	16.452665
				C	16.183183	4.766793	17.208378

C	15.800145	5.471672	19.516561
C	15.366246	6.775216	19.350410
H	15.299065	7.158101	18.348929
C	15.048676	7.519663	20.476004
H	14.705766	8.537730	20.359616
C	15.183813	6.977569	21.744164
H	14.980816	7.525639	22.646989
C	15.653181	5.679707	21.869841
C	15.832626	5.474502	24.287314
C	16.217716	4.986803	26.525537
H	15.221960	5.386355	26.715187
H	16.931020	5.793391	26.669636
C	16.537379	3.850314	27.439109
C	16.883978	4.157223	28.753251
H	16.963170	5.196015	29.047135
C	16.466045	2.518034	27.046214
H	16.232693	2.281793	26.017161
C	16.721496	1.505363	27.966275
H	16.679408	0.470481	27.650025
C	17.043124	1.816458	29.281614
H	17.229631	1.026876	29.998670
C	17.126394	3.149725	29.673862
H	17.375567	3.402718	30.695985