Supporting Information

Intramolecular CH…π attraction mediated conformational polymorphism of constraint helical peptides

Jinming Sun,[a, ‡]Zi-You Tian,[a, ‡] Jianbo Liu,[b, ‡] Chuan Wan,[d] Chuan Dai,[b] Zhihong Liu,[b] Yun Xing,[a] Yujie Wu,[e] Zhanfeng Hou,[a] Wei Han,[c] Feng Yin,[a,b*] Yuxin Ye,[b*] Zigang Li[a,b*]

Contents

1. Materials and methods

General: All chemicals and solvents were purchased from commercial suppliers and used without further purification. The ^{1}H NMR spectra were recorded with a Zhongke-Niujin AS400 400 MHz spectrometer in MeOD at 298K and calibrated against the residual proton signal or natural abundance carbon resonance of the used deuterated solvent from tetramethylsilane (TMS) as the internal standard. Peptides were analyzed and purified by RP-HPLC (SHIMAZU Prominence LC-20AT) using a C_{18} analytic column (Agilent ZORBAX SB-Aq, 4.6 × 250 mm, 5 μm, flow rate 0.8 mL/min). H_2O (containing 0.1% TFA) and pure acetonitrile were utilized as solvents in linear gradient mixtures. LC-MS spectra were carried out on SHIMAZU LC-MS 8030 (Electrospray Ionization).

Preparation of peptide assemblies: Lyophilized pentapeptide powder was dissolved in deionized water and diluted to the 5-millimole concentration. Preheat the water bath to the target temperature in advance, take an appropriate amount of peptide solution (about 150 μL) in a 2 ml glass bottle, and seal the bottle with Teflon tape, which was heated in a water bath for at least four hours, then naturally cooled to room temperature about 0.2K/min.

Circular Dichroism (CD) Spectroscopy: CD spectra were recorded by Chirascan Plus Circular Dichroism Spectrometer (Applied Photophysics) at the preset temperature level. Peptides were dissolved in deionized water at 100 micromole concentration. Parameters used in the experiment are as follows: wavelengths from 250 to 190 nm were measured with a resolution of 1.5 nm at a scan speed of 1 nm/sec. Each sample was scanned twice and the averaged spectrum was smoothed using Pro-Data Viewer by Applied Photophysics with a smooth window. CD data were presented as mean residual ellipticity [θ] in $deg \cdot cm^{2} \cdot dmol^{-1}$.

Scanning Electron Microscopy (SEM): The samples (20 μL) of peptide assemblies were placed on polished silicon slides and stood for 10 minutes before removing the remaining solvent, then were viewed using a scanning electron microscope (ZEISS Supra 55, Oxford X-Max 20, 5 kV).

Atomic Force Microscope (AFM): Samples of peptide assemblies were diluted five times with deionized water before 5 μL liquid was dispersed on Mica flakes. After adsorption on mica flakes for 30 minutes, the remaining solvent was removed and then dried in the oven at 398 K. The samples were then characterized by Bruker Dimension Icon atomic force microscope, and AFM analysis was performed in AFM, Bruker, and Multimode 8 modes. The probe material used by AFM is an antimony-doped silicon cantilever with a spring constant of 0.4 N/m and a resonance frequency of 300 kHz. The acquired image data is analyzed using nasoscope analysis.

Single Crystal X-ray diffraction (SCXRD): The crystals were quick-frozen with liquid nitrogen and protected with 30% glycerin. The selected crystals are collected under 100K, and the collection device is an indoor X-ray diffraction system. The system parameters are as follows: high-strength sealed copper tube X -ray generator (Rigaku® MicroMax-002^{+}), an AFC^{11} goniometer, a Saturn 944^{+} CCD detector (Rigaku®), and an Oxford refrigeration system. Diffraction data collection, integration, scaling, and empirical correction are

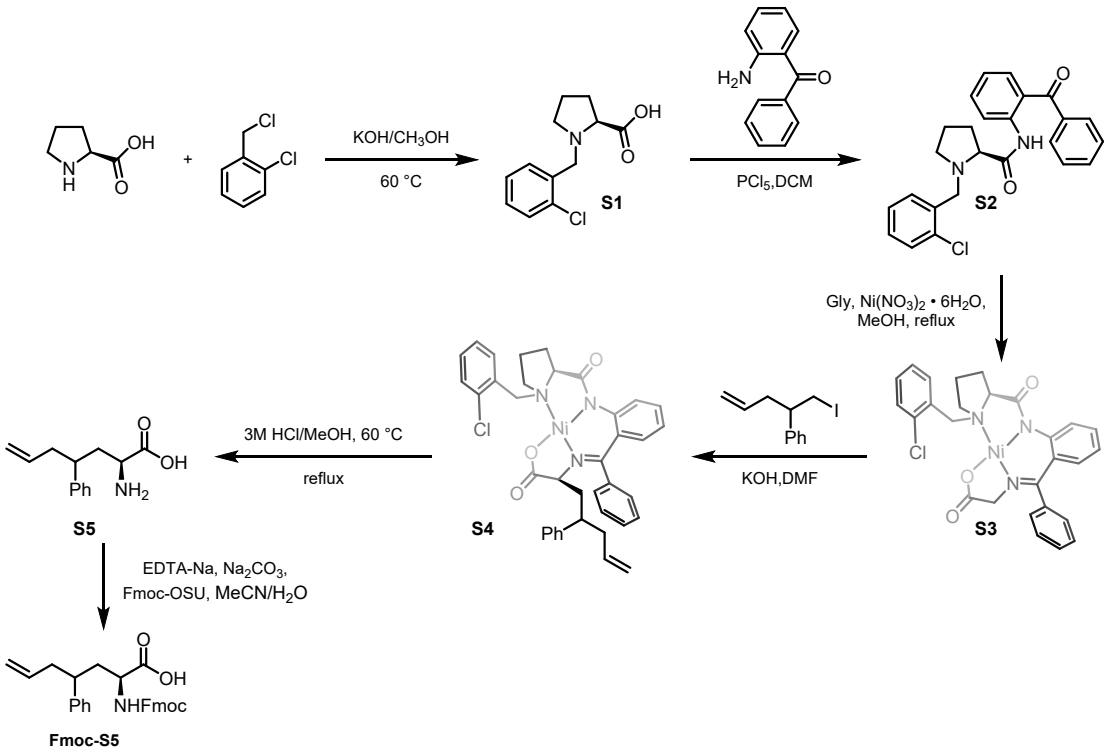
completed through the Rigaku CrystalClear-2.054 program package. The resolution of the crystal obtained by the software SIR201155 is 0.8Å and the structure is refined by the SHELXTL97 software using Full-Matrix-Least-Squares against F^2. Non-hydrogen atoms are defined as anisotropy, and hydrogen atoms are placed in the most ideal position. The absolute configuration of the crystal is determined using the Flack method.

Power X-ray diffraction (PXRD): The crystals were mounted vertically onto the goniometer of a Bruker Instruments Gemini X-ray diffractometer equipped with a Sapphire 3 charge-coupled device (CCD) detector. The sample-to-detector distance was 15mm. Jade 6 software was used to study the peptide structures of the samples. The sample powders were scanned in the range of $2\theta = 5°$ to $30°$ with a step size of $0.15°$.

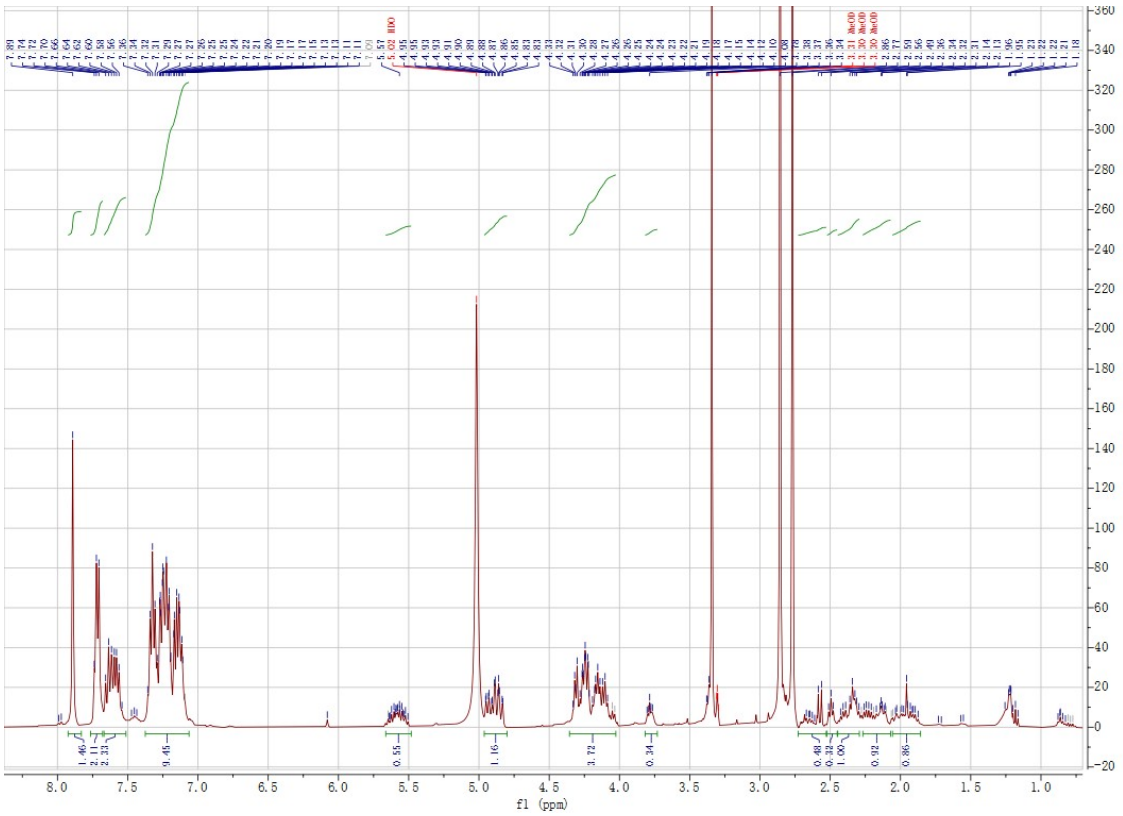
2. Synthesis of peptides

2.1 Fmoc-S5 unnatural amino acid synthesis.

The unnatural amino acid (S5) was synthesized based on the previous literature,[1] as shown in following flow chart scheme.

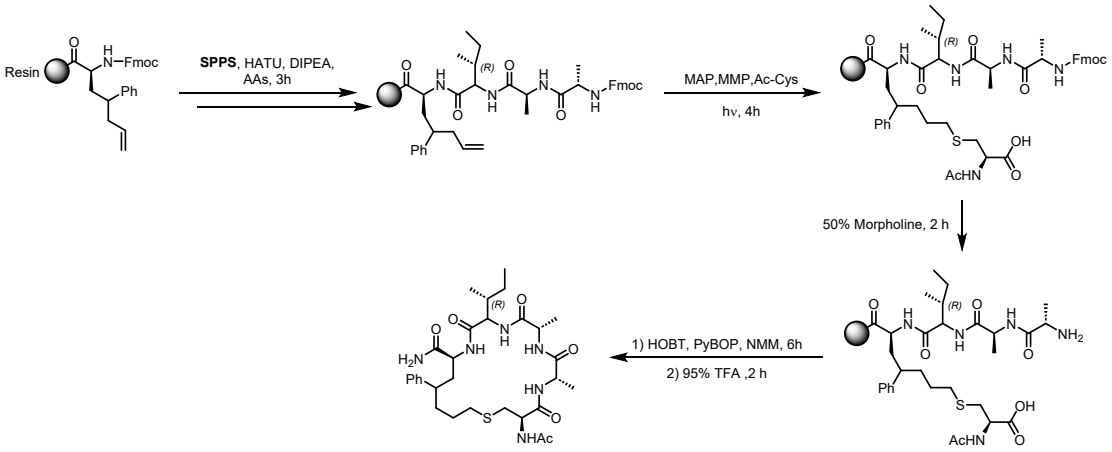


2.2 NMR spectral data of Fmoc-S5 unnatural amino acid



2.3 Solid-phase peptide synthesis.

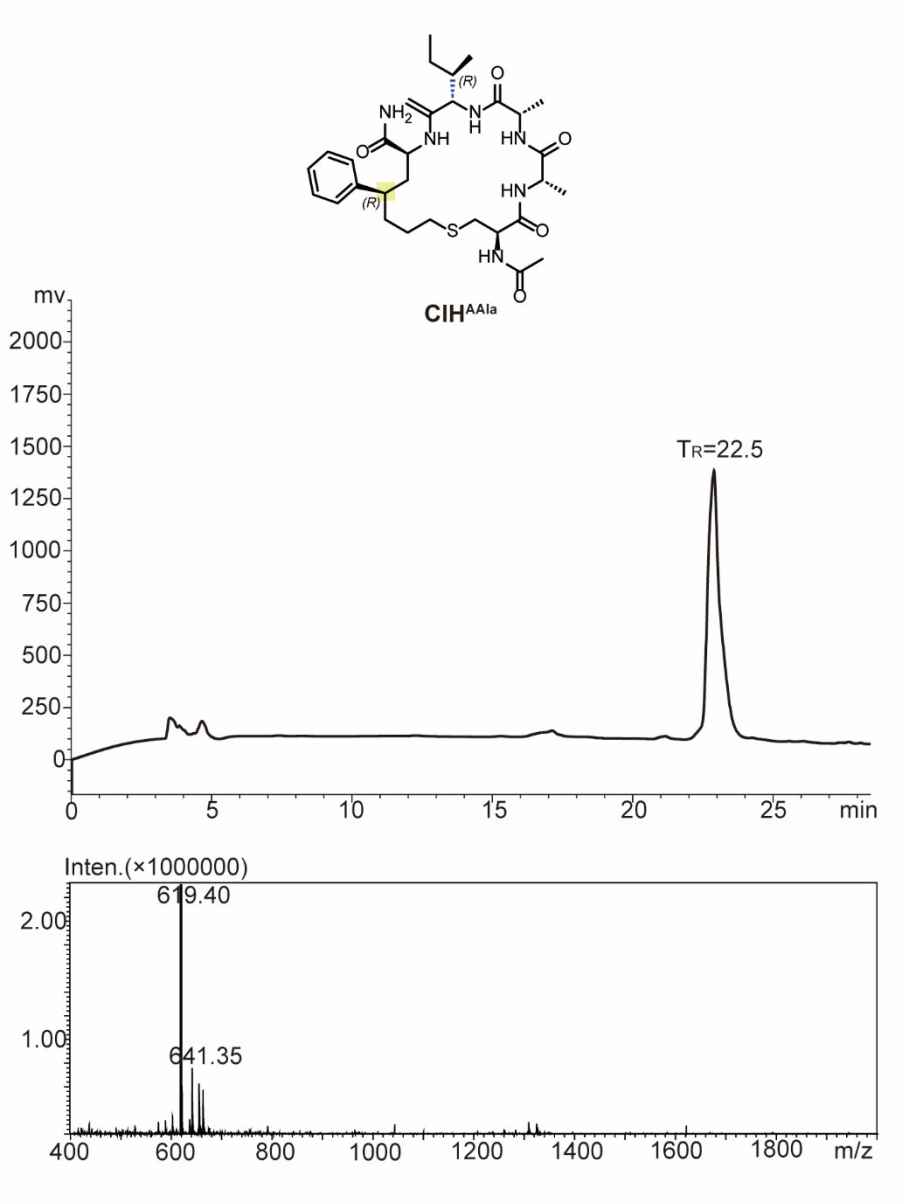
All peptides were synthesized by manual Fmoc-based solid-phase synthesis, as shown in following scheme. Intramolecular thiol-ene reactions were used for constructing target cyclic peptides. The thiol-ene reaction is conducted at ultraviolet light (365 nm) with 3 eq MAP/MMP (1:1) catalysis in dry DMF for 4 hours. The photoreaction efficiency is generally >90% for pentapeptides. The resulting cyclic diastereomers were separated by HPLC. The purified peptides were tested by ESI/LC-MS and the pure fractions were combined and then lyophilized.

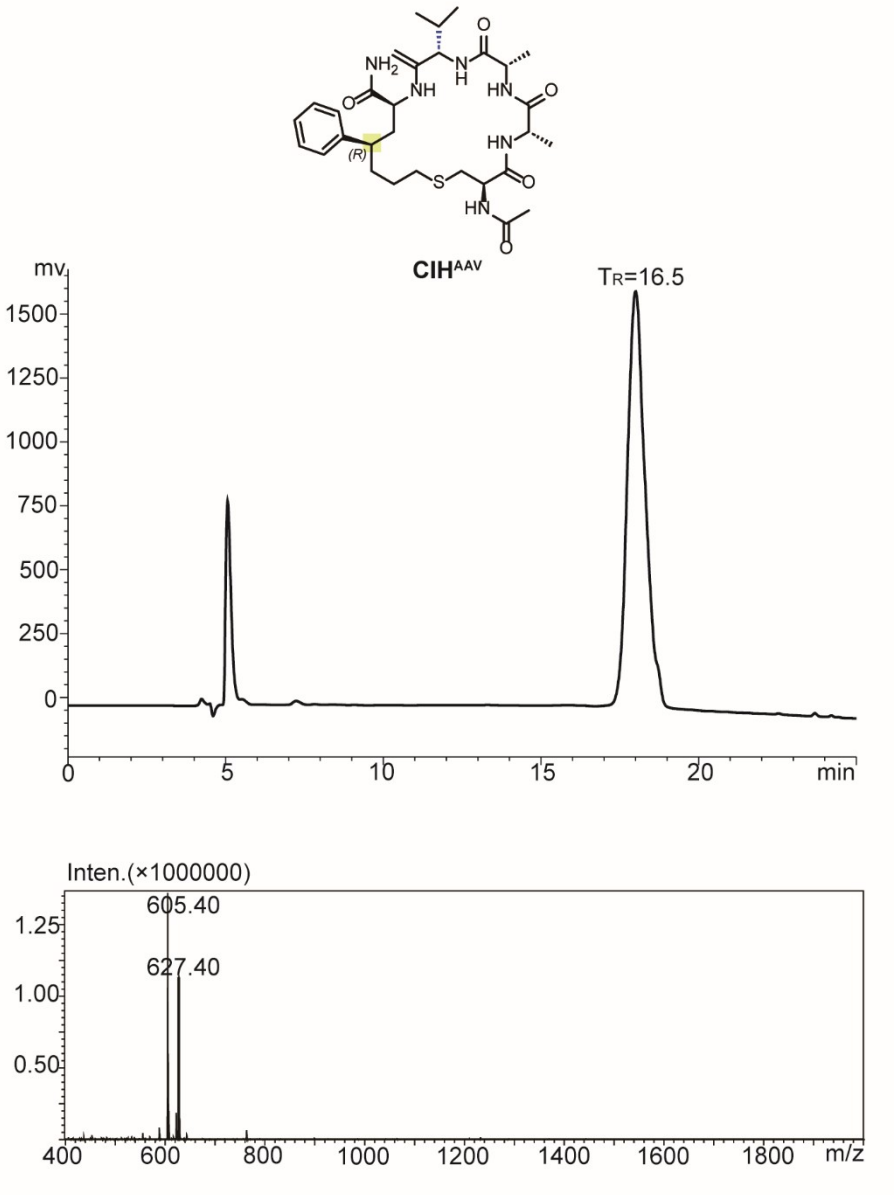


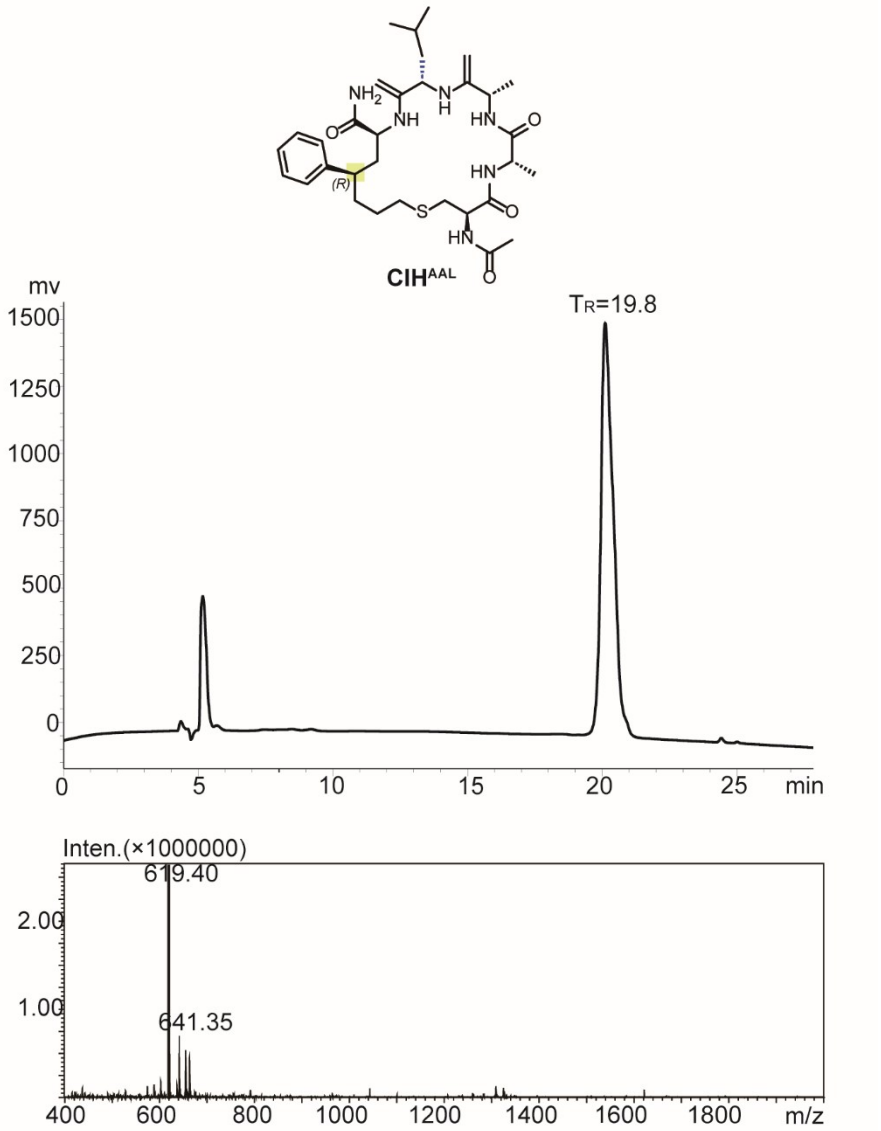
(MAP:4-methoxy acetophenone, MMP: 2-hydroxy-4'-(2-hydroxyethoxy)-2-methylpropiophenone, AC-Cys: Acetylcysteine, DIPEA: N, N-diisopropylethylamine, PyBOP: Benzotriazol-1-yl-oxytripyrrolidino-phosphonium Hexafluorophosphate, HOBT: 1-Hydroxybenzotriazole.

2.4 HPLC and MS spectral data of CIH peptides

The resulting HPLC and ESI/LC-MS spectral were showed as following. The calculated and found m/z ($[M+H]^+$/$[M+Na]^+$), the HPLC spectra (line 220 nm), retention time T_R are presented.




NH2
NH
N
H
O
HN
HN
HN
S
(R)
HN
CIHAAV
mv
1500
1250
1000
750
500
250
0
TR=16.5
0
5
10
15
20
min
Inten.(×1000000)
605.40
627.40
1.25
1.00
0.50
400
600
800
1000
1200
1400
1600
1800
m/z


ClH^AAL
mv
1500
1250
1000
750
500
250
0
TR=19.8
0
5
10
15
20
25
min
Inten.(×1000000)
619.40
2.00
1.00
641.35
400
600
800
1000
1200
1400
1600
1800
m/z

2.5 CD spectral data of CIH peptides

The CIH peptides were characterized by CD spectral, the results were showed as following.

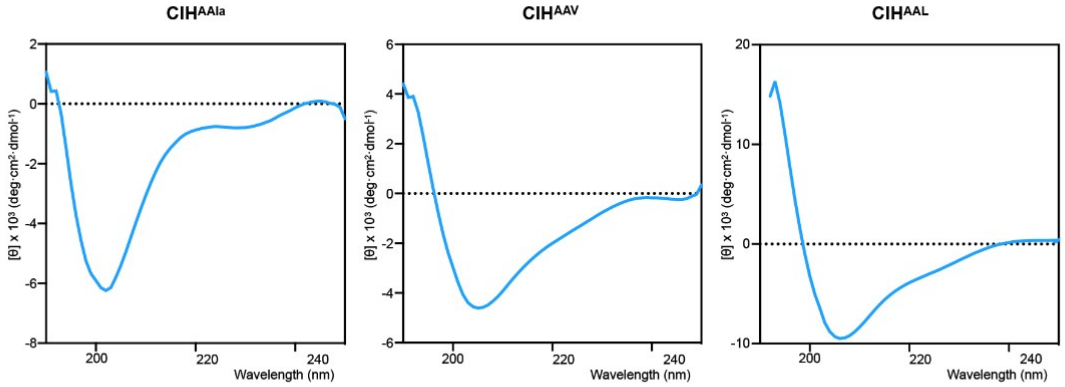


Figure S1. CD spectra of CIH peptides in ddH_2O at room temperature.

3. Polymorphs characterization of the ClH^{AAla}

3.1 Optical microscope images for ClH^{AAla} self-assembly process

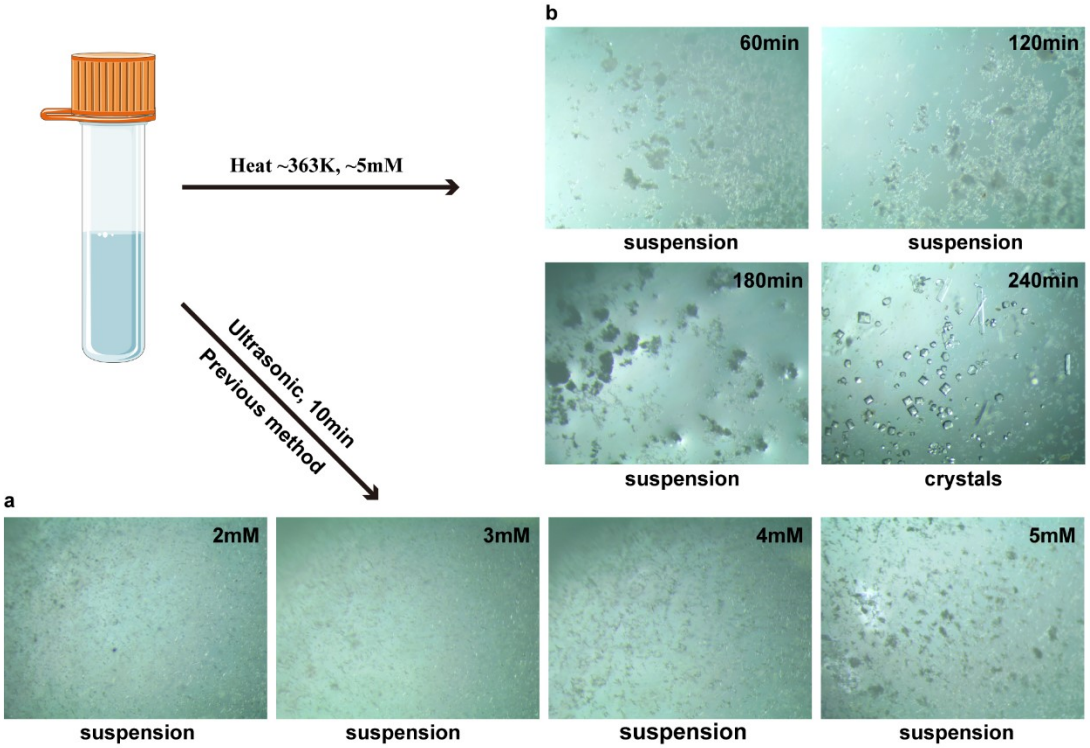


Figure S2. The self-assembly results of ClH^{AAla} by two different methods. (a) the peptide was dissolved in double distilled water as a reserve liquid about 5mM. Different morphologies of the peptides after annealing at different heating times were presented. Obvious crystals appeared after 240 minutes of heating durations. (b) the peptide was dissolved in different concentration. No obvious crystals appeared after 10 minutes ultrasonic.

3.2 Crystal packing of ClH^{AAla}

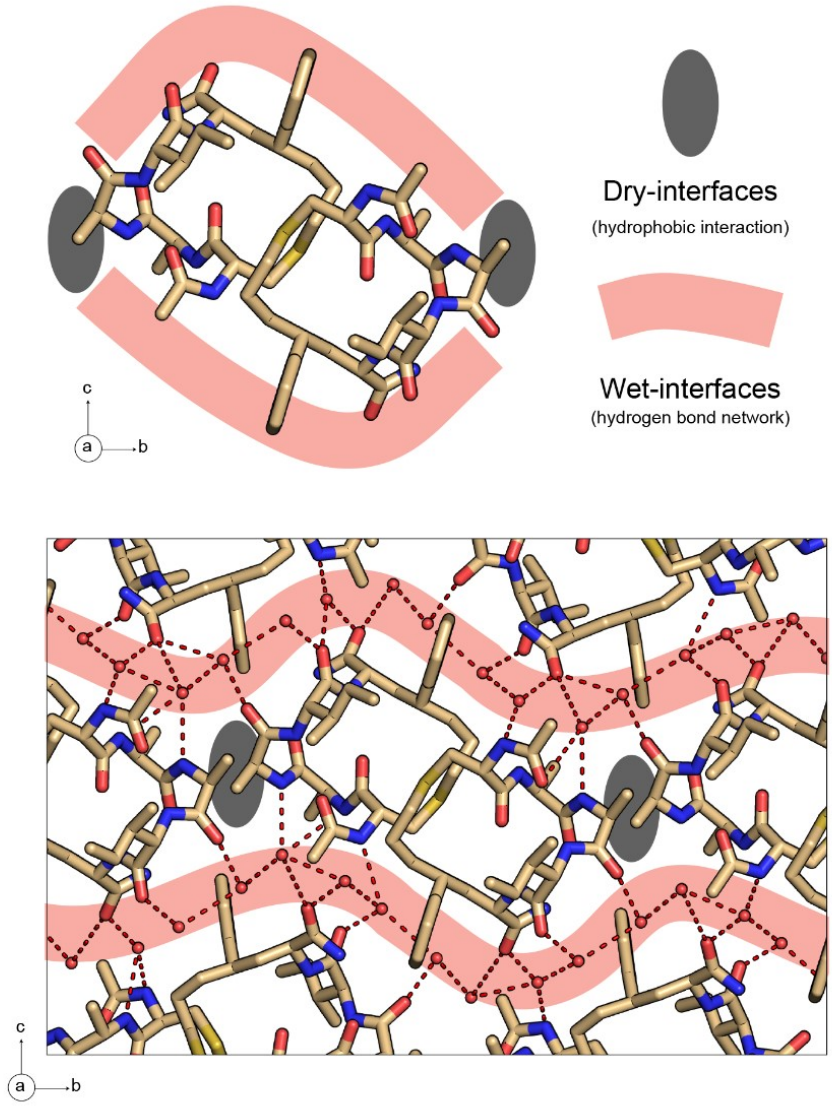


Figure S3. The dry-interface and wet-interface of **ClH^{AAla}** cuboid column in polymorph-**α**. The wet interface constitutes the major portion of the column interface, primarily formed by a hydrogen bond network between solvent water molecules and the peptide. The dry interface at the column's corners is relatively small and primarily stems from the hydrophobic interactions along the b-axis contributed by the methyl group of the third alanine residue's side chain.

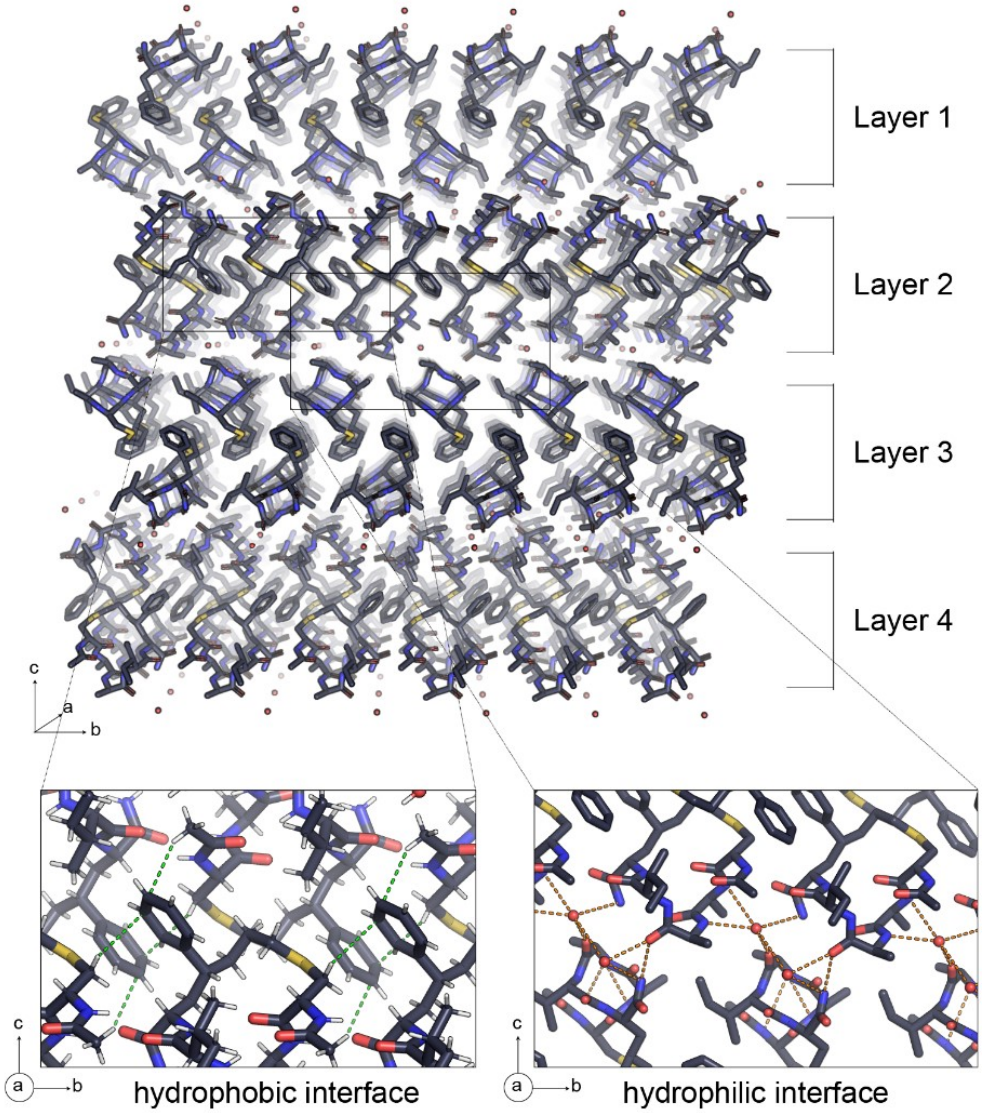


Figure S4. The crystal packing mode of **ClH^{AAla}** in polymorph-**β**. The helical columns stack into 2D layers through the zipper-type hydrophobic interaction along the a- and b- axis, and the layers further stack along the c-axis through hydrogen bonds networks. The magnified view of hydrophobic-interface and hydrophilic-interface were showed in bottom frames. The intramolecular C-H...π interactions formed between the benzene ring with the neighboring linker regions and acetyl groups were showed by green dashes. The hydrogen bonds between hydrophilic interface and solvent water molecule were showed by orange dashes.

4. DFT calculation

The DFT calculation was performed in Gaussian 09 program. Becke3LYP functional with dispersion correction was used to locate all the stationary points and frequency analysis was executed in the aqueous phase with 6-311G* basis set. The thermodynamics correction with temperature was also employed to discuss the Gibbs free energy in 1 M concentration. Specifically, high accuracy single point energy calculation was performed at M06-2X/def2-TZVPP level in aqueous phase and the ultrafine integrated grid was used and discussed in SI to validate the result based on the Becke3LYP level. The IRC calculation was executed to confirm the transition state. The wavefunction analysis with AIM was conducted by Multiwfn software to confirm the CH…π interaction. The 3D molecular graphs were presented by CYLview and VMD software.

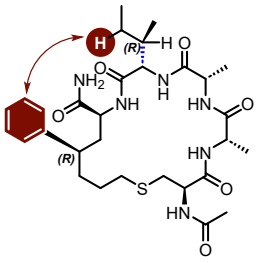
4.1 Benchmark calculation of ClH^{AAIa}

The simple benchmark calculation was employed to validate whether the calculated aqueous structure was consistent with the X-ray structure. We chose the **ClH^{AAIa}** X-ray structure as the standard and focused on the C…H distance to confirm that the functional and basis set was adequate (as following table).

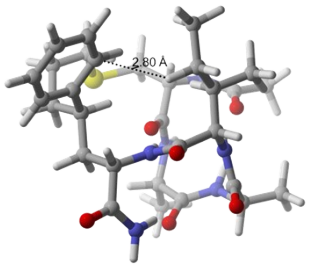
Distance of C…H in X-ray structure and calculated data

Crystal of isoleucine	2.88 Å (Distance of C…H)
B3LYP-D3(BJ)(SMD, H_2O)/6-311G*	2.80 Å
B3LYP(SMD, H_2O)/6-311G**	3.23 Å
B3LYP(SMD, H_2O)/6-31+G**	3.23 Å
B3LYP-D3(BJ)(SMD, H_2O)/6-31+G**	2.80 Å

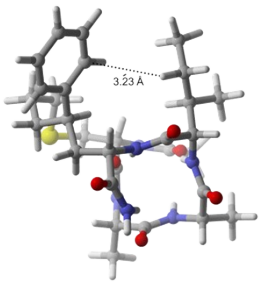
The combination with B3LYP-D3(BJ)/6-311G* and B3LYP-D3(BJ)/6-311+G** in aqueous phase provided adequate calculated structure with X-ray result (benchmark DFT calculation of ClH^{AAIa} is shown as following figure,), in which the C…H distances were all 2.80 Å that were in agreement with 2.88 Å in X-ray's. However, the C...H distance without dispersion correction was prolonged all to 3.23 Å, demonstrating the weak CH…π interaction lost. The effect of basis set considering the diffuse functions was subtle, underlying that the DFT study could be employed in high efficiency with simple 6-311G*. Ultimately, the B3LYP-D3(BJ) functional and 6-311G* basis set was used.



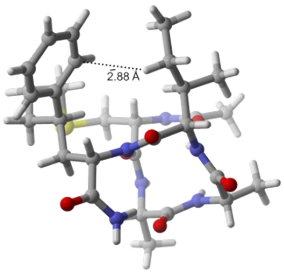
ClH^{AAla}



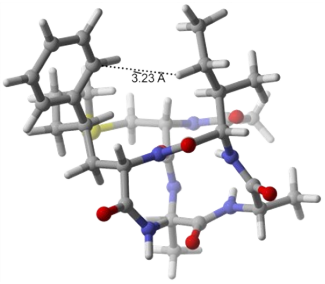
B3LYP-D3(BJ)(SMD, H_2O)/6-311G*



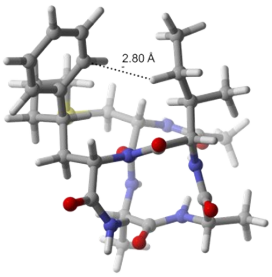
B3LYP(SMD, H_2O)/6-311G**



Crystal of ClH^{AAla}



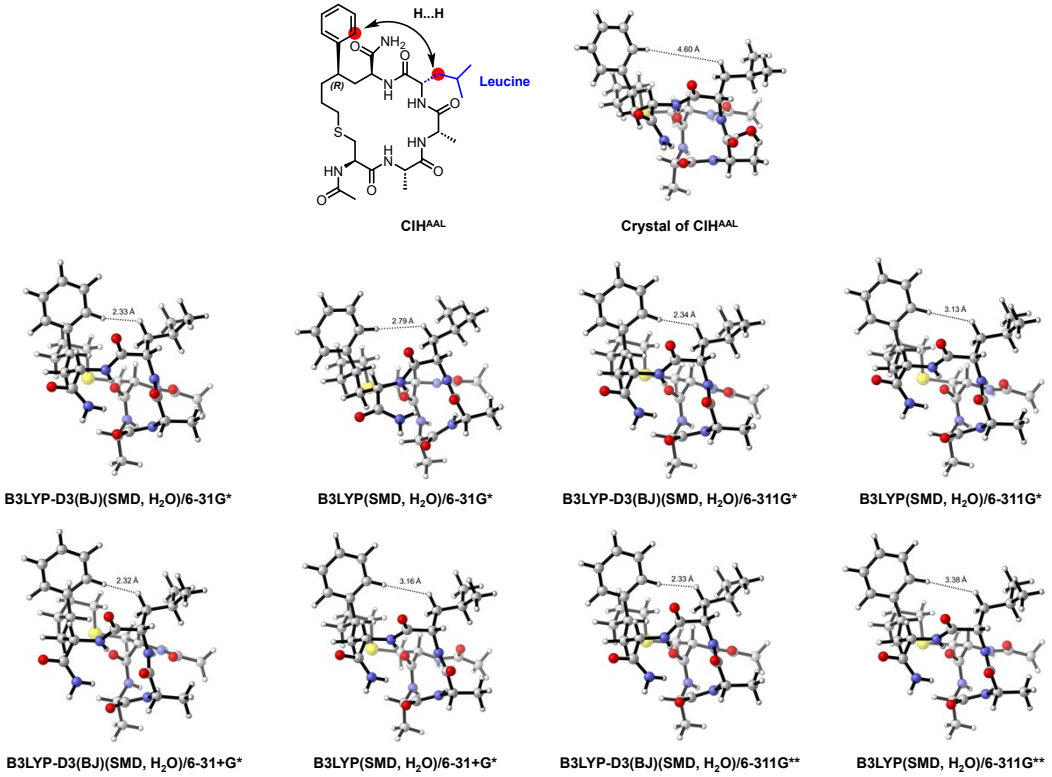
B3LYP(SMD, H_2O)/6-31+G**



B3LYP-D3(BJ)(SMD, H_2O)/6-31+G**

4.2 DFT analyses of CIH^{AAL}

For the leucine side chain in **CIH^{AAL}** case, it is vital to demonstrate that the error was induced by the dispersion correction compared with related X-ray structure. The H...H distance was 4.6 Å in X-ray structure but decreased to 2.3 Å in calculated one. The inferior distance offered imposed dispersion interaction, generating crucial Gibbs free energy gap error. The simulation of Leucine side chain case was distinct from previous examples (as following figure).



We found that once the DFT functional was corrected with dispersion, the H…H distance we focused on was evidently shorter than the crystal one, implying that the overestimated dispersion interaction in another conformation (as following table). The calculation without the dispersion correction provided the consistent result with experiment. Meanwhile, the screening of the combination with dispersion and basis set revealed that the basis set has subtle effect compared with dispersion correction.

DFT benchmark calculation for leucine case

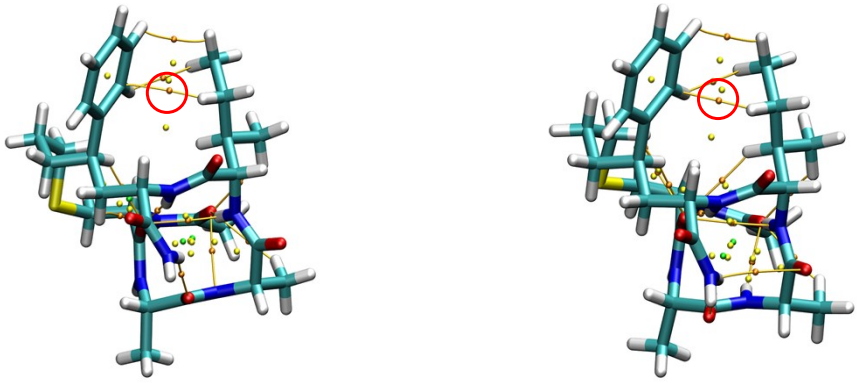
	ΔG/(kcal/mol)			*High accuracy* *ΔG*$^{\#}$/(kcal/mol)		
	L1	L2	L3	L1	L2	L3
B3LYP-D3(BJ)(SMD, H_2O)/6-31G*	0.0	2.6	0.6	0.0	1.5	0.1
B3LYP(SMD, H_2O)/6-31G*	0.0	2.9	1.3	0.0	2.9	0.8
B3LYP-D3(BJ)(SMD, H_2O)/6-31+G*	0.0	2.8	0.4	0.0	1.8	-0.2
B3LYP(SMD, H_2O)/6-31+G*	0.0	4.9	1.7	0.0	3.8	1.3
B3LYP-D3(BJ)(SMD, H_2O)/6-311G*	0.0	1.7	0.4	0.0	0.4	-0.1
B3LYP(SMD, H_2O)/6-311G*	0.0	4.3	2.6	0.0	4.0	1.7

B3LYP-D3(BJ)(SMD, H_2O)/6-311G**	0.0	1.9	0.5	0.0	0.6	-0.2
B3LYP(SMD, H_2O)/6-311G**	0.0	3.4	2.4	0.0	2.9	1.0

#: High accuracy Gibbs energy was obtained with M06-2X(SMD, H_2O)/def2-TZVPP single point energy level

4.3 AIM analyses

Atoms in molecules analyses for X-ray structure conformer-**1** and calculated **iL1** structure were executed in **Figure S5**. The bond critical point (CP) at conformer **1** revealed that there existed a weak CH…π interaction between H and C, where the electron density (ρ_b) was 0.0055 au and the Laplacian values ($\Delta^2\rho_b$) was 0.01634 au. The relevant CH…π interaction was also present in **iL1** simulation with 0.0067 au ρ_b and 0.02098 au $\Delta^2\rho_b$ values.



CH…π interaction in X-ray structure

CH…π interaction in calculated iL1 structure

Figure S5. AIM analyses of CH…π interaction in conformer-**1** and calculated **iL1**.

4.4 Thermodynamic correction with temperature elevation

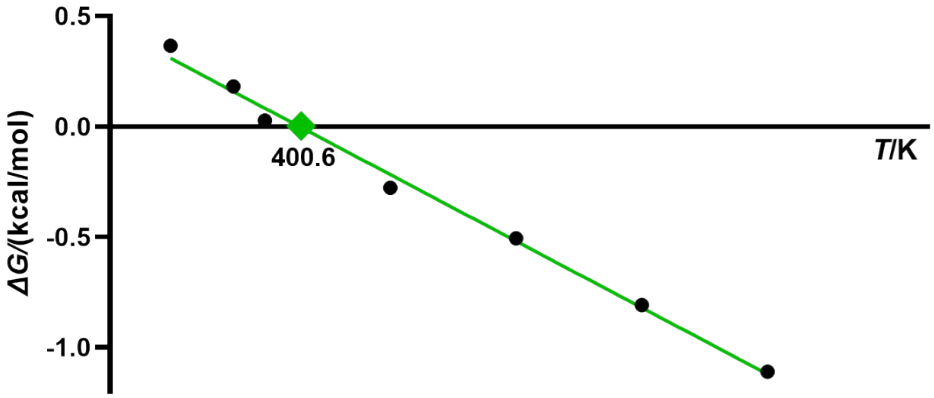


Figure S6. Linear regression of Gibbs energy with respective to temperature

T/K	298	348	373	473	573	673	773
ΔG/(kcal/mol)	0.4	0.2	0.0	-0.3	-0.5	-0.8	-1.1

The calculated critical temperature was 373 K, nonetheless the linear regression offered that the critical temperature was 400 K. The tendency of Gibbs free energy with respect to temperature was diminished, even the adequate Gibbs energy prediction was not acceptable due to the calculation model used.

5. Crystal data

Table S1. Crystal data for polymorph-**α** and polymorph-**β** of **ClH^{AAla}**

	Polymorph-**α**	Polymorph-**β**
CCDC	2292337	2292338
Formula	C_{30} H_{46} N_6 O_6 S	C_{30} H_{46} N_6 O_6 S
Formula Weight	618.32	618.32
Crystal System	orthorhombic	tetragonal
Temperature / K	100	100
Wavelength/ Å	1.54184	1.54184
a / Å	9.8076(2)	10.30099(6)
b / Å	16.1235(3)	10.30099(6)
c / Å	22.4399(4)	63.8033(6)
α / °	90	90
β / °	90	90
γ / °	90	90
Space Group	$P2_12_12_1$ #19	P 4_12_12 #92
Z value	4	8
D calc / g cm $^{-3}$	1.293	1.251
Reflections collected	19530	41777
Independent reflections	7110 [Rint = 0.0473, Rsigma = 0.0442]	6970 [Rint = 0.0345, Rsigma = 0.0225]
F (000)	1488	2736
2Θ range for data collection/°	6.75 to 156.338	5.54 to 154.038
Goodness-of-fit on F^2	0.995	1.067
Final R indexes [I>=2σ (I)]	R1 = 0.0522, wR2 = 0.1406	R1 = 0.0367, wR2 = 0.0973
Final R indexes [all data]	R1 = 0.0551, wR2 = 0.1427	R1 = 0.0379, wR2 = 0.0980
Largest diff. peak and hole e.Å^{-3}	0.90 and -0.61	0.53 and -0.26

Table S2. Crystal data for **ClH^{AAV}** and **ClH^{AAL}**

	ClH^{AAV}	**ClH^{AAL}**
CCDC	2292339	2292343
Formula	C_{29} H_{44} N_6 O_6 S	C_{30} H_{46} N_6 O_6 S
Formula Weight	604.30	618.32
Crystal System	orthorhombic	tetragonal
Temperature / K	100	100
Wavelength/ Å	1.54184	1.54184
a / Å	9.64330(10)	10.47390(10)
b / Å	16.0251(2)	10.47390(10)
c / Å	22.6439(3)	61.7275(8)
α / °	90	90
β / °	90	90
γ / °	90	90
Space Group	P212121 #19	P41212 #92
Z value	4	8
D calc / g cm −3	1.256	1.214
Reflections collected	20927	40369
Independent reflections	7023 [Rint = 0.0418, Rsigma = 0.0432]	7029 [Rint = 0.0667, Rsigma = 0.0372]
F (000)	1396	2656
2Θ range for data collection/°	6.758 to 153.064	5.726 to 154.154
Goodness-of-fit on F^2	1.033	1.037
Final R indexes [I>=2σ (I)]	R1 = 0.0394, wR2 = 0.1031	R1 = 0.0457, wR2 = 0.1075
Final R indexes [all data]	R1 = 0.0412, wR2 = 0.1043	R1 = 0.0529, wR2 = 0.1107
Largest diff. peak and hole e.Å^{-3}	0.28 and -0.52	0.28 and -0.28

6. Crystal structures of the ClH^{AAV} and ClH^{AAL}

6.1 X-ray structure superpositions of ClH^{AAIa} (conformer-1) / ClH^{AAV}, and ClH^{AAIa} (conformer-2) / ClH^{AAL}

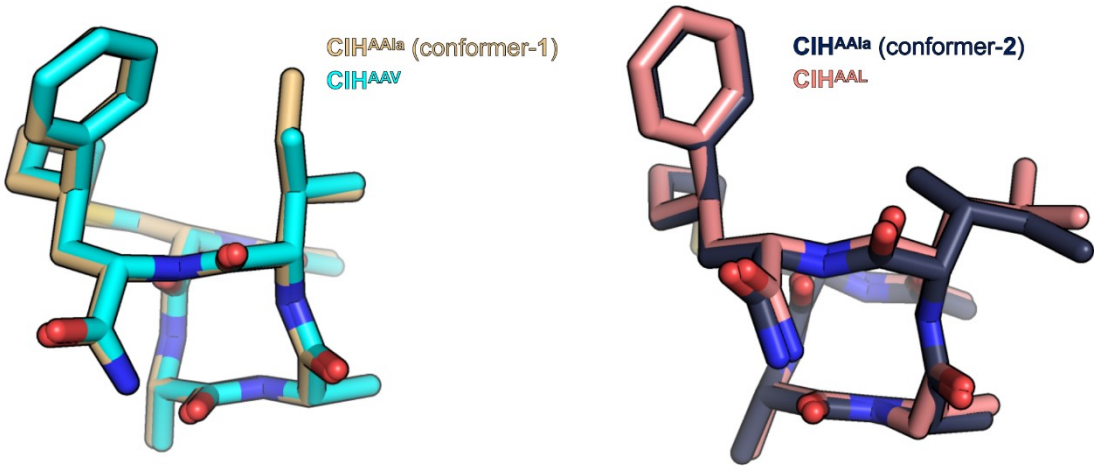


Figure S7. Superpositions of the single molecule X-ray structures of **ClH^{AAIa}** (conformer-**1**) / **ClH^{AAV}**, and **ClH^{AAIa}** (conformer-**2**) / **ClH^{AAL}**.

6.2 Crystal packing of ClH^{AAV} and ClH^{AAL}

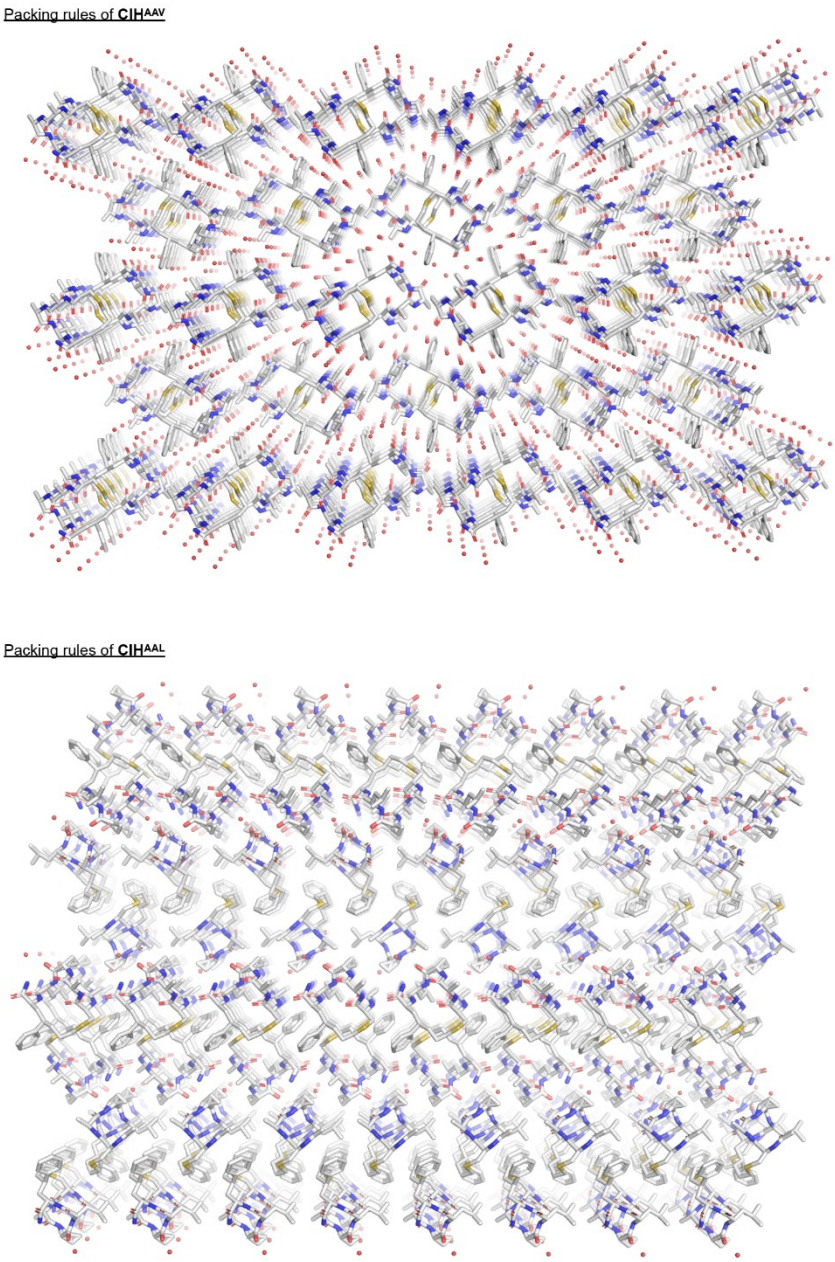


Figure S8. The crystal packing mode of **ClH^{AAV}** and **ClH^{AAL}**. The **ClH^{AAV}** molecules packed as **ClH^{AAIa}** in polymorph-**α**, and The **ClH^{AAL}** molecules packed as **ClH^{AAIa}** in polymorph-**β**.

6.3 Temperature-dependent CD of ClH^{AAV} and ClH^{AAL}

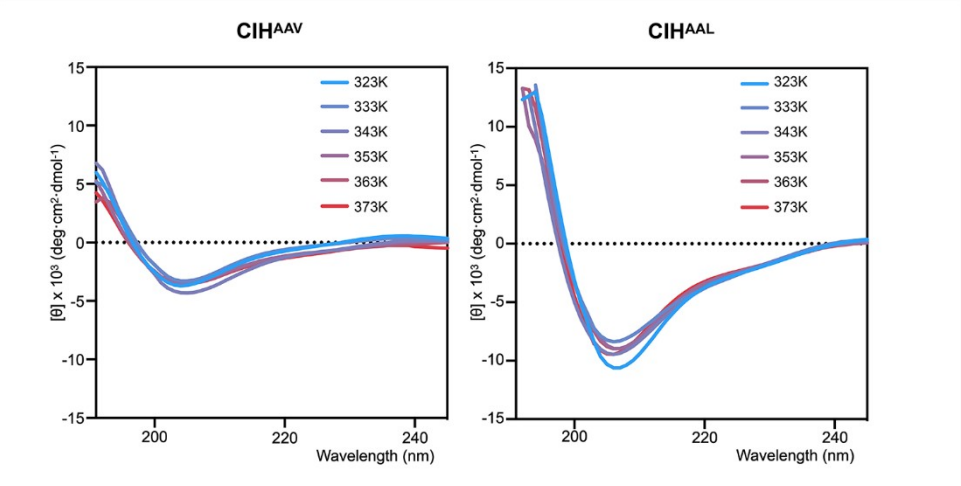


Figure S9. CD spectra of **CIH^{AAV}** and **CIH^{AAL}** in ddH_2O at variable temperatures.

7. Cartesian Coordinates and Energy of Stationary Points

7.1 Energy data summary

Structure	CH	CG	E	U	H	G	SP
iL1	0.804996	0.679329	-2349.097395	-2349.051851	-2349.050907	-2349.176574	-2349.14046
iL2	0.80548	0.678335	-2349.095455	-2349.049789	-2349.048845	-2349.17599	-2349.138581
TS	0.804565	0.681456	-2349.088688	-2349.044271	-2349.043327	-2349.166437	-2349.129512
V1	0.775141	0.651885	-2309.799095	-2309.754842	-2309.753897	-2309.877153	-2309.83275
V2	0.775328	0.652056	-2309.797419	-2309.753127	-2309.752183	-2309.875455	-2309.830837
V3	0.775177	0.652473	-2309.796492	-2309.752346	-2309.751402	-2309.874107	-2309.830209
L1	0.802628	0.671421	-2348.88392	-2348.837468	-2348.836524	-2348.96773	-2349.133275
L2	0.802917	0.674096	-2348.879149	-2348.832936	-2348.831992	-2348.960813	-2349.129581
L3	0.803024	0.675322	-2348.882877	-2348.836851	-2348.835907	-2348.963608	-2349.134406

CH = Thermal correction to Enthalpy

CG = Thermal correction to Gibbs Free Energy

E = Sum of electronic and zero-point Energies

U = Sum of electronic and thermal Energies

H = Sum of electronic and thermal Enthalpies

G = Sum of electronic and thermal Free Energies

SP = Single point energy at M06-2X (SMD, H_2O)/def2-TZVPP level

7.2 Coordinates

iL1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.010467	4.138001	-1.127066
2	8	0	-1.729145	-3.331267	0.897796
3	8	0	2.019310	-1.693830	-2.619220
4	8	0	0.692653	0.824891	-0.547650
5	8	0	-2.861685	-3.212711	-2.893092
6	8	0	1.640119	-4.004924	0.179368
7	8	0	3.103985	0.526984	1.699253
8	7	0	-0.949294	-1.584012	-0.318757
9	1	0	-0.250078	-0.853167	-0.403695
10	7	0	2.658937	1.568214	-1.359606
11	1	0	3.434414	2.208757	-1.262362
12	7	0	3.388843	-1.123924	-0.905821
13	1	0	3.749611	-0.366422	-0.340191
14	7	0	1.491013	-1.924274	1.061997
15	1	0	1.900645	-0.999447	1.138980
16	7	0	3.011012	2.738807	1.256646
17	1	0	3.462289	3.639441	1.330956
18	6	0	-0.899940	-2.431050	0.724109
19	7	0	-0.614372	-3.168437	-2.591536
20	1	0	-0.476516	-3.846639	-3.326544
21	1	0	0.204442	-2.721775	-2.200027
22	6	0	2.640779	-0.834185	-1.984464
23	6	0	-2.027056	-1.642332	-1.291008
24	1	0	-2.951521	-1.878149	-0.762273
25	6	0	0.227211	-2.193649	1.735258
26	1	0	0.314437	-3.129126	2.291883
27	6	0	2.093185	-2.862138	0.313306
28	6	0	-1.861313	-2.756585	-2.325376
29	6	0	1.650261	1.599028	-0.476016
30	6	0	-3.768792	0.621628	-0.242651
31	6	0	3.620226	1.653132	1.769636
32	6	0	2.646233	0.620312	-2.465759
33	1	0	1.714008	0.740904	-3.020146
34	6	0	-0.101389	-1.047714	2.720244
35	1	0	-0.047351	-0.109248	2.154428
36	6	0	-2.182736	-0.295473	-2.008955

37	1	0	-1.253834	-0.064305	-2.539151
38	1	0	-2.962251	-0.406961	-2.765930
39	6	0	-2.515179	0.864568	-1.056855
40	1	0	-1.687808	0.947406	-0.353257
41	6	0	1.702049	2.667077	0.616554
42	1	0	0.953028	2.364032	1.349217
43	6	0	-3.737651	0.763523	1.147073
44	1	0	-2.804791	1.035426	1.628436
45	6	0	-4.982128	0.273938	-0.848347
46	1	0	-5.032311	0.157850	-1.925863
47	6	0	3.420117	-2.469242	-0.347540
48	1	0	3.552103	-3.173899	-1.167660
49	6	0	3.832779	0.874547	-3.390250
50	1	0	3.767012	1.876803	-3.818223
51	1	0	3.828181	0.150561	-4.205993
52	1	0	4.777865	0.784352	-2.850175
53	6	0	4.573113	-2.603722	0.643734
54	1	0	5.526472	-2.450141	0.134482
55	1	0	4.572024	-3.603071	1.081715
56	1	0	4.484198	-1.871431	1.448278
57	6	0	-6.128194	0.068441	-0.083630
58	1	0	-7.058680	-0.204808	-0.570522
59	6	0	1.364053	4.064168	0.067222
60	1	0	2.222822	4.453997	-0.483352
61	1	0	1.169645	4.738296	0.902854
62	6	0	-1.525778	-1.183428	3.279676
63	1	0	-2.239598	-1.212187	2.453483
64	1	0	-1.615900	-2.145435	3.797816
65	6	0	-6.082394	0.210489	1.304022
66	1	0	-6.974703	0.047804	1.899106
67	6	0	-1.456586	3.690759	-0.078095
68	1	0	-1.201134	2.809786	0.509369
69	1	0	-1.645589	4.515115	0.611257
70	6	0	-2.684013	3.434573	-0.954598
71	1	0	-3.548977	3.351809	-0.288813
72	1	0	-2.869318	4.312586	-1.582436
73	6	0	-2.595887	2.187496	-1.841855
74	1	0	-1.716842	2.259191	-2.489192
75	1	0	-3.468515	2.158142	-2.502731
76	6	0	-1.924351	-0.048694	4.221995
77	1	0	-1.771325	0.927578	3.751401
78	1	0	-1.351310	-0.062069	5.151777
79	1	0	-2.981763	-0.124600	4.487996
80	6	0	0.943253	-1.013783	3.839801

81	1	0	0.854450	-1.904421	4.470167
82	1	0	0.808338	-0.136715	4.474953
83	1	0	1.960934	-0.974632	3.451804
84	6	0	4.962415	1.861238	2.412699
85	1	0	4.920064	1.493622	3.440084
86	1	0	5.283123	2.902789	2.416553
87	1	0	5.701583	1.260283	1.877916
88	6	0	-4.881820	0.560806	1.918181
89	1	0	-4.831787	0.673972	2.995895

##

iL2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.487499	4.326534	0.314042
2	8	0	-0.486569	1.019701	0.431250
3	8	0	-1.864379	-3.777901	0.741789
4	8	0	3.039930	-2.603877	3.264074
5	8	0	1.742831	-3.371850	-0.613419
6	8	0	-1.840933	-1.036730	3.036483
7	7	0	0.977841	-1.548665	0.505055
8	1	0	0.256270	-0.838501	0.568966
9	7	0	-1.554791	-1.956759	-0.573543
10	1	0	-1.897797	-1.046629	-0.861096
11	8	0	-3.069860	0.530533	-1.585418
12	7	0	-2.294815	2.046848	1.300755
13	1	0	-3.030268	2.728735	1.175917
14	7	0	-2.875703	2.775013	-1.432031
15	1	0	-3.315805	3.675682	-1.555270
16	7	0	-3.240959	-0.588231	1.311573
17	1	0	-3.549170	0.105105	0.643503
18	7	0	0.780645	-2.588677	3.065481
19	1	0	0.674002	-3.059954	3.951933
20	6	0	-2.209341	-2.647700	0.379609
21	6	0	3.977666	0.386235	-0.256096
22	6	0	-1.390057	1.852079	0.327689
23	6	0	2.016353	-2.276370	2.650906
24	6	0	-0.416471	-2.559153	-1.249763
25	1	0	-0.629521	-3.622587	-1.352570
26	6	0	0.865271	-2.522766	-0.414092

27	6	0	2.792035	0.896606	0.538806
28	1	0	1.930468	0.901187	-0.129615
29	6	0	2.139579	-1.446795	1.371230
30	1	0	2.992973	-1.862840	0.836522
31	6	0	-1.510072	2.730210	-0.920350
32	1	0	-0.862804	2.267490	-1.664411
33	6	0	3.060445	3.389887	-0.097934
34	1	0	3.807829	3.111066	-0.847286
35	1	0	3.390164	4.349353	0.314382
36	6	0	-2.404967	-0.221372	2.297988
37	6	0	2.429719	0.012678	1.741296
38	1	0	3.235341	0.019178	2.478243
39	1	0	1.549661	0.435102	2.234149
40	6	0	-1.048197	4.170968	-0.654115
41	1	0	-1.802136	4.692830	-0.060723
42	1	0	-0.946707	4.695981	-1.605240
43	6	0	5.134504	-0.094385	0.369609
44	1	0	5.184917	-0.139825	1.451945
45	6	0	3.952565	0.427382	-1.654182
46	1	0	3.067288	0.802429	-2.155784
47	6	0	-3.562703	1.659179	-1.741563
48	6	0	3.031051	2.343306	1.021383
49	1	0	2.246938	2.601740	1.738839
50	1	0	3.977821	2.378555	1.570195
51	6	0	-2.230738	1.280986	2.537329
52	1	0	-1.234061	1.391166	2.968403
53	6	0	5.044313	-0.000040	-2.408929
54	1	0	4.999877	0.041109	-3.492336
55	6	0	1.729462	3.583724	-0.825534
56	1	0	1.342090	2.633992	-1.192742
57	1	0	1.852919	4.252871	-1.678392
58	6	0	6.186849	-0.481391	-1.773005
59	1	0	7.037022	-0.819410	-2.355865
60	6	0	-0.181976	-1.988217	-2.665016
61	1	0	0.612950	-2.615208	-3.083495
62	6	0	6.227155	-0.526292	-0.379500
63	1	0	7.111448	-0.900309	0.126066
64	6	0	-3.453468	-1.991647	0.988303
65	1	0	-3.632306	-2.529879	1.918347
66	6	0	0.305748	-0.538368	-2.661475
67	1	0	-0.445730	0.139105	-2.254210
68	1	0	0.522605	-0.214823	-3.682962
69	1	0	1.217401	-0.420338	-2.075887
70	6	0	-4.961160	1.838915	-2.262622

71	1	0	-5.045954	1.330456	-3.225144
72	1	0	-5.247756	2.883846	-2.381032
73	1	0	-5.654417	1.353248	-1.571731
74	6	0	-3.279115	1.784560	3.525378
75	1	0	-3.087267	2.829353	3.777362
76	1	0	-3.236506	1.195368	4.442059
77	1	0	-4.284418	1.703030	3.106036
78	6	0	-1.426718	-2.149445	-3.552787
79	1	0	-2.206921	-1.460763	-3.213329
80	1	0	-1.151511	-1.818968	-4.560032
81	6	0	-1.985814	-3.569224	-3.620348
82	1	0	-1.211620	-4.288784	-3.905207
83	1	0	-2.787293	-3.634723	-4.361262
84	1	0	-2.402905	-3.892155	-2.662694
85	6	0	-4.655369	-2.149074	0.060562
86	1	0	-5.561704	-1.799555	0.558887
87	1	0	-4.787780	-3.200510	-0.199504
88	1	0	-4.518701	-1.577300	-0.858619
89	1	0	-0.051891	-2.222036	2.624234

##

TS

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.601793	4.189691	0.526173
2	8	0	-0.859881	0.782690	0.016353
3	8	0	-1.254448	-4.464323	-0.153117
4	8	0	2.985938	-1.273759	4.050804
5	8	0	2.398176	-2.998474	0.449266
6	8	0	-1.902053	-1.981367	2.503055
7	7	0	1.227963	-1.114413	0.893948
8	1	0	0.458072	-0.502208	0.642966
9	7	0	-0.845421	-2.290481	-0.694741
10	1	0	-1.202922	-1.345627	-0.660659
11	8	0	-3.466539	0.105875	-1.871277
12	7	0	-2.795093	1.220727	1.098146
13	1	0	-3.667036	1.732574	1.097600
14	7	0	-3.668009	2.307459	-1.426225
15	1	0	-4.259773	3.126141	-1.431795
16	7	0	-3.136407	-1.527596	0.665317

17	1	0	-3.477473	-0.823276	0.019369
18	7	0	0.843792	-1.830797	3.561330
19	1	0	0.708998	-2.213993	4.485555
20	6	0	-1.617485	-3.286220	-0.221280
21	6	0	3.406525	1.213568	-0.175890
22	6	0	-1.926363	1.402209	0.093459
23	6	0	2.033752	-1.298468	3.259160
24	6	0	0.556716	-2.490225	-1.030194
25	1	0	0.663692	-3.547299	-1.262409
26	6	0	1.463887	-2.235541	0.181701
27	6	0	2.280034	1.663904	0.729664
28	1	0	1.351490	1.514416	0.180811
29	6	0	2.190935	-0.655994	1.881715
30	1	0	3.181071	-0.956006	1.538405
31	6	0	-2.291319	2.446753	-0.964303
32	1	0	-1.607525	2.264265	-1.793840
33	6	0	2.094898	4.095948	-0.128537
34	1	0	2.824087	3.928079	-0.927815
35	1	0	2.225590	5.134048	0.193255
36	6	0	-2.486683	-1.161187	1.783177
37	6	0	2.156370	0.870720	2.041739
38	1	0	2.958066	1.140003	2.732940
39	1	0	1.216591	1.161950	2.521648
40	6	0	-2.111407	3.883278	-0.445739
41	1	0	-2.930510	4.130389	0.232950
42	1	0	-2.157057	4.572636	-1.290495
43	6	0	4.676154	0.897946	0.321432
44	1	0	4.868391	0.961042	1.387296
45	6	0	3.196629	1.129869	-1.556198
46	1	0	2.218630	1.375371	-1.957046
47	6	0	-4.160120	1.134453	-1.870304
48	6	0	2.393985	3.168011	1.054486
49	1	0	1.709621	3.396351	1.877289
50	1	0	3.401597	3.377199	1.428114
51	6	0	-2.514909	0.309463	2.197985
52	1	0	-1.510498	0.518366	2.572491
53	6	0	4.216084	0.728664	-2.417996
54	1	0	4.025190	0.660910	-3.483861
55	6	0	0.704847	3.928447	-0.743632
56	1	0	0.580704	2.932045	-1.165889
57	1	0	0.553648	4.656649	-1.542344
58	6	0	5.471806	0.403469	-1.908251
59	1	0	6.266179	0.082405	-2.573434
60	6	0	1.044776	-1.633311	-2.249016

61	1	0	1.737559	-0.883934	-1.860962
62	6	0	5.698817	0.493668	-0.534700
63	1	0	6.673358	0.243842	-0.128226
64	6	0	-3.044620	-2.904017	0.193249
65	1	0	-3.284447	-3.566188	1.024937
66	6	0	-0.078079	-0.877220	-2.962729
67	1	0	1.157352	-3.282770	-3.634749
68	1	0	0.347458	-0.314576	-3.797780
69	1	0	-0.576859	-0.159073	-2.312536
70	6	0	-5.589917	1.126047	-2.333594
71	1	0	-5.632871	0.697731	-3.336741
72	1	0	-6.045069	2.116270	-2.343398
73	1	0	-6.166056	0.474949	-1.671455
74	6	0	-3.530440	0.513506	3.320025
75	1	0	-3.476996	1.537880	3.692781
76	1	0	-3.313054	-0.166947	4.143110
77	1	0	-4.545648	0.319274	2.965641
78	6	0	1.820920	-2.494301	-3.258566
79	1	0	-0.833602	-1.555066	-3.368687
80	1	0	2.059575	-1.858063	-4.117468
81	6	0	3.114748	-3.110844	-2.730311
82	1	0	3.781483	-2.340108	-2.331663
83	1	0	3.647064	-3.632716	-3.530739
84	1	0	2.931342	-3.829904	-1.930621
85	6	0	-4.018531	-3.153715	-0.954992
86	1	0	-5.044208	-2.983869	-0.621736
87	1	0	-3.930857	-4.188493	-1.288348
88	1	0	-3.813205	-2.495295	-1.799724
89	1	0	0.048191	-1.817124	2.934044

##

V1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.054640	4.156747	-0.980258
2	8	0	0.643621	0.819239	-0.443642
3	8	0	1.909467	-1.699157	-2.594222
4	8	0	-1.818579	-3.342515	0.914497
5	8	0	-3.046317	-3.059497	-2.840644

6	8	0	3.092829	0.488655	1.723697
7	8	0	1.560376	-4.021591	0.156521
8	7	0	-1.037026	-1.565544	-0.257016
9	1	0	-0.329224	-0.841946	-0.331766
10	7	0	1.420299	-1.961385	1.086168
11	1	0	1.828922	-1.037835	1.179670
12	7	0	2.580066	1.560029	-1.326771
13	1	0	3.361201	2.197061	-1.254530
14	7	0	3.301173	-1.132295	-0.898464
15	1	0	3.662190	-0.377158	-0.329901
16	7	0	3.028577	2.703280	1.292236
17	1	0	3.494815	3.596679	1.361651
18	7	0	-0.791591	-3.061873	-2.594694
19	1	0	-0.681185	-3.712807	-3.358335
20	1	0	0.042719	-2.649178	-2.199182
21	6	0	-0.979821	-2.448418	0.755875
22	6	0	-2.024807	-2.642849	-2.280348
23	6	0	2.535077	-0.839511	-1.963492
24	6	0	1.604912	1.591083	-0.406311
25	6	0	2.017484	-2.883409	0.312243
26	6	0	1.702181	2.655354	0.686919
27	1	0	0.969067	2.361678	1.439199
28	6	0	-2.143975	-1.569098	-1.197796
29	1	0	-3.054701	-1.813019	-0.649503
30	6	0	3.629532	1.605816	1.789743
31	6	0	0.163035	-2.256599	1.759909
32	1	0	0.257365	-3.213757	2.276904
33	6	0	2.522762	0.617501	-2.435832
34	1	0	1.569412	0.741958	-2.952397
35	6	0	-3.589090	0.716893	1.437564
36	1	0	-2.609120	0.930652	1.851267
37	6	0	3.341181	-2.480965	-0.348917
38	1	0	3.472284	-3.179651	-1.174208
39	6	0	1.371017	4.058607	0.151077
40	1	0	2.212477	4.430334	-0.437280
41	1	0	1.227049	4.736918	0.993482
42	6	0	-3.745452	0.674248	0.050173
43	6	0	3.671506	0.875028	-3.405991
44	1	0	3.590953	1.880039	-3.824807
45	1	0	3.631946	0.156032	-4.225087
46	1	0	4.637265	0.779237	-2.904858
47	6	0	-2.731944	3.506473	-0.676781
48	1	0	-2.945462	4.401488	-1.270571
49	1	0	-3.558072	3.411446	0.035315

50	6	0	-0.171562	-1.160621	2.795392
51	1	0	-0.206431	-0.204376	2.259919
52	6	0	-2.307130	-0.194392	-1.859284
53	1	0	-3.131730	-0.264796	-2.572352
54	1	0	-1.404887	0.037468	-2.433533
55	6	0	4.498874	-2.617878	0.636339
56	1	0	5.449192	-2.456456	0.123762
57	1	0	4.504080	-3.620682	1.066367
58	1	0	4.410883	-1.892138	1.446688
59	6	0	-1.455914	3.730945	0.136025
60	1	0	-1.190270	2.839776	0.703207
61	1	0	-1.591717	4.553013	0.840517
62	6	0	-1.534340	-1.411789	3.444363
63	1	0	-2.349717	-1.426714	2.721856
64	1	0	-1.751780	-0.623501	4.169211
65	1	0	-1.538165	-2.367883	3.976870
66	6	0	-2.561583	0.941769	-0.854489
67	1	0	-1.680958	1.009592	-0.217971
68	6	0	-2.705224	2.281936	-1.598813
69	1	0	-1.878318	2.373132	-2.309442
70	1	0	-3.624558	2.264909	-2.193290
71	6	0	4.986327	1.789421	2.409430
72	1	0	4.954217	1.424523	3.438193
73	1	0	5.326447	2.824878	2.406249
74	1	0	5.705154	1.173747	1.863843
75	6	0	-5.015655	0.394050	-0.468093
76	1	0	-5.161414	0.354971	-1.542756
77	6	0	-4.667092	0.483741	2.291331
78	1	0	-4.519729	0.515235	3.365801
79	6	0	0.914598	-1.087997	3.872145
80	1	0	0.988477	-2.041096	4.405353
81	1	0	0.666002	-0.313818	4.602904
82	1	0	1.896093	-0.849857	3.462841
83	6	0	-6.095903	0.159270	0.379134
84	1	0	-7.072105	-0.060633	-0.040585
85	6	0	-5.925587	0.203132	1.763830
86	1	0	-6.766532	0.017591	2.423483

##

V2

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	16	0	-0.049186	4.182223	-0.847866
2	8	0	0.651969	0.856687	-0.543506
3	8	0	1.855267	-1.747027	-2.680397
4	8	0	-2.110811	-2.894795	1.310087
5	8	0	-3.142198	-2.817288	-2.873162
6	8	0	3.214554	0.425153	1.616357
7	8	0	1.408587	-4.029030	0.098575
8	7	0	-1.067309	-1.553163	-0.199002
9	1	0	-0.258500	-0.969737	-0.385584
10	7	0	1.364534	-1.986493	1.081979
11	1	0	1.827756	-1.093053	1.205237
12	7	0	2.618958	1.506136	-1.434376
13	1	0	3.445636	2.080232	-1.342785
14	7	0	3.230711	-1.202976	-0.962982
15	1	0	3.589278	-0.456499	-0.381219
16	7	0	3.186746	2.632892	1.136441
17	1	0	3.686022	3.511041	1.152928
18	7	0	-0.914498	-3.052527	-2.526388
19	1	0	-0.829873	-3.666035	-3.323720
20	1	0	-0.063316	-2.727387	-2.090591
21	6	0	-1.112940	-2.263613	0.941515
22	6	0	-2.114651	-2.525605	-2.248498
23	6	0	2.490603	-0.899032	-2.044217
24	6	0	1.653553	1.575101	-0.503818
25	6	0	1.911361	-2.913353	0.270751
26	6	0	1.827912	2.614934	0.604664
27	1	0	1.139257	2.317810	1.393116
28	6	0	-2.194518	-1.500780	-1.115876
29	1	0	-3.087831	-1.764962	-0.550844
30	6	0	3.784031	1.528706	1.623698
31	6	0	0.145688	-2.289006	1.817149
32	1	0	0.212972	-3.328474	2.142611
33	6	0	2.524928	0.553077	-2.530712
34	1	0	1.575000	0.704048	-3.045951
35	6	0	-3.896039	0.366728	1.499296
36	1	0	-2.945894	0.427413	2.017004
37	6	0	3.234122	-2.551582	-0.414281
38	1	0	3.324168	-3.250940	-1.244084
39	6	0	1.482352	4.034372	0.128653
40	1	0	2.269786	4.401178	-0.533210
41	1	0	1.436659	4.696067	0.995152
42	6	0	-3.945215	0.626027	0.127070

43	6	0	3.678024	0.757775	-3.508360
44	1	0	3.631413	1.759423	-3.940063
45	1	0	3.610263	0.029773	-4.317536
46	1	0	4.641864	0.634699	-3.009281
47	6	0	-2.685744	3.520301	-0.298305
48	1	0	-2.952140	4.454722	-0.803257
49	1	0	-3.433352	3.376623	0.489292
50	6	0	-0.031585	-1.424350	3.083404
51	1	0	-0.982166	-1.758347	3.510172
52	6	0	-2.368673	-0.096690	-1.707929
53	1	0	-3.171661	-0.139942	-2.446915
54	1	0	-1.454488	0.183541	-2.239260
55	6	0	4.406599	-2.736518	0.545879
56	1	0	5.350627	-2.609555	0.012453
57	1	0	4.382505	-3.740981	0.971647
58	1	0	4.365902	-2.012271	1.360998
59	6	0	-1.326667	3.684643	0.383295
60	1	0	-1.011473	2.754089	0.852801
61	1	0	-1.374313	4.455339	1.154132
62	6	0	1.079297	-1.715098	4.094355
63	1	0	1.150201	-2.783596	4.315388
64	1	0	0.886560	-1.187696	5.032399
65	1	0	2.050960	-1.379284	3.722241
66	6	0	-2.685193	0.968213	-0.644356
67	1	0	-1.857298	0.969246	0.065302
68	6	0	-2.760675	2.360285	-1.297874
69	1	0	-1.945877	2.450983	-2.021685
70	1	0	-3.689182	2.438530	-1.871088
71	6	0	5.181868	1.685274	2.153883
72	1	0	5.213802	1.306546	3.177386
73	1	0	5.536810	2.715679	2.139669
74	1	0	5.852818	1.067100	1.552550
75	6	0	-5.183843	0.532246	-0.520506
76	1	0	-5.248177	0.721596	-1.587060
77	6	0	-5.046992	0.025379	2.209969
78	1	0	-4.982866	-0.174094	3.274632
79	6	0	-0.129966	0.075380	2.797015
80	1	0	0.835222	0.483220	2.495859
81	1	0	-0.442747	0.606942	3.699460
82	1	0	-0.850165	0.300346	2.010337
83	6	0	-6.336124	0.192221	0.183395
84	1	0	-7.285337	0.123860	-0.337965
85	6	0	-6.272394	-0.063247	1.553978
86	1	0	-7.169495	-0.330191	2.102414

##

V3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.112885	4.161978	0.928811
2	8	0	-0.756026	0.836405	0.528273
3	8	0	-2.109390	-1.860262	2.510753
4	8	0	2.049337	-3.186789	-0.895698
5	8	0	2.917585	-2.770099	3.036482
6	8	0	-3.190879	0.416943	-1.793157
7	8	0	-1.401852	-4.090596	-0.222615
8	7	0	1.053630	-1.489511	0.226336
9	1	0	0.288556	-0.824516	0.269783
10	7	0	-1.301497	-2.067266	-1.236208
11	1	0	-1.741079	-1.165789	-1.377595
12	7	0	-2.800482	1.420349	1.275935
13	1	0	-3.628726	1.982182	1.135459
14	7	0	-3.316031	-1.282707	0.681351
15	1	0	-3.624808	-0.526191	0.083096
16	7	0	-3.199865	2.618902	-1.286886
17	1	0	-3.697507	3.497078	-1.330204
18	7	0	0.701362	-2.925920	2.584851
19	1	0	0.557580	-3.536659	3.375790
20	1	0	-0.118324	-2.582639	2.102845
21	6	0	1.121954	-2.376408	-0.782931
22	6	0	1.931909	-2.445893	2.362149
23	6	0	-2.685544	-1.000431	1.834270
24	6	0	-1.768132	1.534096	0.425787
25	6	0	-1.901750	-2.984625	-0.453130
26	6	0	-1.878823	2.599320	-0.666347
27	1	0	-1.133369	2.331011	-1.412990
28	6	0	2.098948	-1.425754	1.234951
29	1	0	3.042226	-1.684382	0.753937
30	6	0	-3.760801	1.519621	-1.825723
31	6	0	-0.001436	-2.353742	-1.829487
32	1	0	-0.030311	-3.377573	-2.202898
33	6	0	-2.776692	0.438674	2.350802
34	1	0	-1.872489	0.587692	2.942850
35	6	0	3.848561	0.713194	-1.359999

36	1	0	2.932630	0.925589	-1.898840
37	6	0	-3.279021	-2.624102	0.114738
38	1	0	-3.445638	-3.334117	0.923354
39	6	0	-1.585251	4.011068	-0.132651
40	1	0	-2.414885	4.346614	0.493113
41	1	0	-1.504884	4.696242	-0.978225
42	6	0	3.840182	0.738210	0.037455
43	6	0	-4.005885	0.601966	3.239868
44	1	0	-4.009334	1.592780	3.698213
45	1	0	-3.989516	-0.145570	4.033658
46	1	0	-4.925833	0.477820	2.664068
47	6	0	2.570979	3.614636	0.487960
48	1	0	2.788174	4.545758	1.021625
49	1	0	3.356422	3.506278	-0.267569
50	6	0	0.297605	-1.432129	-3.035702
51	1	0	-0.487543	-1.662827	-3.764178
52	6	0	2.207953	-0.018350	1.831899
53	1	0	2.959909	-0.049126	2.623268
54	1	0	1.257631	0.247447	2.302991
55	6	0	-4.362437	-2.785803	-0.948388
56	1	0	-5.349231	-2.657868	-0.499194
57	1	0	-4.308146	-3.784791	-1.384254
58	1	0	-4.244388	-2.051218	-1.746376
59	6	0	1.240595	3.754908	-0.253017
60	1	0	0.983829	2.831952	-0.771528
61	1	0	1.297349	4.554786	-0.992953
62	6	0	0.220045	0.061988	-2.715478
63	1	0	-0.789130	0.373131	-2.449237
64	1	0	0.515173	0.641803	-3.594035
65	1	0	0.888088	0.335731	-1.898657
66	6	0	2.565615	1.056787	0.792905
67	1	0	1.756148	1.078065	0.063473
68	6	0	2.633695	2.439271	1.469985
69	1	0	1.810253	2.518359	2.185527
70	1	0	3.557182	2.506117	2.053603
71	6	0	-5.121436	1.681226	-2.443473
72	1	0	-5.088782	1.305703	-3.468079
73	1	0	-5.474060	2.712393	-2.447985
74	1	0	-5.830912	1.062977	-1.888097
75	6	0	5.036389	0.463853	0.712360
76	1	0	5.057137	0.476286	1.797051
77	6	0	5.012990	0.416436	-2.068776
78	1	0	4.993254	0.399568	-3.153528
79	6	0	1.645786	-1.784441	-3.670464

80	1	0	2.480764	-1.502648	-3.024330
81	1	0	1.761043	-1.244979	-4.613741
82	1	0	1.728207	-2.853884	-3.879742
83	6	0	6.201872	0.166899	0.010287
84	1	0	7.117305	-0.046980	0.552299
85	6	0	6.194544	0.139579	-1.385039
86	1	0	7.101699	-0.095330	-1.931568

##

L1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.402862	4.376159	-0.279222
2	8	0	0.587944	1.082787	-0.638484
3	8	0	-3.167965	-2.402994	-3.436440
4	7	0	1.545803	-2.052092	0.439926
5	1	0	1.913712	-1.152311	0.729863
6	7	0	-1.061152	-1.490181	-0.640546
7	1	0	-0.373462	-0.743505	-0.639480
8	7	0	2.937236	2.694076	1.451099
9	1	0	3.390940	3.587421	1.581897
10	8	0	-1.717510	-3.471078	0.254067
11	7	0	2.542238	1.991877	-1.311468
12	1	0	3.319003	2.599267	-1.087318
13	8	0	1.797484	-3.874036	-0.885962
14	8	0	3.039567	0.453364	1.738563
15	7	0	3.356674	-0.728359	-1.371018
16	1	0	3.699651	-0.079110	-0.675160
17	7	0	-0.909085	-2.432221	-3.257418
18	1	0	-0.813921	-2.890525	-4.152047
19	8	0	2.059154	-0.998689	-3.212836
20	6	0	1.539647	1.841055	-0.427640
21	6	0	-2.888501	0.984430	-0.556160
22	1	0	-2.031691	0.931282	0.118612
23	6	0	-2.136425	-2.123868	-2.813715
24	6	0	-4.097603	0.476007	0.215211
25	6	0	-5.357300	0.362345	-0.390854
26	1	0	-5.480597	0.633156	-1.435047
27	6	0	-2.240673	-1.356072	-1.487912

28	1	0	-3.083056	-1.807904	-0.962423
29	6	0	1.600522	2.669513	0.863811
30	1	0	0.921831	2.166578	1.553974
31	6	0	-3.055036	2.458502	-0.997056
32	1	0	-2.269012	2.694464	-1.720639
33	1	0	-4.002784	2.564090	-1.535162
34	6	0	-2.557466	0.119086	-1.791056
35	1	0	-3.394907	0.136945	-2.493015
36	1	0	-1.701734	0.562103	-2.309577
37	6	0	-0.896156	-2.550561	0.177217
38	6	0	0.342467	-2.561960	1.088947
39	1	0	0.497409	-3.616463	1.318252
40	6	0	2.619873	-0.259140	-2.396854
41	6	0	-3.017477	3.488390	0.142556
42	1	0	-3.333113	4.462458	-0.247398
43	1	0	-3.754466	3.221138	0.908112
44	6	0	2.552282	1.265988	-2.578131
45	1	0	1.605463	1.445407	-3.090483
46	6	0	2.185824	-2.762482	-0.509711
47	6	0	1.143183	4.127926	0.661259
48	1	0	1.898820	4.673506	0.091079
49	1	0	1.058619	4.604381	1.639931
50	6	0	-3.981390	0.113644	1.562474
51	1	0	-3.014207	0.189802	2.050884
52	6	0	3.558464	1.572175	1.874103
53	6	0	-6.460991	-0.094310	0.326969
54	1	0	-7.426036	-0.174443	-0.163565
55	6	0	-1.667527	3.643659	0.851150
56	1	0	-1.297648	2.681306	1.204227
57	1	0	-1.770037	4.303293	1.714729
58	6	0	-6.329520	-0.448452	1.670769
59	1	0	-7.189267	-0.803504	2.229662
60	6	0	0.040054	-1.779216	2.378440
61	1	0	-0.960119	-2.070044	2.716772
62	1	0	-0.010413	-0.713209	2.130895
63	6	0	-5.084061	-0.343140	2.286663
64	1	0	-4.967308	-0.616686	3.330607
65	6	0	3.704173	1.752075	-3.457724
66	1	0	3.582566	2.813367	-3.684653
67	1	0	3.710266	1.199357	-4.398242
68	1	0	4.668528	1.607462	-2.964670
69	6	0	1.036266	-1.992126	3.534220
70	1	0	2.044606	-1.763297	3.171258
71	6	0	4.913475	1.743478	2.509388

72	1	0	5.649286	1.182005	1.928818
73	1	0	4.888216	1.311809	3.512478
74	1	0	5.232092	2.783973	2.576486
75	6	0	3.472243	-2.156923	-1.097889
76	1	0	3.613261	-2.669358	-2.049193
77	6	0	1.028079	-3.434155	4.052350
78	1	0	0.032785	-3.714317	4.414883
79	1	0	1.728906	-3.550333	4.884473
80	1	0	1.316766	-4.154962	3.282732
81	6	0	0.719767	-1.008355	4.666627
82	1	0	1.425475	-1.121402	5.495030
83	1	0	-0.287541	-1.174983	5.064231
84	1	0	0.774645	0.028448	4.321385
85	6	0	4.668181	-2.431698	-0.185455
86	1	0	5.594304	-2.130262	-0.679306
87	1	0	4.729722	-3.498450	0.037377
88	1	0	4.581206	-1.886155	0.756979
89	1	0	-0.068590	-2.161779	-2.767961

##

L2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.001164	4.435173	-0.105600
2	8	0	0.816169	1.077016	-0.502799
3	8	0	-2.901197	-2.463968	-3.399915
4	7	0	1.651255	-2.156189	0.466923
5	1	0	2.033033	-1.292760	0.839738
6	7	0	-0.923384	-1.459250	-0.562920
7	1	0	-0.216969	-0.732931	-0.502724
8	7	0	2.994374	2.447159	1.905640
9	1	0	3.477896	3.301737	2.143793
10	8	0	-1.603119	-3.517365	0.101438
11	7	0	2.840375	1.968033	-0.953395
12	1	0	3.602641	2.552152	-0.637204
13	8	0	1.910919	-3.894731	-0.966180
14	8	0	2.971456	0.188228	2.034072
15	7	0	3.585021	-0.771682	-1.174686
16	1	0	3.949736	-0.184661	-0.436219

17	7	0	-0.646153	-2.428955	-3.182823
18	1	0	-0.523803	-2.941619	-4.043943
19	8	0	2.341344	-0.854291	-3.070905
20	6	0	1.764843	1.792727	-0.165807
21	6	0	-2.650134	1.129563	-0.758879
22	1	0	-1.931386	1.018057	0.056714
23	6	0	-1.888478	-2.130274	-2.774084
24	6	0	-4.023205	0.778683	-0.202860
25	6	0	-5.153427	0.717060	-1.031091
26	1	0	-5.054305	0.907458	-2.095155
27	6	0	-2.031966	-1.286892	-1.497337
28	1	0	-2.944613	-1.647354	-1.020463
29	6	0	1.732345	2.539569	1.176153
30	1	0	0.953164	2.040199	1.753431
31	6	0	-2.587961	2.597080	-1.249156
32	1	0	-1.657361	2.737746	-1.806878
33	1	0	-3.399947	2.765773	-1.964458
34	6	0	-2.207478	0.188034	-1.899618
35	1	0	-2.937116	0.222634	-2.712398
36	1	0	-1.262062	0.550964	-2.312833
37	6	0	-0.783436	-2.592816	0.155165
38	6	0	0.442448	-2.707371	1.077046
39	1	0	0.589500	-3.782049	1.197234
40	6	0	2.909880	-0.199900	-2.190457
41	6	0	-2.675996	3.655586	-0.138776
42	1	0	-2.850073	4.637443	-0.593003
43	1	0	-3.551266	3.460229	0.490179
44	6	0	2.929084	1.335895	-2.266947
45	1	0	2.039744	1.598484	-2.842631
46	6	0	2.309121	-2.819437	-0.504169
47	6	0	1.382534	4.033293	1.020636
48	1	0	2.237165	4.568857	0.599978
49	1	0	1.185187	4.451069	2.009598
50	6	0	-4.196331	0.531867	1.163937
51	1	0	-3.335728	0.575762	1.823863
52	6	0	3.518980	1.267992	2.303065
53	6	0	-6.410545	0.416799	-0.510015
54	1	0	-7.270403	0.373257	-1.171155
55	6	0	-1.458115	3.738533	0.788076
56	1	0	-1.189899	2.754814	1.172500
57	1	0	-1.672966	4.387009	1.639176
58	6	0	-6.566637	0.173222	0.855550
59	1	0	-7.545491	-0.060809	1.261347
60	6	0	0.246836	-2.082092	2.473197

61	1	0	0.056977	-1.007675	2.375233
62	1	0	1.215549	-2.178460	2.972270
63	6	0	-5.453776	0.232762	1.691815
64	1	0	-5.560960	0.045991	2.755716
65	6	0	4.174888	1.824782	-3.004797
66	1	0	4.119851	2.904210	-3.161701
67	1	0	4.241393	1.340854	-3.980375
68	1	0	5.084366	1.598620	-2.443134
69	6	0	-0.834743	-2.734636	3.363335
70	1	0	-0.886402	-3.800689	3.110103
71	6	0	4.809553	1.326566	3.078573
72	1	0	5.594241	0.839652	2.493990
73	1	0	4.689476	0.759552	4.003957
74	1	0	5.125296	2.342202	3.318188
75	6	0	3.636925	-2.218308	-0.996547
76	1	0	3.806512	-2.672936	-1.972411
77	6	0	-2.226813	-2.123908	3.160089
78	1	0	-2.221592	-1.060426	3.421426
79	1	0	-2.962853	-2.618449	3.801594
80	1	0	-2.579344	-2.214966	2.131662
81	6	0	-0.427457	-2.622858	4.838508
82	1	0	-1.179704	-3.076445	5.490884
83	1	0	-0.320019	-1.574007	5.137069
84	1	0	0.526987	-3.122295	5.029724
85	6	0	4.776752	-2.594745	-0.048793
86	1	0	5.735983	-2.293271	-0.474720
87	1	0	4.793244	-3.675171	0.104808
88	1	0	4.657283	-2.109566	0.922965
89	1	0	0.179283	-2.124532	-2.687860

##

L3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.099126	4.375432	-0.401007
2	8	0	0.863564	1.007437	-0.543962
3	8	0	-2.821867	-2.456664	-3.513910
4	7	0	1.536535	-2.123313	0.685568
5	1	0	1.936777	-1.232443	0.960736
6	7	0	-0.943774	-1.438457	-0.605620

7	1	0	-0.227595	-0.720743	-0.553681
8	7	0	3.070885	2.517271	1.762758
9	1	0	3.558349	3.383787	1.943469
10	8	0	-1.737035	-3.397460	0.217945
11	7	0	2.931062	1.772403	-1.030838
12	1	0	3.716354	2.343155	-0.747941
13	8	0	1.780200	-4.025667	-0.524881
14	8	0	3.021414	0.274775	2.062961
15	7	0	3.584062	-0.997237	-0.984858
16	1	0	3.935117	-0.356653	-0.285100
17	7	0	-0.581368	-2.491136	-3.175749
18	1	0	-0.431547	-3.007303	-4.030526
19	8	0	2.385769	-1.216893	-2.899191
20	6	0	1.837255	1.709161	-0.251358
21	6	0	-2.606349	1.144311	-0.867008
22	1	0	-1.861211	1.054589	-0.073392
23	6	0	-1.833008	-2.145765	-2.839373
24	6	0	-3.955859	0.791152	-0.258360
25	6	0	-5.117317	0.733385	-1.042526
26	1	0	-5.058793	0.932412	-2.108091
27	6	0	-2.019063	-1.287197	-1.579356
28	1	0	-2.942686	-1.646955	-1.123542
29	6	0	1.813621	2.567173	1.021473
30	1	0	1.023621	2.133394	1.635988
31	6	0	-2.570291	2.600951	-1.389981
32	1	0	-1.668357	2.729441	-1.995768
33	1	0	-3.415459	2.755963	-2.068672
34	6	0	-2.190918	0.182650	-2.002083
35	1	0	-2.933009	0.210012	-2.803866
36	1	0	-1.248716	0.533944	-2.433241
37	6	0	-0.890553	-2.496109	0.229565
38	6	0	0.253398	-2.521877	1.259031
39	1	0	0.331120	-3.564791	1.566166
40	6	0	2.950946	-0.500639	-2.065526
41	6	0	-2.604134	3.685494	-0.301857
42	1	0	-2.786511	4.657448	-0.773736
43	1	0	-3.455497	3.515016	0.366315
44	6	0	3.013653	1.020584	-2.280079
45	1	0	2.136603	1.254095	-2.886153
46	6	0	2.204175	-2.919780	-0.170951
47	6	0	1.491114	4.047558	0.735600
48	1	0	2.350169	4.524560	0.257710
49	1	0	1.316662	4.556422	1.685569
50	6	0	-4.074517	0.531191	1.112143

51	1	0	-3.189505	0.572053	1.740238
52	6	0	3.578457	1.366421	2.254350
53	6	0	-6.352567	0.426064	-0.475459
54	1	0	-7.237643	0.386599	-1.102702
55	6	0	-1.351722	3.780980	0.576216
56	1	0	-1.101731	2.813442	1.010711
57	1	0	-1.518422	4.484520	1.393932
58	6	0	-6.454677	0.170437	0.893037
59	1	0	-7.416581	-0.068515	1.334876
60	6	0	-0.054562	-1.632661	2.478190
61	1	0	-0.075708	-0.588718	2.147822
62	1	0	0.791230	-1.724508	3.169021
63	6	0	-5.310094	0.224517	1.685732
64	1	0	-5.375317	0.028233	2.751282
65	6	0	4.278040	1.406000	-3.047176
66	1	0	4.254059	2.467688	-3.301953
67	1	0	4.337851	0.833090	-3.973696
68	1	0	5.176718	1.207494	-2.458333
69	6	0	-1.354545	-1.949854	3.237038
70	1	0	-2.196253	-1.856728	2.540134
71	6	0	4.864138	1.471580	3.032402
72	1	0	5.652258	0.950519	2.482726
73	1	0	4.738828	0.961926	3.989804
74	1	0	5.178144	2.500280	3.210528
75	6	0	3.571506	-2.422555	-0.671846
76	1	0	3.749727	-2.971758	-1.596156
77	6	0	-1.557254	-0.914165	4.349381
78	1	0	-0.748536	-0.966146	5.086691
79	1	0	-2.499156	-1.085426	4.878632
80	1	0	-1.578455	0.104784	3.951056
81	6	0	-1.368635	-3.370658	3.813521
82	1	0	-2.277413	-3.540804	4.398627
83	1	0	-0.511936	-3.533369	4.477003
84	1	0	-1.337380	-4.132745	3.031607
85	6	0	4.667880	-2.755588	0.340962
86	1	0	5.649962	-2.528196	-0.078876
87	1	0	4.637234	-3.818589	0.586494
88	1	0	4.540264	-2.183821	1.263159
89	1	0	0.229489	-2.191040	-2.653490

##

References

1. Hu, K.; Geng, H.; Zhang, Q.; Liu, Q.; Xie, M.; Sun, C.; Li, W.; Lin, H.; Jiang, F.; Wang, T.; Wu, Y. D.; Li, Z., An In-tether Chiral Center Modulates the Helicity, Cell Permeability, and Target Binding Affinity of a Peptide. *Angew Chem Int Ed Engl* **2016,** *55* (28), 8013-7.