Supplementary Materials

A Peptide Potential Based on a Bond Dipole Representation of Electrostatics

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This Supporting Information includes:

Figure S1 Two clusters which contain one glycine tetrapeptide and 30 water molecules.

Figure S2 79 conformations used to derive the scale factors for intramolecular dipole-dipole interactions.

Table S1 RMSEs of different methods with respect to the benchmark QM conformational energies.

Figure S3 The linear correlations between the QM conformational energies and the force field ones for all the structures included in Table S1.

Table S2 Bond stretching, angle bending and dihedral angle parameters used in our potential.

Table S3 The backbone dihedral angles and hydrogen bond lengths for polypeptides AcAla$_4$XAla$_4$NHMe (X=Val, Ile, Leu, Asn, Gln, Ser, Thr, Phe, Cys, Met, Hid, Hie, Trp and Tyr), AcAla$_{13}$NH$_2$ and Ac(Ala$_2$GlnAla$_2$)$_3$NH$_2$.

Figure S4 The hydrogen-bonded dimers.

Table S4 Physical components of the interaction energy (*IE*) for eight hydrogen-bonded dimers.

Table S5 Cartesian coordinates in angstroms for Cluster A and B, 28 glycine tetrapeptide conformers, 51 alanine tetrapeptide conformers, AcAla$_4$XAla$_4$NHMe (X=Val, Ile, Leu, Asn, Gln, Ser, Thr, Phe, Cys, Met, Hid, Hie, Trp and Tyr), AcAla$_{13}$NH$_2$, Ac(Ala$_2$GlnAla$_2$)$_3$NH$_2$ and hydrogen-bonded dimers.

Cluster A

$IE_{3B,MP2}$=-18.64 kcal/mol
$IE_{3B,This\ work}$=-18.41 kcal/mol

Cluster B

$IE_{3B,MP2}$=-6.08 kcal/mol
$IE_{3B,This\ work}$=-6.49 kcal/mol
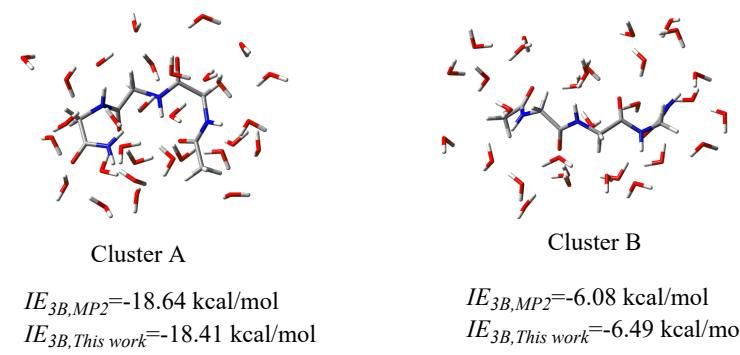
Figure S1. Two clusters which contain one glycine tetrapeptide and 30 water molecules.

The total 3-body interaction energies (*IE*$_{3B}$) are calculated using the counterpoise-corrected MP2/aug-cc-pVDZ method and our peptide potential. The relevant parameters for water molecules are taken from our previous work (J. Comput. Chem. 2023, 44, 677-686)

A) 28 conformations of the glycine tetrapeptide
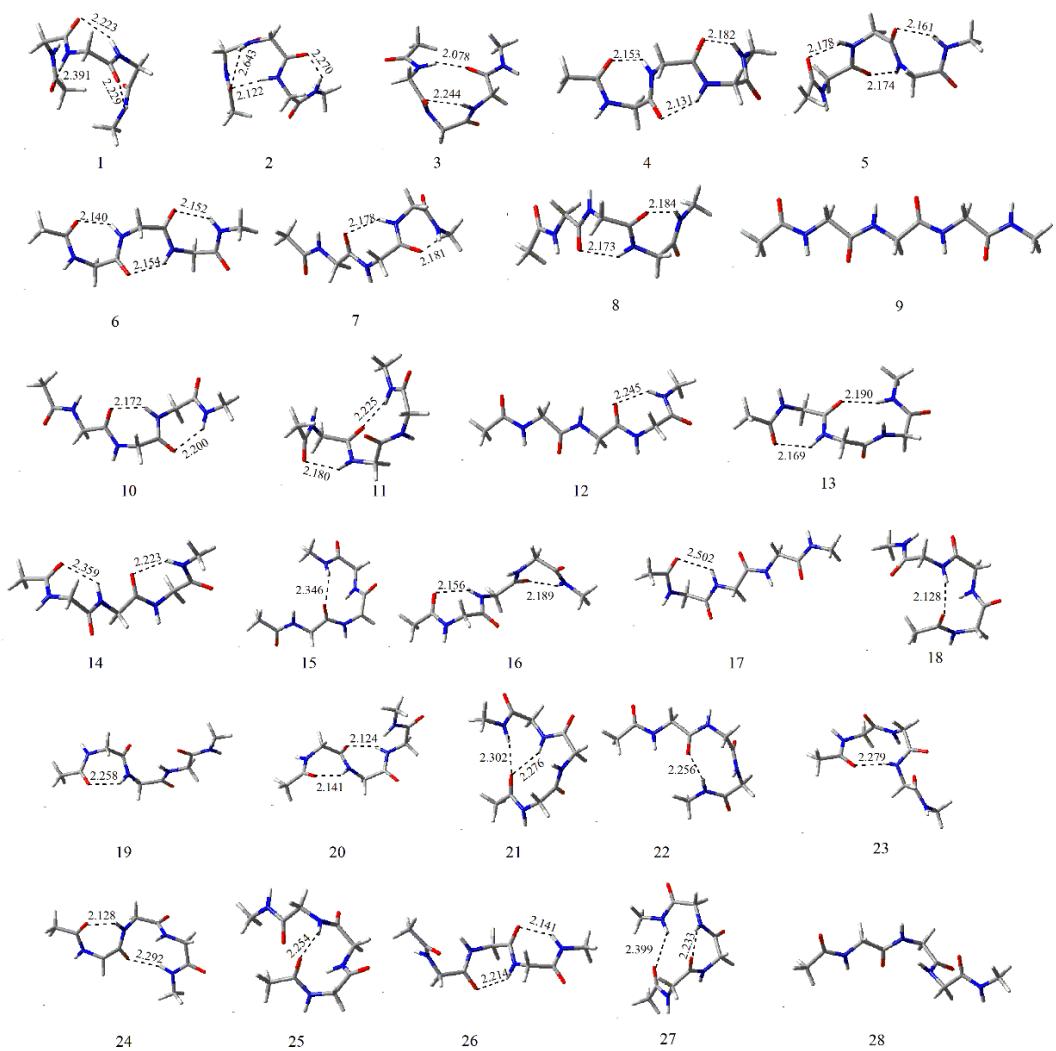
B) 51 conformations of the alanine tetrapeptide
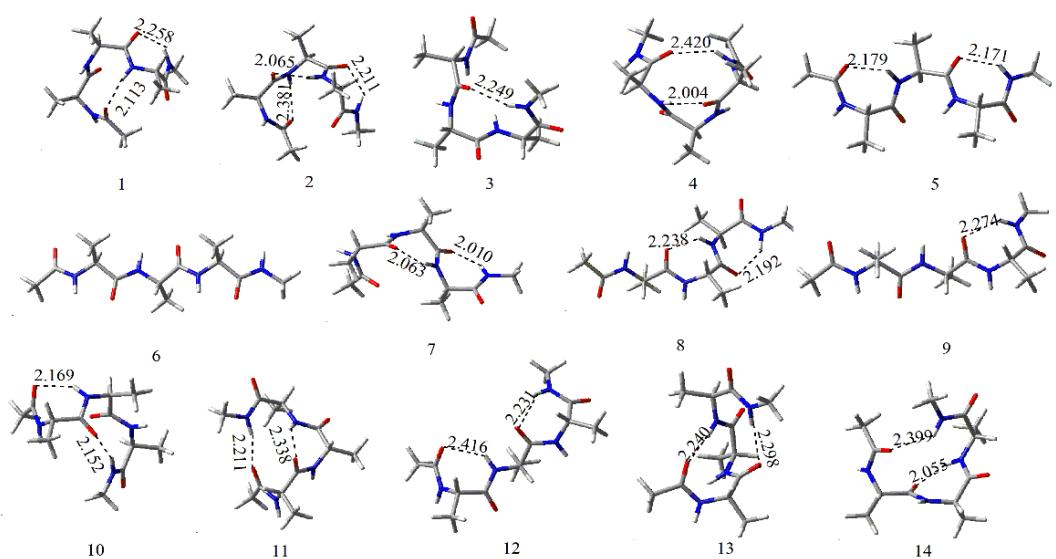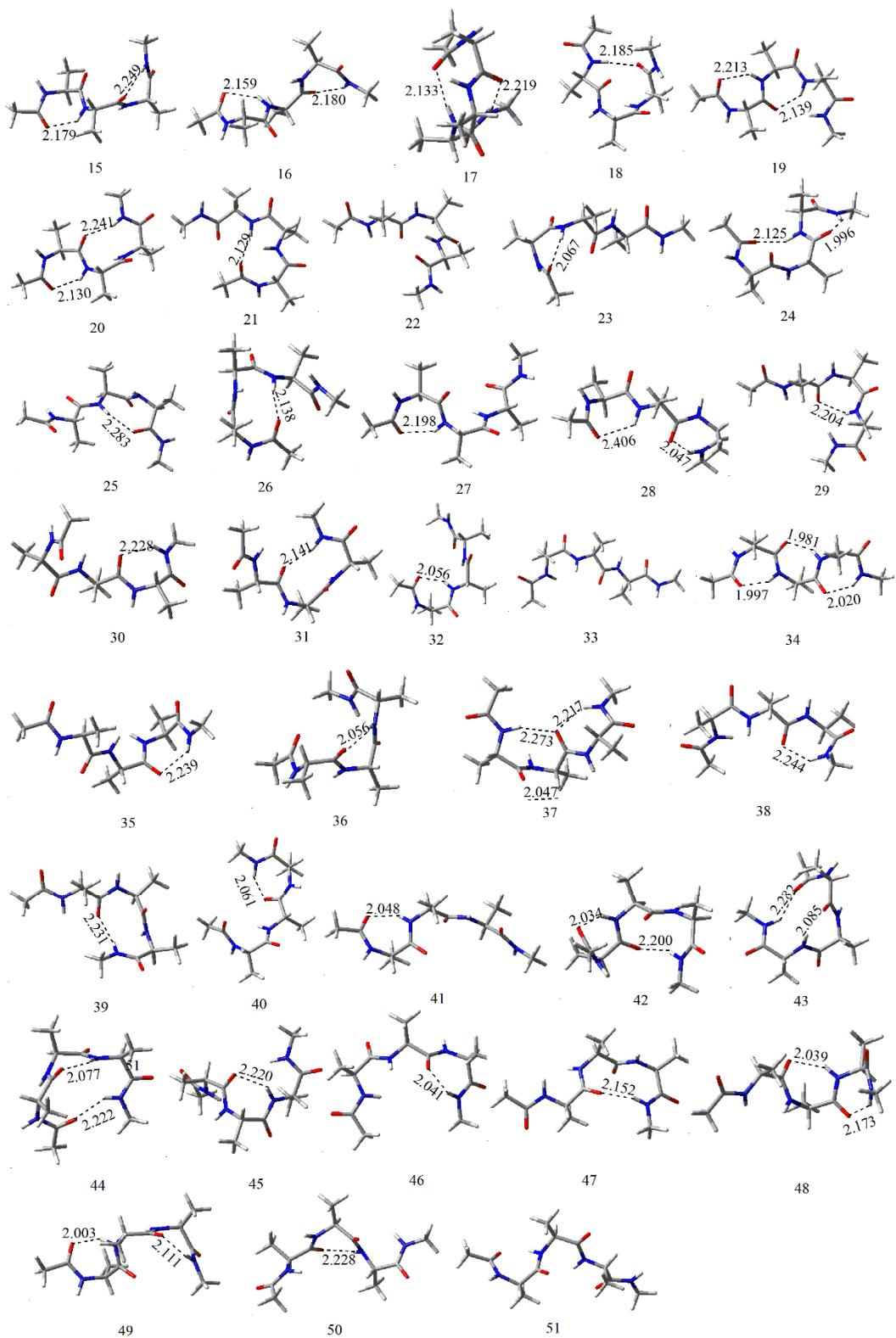
Figure S2. 79 conformations used to derive the scale factors for intramolecular dipole-dipole interactions.

Table S1. RMSEs of different methods with respect to the benchmark QM conformational energies (kcal/mol) dipeptides: QM=RIMP2/CBS[a], tetrapeptides: QM=LMP2/cc-pVQZ(-g)[b].

	Number of conformers	AM-BER99sb	AMOBEA-bio18	This work
AcGlyNHMe	325	3.71	3.96	2.36
AcAlaNHMe	625	5.12	3.99	3.87
AcGly$_3$NHMe	28	2.90	3.10	2.12
AcAla$_3$NHMe	51	2.14	2.08	1.84

[a]Lopes, P. E. M.; Huang, J.; Shim, J.; Luo, Y.; Li, H.; Roux, B.; MacKerell, A. D. Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator. *Journal of Chemical Theory and Computation* **2013**, *9*, 5430-5449.
[b]Hornak, V.; Abel, R.; Okur, A.; Strockbine, B.; Roitberg, A.; Simmerling, C. Comparison of multiple Amber force fields and development of improved protein backbone parameters. *Proteins: Structure, Function, and Bioinformatics* **2006**, *65*, 712-725.
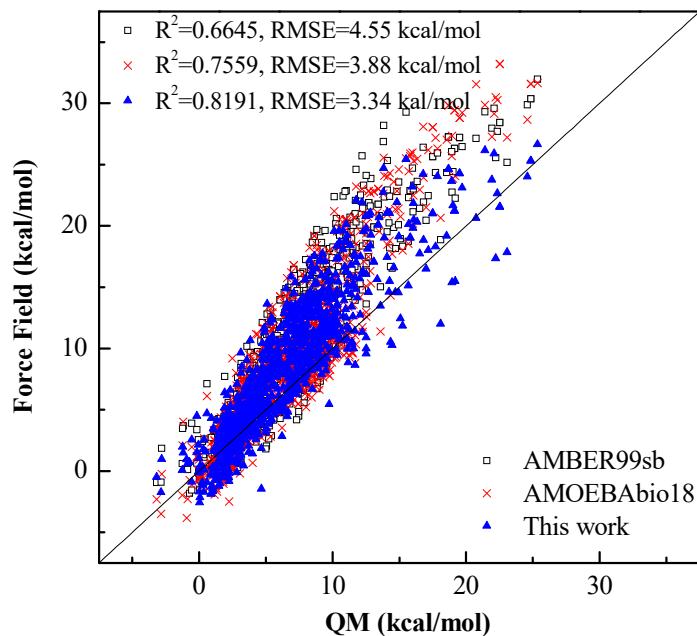

Figure S3. The linear correlations between the QM conformational energies and the force field ones for all the structures included in Table S1.

Table S2. (a) Bond stretching parameters used in our potential.[a.]

Bond	k_b	b_0	Bond	k_b	b_0	Bond	k_b	b_0
CA-CA	469.00	1.4000	C-O(Ac)	570.00	1.2290	CT-S	227.00	1.8100
CA-CB	469.00	1.4040	CR-H5	367.00	1.0800	CT-SH	237.00	1.8100
CA-CN	469.00	1.4000	CR-NA	477.00	1.3430	CV-H4	367.00	1.0800
CA-HA	367.00	1.0800	CR-NB	488.00	1.3350	CV-NB	410.00	1.3940
CA-OH	450.00	1.3640	CT-C	317.00	1.5220	CW-C*	546.00	1.3520
CB-C*	388.00	1.4590	CT-C*	317.00	1.4950	CW-H4	367.00	1.0800
CB-CN	447.00	1.4190	CT-CA	317.00	1.5100	CW-NA	427.00	1.3810
CC-CV	512.00	1.3750	CT-CC	317.00	1.5040	NA-H	434.00	1.0100
CC-CW	518.00	1.3710	CT-CT	310.00	1.5260	N-H	434.00	1.0100
CC-NA	422.00	1.3850	CT-H1	340.00	1.0900	N-HQ	434.00	1.0100
CC-NB	410.00	1.3940	CT-H2	340.00	1.0900	OH-HO	553.00	0.9600
C-N	490.00	1.3350	CT-HC	340.00	1.0900	SH-HS	274.00	1.3360
CN-NA	428.00	1.3800	CT-N	337.00	1.4490			
C-O	570.00	1.2290	CT-OH	320.00	1.4100			

[a]The unit for the stretching force constant is kcal/(mol Å^2). The unit for the equilibrium bond length is Å.

Table S2. (b) Angle bending parameters used in our potential.[b.]

Angle	k_θ	θ_0	Angle	k_θ	θ_0	Angle	k_θ	θ_0
C*-CB-CN	63.00	108.80	C-N- H	50.00	120.00	CT-N-CT	50.00	118.00
C*-CT-HC	50.00	109.50	CN-CA-HA	50.00	120.00	CT-OH-HO	55.00	108.50
C*-CW-H4	50.00	120.00	C-N-HQ	50.00	120.00	CT-S-CT	62.00	98.90
C*-CW-NA	70.00	108.70	CN-NA-H	50.00	123.10	CT-SH-HS	43.00	96.00
CA-CA-CA	63.00	120.00	CR-NA-H	50.00	120.00	CV-CC-NA	70.00	120.00
CA-CA-CB	63.00	120.00	CT-C*-CB	70.00	128.60	CV-NB-CR	70.00	117.00
CA-CA-CN	63.00	120.00	CT-C*-CW	70.00	125.00	CW-C*-CB	63.00	106.40
CA-CA-H4	50.00	120.00	CT-CA-CA	70.00	120.00	CW-CC-NA	70.00	120.00
CA-CA-HA	50.00	120.00	CT-CC-CV	70.00	120.00	CW-CC-NB	70.00	120.00
CA-CA-OH	70.00	120.00	CT-CC-CW	70.00	120.00	CW-NA-CN	70.00	111.60
CA-CB-C*	63.00	134.90	CT-CC-NA	70.00	120.00	CW-NA-CR	70.00	120.00
CA-CB-CN	63.00	116.20	CT-CC-NB	70.00	120.00	CW-NA-H	50.00	120.00
CA-CB-NB	70.00	132.40	CT-C-N	70.00	116.60	H1-CT-H1	35.00	109.50
CA-CN-CB	63.00	122.70	CT-C-O	80.00	120.40	H2-CT-H2	35.00	109.50
CA-CN-NA	70.00	132.80	CT-C-O(Ac)	80.00	120.40	HC-CT-HC	35.00	109.50
CA-CT-HC	50.00	109.50	CT-CT-C	63.00	111.10	HC-CT-OH	50.00	109.50
CA-OH-HO	50.00	113.00	CT-CT-C*	63.00	115.60	HQ-N-HQ	35.00	120.00
CB-CA-HA	50.00	120.00	CT-CT-CA	63.00	114.00	NA-CR-H5	50.00	120.00
CB-CN-NA	70.00	104.40	CT-CT-CC	63.00	113.10	NA-CR-NA	70.00	120.00
CC-CT-HC	50.00	109.50	CT-CT-CT	40.00	109.50	NA-CR-NB	70.00	120.00
CC-CV-H4	50.00	120.00	CT-CT-H1	50.00	109.50	NA-CW-H4	50.00	120.00
CC-CV-NB	70.00	120.00	CT-CT-H2	50.00	109.50	NB-CR-H5	50.00	120.00
CC-CW-H4	50.00	120.00	CT-CT-HC	50.00	109.50	NB-CV-H4	50.00	120.00
CC-CW-NA	70.00	120.00	CT-CT-N	80.00	109.70	N-C-O	80.00	122.90
CC-NA-CR	70.00	120.00	CT-CT-N	80.00	109.70	N-C-O(Ac)	80.00	122.90
CC-NA-H	50.00	120.00	CT-CT-OH	50.00	109.50	N-CT-H1	50.00	109.50
CC-NB-CR	70.00	117.00	CT-CT-S	50.00	114.70	N-CT-HC	50.00	109.50
C-CT-H1	50.00	109.50	CT-CT-SH	50.00	108.60	S-CT-H2	50.00	109.50
C-CT-HC	50.00	109.50	CT-N- C	50.00	121.90	S-CT-HC	50.00	109.50
C-CT-N	63.00	110.10	CT-N- H	50.00	118.04	SH-CT-HC	50.00	109.50

Table S2. (c) Dihedral angle parameters used in our potential.[c]

Dihedral angle	$V_1/2$	γ_1	$V_1/2$	γ_1	$V_1/2$	γ_1
N-CT-C-N	0.450	180.0	1.580	180.0	0.550	180.0
CT-CT-C-N	0.200	0.0	0.200	0.0	0.400	0.0
CT-CT-N-C	2.000	0.0	2.000	0.0	0.400	0.0
CT-CT-CT-CT	0.200	180.0	0.250	180.0	0.180	0.0
HC-CT-C-O	0.800	0.0	--	--	0.080	180.0
H1-CT-C-O	0.800	0.0	--	--	0.080	180.0
H1-CT-C-O(Ac)	0.800	0.0	--	--	0.080	180.0
HC-CT-C-O(Ac)	0.800	0.0	--	--	0.080	180.0
CT-CT-OH-HO	0.025	0.0	--	--	0.160	0.0
OH-CT-CT-HC	0.250	0.0	--	--	0.156	0.0
C-CT-N-C	--	--	0.270	0.0	0.420	0.0
O-C-N-H	2.000	0.0	2.500	180.0	--	--
O-C-N-HQ	2.000	0.0	2.500	180.0	--	--
O(Ac)-C-N-H	2.000	0.0	2.500	180.0	--	--
C-CT-CT-HC	--	--	--	--	0.156	0.0
N-CT-CT-HC	--	--	--	--	0.156	0.0
H1-CT-CT-HC	--	--	--	--	0.156	0.0
N-CT-CT-CT	--	--	--	--	0.156	0.0
HC-CT-CT-HC	--	--	--	--	0.150	0.0
C-CT-CT-CT	--	--	--	--	0.156	0.0
HC-CT-CT-CT	--	--	--	--	0.160	0.0
H1-CT-CT-CT	--	--	--	--	0.156	0.0
C-CT-CT-C	--	--	--	--	0.156	0.0
C-CT-CT-N	--	--	--	--	0.156	0.0
N-CT-CT-CA	--	--	--	--	0.156	0.0
C-CT-CT-CA	--	--	--	--	0.156	0.0
CA-CT-CT-H1	--	--	--	--	0.156	0.0
N-CT-CT-HC	--	--	--	--	0.156	0.0
C-CT-CT-HC	--	--	--	--	0.156	0.0
H1-CT-CT-HC	--	--	--	--	0.156	0.0
OH-CT-CT-N	--	--	--	--	0.156	0.0
OH-CT-CT-C	--	--	--	--	0.156	0.0
OH-CT-CT-H1	--	--	--	--	0.156	0.0
HO-OH-CT-HC	--	--	--	--	0.167	0.0
C-CT-CT-SH	--	--	--	--	0.156	0.0
N-CT-CT-SH	--	--	--	--	0.156	0.0
SH-CT-CT-H1	--	--	--	--	0.156	0.0
CT-CT-SH-HS	--	--	--	--	0.250	0.0
HC-CT-SH-HS	--	--	--	--	0.250	0.0
CT-CT-CT-S	--	--	--	--	0.156	0.0
S-CT-CT-HC	--	--	--	--	0.156	0.0
CT-CT-S-CT	--	--	--	--	0.333	0.0
HC-CT-S-CT	--	--	--	--	0.333	0.0
CT-CT-CT-H2	--	--	--	--	0.156	0.0
HC-CT-CT-H2	--	--	--	--	0.156	0.0
H2-CT-S-CT	--	--	--	--	0.333	0.0
C-CT-CT-CC	--	--	--	--	0.156	0.0

C-CT-CT-C*	--	--	--	--	0.156	0.0
CC-CT-CT-N	--	--	--	--	0.156	0.0
CC-CT-CT-H1	--	--	--	--	0.156	0.0
C*-CT-CT-N	--	--	--	--	0.156	0.0
C*-CT-CT-H1	--	--	--	--	0.156	0.0
N-CT-C-O	--	--	--	--	--	--
HC-CT-C-N	--	--	--	--	--	--
H1-CT-C-N	--	--	--	--		
C-CT-N-H	--	--	--	--	--	--
H1-CT-N-C	--	--	--	--	--	--
H1-CT-N-H	--	--	--	--	--	--
CT-CT-C-O	--	--	--	--	--	--
CT-CT-N-H	--	--	--	--	--	--
HC-CT-N-H	--	--	--	--	--	--
HC-CT-N-C	--	--	--	--	--	--
CT-N-CT-CT	--	--	--	--	--	--
CT-N-CT-C	--	--	--	--	--	--
CT-N-CT-H1	--	--	--	--	--	--
CT-CT-CA-CA	--	--	--	--	--	--
CA-CA-CT-HC	--	--	--	--	--	--
CT-CT-CC-CV	--	--	--	--	--	--
CT-CT-CC-CW	--	--	--	--	--	--
CT-CT-CC-NA	--	--	--	--	--	--
CT-CT-CC-NB	--	--	--	--	--	--
HC-CT-CC-CV	--	--	--	--	--	--
HC-CT-CC-CW	--	--	--	--	--	--
HC-CT-CC-NA	--	--	--	--	--	--
HC-CT-CC-NB	--	--	--	--	--	--
CT-CT-C*-CW	--	--	--	--	--	--
CT-CT-C*-CB	--	--	--	--	--	--
HC-CT-C*-CW	--	--	--	--	--	--
HC-CT-C*-CB	--	--	--	--	--	--
O(Ac)-C-N-CT	--	--	2.500	180.0	--	--
CT-C-N-CT	--	--	2.500	180.0	--	--
CT-C-N-H	--	--	2.500	180.0	--	--
O-C-N-CT	--	--	2.500	180.0	--	--
CT-C-N-HQ	--	--	2.500	180.0	--	--
CT-CA-CA-CA	--	--	3.625	180.0	--	--
CT-CA-CA-HA	--	--	3.625	180.0	--	--
CA-CA-CA-HA	--	--	3.625	180.0	--	--
CA-CA-CA-CA	--	--	3.625	180.0	--	--
HA-CA-CA-HA	--	--	3.625	180.0	--	--
CA-CA-CA-OH	--	--	3.625	180.0	--	--
OH-CA-CA-HA	--	--	3.625	180.0	--	--
CA-CA-OH-HO	--	--	0.900	180.0	--	--
CA-CA-CA-CB	--	--	3.625	180.0	--	--
CA-CA-CA-CN	--	--	3.625	180.0	--	--
CB-CA-CA-HA	--	--	3.625	180.0	--	--
CN-CA-CA-HA	--	--	3.625	180.0	--	--
CA-CA-CB-C*	--	--	3.500	180.0	--	--
CA-CA-CB-CN	--	--	3.500	180.0	--	--
HA-CA-CB-C*	--	--	3.500	180.0	--	--
HA-CA-CB-CN	--	--	3.500	180.0	--	--

CA-CA-CN-CB	--	--	3.625	180.0	--	--
CA-CA-CN-NA	--	--	3.625	180.0	--	--
HA-CA-CN-CB	--	--	3.625	180.0	--	--
HA-CA-CN-NA	--	--	3.625	180.0	--	--
CT-CC-CV-NB	--	--	5.150	180.0	--	--
CT-CC-CV-H4	--	--	5.150	180.0	--	--
NA-CC-CV-NB	--	--	5.150	180.0	--	--
NA-CC-CV-H4	--	--	5.150	180.0	--	--
CT-CC-CW-NA	--	--	5.375	180.0	--	--
CT-CC-CW-H4	--	--	5.375	180.0	--	--
NA-CC-CW-NA	--	--	5.375	180.0	--	--
NA-CC-CW-H4	--	--	5.375	180.0	--	--
NB-CC-CW-NA	--	--	5.375	180.0	--	--
NB-CC-CW-H4	--	--	5.375	180.0	--	--
CT-CC-NA-CR	--	--	1.400	180.0	--	--
CT-CC-NA-H	--	--	1.400	180.0	--	--
CV-CC-NA-CR	--	--	1.400	180.0	--	--
CV-CC-NA-H	--	--	1.400	180.0	--	--
CW-CC-NA-CR	--	--	1.400	180.0	--	--
CW-CC-NA-H	--	--	1.400	180.0	--	--
CT-CC-NB-CR	--	--	2.400	180.0	--	--
CW-CC-NB-CR	--	--	2.400	180.0	--	--
CC-CV-NB-CR	--	--	2.400	180.0	--	--
H4-CV-NB-CR	--	--	2.400	180.0	--	--
NA-CW-C*-CT	--	--	6.525	180.0	--	--
NA-CW-C*-CB	--	--	6.525	180.0	--	--
H4-CW-C*-CT	--	--	6.525	180.0	--	--
H4-CW-C*-CB	--	--	6.525	180.0	--	--
CC-CW-NA-CR	--	--	1.500	180.0	--	--
CC-CW-NA-H	--	--	1.500	180.0	--	--
C*-CW-NA-CN	--	--	1.500	180.0	--	--
C*-CW-NA-H	--	--	1.500	180.0	--	--
H4-CW-NA-CR	--	--	1.500	180.0	--	--
H4-CW-NA-CN	--	--	1.500	180.0	--	--
H4-CW-NA-H	--	--	1.500	180.0	--	--
NA-CR-NA-CC	--	--	2.325	180.0	--	--
NA-CR-NA-CW	--	--	2.325	180.0	--	--
NA-CR-NA-H	--	--	2.325	180.0	--	--
NB-CR-NA-CC	--	--	2.325	180.0	--	--
NB-CR-NA-CW	--	--	2.325	180.0	--	--
NB-CR-NA-H	--	--	2.325	180.0	--	--
H5-CR-NA-CC	--	--	2.325	180.0	--	--
H5-CR-NA-CW	--	--	2.325	180.0	--	--
H5-CR-NA-H	--	--	2.325	180.0	--	--
NA-CR-NB-CC	--	--	5.000	180.0	--	--
NA-CR-NB-CV	--	--	5.000	180.0	--	--
H5-CR-NB-CC	--	--	5.000	180.0	--	--
H5-CR-NB-CV	--	--	5.000	180.0	--	--
CA-CB-C*-CT	--	--	1.675	180.0	--	--
CA-CB-C*-CW	--	--	1.675	180.0	--	--
CN-CB-C*-CT	--	--	1.675	180.0	--	--
CN-CB-C*-CW	--	--	1.675	180.0	--	--
CA-CB-CN-CA	--	--	3.000	180.0	--	--

CA-CB-CN-NA	--	--	3.000	180.0	--	--
C*-CB-CN-CA	--	--	3.000	180.0	--	--
C*-CB-CN-NA	--	--	3.000	180.0	--	--
CA-CN-NA-CW	--	--	1.525	180.0	--	--
CA-CN-NA-H	--	--	1.525	180.0	--	--
CB-CN-NA-CW	--	--	1.525	180.0	--	--
CB-CN-NA-H	--	--	1.525	180.0	--	--
C*-NA-CW-H4	--	--	1.100	180.0	--	--
CA-CA-CA-HA	--	--	1.100	180.0	--	--
CA-CA-CA-OH	--	--	1.100	180.0	--	--
CA-CB-CA-HA	--	--	1.100	180.0	--	--
CC-CR-NA-H	--	--	1.000	180.0	--	--
CC-NA-CW-H4	--	--	1.100	180.0	--	--
CC-NB-CV-H4	--	--	1.100	180.0	--	--
C-CT-N-CT	--	--	1.000	180.0	--	--
C-H-N-CT	--	--	1.000	180.0	--	--
C-H-N-H	--	--	1.000	180.0	--	--
C-HQ-N-HQ	--	--	1.000	180.0	--	--
CN-CA-CA-HA	--	--	1.100	180.0	--	--
CR-CW-NA-H	--	--	1.000	180.0	--	--
CT-CA-CA-CA	--	--	1.100	180.0	--	--
CT-O(Ac)-C-N	--	--	10.500	180.0	--	--
CW-CB-C*-CT	--	--	1.100	180.0	--	--
CW-CN-NA-H	--	--	1.000	180.0	--	--
NA-CV-CC-CT	--	--	1.100	180.0	--	--
NA-CW-CC-CT	--	--	1.100	180.0	--	--
NA-NA-CR-H5	--	--	1.100	180.0	--	--
NA-NB-CR-H5	--	--	1.100	180.0	--	--
NB-CW-CC-CT	--	--	1.100	180.0	--	--
NB-NA-CR-H5	--	--	1.100	180.0	--	--
N-O-C-CT	--	--	10.500	180.0	--	--

[c]The unit for the Fourier coefficient is kcal/mol, and the unit for the phase angle is degree.

Table S3. The backbone dihedral angles and hydrogen bond lengths for polypeptides AcAla$_4$XAla$_4$NHMe (X=Val, Ile, Leu, Asn, Gln, Ser, Thr, Phe, Cys, Met, Hid, Hie, Trp and Tyr), AcAla$_{13}$NH$_2$ and Ac(Ala$_2$GlnAla$_2$)$_3$NH$_2$.

		φ (degree)				ψ (degree)			R(O···H) (Å)	
		helix	C5	C7$_{eq}$		helix	C5	C7$_{eq}$	helix	C7$_{eq}$
	φ$_1$	-65.1	-159.1	-82.4	ψ$_1$	-25.5	165.6	68.8	2.04	1.97
	φ$_2$	-58.8	-159.3	-83.7	ψ$_2$	-23.1	166.6	66.5	2.13	1.97
	φ$_3$	-59.6	-159.6	-83.8	ψ$_3$	-29.8	166.3	66.6	2.19	1.96
	φ$_4$	-68.3	-160.5	-83.8	ψ$_4$	-29.8	165.0	67.0	2.18	1.98
AcAla$_4$ValAla$_4$NHMe	φ$_5$	-73.5	-132.8	-83.4	ψ$_5$	-43.3	162.2	75.2	2.21	1.99
	φ$_6$	-58.1	-161.4	-85.2	ψ$_6$	-32.9	167.5	66.6	2.16	1.97
	φ$_7$	-60.0	-158.4	-83.7	ψ$_7$	-25.5	167.4	66.7	2.08	1.97
	φ$_8$	-71.2	-159.9	-84.5	ψ$_8$	-7.4	168.0	66.4	2.14	1.99
	φ$_9$	-101.2	-158.3	-84.7	ψ$_9$	8.8	165.2	68.8		2.00
	φ$_1$	-65.0	-158.6	-82.4	ψ$_1$	-25.5	166.9	68.4	2.05	1.97
	φ$_2$	-58.7	-158.8	-83.7	ψ$_2$	-22.5	167.3	66.8	2.11	1.97
	φ$_3$	-58.9	-158.8	-83.8	ψ$_3$	-30.4	168.6	67.4	2.21	1.96
	φ$_4$	-67.9	-158.5	-83.2	ψ$_4$	-31.0	168.4	67.7	2.20	1.96
AcAla$_4$LeuAla$_4$NHMe	φ$_5$	-71.2	-153.9	-84.2	ψ$_5$	-44.1	142.7	74.4	2.16	1.98
	φ$_6$	-58.1	-159.5	-85.0	ψ$_6$	-33.7	169.7	65.7	2.17	1.96
	φ$_7$	-60.2	-158.3	-83.0	ψ$_7$	-25.8	167.3	67.8	2.08	1.97
	φ$_8$	-70.7	-160.1	-84.4	ψ$_8$	-7.9	167.7	65.6	2.13	1.98
	φ$_9$	-101.2	-158.3	-84.6	ψ$_9$	8.8	165.5	68.8		2.00
	φ$_1$	-65.1	-158.5	-82.3	ψ$_1$	-25.8	167.5	68.4	2.04	1.97
	φ$_2$	-57.9	-158.1	-83.9	ψ$_2$	-25.1	166.8	66.6	2.13	1.97
	φ$_3$	-60.2	-159.5	-83.8	ψ$_3$	-30.5	168.0	67.0	2.19	1.96
	φ$_4$	-69.0	-158.7	-84.3	ψ$_4$	-29.2	167.7	61.6	2.24	1.95
AcAla$_4$IleAla$_4$NHMe	φ$_5$	-72.9	-153.8	-85.0	ψ$_5$	-43.9	158.6	68.9	2.17	1.97
	φ$_6$	-58.4	-157.2	-84.8	ψ$_6$	-33.3	169.0	66.4	2.16	1.97
	φ$_7$	-60.2	-159.3	-83.7	ψ$_7$	-25.4	167.0	66.8	2.08	1.97
	φ$_8$	-71.0	-159.3	-84.5	ψ$_8$	-7.5	167.4	67.1	2.13	1.99
	φ$_9$	-101.7	-159.1	-84.7	ψ$_9$	9.4	165.4	69.0		2.00
	φ$_1$	-65.3	-158.4	-82.3	ψ$_1$	-25.3	167.0	69.4	2.04	1.98
	φ$_2$	-58.9	-159.0	-83.6	ψ$_2$	-22.1	166.4	67.4	2.13	1.97
	φ$_3$	-59.5	-159.3	-83.5	ψ$_3$	-28.8	167.9	67.4	2.18	1.95
	φ$_4$	-68.7	-158.7	-83.0	ψ$_4$	-27.3	167.4	66.9	2.24	1.93
AcAla$_4$SerAla$_4$NHMe	φ$_5$	-75.5	-160.6	-83.1	ψ$_5$	-45.8	173.3	59.4	2.14	1.92
	φ$_6$	-57.1	-156.7	-83.0	ψ$_6$	-32.6	168.2	68.0	2.10	1.99
	φ$_7$	-59.4	-160.5	-84.7	ψ$_7$	-25.4	167.7	66.6	2.08	1.98
	φ$_8$	-70.7	-158.2	-84.4	ψ$_8$	-8.3	167.0	66.2	2.13	1.99
	φ$_9$	-101.2	-158.9	-84.6	ψ$_9$	9.1	165.6	69.6		2.01
	φ$_1$	-65.3	-158.6	-82.3	ψ$_1$	-25.3	167.0	69.4	2.04	1.98
	φ$_2$	-58.9	-158.7	-83.6	ψ$_2$	-22.1	166.4	67.4	2.13	1.96
	φ$_3$	-60.0	-160.5	-83.5	ψ$_3$	-28.8	167.9	67.4	2.18	1.96
	φ$_4$	-69.8	-158.7	-82.9	ψ$_4$	-27.3	167.4	66.9	2.23	1.96
AcAla$_4$ThrAla$_4$NHMe	φ$_5$	-75.7	-133.0	-82.7	ψ$_5$	-45.8	173.3	59.4	2.15	1.92
	φ$_6$	-57.2	-157.7	-83.1	ψ$_6$	-32.6	168.2	68.0	2.09	1.99
	φ$_7$	-58.8	-159.0	-85.4	ψ$_7$	-25.4	167.7	66.6	2.07	1.98
	φ$_8$	-70.3	-159.5	-84.2	ψ$_8$	-8.3	167.0	66.2	2.12	1.99
	φ$_9$	-101.1	-158.7	-84.6	ψ$_9$	9.1	165.6	69.6		2.00
AcAla$_4$PheAla$_4$NHMe	φ$_1$	-65.0	-158.9	-82.3	ψ$_1$	-25.5	166.4	69.6	2.04	1.98

	φ_2	-58.5	-159.1	-83.5	ψ_2	-23.0	167.1	66.1	2.11	1.96
	φ_3	-59.1	-158.1	-83.8	ψ_3	-30.6	166.1	67.1	2.21	1.96
	φ_4	-68.4	-161.0	-83.4	ψ_4	-29.5	168.2	66.0	2.21	1.95
	φ_5	-72.4	-158.1	-84.8	ψ_5	-45.2	155.7	73.2	2.17	2.00
	φ_6	-57.9	-161.2	-85.4	ψ_6	-32.4	163.3	66.3	2.14	1.98
	φ_7	-59.8	-159.2	-83.5	ψ_7	-25.6	166.4	66.7	2.08	1.96
	φ_8	-70.0	-159.4	-84.5	ψ_8	-9.2	167.3	66.4	2.12	1.99
	φ_9	-101.8	-159.0	-84.6	ψ_9	9.8	165.2	69.4		2.00
	φ_1	-65.0	-158.6	-82.6	ψ_1	-25.6	166.6	68.5	2.04	1.98
	φ_2	-58.4	-158.7	-83.9	ψ_2	-23.5	166.7	65.6	2.12	1.97
	φ_3	-59.4	-158.8	-83.7	ψ_3	-30.1	167.5	66.6	2.22	1.96
	φ_4	-67.9	-159.9	-83.7	ψ_4	-30.4	168.4	66.0	2.19	1.95
AcAla4TyrAla4NHMe	φ_5	-72.9	-154.9	-84.8	ψ_5	-44.5	175.2	72.5	2.17	1.99
	φ_6	-58.0	-149.2	-85.6	ψ_6	-32.3	175.8	66.8	2.12	1.99
	φ_7	-59.8	-159.1	-83.6	ψ_7	-25.4	166.1	66.4	2.09	1.96
	φ_8	-70.9	-159.3	-84.5	ψ_8	-8.0	166.6	66.7	2.13	1.99
	φ_9	-102.0	-158.7	-84.6	ψ_9	9.6	165.7	69.4		2.00
	φ_1	-62.8	-158.4	-82.3	ψ_1	-30.8	167.3	69.85	2.07	1.98
	φ_2	-57.6	-157.7	-83.4	ψ_2	-31.8	166.4	67.83	2.32	1.97
	φ_3	-65.4	-159.8	-83.6	ψ_3	-40.1	168.3	68.25	2.19	1.96
	φ_4	-64.5	-157.7	-82.5	ψ_4	-39.8	166.3	68.37	2.10	1.94
AcAla4AsnAla4NHMe	φ_5	-61.6	-165.0	-83.0	ψ_5	-39.0	177.1	65.42	2.17	1.96
	φ_6	-68.1	-155.5	-82.9	ψ_6	-39.4	158.0	64.79	2.47	1.98
	φ_7	-61.5	-157.9	-85.4	ψ_7	-29.3	166.6	66.69	2.12	1.97
	φ_8	-68.4	-159.1	-84.3	ψ_8	-9.9	167.4	65.67	2.11	1.98
	φ_9	-99.5	-158.3	-84.7	ψ_9	7.5	165.0	69.55		2.00
	φ_1	-63.2	-158.8	-82.2	ψ_1	-30.4	166.7	69.6	2.07	1.98
	φ_2	-57.4	-158.7	-83.7	ψ_2	-31.9	166.2	67.3	2.28	1.98
	φ_3	-65.4	-159.5	-83.0	ψ_3	-38.7	166.5	69.8	2.24	1.97
	φ_4	-65.6	-158.7	-82.2	ψ_4	-39.7	165.4	58.0	2.16	1.88
AcAla4GlnAla4NHMe	φ_5	-61.8	-156.2	-88.3	ψ_5	-39.4	162.9	60.4	2.12	2.00
	φ_6	-67.3	-160.6	-83.8	ψ_6	-42.2	163.5	65.2	2.31	1.97
	φ_7	-61.5	-160.5	-83.6	ψ_7	-31.7	166.3	67.6	2.15	1.97
	φ_8	-69.8	-158.9	-84.5	ψ_8	-8.5	166.2	66.9	2.12	1.99
	φ_9	-99.5	-159.0	-84.6	ψ_9	6.6	165.6	69.3		2.00
	φ_1	-65.0	-158.9	-82.3	ψ_1	-25.5	166.4	69.6	2.04	1.98
	φ_2	-58.5	-159.1	-83.5	ψ_2	-23.0	167.1	66.1	2.11	1.96
	φ_3	-59.1	-158.1	-83.8	ψ_3	-30.6	166.1	67.1	2.21	1.96
	φ_4	-68.4	-161.0	-83.4	ψ_4	-29.5	168.2	66.0	2.21	1.95
AcAla4PheAla4NHMe	φ_5	-72.4	-158.1	-84.8	ψ_5	-45.2	155.7	73.2	2.17	2.00
	φ_6	-57.9	-161.2	-85.4	ψ_6	-32.4	163.3	66.3	2.14	1.98
	φ_7	-59.8	-159.2	-83.5	ψ_7	-25.6	166.4	66.7	2.08	1.96
	φ_8	-70.0	-159.4	-84.5	ψ_8	-9.2	167.3	66.4	2.12	1.99
	φ_9	-101.8	-159.0	-84.6	ψ_9	9.8	165.2	69.4		2.00
	φ_1	-65.2	-158.5	-82.3	ψ_1	-25.6	166.5	69.1	2.03	1.97
	φ_2	-58.2	-159.5	-83.6	ψ_2	-23.5	167.3	66.5	2.13	1.96
	φ_3	-57.9	-158.4	-83.8	ψ_3	-31.5	166.8	68.1	2.17	1.96
	φ_4	-65.7	-160.0	-83.1	ψ_4	-33.0	168.0	65.6	2.21	1.93
AcAla4CysAla4NHMe	φ_5	-72.7	-159.9	-84.7	ψ_5	-39.3	164.4	68.2	2.21	1.97
	φ_6	-60.8	-162.4	-84.6	ψ_6	-31.7	162.3	66.3	2.25	1.99
	φ_7	-60.9	-159.8	-84.2	ψ_7	-25.3	167.3	66.6	2.09	1.97
	φ_8	-71.5	-159.4	-84.6	ψ_8	-6.9	167.0	67.6	2.16	2.00

	φ_9	-101.7	-159.5	-84.7	ψ_9	8.9	166.0	69.0		2.00
AcAla4MetAla4NHMe	φ_1	-65.5	-158.5	-82.2	ψ_1	-24.9	167.1	69.3	2.04	1.98
	φ_2	-58.9	-158.2	-83.6	ψ_2	-21.8	166.3	66.9	2.13	1.97
	φ_3	-58.7	-159.0	-83.9	ψ_3	-28.4	167.1	67.0	2.15	1.96
	φ_4	-66.5	-158.2	-83.0	ψ_4	-32.2	167.3	68.1	==2.20==	1.95
	φ_5	-74.4	-157.0	-84.9	ψ_5	-38.5	152.6	72.3	==2.20==	2.00
	φ_6	-61.6	-155.7	-84.3	ψ_6	-32.3	170.4	69.8	2.16	1.99
	φ_7	-60.1	-158.6	-82.8	ψ_7	-25.4	167.7	66.8	2.09	1.95
	φ_8	-72.9	-159.3	-84.6	ψ_8	-5.1	168.3	66.8	2.15	1.99
	φ_9	-102.4	-157.8	-84.6	ψ_9	9.3	165.6	69.2		2.00
AcAla4HidAla4NHMe	φ_1	-62.7	--	-82.3	ψ_1	-31.4	--	69.0	2.07	1.97
	φ_2	-58.1	--	-83.7	ψ_2	-32.6	--	66.2	==2.38==	1.96
	φ_3	-65.6	--	-83.7	ψ_3	-40.0	--	67.5	==2.12==	1.95
	φ_4	-64.1	--	-83.2	ψ_4	-40.7	--	67.8	==2.18==	1.93
	φ_5	-63.6	--	-84.7	ψ_5	-36.4	--	63.3	2.51	1.91
	φ_6	-68.8	--	-85.7	ψ_6	-39.2	--	68.8	2.13	2.04
	φ_7	-61.8	--	-83.7	ψ_7	-29.1	--	66.9	2.11	1.98
	φ_8	-68.4	--	-84.6	ψ_8	-9.9	--	66.9		2.00
	φ_9	-99.8	--	-84.8	ψ_9	7.6	--	69.3		2.01
AcAla4HieAla4NHMe	φ_1	-63.7	-159.0	-82.3	ψ_1	-29.2	165.9	69.2	2.07	1.98
	φ_2	-57.9	-159.4	-83.8	ψ_2	-30.1	167.3	66.5	2.25	1.97
	φ_3	-66.9	-158.1	-83.8	ψ_3	-37.5	166.0	67.9	==2.28==	1.97
	φ_4	-66.0	-161.4	-83.1	ψ_4	-39.8	168.3	69.1	==2.06==	1.96
	φ_5	-59.8	-158.0	-84.3	ψ_5	-46.2	156.4	71.1	==2.25==	1.96
	φ_6	-61.5	-157.4	-84.7	ψ_6	-36.6	168.8	64.7	2.32	1.95
	φ_7	-61.5	-158.9	-84.2	ψ_7	-26.5	166.2	66.8	2.10	1.97
	φ_8	-71.1	-159.2	-84.2	ψ_8	-6.9	167.2	66.4	2.13	1.98
	φ_9	-100.5	-159.1	-84.9	ψ_9	8.0	165.3	69.7		2.01
AcAla4TrpAla4NHMe	φ_1	-63.9	-158.5	-82.3	ψ_1	-29.1	167.2	69.1	2.07	1.97
	φ_2	-57.4	-158.2	-83.8	ψ_2	-31.0	166.3	66.5	2.27	1.97
	φ_3	-67.2	-159.1	-83.9	ψ_3	-36.7	167.2	67.2	==2.32==	1.96
	φ_4	-66.6	-158.1	-83.3	ψ_4	-39.6	167.6	66.8	==2.07==	1.95
	φ_5	-60.4	-159.3	-83.8	ψ_5	-46.9	146.3	78.8	2.21	2.02
	φ_6	-60.8	-159.7	-84.7	ψ_6	-37.5	168.5	67.1	2.32	1.96
	φ_7	-60.7	-161.8	-83.6	ψ_7	-28.2	166.1	65.6	2.09	1.96
	φ_8	-72.6	-158.1	-84.3	ψ_8	-5.3	165.6	66.8	2.14	1.99
	φ_9	-102.0	-159.6	-84.7	ψ_9	8.7	165.1	69.3		2.00
AcAla13NH2	φ_1	-63.4	-158.5	-82.1	ψ_1	-29.6	167.8	69.6	2.05	1.98
	φ_2	-56.5	-157.9	-83.6	ψ_2	-32.3	167.2	66.8	2.24	1.96
	φ_3	-65.5	-159.2	-83.7	ψ_3	-36.2	167.5	66.7	==2.38==	1.96
	φ_4	-66.0	-159.0	-83.8	ψ_4	-40.1	168.3	67.7	==2.08==	1.96
	φ_5	-61.1	-158.3	-83.9	ψ_5	-43.1	167.4	65.7	==2.12==	1.94
	φ_6	-61.5	-160.5	-83.5	ψ_6	-42.9	168.3	66.4	==2.10==	1.95
	φ_7	-61.3	-158.2	-83.9	ψ_7	-43.0	166.8	67.1	==2.09==	1.95
	φ_8	-61.8	-160.9	-83.6	ψ_8	-42.0	168.7	66.2	==2.12==	1.94
	φ_9	-61.1	-158.2	-84.1	ψ_9	-42.3	166.9	67.0	==2.12==	1.96
	φ_{10}	-65.4	-160.8	-83.9	ψ_{10}	-36.2	168.2	66.1	==2.28==	1.95
	φ_{11}	-67.8	-158.1	-83.8	ψ_{11}	-31.2	166.8	67.1	==2.02==	1.96
	φ_{12}	-94.1	-159.5	-84.3	ψ_{12}	-23.6	167.5	66.5	==2.13==	1.98
	φ_{13}	-139.4	-158.3	-83.6	ψ_{13}	11.4	168.4	71.6		2.00
Ac(Ala2GlnAla2)3NH2	φ_1	-64.6	-158.2	-82.0	ψ_1	-24.7	166.3	70.2	2.06	1.98
	φ_2	-53.7	-158.6	-83.4	ψ_2	-28.1	167.2	66.4	2.15	1.95

							R(O···H)	
φ_3	-66.1	-154.9	-85.2	ψ_3	-25.1	157.3	67.2	2.15	1.95
φ_4	-69.6	-141.0	-84.1	ψ_4	-25.9	173.5	65.2	2.09	1.95
φ_5	-78.9	-157.8	-84.1	ψ_5	-44.1	168.4	67.4	2.05	1.97
φ_6	-56.3	-158.3	-83.3	ψ_6	-38.4	169.0	67.1	2.38	1.95
φ_7	-61.5	-158.1	-83.7	ψ_7	-36.3	168.5	66.3	2.24	1.94
φ_8	-66.4	-155.6	-84.3	ψ_8	-42.0	158.3	67.0	2.04	1.93
φ_9	-61.8	-140.2	-84.6	ψ_9	-43.3	171.1	65.6	2.14	1.96
φ_{10}	-63.5	-160.4	-83.9	ψ_{10}	-34.3	167.5	66.3	1.98	1.96
φ_{11}	-58.5	-159.0	-83.9	ψ_{11}	-30.0	167.8	66.1	2.04	1.96
φ_{12}	-68.4	-159.0	-83.7	ψ_{12}	-15.6	167.1	65.1	2.13	1.94
φ_{13}	-78.4	-156.9	-84.9	ψ_{13}	-10.7	158.6	67.5		1.96
φ_{14}	-106.0	-144.3	-84.7	ψ_{14}	-32.4	171.9	64.9		1.98
φ_{15}	-134.2	-159.3	-83.9	ψ_{15}	9.5	168.4	71.4		2.01

In Table S3, R(O···H) is the hydrogen bond length in Å. The 10-membered-ring hydrogen bonds formed between backbone O and H atoms are denoted by white background. The 13-membered-ring hydrogen bonds formed between two backbone atoms are denoted by yellow background. It can be seen from Table S3 that there exist both 10-membered-ring and 13-membered-ring hydrogen bonds for the helix conformers, indicating that these helices are neither pure α-helices nor pure 3$_{10}$-helices..

antiparallel Gly tripeptide

parallel Gly tripeptide

antiparallel Gly pentapeptide

parallel Gly pentapeptide

antiparallel Ala tripeptide

parallel Ala tripeptide

antiparallel Ala tetrapeptide

parallel Ala tetrapeptide
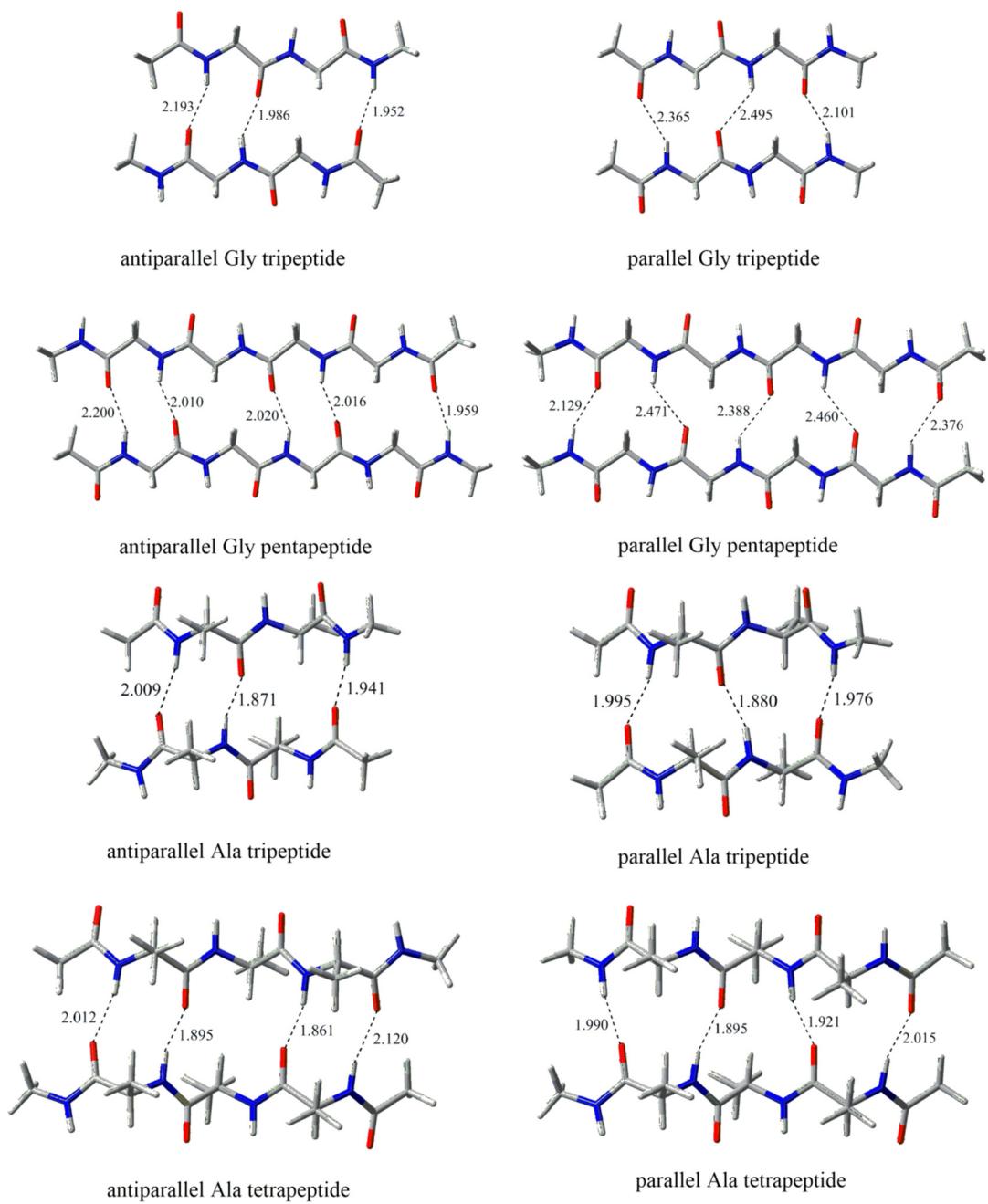
Figure S4. The hydrogen-bonded dimers. All distances are in Å.

Table S4. Physical components of the interaction energy (*IE*) for eight hydrogen-bonded dimers.

Dimers	AMBER99sb			AMOEBAbio18			This work		
	IE	*IE*$_{elec}$	*IE*$_{vdw}$	*IE*	*IE*$_{elec}$	*IE*$_{vdw}$	*IE*	*IE*$_{elec}$	*IE*$_{vdw}$
antiparallel Gly tripeptide	-21.77	-18.37	-3.40	-21.54	-22.84	1.29	-22.62	-18.86	-3.76
parallel Gly tripeptide	-15.31	-14.78	-0.53	-15.61	-15.34	-0.27	-17.25	-15.30	-1.95
antiparallel Gly pentapeptide	-36.08	-29.51	-6.57	-36.10	-37.64	1.54	-36.26	-29.38	-6.88
parallel Gly pentapeptide	-25.34	-23.70	-1.63	-26.42	-25.32	-1.10	-27.30	-23.84	-3.46
antiparallel Ala tripeptide	-23.34	-19.93	-3.41	-23.10	-26.32	3.22	-24.61	-21.22	-3.39
parallel Ala tripeptide	-22.92	-19.49	-3.44	-21.17	-23.79	2.62	-24.88	-21.28	-3.60
antiparallel Ala tetrapeptide	-29.12	-23.59	-5.53	-29.60	-32.41	2.81	-30.12	-24.66	-5.46
parallel Ala tetrapeptide	-30.20	-25.78	-4.42	-28.47	-31.86	3.39	-32.46	-27.61	-4.86

IE$_{elec}$ represents the electrostatic interaction energy, *IE*$_{vdw}$ represents the van der Waals interaction energy. All energies are in kcal/mol.

Table S5. Cartesian coordinates in angstroms for Cluster A and B, 28 glycine tetrapeptide conformers, 51 alanine tetrapeptide conformers, AcAla4XAla4NHMe (X=Val, Ile, Leu, Asn, Gln, Ser, Thr, Phe, Cys, Met, Hid, Hie, Trp and Tyr), AcAla13NH2, Ac(Ala2GlnAla2)3NH2 and hydrogen-bonded dimers.

H	7.428125	-5.736182	2.448523			Cluster A		
O	6.930235	-9.082793	2.721394		C	6.302080	-7.386495	-1.169027
H	6.840812	-8.296750	2.202163		C	7.321943	-6.638735	-0.277317
H	7.852764	-9.244880	2.518455		N	8.177252	-5.779331	-0.879713
O	12.413877	-4.817676	4.379024		O	7.251651	-6.898668	0.955201
H	13.027583	-4.857954	3.596039		C	9.170686	-4.965645	-0.101378
H	12.916836	-4.286894	5.067079		C	10.403180	-5.652339	0.559308
O	9.694455	-4.479460	5.203573		N	10.248867	-6.938369	0.823622
H	9.158254	-4.881459	4.504486		O	11.521173	-5.051384	0.665163
H	10.579847	-4.773380	4.927083		C	11.148831	-7.712026	1.681810
O	8.599703	-5.173472	-4.408102		C	10.784546	-9.153755	1.547068
H	7.824540	-4.742767	-4.847238		N	11.784927	-9.995402	1.171062
H	8.474138	-6.079500	-4.771272		O	9.645513	-9.477291	1.758791
O	8.054009	-2.945469	3.230178		C	11.830621	-11.458715	1.471327
H	7.894160	-2.102845	3.754876		C	11.000873	-12.245001	0.384262
H	8.340329	-2.646981	2.395533		N	10.612006	-11.613164	-0.674912
O	8.570575	-7.731266	-5.197466		O	10.462752	-13.315189	0.600634
H	7.654327	-7.922488	-5.420649		H	6.045551	-8.275584	-0.633369
H	8.712941	-8.275055	-4.416252		H	6.591146	-7.684718	-2.156745
O	12.377161	-9.595068	4.859796		H	5.502663	-6.682782	-1.392112
H	12.405215	-8.697690	5.251341		H	8.122831	-5.604404	-1.898743
H	11.401476	-9.693684	4.794373		H	9.561310	-4.212686	-0.799625
O	4.661790	-5.969657	3.933004		H	8.713655	-4.503766	0.711170
H	5.661536	-6.048906	3.836576		H	9.425428	-7.421759	0.518542
H	4.572207	-5.024243	4.072036		H	12.213445	-7.529663	1.396897
O	10.652834	-1.949144	-0.827218		H	10.982484	-7.386537	2.729375
H	9.745921	-1.784004	-0.532473		H	12.687644	-9.596204	0.903637
H	10.476395	-2.160406	-1.723586		H	12.807709	-11.934415	1.445797
O	13.787652	-10.292543	7.173515		H	11.381023	-11.638442	2.418879
H	13.293494	-9.570550	7.474343		H	10.865320	-10.609670	-0.839404
H	13.442597	-10.469542	6.279317		H	9.917002	-12.037994	-1.243737
O	12.894899	-11.784639	-3.455633		O	11.104209	-5.319346	-3.440043
H	13.672856	-11.749215	-2.954780		H	10.244940	-5.279256	-3.883518
H	13.219766	-12.106971	-4.344629		H	11.728181	-5.405517	-4.193522
O	6.697679	-8.130031	5.476412		O	13.504079	-13.441606	-1.062576
H	6.465719	-7.336212	4.979129		H	13.202344	-13.859469	-0.282367
H	6.289182	-8.824942	4.916137		H	13.509311	-12.507758	-0.918408
O	12.452970	-6.935420	-1.948327		O	8.465976	-13.241327	2.738740
H	13.324602	-6.546706	-2.095047		H	9.216123	-13.409470	2.136565
H	11.870047	-6.337453	-2.421172		H	8.001368	-14.069650	2.812919
O	4.768359	-3.904768	1.543483		O	11.428506	-7.104432	5.731743
H	5.033198	-3.041879	1.196948		H	11.710004	-6.387488	5.196702
H	4.650383	-3.734135	2.513353		H	10.998504	-6.691315	6.536577
O	6.232950	-12.094996	2.034114		O	6.039739	-8.310659	-5.000306
H	7.089479	-12.533939	2.296277		H	5.561625	-7.539509	-5.353748
H	6.105209	-12.449960	1.159826		H	5.640537	-8.282376	-4.121546
O	8.158667	-12.101521	-2.402201		O	7.451729	-5.614892	3.386289
H	7.402036	-12.658624	-2.429643		H	7.514444	-4.615983	3.420495
H	7.902242	-11.556860	-1.670815					

H	10.867554	0.199428	5.034044
H	11.385114	1.888062	5.018278
O	11.315079	-3.592515	-1.366748
H	10.721377	-3.676065	-0.585791
H	10.959981	-2.833011	-1.834290
O	3.113263	4.558958	2.031779
H	3.945708	4.998747	2.023437
H	3.123287	3.914944	1.305239
O	7.545300	-1.606277	6.408733
H	7.034466	-1.318159	5.588899
H	8.491407	-1.569348	6.114493
O	4.993031	8.955975	-3.555734
H	5.421037	8.630045	-4.338141
H	5.791458	9.285748	-3.138565
O	6.097576	-0.663939	4.473505
H	5.182686	-1.117884	4.410736
H	5.796220	0.222166	4.569134
O	10.736773	5.134732	-1.009684
H	10.015237	4.543790	-1.290519
H	10.434791	5.998500	-1.305867
O	10.794023	4.098817	5.160318
H	11.286016	4.904158	5.314705
H	10.355045	4.321028	4.284609
O	5.535123	-0.446433	0.496344
H	5.699484	-0.383820	-0.470418
H	4.678129	-0.859360	0.530089
O	12.445054	3.098087	0.158133
H	12.139778	2.804618	1.045480
H	11.904993	3.951911	-0.046640
O	12.436559	2.187944	6.917008
H	12.378355	2.512605	7.817063
H	11.903218	2.846782	6.458806
O	12.202055	-0.140491	-1.351461
H	12.839485	-0.817416	-1.159456
H	12.683978	0.636416	-1.734878
O	9.898352	4.978490	2.252537
H	9.686741	4.070348	2.209024
H	9.094382	5.454365	2.634079
O	6.662616	5.016120	-4.632396
H	6.978794	5.933200	-4.726880
H	5.867231	5.122914	-4.061991
O	8.956953	2.992523	6.555815
H	9.573548	3.560366	6.143733
H	8.254459	3.574797	6.797130
O	10.022757	5.177279	-4.660873
H	10.059238	4.951926	-5.588637
H	9.700142	4.331272	-4.282337
O	1.971732	6.710568	0.435800
H	2.460868	6.138767	0.998770
H	1.041072	6.442334	0.726460
O	7.764423	0.703224	8.083678
H	8.161753	1.187369	7.340018
H	7.711380	-0.246990	7.866874

O	9.521392	-2.352520	-3.365683
H	9.555928	-3.305505	-3.535092
H	9.043118	-1.963659	-4.098993
O	7.641703	-10.840596	-0.150839
H	6.918301	-10.247130	0.223366
H	8.204502	-10.993592	0.617016
O	11.803533	-9.509215	-1.867828
H	11.974662	-8.540258	-1.923447
H	12.356749	-9.826632	-2.602737
O	13.428031	-3.234547	-0.740111
H	13.103840	-3.913041	-0.160066
H	12.667971	-2.676579	-1.045895
O	8.927948	-9.601405	-3.186161
H	9.612526	-9.693578	-2.557523
H	8.404236	-10.393870	-3.013173
O	11.124517	-13.791954	-3.333548
H	11.417116	-12.976745	-2.952904
H	10.894732	-13.513032	-4.238652
O	10.320041	-12.043584	4.469978
H	10.097326	-12.097727	5.412137
H	9.399218	-12.161576	4.181204
O	5.143562	-4.011618	-1.380518
H	4.587826	-3.915217	-0.602964
H	5.925908	-3.531303	-1.121910

Cluster B

C	6.355813	7.275061	-0.530067
C	6.213335	5.906639	-0.056199
N	6.228787	4.979980	-1.023214
O	5.877260	5.666779	1.105990
C	6.350798	3.524820	-0.868046
C	7.728901	2.796785	-1.085297
N	7.732334	1.506967	-0.708224
O	8.692941	3.426604	-1.528569
C	8.973662	0.735443	-0.546176
C	9.254637	0.320685	0.916655
N	10.512865	-0.067613	1.198251
O	8.333873	0.362452	1.748433
C	10.990427	-0.244781	2.523580
C	11.297086	1.054485	3.251610
N	11.119381	1.003125	4.538479
O	11.531900	2.048363	2.585299
H	6.280536	7.938035	0.318556
H	5.674128	7.434139	-1.388746
H	7.356365	7.408882	-0.960835
H	6.448542	5.325314	-1.958454
H	5.837908	3.307043	0.036586
H	5.699021	2.996653	-1.542339
H	6.855499	1.215608	-0.379579
H	8.932435	-0.092485	-1.194091
H	9.788224	1.303864	-0.955183
H	11.208844	-0.093321	0.449357
H	10.217148	-0.705045	3.068693
H	11.786444	-0.941023	2.562816

N	0.152000	1.009000	2.451000		O	2.702832	3.656984	-2.297571
H	0.947000	1.602000	2.342000		H	3.075989	4.511471	-2.617015
C	-1.073000	1.584000	2.971000		H	1.751364	3.646194	-2.469734
H	-1.722000	0.778000	3.286000		O	2.648545	2.530973	0.162011
H	-0.842000	2.211000	3.819000		H	2.563561	1.596874	-0.001688
C	-1.783000	2.462000	1.947000		H	2.714836	2.968796	-0.707284
O	-1.937000	3.643000	2.136000		O	10.064997	2.098539	-3.454155
N	-2.192000	1.838000	0.827000		H	9.598025	2.654989	-2.757979
H	-2.021000	0.860000	0.733000		H	9.355308	1.523914	-3.732647
C	-2.722000	2.575000	-0.304000		O	7.346761	3.991353	2.638074
H	-3.273000	1.894000	-0.936000		H	6.682933	3.341356	2.497000
H	-3.383000	3.351000	0.055000		H	6.962068	4.779361	2.238042
C	-1.583000	3.160000	-1.138000		O	12.651494	-3.213804	1.884144
O	-1.168000	2.581000	-2.111000		H	13.459010	-3.137704	2.473945
N	-1.085000	4.323000	-0.689000		H	12.843142	-2.456582	1.335297
H	-1.379000	4.625000	0.214000		O	10.024563	-1.873309	5.388304
C	0.112000	4.908000	-1.258000		H	10.309292	-2.321688	4.553274
H	0.076000	4.826000	-2.334000		H	10.887503	-1.950199	5.859498
H	0.152000	5.955000	-0.986000		O	7.863533	0.318779	-4.074117
H	1.010000	4.416000	-0.898000		H	7.603964	0.770985	-4.933744

Glycine tetrapeptide_02

H	3.870000	2.470000	-0.268000		H	8.438106	-0.473501	-4.316939
C	3.736000	1.432000	0.018000		O	10.078172	-1.592151	-3.567632
H	3.925000	0.793000	-0.836000		H	10.668849	-0.948181	-3.073829
H	4.444000	1.206000	0.805000		H	10.613301	-1.782454	-4.354365
C	2.345000	1.273000	0.571000		O	9.928119	7.663160	-2.145275
O	2.027000	1.729000	1.648000		H	9.212567	8.262818	-1.970629
N	1.449000	0.614000	-0.194000		H	10.637394	8.129479	-2.545957
H	1.677000	0.410000	-1.139000		O	5.999184	1.549003	2.103643
C	0.062000	0.519000	0.210000		H	5.587381	0.682085	1.882814
H	-0.435000	-0.188000	-0.441000		H	6.938766	1.299873	2.087769
H	0.012000	0.155000	1.227000		O	2.797888	9.286272	-0.281346
C	-0.638000	1.864000	0.045000		H	3.471538	9.276860	0.462598
O	-0.875000	2.301000	-1.046000		H	2.292796	8.513215	0.001342
N	-0.942000	2.521000	1.190000		O	4.420023	2.101187	-3.439751
H	-0.549000	2.174000	2.035000		H	3.780304	2.851833	-3.350258
C	-1.411000	3.884000	1.151000		H	4.244977	1.789408	-4.328720
H	-2.101000	4.002000	0.330000		O	13.592272	-0.157390	6.481155
H	-1.939000	4.110000	2.069000		H	14.377490	0.029687	5.866942
C	-0.336000	4.951000	0.972000		H	13.200698	0.751969	6.599603
O	-0.658000	6.064000	0.636000		Glycine tetrapeptide_01			
N	0.932000	4.603000	1.245000		H	1.154000	1.768000	-2.273000
H	1.166000	3.659000	1.462000		C	2.117000	1.386000	-1.949000
C	2.026000	5.543000	1.113000		H	2.368000	0.512000	-2.538000
H	1.688000	6.524000	1.420000		H	2.865000	2.153000	-2.098000
H	2.836000	5.221000	1.751000		C	2.038000	1.075000	-0.476000
C	2.558000	5.575000	-0.318000		O	2.277000	1.893000	0.377000
O	3.559000	4.977000	-0.625000		N	1.664000	-0.188000	-0.156000
N	1.827000	6.295000	-1.184000		H	1.333000	-0.795000	-0.870000
H	0.939000	6.628000	-0.875000		C	1.506000	-0.598000	1.222000
C	2.132000	6.305000	-2.598000		H	1.532000	-1.677000	1.270000
H	3.194000	6.445000	-2.741000		H	2.323000	-0.194000	1.803000
H	1.840000	5.378000	-3.083000		C	0.157000	-0.156000	1.776000
					O	-0.836000	-0.815000	1.588000

H	-2.442000	-0.664000	1.456000
H	-2.106000	-2.092000	0.477000
C	-1.936000	-2.361000	2.598000
O	-2.600000	-1.974000	3.530000
N	-1.305000	-3.545000	2.584000
H	-0.737000	-3.769000	1.795000
C	-1.399000	-4.488000	3.681000
H	-2.406000	-4.460000	4.079000
H	-1.195000	-5.478000	3.301000
C	-0.395000	-4.228000	4.802000
O	0.487000	-5.009000	5.041000
N	-0.579000	-3.089000	5.492000
H	-1.325000	-2.485000	5.226000
C	0.325000	-2.707000	6.554000
H	1.339000	-2.599000	6.187000
H	-0.004000	-1.761000	6.962000
H	0.332000	-3.448000	7.344000

Glycine tetrapeptide_05

H	-0.127000	2.409000	-1.487000
C	0.952000	2.296000	-1.517000
H	1.247000	2.143000	-2.550000
H	1.417000	3.193000	-1.136000
C	1.380000	1.127000	-0.663000
O	2.115000	1.247000	0.283000
N	0.882000	-0.079000	-1.027000
H	0.235000	-0.136000	-1.779000
C	1.246000	-1.300000	-0.337000
H	1.093000	-2.137000	-1.002000
H	2.290000	-1.247000	-0.058000
C	0.378000	-1.543000	0.893000
O	-0.500000	-2.371000	0.883000
N	0.652000	-0.772000	1.959000
H	1.317000	-0.036000	1.851000
C	-0.088000	-0.880000	3.199000
H	-0.320000	-1.922000	3.379000
H	0.526000	-0.508000	4.006000
C	-1.376000	-0.063000	3.209000
O	-1.524000	0.856000	3.978000
N	-2.311000	-0.436000	2.320000
H	-2.138000	-1.243000	1.761000
C	-3.529000	0.321000	2.109000
H	-3.306000	1.377000	2.207000
H	-3.888000	0.126000	1.109000
C	-4.668000	-0.042000	3.059000
O	-5.700000	-0.495000	2.639000
N	-4.441000	0.199000	4.361000
H	-3.568000	0.596000	4.628000
C	-5.442000	-0.100000	5.360000
H	-5.060000	0.191000	6.330000
H	-6.360000	0.442000	5.166000
H	-5.674000	-1.159000	5.377000

Glycine tetrapeptide_06

H	1.601000	7.125000	-3.064000

Glycine tetrapeptide_03

H	1.825000	3.410000	-0.559000
C	1.815000	2.458000	-1.071000
H	0.909000	2.358000	-1.657000
H	2.668000	2.427000	-1.742000
C	1.972000	1.355000	-0.048000
O	2.665000	1.484000	0.923000
N	1.280000	0.219000	-0.318000
H	0.806000	0.133000	-1.192000
C	1.453000	-0.986000	0.456000
H	2.112000	-1.695000	-0.031000
H	1.883000	-0.718000	1.412000
C	0.133000	-1.706000	0.674000
O	0.043000	-2.901000	0.547000
N	-0.916000	-0.930000	1.026000
H	-0.801000	0.055000	0.942000
C	-2.269000	-1.449000	1.036000
H	-2.244000	-2.473000	1.383000
H	-2.880000	-0.854000	1.699000
C	-2.858000	-1.347000	-0.364000
O	-3.652000	-0.497000	-0.661000
N	-2.372000	-2.238000	-1.266000
H	-1.590000	-2.791000	-0.988000
C	-2.532000	-1.952000	-2.663000
H	-2.223000	-2.817000	-3.239000
H	-3.575000	-1.763000	-2.877000
C	-1.674000	-0.769000	-3.111000
O	-0.651000	-0.478000	-2.542000
N	-2.101000	-0.126000	-4.209000
H	-3.023000	-0.303000	-4.534000
C	-1.392000	1.021000	-4.740000
H	-0.337000	0.797000	-4.810000
H	-1.771000	1.239000	-5.730000
H	-1.520000	1.897000	-4.112000

Glycine tetrapeptide_04

H	0.581000	1.890000	-2.433000
C	1.277000	2.217000	-1.667000
H	2.263000	2.290000	-2.115000
H	0.975000	3.184000	-1.297000
C	1.287000	1.238000	-0.517000
O	0.966000	1.549000	0.602000
N	1.672000	-0.023000	-0.822000
H	1.890000	-0.253000	-1.763000
C	1.805000	-1.056000	0.185000
H	2.495000	-1.806000	-0.170000
H	2.194000	-0.614000	1.093000
C	0.487000	-1.766000	0.477000
O	0.308000	-2.913000	0.147000
N	-0.439000	-1.033000	1.117000
H	-0.217000	-0.088000	1.348000
C	-1.789000	-1.514000	1.336000

O	-1.779000	-3.213000	3.722000
N	-2.411000	-1.476000	2.447000
H	-2.312000	-1.033000	1.560000
C	-3.312000	-0.898000	3.427000
H	-4.025000	-0.273000	2.910000
H	-3.839000	-1.696000	3.934000
C	-2.607000	-0.010000	4.451000
O	-2.791000	1.178000	4.473000
N	-1.792000	-0.648000	5.308000
H	-1.687000	-1.634000	5.223000
C	-1.055000	0.079000	6.319000
H	-0.341000	0.763000	5.873000
H	-1.725000	0.654000	6.946000
H	-0.521000	-0.633000	6.935000

Glycine tetrapeptide_08

H	2.771000	1.901000	-1.613000
C	3.091000	1.283000	-0.787000
H	3.755000	0.506000	-1.150000
H	3.640000	1.889000	-0.074000
C	1.870000	0.679000	-0.131000
O	0.749000	0.934000	-0.478000
N	2.122000	-0.175000	0.887000
H	3.048000	-0.408000	1.164000
C	1.048000	-0.820000	1.584000
H	0.429000	-0.100000	2.113000
H	0.397000	-1.347000	0.893000
C	1.621000	-1.806000	2.584000
O	2.810000	-1.952000	2.731000
N	0.717000	-2.503000	3.296000
H	-0.251000	-2.313000	3.174000
C	1.100000	-3.554000	4.221000
H	0.277000	-4.246000	4.320000
H	1.958000	-4.075000	3.818000
C	1.419000	-3.044000	5.623000
O	0.741000	-3.373000	6.566000
N	2.487000	-2.238000	5.726000
H	2.988000	-2.004000	4.896000
C	2.948000	-1.716000	6.999000
H	2.837000	-2.485000	7.754000
H	3.991000	-1.456000	6.905000
C	2.213000	-0.449000	7.434000
O	2.774000	0.614000	7.463000
N	0.925000	-0.616000	7.781000
H	0.525000	-1.524000	7.708000
C	0.110000	0.508000	8.187000
H	-0.859000	0.137000	8.498000
H	0.568000	1.034000	9.016000
H	-0.028000	1.214000	7.376000

Glycine tetrapeptide_09

H	2.385000	-1.781000	-3.142000
C	2.516000	-1.828000	-2.071000
H	2.213000	-2.806000	-1.711000

H	1.124000	3.354000	-1.518000
C	2.118000	2.976000	-1.296000
H	2.658000	2.876000	-2.231000
H	2.632000	3.675000	-0.653000
C	2.026000	1.645000	-0.589000
O	2.456000	1.471000	0.523000
N	1.423000	0.652000	-1.282000
H	1.039000	0.846000	-2.178000
C	1.329000	-0.702000	-0.775000
H	1.218000	-1.382000	-1.607000
H	2.240000	-0.940000	-0.240000
C	0.129000	-0.921000	0.140000
O	-0.772000	-1.657000	-0.182000
N	0.156000	-0.258000	1.307000
H	0.945000	0.319000	1.507000
C	-0.963000	-0.266000	2.227000
H	-0.922000	0.627000	2.833000
H	-1.888000	-0.272000	1.662000
C	-0.952000	-1.451000	3.187000
O	-0.825000	-1.283000	4.376000
N	-1.107000	-2.660000	2.626000
H	-1.239000	-2.710000	1.638000
C	-1.009000	-3.890000	3.387000
H	-0.733000	-4.690000	2.716000
H	-0.240000	-3.776000	4.142000
C	-2.319000	-4.308000	4.054000
O	-2.876000	-5.326000	3.739000
N	-2.775000	-3.480000	5.008000
H	-2.256000	-2.655000	5.212000
C	-4.012000	-3.753000	5.706000
H	-3.971000	-4.714000	6.205000
H	-4.170000	-2.979000	6.445000
H	-4.854000	-3.765000	5.023000

Glycine tetrapeptide_07

H	0.862000	3.084000	-2.063000
C	1.525000	2.371000	-2.541000
H	0.984000	1.902000	-3.356000
H	2.389000	2.888000	-2.930000
C	1.988000	1.335000	-1.542000
O	3.139000	1.195000	-1.231000
N	1.011000	0.565000	-1.010000
H	0.057000	0.664000	-1.275000
C	1.322000	-0.459000	-0.056000
H	2.060000	-1.149000	-0.453000
H	1.743000	-0.037000	0.853000
C	0.058000	-1.221000	0.291000
O	-1.014000	-0.938000	-0.186000
N	0.212000	-2.233000	1.165000
H	1.105000	-2.395000	1.571000
C	-0.877000	-3.123000	1.522000
H	-1.500000	-3.277000	0.651000
H	-0.464000	-4.070000	1.837000
C	-1.730000	-2.609000	2.678000

C	-1.064000	-4.684000	3.147000
H	-1.039000	-4.427000	4.199000
H	-1.806000	-4.076000	2.650000
C	-1.503000	-6.138000	2.984000
O	-2.467000	-6.423000	2.324000
N	-0.752000	-7.048000	3.629000
H	0.023000	-6.733000	4.168000
C	-1.051000	-8.460000	3.539000
H	-0.969000	-8.814000	2.518000
H	-0.346000	-9.002000	4.156000
H	-2.056000	-8.666000	3.887000

Glycine tetrapeptide_11

H	2.791000	-1.500000	-0.458000
C	3.276000	-0.540000	-0.332000
H	4.063000	-0.639000	0.409000
H	3.716000	-0.222000	-1.267000
C	2.324000	0.526000	0.145000
O	2.458000	1.689000	-0.143000
N	1.310000	0.102000	0.942000
H	1.345000	-0.826000	1.298000
C	0.444000	1.045000	1.621000
H	0.230000	1.864000	0.950000
H	-0.475000	0.550000	1.898000
C	1.118000	1.532000	2.895000
O	0.867000	1.043000	3.970000
N	2.054000	2.489000	2.736000
H	2.368000	2.664000	1.805000
C	2.973000	2.728000	3.820000
H	3.675000	3.494000	3.515000
H	2.435000	3.085000	4.688000
C	3.765000	1.460000	4.137000
O	4.199000	0.769000	3.256000
N	3.937000	1.185000	5.447000
H	3.433000	1.722000	6.114000
C	4.582000	-0.028000	5.889000
H	5.370000	-0.279000	5.194000
H	5.037000	0.137000	6.858000
C	3.701000	-1.266000	6.023000
O	4.195000	-2.273000	6.458000
N	2.414000	-1.172000	5.659000
H	2.063000	-0.344000	5.234000
C	1.549000	-2.330000	5.714000
H	1.895000	-3.115000	5.049000
H	1.513000	-2.735000	6.717000
H	0.554000	-2.026000	5.417000

Glycine tetrapeptide_12

H	5.058000	-0.958000	-1.972000
C	4.999000	0.039000	-1.561000
H	5.862000	0.223000	-0.929000
H	5.013000	0.766000	-2.367000
C	3.722000	0.162000	-0.760000
O	2.941000	-0.744000	-0.638000

H	3.565000	-1.691000	-1.827000
C	1.677000	-0.745000	-1.429000
O	0.997000	0.012000	-2.068000
N	1.745000	-0.685000	-0.083000
H	2.308000	-1.312000	0.447000
C	1.002000	0.292000	0.660000
H	1.276000	1.301000	0.366000
H	-0.065000	0.193000	0.484000
C	1.287000	0.104000	2.141000
O	2.032000	-0.754000	2.542000
N	0.656000	0.956000	2.963000
H	0.041000	1.663000	2.625000
C	0.838000	0.886000	4.387000
H	0.540000	-0.084000	4.771000
H	1.882000	1.025000	4.653000
C	0.000000	1.970000	5.042000
O	-0.683000	2.723000	4.396000
N	0.076000	2.023000	6.380000
H	0.643000	1.396000	6.907000
C	-0.666000	2.999000	7.130000
H	-0.393000	4.006000	6.832000
H	-1.733000	2.894000	6.954000
C	-0.372000	2.807000	8.609000
O	0.376000	1.949000	8.997000
N	-1.004000	3.656000	9.436000
H	-1.611000	4.345000	9.058000
C	-0.817000	3.589000	10.873000
H	-1.418000	4.361000	11.334000
H	-1.126000	2.625000	11.256000
H	0.222000	3.745000	11.134000

Glycine tetrapeptide_10

H	-0.094000	0.939000	-1.938000
C	0.948000	1.228000	-2.030000
H	1.382000	0.664000	-2.849000
H	1.012000	2.284000	-2.245000
C	1.691000	0.947000	-0.744000
O	2.248000	1.802000	-0.110000
N	1.689000	-0.345000	-0.344000
H	1.238000	-1.060000	-0.868000
C	2.362000	-0.742000	0.858000
H	3.428000	-0.538000	0.801000
H	1.984000	-0.193000	1.716000
C	2.153000	-2.227000	1.080000
O	1.544000	-2.912000	0.295000
N	2.693000	-2.728000	2.206000
H	3.134000	-2.113000	2.851000
C	2.654000	-4.143000	2.524000
H	2.759000	-4.709000	1.607000
H	3.478000	-4.376000	3.180000
C	1.380000	-4.575000	3.244000
O	1.432000	-5.053000	4.351000
N	0.234000	-4.400000	2.567000
H	0.283000	-4.079000	1.624000

C	-3.033000	-5.700000	2.274000		N	3.515000	1.365000	-0.183000
O	-3.376000	-6.781000	2.677000		H	4.158000	2.118000	-0.285000
N	-2.126000	-4.930000	2.894000		C	2.347000	1.619000	0.609000
H	-1.797000	-4.093000	2.467000		H	1.439000	1.501000	0.024000
C	-1.437000	-5.410000	4.072000		H	2.278000	0.922000	1.439000
H	-0.864000	-4.592000	4.489000		C	2.414000	3.038000	1.144000
H	-2.151000	-5.757000	4.808000		O	3.317000	3.786000	0.867000
H	-0.767000	-6.231000	3.839000		N	1.398000	3.404000	1.943000

Glycine tetrapeptide_14

H	2.946000	-0.664000	-3.019000		H	0.659000	2.780000	2.182000
C	3.269000	0.112000	-2.336000		C	1.354000	4.718000	2.520000
H	4.251000	-0.146000	-1.952000		H	2.250000	4.918000	3.099000
H	3.353000	1.052000	-2.863000		H	1.298000	5.482000	1.749000
C	2.331000	0.299000	-1.168000		C	0.136000	4.827000	3.418000
O	2.307000	1.319000	-0.529000		O	-0.642000	3.913000	3.545000
N	1.535000	-0.753000	-0.869000		N	-0.007000	6.001000	4.053000
H	1.647000	-1.609000	-1.360000		H	0.626000	6.742000	3.856000
C	0.617000	-0.721000	0.252000		C	-1.094000	6.260000	4.982000
H	0.223000	0.281000	0.343000		H	-1.305000	5.349000	5.526000
H	-0.192000	-1.412000	0.063000		H	-0.781000	7.025000	5.675000
C	1.289000	-1.162000	1.547000		C	-2.356000	6.771000	4.289000
O	1.145000	-2.278000	1.975000		O	-2.723000	7.906000	4.437000
N	2.049000	-0.231000	2.152000		N	-3.000000	5.875000	3.523000
H	2.180000	0.666000	1.734000		H	-2.627000	4.957000	3.442000
C	2.762000	-0.532000	3.361000		C	-4.188000	6.243000	2.781000
H	2.185000	-1.232000	3.950000		H	-3.970000	7.009000	2.045000
H	3.725000	-1.000000	3.162000		H	-4.564000	5.365000	2.274000
C	3.020000	0.742000	4.143000		H	-4.954000	6.623000	3.445000
O	2.896000	1.832000	3.644000					

Glycine tetrapeptide_13

N	3.431000	0.565000	5.413000		H	2.484000	2.454000	-1.030000
H	3.413000	-0.347000	5.809000		C	1.803000	2.210000	-0.226000
C	3.791000	1.678000	6.274000		H	2.230000	2.522000	0.720000
H	4.482000	1.326000	7.026000		H	0.881000	2.755000	-0.394000
H	4.274000	2.434000	5.670000		C	1.503000	0.732000	-0.288000
C	2.591000	2.272000	7.009000		O	1.268000	0.178000	-1.332000
O	2.476000	2.152000	8.200000		N	1.490000	0.070000	0.890000
N	1.701000	2.917000	6.238000		H	1.635000	0.573000	1.734000
H	1.856000	2.955000	5.256000		C	1.256000	-1.357000	0.975000
C	0.490000	3.475000	6.802000		H	1.738000	-1.843000	0.136000
H	-0.049000	3.991000	6.018000		H	1.684000	-1.728000	1.894000
H	-0.146000	2.700000	7.216000		C	-0.222000	-1.730000	0.991000
H	0.723000	4.178000	7.592000		O	-0.724000	-2.253000	1.957000

Glycine tetrapeptide_15

H	2.490000	1.709000	-1.254000		N	-0.917000	-1.443000	-0.118000
C	3.112000	1.616000	-0.372000		H	-0.427000	-1.112000	-0.921000
H	4.139000	1.443000	-0.663000		C	-2.302000	-1.825000	-0.217000
H	3.071000	2.549000	0.181000		H	-2.883000	-1.320000	0.546000
C	2.673000	0.497000	0.542000		H	-2.672000	-1.514000	-1.186000
O	3.417000	-0.019000	1.332000		C	-2.469000	-3.341000	-0.127000
N	1.375000	0.131000	0.447000		O	-1.788000	-4.076000	-0.784000
H	0.759000	0.538000	-0.218000		N	-3.441000	-3.765000	0.712000
C	0.835000	-0.883000	1.304000		H	-3.863000	-3.099000	1.316000
					C	-3.663000	-5.164000	0.992000
					H	-4.723000	-5.370000	1.059000
					H	-3.264000	-5.741000	0.170000

H	8.819000	-0.714000	-1.478000
C	9.808000	-2.179000	-0.293000
H	10.018000	-2.666000	-1.236000
H	10.739000	-2.020000	0.236000
H	9.183000	-2.831000	0.308000

Glycine tetrapeptide_17

H	1.543000	-0.881000	-2.229000
C	2.347000	-0.500000	-1.608000
H	3.128000	-1.242000	-1.530000
H	2.745000	0.393000	-2.081000
C	1.841000	-0.179000	-0.220000
O	2.300000	-0.684000	0.769000
N	0.821000	0.712000	-0.166000
H	0.546000	1.191000	-0.993000
C	0.247000	1.140000	1.092000
H	-0.781000	1.431000	0.929000
H	0.282000	0.309000	1.782000
C	0.972000	2.356000	1.657000
O	0.555000	3.470000	1.469000
N	2.096000	2.099000	2.347000
H	2.438000	1.167000	2.446000
C	2.879000	3.167000	2.903000
H	3.438000	3.700000	2.136000
H	2.230000	3.893000	3.378000
C	3.862000	2.604000	3.914000
O	4.015000	1.421000	4.068000
N	4.558000	3.520000	4.610000
H	4.431000	4.499000	4.483000
C	5.536000	3.116000	5.581000
H	5.079000	2.523000	6.369000
H	6.302000	2.497000	5.125000
C	6.177000	4.354000	6.186000
O	5.867000	5.463000	5.840000
N	7.107000	4.114000	7.126000
H	7.322000	3.177000	7.372000
C	7.806000	5.198000	7.790000
H	8.373000	5.786000	7.079000
H	7.108000	5.853000	8.295000
H	8.484000	4.774000	8.519000

Glycine tetrapeptide_18

H	1.235000	2.711000	-1.070000
C	1.667000	1.732000	-1.243000
H	1.095000	1.217000	-2.005000
H	2.686000	1.876000	-1.583000
C	1.710000	0.995000	0.071000
O	2.365000	1.389000	1.002000
N	1.011000	-0.167000	0.159000
H	0.369000	-0.395000	-0.564000
C	0.878000	-0.839000	1.437000
H	0.506000	-0.169000	2.200000
H	0.171000	-1.652000	1.324000
C	2.170000	-1.423000	1.995000

H	1.220000	-1.870000	1.054000
H	1.110000	-0.693000	2.336000
C	-0.674000	-0.909000	1.164000
O	-1.250000	-0.299000	0.301000
N	-1.334000	-1.652000	2.082000
H	-0.804000	-2.211000	2.710000
C	-2.743000	-1.952000	1.915000
H	-2.948000	-2.312000	0.916000
H	-3.010000	-2.734000	2.614000
C	-3.706000	-0.793000	2.143000
O	-4.831000	-0.893000	1.742000
N	-3.235000	0.276000	2.817000
H	-2.291000	0.262000	3.123000
C	-4.019000	1.468000	3.034000
H	-5.051000	1.237000	2.811000
H	-3.965000	1.778000	4.070000
C	-3.627000	2.679000	2.196000
O	-4.051000	3.761000	2.505000
N	-2.819000	2.473000	1.143000
H	-2.584000	1.545000	0.872000
C	-2.479000	3.561000	0.251000
H	-3.328000	3.873000	-0.347000
H	-2.135000	4.414000	0.820000
H	-1.687000	3.231000	-0.409000

Glycine tetrapeptide_16

H	-1.166000	-0.010000	-1.308000
C	-0.538000	0.814000	-1.624000
H	-0.287000	0.681000	-2.672000
H	-1.077000	1.746000	-1.525000
C	0.745000	0.916000	-0.835000
O	1.386000	1.937000	-0.797000
N	1.149000	-0.204000	-0.198000
H	0.638000	-1.047000	-0.319000
C	2.368000	-0.250000	0.584000
H	2.473000	0.685000	1.119000
H	2.299000	-1.063000	1.292000
C	3.590000	-0.513000	-0.290000
O	4.102000	-1.595000	-0.344000
N	4.039000	0.559000	-0.992000
H	3.456000	1.370000	-0.999000
C	5.005000	0.393000	-2.053000
H	4.935000	-0.603000	-2.468000
H	4.792000	1.099000	-2.846000
C	6.467000	0.597000	-1.687000
O	7.305000	0.453000	-2.544000
N	6.757000	0.946000	-0.427000
H	6.022000	0.972000	0.239000
C	8.115000	1.204000	0.013000
H	8.647000	1.703000	-0.787000
H	8.083000	1.850000	0.878000
C	8.869000	-0.058000	0.430000
O	9.186000	-0.236000	1.577000
N	9.154000	-0.917000	-0.562000

H	-5.537000	-1.984000	-6.638000
H	-5.918000	-3.631000	-7.134000

Glycine tetrapeptide_20

H	3.163000	0.882000	1.309000
C	3.251000	1.249000	0.294000
H	3.347000	2.327000	0.303000
H	4.149000	0.840000	-0.155000
C	2.075000	0.883000	-0.578000
O	1.917000	1.378000	-1.667000
N	1.220000	-0.039000	-0.085000
H	1.412000	-0.468000	0.789000
C	0.033000	-0.453000	-0.805000
H	-0.684000	-0.849000	-0.102000
H	-0.392000	0.410000	-1.302000
C	0.318000	-1.553000	-1.822000
O	-0.074000	-2.681000	-1.644000
N	1.015000	-1.178000	-2.908000
H	1.338000	-0.235000	-2.951000
C	1.544000	-2.138000	-3.858000
H	2.409000	-1.708000	-4.338000
H	1.841000	-3.038000	-3.331000
C	0.574000	-2.518000	-4.973000
O	0.866000	-2.349000	-6.124000
N	-0.599000	-3.057000	-4.564000
H	-0.703000	-3.251000	-3.591000
C	-1.569000	-3.583000	-5.494000
H	-1.112000	-3.646000	-6.472000
H	-1.868000	-4.582000	-5.203000
C	-2.853000	-2.780000	-5.654000
O	-3.784000	-3.272000	-6.234000
N	-2.873000	-1.540000	-5.134000
H	-2.030000	-1.172000	-4.764000
C	-4.005000	-0.661000	-5.333000
H	-4.004000	-0.214000	-6.322000
H	-4.921000	-1.221000	-5.213000
H	-3.973000	0.129000	-4.592000

Glycine tetrapeptide_21

H	0.563000	2.487000	-2.651000
C	1.184000	1.708000	-2.231000
H	1.000000	0.773000	-2.744000
H	2.223000	1.989000	-2.374000
C	0.919000	1.622000	-0.750000
O	0.698000	2.605000	-0.081000
N	0.952000	0.395000	-0.192000
H	1.358000	-0.351000	-0.708000
C	0.894000	0.275000	1.244000
H	-0.051000	0.663000	1.602000
H	0.950000	-0.775000	1.505000
C	2.077000	0.987000	1.896000
O	3.184000	0.864000	1.449000
N	1.784000	1.737000	2.977000
H	0.827000	1.893000	3.198000

O	2.273000	-1.619000	3.172000
N	3.132000	-1.726000	1.094000
H	2.944000	-1.541000	0.137000
C	4.464000	-2.129000	1.470000
H	4.499000	-2.209000	2.548000
H	4.723000	-3.093000	1.051000
C	5.544000	-1.155000	1.013000
O	6.658000	-1.559000	0.776000
N	5.187000	0.132000	0.891000
H	4.259000	0.424000	1.110000
C	6.110000	1.142000	0.412000
H	5.753000	2.109000	0.732000
H	7.093000	0.959000	0.826000
C	6.146000	1.147000	-1.114000
O	5.463000	1.905000	-1.756000
N	6.965000	0.237000	-1.671000
H	7.353000	-0.460000	-1.074000
C	7.001000	0.040000	-3.104000
H	7.099000	0.993000	-3.603000
H	7.855000	-0.578000	-3.349000
H	6.100000	-0.445000	-3.471000

Glycine tetrapeptide_19

H	2.835000	0.790000	1.313000
C	3.052000	1.002000	0.273000
H	3.350000	2.035000	0.162000
H	3.880000	0.374000	-0.044000
C	1.874000	0.738000	-0.634000
O	1.735000	1.315000	-1.683000
N	0.999000	-0.202000	-0.211000
H	1.208000	-0.733000	0.602000
C	-0.137000	-0.610000	-1.016000
H	-0.876000	-1.062000	-0.372000
H	-0.559000	0.265000	-1.490000
C	0.275000	-1.655000	-2.047000
O	0.161000	-2.829000	-1.829000
N	0.792000	-1.161000	-3.198000
H	1.021000	-0.190000	-3.208000
C	1.466000	-2.035000	-4.131000
H	2.153000	-1.444000	-4.723000
H	2.039000	-2.788000	-3.609000
C	0.586000	-2.791000	-5.115000
O	1.083000	-3.639000	-5.810000
N	-0.709000	-2.453000	-5.191000
H	-1.111000	-1.786000	-4.573000
C	-1.597000	-3.178000	-6.053000
H	-1.338000	-3.026000	-7.097000
H	-1.527000	-4.246000	-5.865000
C	-3.024000	-2.712000	-5.820000
O	-3.292000	-1.831000	-5.047000
N	-3.957000	-3.352000	-6.549000
H	-3.682000	-4.098000	-7.144000
C	-5.364000	-3.031000	-6.425000
H	-5.727000	-3.241000	-5.425000

Glycine tetrapeptide_23

H	2.394000	1.383000	-3.107000
C	2.349000	0.622000	-2.340000
H	1.853000	-0.262000	-2.724000
H	3.363000	0.358000	-2.058000
C	1.653000	1.190000	-1.128000
O	1.702000	2.362000	-0.852000
N	0.974000	0.305000	-0.357000
H	1.198000	-0.658000	-0.461000
C	0.497000	0.734000	0.936000
H	-0.197000	1.553000	0.808000
H	-0.028000	-0.091000	1.401000
C	1.668000	1.130000	1.833000
O	2.668000	0.466000	1.857000
N	1.484000	2.248000	2.561000
H	0.682000	2.811000	2.371000
C	2.573000	2.902000	3.253000
H	2.391000	2.969000	4.317000
H	3.474000	2.327000	3.088000
C	2.752000	4.328000	2.748000
O	2.965000	5.230000	3.508000
N	2.644000	4.507000	1.403000
H	2.329000	3.733000	0.857000
C	2.192000	5.786000	0.939000
H	2.786000	6.571000	1.388000
H	2.311000	5.839000	-0.137000
C	0.713000	5.995000	1.276000
O	0.022000	5.101000	1.695000
N	0.237000	7.231000	1.040000
H	0.881000	7.957000	0.831000
C	-1.128000	7.590000	1.369000
H	-1.283000	7.641000	2.441000
H	-1.348000	8.556000	0.933000
H	-1.808000	6.856000	0.960000
C	2.768000	2.553000	3.651000
H	2.618000	2.514000	4.720000
H	3.747000	2.153000	3.428000
C	2.760000	4.031000	3.269000
O	3.102000	4.845000	4.082000
N	2.387000	4.333000	2.007000
H	2.184000	3.597000	1.370000
C	2.357000	5.694000	1.525000
H	2.874000	6.324000	2.231000
H	2.878000	5.762000	0.575000
C	0.976000	6.305000	1.317000
O	0.868000	7.501000	1.250000
N	-0.068000	5.464000	1.186000
H	0.107000	4.497000	1.037000
C	-1.381000	5.978000	0.864000
H	-1.432000	6.366000	-0.149000
H	-2.103000	5.177000	0.971000
H	-1.639000	6.778000	1.544000

Glycine tetrapeptide_22

H	4.040000	-0.679000	-2.137000
C	4.071000	0.317000	-1.718000
H	5.049000	0.506000	-1.291000
H	3.901000	1.027000	-2.521000
C	2.954000	0.453000	-0.709000
O	1.888000	-0.082000	-0.857000
N	3.217000	1.236000	0.360000
H	4.097000	1.681000	0.481000
C	2.222000	1.475000	1.365000
H	1.396000	2.069000	0.978000
H	1.801000	0.540000	1.717000
C	2.850000	2.226000	2.520000
O	3.968000	2.681000	2.458000
N	2.094000	2.351000	3.627000
H	1.120000	2.161000	3.569000
C	2.568000	3.170000	4.718000
H	1.855000	3.103000	5.530000
H	3.517000	2.787000	5.067000
C	2.663000	4.636000	4.301000
O	1.746000	5.168000	3.742000
N	3.818000	5.261000	4.612000
H	4.575000	4.713000	4.950000
C	4.087000	6.620000	4.205000
H	3.150000	7.153000	4.143000
H	4.700000	7.112000	4.949000
C	4.793000	6.804000	2.864000
O	5.133000	7.912000	2.544000
N	5.011000	5.715000	2.111000
H	4.639000	4.833000	2.379000
C	5.607000	5.837000	0.798000
H	6.532000	6.396000	0.855000
H	5.815000	4.844000	0.423000
H	4.946000	6.346000	0.105000

Glycine tetrapeptide_24

H	0.954000	2.841000	-1.113000
C	1.649000	2.387000	-0.419000
H	2.654000	2.554000	-0.793000
H	1.555000	2.857000	0.552000
C	1.395000	0.901000	-0.386000
O	1.153000	0.275000	-1.388000
N	1.475000	0.303000	0.823000
H	1.615000	0.855000	1.636000
C	1.343000	-1.132000	0.984000
H	1.826000	-1.623000	0.149000
H	1.827000	-1.427000	1.903000
C	-0.116000	-1.564000	1.081000
O	-0.601000	-1.906000	2.128000
N	-0.808000	-1.549000	-0.079000
H	-0.361000	-1.127000	-0.867000
C	-2.251000	-1.657000	-0.076000
H	-2.695000	-0.980000	0.643000

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C	-0.304000	1.048000	-2.253000
H	-0.082000	0.359000	-3.061000
H	-0.079000	2.059000	-2.561000
C	0.481000	0.737000	-1.001000
O	0.863000	1.584000	-0.248000
N	0.730000	-0.588000	-0.773000
H	0.283000	-1.259000	-1.354000
C	1.246000	-1.032000	0.502000
H	0.919000	-0.366000	1.288000
H	0.862000	-2.020000	0.723000
C	2.759000	-1.127000	0.625000
O	3.241000	-1.441000	1.685000
N	3.495000	-0.888000	-0.472000
H	3.042000	-0.527000	-1.279000
C	4.940000	-0.983000	-0.463000
H	5.227000	-1.806000	0.178000
H	5.285000	-1.175000	-1.468000
C	5.619000	0.301000	0.004000
O	6.251000	0.981000	-0.769000
N	5.468000	0.602000	1.301000
H	4.923000	-0.013000	1.867000
C	5.911000	1.863000	1.867000
H	5.749000	2.652000	1.142000
H	5.324000	2.068000	2.749000
C	7.375000	1.871000	2.302000
O	7.677000	2.060000	3.451000
N	8.277000	1.682000	1.324000
H	7.951000	1.574000	0.389000
C	9.695000	1.691000	1.605000
H	10.014000	2.653000	1.993000
H	9.950000	0.934000	2.336000
H	10.231000	1.488000	0.687000

Glycine tetrapeptide_27

H	0.774000	3.104000	1.028000
C	1.515000	2.319000	1.067000
H	2.346000	2.601000	0.428000
H	1.881000	2.208000	2.081000
C	0.906000	1.047000	0.531000
O	0.042000	1.044000	-0.303000
N	1.392000	-0.118000	1.043000
H	2.197000	-0.078000	1.624000
C	1.075000	-1.376000	0.402000
H	1.177000	-1.306000	-0.672000
H	1.769000	-2.129000	0.758000
C	-0.324000	-1.914000	0.657000
O	-0.760000	-2.777000	-0.063000
N	-0.995000	-1.430000	1.713000
H	-0.616000	-0.655000	2.204000
C	-2.327000	-1.885000	2.059000
H	-2.395000	-2.943000	1.842000
H	-2.489000	-1.728000	3.115000
C	-3.439000	-1.136000	1.327000
O	-4.246000	-0.494000	1.940000

H	-2.614000	-1.385000	-1.059000
C	-2.824000	-3.029000	0.250000
O	-3.982000	-3.119000	0.548000
N	-1.988000	-4.084000	0.157000
H	-1.046000	-3.914000	-0.105000
C	-2.385000	-5.420000	0.527000
H	-3.464000	-5.470000	0.519000
H	-2.015000	-6.137000	-0.196000
C	-1.921000	-5.903000	1.897000
O	-2.056000	-7.066000	2.176000
N	-1.378000	-4.999000	2.728000
H	-1.369000	-4.036000	2.482000
C	-0.995000	-5.371000	4.072000
H	-1.860000	-5.571000	4.696000
H	-0.380000	-6.261000	4.053000
H	-0.429000	-4.556000	4.505000

Glycine tetrapeptide_25

H	1.010000	-0.519000	-1.849000
C	1.293000	0.518000	-1.710000
H	2.334000	0.646000	-1.985000
H	0.689000	1.149000	-2.347000
C	1.135000	0.986000	-0.286000
O	1.076000	2.154000	0.004000
N	1.117000	0.024000	0.672000
H	1.075000	-0.928000	0.394000
C	0.827000	0.357000	2.050000
H	-0.060000	0.971000	2.123000
H	0.646000	-0.561000	2.595000
C	1.915000	1.120000	2.796000
O	1.636000	1.688000	3.815000
N	3.155000	1.086000	2.267000
H	3.291000	0.602000	1.409000
C	4.242000	1.889000	2.772000
H	3.869000	2.478000	3.599000
H	5.061000	1.278000	3.127000
C	4.819000	2.812000	1.707000
O	5.997000	3.045000	1.668000
N	3.936000	3.352000	0.834000
H	3.007000	2.993000	0.808000
C	4.436000	3.900000	-0.392000
H	3.640000	4.452000	-0.881000
H	5.246000	4.585000	-0.184000
C	4.900000	2.802000	-1.349000
O	4.513000	1.665000	-1.249000
N	5.718000	3.209000	-2.336000
H	6.132000	4.109000	-2.266000
C	6.267000	2.273000	-3.296000
H	6.995000	1.610000	-2.840000
H	5.473000	1.672000	-3.716000
H	6.744000	2.830000	-4.092000

Glycine tetrapeptide_26

H	-1.364000	0.984000	-2.029000

H	-2.129000	0.044000	-3.651000
H	-1.965000	-1.704000	-3.604000
N	-1.449000	-1.044000	-0.698000
C	-1.899000	-1.220000	0.678000
C	-2.813000	-2.453000	0.769000
O	-2.332000	-3.547000	0.652000
C	-2.427000	0.077000	1.289000
H	-0.524000	-1.335000	-0.913000
H	-1.020000	-1.524000	1.232000
H	-2.742000	-0.090000	2.314000
H	-1.634000	0.815000	1.295000
H	-3.255000	0.484000	0.725000
N	-4.131000	-2.260000	0.994000
C	-5.046000	-3.384000	1.016000
C	-5.285000	-4.030000	-0.350000
O	-5.663000	-5.176000	-0.399000
C	-6.386000	-2.965000	1.621000
H	-4.502000	-1.346000	0.872000
H	-4.603000	-4.165000	1.616000
H	-7.057000	-3.814000	1.643000
H	-6.243000	-2.603000	2.633000
H	-6.851000	-2.179000	1.033000
N	-5.122000	-3.260000	-1.438000
C	-5.285000	-3.789000	-2.786000
C	-3.951000	-4.405000	-3.228000
O	-3.174000	-3.807000	-3.932000
C	-5.743000	-2.691000	-3.734000
H	-4.695000	-2.362000	-1.354000
H	-6.030000	-4.571000	-2.731000
H	-5.845000	-3.080000	-4.740000
H	-6.702000	-2.304000	-3.408000
H	-5.027000	-1.880000	-3.759000
N	-3.718000	-5.638000	-2.749000
C	-2.425000	-6.270000	-2.899000
H	-4.333000	-5.975000	-2.039000
H	-1.689000	-5.848000	-2.220000
H	-2.527000	-7.328000	-2.691000
H	-2.075000	-6.141000	-3.913000

Alanine tetrapeptide_02

C	1.018000	-0.225000	2.755000
C	-0.180000	-0.929000	2.169000
O	-0.941000	-0.391000	1.404000
H	1.316000	0.567000	2.083000
H	1.849000	-0.904000	2.912000
H	0.734000	0.209000	3.709000
N	-0.361000	-2.213000	2.566000
C	-1.501000	-2.998000	2.129000
C	-2.717000	-2.634000	2.987000
O	-2.876000	-3.135000	4.076000
C	-1.194000	-4.486000	2.235000
H	0.190000	-2.568000	3.315000
H	-1.691000	-2.733000	1.099000
H	-2.033000	-5.071000	1.876000

N	-3.433000	-1.261000	-0.019000
H	-2.779000	-1.895000	-0.425000
C	-4.477000	-0.700000	-0.846000
H	-4.871000	-1.456000	-1.515000
H	-5.285000	-0.377000	-0.206000
C	-4.106000	0.490000	-1.721000
O	-4.927000	0.904000	-2.499000
N	-2.886000	1.025000	-1.584000
H	-2.241000	0.654000	-0.927000
C	-2.487000	2.169000	-2.376000
H	-1.469000	2.419000	-2.116000
H	-2.544000	1.944000	-3.434000
H	-3.129000	3.020000	-2.179000

Glycine tetrapeptide_28

H	4.387000	-1.616000	-0.678000
C	3.364000	-1.538000	-1.034000
H	3.386000	-1.409000	-2.106000
H	2.843000	-2.455000	-0.783000
C	2.725000	-0.318000	-0.412000
O	2.812000	0.775000	-0.905000
N	2.069000	-0.526000	0.749000
H	2.020000	-1.424000	1.176000
C	1.467000	0.560000	1.466000
H	2.209000	1.299000	1.760000
H	0.738000	1.077000	0.850000
C	0.796000	0.014000	2.713000
O	0.913000	-1.131000	3.050000
N	0.056000	0.907000	3.415000
H	0.076000	1.864000	3.147000
C	-0.498000	0.560000	4.705000
H	0.170000	-0.108000	5.230000
H	-0.604000	1.460000	5.297000
C	-1.862000	-0.115000	4.699000
O	-2.314000	-0.521000	5.735000
N	-2.504000	-0.226000	3.517000
H	-2.185000	0.335000	2.763000
C	-3.875000	-0.654000	3.494000
H	-4.116000	-1.020000	2.501000
H	-3.995000	-1.471000	4.191000
C	-4.837000	0.488000	3.811000
O	-4.545000	1.629000	3.573000
N	-6.038000	0.110000	4.294000
H	-6.134000	-0.817000	4.639000
C	-7.045000	1.082000	4.666000
H	-7.052000	1.881000	3.939000
H	-8.015000	0.601000	4.673000
H	-6.855000	1.510000	5.645000

Alanine tetrapeptide_01

C	-1.692000	-0.781000	-3.104000
C	-2.293000	-0.809000	-1.724000
O	-3.480000	-0.644000	-1.543000
H	-0.613000	-0.679000	-3.092000

H	3.062000	-1.115000	1.373000
H	3.156000	-0.272000	2.921000
N	1.270000	-1.577000	5.283000
C	1.301000	-1.790000	6.717000
C	0.214000	-2.732000	7.244000
O	0.134000	-2.918000	8.432000
C	1.227000	-0.454000	7.452000
H	0.642000	-0.902000	4.916000
H	2.239000	-2.276000	6.943000
H	1.246000	-0.621000	8.519000
H	2.064000	0.175000	7.170000
H	0.305000	0.072000	7.211000
N	-0.614000	-3.299000	6.356000
C	-1.621000	-4.244000	6.788000
H	-0.462000	-3.185000	5.381000
H	-2.212000	-4.527000	5.928000
H	-1.172000	-5.131000	7.220000
H	-2.267000	-3.796000	7.532000

Alanine tetrapeptide_04

C	0.277000	0.362000	2.332000
C	-0.416000	-0.868000	2.862000
O	-0.571000	-1.061000	4.044000
H	-0.475000	1.112000	2.104000
H	0.837000	0.145000	1.432000
H	0.932000	0.750000	3.099000
N	-0.893000	-1.717000	1.920000
C	-1.596000	-2.940000	2.273000
C	-0.577000	-4.077000	2.395000
O	-0.526000	-4.970000	1.583000
C	-2.670000	-3.260000	1.245000
H	-0.483000	-1.671000	1.012000
H	-2.044000	-2.771000	3.243000
H	-3.194000	-4.169000	1.514000
H	-3.379000	-2.443000	1.198000
H	-2.235000	-3.410000	0.264000
N	0.273000	-3.955000	3.434000
C	1.517000	-4.702000	3.608000
C	2.556000	-4.249000	2.575000
O	3.531000	-3.626000	2.908000
C	1.330000	-6.217000	3.667000
H	0.170000	-3.134000	3.993000
H	1.924000	-4.368000	4.551000
H	2.286000	-6.689000	3.874000
H	0.647000	-6.463000	4.472000
H	0.932000	-6.617000	2.747000
N	2.312000	-4.565000	1.285000
C	3.099000	-3.954000	0.242000
C	2.877000	-2.439000	0.216000
O	1.765000	-1.970000	0.168000
C	2.707000	-4.539000	-1.113000
H	1.405000	-4.911000	1.051000
H	4.143000	-4.162000	0.439000
H	3.305000	-4.100000	-1.904000

H	-0.323000	-4.725000	1.635000
H	-1.011000	-4.767000	3.265000
N	-3.539000	-1.715000	2.450000
C	-4.720000	-1.134000	3.084000
C	-4.370000	-0.079000	4.138000
O	-4.850000	1.027000	4.060000
C	-5.712000	-2.171000	3.617000
H	-3.162000	-1.203000	1.681000
H	-5.213000	-0.566000	2.308000
H	-6.602000	-1.658000	3.967000
H	-5.997000	-2.845000	2.817000
H	-5.297000	-2.753000	4.426000
N	-3.529000	-0.447000	5.119000
C	-3.018000	0.504000	6.097000
C	-1.849000	1.265000	5.455000
O	-0.706000	0.908000	5.601000
C	-2.581000	-0.224000	7.359000
H	-3.168000	-1.377000	5.120000
H	-3.815000	1.199000	6.323000
H	-2.214000	0.484000	8.093000
H	-3.420000	-0.764000	7.783000
H	-1.779000	-0.919000	7.143000
N	-2.210000	2.321000	4.705000
C	-1.255000	3.017000	3.868000
H	-3.179000	2.410000	4.489000
H	-0.336000	3.167000	4.417000
H	-1.034000	2.463000	2.961000
H	-1.665000	3.982000	3.598000

Alanine tetrapeptide_03

C	-2.979000	2.248000	3.489000
C	-3.035000	0.904000	2.799000
O	-4.053000	0.425000	2.389000
H	-2.290000	2.914000	2.979000
H	-2.640000	2.130000	4.513000
H	-3.967000	2.682000	3.485000
N	-1.837000	0.264000	2.688000
C	-1.737000	-1.035000	2.041000
C	-0.581000	-1.820000	2.648000
O	-0.745000	-2.888000	3.170000
C	-1.627000	-0.935000	0.517000
H	-1.012000	0.744000	2.964000
H	-2.627000	-1.588000	2.294000
H	-1.535000	-1.922000	0.075000
H	-2.521000	-0.466000	0.129000
H	-0.772000	-0.340000	0.210000
N	0.650000	-1.235000	2.592000
C	1.846000	-1.999000	2.928000
C	1.993000	-2.313000	4.416000
O	2.769000	-3.166000	4.749000
C	3.087000	-1.249000	2.450000
H	0.773000	-0.491000	1.942000
H	1.801000	-2.969000	2.449000
H	3.970000	-1.817000	2.705000

C	-1.243000	2.746000	0.224000
C	-1.558000	1.811000	1.372000
O	-1.462000	2.148000	2.523000
H	-0.444000	2.340000	-0.388000
H	-0.941000	3.701000	0.626000
H	-2.115000	2.877000	-0.408000
N	-1.956000	0.572000	1.010000
C	-2.246000	-0.455000	1.980000
C	-2.110000	-1.800000	1.272000
O	-2.128000	-1.884000	0.068000
C	-3.648000	-0.302000	2.585000
H	-1.981000	0.295000	0.054000
H	-1.513000	-0.397000	2.777000
H	-3.841000	-1.061000	3.336000
H	-3.726000	0.671000	3.052000
H	-4.403000	-0.382000	1.810000
N	-1.996000	-2.870000	2.073000
C	-1.943000	-4.217000	1.551000
C	-2.382000	-5.156000	2.671000
O	-2.383000	-4.803000	3.825000
C	-0.538000	-4.586000	1.057000
H	-2.008000	-2.782000	3.065000
H	-2.640000	-4.294000	0.725000
H	-0.518000	-5.587000	0.638000
H	-0.238000	-3.886000	0.289000
H	0.172000	-4.538000	1.875000
N	-2.733000	-6.392000	2.286000
C	-3.075000	-7.426000	3.236000
C	-2.833000	-8.767000	2.549000
O	-2.783000	-8.857000	1.349000
C	-4.532000	-7.314000	3.703000
H	-2.701000	-6.669000	1.329000
H	-2.419000	-7.331000	4.094000
H	-4.771000	-8.078000	4.436000
H	-4.687000	-6.343000	4.156000
H	-5.206000	-7.422000	2.860000
N	-2.714000	-9.830000	3.362000
C	-2.541000	-11.169000	2.833000
H	-2.733000	-9.697000	4.346000
H	-1.642000	-11.233000	2.234000
H	-2.466000	-11.859000	3.662000
H	-3.384000	-11.450000	2.214000

Alanine tetrapeptide_07

C	-1.523000	1.529000	-0.446000
C	-2.039000	1.029000	0.882000
O	-2.793000	1.661000	1.566000
H	-1.444000	0.731000	-1.176000
H	-0.537000	1.961000	-0.304000
H	-2.189000	2.297000	-0.812000
N	-1.601000	-0.210000	1.256000
C	-1.791000	-0.700000	2.617000
C	-3.277000	-0.809000	2.979000
O	-3.650000	-0.593000	4.104000

H	2.865000	-5.612000	-1.114000
H	1.663000	-4.337000	-1.322000
N	3.994000	-1.692000	0.174000
C	3.937000	-0.246000	0.193000
H	4.834000	-2.123000	0.487000
H	3.197000	0.094000	-0.518000
H	3.679000	0.137000	1.175000
H	4.904000	0.146000	-0.094000

Alanine tetrapeptide_05

C	-2.374000	1.643000	-0.358000
C	-1.293000	0.989000	0.470000
O	-0.330000	1.593000	0.868000
H	-2.493000	1.127000	-1.305000
H	-2.099000	2.671000	-0.541000
H	-3.323000	1.609000	0.166000
N	-1.482000	-0.323000	0.738000
C	-0.577000	-1.092000	1.579000
C	0.580000	-1.642000	0.737000
O	0.640000	-2.806000	0.419000
C	-1.329000	-2.211000	2.284000
H	-2.262000	-0.794000	0.340000
H	-0.167000	-0.405000	2.308000
H	-0.661000	-2.764000	2.931000
H	-2.130000	-1.793000	2.884000
H	-1.741000	-2.912000	1.568000
N	1.504000	-0.733000	0.385000
C	2.587000	-1.036000	-0.541000
C	3.793000	-1.595000	0.225000
O	4.807000	-0.956000	0.372000
C	2.962000	0.206000	-1.334000
H	1.346000	0.219000	0.640000
H	2.233000	-1.811000	-1.209000
H	3.749000	-0.023000	-2.041000
H	2.097000	0.570000	-1.877000
H	3.326000	0.988000	-0.678000
N	3.627000	-2.836000	0.709000
C	4.597000	-3.475000	1.589000
C	5.657000	-4.212000	0.759000
O	5.679000	-5.412000	0.671000
C	3.888000	-4.422000	2.545000
H	2.746000	-3.283000	0.565000
H	5.092000	-2.688000	2.145000
H	4.601000	-4.881000	3.217000
H	3.155000	-3.876000	3.129000
H	3.393000	-5.217000	2.001000
N	6.552000	-3.410000	0.155000
C	7.549000	-3.948000	-0.743000
H	6.392000	-2.427000	0.181000
H	8.266000	-3.171000	-0.971000
H	8.063000	-4.776000	-0.273000
H	7.111000	-4.305000	-1.670000

Alanine tetrapeptide_06

C	1.152000	3.726000	4.590000
H	0.679000	2.508000	2.360000
H	-0.871000	3.027000	4.761000
H	1.086000	4.414000	5.423000
H	1.584000	2.795000	4.939000
H	1.805000	4.174000	3.850000
N	-2.209000	4.696000	3.332000
C	-2.977000	5.771000	2.713000
C	-3.423000	6.778000	3.782000
O	-4.556000	6.821000	4.182000
C	-4.169000	5.194000	1.966000
H	-2.665000	3.827000	3.509000
H	-2.315000	6.279000	2.023000
H	-4.728000	5.987000	1.485000
H	-3.830000	4.496000	1.209000
H	-4.842000	4.688000	2.647000
N	-2.450000	7.599000	4.217000
C	-2.690000	8.534000	5.293000
H	-1.515000	7.411000	3.930000
H	-3.607000	9.077000	5.111000
H	-2.777000	8.037000	6.255000
H	-1.866000	9.235000	5.335000

Alanine tetrapeptide_09

C	-2.457000	3.010000	0.164000
C	-2.584000	1.527000	-0.098000
O	-3.304000	1.092000	-0.958000
H	-1.730000	3.423000	-0.529000
H	-2.134000	3.232000	1.174000
H	-3.411000	3.480000	-0.028000
N	-1.816000	0.731000	0.674000
C	-1.817000	-0.703000	0.530000
C	-1.300000	-1.294000	1.836000
O	-0.655000	-0.641000	2.618000
C	-0.950000	-1.170000	-0.647000
H	-1.253000	1.103000	1.406000
H	-2.836000	-1.032000	0.366000
H	-0.985000	-2.248000	-0.761000
H	-1.319000	-0.716000	-1.557000
H	0.082000	-0.872000	-0.496000
N	-1.585000	-2.592000	2.034000
C	-1.088000	-3.317000	3.179000
C	-1.060000	-4.794000	2.809000
O	-1.754000	-5.231000	1.921000
C	-1.960000	-3.098000	4.422000
H	-2.112000	-3.115000	1.370000
H	-0.081000	-2.975000	3.388000
H	-1.565000	-3.629000	5.282000
H	-1.987000	-2.042000	4.653000
H	-2.971000	-3.445000	4.238000
N	-0.249000	-5.565000	3.551000
C	-0.147000	-7.010000	3.371000
C	-1.251000	-7.702000	4.182000
O	-1.036000	-8.172000	5.267000

C	-1.016000	0.093000	3.664000
H	-0.848000	-0.604000	0.740000
H	-1.429000	-1.725000	2.612000
H	-1.143000	-0.356000	4.639000
H	0.039000	0.091000	3.410000
H	-1.369000	1.113000	3.710000
N	-4.084000	-1.247000	1.994000
C	-5.528000	-1.442000	2.080000
C	-6.323000	-0.130000	2.059000
O	-7.163000	0.026000	1.201000
C	-5.962000	-2.354000	3.229000
H	-3.694000	-1.263000	1.081000
H	-5.806000	-1.919000	1.151000
H	-7.031000	-2.525000	3.160000
H	-5.456000	-3.310000	3.146000
H	-5.737000	-1.929000	4.195000
N	-6.061000	0.751000	3.031000
C	-6.549000	2.127000	3.115000
C	-8.001000	2.263000	3.584000
O	-8.269000	3.034000	4.470000
C	-6.303000	2.937000	1.839000
H	-5.345000	0.503000	3.680000
H	-5.979000	2.577000	3.915000
H	-6.601000	3.966000	2.010000
H	-5.248000	2.914000	1.595000
H	-6.865000	2.545000	1.003000
N	-8.930000	1.540000	2.939000
C	-10.329000	1.667000	3.276000
H	-8.648000	0.969000	2.173000
H	-10.898000	1.004000	2.637000
H	-10.506000	1.396000	4.310000
H	-10.680000	2.682000	3.132000

Alanine tetrapeptide_08

C	-2.583000	-2.588000	1.046000
C	-1.556000	-1.499000	0.835000
O	-0.597000	-1.639000	0.124000
H	-2.220000	-3.500000	0.597000
H	-3.520000	-2.305000	0.576000
H	-2.772000	-2.747000	2.102000
N	-1.798000	-0.345000	1.499000
C	-0.923000	0.793000	1.381000
C	-1.156000	1.681000	2.595000
O	-2.200000	1.659000	3.202000
C	-1.174000	1.594000	0.096000
H	-2.601000	-0.237000	2.077000
H	0.100000	0.437000	1.379000
H	-0.494000	2.436000	0.013000
H	-1.023000	0.946000	-0.757000
H	-2.192000	1.969000	0.079000
N	-0.147000	2.512000	2.914000
C	-0.229000	3.468000	4.010000
C	-0.881000	4.765000	3.512000
O	-0.229000	5.756000	3.289000

H	-0.631000	3.875000	7.003000
H	0.160000	2.605000	6.069000

Alanine tetrapeptide_11

C	-3.471000	1.989000	4.097000
C	-3.546000	1.070000	2.902000
O	-4.357000	1.217000	2.028000
H	-2.809000	2.816000	3.860000
H	-3.093000	1.488000	4.981000
H	-4.456000	2.387000	4.294000
N	-2.634000	0.062000	2.862000
C	-2.456000	-0.721000	1.650000
C	-3.614000	-1.679000	1.377000
O	-3.884000	-1.967000	0.239000
C	-1.151000	-1.513000	1.720000
H	-1.890000	0.075000	3.522000
H	-2.439000	-0.062000	0.792000
H	-1.034000	-2.101000	0.819000
H	-0.303000	-0.840000	1.802000
H	-1.147000	-2.186000	2.572000
N	-4.236000	-2.213000	2.443000
C	-5.365000	-3.126000	2.316000
C	-6.693000	-2.351000	2.328000
O	-7.553000	-2.595000	3.131000
C	-5.328000	-4.178000	3.415000
H	-4.046000	-1.826000	3.338000
H	-5.266000	-3.599000	1.347000
H	-6.162000	-4.858000	3.311000
H	-4.401000	-4.738000	3.355000
H	-5.405000	-3.721000	4.395000
N	-6.792000	-1.388000	1.391000
C	-7.979000	-0.555000	1.239000
C	-7.841000	0.322000	-0.003000
O	-8.771000	0.476000	-0.749000
C	-8.233000	0.337000	2.461000
H	-6.104000	-1.371000	0.669000
H	-8.846000	-1.178000	1.067000
H	-9.089000	0.976000	2.269000
H	-8.440000	-0.272000	3.329000
H	-7.370000	0.962000	2.664000
N	-6.647000	0.922000	-0.183000
C	-6.446000	1.850000	-1.275000
H	-5.971000	0.908000	0.549000
H	-5.388000	2.066000	-1.351000
H	-6.786000	1.408000	-2.201000
H	-6.988000	2.778000	-1.124000

Alanine tetrapeptide_12

C	-2.973000	1.291000	1.949000
C	-2.031000	0.487000	1.085000
O	-2.274000	0.245000	-0.069000
H	-3.671000	0.611000	2.429000
H	-3.534000	1.965000	1.318000
H	-2.454000	1.851000	2.718000

C	1.233000	-7.492000	3.789000
H	0.260000	-5.154000	4.301000
H	-0.307000	-7.204000	2.319000
H	1.322000	-8.558000	3.623000
H	1.995000	-6.983000	3.209000
H	1.400000	-7.313000	4.844000
N	-2.457000	-7.721000	3.586000
C	-3.624000	-8.226000	4.275000
H	-2.577000	-7.177000	2.761000
H	-3.969000	-7.543000	5.046000
H	-4.418000	-8.372000	3.555000
H	-3.391000	-9.172000	4.742000

Alanine tetrapeptide_10

C	-2.337000	1.598000	0.163000
C	-1.840000	0.323000	0.792000
O	-2.306000	-0.756000	0.519000
H	-2.769000	1.369000	-0.801000
H	-1.549000	2.335000	0.051000
H	-3.108000	2.006000	0.808000
N	-0.845000	0.464000	1.706000
C	-0.412000	-0.643000	2.547000
C	-1.382000	-0.722000	3.727000
O	-1.133000	-0.207000	4.792000
C	1.025000	-0.446000	3.002000
H	-0.641000	1.383000	2.031000
H	-0.499000	-1.541000	1.951000
H	1.342000	-1.275000	3.624000
H	1.677000	-0.387000	2.138000
H	1.126000	0.460000	3.588000
N	-2.555000	-1.333000	3.467000
C	-3.703000	-1.103000	4.328000
C	-3.917000	0.416000	4.458000
O	-3.901000	1.098000	3.467000
C	-3.624000	-1.910000	5.623000
H	-2.745000	-1.514000	2.503000
H	-4.566000	-1.445000	3.767000
H	-4.541000	-1.814000	6.197000
H	-3.499000	-2.958000	5.376000
H	-2.782000	-1.605000	6.231000
N	-4.141000	0.923000	5.685000
C	-4.358000	2.340000	5.910000
C	-3.081000	3.175000	6.062000
O	-3.187000	4.361000	6.244000
C	-5.257000	2.549000	7.127000
H	-4.037000	0.335000	6.479000
H	-4.848000	2.731000	5.029000
H	-5.421000	3.606000	7.281000
H	-6.211000	2.056000	6.976000
H	-4.798000	2.144000	8.026000
N	-1.899000	2.547000	6.004000
C	-0.667000	3.302000	6.085000
H	-1.843000	1.589000	5.741000
H	-0.568000	3.993000	5.255000

N	-1.328000	-0.321000	0.513000
C	0.053000	0.123000	0.501000
C	0.241000	1.636000	0.349000
O	1.332000	2.095000	0.563000
C	0.819000	-0.598000	-0.606000
H	-1.691000	-0.811000	-0.271000
H	0.497000	-0.110000	1.459000
H	0.792000	-1.671000	-0.448000
H	0.391000	-0.379000	-1.581000
H	1.848000	-0.268000	-0.605000
N	-0.821000	2.363000	-0.042000
C	-0.774000	3.807000	-0.165000
C	-1.301000	4.556000	1.063000
O	-1.363000	5.760000	1.034000
C	-1.527000	4.259000	-1.415000
H	-1.695000	1.914000	-0.205000
H	0.267000	4.086000	-0.247000
H	-1.065000	3.832000	-2.298000
H	-2.563000	3.935000	-1.379000
H	-1.506000	5.337000	-1.485000
N	-1.673000	3.834000	2.128000
C	-2.139000	4.483000	3.333000
H	-1.566000	2.846000	2.132000
H	-2.980000	5.130000	3.117000
H	-2.448000	3.719000	4.033000
H	-1.358000	5.084000	3.786000

Alanine tetrapeptide_14

C	-5.341000	3.386000	3.270000
C	-5.527000	1.927000	3.604000
O	-6.133000	1.567000	4.583000
H	-6.294000	3.888000	3.376000
H	-4.954000	3.548000	2.272000
H	-4.657000	3.815000	3.993000
N	-4.977000	1.031000	2.752000
C	-4.979000	-0.375000	3.092000
C	-4.083000	-0.622000	4.309000
O	-2.955000	-0.189000	4.323000
C	-4.468000	-1.202000	1.915000
H	-4.301000	1.349000	2.097000
H	-5.999000	-0.655000	3.320000
H	-4.494000	-2.258000	2.157000
H	-5.089000	-1.034000	1.042000
H	-3.443000	-0.936000	1.681000
N	-4.623000	-1.364000	5.289000
C	-3.972000	-1.792000	6.526000
C	-3.820000	-0.682000	7.575000
O	-4.199000	-0.882000	8.697000
C	-2.646000	-2.522000	6.293000
H	-5.612000	-1.471000	5.266000
H	-4.661000	-2.485000	6.987000
H	-2.277000	-2.890000	7.244000
H	-2.806000	-3.370000	5.636000
H	-1.901000	-1.877000	5.852000

N	-0.910000	0.040000	1.698000
C	0.060000	-0.809000	1.023000
C	-0.380000	-2.269000	1.160000
O	0.002000	-2.963000	2.067000
C	1.449000	-0.597000	1.603000
H	-0.807000	0.172000	2.679000
H	0.044000	-0.527000	-0.021000
H	2.174000	-1.205000	1.075000
H	1.734000	0.445000	1.508000
H	1.479000	-0.887000	2.647000
N	-1.235000	-2.695000	0.213000
C	-1.827000	-4.008000	0.277000
C	-2.256000	-4.402000	-1.129000
O	-2.526000	-3.572000	-1.962000
C	-3.037000	-4.055000	1.221000
H	-1.613000	-2.048000	-0.446000
H	-1.071000	-4.696000	0.636000
H	-3.466000	-5.051000	1.269000
H	-2.720000	-3.771000	2.216000
H	-3.803000	-3.366000	0.882000
N	-2.353000	-5.725000	-1.357000
C	-2.822000	-6.275000	-2.624000
C	-4.356000	-6.318000	-2.626000
O	-4.960000	-7.328000	-2.378000
C	-2.229000	-7.657000	-2.845000
H	-2.167000	-6.361000	-0.615000
H	-2.488000	-5.598000	-3.399000
H	-2.548000	-8.052000	-3.801000
H	-1.146000	-7.602000	-2.833000
H	-2.566000	-8.347000	-2.081000
N	-4.950000	-5.146000	-2.913000
C	-6.387000	-4.995000	-2.829000
H	-4.378000	-4.331000	-2.948000
H	-6.735000	-4.973000	-1.801000
H	-6.668000	-4.069000	-3.314000
H	-6.871000	-5.819000	-3.333000

Alanine tetrapeptide_13

C	-5.032000	-0.135000	-2.018000
C	-4.247000	0.197000	-0.774000
O	-3.820000	1.300000	-0.557000
H	-4.729000	0.532000	-2.812000
H	-6.086000	0.027000	-1.818000
H	-4.896000	-1.165000	-2.329000
N	-4.044000	-0.825000	0.101000
C	-3.587000	-0.557000	1.456000
C	-2.158000	-0.030000	1.529000
O	-1.811000	0.591000	2.501000
C	-3.701000	-1.822000	2.304000
H	-4.534000	-1.676000	-0.057000
H	-4.188000	0.230000	1.895000
H	-3.355000	-1.616000	3.308000
H	-4.733000	-2.153000	2.358000
H	-3.099000	-2.625000	1.890000

N	3.029000	-2.634000	5.896000
C	3.429000	-1.505000	6.709000
H	2.193000	-3.122000	6.135000
H	4.500000	-1.375000	6.646000
H	2.949000	-0.585000	6.388000
H	3.157000	-1.703000	7.738000

Alanine tetrapeptide_16

C	-1.778000	1.133000	-1.434000
C	-1.752000	0.811000	0.042000
O	-2.561000	1.260000	0.815000
H	-2.673000	1.697000	-1.651000
H	-1.760000	0.227000	-2.030000
H	-0.908000	1.728000	-1.697000
N	-0.753000	-0.008000	0.444000
C	-0.601000	-0.453000	1.823000
C	0.196000	0.595000	2.611000
O	1.365000	0.460000	2.841000
C	0.082000	-1.812000	1.866000
H	-0.068000	-0.298000	-0.216000
H	-1.596000	-0.523000	2.241000
H	0.174000	-2.154000	2.890000
H	-0.500000	-2.536000	1.307000
H	1.082000	-1.755000	1.453000
N	-0.533000	1.671000	3.008000
C	0.101000	2.877000	3.508000
C	-0.366000	3.275000	4.908000
O	-0.058000	4.355000	5.356000
C	-0.073000	4.047000	2.538000
H	-1.437000	1.765000	2.588000
H	1.155000	2.653000	3.613000
H	0.399000	4.935000	2.935000
H	0.377000	3.798000	1.584000
H	-1.125000	4.262000	2.375000
N	-1.083000	2.378000	5.600000
C	-1.582000	2.635000	6.945000
C	-0.508000	2.280000	7.985000
O	-0.584000	1.287000	8.660000
C	-2.863000	1.850000	7.186000
H	-1.236000	1.483000	5.196000
H	-1.778000	3.698000	7.006000
H	-3.252000	2.059000	8.174000
H	-3.610000	2.126000	6.449000
H	-2.677000	0.784000	7.131000
N	0.504000	3.161000	8.074000
C	1.643000	2.907000	8.930000
H	0.550000	3.892000	7.398000
H	2.245000	3.805000	8.981000
H	1.309000	2.649000	9.925000
H	2.257000	2.093000	8.557000

Alanine tetrapeptide_17

C	-4.706000	1.289000	1.665000
C	-3.767000	0.119000	1.527000

N	-3.228000	0.464000	7.178000
C	-2.909000	1.525000	8.115000
C	-3.968000	2.624000	8.232000
O	-3.824000	3.481000	9.067000
C	-1.561000	2.155000	7.762000
H	-2.852000	0.503000	6.255000
H	-2.853000	1.087000	9.102000
H	-1.332000	2.944000	8.464000
H	-0.778000	1.406000	7.796000
H	-1.582000	2.582000	6.762000
N	-5.000000	2.606000	7.378000
C	-6.058000	3.589000	7.474000
H	-5.107000	1.861000	6.731000
H	-5.660000	4.592000	7.376000
H	-6.762000	3.401000	6.676000
H	-6.569000	3.524000	8.428000

Alanine tetrapeptide_15

C	-4.108000	0.798000	0.912000
C	-2.731000	0.178000	0.951000
O	-2.462000	-0.834000	0.353000
H	-4.540000	0.816000	1.907000
H	-4.736000	0.210000	0.259000
H	-4.059000	1.819000	0.547000
N	-1.818000	0.832000	1.704000
C	-0.432000	0.399000	1.820000
C	-0.329000	-0.678000	2.906000
O	0.018000	-0.428000	4.027000
C	0.469000	1.584000	2.134000
H	-2.104000	1.622000	2.236000
H	-0.157000	-0.038000	0.869000
H	1.502000	1.264000	2.197000
H	0.382000	2.331000	1.353000
H	0.207000	2.025000	3.088000
N	-0.664000	-1.932000	2.505000
C	-0.880000	-2.972000	3.495000
C	0.410000	-3.509000	4.108000
O	0.373000	-4.044000	5.189000
C	-1.657000	-4.132000	2.870000
H	-1.145000	-2.007000	1.633000
H	-1.434000	-2.571000	4.334000
H	-1.816000	-4.905000	3.611000
H	-2.621000	-3.789000	2.511000
H	-1.110000	-4.559000	2.035000
N	1.527000	-3.427000	3.365000
C	2.819000	-3.904000	3.839000
C	3.504000	-2.793000	4.647000
O	4.385000	-2.122000	4.176000
C	3.680000	-4.352000	2.667000
H	1.502000	-2.866000	2.545000
H	2.618000	-4.741000	4.495000
H	4.631000	-4.728000	3.023000
H	3.175000	-5.138000	2.117000
H	3.888000	-3.522000	2.003000

H	-0.492000	0.035000	2.998000
H	1.860000	0.418000	3.633000
H	1.715000	-0.907000	2.501000
H	2.299000	0.649000	1.931000
N	0.761000	2.881000	2.804000
C	0.468000	4.302000	2.865000
C	0.106000	4.861000	1.487000
O	-0.680000	5.762000	1.382000
C	1.651000	5.064000	3.455000
H	1.620000	2.543000	3.169000
H	-0.415000	4.468000	3.467000
H	1.423000	6.122000	3.485000
H	1.852000	4.729000	4.467000
H	2.547000	4.925000	2.857000
N	0.767000	4.323000	0.430000
C	0.260000	4.483000	-0.924000
C	-0.825000	3.419000	-1.113000
O	-0.523000	2.268000	-1.342000
C	1.380000	4.324000	-1.940000
H	1.269000	3.481000	0.600000
H	-0.166000	5.473000	-0.988000
H	1.000000	4.464000	-2.946000
H	2.151000	5.062000	-1.754000
H	1.811000	3.332000	-1.884000
N	-2.085000	3.840000	-0.962000
C	-3.183000	2.894000	-0.882000
H	-2.212000	4.733000	-0.539000
H	-3.136000	2.216000	-1.723000
H	-3.143000	2.324000	0.038000
H	-4.114000	3.443000	-0.926000

Alanine tetrapeptide_19

C	-3.350000	-0.464000	0.958000
C	-2.463000	0.197000	1.986000
O	-2.905000	0.837000	2.906000
H	-3.165000	-1.532000	0.923000
H	-3.153000	-0.054000	-0.028000
H	-4.382000	-0.283000	1.221000
N	-1.132000	0.024000	1.806000
C	-0.141000	0.563000	2.726000
C	0.189000	2.010000	2.337000
O	1.198000	2.287000	1.729000
C	1.106000	-0.308000	2.732000
H	-0.807000	-0.449000	0.994000
H	-0.595000	0.566000	3.708000
H	1.828000	0.073000	3.444000
H	0.845000	-1.322000	3.014000
H	1.580000	-0.315000	1.758000
N	-0.728000	2.916000	2.705000
C	-0.691000	4.314000	2.288000
C	0.225000	5.121000	3.223000
O	-0.213000	5.894000	4.031000
C	-2.101000	4.886000	2.278000
H	-1.561000	2.579000	3.141000

O	-3.996000	-0.795000	0.770000
H	-4.590000	1.917000	0.789000
H	-4.520000	1.878000	2.554000
H	-5.721000	0.916000	1.680000
N	-2.647000	0.146000	2.279000
C	-1.606000	-0.861000	2.138000
C	-1.107000	-0.870000	0.685000
O	-0.633000	0.139000	0.226000
C	-2.022000	-2.201000	2.740000
H	-2.416000	0.987000	2.753000
H	-0.756000	-0.486000	2.695000
H	-1.214000	-2.922000	2.665000
H	-2.250000	-2.062000	3.790000
H	-2.905000	-2.599000	2.257000
N	-1.195000	-2.011000	-0.018000
C	-0.723000	-2.100000	-1.389000
C	-1.494000	-1.246000	-2.400000
O	-0.984000	-1.025000	-3.466000
C	-0.730000	-3.557000	-1.844000
H	-1.737000	-2.759000	0.346000
H	0.287000	-1.714000	-1.425000
H	-0.361000	-3.620000	-2.858000
H	-0.095000	-4.158000	-1.200000
H	-1.736000	-3.967000	-1.821000
N	-2.719000	-0.818000	-2.046000
C	-3.521000	0.040000	-2.895000
C	-3.414000	1.530000	-2.554000
O	-4.110000	2.323000	-3.136000
C	-4.984000	-0.400000	-2.868000
H	-3.076000	-1.030000	-1.140000
H	-3.133000	-0.052000	-3.900000
H	-5.579000	0.261000	-3.483000
H	-5.070000	-1.414000	-3.242000
H	-5.374000	-0.376000	-1.855000
N	-2.539000	1.896000	-1.599000
C	-2.287000	3.296000	-1.339000
H	-1.892000	1.231000	-1.239000
H	-1.639000	3.370000	-0.475000
H	-1.808000	3.783000	-2.182000
H	-3.215000	3.814000	-1.137000

Alanine tetrapeptide_18

C	-0.996000	-1.510000	-0.690000
C	-0.540000	-1.197000	0.717000
O	-0.454000	-2.050000	1.563000
H	-0.305000	-2.223000	-1.123000
H	-1.053000	-0.634000	-1.322000
H	-1.968000	-1.986000	-0.635000
N	-0.221000	0.094000	0.954000
C	0.155000	0.531000	2.282000
C	-0.190000	2.018000	2.372000
O	-1.267000	2.422000	2.020000
C	1.603000	0.162000	2.608000
H	-0.410000	0.777000	0.251000

H	1.233000	3.769000	-0.077000
H	0.864000	2.621000	-2.226000
H	-0.805000	3.182000	-2.274000
H	0.504000	4.344000	-2.392000
N	-1.487000	4.663000	0.998000
C	-2.214000	5.808000	1.500000
H	-1.526000	3.816000	1.518000
H	-2.704000	6.327000	0.687000
H	-2.959000	5.457000	2.201000
H	-1.558000	6.512000	2.002000

Alanine tetrapeptide_21

C	-3.288000	1.513000	1.071000
C	-2.008000	0.920000	1.601000
O	-1.693000	1.037000	2.762000
H	-3.237000	2.588000	1.195000
H	-4.107000	1.143000	1.676000
H	-3.475000	1.273000	0.031000
N	-1.227000	0.270000	0.713000
C	0.000000	-0.420000	1.084000
C	1.227000	0.506000	1.059000
O	2.236000	0.194000	0.489000
C	0.210000	-1.631000	0.186000
H	-1.497000	0.254000	-0.243000
H	-0.126000	-0.743000	2.111000
H	1.109000	-2.159000	0.472000
H	-0.639000	-2.301000	0.271000
H	0.325000	-1.333000	-0.850000
N	1.067000	1.666000	1.738000
C	2.155000	2.608000	1.969000
C	1.644000	3.768000	2.818000
O	2.323000	4.261000	3.679000
C	2.742000	3.176000	0.672000
H	0.295000	1.690000	2.372000
H	2.947000	2.144000	2.544000
H	3.489000	3.924000	0.914000
H	3.205000	2.390000	0.094000
H	1.967000	3.641000	0.072000
N	0.412000	4.218000	2.507000
C	-0.215000	5.310000	3.209000
C	-1.718000	5.169000	2.998000
O	-2.162000	4.722000	1.969000
C	0.256000	6.679000	2.705000
H	-0.099000	3.824000	1.750000
H	0.028000	5.216000	4.261000
H	-0.222000	7.483000	3.256000
H	1.327000	6.757000	2.838000
H	0.019000	6.791000	1.653000
N	-2.496000	5.625000	3.992000
C	-3.941000	5.562000	3.912000
H	-2.074000	5.876000	4.855000
H	-4.358000	6.149000	4.719000
H	-4.275000	5.971000	2.968000
H	-4.300000	4.542000	3.992000

H	-0.270000	4.347000	1.289000
H	-2.085000	5.916000	1.945000
H	-2.731000	4.309000	1.608000
H	-2.528000	4.870000	3.273000
N	1.537000	4.870000	3.053000
C	2.581000	5.516000	3.833000
C	3.961000	5.186000	3.272000
O	4.844000	5.998000	3.323000
C	2.541000	5.123000	5.316000
H	1.782000	4.263000	2.304000
H	2.479000	6.590000	3.753000
H	3.348000	5.619000	5.845000
H	1.598000	5.422000	5.751000
H	2.658000	4.049000	5.432000
N	4.147000	3.945000	2.772000
C	5.452000	3.524000	2.305000
H	3.429000	3.262000	2.842000
H	6.153000	3.406000	3.125000
H	5.345000	2.579000	1.789000
H	5.854000	4.258000	1.620000

Alanine tetrapeptide_20

C	-4.254000	-2.957000	3.458000
C	-3.826000	-1.900000	2.471000
O	-3.218000	-2.180000	1.467000
H	-3.461000	-3.687000	3.550000
H	-5.130000	-3.459000	3.062000
H	-4.495000	-2.554000	4.434000
N	-4.186000	-0.630000	2.760000
C	-3.950000	0.482000	1.850000
C	-2.537000	1.035000	2.067000
O	-2.336000	2.065000	2.659000
C	-5.003000	1.561000	2.047000
H	-4.635000	-0.436000	3.625000
H	-4.008000	0.082000	0.846000
H	-4.843000	2.373000	1.349000
H	-5.990000	1.147000	1.878000
H	-4.951000	1.975000	3.046000
N	-1.543000	0.289000	1.539000
C	-0.156000	0.538000	1.897000
C	0.412000	1.838000	1.328000
O	1.385000	2.323000	1.836000
C	0.711000	-0.634000	1.440000
H	-1.791000	-0.620000	1.205000
H	-0.072000	0.655000	2.971000
H	0.381000	-1.554000	1.910000
H	0.658000	-0.758000	0.363000
H	1.740000	-0.451000	1.717000
N	-0.199000	2.347000	0.239000
C	0.221000	3.575000	-0.404000
C	-0.589000	4.808000	0.011000
O	-0.402000	5.854000	-0.557000
C	0.196000	3.421000	-1.923000
H	-0.994000	1.868000	-0.116000

C	-5.362000	0.348000	2.404000
O	-6.460000	0.313000	1.918000
C	-4.049000	2.242000	3.537000
H	-5.691000	-0.080000	5.266000
H	-6.054000	1.620000	3.893000
H	-4.356000	2.925000	2.751000
H	-3.973000	2.799000	4.464000
H	-3.075000	1.845000	3.297000
N	-4.303000	-0.314000	1.877000
C	-4.548000	-1.384000	0.944000
C	-5.215000	-2.567000	1.659000
O	-5.101000	-2.741000	2.847000
C	-3.230000	-1.830000	0.306000
H	-3.503000	-0.410000	2.467000
H	-5.222000	-1.019000	0.180000
H	-3.397000	-2.618000	-0.419000
H	-2.764000	-0.990000	-0.195000
H	-2.547000	-2.203000	1.062000
N	-5.890000	-3.414000	0.864000
C	-6.550000	-4.589000	1.382000
C	-6.732000	-5.561000	0.221000
O	-6.764000	-5.178000	-0.920000
C	-7.909000	-4.255000	2.012000
H	-6.018000	-3.227000	-0.105000
H	-5.908000	-5.031000	2.135000
H	-8.381000	-5.141000	2.425000
H	-7.764000	-3.536000	2.808000
H	-8.572000	-3.825000	1.269000
N	-6.892000	-6.853000	0.559000
C	-7.142000	-7.869000	-0.444000
H	-6.820000	-7.120000	1.511000
H	-8.045000	-7.649000	-0.999000
H	-6.318000	-7.933000	-1.145000
H	-7.257000	-8.823000	0.054000

Alanine tetrapeptide_24

C	-4.224000	1.504000	1.734000
C	-3.613000	0.248000	2.303000
O	-4.288000	-0.618000	2.805000
H	-3.541000	2.345000	1.758000
H	-5.119000	1.740000	2.290000
H	-4.502000	1.311000	0.702000
N	-2.270000	0.137000	2.207000
C	-1.591000	-1.108000	2.532000
C	-2.197000	-2.242000	1.687000
O	-2.264000	-2.109000	0.496000
C	-1.499000	-1.330000	4.040000
H	-1.798000	0.766000	1.600000
H	-0.584000	-1.006000	2.142000
H	-0.916000	-2.217000	4.265000
H	-0.999000	-0.482000	4.493000
H	-2.480000	-1.419000	4.490000
N	-2.601000	-3.362000	2.322000
C	-3.183000	-4.481000	1.608000

Alanine tetrapeptide_22

C	-3.683000	2.426000	3.033000
C	-2.789000	1.229000	3.268000
O	-2.583000	0.780000	4.365000
H	-3.142000	3.213000	2.519000
H	-4.037000	2.790000	3.986000
H	-4.531000	2.145000	2.416000
N	-2.244000	0.695000	2.153000
C	-1.335000	-0.421000	2.212000
C	-0.493000	-0.394000	0.942000
O	-0.797000	0.268000	-0.014000
C	-2.070000	-1.763000	2.346000
H	-2.371000	1.119000	1.261000
H	-0.686000	-0.291000	3.071000
H	-1.374000	-2.587000	2.468000
H	-2.705000	-1.725000	3.220000
H	-2.678000	-1.960000	1.470000
N	0.596000	-1.198000	0.946000
C	1.529000	-1.222000	-0.166000
C	1.061000	-2.053000	-1.361000
O	1.645000	-1.951000	-2.411000
C	2.888000	-1.738000	0.302000
H	0.860000	-1.641000	1.796000
H	1.634000	-0.217000	-0.551000
H	3.576000	-1.753000	-0.532000
H	3.289000	-1.095000	1.078000
H	2.806000	-2.748000	0.696000
N	0.042000	-2.901000	-1.163000
C	-0.516000	-3.682000	-2.240000
C	-1.960000	-4.002000	-1.871000
O	-2.334000	-3.997000	-0.725000
C	0.273000	-4.975000	-2.480000
H	-0.451000	-2.915000	-0.300000
H	-0.493000	-3.082000	-3.143000
H	-0.141000	-5.541000	-3.308000
H	1.299000	-4.724000	-2.714000
H	0.254000	-5.597000	-1.592000
N	-2.766000	-4.327000	-2.895000
C	-4.149000	-4.700000	-2.679000
H	-2.423000	-4.256000	-3.824000
H	-4.592000	-4.948000	-3.634000
H	-4.215000	-5.560000	-2.025000
H	-4.706000	-3.886000	-2.230000

Alanine tetrapeptide_23

C	-3.853000	-1.532000	6.106000
C	-3.747000	-0.490000	5.020000
O	-2.734000	-0.345000	4.382000
H	-4.529000	-1.240000	6.901000
H	-2.867000	-1.715000	6.510000
H	-4.220000	-2.445000	5.649000
N	-4.868000	0.242000	4.810000
C	-5.105000	1.148000	3.686000

C	4.813000	-3.260000	1.635000
O	4.028000	-2.345000	1.567000
C	5.447000	-4.469000	-0.479000
H	2.881000	-4.046000	-0.221000
H	4.903000	-5.395000	1.387000
H	6.504000	-4.392000	-0.250000
H	5.283000	-5.364000	-1.068000
H	5.171000	-3.605000	-1.076000
N	5.925000	-3.216000	2.384000
C	6.218000	-2.087000	3.247000
H	6.433000	-4.059000	2.524000
H	7.261000	-2.128000	3.533000
H	6.034000	-1.168000	2.711000
H	5.603000	-2.096000	4.141000

Alanine tetrapeptide_26

C	-1.189000	0.145000	5.515000
C	-2.424000	0.782000	4.934000
O	-2.409000	1.912000	4.498000
H	-0.923000	0.685000	6.416000
H	-0.380000	0.262000	4.806000
H	-1.324000	-0.901000	5.758000
N	-3.557000	0.050000	4.944000
C	-4.778000	0.524000	4.308000
C	-4.500000	0.775000	2.818000
O	-4.138000	-0.140000	2.131000
C	-5.438000	1.652000	5.097000
H	-3.483000	-0.924000	5.122000
H	-5.452000	-0.324000	4.300000
H	-6.367000	1.955000	4.625000
H	-5.670000	1.299000	6.095000
H	-4.787000	2.511000	5.190000
N	-4.694000	2.017000	2.325000
C	-4.431000	2.309000	0.930000
C	-2.958000	2.221000	0.517000
O	-2.693000	1.998000	-0.631000
C	-4.970000	3.695000	0.580000
H	-4.822000	2.772000	2.957000
H	-4.926000	1.562000	0.327000
H	-4.790000	3.903000	-0.466000
H	-6.037000	3.743000	0.767000
H	-4.479000	4.465000	1.169000
N	-2.034000	2.501000	1.471000
C	-0.612000	2.243000	1.237000
C	0.146000	2.447000	2.548000
O	0.874000	1.595000	2.987000
C	-0.013000	3.134000	0.146000
H	-2.336000	2.399000	2.417000
H	-0.466000	1.204000	0.970000
H	1.057000	2.963000	0.089000
H	-0.458000	2.902000	-0.809000
H	-0.181000	4.183000	0.365000
N	-0.009000	3.654000	3.128000
C	0.529000	3.935000	4.441000

C	-4.683000	-4.359000	1.316000
O	-5.200000	-5.238000	0.661000
C	-2.915000	-5.783000	2.362000
H	-2.624000	-3.376000	3.315000
H	-2.714000	-4.523000	0.635000
H	-3.334000	-6.616000	1.816000
H	-1.847000	-5.933000	2.478000
H	-3.369000	-5.763000	3.350000
N	-5.338000	-3.316000	1.831000
C	-6.727000	-2.942000	1.561000
C	-7.773000	-3.810000	2.273000
O	-8.648000	-3.278000	2.908000
C	-7.045000	-2.811000	0.069000
H	-4.811000	-2.615000	2.302000
H	-6.843000	-1.973000	2.022000
H	-8.060000	-2.445000	-0.049000
H	-6.366000	-2.099000	-0.387000
H	-6.950000	-3.756000	-0.447000
N	-7.692000	-5.139000	2.114000
C	-8.682000	-6.015000	2.700000
H	-6.976000	-5.511000	1.530000
H	-8.408000	-7.039000	2.482000
H	-8.726000	-5.884000	3.775000
H	-9.670000	-5.822000	2.298000

Alanine tetrapeptide_25

C	-3.000000	1.417000	0.606000
C	-1.551000	1.001000	0.733000
O	-0.642000	1.724000	0.422000
H	-3.525000	0.756000	-0.077000
H	-3.042000	2.429000	0.232000
H	-3.497000	1.364000	1.570000
N	-1.355000	-0.242000	1.224000
C	-0.039000	-0.824000	1.339000
C	-0.215000	-2.341000	1.327000
O	-1.293000	-2.854000	1.491000
C	0.690000	-0.364000	2.609000
H	-2.122000	-0.851000	1.401000
H	0.548000	-0.533000	0.476000
H	1.697000	-0.766000	2.659000
H	0.756000	0.716000	2.600000
H	0.144000	-0.676000	3.493000
N	0.911000	-3.058000	1.124000
C	0.900000	-4.513000	1.266000
C	2.340000	-4.953000	1.493000
O	2.690000	-5.496000	2.501000
C	0.258000	-5.213000	0.066000
H	1.790000	-2.586000	1.183000
H	0.362000	-4.780000	2.165000
H	0.304000	-6.290000	0.195000
H	-0.779000	-4.917000	-0.010000
H	0.761000	-4.956000	-0.861000
N	3.213000	-4.672000	0.479000
C	4.613000	-4.533000	0.801000

H	-8.025000	2.457000	1.394000
H	-6.505000	2.960000	2.149000
N	-5.588000	0.436000	2.379000
C	-4.877000	-0.796000	2.075000
C	-5.590000	-1.971000	2.754000
O	-5.264000	-2.361000	3.846000
C	-3.429000	-0.700000	2.531000
H	-5.356000	0.912000	3.222000
H	-4.923000	-0.926000	1.003000
H	-2.894000	-1.608000	2.278000
H	-2.943000	0.137000	2.043000
H	-3.371000	-0.578000	3.605000
N	-6.601000	-2.510000	2.048000
C	-7.423000	-3.563000	2.595000
C	-7.875000	-4.459000	1.449000
O	-8.139000	-3.989000	0.368000
C	-8.653000	-3.021000	3.334000
H	-6.909000	-2.067000	1.207000
H	-6.807000	-4.119000	3.288000
H	-9.255000	-3.829000	3.738000
H	-8.330000	-2.391000	4.154000
H	-9.268000	-2.435000	2.660000
N	-7.994000	-5.764000	1.749000
C	-8.536000	-6.819000	0.890000
C	-7.572000	-7.268000	-0.217000
O	-7.263000	-8.429000	-0.297000
C	-9.928000	-6.499000	0.339000
H	-7.651000	-6.059000	2.634000
H	-8.614000	-7.689000	1.526000
H	-10.294000	-7.357000	-0.214000
H	-10.611000	-6.303000	1.159000
H	-9.916000	-5.640000	-0.314000
N	-7.147000	-6.334000	-1.080000
C	-6.241000	-6.675000	-2.155000
H	-7.430000	-5.388000	-0.948000
H	-5.293000	-7.035000	-1.772000
H	-6.664000	-7.448000	-2.786000
H	-6.066000	-5.789000	-2.751000

Alanine tetrapeptide_29

C	-2.741000	1.816000	-0.874000
C	-1.893000	0.947000	0.027000
O	-0.780000	0.600000	-0.263000
H	-3.673000	1.317000	-1.119000
H	-2.190000	2.019000	-1.781000
H	-2.981000	2.752000	-0.379000
N	-2.477000	0.587000	1.194000
C	-1.812000	-0.271000	2.143000
C	-2.888000	-0.931000	2.997000
O	-3.975000	-0.416000	3.140000
C	-0.829000	0.500000	3.037000
H	-3.412000	0.853000	1.407000
H	-1.266000	-1.030000	1.595000
H	-0.323000	-0.160000	3.734000

H	-0.748000	4.229000	2.796000
H	-0.089000	3.508000	5.223000
H	1.523000	3.521000	4.514000
H	0.584000	5.008000	4.578000

Alanine tetrapeptide_27

C	-1.913000	-0.282000	-1.189000
C	-1.128000	0.557000	-0.210000
O	-0.043000	1.005000	-0.489000
H	-1.568000	-1.309000	-1.117000
H	-1.709000	0.073000	-2.189000
H	-2.979000	-0.261000	-1.001000
N	-1.700000	0.747000	0.998000
C	-1.057000	1.509000	2.061000
C	-0.089000	0.601000	2.827000
O	-0.388000	0.073000	3.862000
C	-2.098000	2.110000	2.992000
H	-2.555000	0.286000	1.209000
H	-0.491000	2.296000	1.582000
H	-1.612000	2.706000	3.754000
H	-2.773000	2.745000	2.429000
H	-2.662000	1.334000	3.493000
N	1.120000	0.444000	2.239000
C	2.083000	-0.510000	2.752000
C	2.846000	-0.016000	3.980000
O	3.481000	-0.799000	4.640000
C	3.082000	-0.882000	1.658000
H	1.215000	0.766000	1.298000
H	1.563000	-1.398000	3.089000
H	3.796000	-1.596000	2.045000
H	2.567000	-1.321000	0.811000
H	3.623000	-0.006000	1.313000
N	2.809000	1.301000	4.230000
C	3.429000	1.870000	5.399000
C	2.648000	3.126000	5.770000
O	1.976000	3.715000	4.962000
C	4.905000	2.210000	5.157000
H	2.221000	1.899000	3.697000
H	3.362000	1.147000	6.204000
H	5.370000	2.614000	6.050000
H	5.432000	1.308000	4.872000
H	4.997000	2.939000	4.359000
N	2.804000	3.552000	7.037000
C	2.131000	4.737000	7.527000
H	3.268000	2.962000	7.687000
H	1.072000	4.563000	7.682000
H	2.582000	5.031000	8.465000
H	2.244000	5.541000	6.814000

Alanine tetrapeptide_28

C	-7.252000	2.175000	2.094000
C	-6.630000	0.876000	1.634000
O	-7.028000	0.275000	0.671000
H	-7.688000	2.054000	3.081000

H	-5.019000	-2.376000	5.553000		H	-0.085000	0.975000	2.411000
H	-5.817000	-0.805000	5.455000		H	-1.353000	1.264000	3.603000
N	-7.393000	-1.423000	2.376000		N	-2.542000	-2.081000	3.593000
C	-8.447000	-0.748000	1.625000		C	-3.438000	-2.843000	4.460000
C	-9.383000	-0.016000	2.596000		C	-3.397000	-2.271000	5.886000
O	-10.447000	-0.472000	2.917000		O	-2.831000	-2.840000	6.779000
C	-9.207000	-1.754000	0.776000		C	-3.048000	-4.313000	4.444000
H	-7.539000	-2.374000	2.629000		H	-1.623000	-2.437000	3.455000
H	-7.960000	-0.019000	0.991000		H	-4.438000	-2.720000	4.063000
H	-9.967000	-1.251000	0.192000		H	-3.723000	-4.885000	5.067000
H	-8.525000	-2.260000	0.102000		H	-3.093000	-4.698000	3.431000
H	-9.708000	-2.484000	1.400000		H	-2.049000	-4.451000	4.841000
N	-8.910000	1.159000	3.052000		N	-4.020000	-1.084000	6.019000
C	-9.621000	1.909000	4.063000		C	-4.111000	-0.363000	7.281000
H	-7.962000	1.389000	2.849000		C	-5.009000	0.863000	7.139000
H	-9.573000	1.427000	5.035000		O	-5.676000	1.234000	8.066000
H	-9.182000	2.895000	4.138000		C	-2.742000	0.090000	7.805000
H	-10.661000	2.005000	3.785000		H	-4.550000	-0.766000	5.239000

Alanine tetrapeptide_31

C	-0.917000	0.861000	-0.956000		H	-4.584000	-0.989000	8.027000
C	-1.176000	0.649000	0.518000		H	-2.875000	0.645000	8.727000
O	-1.205000	1.557000	1.305000		H	-2.116000	-0.768000	7.997000
H	-1.488000	0.175000	-1.572000		H	-2.248000	0.732000	7.081000
H	0.138000	0.701000	-1.156000		N	-4.975000	1.521000	5.959000
H	-1.168000	1.880000	-1.211000		C	-5.716000	2.753000	5.775000
N	-1.343000	-0.638000	0.896000		H	-4.327000	1.252000	5.256000
C	-1.503000	-1.004000	2.281000		H	-5.274000	3.574000	6.329000
C	-1.054000	-2.449000	2.436000		H	-5.721000	2.998000	4.721000
O	-1.114000	-3.230000	1.515000		H	-6.734000	2.624000	6.114000
C	-2.954000	-0.858000	2.758000					

Alanine tetrapeptide_30

H	-1.299000	-1.380000	0.235000		C	-1.949000	1.865000	0.896000
H	-0.869000	-0.358000	2.877000		C	-1.837000	0.439000	1.383000
H	-3.050000	-1.117000	3.807000		O	-1.924000	-0.500000	0.644000
H	-3.265000	0.169000	2.624000		H	-1.368000	2.558000	1.495000
H	-3.606000	-1.504000	2.180000		H	-2.992000	2.165000	0.941000
N	-0.657000	-2.815000	3.667000		H	-1.624000	1.909000	-0.133000
C	-0.160000	-4.155000	3.938000		N	-1.687000	0.288000	2.728000
C	1.032000	-4.442000	3.009000		C	-1.533000	-1.019000	3.335000
O	1.930000	-3.648000	2.955000		C	-2.849000	-1.764000	3.557000
C	-1.291000	-5.181000	3.971000		O	-2.830000	-2.928000	3.867000
H	-0.411000	-2.097000	4.308000		C	-0.793000	-0.901000	4.666000
H	0.285000	-4.110000	4.925000		H	-1.535000	1.094000	3.289000
H	-0.920000	-6.156000	4.268000		H	-0.968000	-1.646000	2.659000
H	-2.029000	-4.872000	4.702000		H	-0.686000	-1.881000	5.110000
H	-1.785000	-5.262000	3.011000		H	0.192000	-0.474000	4.513000
N	1.029000	-5.603000	2.325000		H	-1.341000	-0.271000	5.362000
C	2.106000	-5.983000	1.430000		N	-3.981000	-1.052000	3.439000
C	1.962000	-5.472000	-0.007000		C	-5.279000	-1.670000	3.545000
O	2.818000	-5.748000	-0.809000		C	-6.257000	-0.815000	2.749000
C	2.265000	-7.502000	1.418000		O	-6.023000	0.347000	2.504000
H	0.208000	-6.162000	2.325000		C	-5.742000	-1.788000	5.003000
H	3.010000	-5.527000	1.807000		H	-3.955000	-0.117000	3.107000
H	3.071000	-7.779000	0.753000		H	-5.225000	-2.661000	3.110000
					H	-6.709000	-2.276000	5.075000

C	-2.045000	2.892000	-0.281000
C	-2.250000	1.458000	0.158000
O	-2.727000	0.630000	-0.566000
H	-2.895000	3.487000	0.042000
H	-1.995000	2.921000	-1.360000
H	-1.145000	3.322000	0.143000
N	-1.866000	1.185000	1.434000
C	-2.194000	-0.086000	2.072000
C	-1.992000	0.017000	3.580000
O	-2.767000	-0.486000	4.348000
C	-1.356000	-1.246000	1.521000
H	-1.688000	1.965000	2.025000
H	-3.243000	-0.309000	1.929000
H	-1.615000	-2.163000	2.041000
H	-1.558000	-1.372000	0.467000
H	-0.296000	-1.056000	1.655000
N	-0.889000	0.681000	3.985000
C	-0.561000	0.861000	5.380000
C	0.329000	2.097000	5.467000
O	0.958000	2.483000	4.511000
C	0.148000	-0.361000	5.979000
H	-0.213000	1.008000	3.331000
H	-1.482000	1.036000	5.922000
H	0.365000	-0.212000	7.031000
H	-0.494000	-1.227000	5.879000
H	1.080000	-0.550000	5.456000
N	0.384000	2.698000	6.664000
C	1.233000	3.843000	6.905000
C	1.458000	3.931000	8.412000
O	0.716000	3.389000	9.189000
C	0.605000	5.141000	6.379000
H	-0.136000	2.362000	7.444000
H	2.179000	3.678000	6.403000
H	1.261000	5.990000	6.540000
H	0.424000	5.043000	5.317000
H	-0.337000	5.332000	6.883000
N	2.503000	4.680000	8.803000
C	2.800000	4.888000	10.207000
H	3.118000	5.053000	8.119000
H	3.094000	3.963000	10.688000
H	3.611000	5.600000	10.285000
H	1.934000	5.282000	10.721000

Alanine tetrapeptide_34

C	-2.694000	1.748000	-0.327000
C	-3.027000	0.429000	0.332000
O	-3.076000	-0.594000	-0.305000
H	-3.609000	2.172000	-0.729000
H	-2.017000	1.562000	-1.148000
H	-2.254000	2.463000	0.358000
N	-3.282000	0.484000	1.657000
C	-3.767000	-0.607000	2.499000
C	-2.690000	-1.641000	2.853000
O	-2.458000	-1.862000	4.020000

H	2.482000	-7.863000	2.417000
H	1.357000	-7.985000	1.066000
N	0.863000	-4.766000	-0.316000
C	0.709000	-4.191000	-1.633000
H	0.264000	-4.437000	0.407000
H	0.922000	-4.935000	-2.388000
H	-0.314000	-3.856000	-1.744000
H	1.377000	-3.350000	-1.789000

Alanine tetrapeptide_32

C	-3.227000	0.713000	0.656000
C	-1.794000	0.894000	1.101000
O	-1.437000	1.905000	1.654000
H	-3.609000	1.671000	0.332000
H	-3.813000	0.387000	1.510000
H	-3.337000	-0.014000	-0.140000
N	-0.971000	-0.150000	0.864000
C	0.447000	-0.233000	1.217000
C	0.647000	-0.441000	2.725000
O	0.989000	-1.517000	3.137000
C	1.288000	0.904000	0.636000
H	-1.375000	-0.974000	0.484000
H	0.790000	-1.164000	0.789000
H	2.332000	0.738000	0.881000
H	1.188000	0.913000	-0.444000
H	0.992000	1.871000	1.015000
N	0.437000	0.633000	3.518000
C	0.422000	0.503000	4.971000
C	-0.151000	1.770000	5.598000
O	-0.958000	1.710000	6.489000
C	1.813000	0.228000	5.552000
H	-0.078000	1.385000	3.107000
H	-0.246000	-0.297000	5.263000
H	1.754000	0.188000	6.635000
H	2.183000	-0.720000	5.188000
H	2.512000	1.009000	5.270000
N	0.328000	2.936000	5.124000
C	-0.108000	4.211000	5.642000
C	0.254000	5.267000	4.602000
O	1.170000	5.104000	3.839000
C	0.554000	4.552000	6.984000
H	1.031000	2.961000	4.419000
H	-1.182000	4.174000	5.777000
H	0.199000	5.505000	7.364000
H	0.314000	3.782000	7.706000
H	1.631000	4.606000	6.867000
N	-0.474000	6.397000	4.637000
C	-0.217000	7.488000	3.718000
H	-1.283000	6.432000	5.210000
H	-0.782000	8.353000	4.040000
H	0.836000	7.732000	3.721000
H	-0.507000	7.232000	2.705000

Alanine tetrapeptide_33

C	-2.901000	3.025000	5.018000
H	-2.220000	-0.163000	4.761000
H	-1.129000	2.133000	5.834000
H	-2.994000	3.755000	5.815000
H	-2.381000	3.479000	4.188000
H	-3.895000	2.736000	4.693000
N	-3.870000	0.474000	6.567000
C	-4.675000	-0.048000	7.669000
C	-4.069000	-1.375000	8.146000
O	-4.500000	-2.434000	7.777000
C	-6.116000	-0.230000	7.220000
H	-4.222000	0.361000	5.643000
H	-4.622000	0.674000	8.472000
H	-6.720000	-0.591000	8.043000
H	-6.522000	0.717000	6.880000
H	-6.181000	-0.961000	6.424000
N	-3.028000	-1.245000	8.987000
C	-2.274000	-2.397000	9.432000
H	-2.638000	-0.335000	9.107000
H	-1.665000	-2.109000	10.278000
H	-2.953000	-3.181000	9.734000
H	-1.629000	-2.788000	8.651000

Alanine tetrapeptide_36

C	-0.379000	3.626000	1.062000
C	-1.423000	2.561000	0.822000
O	-2.283000	2.667000	-0.004000
H	-0.134000	3.725000	2.113000
H	-0.745000	4.567000	0.680000
H	0.527000	3.362000	0.524000
N	-1.328000	1.454000	1.617000
C	-2.083000	0.254000	1.306000
C	-3.542000	0.299000	1.753000
O	-4.306000	-0.543000	1.346000
C	-1.412000	-0.967000	1.934000
H	-0.517000	1.354000	2.184000
H	-2.130000	0.132000	0.232000
H	-1.984000	-1.855000	1.705000
H	-0.408000	-1.088000	1.542000
H	-1.354000	-0.866000	3.014000
N	-3.899000	1.248000	2.633000
C	-5.265000	1.382000	3.117000
C	-6.085000	2.212000	2.118000
O	-6.306000	3.383000	2.321000
C	-5.274000	2.016000	4.499000
H	-3.252000	1.975000	2.831000
H	-5.679000	0.384000	3.163000
H	-6.288000	2.091000	4.873000
H	-4.693000	1.409000	5.185000
H	-4.864000	3.018000	4.468000
N	-6.492000	1.534000	1.036000
C	-7.250000	2.065000	-0.097000
C	-6.419000	2.940000	-1.045000
O	-6.346000	2.648000	-2.211000

C	-5.039000	-1.277000	1.969000
H	-3.170000	1.362000	2.108000
H	-3.997000	-0.153000	3.452000
H	-5.375000	-2.022000	2.682000
H	-5.822000	-0.534000	1.858000
H	-4.879000	-1.754000	1.013000
N	-2.101000	-2.281000	1.835000
C	-0.986000	-3.219000	1.929000
C	-1.364000	-4.616000	2.440000
O	-1.023000	-5.580000	1.792000
C	0.221000	-2.667000	2.695000
H	-2.385000	-2.017000	0.914000
H	-0.684000	-3.402000	0.908000
H	1.031000	-3.387000	2.657000
H	0.558000	-1.747000	2.228000
H	-0.017000	-2.463000	3.729000
N	-2.004000	-4.685000	3.614000
C	-2.506000	-5.893000	4.264000
C	-1.431000	-6.770000	4.919000
O	-1.586000	-7.142000	6.054000
C	-3.421000	-6.734000	3.367000
H	-2.174000	-3.821000	4.084000
H	-3.088000	-5.541000	5.103000
H	-3.823000	-7.561000	3.943000
H	-4.248000	-6.126000	3.015000
H	-2.892000	-7.126000	2.510000
N	-0.373000	-7.120000	4.172000
C	0.642000	-8.006000	4.696000
H	-0.353000	-6.850000	3.213000
H	0.258000	-9.010000	4.850000
H	1.462000	-8.048000	3.991000
H	1.011000	-7.639000	5.645000

Alanine tetrapeptide_35

C	-0.112000	-0.044000	-1.089000
C	-0.640000	-0.654000	0.190000
O	-1.144000	-1.745000	0.228000
H	-0.414000	-0.663000	-1.921000
H	0.971000	0.004000	-1.054000
H	-0.489000	0.964000	-1.225000
N	-0.490000	0.112000	1.294000
C	-0.957000	-0.320000	2.587000
C	-1.171000	0.928000	3.436000
O	-0.637000	1.972000	3.173000
C	0.032000	-1.273000	3.272000
H	-0.105000	1.028000	1.241000
H	-1.904000	-0.831000	2.456000
H	-0.345000	-1.623000	4.228000
H	0.186000	-2.133000	2.635000
H	0.982000	-0.777000	3.435000
N	-1.989000	0.770000	4.505000
C	-2.113000	1.812000	5.521000
C	-2.781000	1.246000	6.768000
O	-2.363000	1.508000	7.866000

H	1.615000	3.148000	-2.658000
H	-0.119000	3.252000	-2.969000

Alanine tetrapeptide_38

C	1.110000	0.587000	0.838000
C	-0.268000	0.474000	1.452000
O	-0.897000	1.434000	1.795000
H	1.262000	-0.141000	0.049000
H	1.859000	0.421000	1.607000
H	1.235000	1.586000	0.446000
N	-0.732000	-0.800000	1.591000
C	-1.940000	-1.091000	2.357000
C	-2.036000	-2.587000	2.631000
O	-2.430000	-3.006000	3.685000
C	-3.212000	-0.625000	1.640000
H	-0.059000	-1.527000	1.504000
H	-1.887000	-0.615000	3.328000
H	-4.082000	-0.892000	2.232000
H	-3.189000	0.447000	1.513000
H	-3.298000	-1.093000	0.664000
N	-1.678000	-3.399000	1.611000
C	-1.724000	-4.837000	1.720000
C	-0.690000	-5.390000	0.746000
O	-0.348000	-4.754000	-0.225000
C	-3.114000	-5.405000	1.405000
H	-1.445000	-3.029000	0.717000
H	-1.455000	-5.102000	2.734000
H	-3.133000	-6.486000	1.507000
H	-3.833000	-4.983000	2.094000
H	-3.406000	-5.151000	0.391000
N	-0.214000	-6.614000	1.019000
C	0.769000	-7.288000	0.175000
C	0.052000	-8.037000	-0.957000
O	-0.129000	-9.224000	-0.911000
C	1.616000	-8.231000	1.016000
H	-0.564000	-7.107000	1.809000
H	1.389000	-6.513000	-0.255000
H	2.369000	-8.706000	0.399000
H	2.110000	-7.680000	1.808000
H	1.006000	-9.017000	1.445000
N	-0.355000	-7.261000	-1.978000
C	-1.145000	-7.806000	-3.062000
H	-0.283000	-6.274000	-1.875000
H	-2.154000	-8.051000	-2.746000
H	-1.194000	-7.073000	-3.857000
H	-0.680000	-8.706000	-3.440000

Alanine tetrapeptide_39

C	-4.329000	1.671000	-0.243000
C	-4.187000	0.302000	0.384000
O	-4.642000	-0.692000	-0.117000
H	-4.768000	2.373000	0.459000
H	-4.958000	1.590000	-1.117000
H	-3.355000	2.051000	-0.534000

C	-8.553000	2.750000	0.317000
H	-6.113000	0.617000	0.923000
H	-7.496000	1.202000	-0.698000
H	-9.102000	3.036000	-0.574000
H	-9.164000	2.060000	0.889000
H	-8.374000	3.630000	0.916000
N	-5.849000	4.035000	-0.518000
C	-4.970000	4.874000	-1.304000
H	-5.907000	4.175000	0.466000
H	-5.409000	5.059000	-2.274000
H	-4.843000	5.818000	-0.788000
H	-3.998000	4.413000	-1.441000

Alanine tetrapeptide_37

C	-3.974000	0.076000	0.966000
C	-3.407000	-0.478000	2.254000
O	-4.057000	-1.154000	3.002000
H	-4.836000	-0.510000	0.683000
H	-3.240000	0.070000	0.167000
H	-4.288000	1.103000	1.128000
N	-2.112000	-0.142000	2.501000
C	-1.504000	-0.395000	3.807000
C	-0.249000	0.465000	3.882000
O	-0.092000	1.304000	4.722000
C	-1.197000	-1.876000	4.039000
H	-1.725000	0.601000	1.957000
H	-2.157000	-0.039000	4.593000
H	-0.704000	-2.006000	4.998000
H	-2.119000	-2.439000	4.042000
H	-0.550000	-2.273000	3.264000
N	0.686000	0.227000	2.911000
C	1.601000	1.283000	2.561000
C	0.838000	2.391000	1.824000
O	-0.220000	2.163000	1.277000
C	2.730000	0.739000	1.681000
H	0.380000	-0.335000	2.148000
H	2.008000	1.687000	3.478000
H	3.442000	1.516000	1.429000
H	3.251000	-0.051000	2.208000
H	2.336000	0.335000	0.754000
N	1.421000	3.595000	1.791000
C	0.809000	4.760000	1.156000
C	1.164000	4.773000	-0.338000
O	2.035000	5.477000	-0.773000
C	1.271000	6.033000	1.847000
H	2.283000	3.729000	2.270000
H	-0.262000	4.647000	1.262000
H	0.793000	6.895000	1.399000
H	1.013000	5.999000	2.900000
H	2.341000	6.163000	1.737000
N	0.432000	3.937000	-1.098000
C	0.723000	3.748000	-2.503000
H	-0.163000	3.288000	-0.633000
H	0.874000	4.708000	-2.976000

N	-6.539000	-1.577000	3.521000
C	-7.362000	-2.633000	4.051000
C	-8.800000	-2.127000	4.068000
O	-9.040000	-0.940000	4.094000
C	-6.929000	-3.048000	5.462000
H	-6.921000	-0.660000	3.528000
H	-7.283000	-3.488000	3.391000
H	-7.541000	-3.860000	5.841000
H	-5.899000	-3.379000	5.430000
H	-7.009000	-2.207000	6.143000
N	-9.745000	-3.079000	4.087000
C	-11.188000	-2.891000	4.239000
C	-11.907000	-2.395000	2.978000
O	-12.931000	-2.931000	2.643000
C	-11.564000	-2.040000	5.455000
H	-9.442000	-4.016000	3.951000
H	-11.589000	-3.883000	4.387000
H	-12.644000	-2.029000	5.554000
H	-11.139000	-2.474000	6.353000
H	-11.209000	-1.024000	5.359000
N	-11.367000	-1.354000	2.328000
C	-12.009000	-0.792000	1.159000
H	-10.582000	-0.891000	2.727000
H	-11.302000	-0.146000	0.655000
H	-12.308000	-1.582000	0.484000
H	-12.891000	-0.216000	1.420000

Alanine tetrapeptide_41

C	-2.764000	2.965000	1.675000
C	-2.700000	1.454000	1.617000
O	-3.196000	0.777000	2.483000
H	-1.934000	3.321000	2.278000
H	-3.685000	3.253000	2.161000
H	-2.703000	3.428000	0.697000
N	-2.036000	0.941000	0.560000
C	-1.709000	-0.465000	0.325000
C	-2.891000	-1.318000	-0.146000
O	-2.772000	-2.000000	-1.132000
C	-0.988000	-1.136000	1.499000
H	-1.713000	1.580000	-0.127000
H	-1.043000	-0.464000	-0.525000
H	-0.722000	-2.149000	1.218000
H	-0.081000	-0.589000	1.731000
H	-1.607000	-1.175000	2.383000
N	-4.011000	-1.294000	0.598000
C	-5.087000	-2.233000	0.353000
C	-4.543000	-3.670000	0.427000
O	-3.783000	-3.978000	1.309000
C	-5.895000	-1.873000	-0.894000
H	-3.973000	-0.831000	1.480000
H	-5.744000	-2.159000	1.215000
H	-6.776000	-2.499000	-0.984000
H	-6.229000	-0.845000	-0.811000
H	-5.296000	-1.966000	-1.790000

N	-3.501000	0.273000	1.549000
C	-3.291000	-0.953000	2.280000
C	-3.049000	-0.583000	3.735000
O	-2.644000	0.513000	4.052000
C	-2.101000	-1.760000	1.740000
H	-3.155000	1.108000	1.965000
H	-4.189000	-1.554000	2.205000
H	-1.959000	-2.682000	2.293000
H	-2.287000	-2.004000	0.702000
H	-1.188000	-1.179000	1.810000
N	-3.287000	-1.541000	4.647000
C	-2.917000	-1.341000	6.035000
C	-1.397000	-1.172000	6.145000
O	-0.660000	-1.986000	5.662000
C	-3.359000	-2.541000	6.868000
H	-3.460000	-2.469000	4.337000
H	-3.419000	-0.447000	6.385000
H	-3.114000	-2.383000	7.912000
H	-4.430000	-2.684000	6.785000
H	-2.848000	-3.437000	6.534000
N	-0.979000	-0.083000	6.822000
C	0.425000	0.259000	7.014000
C	1.180000	0.555000	5.709000
O	2.380000	0.494000	5.688000
C	1.170000	-0.762000	7.871000
H	-1.657000	0.606000	7.051000
H	0.418000	1.206000	7.545000
H	2.180000	-0.418000	8.046000
H	0.660000	-0.876000	8.822000
H	1.213000	-1.721000	7.375000
N	0.454000	0.981000	4.661000
C	1.100000	1.266000	3.398000
H	-0.537000	0.902000	4.672000
H	1.556000	0.378000	2.974000
H	0.355000	1.645000	2.711000
H	1.874000	2.012000	3.527000

Alanine tetrapeptide_40

C	-6.970000	2.270000	1.445000
C	-6.331000	0.907000	1.315000
O	-6.643000	0.127000	0.460000
H	-7.773000	2.215000	2.174000
H	-7.389000	2.550000	0.490000
H	-6.265000	3.025000	1.773000
N	-5.412000	0.600000	2.272000
C	-4.664000	-0.642000	2.245000
C	-5.403000	-1.835000	2.852000
O	-4.938000	-2.940000	2.744000
C	-3.322000	-0.468000	2.954000
H	-5.126000	1.310000	2.906000
H	-4.497000	-0.916000	1.212000
H	-2.775000	-1.400000	2.931000
H	-2.734000	0.299000	2.463000
H	-3.466000	-0.184000	3.994000

N	0.171000	-0.669000	5.068000
C	-0.304000	0.549000	5.685000
H	-0.509000	-1.325000	4.759000
H	-0.255000	1.391000	5.001000
H	-1.332000	0.397000	5.989000
H	0.291000	0.792000	6.556000

Alanine tetrapeptide_43

C	-0.787000	1.248000	-0.230000
C	-1.500000	0.807000	1.024000
O	-2.180000	1.555000	1.673000
H	-0.720000	0.456000	-0.966000
H	0.219000	1.562000	0.032000
H	-1.313000	2.095000	-0.645000
N	-1.329000	-0.497000	1.379000
C	-1.722000	-0.993000	2.694000
C	-3.236000	-0.902000	2.927000
O	-3.664000	-0.757000	4.042000
C	-0.938000	-0.362000	3.844000
H	-0.636000	-1.017000	0.891000
H	-1.514000	-2.059000	2.671000
H	-1.220000	-0.818000	4.783000
H	0.124000	-0.514000	3.683000
H	-1.140000	0.698000	3.907000
N	-4.008000	-1.096000	1.843000
C	-5.469000	-1.147000	1.809000
C	-6.155000	0.220000	1.927000
O	-6.983000	0.522000	1.108000
C	-6.074000	-2.151000	2.793000
H	-3.550000	-1.095000	0.963000
H	-5.720000	-1.465000	0.807000
H	-7.147000	-2.195000	2.637000
H	-5.662000	-3.137000	2.609000
H	-5.879000	-1.882000	3.821000
N	-5.806000	0.996000	2.975000
C	-6.524000	2.214000	3.305000
C	-5.615000	3.430000	3.495000
O	-6.064000	4.430000	3.997000
C	-7.422000	2.019000	4.529000
H	-5.202000	0.600000	3.665000
H	-7.141000	2.445000	2.448000
H	-7.947000	2.936000	4.755000
H	-8.142000	1.231000	4.335000
H	-6.836000	1.740000	5.400000
N	-4.355000	3.350000	3.049000
C	-3.474000	4.494000	3.136000
H	-4.023000	2.528000	2.602000
H	-3.356000	4.814000	4.164000
H	-2.511000	4.206000	2.737000
H	-3.862000	5.332000	2.568000

Alanine tetrapeptide_44

C	-1.251000	-0.338000	-1.755000
C	-0.578000	-0.934000	-0.543000

N	-5.014000	-4.560000	-0.465000
C	-4.511000	-5.914000	-0.494000
C	-4.672000	-6.436000	-1.918000
O	-5.458000	-5.945000	-2.686000
C	-5.257000	-6.818000	0.495000
H	-5.509000	-4.267000	-1.276000
H	-3.459000	-5.895000	-0.230000
H	-4.854000	-7.826000	0.490000
H	-5.153000	-6.411000	1.493000
H	-6.310000	-6.864000	0.240000
N	-3.915000	-7.505000	-2.232000
C	-3.955000	-8.100000	-3.552000
H	-3.192000	-7.778000	-1.608000
H	-3.410000	-7.507000	-4.280000
H	-3.516000	-9.089000	-3.504000
H	-4.981000	-8.185000	-3.879000

Alanine tetrapeptide_42

C	-2.009000	1.547000	0.030000
C	-2.796000	0.336000	0.466000
O	-3.007000	-0.585000	-0.284000
H	-2.306000	2.449000	0.551000
H	-2.135000	1.678000	-1.035000
H	-0.960000	1.353000	0.235000
N	-3.218000	0.349000	1.754000
C	-3.842000	-0.768000	2.462000
C	-2.799000	-1.841000	2.780000
O	-2.423000	-2.009000	3.918000
C	-5.103000	-1.308000	1.787000
H	-2.865000	1.077000	2.331000
H	-4.118000	-0.376000	3.431000
H	-5.548000	-2.068000	2.421000
H	-5.818000	-0.503000	1.665000
H	-4.899000	-1.735000	0.817000
N	-2.309000	-2.552000	1.749000
C	-1.103000	-3.326000	1.942000
C	0.028000	-2.393000	2.392000
O	0.209000	-1.338000	1.845000
C	-0.712000	-4.014000	0.636000
H	-2.500000	-2.210000	0.829000
H	-1.292000	-4.070000	2.707000
H	0.184000	-4.609000	0.775000
H	-1.511000	-4.667000	0.304000
H	-0.516000	-3.276000	-0.133000
N	0.787000	-2.842000	3.413000
C	1.882000	-2.081000	4.000000
C	1.446000	-0.761000	4.654000
O	2.262000	0.098000	4.861000
C	3.043000	-1.867000	3.030000
H	0.483000	-3.658000	3.890000
H	2.241000	-2.687000	4.827000
H	3.853000	-1.366000	3.540000
H	3.389000	-2.827000	2.663000
H	2.734000	-1.260000	2.191000

H	-0.480000	-1.554000	3.098000
H	-2.933000	-1.591000	3.401000
H	-2.358000	0.044000	3.089000
H	-3.159000	-0.864000	1.811000
N	-1.781000	-3.085000	0.499000
C	-2.059000	-4.387000	-0.102000
C	-0.750000	-4.942000	-0.682000
O	-0.496000	-4.874000	-1.854000
C	-3.130000	-4.251000	-1.171000
H	-2.015000	-2.272000	-0.026000
H	-2.405000	-5.039000	0.691000
H	-3.351000	-5.220000	-1.602000
H	-4.039000	-3.847000	-0.738000
H	-2.792000	-3.608000	-1.974000
N	0.078000	-5.449000	0.249000
C	1.422000	-5.930000	-0.036000
C	2.056000	-6.532000	1.216000
O	2.811000	-7.460000	1.120000
C	2.343000	-4.826000	-0.571000
H	-0.268000	-5.497000	1.179000
H	1.375000	-6.732000	-0.759000
H	3.333000	-5.232000	-0.742000
H	1.955000	-4.440000	-1.503000
H	2.422000	-4.013000	0.145000
N	1.765000	-5.946000	2.397000
C	2.392000	-6.397000	3.623000
H	1.236000	-5.105000	2.427000
H	3.432000	-6.093000	3.679000
H	1.853000	-5.975000	4.461000
H	2.350000	-7.475000	3.679000

Alanine tetrapeptide_46

C	-4.587000	2.874000	2.577000
C	-4.927000	1.403000	2.685000
O	-6.035000	1.013000	2.920000
H	-5.504000	3.440000	2.524000
H	-3.979000	3.073000	1.701000
H	-4.029000	3.186000	3.455000
N	-3.876000	0.556000	2.494000
C	-3.994000	-0.871000	2.777000
C	-2.606000	-1.491000	2.884000
O	-2.336000	-2.281000	3.747000
C	-4.815000	-1.609000	1.714000
H	-2.967000	0.957000	2.531000
H	-4.457000	-1.017000	3.744000
H	-4.856000	-2.667000	1.950000
H	-5.821000	-1.216000	1.695000
H	-4.374000	-1.488000	0.729000
N	-1.711000	-1.101000	1.946000
C	-0.359000	-1.610000	1.920000
C	0.499000	-0.540000	1.255000
O	0.050000	0.110000	0.337000
C	-0.236000	-2.932000	1.153000
H	-1.999000	-0.563000	1.160000

O	0.020000	-1.975000	-0.593000
H	-0.616000	-0.494000	-2.616000
H	-1.463000	0.719000	-1.646000
H	-2.183000	-0.867000	-1.924000
N	-0.675000	-0.224000	0.611000
C	-0.287000	-0.798000	1.897000
C	1.196000	-1.187000	1.932000
O	1.559000	-2.129000	2.590000
C	-1.181000	-1.953000	2.336000
H	-1.305000	0.545000	0.632000
H	-0.379000	0.011000	2.616000
H	-0.892000	-2.294000	3.321000
H	-2.214000	-1.619000	2.367000
H	-1.098000	-2.785000	1.650000
N	2.031000	-0.365000	1.274000
C	3.488000	-0.471000	1.206000
C	3.999000	-1.590000	0.290000
O	4.784000	-1.323000	-0.580000
C	4.161000	-0.525000	2.580000
H	1.613000	0.309000	0.677000
H	3.814000	0.431000	0.709000
H	5.237000	-0.504000	2.446000
H	3.871000	0.342000	3.163000
H	3.891000	-1.415000	3.128000
N	3.571000	-2.842000	0.545000
C	4.121000	-3.991000	-0.149000
C	3.453000	-4.322000	-1.484000
O	3.999000	-5.091000	-2.234000
C	4.060000	-5.223000	0.754000
H	2.962000	-2.987000	1.322000
H	5.150000	-3.775000	-0.399000
H	4.473000	-6.076000	0.234000
H	4.626000	-5.052000	1.663000
H	3.033000	-5.453000	1.028000
N	2.254000	-3.781000	-1.734000
C	1.549000	-4.078000	-2.960000
H	1.840000	-3.148000	-1.090000
H	0.578000	-3.606000	-2.913000
H	2.088000	-3.705000	-3.825000
H	1.421000	-5.147000	-3.082000

Alanine tetrapeptide_45

C	0.850000	1.142000	0.358000
C	0.013000	0.539000	1.463000
O	-0.190000	1.100000	2.500000
H	0.354000	1.051000	-0.603000
H	1.804000	0.627000	0.296000
H	1.027000	2.183000	0.583000
N	-0.499000	-0.699000	1.183000
C	-1.127000	-1.498000	2.232000
C	-1.300000	-2.932000	1.749000
O	-1.041000	-3.865000	2.470000
C	-2.487000	-0.937000	2.659000
H	-0.046000	-1.195000	0.447000

H	2.290000	-5.009000	-0.010000
H	2.519000	-7.452000	0.398000
H	3.346000	-6.511000	1.644000
H	1.792000	-7.268000	1.984000
N	-0.768000	-5.371000	0.409000
C	-1.999000	-5.648000	-0.299000
H	-0.777000	-4.652000	1.096000
H	-2.810000	-5.163000	0.228000
H	-1.963000	-5.277000	-1.317000
H	-2.185000	-6.714000	-0.335000

Alanine tetrapeptide_48

C	-0.622000	-0.870000	-1.719000
C	-0.698000	-1.350000	-0.286000
O	-0.464000	-2.481000	0.027000
H	-0.116000	-1.619000	-2.310000
H	-0.096000	0.075000	-1.791000
H	-1.625000	-0.732000	-2.112000
N	-1.051000	-0.388000	0.622000
C	-1.406000	-0.739000	1.995000
C	-2.027000	0.463000	2.696000
O	-2.948000	0.315000	3.459000
C	-0.199000	-1.221000	2.810000
H	-1.508000	0.409000	0.238000
H	-2.167000	-1.509000	2.004000
H	-0.505000	-1.413000	3.833000
H	0.192000	-2.131000	2.383000
H	0.587000	-0.472000	2.818000
N	-1.459000	1.662000	2.438000
C	-1.889000	2.963000	2.948000
C	-1.526000	3.223000	4.415000
O	-0.912000	4.227000	4.695000
C	-3.368000	3.258000	2.683000
H	-0.606000	1.652000	1.927000
H	-1.297000	3.689000	2.410000
H	-3.591000	4.269000	3.009000
H	-3.570000	3.190000	1.620000
H	-4.016000	2.569000	3.204000
N	-1.949000	2.339000	5.327000
C	-1.764000	2.542000	6.760000
C	-0.382000	2.033000	7.195000
O	-0.244000	1.001000	7.797000
C	-2.874000	1.840000	7.529000
H	-2.449000	1.532000	5.017000
H	-1.805000	3.609000	6.939000
H	-2.757000	2.007000	8.592000
H	-3.840000	2.225000	7.218000
H	-2.842000	0.771000	7.360000
N	0.647000	2.829000	6.853000
C	2.014000	2.439000	7.121000
H	0.462000	3.610000	6.262000
H	2.664000	3.271000	6.883000
H	2.133000	2.187000	8.167000
H	2.312000	1.578000	6.531000

H	-0.050000	-1.763000	2.945000
H	0.790000	-3.289000	1.157000
H	-0.862000	-3.678000	1.625000
H	-0.552000	-2.802000	0.124000
N	1.743000	-0.403000	1.734000
C	2.791000	0.484000	1.221000
C	2.571000	1.960000	1.580000
O	3.414000	2.550000	2.203000
C	3.073000	0.289000	-0.271000
H	1.973000	-0.920000	2.551000
H	3.681000	0.219000	1.773000
H	3.910000	0.917000	-0.557000
H	3.341000	-0.745000	-0.462000
H	2.219000	0.543000	-0.882000
N	1.442000	2.539000	1.142000
C	1.165000	3.932000	1.421000
H	0.784000	1.991000	0.634000
H	1.094000	4.112000	2.488000
H	1.945000	4.570000	1.024000
H	0.224000	4.195000	0.956000

Alanine tetrapeptide_47

C	-2.505000	2.620000	3.497000
C	-2.677000	1.536000	2.457000
O	-3.562000	1.551000	1.650000
H	-1.465000	2.907000	3.603000
H	-2.858000	2.259000	4.459000
H	-3.096000	3.477000	3.209000
N	-1.747000	0.538000	2.510000
C	-1.914000	-0.679000	1.724000
C	-0.977000	-1.763000	2.228000
O	-1.319000	-2.918000	2.250000
C	-1.647000	-0.453000	0.230000
H	-1.225000	0.465000	3.354000
H	-2.917000	-1.067000	1.848000
H	-1.764000	-1.387000	-0.308000
H	-2.353000	0.268000	-0.157000
H	-0.640000	-0.087000	0.065000
N	0.258000	-1.367000	2.626000
C	1.292000	-2.357000	2.898000
C	1.474000	-3.242000	1.654000
O	1.628000	-2.711000	0.587000
C	1.064000	-3.056000	4.236000
H	0.573000	-0.494000	2.265000
H	2.221000	-1.801000	2.962000
H	1.896000	-3.712000	4.473000
H	1.001000	-2.310000	5.019000
H	0.145000	-3.626000	4.239000
N	1.490000	-4.577000	1.827000
C	1.674000	-5.505000	0.726000
C	0.390000	-5.893000	-0.015000
O	0.468000	-6.667000	-0.935000
C	2.381000	-6.765000	1.220000
H	1.240000	-4.951000	2.712000

C	-0.419000	1.049000	3.659000
O	-0.440000	1.876000	4.535000
C	-1.257000	-1.277000	4.026000
H	-1.517000	0.754000	1.436000
H	-2.421000	0.525000	3.984000
H	-0.983000	-1.170000	5.071000
H	-2.119000	-1.923000	3.955000
H	-0.430000	-1.737000	3.496000
N	0.638000	0.896000	2.832000
C	1.848000	1.704000	2.945000
C	1.628000	2.997000	2.152000
O	2.008000	3.120000	1.021000
C	3.051000	0.931000	2.426000
H	0.618000	0.176000	2.146000
H	1.977000	1.942000	3.993000
H	3.951000	1.526000	2.530000
H	3.175000	0.013000	2.990000
H	2.934000	0.700000	1.374000
N	0.948000	3.965000	2.814000
C	0.368000	5.087000	2.092000
C	1.359000	6.194000	1.734000
O	1.048000	7.008000	0.905000
C	-0.777000	5.687000	2.908000
H	0.513000	3.695000	3.672000
H	-0.008000	4.741000	1.137000
H	-1.216000	6.512000	2.364000
H	-1.542000	4.940000	3.094000
H	-0.419000	6.056000	3.864000
N	2.510000	6.248000	2.428000
C	3.526000	7.228000	2.110000
H	2.743000	5.476000	3.004000
H	4.056000	6.978000	1.196000
H	3.066000	8.197000	1.983000
H	4.235000	7.276000	2.927000

Alanine tetrapeptide_51

C	-0.897000	0.697000	-1.590000
C	-0.898000	-0.402000	-0.551000
O	-1.120000	-1.550000	-0.843000
H	-1.020000	0.252000	-2.565000
H	0.034000	1.255000	-1.561000
H	-1.711000	1.390000	-1.404000
N	-0.637000	0.004000	0.712000
C	-0.621000	-0.834000	1.912000
C	0.634000	-1.712000	1.984000
O	1.467000	-1.501000	2.825000
C	-1.918000	-1.616000	2.131000
H	-0.393000	0.958000	0.843000
H	-0.494000	-0.147000	2.736000
H	-1.855000	-2.165000	3.064000
H	-2.751000	-0.924000	2.198000
H	-2.115000	-2.313000	1.330000
N	0.718000	-2.731000	1.099000
C	1.941000	-3.501000	0.922000

Alanine tetrapeptide_49

C	-1.201000	1.411000	-0.758000
C	-1.362000	0.340000	0.296000
O	-0.765000	-0.707000	0.221000
H	-1.860000	1.178000	-1.588000
H	-0.182000	1.387000	-1.117000
H	-1.442000	2.402000	-0.394000
N	-2.224000	0.627000	1.294000
C	-2.666000	-0.278000	2.354000
C	-1.603000	-0.480000	3.443000
O	-1.826000	-0.131000	4.571000
C	-3.232000	-1.604000	1.838000
H	-2.646000	1.526000	1.289000
H	-3.454000	0.250000	2.871000
H	-3.601000	-2.186000	2.677000
H	-4.065000	-1.410000	1.170000
H	-2.492000	-2.182000	1.304000
N	-0.461000	-1.111000	3.080000
C	0.678000	-1.203000	3.984000
C	0.335000	-1.974000	5.263000
O	0.821000	-1.656000	6.319000
C	1.310000	0.149000	4.301000
H	-0.292000	-1.215000	2.100000
H	1.410000	-1.819000	3.469000
H	2.190000	0.013000	4.915000
H	1.597000	0.636000	3.375000
H	0.615000	0.781000	4.838000
N	-0.446000	-3.057000	5.092000
C	-0.920000	-3.963000	6.138000
C	-2.046000	-3.358000	6.989000
O	-3.134000	-3.877000	6.987000
C	0.203000	-4.559000	6.990000
H	-0.883000	-3.147000	4.204000
H	-1.407000	-4.772000	5.611000
H	-0.220000	-5.291000	7.671000
H	0.920000	-5.062000	6.350000
H	0.723000	-3.807000	7.563000
N	-1.741000	-2.283000	7.733000
C	-2.765000	-1.576000	8.472000
H	-0.866000	-1.834000	7.576000
H	-2.287000	-0.883000	9.153000
H	-3.427000	-1.022000	7.814000
H	-3.358000	-2.278000	9.041000

Alanine tetrapeptide_50

C	-3.395000	-0.254000	0.118000
C	-3.072000	-0.513000	1.573000
O	-3.794000	-1.144000	2.289000
H	-4.084000	-1.012000	-0.224000
H	-2.506000	-0.254000	-0.502000
H	-3.876000	0.716000	0.029000
N	-1.900000	0.038000	2.012000
C	-1.589000	0.099000	3.439000

C	-2.951012	-2.154705	0.419877		C	2.355000	-4.264000	2.184000
H	-2.277632	-2.338019	1.262200		O	3.512000	-4.510000	2.402000
C	-3.505652	-3.488284	-0.092324		C	3.100000	-2.675000	0.367000
H	-4.046393	-4.011010	0.702950		H	0.067000	-2.723000	0.342000
H	-4.191914	-3.337081	-0.931607		H	1.691000	-4.275000	0.202000
H	-2.676564	-4.118060	-0.424820		H	3.958000	-3.309000	0.192000
C	-2.059810	-1.492764	-0.651660		H	2.799000	-2.218000	-0.570000
O	-0.880034	-1.836558	-0.748113		H	3.385000	-1.901000	1.066000
N	-2.636670	-0.581860	-1.472658		N	1.355000	-4.728000	2.955000
H	-3.588570	-0.268390	-1.302305		C	1.625000	-5.425000	4.189000
C	-1.847137	0.109991	-2.489256		C	0.370000	-6.205000	4.563000
H	-1.244472	-0.635587	-3.013914		O	-0.727000	-5.830000	4.237000
C	-2.764475	0.828833	-3.484073		C	2.002000	-4.467000	5.327000
H	-3.396446	0.108005	-4.013596		H	0.414000	-4.453000	2.788000
H	-3.412215	1.550244	-2.974878		H	2.447000	-6.108000	4.014000
H	-2.153080	1.361803	-4.216954		H	2.223000	-5.011000	6.241000
C	-0.811817	1.093184	-1.898836		H	2.877000	-3.899000	5.040000
O	0.210648	1.351641	-2.524662		H	1.189000	-3.777000	5.521000
N	-1.129685	1.671593	-0.705824		N	0.568000	-7.300000	5.319000
H	-1.909271	1.297379	-0.177112		C	-0.541000	-8.101000	5.796000
C	-0.157675	2.491071	0.014047		H	1.495000	-7.597000	5.509000
H	0.369141	3.099959	-0.724821		H	-0.155000	-8.867000	6.457000
C	0.943275	1.622085	0.659050		H	-1.246000	-7.487000	6.341000
O	2.129282	1.950566	0.602628		H	-1.066000	-8.575000	4.975000
N	0.538082	0.485079	1.283366		Ac-(Ala)₄-Val-(Ala)₄-NHMe _αR
H	-0.448916	0.255138	1.334873		C	-8.965363	-2.950402	0.652913
C	1.508558	-0.420614	1.892380		H	-9.887208	-2.465621	0.987616
H	2.098547	0.126764	2.634471		H	-8.532751	-3.519138	1.479717
C	0.788930	-1.597312	2.559699		H	-9.213652	-3.664581	-0.140169
H	0.095656	-1.241229	3.330005		C	-7.928952	-1.978304	0.125410
H	0.228930	-2.176037	1.816845		O	-6.756594	-2.304273	-0.055720
H	1.524420	-2.254502	3.031671		N	-8.363045	-0.703540	-0.133588
C	2.552443	-0.938349	0.882486		H	-9.358391	-0.524053	-0.094110
O	3.701796	-1.183988	1.252481		C	-7.550479	0.224995	-0.924757
N	2.130753	-1.113878	-0.392019		H	-7.245963	-0.264658	-1.856693
H	1.142096	-1.025476	-0.606090		C	-8.354047	1.489215	-1.249926
C	3.023323	-1.618292	-1.429449		H	-9.241592	1.243096	-1.843373
H	3.442093	-2.580535	-1.114548		H	-8.671666	2.003495	-0.335918
C	2.248161	-1.791237	-2.741006		H	-7.733303	2.173787	-1.832933
H	1.434219	-2.512681	-2.610871		C	-6.225800	0.600516	-0.243636
H	1.819492	-0.836383	-3.065100		O	-5.270958	0.978382	-0.922713
H	2.926101	-2.158083	-3.516068		N	-6.175951	0.518871	1.108094
C	4.258656	-0.725816	-1.661692		H	-6.982891	0.160366	1.600862
O	5.275562	-1.225739	-2.152115		C	-4.950895	0.807207	1.844393
N	4.153592	0.584654	-1.343300		H	-4.620195	1.818956	1.589321
H	3.318775	0.930107	-0.877680		C	-5.199507	0.717350	3.353545
C	5.275480	1.502299	-1.508944		H	-5.955560	1.445928	3.664487
H	5.736301	1.287225	-2.478610		H	-5.535198	-0.286030	3.641399
C	4.787981	2.954010	-1.485475		H	-4.271257	0.932927	3.887774
H	4.112573	3.145050	-2.326017		C	-3.769224	-0.095045	1.440384
H	4.249888	3.171883	-0.556835		O	-2.617810	0.302298	1.661949
H	5.651935	3.618283	-1.560571		N	-4.037755	-1.289187	0.874218
C	6.430365	1.299324	-0.499273		H	-4.995618	-1.555249	0.652734

O	-9.402037	-0.134355	-1.587369		O	7.477713	1.919777	-0.664889
N	-8.161424	0.103356	0.303489		N	6.218117	0.415480	0.510638
H	-8.054951	-0.051055	1.301942		H	5.312697	-0.035665	0.612038
C	-6.961040	0.583994	-0.359771		C	7.273311	-0.001876	1.421836
H	-6.785374	-0.030653	-1.251118		H	8.093042	0.710314	1.282739
C	-7.088481	2.056529	-0.793379		C	6.796590	0.032953	2.878220
H	-7.939718	2.156644	-1.471258		H	6.565708	1.060592	3.177268
H	-7.247977	2.699691	0.078360		H	5.892240	-0.574047	3.001211
H	-6.186634	2.394186	-1.315355		H	7.578686	-0.369800	3.525560
C	-5.808076	0.386391	0.641674		C	7.861001	-1.393967	1.083727
O	-6.029130	0.158586	1.833195		O	8.654995	-1.933296	1.854429
N	-4.566889	0.500564	0.124794		N	7.470763	-1.953419	-0.086031
H	-4.404897	0.727527	-0.852098		H	6.821174	-1.473781	-0.699770
C	-3.360706	0.449481	0.934113		C	7.989832	-3.239369	-0.508872
H	-3.524616	1.037755	1.844922		H	7.978931	-3.942052	0.329754
C	-2.991572	-0.992193	1.334035		H	7.359527	-3.618798	-1.316725
H	-3.814093	-1.425023	1.908676		H	9.024540	-3.163939	-0.868623
H	-2.819507	-1.602647	0.441374		C	-0.864377	3.411632	1.041127
H	-2.086036	-1.014554	1.950025		H	-1.427191	2.763886	1.729333
C	-2.248644	1.097379	0.089192		C	-1.857869	4.349492	0.337538
O	-2.393552	1.277502	-1.120118		H	-2.608106	3.797719	-0.237910
N	-1.128873	1.434855	0.774401		H	-2.380667	4.972633	1.072672
H	-1.000957	1.093474	1.723272		H	-1.333865	5.020497	-0.354604
C	0.125595	1.778800	0.118755		C	0.152840	4.219754	1.860972
H	0.054308	1.451050	-0.924119		H	0.829617	3.577570	2.431511
C	1.226195	0.981490	0.845930		H	0.769945	4.849877	1.209857
O	1.036247	0.516805	1.973206		H	-0.369877	4.874513	2.567340
N	2.393237	0.858048	0.180048		Ac-(Ala)₄-Val-(Ala)₄-NHMe_C5			
H	2.545497	1.281509	-0.731072		C	-17.447492	-2.170774	-0.035612
C	3.572649	0.227765	0.749992		H	-17.247946	-2.144449	1.040097
H	3.692244	0.577176	1.782847		H	-17.678692	-3.199057	-0.330947
C	3.461722	-1.308677	0.757464		H	-18.333327	-1.564259	-0.248572
H	2.584656	-1.601081	1.339909		C	-16.289574	-1.665228	-0.885274
H	3.355855	-1.689140	-0.263844		O	-16.351073	-1.628012	-2.111672
H	4.347598	-1.767150	1.209907		N	-15.191563	-1.255467	-0.193475
C	4.765120	0.705086	-0.100164		H	-15.114899	-1.355947	0.812362
O	4.591605	1.266156	-1.184366		C	-13.978683	-0.813572	-0.854064
N	5.984850	0.447563	0.416372		H	-13.786498	-1.476254	-1.707270
H	6.108424	-0.074072	1.279703		C	-14.096945	0.631218	-1.377951
C	7.220056	0.704187	-0.305506		H	-14.936702	0.684183	-2.075102
H	7.079813	0.409206	-1.352663		H	-14.274482	1.325050	-0.549382
C	7.619059	2.190998	-0.261074		H	-13.186615	0.940685	-1.903440
H	6.815853	2.789029	-0.698667		C	-12.841136	-0.947272	0.172326
H	7.782239	2.513916	0.772402		O	-13.070947	-1.092315	1.375032
H	8.536397	2.372159	-0.831599		N	-11.590781	-0.874545	-0.336151
C	8.289191	-0.194054	0.345006		H	-11.417078	-0.703326	-1.322012
O	8.083484	-0.749585	1.426389		C	-10.399674	-0.862236	0.494883
N	9.446049	-0.308571	-0.340092		H	-10.586105	-0.218777	1.363462
H	9.619068	0.202868	-1.200693		C	-10.029326	-2.271075	0.996357
C	10.600370	-1.028531	0.171738		H	-10.865853	-2.675145	1.571724
H	10.721195	-0.784393	1.234334		H	-9.823216	-2.935676	0.150844
C	10.441503	-2.554084	0.030287		H	-9.144320	-2.242404	1.641263
H	9.547354	-2.871725	0.572122		C	-9.276907	-0.256312	-0.366891

H	-8.927112	-2.543139	-1.738523		H	10.338693	-2.832597	-1.023663
H	-7.920895	-3.415914	-0.584620		H	11.305315	-3.082538	0.447605
C	-7.258958	-0.731017	-0.427067		C	11.815000	-0.508025	-0.618489
O	-6.666996	-1.101426	-1.446197		O	11.672346	0.170521	-1.637991
N	-6.852735	0.313537	0.331837		N	13.021866	-0.862475	-0.128096
H	-7.433762	0.564653	1.133239		H	13.122934	-1.465899	0.682871
C	-5.789062	1.231834	-0.089400		C	14.268879	-0.555795	-0.807273
H	-5.847979	1.308030	-1.182583		H	14.122814	-0.710527	-1.883559
C	-5.996993	2.602234	0.547729		C	14.710996	0.900960	-0.571350
H	-6.986309	2.991072	0.287286		H	13.928371	1.574512	-0.929232
H	-5.907798	2.543820	1.636298		H	14.878701	1.081521	0.495288
H	-5.238508	3.304765	0.193802		H	15.636907	1.128132	-1.111344
C	-4.392388	0.658182	0.252799		C	15.308426	-1.556786	-0.268906
O	-3.647462	1.193253	1.082338		O	15.098317	-2.196241	0.759719
N	-4.057653	-0.454932	-0.438585		N	16.451883	-1.647829	-0.993788
H	-4.762689	-0.842737	-1.068270		H	16.527970	-1.105802	-1.843074
C	-2.873336	-1.258150	-0.119849		C	17.563805	-2.506620	-0.616186
H	-2.728381	-1.195093	0.966336		H	17.750867	-3.266100	-1.383513
C	-3.098313	-2.708350	-0.537531		H	18.477206	-1.920936	-0.464108
H	-3.990524	-3.107629	-0.045193		H	17.294331	-3.000998	0.317465
H	-3.219688	-2.787449	-1.621657		C	0.429929	3.306553	0.131624
H	-2.237258	-3.320946	-0.259376		H	1.416534	3.421000	-0.340930
C	-1.598502	-0.678642	-0.780795		C	-0.590785	4.079415	-0.714406
O	-0.984189	-1.291427	-1.660617		H	-0.638396	3.698288	-1.739700
N	-1.207713	0.525068	-0.298941		H	-1.596011	4.001516	-0.286848
H	-1.793832	0.956902	0.416183		H	-0.323002	5.141590	-0.753515
C	-0.074887	1.263139	-0.869061		C	0.514603	3.870972	1.556908
H	-0.054853	1.024181	-1.940059		H	-0.451949	3.785216	2.066845
C	1.231580	0.719039	-0.238073		H	1.261702	3.350413	2.165480
O	1.855910	1.326997	0.638488		H	0.782080	4.932972	1.528945
N	1.614212	-0.489125	-0.718415		Ac-(Ala)₄-Val-(Ala)₄-NHMe_C7eq			

Ac-(Ala)₄-Val-(Ala)₄-NHMe_C7_{eq}

H	0.955200	-0.961955	-1.338396		C	-14.128777	-1.678627	0.474481
C	2.660763	-1.294432	-0.077172		H	-14.469794	-1.531361	1.503505
H	2.618426	-1.080193	0.998869		H	-13.891368	-2.735379	0.321852
C	2.408467	-2.777324	-0.331591		H	-14.946178	-1.426719	-0.208749
H	1.413715	-3.057699	0.028630		C	-12.916434	-0.843707	0.107823
H	2.481552	-3.007197	-1.398412		O	-12.370836	-0.942982	-0.994362
H	3.156601	-3.382978	0.185647		N	-12.472584	0.026232	1.056308
C	4.067455	-0.874433	-0.566762		H	-12.916438	0.041662	1.964244
O	4.786651	-1.634757	-1.223895		C	-11.393815	0.990001	0.810801
N	4.442926	0.371377	-0.195662		H	-11.491939	1.296639	-0.236996
H	3.758976	0.932714	0.314596		C	-11.543496	2.195561	1.732660
C	5.665184	1.011346	-0.692758		H	-12.522655	2.663185	1.589249
H	5.818440	0.649896	-1.717507		H	-11.427492	1.903564	2.781119
C	5.506595	2.528426	-0.686205		H	-10.767643	2.934327	1.517593
H	4.648615	2.821313	-1.299668		C	-10.004816	0.325352	0.973952
H	5.366093	2.901553	0.332417		O	-9.244739	0.620076	1.902588
H	6.405489	3.003866	-1.086343		N	-9.702217	-0.581691	0.017503
C	6.899776	0.574496	0.133885		H	-10.429256	-0.795204	-0.667558
O	7.532683	1.368629	0.837234		C	-8.524533	-1.453728	0.095272
N	7.227630	-0.732083	0.003842		H	-8.356356	-1.669877	1.158161
H	6.613205	-1.313480	-0.568234		C	-8.779614	-2.746208	-0.673971
C	8.248313	-1.377897	0.835497		H	-9.665789	-3.251855	-0.278217

N	-6.204504	0.718846	0.802551
H	-7.017951	0.537016	1.375089
C	-4.982158	1.214334	1.424547
H	-4.642123	2.095848	0.871864
C	-5.241903	1.598028	2.884826
H	-5.995643	2.389870	2.947892
H	-5.585463	0.734803	3.467141
H	-4.316028	1.965411	3.333456
C	-3.804268	0.225429	1.329741
O	-2.651863	0.665545	1.433748
N	-4.077580	-1.082303	1.146769
H	-5.036334	-1.398591	1.012214
C	-2.994492	-2.049296	0.979278
H	-2.331357	-1.983663	1.846804
C	-3.557400	-3.470343	0.870326
H	-4.111063	-3.735689	1.776497
H	-4.234249	-3.564122	0.015164
H	-2.731777	-4.175473	0.744929
C	-2.085948	-1.734030	-0.227242
O	-0.906096	-2.090385	-0.199388
N	-2.646789	-1.109351	-1.291211
H	-3.599634	-0.758390	-1.236945
C	-1.839142	-0.751223	-2.455269
H	-1.237831	-1.621175	-2.731083
C	-2.739038	-0.350633	-3.629126
H	-3.373017	-1.191201	-3.930557
H	-3.384520	0.493163	-3.363502
H	-2.115310	-0.061584	-4.479145
C	-0.801724	0.355836	-2.163533
O	0.240548	0.403305	-2.808275
N	-1.139598	1.275266	-1.215596
H	-1.934997	1.088150	-0.615957
C	-0.168088	2.266862	-0.752377
H	0.363604	2.638343	-1.631346
C	-0.919766	3.426853	-0.066091
H	-1.708973	3.720237	-0.771323
H	-1.430481	3.051803	0.832269
C	-0.087595	4.680698	0.288056
H	0.604199	4.871769	-0.545029
C	-1.021903	5.896061	0.409163
H	-0.455954	6.804271	0.645603
H	-1.572986	6.075671	-0.521898
H	-1.758270	5.747986	1.210774
C	0.745908	4.524627	1.570580
H	1.263588	5.462572	1.803659
H	0.101899	4.281812	2.426575
H	1.507085	3.746977	1.476182
C	0.927021	1.610057	0.112386
O	2.117299	1.890451	-0.045647
N	0.516713	0.707504	1.040053
H	-0.471986	0.511737	1.159740
C	1.483367	0.013941	1.887648
H	2.075917	0.751598	2.438391

H	8.218951	-0.883266	1.814627
C	7.939373	-2.864247	0.984916
H	6.942605	-3.001368	1.415977
H	7.985315	-3.370502	0.016288
H	8.676104	-3.339730	1.637047
C	9.667922	-1.156727	0.256610
O	10.349799	-2.092098	-0.176644
N	10.090127	0.127220	0.285216
H	9.437741	0.827330	0.639786
C	11.338440	0.571144	-0.346450
H	11.486500	-0.063963	-1.228388
C	11.223789	2.034584	-0.759406
H	10.369746	2.175603	-1.429808
H	11.104759	2.676310	0.118388
H	12.134675	2.352910	-1.272637
C	12.550998	0.352874	0.598546
O	13.171598	1.290000	1.090396
N	12.851459	-0.958681	0.798499
H	12.210383	-1.645089	0.405097
C	13.896665	-1.385341	1.708697
H	13.482089	-1.850424	2.612976
H	14.564138	-2.105919	1.222180
H	14.468912	-0.502432	1.997836
C	-0.219371	2.787091	-0.692107
H	-0.109481	3.006002	0.377819
C	0.907485	3.516787	-1.441571
H	1.893201	3.211702	-1.081350
H	0.852256	3.322896	-2.520932
H	0.818942	4.598843	-1.295639
C	-1.590021	3.292627	-1.169876
H	-1.765101	3.026920	-2.220462
H	-2.414161	2.889915	-0.574237
H	-1.629830	4.385051	-1.093213
H	-1.765101	3.026920	-2.220462
H	-2.414161	2.889915	-0.574237
H	-1.629830	4.385051	-1.093213

Ac-(Ala)4-Leu-(Ala)4-NHMe_αR

C	-9.028654	-2.694123	1.430321
H	-9.937783	-2.111773	1.607327
H	-8.600684	-3.000909	2.387773
H	-9.298635	-3.605794	0.885450
C	-7.978007	-1.944208	0.635875
O	-6.808334	-2.320373	0.575390
N	-8.397448	-0.810325	-0.011906
H	-9.391014	-0.618748	-0.037849
C	-7.571774	-0.182436	-1.047485
H	-7.268981	-0.941081	-1.778007
C	-8.360294	0.924329	-1.756720
H	-9.246891	0.513005	-2.251896
H	-8.677743	1.700070	-1.050903
H	-7.729054	1.388291	-2.518350
C	-6.246160	0.375059	-0.507529
O	-5.284584	0.513757	-1.263610

C	14.121009	0.924294	1.354806		C	0.758632	-0.912498	2.869554
H	14.951760	1.102346	2.041959		H	0.071487	-0.342253	3.504790
H	14.252140	1.549562	0.465227		H	0.191473	-1.677892	2.328553
H	13.189105	1.215751	1.851996		H	1.491969	-1.409321	3.510687
C	12.988807	-0.882330	-0.037532		C	2.524765	-0.781314	1.074256
O	13.234882	-1.149837	-1.215800		O	3.676140	-0.903668	1.495893
N	11.732620	-0.827622	0.458898		N	2.097432	-1.333503	-0.085529
H	11.541601	-0.545546	1.415650		H	1.108060	-1.310579	-0.313814
C	10.549978	-0.978999	-0.370525		C	2.985040	-2.132068	-0.923666
H	10.709095	-0.431633	-1.307825		H	3.404726	-2.953047	-0.331849
C	10.263432	-2.454955	-0.705790		C	2.203624	-2.695900	-2.116385
H	11.128963	-2.875834	-1.223387		H	1.388215	-3.339419	-1.768696
H	10.081800	-3.027458	0.209833		H	1.776842	-1.884324	-2.716020
H	9.387867	-2.551828	-1.357031		H	2.877106	-3.285544	-2.743872
C	9.388156	-0.337620	0.410206		C	4.219078	-1.355414	-1.423590
O	9.500773	-0.048580	1.603445		O	5.235885	-1.981485	-1.737741
N	8.255783	-0.135616	-0.297125		N	4.112627	-0.010926	-1.525988
H	8.156229	-0.443672	-1.260175		H	3.277605	0.459621	-1.188321
C	7.024497	0.346771	0.304841		C	5.233352	0.812022	-1.967600
H	6.889455	-0.153099	1.271977		H	5.689244	0.313916	-2.829560
C	7.051152	1.869211	0.536525		C	4.745497	2.203963	-2.380188
H	7.893700	2.116280	1.187088		H	4.064173	2.134035	-3.234672
H	7.166474	2.399865	-0.414331		H	4.213995	2.692406	-1.556595
H	6.129241	2.213339	1.017601		H	5.608837	2.813092	-2.657546
C	5.888581	-0.065845	-0.650367		C	6.393200	0.922680	-0.948808
O	6.127744	-0.483445	-1.785703		O	7.442027	1.456709	-1.301053
N	4.639443	0.077511	-0.159981		N	6.181020	0.395448	0.285056
H	4.459401	0.488070	0.751992		H	5.274033	0.001873	0.521497
C	3.445010	-0.148818	-0.956313		C	7.236579	0.277368	1.279699
H	3.608830	0.270571	-1.956728		H	8.057718	0.909471	0.926577
C	3.117684	-1.647068	-1.096357		C	6.761466	0.762534	2.653996
H	3.963334	-2.155849	-1.565789		H	6.535000	1.833254	2.620895
H	2.934171	-2.092071	-0.112907		H	5.854825	0.226871	2.957917
H	2.230070	-1.801091	-1.719239		H	7.542679	0.576335	3.394229
C	2.310438	0.620111	-0.252094		C	7.820427	-1.152156	1.388940
O	2.453394	1.061470	0.890292		O	8.615230	-1.428418	2.287489
N	1.167507	0.743880	-0.959223		N	7.428550	-2.046264	0.450682
H	1.082475	0.393984	-1.907647		H	6.775453	-1.782682	-0.279251
C	-0.027128	1.401742	-0.440658		C	7.946952	-3.400269	0.450508
H	-0.093417	1.179500	0.629498		H	7.882483	-3.831335	1.454649
C	0.075522	2.937503	-0.623487		H	7.352316	-3.997461	-0.244742
H	1.005894	3.222135	-0.119619		H	8.999636	-3.432093	0.140984

Ac-(Ala)₄-Leu-(Ala)₄-NHMe_C5

H	0.211649	3.149006	-1.692111		C	17.666915	-1.752099	0.272114
C	-1.097093	3.776520	-0.059685		H	17.465963	-1.853455	-0.798870
H	-1.547363	3.226823	0.781370		H	17.975655	-2.723168	0.671594
C	-0.578618	5.113078	0.495330		H	18.504205	-1.061342	0.413169
H	-1.399196	5.720271	0.895218		C	16.473907	-1.249310	1.073510
H	0.149186	4.956239	1.299708		O	16.528096	-1.092602	2.290741
H	-0.086104	5.697696	-0.292594		N	15.354004	-0.979816	0.348464
C	-2.194516	4.029326	-1.106472		H	15.284610	-1.192053	-0.640491
H	-3.040650	4.566970	-0.663082		C	14.109660	-0.567613	0.968156
H	-1.804070	4.641245	-1.929662		H	13.962024	-1.159938	1.880154
H	-2.579505	3.101186	-1.539528					

C	-12.979796	-0.836240	0.046545		C	-1.202750	0.770171	-1.199975
O	-12.416466	-0.888371	-1.049971		O	-1.086921	0.467373	-2.389840
N	-12.531585	-0.032693	1.049834		N	-2.330876	0.570052	-0.485952
H	-12.991347	-0.056755	1.949595		H	-2.422779	0.880898	0.477105
C	-11.425470	0.915753	0.876997		C	-3.567242	0.084935	-1.076405
H	-11.497213	1.283089	-0.153318		H	-3.718099	0.589900	-2.038846
C	-11.562689	2.071486	1.862424		C	-3.533601	-1.435654	-1.317916
H	-12.526755	2.571886	1.727640		H	-2.698001	-1.672853	-1.980809
H	-11.474815	1.718644	2.894805		H	-3.403091	-1.971587	-0.372033
H	-10.764288	2.800342	1.703558		H	-4.459150	-1.782705	-1.789615
C	-10.055294	0.209546	1.024851		C	-4.692259	0.487424	-0.103254
O	-9.301462	0.439649	1.976525		O	-4.437847	0.918481	1.023694
N	-9.760391	-0.656355	0.028650		N	-5.948089	0.320749	-0.567870
H	-10.480386	-0.816409	-0.678104		H	-6.140173	-0.099840	-1.472734
C	-8.601523	-1.555121	0.077065		C	-7.129148	0.535914	0.251483
H	-8.449568	-1.823753	1.130312		H	-6.936595	0.131698	1.252731
C	-8.872668	-2.805481	-0.753831		C	-7.480398	2.029842	0.380722
H	-9.773313	-3.310800	-0.391752		H	-6.634950	2.558792	0.827633
H	-9.002744	-2.551386	-1.809657		H	-7.690782	2.460263	-0.603846
H	-8.028385	-3.495765	-0.685195		H	-8.357895	2.176130	1.019784
C	-7.317070	-0.833463	-0.398123		C	-8.265156	-0.260192	-0.418192
O	-6.724769	-1.161989	-1.431229		O	-8.144926	-0.703898	-1.562272
N	-6.896676	0.162327	0.416845		N	-9.380855	-0.414056	0.324975
H	-7.479507	0.383930	1.225529		H	-9.481250	0.005907	1.244635
C	-5.812524	1.079622	0.050069		C	-10.589766	-1.042757	-0.180967
H	-5.862286	1.212377	-1.038116		H	-10.770517	-0.683034	-1.201345
C	-5.997751	2.419841	0.754715		C	-10.475236	-2.578638	-0.211579
H	-6.974936	2.844327	0.504360		H	-9.632983	-2.861556	-0.847660
H	-5.922074	2.303754	1.839678		H	-10.308341	-2.970275	0.797248
H	-5.218930	3.121396	0.445747		H	-11.384332	-3.035684	-0.616929
C	-4.429850	0.462354	0.371682		C	-11.731548	-0.577323	0.741242
O	-3.689005	0.931012	1.242879		O	-11.498636	-0.022835	1.817601
N	-4.104986	-0.610330	-0.387041		N	-12.979822	-0.836862	0.297334
H	-4.812028	-0.948244	-1.042512		H	-13.155620	-1.343414	-0.565491
C	-2.931615	-1.447970	-0.116487		C	-14.167810	-0.574747	1.091280
H	-2.794409	-1.464605	0.972342		H	-13.958341	-0.858658	2.130177
C	-3.164041	-2.861100	-0.641676		C	-14.569211	0.912126	1.055540
H	-4.066227	-3.287149	-0.191815		H	-13.739910	1.514965	1.433710
H	-3.270653	-2.859057	-1.730146		H	-14.799051	1.221900	0.031022
H	-2.312121	-3.500583	-0.397468		H	-15.448488	1.102045	1.681049
C	-1.652178	-0.826543	-0.728404		C	-15.276509	-1.475388	0.514665
O	-1.046426	-1.359828	-1.664462		O	-15.154437	-2.001731	-0.589552
N	-1.257856	0.328793	-0.144520		N	-16.375757	-1.612066	1.298332
H	-1.859882	0.712262	0.586089		H	-16.380080	-1.164724	2.204249
C	-0.174401	1.156664	-0.689130		C	-17.540662	-2.388258	0.902068
H	-0.198780	1.027305	-1.778581		H	-17.713482	-3.217427	1.597105
C	-0.386014	2.632823	-0.320205		H	-18.437419	-1.759659	0.866770
H	-1.462467	2.797308	-0.187124		H	-17.344533	-2.790255	-0.092267
H	0.095047	2.823509	0.646211		Ac-(Ala)₄-Leu-(Ala)₄-NHMe_C7ₑq			

Ac-(Ala)$_4$-Leu-(Ala)$_4$-NHMe_C7$_{eq}$

C	0.126736	3.640593	-1.369645
H	-0.409810	3.437569	-2.309969
C	-0.220109	5.071118	-0.931595
H	0.084364	5.800682	-1.690913

C	-14.219844	-1.657674	0.344691
H	-14.575913	-1.559639	1.374513
H	-14.007256	-2.710130	0.136118
H	-15.017744	-1.345555	-0.336754

H	14.356023	-0.783416	2.181453
H	14.356023	-0.783416	2.181453

Ac-(Ala)₄-Ile-(Ala)4-NHMe_αR

C	-8.959149	-2.846824	1.097236
H	-9.872027	-2.291077	1.331383
H	-8.545343	-3.270797	2.015327
H	-9.219119	-3.683167	0.438485
C	-7.898045	-2.003311	0.419138
O	-6.725142	-2.365025	0.336429
N	-8.311637	-0.801781	-0.096569
H	-9.305837	-0.612992	-0.120167
C	-7.470141	-0.052867	-1.034611
H	-7.148448	-0.718877	-1.843234
C	-8.251717	1.127099	-1.623319
H	-9.128127	0.774029	-2.177967
H	-8.584275	1.814668	-0.837552
H	-7.610152	1.678439	-2.314900
C	-6.158438	0.441629	-0.406348
O	-5.180821	0.667102	-1.120340
N	-6.145107	0.633494	0.934715
H	-6.969461	0.386365	1.465757
C	-4.934326	1.051828	1.631920
H	-4.590761	1.997510	1.201185
C	-5.216342	1.244050	3.125458
H	-5.978936	2.014971	3.278637
H	-5.557820	0.310549	3.588154
H	-4.300262	1.559920	3.630142
C	-3.752325	0.084423	1.429973
O	-2.600884	0.516538	1.568069
N	-4.022611	-1.203650	1.132762
H	-4.978727	-1.505893	0.954453
C	-2.935336	-2.150707	0.892492
H	-2.269103	-2.139693	1.759857
C	-3.490154	-3.564599	0.689642
H	-4.030333	-3.897328	1.581693
H	-4.176813	-3.603176	-0.161890
H	-2.661308	-4.252934	0.505660
C	-2.034865	-1.748527	-0.293446
O	-0.853278	-2.099742	-0.297367
N	-2.607547	-1.056254	-1.308327
H	-3.556890	-0.704806	-1.216025
C	-1.814764	-0.617959	-2.454504
H	-1.199187	-1.460318	-2.779968
C	-2.728769	-0.172526	-3.601036
H	-3.342487	-1.010071	-3.949305
H	-3.393895	0.638257	-3.285415
H	-2.115141	0.180697	-4.433912
C	-0.797344	0.491641	-2.109078
O	0.224755	0.612634	-2.775997
N	-1.129729	1.326122	-1.084010
H	-1.909464	1.076179	-0.487139
C	-0.173497	2.304278	-0.569322
H	0.345337	2.738228	-1.427863
H	-1.297358	5.190009	-0.763971
H	0.293626	5.328887	0.003218
C	1.631235	3.511296	-1.651803
H	1.949185	4.259809	-2.387181
H	2.215076	3.661318	-0.736606
H	1.892210	2.525837	-2.055028
C	1.181523	0.602909	-0.179260
O	1.835267	1.154825	0.711799
N	1.569095	-0.546593	-0.783482
H	0.882189	-0.984916	-1.399671
C	2.643419	-1.393338	-0.248420
H	2.623409	-1.288930	0.844747
C	2.401326	-2.847062	-0.643850
H	1.417360	-3.174233	-0.293607
H	2.453197	-2.967560	-1.729669
H	3.167014	-3.491648	-0.205813
C	4.039476	-0.915568	-0.716754
O	4.762495	-1.616538	-1.433535
N	4.408549	0.298867	-0.249345
H	3.726936	0.812845	0.311681
C	5.644007	0.966223	-0.672501
H	5.812185	0.686309	-1.719930
C	5.500811	2.479168	-0.545592
H	4.655079	2.830503	-1.144134
H	5.350766	2.769389	0.498373
H	6.410869	2.974248	-0.893625
C	6.857975	0.451364	0.140043
O	7.468970	1.173285	0.934704
N	7.192777	-0.836842	-0.106089
H	6.589634	-1.361311	-0.741507
C	8.184432	-1.563099	0.694266
H	8.117975	-1.168402	1.716222
C	7.872942	-3.056428	0.683897
H	6.860828	-3.233698	1.061211
H	7.956217	-3.463898	-0.327802
H	8.585535	-3.595626	1.312728
C	9.625171	-1.289539	0.194755
O	10.329424	-2.183884	-0.286986
N	10.039718	-0.012385	0.350075
H	9.371956	0.653433	0.740563
C	11.313602	0.484028	-0.183772
H	11.504842	-0.074213	-1.108376
C	11.211371	1.977000	-0.476738
H	10.389612	2.173140	-1.173140
H	11.047183	2.542157	0.445310
H	12.144092	2.338410	-0.917020
C	12.482699	0.187199	0.793918
O	13.076034	1.079356	1.391642
N	12.780377	-1.136309	0.894745
H	12.160066	-1.787306	0.416919
C	13.785649	-1.637132	1.812123
H	13.333325	-2.156651	2.667505
H	14.462532	-2.331864	1.301918

H	-1.480534	4.615501	-1.505168
C	0.113552	4.438730	0.796654
H	0.903628	3.906058	1.336607
H	0.615746	4.946227	-0.038815
C	-0.504749	5.480651	1.736545
H	0.274705	6.121216	2.163381
H	-1.218998	6.133647	1.223567
H	-1.030623	4.999549	2.571360

Ac-(Ala)$_4$-Ile-(Ala)$_4$-NHMe_C5

C	17.825168	-1.125541	-0.037981
H	17.560550	-1.543848	-1.014007
H	18.207707	-1.927252	0.601817
H	18.633603	-0.399562	-0.168123
C	16.662375	-0.444326	0.670688
O	16.797763	0.105826	1.760711
N	15.471882	-0.484920	0.012188
H	15.343205	-1.016271	-0.841707
C	14.249317	0.041255	0.587366
H	14.221162	-0.227216	1.651132
C	14.168755	1.576031	0.471862
H	15.034178	2.011524	0.977174
H	14.176869	1.882083	-0.579701
H	13.258677	1.965485	0.941597
C	13.084091	-0.643513	-0.147730
O	13.261982	-1.278099	-1.189896
N	11.867224	-0.484736	0.419422
H	11.726464	0.093349	1.242500
C	10.641859	-0.957073	-0.200910
H	10.697759	-0.757799	-1.278102
C	10.432367	-2.468677	0.009308
H	11.286547	-3.007129	-0.408727
H	10.352548	-2.699448	1.076770
H	9.522510	-2.816811	-0.491731
C	9.496961	-0.134284	0.417619
O	9.670302	0.540216	1.435028
N	8.310315	-0.222564	-0.220421
H	8.169889	-0.831042	-1.021927
C	7.093583	0.392846	0.281830
H	7.045257	0.237451	1.366640
C	7.051046	1.906066	-0.002139
H	7.916909	2.381049	0.465646
H	7.079600	2.094400	-1.080446
H	6.142464	2.360985	0.406905
C	5.926524	-0.347681	-0.398147
O	6.119102	-1.098788	-1.357094
N	4.704161	-0.101309	0.117620
H	4.556451	0.570104	0.865927
C	3.478882	-0.616793	-0.469918
H	3.553402	-0.533600	-1.561070
C	3.237190	-2.092955	-0.102749
H	4.082891	-2.691211	-0.450876
H	3.141575	-2.207432	0.982071
H	2.325187	-2.474323	-0.574589
C	-0.898724	3.421984	0.226355
H	-1.413687	2.941085	1.072116
C	0.937347	1.612642	0.249397
O	2.121655	1.923377	0.110851
N	0.543537	0.646274	1.119837
H	-0.441334	0.428146	1.231451
C	1.523675	-0.083384	1.919648
H	2.110166	0.628088	2.509829
C	0.816576	-1.076412	2.847932
H	0.123938	-0.554262	3.517475
H	0.257785	-1.816625	2.264731
H	1.559451	-1.599948	3.455945
C	2.570562	-0.814512	1.054923
O	3.724740	-0.950818	1.464320
N	2.145475	-1.294600	-0.137774
H	1.154706	-1.271302	-0.359880
C	3.039675	-2.022485	-1.031469
H	3.473980	-2.875165	-0.497864
C	2.259261	-2.516068	-2.255633
H	1.455070	-3.193326	-1.948317
H	1.817577	-1.672250	-2.797444
H	2.937235	-3.051966	-2.925030
C	4.259609	-1.196615	-1.484496
O	5.280507	-1.786493	-1.851282
N	4.136722	0.150331	-1.489133
H	3.301428	0.585716	-1.107396
C	5.244567	1.015123	-1.880178
H	5.701417	0.579979	-2.775032
C	4.738364	2.425106	-2.198299
H	4.054567	2.403129	-3.053339
H	4.204221	2.851966	-1.342876
H	5.593355	3.061545	-2.437599
C	6.408810	1.071347	-0.861880
O	7.447195	1.645548	-1.180293
N	6.213116	0.452622	0.331677
H	5.313154	0.030603	0.544662
C	7.277338	0.277427	1.308346
H	8.091027	0.937077	0.989848
C	6.811805	0.669023	2.715181
H	6.580527	1.738490	2.753940
H	5.909957	0.110430	2.990987
H	7.599955	0.438376	3.435275
C	7.871896	-1.151738	1.318223
O	8.669618	-1.483953	2.194970
N	7.488051	-1.980901	0.318908
H	6.831529	-1.673149	-0.390329
C	8.019647	-3.326445	0.222833
H	7.962610	-3.826998	1.194605
H	7.428668	-3.879569	-0.510938
H	9.071574	-3.325981	-0.090896
C	-1.955771	4.103997	-0.658445
H	-2.671093	3.383162	-1.066637
H	-2.521158	4.850917	-0.092093

H	-18.238767	-1.738649	1.630009	C	2.343589	0.290678	0.041384
H	-18.697818	-0.762910	0.208967	O	2.527637	1.078308	0.972222
H	-17.632596	-2.177872	0.013550	N	1.158200	0.143749	-0.586928
C	-0.260580	2.331009	-2.226598	H	1.014804	-0.558693	-1.306300
H	-0.132199	3.351333	-2.600867	C	-0.058069	0.820475	-0.159694
H	0.496287	1.705101	-2.710376	H	-0.054757	0.866712	0.935583
H	-1.245576	1.975900	-2.553090	C	-0.123252	2.286253	-0.698441
C	-1.196501	3.123821	0.026352	H	0.852706	2.707702	-0.423729
H	-2.200803	2.797308	-0.273443	C	-1.215232	-0.072538	-0.645486
H	-1.119022	2.938142	1.107662	O	-1.048475	-0.875800	-1.567474
C	-1.067895	4.633453	-0.212508	N	-2.395938	0.082755	-0.009959
H	-1.810321	5.182136	0.377357	H	-2.537041	0.793400	0.701853
H	-0.074877	4.996137	0.079444	C	-3.611130	-0.597237	-0.428103
H	-1.224612	4.897284	-1.264061	H	-3.646631	-0.602273	-1.524259

C	14.206455	-1.548211	-0.104879	C	-3.659535	-2.052842	0.072399
H	14.581154	-1.488279	-1.131009	H	-2.793103	-2.592802	-0.317550
H	13.998368	-2.593449	0.141502	H	-3.636407	-2.083972	1.166711
H	14.988661	-1.202431	0.578413	H	-4.567056	-2.560832	-0.271114
C	12.954514	-0.726509	0.137470	C	-4.781745	0.239742	0.121658
O	12.378260	-0.730736	1.228492	O	-4.592706	1.138129	0.945418
N	12.509929	0.021108	-0.909717	N	-6.002588	-0.089947	-0.348714
H	12.979937	-0.043177	-1.802149	H	-6.147699	-0.870628	-0.982751
C	11.389829	0.962141	-0.797977	C	-7.229553	0.518498	0.138094
H	11.443574	1.381158	0.213507	H	-7.163041	0.613177	1.228778
C	11.524974	2.069116	-1.838266	C	-7.462420	1.915676	-0.466587
H	12.480774	2.588350	-1.716657	H	-6.615179	2.559011	-0.216577
H	11.455104	1.663958	-2.852674	H	-7.553101	1.850996	-1.555871
H	10.715305	2.794196	-1.726044	H	-8.374484	2.372199	-0.067388
C	10.030956	0.231020	-0.927200	C	-8.364677	-0.455397	-0.229754
O	9.287067	0.402215	-1.898922	O	-8.182225	-1.373411	-1.032374
N	9.733654	-0.587834	0.107489	N	-9.550592	-0.216735	0.368324
H	10.446166	-0.702762	0.830446	H	-9.697096	0.578867	0.983070
C	8.589032	-1.505601	0.086733	C	-10.759824	-0.958302	0.051173
H	8.456560	-1.826340	-0.954541	H	-10.809028	-1.096928	-1.035822
C	8.865891	-2.710774	0.980188	C	-10.785666	-2.342015	0.727322
H	9.780091	-3.218042	0.656848	H	-9.914416	-2.915158	0.400928
H	8.974309	-2.405285	2.024784	H	-10.756381	-2.236867	1.816855
H	8.033596	-3.417077	0.930876	H	-11.688702	-2.899022	0.455206
C	7.286912	-0.782407	0.508387	C	-11.935191	-0.077930	0.513859
O	6.682556	-1.072975	1.545941	O	-11.754609	0.895062	1.249408
N	6.865205	0.168879	-0.357481	N	-13.153973	-0.458713	0.075791
H	7.456955	0.361034	-1.167267	H	-13.292763	-1.291242	-0.489639
C	5.761487	1.084802	-0.050072	C	-14.382233	0.190195	0.500759
H	5.791464	1.267111	1.031642	H	-14.309992	0.396842	1.575867
C	5.937942	2.394393	-0.812200	C	-14.621384	1.517466	-0.243997
H	6.903733	2.846051	-0.565198	H	-13.778227	2.187786	-0.059978
H	5.883655	2.227489	-1.891835	H	-14.710578	1.341213	-1.320757
H	5.142667	3.096171	-0.549242	H	-15.536723	2.008693	0.104067
C	4.393879	0.432031	-0.364356	C	-15.514833	-0.819439	0.235446
O	3.655727	0.851968	-1.262915	O	-15.338063	-1.792063	-0.495185
N	4.074456	-0.614708	0.431150	N	-16.695208	-0.535368	0.841523
H	4.777313	-0.914259	1.109558	H	-16.744864	0.274307	1.443869
				C	-17.891217	-1.345327	0.668390

H	-12.045304	2.174591	1.630084
C	-12.546962	0.308330	-0.355217
O	-13.183368	1.277123	-0.757375
N	-12.862281	-0.986610	-0.627458
H	-12.206742	-1.698262	-0.310106
C	-13.946681	-1.350201	-1.519069
H	-13.572251	-1.763063	-2.465193
H	-14.601705	-2.093838	-1.050553
H	-14.521228	-0.447284	-1.731677
C	0.665452	3.087492	-0.809556
H	0.875840	4.161937	-0.801306
H	1.545255	2.604047	-1.249259
H	-0.193840	2.908106	-1.459664
C	-0.749207	3.380370	1.311887
H	-1.645729	3.340558	0.683862
H	-1.005128	2.876063	2.255280
C	-0.393793	4.838492	1.624255
H	-1.212039	5.328388	2.163848
H	0.503881	4.904254	2.251984
H	-0.208605	5.420921	0.715361
H	-0.208605	5.420921	0.715361

Ac-(Ala)₄-Phe-(Ala)₄-NHMe_αR

C	-9.175996	-2.594968	1.604094
H	-10.075936	-1.987752	1.739101
H	-8.754889	-2.843690	2.581291
H	-9.459192	-3.536825	1.120861
C	-8.111626	-1.917647	0.764120
O	-6.950738	-2.322899	0.724688
N	-8.507442	-0.815720	0.049699
H	-9.496572	-0.603976	0.013192
C	-7.671444	-0.271540	-1.024168
H	-7.389401	-1.080088	-1.708052
C	-8.436089	0.808409	-1.797952
H	-9.335852	0.389649	-2.262240
H	-8.729483	1.635125	-1.141266
H	-7.798050	1.207133	-2.590269
C	-6.330796	0.286025	-0.523182
O	-5.369638	0.356135	-1.289229
N	-6.274319	0.707353	0.763459
H	-7.089319	0.582247	1.348751
C	-5.037207	1.210419	1.349069
H	-4.681003	2.050520	0.744591
C	-5.278978	1.683167	2.786172
H	-6.014503	2.494111	2.807342
H	-5.637887	0.862593	3.418723
H	-4.342518	2.055156	3.208283
C	-3.883263	0.190124	1.305990
O	-2.719304	0.607862	1.370292
N	-4.189867	-1.119483	1.212014
H	-5.157547	-1.418767	1.104765
C	-3.133902	-2.124364	1.100773
H	-2.460312	-2.019055	1.956227
C	-3.735843	-3.533532	1.091669

C	2.926315	-1.488745	0.169259
H	2.803632	-1.533618	-0.920959
C	3.192306	-2.883722	0.727116
H	4.102503	-3.299289	0.283655
H	3.304883	-2.854411	1.814900
H	2.353547	-3.546849	0.503592
C	1.613991	-0.897982	0.741323
O	0.946209	-1.495095	1.593064
N	1.254849	0.294791	0.212994
H	1.860618	0.689198	-0.507005
C	0.117744	1.069839	0.718472
H	0.030780	0.813323	1.781576
C	0.384558	2.590379	0.620245
H	1.298056	2.746859	1.214827
C	-1.194856	0.582069	0.053610
O	-1.853355	1.254545	-0.749324
N	-1.564846	-0.662733	0.441945
H	-0.927118	-1.167243	1.060405
C	-2.642623	-1.408900	-0.215869
H	-2.642323	-1.106831	-1.271107
C	-2.391092	-2.908885	-0.095645
H	-1.418073	-3.163693	-0.527072
H	-2.414480	-3.224876	0.951193
H	-3.169011	-3.466485	-0.622932
C	-4.025949	-1.026661	0.364519
O	-4.721920	-1.836511	0.986666
N	-4.408280	0.246831	0.114141
H	-3.742154	0.846506	-0.375465
C	-5.602902	0.848586	0.715452
H	-5.714516	0.404467	1.712722
C	-5.431290	2.360203	0.826232
H	-4.539196	2.596367	1.414875
H	-5.340696	2.815386	-0.164346
H	-6.303511	2.805404	1.311251
C	-6.874386	0.486148	-0.090854
O	-7.528643	1.336975	-0.702219
N	-7.206426	-0.825347	-0.052254
H	-6.572006	-1.453339	0.443921
C	-8.261709	-1.399107	-0.893426
H	-8.265818	-0.828685	-1.830885
C	-7.968613	-2.870079	-1.172012
H	-6.988171	-2.976233	-1.646975
H	-7.985259	-3.452285	-0.246166
H	-8.730503	-3.288209	-1.834543
C	-9.655988	-1.219553	-0.243742
O	-10.321928	-2.183114	0.150692
N	-10.075645	0.063284	-0.165375
H	-9.433252	0.786676	-0.490196
C	-11.294311	0.461615	0.549384
H	-11.405212	-0.232971	1.390953
C	-11.158625	1.893359	1.056349
H	-10.275386	1.989386	1.696190
H	-11.077792	2.593543	0.219884

O	7.429709	0.837878	-1.434479
N	6.125844	-0.032186	0.231179
H	5.200950	-0.357236	0.500121
C	7.182663	-0.139275	1.225707
H	8.038013	0.408868	0.817524
C	6.755417	0.483280	2.559649
H	6.596651	1.560212	2.442270
H	5.820211	0.032569	2.911577
H	7.531200	0.306683	3.307917
C	7.674407	-1.590568	1.445202
O	8.446376	-1.849661	2.368525
N	7.231068	-2.524327	0.570649
H	6.598665	-2.273975	-0.181896
C	7.659144	-3.905522	0.674886
H	7.577338	-4.249428	1.710741
H	7.018552	-4.514812	0.032931
H	8.703890	-4.032737	0.362545
C	0.004247	4.306489	0.084708
C	0.472234	5.204385	-0.884086
C	0.423791	4.474120	1.409656
C	1.340343	6.239428	-0.539422
H	0.153265	5.090817	-1.918253
C	1.292502	5.509124	1.759659
H	0.069968	3.784862	2.173253
C	1.753659	6.394744	0.785483
H	1.694158	6.925028	-1.304863
H	1.609839	5.621457	2.793029
H	2.431277	7.200123	1.055482

Ac-(Ala)₄-Phe-(Ala)₄-NHMe_C5

C	17.966465	-1.309244	0.462844
H	17.730017	-1.968379	-0.378164
H	18.324626	-1.914117	1.301722
H	18.782779	-0.640474	0.172244
C	16.786559	-0.469482	0.932703
O	16.880478	0.313683	1.874527
N	15.630975	-0.641327	0.234563
H	15.532938	-1.346145	-0.487526
C	14.397767	0.028190	0.599956
H	14.304292	0.012666	1.693260
C	14.373987	1.496333	0.131520
H	15.222987	2.020662	0.576819
H	14.451183	1.551486	-0.959580
H	13.451476	1.999508	0.441879
C	13.250920	-0.782133	-0.027902
O	13.460231	-1.626895	-0.901341
N	12.014174	-0.487460	0.431668
H	11.851433	0.250560	1.110096
C	10.805484	-1.063939	-0.130377
H	10.904648	-1.087259	-1.222625
C	10.560689	-2.499626	0.372129
H	11.418732	-3.121257	0.104795
H	10.438680	-2.508396	1.460315
H	9.662720	-2.931732	-0.082883

H	-4.291224	-3.721119	2.016014
H	-4.419879	-3.666269	0.247499
H	-2.930514	-4.268067	1.011411
C	-2.230928	-1.916572	-0.132649
O	-1.060364	-2.300069	-0.091615
N	-2.789226	-1.354408	-1.232625
H	-3.732113	-0.975796	-1.194003
C	-1.989670	-1.107823	-2.430965
H	-1.412173	-2.010918	-2.644393
C	-2.896326	-0.780052	-3.622199
H	-3.551383	-1.627591	-3.850171
H	-3.520803	0.095520	-3.415560
H	-2.277572	-0.571502	-4.498935
C	-0.923874	-0.005573	-2.240188
O	0.097949	-0.017138	-2.917205
N	-1.218771	0.974226	-1.338336
H	-2.001249	0.832042	-0.710037
C	-0.220078	1.966858	-0.951023
H	0.308372	2.280247	-1.853264
C	-0.929190	3.178061	-0.299044
H	-1.673381	3.536154	-1.021940
H	-1.481738	2.829359	0.581862
C	0.874530	1.360690	-0.046306
O	2.065885	1.590986	-0.245747
N	0.451168	0.555806	0.965833
H	-0.539815	0.390133	1.108398
C	1.411259	-0.093583	1.854305
H	2.035994	0.669569	2.329172
C	0.675825	-0.908468	2.923436
H	0.016729	-0.264675	3.516693
H	0.076355	-1.699605	2.459342
H	1.404406	-1.371832	3.594238
C	2.414422	-0.989340	1.099335
O	3.561486	-1.127223	1.527994
N	1.960927	-1.604880	-0.017541
H	0.972355	-1.559214	-0.244845
C	2.813732	-2.489192	-0.803785
H	3.203880	-3.286445	-0.161423
C	2.006229	-3.097616	-1.956622
H	1.167304	-3.684200	-1.566981
H	1.609448	-2.310504	-2.607419
H	2.653927	-3.752539	-2.545249
C	4.075075	-1.795493	-1.355038
O	5.062817	-2.482363	-1.633517
N	4.025026	-0.456815	-1.540463
H	3.212893	0.070630	-1.231258
C	5.178306	0.286051	-2.037663
H	5.598849	-0.277707	-2.876752
C	4.752545	1.676967	-2.517463
H	4.055090	1.595926	-3.357844
H	4.258843	2.235341	-1.715209
H	5.640222	2.226342	-2.839443
C	6.355108	0.393267	-1.038543

C	-10.592854	-1.202296	0.052366
H	-10.660243	-1.293606	-1.038693
C	-10.617489	-2.614244	0.667800
H	-9.756092	-3.177904	0.301287
H	-10.568602	-2.557226	1.760197
H	-11.529063	-3.152895	0.387269
C	-11.755031	-0.336114	0.571238
O	-11.557449	0.602259	1.346280
N	-12.982951	-0.689592	0.135148
H	-13.135540	-1.494929	-0.464927
C	-14.200101	-0.052641	0.607436
H	-14.109097	0.107163	1.689077
C	-14.442297	1.306766	-0.075723
H	-13.590515	1.962301	0.121357
H	-14.551971	1.177020	-1.157197
H	-15.347344	1.789308	0.309469
C	-15.343513	-1.042954	0.317431
O	-15.186851	-1.980989	-0.461369
N	-16.510531	-0.781158	0.958557
H	-16.542740	-0.002180	1.601223
C	-17.714270	-1.576345	0.771513
H	-18.039047	-2.022513	1.717979
H	-18.529557	-0.966164	0.366814
H	-17.476410	-2.371407	0.064304
C	-1.052600	2.865606	-0.718420
C	-2.204869	3.106425	-1.477096
C	-0.921282	3.507915	0.522684
C	-3.202185	3.964645	-1.010481
H	-2.318626	2.620210	-2.443555
C	-1.918689	4.361311	0.993973
H	-0.023616	3.343271	1.115496
C	-3.063095	4.592264	0.227838
H	-4.086655	4.143490	-1.616491
H	-1.799469	4.850888	1.956874
H	-3.839428	5.258862	0.593343

Ac-(Ala)$_4$-Phe-(Ala)$_4$-NHMe_C7$_{eq}$

C	14.338472	-1.732202	-0.091212
H	14.686287	-1.820262	-1.124731
H	14.131127	-2.730510	0.304839
H	15.140360	-1.301072	0.516608
C	13.097655	-0.873463	0.064386
O	12.546681	-0.723253	1.158063
N	12.634337	-0.270967	-1.065212
H	13.082155	-0.461741	-1.950993
C	11.519348	0.682495	-1.058384
H	11.595459	1.232917	-0.113655
C	11.633957	1.639009	-2.240657
H	12.595067	2.161885	-2.213201
H	11.535872	1.102248	-3.189426
H	10.831192	2.379573	-2.206222
C	10.158530	-0.055932	-1.060880
O	9.405404	-0.034512	-2.040321
N	9.872958	-0.706410	0.090220

C	9.652507	-0.123153	0.264713
O	9.800221	0.742281	1.130217
N	8.486286	-0.330554	-0.383673
H	8.364214	-1.087337	-1.050334
C	7.260562	0.373885	-0.047279
H	7.192970	0.452529	1.044589
C	7.224280	1.792339	-0.646686
H	8.080012	2.359811	-0.272445
H	7.275582	1.747930	-1.739581
H	6.306916	2.318944	-0.361893
C	6.105599	-0.495910	-0.577053
O	6.310546	-1.409344	-1.379666
N	4.879149	-0.173060	-0.115917
H	4.724230	0.613880	0.507911
C	3.660975	-0.815000	-0.580801
H	3.711845	-0.914558	-1.672173
C	3.472076	-2.214136	0.034925
H	4.332496	-2.836569	-0.222325
H	3.393475	-2.144882	1.124859
H	2.566953	-2.695823	-0.349884
C	2.507339	0.131647	-0.200534
O	2.682114	1.068698	0.582993
N	1.312102	-0.152934	-0.757567
H	1.177239	-0.932338	-1.394720
C	0.098631	0.578075	-0.433831
H	0.096699	0.789599	0.640391
C	0.033114	1.931101	-1.204426
H	1.012769	2.401312	-1.069260
H	-0.085944	1.716003	-2.272501
C	-1.065917	-0.356416	-0.804626
O	-0.911542	-1.236095	-1.657167
N	-2.228248	-0.142799	-0.157590
H	-2.350185	0.629340	0.492610
C	-3.446559	-0.874005	-0.470344
H	-3.543197	-0.945302	-1.560518
C	-3.432840	-2.297382	0.118631
H	-2.576444	-2.844056	-0.283417
H	-3.353043	-2.257434	1.209904
H	-4.347370	-2.839683	-0.144846
C	-4.607599	-0.044962	0.105813
O	-4.411193	0.821619	0.958584
N	-5.833127	-0.354288	-0.370845
H	-5.984677	-1.108926	-1.033786
C	-7.051575	0.245369	0.145756
H	-6.974875	0.304880	1.238236
C	-7.277409	1.663766	-0.411387
H	-6.417615	2.287975	-0.155218
H	-7.385816	1.633451	-1.500673
H	-8.177866	2.118145	0.015961
C	-8.198437	-0.704813	-0.244087
O	-8.036032	-1.589629	-1.087133
N	-9.373693	-0.483070	0.381902
H	-9.504059	0.286257	1.032504

H	-4.504165	2.656240	0.521252
H	-5.262414	2.375503	-1.069612
H	-6.267764	2.791106	0.316144
C	-6.772461	0.151924	-0.348079
O	-7.412038	0.771721	-1.204239
N	-7.097462	-1.094246	0.067932
H	-6.477220	-1.535730	0.748643
C	-8.122055	-1.907008	-0.595283
H	-8.099266	-1.639124	-1.659273
C	-7.811718	-3.389975	-0.417613
H	-6.816205	-3.617141	-0.811901
H	-7.854096	-3.672784	0.638189
H	-8.549912	-3.996609	-0.947943
C	-9.538454	-1.564942	-0.070032
O	-10.215993	-2.382696	0.562352
N	-9.962785	-0.318518	-0.376981
H	-9.312582	0.287008	-0.879232
C	-11.207111	0.253307	0.151141
H	-11.346881	-0.171241	1.152792
C	-11.092732	1.771904	0.229470
H	-10.234784	2.058416	0.846391
H	-10.980636	2.203530	-0.769365
H	-12.001007	2.195290	0.665713
C	-12.425933	-0.168947	-0.712880
O	-13.046671	0.634190	-1.402067
N	-12.732642	-1.489943	-0.605953
H	-12.087062	-2.072188	-0.075714
C	-13.784358	-2.107722	-1.390407
H	-13.376630	-2.763050	-2.171595
H	-14.447499	-2.700847	-0.750236
H	-14.359298	-1.310739	-1.864570
C	-0.411293	3.453556	0.408495
C	-1.592123	3.896878	-0.200378
C	-0.035931	4.021273	1.634442
C	-2.375223	4.885475	0.399522
H	-1.897110	3.454602	-1.143789
C	-0.819125	5.004339	2.239625
H	0.883884	3.694836	2.116388
C	-1.992558	5.440891	1.621795
H	-3.283669	5.224080	-0.091944
H	-0.509558	5.433770	3.188930
H	-2.601648	6.211044	2.087501
H	-2.601648	6.211044	2.087501

Ac-(Ala)₄-Asn-(Ala)₄-NHMe_αR

C	-8.923612	-2.144836	0.133455
H	-9.807127	-1.508162	0.236414
H	-8.737951	-2.663679	1.077264
H	-9.128768	-2.909259	-0.624300
C	-7.675473	-1.385325	-0.267130
O	-6.550707	-1.881392	-0.193297
N	-7.854494	-0.101920	-0.712408
H	-8.799049	0.215011	-0.891571
C	-6.768964	0.613723	-1.388025

H	10.599013	-0.716965	0.808698
C	8.733234	-1.621751	0.223559
H	8.597256	-2.107433	-0.751434
C	9.023414	-2.664367	1.298523
H	9.938025	-3.213807	1.054997
H	9.138270	-2.191974	2.278269
H	8.194594	-3.372487	1.371945
C	7.427694	-0.847926	0.531321
O	6.824976	-0.979489	1.601755
N	7.000605	-0.043345	-0.469518
H	7.591356	0.025699	-1.299819
C	5.892063	0.902868	-0.305208
H	5.921564	1.250201	0.735437
C	6.060593	2.079897	-1.260715
H	7.020992	2.574149	-1.084186
H	6.013004	1.746776	-2.301467
H	5.257634	2.806234	-1.112950
C	4.527249	0.202755	-0.514156
O	3.788778	0.478036	-1.466273
N	4.212747	-0.710116	0.434017
H	4.917524	-0.899694	1.149004
C	3.064010	-1.614704	0.314596
H	2.945821	-1.842606	-0.752659
C	3.322843	-2.894995	1.102759
H	4.237179	-3.378552	0.745181
H	3.423311	-2.681236	2.170759
H	2.486628	-3.588416	0.985011
C	1.757192	-0.925979	0.777987
O	1.127796	-1.309215	1.769328
N	1.361808	0.108133	-0.001902
H	1.970697	0.369493	-0.779930
C	0.245528	0.984386	0.365691
H	0.230083	1.044293	1.460120
C	0.452964	2.386146	-0.233859
H	1.510442	2.643858	-0.099901
H	0.257519	2.337505	-1.309497
C	-1.086608	0.344185	-0.093980
O	-1.721701	0.755702	-1.071144
N	-1.473084	-0.717640	0.652088
H	-0.811415	-1.043813	1.358076
C	-2.535651	-1.636055	0.225123
H	-2.509253	-1.670094	-0.872056
C	-2.285883	-3.025869	0.802764
H	-1.298643	-3.388484	0.499865
H	-2.342623	-3.008718	1.894857
H	-3.045595	-3.725847	0.446725
C	-3.934686	-1.109207	0.626200
O	-4.648858	-1.706388	1.439172
N	-4.312420	0.026255	-0.004133
H	-3.632479	0.464456	-0.627214
C	-5.531944	0.760132	0.351888
H	-5.674519	0.632678	1.432398
C	-5.376199	2.238055	0.009920

H	1.626551	-1.210343	3.879257		H	-6.392297	0.004850	-2.217415
C	2.540826	-0.810861	1.339267		C	-7.271276	1.958987	-1.925158
O	3.730314	-0.745191	1.652399		H	-8.070764	1.808343	-2.659054
N	2.086809	-1.609053	0.341916		H	-7.649116	2.594687	-1.116827
H	1.090440	-1.682097	0.160524		H	-6.451119	2.484559	-2.420580
C	3.001029	-2.452452	-0.421718		C	-5.548245	0.825049	-0.480411
H	3.577396	-3.076548	0.269231		O	-4.419741	0.892089	-0.976042
C	2.215126	-3.336618	-1.396059		N	-5.777509	0.960021	0.844411
H	1.511924	-3.977933	-0.854225		H	-6.727501	0.870991	1.180606
H	1.652780	-2.718174	-2.103796		C	-4.689424	1.159138	1.798041
H	2.911676	-3.967915	-1.954432		H	-4.137697	2.061591	1.518796
C	4.067624	-1.641864	-1.184940		C	-5.248073	1.322415	3.215041
O	5.166230	-2.147208	-1.427382		H	-5.911296	2.192177	3.271269
N	3.717121	-0.394671	-1.573538		H	-5.801938	0.429997	3.529168
H	2.778111	-0.064515	-1.380587		H	-4.422828	1.476387	3.914495
C	4.631223	0.486107	-2.291198		C	-3.642248	0.028069	1.757448
H	5.093070	-0.087401	-3.102371		O	-2.474104	0.285922	2.053593
C	3.861881	1.675117	-2.874129		N	-4.067498	-1.220422	1.445246
H	3.109456	1.332844	-3.592769		H	-5.006850	-1.367101	1.083382
H	3.353630	2.232271	-2.078978		C	-3.109264	-2.322735	1.358239
H	4.565172	2.341127	-3.378987		H	-2.493817	-2.309075	2.260896
C	5.834559	0.985624	-1.456617		C	-3.843802	-3.663147	1.246637
O	6.746552	1.571273	-2.034935		H	-4.447513	-3.841293	2.142559
N	5.810289	0.736878	-0.122089		H	-4.504146	-3.684683	0.373783
H	5.007714	0.274309	0.295415		H	-3.115156	-4.473458	1.155135
C	6.941769	1.023204	0.748384		C	-2.103846	-2.140364	0.201453
H	7.594085	1.698346	0.185544		O	-0.925912	-2.470090	0.344121
C	6.485326	1.701113	2.045066		N	-2.599308	-1.648823	-0.963281
H	6.048336	2.681430	1.828837		H	-3.532600	-1.254452	-0.971308
H	5.729918	1.090329	2.552805		C	-1.714059	-1.330629	-2.081764
H	7.343025	1.821082	2.710478		H	-1.072129	-2.195647	-2.262976
C	7.805098	-0.220395	1.072058		C	-2.534180	-1.014241	-3.336955
O	8.718853	-0.138861	1.892841		H	-3.131013	-1.884080	-3.631355
N	7.512419	-1.359935	0.403172		H	-3.206589	-0.167153	-3.163198
H	6.749724	-1.389311	-0.264765		H	-1.862214	-0.761171	-4.161903
C	8.282581	-2.569207	0.619000		C	-0.740332	-0.181107	-1.744842
H	8.417210	-2.745359	1.690750		O	0.428476	-0.213995	-2.125395
H	7.742269	-3.407745	0.173295		N	-1.254418	0.847413	-1.021619
H	9.279255	-2.503147	0.163520		H	-2.240699	0.857596	-0.784051
C	-0.746767	4.466793	0.217419		C	-0.412870	1.965899	-0.609982
O	-1.527987	5.374737	0.477981		H	0.085266	2.375680	-1.494268
N	0.588322	4.651370	0.052099		C	-1.297260	3.041805	0.050851
H	0.940276	5.581306	0.236363		H	-2.207703	3.160309	-0.547014
H	1.251607	3.879426	0.004746		H	-1.619026	2.695415	1.041087

Ac-(Ala)₄-Asn-(Ala)₄-NHMe_C5

C	17.670116	-1.352769	-1.340535		C	0.736222	1.500324	0.310835
H	17.266870	-2.222168	-1.868898		O	1.855852	2.017483	0.215657
H	18.231284	-1.695482	-0.465359		N	0.449337	0.543335	1.218397
H	18.375619	-0.832907	-1.996043		H	-0.505191	0.209573	1.316676
C	16.604373	-0.365713	-0.884650		C	1.483061	0.012118	2.104416
O	16.890355	0.674333	-0.296759		H	2.042776	0.848293	2.531877
N	15.321323	-0.712522	-1.178614		C	0.845386	-0.827848	3.216206
H	15.081803	-1.611757	-1.581061		H	0.150506	-0.220889	3.805741
					H	0.297710	-1.677977	2.795037

H	-3.986631	-0.447579	3.218322
H	-4.768329	-1.786612	2.347409
C	-4.842604	0.523988	0.767809
O	-4.796638	1.727425	1.013095
N	-5.935758	-0.089845	0.253208
H	-5.977237	-1.094652	0.111819
C	-7.199274	0.598523	0.056880
H	-7.373960	1.257940	0.916018
C	-7.199518	1.453115	-1.224902
H	-6.392820	2.187520	-1.160929
H	-7.040102	0.822270	-2.105707
H	-8.148130	1.987639	-1.345614
C	-8.285948	-0.490723	0.011073
O	-7.995989	-1.680459	-0.130624
N	-9.557181	-0.046294	0.117126
H	-9.781029	0.942593	0.177181
C	-10.711797	-0.916530	-0.026705
H	-10.526509	-1.606760	-0.858933
C	-10.978813	-1.741064	1.247033
H	-10.096091	-2.344572	1.472020
H	-11.184908	-1.079812	2.095113
H	-11.833472	-2.413032	1.112971
C	-11.900843	-0.001273	-0.369841
O	-11.828170	1.221948	-0.234106
N	-13.013687	-0.631550	-0.804009
H	-13.076884	-1.643521	-0.862552
C	-14.260051	0.066895	-1.066095
H	-14.406270	0.817671	-0.279531
C	-14.245638	0.778431	-2.432515
H	-13.417342	1.490869	-2.454621
H	-14.114805	0.051741	-3.240750
H	-15.178642	1.326123	-2.605765
C	-15.373314	-0.994432	-0.993178
O	-15.110521	-2.193950	-1.047836
N	-16.634361	-0.502183	-0.894625
H	-16.756525	0.498175	-0.822844
C	-17.815523	-1.350439	-0.858001
H	-18.348820	-1.241309	0.093081
H	-18.498186	-1.106158	-1.679367
H	-17.481029	-2.382830	-0.963128
C	-0.857956	3.215912	0.414196
O	-1.641581	3.153768	1.358342
N	-0.613238	4.384104	-0.239393
H	-1.045780	5.223976	0.120759
H	0.146516	4.481507	-0.896003

Ac-(Ala)₄-Asn-(Ala)₄-NHMe_C7eq

C	14.278806	-1.129442	0.782319
H	14.791358	-0.823528	-0.134496
H	14.111162	-2.210207	0.756861
H	14.928382	-0.921117	1.638261
C	12.950655	-0.429576	1.001128
O	12.235183	-0.685824	1.972904
N	12.598769	0.500741	0.071379
C	14.186653	0.076537	-0.740061
H	14.374355	0.415204	0.286830
C	13.966616	1.317362	-1.627411
H	14.872991	1.927469	-1.608406
H	13.758363	1.017911	-2.660134
H	13.130025	1.925445	-1.265194
C	12.963871	-0.856671	-0.759305
O	12.995700	-1.951580	-1.325325
N	11.863721	-0.383710	-0.131612
H	11.832436	0.546242	0.275100
C	10.586326	-1.074469	-0.155132
H	10.430073	-1.482207	-1.161340
C	10.536879	-2.233999	0.857925
H	11.337058	-2.941634	0.627129
H	10.675492	-1.858426	1.877128
H	9.579258	-2.763689	0.808485
C	9.512760	-0.012797	0.144534
O	9.814563	1.092589	0.599562
N	8.240381	-0.386686	-0.110398
H	8.003248	-1.322356	-0.427532
C	7.093206	0.444196	0.212874
H	7.250567	0.887724	1.203778
C	6.895290	1.578915	-0.809689
H	7.796670	2.196080	-0.836801
H	6.713946	1.167157	-1.808044
H	6.046940	2.215400	-0.535702
C	5.876665	-0.499663	0.256643
O	5.944875	-1.650702	-0.179800
N	4.751487	0.029820	0.781220
H	4.697524	0.999182	1.080524
C	3.477733	-0.670275	0.793953
H	3.360250	-1.196076	-0.161152
C	3.391970	-1.698068	1.937653
H	4.199333	-2.426235	1.825931
H	3.491787	-1.200812	2.908080
H	2.436507	-2.233014	1.916943
C	2.392721	0.414721	0.925711
O	2.682226	1.570260	1.250692
N	1.133080	0.008791	0.670257
H	0.901370	-0.962194	0.469432
C	-0.036081	0.841909	0.898300
H	0.018520	1.286198	1.898813
C	-0.115908	1.998267	-0.129181
H	0.906562	2.289298	-0.386322
H	-0.604363	1.665177	-1.053818
C	-1.243859	-0.128224	0.846157
O	-1.063624	-1.323355	0.582904
N	-2.450710	0.407177	1.093366
H	-2.539985	1.402812	1.313362
C	-3.657094	-0.406168	1.064706
H	-3.545424	-1.141356	0.260404
C	-3.872322	-1.158005	2.393038
H	-3.008850	-1.799030	2.590368

H	-1.622841	-3.473012	-1.658164
H	-2.395389	-3.570468	-0.053228
H	-3.380556	-3.710116	-1.507251
C	-3.984871	-1.285838	-0.307693
O	-4.627023	-2.098352	0.365718
N	-4.321348	0.020293	-0.422133
H	-3.703617	0.616661	-0.972913
C	-5.323535	0.658458	0.439914
H	-5.280587	0.145849	1.409199
C	-5.000032	2.139388	0.612778
H	-3.988096	2.265963	1.010175
H	-5.085157	2.664562	-0.343845
H	-5.714137	2.600745	1.299922
C	-6.750361	0.450841	-0.122543
O	-7.437685	1.389990	-0.537783
N	-7.177789	-0.833308	-0.103702
H	-6.514845	-1.541229	0.216430
C	-8.421289	-1.262971	-0.750896
H	-8.558771	-0.621190	-1.630501
C	-8.314357	-2.724303	-1.175286
H	-7.458417	-2.861392	-1.843636
H	-8.197904	-3.375216	-0.303874
H	-9.224043	-3.034530	-1.695252
C	-9.644155	-1.035908	0.172708
O	-10.316238	-1.976505	0.610224
N	-9.912374	0.262693	0.436200
H	-9.279252	0.960712	0.043680
C	-10.928877	0.687004	1.406276
H	-10.947796	-0.075044	2.194961
C	-10.558845	2.046165	1.990113
H	-9.565878	2.006189	2.449505
H	-10.567783	2.816049	1.213171
H	-11.289080	2.341341	2.747888
C	-12.337839	0.725364	0.755763
O	-12.936688	1.777524	0.556289
N	-12.828861	-0.507962	0.457771
H	-12.198474	-1.297990	0.582824
C	-14.090635	-0.693823	-0.232350
H	-13.941968	-1.030708	-1.266987
H	-14.711383	-1.432383	0.287792
H	-14.608401	0.266538	-0.246277
C	-0.877559	3.067380	0.072106
O	-1.366885	2.756235	1.150843
N	-1.245533	4.194287	-0.608752
H	-2.071681	4.669025	-0.267083
H	-1.069603	4.258118	-1.601483

Ac-(Ala)₄-Gln-(Ala)₄-NHMe_αR

C	-9.000955	-2.099642	-0.223804
H	-9.879194	-1.470812	-0.051040
H	-8.846631	-2.752886	0.638753
H	-9.194982	-2.742904	-1.089319
C	-7.733668	-1.309765	-0.479385
O	-6.618018	-1.830591	-0.460527

H	13.188125	0.643697	-0.737164
C	11.405707	1.344475	0.201185
H	11.288916	1.544193	1.272476
C	11.596500	2.649535	-0.564473
H	12.484766	3.175530	-0.200900
H	11.695805	2.462302	-1.638286
H	10.726665	3.297195	-0.430182
C	10.139778	0.591341	-0.274582
O	9.540420	0.908024	-1.307825
N	9.753391	-0.420494	0.535922
H	10.362289	-0.641465	1.325726
C	8.696903	-1.371014	0.169402
H	8.750558	-1.505390	-0.918571
C	8.921225	-2.702496	0.879028
H	9.911716	-3.098192	0.634175
H	8.838424	-2.584721	1.963161
H	8.164968	-3.428185	0.569878
C	7.296618	-0.793256	0.489463
O	6.571931	-1.277154	1.364819
N	6.936447	0.262888	-0.277319
H	7.631946	0.622061	-0.933288
C	5.738527	1.064519	-0.006210
H	5.602702	1.079555	1.082716
C	5.925445	2.483163	-0.534737
H	6.815648	2.937255	-0.088581
H	6.028057	2.482755	-1.623617
H	5.055717	3.096981	-0.287385
C	4.478671	0.401433	-0.614396
O	3.859689	0.911188	-1.555888
N	4.113620	-0.757639	-0.020423
H	4.730670	-1.119608	0.709116
C	3.062292	-1.630658	-0.554908
H	3.110166	-1.558591	-1.649136
C	3.299202	-3.069559	-0.108078
H	4.289394	-3.406898	-0.429809
H	3.225410	-3.155582	0.979713
H	2.543200	-3.729343	-0.540950
C	1.659894	-1.134685	-0.124473
O	0.946407	-1.774905	0.653049
N	1.286973	0.039590	-0.687897
H	1.985273	0.514509	-1.263231
C	0.099743	0.776523	-0.252860
H	-0.012013	0.647076	0.829193
C	0.262335	2.265225	-0.556150
H	1.204954	2.616910	-0.118699
H	0.312233	2.430143	-1.636994
C	-1.195949	0.244995	-0.908246
O	-1.875379	0.952295	-1.665031
N	-1.536116	-1.012108	-0.559496
H	-0.905279	-1.511428	0.070385
C	-2.716398	-1.694613	-1.097566
H	-2.842709	-1.339553	-2.127484
C	-2.511423	-3.205640	-1.077961

C	0.773431	-1.436779	3.147131		N	-7.885290	0.029951	-0.725651
H	0.098910	-0.897132	3.820072		H	-8.821554	0.385715	-0.872547
H	0.193969	-2.188385	2.599937		C	-6.777303	0.821929	-1.266390
H	1.530024	-1.950347	3.747307		H	-6.390116	0.337164	-2.169528
C	2.484988	-1.203975	1.295758		C	-7.252691	2.238863	-1.608381
O	3.681678	-1.197581	1.586757		H	-8.037056	2.209638	-2.372759
N	1.996419	-1.865494	0.217589		H	-7.641884	2.752872	-0.722592
H	0.995977	-1.897151	0.044320		H	-6.415942	2.820015	-2.003843
C	2.882594	-2.623138	-0.660623		C	-5.572863	0.879127	-0.315836
H	3.459752	-3.336537	-0.063282		O	-4.434987	1.011280	-0.774760
C	2.063123	-3.366195	-1.721434		N	-5.824635	0.810727	1.010747
H	1.350517	-4.050897	-1.249963		H	-6.779802	0.672403	1.313832
H	1.507169	-2.654853	-2.341704		C	-4.748613	0.842556	1.997786
H	2.735854	-3.941773	-2.363204		H	-4.182606	1.769901	1.869026
C	3.949553	-1.739401	-1.337795		C	-5.326678	0.789657	3.415472
O	5.052113	-2.211520	-1.624164		H	-5.982301	1.647718	3.598718
N	3.589866	-0.463114	-1.607506		H	-5.895044	-0.133403	3.578720
H	2.645260	-0.160105	-1.394481		H	-4.510896	0.820474	4.141886
C	4.495555	0.480689	-2.251201		C	-3.712047	-0.280719	1.794087
H	4.969323	-0.025557	-3.099652		O	-2.545096	-0.086994	2.139043
C	3.715645	1.699808	-2.751193		N	-4.147173	-1.459693	1.286985
H	2.963263	1.402802	-3.489070		H	-5.082891	-1.538400	0.895862
H	3.204236	2.195925	-1.918382		C	-3.198877	-2.545638	1.043055
H	4.413429	2.404994	-3.208148		H	-2.597953	-2.681100	1.945436
C	5.687458	0.933013	-1.374574		C	-3.942589	-3.844241	0.712588
O	6.582770	1.593151	-1.896377		H	-4.561584	-4.154422	1.560870
N	5.673700	0.558907	-0.069945		H	-4.588900	-3.722134	-0.162371
H	4.881880	0.043336	0.302601		H	-3.218497	-4.637140	0.505720
C	6.799279	0.788711	0.824333		C	-2.174754	-2.198124	-0.057758
H	7.434056	1.530858	0.330085		O	-1.010320	-2.588946	0.035299
C	6.327089	1.325880	2.180048		N	-2.642074	-1.500726	-1.123982
H	5.856451	2.306802	2.057989		H	-3.559621	-1.074256	-1.066185
H	5.595165	0.644228	2.628397		C	-1.740452	-1.039360	-2.177708
H	7.183549	1.411279	2.852452		H	-1.120180	-1.885013	-2.483027
C	7.691757	-0.459166	1.028478		C	-2.540883	-0.518681	-3.376011
O	8.613278	-0.430249	1.844061		H	-3.153225	-1.320777	-3.801710
N	7.413971	-1.542993	0.267138		H	-3.197088	0.307642	-3.082367
H	6.640452	-1.533453	-0.388707		H	-1.855207	-0.160259	-4.149015
C	8.207072	-2.751727	0.378199		C	-0.736821	0.016853	-1.669804
H	8.313127	-3.043577	1.428115		O	0.432488	0.001555	-2.052578
H	7.702453	-3.547717	-0.174235		N	-1.216175	0.940432	-0.798126
H	9.215273	-2.612903	-0.032508		H	-2.201854	0.950641	-0.558910
C	-0.302028	4.082606	1.228661		C	-0.330620	1.945399	-0.221442
H	0.454979	3.663138	1.898842		H	0.190554	2.460480	-1.033233
H	-0.960943	4.723019	1.822148		C	-1.149193	2.958697	0.602236
C	0.339286	4.979665	0.164652		H	-1.902591	3.408207	-0.056426
O	-0.292022	5.880081	-0.376936		H	-1.677951	2.418540	1.397863
N	1.640564	4.689768	-0.120290		C	0.791405	1.304758	0.621488
H	2.064114	5.183253	-0.895209		O	1.933779	1.777219	0.609230
H	2.041708	3.797330	0.160742		N	0.453868	0.240219	1.384271

Ac-(Ala)4-Gln-(Ala)4-NHMe_C5

C	-17.854858	-0.824268	0.357975		H	-0.512562	-0.069771	1.421930
H	-17.576694	-1.099712	1.379940		C	1.456579	-0.464953	2.179231
					H	2.048338	0.269905	2.731604

N	2.421961	-0.353040	-0.255136
H	2.551247	0.106830	-1.152639
C	3.649895	-0.862851	0.334486
H	3.698937	-0.533981	1.379429
C	3.718774	-2.400872	0.293605
H	2.866312	-2.813792	0.838568
H	3.688368	-2.756450	-0.741511
H	4.640353	-2.764608	0.760570
C	4.800171	-0.229163	-0.470080
O	4.598230	0.270280	-1.578695
N	6.015836	-0.286306	0.111539
H	6.169154	-0.739179	1.008065
C	7.230971	0.166986	-0.545235
H	7.212702	-0.173963	-1.587479
C	7.360072	1.701950	-0.528469
H	6.493058	2.140092	-1.028723
H	7.402027	2.071111	0.501494
H	8.265040	2.027339	-1.052785
C	8.396426	-0.506279	0.202486
O	8.226949	-1.036409	1.302793
N	9.593469	-0.451560	-0.418511
H	9.724208	0.035155	-1.300628
C	10.824544	-0.922809	0.193906
H	10.829009	-0.617376	1.247268
C	10.957346	-2.455837	0.123252
H	10.103820	-2.911608	0.631069
H	10.973617	-2.791066	-0.918988
H	11.875525	-2.796362	0.613874
C	11.971349	-0.220785	-0.555581
O	11.777942	0.345491	-1.633535
N	13.182499	-0.290829	0.036987
H	13.336100	-0.802205	0.901172
C	14.393431	0.216496	-0.584834
H	14.370435	-0.045246	-1.650099
C	14.511885	1.746927	-0.453448
H	13.639004	2.213529	-0.916489
H	14.556552	2.038170	0.600907
H	15.411279	2.120777	-0.955239
C	15.565862	-0.503176	0.107664
O	15.404924	-1.098505	1.171056
N	16.761317	-0.401584	-0.526381
H	16.796938	0.081843	-1.412881
C	17.989834	-0.975144	0.000967
H	18.383868	-1.746500	-0.670300
H	18.752976	-0.201807	0.141942
H	17.754030	-1.427375	0.964650
C	0.235680	2.465320	1.123683
H	-0.738051	2.320533	1.606268
H	0.971943	1.942096	1.749800
C	0.623116	3.944751	1.115159
O	1.418880	4.414647	0.314311
N	0.028918	4.705290	2.083333
H	0.315995	5.669605	2.176227
H	-18.313637	-1.687933	-0.133357
H	-18.610058	-0.032819	0.396152
C	-16.682711	-0.344614	-0.486993
O	-16.820372	-0.016213	-1.662723
N	-15.481602	-0.296502	0.151513
H	-15.353897	-0.646232	1.094458
C	-14.256207	0.071205	-0.530872
H	-14.255892	-0.399136	-1.522344
C	-14.131702	1.596128	-0.717009
H	-14.991158	1.950934	-1.290987
H	-14.117420	2.100628	0.254999
H	-13.216936	1.858932	-1.259824
C	-13.095629	-0.491122	0.307366
O	-13.266178	-0.890044	1.461498
N	-11.889603	-0.496469	-0.303680
H	-11.754008	-0.113962	-1.234604
C	-10.663953	-0.880031	0.374594
H	-10.678784	-0.457016	1.386553
C	-10.516224	-2.409634	0.483107
H	-11.372172	-2.811678	1.030739
H	-10.485085	-2.862825	-0.513262
H	-9.600450	-2.682344	1.018866
C	-9.509288	-0.256842	-0.430454
O	-9.686562	0.183213	-1.568247
N	-8.309024	-0.249420	0.188493
H	-8.169537	-0.663356	1.105646
C	-7.086273	0.188989	-0.462973
H	-7.076236	-0.203742	-1.487048
C	-6.979562	1.724477	-0.522894
H	-7.838917	2.120921	-1.069167
H	-6.972472	2.147354	0.487203
H	-6.065338	2.037465	-1.038643
C	-5.926462	-0.427823	0.340374
O	-6.110533	-0.909928	1.460391
N	-4.717508	-0.380294	-0.257498
H	-4.575214	0.065592	-1.159358
C	-3.492387	-0.808731	0.396649
H	-3.516181	-0.467312	1.438566
C	-3.333433	-2.340760	0.382585
H	-4.189494	-2.793867	0.888752
H	-3.289839	-2.711326	-0.646805
H	-2.419706	-2.648051	0.902695
C	-2.341052	-0.114553	-0.354771
O	-2.521403	0.398065	-1.460994
N	-1.145562	-0.128930	0.273046
H	-1.005096	-0.616641	1.153225
C	0.082119	0.345799	-0.348725
H	0.071004	0.049647	-1.404292
C	0.231732	1.883511	-0.293730
H	1.159579	2.178500	-0.794641
H	-0.591065	2.313428	-0.874130
C	1.234846	-0.365765	0.382236
O	1.061421	-0.878799	1.492004

H	0.328919	2.456705	-1.102558		H	-0.580904	4.313233	2.784152

Ac-(Ala)$_4$-Gln-(Ala)$_4$-NHMe_C7$_{eq}$

H	-1.369474	1.999376	-1.230129		C	-14.133682	-1.058731	-0.565582
C	1.268735	0.242306	0.237454		H	-14.611418	-0.726624	0.360899
O	1.931923	1.168148	0.723304		H	-14.023936	-2.146951	-0.543234
N	1.685953	-1.044253	0.229824		H	-14.787594	-0.814908	-1.408791
H	1.079424	-1.733697	-0.219335		C	-12.773957	-0.431458	-0.810305
C	2.872909	-1.503079	0.957043		O	-12.091520	-0.728525	-1.794124
H	2.946655	-0.883571	1.859786		N	-12.356346	0.481075	0.109620
C	2.721438	-2.972847	1.336724		H	-12.921811	0.655786	0.928895
H	1.823546	-3.113016	1.946506		C	-11.121021	1.257800	-0.042334
H	2.651831	-3.601670	0.444244		H	-11.011304	1.448158	-1.116064
H	3.592003	-3.308432	1.905408		C	-11.226540	2.573395	0.721761
C	4.165083	-1.264763	0.137759		H	-12.090949	3.146715	0.372307
O	4.868753	-2.197933	-0.262712		H	-11.316304	2.394725	1.797913
N	4.460142	0.038188	-0.079143		H	-10.324660	3.171263	0.569690
H	3.797997	0.733358	0.268947		C	-9.889464	0.438633	0.414962
C	5.545938	0.467819	-0.966535		O	-9.253558	0.728503	1.433703
H	5.608444	-0.272785	-1.773725		N	-9.574851	-0.597966	-0.395212
C	5.242260	1.848924	-1.538306		H	-10.206376	-0.787961	-1.174885
H	4.284888	1.835839	-2.068562		C	-8.556509	-1.595169	-0.046371
H	5.204627	2.599156	-0.743165		H	-8.584684	-1.711236	1.044591
H	6.028035	2.151076	-2.235112		C	-8.867258	-2.923186	-0.729223
C	6.905901	0.454420	-0.226046		H	-9.865594	-3.270068	-0.445029
O	7.529320	1.492012	0.020097		H	-8.817600	-2.822340	-1.817156
N	7.347429	-0.779888	0.110182		H	-8.134043	-3.678921	-0.437111
H	6.730716	-1.567743	-0.093858		C	-7.139097	-1.092793	-0.415767
C	8.513216	-0.995600	0.973809		O	-6.464464	-1.631771	-1.299768
H	8.541409	-0.159148	1.683582		N	-6.706580	-0.039251	0.314490
C	8.373608	-2.318280	1.720769		H	-7.358945	0.366147	0.986865
H	7.446167	-2.327790	2.302050		C	-5.477418	0.692970	-0.011121
H	8.369684	-3.160308	1.022606		H	-5.376578	0.675909	-1.103600
H	9.218518	-2.460491	2.399098		C	-5.559758	2.133458	0.484220
C	9.829873	-0.949124	0.159245		H	-6.436384	2.626403	0.051775
O	10.545034	-1.946871	0.016570		H	-5.633088	2.164963	1.575481
N	10.125580	0.264829	-0.357158		H	-4.663339	2.688409	0.193131
H	9.448904	1.014043	-0.208508		C	-4.235783	-0.024729	0.566206
C	11.240231	0.487037	-1.286332		O	-3.561072	0.461945	1.483163
H	11.341911	-0.429750	-1.879945		N	-3.925471	-1.196619	-0.034521
C	10.935653	1.675198	-2.192185		H	-4.580353	-1.545853	-0.736865
H	9.999151	1.510922	-2.735074		C	-2.832049	-2.063448	0.419641
H	10.858785	2.596876	-1.608127		H	-2.781803	-1.968420	1.512308
H	11.744653	1.815063	-2.913544		C	-3.105659	-3.511685	0.027160
C	12.573184	0.700683	-0.519135		H	-4.049223	-3.849581	0.466446
O	13.150590	1.783139	-0.504472		H	-3.159965	-3.618402	-1.060522
N	13.026741	-0.422218	0.100192		H	-2.297664	-4.157346	0.378601
H	12.412409	-1.234279	0.091337		C	-1.472024	-1.573030	-0.139328
C	14.211948	-0.422098	0.935955		O	-0.738334	-2.290017	-0.827377
H	13.958672	-0.521501	1.999864		N	-1.162221	-0.299962	0.200227
H	14.880674	-1.245274	0.659454		H	-1.824065	0.185505	0.807154
H	14.727366	0.527576	0.784343		C	-0.097360	0.462283	-0.450365
C	-0.800483	2.685516	0.724850		H	0.006566	0.044718	-1.460822
H	-1.519300	2.122808	1.333675		C	-0.487072	1.940806	-0.584812
H	0.110192	2.810541	1.315898					

H	-1.894487	1.433988	-0.017315
C	-0.159540	2.622822	0.278752
H	0.361799	3.325345	-0.373185
C	-0.883427	3.392547	1.390355
H	-1.593842	4.089044	0.916709
H	-1.463545	2.687377	2.006490
C	0.943832	1.691858	0.829883
O	2.133226	1.984362	0.735374
N	0.526631	0.522212	1.387044
H	-0.463205	0.311519	1.457869
C	1.491224	-0.443113	1.906701
H	2.098686	0.033921	2.682594
C	0.762394	-1.659634	2.486440
H	0.083734	-1.358704	3.292553
H	0.185259	-2.169158	1.706468
H	1.493682	-2.363373	2.893131
C	2.515364	-0.896825	0.846089
O	3.661263	-1.197307	1.185062
N	2.079359	-0.959940	-0.433797
H	1.091684	-0.829373	-0.630243
C	2.951010	-1.391648	-1.520394
H	3.346010	-2.389194	-1.297982
C	2.161947	-1.424793	-2.834928
H	1.326477	-2.129059	-2.762265
H	1.761643	-0.432038	-3.070262
H	2.823807	-1.740471	-3.645541
C	4.207942	-0.515215	-1.688219
O	5.203475	-0.997809	-2.237037
N	4.144492	0.763703	-1.253855
H	3.327566	1.090099	-0.743355
C	5.291387	1.660080	-1.357626
H	5.726309	1.525303	-2.353368
C	4.850683	3.116616	-1.183985
H	4.162495	3.406931	-1.984691
H	4.340875	3.261846	-0.225802
H	5.733442	3.759267	-1.218241
C	6.458149	1.326367	-0.397327
O	7.526435	1.917285	-0.534103
N	6.229059	0.370464	0.540816
H	5.308154	-0.052323	0.621923
C	7.281825	-0.158286	1.394827
H	8.125378	0.532939	1.298381
C	6.829565	-0.225066	2.857857
H	6.643967	0.782535	3.243875
H	5.903827	-0.805093	2.947810
H	7.604875	-0.709270	3.455689
C	7.812100	-1.537475	0.934110
O	8.593704	-2.169096	1.645240
N	7.389518	-1.981922	-0.273288
H	6.752070	-1.429735	-0.836944
C	7.860222	-3.243789	-0.809880
H	7.816751	-4.019897	-0.039647
H	7.220665	-3.522470	-1.650815

C	-1.489096	4.015815	0.427170
O	-2.461033	4.098923	-0.316595
N	-0.966853	5.103999	1.061405
H	-1.390799	6.006725	0.898701
H	-0.139144	5.051088	1.634610

Ac-(Ala)4-Ser-(Ala)4-NHMe αR

C	-8.955650	-2.989700	0.435423
H	-9.875294	-2.557056	0.840531
H	-8.493581	-3.633367	1.187768
H	-9.215249	-3.621771	-0.421384
C	-7.948161	-1.949930	-0.012851
O	-6.768846	-2.227546	-0.226236
N	-8.418170	-0.670244	-0.162701
H	-9.417793	-0.522569	-0.103177
C	-7.638558	0.341462	-0.881842
H	-7.327722	-0.063448	-1.851611
C	-8.480060	1.603829	-1.100878
H	-9.364852	1.380248	-1.707179
H	-8.805082	2.034765	-0.147207
H	-7.883266	2.349891	-1.631030
C	-6.319451	0.699866	-0.181114
O	-5.383392	1.161718	-0.833056
N	-6.254996	0.507485	1.159394
H	-7.044915	0.079681	1.623738
C	-5.032677	0.768262	1.909835
H	-4.732118	1.806394	1.735949
C	-5.266508	0.548207	3.407928
H	-6.042360	1.224603	3.781604
H	-5.568598	-0.485417	3.614298
H	-4.340985	0.747436	3.953088
C	-3.828912	-0.064053	1.427886
O	-2.686784	0.338658	1.689057
N	-4.069541	-1.204519	0.751214
H	-5.021740	-1.474011	0.509586
C	-2.965707	-2.000163	0.217370
H	-2.289035	-2.251496	1.039373
C	-3.493903	-3.288097	-0.423394
H	-4.023685	-3.897063	0.315833
H	-4.183825	-3.068397	-1.244372
H	-2.652401	-3.864902	-0.815255
C	-2.087853	-1.222148	-0.784107
O	-0.907332	-1.547254	-0.922262
N	-2.674430	-0.233448	-1.501826
H	-3.631444	0.047252	-1.304210
C	-1.899947	0.558592	-2.455116
H	-1.300560	-0.128708	-3.057861
C	-2.832566	1.365334	-3.364615
H	-3.468688	0.695789	-3.953011
H	-3.476586	2.031536	-2.780725
H	-2.232134	1.969390	-4.049678
C	-0.861183	1.487153	-1.786525
O	0.128201	1.845924	-2.412341
N	-1.147194	1.903212	-0.517340

H	0.060358	0.334080	-1.778971	H	8.899398	-3.176759	-1.158056
C	0.270992	1.746967	-0.189740	O	0.099290	4.070351	2.151920
H	1.131117	2.206148	-0.704638	H	-0.339828	4.496341	2.902665

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<tr><td colspan="4">Ac-(Ala)₄-Ser-(Ala)₄-NHMe_C5</td></tr>
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H	-0.629253	2.306445	-0.475216	C	-17.792191	-0.340417	0.919567
C	1.274102	-0.602146	-0.235522	H	-17.466669	-0.886287	1.810451
O	1.084201	-1.564582	0.507587	H	-18.317619	-1.028694	0.250200
N	2.485216	-0.269070	-0.729057	H	-18.507360	0.432781	1.217584
H	2.636429	0.578843	-1.268166	C	-16.651528	0.314261	0.152329
C	3.711475	-0.922956	-0.303581	O	-16.844682	0.954583	-0.878160
H	3.652603	-1.103413	0.776806	N	-15.412736	0.147991	0.691059
C	3.927520	-2.269155	-1.019093	H	-15.245758	-0.452469	1.490748
H	3.078591	-2.924561	-0.809095	C	-14.213161	0.641368	0.042918
H	4.004675	-2.120771	-2.101246	H	-14.299861	0.457678	-1.035561
H	4.840817	-2.762027	-0.668951	C	-14.015901	2.153928	0.263181
C	4.850124	0.072107	-0.597259	H	-14.891693	2.681287	-0.122764
O	4.661833	1.070130	-1.297405	H	-13.906272	2.374720	1.330279
N	6.044874	-0.235776	-0.051366	H	-13.127610	2.521858	-0.262326
H	6.194988	-1.088119	0.480988	C	-13.036852	-0.171240	0.610882
C	7.252147	0.534229	-0.299305	O	-13.161197	-0.867271	1.621093
H	7.295733	0.782324	-1.366891	N	-11.870878	-0.051665	-0.062475
C	7.282280	1.841834	0.514207	H	-11.768117	0.567289	-0.861035
H	6.408628	2.444306	0.253885	C	-10.632086	-0.659006	0.391523
H	7.260276	1.625378	1.587340	H	-10.560569	-0.534045	1.478875
H	8.183701	2.424072	0.294667	C	-10.571055	-2.163040	0.063456
C	8.430528	-0.387603	0.066579	H	-11.416964	-2.665605	0.538951
O	8.252635	-1.430993	0.698609	H	-10.624451	-2.320560	-1.018850
N	9.646871	0.039448	-0.333552	H	-9.644443	-2.613067	0.436112
H	9.781105	0.932120	-0.799659	C	-9.492463	0.115514	-0.295079
C	10.881023	-0.634196	0.034684	O	-9.712065	0.864199	-1.249799
H	10.808427	-0.944831	1.084098	N	-8.259007	-0.101388	0.209319
C	11.143450	-1.880152	-0.832028	H	-8.088892	-0.767626	0.957419
H	10.310248	-2.577912	-0.717115	C	-7.052209	0.444397	-0.388192
H	11.232345	-1.601387	-1.887175	H	-7.128246	0.350163	-1.478474
H	12.064942	-2.387380	-0.526684	C	-6.851946	1.930162	-0.034633
C	12.001252	0.410756	-0.119129	H	-7.717144	2.499508	-0.383135
O	11.810738	1.468597	-0.723346	H	-6.754106	2.056415	1.048691
N	13.187586	0.076354	0.431740	H	-5.954011	2.334059	-0.514735
H	13.344010	-0.820157	0.883152	C	-5.888609	-0.424844	0.125302
C	14.380460	0.893126	0.288611	O	-6.044865	-1.211698	1.061808
H	14.424265	1.262861	-0.743453	N	-4.709809	-0.247370	-0.506652
C	14.371979	2.099302	1.246985	H	-4.584429	0.450690	-1.234263
H	13.487481	2.708532	1.045749	C	-3.477889	-0.891738	-0.081504
H	14.344815	1.760795	2.287697	H	-3.429707	-0.864071	1.013853
H	15.261567	2.723514	1.108164	C	-3.402104	-2.358960	-0.543092
C	15.575061	-0.039677	0.563071	H	-4.251469	-2.908221	-0.129278
O	15.415380	-1.129957	1.107913	H	-3.436450	-2.418889	-1.635921
N	16.785032	0.444882	0.185369	H	-2.478440	-2.834866	-0.196983
H	16.821266	1.340903	-0.280119	C	-2.330204	-0.049693	-0.668988
C	18.030718	-0.273402	0.406465	O	-2.541831	0.797450	-1.541647
H	18.524624	-0.503658	-0.544111	N	-1.104602	-0.318695	-0.178348
H	18.714970	0.311482	1.031152	H	-0.940167	-1.048797	0.508466
H	17.785920	-1.205189	0.916953	C	0.103940	0.302333	-0.682692
O	0.459846	1.712632	1.215590				

H	-1.275703	2.875465	-0.096195		H	0.454915	2.624286	1.542781

H	-0.537044	2.730611	1.510748
C	1.225272	0.640377	0.817256
O	1.935797	1.435326	1.458780
N	1.565874	-0.644939	0.608900
H	0.928146	-1.211567	0.043745
C	2.750273	-1.269188	1.208621
H	2.884900	-0.806484	2.193572
C	2.535718	-2.772228	1.353699
H	1.648248	-2.969055	1.962991
H	2.413879	-3.244752	0.374796
H	3.402949	-3.232625	1.833641
C	4.015225	-0.957904	0.371600
O	4.618041	-1.833430	-0.256416
N	4.396506	0.340924	0.396380
H	3.799591	0.991951	0.906254
C	5.425150	0.884394	-0.498157
H	5.361376	0.319517	-1.436858
C	5.164813	2.365737	-0.753911
H	4.159915	2.508530	-1.164153
H	5.264460	2.942874	0.170103
H	5.895222	2.761062	-1.463950
C	6.843861	0.654199	0.077387
O	7.567258	1.590489	0.431609
N	7.220000	-0.644211	0.139261
H	6.532951	-1.345481	-0.140878
C	8.450901	-1.079943	0.807013
H	8.618837	-0.388510	1.642319
C	8.290222	-2.505668	1.325238
H	7.434193	-2.566523	2.004688
H	8.144136	-3.206161	0.497888
H	9.190674	-2.816525	1.860606
C	9.674379	-0.961860	-0.136001
O	10.299254	-1.956023	-0.521394
N	9.998699	0.305370	-0.477272
H	9.402919	1.054255	-0.123031
C	11.031122	0.624463	-1.470888
H	11.013591	-0.184372	-2.211386
C	10.721421	1.961084	-2.136154
H	9.727005	1.938129	-2.593685
H	10.766337	2.775496	-1.407333
H	11.463043	2.176692	-2.909458
C	12.442070	0.638723	-0.823143
O	13.086987	1.673454	-0.687147
N	12.878637	-0.594844	-0.450965
H	12.215159	-1.363072	-0.530500
C	14.133566	-0.794880	0.247936
H	13.973576	-1.064372	1.300418
H	14.720117	-1.588537	-0.228883
H	14.692359	0.141324	0.205639
O	0.685125	3.387471	-0.048027
H	1.444300	3.163801	0.520762

Ac-(Ala)₄-Thr-(Ala)₄-NHMe_αR

Right column:

C	-14.186271	-1.247029	-0.853068
H	-14.713840	-0.975530	0.066087
H	-13.988615	-2.322977	-0.849548
H	-14.835415	-1.038408	-1.709308
C	-12.876697	-0.506158	-1.046988
O	-12.145090	-0.726207	-2.015723
N	-12.559992	0.418440	-0.099299
H	-13.161543	0.533374	0.704718
C	-11.391961	1.299888	-0.205555
H	-11.272698	1.520944	-1.272434
C	-11.628443	2.585914	0.579426
H	-12.529930	3.089905	0.217252
H	-11.729787	2.378494	1.649315
H	-10.778202	3.262274	0.462417
C	-10.107015	0.578336	0.268287
O	-9.520965	0.901825	1.307000
N	-9.687767	-0.414065	-0.549945
H	-10.284355	-0.643213	-1.346854
C	-8.606655	-1.337344	-0.186084
H	-8.660551	-1.480282	0.900782
C	-8.791708	-2.669997	-0.904944
H	-9.771834	-3.094124	-0.666077
H	-8.708621	-2.543277	-1.988074
H	-8.016976	-3.376746	-0.597659
C	-7.221715	-0.719099	-0.496378
O	-6.477671	-1.181215	-1.367664
N	-6.896885	0.346247	0.273246
H	-7.605362	0.682204	0.927804
C	-5.724543	1.186837	0.007311
H	-5.586513	1.208576	-1.081329
C	-5.958395	2.597537	0.538462
H	-6.859051	3.025235	0.087225
H	-6.068868	2.591029	1.626577
H	-5.106147	3.238410	0.299577
C	-4.444401	0.564548	0.615281
O	-3.833555	1.100036	1.547376
N	-4.048102	-0.589521	0.030505
H	-4.656350	-0.975738	-0.694366
C	-2.971650	-1.425245	0.572939
H	-3.014812	-1.334944	1.666123
C	-3.172864	-2.877876	0.153394
H	-4.150055	-3.235807	0.491923
H	-3.109103	-2.981386	-0.933565
H	-2.394701	-3.509347	0.589010
C	-1.584851	-0.900404	0.128231
O	-0.845113	-1.548984	-0.618713
N	-1.249147	0.306267	0.644389
H	-1.961206	0.774865	1.210510
C	-0.105945	1.085618	0.169962
H	-0.003703	0.928537	-0.911489
C	-0.364580	2.579942	0.433508

O	2.140888	1.966012	0.556137	C	-8.903771	-3.079767	0.600745
N	0.558093	0.543176	1.339511	H	-9.841521	-2.624278	0.932443
H	-0.428644	0.331221	1.441013	H	-8.460303	-3.641578	1.426562
C	1.537253	-0.364057	1.931315	H	-9.125855	-3.795334	-0.198818
H	2.141811	0.181838	2.662866	C	-7.892752	-2.074285	0.086913
C	0.825311	-1.537576	2.612346	O	-6.711097	-2.365766	-0.092598
H	0.148457	-1.179581	3.396376	N	-8.360993	-0.809345	-0.160858
H	0.248548	-2.114061	1.880216	H	-9.361137	-0.658239	-0.123502
H	1.566427	-2.198703	3.069672	C	-7.572676	0.148818	-0.941103
C	2.562572	-0.889863	0.906474	H	-7.249576	-0.324567	-1.875206
O	3.713942	-1.145958	1.263088	C	-8.412033	1.390907	-1.261180
N	2.122962	-1.062622	-0.362052	H	-9.288611	1.122780	-1.861300
H	1.131939	-0.967935	-0.562034	H	-8.749817	1.888429	-0.345101
C	2.996765	-1.566373	-1.415403	H	-7.808891	2.098003	-1.835680
H	3.400345	-2.541959	-1.122139	C	-6.262665	0.558661	-0.251378
C	2.206139	-1.701597	-2.722424	O	-5.318723	0.975261	-0.922562
H	1.375918	-2.404693	-2.596740	N	-6.213700	0.461640	1.099793
H	1.798586	-0.731453	-3.028899	H	-7.008907	0.068050	1.584871
H	2.868898	-2.071290	-3.509131	C	-4.999024	0.775206	1.842660
C	4.245992	-0.694092	-1.649843	H	-4.695797	1.798362	1.599003
O	5.246218	-1.208794	-2.159845	C	-5.249315	0.661795	3.349969
N	4.170581	0.614145	-1.316869	H	-6.025855	1.365890	3.666765
H	3.349868	0.972641	-0.834487	H	-5.558723	-0.353491	3.625162
C	5.309115	1.510186	-1.490715	H	-4.328726	0.895386	3.889870
H	5.741423	1.308431	-2.476225	C	-3.791035	-0.089057	1.432910
C	4.855807	2.971565	-1.420158	O	-2.651494	0.335384	1.668391
H	4.158633	3.196499	-2.234046	N	-4.025046	-1.280225	0.847022
H	4.352036	3.181748	-0.470891	H	-4.974930	-1.568340	0.618383
H	5.732072	3.617890	-1.508931	C	-2.915175	-2.112524	0.386750
C	6.483212	1.258268	-0.514921	H	-2.239186	-2.285857	1.229155
O	7.547292	1.842177	-0.704757	C	-3.433174	-3.455676	-0.138627
N	6.265199	0.378968	0.497917	H	-3.960510	-4.000309	0.650879
H	5.348353	-0.044039	0.617244	H	-4.122281	-3.315109	-0.977442
C	7.326728	-0.076036	1.383084	H	-2.586700	-4.059105	-0.475867
H	8.165824	0.609746	1.227239	C	-2.038010	-1.419775	-0.676642
C	6.884708	-0.030249	2.850088	O	-0.856425	-1.751969	-0.785495
H	6.694784	1.003421	3.156964	N	-2.627166	-0.496122	-1.474628
H	5.963661	-0.607293	2.992237	H	-3.584498	-0.202487	-1.299311
H	7.667294	-0.461043	3.478510	C	-1.854664	0.221022	-2.486722
C	7.860995	-1.485021	1.028214	H	-1.234400	-0.507793	-3.014679
O	8.648734	-2.056147	1.782516	C	-2.788198	0.921099	-3.479854
N	7.433918	-2.023817	-0.138324	H	-3.398499	0.187066	-4.016447
H	6.791490	-1.519535	-0.740073	H	-3.457318	1.620904	-2.967930
C	7.904194	-3.323327	-0.576171	H	-2.188135	1.475683	-4.205752
H	7.871332	-4.034504	0.254854	C	-0.842091	1.228541	-1.896331
H	7.257138	-3.670925	-1.385103	O	0.135333	1.563699	-2.553721
H	8.939528	-3.281738	-0.939550	N	-1.135374	1.734874	-0.662412
O	0.140683	4.005536	1.897893	H	-1.870542	1.288964	-0.124477
H	-0.279681	4.530112	2.596245	C	-0.164666	2.539175	0.071587
C	-1.814217	4.434867	0.500177	H	0.344593	3.192659	-0.639204
H	-2.585859	3.966106	-0.119395	C	-0.889851	3.392529	1.131292
H	-2.316944	5.020953	1.280467	H	-1.484522	2.715145	1.766596
H	-1.234250	5.123262	-0.123661	C	0.956116	1.670612	0.689006

C	1.217664	0.307280	0.639441		Ac-(Ala)₄-Thr-(Ala)₄-NHMe_C5			
O	0.992919	-0.505350	1.535471		C	-17.675621	-1.422655	0.045225
N	2.410199	0.418117	0.015311		H	-17.434526	-1.595019	1.098693
H	2.599241	1.146678	-0.667106		H	-17.996631	-2.366950	-0.406107
C	3.594440	-0.304369	0.448377		H	-18.518912	-0.728217	-0.019039
H	3.623981	-0.300082	1.545074		C	-16.514507	-0.861539	-0.764133
C	3.592314	-1.764896	-0.039578		O	-16.628684	-0.577944	-1.954003
H	2.702171	-2.267387	0.346789		N	-15.350176	-0.694531	-0.079318
H	3.577656	-1.804343	-1.133782		H	-15.233884	-1.007971	0.877841
H	4.476601	-2.304332	0.316723		C	-14.129978	-0.249558	-0.723864
C	4.799375	0.483124	-0.100659		H	-14.049606	-0.748178	-1.698169
O	4.650221	1.385192	-0.928763		C	-14.119381	1.274115	-0.955914
N	6.005341	0.107480	0.374442		H	-14.980715	1.541563	-1.572828
H	6.117343	-0.675392	1.012206		H	-14.183129	1.807211	-0.001341
C	7.255246	0.665789	-0.113289		H	-13.207451	1.592689	-1.473009
H	7.191448	0.762426	-1.203953		C	-12.965255	-0.690130	0.179252
C	7.543653	2.053380	0.489781		O	-13.153741	-1.070335	1.336922
H	6.722006	2.728939	0.239267		N	-11.737000	-0.611035	-0.379955
H	7.631759	1.986364	1.579132		H	-11.592058	-0.243991	-1.315744
H	8.472938	2.473399	0.089913		C	-10.514877	-0.868742	0.361430
C	8.352095	-0.350854	0.253786		H	-10.610579	-0.419775	1.357651
O	8.138567	-1.256117	1.062906		C	-10.243106	-2.376356	0.524817
N	9.542769	-0.163110	-0.353570		H	-11.086294	-2.835699	1.046649
H	9.715940	0.622271	-0.974374		H	-10.127045	-2.852212	-0.454554
C	10.723233	-0.951560	-0.041729		H	-9.333358	-2.553752	1.108722
H	10.776086	-1.085611	1.045709		C	-9.382079	-0.172252	-0.414276
C	10.686564	-2.339377	-0.709081		O	-9.544551	0.215512	-1.573354
H	9.796296	-2.874904	-0.370429		N	-8.216935	-0.041665	0.255061
H	10.650565	-2.239599	-1.798911		H	-8.084556	-0.412171	1.191884
H	11.569227	-2.930442	-0.442163		C	-7.007729	0.484715	-0.354939
C	11.929807	-0.123173	-0.519611		H	-6.903971	0.051111	-1.357319
O	11.783358	0.853195	-1.258262		C	-7.043339	2.019351	-0.482324
N	13.136163	-0.551944	-0.091135		H	-7.906440	2.307801	-1.087212
H	13.246428	-1.386917	0.476842		H	-7.128091	2.483452	0.505875
C	14.385149	0.045409	-0.531164		H	-6.136871	2.396752	-0.967745
H	14.306968	0.257167	-1.604784		C	-5.840334	0.016850	0.534434
C	14.689466	1.359931	0.212504		O	-6.041120	-0.450300	1.657694
H	13.872194	2.064929	0.041553		N	-4.609421	0.175487	0.004718
H	14.785985	1.177443	1.287595		H	-4.462889	0.606472	-0.903336
H	15.619559	1.813676	-0.147215		C	-3.386638	-0.096582	0.742122
C	15.478055	-1.010615	-0.281757		H	-3.507466	0.273720	1.767071
O	15.273819	-1.971216	0.457500		C	-3.059367	-1.601544	0.793138
N	16.658132	-0.779560	-0.910699		H	-3.878545	-2.129479	1.287676
H	16.729277	0.022132	-1.521485		H	-2.938587	-1.999371	-0.219901
C	17.820809	-1.640329	-0.757239		H	-2.135002	-1.787205	1.350674
H	18.121403	-2.067168	-1.720494		C	-2.270746	0.690584	0.033557
H	18.666179	-1.086831	-0.333318		O	-2.431435	1.142206	-1.101696
H	17.544434	-2.447984	-0.078916		N	-1.127075	0.830726	0.743805
C	-0.628529	3.724374	0.092292		H	-0.992440	0.298926	1.598617
H	-0.862978	3.656663	-0.974519		C	0.116688	1.273770	0.142984
H	-1.541062	3.522755	0.660140		H	0.012213	1.199235	-0.944909
H	-0.306553	4.751534	0.306883		C	0.468177	2.738235	0.487145
O	0.726348	2.763812	1.888444		H	1.387571	2.987719	-0.070134

H	-0.412899	2.767798	1.348975
C	1.262649	0.579544	0.741963
O	1.949576	1.306203	1.482766
N	1.589973	-0.696755	0.465320
H	0.961823	-1.217025	-0.152231
C	2.732401	-1.383391	1.079334
H	2.827998	-0.989479	2.098077
C	2.488999	-2.888386	1.111423
H	1.569872	-3.110857	1.662175
H	2.409104	-3.291872	0.097947
H	3.325051	-3.394913	1.600307
C	4.035977	-1.037511	0.318485
O	4.646635	-1.874145	-0.353143
N	4.434861	0.249490	0.452679
H	3.828691	0.869500	0.989112
C	5.480008	0.848736	-0.385456
H	5.426508	0.353067	-1.363248
C	5.229428	2.346062	-0.537518
H	4.228234	2.523476	-0.943784
H	5.324958	2.855307	0.426066
H	5.967261	2.787078	-1.212098
C	6.889321	0.567816	0.189765
O	7.616766	1.471796	0.613129
N	7.253702	-0.735143	0.168789
H	6.564991	-1.409964	-0.166836
C	8.475697	-1.225378	0.814650
H	8.642569	-0.593404	1.696078
C	8.299512	-2.681314	1.234290
H	7.438224	-2.780232	1.902516
H	8.153219	-3.323194	0.360673
H	9.193528	-3.035530	1.753255
C	9.707951	-1.053922	-0.108867
O	10.330531	-2.024662	-0.553199
N	10.041482	0.230900	-0.364660
H	9.447392	0.958345	0.034427
C	11.081575	0.609220	-1.329033
H	11.064139	-0.148155	-2.122195
C	10.782442	1.988841	-1.905489
H	9.790938	2.001374	-2.369666
H	10.826126	2.752533	-1.123633
H	11.530042	2.252019	-2.658021
C	12.488912	0.572736	-0.674353
O	13.139570	1.592420	-0.469448
N	12.915524	-0.684931	-0.379292
H	12.247942	-1.442176	-0.512172
C	14.164856	-0.937914	0.312343
H	13.996083	-1.282539	1.341234
H	14.753945	-1.696344	-0.216029
H	14.725670	-0.002404	0.342114
O	0.971646	3.295486	-0.104859
H	1.644877	3.003081	0.537097
C	-1.357454	3.190371	-0.542649
H	-1.204501	2.994957	-1.610063

H	0.887077	3.684693	2.145784
Ac-(Ala)₄-Thr-(Ala)₄-NHMe_C7ₑ𝓆			
C	-14.178193	-1.470077	-0.494729
H	-14.658337	-1.174324	0.442726
H	-13.955935	-2.540681	-0.462909
H	-14.880008	-1.307753	-1.318919
C	-12.899173	-0.709781	-0.790796
O	-12.212950	-0.957552	-1.785614
N	-12.558622	0.265798	0.095872
H	-13.118144	0.400579	0.926708
C	-11.417639	1.164727	-0.109566
H	-11.356223	1.336732	-1.190173
C	-11.643548	2.481524	0.625750
H	-12.573973	2.948517	0.288063
H	-11.684791	2.323479	1.707971
H	-10.816616	3.169300	0.432444
C	-10.096912	0.490060	0.333481
O	-9.478023	0.860305	1.336851
N	-9.687893	-0.519453	-0.469137
H	-10.316258	-0.793520	-1.226357
C	-8.575823	-1.410314	-0.117189
H	-8.587303	-1.521244	0.974759
C	-8.759733	-2.767521	-0.788823
H	-9.722125	-3.202554	-0.502244
H	-8.717663	-2.672307	-1.877508
H	-7.960590	-3.449742	-0.488676
C	-7.215624	-0.775723	-0.496586
O	-6.496299	-1.247844	-1.382997
N	-6.882297	0.315423	0.232226
H	-7.573255	0.657891	0.901985
C	-5.735418	1.168186	-0.098528
H	-5.636562	1.163638	-1.191532
C	-5.975707	2.587972	0.404889
H	-6.906586	2.982701	-0.013976
H	-6.034031	2.609563	1.496783
H	-5.151989	3.241522	0.107019
C	-4.426178	0.580013	0.480964
O	-3.800809	1.138658	1.390321
N	-4.023724	-0.573460	-0.099308
H	-4.649366	-0.984939	-0.794867
C	-2.927360	-1.388053	0.434968
H	-2.956567	-1.289648	1.527903
C	-3.116515	-2.846895	0.030687
H	-4.087449	-3.211496	0.380075
H	-3.059605	-2.959490	-1.055636
H	-2.328879	-3.466487	0.466389
C	-1.550518	-0.854484	-0.031563
O	-0.826617	-1.497757	-0.798933
N	-1.200506	0.344209	0.492977
H	-1.899102	0.811822	1.074333
C	-0.023121	1.091631	0.046425
H	0.103078	0.917085	-1.029712
C	-0.210226	2.610879	0.276675

H	0.323493	2.013074	-2.017778
C	-0.886977	3.049686	-0.530112
H	-1.592169	3.405700	-1.292897
H	-1.484513	2.769484	0.346068
C	0.851337	1.190160	-0.156147
O	2.049922	1.378184	-0.359628
N	0.402132	0.450845	0.893012
H	-0.593760	0.324528	1.041540
C	1.340805	-0.172558	1.821837
H	1.981635	0.599667	2.259152
C	0.579738	-0.910861	2.927998
H	-0.073252	-0.221907	3.475438
H	-0.029262	-1.716909	2.503568
H	1.292745	-1.347737	3.632459
C	2.325034	-1.132453	1.122347
O	3.465906	-1.276804	1.565223
N	1.861846	-1.794412	0.036297
H	0.877135	-1.731429	-0.202978
C	2.697121	-2.734531	-0.702377
H	3.068985	-3.506774	-0.019890
C	1.878355	-3.382211	-1.825533
H	1.028254	-3.933172	-1.409122
H	1.496242	-2.619825	-2.513467
H	2.513451	-4.076810	-2.381490
C	3.973407	-2.095467	-1.284326
O	4.946124	-2.815873	-1.529177
N	3.951658	-0.766274	-1.533095
H	3.153474	-0.206471	-1.244391
C	5.119947	-0.073819	-2.065826
H	5.535460	-0.696298	-2.864980
C	4.721718	1.290998	-2.635544
H	4.031834	1.168190	-3.477137
H	4.228587	1.905628	-1.875168
H	5.621682	1.805077	-2.980936
C	6.293136	0.073759	-1.067658
O	7.372476	0.491532	-1.480129
N	6.058075	-0.294261	0.218751
H	5.128593	-0.593569	0.501352
C	7.113533	-0.371206	1.217646
H	7.976434	0.145017	0.784528
C	6.696939	0.317656	2.521839
H	6.553551	1.390215	2.355304
H	5.755711	-0.102535	2.894925
H	7.471099	0.164611	3.276986
C	7.584190	-1.818377	1.501347
O	8.355414	-2.046993	2.433196
N	7.123960	-2.783636	0.670594
H	6.492720	-2.557420	-0.090492
C	7.532921	-4.164988	0.833302
H	7.463075	-4.457601	1.885548
H	6.872803	-4.793963	0.231310
H	8.570307	-4.323510	0.510638
C	0.085234	4.148301	-0.157928

H	-2.321273	2.775022	-0.235944
H	-1.383449	4.274154	-0.395722
H	-1.383449	4.274154	-0.395722

Ac-(Ala)4-Tyr-(Ala)4-NHMe_αR

C	-9.264692	-2.447086	1.750773
H	-10.153438	-1.819830	1.866856
H	-8.837330	-2.657933	2.734179
H	-9.567618	-3.405279	1.313889
C	-8.198477	-1.826226	0.870498
O	-7.045875	-2.254829	0.835101
N	-8.582307	-0.747885	0.114855
H	-9.567772	-0.519364	0.080441
C	-7.749725	-0.264953	-0.990579
H	-7.491903	-1.106254	-1.643878
C	-8.503465	0.797386	-1.798676
H	-9.418292	0.378590	-2.232565
H	-8.770316	1.656763	-1.173319
H	-7.869174	1.149359	-2.615795
C	-6.392423	0.286563	-0.529078
O	-5.439244	0.304641	-1.307913
N	-6.313197	0.762122	0.737351
H	-7.123046	0.675991	1.336662
C	-5.059416	1.264037	1.287517
H	-4.694217	2.071346	0.644979
C	-5.274630	1.799385	2.706777
H	-5.994911	2.624176	2.703451
H	-5.640573	1.011802	3.376162
H	-4.326410	2.170517	3.102610
C	-3.926864	0.219213	1.274176
O	-2.753734	0.614565	1.302257
N	-4.262255	-1.086639	1.247439
H	-5.236965	-1.370292	1.163936
C	-3.229484	-2.118754	1.175554
H	-2.542615	-1.983129	2.016056
C	-3.860486	-3.513305	1.249131
H	-4.406321	-3.639946	2.189386
H	-4.559070	-3.675995	0.422289
H	-3.071351	-4.267695	1.197518
C	-2.339290	-1.997393	-0.078026
O	-1.180246	-2.413763	-0.033339
N	-2.895717	-1.472193	-1.197039
H	-3.826271	-1.063772	-1.165725
C	-2.103439	-1.307368	-2.414142
H	-1.562227	-2.239503	-2.595368
C	-3.013265	-0.996374	-3.607369
H	-3.702135	-1.827627	-3.791553
H	-3.602478	-0.090251	-3.430974
H	-2.399295	-0.848097	-4.499653
C	-0.995496	-0.238773	-2.282077
O	0.023907	-0.324639	-2.957547
N	-1.251634	0.798076	-1.433820
H	-2.039895	0.721954	-0.801302
C	-0.219468	1.775695	-1.100988

H	4.298292	-2.193598	-1.941561
H	3.458710	-2.938418	-0.558141
H	2.526256	-2.141453	-1.844972
C	2.425345	-0.586948	0.521263
O	2.642548	-0.628296	1.734626
N	1.198483	-0.396878	-0.008707
H	1.029338	-0.483328	-1.007376
C	-0.012500	-0.391615	0.792520
H	0.084317	-1.159266	1.571104
C	-0.252528	0.966736	1.516393
H	-1.076904	0.834985	2.228201
H	0.644498	1.148438	2.117445
C	-1.154685	-0.788630	-0.163796
O	-0.948331	-0.964821	-1.365385
N	-2.369503	-0.942672	0.408616
H	-2.546938	-0.632830	1.359749
C	-3.576215	-1.135758	-0.379524
H	-3.461676	-0.583606	-1.320580
C	-3.815617	-2.620449	-0.705193
H	-2.949972	-3.008229	-1.248641
H	-3.946965	-3.202651	0.212853
H	-4.702444	-2.757504	-1.333222
C	-4.726814	-0.507612	0.432324
O	-4.533893	-0.042610	1.560269
N	-5.932858	-0.502745	-0.169757
H	-6.091577	-0.939314	-1.073343
C	-7.141677	-0.022341	0.479674
H	-7.141569	-0.373605	1.518453
C	-7.230411	1.515272	0.476581
H	-6.361361	1.925802	0.996660
H	-7.245453	1.895820	-0.549972
H	-8.135112	1.859376	0.989181
C	-8.317532	-0.658305	-0.285039
O	-8.150881	-1.181677	-1.388880
N	-9.517557	-0.580027	0.327041
H	-9.643599	-0.099565	1.213335
C	-10.755124	-1.019475	-0.296122
H	-10.749269	-0.701931	-1.345898
C	-10.918612	-2.550229	-0.243361
H	-10.072097	-3.017287	-0.752641
H	-10.946364	-2.896759	0.794930
H	-11.841086	-2.866950	-0.741712
C	-11.890472	-0.302560	0.457104
O	-11.687789	0.253941	1.538555
N	-13.102201	-0.348504	-0.136181
H	-13.264645	-0.854141	-1.002181
C	-14.305031	0.173930	0.489029
H	-14.284463	-0.092271	1.553222
C	-14.401639	1.706344	0.363508
H	-13.522332	2.159022	0.828255
H	-14.442214	2.002241	-0.689709
H	-15.295638	2.091029	0.866738
C	-15.488371	-0.526571	-0.204835

C	0.736869	4.900192	-1.142974
C	0.367754	4.440865	1.182810
C	1.641558	5.904648	-0.806891
H	0.538968	4.699760	-2.193778
C	1.267368	5.442533	1.537230
H	-0.123260	3.870339	1.968080
C	1.911996	6.177646	0.538529
H	2.138430	6.475950	-1.589154
H	1.486034	5.663324	2.577202
O	2.785261	7.152557	0.934785
H	3.203729	7.538899	0.149853

Ac-(Ala)$_4$-Tyr-(Ala)$_4$-NHMe_C5

C	17.916577	-0.390830	-0.771826
H	17.615656	-0.084306	-1.778384
H	18.371379	-1.385210	-0.822446
H	18.682402	0.298643	-0.403173
C	16.766869	-0.427457	0.225674
O	16.936700	-0.737733	1.402124
N	15.547163	-0.088815	-0.274507
H	15.395016	0.084301	-1.261804
C	14.338022	-0.150920	0.523357
H	14.372040	-1.060585	1.136273
C	14.200186	1.062843	1.463176
H	15.072656	1.098752	2.120046
H	14.148992	1.991349	0.884611
H	13.299682	0.987761	2.082881
C	13.160527	-0.236474	-0.462889
O	13.302599	0.014886	-1.661635
N	11.973336	-0.584747	0.081939
H	11.859970	-0.731018	1.080549
C	10.731522	-0.593640	-0.671239
H	10.710772	0.290531	-1.320239
C	10.596391	-1.851791	-1.549952
H	11.441465	-1.894030	-2.241463
H	10.597393	-2.753951	-0.929342
H	9.669650	-1.830874	-2.133779
C	9.596409	-0.501394	0.364918
O	9.807277	-0.694864	1.564130
N	8.375654	-0.215515	-0.136406
H	8.208356	-0.122521	-1.134215
C	7.168990	-0.213738	0.673276
H	7.204663	-1.072324	1.355047
C	7.034101	1.073219	1.508598
H	7.907284	1.169126	2.158588
H	6.977467	1.950097	0.855149
H	6.136177	1.046738	2.135486
C	5.993909	-0.383020	-0.308306
O	6.152548	-0.247606	-1.523789
N	4.803149	-0.669516	0.257874
H	4.679291	-0.715635	1.265359
C	3.565971	-0.762052	-0.499163
H	3.537383	0.059205	-1.225787
C	3.450488	-2.097039	-1.258898

H	-5.314860	2.654466	1.328017		O	-15.336325	-1.121809	-1.269581
C	-4.594492	0.088072	0.580123		N	-16.681933	-0.408841	0.429822
O	-3.866074	0.303253	1.555109		H	-16.710297	0.073480	1.317192
N	-4.275034	-0.774441	-0.412561		C	-17.918931	-0.963365	-0.098201
H	-4.968334	-0.914300	-1.149830		H	-18.325351	-1.727969	0.573361
C	-3.136410	-1.694991	-0.326309		H	-18.669776	-0.178280	-0.240254
H	-3.032523	-1.976095	0.729655		H	-17.689524	-1.419835	-1.061420
C	-3.397718	-2.932812	-1.179015		C	-0.541761	2.141768	0.608798
H	-4.320914	-3.424046	-0.856317		C	0.494982	2.857881	-0.002573
H	-3.482632	-2.666733	-2.236571		C	-1.860290	2.548984	0.349550
H	-2.569603	-3.639516	-1.085112		C	0.232647	3.929643	-0.855285
C	-1.818284	-0.997298	-0.740876		H	1.527241	2.581779	0.195257
O	-1.181792	-1.338278	-1.743227		C	-2.138006	3.617928	-0.497605
N	-1.421472	-0.006628	0.092745		H	-2.686325	2.023472	0.823486
H	-2.036079	0.221800	0.876507		C	-1.088428	4.310821	-1.108735
C	-0.294223	0.877528	-0.219877		H	1.055163	4.474087	-1.316474
H	-0.267452	0.991320	-1.309873		H	-3.158671	3.932806	-0.691390
C	-0.497748	2.250090	0.445176		O	-1.414111	5.354163	-1.932138
H	-1.549673	2.526022	0.301837		H	-0.598518	5.740702	-2.286989
H	-0.330079	2.143672	1.521561			Ac-(Ala)4-Tyr-(Ala)4-NHMe_C7eq		
C	1.028900	0.204675	0.217833		C	-14.405369	-1.735710	-0.177375
O	1.667312	0.569173	1.211589		H	-14.765801	-1.932250	0.836729
N	1.405408	-0.831008	-0.569298		H	-14.203724	-2.686733	-0.678449
H	0.745086	-1.118278	-1.293501		H	-15.196114	-1.231272	-0.742020
C	2.460037	-1.774207	-0.179878		C	-13.154028	-0.879409	-0.225048
H	2.437244	-1.847009	0.915388		O	-12.577870	-0.632579	-1.287747
C	2.196150	-3.140203	-0.805964		N	-12.711033	-0.390350	0.965740
H	1.206906	-3.504853	-0.512300		H	-13.182134	-0.656933	1.819284
H	2.249179	-3.084518	-1.896939		C	-11.593304	0.554418	1.072852
H	2.950801	-3.859186	-0.477904		H	-11.645887	1.190872	0.181962
C	3.860686	-1.243785	-0.568827		C	-11.733348	1.397298	2.336040
O	4.562174	-1.808875	-1.414942		H	-12.691952	1.925470	2.334760
N	4.253994	-0.140615	0.108365		H	-11.659882	0.774133	3.232835
H	3.580312	0.277684	0.751660		H	-10.927634	2.133407	2.389936
C	5.470775	0.603948	-0.234183		C	-10.234130	-0.186159	1.037201
H	5.594737	0.526541	-1.321817		O	-9.493645	-0.241220	2.024934
C	5.327830	2.065126	0.178041		N	-9.933918	-0.748222	-0.155884
H	4.446003	2.508283	-0.294079		H	-10.644121	-0.692542	-0.888003
H	5.238567	2.153245	1.265033		C	-8.796475	-1.656887	-0.341675
H	6.215101	2.628347	-0.122395		H	-8.673928	-2.211124	0.597867
C	6.721816	-0.038500	0.414939		C	-9.078813	-2.619389	-1.490893
O	7.382594	0.544147	1.281268		H	-9.995839	-3.183337	-1.294228
N	7.031539	-1.267992	-0.057391		H	-9.185805	-2.078059	-2.435293
H	6.397257	-1.678183	-0.744811		H	-8.249982	-3.321431	-1.608610
C	8.069486	-2.108977	0.547252		C	-7.483570	-0.871124	-0.578514
H	8.074606	-1.882671	1.621006		O	-6.864034	-0.938084	-1.645375
C	7.749313	-3.582932	0.319445		N	-7.069142	-0.133541	0.477765
H	6.763745	-3.822926	0.730714		H	-7.668764	-0.119095	1.304351
H	7.762636	-3.823736	-0.747493		C	-5.950609	0.811209	0.392672
H	8.499012	-4.212045	0.805651		H	-5.958975	1.222801	-0.624623
C	9.472577	-1.749094	-0.001103		C	-6.126676	1.928379	1.416335
O	10.128523	-2.539505	-0.688377		H	-7.079447	2.441723	1.253480
N	9.910431	-0.518710	0.349236		H	-6.100884	1.531324	2.435238

O	2.659377	0.523425	-1.526179		H	9.275913	0.066173	0.894054
N	4.104733	-1.142686	-0.973466		C	11.139767	0.074487	-0.190254
H	5.068797	-1.426847	-0.807552		H	11.247497	-0.303245	-1.214376
C	3.034026	-2.068373	-0.607527		C	11.027829	1.595295	-0.194335
H	2.359915	-2.178436	-1.462043		H	10.150504	1.911567	-0.767970
C	3.613456	-3.436447	-0.231971		H	10.951110	1.979630	0.826859
H	4.166183	-3.864790	-1.073958		H	11.922297	2.036982	-0.640814
H	4.295057	-3.358036	0.620878		C	12.383360	-0.388775	0.615666
H	2.796512	-4.113231	0.031203		O	13.026926	0.381379	1.321440
C	2.139092	-1.531162	0.527440		N	12.682955	-1.703864	0.439491
O	0.956099	-1.874486	0.576388		H	12.020107	-2.260436	-0.096972
N	2.714098	-0.726097	1.454049		C	13.756497	-2.358271	1.162241
H	3.667652	-0.396106	1.328340		H	13.370916	-3.050659	1.922395
C	1.917048	-0.159117	2.539844		H	14.400163	-2.919679	0.475278
H	1.343878	-0.966915	3.002153		H	14.345836	-1.584896	1.657351
C	2.825503	0.497233	3.584989		C	0.392802	3.339584	-0.117212
H	3.493772	-0.245898	4.032778		C	1.558841	3.744198	0.541455
H	3.436042	1.288780	3.138217		C	0.063792	3.980120	-1.321931
H	2.209862	0.933220	4.376257		C	2.369235	4.754343	0.020983
C	0.847050	0.838937	2.047757		H	1.841163	3.255453	1.468705
O	-0.202431	0.975185	2.665681		C	0.863683	4.984696	-1.857565
N	1.167739	1.580650	0.946103		H	-0.842757	3.692066	-1.850952
H	1.958319	1.295295	0.378486		C	2.024463	5.377120	-1.182378
C	0.169714	2.450487	0.331129		H	3.267372	5.060793	0.554876
H	-0.362291	2.970623	1.129275		H	0.602877	5.479166	-2.788009
C	0.874069	3.467705	-0.584286		O	2.775021	6.373479	-1.743856
H	1.676402	3.948726	-0.016720		H	3.543806	6.544914	-1.177960
H	1.326295	2.956955	-1.440110		Ac-(Ala)$_4$-Cys-(Ala)$_4$-NHMe_αR			
C	-0.913229	1.655335	-0.430676		C	9.040906	-2.782551	-1.055468
O	-2.094233	2.009401	-0.403449		H	9.943468	-2.247328	-1.364881
N	-0.496816	0.573518	-1.134446		H	8.590080	-3.268444	-1.924149
H	0.487133	0.327508	-1.159589		H	9.327353	-3.571684	-0.351069
C	-1.454041	-0.260566	-1.856577		C	8.008097	-1.891511	-0.395055
H	-2.040764	0.371168	-2.530488		O	6.840731	-2.246372	-0.236168
C	-0.719553	-1.341872	-2.655741		N	8.439541	-0.656094	0.014883
H	-0.028491	-0.888040	-3.374640		H	9.432980	-0.464915	-0.019392
H	-0.155520	-1.998997	-1.984624		C	7.636649	0.157623	0.932408
H	-1.446586	-1.945654	-3.205555		H	7.351165	-0.450252	1.798427
C	-2.501904	-0.901056	-0.924053		C	8.439339	1.375183	1.404352
O	-3.640769	-1.125035	-1.336698		H	9.338170	1.060828	1.946236
N	-2.097256	-1.198728	0.333723		H	8.738756	2.005871	0.559699
H	-1.114757	-1.113738	0.575476		H	7.825635	1.974427	2.081238
C	-2.998212	-1.824806	1.295669		C	6.297903	0.606527	0.327313
H	-3.403581	-2.747823	0.866857		O	5.352208	0.885254	1.064610
C	-2.237770	-2.140713	2.588954		N	6.226059	0.697760	-1.022930
H	-1.420683	-2.842698	2.389616		H	7.027666	0.411998	-1.569198
H	-1.814674	-1.227656	3.021958		C	4.986445	1.062319	-1.698505
H	-2.923232	-2.592698	3.310557		H	4.655088	2.034746	-1.320772
C	-4.244058	-0.972565	1.608473		C	5.206976	1.150972	-3.212041
O	-5.263314	-1.528662	2.026417		H	5.956800	1.912931	-3.449123
N	-4.143691	0.365869	1.435753		H	5.537243	0.188760	-3.620947
H	-3.303077	0.760655	1.025430		H	4.269209	1.425945	-3.700418
C	-5.272067	1.256829	1.683625		C	3.818167	0.109659	-1.382051

H	8.161276	-0.975421	-0.951200		H	-5.747829	0.932246	2.614836
C	7.124129	0.553680	0.021790		C	-4.789991	2.702726	1.832574
H	7.126377	0.701780	1.108609		H	-4.134126	2.800929	2.703939
C	7.049618	1.931129	-0.663561		H	-4.233441	3.024702	0.945866
H	7.930275	2.515517	-0.385772		H	-5.657960	3.353147	1.961830
H	7.025848	1.816633	-1.752305		C	-6.408307	1.165432	0.637176
H	6.155369	2.481516	-0.351376		O	-7.457885	1.767234	0.849114
C	5.937296	-0.342939	-0.376114		N	-6.178648	0.392549	-0.456554
O	6.090838	-1.313986	-1.120015		H	-5.271389	-0.045336	-0.590306
N	4.739748	0.022577	0.128983		C	-7.215150	0.084495	-1.430572
H	4.623830	0.857025	0.696539		H	-8.036477	0.779178	-1.227268
C	3.495822	-0.639313	-0.226462		C	-6.709516	0.283573	-2.863766
H	3.495722	-0.826670	-1.307372		H	-6.475091	1.338358	-3.040424
C	3.323305	-1.982930	0.506943		H	-5.801670	-0.305873	-3.036779
H	4.163894	-2.634982	0.257656		H	-7.477805	-0.043229	-3.567919
H	3.300075	-1.828044	1.590631		C	-7.810580	-1.334637	-1.264139
H	2.395958	-2.481932	0.206047		O	-8.587534	-1.781972	-2.107307
C	2.368460	0.347884	0.124869		N	-7.446924	-2.022286	-0.155285
O	2.583100	1.347178	0.815324		H	-6.810324	-1.614894	0.520653
N	1.147042	0.032900	-0.357242		C	-7.978591	-3.344249	0.112941
H	0.967859	-0.814682	-0.889796		H	-7.965738	-3.944713	-0.801445
C	-0.050519	0.780430	-0.013978		H	-7.357933	-3.820022	0.876094
H	-0.023980	1.025536	1.053468		H	-9.015599	-3.302472	0.471636
C	-0.104463	2.102182	-0.822138		S	-0.195332	4.852823	-1.154244
H	0.886893	2.556533	-0.800712		H	-1.283761	4.109148	-1.446046
H	-0.365026	1.898106	-1.864773		Ac-(Ala)₄-Cys-(Ala)₄-NHMe_C5			
C	-1.232777	-0.165883	-0.322021		C	17.839674	-1.147551	-0.024355
O	-1.054356	-1.168471	-1.021147		H	17.558088	-1.839056	-0.824505
N	-2.423605	0.167308	0.208086		H	18.226888	-1.721151	0.823676
H	-2.562722	1.041766	0.710667		H	18.650745	-0.503897	-0.378925
C	-3.631829	-0.604939	-0.047145		C	16.692502	-0.271223	0.459249
H	-3.673169	-0.849201	-1.115403		O	16.842660	0.564264	1.347237
C	-3.658209	-1.915239	0.762458		N	15.498618	-0.473387	-0.162399
H	-2.785923	-2.518988	0.500792		H	15.355750	-1.220249	-0.832890
H	-3.637413	-1.699439	1.835658		C	14.291204	0.224112	0.235368
H	-4.561397	-2.493489	0.540239		H	14.264300	0.274931	1.331246
C	-4.816598	0.300351	0.331839		C	14.243230	1.661895	-0.318016
O	-4.663483	1.278383	1.064058		H	15.119315	2.206154	0.042972
N	-6.013006	-0.075595	-0.169998		H	14.254156	1.651689	-1.413119
H	-6.128165	-0.915070	-0.730638		H	13.343004	2.189066	0.017140
C	-7.259237	0.582129	0.184909		C	13.106529	-0.615771	-0.271525
H	-7.255248	0.779447	1.264007		O	13.260370	-1.515202	-1.100751
C	-7.441582	1.917928	-0.560166		N	11.900527	-0.284993	0.242287
H	-6.603662	2.577142	-0.320751		H	11.781428	0.495487	0.881053
H	-7.468343	1.752371	-1.642230		C	10.659159	-0.893401	-0.202395
H	-8.370884	2.414328	-0.260548		H	10.686739	-0.985403	-1.295218
C	-8.382130	-0.415763	-0.153798		C	10.451471	-2.294228	0.404296
O	-8.164256	-1.411413	-0.847726		H	11.293352	-2.931525	0.122999
N	-9.599282	-0.109868	0.343246		H	10.398204	-2.233972	1.496344
H	-9.771283	0.743007	0.867782		H	9.528422	-2.753947	0.034716
C	-10.796296	-0.872276	0.030071		C	9.532342	0.072677	0.206622
H	-10.782727	-1.120088	-1.038378		O	9.734786	0.993681	1.000665
C	-10.878724	-2.180224	0.839408		N	8.325548	-0.175739	-0.346666

H	-5.801137	1.229661	-1.166316	H	-9.997057	-2.788543	0.623490
C	-5.991908	2.544682	0.544126	H	-10.910519	-1.965210	1.912580
H	-6.945608	2.973503	0.221396	H	-11.771432	-2.756157	0.572551
H	-5.971537	2.491835	1.636381	C	-11.986573	0.056859	0.330386
H	-5.183198	3.210743	0.233244	O	-11.840406	1.093840	0.981179
C	-4.453362	0.536839	0.351873	N	-13.180249	-0.354650	-0.147662
O	-3.748114	1.035894	1.236317	H	-13.294683	-1.236006	-0.639680
N	-4.110695	-0.578089	-0.334591	C	-14.423710	0.341071	0.135044
H	-4.795691	-0.940159	-1.001035	H	-14.420265	0.641398	1.190400
C	-2.982466	-1.433070	0.050639	C	-14.591922	1.599698	-0.737448
H	-2.916469	-1.403802	1.146241	H	-13.752361	2.275199	-0.556120
C	-3.222303	-2.862227	-0.425911	H	-14.611871	1.329725	-1.798194
H	-4.161383	-3.244109	-0.013602	H	-15.520310	2.129764	-0.497030
H	-3.265102	-2.906752	-1.517936	C	-15.552070	-0.676906	-0.116000
H	-2.404525	-3.511244	-0.103652	O	-15.340985	-1.717358	-0.735662
C	-1.644448	-0.878470	-0.496393	N	-16.767829	-0.322623	0.371732
O	-0.968127	-1.492426	-1.327291	H	-16.846146	0.542286	0.888083
N	-1.273975	0.313309	0.031136	C	-17.962257	-1.133019	0.190250
H	-1.923945	0.753637	0.686800	H	-18.380264	-1.434976	1.156901
C	-0.138414	1.082414	-0.489060	H	-18.726557	-0.586226	-0.373394
H	-0.081453	0.899223	-1.567999	H	-17.673262	-2.023570	-0.368529
C	-0.377802	2.571686	-0.228226	S	-1.328585	3.335179	-0.216157
H	-1.371848	2.840511	-0.595982	H	-0.595554	3.767278	0.832973
H	-0.338259	2.783664	0.842752	Ac-(Ala)₄-Cys-(Ala)₄-NHMe_C7$_{eq}$			
C	1.184922	0.591717	0.145749	C	-14.273214	-1.400413	0.047508
O	1.837132	1.289047	0.933656	H	-14.661788	-1.225580	1.055136
N	1.553522	-0.652035	-0.230075	H	-14.075990	-2.468394	-0.082075
H	0.909691	-1.163350	-0.836873	H	-15.040842	-1.120382	-0.681071
C	2.655470	-1.381531	0.407162	C	-13.006675	-0.624637	-0.261195
H	2.680863	-1.065972	1.457945	O	-12.403997	-0.766195	-1.328487
C	2.412695	-2.884553	0.311934	N	-12.580578	0.242571	0.697868
H	1.454327	-3.142095	0.773397	H	-13.074380	0.292781	1.578338
H	2.410127	-3.212715	-0.731385	C	-11.450363	1.157024	0.499613
H	3.209886	-3.428933	0.823889	H	-11.477526	1.450873	-0.556066
C	4.017265	-0.994329	-0.218878	C	-11.599787	2.381980	1.395597
O	4.701228	-1.805872	-0.850760	H	-12.549529	2.886732	1.192610
N	4.393704	0.286688	0.000961	H	-11.552841	2.101595	2.452536
H	3.741998	0.886412	0.507810	H	-10.783745	3.085471	1.213472
C	5.557562	0.893273	-0.654457	C	-10.102075	0.437930	0.749759
H	5.638810	0.430317	-1.645908	O	-9.385240	0.712940	1.718116
C	5.358989	2.399419	-0.790568	N	-9.782842	-0.493142	-0.177812
H	4.446058	2.608987	-1.357154	H	-10.479392	-0.687601	-0.899362
H	5.294237	2.874282	0.193015	C	-8.649312	-1.412178	-0.021722
H	6.208232	2.847286	-1.312288	H	-8.553391	-1.622262	1.051329
C	6.862207	0.564843	0.112217	C	-8.912309	-2.701983	-0.792650
O	7.526969	1.437114	0.680075	H	-9.840409	-3.166092	-0.445130
N	7.209752	-0.743037	0.090362	H	-8.988817	-2.505459	-1.865846
H	6.571439	-1.390042	-0.374768	H	-8.089000	-3.405321	-0.646420
C	8.308903	-1.282679	0.897118	C	-7.326760	-0.747175	-0.474725
H	8.346585	-0.688056	1.818490	O	-6.692059	-1.150573	-1.454817
C	8.048693	-2.749456	1.225417	N	-6.923572	0.288240	0.298621
H	7.092793	-2.855557	1.748033	H	-7.541701	0.572498	1.060491
H	8.030744	-3.354994	0.314678	C	-5.804708	1.161365	-0.071016

H	4.197664	-3.218907	-2.404541
H	4.380874	-3.429361	-0.653216
H	2.858006	-3.891032	-1.447818
C	2.231355	-1.727597	0.050511
O	1.064578	-2.120586	-0.005470
N	2.813757	-1.295374	1.195472
H	3.758105	-0.918932	1.182372
C	2.038575	-1.194273	2.429844
H	1.492109	-2.130694	2.568447
C	2.965820	-0.952860	3.625728
H	3.656877	-1.793013	3.751574
H	3.553438	-0.038282	3.493548
H	2.365567	-0.855895	4.534295
C	0.936664	-0.113603	2.370084
O	-0.087677	-0.246222	3.030786
N	1.200933	0.987793	1.607566
H	1.980296	0.956790	0.959267
C	0.162625	1.982724	1.359872
H	-0.400780	2.097029	2.288563
C	0.805910	3.332218	0.983340
H	1.421292	3.638663	1.838821
H	1.489816	3.190753	0.136660
C	-0.889365	1.490601	0.344069
O	-2.088501	1.725899	0.525480
N	-0.443648	0.760609	-0.705513
H	0.553444	0.668111	-0.870112
C	-1.375953	0.259654	-1.710185
H	-1.965828	1.093554	-2.103777
C	-0.614330	-0.426312	-2.848811
H	0.079867	0.274945	-3.325063
H	-0.051463	-1.286940	-2.470937
H	-1.324160	-0.778001	-3.602550
C	-2.414269	-0.704893	-1.105253
O	-3.551364	-0.771289	-1.575778
N	-1.997467	-1.461336	-0.062096
H	-1.016802	-1.445054	0.201574
C	-2.879096	-2.421277	0.591123
H	-3.268371	-3.124853	-0.153065
C	-2.102704	-3.181924	1.672798
H	-1.271029	-3.737408	1.226173
H	-1.696761	-2.487730	2.417162
H	-2.772550	-3.887041	2.171712
C	-4.139319	-1.777801	1.202008
O	-5.143942	-2.473082	1.379084
N	-4.066968	-0.472091	1.550550
H	-3.244379	0.073082	1.307464
C	-5.211695	0.228815	2.120397
H	-5.685106	-0.450592	2.836845
C	-4.759434	1.499458	2.845299
H	-4.111020	1.247940	3.691067
H	-4.202433	2.158465	2.170642
H	-5.640777	2.029951	3.212777
C	-6.342991	0.545117	1.112694

H	8.845789	-3.141133	1.862254
C	9.668842	-1.102158	0.178694
O	10.322718	-2.066534	-0.233196
N	10.072290	0.182817	0.059342
H	9.438130	0.905904	0.399929
C	11.246389	0.580825	-0.727184
H	11.317012	-0.124335	-1.564403
C	11.069687	2.004140	-1.245098
H	10.152199	2.083711	-1.837254
H	11.027825	2.715169	-0.414940
H	11.921215	2.284993	-1.869888
C	12.549413	0.451053	0.107471
O	13.199492	1.430927	0.457462
N	12.891206	-0.836835	0.380571
H	12.224884	-1.558543	0.112267
C	14.030935	-1.177635	1.210039
H	13.719491	-1.563083	2.190031
H	14.653229	-1.935422	0.720322
H	14.618329	-0.270345	1.359413
S	0.787270	3.689379	-1.103317
H	1.841219	3.433725	-0.302045

Ac-(Ala)4-Met-(Ala)4-NHMe_αR

C	9.080185	-2.205357	-2.154521
H	9.983272	-1.593496	-2.237623
H	8.600138	-2.280032	-3.133362
H	9.370562	-3.218569	-1.854763
C	8.078206	-1.668971	-1.151670
O	6.914542	-2.065975	-1.111196
N	8.533825	-0.704496	-0.289610
H	9.527007	-0.509747	-0.277542
C	7.769603	-0.337917	0.906076
H	7.501912	-1.247268	1.455940
C	8.602454	0.578675	1.809362
H	9.511682	0.068986	2.146887
H	8.886801	1.499458	1.287601
H	8.015768	0.849080	2.690558
C	6.418870	0.320100	0.584338
O	5.506108	0.280223	1.409157
N	6.301898	0.945048	-0.612581
H	7.079647	0.900292	-1.257407
C	5.046238	1.550504	-1.040824
H	4.736491	2.281050	-0.286848
C	5.222272	2.254973	-2.389922
H	5.972268	3.049344	-2.315703
H	5.530687	1.547815	-3.169110
H	4.272551	2.702518	-2.691842
C	3.877065	0.549550	-1.108031
O	2.719545	0.987881	-1.062482
N	4.163075	-0.762745	-1.223671
H	5.128815	-1.086202	-1.207251
C	3.095530	-1.761361	-1.226576
H	2.399183	-1.523884	-2.036157
C	3.673612	-3.163582	-1.445286

H	-8.242419	-0.800204	1.126172	O	-7.395145	1.020730	1.532582
C	-7.122737	0.193107	-0.329266	N	-6.108994	0.240730	-0.190591
H	-7.064044	-0.119262	-1.379046	H	-5.197505	-0.106022	-0.477702
C	-7.053752	1.730747	-0.267072	C	-7.146815	0.302388	-1.208919
H	-7.903001	2.148159	-0.813579	H	-7.982109	0.845718	-0.755429
H	-7.094290	2.073862	0.771970	C	-6.660635	1.045760	-2.457941
H	-6.130393	2.105178	-0.722016	H	-6.458823	2.095363	-2.220103
C	-5.978986	-0.458853	0.469575	H	-5.737490	0.594189	-2.839231
O	-6.194679	-1.042865	1.533900	H	-7.425794	0.987537	-3.235125
N	-4.747927	-0.327089	-0.068275	C	-7.706076	-1.088623	-1.595970
H	-4.581603	0.212473	-0.913014	O	-8.475615	-1.201719	-2.549808
C	-3.538738	-0.768347	0.606516	N	-7.320267	-2.135528	-0.828272
H	-3.621627	-0.515130	1.670622	H	-6.690127	-1.999725	-0.045406
C	-3.324632	-2.287788	0.475949	C	-7.810628	-3.475294	-1.086877
H	-4.187949	-2.807207	0.899293	H	-7.806019	-3.671503	-2.162911
H	-3.218353	-2.570663	-0.576480	H	-7.157715	-4.188449	-0.577813
H	-2.427112	-2.608586	1.015643	H	-8.838462	-3.612200	-0.725122
C	-2.381747	0.027060	-0.026151	C	-0.210697	4.444076	0.665755
O	-2.536283	0.653002	-1.076781	H	-1.141920	4.279729	1.215886
N	-1.205202	-0.032976	0.633635	H	0.192073	5.414438	0.970467
H	-1.093332	-0.552956	1.498203	S	-0.626303	4.524018	-1.132386
C	0.007659	0.609478	0.150348	C	-2.442637	4.729436	-1.065342
H	0.040204	0.505990	-0.940134	H	-2.791107	4.771229	-2.100957
C	0.014697	2.119475	0.515590	H	-2.897590	3.870511	-0.565952
H	-0.959273	2.520719	0.220503	H	-2.722520	5.660425	-0.564306
H	0.091515	2.207608	1.605859	Ac-(Ala)₄-Met-(Ala)₄-NHMe_C5			
C	1.171736	-0.149851	0.808907	C	-17.883940	-1.098701	-0.009601
O	1.020928	-0.700459	1.901921	H	-17.640703	-1.411073	1.010666
N	2.338845	-0.152368	0.130875	H	-18.292253	-1.953565	-0.557742
H	2.460743	0.364471	-0.735457	H	-18.665865	-0.333806	0.029182
C	3.572214	-0.691806	0.680612	C	-16.693030	-0.545495	-0.780226
H	3.616583	-0.436615	1.746326	O	-16.794835	-0.153046	-1.939867
C	3.646628	-2.222835	0.536750	N	-15.517873	-0.509715	-0.094493
H	2.793791	-2.671322	1.052516	H	-15.416907	-0.914864	0.829364
H	3.616961	-2.512332	-0.518862	C	-14.275258	-0.084382	-0.708921
H	4.565914	-2.619980	0.980346	H	-14.229980	-0.498573	-1.724193
C	4.717549	0.019248	-0.066681	C	-14.171838	1.450241	-0.806172
O	4.492622	0.720005	-1.056801	H	-15.017052	1.822619	-1.390102
N	5.954100	-0.187314	0.430125	H	-14.200180	1.900593	0.191772
H	6.129689	-0.821749	1.204405	H	-13.243898	1.757557	-1.301159
C	7.157773	0.317190	-0.210560	C	-13.136248	-0.675285	0.139585
H	7.057474	0.183396	-1.294490	O	-13.343478	-1.149652	1.258642
C	7.387617	1.811248	0.083882	N	-11.907460	-0.619906	-0.421503
H	6.525568	2.382490	-0.269518	H	-11.742942	-0.171650	-1.317791
H	7.509208	1.975864	1.159583	C	-10.700901	-1.019446	0.281438
H	8.281903	2.182459	-0.428053	H	-10.768743	-0.667499	1.318065
C	8.316457	-0.552715	0.312481	C	-10.517339	-2.548999	0.292382
O	8.165686	-1.300308	1.281425	H	-11.385941	-3.008139	0.770959
N	9.484208	-0.421281	-0.350292	H	-10.429521	-2.931175	-0.730026
H	9.605945	0.246481	-1.106445	H	-9.619769	-2.836836	0.850627
C	10.711208	-1.079371	0.067416	C	-9.531515	-0.314657	-0.429866
H	10.790655	-1.009960	1.159262	O	-9.675127	0.199458	-1.541139
C	10.737806	-2.565250	-0.336859	N	-8.357790	-0.321281	0.237759

H	8.120957	-3.417800	1.095185		H	9.885037	-3.074617	0.118623
C	7.402259	-0.813262	0.475760		H	10.675032	-2.667341	-1.425215
O	6.784653	-1.018922	1.525729		H	11.656243	-3.053251	0.006468
N	6.997428	0.071290	-0.465380		C	11.861576	-0.289986	-0.584742
H	7.603231	0.200099	-1.277432		O	11.645705	0.538208	-1.472354
C	5.900499	1.018626	-0.240311		N	13.098961	-0.582271	-0.131005
H	5.922903	1.284255	0.824301		H	13.268019	-1.308834	0.558550
C	6.098442	2.262570	-1.100847		C	14.303419	-0.016708	-0.714087
H	7.066045	2.723581	-0.879522		H	14.178048	0.012672	-1.803558
H	6.054151	2.011154	-2.164397		C	14.572766	1.412975	-0.207355
H	5.307583	2.990422	-0.903536		H	13.718039	2.047326	-0.454996
C	4.528080	0.357791	-0.516904		H	14.716211	1.413335	0.877942
O	3.804693	0.718127	-1.452443		H	15.467011	1.839330	-0.675400
N	4.191511	-0.621610	0.353834		C	15.451484	-0.974216	-0.343028
H	4.884957	-0.874028	1.060493		O	15.313762	-1.815061	0.543056
C	3.025934	-1.491697	0.160752		N	16.600959	-0.794910	-1.041449
H	2.912510	-1.639121	-0.920887		H	16.616838	-0.095846	-1.770774
C	3.251201	-2.830243	0.856402		C	17.806886	-1.571190	-0.797208
H	4.161768	-3.303957	0.476676		H	18.093954	-2.140083	-1.688522
H	3.338843	-2.696388	1.938339		H	18.639375	-0.921099	-0.505812
H	2.404713	-3.497602	0.676472		H	17.591511	-2.265001	0.015798
C	1.732810	-0.807054	0.667444		C	1.111970	2.934851	-0.176957
O	1.112006	-1.219337	1.652316		H	2.116909	2.572876	0.065017
N	1.346348	0.263046	-0.066272		H	0.999403	2.868615	-1.265658
H	1.961403	0.550486	-0.829292		S	1.042660	4.734818	0.182584
C	0.253010	1.149097	0.350153		C	1.669440	4.765474	1.899216
H	0.249596	1.156520	1.446748		H	1.724444	5.817271	2.192372
C	0.477638	2.568613	-0.199024		H	1.000220	4.247146	2.591524
H	1.547507	2.698385	-0.401720		H	2.672664	4.331885	1.960050
H	-0.052720	2.667436	-1.151180		Ac-(Ala)₄-Met-(Ala)₄-NHMe_C7eq		

C	-1.097690	0.547649	-0.118276		C	14.317334	-1.704173	-0.057295
O	-1.737392	1.014032	-1.066279		H	14.704465	-1.692127	-1.080465
N	-1.486355	-0.545206	0.578478		H	14.087354	-2.735014	0.227716
H	-0.827499	-0.908446	1.268059		H	15.097801	-1.345611	0.621223
C	-2.563985	-1.428834	0.118947		C	13.078109	-0.851179	0.137398
H	-2.536454	-1.426208	-0.978589		O	12.500017	-0.787634	1.225571
C	-2.336851	-2.841452	0.648917		N	12.646485	-0.154881	-0.949997
H	-1.351988	-3.206343	0.340768		H	13.115438	-0.275632	-1.837120
H	-2.402530	-2.861005	1.740361		C	11.536398	0.802416	-0.892706
H	-3.102326	-3.518949	0.262518		H	11.591982	1.274185	0.095062
C	-3.956788	-0.896970	0.537069		C	11.685350	1.850635	-1.990433
O	-4.655400	-1.487050	1.369171		H	12.646953	2.364583	-1.895187
N	-4.349807	0.225710	-0.106018		H	11.611504	1.392671	-2.981788
H	-3.663159	0.679848	-0.710291		H	10.884097	2.590060	-1.917956
C	-5.570161	0.958349	0.253279		C	10.171441	0.077629	-0.987591
H	-5.693776	0.860852	1.339507		O	9.439900	0.189777	-1.977181
C	-5.435469	2.426827	-0.135206		N	9.855689	-0.667318	0.096487
H	-4.556816	2.866711	0.345178		H	10.563511	-0.745066	0.828891
H	-5.341643	2.534212	-1.219730		C	8.703476	-1.575724	0.125172
H	-6.326900	2.980092	0.171162		H	8.582305	-1.969846	-0.892069
C	-6.817145	0.319347	-0.407825		C	8.957377	-2.714764	1.107579
O	-7.478201	0.909559	-1.268654		H	9.873064	-3.249890	0.837621
N	-7.125068	-0.917446	0.047874		H	9.050501	-2.334884	2.128929

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H	4.198959	1.402318	-1.237754		H	-6.486074	-1.337262	0.725216
C	5.193269	0.789408	-3.053113		C	-8.152332	-1.756064	-0.577560
H	5.925388	1.603863	-3.035155		H	-8.149189	-1.516176	-1.648474
H	5.660748	-0.099837	-3.491953		C	-7.825956	-3.231100	-0.365751
H	4.361869	1.090194	-3.695168		H	-6.834278	-3.459639	-0.768816
C	3.533155	-0.541290	-1.693432		H	-7.849604	-3.486048	0.697692
O	2.384793	-0.159106	-1.926672		H	-8.566275	-3.858219	-0.868693
N	3.861211	-1.844905	-1.529774		C	-9.562748	-1.411828	-0.038358
H	4.796804	-2.106391	-1.227731		O	-10.220658	-2.215200	0.632298
C	2.821163	-2.873362	-1.541300		N	-10.005101	-0.180117	-0.377716
H	2.180281	-2.695057	-2.407958		H	-9.366976	0.416207	-0.906165
C	3.448194	-4.268614	-1.635467		C	-11.242974	0.398816	0.157669
H	4.005999	-4.373187	-2.571899		H	-11.357615	0.008080	1.176224
H	4.132350	-4.455060	-0.801400		C	-11.140750	1.920137	0.180912
H	2.658401	-5.024547	-1.617083		H	-10.271274	2.235067	0.767040
C	1.871488	-2.777470	-0.328073		H	-11.055635	2.317277	-0.834694
O	0.682952	-3.072437	-0.451956		H	-12.042557	2.350925	0.623282
N	2.429632	-2.414590	0.855447		C	-12.476735	-0.062783	-0.664191
H	3.369055	-2.034686	0.859770		O	-13.121800	0.711919	-1.363612
C	1.606445	-2.211364	2.045751		N	-12.766996	-1.382680	-0.508710
H	0.936465	-3.068778	2.140963		H	-12.103494	-1.941220	0.025079
C	2.489576	-2.096042	3.292410		C	-13.829284	-2.035436	-1.249148
H	3.055664	-3.021118	3.445747		H	-13.432015	-2.715350	-2.014563
H	3.195172	-1.263101	3.200433		H	-14.475093	-2.610201	-0.575278
H	1.862604	-1.924482	4.172025		H	-14.419768	-1.259985	-1.739668
C	0.664152	-0.996205	1.908793		C	0.064959	3.688836	0.762050
O	-0.483236	-1.040126	2.344438		H	0.332486	4.657972	0.326045
N	1.180337	0.101490	1.295272		H	0.607600	3.585705	1.710399
H	2.143663	0.098417	0.979950		S	-1.736725	3.682336	1.131919
C	0.348077	1.269965	1.014884		C	-1.751265	4.921114	2.473593
H	-0.124597	1.602017	1.943572		H	-2.788033	5.024218	2.804343
C	1.246895	2.386054	0.447648		H	-1.142004	4.595530	3.322824
H	2.122702	2.454351	1.110244		H	-1.398506	5.895067	2.120064
H	1.633442	2.056803	-0.528717		Ac-(Ala)₄-Trp-(Ala)₄-NHMe_αR			
C	-0.828063	0.893851	0.082421		C	8.708696	-3.262490	-0.565922
O	-1.981059	1.254066	0.331937		H	9.633140	-2.678864	-0.602918
N	-0.525382	0.148449	-1.007726		H	8.471822	-3.631204	-1.567177
H	0.439975	-0.091290	-1.215808		H	8.871415	-4.137214	0.073502
C	-1.566714	-0.237967	-1.956886		C	7.523403	-2.484121	-0.032173
H	-2.088700	0.659344	-2.303857		O	6.366985	-2.893103	-0.135332
C	-0.947064	-0.980038	-3.146364		N	7.798999	-1.283701	0.570067
H	-0.210165	-0.348452	-3.653591		H	8.766934	-1.054735	0.758006
H	-0.452489	-1.898738	-2.812928		C	6.782445	-0.597822	1.372119
H	-1.732294	-1.244638	-3.860113		H	6.376554	-1.292810	2.115696
C	-2.670647	-1.096072	-1.308389		C	7.394505	0.614334	2.083731
O	-3.844597	-0.971893	-1.663402		H	8.193154	0.300781	2.765130
N	-2.276656	-1.993483	-0.373740		H	7.805073	1.332325	1.365103
H	-1.289111	-2.115681	-0.172227		H	6.624681	1.118729	2.672942
C	-3.236271	-2.883022	0.271554		C	5.562638	-0.167665	0.544254
H	-3.785116	-3.440325	-0.495205		O	4.460025	-0.060676	1.087411
C	-2.505010	-3.856691	1.202660		N	5.765928	0.108505	-0.763697
H	-1.789762	-4.463972	0.637739		H	6.690263	-0.035892	-1.148274
H	-1.961444	-3.307336	1.978581		C	4.668444	0.501120	-1.643187

C	-14.589486	-0.111297	-0.726567
H	-14.547446	-0.535029	-1.738055
C	-14.473769	1.421477	-0.837753
H	-15.315943	1.795251	-1.425168
H	-14.498589	1.881122	0.156044
H	-13.543335	1.716856	-1.335336
C	-13.455327	-0.703893	0.127335
O	-13.666928	-1.168807	1.249526
N	-12.225709	-0.661103	-0.432957
H	-12.057172	-0.220480	-1.332278
C	-11.022687	-1.065012	0.273593
H	-11.088138	-0.704713	1.307502
C	-10.851304	-2.595845	0.296260
H	-11.723538	-3.044405	0.778236
H	-10.766399	-2.986539	-0.723171
H	-9.956111	-2.886509	0.856822
C	-9.847332	-0.374913	-0.442285
O	-9.986500	0.132984	-1.557086
N	-8.674016	-0.386966	0.225751
H	-8.562610	-0.861616	1.117073
C	-7.433717	0.110918	-0.344426
H	-7.376773	-0.210820	-1.391475
C	-7.350503	1.648261	-0.295058
H	-8.195375	2.069094	-0.845752
H	-7.388580	2.000383	0.741058
H	-6.423084	2.009843	-0.752205
C	-6.297012	-0.545208	0.461579
O	-6.520860	-1.119382	1.529625
N	-5.064071	-0.427924	-0.074420
H	-4.890777	0.103257	-0.923105
C	-3.859220	-0.875543	0.604270
H	-3.941802	-0.615948	1.666889
C	-3.657502	-2.397237	0.482210
H	-4.525349	-2.907796	0.907198
H	-3.551850	-2.686551	-0.568526
H	-2.762923	-2.721501	1.024447
C	-2.694800	-0.092310	-0.031244
O	-2.845513	0.529019	-1.086172
N	-1.519342	-0.163349	0.627357
H	-1.427437	-0.643738	1.516872
C	-0.303455	0.488775	0.163523
H	-0.246805	0.386270	-0.924282
C	-0.318862	2.005798	0.523105
H	-1.220826	2.417440	0.058862
H	-0.447466	2.085863	1.609169
C	0.856850	-0.242635	0.851232
O	0.717176	-0.684996	1.996078
N	1.994789	-0.347294	0.138357
H	2.103220	0.119598	-0.758351
C	3.239146	-0.838560	0.708452
H	3.364574	-0.398928	1.705751
C	3.251083	-2.373183	0.830489
H	2.417782	-2.688780	1.462892

H	-3.233781	-4.518284	1.678736
C	-4.330710	-2.129384	1.052151
O	-5.431909	-2.660515	1.222825
N	-4.004683	-0.914268	1.549115
H	-3.099895	-0.509586	1.330660
C	-4.960208	-0.106706	2.296581
H	-5.498544	-0.778673	2.973453
C	-4.230846	0.965209	3.111151
H	-3.570747	0.501149	3.851335
H	-3.622418	1.600136	2.458088
H	-4.969380	1.585545	3.623963
C	-6.081795	0.526847	1.438971
O	-6.999512	1.115697	2.005903
N	-5.995730	0.361033	0.093829
H	-5.182647	-0.093866	-0.312894
C	-7.071651	0.732776	-0.812502
H	-7.758464	1.353191	-0.227791
C	-6.541424	1.530058	-2.009352
H	-6.121443	2.483787	-1.673148
H	-7.356737	1.716624	-2.711861
H	-5.754218	0.968890	-2.525851
C	-7.906451	-0.475647	-1.301280
O	-8.755951	-0.324479	-2.179263
N	-7.665766	-1.666712	-0.704256
H	-6.953169	-1.754907	0.011997
C	-8.413727	-2.851694	-1.076551
H	-8.461733	-2.941945	-2.166272
H	-7.908937	-3.724952	-0.656788
H	-9.443838	-2.817420	-0.698570
C	0.621784	3.748925	0.331991
C	-0.693137	4.118486	0.481683
C	1.353221	4.957044	0.033525
H	-1.558643	3.506263	0.691189
N	-0.819532	5.482282	0.297455
C	0.415262	6.026842	0.018069
C	2.706192	5.242026	-0.218041
H	-1.690015	5.988756	0.340524
C	0.793426	7.347853	-0.241304
C	3.087474	6.553420	-0.476713
H	3.448155	4.446372	-0.210205
H	0.062860	8.152700	-0.249655
C	2.139156	7.596282	-0.489095
H	4.131697	6.782950	-0.672731
H	2.464504	8.612400	-0.694929

Ac-(Ala)$_4$-Trp-(Ala)$_4$-NHMe_C5

C	-18.206477	-1.089072	-0.018247
H	-17.965010	-1.397976	1.003494
H	-18.624599	-1.942738	-0.560798
H	-18.980275	-0.315770	0.017266
C	-17.011004	-0.552865	-0.793796
O	-17.109697	-0.169457	-1.956752
N	-15.835519	-0.520977	-0.108459
H	-15.737617	-0.919795	0.818497

H	4.124168	2.776109	3.560294		H	3.146730	-2.836790	-0.156039
H	5.585578	4.163150	2.122049		H	4.184001	-2.725245	1.283572

Ac-(Ala)4-Trp-(Ala)4-NHMe_C7eq

C	-14.422750	-1.790030	0.053648		C	4.363573	-0.330352	-0.213267
H	-14.809336	-1.748413	1.076271		O	4.117000	0.151346	-1.320950
H	-14.238992	-2.833360	-0.218968		N	5.614303	-0.472992	0.272798
H	-15.186310	-1.404918	-0.629632		H	5.799735	-0.894045	1.178093
C	-13.146364	-0.995850	-0.149935		C	6.804409	-0.116591	-0.479368
O	-12.560021	-0.979534	-1.235398		H	6.691210	-0.482669	-1.507117
N	-12.691310	-0.296827	0.925998		C	7.031392	1.406795	-0.517064
H	-13.170293	-0.379029	1.812157		H	6.155677	1.888155	-0.958333
C	-11.541283	0.611415	0.856773		H	7.171449	1.796829	0.496113
H	-11.571113	1.065174	-0.140514		H	7.912856	1.659538	-1.116652
C	-11.652492	1.686994	1.932302		C	7.977808	-0.840931	0.204659
H	-12.591628	2.237925	1.820873		O	7.860892	-1.323694	1.332828
H	-11.602823	1.246631	2.933099		N	9.127266	-0.882146	-0.503241
H	-10.821204	2.391413	1.850032		H	9.222074	-0.430885	-1.408185
C	-10.208476	-0.167648	0.975020		C	10.369143	-1.406197	0.039868
O	-9.476524	-0.063163	1.965090		H	10.459573	-1.075957	1.081791
N	-9.919633	-0.949999	-0.090028		C	10.413752	-2.945575	0.004353
H	-10.625557	-1.013469	-0.825596		H	9.575036	-3.340031	0.583272
C	-8.804787	-1.904235	-0.092340		H	10.337492	-3.306995	-1.026399
H	-8.700776	-2.275090	0.935461		H	11.344811	-3.324684	0.439344
C	-9.103744	-3.058398	-1.044020		C	11.500821	-0.788394	-0.800629
H	-10.040034	-3.548841	-0.760357		O	11.270658	-0.245894	-1.883661
H	-9.181958	-2.702831	-2.075361		N	12.740976	-0.903329	-0.278897
H	-8.295905	-3.793466	-1.011952		H	12.919868	-1.389297	0.594993
C	-7.473668	-1.204313	-0.460208		C	13.936133	-0.473409	-0.983784
O	-6.860586	-1.467314	-1.499982		H	13.842808	-0.769391	-2.036185
N	-7.039053	-0.305917	0.454186		C	14.129133	1.053560	-0.913927
H	-7.639601	-0.131877	1.261603		H	13.253413	1.544013	-1.345921
C	-5.905689	0.591410	0.205355		H	14.244682	1.376985	0.125550
H	-5.913379	0.823673	-0.867157		H	15.015325	1.368444	-1.476091
C	-6.058190	1.868949	1.024812		C	15.113006	-1.220920	-0.329551
H	-7.005679	2.360687	0.783453		O	14.988437	-1.762971	0.766622
H	-6.028284	1.650199	2.096083		N	16.271933	-1.204599	-1.035485
H	-5.238314	2.558122	0.808207		H	16.277279	-0.760082	-1.942790
C	-4.561226	-0.112584	0.509754		C	17.502261	-1.813323	-0.553735
O	-3.828864	0.246107	1.438427		H	17.829506	-2.618716	-1.220787
N	-4.256965	-1.129097	-0.330410		H	18.302533	-1.069141	-0.474535
H	-4.955397	-1.376594	-1.033776		H	17.298431	-2.228129	0.433773
C	-3.126986	-2.035901	-0.101342		C	0.891689	2.778117	0.085603
H	-3.023477	-2.149060	0.985498		C	1.066006	3.413519	-1.120619
C	-3.400417	-3.388640	-0.750795		C	2.097933	3.014336	0.844431
H	-4.328662	-3.814612	-0.357527		H	0.390743	3.486737	-1.962831
H	-3.481999	-3.289663	-1.837014		N	2.300234	4.031928	-1.156581
H	-2.579531	-4.080150	-0.545589		C	2.958544	3.805145	0.034254
C	-1.805768	-1.420285	-0.622805		C	2.530572	2.639757	2.129504
O	-1.183999	-1.905259	-1.573932		H	2.670535	4.544012	-1.941733
N	-1.391692	-0.324746	0.056837		C	4.217419	4.229674	0.472830
H	-1.999582	0.028205	0.798394		C	3.781609	3.056872	2.568039
C	-0.256863	0.482108	-0.396823		H	1.899107	2.025070	2.765877
H	-0.261129	0.444399	-1.492393		H	4.859156	4.840313	-0.157272
					C	4.615715	3.845834	1.748490

C	0.529733	4.326494	-0.395083
H	1.728980	1.721900	-2.066380
N	2.042890	3.837269	-1.990212
C	1.505143	4.881670	-1.267358
C	-0.175375	5.183205	0.467991
H	2.745715	3.920936	-2.707484
C	1.785390	6.251742	-1.299562
C	0.099840	6.544534	0.440591
H	-0.923196	4.786132	1.149885
H	2.534805	6.660260	-1.972691
C	1.070397	7.072979	-0.435455
H	-0.437746	7.215811	1.104696
H	1.264902	8.142014	-0.434225

Ac-(Ala)$_4$-Hid-(Ala)$_4$-NHMe_αR

C	-8.914083	-2.327653	0.043577
H	-9.806765	-1.709620	0.176537
H	-8.722333	-2.890448	0.960702
H	-9.107000	-3.056380	-0.751571
C	-7.676552	-1.531600	-0.316241
O	-6.545808	-2.018662	-0.277973
N	-7.871117	-0.225313	-0.680675
H	-8.819787	0.090909	-0.838107
C	-6.795967	0.542096	-1.314757
H	-6.417892	-0.008700	-2.183170
C	-7.314177	1.913559	-1.763256
H	-8.116551	1.801688	-2.500910
H	-7.693525	2.493297	-0.914542
H	-6.502193	2.476962	-2.229784
C	-5.572554	0.707208	-0.400911
O	-4.446539	0.810253	-0.895202
N	-5.797581	0.767151	0.930785
H	-6.745057	0.650916	1.265874
C	-4.704990	0.914769	1.888777
H	-4.149553	1.826613	1.650567
C	-5.257883	1.010709	3.314147
H	-5.918287	1.878533	3.415978
H	-5.813943	0.105865	3.585901
H	-4.429841	1.126279	4.017759
C	-3.660932	-0.215650	1.789208
O	-2.489370	0.026737	2.082456
N	-4.095671	-1.449445	1.433219
H	-5.035063	-1.575363	1.064294
C	-3.143137	-2.551397	1.294990
H	-2.517604	-2.572063	2.190489
C	-3.883920	-3.884506	1.144279
H	-4.475096	-4.093930	2.041833
H	-4.556628	-3.871914	0.280724
H	-3.159548	-4.693101	1.012490
C	-2.151264	-2.329046	0.134238
O	-0.972393	-2.665698	0.249545
N	-2.658831	-1.790724	-1.004091
H	-3.595376	-1.405081	-0.990056
C	-1.786952	-1.439012	-2.122823

C	-0.401966	1.929581	0.077737
H	-1.449788	2.227740	-0.064928
H	-0.206849	1.960076	1.157351
C	1.060668	-0.157277	0.103546
O	1.672782	0.266867	1.086967
N	1.469286	-1.223479	-0.629987
H	0.790692	-1.594896	-1.296401
C	2.544031	-2.115999	-0.175491
H	2.499833	-2.146449	0.921337
C	2.340149	-3.513215	-0.752332
H	1.354891	-3.897102	-0.469759
H	2.421022	-3.498795	-1.842912
H	3.107244	-4.194345	-0.375874
C	3.932024	-1.548578	-0.559543
O	4.666995	-2.114606	-1.376600
N	4.272137	-0.407687	0.082877
H	3.573661	0.005421	0.703728
C	5.461759	0.375842	-0.267349
H	5.608266	0.264153	-1.349583
C	5.246774	1.843361	0.090221
H	4.357946	2.232091	-0.416389
H	5.122800	1.966589	1.169918
H	6.116028	2.435384	-0.206950
C	6.729926	-0.188170	0.420236
O	7.361262	0.458564	1.262129
N	7.089875	-1.425574	0.006885
H	6.481185	-1.889171	-0.669600
C	8.158741	-2.194772	0.651721
H	8.149070	-1.920800	1.714211
C	7.901402	-3.689622	0.489906
H	6.924297	-3.951854	0.907739
H	7.931677	-3.977981	-0.564819
H	8.673621	-4.264043	1.007598
C	9.548118	-1.801857	0.091064
O	10.237814	-2.593858	-0.560554
N	9.934435	-0.540616	0.387825
H	9.274783	0.041322	0.905327
C	11.139893	0.078213	-0.176221
H	11.266173	-0.340505	-1.182171
C	10.965062	1.591323	-0.249328
H	10.077286	1.844414	-0.838099
H	10.868433	2.018676	0.752921
H	11.841951	2.049177	-0.714016
C	12.399312	-0.296706	0.650542
O	13.010037	0.530590	1.319762
N	12.752136	-1.605428	0.535259
H	12.113944	-2.212668	0.024455
C	13.850496	-2.181439	1.286980
H	13.492417	-2.853086	2.078515
H	14.517467	-2.747250	0.626352
H	14.407087	-1.362509	1.745337
C	0.498890	2.903010	-0.630609
C	1.431038	2.654668	-1.607313

H	7.321961	1.488727	2.775993
C	7.771826	-0.513306	1.085536
O	8.679497	-0.465018	1.915548
N	7.472604	-1.630129	0.381888
H	6.716083	-1.631469	-0.293590
C	8.228752	-2.853152	0.568007
H	8.363933	-3.053876	1.635228
H	7.677258	-3.675225	0.105567
H	9.224943	-2.789273	0.111017
C	-0.609799	4.259395	0.109897
N	0.742847	4.482097	0.289453
C	-1.158117	5.517943	-0.000810
C	0.935262	5.831855	0.266235
N	-0.192936	6.492778	0.100677
H	-2.200567	5.772583	-0.148764
H	1.917194	6.274330	0.369211
H	1.448270	3.746626	0.332303

Ac-(Ala)$_4$-Hid-(Ala)$_4$-NHMe_C7$_{eq}$

C	14.303335	-1.654834	0.466437
H	14.752405	-1.565159	-0.527181
H	14.082142	-2.706915	0.667780
H	15.031825	-1.326402	1.214683
C	13.033416	-0.843164	0.638348
O	12.370424	-0.890086	1.677836
N	12.673700	-0.053767	-0.410931
H	13.214607	-0.082559	-1.264155
C	11.546156	0.883063	-0.352250
H	11.517201	1.261022	0.676270
C	11.760843	2.031148	-1.332940
H	12.704624	2.541991	-1.117797
H	11.768024	1.668188	-2.365497
H	10.945413	2.754101	-1.252602
C	10.205000	0.157131	-0.620325
O	9.546433	0.358916	-1.646424
N	9.822731	-0.694083	0.358771
H	10.474018	-0.834259	1.133215
C	8.690692	-1.616111	0.210207
H	8.654172	-1.909254	-0.846993
C	8.896054	-2.842827	1.093492
H	9.837776	-3.338488	0.838335
H	8.912497	-2.562928	2.150685
H	8.075388	-3.550863	0.955244
C	7.350574	-0.911381	0.532632
O	6.654365	-1.238703	1.499385
N	7.004692	0.066790	-0.336875
H	7.669403	0.288613	-1.080108
C	5.874393	0.971114	-0.100345
H	5.807080	1.120095	0.984846
C	6.111862	2.303807	-0.803396
H	7.047959	2.750668	-0.454728
H	6.158584	2.169950	-1.887932
H	5.292121	2.995241	-0.593367
C	4.543877	0.324608	-0.554783

H	-1.159858	-2.304107	-2.350241
C	-2.622467	-1.059059	-3.349770
H	-3.236622	-1.907463	-3.670082
H	-3.279350	-0.210514	-3.129610
H	-1.960657	-0.781096	-4.174884
C	-0.792056	-0.318214	-1.754198
O	0.373358	-0.357745	-2.144324
N	-1.282214	0.697042	-0.995329
H	-2.266196	0.719386	-0.748854
C	-0.415049	1.793839	-0.582215
H	0.089739	2.196805	-1.465206
C	-1.253340	2.903637	0.098129
H	-2.201234	2.994306	-0.446428
H	-1.509655	2.565628	1.113254
C	0.724011	1.300892	0.339643
O	1.845763	1.821016	0.284601
N	0.425578	0.313077	1.209034
H	-0.529491	-0.024583	1.283445
C	1.448620	-0.250306	2.087889
H	2.012171	0.569821	2.540365
C	0.798250	-1.114220	3.173521
H	0.103268	-0.518211	3.773816
H	0.248065	-1.949963	2.727692
H	1.573147	-1.518388	3.831066
C	2.503655	-1.061178	1.305838
O	3.691287	-1.018453	1.629357
N	2.048212	-1.822540	0.280686
H	1.052685	-1.878167	0.089493
C	2.957981	-2.652742	-0.502353
H	3.525989	-3.300493	0.173523
C	2.167452	-3.502614	-1.503188
H	1.459303	-4.154445	-0.980751
H	1.609645	-2.860204	-2.192941
H	2.860353	-4.122148	-2.078963
C	4.035025	-1.830649	-1.238206
O	5.129393	-2.339129	-1.492115
N	3.698180	-0.568567	-1.589678
H	2.762614	-0.234798	-1.387379
C	4.623857	0.325817	-2.275146
H	5.084020	-0.226403	-3.101839
C	3.868143	1.539686	-2.823764
H	3.116793	1.227359	-3.557022
H	3.360494	2.076400	-2.014128
H	4.579758	2.215250	-3.303551
C	5.827727	0.787464	-1.419809
O	6.747663	1.382378	-1.975382
N	5.794928	0.497548	-0.093669
H	4.986753	0.029137	0.305873
C	6.924031	0.748011	0.790958
H	7.586658	1.431330	0.250462
C	6.466949	1.395405	2.102918
H	6.041319	2.385671	1.910714
H	5.702625	0.778886	2.589958

H	-11.137075	-0.371120	1.814348
C	-10.963534	1.733834	1.332899
H	-10.013346	1.872636	1.858872
H	-10.990317	2.385726	0.454895
H	-11.780839	2.041480	1.989978
C	-12.487639	0.058908	0.190563
O	-13.179629	0.997589	-0.190203
N	-12.817512	-1.251855	0.038055
H	-12.118872	-1.939366	0.313331
C	-13.999193	-1.674079	-0.689205
H	-13.745360	-2.091726	-1.672774
H	-14.550211	-2.432002	-0.121144
H	-14.634189	-0.798572	-0.833557
C	-0.342218	3.482300	0.225448
N	-1.649415	3.706724	-0.159871
C	-0.103790	4.424995	1.201263
C	-2.125208	4.742953	0.589230
N	-1.215618	5.204827	1.423186
H	0.815621	4.588942	1.749278
H	-3.133240	5.121154	0.481397
H	-2.130274	3.130187	-0.840261

Ac-(Ala)₄-Hie-(Ala)₄-NHMe_αR

C	8.997600	-2.369110	-0.467577
H	9.875921	-1.724925	-0.569086
H	8.771828	-2.830372	-1.432204
H	9.235188	-3.177124	0.233418
C	7.767505	-1.637777	0.030521
O	6.638822	-2.123572	-0.040590
N	7.969976	-0.390991	0.563339
H	8.922437	-0.091930	0.730797
C	6.914980	0.275259	1.331739
H	6.556906	-0.398817	2.117881
C	7.451297	1.563936	1.965817
H	8.271834	1.342814	2.657395
H	7.810864	2.263132	1.202766
H	6.653232	2.052079	2.530608
C	5.667491	0.577642	0.488394
O	4.561411	0.640813	1.031839
N	5.849763	0.792071	-0.833540
H	6.782247	0.692071	-1.212501
C	4.730071	1.070681	-1.728565
H	4.205203	1.960166	-1.367640
C	5.236565	1.322162	-3.152147
H	5.912040	2.183982	-3.175757
H	5.763016	0.445505	-3.547592
H	4.387246	1.534555	-3.805882
C	3.663501	-0.043277	-1.724523
O	2.495662	0.252122	-1.985727
N	4.068604	-1.312363	-1.480319
H	5.017736	-1.497882	-1.164668
C	3.091526	-2.399821	-1.422094
H	2.442448	-2.318246	-2.297119
C	3.801163	-3.758050	-1.423516

O	3.890493	0.765866	-1.507267
N	4.156837	-0.741598	0.183668
H	4.798561	-1.058825	0.913287
C	3.040399	-1.610589	-0.203194
H	3.028962	-1.650376	-1.300201
C	3.238889	-3.008397	0.374447
H	4.193410	-3.423017	0.036029
H	3.224801	-2.983561	1.467723
H	2.431790	-3.670408	0.051049
C	1.687452	-1.006357	0.243945
O	0.984733	-1.536309	1.110974
N	1.337899	0.128193	-0.408430
H	2.026471	0.511871	-1.060439
C	0.225883	0.983722	0.020918
H	0.160506	0.920276	1.114138
C	0.529290	2.437527	-0.396180
H	1.564339	2.645387	-0.105203
H	0.485690	2.501628	-1.490828
C	-1.115849	0.460422	-0.551770
O	-1.807449	1.114431	-1.350350
N	-1.463098	-0.765208	-0.112245
H	-0.811901	-1.232509	0.524542
C	-2.581422	-1.533274	-0.670567
H	-2.661066	-1.253308	-1.728105
C	-2.308238	-3.028158	-0.536893
H	-1.369177	-3.286449	-1.035846
H	-2.250221	-3.320092	0.515422
H	-3.119480	-3.601932	-0.991910
C	-3.915126	-1.145333	0.011638
O	-4.528839	-1.926307	0.744293
N	-4.347857	0.104887	-0.276178
H	-3.741157	0.684786	-0.853807
C	-5.486348	0.728609	0.408746
H	-5.483001	0.350460	1.438709
C	-5.335645	2.246286	0.403173
H	-4.388512	2.535540	0.869484
H	-5.376684	2.634372	-0.619438
H	-6.155863	2.709377	0.956872
C	-6.828292	0.299151	-0.235052
O	-7.555926	1.102737	-0.826796
N	-7.132464	-1.009721	-0.079278
H	-6.444554	-1.598507	0.392011
C	-8.268793	-1.644096	-0.755554
H	-8.389529	-1.131819	-1.718289
C	-7.985852	-3.126610	-0.977150
H	-7.066401	-3.253112	-1.557457
H	-7.884323	-3.650037	-0.022078
H	-8.813194	-3.592278	-1.518259
C	-9.580260	-1.437304	0.042074
O	-10.178890	-2.381247	0.568731
N	-10.007664	-0.155707	0.095066
H	-9.422850	0.552718	-0.348411
C	-11.138226	0.274268	0.927470

O	-6.974931	1.335356	1.873160		H	4.369121	-3.890703	-2.350250
N	-5.931680	0.482996	0.024639		H	4.490836	-3.847210	-0.578025
H	-5.092181	0.048550	-0.349736		H	3.058109	-4.557374	-1.355734
C	-7.040348	0.689220	-0.895235		C	2.135489	-2.279355	-0.215270
H	-7.755140	1.330370	-0.369514		O	0.962138	-2.635884	-0.318793
C	-6.574566	1.377502	-2.183152		N	2.674864	-1.821523	0.944559
H	-6.213690	2.387960	-1.964553		H	3.592325	-1.391687	0.923066
H	-5.758330	0.812478	-2.647644		C	1.836263	-1.573566	2.115652
H	-7.408670	1.430916	-2.886265		H	1.205797	-2.452012	2.269871
C	-7.810912	-0.610733	-1.231833		C	2.706527	-1.329865	3.353048
O	-8.688148	-0.601548	-2.095543		H	3.315415	-2.213880	3.571100
N	-7.483072	-1.717058	-0.524088		H	3.371670	-0.472413	3.203798
H	-6.753643	-1.687434	0.180241		H	2.067719	-1.128013	4.217623
C	-8.169531	-2.974628	-0.746646		C	0.841128	-0.414833	1.889796
H	-8.247220	-3.177766	-1.819224		O	-0.308135	-0.481786	2.318662
H	-7.599480	-3.770347	-0.261321		N	1.313293	0.660191	1.206144
H	-9.187085	-2.960960	-0.334699		H	2.282341	0.684861	0.909231
C	0.618166	4.202508	-0.001894		C	0.437525	1.774700	0.850187
N	1.388197	5.310470	-0.313230		H	-0.042331	2.158817	1.755207
C	-0.709951	4.551737	0.073014		C	1.292795	2.874122	0.192813
C	0.538957	6.308215	-0.423539		H	2.174389	3.035663	0.827413
N	-0.744712	5.904391	-0.198523		H	1.672162	2.499991	-0.768503
H	-1.597932	3.972385	0.272948		C	-0.730209	1.292522	-0.043372
H	0.792131	7.333781	-0.657748		O	-1.892187	1.641370	0.180464
H	-1.573693	6.480272	-0.224067		N	-0.408494	0.471581	-1.071894

Ac-(Ala)$_4$-Hie-(Ala)$_4$-NHMe_C5

C	17.949640	-1.256097	0.425473		H	0.563569	0.246606	-1.265252
H	17.711420	-1.896307	-0.429538		C	-1.439718	-0.023868	-1.979787
H	18.312549	-1.879014	1.248890		H	-2.000425	0.824274	-2.384980
H	18.763280	-0.578897	0.146924		C	-0.799268	-0.825436	-3.118539
C	16.769655	-0.430270	0.919295		H	-0.092161	-0.203608	-3.677579
O	16.862869	0.323272	1.885092		H	-0.265227	-1.696584	-2.723879
N	15.615134	-0.579249	0.214354		H	-1.578355	-1.172647	-3.802975
H	15.518496	-1.258136	-0.532332		C	-2.503070	-0.876212	-1.260506
C	14.382519	0.082497	0.595734		O	-3.680710	-0.838312	-1.623648
H	14.285891	0.034955	1.687769		N	-2.070038	-1.672713	-0.254617
C	14.363399	1.563671	0.170026		H	-1.079731	-1.724030	-0.038145
H	15.212125	2.073257	0.632653		C	-2.988379	-2.547674	0.465069
H	14.443904	1.649773	-0.918820		H	-3.519855	-3.180057	-0.254130
H	13.440791	2.059312	0.491971		C	-2.213170	-3.422472	1.456777
C	13.235666	-0.705213	-0.060171		H	-1.481254	-4.043078	0.928836
O	13.445105	-1.516222	-0.965042		H	-1.683171	-2.797878	2.183565
N	11.999369	-0.428604	0.411274		H	-2.912885	-4.073051	1.988177
H	11.837120	0.281912	1.118647		C	-4.108157	-1.783492	1.197779
C	10.789755	-0.982180	-0.171591		O	-5.175626	-2.355490	1.438453
H	10.885163	-0.957832	-1.264198		N	-3.846399	-0.509969	1.569912
C	10.548186	-2.438746	0.268521		H	-2.966336	-0.079568	1.304333
H	11.405292	-3.047470	-0.029681		C	-4.841890	0.312639	2.245804
H	10.430992	-2.495677	1.355806		H	-5.320228	-0.308122	3.010861
H	9.648366	-2.851028	-0.200982		C	-4.174137	1.519721	2.910462
C	9.636923	-0.060618	0.267346		H	-3.471470	1.191707	3.683707
O	9.788050	0.769912	1.166015		H	-3.621337	2.111543	2.173135
N	8.467896	-0.244440	-0.382528		H	-4.945312	2.145342	3.365611
					C	-6.019420	0.766567	1.350022

H	-9.778144	-3.062809	0.383701
H	-10.595538	-2.397915	1.820230
H	-11.551394	-3.039923	0.465095
C	-11.784556	-0.219051	0.559032
O	-11.590705	0.743303	1.305307
N	-13.010543	-0.588454	0.131066
H	-13.159552	-1.411990	-0.444811
C	-14.230620	0.059971	0.579411
H	-14.144987	0.251083	1.656426
C	-14.471971	1.398713	-0.143791
H	-13.622866	2.061801	0.039059
H	-14.575300	1.237900	-1.221701
H	-15.380308	1.889817	0.222365
C	-15.371211	-0.940345	0.313087
O	-15.208360	-1.902348	-0.434522
N	-16.542649	-0.660153	0.938193
H	-16.580693	0.139865	1.554113
C	-17.744442	-1.462067	0.767801
H	-18.079890	-1.871574	1.726983
H	-18.555052	-0.868149	0.330717
H	-17.498774	-2.283563	0.094279
C	-1.192544	2.847110	-0.621296
N	-2.332780	2.920423	-1.401780
C	-1.357841	3.595981	0.522969
C	-3.163533	3.697803	-0.743438
N	-2.622034	4.138926	0.428095
H	-0.705907	3.800649	1.359313
H	-4.158524	3.977433	-1.062169
H	-3.075157	4.718742	1.119370

Ac-(Ala)4-Hie-(Ala)4-NHMe_C7eq

C	14.367474	-1.377399	0.256760
H	14.795873	-1.281026	-0.745336
H	14.184043	-2.434573	0.469329
H	15.097792	-1.019949	0.989716
C	13.074758	-0.606043	0.445254
O	12.435855	-0.660676	1.499196
N	12.667247	0.155999	-0.606707
H	13.188571	0.129853	-1.472126
C	11.505162	1.048997	-0.539698
H	11.479448	1.438943	0.484316
C	11.658114	2.191363	-1.538322
H	12.585306	2.740598	-1.346825
H	11.660773	1.815119	-2.566126
H	10.816929	2.883536	-1.452336
C	10.189054	0.267925	-0.775652
O	9.508966	0.427491	-1.794920
N	9.854216	-0.581239	0.222274
H	10.520021	-0.683820	0.989809
C	8.750669	-1.541966	0.108331
H	8.702979	-1.849143	-0.944300
C	9.013755	-2.750639	1.001129
H	9.967456	-3.216553	0.734527
H	9.038168	-2.458594	2.054877

H	8.343152	-0.974309	-1.078206
C	7.242131	0.443182	-0.012762
H	7.179218	0.477832	1.081659
C	7.199910	1.884224	-0.554796
H	8.054962	2.439221	-0.160728
H	7.247866	1.883735	-1.648736
H	6.281558	2.395615	-0.246586
C	6.086884	-0.408159	-0.572053
O	6.291782	-1.287596	-1.411980
N	4.862424	-0.107868	-0.092233
H	4.708129	0.651940	0.564775
C	3.641761	-0.732185	-0.574880
H	3.681424	-0.780532	-1.670131
C	3.463314	-2.158933	-0.022857
H	4.321723	-2.766940	-0.318575
H	3.397447	-2.140558	1.070012
H	2.554434	-2.624198	-0.418783
C	2.489371	0.192513	-0.138293
O	2.672346	1.092448	0.686260
N	1.290345	-0.071256	-0.694918
H	1.152324	-0.825069	-1.362072
C	0.071661	0.630773	-0.328666
H	0.073880	0.792572	0.754538
C	-0.012619	2.018342	-1.032702
H	0.922081	2.536529	-0.795839
H	-0.049535	1.859764	-2.115112
C	-1.086314	-0.298392	-0.731405
O	-0.925170	-1.155895	-1.603881
N	-2.248180	-0.112894	-0.072112
H	-2.378760	0.682692	0.546531
C	-3.479752	-0.772986	-0.473517
H	-3.533490	-0.777859	-1.569373
C	-3.540450	-2.226621	0.031829
H	-2.684985	-2.777195	-0.366829
H	-3.504261	-2.254087	1.125914
H	-4.458019	-2.724573	-0.299614
C	-4.636422	0.073226	0.087741
O	-4.443805	0.964854	0.917511
N	-5.862547	-0.247770	-0.379977
H	-6.011352	-1.018010	-1.025124
C	-7.082960	0.363294	0.115668
H	-7.007491	0.458516	1.205755
C	-7.316447	1.761234	-0.487840
H	-6.461360	2.397898	-0.247118
H	-7.416886	1.696145	-1.576136
H	-8.222016	2.223423	-0.080023
C	-8.226951	-0.603139	-0.243041
O	-8.062686	-1.512500	-1.058536
N	-9.402523	-0.366275	0.377523
H	-9.535133	0.421822	1.004635
C	-10.619608	-1.098535	0.069806
H	-10.685025	-1.224765	-1.017865
C	-10.641865	-2.490055	0.730101

H	-6.518936	-1.564924	0.573997		H	8.215441	-3.487605	0.884751
C	-8.268742	-1.655532	-0.683593		C	7.395130	-0.876585	0.450532
H	-8.299058	-1.236263	-1.697329		O	6.734298	-1.208586	1.439799
C	-8.033882	-3.161565	-0.741106		N	6.997430	0.073725	-0.427548
H	-7.080871	-3.376837	-1.234579		H	7.635496	0.302952	-1.190980
H	-8.023767	-3.592119	0.264422		C	5.839390	0.940490	-0.183954
H	-8.838932	-3.648545	-1.296902		H	5.786606	1.104185	0.899720
C	-9.626105	-1.325777	-0.013580		C	6.015231	2.269910	-0.910820
O	-10.307689	-2.192688	0.544136		H	6.941239	2.755712	-0.587841
N	-9.995824	-0.028637	-0.108352		H	6.044618	2.121263	-1.994090
H	-9.346212	0.611185	-0.566852		H	5.174742	2.933614	-0.693503
C	-11.164829	0.520281	0.588580		C	4.524195	0.241066	-0.603723
H	-11.262925	-0.040824	1.525931		O	3.842763	0.640021	-1.554488
C	-10.952850	2.002563	0.877430		N	4.185199	-0.820833	0.163678
H	-10.039968	2.149544	1.463814		H	4.842976	-1.098464	0.894077
H	-10.880922	2.571670	-0.053907		C	3.068529	-1.712631	-0.165346
H	-11.802534	2.401964	1.436976		H	3.015696	-1.768515	-1.260028
C	-12.461333	0.293676	-0.234350		C	3.310313	-3.098013	0.424917
O	-13.072958	1.220333	-0.756446		H	4.258447	-3.503954	0.058708
N	-12.843364	-1.010532	-0.292644		H	3.333809	-3.056274	1.517514
H	-12.202205	-1.697404	0.099722		H	2.502350	-3.776922	0.140492
C	-13.979455	-1.451387	-1.079019		C	1.728473	-1.116745	0.330986
H	-13.664188	-1.990890	-1.982139		O	1.087997	-1.624994	1.257033
H	-14.625644	-2.110384	-0.488084		N	1.325630	-0.012361	-0.340889
H	-14.543420	-0.566343	-1.377808		H	1.971272	0.365030	-1.036869
C	-0.454636	3.254614	0.367398		C	0.215224	0.828446	0.120752
N	-0.143685	3.653943	1.655225		H	0.219060	0.809418	1.216865
C	-1.606781	3.872724	-0.054138		C	0.409935	2.273170	-0.365580
C	-1.088213	4.499951	2.001234		H	1.460827	2.540386	-0.206293
N	-2.003502	4.670253	1.000989		H	0.204448	2.318013	-1.439147
H	-2.165988	3.806094	-0.974318		C	-1.133480	0.243614	-0.363324
H	-1.162172	5.017338	2.948568		O	-1.812176	0.779595	-1.248152
H	-2.811753	5.275242	1.019887		N	-1.498056	-0.900809	0.259971

Ac-(Ala)₁₃-NH₂ αR

					H	-0.813727	-1.311067	0.898828
C	-11.812373	-0.253462	1.390075		C	-2.607739	-1.738431	-0.208185
C	-10.526084	-0.393969	0.602853		H	-2.648954	-1.636492	-1.300734
N	-10.636597	-0.367804	-0.763516		C	-2.363036	-3.193849	0.178240
O	-9.429175	-0.517592	1.148542		H	-1.410289	-3.538133	-0.235789
C	-9.520281	-0.791128	-1.612974		H	-2.343170	-3.309325	1.265755
C	-8.282146	0.102953	-1.452256		H	-3.166571	-3.827956	-0.204023
N	-8.490110	1.397275	-1.120954		C	-3.962872	-1.233236	0.342336
O	-7.156057	-0.361971	-1.651185		O	-4.657905	-1.914837	1.103710
C	-7.379524	2.322684	-0.916144		N	-4.325291	-0.005371	-0.096568
C	-6.384927	1.837672	0.157541		H	-3.662002	0.490432	-0.695450
N	-6.874370	1.113775	1.191316		C	-5.476620	0.717922	0.450705
O	-5.198694	2.162653	0.062424		H	-5.555198	0.436420	1.508459
C	-5.977598	0.610902	2.231285		C	-5.264748	2.222716	0.319715
C	-4.977145	-0.435791	1.700038		H	-4.331442	2.515305	0.810625
N	-5.429481	-1.287215	0.744792		H	-5.228916	2.516952	-0.733485
O	-3.841892	-0.498989	2.174298		H	-6.096925	2.761456	0.780381
C	-4.533075	-2.254346	0.117031		C	-6.791982	0.279250	-0.238311
C	-3.438976	-1.568947	-0.726244		O	-7.448927	1.050253	-0.946204
N	-3.819388	-0.494907	-1.460767		N	-7.158301	-0.998411	0.013744

H	0.643017	-0.885322	3.043196	O	-2.285865	-2.002670	-0.722024
H	-0.253876	-1.619106	-0.368801	C	-2.841381	0.283105	-2.216730
H	2.191977	-3.035398	-0.923674	C	-1.774325	0.913532	-1.295498
H	1.398100	0.467112	-1.146982	N	-2.217125	1.472848	-0.145034
H	3.941491	1.193544	-2.287169	O	-0.587222	0.903343	-1.627422
H	2.936662	0.830721	1.152131	C	-1.284625	2.063931	0.811742
H	5.496682	1.734804	2.152033	C	-0.286846	1.022859	1.361050
H	4.352111	-1.515374	1.165304	N	-0.794588	-0.186814	1.693075
H	6.694921	-2.841340	2.203703	O	0.903253	1.315531	1.498401
H	6.104784	-1.207763	-0.890361	C	0.068970	-1.254721	2.188099
H	8.680732	-2.214818	-1.873094	C	1.136764	-1.659671	1.150030
H	7.499991	0.840460	-0.555656	N	0.721885	-1.777054	-0.132689
H	10.202930	1.924643	-1.067703	O	2.295838	-1.882661	1.507719
H	8.487965	0.961094	1.578244	C	1.660269	-2.119296	-1.197587
H	8.966850	2.246029	2.629278	C	2.769263	-1.057627	-1.355712
C	-9.956063	-0.834883	-3.082252	N	2.378726	0.236633	-1.280222
H	-10.769175	-1.555423	-3.223343	O	3.935843	-1.398460	-1.562061
H	-10.292699	0.149069	-3.426943	C	3.352983	1.317369	-1.372942
H	-9.113854	-1.148702	-3.703907	C	4.394938	1.254370	-0.237276
C	-7.907607	3.717798	-0.567223	N	3.932336	0.969256	1.001033
H	-7.066262	4.399796	-0.421764	O	5.583084	1.483999	-0.474720
H	-8.531114	4.109919	-1.377801	C	4.845595	0.855561	2.133419
H	-8.496498	3.699003	0.357096	C	5.817218	-0.337475	2.004189
C	-6.781838	0.050081	3.409318	N	5.330401	-1.463195	1.433918
H	-7.385304	0.840115	3.867939	O	6.966432	-0.250553	2.441609
H	-7.450499	-0.754809	3.088138	C	6.175678	-2.638664	1.262344
H	-6.095867	-0.342928	4.164613	C	7.311313	-2.433980	0.234921
C	-5.330722	-3.265327	-0.713912	N	7.043312	-1.582148	-0.794453
H	-6.008640	-3.834221	-0.068967	O	8.356441	-3.064707	0.348255
H	-5.920792	-2.762934	-1.487700	C	8.006430	-1.355100	-1.860869
H	-4.645563	-3.967229	-1.197754	C	8.931856	-0.134513	-1.656772
C	-3.546726	1.351064	-3.058788	N	8.477248	0.854632	-0.835571
H	-4.240648	0.883669	-3.766035	O	10.000876	-0.085806	-2.260301
H	-4.102738	2.046722	-2.421027	C	9.175355	2.132091	-0.751114
H	-2.806389	1.919542	-3.628809	C	9.272440	2.694567	0.679600
C	-2.055435	2.736589	1.952891	N	8.932208	1.863825	1.695103
H	-2.713851	3.519567	1.562118	O	9.680327	3.839506	0.864204
H	-2.663174	2.004971	2.495857	H	-12.660060	0.079437	0.784165
H	-1.350478	3.193115	2.653592	H	-11.653857	0.450122	2.211220
C	-0.774000	-2.465093	2.603950	H	-12.059688	-1.223668	1.835302
H	-1.487126	-2.185454	3.386384	H	-11.564093	-0.408075	-1.167188
H	-1.330360	-2.860901	1.748066	H	-9.181894	-1.785686	-1.301342
H	-0.120737	-3.252214	2.991467	H	-9.437321	1.701625	-0.937368
C	0.909225	-2.323456	-2.517674	H	-6.790569	2.374087	-1.836739
H	0.170839	-3.126070	-2.418667	H	-7.829647	0.763355	1.167474
H	0.390507	-1.405831	-2.813775	H	-5.353393	1.440871	2.571448
H	1.618594	-2.595182	-3.304806	H	-6.313836	-1.094106	0.288069
C	2.640468	2.674035	-1.385887	H	-3.986734	-2.771798	0.908855
H	1.955554	2.738161	-2.238050	H	-4.785005	-0.186689	-1.437854
H	2.066620	2.817634	-0.464670	H	-2.278935	-0.393774	-2.865670
H	3.379419	3.476356	-1.469093	H	-3.213978	1.524205	0.046190
C	4.052163	0.755818	3.440818	H	-0.660334	2.800027	0.296611
H	3.421737	1.640882	3.577213	H	-1.794513	-0.355718	1.627309

N	-10.023733	-0.200914	0.044277		H	3.411516	-0.132512	3.434792
O	-8.645519	1.159197	1.238248		H	4.744834	0.683108	4.284198
C	-11.236719	0.570435	0.261108		C	5.321826	-3.846453	0.860038
C	-12.407012	-0.371874	-0.079577		H	4.565100	-4.056618	1.623369
N	-13.629115	0.064025	0.289883		H	4.813064	-3.656461	-0.091433
O	-12.215828	-1.439295	-0.666721		H	5.965922	-4.722805	0.745743
C	-14.856853	-0.628086	-0.066065		C	7.294507	-1.228768	-3.215138
C	-15.981212	0.420265	0.031334		H	6.743207	-2.146403	-3.444362
N	-17.158269	0.061461	-0.522553		H	6.580877	-0.396284	-3.204314
O	-15.798244	1.500895	0.596115		H	8.032363	-1.045185	-4.001001
C	-18.359511	0.874137	-0.424716		C	8.570667	3.181072	-1.696515
C	-19.540822	-0.074743	-0.697567		H	8.679379	2.849159	-2.734084
N	-20.762972	0.416579	-0.399606		H	7.504588	3.318139	-1.484040
O	-19.362399	-1.198690	-1.171609		H	9.083078	4.136703	-1.563658

Ac-(Ala)13-NH2_C5

C	24.577886	0.900097	-0.209542
C	23.398533	0.220711	-0.892107
N	22.217042	0.285516	-0.219502
O	23.514147	-0.349624	-1.974033
C	20.981570	-0.235879	-0.770982
C	19.833440	0.474811	-0.033438
N	18.606995	0.316102	-0.579530
O	20.032592	1.129943	0.992079
C	17.395580	0.813632	0.048413
C	16.233919	-0.012596	-0.533499
N	15.055877	0.108543	0.114850
O	16.387617	-0.718506	-1.532588
C	13.826508	-0.507891	-0.354515
C	12.675714	0.271516	0.309483
N	11.446893	0.031860	-0.193715
O	12.886332	1.045590	1.246160
C	10.232963	0.583136	0.384924
C	9.080108	-0.314189	-0.104421
N	7.896279	-0.125071	0.514058
O	9.249612	-1.132723	-1.011137
C	6.671888	-0.792560	0.103415
C	5.514907	0.067089	0.647933
N	4.293674	-0.227476	0.157559
O	5.717092	0.950346	1.484784
C	3.073577	0.408633	0.626363
C	1.919621	-0.521219	0.204335
N	0.720115	-0.242587	0.754357
O	2.103067	-1.440546	-0.597098
C	-0.504820	-0.928036	0.376032
C	-1.658830	0.010203	0.778688
N	-2.866816	-0.305369	0.269368
O	-1.465988	0.969384	1.529829
C	-4.088148	0.399558	0.622221
C	-5.247551	-0.539215	0.235942
N	-6.462766	-0.178848	0.696736
O	-5.053604	-1.537146	-0.462334
C	-7.688181	-0.867612	0.326221
C	-8.831481	0.134081	0.578108

Left column continued:

C	-21.990795	-0.295365	-0.708141
C	-23.105810	0.764852	-0.739380
N	-24.292770	0.349467	-1.251054
O	-22.926404	1.897203	-0.305277
H	25.376901	0.165248	-0.070918
H	24.329032	1.343462	0.759545
H	24.965893	1.681721	-0.870502
H	22.104218	0.834716	0.625336
H	20.943189	0.015656	-1.838588
H	18.448138	-0.281188	-1.385455
H	17.466069	0.637951	1.128878
H	14.931580	0.741733	0.899660
H	13.770506	-0.390471	-1.443635
H	11.283929	-0.658515	-0.921419
H	10.307678	0.522004	1.477589
H	7.758390	0.601854	1.210765
H	6.634170	-0.808359	-0.992641
H	4.138534	-0.996648	-0.488444
H	3.111461	0.475831	1.720555
H	0.575538	0.557888	1.363726
H	-0.504525	-1.067069	-0.711856
H	-3.015589	-1.131075	-0.304448
H	-4.096057	0.566621	1.706397
H	-6.612233	0.681479	1.216842
H	-7.641294	-1.112136	-0.741927
H	-10.170487	-1.075622	-0.451984
H	-11.287659	0.853435	1.319674
H	-13.773994	0.975207	0.715837
H	-14.770070	-0.981140	-1.100819
H	-17.305923	-0.855512	-0.934347
H	-18.432225	1.268213	0.596360
H	-20.899449	1.368514	-0.072135
H	-21.887272	-0.751760	-1.700627
H	-24.424125	-0.567825	-1.649437
H	-25.060594	1.005720	-1.280525
C	-18.340460	2.057589	-1.410549
H	-17.465102	2.678200	-1.204445
H	-18.287442	1.696245	-2.442782
H	-19.237299	2.677088	-1.303603

C	16.778412	1.376967	-0.283406		C	20.885507	-1.767558	-0.629766
C	15.465759	0.591260	-0.522512		H	19.965666	-2.154520	-1.082227
N	15.085209	-0.192656	0.512006		H	21.739943	-2.220510	-1.138421
O	14.826585	0.691842	-1.575386		H	20.903106	-2.057164	0.426340
C	13.982421	-1.155831	0.412347		C	-15.126943	-1.837700	0.848073
C	12.617001	-0.465389	0.649989		H	-14.289921	-2.536554	0.774360
N	12.260530	0.421953	-0.307866		H	-15.232044	-1.515441	1.889242
O	11.912681	-0.726877	1.630722		H	-16.042327	-2.360949	0.551280
C	11.102406	1.311689	-0.170985		C	-7.884940	-2.170283	1.123568
C	9.795204	0.595028	-0.587166		H	-7.036202	-2.833987	0.940338
N	9.428353	-0.422043	0.227132		H	-7.946918	-1.957653	2.195897
O	9.140681	0.945190	-1.575245		H	-8.801254	-2.686328	0.817405
C	8.328878	-1.336871	-0.096665		C	6.600727	-2.241202	0.620863
C	6.966079	-0.732635	0.319541		H	7.458096	-2.800317	0.237805
N	6.590428	0.351880	-0.398384		H	6.623157	-2.259023	1.715467
O	6.280820	-1.219345	1.225579		H	5.684529	-2.737352	0.283171
C	5.448018	1.192015	-0.023626		C	-11.270033	1.849823	-0.595696
C	4.117506	0.600432	-0.549386		H	-10.401581	2.466246	-0.351250
N	3.770602	-0.584128	0.004949		H	-11.241514	1.597828	-1.660890
O	3.426999	1.185512	-1.391440		H	-12.175885	2.433503	-0.400128
C	2.643523	-1.386581	-0.481021		C	2.901696	1.826015	0.048844
C	1.307863	-0.896313	0.128633		H	3.761839	2.435941	0.335642
N	0.932394	0.342618	-0.266782		H	2.838092	1.788958	-1.043660
O	0.641348	-1.595261	0.899889		H	1.994406	2.303032	0.434486
C	-0.188009	1.062748	0.346345		C	17.197070	2.322150	-0.192387
C	-1.535781	0.638952	-0.285441		H	18.062591	2.861343	0.200619
N	-1.898287	-0.640059	-0.031287		H	17.103132	2.530054	-1.263384
O	-2.223349	1.421392	-0.951048		H	16.298380	2.690487	0.314326
C	-3.035659	-1.286777	-0.693955		C	-4.196834	1.761128	-0.089240
C	-4.366439	-0.944083	0.019193		H	-3.332979	2.374282	0.178690
N	-4.724624	0.358832	-0.057654		H	-4.215776	1.625236	-1.175617
O	-5.044982	-1.803254	0.592821		H	-5.105889	2.293373	0.210653
C	-5.840668	0.919106	0.710590		C	-0.629729	-2.306368	1.051179
C	-7.187724	0.687137	-0.014932		H	0.229630	-2.920960	0.771535
N	-7.568147	-0.609578	-0.091906		H	-0.652573	-2.198782	2.140616
O	-7.859169	1.620904	-0.467490		H	-1.542558	-2.821213	0.732847
C	-8.706168	-1.052975	-0.903967		C	10.018361	2.055329	-0.013546
C	-10.040982	-0.886924	-0.137200		H	10.875762	2.644735	0.320692
N	-10.386016	0.396413	0.117553		H	9.923221	2.148469	-1.100444
O	-10.732892	-1.856512	0.192533		H	9.114500	2.463956	0.451037
C	-11.514225	0.756381	0.982272		C	13.766722	-2.009236	-0.015858
C	-12.848976	0.731931	0.197685		H	14.620912	-2.512933	-0.475104
N	-13.235739	-0.498772	-0.211213		H	13.804552	-2.158626	1.068225
O	-13.503377	1.757726	-0.016249		H	12.847541	-2.465724	-0.398594
C	-14.368254	-0.711293	-1.118565		C	-22.289327	-1.405148	0.317840
C	-15.708939	-0.748009	-0.343281		H	-21.453378	-2.108569	0.333112
N	-16.056003	0.427697	0.227359		H	-22.416804	-0.978530	1.317860
O	-16.396626	-1.772649	-0.275721		H	-23.199862	-1.955587	0.056816

Ac-(Ala)$_{13}$-NH$_2$_C7$_{eq}$

C	-17.204738	0.573123	1.129665	C	19.588363	-1.020143	0.752180
C	-18.514852	0.766205	0.320190	C	18.296252	-0.231346	0.848849
N	-18.929124	-0.364161	-0.316094	N	17.934688	0.474649	-0.257803
O	-19.116940	1.830845	0.285866	O	17.616971	-0.224919	1.878781
H	20.286874	-0.639356	1.504009				

H	-12.090464	2.371138	2.300123		H	19.384767	-2.066464	0.997977
C	-16.974785	1.738775	2.084714		H	20.064084	-0.967971	-0.231629
H	-16.046682	1.594745	2.647229		H	18.488875	0.399380	-1.099611
H	-16.922549	2.683157	1.535278		H	16.718793	1.823909	0.715589
H	-17.807411	1.817568	2.788499		H	15.723611	-0.255496	1.306893
C	14.198684	-2.303490	1.393751		H	13.978694	-1.531980	-0.618848
H	15.160401	-2.789059	1.201363		H	12.935720	0.601647	-1.052813
H	14.178486	-1.942389	2.425939		H	11.010991	1.554673	0.895398
H	13.402035	-3.044265	1.290822		H	10.063921	-0.661167	0.990709
C	8.559423	-2.691191	0.566223		H	8.314850	-1.445166	-1.188713
H	9.520653	-3.106648	0.248317		H	7.259723	0.709052	-1.083110
H	8.549979	-2.598414	1.655959		H	5.390276	1.183596	1.072717
H	7.764679	-3.388604	0.289966		H	4.432227	-1.002707	0.662220
C	2.881482	-2.862694	-0.178518		H	2.581099	-1.225524	-1.564939
H	3.816911	-3.194962	-0.639155		H	1.580632	0.855310	-0.868265
H	2.930899	-3.036179	0.900327		H	-0.219822	0.765702	1.402574
H	2.059997	-3.467429	-0.570413		H	-1.230852	-1.218639	0.483147
C	-2.816540	-2.794938	-0.759174		H	-3.096684	-0.866931	-1.706389
H	-1.881629	-3.017280	-1.282826		H	-4.070147	0.995462	-0.517296
H	-2.777052	-3.226505	0.245130		H	-5.885141	0.366713	1.657990
H	-3.642338	-3.275267	-1.289672		H	-6.914659	-1.308317	0.267250
C	-8.501506	-2.497627	-1.349073		H	-8.752820	-0.389270	-1.777052
H	-7.566750	-2.589879	-1.910778		H	-9.722399	1.121829	-0.161009
H	-8.470509	-3.170309	-0.487075		H	-11.581165	-0.017907	1.757182
H	-9.330076	-2.818722	-1.984989		H	-12.596652	-1.273752	-0.026096
C	-14.161478	-1.990543	-1.923364		H	-14.405544	0.157066	-1.788610
H	-13.220241	-1.938415	-2.479601		H	-15.399610	1.203917	0.134327
H	-14.143143	-2.864801	-1.266197		H	-17.293068	-0.368402	1.685268
H	-14.983546	-2.129940	-2.629746		H	-18.293825	-1.156299	-0.388947

Ac-(Ala-Ala-Gln-Ala-Ala)₃-NH₂_αR

H	-14.141746	-2.103727	-1.429453		H	-19.699334	-0.277523	-0.965181
C	-13.142110	-2.308339	-1.823066		C	16.976159	2.460379	-1.338411
H	-13.207914	-2.430817	-2.909169		H	17.012019	2.027041	-2.342806
H	-12.781128	-3.254951	-1.410571		H	16.138417	3.161783	-1.321086
C	-12.133923	-1.219400	-1.518589		H	17.900539	3.013516	-1.144813
O	-10.940314	-1.332870	-1.804557		C	11.319411	2.582591	-0.986463
N	-12.609347	-0.102638	-0.886580		H	12.234622	3.086891	-0.661234
H	-13.611198	-0.002170	-0.784944		H	11.394891	2.352670	-2.053179
C	-11.799227	1.113379	-0.771553		H	10.475524	3.264699	-0.857633
H	-11.416512	1.384945	-1.761763		C	5.656464	2.615734	-0.530429
C	-12.646277	2.264633	-0.217513		H	6.590726	3.023912	-0.132599
H	-13.046239	2.022726	0.773600		H	5.690873	2.639056	-1.623410
H	-12.027526	3.160842	-0.129584		H	4.828324	3.255179	-0.215445
H	-13.481092	2.490340	-0.889972		C	0.027748	2.568262	0.227436
C	-10.536409	0.921097	0.083028		H	0.976645	2.850437	0.693931
O	-9.565112	1.660933	-0.081709		H	0.035874	2.878767	-0.821239
N	-10.558126	-0.069057	1.006702		H	-0.783690	3.107546	0.722387
H	-11.376608	-0.660414	1.061471		C	-5.603688	2.402847	0.974934
C	-9.392067	-0.391751	1.823088		H	-4.656695	2.543956	1.504995
H	-9.141172	0.470926	2.448227		H	-5.578657	2.966465	0.037946
C	-9.680236	-1.613842	2.704433		H	-6.413770	2.813644	1.582605
H	-10.559031	-1.436894	3.334145		C	-11.273366	2.121728	1.618645
H	-9.838028	-2.509804	2.093984		H	-10.333495	2.115710	2.179461
					H	-11.232728	2.904730	0.856046

H	-0.695884	-1.145810	-1.999722	H	-8.823400	-1.800336	3.356162
C	-1.851382	0.414098	-2.962582	C	-8.137962	-0.660639	0.979252
H	-2.608128	-0.262583	-3.372317	O	-7.019309	-0.459320	1.476818
H	-2.334787	1.363850	-2.708267	N	-8.307917	-1.139915	-0.266728
H	-1.094347	0.601431	-3.728880	H	-9.242783	-1.270857	-0.646231
C	-0.049568	0.704472	-1.222763	C	-7.151232	-1.522838	-1.061511
O	1.096303	0.550574	-1.651169	H	-6.517828	-2.164875	-0.443225
N	-0.399469	1.692683	-0.366158	C	-7.548078	-2.289704	-2.335298
H	-1.320404	1.668208	0.058325	H	-6.612486	-2.537962	-2.847060
C	0.595109	2.599267	0.205960	H	-8.115177	-1.630028	-3.002973
H	1.225538	2.968645	-0.607280	C	-8.386042	-3.568578	-2.095840
C	-0.100696	3.773929	0.912309	H	-8.440047	-4.122289	-3.041169
H	0.656249	4.385849	1.411990	H	-9.407843	-3.293684	-1.824615
H	-0.762832	3.377562	1.691922	C	-7.842246	-4.445862	-0.971038
C	-0.904231	4.655310	-0.059567	O	-8.149945	-4.262197	0.202281
H	-1.581564	4.044453	-0.664021	N	-6.950859	-5.407553	-1.347078
H	-0.214831	5.164162	-0.744023	H	-6.573459	-6.018330	-0.635256
C	-1.676169	5.730813	0.700677	H	-6.750710	-5.617814	-2.313087
O	-1.117935	6.586091	1.375067	C	-6.262670	-0.317859	-1.423559
N	-3.035068	5.644445	0.585828	O	-5.069452	-0.498739	-1.682532
H	-3.593072	6.338077	1.063913	N	-6.853192	0.900718	-1.459206
H	-3.487998	4.916409	0.043578	H	-7.820113	1.002986	-1.159569
C	1.563477	1.865510	1.154753	C	-6.075251	2.107367	-1.717861
O	2.768785	2.109039	1.144461	H	-5.408601	1.906597	-2.560643
N	1.007597	0.951752	1.994350	C	-6.999081	3.282540	-2.057870
H	0.011662	0.765260	1.953862	H	-7.715110	3.469476	-1.250529
C	1.852763	0.126670	2.848461	H	-6.398542	4.182465	-2.213239
H	2.521287	0.779682	3.416217	H	-7.557801	3.073851	-2.975801
C	0.992536	-0.707472	3.803469	C	-5.124877	2.481994	-0.560186
H	0.393027	-0.052679	4.445018	O	-4.128795	3.169047	-0.800926
H	0.320198	-1.367969	3.245527	N	-5.469485	2.058922	0.680614
H	1.634405	-1.322800	4.440751	H	-6.253086	1.420371	0.774760
C	2.803624	-0.773096	2.030963	C	-4.559183	2.162942	1.820172
O	3.985133	-0.902597	2.381030	H	-3.992971	3.089481	1.713054
N	2.286138	-1.399120	0.954644	C	-5.341346	2.173303	3.139054
H	1.298067	-1.293541	0.737012	H	-4.647241	2.221960	3.983434
C	3.107480	-2.271805	0.110829	H	-5.996887	3.048979	3.179113
H	3.606422	-3.020768	0.734590	H	-5.954639	1.271881	3.241298
C	2.230062	-2.969367	-0.934618	C	-3.502013	1.038197	1.802409
H	1.455112	-3.566360	-0.442719	O	-2.312422	1.285630	2.028674
H	1.748629	-2.239340	-1.595009	N	-3.940980	-0.211669	1.519041
H	2.850347	-3.636942	-1.538987	H	-4.933848	-0.388838	1.388375
C	4.244420	-1.498712	-0.579807	C	-3.010777	-1.336000	1.460040
O	5.339614	-2.032620	-0.788839	H	-2.507110	-1.442466	2.426257
N	3.990204	-0.220694	-0.948546	C	-3.759161	-2.629267	1.119192
H	3.050966	0.158943	-0.867282	H	-3.058102	-3.468567	1.120861
C	5.009656	0.575100	-1.619134	H	-4.541884	-2.830223	1.858367
H	5.336913	0.062287	-2.530391	H	-4.218235	-2.560668	0.127281
C	4.455166	1.961427	-1.969762	C	-1.870571	-1.093947	0.452144
H	5.232561	2.553233	-2.460934	O	-0.729572	-1.486429	0.709503
H	3.602943	1.863124	-2.650004	N	-2.194532	-0.463474	-0.700725
H	4.120628	2.481923	-1.066881	H	-3.172785	-0.290423	-0.923039
C	6.289521	0.706392	-0.777436	C	-1.187835	-0.206553	-1.727271

O	-27.263205	-0.295738	-1.731083		O	7.382359	0.853659	-1.346226
C	-28.368592	-0.688531	0.373580		N	6.157434	0.679968	0.563468
H	-28.797696	-1.644859	0.058623		H	5.242474	0.509904	0.971400
H	-28.129486	-0.737581	1.440381		C	7.309279	0.771565	1.450609
H	-29.132937	0.078846	0.215402		H	7.945521	1.591007	1.100795
N	-25.992160	-0.184623	0.149438		C	6.854273	1.071613	2.883615
C	-24.741714	0.047937	-0.547126		H	7.725567	1.080079	3.543118
C	-23.614570	-0.332634	0.427958		H	6.367877	2.051341	2.927058
O	-23.829163	-0.492414	1.631695		H	6.138310	0.322036	3.236391
C	-24.606412	1.507039	-1.024742		C	8.243328	-0.458538	1.415259
H	-25.899082	-0.335420	1.147663		O	9.372662	-0.352240	1.901077
H	-24.706439	-0.608500	-1.425728		N	7.785842	-1.607778	0.854935
H	-25.444843	1.739308	-1.685987		H	6.865951	-1.640211	0.415355
H	-24.623129	2.192955	-0.171138		C	8.693264	-2.730275	0.631766
H	-23.673343	1.661921	-1.577723		H	9.401592	-2.735861	1.465839
N	-22.387707	-0.459610	-0.125450		C	7.972147	-4.089062	0.573652
C	-21.187939	-0.685441	0.661355		H	8.722740	-4.804686	0.225885
C	-20.005103	-0.236223	-0.215734		H	7.171122	-4.063108	-0.174686
O	-20.144475	-0.030122	-1.422676		C	7.396658	-4.590531	1.919072
C	-21.047186	-2.157493	1.093165		H	8.100311	-4.380181	2.734587
H	-22.215072	-0.260643	-1.106407		H	7.276410	-5.676811	1.858082
H	-21.237526	-0.059711	1.561110		C	6.008951	-4.029369	2.215992
H	-21.926903	-2.442685	1.675322		O	5.012346	-4.476155	1.652863
H	-20.973158	-2.808580	0.215808		N	5.941692	-3.025137	3.141992
H	-20.156510	-2.305726	1.713591		H	5.113367	-2.434882	3.095777
N	-18.822249	-0.111181	0.424818		H	6.797811	-2.539097	3.372063
C	-17.585193	0.224492	-0.261444		C	9.599289	-2.564504	-0.616329
C	-16.451467	-0.340758	0.611947		O	10.530326	-3.346198	-0.784178
O	-16.619802	-0.545185	1.814703		N	9.295931	-1.542079	-1.459013
C	-17.458145	1.755611	-0.468211		H	8.474562	-0.975556	-1.278981
C	-16.320493	2.173239	-1.403381		C	10.127396	-1.198524	-2.603253
C	-16.339601	3.674507	-1.696589		H	10.858396	-2.002037	-2.706790
N	-15.133296	4.180798	-2.099069		C	9.284328	-1.083296	-3.883530
O	-17.339097	4.368585	-1.585897		H	8.804235	-2.041820	-4.105621
H	-18.717639	-0.317952	1.412772		H	8.503189	-0.323293	-3.765512
H	-17.593907	-0.266097	-1.242065		H	9.922329	-0.801820	-4.727049
H	-17.347015	2.239810	0.509290		C	10.958781	0.089499	-2.414346
H	-18.401395	2.108147	-0.893016		O	12.044268	0.201681	-2.974377
H	-16.425487	1.654404	-2.368954		N	10.400861	1.074151	-1.643263
H	-15.336553	1.897457	-1.009936		H	9.414800	1.003652	-1.403627
H	-15.103086	5.137881	-2.421357		C	11.005810	2.399179	-1.568692
H	-14.336927	3.586027	-2.275307		H	12.032975	2.270714	-1.925431
N	-15.277259	-0.577822	-0.021705		C	10.288879	3.410529	-2.474770
C	-14.047717	-0.866515	0.698618		H	10.373680	3.100168	-3.520933
C	-12.911951	-0.139943	-0.051326		H	9.224803	3.474782	-2.217363
O	-13.114443	0.429105	-1.129570		H	10.735514	4.399414	-2.349780
C	-13.799746	-2.380734	0.823251		C	11.112436	2.951355	-0.134250
H	-15.135494	-0.265588	-0.976507		O	11.442511	4.117979	0.056875
H	-14.143974	-0.442674	1.704929		N	10.831098	2.090835	0.877941
H	-14.646244	-2.838686	1.342218		H	10.605727	1.112169	0.754731
H	-13.703507	-2.840886	-0.165804		H	10.954053	2.427144	1.822379
H	-12.890405	-2.595676	1.394742		Ac-(Ala-Ala-Gln-Ala-Ala)$_3$-NH$_2$_C5			
N	-11.705244	-0.176480	0.547590		C	-27.167726	-0.375708	-0.508913

H	3.212071	2.933912	0.854075	C	-10.498948	0.364496	-0.057124
H	4.133459	2.088241	2.118698	C	-9.320058	-0.351498	0.631643
H	4.969365	2.748601	0.696798	O	-9.493225	-1.024265	1.650696
N	6.142737	0.256988	0.019905	C	-10.409201	1.893529	0.100172
C	7.347902	-0.534491	0.208468	H	-11.535826	-0.714245	1.393365
C	8.527811	0.417216	-0.071398	H	-10.504780	0.118384	-1.125800
O	8.346677	1.509254	-0.615107	H	-11.286616	2.353555	-0.361487
C	7.382057	-1.765526	-0.716047	H	-10.379845	2.169754	1.159270
H	6.304080	1.149539	-0.439411	H	-9.512670	2.290625	-0.387754
H	7.384852	-0.872642	1.251045	N	-8.116866	-0.173882	0.050495
H	6.505903	-2.387616	-0.517209	C	-6.875911	-0.672678	0.620882
H	7.367939	-1.456428	-1.766276	C	-5.751537	0.177713	-0.002367
H	8.281372	-2.365591	-0.541762	O	-5.973453	0.922467	-0.960486
N	9.740211	-0.040211	0.299054	C	-6.677285	-2.175262	0.349063
C	10.980308	0.659410	0.003379	H	-7.985300	0.445068	-0.745146
C	12.095642	-0.400061	0.097542	H	-6.900067	-0.510271	1.705353
O	11.882353	-1.504870	0.603146	H	-7.518373	-2.729741	0.772856
C	11.227329	1.834414	0.967392	H	-6.629300	-2.367565	-0.727783
H	9.874334	-0.969229	0.689424	H	-5.753783	-2.543268	0.808533
H	10.926403	1.047873	-1.020919	N	-4.536025	0.035950	0.563439
H	10.394498	2.538480	0.895674	C	-3.336418	0.662959	0.032608
H	11.302888	1.474768	1.998803	C	-2.152339	-0.157835	0.579330
H	12.151758	2.365275	0.716170	O	-2.311939	-0.981913	1.482309
N	13.295006	-0.023777	-0.389850	C	-3.237576	2.147800	0.427565
C	14.492114	-0.840320	-0.270502	H	-4.356246	-0.641513	1.299751
C	15.680965	0.123486	-0.444572	H	-3.359299	0.589474	-1.061557
O	15.517589	1.262968	-0.885720	H	-4.114958	2.678004	0.048719
C	14.523354	-1.978763	-1.307069	H	-3.199758	2.252947	1.516802
H	13.465985	0.912737	-0.746079	H	-2.341543	2.612112	0.001992
H	14.517115	-1.278145	0.734845	N	-0.954777	0.104328	0.016208
H	13.642908	-2.611421	-1.170110	C	0.279359	-0.533023	0.447830
H	14.516458	-1.571876	-2.323609	C	1.411141	0.429336	0.044638
H	15.418422	-2.598202	-1.185856	O	1.247283	1.257147	-0.852551
N	16.888049	-0.373615	-0.102932	C	0.439910	-1.932150	-0.200085
C	18.123405	0.378736	-0.255734	C	1.566045	-2.779969	0.396568
C	19.246058	-0.670809	-0.333125	C	1.569045	-4.203665	-0.163972
O	19.087423	-1.803306	0.124184	N	2.773845	-4.843371	-0.059060
C	18.321780	1.368135	0.920862	O	0.585222	-4.731444	-0.660775
C	19.436780	2.394807	0.707408	H	-0.835646	0.813616	-0.700194
C	19.447610	3.458303	1.808479	H	0.243704	-0.647246	1.537725
N	20.636408	4.125476	1.934911	H	0.584223	-1.810216	-1.280204
O	18.483343	3.696007	2.519679	H	-0.502853	-2.467813	-0.063581
H	17.008899	-1.324322	0.231794	H	1.430404	-2.862469	1.486214
H	18.065704	0.946836	-1.191983	H	2.552248	-2.330500	0.240518
H	18.496798	0.798956	1.841470	H	2.815898	-5.822628	-0.304217
H	17.381629	1.908601	1.055069	H	3.555695	-4.433246	0.430317
H	19.280360	2.919332	-0.248099	N	2.575874	0.290278	0.721824
H	20.426760	1.929567	0.647411	C	3.808758	0.933407	0.295847
H	20.665011	4.924897	2.552493	C	4.943252	-0.086020	0.527754
H	21.386012	4.007293	1.269218	O	4.744669	-1.137657	1.146300
N	20.400270	-0.263006	-0.912239	C	4.051948	2.258832	1.040048
C	21.619830	-1.052142	-0.856729	H	2.714166	-0.491607	1.353600
C	22.788123	-0.053122	-0.745872	H	3.721871	1.142140	-0.776483

C	-13.887363	-4.211640	-2.342674		O	22.611654	1.162591	-0.873302
N	-12.925952	-4.910562	-3.017999		C	21.757442	-1.982906	-2.075527
O	-15.079278	-4.461073	-2.458500		H	20.540967	0.709284	-1.165319
H	-15.803912	0.048415	-0.797004		H	21.581080	-1.666012	0.050755
H	-13.979318	-1.551517	0.783797		H	20.891565	-2.649252	-2.113363
H	-14.265083	-1.385866	-2.263899		H	21.796819	-1.403076	-3.003593
H	-15.333514	-2.327230	-1.219023		H	22.661206	-2.598354	-2.012210
H	-13.282356	-3.611414	-0.396397		N	23.999060	-0.600265	-0.511683
H	-12.353571	-2.813051	-1.668093		C	25.225375	0.177446	-0.475406
H	-13.230122	-5.596030	-3.695810		C	26.371315	-0.822485	-0.714919
H	-11.964430	-4.607196	-3.045776		O	26.186546	-2.032829	-0.655425
N	-12.288595	0.441340	0.777198		C	25.396847	0.926930	0.859560
C	-11.154753	1.372327	0.768312		H	24.140386	-1.605594	-0.469937
C	-9.815050	0.625199	0.976256		H	25.197043	0.910077	-1.291700
O	-9.104215	0.811738	1.969274		H	24.539398	1.587307	1.009778
C	-11.354347	2.452839	1.826530		H	25.452027	0.219160	1.692708
H	-12.939225	0.464860	1.565749		H	26.307584	1.535626	0.860829
H	-11.118371	1.822265	-0.232317		N	27.586310	-0.271391	-0.964373
H	-12.294682	2.983943	1.649642		H	27.725608	0.722880	-1.061337
H	-11.370778	2.017775	2.829934		H	28.372704	-0.887930	-1.115193
H	-10.531054	3.170452	1.794209		Ac-(Ala-Ala-Gln-Ala-Ala)$_3$-NH$_2$_C7$_{eq}$			
N	-9.485306	-0.225371	-0.024154		C	-21.169531	0.285100	1.190967
C	-8.353805	-1.151777	0.069746		O	-20.503744	-0.038143	2.178294
C	-7.029342	-0.454711	-0.323660		C	-22.467414	1.059163	1.325886
O	-6.398117	-0.772344	-1.338069		H	-22.278992	1.970284	1.901058
C	-8.607506	-2.382429	-0.795538		H	-22.922765	1.326294	0.367625
H	-10.155731	-0.331397	-0.787773		H	-23.177352	0.453699	1.898389
H	-8.266122	-1.441419	1.124547		N	-20.789238	-0.040435	-0.074654
H	-9.535823	-2.873123	-0.485785		C	-19.627476	-0.888816	-0.364117
H	-8.676842	-2.106618	-1.851972		C	-18.317653	-0.065445	-0.323181
H	-7.782904	-3.092783	-0.696627		O	-17.666657	0.179649	-1.344559
N	-6.624227	0.506580	0.538030		C	-19.801704	-1.587199	-1.708674
C	-5.507010	1.412660	0.247838		H	-21.336922	0.286026	-0.858810
C	-4.151621	0.752915	0.596978		H	-19.579117	-1.626976	0.444549
O	-3.428812	1.174458	1.506454		H	-20.726432	-2.172780	-1.713244
C	-5.690226	2.729844	0.995020		H	-19.824053	-0.860752	-2.527037
H	-7.248728	0.726774	1.316273		H	-18.961322	-2.259668	-1.897759
H	-5.509835	1.587220	-0.835724		N	-17.949387	0.343452	0.913036
H	-6.647066	3.185840	0.722623		C	-16.835763	1.271689	1.140308
H	-5.662247	2.571217	2.076894		C	-15.486322	0.513624	1.158114
H	-4.884400	3.423736	0.743656		O	-14.792009	0.430403	2.176832
N	-3.821445	-0.301397	-0.186056		C	-17.053580	2.047349	2.435438
C	-2.674660	-1.168612	0.099781		H	-18.597846	0.151490	1.678522
C	-1.366203	-0.556942	-0.456029		H	-16.810888	1.957720	0.283914
O	-0.725333	-1.092864	-1.367491		H	-18.005541	2.585735	2.397136
C	-2.916238	-2.564610	-0.465594		H	-17.056327	1.373729	3.297121
H	-4.513313	-0.604686	-0.874517		H	-16.245819	2.767842	2.585658
H	-2.570832	-1.212717	1.191678		N	-15.134266	-0.033574	-0.029303
H	-3.836228	-2.985261	-0.048062		C	-14.029541	-0.990073	-0.158989
H	-2.997232	-2.534761	-1.555940		C	-12.681366	-0.246080	-0.319157
H	-2.081152	-3.224226	-0.217050		O	-12.019675	-0.293201	-1.364411
N	-0.983031	0.592180	0.147967		C	-14.313969	-1.943464	-1.321893
C	0.098205	1.435930	-0.372400		C	-13.359427	-3.139181	-1.386935

H	11.184790	3.275379	-0.909334
H	12.055986	2.956482	-2.407882
N	13.130142	-0.280367	-0.335898
C	14.232951	-0.635687	0.562979
C	15.583355	-0.613042	-0.195484
O	16.242891	-1.639377	-0.403481
C	13.950853	-1.993552	1.210056
C	14.913129	-2.338603	2.351183
C	14.427322	-3.560985	3.131295
N	15.417626	-4.380765	3.598772
O	13.244380	-3.767353	3.364498
H	12.471534	-1.007618	-0.623287
H	14.281082	0.145601	1.333413
H	14.001554	-2.774222	0.442800
H	12.931988	-1.989314	1.609161
H	14.957778	-1.504790	3.067066
H	15.925519	-2.487654	1.964422
H	15.139821	-5.231493	4.068799
H	16.368236	-4.308578	3.268966
N	15.978658	0.616958	-0.594122
C	17.123076	0.833011	-1.486470
C	18.453284	0.874046	-0.693912
O	19.152357	1.891207	-0.640300
C	16.922368	2.110948	-2.294856
H	15.330590	1.389228	-0.425675
H	17.172754	-0.035610	-2.155521
H	15.990606	2.053279	-2.866137
H	16.887929	2.985493	-1.638653
H	17.755147	2.254564	-2.987534
N	18.779407	-0.291749	-0.090297
C	19.917274	-0.428227	0.825719
C	21.231492	-0.666663	0.035416
O	21.816429	-1.741475	0.041356
C	19.661663	-1.560492	1.813970
H	18.127159	-1.069971	-0.192316
H	20.014670	0.527874	1.353810
H	18.733897	-1.380754	2.367558
H	19.596694	-2.519608	1.291450
H	20.489081	-1.633491	2.524458
N	21.666861	0.435779	-0.633544
H	21.047859	1.237877	-0.731322
H	22.443583	0.320148	-1.270190

antiparallel Gly tripeptide

C	-6.207572	1.115760	0.000000
N	-5.410257	-0.098667	0.000000
C	-4.053948	-0.099734	0.000000
O	-3.362346	0.925585	0.000000
C	-3.442924	-1.493176	0.000000
N	-2.005189	-1.400888	0.000000
C	-1.280164	-2.536815	0.000000
O	-1.794790	-3.667364	0.000000
C	0.229940	-2.350071	0.000000
N	0.837886	-3.659589	0.000000
C	1.473397	0.919206	0.118486
O	2.187197	1.567899	0.894753
C	-0.154811	2.892538	0.023219
C	0.777358	3.890391	-0.671462
C	0.288655	5.326579	-0.474473
N	1.276497	6.262839	-0.336596
O	-0.897091	5.625778	-0.489432
H	-1.615227	0.979030	0.852802
H	0.086605	1.335654	-1.466244
H	-0.051006	2.992240	1.109563
H	-1.186327	3.151993	-0.233876
H	0.781371	3.706113	-1.755833
H	1.804849	3.763741	-0.317825
H	0.995858	7.214651	-0.143271
H	2.233260	6.003390	-0.149941
N	1.827282	-0.286734	-0.380821
C	2.978370	-1.045781	0.119852
C	4.288982	-0.588964	-0.564069
O	4.946746	-1.338695	-1.293312
C	2.745521	-2.540741	-0.074998
H	1.136231	-0.766094	-0.963215
H	3.075413	-0.811937	1.187984
H	1.827563	-2.848044	0.435283
H	2.665353	-2.787162	-1.137625
H	3.584414	-3.110789	0.331504
N	4.657201	0.682656	-0.280087
C	5.763639	1.355909	-0.966210
C	7.123291	1.001022	-0.316263
O	7.814844	1.848180	0.260312
C	5.536263	2.864258	-0.977677
H	4.026037	1.230685	0.307427
H	5.785538	0.967279	-1.992334
H	4.584032	3.096772	-1.465201
H	5.529885	3.263052	0.041105
H	6.342283	3.365186	-1.519458
N	7.487271	-0.295020	-0.448878
C	8.631763	-0.874070	0.263107
C	9.955222	-0.605484	-0.491912
O	10.630981	-1.518479	-0.978875
C	8.414305	-2.368117	0.482217
H	6.822345	-0.921385	-0.906868
H	8.702360	-0.355920	1.228085
H	7.485986	-2.534897	1.037316
H	8.362275	-2.898792	-0.472863
H	9.246156	-2.792912	1.049157
N	10.317275	0.697756	-0.550492
C	11.448346	1.167206	-1.356506
C	12.782695	1.003025	-0.589133
O	13.470514	1.973119	-0.251633
C	11.228410	2.615733	-1.780915
H	9.671542	1.381530	-0.151073
H	11.502184	0.516177	-2.238509
H	10.295296	2.704636	-2.345834

C	4.416301	1.156350	0.000000		C	2.174252	-3.821084	0.000000
O	3.640946	2.126778	0.000000		O	2.953713	-2.850545	0.000000
C	5.917251	1.333082	0.000000		C	2.682247	-5.244125	0.000000
H	-2.812818	-6.176306	0.891836		H	-6.837890	1.164653	0.891696
H	-2.812818	-6.176306	-0.891836		H	-6.837890	1.164653	-0.891696
H	-3.238873	-4.699086	0.000000		H	-5.520898	1.959813	0.000000
H	-0.486543	-5.823786	0.000000		H	-5.889313	-0.990371	0.000000
H	1.080977	-4.091065	-0.877426		H	-3.792057	-2.051928	0.878566
H	1.080977	-4.091065	0.877426		H	-3.792057	-2.051928	-0.878566
H	0.224889	-1.496842	0.000000		H	-1.564261	-0.478806	0.000000
H	2.061000	0.122378	-0.868716		H	0.535974	-1.768961	0.875324
H	2.061000	0.122378	0.868716		H	0.535974	-1.768961	-0.875324
H	4.554303	-0.931537	0.000000		H	0.185731	-4.438956	0.000000
H	6.202846	1.911010	0.881826		H	3.309257	-5.393105	0.882075
H	6.202846	1.911010	-0.881826		H	3.309257	-5.393105	-0.882075
H	6.458029	0.383965	0.000000		H	1.878979	-5.983847	0.000000
N	-4.395747	-1.481511	0.000000		N	4.946087	-0.692986	0.000000
C	-5.786350	-1.891987	0.000000		C	6.396899	-0.712227	0.000000
C	-4.026860	-0.178040	0.000000		C	4.246887	0.461271	0.000000
O	-4.807206	0.782059	0.000000		O	4.743679	1.597608	0.000000
C	-2.518908	0.014381	0.000000		C	2.733927	0.266544	0.000000
N	-2.216905	1.422061	0.000000		N	2.113808	1.569386	0.000000
C	-0.928261	1.815799	0.000000		C	0.778789	1.716833	0.000000
O	0.000000	0.987662	0.000000		O	0.000000	0.744734	0.000000
C	-0.696449	3.313070	0.000000		C	0.288745	3.153611	0.000000
N	0.711624	3.624335	0.000000		N	-1.151176	3.187368	0.000000
C	1.069190	4.939393	0.000000		C	-1.776906	4.394656	0.000000
O	0.213030	5.833793	0.000000		O	-1.141920	5.456183	0.000000
C	2.550823	5.238198	0.000000		C	-3.289224	4.353883	0.000000
H	-3.653299	-2.176204	0.000000		H	4.426144	-1.569332	0.000000
H	-6.021350	-2.481025	-0.891381		H	6.778146	-1.220204	0.890349
H	-6.392437	-0.986388	0.000000		H	6.740067	0.321697	0.000000
H	-6.021350	-2.481025	0.891381		H	6.778146	-1.220204	-0.890349
H	-2.080607	-0.476919	-0.875330		H	2.432085	-0.315488	0.876284
H	-2.080607	-0.476919	0.875330		H	2.432085	-0.315488	-0.876284
H	-3.008744	2.059275	0.000000		H	2.760600	2.355813	0.000000
H	-1.187476	3.760142	-0.874897		H	0.687693	3.681354	0.876454
H	-1.187476	3.760142	0.874897		H	0.687693	3.681354	-0.876454
H	1.396495	2.871144	0.000000		H	-1.657660	2.305529	0.000000
H	2.776441	5.845826	0.880134		H	-3.651441	4.889029	-0.881402
H	2.776441	5.845826	-0.880134		H	-3.651441	4.889029	0.881402
H	3.169236	4.340802	0.000000		H	-3.673418	3.333814	0.000000

antiparallel Gly pentapeptide					parallel Gly tripeptide			
N	8.320866	1.425969	0.000000		C	-2.601376	-5.581173	0.000000
C	9.762237	1.260197	0.000000		N	-1.221508	-5.127277	0.000000
C	7.480240	0.370792	0.000000		C	-0.863864	-3.820750	0.000000
O	7.825034	-0.820781	0.000000		O	-1.674546	-2.883198	0.000000
C	6.006032	0.759069	0.000000		C	0.640062	-3.599163	0.000000
N	5.220426	-0.453274	0.000000		N	0.965641	-2.195204	0.000000
C	3.879977	-0.405690	0.000000		C	2.273502	-1.836770	0.000000
O	3.251788	0.669045	0.000000		O	3.188286	-2.673619	0.000000
C	3.163221	-1.748478	0.000000		C	2.533072	-0.345683	0.000000
N	1.740199	-1.510326	0.000000		N	3.954902	-0.113470	0.000000

H	7.332865	6.286599	-0.882133		C	0.871916	-2.539763	0.000000
H	4.101425	5.795419	0.000000		O	1.216622	-3.731440	0.000000
H	4.071056	3.103294	0.875409		C	-0.596635	-2.132795	0.000000
H	4.071056	3.103294	-0.875409		N	-1.395229	-3.334935	0.000000
H	1.843746	2.112349	0.000000		C	-2.738730	-3.291629	0.000000
H	-0.207266	3.899180	0.879304		O	-3.372075	-2.219284	0.000000
H	-0.207266	3.899180	-0.879304		C	-3.424549	-4.645706	0.000000
H	-2.497840	2.890025	0.000000		N	-4.855324	-4.480809	0.000000
H	-2.534276	0.192570	0.875372		C	-5.639632	-5.592095	0.000000
H	-2.534276	0.192570	-0.875372		O	-5.153888	-6.729555	0.000000
H	-4.787694	-0.791821	0.000000		C	-7.132372	-5.347193	0.000000
H	-6.781372	1.067123	-0.878840		H	7.916767	2.361916	0.000000
H	-6.781372	1.067123	0.878840		H	10.204612	1.715528	0.890392
H	-9.002333	0.290948	0.000000		H	10.204612	1.715528	-0.890392
H	-10.226471	-1.720013	-0.891716		H	9.971630	0.191017	0.000000
H	-10.226471	-1.720013	0.891716		H	5.779366	1.374696	0.875817
H	-9.026132	-2.682233	0.000000		H	5.779366	1.374696	-0.875817
parallel Gly pentapeptide					H	5.756553	-1.319056	0.000000
N	-8.313542	-1.706309	0.000000		H	3.461176	-2.333770	0.879437
C	-6.959908	-1.715946	0.000000		H	3.461176	-2.333770	-0.879437
O	-6.275204	-2.749726	0.000000		H	1.418036	-0.541883	0.000000
C	-6.339538	-0.327406	0.000000		H	-0.812366	-1.513514	0.876171
N	-4.899038	-0.396032	0.000000		H	-0.812366	-1.513514	-0.876171
C	-4.197730	0.763293	0.000000		H	-0.869442	-4.206677	0.000000
O	-4.747238	1.874078	0.000000		H	-3.102451	-5.223758	-0.876369
C	-2.690464	0.607316	0.000000		H	-3.102451	-5.223758	0.876369
N	-2.084781	1.916824	0.000000		H	-5.237290	-3.538476	0.000000
C	-0.743273	2.025517	0.000000		H	-7.563475	-5.828589	0.881301
O	0.000000	1.028658	0.000000		H	-7.563475	-5.828589	-0.881301
C	-0.195587	3.442534	0.000000		H	-7.375677	-4.284707	0.000000
N	1.246370	3.410503	0.000000		O	6.610842	3.822209	0.000000
C	1.939851	4.571558	0.000000		C	5.981006	4.896697	0.000000
O	1.389483	5.683071	0.000000		C	6.690918	6.230328	0.000000
C	3.446526	4.410205	0.000000		N	4.635476	4.930654	0.000000
N	4.058502	5.714438	0.000000		C	3.847951	3.721163	0.000000
C	5.404568	5.814192	0.000000		C	2.376284	4.114567	0.000000
O	6.129218	4.804771	0.000000		O	2.019884	5.303490	0.000000
C	-9.125711	-2.911097	0.000000		N	1.514998	3.079162	0.000000
C	5.982292	7.210912	0.000000		C	0.091412	3.313911	0.000000
H	-8.785126	-0.810110	0.000000		C	-0.625466	1.971649	0.000000
H	-6.692226	0.230325	0.877722		O	0.000000	0.896854	0.000000
H	-6.692226	0.230325	-0.877722		N	-1.967305	2.021427	0.000000
H	-4.431440	-1.300428	0.000000		C	-2.756334	0.810361	0.000000
H	-2.369791	0.028997	0.871314		C	-4.224215	1.207371	0.000000
H	-2.369791	0.028997	-0.871314		O	-4.574130	2.398809	0.000000
H	-2.716422	2.713066	0.000000		N	-5.098132	0.181909	0.000000
H	-0.569517	3.985019	0.878217		C	-6.510427	0.467091	0.000000
H	-0.569517	3.985019	-0.878217		C	-7.300532	-0.833421	0.000000
H	1.722194	2.509407	0.000000		O	-6.748896	-1.940518	0.000000
H	3.766699	3.828476	-0.869505		N	-8.644769	-0.656081	0.000000
H	3.766699	3.828476	0.869505		C	-9.595333	-1.754920	0.000000
H	3.431530	6.511992	0.000000		H	7.332865	6.286599	0.882133
H	-9.755742	-2.952002	-0.891855		H	6.003741	7.078951	0.000000

C	-0.666609	2.570699	2.144962	H	-9.755742	-2.952002	0.891855
N	1.560715	2.317201	-0.326356	H	-8.450688	-3.764709	0.000000
C	2.685989	1.486275	-0.731422	H	6.616007	7.329034	0.881867
C	3.831905	1.805504	0.222592	H	5.215350	7.988787	0.000000
O	4.090039	2.986572	0.502057	H	6.616007	7.329034	-0.881867
C	3.098320	1.781902	-2.170684	N	-5.692660	-5.779277	0.000000
N	4.508900	0.731402	0.684239	C	-4.339123	-5.775618	0.000000
C	5.652178	0.873107	1.566144	O	-3.621201	-6.783382	0.000000
H	-4.213512	2.175225	-0.940752	C	-3.748281	-4.375250	0.000000
H	-4.692103	3.895697	-0.836849	N	-2.309804	-4.466138	0.000000
H	-3.865239	3.305896	-2.277549	C	-1.588896	-3.332517	0.000000
H	-2.322336	1.643893	0.052373	O	-2.134941	-2.213570	0.000000
H	-0.352823	3.822264	0.402179	C	-0.078428	-3.488928	0.000000
H	0.323632	2.721908	2.587179	N	0.539574	-2.184786	0.000000
H	-1.369646	3.273886	2.597990	C	1.887594	-2.080750	0.000000
H	-0.994755	1.549893	2.361510	O	2.640554	-3.065000	0.000000
H	1.794405	3.276043	-0.081576	C	2.414817	-0.657193	0.000000
H	2.373872	0.445292	-0.629688	N	3.855564	-0.694087	0.000000
H	2.257926	1.597227	-2.844774	C	4.556645	0.457449	0.000000
H	3.935261	1.139752	-2.461681	O	3.993964	1.566236	0.000000
H	3.409113	2.826347	-2.260919	C	6.063831	0.293006	0.000000
H	4.173276	-0.199739	0.441117	N	6.739688	1.567011	0.000000
H	5.426189	0.494160	2.567594	C	8.102545	1.555709	0.000000
H	6.512675	0.330134	1.166154	O	8.731532	0.488883	0.000000
H	5.888443	1.934874	1.631453	C	-6.464539	-7.007488	0.000000
C	3.741428	-4.040708	0.305265	C	8.794107	2.899463	0.000000
C	2.827236	-2.944112	-0.192509	H	-6.160611	-4.876454	0.000000
O	3.177062	-1.751675	-0.162578	H	-4.100365	-3.819750	0.875344
N	1.634115	-3.344798	-0.690111	H	-4.100365	-3.819750	-0.875344
C	0.567332	-2.413313	-1.024861	H	-1.912422	-5.402331	0.000000
C	-0.654962	-2.835248	-0.219466	H	0.236748	-4.066975	0.878442
O	-0.968979	-4.035266	-0.146212	H	0.236748	-4.066975	-0.878442
C	0.245357	-2.439646	-2.516639	H	-0.057589	-1.358979	0.000000
N	-1.336994	-1.827208	0.371142	H	2.035989	-0.116121	-0.872840
C	-2.585760	-2.071020	1.064262	H	2.035989	-0.116121	0.872840
C	-3.664677	-1.197011	0.441205	H	4.286010	-1.614774	0.000000
O	-3.477641	0.009721	0.222156	H	6.366349	-0.298556	0.874593
C	-2.467061	-1.763809	2.557407	H	6.366349	-0.298556	-0.874593
N	-4.855382	-1.796481	0.212640	H	6.199929	2.430115	0.000000
C	-5.968286	-1.057886	-0.363211	H	-7.094761	-7.073349	-0.891483
H	4.702950	-3.952808	-0.205093	H	-7.094761	-7.073349	0.891483
H	3.916752	-3.891913	1.373771	H	-5.757080	-7.836234	0.000000
H	3.337578	-5.042410	0.144007	H	9.440457	2.949867	0.880079
H	1.333969	-4.307133	-0.564522	H	8.100444	3.739780	0.000000
H	0.896276	-1.416099	-0.728964	H	9.440457	2.949867	-0.880079
H	-0.544384	-1.716540	-2.742558	antiparallel Ala tripeptide			
H	-0.092387	-3.437576	-2.810208	C	-3.929231	3.198935	-1.191383
H	1.137071	-2.177918	-3.092007	C	-2.598163	3.597145	-0.587814
H	-1.024444	-0.859813	0.243345	O	-2.160517	4.750556	-0.664115
H	-2.808801	-3.133011	0.918920	N	-1.929231	2.582659	0.033106
H	-3.416733	-1.950851	3.068780	C	-0.629754	2.788446	0.631169
H	-2.193417	-0.715594	2.701656	C	0.357970	1.814587	0.008947
H	-1.694356	-2.397475	2.999266	O	0.053167	0.616857	-0.153453

H	-5.049145	-3.131153	-1.172277
H	-4.650719	-4.241954	0.163391
H	-2.528330	-3.866836	0.785269
H	-1.507552	-1.125982	0.626158
H	-0.126582	-1.501423	2.681577
H	-0.907387	-3.083290	2.912822
H	-1.862541	-1.587472	3.063721
H	0.422685	-1.055792	-0.424465
H	1.708262	-3.691085	-0.915192
H	2.452650	-2.760045	-3.157353
H	1.542126	-1.274934	-2.797711
H	0.680149	-2.819389	-2.994936
H	3.871389	-3.802831	-0.383883
H	5.257698	-1.944551	1.119545
H	6.056266	-3.095626	0.017589
H	5.625111	-1.464227	-0.549444

antiparallel Ala tetrapeptide

C	-6.246146	2.324525	-1.296926
C	-5.025495	3.048830	-0.768779
O	-4.860261	4.263123	-0.930611
N	-4.132152	2.254861	-0.109337
C	-2.899678	2.790084	0.422914
C	-1.732019	2.020125	-0.171856
O	-1.760128	0.776940	-0.240860
C	-2.850490	2.678282	1.947999
N	-0.679925	2.754186	-0.587265
C	0.588498	2.159718	-0.982127
C	1.668336	2.780069	-0.104808
O	1.688022	4.004077	0.099483
C	0.891083	2.424758	-2.454776
N	2.569403	1.899476	0.387338
C	3.698617	2.323360	1.186229
C	3.615464	1.748045	2.600685
C	4.980024	1.840435	0.520813
O	5.108262	0.670404	0.127403
N	5.986880	2.742061	0.464907
C	7.278256	2.402763	-0.111768
H	-6.273179	1.275256	-0.997590
H	-7.138291	2.839329	-0.932928
H	-6.247834	2.395907	-2.387779
H	-4.297475	1.253552	-0.025609
H	-2.870572	3.840559	0.116909
H	-1.910588	3.079949	2.340971
H	-3.684329	3.235523	2.381721
H	-2.932453	1.627876	2.242274
H	-0.667749	3.757363	-0.424815
H	0.513934	1.086999	-0.793756
H	0.095199	2.008693	-3.077731
H	1.840999	1.958546	-2.734259
H	0.960932	3.501406	-2.633350
H	2.463692	0.902217	0.190729
H	3.656051	3.416923	1.216943
H	4.477477	2.058498	3.199684

H	-4.914418	-2.803348	0.286516
H	-5.798668	-0.840453	-1.421762
H	-6.875848	-1.652356	-0.254662
H	-6.084714	-0.114075	0.170500

parallel Ala tripeptide

C	-5.022037	1.924695	-1.396792
C	-3.889160	2.645375	-0.696434
O	-3.800720	3.878677	-0.679601
N	-2.965890	1.822064	-0.119738
C	-1.828165	2.350166	0.596035
C	-0.553075	1.805982	-0.029158
O	-0.463782	0.598831	-0.325109
C	-1.871628	1.968691	2.077051
N	0.444916	2.690773	-0.218705
C	1.773724	2.299702	-0.661703
C	2.760641	2.796533	0.388295
O	2.662331	3.947186	0.837884
C	2.101387	2.916679	-2.019298
N	3.720592	1.906497	0.732221
C	4.752639	2.230806	1.698603
H	-5.070064	0.866696	-1.131862
H	-5.959526	2.420865	-1.138164
H	-4.883244	2.020724	-2.477499
H	-3.105895	0.812261	-0.122352
H	-1.879620	3.437621	0.481590
H	-0.993243	2.351187	2.607650
H	-2.772072	2.386665	2.533909
H	-1.897753	0.880282	2.178110
H	0.352192	3.643120	0.123486
H	1.782154	1.210142	-0.723423
H	1.366498	2.596625	-2.762291
H	3.098115	2.604335	-2.345972
H	2.084323	4.007433	-1.944091
H	3.658225	0.961060	0.360899
H	4.645590	1.627188	2.605212
H	5.746154	2.062694	1.273493
H	4.641261	3.283850	1.955789
C	-4.850966	-3.201084	-0.100077
C	-3.709935	-2.269290	0.242363
O	-3.806701	-1.046809	0.053264
N	-2.613516	-2.855216	0.787552
C	-1.377965	-2.131015	1.030792
C	-0.270012	-2.862777	0.284696
O	-0.185547	-4.100483	0.341213
C	-1.046977	-2.071872	2.520457
N	0.587618	-2.065671	-0.395519
C	1.716815	-2.614838	-1.115443
C	2.994523	-1.973075	-0.597013
O	3.086654	-0.741844	-0.462950
C	1.592457	-2.352034	-2.617012
N	4.036344	-2.804919	-0.376819
C	5.317870	-2.296564	0.085453
H	-5.746344	-2.861791	0.425244

C	3.488032	-2.490941	0.419814
C	2.238725	-1.845986	-0.157348
O	2.149323	-0.607349	-0.235435
C	3.458930	-2.358661	1.944191
N	1.251705	-2.686431	-0.537146
C	-0.062526	-2.214879	-0.939795
C	-1.093900	-2.882759	-0.041215
O	-1.037371	-4.099702	0.191092
C	-0.351141	-2.557411	-2.400057
N	-2.063771	-2.055587	0.421500
C	-3.163594	-2.550789	1.220581
C	-3.140952	-1.949807	2.626944
C	-4.472924	-2.185510	0.536895
O	-4.682124	-1.033183	0.122824
N	-5.412404	-3.154935	0.486385
C	-6.710820	-2.912602	-0.122311
H	6.728273	-0.734313	-1.048797
H	7.687556	-2.245276	-1.041338
H	6.721526	-1.832949	-2.456276
H	4.755280	-0.843123	-0.057121
H	3.552060	-3.544404	0.129988
H	2.566531	-2.835954	2.363052
H	4.347468	-2.833292	2.367525
H	3.454655	-1.300718	2.222266
H	1.346881	-3.684945	-0.377322
H	-0.068778	-1.133948	-0.792453
H	0.405951	-2.102330	-3.043822
H	-1.337327	-2.180514	-2.689299
H	-0.334864	-3.641983	-2.539692
H	-2.001333	-1.052102	0.235468
H	-3.035045	-3.636953	1.270411
H	-3.981993	-2.318118	3.223040
H	-2.206553	-2.220468	3.124236
H	-3.206977	-0.860108	2.562790
H	-5.144087	-4.102068	0.719393
H	-7.134065	-1.994382	0.287248
H	-7.368263	-3.749971	0.111864
H	-6.628665	-2.806590	-1.207867
C	6.520459	3.169898	-0.236013
C	5.395041	2.264791	0.212737
O	5.476901	1.032821	0.084627
N	4.325998	2.884052	0.773257
C	3.089970	2.182156	1.075406
C	1.967445	2.905545	0.341813
O	1.896185	4.144534	0.365932
C	2.804436	2.171430	2.575423
N	1.085192	2.094162	-0.284993
C	-0.114478	2.600232	-0.919702
C	-1.307312	1.889380	-0.297728
O	-1.264713	0.657646	-0.118233
C	-0.096308	2.345596	-2.427190
N	-2.371507	2.650930	0.018347
C	-3.632773	2.085514	0.473966
H	2.700193	2.096150	3.085446
H	3.599172	0.655948	2.549301
H	5.784106	3.707098	0.688318
H	7.705666	1.546856	0.413198
H	7.941793	3.260532	-0.000111
H	7.182984	2.153032	-1.171641
C	6.215467	-2.268351	-1.391578
C	5.011765	-3.023429	-0.872100
O	4.844710	-4.226955	-1.099359
N	4.142520	-2.280758	-0.122646
C	2.921420	-2.867155	0.386226
C	1.741645	-2.047386	-0.109922
O	1.768323	-0.802999	-0.075929
C	2.909138	-2.935803	1.914465
N	0.682210	-2.744695	-0.567815
C	-0.578190	-2.112742	-0.925496
C	-1.671275	-2.765321	-0.091116
O	-1.709726	-3.998607	0.041647
C	-0.884278	-2.282679	-2.411522
N	-2.565089	-1.904545	0.452643
C	-3.732820	-2.381466	1.164511
C	-3.694080	-1.975347	2.638162
C	-4.973987	-1.799952	0.503367
O	-5.055432	-0.593835	0.222882
N	-6.002412	-2.656940	0.312332
C	-7.246800	-2.211895	-0.295232
H	6.175933	-1.204152	-1.157852
H	7.116304	-2.707092	-0.954748
H	6.271767	-2.412141	-2.473088
H	4.283179	-1.276948	-0.015856
H	2.885376	-3.879184	-0.029322
H	1.977022	-3.381897	2.276995
H	3.749260	-3.546228	2.254538
H	3.005165	-1.933790	2.341047
H	0.669391	-3.757563	-0.488384
H	-0.488890	-1.054233	-0.678761
H	-0.078658	-1.846898	-3.008025
H	-1.822032	-1.776359	-2.660425
H	-0.978797	-3.344325	-2.656838
H	-2.477884	-0.901171	0.269303
H	-3.714787	-3.472738	1.076805
H	-4.581203	-2.340283	3.165639
H	-2.802105	-2.396026	3.108503
H	-3.661345	-0.885947	2.722023
H	-5.838343	-3.647153	0.436485
H	-7.575699	-1.294634	0.194374
H	-7.999848	-2.988334	-0.157890
H	-7.120469	-2.010635	-1.362969

parallel Ala tetrapeptide

C	6.754526	-1.778210	-1.364681
C	5.600156	-2.584404	-0.809102
O	5.522071	-3.809960	-0.958554
N	4.656132	-1.854378	-0.144856

C	-3.947757	2.525535	1.901217
C	-4.715173	2.577087	-0.479317
O	-4.748665	3.769634	-0.815771
N	-5.599024	1.631065	-0.870515
C	-6.710361	1.940746	-1.750846
H	6.370621	4.213843	0.047950
H	7.453848	2.806244	0.198252
H	6.611012	3.102486	-1.323190
H	4.242906	3.894790	0.718799
H	3.197823	1.162826	0.700406
H	1.876616	1.627641	2.780075
H	3.626127	1.682678	3.105681
H	2.699524	3.196150	2.942949
H	1.237663	1.083082	-0.276244
H	-0.144081	3.674791	-0.712531
H	0.762435	2.852595	-2.873564
H	-1.013004	2.717283	-2.896572
H	-0.013400	1.271789	-2.617072
H	-2.395996	3.631776	-0.247533
H	-3.534467	1.000093	0.420886
H	-4.889858	2.078923	2.234009
H	-3.146901	2.210953	2.575729
H	-4.043896	3.614008	1.941992
H	-5.430793	0.666968	-0.591491
H	-6.729340	3.021674	-1.887140
H	-7.654224	1.612109	-1.307446
H	-6.586142	1.458436	-2.725018