SUPPORTING INFORMATION

Title: Synthesis of Intrinsically Blue-Colored bis-Nitronyl Nitroxide Peptidomimetic Templates and Their Conformational Preferences as Revealed by a Combined Spectroscopic Analysis

Authors: Marta De Zotti,* Karen Wright,* Edouard d'Aboville, Antonio Toffoletti, Claudio Toniolo, Giovanna Longhi, Giuseppe Mazzeo, Sergio Abbate, Fernando Formaggio

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I) *bis*-(*R*)-Aic(CN) pentapeptide

Table S1. Gibbs free energy and backbone dihedral angles for the right- and left-handed 3_{10}-helical conformers of the *bis*-(*R*)-Aic(CN) pentapeptide. Initial conditions with α-helix dihedral angles give the same structures

	G (Kcal/mole)	φ_1	ψ_1	φ_2	ψ_2	φ_3	ψ_3	φ_4	ψ_4	φ_5
a	0.0	-66.2	-26.8	-61.8	-20.3	-65.6	-16.6	-65.2	-23.8	-98.0
b	2.1	-64.0	-31.5	-59.2	-24.8	-69.0	-12.1	-66.0	-27.7	-92.9
c	0.5	-64.9	-29.1	-62.4	-19.9	-67.1	-13.7	-64.8	-28.8	-93.4
left1	4.4	64.4	29.8	55.3	28.0	55.9	29.6	66.7	19.3	51.2
left2	5.5	62.8	33.6	55.0	27.8	57.4	24.5	64.7	25.0	51.0

The three conformers **a-c** differ in the puckering of the five-membered rings of their Aic(CN) goups, while the backbone structures are nearly superimposable and of the right-handed 3_{10}-helix type. Identical geometries are obtained when optimization starts from either the 3_{10}- or the α-helix geometry. Left-handed structures present considerably higher energy.

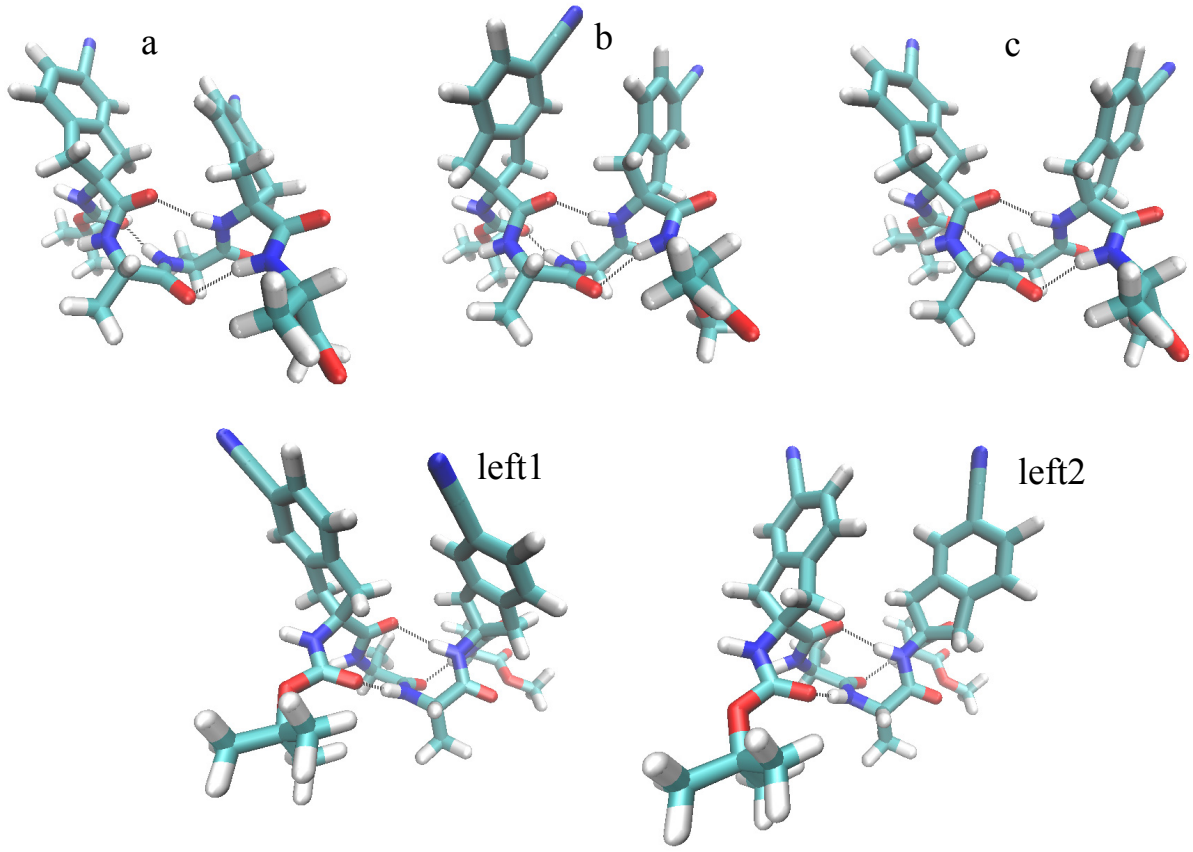
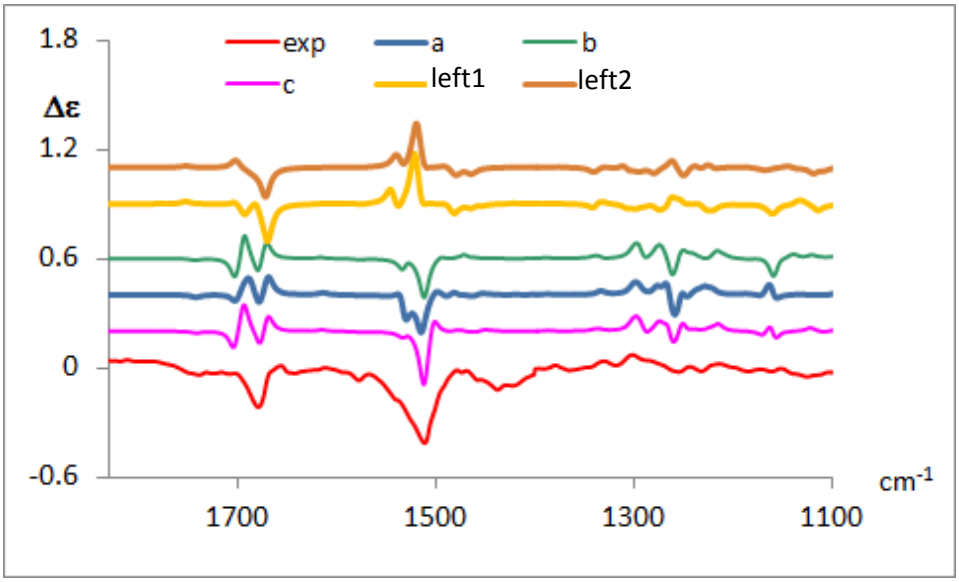


Figure S1. *Optimized 3D-structures for the bis-(R)-Aic(CN) pentapeptide, with the intramolecular H-bonds (distance cutoff 3.1 Å, angle cut-off 20°) highlighted.*



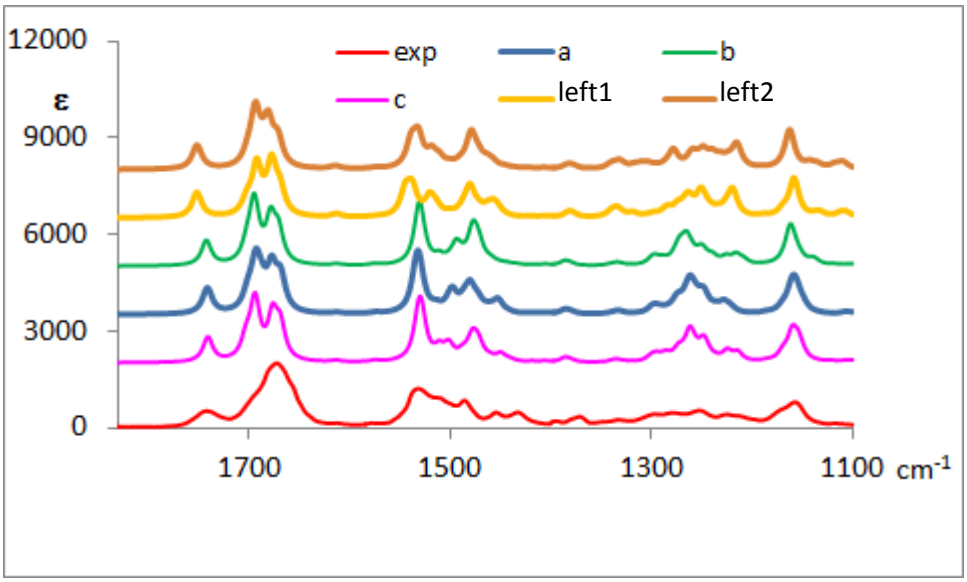


Figure S2. *Calculated IR absorption and VCD spectra for the bis-(R)-Aic(CN) pentapeptide. The calculated spectra correspond to the three right-handed 3_{10}-helix conformers* ***a-c*** *[with different Aic(CN) group orientation] and two left-handed conformers, with the geometrical and energetic characteristics reported in Table S1.*

II) *bis*-(*R*)-Aic(NN) hexapeptide

IR absorption and VCD spectra [optimization starting from the bis-(*R*)-Aic(CN) pentapeptide right-handed 3_{10}-helix structures].

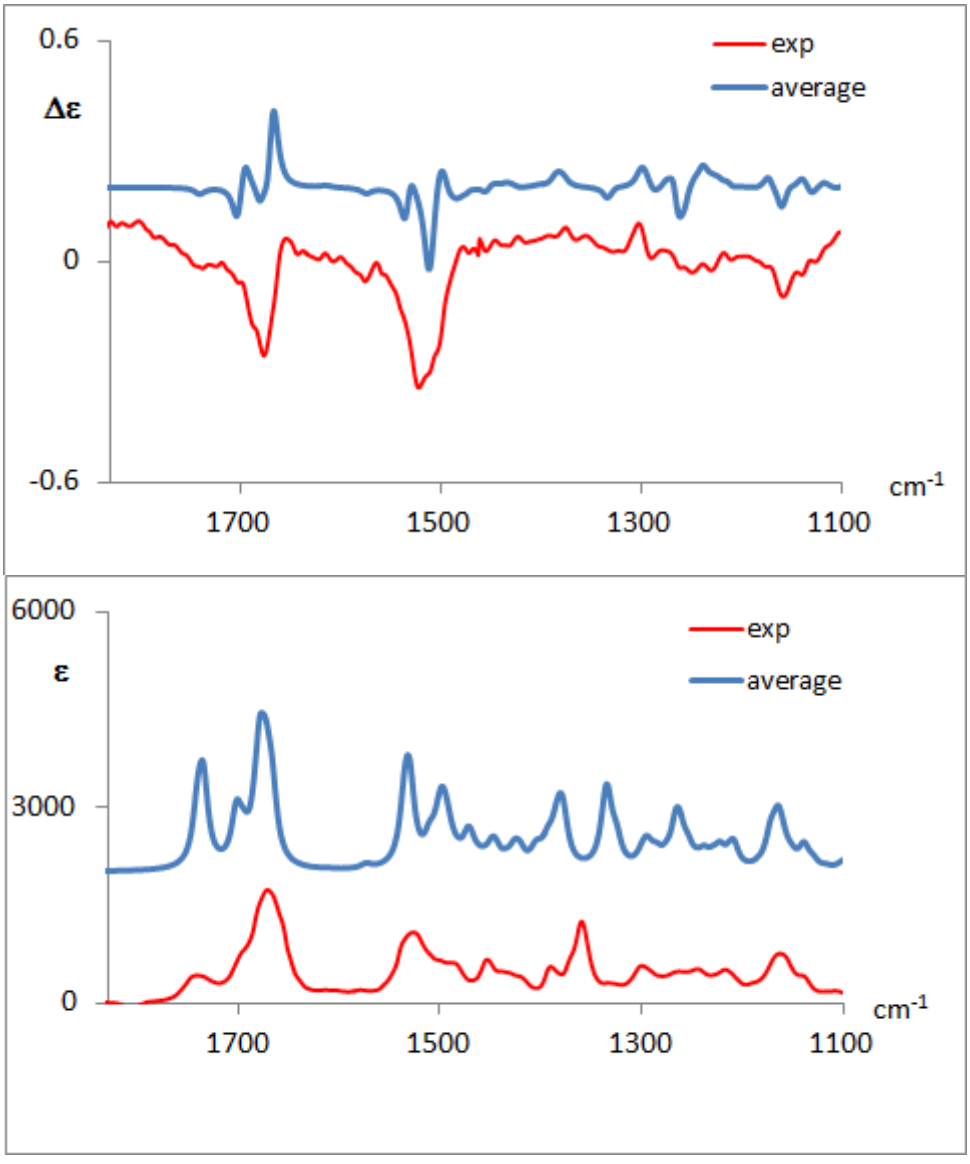


Figure S3. *Experimental and calculated IR absorption and VCD spectra for the bis-(R)-Aic(NN) hexapeptide. The calculated spectra correspond to a weighted average of the two conformers* ***a*** *and* ***c*** *(37%,63%). For a better comparison, the calculated wavenumbers have been scaled by 0.97.*

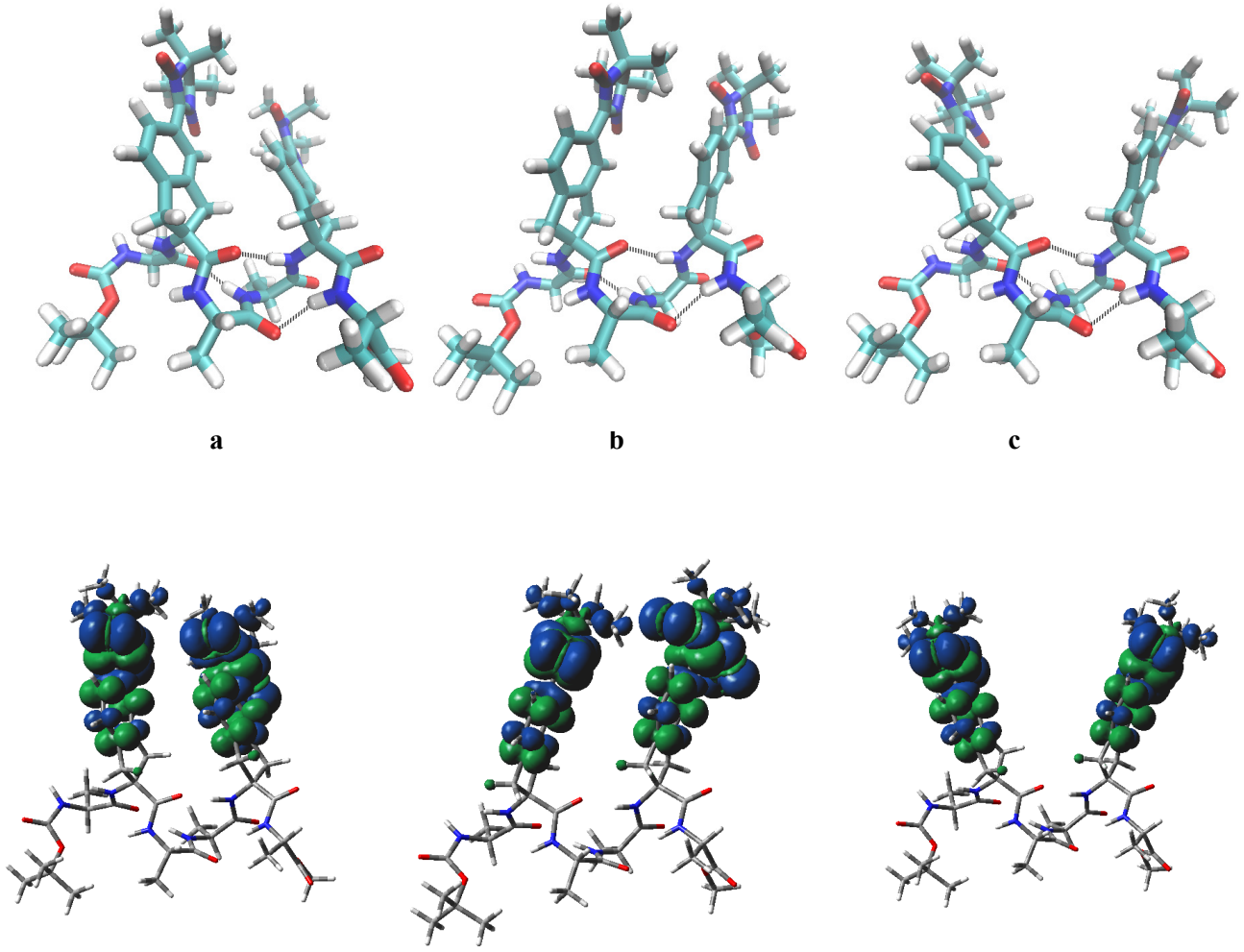


Figure S4. *Top: optimized 3D-structures for the bis-(R)-Aic(NN) hexapeptide with the intramolecular H-bonds highlighted (distance cutoff 3.1 Å, angle cut-off 20°). Considering the Gibbs free energy:* ***c*** *is the most stable structure,* ***a*** *is 0.3 kcal/mol higher, and* ***b*** *is 2.2 kcal/mol higher. Bottom: spin densities are highlighted (in green and blue, respectively, according to the phase).*

Table S2. Calculated distances (Å) for the right-handed 3_{10}-helical conformers of the *bis*-(*R*)-Aic(NN) hexapeptide

distance	***a***	***b***	***c***
C(NN)···C(NN)	*6.53*	*6.89*	*10.60*

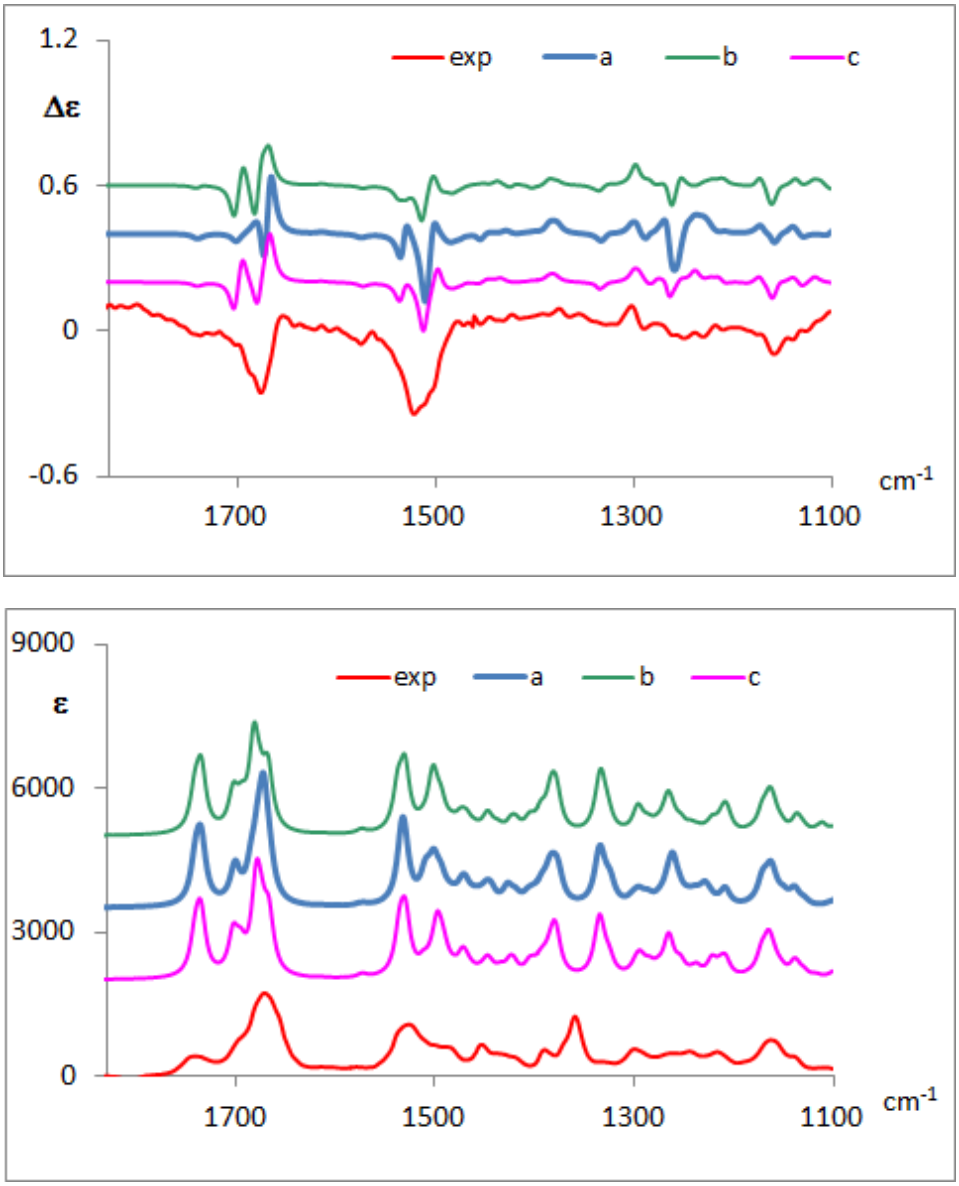
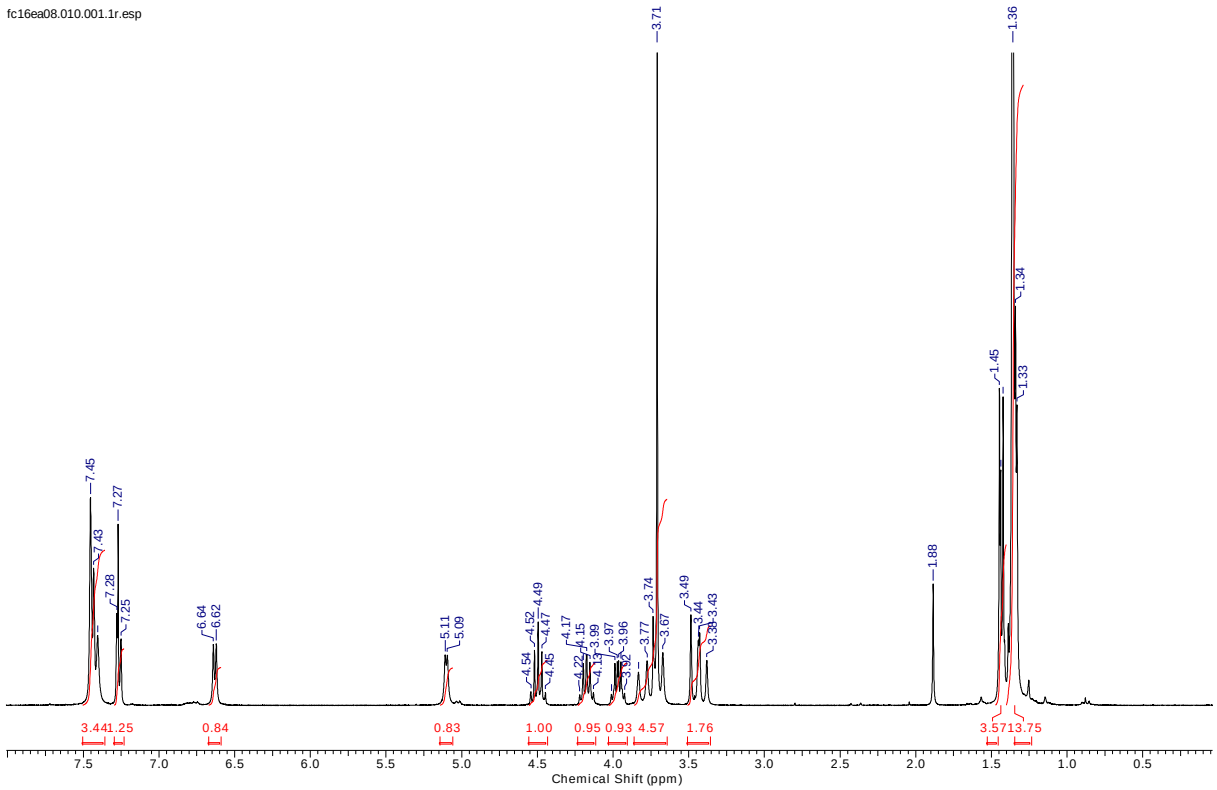
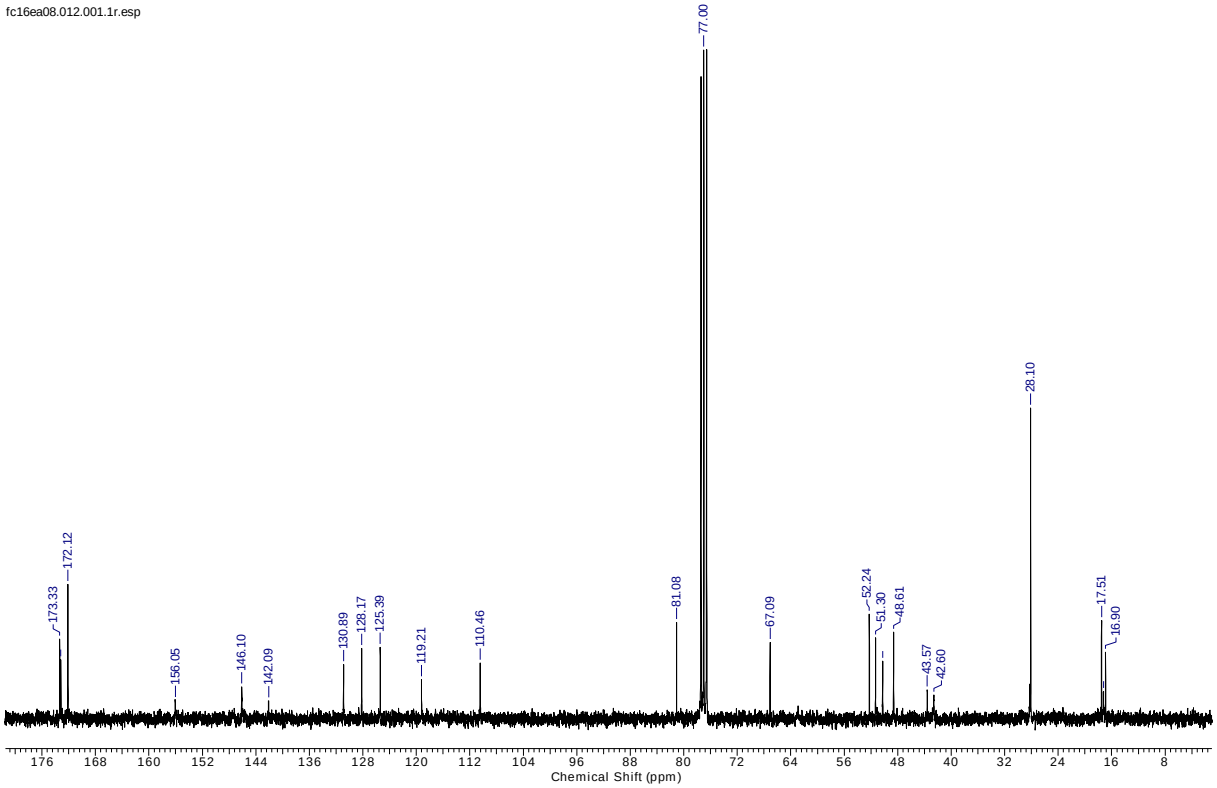


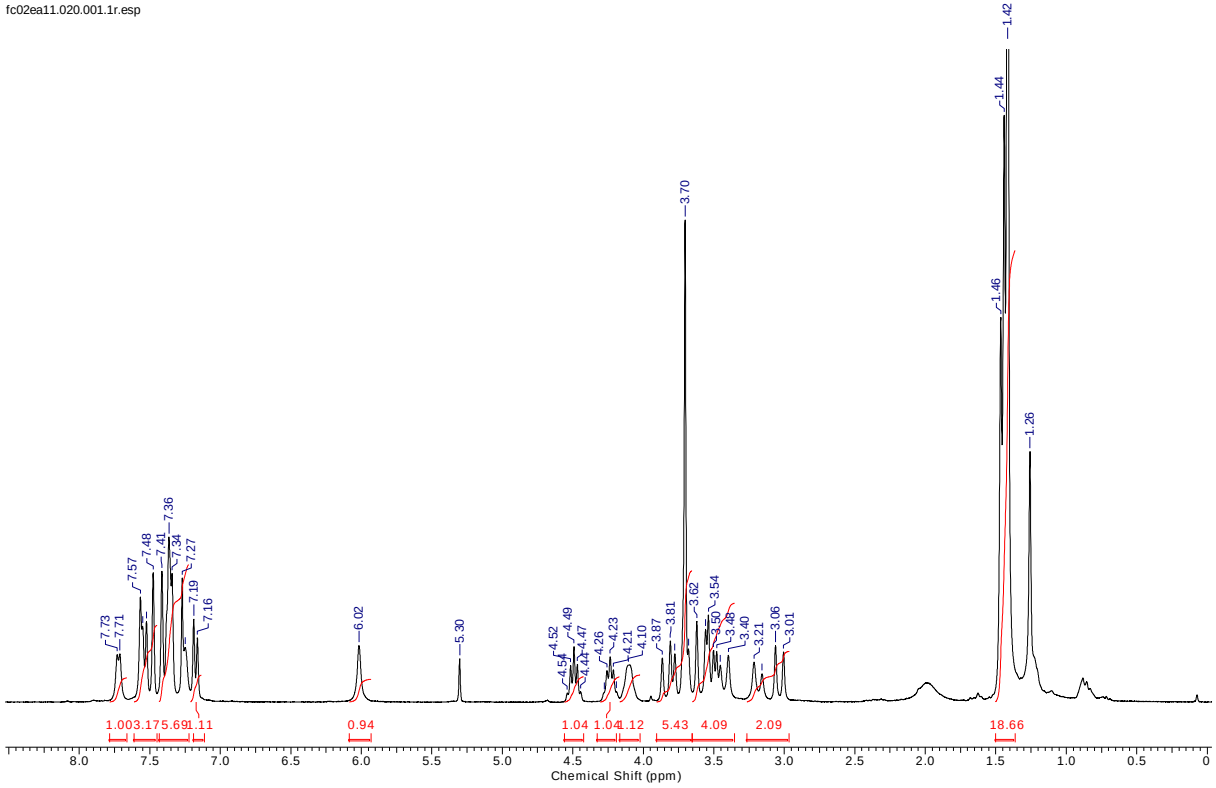
Figure S5. *Experimental and calculated VCD spectra for the bis-(R)-Aic(NN) hexapeptide. The calculated spectra correspond to each of the three right-handed 3_{10}-helical conformers* ***a*****-****c** *(with different Aic(NN) group orientation). Considering the Gibbs free energy:* ***c*** *is the most stable structure,* ***a*** *is 0.3 kcal/mol higher, and* ***b*** *is 2.2 kcal/mol higher.*

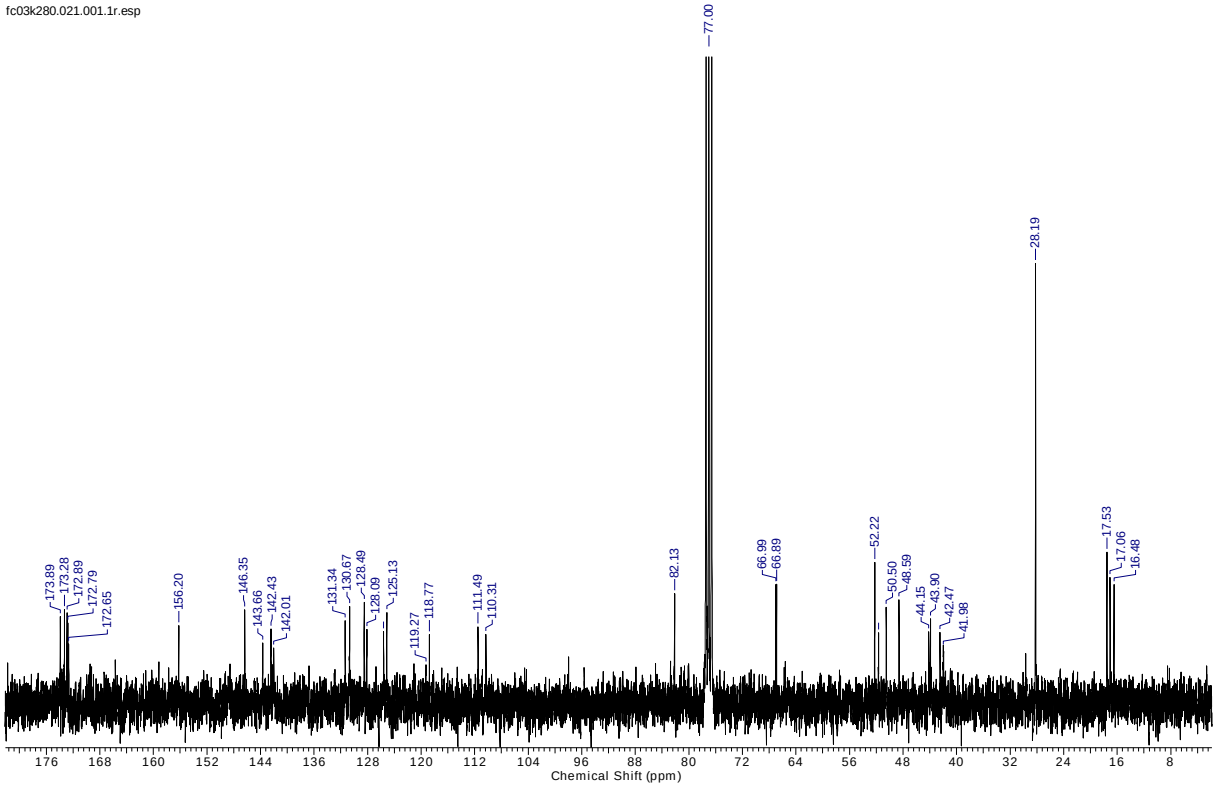
Boc-Ala-Ala-(*R*)-Aic(CN)-Ala-OMe



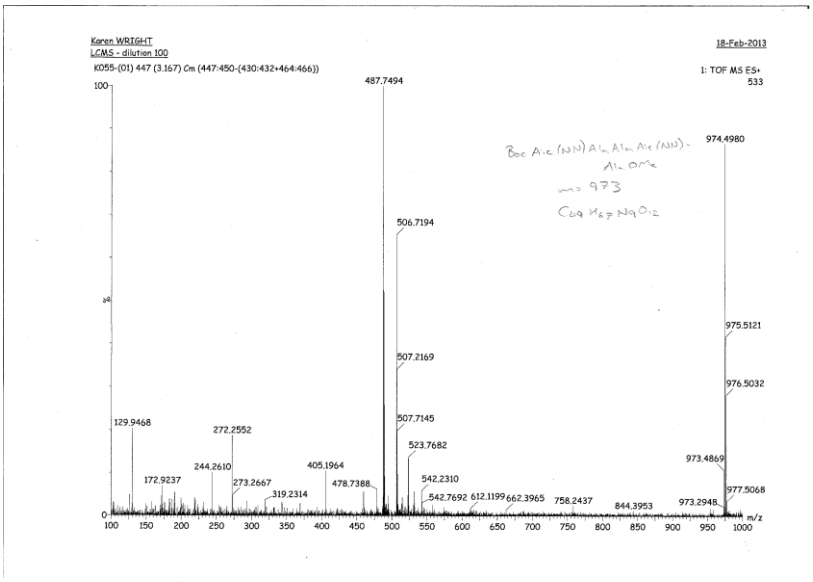


Boc-(*R*)-Aic(CN)-Ala-Ala-(*R*)-Aic(CN)-Ala-OMe





Boc-(*R*)-Aic(NN)-Ala-Ala-(*R*)-Aic(NN)-Ala-OMe

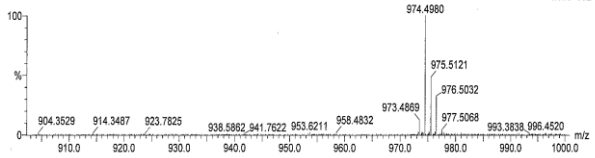


Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 0.8 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

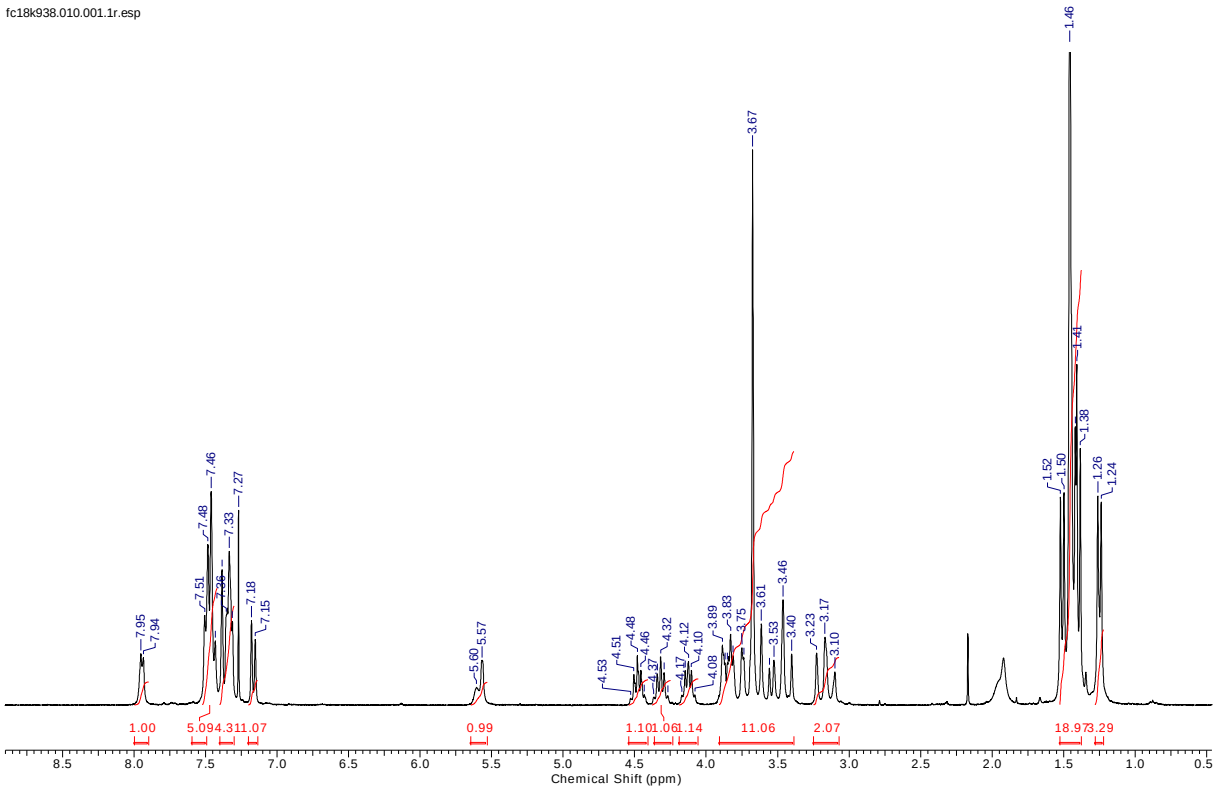
Monoisotopic Mass, Even Electron Ions
13158 formula(e) evaluated with 9 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-150 H: 0-150 N: 0-50 O: 0-50

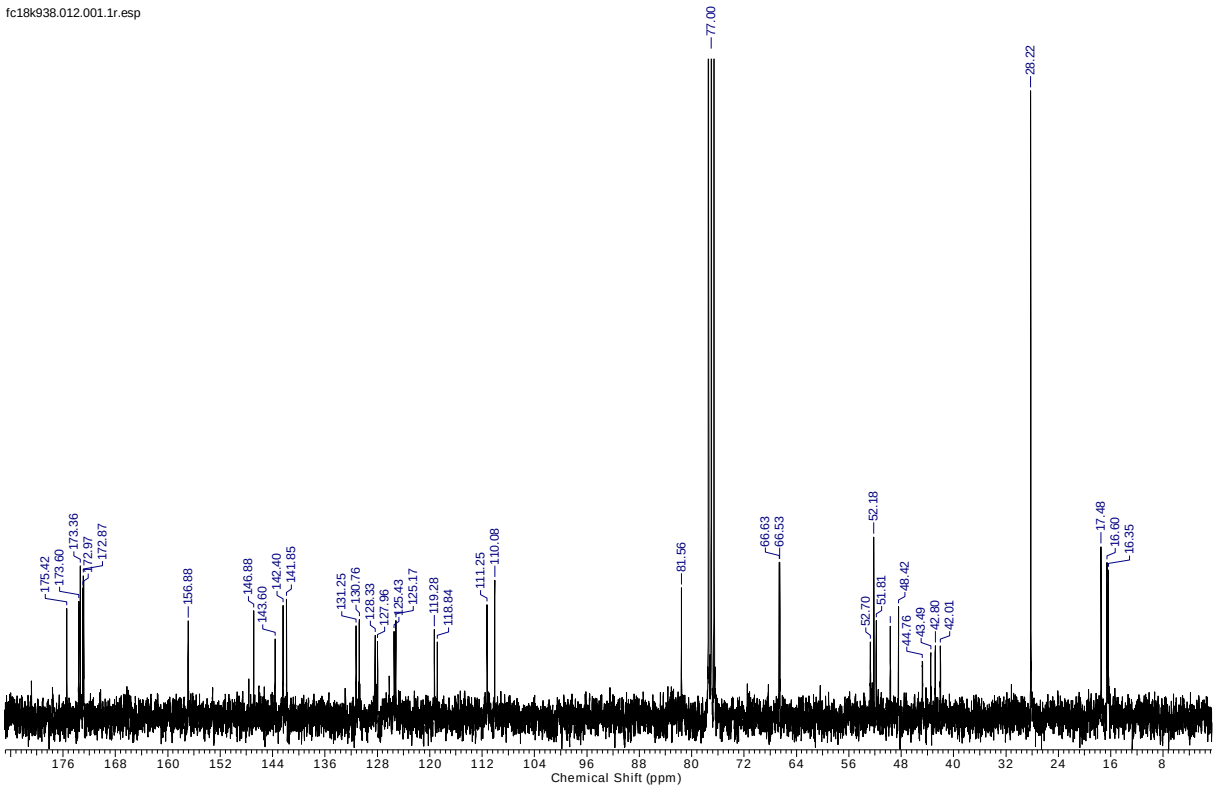
Karen WRIGHT
LCMS - dilution 100
K055-(01) 447 (3.167) Cm (447:450-(430:432+464:466))
18-Feb-2013
1: TOF MS ES+
4.62e+002



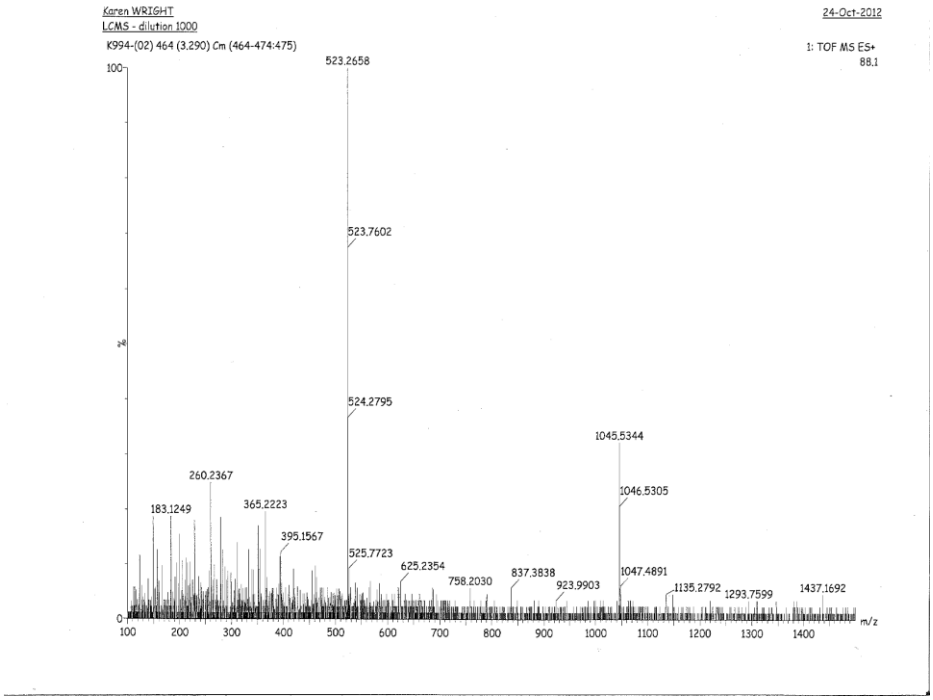
Minimum:				-1.5							
Maximum:		10.0	0.8	500.0							
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula				
974.4980	974.4987	-0.7	-0.7	20.5	73.3	1.4	C49	H68	N9	O12	
	974.4974	0.6	0.6	15.5	73.5	1.6	C48	H72	N5	O16	
	974.4987	-0.7	-0.7	31.5	73.8	1.9	C47	H56	N23	O2	
	974.4982	-0.2	-0.2	38.5	73.9	2.0	C62	H60	N11	O	
	974.4974	0.6	0.6	26.5	74.1	2.2	C46	H60	N19	O6	
	974.4979	0.1	0.1	8.5	74.4	2.5	C33	H68	N17	O17	
	974.4979	0.1	0.1	19.5	74.9	3.0	C31	H56	N31	O7	
	974.4984	-0.4	-0.4	1.5	75.9	4.0	C18	H64	N29	O18	
	974.4984	-0.4	-0.4	12.5	76.3	4.4	C16	H52	N43	O8	

Boc-Ala-(*R*)-Aic(CN)-Ala-Ala-(*R*)-Aic(CN)-Ala-OMe





Boc-Ala-(*R*)-Aic(NN)-Ala-Ala-(*R*)-Aic(NN)-Ala-OMe



Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 1.5 PPM / DBE: min = -1.5, max = 500.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
4049 formula(e) evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 30-60 H: 30-80 N: 1-50 O: 1-50

Karen WRIGHT
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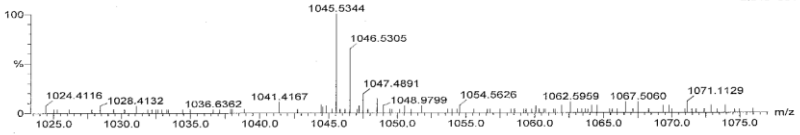
K994-(02) 464 (3.290) Cm (464-474:475)
24-Oct-2012
1: TOF MS ES+
2.84e+001



Minimum:				-1.5								
Maximum:		10.0	1.5	500.0								
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula					
1045.5344	1045.5359	-1.5	-1.4	21.5	19.9	2.5		C52	H73	N10	O13	
	1045.5345	-0.1	-0.1	16.5	19.8	2.4		C51	H77	N6	O17	
	1045.5358	-1.4	-1.3	32.5	19.8	2.4		C50	H61	N24	O3	
	1045.5345	-0.1	-0.1	27.5	19.7	2.3		C49	H65	N20	O7	
	1045.5332	1.2	1.1	22.5	19.6	2.2		C48	H69	N16	O11	
	1045.5332	1.2	1.1	33.5	19.5	2.1		C46	H57	N30	O	
	1045.5350	-0.6	-0.6	9.5	20.0	2.6		C36	H73	N18	O18	
	1045.5337	0.7	0.7	4.5	20.0	2.6		C35	H77	N14	O22	
	1045.5350	-0.6	-0.6	20.5	19.9	2.5		C34	H61	N32	O8	
	1045.5337	0.7	0.7	15.5	19.9	2.5		C33	H65	N28	O12	
	1045.5337	0.7	0.7	26.5	19.8	2.4		C31	H53	N42	O2	

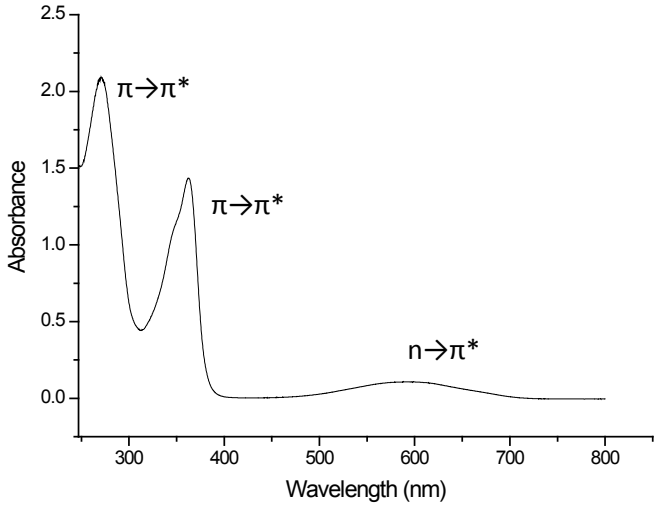


Figure S6. Near-UV/Vis absorption spectrum of the *bis*-(*R*)-Aic(NN) pentapeptide in MeOH solution. Peptide concentration: 1 mM. The specific electronic transitions of the nitronyl nitroxide chromophore for the three absorption bands are indicated.

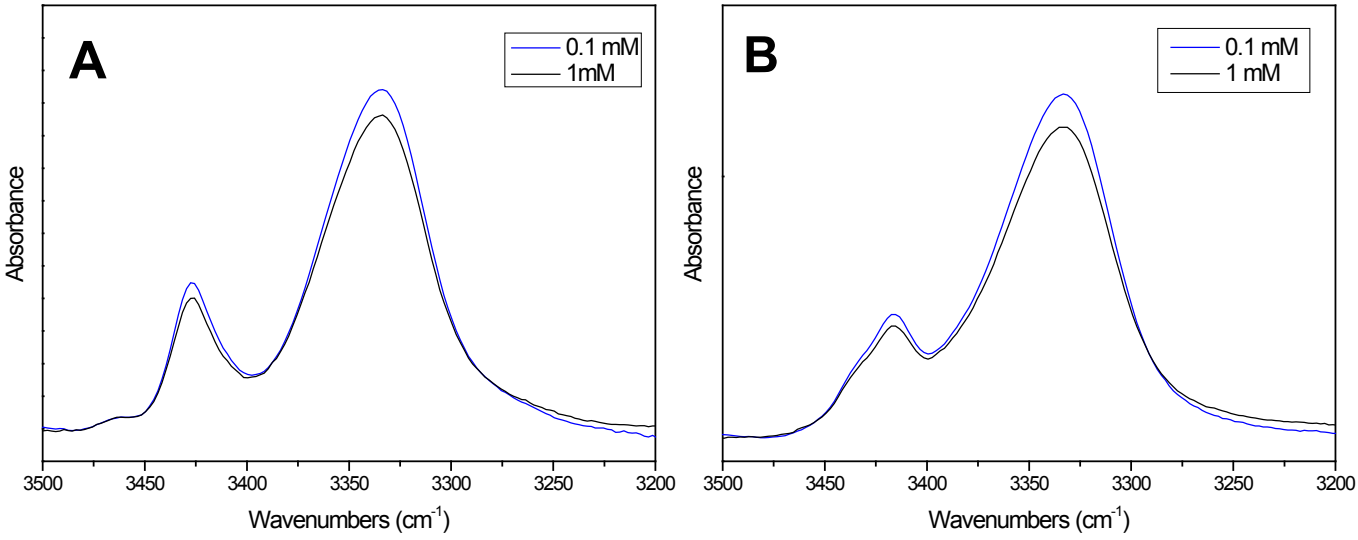


Figure S7. FTIR absorption spectra (N-H stretching region) for the *bis*-(*R*)-Aic(NN) penta- (**A**) and hexapeptides (**B**) in $CDCl_3$ solution [peptide concentrations: 1×10^{-3} M (black line), and 1×10^{-4} M (blue line)].

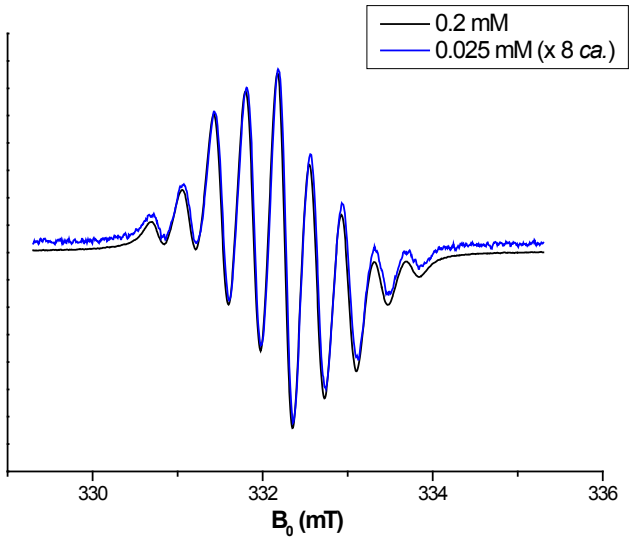
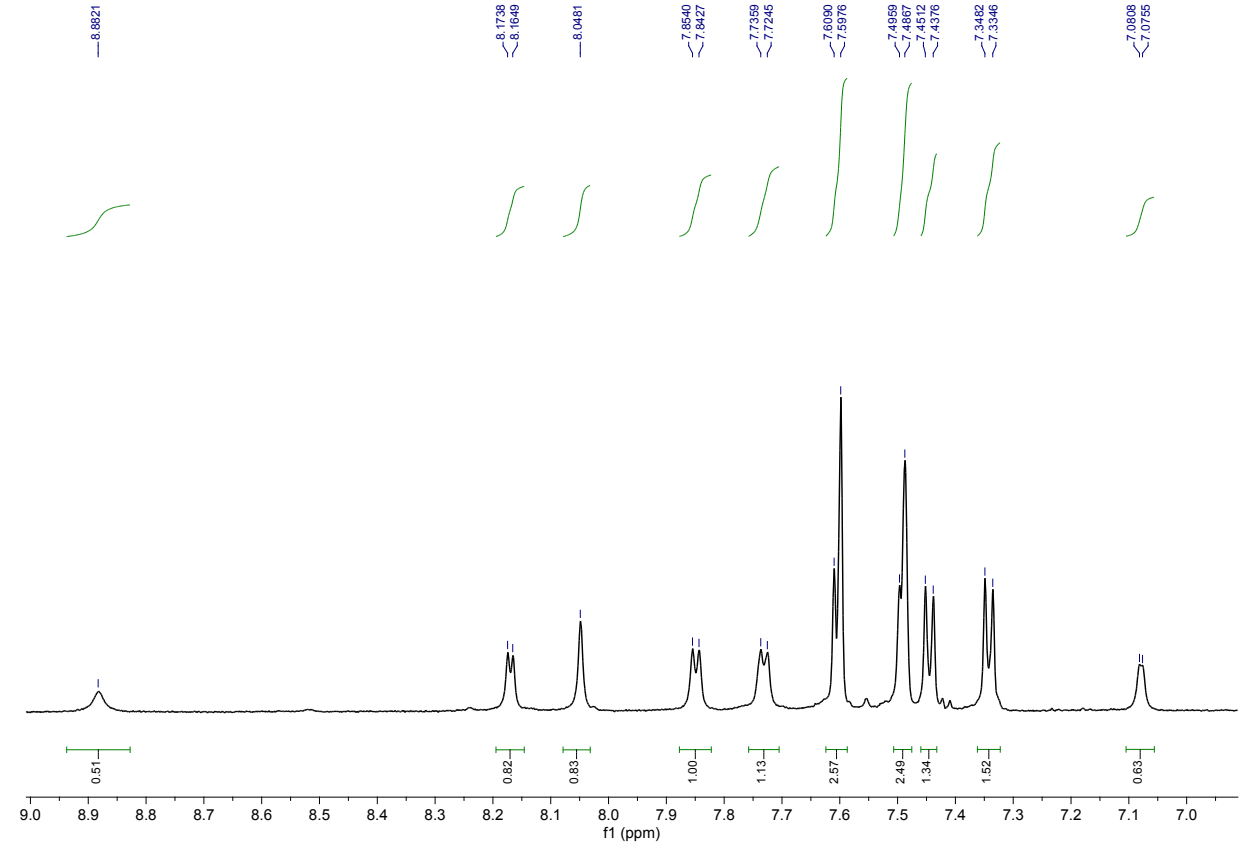


Figure S8. Experimental cw EPR spectrum of the bis-(R)-Aic(NN) hexapeptide in toluene at room temperature (293 K) at two peptide concentrations: 0.2 mM (black line) and 0.025 mM (blue line). The signal at low concentration is amplified for a better comparison. The dilution does not modify the overall hyperfine pattern, but just reduces the signal intensities.

1D ^{1}H NMR spectra of the *bis*-(*R*)-Aic(CN) hexapeptide in CD_3OH solution at two different concentrations (top, 2 mM; bottom, 0.5 mM). No self-association propensity was observed.



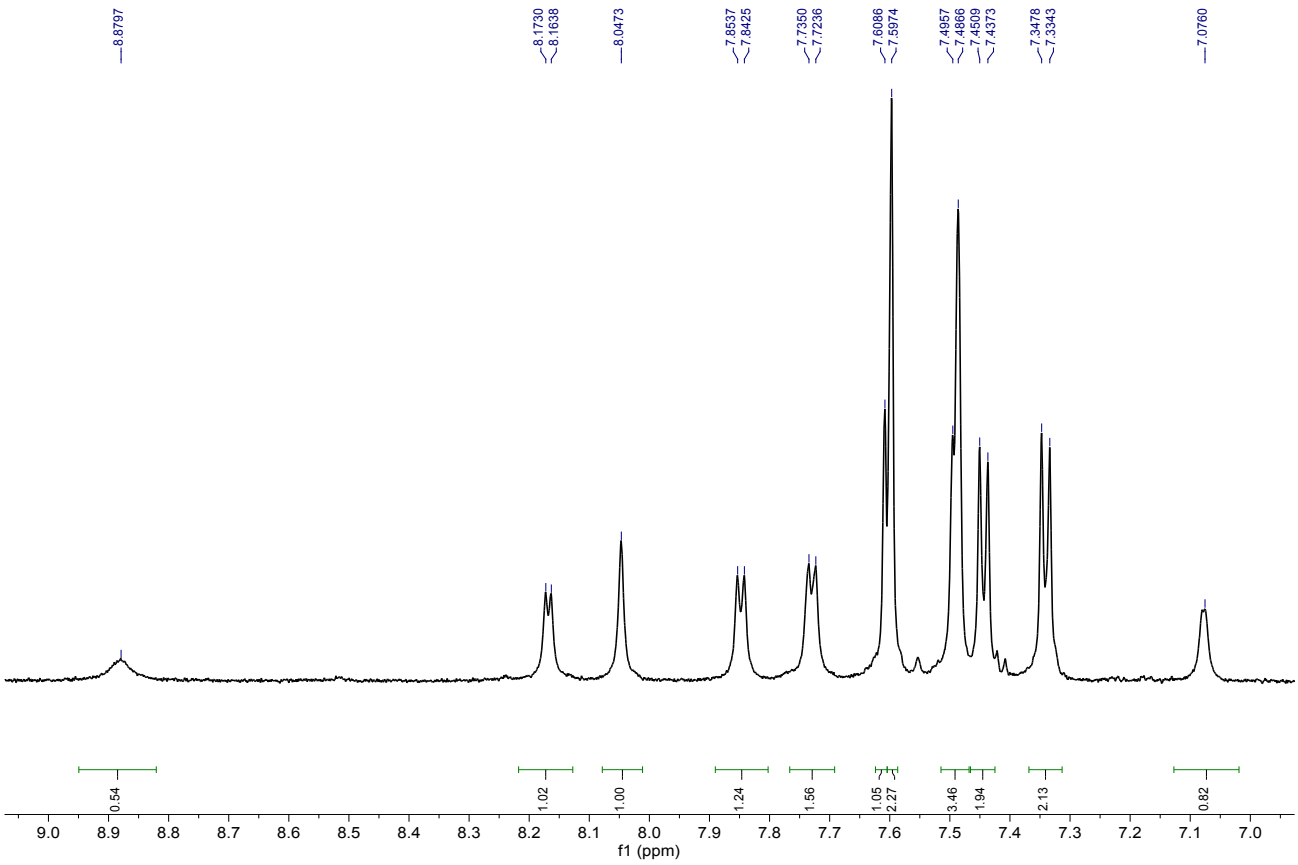


Table S3. Cartesian coordinates, computed total energies and lowest frequency values for the optimized structures discussed in text

***bis*-(*R*)-Aic(NN) hexapeptide: conformer a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.856534	2.253223	-1.093164
2	6	0	-0.303284	3.089482	-2.068935
3	6	0	-1.127792	3.875494	-2.871419
4	6	0	-2.510923	3.811816	-2.700552
5	6	0	-3.074013	2.975531	-1.714346
6	6	0	-2.229794	2.196579	-0.896102
7	1	0	-0.708741	4.529039	-3.632071
8	1	0	-2.658367	1.559718	-0.133207
9	6	0	0.215556	1.449858	-0.399020
10	6	0	1.200001	2.931149	-2.111094
11	6	0	1.540646	2.181387	-0.780583
12	1	0	1.494423	2.310167	-2.966171
13	1	0	1.752758	3.873581	-2.199290
14	1	0	0.095231	1.382037	0.684818
15	1	0	0.241871	0.426801	-0.787078
16	7	0	1.897589	3.180990	0.237234
17	6	0	2.679115	1.174570	-1.029487
18	1	0	1.682929	4.155102	0.053506
19	6	0	2.159706	2.873007	1.532045
20	8	0	2.359625	1.721433	1.932793
21	8	0	2.445914	0.081272	-1.555767
22	7	0	3.933758	1.540967	-0.686321
23	1	0	4.082365	2.435579	-0.238433
24	6	0	5.048416	0.611338	-0.833511
25	1	0	5.099924	0.288460	-1.877668
26	6	0	4.852103	-0.692288	-0.033887
27	8	0	5.453817	-1.714517	-0.385193
28	6	0	6.365977	1.285497	-0.439802
29	1	0	6.344493	1.617513	0.604433
30	1	0	7.187329	0.574449	-0.557152
31	1	0	6.562032	2.149373	-1.083240
32	7	0	4.038341	-0.653232	1.044074
33	1	0	3.535962	0.202009	1.280436
34	6	0	3.815589	-1.840047	1.863605
35	1	0	4.789201	-2.270201	2.118874
36	6	0	3.081184	-2.990628	1.137983
37	8	0	3.163134	-4.126778	1.601643
38	7	0	2.362849	-2.666360	0.028869
39	6	0	3.069346	-1.465506	3.149120
40	1	0	3.652929	-0.749420	3.736110
41	1	0	2.096748	-1.015833	2.923889
42	1	0	2.909808	-2.364846	3.748558
43	1	0	2.398300	-1.706958	-0.303488
44	6	0	1.699823	-3.651945	-0.836310
45	6	0	0.656423	-4.496994	-0.045377

46	6	0	0.823737	-2.874368	-1.875275
47	6	0	2.710034	-4.543480	-1.605752
48	6	0	-0.620420	-3.696736	-0.159945
49	1	0	0.983408	-4.681148	0.978292
50	1	0	0.553942	-5.467517	-0.544234
51	6	0	-0.525167	-2.767614	-1.203029
52	1	0	0.742287	-3.477613	-2.788433
53	1	0	1.263980	-1.912771	-2.154049
54	8	0	2.327888	-5.581238	-2.150353
55	7	0	3.968825	-4.057640	-1.733533
56	6	0	-1.780304	-3.806847	0.594583
57	6	0	-1.604422	-1.939198	-1.502713
58	1	0	4.264488	-3.254018	-1.185939
59	6	0	5.002634	-4.776234	-2.453553
60	6	0	-2.885002	-2.974330	0.297568
61	1	0	-1.848742	-4.515613	1.408516
62	6	0	-2.780859	-2.042915	-0.758245
63	1	0	-1.544420	-1.212540	-2.309173
64	1	0	4.485156	-5.509320	-3.082137
65	6	0	-4.525164	2.881165	-1.554330
66	1	0	-3.163353	4.399438	-3.332235
67	6	0	-4.122238	-3.085137	1.072914
68	1	0	-3.625231	-1.407748	-0.986565
69	6	0	5.926555	-5.602274	-1.544819
70	6	0	5.824980	-3.825106	-3.333462
71	1	0	6.254818	-3.019414	-2.728721
72	1	0	6.635921	-4.370217	-3.821602
73	1	0	5.181976	-3.378757	-4.097556
74	8	0	6.960755	-6.110142	-1.934872
75	8	0	5.453804	-5.724517	-0.299144
76	6	0	6.243954	-6.517532	0.605284
77	1	0	5.721203	-6.468935	1.559673
78	1	0	6.306900	-7.549751	0.251370
79	1	0	7.251413	-6.103650	0.694691
80	6	0	2.210016	4.051675	2.523129
81	1	0	3.191345	3.992791	3.001379
82	7	0	2.077189	5.358135	1.882925
83	6	0	1.120294	3.864411	3.588662
84	1	0	1.211657	2.874521	4.040208
85	1	0	1.224872	4.622986	4.369811
86	1	0	0.120719	3.950164	3.146652
87	1	0	1.208819	5.859005	2.025964
88	6	0	3.118789	6.194734	1.538245
89	8	0	2.947737	7.370243	1.256355
90	8	0	4.288095	5.524255	1.527877
91	6	0	5.568304	6.221029	1.256989
92	6	0	5.569413	6.763838	-0.174635
93	1	0	4.826880	7.553361	-0.298852
94	1	0	6.558874	7.171529	-0.408277
95	1	0	5.357635	5.959991	-0.888425
96	6	0	6.595661	5.098963	1.414993
97	1	0	6.562536	4.679860	2.425878
98	1	0	6.406398	4.294339	0.697092
99	1	0	7.602575	5.488577	1.235358
100	6	0	5.798639	7.316533	2.301633

101	1	0	6.799151	7.740907	2.165738
102	1	0	5.063568	8.116985	2.206500
103	1	0	5.742234	6.898082	3.312454
104	7	0	-5.445329	3.102124	-2.531038
105	7	0	-5.170715	2.512821	-0.416968
106	6	0	-6.822434	2.644092	-2.112430
107	6	0	-6.669109	2.629405	-0.556652
108	6	0	-7.016064	1.250234	-2.737692
109	1	0	-6.900572	1.334367	-3.821772
110	1	0	-6.282684	0.528609	-2.366629
111	1	0	-8.018294	0.868997	-2.522645
112	6	0	-7.871090	3.611202	-2.662185
113	1	0	-7.837229	3.596671	-3.753781
114	1	0	-8.869565	3.296980	-2.342336
115	1	0	-7.704862	4.638491	-2.331134
116	6	0	-7.062736	3.950207	0.128692
117	1	0	-6.727462	3.916861	1.168842
118	1	0	-6.599014	4.815517	-0.354296
119	1	0	-8.148422	4.082655	0.116409
120	6	0	-7.333224	1.450306	0.155978
121	1	0	-7.146156	1.527726	1.229563
122	1	0	-8.415178	1.479906	-0.008075
123	1	0	-6.946995	0.486875	-0.184078
124	8	0	-5.216533	3.461268	-3.735037
125	8	0	-4.645022	2.253945	0.718204
126	7	0	-4.244740	-3.689549	2.288753
127	7	0	-5.349171	-2.620629	0.702389
128	6	0	-5.611376	-3.477084	2.890509
129	6	0	-6.439177	-3.129770	1.616459
130	6	0	-7.050437	-4.353220	0.908335
131	1	0	-7.885570	-4.756666	1.487925
132	1	0	-7.424435	-4.039318	-0.070048
133	1	0	-6.313929	-5.147551	0.755334
134	6	0	-7.508423	-2.054680	1.805351
135	1	0	-7.987526	-1.846241	0.846439
136	1	0	-8.272999	-2.414516	2.501430
137	1	0	-7.095897	-1.120326	2.190714
138	6	0	-5.462205	-2.310868	3.885399
139	1	0	-6.403051	-2.128541	4.412416
140	1	0	-4.697815	-2.577589	4.620241
141	1	0	-5.153153	-1.386984	3.387704
142	6	0	-6.043896	-4.741439	3.634011
143	1	0	-5.354689	-4.926759	4.460552
144	1	0	-7.049365	-4.605035	4.044665
145	1	0	-6.045271	-5.623119	2.989846
146	8	0	-3.319157	-4.226175	2.986624
147	8	0	-5.653194	-2.004970	-0.377789

SCF Done: E(UB3LYP) = -3550.30976456

Full mass-weighted force constant matrix:
Low frequencies --- -5.2221 -1.8909 -1.1605 -0.0041 -0.0027
0.0038
Low frequencies --- 5.5828 10.3010 11.9538

***bis*-(*R*)-Aic(NN) hexapeptide: conformer b**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.016908	-2.965731	-0.255073
2	6	0	-1.750074	-3.393626	-1.365978
3	6	0	-1.124127	-4.106497	-2.385849
4	6	0	0.237198	-4.390224	-2.290065
5	6	0	0.984701	-3.971975	-1.166463
6	6	0	0.338257	-3.248632	-0.139704
7	1	0	-1.681818	-4.440936	-3.256870
8	1	0	0.903749	-2.925983	0.723878
9	6	0	-1.899081	-2.233705	0.728311
10	6	0	-3.202671	-3.004330	-1.239956
11	6	0	-3.218272	-1.965569	-0.065434
12	1	0	-3.629153	-2.596355	-2.162606
13	1	0	-3.815052	-3.877756	-0.971687
14	1	0	-2.126612	-2.864022	1.597135
15	1	0	-1.457316	-1.306455	1.097571
16	7	0	-4.426060	-2.141707	0.743870
17	6	0	-3.174938	-0.544442	-0.677740
18	1	0	-4.936326	-3.015292	0.675696
19	6	0	-4.719509	-1.364529	1.814152
20	8	0	-4.104013	-0.328176	2.085980
21	8	0	-2.103868	0.015826	-0.921989
22	7	0	-4.366493	0.028609	-0.973325
23	1	0	-5.218762	-0.459342	-0.729745
24	6	0	-4.448281	1.348124	-1.590206
25	1	0	-3.841499	1.343518	-2.501585
26	6	0	-3.838741	2.474200	-0.731600
27	8	0	-3.526462	3.539441	-1.278302
28	6	0	-5.899762	1.680407	-1.949373
29	1	0	-6.534737	1.693806	-1.056231
30	1	0	-5.940962	2.667616	-2.415204
31	1	0	-6.298302	0.945566	-2.656321
32	7	0	-3.681045	2.249828	0.590998
33	1	0	-3.896364	1.335893	0.987434
34	6	0	-3.066153	3.246996	1.461111
35	1	0	-3.495041	4.221063	1.203682
36	6	0	-1.550110	3.446132	1.232163
37	8	0	-0.979526	4.383414	1.787969
38	7	0	-0.923918	2.582486	0.391319
39	6	0	-3.356173	2.934553	2.932239
40	1	0	-4.432997	2.965756	3.125166
41	1	0	-2.985785	1.941388	3.205706
42	1	0	-2.862340	3.679708	3.559725
43	1	0	-1.443162	1.805357	-0.007850
44	6	0	0.438305	2.813434	-0.087438
45	6	0	1.512794	2.831621	1.043774
46	6	0	0.868576	1.637405	-1.032486
47	6	0	0.522657	4.125676	-0.921044
48	6	0	2.690344	2.088862	0.455426

49	1	0	1.117555	2.309711	1.923545
50	1	0	1.757850	3.851119	1.345644
51	6	0	2.329129	1.431669	-0.725826
52	1	0	0.669847	1.861439	-2.086007
53	1	0	0.292052	0.735155	-0.791231
54	8	0	1.574620	4.756538	-1.002487
55	7	0	-0.590867	4.434918	-1.639769
56	6	0	3.984971	1.998145	0.951858
57	6	0	3.269610	0.685029	-1.432451
58	1	0	-1.476779	3.991053	-1.410994
59	6	0	-0.655212	5.611177	-2.484869
60	6	0	4.941969	1.228539	0.254624
61	1	0	4.272909	2.519574	1.855418
62	6	0	4.570140	0.580659	-0.943265
63	1	0	3.000266	0.183185	-2.358372
64	1	0	0.377303	5.876430	-2.734032
65	6	0	2.411800	-4.285836	-1.065730
66	1	0	0.735847	-4.929405	-3.082952
67	6	0	6.308099	1.101017	0.761903
68	1	0	5.306835	-0.002005	-1.478696
69	6	0	-1.233276	6.851658	-1.786967
70	6	0	-1.439328	5.319761	-3.773190
71	1	0	-2.446657	4.959042	-3.537857
72	1	0	-1.522711	6.227371	-4.375787
73	1	0	-0.923910	4.550165	-4.355064
74	8	0	-1.385176	7.917339	-2.353592
75	8	0	-1.536461	6.633525	-0.502463
76	6	0	-2.035487	7.762733	0.236538
77	1	0	-2.155837	7.402865	1.257632
78	1	0	-1.320693	8.588210	0.198967
79	1	0	-2.992974	8.094252	-0.174074
80	6	0	-5.909558	-1.811391	2.685042
81	1	0	-6.654706	-1.016749	2.588220
82	7	0	-6.517857	-3.064449	2.241027
83	6	0	-5.473148	-1.909915	4.152957
84	1	0	-4.990695	-0.979437	4.458239
85	1	0	-6.343113	-2.087733	4.791481
86	1	0	-4.759234	-2.729235	4.297129
87	1	0	-6.316143	-3.892180	2.788989
88	6	0	-7.694499	-3.183499	1.528886
89	8	0	-8.301017	-4.239569	1.442931
90	8	0	-8.021012	-2.015529	0.941167
91	6	0	-9.277580	-1.871720	0.166759
92	6	0	-9.246677	-2.796668	-1.052996
93	1	0	-9.260699	-3.845727	-0.754817
94	1	0	-10.121331	-2.596701	-1.681139
95	1	0	-8.349417	-2.608376	-1.652959
96	6	0	-9.234517	-0.404408	-0.263051
97	1	0	-9.201001	0.256766	0.608967
98	1	0	-8.355137	-0.207548	-0.885305
99	1	0	-10.128074	-0.161250	-0.846454
100	6	0	-10.480516	-2.136910	1.075923
101	1	0	-11.403831	-1.913197	0.530902
102	1	0	-10.510552	-3.178338	1.399859
103	1	0	-10.442535	-1.489635	1.958886

104	7	0	3.217093	-4.681121	-2.090419
105	7	0	3.156636	-4.242305	0.074547
106	6	0	4.669579	-4.732788	-1.678994
107	6	0	4.533224	-4.831116	-0.127647
108	6	0	5.298974	-3.418245	-2.173206
109	1	0	5.166415	-3.354565	-3.256956
110	1	0	4.831695	-2.543733	-1.712877
111	1	0	6.368216	-3.391482	-1.947800
112	6	0	5.349383	-5.923412	-2.355763
113	1	0	5.330083	-5.783631	-3.438720
114	1	0	6.393573	-5.984093	-2.033290
115	1	0	4.856606	-6.870610	-2.126517
116	6	0	4.454771	-6.272754	0.409728
117	1	0	4.157543	-6.236412	1.461368
118	1	0	3.719348	-6.872996	-0.134644
119	1	0	5.428490	-6.765988	0.340184
120	6	0	5.559341	-4.033000	0.677301
121	1	0	5.295543	-4.081634	1.736485
122	1	0	6.551023	-4.479174	0.548955
123	1	0	5.614555	-2.983197	0.382078
124	8	0	2.894265	-4.830618	-3.317634
125	8	0	2.754686	-3.945342	1.250060
126	7	0	6.917791	1.949346	1.636453
127	7	0	7.184923	0.111712	0.442588
128	6	0	8.250694	1.417179	2.104646
129	6	0	8.570557	0.392019	0.970019
130	6	0	9.365304	0.981437	-0.210035
131	1	0	10.404485	1.167430	0.076167
132	1	0	9.355029	0.259602	-1.031477
133	1	0	8.928761	1.917563	-0.570336
134	6	0	9.217601	-0.915373	1.427822
135	1	0	9.327604	-1.583456	0.571066
136	1	0	10.211399	-0.712570	1.839234
137	1	0	8.623679	-1.430340	2.185619
138	6	0	7.995744	0.777165	3.481547
139	1	0	8.928808	0.407077	3.916331
140	1	0	7.580128	1.538545	4.147411
141	1	0	7.283914	-0.051432	3.420961
142	6	0	9.241040	2.573177	2.244143
143	1	0	8.884361	3.264854	3.010318
144	1	0	10.218253	2.187985	2.552037
145	1	0	9.361814	3.131549	1.313754
146	8	0	6.430931	3.011742	2.150662
147	8	0	6.978573	-0.893309	-0.323958

SCF Done: E(UB3LYP) = -3550.30696789

Full mass-weighted force constant matrix:
Low frequencies --- -0.0040 -0.0034 -0.0021 1.5215 3.1141
4.4031
Low frequencies --- 7.2993 10.8598 13.6267

***bis*-(*R*)-Aic(NN) hexapeptide: conformer c**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.465187	2.267227	-0.786201
2	6	0	3.325107	2.030274	-1.866082
3	6	0	3.905114	3.095009	-2.550054
4	6	0	3.622621	4.400795	-2.149711
5	6	0	2.765861	4.650200	-1.055760
6	6	0	2.183561	3.561228	-0.368790
7	1	0	4.575667	2.922774	-3.387891
8	1	0	1.534279	3.747206	0.476180
9	6	0	1.939330	0.961221	-0.232888
10	6	0	3.452040	0.544804	-2.118981
11	6	0	2.945406	-0.090763	-0.784399
12	1	0	2.794650	0.236783	-2.942347
13	1	0	4.463779	0.211117	-2.375008
14	1	0	1.874899	0.923510	0.857449
15	1	0	0.941928	0.739669	-0.628037
16	7	0	4.100536	-0.232156	0.114956
17	6	0	2.283809	-1.453609	-1.062734
18	1	0	4.928930	0.321362	-0.075921
19	6	0	4.009100	-0.746557	1.366057
20	8	0	3.013750	-1.351531	1.778644
21	8	0	1.080745	-1.544834	-1.323143
22	7	0	3.103567	-2.531573	-1.072957
23	1	0	4.076716	-2.410287	-0.822452
24	6	0	2.604319	-3.864663	-1.387561
25	1	0	2.053994	-3.811459	-2.332482
26	6	0	1.571648	-4.394166	-0.374145
27	8	0	0.835445	-5.332297	-0.704636
28	6	0	3.765894	-4.852071	-1.532133
29	1	0	4.339900	-4.924728	-0.601547
30	1	0	3.372486	-5.842790	-1.770750
31	1	0	4.436989	-4.539918	-2.338731
32	7	0	1.518886	-3.809645	0.842323
33	1	0	2.106210	-3.003397	1.052520
34	6	0	0.539336	-4.230039	1.839506
35	1	0	0.557818	-5.323246	1.891593
36	6	0	-0.923596	-3.900074	1.467865
37	8	0	-1.836395	-4.426689	2.101670
38	7	0	-1.126226	-3.032179	0.442264
39	6	0	0.886569	-3.649324	3.214220
40	1	0	1.865883	-4.008235	3.545865
41	1	0	0.912367	-2.555305	3.186122
42	1	0	0.131439	-3.965634	3.937456
43	1	0	-0.324753	-2.628657	-0.034257
44	6	0	-2.455038	-2.769190	-0.110156
45	6	0	-3.460758	-2.186051	0.932688
46	6	0	-2.345908	-1.673178	-1.229592

47	6	0	-3.058228	-4.042862	-0.769682
48	6	0	-4.184931	-1.086751	0.191022
49	1	0	-2.904352	-1.784751	1.787672
50	1	0	-4.132815	-2.957982	1.310714
51	6	0	-3.562423	-0.806845	-1.029286
52	1	0	-2.287960	-2.113154	-2.231148
53	1	0	-1.424594	-1.092660	-1.092528
54	8	0	-4.275283	-4.170149	-0.891888
55	7	0	-2.159961	-4.915914	-1.299774
56	6	0	-5.307910	-0.376415	0.597521
57	6	0	-4.070333	0.186800	-1.863775
58	1	0	-1.183679	-4.862156	-1.020649
59	6	0	-2.579364	-6.140680	-1.953844
60	6	0	-5.833587	0.632108	-0.240723
61	1	0	-5.784575	-0.586017	1.545655
62	6	0	-5.203479	0.899464	-1.476330
63	1	0	-3.596525	0.409798	-2.816603
64	1	0	-3.598340	-5.972716	-2.316598
65	6	0	2.485946	6.024400	-0.634905
66	1	0	4.061704	5.235965	-2.677177
67	6	0	-7.018817	1.389972	0.164223
68	1	0	-5.614647	1.660295	-2.124707
69	6	0	-2.680666	-7.350243	-1.011267
70	6	0	-1.657183	-6.473190	-3.136138
71	1	0	-0.616099	-6.545267	-2.802990
72	1	0	-1.951252	-7.425240	-3.584232
73	1	0	-1.724791	-5.686011	-3.892656
74	8	0	-3.003608	-8.459218	-1.393203
75	8	0	-2.383842	-7.048244	0.256989
76	6	0	-2.489653	-8.118603	1.212220
77	1	0	-2.249933	-7.665386	2.173329
78	1	0	-3.504032	-8.524808	1.218192
79	1	0	-1.781784	-8.916033	0.971205
80	6	0	5.236183	-0.563750	2.279571
81	1	0	5.546559	-1.574349	2.558191
82	7	0	6.358536	0.100478	1.621514
83	6	0	4.823947	0.200438	3.545729
84	1	0	3.965520	-0.289371	4.009794
85	1	0	5.652782	0.217978	4.259234
86	1	0	4.543400	1.233122	3.308127
87	1	0	6.545260	1.062345	1.877220
88	6	0	7.459888	-0.527661	1.078476
89	8	0	8.476256	0.077880	0.776570
90	8	0	7.225169	-1.844545	0.910729
91	6	0	8.280865	-2.754800	0.407104
92	6	0	8.652797	-2.371800	-1.027729
93	1	0	9.131117	-1.391911	-1.062565
94	1	0	9.344917	-3.116298	-1.435577
95	1	0	7.760556	-2.355168	-1.663512
96	6	0	7.588528	-4.118240	0.447479
97	1	0	7.280781	-4.368374	1.467959
98	1	0	6.701955	-4.124467	-0.195309
99	1	0	8.274117	-4.894460	0.093419
100	6	0	9.485202	-2.731024	1.352150
101	1	0	10.207561	-3.491663	1.037151

102	1	0	9.976454	-1.757031	1.343187
103	1	0	9.171927	-2.963585	2.375707
104	7	0	2.653027	7.139810	-1.397424
105	7	0	2.012984	6.400630	0.585025
106	6	0	2.074541	8.367666	-0.735341
107	6	0	2.019153	7.901697	0.754712
108	6	0	0.694231	8.588556	-1.380757
109	1	0	0.828270	8.706118	-2.459507
110	1	0	0.022723	7.742460	-1.207943
111	1	0	0.224603	9.494434	-0.987142
112	6	0	2.976605	9.570123	-1.015966
113	1	0	2.997466	9.762271	-2.090871
114	1	0	2.579285	10.457218	-0.512968
115	1	0	4.002731	9.407552	-0.680074
116	6	0	3.283497	8.232040	1.568299
117	1	0	3.234806	7.697329	2.520786
118	1	0	4.195561	7.924837	1.048018
119	1	0	3.342057	9.304642	1.773684
120	6	0	0.774373	8.331753	1.531672
121	1	0	0.798711	7.885459	2.528192
122	1	0	0.762521	9.420927	1.639395
123	1	0	-0.149837	8.018900	1.041689
124	8	0	3.066833	7.197060	-2.604409
125	8	0	1.755834	5.643624	1.581516
126	7	0	-7.503467	1.491647	1.433438
127	7	0	-7.822721	2.117284	-0.660884
128	6	0	-8.613647	2.509198	1.535030
129	6	0	-9.065800	2.602598	0.044368
130	6	0	-10.184988	1.617614	-0.340756
131	1	0	-11.140171	1.926676	0.093340
132	1	0	-10.283012	1.611230	-1.429747
133	1	0	-9.962944	0.598694	-0.010351
134	6	0	-9.418471	4.006397	-0.449274
135	1	0	-9.644264	3.967400	-1.517085
136	1	0	-10.303953	4.373338	0.079356
137	1	0	-8.602761	4.716787	-0.299995
138	6	0	-7.963727	3.794257	2.080447
139	1	0	-8.715110	4.575116	2.228772
140	1	0	-7.501214	3.568398	3.045110
141	1	0	-7.188462	4.175964	1.409415
142	6	0	-9.675993	2.010928	2.515351
143	1	0	-9.231351	1.908687	3.507639
144	1	0	-10.494573	2.735379	2.574905
145	1	0	-10.086547	1.041438	2.226058
146	8	0	-7.013745	0.974322	2.494393
147	8	0	-7.711164	2.260291	-1.926085

SCF Done: E(UB3LYP) = -3550.30713568

Full mass-weighted force constant matrix:
Low frequencies --- -4.5274 -0.0043 -0.0031 -0.0013 1.7643
2.6300
Low frequencies --- 4.0716 7.3037 10.3623

***bis*-(*R*)-Aic(CN) penta peptide conformer a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.104510	0.744096	1.178224
2	6	0	-4.305365	0.106547	2.411531
3	6	0	-5.436920	0.370233	3.180717
4	6	0	-6.382502	1.278233	2.705197
5	6	0	-6.185271	1.915505	1.466570
6	6	0	-5.038059	1.650666	0.693413
7	1	0	-5.591670	-0.123657	4.135708
8	1	0	-4.900374	2.148501	-0.261389
9	6	0	-2.796382	0.308060	0.561651
10	6	0	-3.144374	-0.813096	2.715872
11	6	0	-2.456352	-1.006035	1.326291
12	1	0	-2.444176	-0.325247	3.405732
13	1	0	-3.429434	-1.768613	3.168998
14	1	0	-2.838438	0.148029	-0.518395
15	1	0	-2.008974	1.046078	0.750684
16	7	0	-3.059859	-2.186471	0.690010
17	6	0	-0.938008	-1.193138	1.513843
18	1	0	-3.989810	-2.446872	0.996372
19	6	0	-2.754320	-2.534801	-0.606128
20	8	0	-1.748721	-2.137690	-1.190131
21	8	0	-3.679496	-3.374758	-1.085328
22	6	0	-3.573253	-3.981988	-2.437825
23	6	0	-3.613486	-2.881643	-3.500599
24	1	0	-4.506124	-2.260140	-3.372847
25	1	0	-2.727773	-2.246272	-3.451461
26	1	0	-3.659382	-3.340126	-4.494185
27	6	0	-2.309819	-4.841549	-2.521302
28	1	0	-2.292620	-5.576123	-1.708849
29	1	0	-2.305984	-5.387335	-3.470703
30	1	0	-1.406750	-4.230795	-2.469628
31	6	0	-4.830442	-4.850799	-2.501981
32	1	0	-4.877907	-5.361826	-3.468595
33	1	0	-4.821178	-5.606873	-1.710374
34	1	0	-5.731050	-4.238870	-2.389569
35	8	0	-0.179323	-0.222826	1.600356
36	7	0	-0.500361	-2.466974	1.627688
37	1	0	-1.174614	-3.215898	1.534238
38	6	0	0.907168	-2.784099	1.833948
39	1	0	1.266812	-2.227369	2.705357
40	6	0	1.814084	-2.318495	0.679613
41	8	0	3.027306	-2.186689	0.883249
42	6	0	1.083539	-4.286120	2.080307
43	1	0	0.726801	-4.871017	1.225000
44	1	0	2.142507	-4.507497	2.231383
45	1	0	0.532021	-4.594812	2.973924
46	7	0	1.241461	-2.079722	-0.520604
47	1	0	0.233148	-2.166675	-0.637003
48	6	0	2.036932	-1.616001	-1.652751

49	1	0	2.912498	-2.266550	-1.744694
50	6	0	2.642313	-0.206300	-1.466338
51	8	0	3.559935	0.146827	-2.204752
52	7	0	2.115047	0.572433	-0.483266
53	6	0	1.220168	-1.676913	-2.947550
54	1	0	0.921268	-2.707226	-3.164577
55	1	0	0.317270	-1.061829	-2.875693
56	1	0	1.831541	-1.308078	-3.774382
57	1	0	1.360145	0.196166	0.083351
58	6	0	2.678977	1.869714	-0.092571
59	6	0	2.646652	2.883223	-1.273809
60	6	0	1.724601	2.514164	0.965020
61	6	0	4.095887	1.741739	0.527778
62	6	0	1.290591	3.535092	-1.149014
63	1	0	2.824248	2.391213	-2.230493
64	1	0	3.446165	3.616795	-1.119536
65	6	0	0.760513	3.325813	0.133032
66	1	0	2.309790	3.178145	1.613748
67	1	0	1.242192	1.768465	1.602854
68	8	0	4.827794	2.730151	0.601050
69	7	0	4.403728	0.541975	1.077461
70	6	0	0.584418	4.271537	-2.090391
71	6	0	-0.476162	3.857886	0.493712
72	1	0	3.813855	-0.267478	0.900360
73	6	0	5.679080	0.294362	1.724067
74	6	0	-0.670163	4.804267	-1.731192
75	1	0	0.977950	4.438825	-3.088409
76	6	0	-1.197101	4.599094	-0.443174
77	1	0	-0.882022	3.700975	1.489273
78	1	0	6.112835	1.278171	1.934926
79	6	0	-7.168988	2.839904	0.983526
80	1	0	-7.275779	1.493520	3.281959
81	7	0	-7.968816	3.589355	0.592095
82	6	0	-1.421760	5.557949	-2.690866
83	1	0	-2.165083	5.017466	-0.187259
84	7	0	-2.033047	6.168164	-3.471594
85	6	0	6.701215	-0.414680	0.821550
86	6	0	5.493286	-0.481856	3.034794
87	1	0	4.961873	-1.422241	2.852892
88	1	0	6.465701	-0.708583	3.477474
89	1	0	4.908717	0.115528	3.740411
90	8	0	7.745727	-0.877298	1.238925
91	8	0	6.329851	-0.437695	-0.463364
92	6	0	7.254116	-1.048693	-1.382158
93	1	0	6.767559	-0.994150	-2.355273
94	1	0	8.199694	-0.500655	-1.391811
95	1	0	7.441085	-2.087826	-1.100143

SCF Done: E(RB3LYP) = -2421.04300394

Full mass-weighted force constant matrix:
Low frequencies --- -5.6687 -0.0010 -0.0006 0.0006 4.1640
5.3152
Low frequencies --- 9.2158 12.3387 16.4841

***bis*-(*R*)-Aic(CN) penta peptide conformer b**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.650758	3.338444	-0.993172
2	6	0	2.200750	3.257020	-2.280204
3	6	0	1.725401	4.058661	-3.315799
4	6	0	0.680087	4.945968	-3.061803
5	6	0	0.121884	5.023119	-1.772992
6	6	0	0.610807	4.218094	-0.725575
7	1	0	2.149633	3.992567	-4.313561
8	1	0	0.166068	4.285108	0.262352
9	6	0	2.344302	2.381321	-0.054010
10	6	0	3.310357	2.233789	-2.317983
11	6	0	3.086344	1.398294	-1.012384
12	1	0	3.308907	1.615161	-3.220841
13	1	0	4.290259	2.731384	-2.273199
14	1	0	1.662352	1.861328	0.620658
15	1	0	3.087645	2.909001	0.557860
16	7	0	4.366509	0.903684	-0.509385
17	6	0	2.150851	0.214610	-1.357496
18	1	0	5.194534	1.435981	-0.747783
19	6	0	4.442573	0.190632	0.665181
20	8	0	3.472710	-0.356939	1.183645
21	8	0	5.706896	0.170153	1.104404
22	6	0	6.112877	-0.580337	2.320994
23	6	0	5.395539	-0.004742	3.543991
24	1	0	5.577977	1.072420	3.621538
25	1	0	4.319642	-0.179901	3.494969
26	1	0	5.785965	-0.480681	4.449790
27	6	0	5.842942	-2.073436	2.122143
28	1	0	6.328427	-2.431492	1.207787
29	1	0	6.259724	-2.631723	2.967110
30	1	0	4.773330	-2.282128	2.063956
31	6	0	7.615509	-0.301464	2.386132
32	1	0	8.048420	-0.806506	3.255192
33	1	0	8.118277	-0.669500	1.486027
34	1	0	7.807142	0.772217	2.478984
35	8	0	0.923931	0.322595	-1.282068
36	7	0	2.747532	-0.920079	-1.787962
37	1	0	3.758670	-0.958023	-1.807876
38	6	0	1.972969	-2.084110	-2.204406
39	1	0	1.287217	-1.784407	-3.003392
40	6	0	1.055539	-2.638060	-1.098309
41	8	0	0.062459	-3.303055	-1.416550
42	6	0	2.908401	-3.183557	-2.719271
43	1	0	3.603101	-3.508537	-1.936742
44	1	0	2.317101	-4.046137	-3.035468
45	1	0	3.485565	-2.825656	-3.577970
46	7	0	1.394682	-2.393375	0.187496
47	1	0	2.175307	-1.775907	0.402858
48	6	0	0.571751	-2.880481	1.290202
49	1	0	0.322787	-3.926385	1.084512

50	6	0	-0.805839	-2.190673	1.416491
51	8	0	-1.651775	-2.680228	2.162732
52	7	0	-1.010674	-1.063642	0.684969
53	6	0	1.337031	-2.789535	2.614141
54	1	0	2.233817	-3.416465	2.582468
55	1	0	1.641127	-1.758618	2.823558
56	1	0	0.693569	-3.137539	3.425294
57	1	0	-0.270373	-0.725098	0.075990
58	6	0	-2.324256	-0.428194	0.577029
59	6	0	-2.921157	-0.004968	1.957584
60	6	0	-2.193103	0.905178	-0.243032
61	6	0	-3.340880	-1.330925	-0.178631
62	6	0	-3.461754	1.386071	1.732434
63	1	0	-3.686968	-0.706654	2.291678
64	1	0	-2.127947	0.000930	2.713116
65	6	0	-3.055218	1.896969	0.493751
66	1	0	-2.492677	0.775025	-1.288428
67	1	0	-1.147352	1.234229	-0.262417
68	8	0	-4.550522	-1.167689	-0.025416
69	7	0	-2.809649	-2.194790	-1.082340
70	6	0	-4.243987	2.153926	2.586558
71	6	0	-3.422550	3.181822	0.092655
72	1	0	-1.814325	-2.400326	-1.057517
73	6	0	-3.636800	-3.095875	-1.862198
74	6	0	-4.616673	3.450988	2.184489
75	1	0	-4.571200	1.770803	3.548453
76	6	0	-4.205147	3.963686	0.940099
77	1	0	-3.108273	3.579059	-0.868264
78	1	0	-4.640577	-2.659233	-1.886198
79	6	0	-0.971712	5.916599	-1.526129
80	1	0	0.285537	5.571849	-3.855218
81	7	0	-1.865957	6.634015	-1.323957
82	6	0	-5.422732	4.257946	3.052187
83	1	0	-4.499154	4.965898	0.646303
84	7	0	-6.074433	4.913445	3.760211
85	6	0	-3.812840	-4.482976	-1.224230
86	6	0	-3.097261	-3.236310	-3.292924
87	1	0	-2.054599	-3.572106	-3.278421
88	1	0	-3.693832	-3.962746	-3.849623
89	1	0	-3.142660	-2.269881	-3.803314
90	8	0	-4.414180	-5.389286	-1.768403
91	8	0	-3.249238	-4.574243	-0.014375
92	6	0	-3.401078	-5.832174	0.667584
93	1	0	-2.887271	-5.702563	1.619360
94	1	0	-4.459347	-6.053676	0.826400
95	1	0	-2.945967	-6.638268	0.086455

SCF Done: E(RB3LYP) = -2421.03928927

Full mass-weighted force constant matrix:
Low frequencies --- -0.0008 -0.0004 0.0002 2.0466 3.8321
5.9516
Low frequencies --- 10.3485 14.6536 18.4011

***bis*-(*R*)-Aic(CN) penta peptide conformer c**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.136124	1.881262	-0.770812
2	6	0	4.518346	1.449872	-2.049781
3	6	0	5.552039	2.078663	-2.741169
4	6	0	6.215294	3.148582	-2.141176
5	6	0	5.835876	3.580483	-0.857175
6	6	0	4.787693	2.945852	-0.162528
7	1	0	5.847390	1.743871	-3.731463
8	1	0	4.507601	3.289454	0.828359
9	6	0	2.981550	1.054249	-0.255562
10	6	0	3.647360	0.294567	-2.489603
11	6	0	3.019778	-0.217331	-1.153234
12	1	0	2.850591	0.652028	-3.154273
13	1	0	4.181323	-0.498588	-3.023813
14	1	0	3.045366	0.803351	0.806135
15	1	0	2.029912	1.573815	-0.413146
16	7	0	3.912879	-1.250627	-0.608982
17	6	0	1.613889	-0.791787	-1.418338
18	1	0	4.886916	-1.206688	-0.884562
19	6	0	3.679468	-1.818561	0.622708
20	8	0	2.586360	-1.781746	1.183193
21	8	0	4.787371	-2.423924	1.066049
22	6	0	4.813977	-3.198895	2.334033
23	6	0	4.517716	-2.268587	3.512439
24	1	0	5.208423	-1.418582	3.512130
25	1	0	3.493369	-1.894120	3.477393
26	1	0	4.656413	-2.817812	4.449808
27	6	0	3.834701	-4.371482	2.244322
28	1	0	4.046708	-4.980391	1.358719
29	1	0	3.951014	-5.007806	3.127906
30	1	0	2.800395	-4.025770	2.200611
31	6	0	6.259560	-3.696525	2.379256
32	1	0	6.418788	-4.287830	3.286356
33	1	0	6.481283	-4.326620	1.511962
34	1	0	6.959589	-2.855103	2.387431
35	8	0	0.610877	-0.071424	-1.408646
36	7	0	1.556942	-2.108848	-1.718533
37	1	0	2.415364	-2.644373	-1.692665
38	6	0	0.302312	-2.775122	-2.044440
39	1	0	-0.188159	-2.219149	-2.850209
40	6	0	-0.719831	-2.759884	-0.892990
41	8	0	-1.914763	-2.952777	-1.149190
42	6	0	0.567275	-4.212000	-2.505835
43	1	0	1.058400	-4.795652	-1.718970
44	1	0	-0.381088	-4.695161	-2.751593
45	1	0	1.201879	-4.216439	-3.397653
46	7	0	-0.264407	-2.539916	0.359880
47	1	0	0.721844	-2.343779	0.522772
48	6	0	-1.183411	-2.467682	1.491661
49	1	0	-1.862568	-3.324106	1.432271

50	6	0	-2.126884	-1.244131	1.463816
51	8	0	-3.097884	-1.220042	2.217183
52	7	0	-1.828482	-0.242810	0.593681
53	6	0	-0.414692	-2.518331	2.815747
54	1	0	0.134500	-3.460919	2.904772
55	1	0	0.300349	-1.692433	2.889979
56	1	0	-1.122820	-2.444886	3.644243
57	1	0	-1.007468	-0.325768	0.000235
58	6	0	-2.736325	0.876655	0.351669
59	6	0	-3.056160	1.713327	1.630040
60	6	0	-2.062484	1.893270	-0.635001
61	6	0	-4.066061	0.410056	-0.309761
62	6	0	-3.045116	3.145689	1.153507
63	1	0	-2.273276	1.544823	2.378793
64	1	0	-4.007697	1.418589	2.074024
65	6	0	-2.490916	3.247028	-0.129378
66	1	0	-2.347052	1.709969	-1.676354
67	1	0	-0.970904	1.788460	-0.587202
68	8	0	-5.083936	1.093453	-0.210534
69	7	0	-3.983455	-0.702174	-1.084885
70	6	0	-3.482821	4.282178	1.821391
71	6	0	-2.370372	4.483043	-0.763383
72	1	0	-3.177713	-1.316831	-1.001168
73	6	0	-5.135908	-1.236960	-1.785519
74	6	0	-3.361796	5.532313	1.184012
75	1	0	-3.918508	4.220757	2.813985
76	6	0	-2.807892	5.631368	-0.105717
77	1	0	-1.946104	4.558508	-1.760784
78	1	0	-5.848847	-0.411750	-1.888369
79	6	0	6.530593	4.675151	-0.245141
80	1	0	7.028595	3.648896	-2.656223
81	7	0	7.095383	5.562784	0.252611
82	6	0	-3.810083	6.717363	1.853685
83	1	0	-2.729356	6.603060	-0.582215
84	7	0	-4.170302	7.681122	2.398714
85	6	0	-5.887926	-2.325176	-1.003229
86	6	0	-4.741008	-1.756853	-3.174584
87	1	0	-3.950095	-2.510452	-3.092259
88	1	0	-5.605851	-2.207589	-3.666542
89	1	0	-4.369790	-0.930958	-3.788298
90	8	0	-6.791711	-2.981548	-1.484674
91	8	0	-5.457302	-2.449744	0.257063
92	6	0	-6.141265	-3.420560	1.070108
93	1	0	-5.656107	-3.369119	2.043992
94	1	0	-7.201523	-3.168978	1.152586
95	1	0	-6.038693	-4.419263	0.638109

SCF Done: E(RB3LYP) = -2421.04075311

Full mass-weighted force constant matrix:
Low frequencies --- -4.8313 -1.6530 -0.0009 -0.0005 0.0008
5.1967
Low frequencies --- 8.8087 11.5074 16.5813

***bis*-(*R*)-Aic(CN) penta peptide conformer left1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.979208	1.347007	0.552427
2	6	0	4.317227	1.009499	1.871138
3	6	0	5.411359	1.589626	2.498139
4	6	0	6.177504	2.527429	1.779084
5	6	0	5.834627	2.874454	0.459269
6	6	0	4.732035	2.283031	-0.156238
7	1	0	5.682325	1.334704	3.518062
8	1	0	4.467334	2.562825	-1.171684
9	6	0	2.745848	0.596690	0.113128
10	6	0	3.322138	0.018025	2.432084
11	6	0	2.610837	-0.548850	1.160427
12	1	0	2.588178	0.533250	3.064173
13	1	0	3.765864	-0.778198	3.039204
14	1	0	2.800631	0.207132	-0.906806
15	1	0	1.858553	1.237003	0.166268
16	7	0	3.329724	-1.764389	0.750944
17	6	0	1.135255	-0.864212	1.483758
18	1	0	4.303214	-1.834939	1.023592
19	6	0	2.994158	-2.442908	-0.398100
20	8	0	1.911799	-2.312767	-0.966464
21	8	0	3.989856	-3.263281	-0.753737
22	6	0	3.881198	-4.181593	-1.917103
23	6	0	3.721458	-3.365770	-3.202122
24	1	0	4.536021	-2.639879	-3.296985
25	1	0	2.768307	-2.834724	-3.222034
26	1	0	3.764429	-4.038706	-4.065176
27	6	0	2.732453	-5.168053	-1.694778
28	1	0	2.853408	-5.686739	-0.737604
29	1	0	2.744080	-5.919958	-2.490804
30	1	0	1.764304	-4.664618	-1.708378
31	6	0	5.230956	-4.900570	-1.889297
32	1	0	5.284621	-5.618434	-2.713683
33	1	0	5.362536	-5.444144	-0.948200
34	1	0	6.053453	-4.186528	-1.997758
35	8	0	0.255657	-0.007052	1.354993
36	7	0	0.883249	-2.105999	1.953904
37	1	0	1.661763	-2.747874	2.024625
38	6	0	-0.457303	-2.568225	2.320561
39	6	0	-1.467000	-2.408717	1.159490
40	8	0	-2.673731	-2.281340	1.397492
41	7	0	-0.963316	-2.458425	-0.093086
42	1	0	0.043380	-2.512405	-0.230986
43	6	0	-1.798700	-2.355252	-1.291881
44	6	0	-2.661295	-1.069478	-1.323586
45	8	0	-3.720070	-1.043724	-1.946920
46	7	0	-2.142300	0.014451	-0.683345
47	1	0	-1.286121	-0.098588	-0.147902
48	6	0	-2.820095	1.313049	-0.605555
49	6	0	-3.058591	1.911793	-2.023272

50	6	0	-1.823316	2.328820	0.040542
51	6	0	-4.120045	1.273282	0.235327
52	6	0	-1.760241	2.615331	-2.330546
53	1	0	-3.337065	1.144563	-2.746484
54	1	0	-3.885179	2.629524	-1.959165
55	6	0	-1.044220	2.850415	-1.145776
56	1	0	-2.397794	3.140020	0.504400
57	1	0	-1.203418	1.870666	0.815606
58	8	0	-4.931250	2.201041	0.164894
59	7	0	-4.262398	0.240055	1.092976
60	6	0	-1.244191	3.013611	-3.562251
61	6	0	0.192376	3.477508	-1.175248
62	1	0	-3.615579	-0.544223	1.073291
63	6	0	-5.392742	0.155319	2.012305
64	6	0	0.003486	3.636690	-3.610697
65	1	0	-1.794527	2.831913	-4.481136
66	6	0	0.723103	3.863254	-2.423923
67	1	0	0.755850	3.664508	-0.266034
68	6	0	-6.742673	0.337221	1.301588
69	8	0	-7.690525	0.927778	1.777587
70	8	0	-6.779114	-0.319155	0.131541
71	6	0	-8.009810	-0.211889	-0.605361
72	1	0	-7.855903	-0.792020	-1.514809
73	1	0	-8.214782	0.833657	-0.848337
74	1	0	-8.842303	-0.618680	-0.025323
75	6	0	-0.977977	-1.919195	3.607093
76	1	0	-0.360345	-3.647766	2.485532
77	1	0	-1.962768	-2.321651	3.851921
78	1	0	-0.290768	-2.130719	4.431649
79	1	0	-1.063724	-0.837316	3.482514
80	6	0	-2.657478	-3.602675	-1.523667
81	1	0	-3.233902	-3.491010	-2.444086
82	1	0	-2.013735	-4.483588	-1.608696
83	1	0	-3.353464	-3.747509	-0.694112
84	1	0	-1.090532	-2.255982	-2.123485
85	6	0	-5.261551	1.111072	3.202250
86	1	0	-6.103596	0.984888	3.887559
87	1	0	-4.331937	0.902199	3.740303
88	1	0	-5.249311	2.147464	2.856434
89	1	0	-5.391366	-0.878131	2.379806
90	1	0	6.434705	3.602798	-0.075964
91	1	0	0.430689	3.938511	-4.561473
92	6	0	7.320530	3.130959	2.398557
93	7	0	8.249611	3.617271	2.903772
94	6	0	2.024148	4.459573	-2.484050
95	7	0	3.090783	4.925473	-2.527340

SCF Done: E(RB3LYP) = -2421.03973175

Full mass-weighted force constant matrix:
Low frequencies --- -0.0009 0.0007 0.0010 2.4375 3.7284
6.3948
Low frequencies --- 14.7533 15.4043 19.9687

***bis*-(*R*)-Aic(CN) penta peptide conformer left2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.453611	3.046535	0.058260
2	6	0	2.926275	3.168423	1.372458
3	6	0	2.621264	4.284375	2.139007
4	6	0	1.824320	5.295156	1.567976
5	6	0	1.348141	5.174968	0.249473
6	6	0	1.664477	4.047199	-0.507073
7	1	0	2.978405	4.386788	3.159051
8	1	0	1.291843	3.955295	-1.523193
9	6	0	2.935043	1.758907	-0.563506
10	6	0	3.771947	1.975346	1.749753
11	6	0	3.422221	0.912966	0.653249
12	1	0	3.588901	1.607253	2.764069
13	1	0	4.840262	2.228712	1.690581
14	1	0	3.786830	1.948798	-1.229760
15	1	0	2.166842	1.242375	-1.141367
16	7	0	4.589988	0.074065	0.383807
17	6	0	2.251659	0.043707	1.180876
18	1	0	5.501985	0.482211	0.550048
19	6	0	4.552384	-0.916405	-0.569642
20	8	0	3.506229	-1.378161	-1.020238
21	8	0	5.796576	-1.298067	-0.881771
22	6	0	6.069174	-2.399814	-1.841399
23	6	0	5.535492	-2.019924	-3.224511
24	1	0	5.955678	-1.061065	-3.546302
25	1	0	4.446579	-1.948940	-3.225490
26	1	0	5.836385	-2.782787	-3.950420
27	6	0	5.471786	-3.706457	-1.314220
28	1	0	5.831344	-3.909783	-0.299719
29	1	0	5.788728	-4.533952	-1.957680
30	1	0	4.381060	-3.672510	-1.306264
31	6	0	7.597634	-2.458597	-1.840756
32	1	0	7.938593	-3.241198	-2.525688
33	1	0	7.977627	-2.685511	-0.839504
34	1	0	8.022855	-1.504141	-2.166960
35	8	0	1.077248	0.334991	0.940388
36	7	0	2.604701	-1.018457	1.941285
37	1	0	3.592326	-1.191382	2.075937
38	6	0	1.634737	-1.927496	2.557808
39	6	0	0.656104	-2.533997	1.524358
40	8	0	-0.465664	-2.912169	1.881070
41	7	0	1.111963	-2.658461	0.258723
42	1	0	2.017106	-2.266020	0.011310
43	6	0	0.311809	-3.219941	-0.832356
44	6	0	-1.023321	-2.472762	-1.066721
45	8	0	-1.954552	-3.027222	-1.646304
46	7	0	-1.073493	-1.175601	-0.660299
47	1	0	-0.287402	-0.778289	-0.152797
48	6	0	-2.286053	-0.369729	-0.779768
49	6	0	-2.792020	-0.223117	-2.250647

50	6	0	-1.985886	1.097115	-0.305304
51	6	0	-3.442179	-0.906711	0.107340
52	6	0	-3.192146	1.224858	-2.375453
53	1	0	-1.974948	-0.460348	-2.942387
54	1	0	-3.612759	-0.909285	-2.464247
55	6	0	-2.740067	1.969303	-1.278046
56	1	0	-2.281900	1.260284	0.736256
57	1	0	-0.908130	1.293926	-0.356451
58	8	0	-4.609854	-0.597991	-0.139397
59	7	0	-3.090698	-1.631071	1.194323
60	6	0	-3.895628	1.842595	-3.409707
61	6	0	-2.979986	3.334815	-1.198075
62	1	0	-2.137606	-1.966347	1.307375
63	6	0	-4.086247	-2.093959	2.155984
64	6	0	-4.146492	3.211856	-3.344559
65	1	0	-4.253493	1.267007	-4.258810
66	6	0	-3.689560	3.958515	-2.242573
67	1	0	-2.635675	3.921127	-0.351457
68	6	0	-5.260064	-2.822864	1.483280
69	8	0	-6.415774	-2.736833	1.844964
70	8	0	-4.839156	-3.645199	0.509377
71	6	0	-5.868721	-4.382140	-0.172626
72	1	0	-5.351539	-4.974692	-0.926783
73	1	0	-6.576561	-3.696009	-0.644132
74	1	0	-6.404367	-5.030833	0.525593
75	6	0	0.883287	-1.283922	3.727842
76	1	0	2.224500	-2.769590	2.938613
77	1	0	0.197801	-2.008050	4.172270
78	1	0	1.597406	-0.955088	4.488662
79	1	0	0.306047	-0.421983	3.384910
80	6	0	0.082127	-4.727995	-0.682255
81	1	0	-0.497470	-5.099629	-1.529367
82	1	0	1.045101	-5.247007	-0.650716
83	1	0	-0.467903	-4.941117	0.237080
84	1	0	0.905938	-3.045757	-1.737508
85	6	0	-4.584005	-0.974785	3.075703
86	1	0	-5.295820	-1.367766	3.806120
87	1	0	-3.735966	-0.533845	3.608292
88	1	0	-5.082045	-0.197757	2.490873
89	1	0	-3.576367	-2.854791	2.759541
90	1	0	0.731092	5.962504	-0.170311
91	1	0	-4.697084	3.709043	-4.136537
92	6	0	1.493357	6.455851	2.341038
93	7	0	1.229641	7.398115	2.971442
94	6	0	-3.947689	5.366549	-2.183815
95	7	0	-4.151432	6.512099	-2.138682

SCF Done: E(RB3LYP) = -2421.03494763

Full mass-weighted force constant matrix:
Low frequencies --- -5.6895 -0.0008 0.0002 0.0006 5.3535
6.3481
Low frequencies --- 7.3680 12.3857 13.9293