

# Supporting Information

## An improved localized molecular-orbital assembler approach for Hartree-Fock calculations of general large molecules

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### Contents

Cartesian Coordinates (Å):

A . acetyl-(ala) <sub>n</sub> -methylamide	3. 1ALE
1. $\alpha$ -helix acetyl-(ala) <sub>12</sub> -methylamide	4. 2KAM
2 3 <sub>10</sub> -helix acetyl- (ala) <sub>14</sub> -methylamide	
3 3 <sub>10</sub> -helix acetyl- (ala) <sub>19</sub> -methylamid	
4 3 <sub>10</sub> -helix acetyl- (ala) <sub>24</sub> -methylamid	
5 3 <sub>10</sub> -helix acetyl- (ala) <sub>29</sub> -methylamid	
6 3 <sub>10</sub> -helix acetyl- (ala) <sub>34</sub> -methylamid	
B . acetyl-(ala) <sub>n</sub> -NH <sub>2</sub>	A . acetyl-(ala) <sub>n</sub> -methylamide
1. $\alpha$ -helix acetyl-(ala) <sub>15</sub> -NH <sub>2</sub>	1. $\alpha$ -helix acetyl-(ala) <sub>12</sub> -methylamide
2. $\alpha$ -helix acetyl-(ala) <sub>18</sub> - NH <sub>2</sub>	
3. $\beta$ -strand acetyl- (ala) <sub>18</sub> - NH <sub>2</sub>	
4. 3 <sub>10</sub> -helix acetyl- (ala) <sub>18</sub> - NH <sub>2</sub>	
C. water clusters	C      5.40750    5.72410   -2.37140
1. (H <sub>2</sub> O) <sub>32</sub>	N      4.92720    7.09550   -2.37140
2. Ice-like (H <sub>2</sub> O) <sub>48</sub>	C      6.93040    5.71200   -2.22440
3. Ice-like (H <sub>2</sub> O) <sub>64</sub>	C      4.85250    4.99390   -1.14690
4. (H <sub>3</sub> O <sup>+</sup> ) <sub>5</sub> (HO <sup>-</sup> ) <sub>5</sub> (H <sub>2</sub> O) <sub>22</sub>	O      4.35100    3.87670   -1.26270
5. (H <sub>3</sub> O <sup>+</sup> ) <sub>5</sub> (HO <sup>-</sup> ) <sub>5</sub> (H <sub>2</sub> O) <sub>38</sub>	C      0.76450    5.53210    0.41160
6. (H <sub>3</sub> O <sup>+</sup> ) <sub>6</sub> (HO <sup>-</sup> ) <sub>6</sub> (H <sub>2</sub> O) <sub>52</sub>	C     -4.82360   -8.22990   3.36670
D. Protein Molecules	H      5.61890    7.84510   -2.37140
1. 1V4Z	H      5.09330    5.19640   -3.27190
2. 2P5J	H      7.37150    6.26310   -3.05500

H	7.21720	6.19130	-1.28850	H	4.30300	-0.01880	1.18020
H	7.29580	4.68510	-2.22390	N	-1.47920	0.94900	0.36080
N	2.19470	5.70550	0.60090	C	-1.14690	0.34670	1.51660
C	4.45740	5.05150	1.26820	O	-1.74330	-0.63520	1.95600
N	4.94660	5.63620	0.03110	C	-0.74310	-2.63280	-1.70670
C	4.57220	6.07330	2.40120	C	-2.61650	1.27050	-1.77270
C	2.96710	4.73650	1.12400	H	1.49580	2.13000	1.28730
O	2.52480	3.64430	1.47660	H	0.32190	0.25790	3.08170
C	1.12050	3.13820	-2.54560	H	0.36650	2.76520	3.37610
C	0.19310	6.74170	-0.33080	H	-0.79700	2.92420	2.04550
H	5.37150	6.56240	0.07450	H	-1.28420	2.10670	3.54350
H	4.99260	4.13300	1.50870	N	-1.10450	-1.28370	-1.30570
H	5.61680	6.36420	2.51210	C	-2.33360	-0.98030	-0.85170
H	3.98070	6.95780	2.16540	O	-3.23240	-1.81300	-0.74360
H	4.20640	5.63940	3.33170	C	-0.61760	-4.00430	1.85770
N	1.25910	4.23920	-1.60740	C	0.75030	-2.68970	-2.03470
C	0.51690	4.32000	-0.48870	H	-0.95280	1.76130	0.03920
O	-0.32450	3.47740	-0.18050	H	-3.52850	0.55000	0.06770
C	2.83330	0.57510	-0.28750	H	-2.74520	2.32850	-1.54420
C	2.19200	3.24970	-3.63200	H	-1.68070	1.13600	-2.31490
H	2.61000	6.59490	0.32370	H	-3.44060	0.92180	-2.39500
H	0.25680	5.37670	1.36350	N	-0.47690	-3.19090	0.66190
H	0.38690	7.64100	0.25380	C	-0.96030	-3.58570	-0.52950
H	0.67310	6.84110	-1.30430	O	-1.55060	-4.65230	-0.69300
H	-0.88000	6.61640	-0.47540	C	-4.35530	-3.32480	2.26980
N	2.47300	1.76980	-1.03210	C	-0.10100	-3.22890	3.07140
C	1.38280	1.81800	-1.81820	H	-0.39300	-0.55630	-1.37670
O	0.61880	0.86500	-1.96340	H	-1.34600	-2.96800	-2.55060
C	0.03280	0.94440	2.28600	H	0.96320	-1.98940	-2.84240
C	4.02870	0.87460	0.61930	H	1.33430	-2.40870	-1.15840
H	1.94450	4.96450	-1.81830	H	1.02660	-3.70010	-2.33630
H	0.12040	3.11250	-2.97810	N	-2.92460	-3.20730	2.04410
H	2.07360	4.20090	-4.15100	C	-2.10190	-4.26880	2.11770
H	3.18370	3.21260	-3.18120	O	-2.49530	-5.40460	2.37860
H	2.09230	2.42580	-4.33860	C	-5.05950	-5.08790	-1.04640
N	1.13490	1.17950	1.36860	C	-5.03460	-1.98600	1.97490
C	1.67840	0.18900	0.63880	H	0.00570	-2.29620	0.74530
O	1.28700	-0.97580	0.69330	H	-0.10090	-4.95780	1.74890
C	-2.57960	0.47910	-0.46380	H	0.94730	-2.97670	2.91150
C	-0.45710	2.27770	2.85450	H	-0.67230	-2.30900	3.19540
H	3.07560	2.58820	-0.94500	H	-0.20440	-3.83500	3.97140
H	3.04460	-0.25810	-0.95760	N	-4.57260	-4.19650	-0.00730
H	4.86790	1.19970	0.00430	C	-4.94270	-4.33150	1.27870
H	3.77370	1.66940	1.32020	O	-5.71200	-5.20970	1.66580



H	2.98510	3.70900	1.59080	N	-1.81740	-5.26270	1.63970
H	2.49320	6.07160	2.33310	C	-1.57510	-5.90270	0.48180
H	0.95360	6.00870	1.45270	O	-1.79190	-7.10280	0.32160
H	1.21360	4.93610	2.84250	C	-5.47710	-6.95480	0.83290
N	1.01950	1.40450	-1.37590	C	-2.84260	-4.92220	3.82630
C	-0.28130	1.71850	-1.24040	H	-0.73330	-2.94830	-0.55400
O	-1.17340	0.87300	-1.19510	H	-1.34060	-5.47500	-1.61030
C	-0.03620	-0.79730	1.93230	H	0.97220	-4.51100	-1.29910
C	2.98780	-0.03230	-1.27740	H	0.82630	-4.77210	0.45020
H	0.84570	4.75230	-1.05120	H	0.85050	-6.16770	-0.64580
H	-1.51420	3.32820	-0.53050	N	-4.28680	-6.28500	1.32890
H	-1.05950	4.76000	-2.55990	C	-3.59310	-6.75160	2.38250
H	0.02800	3.50270	-3.18120	O	-3.91150	-7.76840	2.99710
H	-1.70430	3.15730	-3.00960	C	-3.48380	-10.14540	0.16320
N	0.55410	-0.13180	0.78340	C	-5.83830	-6.40630	-0.54900
C	0.85520	-0.79490	-0.34740	H	-1.62030	-4.26530	1.72200
O	0.65530	-2.00000	-0.49090	H	-1.62530	-6.62720	3.23530
C	-3.05080	-1.87280	-0.15520	H	-2.00280	-4.29340	4.12180
C	-0.57480	0.24740	2.91180	H	-3.61840	-4.29490	3.38750
H	1.72190	2.14340	-1.40820	H	-3.25020	-5.43230	4.69920
H	1.18400	-0.41080	-2.43530	N	-3.89980	-8.76850	0.36870
H	3.47220	0.57970	-2.03820	C	-5.17640	-8.44240	0.63880
H	3.24670	0.35560	-0.29220	O	-6.07590	-9.27630	0.73080
H	3.33280	-1.06340	-1.35460	C	-4.68400	-11.10080	3.66300
N	-1.89020	-1.18200	0.38080	C	-1.95750	-10.23610	0.22050
C	-1.24300	-1.61950	1.47560	H	-3.98130	-5.43640	0.85260
O	-1.58200	-2.62540	2.09710	H	-6.30840	-6.84870	1.52980
C	-1.00410	-5.05990	-0.66030	H	-6.01790	-5.33410	-0.46940
C	-3.35120	-1.35770	-1.56420	H	-5.01600	-6.57770	-1.24350
H	0.73950	0.86880	0.85270	H	-6.73090	-6.90570	-0.92560
H	0.68180	-1.45950	2.41610	N	-4.19090	-10.39300	2.49370
H	0.24550	0.88980	3.23210	C	-4.00830	-11.00910	1.31210
H	-1.33400	0.85820	2.42350	O	-4.24270	-12.20360	1.13600
H	-1.01880	-0.24700	3.77580	C	4.30150	13.35210	-3.10960
N	-1.43980	-3.68240	-0.50500	C	-5.11010	-10.09340	4.73280
C	-2.73010	-3.36160	-0.30190	H	-3.19010	-8.03890	0.30280
O	-3.62640	-4.20100	-0.23350	H	-3.86780	-10.53670	-0.77890
C	-2.35930	-5.94900	2.80010	H	-1.53470	-9.59760	-0.55520
C	0.51850	-5.13600	-0.53000	H	-1.60130	-9.89630	1.19290
H	-1.56920	-0.34140	-0.09950	H	-1.64020	-11.26750	0.06680
H	-3.91460	-1.75870	0.49970	O	3.70620	11.04230	-3.10970
H	-3.54250	-0.28570	-1.51690	C	-5.94290	-11.88450	3.28610
H	-2.49600	-1.53710	-2.21570	O	-6.24110	-12.91230	3.89250
H	-4.22140	-1.87300	-1.97080	H	-8.03320	-12.95380	2.48430

H	-3.98150	-9.39930	2.58850	C	4.32000	8.61740	0.44270
H	-3.93650	-11.79410	4.04840	C	7.48490	9.33840	-2.63880
H	-4.25200	-9.47770	5.00230	H	5.29810	14.10810	-2.61910
H	-5.90000	-9.45060	4.34450	H	2.92730	12.67520	-2.17730
H	-5.48100	-10.61960	5.61240	H	3.46540	14.06620	-4.21460
N	-6.68080	-11.38930	2.27650	H	4.59040	12.80520	-4.75650
C	4.62320	11.87670	-3.10960	H	2.85470	12.44860	-4.65810
H	3.21900	13.47930	-3.09930	N	4.95830	9.26280	-0.69200
H	4.72290	13.82430	-2.22230	C	5.31690	8.57780	-1.79250
H	4.72280	13.82450	-3.99700	O	5.13320	7.36820	-1.91830
H	-8.74840	-11.41240	1.97200	C	1.41460	7.47060	-1.75850
H	-7.80540	-12.36990	0.81290	C	3.72820	9.67860	1.37260
H	-6.39050	-10.53270	1.80510	H	6.20980	11.49970	-2.87680

### 3<sub>10</sub>-helix acetyl- (ala)<sub>19</sub>-methylamid

C	8.45010	14.47290	-3.72640	H	7.99960	9.93780	-3.38970
N	7.96980	15.84430	-3.72640	H	7.69440	9.74990	-1.65160
C	9.94050	14.44940	-3.38130	H	7.84090	8.30890	-2.67700
C	7.74120	13.68880	-2.62020	N	2.54360	8.18290	-1.18460
O	7.57280	12.47510	-2.72760	C	3.14220	7.77500	-0.05130
C	3.85010	12.54880	-2.74340	O	2.78220	6.78010	0.57590
C	-7.30960	-17.18040	4.72550	C	3.50700	4.29100	-2.09690
H	8.66150	16.59390	-3.72640	C	1.17650	7.95210	-3.19110
H	8.25840	13.98820	-4.68360	H	5.13260	10.26620	-0.63640
H	10.48520	15.03680	-4.12050	H	5.01960	7.97220	0.97400
H	10.10040	14.88430	-2.39480	H	4.52770	10.33490	1.71640
H	10.30580	13.42250	-3.38000	H	2.98810	10.27200	0.83600
N	4.94560	13.28320	-2.13350	H	3.24810	9.19930	2.22580
C	6.64050	13.76850	-0.43530	N	3.05400	5.66780	-1.99270
N	7.32620	14.39450	-1.55300	C	1.75320	5.98180	-1.85710
C	5.99790	14.84460	0.44230	O	0.86110	5.13620	-1.81190
C	5.49360	12.90540	-0.96480	C	1.99830	3.46590	1.31560
O	5.11230	11.92130	-0.33310	C	5.02230	4.23100	-1.89410
C	5.98030	9.38090	-2.91320	H	2.88020	9.01560	-1.66800
C	3.67560	12.99690	-4.19590	H	0.52030	7.59140	-1.14730
H	7.49010	15.40040	-1.51170	H	0.97500	9.02320	-3.17660
H	7.31950	13.14120	0.14230	H	2.06250	7.76600	-3.79790
H	6.77540	15.51510	0.80820	H	0.33020	7.42060	-3.62630
H	5.27910	15.41970	-0.14130	N	2.58860	4.13150	0.16670
H	5.48200	14.37990	1.28260	C	2.88970	3.46840	-0.96410
N	5.51240	10.75560	-2.86080	O	2.68980	2.26330	-1.10760
C	4.20430	11.06120	-2.79300	C	-1.01630	2.39050	-0.77190
O	3.31750	10.20910	-2.77060	C	1.45970	4.51070	2.29510
				H	3.75640	6.40670	-2.02500
				H	3.21850	3.85240	-3.05210

H	5.50670	4.84300	-2.65490	C	-3.14190	-4.17910	0.02210
H	5.28120	4.61890	-0.90900	O	-4.04140	-5.01300	0.11400
H	5.36730	3.19990	-1.97140	C	-2.64950	-6.83760	3.04620
N	0.14430	3.08130	-0.23600	C	0.07700	-5.97280	-0.39630
C	0.79150	2.64370	0.85890	H	-1.94680	-1.17310	0.23590
O	0.45250	1.63790	1.48040	H	-4.27390	-2.58540	0.91310
C	1.03040	-0.79660	-1.27700	H	-3.98340	-1.07090	-1.08610
C	-1.31670	2.90560	-2.18100	H	-2.98150	-2.31440	-1.86020
H	2.77400	5.13210	0.23590	H	-4.69640	-2.64250	-1.54240
H	2.71630	2.80380	1.79940	N	-2.15640	-6.12980	1.87690
H	2.28000	5.15310	2.61530	C	-1.97380	-6.74580	0.69530
H	0.70050	5.12150	1.80670	O	-2.20820	-7.94030	0.51920
H	1.01570	4.01630	3.15910	C	-5.86410	-7.77560	1.20540
N	0.59470	0.58090	-1.12170	C	-3.07560	-5.83020	4.11610
C	-0.69560	0.90170	-0.91870	H	-1.15560	-3.77560	-0.31400
O	-1.59190	0.06220	-0.85030	H	-1.83330	-6.27350	-1.39560
C	-0.32480	-1.68580	2.18340	H	0.49980	-5.33430	-1.17190
C	2.55300	-0.87280	-1.14670	H	0.43320	-5.63310	0.57620
H	0.46530	3.92190	-0.71630	H	0.39430	-7.00420	-0.55000
H	-1.88010	2.50460	-0.11700	N	-4.64630	-7.12600	1.65980
H	-1.50800	3.97760	-2.13370	C	-3.90840	-7.62130	2.66930
H	-0.46150	2.72620	-2.83240	O	-4.20660	-8.64900	3.27570
H	-2.18690	2.39030	-2.58760	C	-3.93190	-10.96570	0.37370
N	0.21710	-0.99940	1.02290	C	-6.28460	-7.19370	-0.14580
C	0.45940	-1.63950	-0.13490	H	-1.94700	-5.13600	1.97170
O	0.24260	-2.83960	-0.29520	H	-1.90200	-7.53090	3.43170
C	-3.44260	-2.69150	0.21610	H	-2.21750	-5.21450	4.38560
C	-0.80810	-0.65900	3.20960	H	-3.86550	-5.18740	3.72770
H	1.30120	1.31490	-1.17070	H	-3.44650	-6.35630	4.99560
H	0.69390	-1.21170	-2.22700	N	-4.32600	-9.59040	0.62850
H	3.00670	-0.24770	-1.91580	C	-5.58580	-9.26070	0.96510
H	2.86080	-0.50880	-0.16650	O	-6.48720	-10.08960	1.08070
H	2.88500	-1.90450	-1.26250	C	-4.97610	-11.98940	3.90410
N	-2.25230	-2.02170	0.71220	C	-2.40550	-11.06920	0.35760
C	-1.55870	-2.48840	1.76580	H	-4.35600	-6.26940	1.18830
O	-1.87700	-3.50520	2.38030	H	-6.66110	-7.67860	1.94260
C	-1.44930	-5.88220	-0.45360	H	-6.45100	-6.12230	-0.03450
C	-3.80380	-2.14300	-1.16570	H	-5.49700	-7.35590	-0.88150
H	0.41420	-0.00210	1.10530	H	-7.19810	-7.67790	-0.49110
H	0.40920	-2.36400	2.61850	N	-4.53180	-11.25960	2.72880
H	0.03170	-0.03010	3.50500	C	-4.40980	-11.85060	1.52680
H	-1.58390	-0.03170	2.77070	O	-4.66250	-13.03910	1.33580
H	-1.21570	-1.16900	4.08240	C	-8.28100	-12.86160	2.19560
N	-1.86530	-4.50520	-0.24800	C	-5.34310	-11.00270	5.01450

H	-3.61380	-8.86500	0.54540	4	3 <sub>10</sub> -helix acetyl-	(ala) <sub>24</sub> -methylamid			
H	-4.36270	-11.33300	-0.55770						
H	-2.01380	-10.41690	-0.42280	C	10.53830	18.68040	-4.52140		
H	-2.00140	-10.75390	1.31950	N	10.05800	20.05180	-4.52140		
H	-2.10470	-12.09930	0.16680	C	12.02870	18.65700	-4.17640		
N	-7.03770	-12.23170	2.60660	C	9.82950	17.89630	-3.41530		
C	-6.25790	-12.75490	3.56950	O	9.66110	16.68270	-3.52260		
O	-6.53640	-13.79350	4.16660	C	5.93840	16.75630	-3.53850		
C	-6.41730	-16.04720	1.20510	C	-9.35410	-22.00820	2.10140		
C	-8.75880	-12.24680	0.87860	H	10.74970	20.80140	-4.52140		
H	-4.30960	-10.26980	2.83540	H	10.34670	18.19570	-5.47870		
H	-4.21750	-12.69670	4.23900	H	12.57350	19.24430	-4.91560		
H	-4.46810	-10.39980	5.25690	H	12.18870	19.09180	-3.18980		
H	-6.14460	-10.34550	4.67760	H	12.39400	17.63000	-4.17510		
H	-5.67720	-11.54550	5.89870	N	7.03380	17.49080	-2.92860		
N	-6.78720	-14.67500	1.50790	C	8.72880	17.97610	-1.23030		
C	-8.02700	-14.34320	1.91010	N	9.41450	18.60200	-2.34810		
O	-8.92910	-15.16750	2.04970	C	8.08620	19.05210	-0.35280		
C	6.33600	17.61530	-3.72640	C	7.58190	17.11290	-1.75990		
C	-4.89430	-16.16200	1.11530	O	7.20060	16.12880	-1.12820		
H	-6.76220	-11.36710	2.14090	C	8.06860	13.58840	-3.70830		
H	-9.04190	-12.77500	2.97120	C	5.76380	17.20440	-4.99100		
H	-8.91060	-11.17680	1.02090	H	9.57840	19.60790	-2.30680		
H	-8.00780	-12.39860	0.10340	H	9.40770	17.34870	-0.65280		
H	-9.69160	-12.71610	0.56590	H	8.86370	19.72260	0.01310		
O	5.74070	15.30560	-3.72650	H	7.36740	19.62720	-0.93640		
C	-6.84860	-16.95380	2.35960	H	7.57030	18.58750	0.48750		
O	-7.12020	-18.13580	2.15470	N	7.60070	14.96310	-3.65590		
H	-7.50820	-18.20160	4.40000	C	6.29260	15.26870	-3.58810		
H	-6.07330	-13.95340	1.40750	O	5.40580	14.41660	-3.56570		
H	-6.89420	-16.39040	0.28700	C	6.40830	12.82490	-0.35240		
H	-4.53370	-15.49550	0.33180	C	9.57320	13.54590	-3.43390		
H	-4.44310	-15.87120	2.06390	H	7.38630	18.31560	-3.41410		
H	-4.61160	-17.18990	0.88820	H	5.01560	16.88270	-2.97240		
N	-6.90940	-16.38870	3.57860	H	5.55370	18.27380	-5.00960		
C	6.65770	16.14000	-3.72640	H	6.67870	17.01270	-5.55160		
H	5.25350	17.74260	-3.71610	H	4.94300	16.65610	-5.45320		
H	6.75740	18.08760	-2.83900	N	7.04650	13.47030	-1.48700		
H	6.75730	18.08770	-4.61370	C	7.40520	12.78540	-2.58760		
H	-6.50970	-17.19310	5.46580	O	7.22150	11.57570	-2.71340		
H	-8.20480	-16.75370	5.17780	C	3.50290	11.67810	-2.55360		
H	-6.67390	-15.40330	3.69630	C	5.81650	13.88610	0.57760		
				H	8.29810	15.70720	-3.67190		
				H	7.82840	13.12650	-4.66590		

H	10.08790	14.14530	-4.18480	C	1.39270	5.10920	-1.71380
H	9.78270	13.95750	-2.44670	O	0.49630	4.26970	-1.64530
H	9.92920	12.51640	-3.47210	C	1.76340	2.52180	1.38830
N	4.63190	12.39040	-1.97970	C	4.64120	3.33470	-1.94180
C	5.23050	11.98250	-0.84640	H	2.55350	8.12940	-1.51140
O	4.87050	10.98760	-0.21920	H	0.20820	6.71210	-0.91210
C	5.59530	8.49860	-2.89190	H	0.58020	8.18510	-2.92870
C	3.26470	12.15960	-3.98620	H	1.62670	6.93370	-3.62750
H	7.22090	14.47370	-1.43140	H	-0.09860	6.59780	-3.38270
H	7.10790	12.17980	0.17900	N	2.30530	3.20810	0.22790
H	6.61600	14.54240	0.92130	C	2.54770	2.56800	-0.93000
H	5.07640	14.47950	0.04090	O	2.33090	1.36790	-1.09020
H	5.33630	13.40690	1.43070	C	-1.35430	1.51600	-0.57890
N	5.14230	9.87530	-2.78770	C	1.28020	3.54850	2.41450
C	3.84150	10.18930	-2.65220	H	3.38940	5.52250	-1.96580
O	2.94930	9.34380	-2.60690	H	2.78220	2.99580	-3.02210
C	4.08650	7.67350	0.52050	H	5.09500	3.95980	-2.71090
C	7.11060	8.43850	-2.68920	H	4.94900	3.69870	-0.96160
H	4.96850	13.22310	-2.46310	H	4.97330	2.30300	-2.05760
H	2.60860	11.79890	-1.94230	N	-0.16400	2.18580	-0.08290
H	3.06330	13.23080	-3.97170	C	0.52960	1.71920	0.97070
H	4.15080	11.97350	-4.59300	O	0.21120	0.70240	1.58530
H	2.41850	11.62810	-4.42140	C	0.63900	-1.67470	-1.24860
N	4.67690	8.33900	-0.62840	C	-1.71550	2.06450	-1.96080
C	4.97790	7.67590	-1.75920	H	2.50250	4.20550	0.31020
O	4.77810	6.47080	-1.90270	H	2.49740	1.84360	1.82350
C	1.07200	6.59800	-1.56700	H	2.12000	4.17740	2.71000
C	3.54800	8.71820	1.50000	H	0.50440	4.17590	1.97560
H	5.84460	10.61420	-2.82000	H	0.87260	3.03850	3.28730
H	5.30670	8.05990	-3.84710	N	0.22290	-0.29770	-1.04310
H	7.59500	9.05050	-3.45000	C	-1.05370	0.02840	-0.77300
H	7.36940	8.82640	-1.70410	O	-1.95310	-0.80550	-0.68100
H	7.45550	7.40740	-2.76640	C	-0.56130	-2.63000	2.25120
N	2.23260	7.28880	-1.03110	C	2.16520	-1.76530	-1.19130
C	2.87980	6.85130	0.06380	H	0.14150	3.03440	-0.55920
O	2.54080	5.84540	0.68530	H	-2.18560	1.62210	0.11800
C	3.11870	3.41090	-2.07210	H	-1.89510	3.13670	-1.88120
C	0.77150	7.11310	-2.97600	H	-0.89320	1.89310	-2.65530
H	4.86230	9.33960	-0.55910	H	-2.60810	1.56500	-2.33740
H	4.80450	7.01130	1.00430	N	-0.06810	-1.92230	1.08190
H	4.36830	9.36060	1.82020	C	0.11450	-2.53830	-0.09970
H	2.78880	9.32900	1.01170	O	-0.11990	-3.73280	-0.27580
H	3.10390	8.22380	2.36400	C	-3.77590	-3.56800	0.41030
N	2.68300	4.78840	-1.91680	C	-0.98730	-1.62260	3.32100



H	0.93270	0.43190	-1.10900	H	-3.58890	-7.33790	5.10370
H	0.25500	-2.06600	-2.19070	N	-4.69890	-10.46750	0.71290
H	2.58800	-1.12680	-1.96700	C	-5.93870	-10.13560	1.11510
H	2.52150	-1.42560	-0.21890	O	-6.84090	-10.96000	1.25470
H	2.48250	-2.79670	-1.34500	C	-5.21650	-12.93350	3.96220
N	-2.55800	-2.91850	0.86470	C	-2.80600	-11.95450	0.32030
C	-1.82010	-3.41370	1.87430	H	-4.67400	-7.15950	1.34580
O	-2.11830	-4.44150	2.48070	H	-6.95360	-8.56750	2.17610
C	-1.84370	-6.75810	-0.42130	H	-6.82230	-6.96930	0.22580
C	-4.19630	-2.98620	-0.94080	H	-5.91950	-8.19110	-0.69160
H	0.14130	-0.92850	1.17670	H	-7.60330	-8.50860	-0.22920
H	0.18630	-3.32330	2.63660	N	-4.82110	-12.18120	2.78350
H	-0.12920	-1.00700	3.59050	C	-4.76030	-12.74630	1.56450
H	-1.77720	-0.97980	2.93270	O	-5.03190	-13.92830	1.35970
H	-1.35820	-2.14880	4.20060	C	-8.60480	-13.74230	2.39140
N	-2.23770	-5.38290	-0.16650	C	-5.52280	-11.96900	5.10970
C	-3.49750	-5.05320	0.17000	H	-3.98510	-9.74580	0.61240
O	-4.39890	-5.88200	0.28570	H	-4.80590	-12.18290	-0.50800
C	-2.88780	-7.78180	3.10910	H	-2.44540	-11.28800	-0.46320
C	-0.31720	-6.86170	-0.43740	H	-2.35480	-11.66370	1.26890
H	-2.26770	-2.06190	0.39320	H	-2.52330	-12.98240	0.09310
H	-4.57280	-3.47110	1.14750	N	-7.33830	-13.13120	2.75740
H	-4.36270	-1.91480	-0.82950	C	-6.51910	-13.68160	3.67120
H	-3.40870	-3.14840	-1.67660	O	-6.77850	-14.73100	4.25790
H	-5.10980	-3.47040	-1.28610	C	-6.81700	-16.91920	1.24550
N	-2.44350	-7.05200	1.93370	C	-9.13810	-13.09480	1.11190
C	-2.32150	-7.64310	0.73170	H	-4.58560	-11.19580	2.90120
O	-2.57420	-8.83160	0.54070	H	-4.44920	-13.65390	4.24560
C	-6.19270	-8.65410	1.40050	H	-4.63220	-11.37830	5.32410
C	-3.25490	-6.79520	4.21940	H	-6.33340	-11.29830	4.82510
H	-1.52550	-4.65750	-0.24970	H	-5.82000	-12.52870	5.99660
H	-2.27450	-7.12550	-1.35270	N	-7.16040	-15.55130	1.59520
H	0.07450	-6.20940	-1.21790	C	-8.37720	-15.21910	2.06210
H	0.08680	-6.54640	0.52440	O	-9.27900	-16.03940	2.22570
H	-0.01640	-7.89180	-0.62830	C	-7.54740	-18.08490	4.81050
N	-4.94940	-8.02420	1.81150	C	-5.30080	-17.04370	1.08220
C	-4.16960	-8.54730	2.77440	H	-7.07730	-12.25860	2.29840
O	-4.44820	-9.58600	3.37150	H	-9.32800	-13.66720	3.20340
C	-4.32900	-11.83970	0.41000	H	-9.27380	-12.02710	1.28450
C	-6.67060	-8.03930	0.08350	H	-8.42540	-13.23510	0.29940
H	-2.22140	-6.06230	2.04030	H	-10.08840	-13.54990	0.83300
H	-2.12920	-8.48920	3.44390	N	-7.20090	-17.30960	3.63140
H	-2.37980	-6.19220	4.46190	C	-7.20190	-17.84790	2.39890
H	-4.05640	-6.13790	3.88250	O	-7.49290	-19.02300	2.18120

C	-11.01210	-18.83280	3.38260	H	12.69770	25.07960	-5.29320
C	-7.79160	-17.14380	5.99190	H	12.29460	22.47390	-6.25050
H	-6.44580	-14.83310	1.47730	H	14.52140	23.52250	-5.68730
H	-7.33910	-17.23840	0.34350	H	14.13660	23.37000	-3.96160
H	-4.97130	-16.36270	0.29740	H	14.34200	21.90820	-4.94690
H	-4.80340	-16.77750	2.01470	N	8.98180	21.76900	-3.70030
H	-5.03790	-18.06840	0.81970	C	10.67670	22.25430	-2.00210
N	-9.72470	-18.23960	3.70230	N	11.36240	22.88020	-3.11990
C	-8.86860	-18.81630	4.56450	C	10.03410	23.33030	-1.12460
O	-9.10950	-19.87660	5.13960	C	9.52980	21.39110	-2.53160
C	8.42430	21.82280	-4.52140	O	9.14850	20.40700	-1.89990
C	-11.59880	-18.15280	2.14390	C	10.01650	17.86660	-4.48010
H	-6.95170	-16.32890	3.75940	C	7.71180	21.48260	-5.76270
H	-6.77410	-18.81720	5.04200	H	11.52630	23.88610	-3.07850
H	-6.88690	-16.56480	6.17730	H	11.35570	21.62690	-1.42460
H	-8.60880	-16.46080	5.76030	H	10.81160	24.00080	-0.75860
H	-8.05200	-17.72070	6.87930	H	9.31530	23.90540	-1.70810
O	7.82900	19.51310	-4.52150	H	9.51820	22.86560	-0.28430
C	-10.81290	-20.30350	3.01090	N	9.54860	19.24130	-4.42770
O	-11.71320	-21.12030	3.19850	C	8.24050	19.54690	-4.35990
H	-10.23580	-22.61320	2.31280	O	7.35370	18.69480	-4.33750
H	-9.47780	-17.35900	3.25070	C	8.35620	17.10310	-1.12410
H	-11.69600	-18.77010	4.22900	C	11.52110	17.82410	-4.20570
H	-11.71700	-17.08830	2.34590	H	9.33430	22.59380	-4.18590
H	-10.92590	-18.28050	1.29610	H	6.96350	21.16090	-3.74420
H	-12.56500	-18.59440	1.89990	H	7.50160	22.55200	-5.78140
N	-9.62210	-20.63460	2.48050	H	8.62660	21.29090	-6.32330
C	8.74590	20.34750	-4.52140	H	6.89090	20.93430	-6.22500
H	7.34180	21.95010	-4.51120	N	8.99450	17.74850	-2.25880
H	8.84560	22.29510	-3.63410	C	9.35310	17.06360	-3.35940
H	8.84560	22.29520	-5.40880	O	9.16940	15.85390	-3.48520
H	-9.13320	-22.06320	1.03540	C	5.45080	15.95630	-3.32540
H	-8.49940	-22.38840	2.66090	C	7.76440	18.16430	-0.19420
H	-8.90760	-19.91950	2.34500	H	10.24600	19.98540	-4.44370
				H	9.77630	17.40470	-5.43770
				H	12.03580	18.42350	-4.95650
				H	11.73060	18.23560	-3.21840
				H	11.87710	16.79460	-4.24390
				N	6.57980	16.66860	-2.75140
				C	7.17840	16.26070	-1.61820
				O	6.81840	15.26580	-0.99100
				C	7.54320	12.77680	-3.66370
				C	5.21270	16.43780	-4.75800
				H	9.16880	18.75190	-2.20320
5	3 <sub>10</sub> -helix	acetyl-	(ala) <sub>29</sub> -methylamid				
C	12.48630	22.95860	-5.29320				
N	12.00600	24.33000	-5.29320				
C	13.97670	22.93520	-4.94820				
C	11.77740	22.17450	-4.18700				
O	11.60900	20.96090	-4.29440				
C	7.88630	21.03450	-4.31030				
C	-13.84880	-24.78060	4.62260				

H	9.05580	16.45790	-0.59280	N	4.25330	7.48630	-0.54390
H	8.56390	18.82060	0.14950	C	4.49560	6.84620	-1.70180
H	7.02430	18.75770	-0.73080	O	4.27880	5.64610	-1.86200
H	7.28430	17.68510	0.65890	C	0.59360	5.79420	-1.35070
N	7.09020	14.15350	-3.55950	C	3.22810	7.82670	1.64280
C	5.78940	14.46750	-3.42400	H	5.33740	9.80070	-2.73760
O	4.89730	13.62200	-3.37870	H	4.73010	7.27400	-3.79390
C	6.03450	11.95170	-0.25130	H	7.04290	8.23800	-3.48270
C	9.05850	12.71670	-3.46090	H	6.89700	7.97690	-1.73340
H	6.91640	17.50130	-3.23480	H	6.92120	6.58120	-2.82930
H	4.55650	16.07710	-2.71410	N	1.78390	6.46400	-0.85470
H	5.01120	17.50900	-4.74340	C	2.47750	5.99730	0.19890
H	6.09870	16.25170	-5.36480	O	2.15920	4.98050	0.81350
H	4.36640	15.90630	-5.19310	C	2.58690	2.60350	-2.02040
N	6.62480	12.61720	-1.40020	C	0.23240	6.34270	-2.73260
C	6.92590	11.95410	-2.53100	H	4.45040	8.48370	-0.46160
O	6.72600	10.74900	-2.67450	H	4.44540	6.12180	1.05170
C	3.01990	10.87620	-2.33880	H	4.06790	8.45560	1.93820
C	5.49590	12.99640	0.72830	H	2.45230	8.45400	1.20390
H	7.79260	14.89240	-3.59180	H	2.82050	7.31670	2.51560
H	7.25470	12.33810	-4.61890	N	2.17090	3.98050	-1.81490
H	9.54290	13.32870	-4.22180	C	0.89430	4.30660	-1.54480
H	9.31740	13.10460	-2.47580	O	-0.00520	3.47270	-1.45280
H	9.40350	11.68560	-3.53820	C	1.38670	1.64810	1.47940
N	4.18050	11.56700	-1.80280	C	4.11320	2.51290	-1.96310
C	4.82770	11.12950	-0.70800	H	2.08940	7.31260	-1.33100
O	4.48870	10.12360	-0.08650	H	-0.23770	5.90030	-0.65380
C	5.06660	7.68910	-2.84390	H	0.05280	7.41480	-2.65300
C	2.71950	11.39130	-3.74780	H	1.05470	6.17130	-3.42710
H	6.81020	13.61780	-1.33090	H	-0.66020	5.84320	-3.10920
H	6.75250	11.28950	0.23260	N	1.87980	2.35590	0.31010
H	6.31620	13.63880	1.04850	C	2.06240	1.73990	-0.87150
H	4.73670	13.60720	0.23990	O	1.82800	0.54540	-1.04760
H	5.05190	12.50200	1.59230	C	-1.82790	0.71020	-0.36140
N	4.63090	9.06660	-2.68860	C	0.96060	2.65550	2.54920
C	3.34060	9.38740	-2.48550	H	2.88060	4.71010	-1.88080
O	2.44430	8.54790	-2.41710	H	2.20290	2.21220	-2.96250
C	3.71140	6.80000	0.61660	H	4.53600	3.15140	-2.73880
C	6.58920	7.61290	-2.71360	H	4.46940	2.85260	-0.99070
H	4.50150	12.40760	-2.28310	H	4.43050	1.48150	-2.11680
H	2.15610	10.99030	-1.68380	N	-0.61010	1.35970	0.09290
H	2.52820	12.46330	-3.70050	C	0.12780	0.86450	1.10250
H	3.57470	11.21190	-4.39930	O	-0.17040	-0.16330	1.70890
H	1.84930	10.87600	-4.15440	C	0.10430	-2.48000	-1.19310

C	-2.24840	1.29200	-1.71260	H	-3.97160	-3.91290	-1.46340
H	2.08920	3.34970	0.40490	H	-5.65540	-4.23040	-1.00100
H	2.13420	0.95490	1.86480	N	-2.87320	-7.90300	2.01180
H	1.81870	3.27120	2.81870	C	-2.81240	-8.46810	0.79270
H	0.17070	3.29840	2.16090	O	-3.08400	-9.65010	0.58790
H	0.58970	2.12940	3.42880	C	-6.65680	-9.46420	1.61960
N	-0.28980	-1.10470	-0.93830	C	-3.57490	-7.69080	4.33790
C	-1.54960	-0.77500	-0.60180	H	-2.03710	-5.46770	-0.15940
O	-2.45100	-1.60380	-0.48610	H	-2.85800	-7.90470	-1.27980
C	-0.93990	-3.50360	2.33730	H	-0.49750	-7.00980	-1.23500
C	1.63070	-2.58350	-1.20920	H	-0.40690	-7.38550	0.49710
H	-0.31980	2.21630	-0.37850	H	-0.57540	-8.70420	-0.67860
H	-2.62490	0.80710	0.37580	N	-5.39040	-8.85300	1.98570
H	-2.41480	2.36340	-1.60130	C	-4.57110	-9.40340	2.89940
H	-1.46080	1.12980	-2.44840	O	-4.83050	-10.45280	3.48610
H	-3.16190	0.80780	-2.05790	C	-4.86900	-12.64100	0.47370
N	-0.49560	-2.77380	1.16200	C	-7.19020	-8.81660	0.34010
C	-0.37360	-3.36490	-0.04010	H	-2.63770	-6.91760	2.12940
O	-0.62630	-4.55340	-0.23100	H	-2.50130	-9.37570	3.47390
C	-4.24480	-4.37590	0.62880	H	-2.68430	-7.10010	4.55230
C	-1.30690	-2.51700	3.44760	H	-4.38550	-7.02010	4.05330
H	0.42240	-0.37930	-1.02140	H	-3.87210	-8.25050	5.22480
H	-0.32650	-2.84730	-2.12450	N	-5.21250	-11.27310	0.82340
H	2.02240	-1.93120	-1.98970	C	-6.42930	-10.94090	1.29030
H	2.03480	-2.26820	-0.24730	O	-7.33110	-11.76120	1.45390
H	1.93150	-3.61360	-1.40000	C	-5.59950	-13.80670	4.03880
N	-3.00150	-3.74600	1.03970	C	-3.35290	-12.76550	0.31040
C	-2.22170	-4.26910	2.00270	H	-5.12940	-7.98040	1.52660
O	-2.50020	-5.30780	2.59980	H	-7.38000	-9.38900	2.43160
C	-2.38110	-7.56150	-0.36180	H	-7.32590	-7.74890	0.51270
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H	-0.27340	-1.78410	1.26850	H	-8.14050	-9.27170	0.06120
H	-0.18130	-4.21100	2.67210	N	-5.25290	-13.03140	2.85970
H	-0.43190	-1.91410	3.69010	C	-5.25390	-13.56980	1.62710
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H	-1.64100	-3.05970	4.33190	C	-9.06420	-14.55460	2.61090
N	-2.75100	-6.18930	-0.05890	C	-5.84370	-12.86560	5.22020
C	-3.99080	-5.85750	0.34330	H	-4.49790	-10.55490	0.70550
O	-4.89300	-6.68180	0.48290	H	-5.39110	-12.96020	-0.42830
C	-3.26860	-8.65530	3.19040	H	-3.02340	-12.08460	-0.47440
C	-0.85810	-7.67630	-0.45150	H	-2.85550	-12.49930	1.24300
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H	16.16690	27.62570	-4.64130	H	9.31450	21.94070	-0.02080
H	16.37220	26.16390	-5.62650	N	9.12040	18.40910	-4.23920
N	11.01200	26.02460	-4.38000	C	7.81960	18.72310	-4.10360
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N	13.39270	27.13590	-3.79960	C	8.06470	16.20730	-0.93090
C	12.06430	27.58590	-1.80420	C	11.08870	16.97230	-4.14060
C	11.56000	25.64680	-3.21130	H	8.94660	21.75700	-3.91450
O	11.17870	24.66260	-2.57960	H	6.58670	20.33280	-3.39380
C	12.04670	22.12230	-5.15980	H	7.04140	21.76460	-5.42310
C	9.74200	25.73820	-6.44240	H	8.12900	20.50740	-6.04450
H	13.55650	28.14180	-3.75820	H	6.39660	20.16190	-5.87280
H	13.38590	25.88260	-2.10430	N	8.65500	16.87280	-2.07990
H	12.84180	28.25650	-1.43830	C	8.95610	16.20980	-3.21070
H	11.34560	28.16110	-2.38780	O	8.75620	15.00460	-3.35420
H	11.54840	27.12130	-0.96400	C	5.05010	15.13190	-3.01850
N	11.57880	23.49690	-5.10740	C	7.52610	17.25200	0.04860
C	10.27080	23.80250	-5.03960	H	9.82280	19.14810	-4.27150
O	9.38390	22.95050	-5.01720	H	9.28490	16.59380	-5.29860
C	10.38640	21.35880	-1.80380	H	11.57320	17.58440	-4.90150
C	13.55130	22.07970	-4.88540	H	11.34760	17.36030	-3.15550
H	11.36450	26.84940	-4.86560	H	11.43370	15.94130	-4.21790
H	8.99380	25.41660	-4.42380	N	6.21070	15.82270	-2.48250
H	9.53180	26.80760	-6.46110	C	6.85790	15.38510	-1.38760
H	10.65680	25.54660	-7.00300	O	6.51890	14.37930	-0.76620
H	8.92110	25.19000	-6.90460	C	7.09680	11.94480	-3.52360
N	11.02470	22.00420	-2.93850	C	4.74970	15.64690	-4.42750
C	11.38340	21.31920	-4.03910	H	8.84040	17.87340	-2.01060
O	11.19960	20.10950	-4.16490	H	8.78270	15.54520	-0.44710
C	7.48100	20.21190	-4.00510	H	8.34640	17.89440	0.36880
C	9.79470	22.41990	-0.87390	H	6.76700	17.86290	-0.43980
H	12.27620	24.24110	-5.12340	H	7.08210	16.75770	0.91260
H	11.80650	21.66040	-6.11740	N	6.66110	13.32220	-3.36830
H	14.06610	22.67920	-5.63620	C	5.37080	13.64310	-3.16520
H	13.76080	22.49130	-3.89810	O	4.47450	12.80360	-3.09680
H	13.90730	21.05030	-4.92360	C	5.74160	11.05560	-0.06310
N	8.61000	20.92430	-3.43110	C	8.61940	11.86860	-3.39320
C	9.20860	20.51640	-2.29790	H	6.53170	16.66330	-2.96280
O	8.84860	19.52140	-1.67070	H	4.18630	15.24600	-2.36350
C	9.57340	17.03240	-4.34340	H	4.55840	16.71900	-4.38020
C	7.24290	20.69350	-5.43770	H	5.60490	15.46760	-5.07900
H	11.19900	23.00760	-2.88290	H	3.87950	15.13170	-4.83410
H	11.08600	20.71360	-1.27250	N	6.28350	11.74200	-1.22360
H	10.59410	23.07630	-0.53020	C	6.52580	11.10190	-2.38150
H	9.05450	23.01340	-1.41050	O	6.30910	9.90180	-2.54170

C	2.62390	10.04990	-2.03040	H	3.84890	7.52690	2.13900
C	5.25830	12.08240	0.96310	H	2.20090	7.55400	1.48120
H	7.36760	14.05630	-3.41730	H	2.61990	6.38510	2.74910
H	6.76030	11.52970	-4.47360	N	1.74040	3.15090	-1.61800
H	9.07310	12.49370	-4.16240	C	0.48060	3.48070	-1.28150
H	8.92720	12.23260	-2.41310	O	-0.42070	2.65180	-1.16580
H	8.95140	10.83690	-3.50900	C	1.09030	0.75200	1.65760
N	3.81410	10.71970	-1.53440	C	3.66090	1.67210	-1.88890
C	4.50780	10.25300	-0.48070	H	1.71050	6.47200	-1.05820
O	4.18940	9.23620	0.13380	H	-0.59470	5.06280	-0.30390
C	4.61710	6.85920	-2.70010	H	-0.38460	6.61910	-2.28100
C	2.26260	10.59840	-3.41230	H	0.56940	5.38540	-3.12810
H	6.48060	12.73930	-1.14130	H	-1.13160	5.06350	-2.73760
H	6.47560	10.37740	0.37200	N	1.53460	1.48180	0.48230
H	6.09820	12.71120	1.25850	C	1.65660	0.89080	-0.71980
H	4.48250	12.70970	0.52420	O	1.40390	-0.29770	-0.91070
H	4.85070	11.57240	1.83590	C	-2.21450	-0.12030	-0.05090
N	4.20110	8.23620	-2.49460	C	0.72330	1.73860	2.76790
C	2.92450	8.56230	-2.22450	H	2.45260	3.87630	-1.70110
O	2.02500	7.72840	-2.13250	H	1.70370	1.40840	-2.80420
C	3.41690	5.90380	0.79970	H	4.05260	2.32450	-2.66940
C	6.14340	6.76850	-2.64280	H	4.06500	1.98750	-0.92700
H	4.11960	11.56830	-2.01070	H	3.96170	0.64200	-2.07970
H	1.79250	10.15600	-1.33350	N	-0.97130	0.50970	0.36000
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C	4.09260	5.99560	-1.55120	H	1.75680	2.47160	0.58880
O	3.85830	4.80100	-1.72730	H	1.84900	0.04470	1.99240
C	0.20230	4.96580	-1.04110	H	1.59830	2.34160	3.01040
C	2.99080	6.91120	1.86950	H	-0.07820	2.39590	2.43110
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H	4.23320	6.46790	-3.64220	N	-0.72070	-1.93360	-0.73860
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H -11.98820 -30.30570 7.20250  
H -13.67850 -29.78990 7.36480  
H -12.45730 -28.32260 5.71620

## B . acetyl-(ala)<sub>n</sub>-NH<sub>2</sub>

### 1. $\alpha$ -helix acetyl-(ala)<sub>15</sub>- NH<sub>2</sub>

C 7.39512 8.03970 -2.20127  
N 7.33260 9.49297 -2.09502  
C 8.85470 7.57357 -2.16560  
C 6.59428 7.33695 -1.11982  
O 6.09284 6.23170 -1.35909

C	2.24833	7.68360	-0.34909	H	4.59716	4.50589	-1.08903
H	8.18415	9.99897	-2.16848	H	4.34778	1.66802	-0.98320
H	6.93974	7.72742	-3.13091	H	6.34040	2.89205	-0.12065
H	9.40317	7.99567	-2.99859	H	5.35628	3.59909	1.15771
H	9.33939	7.86924	-1.24277	H	5.63767	1.86476	1.11716
H	8.89955	6.49679	-2.24714	N	-0.19990	3.04244	-0.08056
N	3.65247	7.87974	-0.01215	C	0.05144	2.51238	1.12516
C	5.74081	7.28765	1.16745	O	-0.64668	1.61032	1.60513
N	6.47430	7.92173	0.08195	C	0.40354	-0.66219	-2.06822
C	5.82574	8.14773	2.43166	C	-1.46686	3.42625	-2.14036
C	4.28551	7.02548	0.80564	H	2.76010	4.20662	1.01659
O	3.71474	6.05041	1.30873	H	1.43297	2.31874	2.67132
C	2.87111	4.97779	-2.97314	H	1.63205	4.74030	3.23293
C	1.69564	8.92080	-1.06242	H	0.57260	5.14377	1.89084
H	6.89946	8.80459	0.23709	H	-0.04485	4.21432	3.25084
H	6.16395	6.31370	1.36295	N	0.13647	0.71328	-1.68145
H	6.85794	8.26015	2.73958	C	-1.08984	1.09248	-1.29364
H	5.39875	9.13026	2.26754	O	-2.04707	0.30814	-1.27746
H	5.28434	7.67156	3.23683	C	0.50211	-2.12593	1.45771
N	2.96828	6.16345	-2.13697	C	1.82197	-0.78731	-2.63035
C	2.04782	6.43472	-1.19620	H	0.33815	3.81292	-0.41726
O	1.05496	5.72024	-1.02398	H	-2.20784	2.55396	-0.31691
C	4.22656	2.54282	-0.36250	H	-1.66957	4.44807	-1.84787
C	3.89027	5.04717	-4.11323	H	-0.57127	3.41450	-2.74758
H	4.15435	8.60275	-0.48118	H	-2.29586	3.06493	-2.73448
H	1.69320	7.50405	0.55821	N	0.66903	-1.26095	0.30050
H	1.74509	9.77779	-0.40288	C	0.20266	-1.62161	-0.90261
H	2.25846	9.14418	-1.95938	O	-0.35175	-2.71183	-1.09579
H	0.66038	8.75870	-1.33050	C	-3.17209	-1.32387	2.11168
N	4.01280	3.70748	-1.20801	C	1.28422	-1.56696	2.64906
C	3.05708	3.70968	-2.15145	H	0.87738	1.37981	-1.74032
O	2.35005	2.72075	-2.37288	H	-0.31550	-0.97212	-2.81171
C	1.21642	3.07326	1.92997	H	1.93534	-0.14648	-3.49480
C	5.47049	2.74194	0.50644	H	2.55761	-0.49886	-1.89127
H	3.78031	6.73106	-2.20927	H	2.00907	-1.81023	-2.92976
H	1.87239	4.91242	-3.37562	N	-1.75927	-1.22575	1.78401
H	3.68424	5.90664	-4.73885	C	-0.96706	-2.30690	1.81934
H	4.90015	5.12601	-3.73053	O	-1.38284	-3.42144	2.16048
H	3.82083	4.15813	-4.72560	C	-4.28167	-2.95508	-1.15510
N	2.39025	3.28291	1.09625	C	-3.80133	0.07100	2.15157
C	3.00462	2.25035	0.50027	H	1.16233	-0.39991	0.41283
O	2.62561	1.08251	0.64988	H	0.85596	-3.11731	1.21778
C	-1.29759	2.54852	-0.89762	H	2.33577	-1.49848	2.40282
C	0.81710	4.38098	2.61842	H	0.92975	-0.57986	2.91500

H	1.16920	-2.22181	3.50289
N	-3.62072	-2.11096	-0.17510
C	-3.91856	-2.21968	1.13231
O	-4.78596	-2.99413	1.54616
C	-2.16321	-6.09159	-0.64708
C	-3.96044	-2.46904	-2.57081
H	-1.38121	-0.32923	1.55912
H	-3.28582	-1.80705	3.07089
H	-3.30154	0.68310	2.89098
H	-3.71750	0.55967	1.18981
H	-4.84820	-0.00759	2.41432
N	-2.60333	-4.71244	-0.76797
C	-3.89391	-4.41970	-0.99415
O	-4.75303	-5.30421	-1.10156
C	-3.66422	-6.66270	2.81880
C	-0.63646	-6.15176	-0.54439
H	-2.96681	-1.42566	-0.49048
H	-5.34781	-2.93167	-0.98697
H	-4.29782	-1.44841	-2.69624
H	-2.89504	-2.50156	-2.75824
H	-4.46275	-3.09377	-3.29812
N	-3.08053	-6.06660	1.63075
C	-2.79162	-6.79610	0.54514
O	-3.00020	-8.01675	0.49664
C	-7.04934	-7.44696	1.21161
C	-3.79236	-5.60406	3.91887
H	-1.91818	-3.98691	-0.72435
H	-2.49719	-6.65409	-1.50720
H	-0.18748	-5.70012	-1.41900
H	-0.29152	-5.61694	0.33098
H	-0.31612	-7.18282	-0.47672
N	-5.74698	-6.88112	1.51630
C	-5.01802	-7.30450	2.55599
O	-5.41413	-8.19554	3.32308
C	-5.62357	-10.78679	-0.01664
C	-7.77935	-6.55878	0.20043
H	-2.82290	-5.10371	1.66464
H	-3.03863	-7.47520	3.16205
H	-2.81531	-5.20498	4.15982
H	-4.42298	-4.78817	3.59021
H	-4.21898	-6.05166	4.80598
N	-5.79239	-9.40287	0.38099
C	-6.98986	-8.88536	0.70690
O	-8.04615	-9.51884	0.61685

C	6.22304	11.65526	-2.33650
C	-4.61101	-10.89738	-1.16010
H	-5.39391	-6.17185	0.91101
H	-7.62539	-7.50419	2.12475
H	-7.92759	-5.57105	0.61923
H	-7.20405	-6.45597	-0.71043
H	-8.74139	-6.99223	-0.03131
O	5.08496	9.55341	-2.14581
C	-5.21656	-11.69699	1.13921
O	-4.98696	-12.89061	0.91263
H	-4.97334	-8.83287	0.40964
H	-6.58564	-11.15169	-0.34714
H	-4.98098	-10.36153	-2.02542
H	-3.65994	-10.46511	-0.87329
H	-4.46104	-11.93484	-1.41913
N	-5.13437	-11.17116	2.36922
C	6.15839	10.16499	-2.18483
H	5.35922	12.10033	-1.86762
H	7.12333	12.07751	-1.91201
H	6.19273	11.90476	-3.39132
H	-5.30891	-10.21397	2.58152
H	-4.89433	-11.78107	3.11355

## 2. $\alpha$ -helix acetyl-(ala)<sub>18</sub>-NH<sub>2</sub>

C	12.98677	-0.51314	-1.81705
C	11.87202	-1.02214	-0.87032
N	12.24586	-1.38290	0.38247
C	11.24662	-1.86670	1.35636
C	10.19196	-0.78589	1.72909
N	10.62477	0.49857	1.75974
C	9.67929	1.61122	1.98640
C	8.65323	1.74849	0.82901
N	9.15718	1.64287	-0.42411
C	8.26756	1.63259	-1.60212
C	7.23062	0.47530	-1.53678
N	7.71431	-0.73560	-1.17651
C	6.81634	-1.89697	-1.02272
C	5.71765	-1.65073	0.04856
N	6.12981	-1.10266	1.21221
C	5.16523	-0.76635	2.27650
C	4.09130	0.24763	1.79373
N	4.54432	1.29921	1.07805
C	3.61120	2.29134	0.51319

C	2.59714	1.64909	-0.47370	O	-3.17738	1.19085	1.41193
N	3.10738	0.77082	-1.36305	O	-4.61036	1.10386	-1.76067
C	2.23060	0.04353	-2.29891	O	-6.05509	-2.03241	-1.20744
C	1.17222	-0.82053	-1.55859	O	-7.69162	-0.91671	1.69568
N	1.62484	-1.54727	-0.51492	O	-9.21347	1.76476	0.07454
C	0.70094	-2.34737	0.30890	O	-10.62720	-0.34747	-2.48512
C	-0.39722	-1.47305	0.97654	O	-11.93916	-3.02989	-0.07360
N	0.02420	-0.32236	1.54201	O	-13.42064	0.13006	2.46259
C	-0.93257	0.62759	2.13815	O	-13.84250	3.48637	-0.96843
C	-1.97932	1.13311	1.10667	N	14.02300	0.27231	-1.10773
N	-1.49625	1.49422	-0.10089	H	12.46241	0.13648	-2.53053
C	-2.40089	1.92284	-1.18237	H	13.21864	-1.29831	0.65026
C	-3.42160	0.81629	-1.57092	H	10.66264	-2.66897	0.88907
N	-2.92262	-0.43279	-1.68405	H	11.52342	0.72906	1.34719
C	-3.79847	-1.58172	-1.97459	H	9.07571	1.37863	2.87033
C	-4.88639	-1.78703	-0.88363	H	10.15321	1.49619	-0.55297
N	-4.47048	-1.68651	0.39677	H	7.65972	2.54561	-1.60367
C	-5.42972	-1.78317	1.51141	H	8.71741	-0.86647	-1.06259
C	-6.50421	-0.65959	1.46519	H	6.25727	-2.05397	-1.95403
N	-6.05092	0.57779	1.16922	H	7.12167	-0.94864	1.38594
C	-6.98406	1.70916	1.03236	H	4.59154	-1.66162	2.54854
C	-8.02192	1.48486	-0.10171	H	5.54493	1.42742	0.93350
N	-7.53932	0.99161	-1.26384	H	2.98531	2.70378	1.31491
C	-8.45084	0.72588	-2.38981	H	4.11351	0.61148	-1.40556
C	-9.45559	-0.42525	-2.09839	H	1.63717	0.76126	-2.87983
N	-8.95610	-1.49410	-1.43572	H	2.62003	-1.55796	-0.29213
C	-9.80741	-2.65892	-1.14729	H	0.14161	-3.03928	-0.33392
C	-10.87918	-2.40523	-0.04835	H	1.02028	-0.10420	1.57785
N	-10.54795	-1.49233	0.90761	H	-1.53100	0.11652	2.90340
C	-11.46356	-1.21028	2.02097	H	-0.48997	1.49602	-0.27050
C	-12.37758	0.03265	1.81395	H	-3.02496	2.75531	-0.83219
N	-11.94815	0.95778	0.90599	H	-1.91957	-0.59256	-1.58772
C	-12.65979	2.22952	0.72357	H	-4.36866	-1.38705	-2.89211
C	-13.17024	2.48163	-0.72103	H	-3.47967	-1.56074	0.60539
N	-12.85624	1.54852	-1.65688	H	-6.00586	-2.71290	1.41956
O	10.70925	-1.09637	-1.27416	H	-5.05036	0.74976	1.07132
O	9.03973	-1.12991	2.00518	H	-7.59155	1.79656	1.94219
O	7.45682	1.93596	1.06634	H	-6.53548	0.86146	-1.38966
O	6.04311	0.68700	-1.80171	H	-9.08638	1.60520	-2.55375
O	4.54214	-1.95320	-0.18655	H	-7.96025	-1.54900	-1.22437
O	2.89919	0.07128	2.07300	H	-10.39844	-2.89687	-2.04064
O	1.39829	1.95084	-0.41898	H	-9.58406	-1.17119	0.97784
O	-0.00664	-0.82104	-1.93520	H	-12.16369	-2.05109	2.09171
O	-1.57809	-1.84387	0.96963	H	-10.98349	0.92013	0.58204

H	-13.56059	2.17005	1.34699
H	-12.20974	0.78346	-1.49923
H	-13.13786	1.74014	-2.60824
C	13.67741	1.44381	-0.47677
O	12.49785	1.74878	-0.25895
H	14.99283	0.15184	-1.37968
C	14.80323	2.33094	-0.02451
H	14.38249	3.17789	0.57234
H	15.53249	1.77109	0.61010
H	15.34123	2.75124	-0.90973
C	13.57217	-1.68466	-2.56040
H	12.74481	-2.24624	-3.06321
H	14.10789	-2.38642	-1.87523
H	14.28903	-1.34038	-3.34625
C	11.87796	-2.38896	2.61885
H	11.06841	-2.73078	3.31227
H	12.54533	-3.25876	2.40086
H	12.47721	-1.60296	3.14044
C	10.38780	2.92429	2.18493
H	9.62785	3.73932	2.27946
H	11.00139	2.90391	3.11882
H	11.06185	3.16231	1.32304
C	9.03900	1.53811	-2.89173
H	8.31923	1.47883	-3.74555
H	9.68202	2.44105	-3.03488
H	9.69257	0.62899	-2.91284
C	7.57449	-3.15111	-0.67420
H	6.84925	-3.99045	-0.53363
H	8.28149	-3.42724	-1.49478
H	8.16166	-3.02534	0.27092
C	5.85114	-0.21585	3.49939
H	5.08057	0.04758	4.26514
H	6.54564	-0.97419	3.93814
H	6.44340	0.70276	3.25581
C	4.33857	3.41043	-0.18541
H	3.59139	4.11461	-0.62732
H	4.97861	3.97604	0.53566
H	4.99364	3.02059	-1.00585
C	3.01749	-0.83601	-3.23534
H	2.30991	-1.39586	-3.89505
H	3.69440	-0.22151	-3.87845
H	3.64308	-1.57410	-2.67119
C	1.42964	-3.12381	1.37461
H	0.68642	-3.68088	1.99631

H	2.13361	-3.86018	0.91463
H	2.01890	-2.44410	2.04197
C	-0.23391	1.81292	2.75219
H	-0.99822	2.52180	3.15518
H	0.42996	1.48849	3.59095
H	0.39340	2.35163	1.99653
C	-1.64101	2.34406	-2.41339
H	-2.36726	2.62294	-3.21580
H	-0.99348	3.22838	-2.19415
H	-0.98811	1.51597	-2.79097
C	-3.01214	-2.85778	-2.12979
H	-3.71833	-3.70459	-2.31178
H	-2.30927	-2.78536	-2.99588
H	-2.41307	-3.07987	-1.20966
C	-4.73905	-1.74513	2.84994
H	-5.50761	-1.78268	3.66050
H	-4.05374	-2.62038	2.96595
H	-4.13624	-0.80878	2.96918
C	-6.25802	3.00579	0.78157
H	-7.00568	3.82560	0.64811
H	-5.59688	3.26119	1.64586
H	-5.62307	2.94406	-0.13913
C	-7.70251	0.39987	-3.65682
H	-8.43768	0.18257	-4.47023
H	-7.06435	1.26150	-3.97205
H	-7.04300	-0.49401	-3.52134
C	-8.99859	-3.86680	-0.74732
H	-9.69374	-4.71410	-0.52754
H	-8.30809	-4.17120	-1.57166
H	-8.38262	-3.66154	0.16346
C	-10.74864	-1.04717	3.33945
H	-11.48503	-0.73350	4.11987
H	-10.28340	-2.01335	3.65323
H	-9.93865	-0.27859	3.27603
C	-11.85571	3.43668	1.14318
H	-12.42465	4.36418	0.88598
H	-11.67357	3.42161	2.24510
H	-10.86486	3.46503	0.62423

### 3. $\beta$ -strand acetyl- (ala)<sub>18</sub>- NH<sub>2</sub>

C	-29.09345	-0.47393	0.20328
O	-29.28242	-1.48399	0.88880
N	-27.87174	-0.07528	-0.22118

H	-27.73657	0.75497	-0.79394	N	4.70644	-0.01745	0.20679
C	-26.63213	-0.76680	0.13536	H	4.86390	-0.90466	0.68201
C	-25.47837	0.18134	-0.28804	C	5.93718	0.72070	-0.08700
O	-25.69463	1.18327	-0.97784	C	7.09866	-0.25755	0.24058
N	-24.25170	-0.17884	0.15054	O	6.88087	-1.33549	0.80490
H	-24.09551	-1.00686	0.72211	N	8.32537	0.16146	-0.13575
C	-23.02702	0.54643	-0.19310	H	8.48372	1.05731	-0.59408
C	-21.85545	-0.37109	0.25047	C	9.55415	-0.58850	0.13548
O	-22.06012	-1.38074	0.93313	C	10.71898	0.39016	-0.17820
N	-20.63132	0.02222	-0.16322	O	10.50453	1.47997	-0.72042
H	-20.48498	0.85673	-0.72837	N	11.94502	-0.04293	0.18438
C	-19.39435	-0.67333	0.19869	H	12.10006	-0.94876	0.62380
C	-18.23976	0.27381	-0.22783	C	13.17743	0.70354	-0.07985
O	-18.46193	1.28217	-0.90698	C	14.33678	-0.28945	0.20799
N	-17.01160	-0.09323	0.19665	O	14.11738	-1.38795	0.73035
H	-16.85136	-0.92926	0.75600	N	15.56430	0.14099	-0.15308
C	-15.78606	0.62996	-0.15018	H	15.72413	1.05310	-0.57739
C	-14.61689	-0.29798	0.27954	C	16.79115	-0.62201	0.08872
O	-14.82660	-1.31679	0.94716	C	17.95863	0.36462	-0.18692
N	-13.39205	0.09618	-0.12912	O	17.74835	1.47368	-0.69004
H	-13.24169	0.94020	-0.67925	N	19.18331	-0.08415	0.16202
C	-12.15696	-0.60931	0.22074	H	19.33493	-1.00442	0.57129
C	-11.00036	0.34150	-0.19290	C	20.41704	0.66971	-0.07304
O	-11.22274	1.36397	-0.85075	C	21.57505	-0.33336	0.18156
N	-9.77196	-0.03819	0.21838	O	21.35581	-1.44781	0.66848
H	-9.61152	-0.88750	0.75752	N	22.80346	0.10723	-0.16594
C	-8.54485	0.68679	-0.11962	H	22.96327	1.03106	-0.56353
C	-7.37822	-0.25604	0.28445	C	24.02804	-0.66632	0.05152
O	-7.59111	-1.29047	0.92667	C	25.19884	0.32463	-0.18934
N	-6.15282	0.14303	-0.11701	O	24.99601	1.44764	-0.66247
H	-5.99946	1.00150	-0.64356	N	26.42165	-0.13716	0.15324
C	-4.91981	-0.57605	0.21230	H	26.56670	-1.06641	0.54290
C	-3.76054	0.38223	-0.17621	C	27.65546	0.62448	-0.05325
O	-3.98106	1.42485	-0.80235	C	28.81447	-0.38213	0.17327
N	-2.53257	-0.01398	0.22012	O	28.60310	-1.50809	0.63465
H	-2.37329	-0.88109	0.73057	N	30.04349	0.06821	-0.16815
C	-1.30365	0.71632	-0.09962	H	30.20002	1.00132	-0.54321
C	-0.13965	-0.24422	0.26899	C	31.26344	-0.71316	0.03705
O	-0.35518	-1.29946	0.87552	C	32.44157	0.27337	-0.16857
N	1.08637	0.16362	-0.12145	O	32.26213	1.40482	-0.61187
H	1.24243	1.04043	-0.61602	N	33.66868	-0.19911	0.19003
C	2.31720	-0.57104	0.18058	H	-26.60421	-0.90661	1.22654
C	3.47931	0.39740	-0.17269	H	-22.98811	0.68168	-1.28443
O	3.26158	1.46389	-0.75832	H	-19.36791	-0.80764	1.29048

H	-15.75334	0.77225	-1.24077	H	14.24248	2.52226	0.40381
H	-12.12950	-0.75993	1.31035	H	13.44885	1.72724	1.82901
H	-8.51688	0.85157	-1.20716	C	9.70194	-1.86000	-0.66295
H	-4.89194	-0.75633	1.29736	H	8.80368	-2.51125	-0.51130
H	-1.27937	0.91572	-1.18143	H	10.60290	-2.42420	-0.31912
H	2.34474	-0.79137	1.25823	H	9.80709	-1.65061	-1.75485
H	5.95955	0.96257	-1.16015	C	6.09574	2.00784	0.68372
H	9.58116	-0.85305	1.20316	H	5.19982	2.66025	0.52351
H	13.20010	0.98840	-1.14240	H	6.99748	2.56017	0.32307
H	16.81725	-0.92809	1.14527	H	6.20611	1.82085	1.77917
H	20.44187	0.99242	-1.12469	C	2.46886	-1.87382	-0.56494
H	24.05146	-1.00811	1.09715	H	1.57221	-2.52069	-0.38726
H	27.68293	0.98084	-1.09392	H	3.37104	-2.42111	-0.19774
H	31.27879	-1.08253	1.07375	H	2.57426	-1.70909	-1.66444
N	-31.49100	-0.30080	0.05306	C	-1.15129	2.03340	0.62007
H	-30.20625	0.62983	-1.31135	H	-2.04889	2.67599	0.43198
H	33.80671	-1.14561	0.51439	H	-0.25035	2.57402	0.24017
H	34.47582	0.38548	0.01785	H	-1.04320	1.89015	1.72232
C	-30.26666	0.44487	-0.22820	C	-4.76354	-1.90501	-0.48450
C	-32.72117	0.11134	-0.38452	H	-5.65810	-2.54787	-0.28322
O	-32.89504	1.13566	-1.04980	H	-3.85963	-2.43526	-0.09713
H	-31.37353	-1.13011	0.62836	H	-4.65832	-1.78068	-1.58932
C	31.41057	-1.90122	-0.88260	C	-8.40086	2.02696	0.55801
H	30.50759	-2.55876	-0.80273	H	-9.29995	2.65965	0.34510
H	32.30522	-2.50221	-0.58966	H	-7.50007	2.55845	0.16514
H	31.52514	-1.58568	-1.94775	H	-8.29755	1.91966	1.66479
C	27.81378	1.82135	0.85188	C	-11.99518	-1.95629	-0.43932
H	26.92224	2.49201	0.75473	H	-12.88734	-2.59685	-0.22077
H	28.72118	2.40383	0.55936	H	-11.08933	-2.47208	-0.03727
H	27.91365	1.51819	1.92204	H	-11.88999	-1.86186	-1.54710
C	24.17135	-1.87747	-0.83679	C	-15.65131	1.98478	0.49982
H	23.27123	-2.53524	-0.73134	H	-16.55152	2.60921	0.26810
H	25.07105	-2.46733	-0.53550	H	-14.75008	2.51126	0.10129
H	24.27599	-1.59022	-1.91090	H	-15.55444	1.90128	1.60923
C	20.57886	1.89429	0.79320	C	-19.22674	-2.02976	-0.44052
H	19.68623	2.56097	0.68017	H	-20.11644	-2.67039	-0.21234
H	21.48413	2.46805	0.47773	H	-18.31886	-2.53545	-0.03036
H	20.68495	1.62465	1.87171	H	-19.12166	-1.95194	-1.54959
C	16.93598	-1.86191	-0.75855	C	-22.90177	1.90676	0.44777
H	16.03664	-2.51690	-0.63142	H	-23.80229	2.52616	0.20401
H	17.83624	-2.44050	-0.43760	H	-21.99904	2.43310	0.05258
H	17.04060	-1.61056	-1.84161	H	-22.81374	1.83189	1.55852
C	13.33921	1.95831	0.74194	C	-26.46008	-2.12084	-0.50895
H	12.44503	2.61896	0.60792	H	-27.34635	-2.76573	-0.27960

H	-25.54833	-2.62344	-0.10388
H	-26.35971	-2.03875	-1.61812
C	-30.16349	1.77933	0.47131
H	-29.24907	2.32083	0.12727
H	-30.11126	1.65956	1.58026
H	-31.05733	2.40657	0.22316
C	-33.88272	-0.77806	-0.01333
H	-33.98950	-0.84355	1.09624
H	-33.74102	-1.80606	-0.42568
H	-34.81863	-0.34304	-0.44128

#### 4. $3_{10}$ -helix acetyl- (ala)<sub>18</sub>- NH<sub>2</sub>

O	0.02750	1.32388	0.94418
H	-0.78901	0.85247	0.61085
H	0.02749	1.32388	1.94419
O	0.02750	3.91664	0.02750
H	0.02750	2.97382	0.36083
H	0.02750	3.91663	-0.97251
O	2.27290	5.21302	0.94418
H	1.45639	4.74161	0.61085
H	2.27289	5.21302	1.94419
O	2.27290	7.80578	0.02750
H	2.27289	6.86296	0.36084
H	1.45639	8.27718	0.36084
O	0.02750	9.10216	0.94418
H	-0.78901	8.63075	0.61085
H	0.02749	9.10216	1.94419
O	0.02750	11.69492	0.02750
H	0.02750	10.75210	0.36083
H	0.02750	11.69491	-0.97251
O	4.51829	1.32388	0.94418
H	3.70178	0.85248	0.61084
H	4.51828	2.26670	0.61084
O	4.51829	3.91664	0.02750
H	3.70178	4.38805	0.36083
H	4.51828	3.91665	-0.97251
O	6.76369	5.21302	0.94418
H	5.94718	4.74162	0.61084
H	6.76368	6.15584	0.61084
O	6.76369	7.80578	0.02750
H	5.94719	8.27720	0.36084
H	7.58019	8.27720	0.36084
O	4.51829	9.10216	0.94418

H	3.70178	8.63075	0.61085
H	4.51828	9.10216	1.94419
O	4.51829	11.69492	0.02750
H	3.70178	12.16632	0.36084
H	4.51828	10.75210	0.36084
O	9.00909	1.32388	0.94418
H	8.19257	0.85247	0.61085
H	9.00908	1.32388	1.94419
O	9.00909	3.91664	0.02750
H	8.19257	4.38804	0.36084
H	9.00908	2.97382	0.36084
O	9.00909	9.10216	0.94418
H	9.82560	8.63076	0.61084
H	9.00910	10.04498	0.61084
O	9.00909	11.69492	0.02750
H	9.82560	12.16633	0.36083
H	9.00910	11.69493	-0.97251
O	0.02750	1.32388	3.69422
H	0.84400	0.85246	4.02756
H	-0.78900	0.85246	4.02756
O	0.02750	3.91664	4.61090
H	0.02749	2.97382	4.27755
H	-0.78901	4.38804	4.27755
O	2.27290	5.21302	3.69422
H	1.45639	4.74162	4.02756
H	2.27289	6.15584	4.02756
O	2.27290	7.80578	4.61090
H	3.08941	8.27719	4.27757
H	2.27291	7.80579	5.61091
O	0.02750	9.10216	3.69422
H	0.84401	8.63076	4.02756
H	0.02751	10.04498	4.02756
O	0.02750	11.69492	4.61090
H	0.84401	12.16633	4.27757
H	0.02751	11.69493	5.61091
O	4.51829	1.32388	3.69422
H	4.51828	1.32388	2.69420
H	3.70178	0.85247	4.02755
O	4.51829	3.91664	4.61090
H	3.70178	4.38804	4.27755
H	4.51828	2.97382	4.27755
O	6.76369	5.21302	3.69422
H	6.76368	5.21302	2.69420
H	5.94718	4.74161	4.02755



O	6.76369	7.80578	4.61090	H	5.33480	4.38805	7.69426
H	6.76369	6.86296	4.27757	O	6.76369	5.21302	8.27761
H	6.76369	7.80577	5.61091	H	7.58020	4.74161	7.94429
O	4.51829	9.10216	3.69422	H	6.76370	5.21302	9.27763
H	5.33480	8.63076	4.02756	O	6.76369	7.80578	7.36093
H	4.51830	10.04498	4.02756	H	6.76368	6.86296	7.69428
O	4.51829	11.69492	4.61090	H	5.94718	8.27718	7.69428
H	5.33480	12.16633	4.27757	O	4.51829	9.10216	8.27761
H	4.51830	11.69493	5.61091	H	4.51829	10.04499	7.94429
O	9.00909	1.32388	3.69422	H	4.51829	9.10217	9.27763
H	8.19257	0.85248	4.02756	O	4.51829	11.69492	7.36093
H	9.00908	2.26670	4.02756	H	3.70179	12.16634	7.69428
O	9.00909	3.91664	4.61090	H	5.33479	12.16634	7.69428
H	8.19258	4.38806	4.27755	O	9.00909	1.32388	8.27761
H	9.82559	4.38806	4.27755	H	9.82560	0.85248	7.94427
O	9.00909	9.10216	3.69422	H	9.00910	2.26670	7.94427
H	9.00908	9.10216	2.69420	O	9.00909	3.91664	7.36093
H	8.19257	8.63075	4.02755	H	9.00910	3.91665	6.36092
O	9.00909	11.69492	4.61090	H	9.82560	4.38805	7.69426
H	8.19257	12.16632	4.27755	O	9.00909	9.10216	8.27761
H	9.00908	10.75210	4.27755	H	8.19257	8.63075	7.94429
O	0.02750	1.32388	8.27761	H	9.00908	9.10216	9.27763
H	0.02749	2.26670	7.94427	O	9.00909	11.69492	7.36093
H	-0.78901	0.85248	7.94427	H	9.00909	11.69491	6.36092
O	0.02750	3.91664	7.36093	H	9.00909	10.75210	7.69426
H	0.02751	3.91665	6.36092	O	0.02750	1.32388	11.02765
H	0.84401	4.38805	7.69426	H	0.02749	1.32388	10.02764
O	2.27290	5.21302	8.27761	H	-0.78901	0.85247	11.36098
H	2.27291	6.15584	7.94427	O	0.02750	3.91664	11.94433
H	3.08941	4.74162	7.94427	H	0.02751	2.97382	11.61099
O	2.27290	7.80578	7.36093	H	0.84401	4.38804	11.61099
H	1.45640	8.27720	7.69428	O	2.27290	5.21302	11.02765
H	3.08940	8.27720	7.69428	H	2.27290	5.21303	10.02764
O	0.02750	9.10216	8.27761	H	2.27290	6.15585	11.36098
H	0.02749	10.04498	7.94427	O	2.27290	7.80578	11.94433
H	-0.78901	8.63076	7.94427	H	2.27291	7.80579	12.94434
O	0.02750	11.69492	7.36093	H	3.08941	8.27719	11.61100
H	0.84400	12.16634	7.69428	O	0.02750	9.10216	11.02765
H	-0.78900	12.16634	7.69428	H	0.02751	9.10216	10.02764
O	4.51829	1.32388	8.27761	H	0.84401	8.63075	11.36098
H	5.33480	0.85248	7.94427	O	0.02750	11.69492	11.94433
H	4.51830	2.26670	7.94427	H	0.02751	10.75210	11.61099
O	4.51829	3.91664	7.36093	H	0.84401	12.16632	11.61099
H	4.51830	3.91665	6.36092	O	4.51829	1.32388	11.02765

H	4.51830	1.32388	10.02764	H	3.91763	7.09514	7.95955
H	5.33480	0.85247	11.36098	O	0.93165	6.78869	6.91871
O	4.51829	3.91664	11.94433	H	0.48814	7.53453	6.48207
H	3.70178	4.38804	11.61099	H	0.36576	6.03024	7.07026
H	4.51828	2.97382	11.61099	O	-0.32959	9.00512	6.13319
O	6.76369	5.21302	11.02765	H	-0.61377	9.39526	6.97575
H	5.94719	4.74160	11.36099	H	-0.12500	9.65264	5.47289
H	7.58019	4.74160	11.36099	O	4.19659	2.29802	7.11199
O	6.76369	7.80578	11.94433	H	4.07035	1.80501	6.31201
H	6.76369	7.80577	12.94434	H	4.78715	3.06824	7.01448
H	6.76369	6.86296	11.61100	O	5.55415	4.57166	7.22076
O	4.51829	9.10216	11.02765	H	4.85277	5.24205	7.20091
H	5.33480	8.63076	11.36099	H	6.11591	4.65768	7.99741
H	4.51830	10.04498	11.36099	O	7.56277	5.13244	9.22607
O	4.51829	11.69492	11.94433	H	8.32139	4.64163	8.90439
H	4.51830	11.69493	12.94434	H	7.44979	5.08614	10.17751
H	5.33480	12.16633	11.61100	O	7.35162	7.46848	7.86600
O	9.00909	1.32388	11.02765	H	7.45995	6.68075	8.41339
H	9.00909	1.32389	10.02764	H	6.45930	7.81941	7.95743
H	9.00909	2.26671	11.36098	O	4.82433	8.39513	8.68953
O	9.00909	3.91664	11.94433	H	4.81397	9.33831	8.45700
H	9.00910	3.91665	12.94434	H	4.82014	8.31727	9.64903
H	9.82560	4.38805	11.61100	O	5.08021	11.06950	8.66960
O	9.00909	9.10216	11.02765	H	4.79882	11.31375	9.54917
H	8.19258	8.63074	11.36099	H	5.93231	11.45369	8.45286
H	9.82559	8.63074	11.36099	O	9.48848	3.83304	7.72982
O	9.00909	11.69492	11.94433	H	10.43044	3.80302	7.62021
H	9.00910	10.75210	11.61099	H	9.03881	4.28388	6.98838
H	9.82560	12.16632	11.61099	O	8.02671	5.30110	6.04438

### C. water clusters

#### 1. (H<sub>2</sub>O)<sub>32</sub>

O	-1.18206	5.99872	10.12279	H	8.94248	9.42093	9.71989
H	-1.04301	5.34940	9.43360	O	7.77690	11.93885	8.44079
H	-0.61569	6.76072	9.97682	H	8.13669	12.55648	7.81805
O	-0.19835	4.39041	7.96368	H	8.22918	11.06597	8.44297
H	-0.68543	3.69530	7.53990	O	-1.34012	5.63684	12.74941
H	0.69831	4.12118	8.22692	H	-1.35871	5.70535	11.77852
O	2.40001	3.93556	8.52329	H	-2.19984	5.66040	13.14482
H	2.83718	4.77364	8.32389	O	1.25056	5.87062	13.42006
H	2.87866	3.20119	8.12841	H	0.28535	5.84451	13.34618
O	3.50710	6.31363	7.55773	H	1.62987	5.02999	13.18006
H	2.66641	6.52283	7.12479	O	2.86314	4.43535	11.30711

H	2.52493	4.06167	10.49218	O	0.02750	1.32388	3.69422
H	2.83675	5.39682	11.27531	H	0.84400	0.85246	4.02756
O	2.53367	7.22883	11.51293	H	-0.78900	0.85246	4.02756
H	2.07128	6.97253	12.32774	O	0.02750	3.91664	4.61090
H	3.33425	7.75259	11.62458	H	0.02749	2.97382	4.27755
O	0.81896	7.87574	9.53768	H	-0.78901	4.38804	4.27755
H	1.07656	7.51304	8.68685	O	2.27290	5.21302	3.69422
H	1.46889	7.71670	10.24204	H	1.45639	4.74162	4.02756
O	-0.82157	9.79106	8.63432	H	2.27289	6.15584	4.02756
H	-0.20468	9.21842	9.11623	O	2.27290	7.80578	4.61090
H	-1.61819	9.96603	9.11698	H	3.08941	8.27719	4.27757
O	5.59120	1.72885	9.47682	H	2.27291	7.80579	5.61091
H	5.02821	1.67584	8.70738	O	0.02750	9.10216	3.69422
H	6.52845	1.59551	9.29095	H	0.84401	8.63076	4.02756
O	5.28781	3.24496	11.59212	H	0.02751	10.04498	4.02756
H	4.39706	3.60025	11.72304	O	0.02750	11.69492	4.61090
H	5.32853	2.70392	10.77606	H	0.84401	12.16633	4.27757
O	7.24807	4.92096	12.01030	H	0.02751	11.69493	5.61091
H	6.42195	4.40082	11.87953	O	4.51829	1.32388	3.69422
H	7.92228	4.32352	12.32751	H	4.51828	1.32388	2.69420
O	7.19713	7.46668	12.77341	H	3.70178	0.85247	4.02755
H	7.00851	7.52184	13.70314	O	4.51829	3.91664	4.61090
H	7.22410	6.53903	12.46508	H	3.70178	4.38804	4.27755
O	4.87608	8.65270	11.50846	H	4.51828	2.97382	4.27755
H	5.66610	8.29102	11.91056	O	6.76369	5.21302	3.69422
H	4.82048	9.61672	11.57837	H	6.76368	5.21302	2.69420
O	4.94468	11.37639	11.58629	H	5.94718	4.74161	4.02755
H	4.41351	11.97198	12.09830	O	6.76369	7.80578	4.61090
H	5.89444	11.61925	11.54629	H	6.76369	6.86296	4.27757
O	8.29196	1.78449	9.38235	H	6.76369	7.80577	5.61091
H	8.76433	2.36742	8.78795	O	4.51829	9.10216	3.69422
H	8.41455	1.97825	10.30991	H	5.33480	8.63076	4.02756
O	7.77657	2.16858	12.26210	H	4.51830	10.04498	4.02756
H	6.82286	2.29457	12.20705	O	4.51829	11.69492	4.61090
H	8.01076	1.38615	12.74594	H	5.33480	12.16633	4.27757
O	8.88933	9.32505	11.67605	H	4.51830	11.69493	5.61091
H	8.28524	8.66034	12.03838	O	9.00909	1.32388	3.69422
H	9.74649	9.29345	12.08279	H	8.19257	0.85248	4.02756
O	7.49022	11.76504	11.20223	H	9.00908	2.26670	4.02756
H	8.05054	11.02323	11.43599	O	9.00909	3.91664	4.61090
H	7.64501	12.06145	10.30160	H	8.19258	4.38806	4.27755
				H	9.82559	4.38806	4.27755
				O	9.00909	9.10216	3.69422
				H	9.00908	9.10216	2.69420

2. Ice-like (H<sub>2</sub>O)<sub>48</sub>

H	8.19257	8.63075	4.02755	H	9.00910	3.91665	6.36092
O	9.00909	11.69492	4.61090	H	9.82560	4.38805	7.69426
H	8.19257	12.16632	4.27755	O	9.00909	9.10216	8.27761
H	9.00908	10.75210	4.27755	H	8.19257	8.63075	7.94429
O	0.02750	1.32388	8.27761	H	9.00908	9.10216	9.27763
H	0.02749	2.26670	7.94427	O	9.00909	11.69492	7.36093
H	-0.78901	0.85248	7.94427	H	9.00909	11.69491	6.36092
O	0.02750	3.91664	7.36093	H	9.00909	10.75210	7.69426
H	0.02751	3.91665	6.36092	O	0.02750	1.32388	11.02765
H	0.84401	4.38805	7.69426	H	0.02749	1.32388	10.02764
O	2.27290	5.21302	8.27761	H	-0.78901	0.85247	11.36098
H	2.27291	6.15584	7.94427	O	0.02750	3.91664	11.94433
H	3.08941	4.74162	7.94427	H	0.02751	2.97382	11.61099
O	2.27290	7.80578	7.36093	H	0.84401	4.38804	11.61099
H	1.45640	8.27720	7.69428	O	2.27290	5.21302	11.02765
H	3.08940	8.27720	7.69428	H	2.27290	5.21303	10.02764
O	0.02750	9.10216	8.27761	H	2.27290	6.15585	11.36098
H	0.02749	10.04498	7.94427	O	2.27290	7.80578	11.94433
H	-0.78901	8.63076	7.94427	H	2.27291	7.80579	12.94434
O	0.02750	11.69492	7.36093	H	3.08941	8.27719	11.61100
H	0.84400	12.16634	7.69428	O	0.02750	9.10216	11.02765
H	-0.78900	12.16634	7.69428	H	0.02751	9.10216	10.02764
O	4.51829	1.32388	8.27761	H	0.84401	8.63075	11.36098
H	5.33480	0.85248	7.94427	O	0.02750	11.69492	11.94433
H	4.51830	2.26670	7.94427	H	0.02751	10.75210	11.61099
O	4.51829	3.91664	7.36093	H	0.84401	12.16632	11.61099
H	4.51830	3.91665	6.36092	O	4.51829	1.32388	11.02765
H	5.33480	4.38805	7.69426	H	4.51830	1.32388	10.02764
O	6.76369	5.21302	8.27761	H	5.33480	0.85247	11.36098
H	7.58020	4.74161	7.94429	O	4.51829	3.91664	11.94433
H	6.76370	5.21302	9.27763	H	3.70178	4.38804	11.61099
O	6.76369	7.80578	7.36093	H	4.51828	2.97382	11.61099
H	6.76368	6.86296	7.69428	O	6.76369	5.21302	11.02765
H	5.94718	8.27718	7.69428	H	5.94719	4.74160	11.36099
O	4.51829	9.10216	8.27761	H	7.58019	4.74160	11.36099
H	4.51829	10.04499	7.94429	O	6.76369	7.80578	11.94433
H	4.51829	9.10217	9.27763	H	6.76369	7.80577	12.94434
O	4.51829	11.69492	7.36093	H	6.76369	6.86296	11.61100
H	3.70179	12.16634	7.69428	O	4.51829	9.10216	11.02765
H	5.33479	12.16634	7.69428	H	5.33480	8.63076	11.36099
O	9.00909	1.32388	8.27761	H	4.51830	10.04498	11.36099
H	9.82560	0.85248	7.94427	O	4.51829	11.69492	11.94433
H	9.00910	2.26670	7.94427	H	4.51830	11.69493	12.94434
O	9.00909	3.91664	7.36093	H	5.33480	12.16633	11.61100

O	9.00909	1.32388	11.02765	H	7.58019	8.27720	0.36084
H	9.00909	1.32389	10.02764	O	4.51829	9.10216	0.94418
H	9.00909	2.26671	11.36098	H	3.70178	8.63075	0.61085
O	9.00909	3.91664	11.94433	H	4.51828	9.10216	1.94419
H	9.00910	3.91665	12.94434	O	4.51829	11.69492	0.02750
H	9.82560	4.38805	11.61100	H	3.70178	12.16632	0.36084
O	9.00909	9.10216	11.02765	H	4.51828	10.75210	0.36084
H	8.19258	8.63074	11.36099	O	9.00909	1.32388	0.94418
H	9.82559	8.63074	11.36099	H	8.19257	0.85247	0.61085
O	9.00909	11.69492	11.94433	H	9.00908	1.32388	1.94419
H	9.00910	10.75210	11.61099	O	9.00909	3.91664	0.02750
H	9.82560	12.16632	11.61099	H	8.19257	4.38804	0.36084

### 3. Ice-like (H<sub>2</sub>O)<sub>64</sub>

O	0.02750	1.32388	0.94418	H	9.00910	10.04498	0.61084
H	-0.78901	0.85247	0.61085	O	9.00909	11.69492	0.02750
H	0.02749	1.32388	1.94419	H	9.82560	12.16633	0.36083
O	0.02750	3.91664	0.02750	H	9.00910	11.69493	-0.97251
H	0.02750	2.97382	0.36083	O	0.02750	1.32388	3.69422
H	0.02750	3.91663	-0.97251	H	0.84400	0.85246	4.02756
O	2.27290	5.21302	0.94418	H	-0.78900	0.85246	4.02756
H	1.45639	4.74161	0.61085	O	0.02750	3.91664	4.61090
H	2.27289	5.21302	1.94419	H	0.02749	2.97382	4.27755
O	2.27290	7.80578	0.02750	H	-0.78901	4.38804	4.27755
H	2.27289	6.86296	0.36084	O	2.27290	5.21302	3.69422
H	1.45639	8.27718	0.36084	H	1.45639	4.74162	4.02756
O	0.02750	9.10216	0.94418	H	2.27289	6.15584	4.02756
H	-0.78901	8.63075	0.61085	O	2.27290	7.80578	4.61090
H	0.02749	9.10216	1.94419	H	3.08941	8.27719	4.27757
O	0.02750	11.69492	0.02750	H	2.27291	7.80579	5.61091
H	0.02750	10.75210	0.36083	O	0.02750	9.10216	3.69422
H	0.02750	11.69491	-0.97251	H	0.84401	8.63076	4.02756
O	4.51829	1.32388	0.94418	H	0.02751	10.04498	4.02756
H	3.70178	0.85248	0.61084	O	0.02750	11.69492	4.61090
H	4.51828	2.26670	0.61084	H	0.84401	12.16633	4.27757
O	4.51829	3.91664	0.02750	H	0.02751	11.69493	5.61091
H	3.70178	4.38805	0.36083	O	4.51829	1.32388	3.69422
H	4.51828	3.91665	-0.97251	H	4.51828	1.32388	2.69420
O	6.76369	5.21302	0.94418	H	3.70178	0.85247	4.02755
H	5.94718	4.74162	0.61084	O	4.51829	3.91664	4.61090
H	6.76368	6.15584	0.61084	H	3.70178	4.38804	4.27755
O	6.76369	7.80578	0.02750	H	4.51828	2.97382	4.27755
H	5.94719	8.27720	0.36084	O	6.76369	5.21302	3.69422

H	6.76368	5.21302	2.69420	O	4.51829	3.91664	7.36093
H	5.94718	4.74161	4.02755	H	4.51830	3.91665	6.36092
O	6.76369	7.80578	4.61090	H	5.33480	4.38805	7.69426
H	6.76369	6.86296	4.27757	O	6.76369	5.21302	8.27761
H	6.76369	7.80577	5.61091	H	7.58020	4.74161	7.94429
O	4.51829	9.10216	3.69422	H	6.76370	5.21302	9.27763
H	5.33480	8.63076	4.02756	O	6.76369	7.80578	7.36093
H	4.51830	10.04498	4.02756	H	6.76368	6.86296	7.69428
O	4.51829	11.69492	4.61090	H	5.94718	8.27718	7.69428
H	5.33480	12.16633	4.27757	O	4.51829	9.10216	8.27761
H	4.51830	11.69493	5.61091	H	4.51829	10.04499	7.94429
O	9.00909	1.32388	3.69422	H	4.51829	9.10217	9.27763
H	8.19257	0.85248	4.02756	O	4.51829	11.69492	7.36093
H	9.00908	2.26670	4.02756	H	3.70179	12.16634	7.69428
O	9.00909	3.91664	4.61090	H	5.33479	12.16634	7.69428
H	8.19258	4.38806	4.27755	O	9.00909	1.32388	8.27761
H	9.82559	4.38806	4.27755	H	9.82560	0.85248	7.94427
O	9.00909	9.10216	3.69422	H	9.00910	2.26670	7.94427
H	9.00908	9.10216	2.69420	O	9.00909	3.91664	7.36093
H	8.19257	8.63075	4.02755	H	9.00910	3.91665	6.36092
O	9.00909	11.69492	4.61090	H	9.82560	4.38805	7.69426
H	8.19257	12.16632	4.27755	O	9.00909	9.10216	8.27761
H	9.00908	10.75210	4.27755	H	8.19257	8.63075	7.94429
O	0.02750	1.32388	8.27761	H	9.00908	9.10216	9.27763
H	0.02749	2.26670	7.94427	O	9.00909	11.69492	7.36093
H	-0.78901	0.85248	7.94427	H	9.00909	11.69491	6.36092
O	0.02750	3.91664	7.36093	H	9.00909	10.75210	7.69426
H	0.02751	3.91665	6.36092	O	0.02750	1.32388	11.02765
H	0.84401	4.38805	7.69426	H	0.02749	1.32388	10.02764
O	2.27290	5.21302	8.27761	H	-0.78901	0.85247	11.36098
H	2.27291	6.15584	7.94427	O	0.02750	3.91664	11.94433
H	3.08941	4.74162	7.94427	H	0.02751	2.97382	11.61099
O	2.27290	7.80578	7.36093	H	0.84401	4.38804	11.61099
H	1.45640	8.27720	7.69428	O	2.27290	5.21302	11.02765
H	3.08940	8.27720	7.69428	H	2.27290	5.21303	10.02764
O	0.02750	9.10216	8.27761	H	2.27290	6.15585	11.36098
H	0.02749	10.04498	7.94427	O	2.27290	7.80578	11.94433
H	-0.78901	8.63076	7.94427	H	2.27291	7.80579	12.94434
O	0.02750	11.69492	7.36093	H	3.08941	8.27719	11.61100
H	0.84400	12.16634	7.69428	O	0.02750	9.10216	11.02765
H	-0.78900	12.16634	7.69428	H	0.02751	9.10216	10.02764
O	4.51829	1.32388	8.27761	H	0.84401	8.63075	11.36098
H	5.33480	0.85248	7.94427	O	0.02750	11.69492	11.94433
H	4.51830	2.26670	7.94427	H	0.02751	10.75210	11.61099

H	0.84401	12.16632	11.61099	O	1.02019	-4.40630	-0.53376
O	4.51829	1.32388	11.02765	O	-1.35018	-4.33904	1.65990
H	4.51830	1.32388	10.02764	O	0.69726	-1.97708	1.66769
H	5.33480	0.85247	11.36098	O	-1.90957	-1.90624	3.66610
O	4.51829	3.91664	11.94433	O	-0.84288	-0.16572	-4.37987
H	3.70178	4.38804	11.61099	O	0.91932	0.31161	-0.42248
H	4.51828	2.97382	11.61099	O	-2.19814	-0.22374	0.72504
O	6.76369	5.21302	11.02765	O	1.05468	-1.03905	4.74789
H	5.94719	4.74160	11.36099	O	-0.05124	1.29018	2.60737
H	7.58019	4.74160	11.36099	O	-0.91858	2.71396	-1.70367
O	6.76369	7.80578	11.94433	O	-1.22504	3.04206	-5.00565
H	6.76369	7.80577	12.94434	O	0.41357	4.14617	0.93424
H	6.76369	6.86296	11.61100	O	-2.26427	4.03785	4.41160
O	4.51829	9.10216	11.02765	O	0.89977	4.11870	4.00638
H	5.33480	8.63076	11.36099	O	3.27977	-2.00038	-0.35267
H	4.51830	10.04498	11.36099	O	2.27276	-0.84536	-3.20613
O	4.51829	11.69492	11.94433	O	3.56422	-0.76920	2.60010
H	4.51830	11.69493	12.94434	O	4.09973	-0.80588	5.75415
H	5.33480	12.16633	11.61100	O	2.22764	3.05925	-1.53155
O	9.00909	1.32388	11.02765	O	1.70382	1.86921	-4.50787
H	9.00909	1.32389	10.02764	O	2.93900	2.14234	1.44405
H	9.00909	2.26671	11.36098	O	2.86721	1.86606	4.61018
O	9.00909	3.91664	11.94433	H	3.31066	1.54439	5.40061
H	9.00910	3.91665	12.94434	H	-4.48178	-3.45425	-3.38400
H	9.82560	4.38805	11.61100	H	-6.13064	-3.61174	-3.23817
O	9.00909	9.10216	11.02765	H	-4.45248	-2.97855	-0.64367
H	8.19258	8.63074	11.36099	H	-2.99664	-2.77747	-0.98094
H	9.82559	8.63074	11.36099	H	-2.75429	-0.73817	-2.87746
O	9.00909	11.69492	11.94433	H	-4.21137	-1.08978	-2.72241
H	9.00910	10.75210	11.61099	H	-3.38542	1.62099	3.33043
H	9.82560	12.16632	11.61099	H	-2.75924	4.40262	-2.43599

4.  $(\text{H}_3\text{O}^+)_5(\text{HO}^-)_5(\text{H}_2\text{O})_{22}$

O	-5.29763	-3.25837	-2.91750	H	-4.11635	4.21081	-3.05611
O	-3.58813	-2.89385	-0.22971	H	-3.35678	3.39450	0.77581
O	-3.55475	-0.45452	-2.42149	H	-2.45747	2.19265	0.81672
O	-3.02412	1.06389	4.02619	H	-3.23522	2.14767	-1.68437
O	-3.23810	4.54406	-3.25711	H	-4.77125	1.62710	-1.31774
O	-2.67550	2.98563	1.31909	H	-0.17282	-2.13096	-0.87016
O	-4.10912	2.32215	-1.32736	H	-0.42695	-1.17668	-2.00962
O	-0.78180	-1.97109	-1.59813	H	-1.90252	-2.36247	-4.67284
O	-2.35281	-3.01606	-4.12967	H	-1.63845	-3.36638	-3.58537
O	0.83412	-3.76101	-3.76076	H	1.00517	-2.86659	-3.44795
				H	0.34913	-4.87350	-0.02488
				H	0.75588	-4.55785	-1.44747
				H	-2.15273	-4.14364	1.16608

H	-1.56808	-4.04504	2.55011				
H	-0.18109	-1.69525	1.93353	O	-1.35178	1.62539	-0.69508
H	0.86004	-2.89723	1.44765	H	-1.20225	1.67557	-1.67654
H	-2.59543	-1.25313	3.84235	H	-0.95246	2.49256	-0.42714
H	-1.23896	-1.69935	4.32559	O	2.15455	1.25623	1.36727
H	-1.25813	0.63647	-4.71369	H	1.23556	1.21153	0.99358
H	0.09537	0.02207	-4.47947	H	2.43548	2.10598	0.94205
H	0.21409	0.40998	0.22797	O	1.47808	-1.19884	-0.95097
H	-2.41149	-0.43127	-0.19153	H	1.64033	-0.43937	-0.34415
H	-2.63232	-0.93516	1.20829	H	1.64412	-0.72537	-1.81217
H	1.67469	-1.02421	5.48334	O	1.09474	2.64610	-0.60236
H	1.57171	-1.41727	4.02816	H	1.78629	2.40905	-1.26961
H	-0.99223	1.28190	2.41744	H	1.30144	3.60127	-0.47270
H	0.33323	0.60465	3.15857	O	-1.93472	-1.99823	0.12783
H	-0.22907	2.04404	-1.76897	H	-2.53139	-2.05051	-0.65526
H	-0.50016	3.39137	-1.16234	H	-1.85861	-2.97523	0.38408
H	-1.89138	3.65846	-5.32407	O	0.17667	-1.12494	3.33971
H	-1.26891	3.16425	-4.05171	H	0.69953	-0.42347	3.80240
H	0.68722	4.73672	1.64253	H	-0.67227	-1.16686	3.84555
H	-2.30395	4.09527	3.45302	O	2.70343	0.86468	-2.40629
H	-1.44626	4.49203	4.63077	H	3.00218	0.87652	-3.35205
H	0.69482	3.17928	3.94330	H	3.56748	1.08965	-1.90734
H	1.72310	4.12021	4.50302	O	-2.68235	0.33652	1.59860
H	2.78405	-2.79635	-0.14699	H	-2.48933	0.72304	0.71635
H	3.49744	-1.79259	-1.26428	H	-2.84104	-0.61586	1.41790
H	2.00141	-0.18626	-2.55747	O	3.79070	-1.34170	2.52438
H	2.62186	-0.30628	-3.92382	H	3.45141	-0.53759	2.04945
H	3.17204	-1.41697	2.00287	H	4.75514	-1.18225	2.43301
H	3.85494	-0.07906	1.99408	O	-3.92930	-4.83722	-0.63056
H	4.35023	-0.97190	4.83830	H	-3.48040	-4.81326	-1.56770
H	2.53704	2.33191	-0.98147	O	0.40048	-0.54461	-4.49585
H	2.06495	3.75612	-0.88862	H	1.27764	-0.24545	-4.83681
H	1.11873	2.41071	-5.04786	H	-0.06401	0.31762	-4.34548
H	1.99596	2.47861	-3.82061	O	-1.62866	1.58883	-3.80154
H	3.20715	2.63105	2.22679	H	-1.86007	2.46941	-4.20046
H	1.97837	2.12558	1.51346	H	-2.53533	1.27616	-3.53996
H	2.70115	1.05696	4.11499	O	-1.11058	4.04441	3.46299
H	-5.28047	-2.70912	-2.13033	H	-1.66273	3.25386	3.23974
H	-4.32090	3.19168	-0.97998	H	-1.57019	4.71543	2.89645
H	1.41283	-1.33875	1.62189	O	5.14983	1.61892	-1.11837
H	0.50527	1.98400	2.24611	H	5.41191	1.33936	-0.14516
H	3.55782	-1.41221	0.35327	O	2.03833	-3.19260	3.56082
				H	1.20518	-3.08955	4.08047
				H	2.41309	-2.27953	3.62046

5.  $(\text{H}_3\text{O}^+)_5(\text{HO}^-)_5(\text{H}_2\text{O})_{38}$



O	-3.08884	4.13887	-1.38873	H	-5.32511	0.78767	-3.44461
H	-3.10065	3.29271	-0.79266	O	-4.93823	-2.59346	-0.13537
O	3.89487	-3.09566	-1.44385	H	-4.48313	-2.76839	-1.00567
H	2.93650	-2.91002	-1.27028	H	-5.34263	-3.50175	-0.03698
H	3.83837	-4.03101	-1.76727	O	5.54742	-2.19515	0.81146
O	-0.99544	-4.67344	0.24219	H	5.28088	-2.46381	-0.10326
H	-0.43672	-5.15123	1.00351	H	6.14349	-1.43914	0.58875
O	0.75718	-3.78976	-2.74662	O	1.75846	-5.42891	1.97528
H	1.38458	-4.50902	-2.48965	H	1.46645	-6.01138	2.71968
H	0.83518	-3.19635	-1.95431	H	1.38729	-4.55366	2.26696
O	4.98053	1.53403	1.93944	O	2.25126	1.65276	-5.21228
H	5.02337	2.52254	1.98252	H	1.55331	2.36507	-5.24022
H	4.05457	1.38238	2.25142	H	2.77196	1.87643	-6.02421
O	-5.23003	2.82030	-0.36947	O	5.93682	-0.97164	-1.57600
H	-5.74056	3.45029	0.28597	H	6.66770	-1.18097	-2.21518
O	3.41587	3.76742	-0.74089	H	5.16254	-1.40083	-2.02586
H	3.65257	4.22985	0.10027	O	-5.31728	-0.07157	-0.35053
H	4.27574	3.28666	-0.98694	H	-6.00272	-0.78691	-0.40710
O	-2.67924	-0.88823	4.51346	H	-4.64634	-0.54628	0.20548
H	-2.93616	-1.44745	5.28295	O	-2.12725	-7.17105	-0.85996
H	-3.13334	-1.32849	3.74650	H	-2.22682	-7.03888	-1.84228
O	-1.58064	4.55560	-3.86415	H	-2.06751	-8.16578	-0.80236
H	-2.28797	5.09703	-4.29779	O	3.59624	4.02889	2.15559
H	-1.94367	4.46548	-2.89323	H	3.04399	3.40249	2.68574
O	2.13977	-4.74875	-0.46558	H	3.62944	4.79518	2.78109
H	2.86574	-4.91686	0.18710	O	-1.71453	-4.95026	-2.59260
H	1.49630	-5.45616	-0.20388	H	-1.18400	-5.11734	-3.42462
O	-5.21553	3.29880	2.40868	H	-1.01858	-4.93235	-1.87106
H	-5.18682	2.30988	2.51158	O	4.11270	0.95125	4.34585
H	-5.75469	3.57426	3.19804	H	5.00305	1.36726	4.25152
O	-2.92269	4.56900	1.39141	H	4.36588	0.00917	4.51128
H	-3.89200	4.38852	1.22776	O	1.48415	5.11237	-2.00217
H	-2.75602	5.14871	0.59226	H	1.46882	6.09903	-2.05642
O	-3.83036	-2.21985	2.15909	H	2.45107	4.91054	-2.05459
H	-3.59721	-2.92371	1.49231	O	-3.18503	-1.89619	-2.54791
H	-4.79633	-2.14806	1.94807	H	-3.18894	-2.51120	-3.32863
O	1.43656	1.12757	4.55199	H	-3.58893	-1.06252	-2.91232
H	2.15083	1.03092	5.23042	O	4.43961	-4.23301	1.95213
H	1.82246	1.86272	4.00844	H	5.38645	-4.27047	2.23610
O	1.51963	3.90871	3.85715	H	4.10043	-3.28423	2.06920
H	0.98421	4.21032	4.63326	H	3.87778	-4.88928	2.45509
H	0.87350	4.09251	3.12908	O	-0.78436	-2.62911	-4.23725
O	-4.44729	0.69771	-2.98873	H	0.21495	-2.62588	-4.29270
H	-4.70778	0.93336	-2.05503	H	-1.11554	-1.73532	-4.50641

H	-1.16928	-3.35694	-4.78651	H	2.23641	-8.05713	3.57250
O	-2.98312	1.19973	3.68478	O	-0.68433	5.54342	1.39640
H	-2.12662	1.08882	4.16958	H	0.07008	5.82750	0.86179
H	-3.19042	2.11985	3.38331	H	-0.33858	5.47781	2.29101
H	-3.70285	0.74006	4.18209	O	-8.15862	5.81346	3.96793
O	0.74903	4.62003	-4.12065	H	-8.41933	5.46498	3.10096
H	1.45163	4.46684	-4.82470	H	-7.97577	5.02276	4.49590
H	-0.01817	5.25199	-4.36497	O	8.40990	-3.29998	-2.82765
H	0.31098	3.76301	-3.78169	H	7.71305	-2.85664	-2.33058
O	0.11642	-1.82168	1.15220	H	9.15490	-2.68472	-2.79459
H	1.00098	-1.61922	1.53171	O	-4.18233	3.21571	5.83892
H	-0.52275	-1.09963	1.40301	H	-3.79617	4.06198	6.08856
H	0.11315	-1.93926	0.15637	H	-3.57871	2.86383	5.18180

6.  $(\text{H}_3\text{O}^+)_6(\text{HO}^-)_6(\text{H}_2\text{O})_{52}$

O	-3.09712	-4.47578	4.17411	O	-4.47908	-5.87883	-4.19468
H	-3.24717	-5.17482	3.52226	H	-4.84995	-6.48702	-3.54131
H	-3.98804	-4.04316	4.23520	O	-0.98370	-10.93288	-0.46528
O	-4.35822	-2.57703	2.80083	H	-1.37797	-10.91158	0.41742
H	-3.55492	-2.05227	2.85388	O	-6.84490	4.62067	1.85751
H	-4.98299	-2.12271	3.38670	H	-6.93416	4.02947	1.10069
O	-1.15455	2.98251	0.20825	H	-6.85251	4.04275	2.63551
H	-1.95617	2.50035	-0.00939	O	-0.36857	-8.43014	-1.35612
H	-1.46311	3.85103	0.48630	H	0.38539	-8.67123	-0.79557
O	5.60800	-3.71642	0.76234	H	-0.71562	-9.29679	-1.64897
H	5.12649	-3.53804	-0.05015	O	-3.90692	-2.45129	-0.84645
H	6.50504	-3.39699	0.58044	H	-3.99375	-1.91525	-1.64560
O	-0.48472	-3.72682	1.06901	H	-3.38193	-3.21538	-1.14046
H	-0.77720	-4.48321	0.54016	O	-4.97849	10.08859	3.66606
H	-0.27170	-4.12146	1.91800	H	-5.76828	9.57528	3.90434
O	2.00354	5.58457	0.31238	O	-2.29024	-10.01288	1.99453
H	2.65178	5.15546	0.88037	H	-2.69383	-10.46006	2.74729
O	-6.26009	7.49193	3.56171	H	-1.63764	-9.42491	2.38402
H	-7.18393	7.49895	3.85738	O	6.08025	-2.20778	-1.31072
H	-5.75161	7.32547	4.36136	H	6.03184	-1.24466	-1.19313
O	3.81725	-4.07034	-1.60357	O	4.16864	0.59125	4.11652
H	2.89740	-4.18288	-1.91366	H	4.41036	-0.22410	4.56883
H	4.34287	-4.45418	-2.31664	H	4.42298	0.45165	3.19735
O	2.26722	1.92221	1.00030	O	-2.32314	4.57206	4.64698
H	2.72656	2.76540	1.00214	H	-1.48817	5.04781	4.56043
H	1.73963	1.93548	0.19562	H	-2.85584	4.88630	3.91240
O	2.03751	-7.56495	2.75718	O	-3.27201	1.45973	3.69283
H	2.55817	-6.75557	2.83461	H	-3.24363	1.58654	2.73632

H	-2.55459	0.86163	3.89149	H	-6.69262	1.66315	0.74230
O	-6.78012	3.27221	4.48686	O	-1.06237	-2.48974	4.33424
H	-7.22296	2.54994	4.95151	H	-0.45589	-3.09309	3.86749
H	-6.06274	3.53242	5.07674	H	-1.81659	-3.06899	4.59026
O	2.26590	-8.07629	-0.00817	O	-6.27921	1.18253	6.24002
H	2.73672	-8.87876	-0.27794	H	-6.66701	0.96653	7.10119
H	1.97699	-8.26025	0.89650	H	-5.51825	1.73606	6.45974
O	-3.61814	2.55879	1.03919	O	-2.86930	9.14012	5.63161
H	-4.40713	2.36887	0.52786	H	-2.63976	9.82486	6.27708
H	-3.78748	3.41901	1.43569	H	-3.43482	9.60878	5.00383
O	4.50469	-2.37721	3.13758	O	4.94749	0.44162	-1.20620
H	3.96188	-1.86400	2.52914	H	5.36400	1.24082	-1.54229
H	5.14067	-2.83375	2.56679	H	4.14834	0.34763	-1.73087
O	3.61384	-5.50691	1.36485	O	-2.89825	-4.80428	-2.20216
H	4.56991	-5.32317	1.45443	H	-3.45754	-5.53300	-1.89069
H	3.25945	-4.74025	0.87777	H	-3.01299	-4.82568	-3.16471
O	3.31500	-4.42742	4.21879	O	-4.91792	-6.82805	-1.52500
H	3.75533	-4.67923	3.39784	H	-5.74277	-6.67332	-1.04752
H	3.76827	-3.61994	4.50546	H	-4.63261	-7.69553	-1.20271
O	-4.32773	6.65581	5.60785	O	-3.06633	-8.32799	-0.03694
H	-3.99941	7.47772	6.01311	H	-3.14234	-9.22052	0.32401
H	-3.54775	6.08763	5.58825	H	-2.25780	-8.34642	-0.55439
O	-5.47849	-0.32787	4.11964	O	-5.58062	-6.00511	0.92933
H	-5.03309	0.53028	4.14608	H	-6.15636	-5.22163	0.94650
H	-6.11035	-0.27557	4.85793	H	-5.24075	-6.02175	1.84593
O	-1.03951	-6.21012	5.38599	O	-3.09992	-6.24264	1.77789
H	-1.90950	-5.82875	5.21575	H	-2.45337	-6.86456	2.14132
H	-1.06696	-6.45392	6.32146	H	-3.52393	-6.74831	1.07451
O	4.76413	-5.70830	-3.87687	O	2.56752	1.17116	-2.56057
H	4.43170	-6.03418	-4.72883	H	1.96096	1.03985	-3.30194
H	5.67107	-5.45293	-4.06385	H	2.30955	2.03265	-2.20301
O	-2.31716	-1.44443	1.37577	O	-0.79737	-7.66066	2.99530
H	-1.71471	-2.19814	1.26629	H	0.07281	-7.74406	2.59514
H	-2.76368	-1.38612	0.51984	H	-0.62237	-7.62190	3.94562
O	0.49273	4.48698	3.98424	O	4.00205	-0.27645	1.34085
H	0.80670	4.60129	4.89553	H	3.27617	0.23744	0.96932
H	0.04070	3.63041	3.99116	H	4.70564	-0.20075	0.68050
O	-6.81213	-0.26487	1.50881	O	1.14764	3.24395	-1.11703
H	-7.10711	-1.15572	1.32770	H	0.21330	3.09451	-1.26540
H	-6.60840	-0.26243	2.45637	H	1.22794	4.19373	-0.98930
O	-3.12015	5.25377	1.93102	O	0.54532	-4.75211	3.58713
H	-4.00619	5.60956	1.93321	H	1.39380	-4.51717	3.97340
H	-2.61243	5.86851	1.38565	H	0.31478	-5.58571	4.02454
O	-6.35933	2.32577	0.12384	O	0.92120	1.79560	3.56922

H	1.07363	1.82678	2.60481	C	-11.79900	4.78500	-1.69000
H	0.03063	1.44574	3.67655	C	-12.78000	4.85300	-0.50900
O	3.97255	4.12171	2.06581	C	-14.05000	5.59600	-0.93600
H	4.88493	4.44090	2.15637	C	-13.81700	7.10900	-0.84100
H	3.59716	4.24271	2.94896	N	-14.76100	7.71300	-1.82600
O	-0.41740	-5.60625	-1.08790	H	-10.82900	5.13500	-1.36700
H	-0.96293	-5.04884	-1.67248	H	-12.15700	5.41900	-2.48800
H	-0.88926	-6.45416	-1.07717	H	-13.03900	3.85300	-0.19500
O	-5.74733	7.19166	1.39071	H	-12.31700	5.37900	0.31200
H	-4.90818	7.37943	1.92357	H	-14.29600	5.33200	-1.95400
H	-6.35142	7.96086	1.56745	H	-14.86500	5.31900	-0.28400
H	-6.16287	6.37717	1.85884	H	-14.03800	7.45900	0.15800
O	-0.89373	-0.67811	2.92023	H	-12.80000	7.35000	-1.10900
H	-0.01083	-0.56092	3.35094	H	-14.66600	8.74800	-1.80600
H	-1.32014	0.15347	2.63292	H	-15.73700	7.44900	-1.57800
H	-1.49452	-1.42300	3.45148	H	-14.53800	7.36600	-2.78000
O	3.06361	2.58182	4.22800	N	-9.86200	2.17100	-1.06500
H	4.00988	2.60046	4.58311	C	-9.26100	1.27000	-0.02800
H	2.52231	3.32337	4.62199	C	-10.00300	-0.07500	0.00200
H	2.65303	1.68779	4.47798	O	-10.56000	-0.48100	1.00700
O	-5.59146	-2.72569	0.91006	H	-9.27900	2.59000	-1.72500
H	-4.64881	-3.07902	0.88699	H	-8.21400	1.11200	-0.23500
H	-5.71083	-1.99947	0.21963	C	-9.42300	2.00600	1.30000
H	-6.21462	-3.46396	0.63381	C	-8.80800	3.41700	1.22600
O	1.93833	-5.94391	-0.99492	C	-8.72900	1.20400	2.40100
H	2.81233	-6.17249	-0.51117	C	-7.33000	3.33800	0.82100
H	1.52366	-5.15016	-0.54425	H	-10.47300	2.07900	1.51600
H	1.29277	-6.71922	-0.94532	H	-9.34800	4.00700	0.50000
O	8.08264	-5.21855	-3.96231	H	-8.88600	3.88900	2.19400
H	9.06543	-5.12649	-3.88836	H	-7.91200	1.77900	2.80800
H	7.57212	-4.38321	-4.17829	H	-8.34900	0.28300	1.98200
H	7.70343	-6.09538	-4.24117	H	-9.43800	0.97800	3.18300

#### D. Protein Molecules

##### 1. 1V4Z

N	-13.04500	2.93900	-2.64400	H	-7.04700	2.30600	0.68100
C	-11.67000	3.34200	-2.20700	H	-6.72100	3.77600	1.59800
C	-11.15800	2.40500	-1.10200	H	-7.18000	3.88100	-0.10100
O	-11.92400	1.90200	-0.30000	N	-10.01700	-0.75200	-1.10700
H	-13.36513	3.56464	-3.36939	C	-10.72200	-2.07300	-1.19600
H	-13.67619	2.98587	-1.85692	C	-10.03500	-3.13000	-0.31500
H	-13.02206	1.99438	-3.00075	O	-10.68700	-3.82900	0.43800
H	-10.99600	3.31900	-3.05000	H	-9.56800	-0.38200	-1.88900
				H	-11.75300	-1.96100	-0.90100
				C	-10.65100	-2.47300	-2.67500
				O	-9.29300	-2.50600	-3.09900
				H	-11.08500	-3.44900	-2.80600

H	-11.20600	-1.75500	-3.26600	O	-1.14600	-0.39100	-0.90700
H	-9.28100	-2.48700	-4.05900	H	-4.12500	-3.48100	-0.50600
N	-8.73000	-3.25900	-0.40700	H	-2.27800	-2.20800	-2.28800
C	-8.00900	-4.27900	0.42000	C	-4.22900	-1.40100	-1.84500
C	-6.81000	-3.64800	1.14500	C	-4.88100	-2.31800	-2.88700
O	-6.27800	-2.64400	0.70600	C	-4.20000	-2.12600	-4.24500
H	-8.22400	-2.69000	-1.02500	O	-4.58400	-1.21200	-4.95600
H	-8.68200	-4.72800	1.13300	O	-3.30500	-2.89800	-4.55100
C	-7.53600	-5.33700	-0.58200	H	-4.87400	-1.32400	-0.98100
O	-6.66800	-4.73500	-1.53700	H	-4.08500	-0.42000	-2.27300
H	-7.00300	-6.11400	-0.06100	H	-4.77800	-3.34700	-2.57400
H	-8.39500	-5.76600	-1.08200	H	-5.92900	-2.07300	-2.97500
H	-7.16400	-4.60500	-2.34900	N	-2.58800	-0.82600	0.71100
N	-6.41800	-4.27200	2.23500	C	-1.91100	0.10400	1.66200
C	-5.26100	-3.77900	3.03300	C	-0.49800	-0.40600	1.97500
C	-3.93900	-3.99400	2.27800	O	0.43600	0.36500	2.06600
O	-2.98000	-3.27400	2.48900	H	-3.37700	-1.32400	1.00800
H	-5.39000	-2.73900	3.28400	H	-1.86800	1.10000	1.24700
C	-5.31200	-4.62900	4.30200	C	-2.77600	0.09800	2.93000
C	-6.03400	-5.87500	3.90100	O	-4.14800	-0.10700	2.59500
C	-7.00900	-5.48500	2.82300	C	-2.62300	1.43600	3.63800
H	-4.31000	-4.86300	4.63700	H	-2.44600	-0.69000	3.58900
H	-5.86000	-4.11700	5.07700	H	-4.42600	0.60700	2.01500
H	-5.33100	-6.60300	3.52100	H	-1.60400	1.77800	3.53500
H	-6.56900	-6.28100	4.74500	H	-2.86400	1.32000	4.68300
H	-7.08800	-6.27000	2.08300	H	-3.29100	2.15300	3.18900
H	-7.97500	-5.26000	3.24600	N	-0.33300	-1.70000	2.12300
N	-3.88300	-4.97300	1.39700	C	1.02800	-2.25600	2.40900
C	-2.62500	-5.22900	0.62000	C	1.98300	-1.89800	1.26700
C	-2.22300	-3.97300	-0.16800	O	3.15000	-1.63100	1.47800
O	-1.05200	-3.68000	-0.32200	H	-1.10000	-2.30500	2.03400
H	-4.67100	-5.53500	1.24300	H	1.40000	-1.87400	3.33800
H	-1.82800	-5.52100	1.28500	C	0.84200	-3.77400	2.49500
C	-2.95400	-6.38300	-0.33900	C	0.28900	-4.14700	3.87300
O	-4.15500	-6.09500	-1.04600	C	-0.42100	-5.50200	3.79200
C	-3.12700	-7.68000	0.45400	O	0.26200	-6.50000	3.63000
H	-2.14500	-6.50600	-1.04300	O	-1.63700	-5.51900	3.89400
H	-3.91600	-5.75700	-1.91200	H	0.15200	-4.09600	1.73000
H	-2.26900	-7.82900	1.09300	H	1.79500	-4.26100	2.34900
H	-3.21600	-8.51100	-0.23000	H	1.10200	-4.20700	4.58200
H	-4.02000	-7.61600	1.05900	H	-0.41400	-3.39300	4.19400
N	-3.19000	-3.22500	-0.65400	N	1.47600	-1.88000	0.06200
C	-2.87300	-1.97600	-1.41900	C	2.32100	-1.53000	-1.12200
C	-2.13000	-0.98900	-0.51000	C	2.62600	-0.02500	-1.14700

O	3.67100	0.38700	-1.61500	H	1.35000	2.09700	3.41400
H	0.52900	-2.09200	-0.06000	H	5.18700	0.95000	4.87200
H	3.23900	-2.09500	-1.10400	H	3.81100	1.03200	5.97100
C	1.48900	-1.93100	-2.34500	H	4.48900	2.51300	5.29600
C	1.86600	-3.35000	-2.78100	H	1.20000	0.01200	4.81900
C	3.10800	-3.30000	-3.68400	H	0.22300	1.35100	5.42100
N	2.73100	-4.03400	-4.92900	H	1.76000	0.96500	6.19400
C	2.63900	-5.34000	-4.92200	N	5.36400	0.44000	1.82700
N	3.72400	-6.07200	-4.95900	C	6.68900	-0.14800	1.44000
N	1.46300	-5.91200	-4.87900	C	7.38000	0.72300	0.37800
H	0.43900	-1.89900	-2.09300	O	8.58100	0.91600	0.41600
H	1.68400	-1.24400	-3.15500	H	4.54200	-0.07300	1.67900
H	2.07900	-3.94800	-1.90700	H	7.32000	-0.25500	2.30900
H	1.04200	-3.78900	-3.32400	C	6.36200	-1.53000	0.86300
H	3.36200	-2.27500	-3.91400	C	6.23200	-2.54600	2.00300
H	3.93900	-3.79300	-3.20300	C	5.75900	-3.89100	1.44200
H	2.56000	-3.53600	-5.75800	O	6.59600	-4.63900	0.96300
H	4.62200	-5.63400	-4.99400	O	4.56800	-4.15100	1.50300
H	3.65500	-7.07000	-4.95400	H	5.43100	-1.48100	0.31600
H	0.63500	-5.35300	-4.85300	H	7.15400	-1.83900	0.19800
H	1.39200	-6.91000	-4.87400	H	7.19300	-2.67300	2.48100
N	1.73300	0.79900	-0.64100	H	5.51500	-2.18700	2.72500
C	1.99600	2.27700	-0.63600	N	6.63000	1.25200	-0.56500
C	2.96400	2.63600	0.50400	C	7.24000	2.11400	-1.62600
O	3.72200	3.58100	0.40600	C	7.77200	3.41900	-1.01600
H	0.90100	0.44500	-0.25700	O	8.83500	3.88700	-1.37800
H	2.42400	2.57300	-1.58200	H	5.66400	1.08500	-0.57200
C	0.62800	2.96100	-0.45400	H	8.03800	1.58300	-2.12200
S	0.18500	3.05300	1.30000	C	6.11100	2.40000	-2.62300
H	0.67900	3.96000	-0.85300	O	4.98600	2.93600	-1.93600
H	-0.12900	2.40600	-0.98800	H	6.44900	3.11300	-3.34900
H	0.62600	3.81700	1.67800	H	5.83400	1.48300	-3.12800
N	2.95400	1.87300	1.57400	H	4.95600	3.88000	-2.10700
C	3.88500	2.14800	2.71300	N	7.04800	4.00100	-0.08400
C	5.28700	1.63700	2.35900	C	7.52100	5.27100	0.56100
O	6.27600	2.31700	2.56100	C	8.82200	5.01200	1.33700
H	2.34300	1.11000	1.62200	O	9.70300	5.85000	1.38000
H	3.91200	3.20200	2.93500	H	6.19800	3.59800	0.19500
C	3.31200	1.36900	3.90700	H	7.67400	6.03700	-0.18300
C	1.95100	1.95600	4.29800	C	6.40100	5.69000	1.52300
C	4.27000	1.47400	5.09900	C	5.25400	6.33500	0.73800
C	1.23100	1.00100	5.25300	C	4.01100	6.41900	1.62800
H	3.19300	0.33000	3.63300	C	5.66000	7.74600	0.30000
H	2.10100	2.90600	4.78100	H	6.03400	4.82100	2.04900

H	6.78900	6.40200	2.23700	O	1.64500	-0.86900	-3.43500
H	5.03200	5.73500	-0.13300	H	1.80700	0.00000	0.85500
H	4.19100	7.11600	2.43300	H	1.38106	-0.91290	0.42883
H	3.79500	5.44400	2.03800	H	0.36309	0.22239	-0.19899
H	3.17000	6.75700	1.04000	H	2.00500	0.98000	-1.68600
H	4.82000	8.23200	-0.17300	C	3.56900	-0.28700	-0.95500
H	6.48000	7.68300	-0.40000	C	3.86400	-1.56900	-0.17600
H	5.96700	8.31700	1.16400	C	3.96100	-2.75700	-1.12100
N	8.94500	3.85100	1.93700	C	5.14600	-1.42000	0.62900
C	10.19000	3.51400	2.70500	H	4.08300	-0.34900	-1.90200
C	11.37000	3.34400	1.73600	H	3.96200	0.54500	-0.38800
O	12.46300	3.81200	1.99300	H	3.05400	-1.75800	0.51400
H	8.21800	3.19500	1.87400	H	3.34200	-3.56100	-0.75300
H	10.40600	4.28700	3.42700	H	4.98700	-3.09000	-1.17600
C	9.88200	2.19000	3.42600	H	3.62500	-2.46300	-2.10400
C	8.86500	2.43700	4.55000	H	5.57600	-2.39400	0.80600
C	11.16200	1.60600	4.02800	H	4.92400	-0.94700	1.57500
C	8.18200	1.12000	4.92800	H	5.84800	-0.81000	0.07900
H	9.47600	1.48600	2.72000	N	0.95900	-2.09900	-1.68100
H	9.37600	2.83800	5.41300	C	0.39900	-3.14300	-2.52000
H	8.11900	3.14200	4.21800	C	-1.10900	-3.04400	-2.64000
H	11.55900	2.28600	4.76600	O	-1.75700	-2.35500	-1.85200
H	11.89100	1.45500	3.24600	H	0.90700	-2.17700	-0.70500
H	10.93600	0.65800	4.49500	H	0.83400	-3.06800	-3.50600
H	7.90500	1.14500	5.97100	H	0.65300	-4.10400	-2.09700
H	8.86300	0.29800	4.75600	N	-1.66800	-3.73500	-3.62800
H	7.29800	0.98600	4.32300	C	-3.10900	-3.72000	-3.84900
N	11.15100	2.67900	0.62400	C	-3.61600	-5.10900	-4.22400
C	12.25300	2.47700	-0.37000	O	-2.82900	-6.03000	-4.44400
C	12.61400	3.80700	-1.04800	H	-1.09900	-4.26600	-4.22300
O	11.70800	4.49200	-1.49900	H	-3.58300	-3.41300	-2.92900
H	10.25800	2.31500	0.44200	C	-3.46700	-2.72000	-4.95100
H	13.12000	2.05600	0.11500	C	-2.78300	-1.37200	-4.79600
C	11.69400	1.48200	-1.39200	C	-3.26700	-0.37800	-5.84000
H	10.76800	1.86400	-1.79800	N	-2.52400	-0.49400	-7.09200
H	11.51200	0.53400	-0.90900	C	-2.83700	0.17400	-8.19700
H	12.40900	1.34700	-2.19100	N	-3.87300	1.00200	-8.20400
O	13.79200	4.11900	-1.10100	N	-2.11300	0.01400	-9.29700
2. 2P5J				H	-3.18000	-3.13600	-5.90600
N	1.32800	0.00000	0.00000	H	-4.53500	-2.56100	-4.94300
C	2.09400	0.00000	-1.24200	H	-3.00000	-0.97900	-3.81300
C	1.54400	-1.03400	-2.22000	H	-1.71700	-1.50500	-4.90500
				H	-4.31300	-0.56200	-6.03500
				H	-3.14300	0.62100	-5.45000

H	-1.75500	-1.10100	-7.10900	H	-5.28800	-0.84700	-10.50800
H	-4.41900	1.12400	-7.37600	H	-5.67900	-1.95200	-9.19500
H	-4.10500	1.50400	-9.03700	H	-7.10000	-0.22800	-11.63600
H	-1.33100	-0.60900	-9.29600	H	-8.51200	-1.25600	-11.87300
H	-2.34900	0.51700	-10.12800	H	-8.10900	-0.67000	-10.25900
N	-4.93600	-5.25300	-4.29500	H	-3.62400	-2.14100	-11.15700
C	-5.54800	-6.53000	-4.64300	H	-3.93600	-3.18000	-9.76600
C	-6.18700	-6.47300	-6.02600	H	-4.70800	-3.52300	-11.31500
O	-7.40000	-6.62700	-6.16800	N	-9.99100	-3.05800	-10.58700
H	-5.51100	-4.48200	-4.10800	C	-11.25700	-3.35800	-11.24600
H	-4.77300	-7.28200	-4.64500	C	-11.15800	-3.11300	-12.74900
C	-6.61700	-6.93900	-3.61300	O	-11.32000	-4.03400	-13.55000
C	-7.09100	-8.36100	-3.87100	H	-9.96500	-2.36600	-9.89300
C	-6.07500	-6.79800	-2.19800	H	-11.48000	-4.40000	-11.07800
H	-7.46300	-6.27700	-3.71900	C	-12.38000	-2.50700	-10.65200
H	-7.30100	-8.84700	-2.92900	C	-13.53400	-3.31100	-10.13900
H	-7.98700	-8.33900	-4.47400	N	-13.37800	-4.48900	-9.43900
H	-6.31900	-8.90800	-4.39300	C	-14.86800	-3.10100	-10.22700
H	-6.23400	-7.71900	-1.65700	C	-14.56700	-4.96900	-9.11900
H	-5.01800	-6.58200	-2.23900	N	-15.48800	-4.14500	-9.58500
H	-6.58800	-5.99100	-1.69500	H	-11.98700	-1.92900	-9.82900
N	-5.36200	-6.25300	-7.04400	H	-12.75400	-1.83500	-11.41100
C	-5.84500	-6.17700	-8.41800	H	-12.52400	-4.91100	-9.21100
C	-6.75800	-4.97000	-8.60700	H	-15.35600	-2.26700	-10.71100
O	-7.42000	-4.52600	-7.66800	H	-14.75400	-5.87900	-8.57000
H	-4.40400	-6.13800	-6.86700	H	-16.49720	-4.25787	-9.48923
H	-4.98800	-6.07000	-9.06600	N	-10.89100	-1.86600	-13.12400
C	-6.59200	-7.46000	-8.78900	C	-10.77000	-1.50100	-14.53100
C	-5.85000	-8.70800	-8.35300	C	-9.58600	-2.20600	-15.18200
O	-4.60300	-8.67100	-8.30600	O	-8.65900	-2.64200	-14.49900
O	-6.51700	-9.72200	-8.05900	H	-10.77300	-1.17600	-12.43900
H	-7.56200	-7.45500	-8.31300	H	-11.67700	-1.80300	-15.03400
H	-6.72100	-7.49500	-9.86100	C	-10.60600	0.02100	-14.70300
N	-6.78700	-4.44200	-9.82600	C	-11.83900	0.75200	-14.19600
C	-7.61900	-3.28600	-10.13800	C	-9.35500	0.50600	-13.98500
C	-8.87100	-3.70000	-10.90300	H	-10.49600	0.23400	-15.75600
O	-8.82400	-4.58100	-11.76300	H	-12.22200	0.24700	-13.32100
H	-6.23800	-4.84000	-10.53300	H	-11.57600	1.76800	-13.94000
H	-7.91500	-2.82800	-9.20600	H	-12.59600	0.75900	-14.96700
C	-6.84600	-2.24400	-10.96700	H	-8.52200	-0.13100	-14.24300
C	-5.54000	-1.86700	-10.26300	H	-9.14000	1.52100	-14.28400
C	-7.70400	-1.01000	-11.20000	H	-9.51700	0.47200	-12.91700
C	-4.36900	-2.74100	-10.65300	N	-9.62300	-2.31300	-16.50500
H	-6.61500	-2.67900	-11.92800	C	-8.55100	-2.96600	-17.24900



C	-8.29400	-2.25200	-18.57100	O	-11.84400	-1.16500	-19.56100
O	-9.22000	-2.00600	-19.34500	H	-10.09600	0.67200	-19.82000
H	-10.38900	-1.94500	-16.99400	H	-11.92100	1.43200	-17.65200
H	-7.65500	-2.91800	-16.64800	C	-12.74900	1.89300	-19.57100
C	-8.90100	-4.43200	-17.50600	C	-12.58500	3.37800	-19.28600
C	-7.69900	-5.29800	-17.73600	C	-12.46900	1.58900	-21.03500
C	-6.93100	-5.35000	-18.86400	H	-13.77200	1.61900	-19.35800
C	-7.12900	-6.23600	-16.81700	H	-13.53300	3.87700	-19.42500
N	-5.91800	-6.26400	-18.70100	H	-12.25100	3.51400	-18.26700
C	-6.01700	-6.82000	-17.45300	H	-11.85600	3.79600	-19.96300
C	-7.44900	-6.63700	-15.51700	H	-12.07100	2.47000	-21.51700
C	-5.22700	-7.78500	-16.83400	H	-11.75100	0.78500	-21.10400
C	-6.66300	-7.59400	-14.90300	H	-13.38600	1.29500	-21.52500
C	-5.56300	-8.15900	-15.56100	N	-13.13100	-0.77000	-17.75900
H	-9.43400	-4.82400	-16.65300	C	-13.63400	-2.13600	-17.68200
H	-9.53100	-4.49600	-18.38100	C	-14.54900	-2.44700	-18.86200
H	-7.10700	-4.75600	-19.74800	O	-15.64500	-1.89700	-18.97300
H	-5.23400	-6.48100	-19.37000	H	-13.43500	-0.11200	-17.09900
H	-8.29300	-6.21300	-14.99300	H	-12.78500	-2.80400	-17.71300
H	-4.37500	-8.22900	-17.32700	C	-14.38600	-2.35200	-16.36800
H	-6.89600	-7.91700	-13.89900	C	-14.99500	-3.73000	-16.23800
H	-4.97800	-8.90300	-15.04300	C	-16.28300	-3.98800	-16.69000
N	-7.03300	-1.92200	-18.82500	C	-14.28100	-4.77500	-15.66400
C	-6.65400	-1.23700	-20.05600	C	-16.84400	-5.24500	-16.57200
C	-7.30500	0.14000	-20.13300	C	-14.83300	-6.03600	-15.54400
O	-7.57800	0.64900	-21.22000	C	-16.11400	-6.26600	-15.99900
H	-6.33900	-2.14500	-18.16900	O	-16.66800	-7.52000	-15.88200
H	-5.58200	-1.11500	-20.05100	H	-13.70400	-2.21300	-15.54300
C	-7.05300	-2.07300	-21.27300	H	-15.18500	-1.62800	-16.29500
C	-6.39300	-1.58900	-22.54900	H	-16.85200	-3.18600	-17.13900
O	-5.64500	-0.59200	-22.48800	H	-13.27700	-4.59200	-15.30900
O	-6.62500	-2.20800	-23.60900	H	-17.84700	-5.42500	-16.92900
H	-6.76400	-3.10000	-21.10700	H	-14.26200	-6.83600	-15.09500
H	-8.12500	-2.02100	-21.40100	H	-17.57600	-7.44100	-15.58000
N	-7.55200	0.73900	-18.97200	N	-14.09100	-3.33200	-19.74100
C	-8.17000	2.05200	-18.93100	C	-14.86800	-3.71900	-20.91200
C	-9.59500	2.00600	-18.41600	C	-16.23000	-4.27300	-20.50900
O	-9.93800	2.69300	-17.45400	O	-16.36300	-4.93500	-19.47900
H	-7.31200	0.28600	-18.13700	H	-13.21000	-3.73600	-19.59700
H	-7.58600	2.69200	-18.28700	H	-15.01600	-2.83700	-21.51900
H	-8.17300	2.46700	-19.92800	C	-14.12700	-4.77100	-21.75700
N	-10.42900	1.19400	-19.06000	C	-12.74800	-4.25100	-22.16500
C	-11.82500	1.06100	-18.66200	C	-14.94700	-5.13500	-22.98600
C	-12.27100	-0.39600	-18.69900	C	-11.84000	-5.32100	-22.72900

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 H -20.14600 -8.27700 -21.61100  
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 C -16.61400 -10.01100 -21.57400  
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 O -14.64200 -8.89800 -20.77600

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 H -14.59600 -11.64900 -22.28100  
 H -15.93400 -12.54500 -20.47100  
 H -16.87900 -13.50200 -21.61100  
 H -14.24900 -14.25200 -21.97700  
 H -16.56500 -14.27000 -19.37700  
 H -15.88600 -15.66600 -18.60800  
 H -13.34600 -16.09100 -20.97400  
 H -14.05500 -16.70100 -19.51700  
 O -15.29865 -8.51948 -22.82889

### 3. 1ALE

N 11.59061 6.22430 -6.37260  
 C 12.12561 6.16130 -5.01560  
 C 11.01461 6.14730 -3.99260  
 O 9.82161 6.24730 -4.31360  
 C 13.08461 7.35130 -4.83760  
 H 10.71461 6.76530 -6.37160  
 H 12.27561 6.68230 -6.99160  
 H 11.40461 5.27030 -6.71460  
 H 12.68761 5.21530 -4.90260  
 H 13.91361 7.32430 -5.57060  
 H 12.57061 8.32330 -4.96560  
 H 13.54961 7.35930 -3.83460  
 N 11.39061 6.00130 -2.73660  
 C 10.42761 5.86130 -1.64560  
 C 9.42061 4.77830 -1.96360  
 O 8.23061 4.85430 -1.63260  
 C 9.74261 7.22530 -1.35060  
 C 10.65761 8.46130 -1.13460  
 C 10.41361 9.57030 -2.17060  
 C 10.46461 9.02330 0.28040

H	12.43861	5.95030	-2.56460	H	13.56061	-3.77470	0.79040
H	10.97061	5.51430	-0.74760	N	7.80361	2.60330	1.09740
H	9.03961	7.45730	-2.17560	C	6.71561	3.22730	1.84440
H	9.09461	7.10730	-0.45960	C	5.44261	3.26030	1.03240
H	11.71561	8.12830	-1.22760	O	4.33161	3.06230	1.54640
H	10.41961	9.16630	-3.19960	C	7.11861	4.65830	2.30240
H	9.42661	10.05030	-2.03660	C	7.77561	4.82030	3.69940
H	11.18161	10.36430	-2.12460	C	6.99061	4.02130	4.74840
H	10.59061	8.24230	1.05440	C	9.25161	4.38730	3.71540
H	11.18361	9.83230	0.51340	H	8.54461	3.17830	0.59440
H	9.44961	9.44130	0.41840	H	6.49961	2.60330	2.73140
N	9.90561	3.72630	-2.60060	H	7.80461	5.09230	1.54640
C	9.05261	2.64230	-3.07960	H	6.21961	5.30430	2.26440
C	8.67761	1.67130	-1.98460	H	7.72561	5.89230	3.98140
O	7.72761	0.87630	-2.12460	H	5.93061	4.33530	4.79640
C	9.74161	1.91730	-4.26960	H	6.99961	2.93430	4.54040
C	8.81661	1.23430	-5.28660	H	7.40761	4.16230	5.76340
O	7.63361	1.89830	-5.45860	H	9.38661	3.34630	3.36940
O	9.12461	0.21530	-5.88860	H	9.86561	5.03330	3.06040
H	10.96661	3.70130	-2.70960	H	9.69461	4.46630	4.72540
H	8.10961	3.11530	-3.41460	N	5.57661	3.53130	-0.25260
H	10.39561	2.60730	-4.82860	C	4.42261	3.68230	-1.13560
H	10.42661	1.14130	-3.87460	C	3.75761	2.35230	-1.39360
N	9.40661	1.68230	-0.88660	O	2.52561	2.23330	-1.45560
C	9.13061	0.79430	0.23940	C	4.88161	4.34830	-2.46260
C	7.95261	1.29230	1.04240	C	5.49661	5.75530	-2.25360
O	7.16961	0.51830	1.61140	C	6.49761	6.18330	-3.33160
C	10.40561	0.68730	1.12240	C	5.89961	7.32730	-4.15960
C	11.30161	-0.52570	0.76640	N	5.68061	6.86930	-5.54260
C	10.98661	-1.81070	1.53740	H	6.57161	3.66930	-0.60260
C	12.29661	-2.54370	1.85440	H	3.68161	4.32830	-0.62960
N	12.92861	-2.98470	0.59840	H	5.62661	3.70130	-2.96660
H	10.18961	2.40130	-0.84560	H	4.02761	4.40730	-3.16860
H	8.86661	-0.20470	-0.15460	H	4.69961	6.52230	-2.23960
H	11.00261	1.61630	1.02740	H	5.97361	5.80730	-1.25460
H	10.11161	0.64530	2.19140	H	7.45261	6.48430	-2.85560
H	11.19961	-0.77470	-0.30660	H	6.73561	5.31930	-3.98660
H	12.36661	-0.25270	0.90640	H	4.94361	7.67330	-3.71060
H	10.42561	-1.56670	2.46040	H	6.56861	8.21230	-4.16260
H	10.32261	-2.45970	0.93040	H	6.37961	6.15130	-5.78160
H	12.98461	-1.88170	2.42240	H	4.73561	6.46830	-5.62760
H	12.11661	-3.42270	2.50840	H	5.77361	7.66630	-6.18760
H	12.20061	-3.28170	-0.06660	N	4.56861	1.32430	-1.56560
H	13.46661	-2.20670	0.19240	C	4.06361	-0.03970	-1.70260

C	3.39561	-0.51270	-0.43260	C	-0.17839	-0.71470	-2.35460
O	2.52361	-1.39970	-0.44960	C	-0.89639	-1.37670	-3.53460
C	5.24961	-0.96470	-2.09460	O	-0.30439	-2.05070	-4.36460
C	5.50261	-1.19170	-3.62160	N	-2.18639	-1.21570	-3.65660
C	4.40561	-1.86770	-4.44860	H	0.82761	0.47230	-0.26360
O	3.34161	-1.05870	-4.71160	H	-1.94139	0.10130	-1.31660
O	4.48061	-3.02570	-4.83560	H	0.22961	0.24830	-2.72360
H	5.60961	1.54830	-1.56060	H	0.71861	-1.31170	-2.10860
H	3.30261	-0.05370	-2.50560	H	-2.66539	-0.71570	-2.90760
H	6.17761	-0.56370	-1.64260	H	-2.57939	-1.76470	-4.42660
H	5.11161	-1.94670	-1.60260	N	-0.76239	-2.17270	0.60840
H	5.71861	-0.22370	-4.11060	C	-1.15239	-3.34370	1.38940
H	6.42561	-1.78370	-3.77160	C	-2.31039	-3.01070	2.30240
N	3.78161	0.05530	0.69340	O	-3.31339	-3.73170	2.39340
C	3.26761	-0.37170	1.99340	C	0.06361	-3.86670	2.22540
C	1.82861	0.04630	2.17440	O	0.82461	-4.80670	1.47940
O	0.99461	-0.68170	2.72940	C	-0.27939	-4.60570	3.53940
C	4.11861	0.26530	3.13540	H	0.11961	-1.61970	0.83740
C	3.77061	-0.15970	4.57040	H	-1.48839	-4.14170	0.70240
C	2.63161	0.37030	5.18940	H	0.71161	-2.99770	2.47540
C	4.60661	-1.01770	5.28740	H	1.58661	-5.02770	2.02340
C	2.32861	0.03730	6.50540	H	-0.92139	-5.48770	3.35740
C	4.30261	-1.35070	6.60540	H	0.62461	-4.95970	4.06540
C	3.16361	-0.82570	7.21240	H	-0.81139	-3.95770	4.26140
H	4.51561	0.82030	0.60740	N	-2.17139	-1.91070	3.02040
H	3.32361	-1.47370	2.05340	C	-3.23539	-1.39270	3.87740
H	5.19361	0.06330	2.94540	C	-4.54039	-1.23970	3.12940
H	4.04861	1.36830	3.07040	O	-5.61439	-1.63870	3.60340
H	1.99861	1.06830	4.65840	C	-2.80439	-0.03470	4.50640
H	5.50161	-1.41570	4.82940	C	-3.80339	0.68530	5.45040
H	1.43861	0.43830	6.96840	C	-3.10239	1.55530	6.50740
H	4.94961	-2.01870	7.15440	C	-4.77539	1.54830	4.63340
H	2.92361	-1.08770	8.23240	H	-1.21039	-1.44270	2.97040
N	1.51861	1.25230	1.72940	H	-3.42739	-2.13270	4.67640
C	0.15661	1.77330	1.78140	H	-1.85439	-0.18370	5.05940
C	-0.77339	1.06930	0.82240	H	-2.53539	0.65630	3.68240
O	-2.00839	1.17330	0.93140	H	-4.39839	-0.08870	5.97840
H	2.33261	1.83730	1.37240	H	-2.30539	0.99130	7.02540
H	-0.24239	1.66830	2.81040	H	-2.60939	2.43630	6.05640
H	0.15161	2.85730	1.55240	H	-3.80239	1.92130	7.28040
N	-0.22539	0.36830	-0.15060	H	-5.26939	0.96630	3.83240
C	-1.01539	-0.45270	-1.06660	H	-5.57639	1.98630	5.25940
C	-1.44439	-1.75870	-0.44060	H	-4.25539	2.38830	4.13540
O	-2.38139	-2.42770	-0.91160	N	-4.47639	-0.63770	1.95740

C	-5.66639	-0.40070	1.14240	H	-4.78839	-5.44470	8.67240
C	-6.28539	-1.71170	0.71540	H	-4.53439	-7.50070	6.61940
O	-7.47739	-1.98170	0.91340	H	-3.16139	-7.18970	7.53940
C	-5.25839	0.45730	-0.08760	H	-4.59439	-7.63970	8.29440
C	-5.05839	1.99130	0.14740	N	-8.94239	-3.59270	3.02640
C	-3.85739	2.67930	-0.50660	C	-10.38939	-3.39770	2.98340
O	-3.42939	2.36730	-1.60960	C	-10.78539	-2.38970	1.92840
O	-3.31239	3.67030	0.25340	O	-11.61539	-1.49670	2.14740
H	-3.50339	-0.37370	1.62140	C	-10.84439	-2.98670	4.39540
H	-6.40939	0.15030	1.74840	H	-8.26339	-2.78570	2.89440
H	-4.32439	0.04530	-0.51460	H	-10.85839	-4.35970	2.70440
H	-6.01039	0.31130	-0.88660	H	-10.58139	-3.75370	5.14940
H	-5.95839	2.53830	-0.19060	H	-10.37939	-2.03770	4.72440
H	-5.00139	2.20530	1.23140	H	-11.93939	-2.85070	4.45240
N	-5.47539	-2.55170	0.09540	N	-10.19339	-2.52270	0.75240
C	-5.87239	-3.90770	-0.26660	C	-10.57239	-1.69670	-0.39160
C	-6.56439	-4.61970	0.87340	C	-11.63539	-2.38270	-1.21860
O	-7.36639	-5.54870	0.65840	O	-12.65039	-1.78670	-1.60460
C	-4.63839	-4.70070	-0.78560	C	-9.32239	-1.36270	-1.25360
C	-4.51739	-4.87570	-2.30560	C	-9.62639	-0.57370	-2.55760
O	-4.95939	-4.06670	-3.10860	C	-8.63039	-0.89570	-3.68060
O	-3.88839	-6.03870	-2.65660	N	-8.23939	0.37430	-4.34160
H	-4.51639	-2.15770	-0.16460	C	-8.67539	0.79430	-5.52160
H	-6.61539	-3.83270	-1.08060	N	-9.51839	0.14230	-6.26660
H	-3.69839	-4.24670	-0.42860	N	-8.23039	1.92130	-5.95160
H	-4.66139	-5.71070	-0.33660	H	-9.40739	-3.23570	0.71240
N	-6.28539	-4.21870	2.09840	H	-11.00539	-0.76070	0.00440
C	-6.89739	-4.83770	3.27240	H	-8.60339	-0.76970	-0.65460
C	-8.40439	-4.78670	3.19040	H	-8.77339	-2.29270	-1.50760
O	-9.10039	-5.80970	3.28940	H	-10.64839	-0.79270	-2.92460
C	-6.38739	-4.13370	4.55940	H	-9.61539	0.51530	-2.35660
C	-5.34639	-4.96970	5.34640	H	-7.73739	-1.40970	-3.26860
C	-5.80739	-5.43870	6.72940	H	-9.09039	-1.58870	-4.41560
C	-4.57839	-5.69570	7.61240	H	-7.57339	0.98130	-3.84160
N	-4.18839	-7.11270	7.50840	H	-9.81739	-0.74070	-5.85360
H	-5.56139	-3.44370	2.18140	H	-9.77839	0.56730	-7.15460
H	-6.60339	-5.90370	3.29440	H	-7.57739	2.35030	-5.29360
H	-5.94139	-3.15470	4.29740	H	-8.56239	2.25130	-6.85560
H	-7.24739	-3.88970	5.21640	N	-11.42839	-3.65870	-1.48060
H	-5.08239	-5.88370	4.77940	C	-12.29539	-4.44570	-2.35560
H	-4.40239	-4.39670	5.43740	C	-12.70039	-3.66370	-3.58360
H	-6.47739	-4.67970	7.17840	O	-13.85439	-3.76470	-4.10360
H	-6.40839	-6.36570	6.63040	C	-13.53839	-4.90870	-1.54260
H	-3.73739	-5.03870	7.30740	C	-13.93639	-4.08370	-0.27360

C	-14.91539	-2.91870	-0.44060
O	-15.72339	-2.85570	-1.35760
O	-14.80139	-1.96370	0.52240
O	-11.81139	-2.89370	-4.06860
H	-10.59439	-4.10370	-0.98060
H	-11.73039	-5.33370	-2.69860
H	-14.41239	-4.94270	-2.22160
H	-13.38739	-5.96670	-1.24560
H	-14.37439	-4.75670	0.49240
H	-13.03139	-3.67870	0.21540

C	15.58800	9.14700	7.86400
O	15.96900	8.19700	7.18100
H	16.18300	11.39500	10.08200
H	17.20900	8.95200	9.23300
C	15.39600	9.02100	10.34300
C	15.06600	7.54000	10.19900
O	15.99000	6.74300	10.21300
O	13.89400	7.22300	10.07600
H	15.92100	9.18500	11.27300
H	14.48500	9.59400	10.34100

#### 4. 2KAM

N	13.37800	13.93400	9.48300
C	13.92300	14.46700	8.24000
C	15.24200	13.77800	7.90300
O	15.44300	13.31600	6.78200
H	12.50603	14.39752	9.69494
H	14.03425	14.09251	10.23420
H	13.21568	12.94225	9.38206
H	13.21900	14.28300	7.44200
C	14.14800	15.97500	8.36700
H	14.98400	16.16100	9.02600
H	13.26100	16.43700	8.77300
H	14.35700	16.39100	7.39300
N	16.13100	13.70100	8.88600
C	17.42200	13.05500	8.68500
C	17.23400	11.56900	8.40400
O	17.72200	11.04200	7.40600
H	15.91300	14.07900	9.76200
H	17.91900	13.51300	7.85200
C	18.27600	13.22800	9.94300
C	18.90400	14.62100	9.97300
C	19.94900	14.75300	8.86900
O	20.85700	13.92600	8.77000
N	19.87200	15.74600	8.02700
H	17.64900	13.10500	10.80700
H	19.05000	12.48700	9.96000
H	18.13400	15.35600	9.82500
H	19.37500	14.78200	10.93000
H	19.14800	16.40000	8.10600
H	20.54000	15.83600	7.31400
N	16.52800	10.90900	9.30500
C	16.27400	9.47900	9.18400

N	14.58200	9.93400	7.50000
C	13.86800	9.69900	6.25000
C	14.82300	9.86300	5.07200
O	14.83400	9.04600	4.15100
H	14.31900	10.68000	8.07800
H	13.49100	8.69500	6.25100
C	12.68800	10.67500	6.12600
C	11.59200	10.31100	7.16000
C	12.11600	10.63700	4.70200
C	10.64900	9.22500	6.61500
H	13.04800	11.66900	6.33100
H	12.05500	9.94800	8.06600
H	11.01500	11.19600	7.38900
H	11.13500	11.08700	4.69600
H	12.04400	9.61200	4.37000
H	12.76800	11.18400	4.03700
H	9.90900	9.68300	5.97500
H	10.15400	8.73400	7.43900
H	11.21200	8.49900	6.05100
N	15.64300	10.90600	5.12100
C	16.61800	11.14500	4.06700
C	17.70100	10.07100	4.12000
O	18.24400	9.66500	3.09500
H	15.60400	11.51400	5.88900
H	16.11800	11.09000	3.11100
C	17.23000	12.53900	4.22700
C	16.15700	13.59100	3.93300
C	18.39200	12.71200	3.24600
C	16.64200	14.96300	4.40400
H	17.58800	12.65900	5.23800
H	15.96900	13.62100	2.86900
H	15.24600	13.33300	4.45200
H	18.65700	13.75700	3.18500
H	18.09500	12.35800	2.27000

H	19.24300	12.14300	3.59200	H	14.11800	7.95000	1.40700
H	17.59000	15.18900	3.94000	H	16.10200	10.11200	-0.65000
H	16.75800	14.95500	5.47700	H	16.65700	11.03400	0.74800
H	15.91700	15.71400	4.12500	H	15.02500	10.36500	0.72300
N	18.00700	9.61400	5.33000	N	18.79800	6.81800	1.05100
C	19.01600	8.57700	5.51600	C	20.19100	6.58100	0.70400
C	18.50000	7.22700	5.01000	C	20.64300	5.22500	1.21900
O	19.26300	6.41400	4.49000	O	21.42500	4.53400	0.57200
H	17.53900	9.97500	6.11200	H	18.56000	7.56300	1.63300
H	19.89700	8.84100	4.96100	H	20.29000	6.59600	-0.37300
C	19.38700	8.46000	6.99600	H	20.80900	7.35200	1.13800
O	20.66700	7.85000	7.11300	N	20.13200	4.83100	2.37500
H	19.41900	9.43900	7.44400	C	20.49200	3.53900	2.92500
H	18.64700	7.86100	7.50600	C	20.14200	2.47300	1.90300
H	20.71900	7.14400	6.46400	O	20.94500	1.59300	1.61100
N	17.20300	6.99500	5.19300	H	19.49600	5.40600	2.85100
C	16.58100	5.73400	4.78700	H	21.55000	3.51100	3.11800
C	16.68600	5.50200	3.28000	C	19.72900	3.28100	4.22400
O	17.04400	4.40800	2.84000	C	20.32600	2.08800	4.96200
H	16.65400	7.67900	5.63000	O	21.47300	1.76800	4.70100
H	17.07400	4.92600	5.29600	O	19.62600	1.51300	5.78100
C	15.11200	5.74000	5.20700	H	19.78500	4.15700	4.85400
O	15.03000	5.83300	6.62400	H	18.69900	3.07500	3.98900
C	14.42600	4.45600	4.73700	N	18.94100	2.59300	1.34500
H	14.62100	6.58800	4.76500	C	18.46600	1.66500	0.32700
H	14.32000	5.25800	6.91800	C	19.36300	1.73200	-0.90500
H	15.02000	3.60300	5.02700	O	19.64400	0.70700	-1.52500
H	14.32300	4.47500	3.66300	H	18.36500	3.33800	1.61300
H	13.44800	4.38600	5.19000	H	18.50400	0.66100	0.72500
N	16.36800	6.52200	2.49100	C	17.01100	1.99900	-0.04300
C	16.42900	6.38700	1.03500	C	16.51700	1.07700	-1.17100
C	17.84300	6.04000	0.59000	C	16.63700	-0.39400	-0.74500
O	18.05700	5.08200	-0.15200	C	15.05000	1.40400	-1.47400
H	16.08200	7.36700	2.88900	H	16.38800	1.85800	0.82800
H	15.77500	5.58200	0.73300	H	16.94600	3.03100	-0.36400
C	15.97200	7.69300	0.35500	H	17.11000	1.24100	-2.06000
C	16.56900	8.91200	1.06900	H	15.95900	-1.00100	-1.32900
C	14.44300	7.79200	0.38900	H	16.39000	-0.49100	0.30300
C	16.05000	10.20000	0.42400	H	17.64800	-0.73500	-0.90700
H	16.31000	7.69100	-0.66100	H	14.46400	1.29100	-0.57600
H	16.28500	8.89400	2.10200	H	14.68000	0.73100	-2.23300
H	17.64300	8.89100	0.98300	H	14.97600	2.42200	-1.82900
H	14.01200	6.87800	0.01100	N	19.81500	2.93300	-1.25900
H	14.12000	8.61800	-0.22400	C	20.67800	3.07300	-2.42200

C	21.94400	2.24600	-2.21900	C	21.62800	-1.47100	3.43100
O	22.35000	1.48900	-3.09900	C	20.59400	-3.40800	3.00700
H	19.57000	3.72900	-0.73600	N	21.69500	-2.28200	4.55100
H	20.15800	2.71800	-3.29200	C	21.06900	-3.49600	4.33400
C	21.04700	4.54200	-2.62900	C	19.90400	-4.49500	2.47100
C	22.09100	4.66700	-3.74000	C	20.86200	-4.63900	5.10700
C	19.79600	5.33600	-3.01000	C	19.69100	-5.65100	3.23900
H	21.45400	4.93300	-1.71600	C	20.16900	-5.72300	4.55700
H	22.17400	5.70100	-4.04100	H	20.32500	-0.55400	1.23600
H	21.78900	4.06900	-4.58600	H	19.91000	-2.12600	0.63200
H	23.04700	4.32000	-3.37700	H	22.04400	-0.47900	3.33400
H	19.49100	5.07000	-4.01000	H	22.12900	-2.04700	5.39600
H	20.01500	6.39200	-2.96800	H	19.54200	-4.43700	1.45600
H	19.00000	5.10500	-2.31700	H	21.23200	-4.68700	6.12100
N	22.55200	2.38800	-1.04500	H	19.15700	-6.48700	2.81300
C	23.76100	1.63800	-0.72800	H	20.00300	-6.61500	5.14500
C	23.45100	0.14800	-0.59400	N	21.31200	-1.47300	-2.05900
O	24.18500	-0.69500	-1.10900	C	21.09600	-2.04500	-3.38300
H	22.17800	2.99900	-0.37800	C	22.42900	-2.51200	-3.96000
H	24.45300	1.75800	-1.54100	O	22.53300	-3.61400	-4.49800
C	24.40200	2.17300	0.56900	H	21.13100	-0.52000	-1.90000
C	25.24500	3.42900	0.28400	H	20.44700	-2.89500	-3.28700
C	24.32900	4.63000	0.04800	C	20.43400	-1.00600	-4.30600
C	25.17400	5.87700	-0.21400	C	18.92200	-0.91300	-3.99500
N	24.27600	7.03900	-0.47300	C	20.64200	-1.38100	-5.78400
H	23.61800	2.42400	1.27500	C	18.13100	-2.01000	-4.73100
H	25.03700	1.41000	1.00000	H	20.89000	-0.04800	-4.12200
H	25.88000	3.62800	1.13600	H	18.76900	-1.02100	-2.93200
H	25.86300	3.27000	-0.58700	H	18.55700	0.05400	-4.30700
H	23.69900	4.44200	-0.80700	H	19.94100	-0.83300	-6.39700
H	23.71800	4.79200	0.92100	H	20.48100	-2.44100	-5.91200
H	25.79000	6.08300	0.65100	H	21.65100	-1.13300	-6.08100
H	25.80500	5.71100	-1.07500	H	17.89100	-1.66800	-5.72700
H	24.84900	7.88000	-0.68100	H	17.21700	-2.21700	-4.19400
H	23.69000	7.21700	0.36900	H	18.72100	-2.91100	-4.79500
H	23.66300	6.82900	-1.28500	N	23.44400	-1.67100	-3.83400
N	22.36100	-0.16900	0.09400	C	24.76600	-2.01100	-4.33700
C	21.96300	-1.54200	0.28400	C	25.30500	-3.21700	-3.58800
C	21.76500	-2.23100	-1.06500	O	25.87700	-4.13100	-4.18100
O	22.02000	-3.42700	-1.20400	H	23.30400	-0.80800	-3.38900
H	21.80700	0.53400	0.48700	H	24.69000	-2.25800	-5.37500
H	22.73900	-2.05700	0.82400	C	25.70900	-0.82300	-4.16900
C	20.67100	-1.55600	1.12000	C	25.26400	0.31600	-5.08800
C	20.94800	-2.11500	2.47100	C	27.13800	-1.23600	-4.53200



C	26.00800	1.59600	-4.70600	C	22.90400	-5.07100	-7.60200
H	25.68000	-0.49300	-3.14600	H	24.87300	-4.71600	-6.83100
H	25.49000	0.06000	-6.11400	H	24.64000	-6.86600	-8.94200
H	24.20000	0.47400	-4.98000	H	26.09300	-6.00900	-8.42700
H	27.53600	-1.87600	-3.75900	H	24.85000	-5.16400	-9.35000
H	27.75400	-0.35400	-4.62400	H	22.35900	-4.95100	-6.67800
H	27.13000	-1.76900	-5.47100	H	22.41600	-5.81600	-8.21400
H	25.64000	2.41900	-5.30000	H	22.92700	-4.13000	-8.13200
H	27.06500	1.46600	-4.88600	N	26.47700	-6.60300	-5.32600
H	25.84500	1.80700	-3.65900	C	27.83900	-7.03400	-5.05600
N	25.11000	-3.20800	-2.28100	C	27.83900	-8.43600	-4.45600
C	25.56800	-4.30100	-1.44400	O	28.66900	-9.27300	-4.81000
C	24.91300	-5.60300	-1.88800	H	26.12700	-5.80100	-4.88100
O	25.51900	-6.67100	-1.81500	H	28.39900	-7.04200	-5.97200
H	24.64300	-2.45200	-1.87000	C	28.50200	-6.06500	-4.08600
H	26.64000	-4.39200	-1.53200	C	29.93500	-6.49700	-3.80800
C	25.20700	-4.01100	0.01500	O	30.20700	-7.68500	-3.63100
C	25.95500	-4.95600	0.95000	N	30.87400	-5.59800	-3.76900
O	26.94300	-5.52800	0.51800	H	28.50100	-5.07400	-4.51300
O	25.52900	-5.09400	2.08400	H	27.95000	-6.05800	-3.16500
H	25.47200	-2.99100	0.25100	H	30.65200	-4.65400	-3.92000
H	24.14200	-4.14500	0.15200	H	31.80000	-5.86400	-3.58700
N	23.66900	-5.50500	-2.34700	N	26.89800	-8.68600	-3.54800
C	22.94000	-6.68500	-2.80000	C	26.79400	-9.99500	-2.90600
C	23.51300	-7.22000	-4.10900	C	26.02300	-10.97600	-3.78400
O	23.74200	-8.42100	-4.25200	O	26.06300	-12.18600	-3.55700
H	23.23900	-4.62300	-2.39100	H	26.26300	-7.97900	-3.30800
H	23.02400	-7.44900	-2.05000	H	27.78400	-10.38200	-2.74200
C	21.46300	-6.35200	-2.98800	C	26.09300	-9.87000	-1.55500
O	20.91000	-5.94200	-1.74500	C	27.00300	-9.14100	-0.56100
C	20.71900	-7.58700	-3.50100	C	26.39700	-9.21200	0.84600
H	21.36600	-5.55600	-3.70200	C	25.11900	-8.37300	0.91800
H	20.16200	-6.51100	-1.55100	N	24.75500	-8.15400	2.34700
H	20.93200	-7.72600	-4.55100	H	25.18300	-9.31000	-1.68800
H	19.65600	-7.44900	-3.36600	H	25.86200	-10.85500	-1.17500
H	21.04100	-8.45800	-2.95000	H	27.97800	-9.61000	-0.55400
N	23.74500	-6.32100	-5.05900	H	27.10600	-8.10800	-0.85500
C	24.29500	-6.71600	-6.34900	H	26.16400	-10.24000	1.08100
C	25.69600	-7.27400	-6.16100	H	27.11100	-8.83500	1.56300
O	26.05900	-8.28900	-6.75700	H	25.28200	-7.42000	0.43700
H	23.54500	-5.37700	-4.88900	H	24.31500	-8.89400	0.42100
H	23.66900	-7.47500	-6.77800	H	23.92400	-8.73100	2.58500
C	24.33300	-5.52000	-7.29600	H	24.53800	-7.14900	2.50000
C	25.03000	-5.91900	-8.59900	H	25.55200	-8.43300	2.95300

N	25.31700	-10.45400	-4.78100	C	28.76200	-13.60500	-3.09200
C	24.54000	-11.30500	-5.67700	C	29.81300	-13.90700	-2.01100
C	25.44600	-12.28600	-6.41300	C	30.75200	-12.70700	-1.83600
O	25.13700	-13.47300	-6.52000	C	31.53800	-12.85500	-0.53200
H	25.31700	-9.48400	-4.91700	N	32.47100	-14.01000	-0.64500
H	23.82700	-11.86100	-5.09700	H	28.30100	-12.65600	-2.87600
C	23.78200	-10.45400	-6.69000	H	28.00800	-14.37700	-3.07700
C	22.89000	-11.34500	-7.52300	H	29.31100	-14.10800	-1.07700
C	21.67400	-11.80100	-6.99900	H	30.39000	-14.77300	-2.29600
C	23.27800	-11.71800	-8.81600	H	31.44300	-12.67000	-2.66000
C	20.84700	-12.62800	-7.76800	H	30.17600	-11.79600	-1.80800
C	22.45000	-12.54400	-9.58400	H	32.10300	-11.95300	-0.35100
C	21.23400	-13.00000	-9.06000	H	30.85400	-13.02000	0.28700
H	23.18000	-9.72300	-6.16900	H	31.96900	-14.88700	-0.40100
H	24.48800	-9.95300	-7.32900	H	33.27000	-13.87400	0.00800
H	21.37400	-11.51500	-6.00200	H	32.82500	-14.07500	-1.62000
H	24.21500	-11.36600	-9.22100	N	29.14600	-15.85700	-5.18500
H	19.90800	-12.98100	-7.36300	C	29.61200	-17.19300	-5.54000
H	22.74900	-12.83100	-10.58200	C	30.79000	-17.10900	-6.50600
H	20.59600	-13.64000	-9.65300	O	31.72200	-17.88000	-6.34000
N	26.57000	-11.78100	-6.92200	H	28.18500	-15.66200	-5.19900
C	27.52600	-12.61700	-7.65300	H	29.93100	-17.70100	-4.64300
C	28.68400	-13.00500	-6.74500	C	28.47600	-17.99200	-6.18300
O	29.82200	-13.14300	-7.19200	C	27.39700	-18.27400	-5.14100
H	26.76200	-10.82900	-6.80200	C	26.25300	-19.04800	-5.79700
H	27.03300	-13.51500	-7.99400	C	25.16100	-19.30600	-4.76400
C	28.06500	-11.85500	-8.86800	N	24.03700	-20.04800	-5.40300
O	29.13900	-12.58400	-9.44300	H	28.04800	-17.42300	-6.99400
C	28.56200	-10.47600	-8.43000	H	28.86300	-18.92800	-6.56000
H	27.27800	-11.73600	-9.59700	H	27.81600	-18.86000	-4.33700
H	29.57400	-13.07600	-8.74200	H	27.02000	-17.34100	-4.75100
H	29.32700	-10.59200	-7.67600	H	25.84900	-18.46900	-6.61500
H	27.73800	-9.90800	-8.02300	H	26.62300	-19.99000	-6.17100
H	28.97100	-9.95400	-9.28300	H	25.56500	-19.89100	-3.95200
N	28.37900	-13.17600	-5.46700	H	24.80000	-18.36200	-4.38300
C	29.39400	-13.54600	-4.48900	H	23.88200	-20.94400	-4.89900
C	30.00300	-14.90000	-4.84100	H	24.27300	-20.24400	-6.39600
O	31.22100	-15.07400	-4.80000	H	23.17200	-19.47300	-5.35800
H	27.45200	-13.04800	-5.17700	O	30.74300	-16.27500	-7.39400
H	30.16600	-12.79800	-4.49600				

