Supporting Information

Conformational Modulation of *Ant-Pro* Oligomers using Chirality alteration of Proline residues

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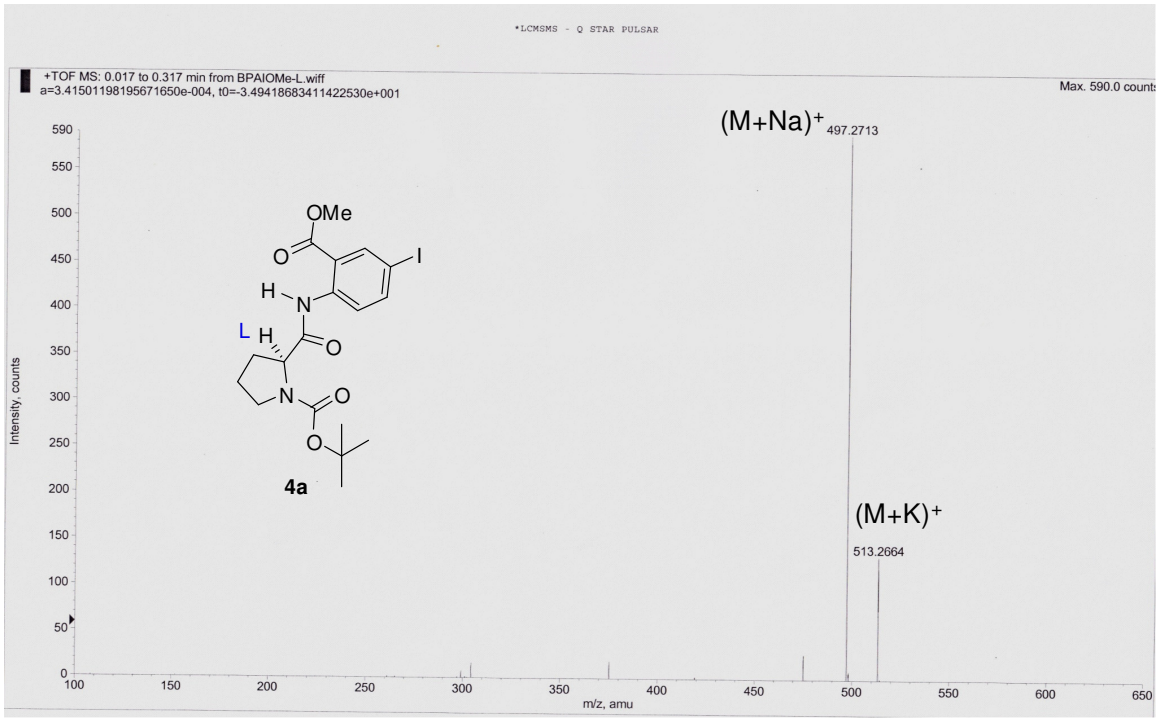
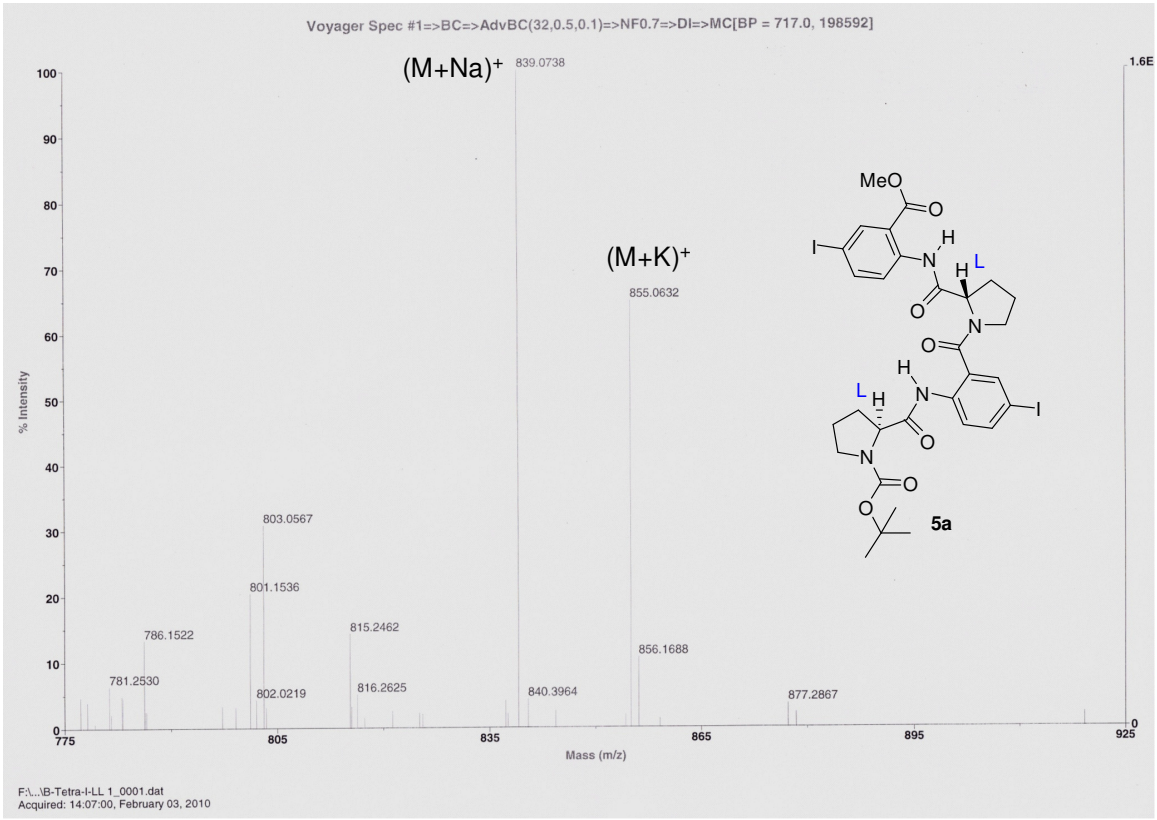
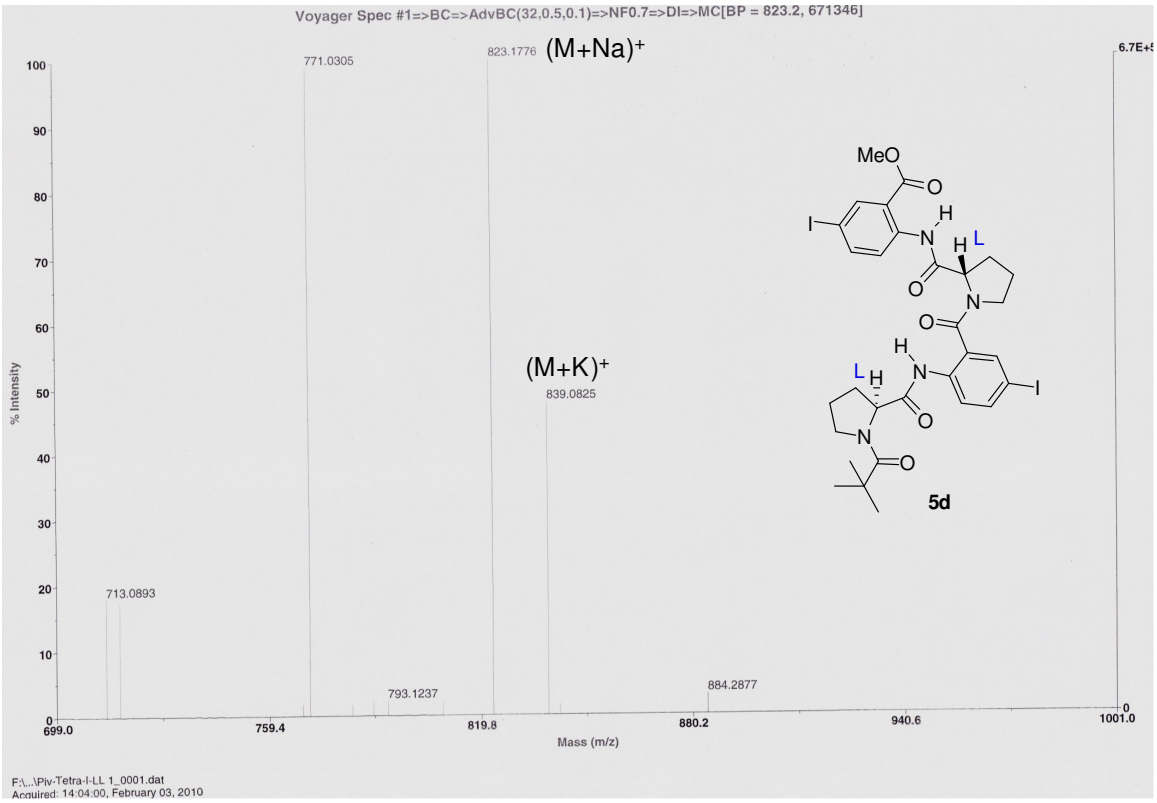
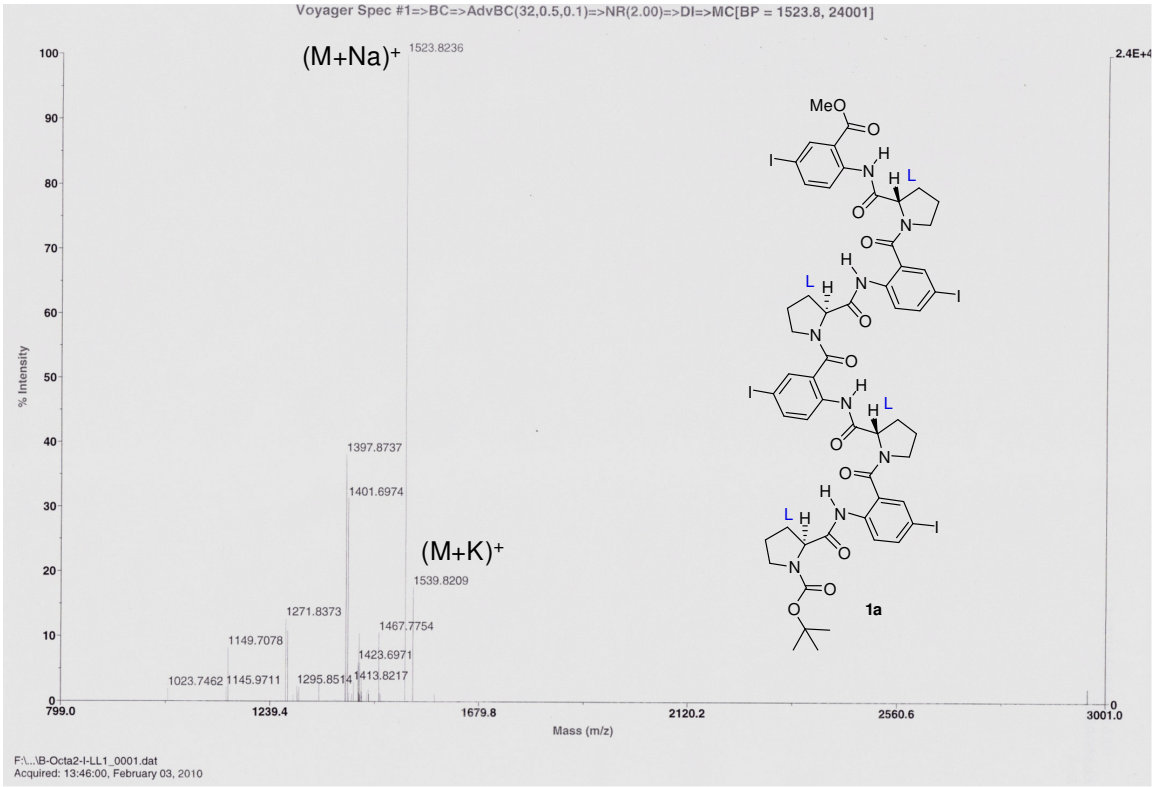
General Methods.

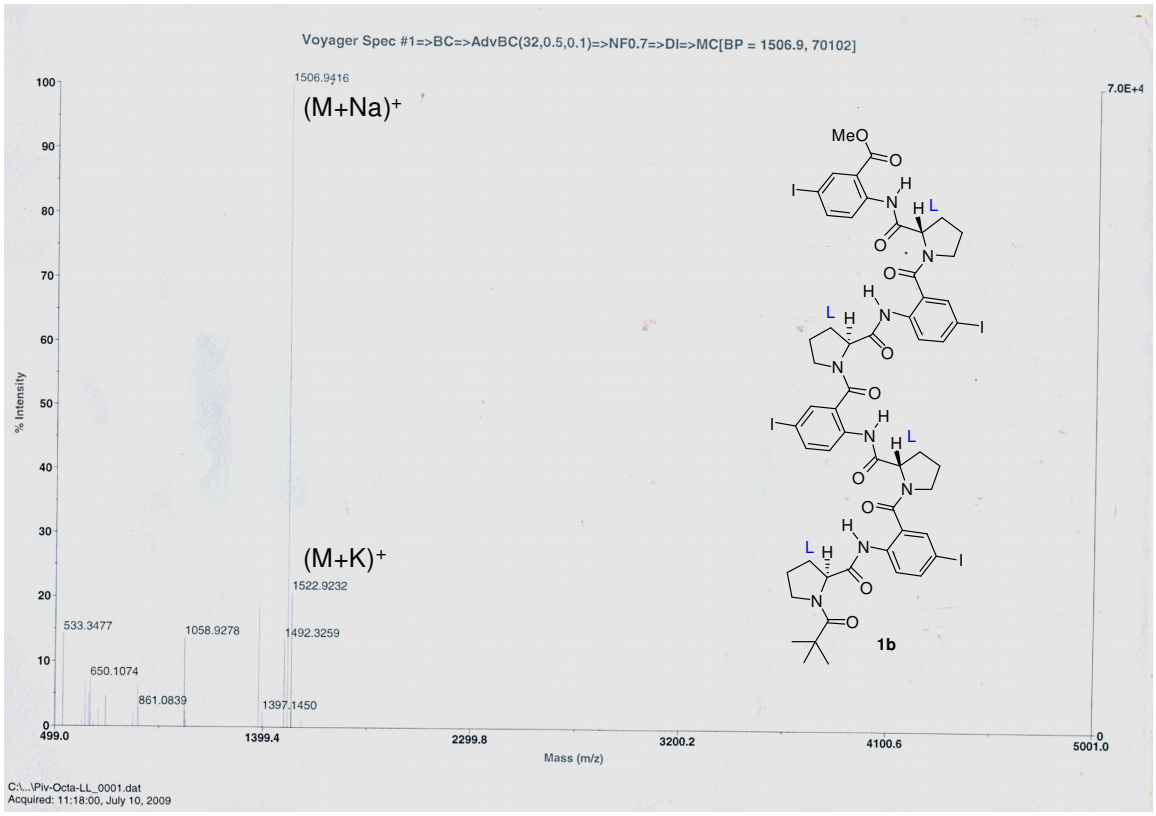
Unless otherwise stated, all the chemicals and reagents were obtained commercially. Dry solvents were prepared by the standard procedures. Analytical Thin Layer Chromatography was done on precoated silica gel plates (Kieselgel $60F_{254}$, Merck). Unless otherwise stated Column Chromatographic purifications were done with 100-200 Mesh Silica gel. NMR spectra were recorded in $CDCl_3$ on AV 200 MHz, AV 400 MHz or AV 500 MHz spectrometers. All chemical shifts are reported in δ ppm downfield to TMS and peak multiplicities as singlet (s), doublet (d), quartet (q), broad singlet (bs), and multiplet (m). The titration studies were done in $CDCl_3$. Elemental analyses were performed on an Elmentar-Vario-EL (Heraeus Company Ltd., Germany). IR spectra were recorded in $CHCl_3$ using Shimadzu FTIR-8400 spectrophotometer. Melting points were determined on a Buchi Melting Point B-540. Electron Scattered Ionization (ESI) Mass Spectrometric measurements were done with API QSTAR Pulsar mass Spectrometer. All spectra have been arranged, as they appear in Scheme 1.

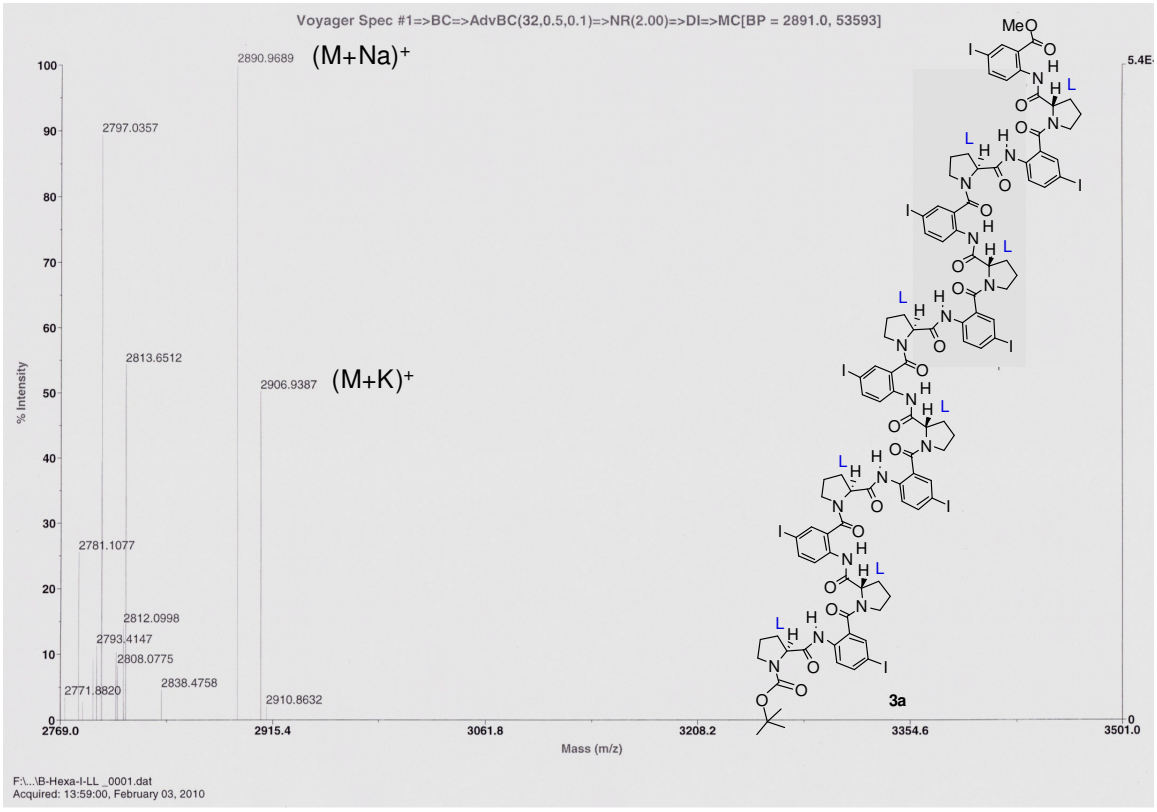


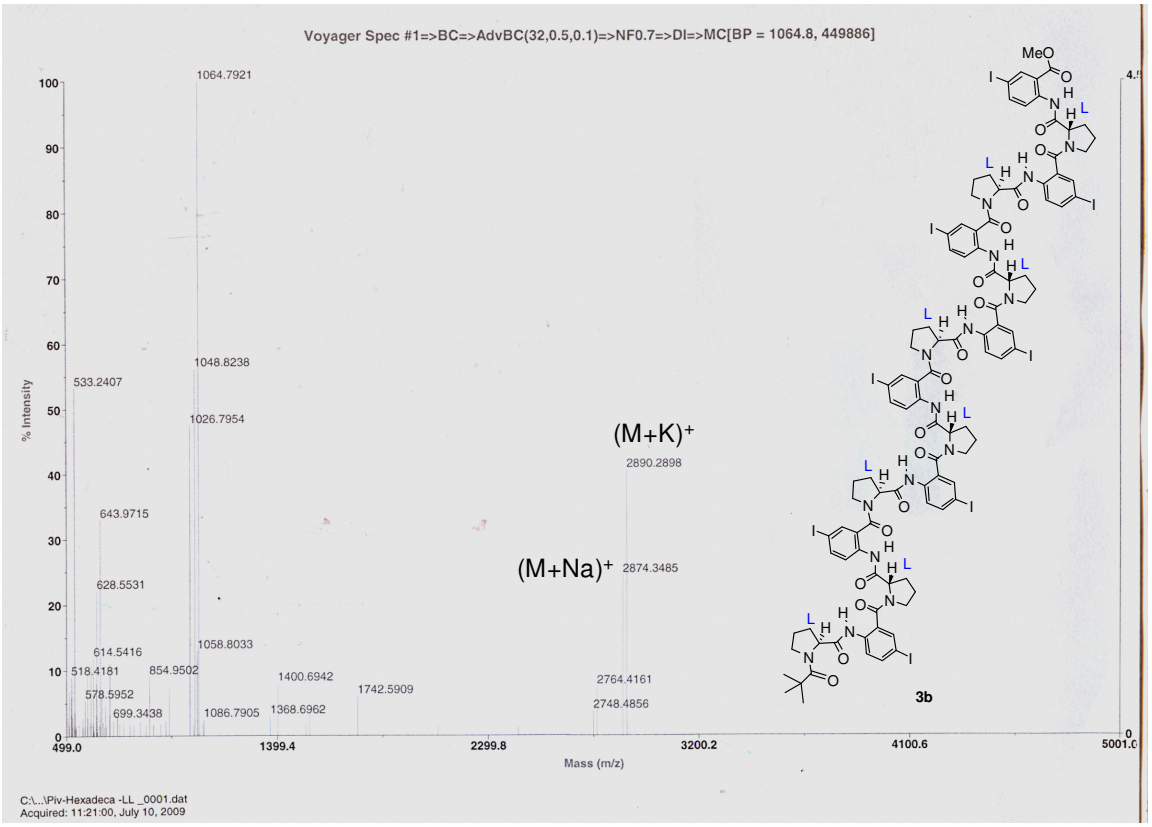








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1048.8238
533.2407
1026.7954
643.9715
628.5531
614.5416
518.4181
854.9502
578.5952
699.3438
1058.8033
1086.7905
1400.6942
1368.6962
1742.5909
(M+K)+
2890.2898
(M+Na)+ 2874.3485
2764.4161
2748.4856
3b
% Intensity
Mass (m/z)
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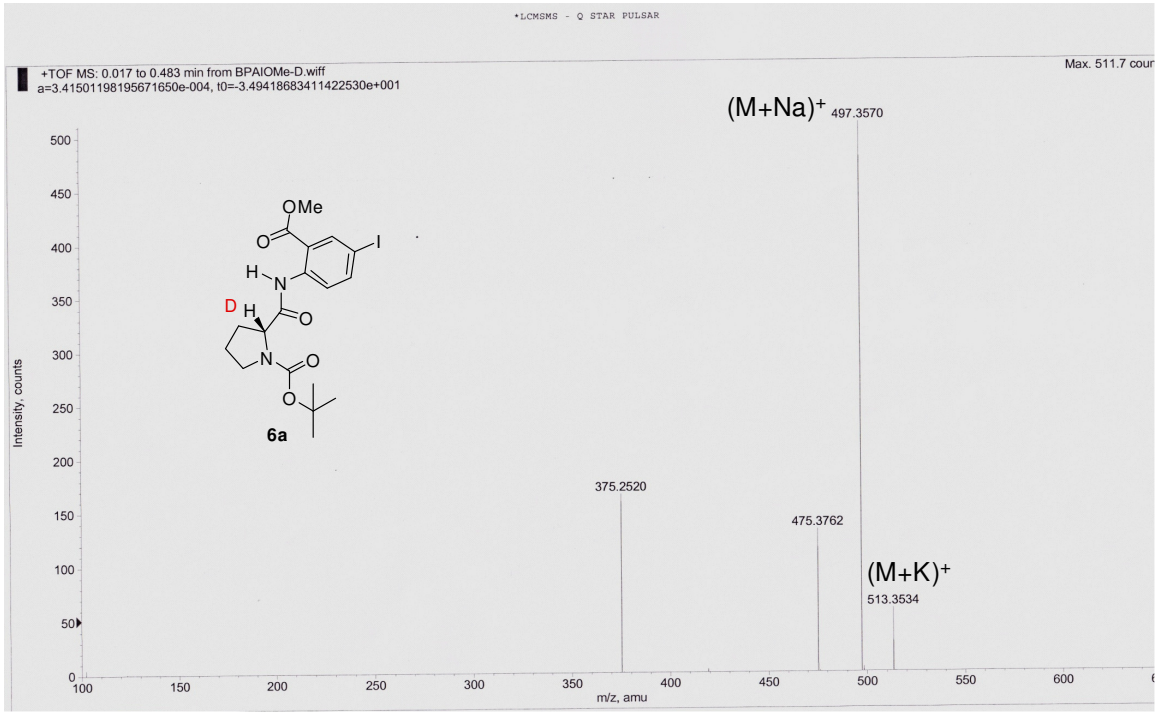
Acquired: 11:21:00, July 10, 2009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+TOF MS: 0.017 to 0.483 min from BPAIOMe-D.wiff
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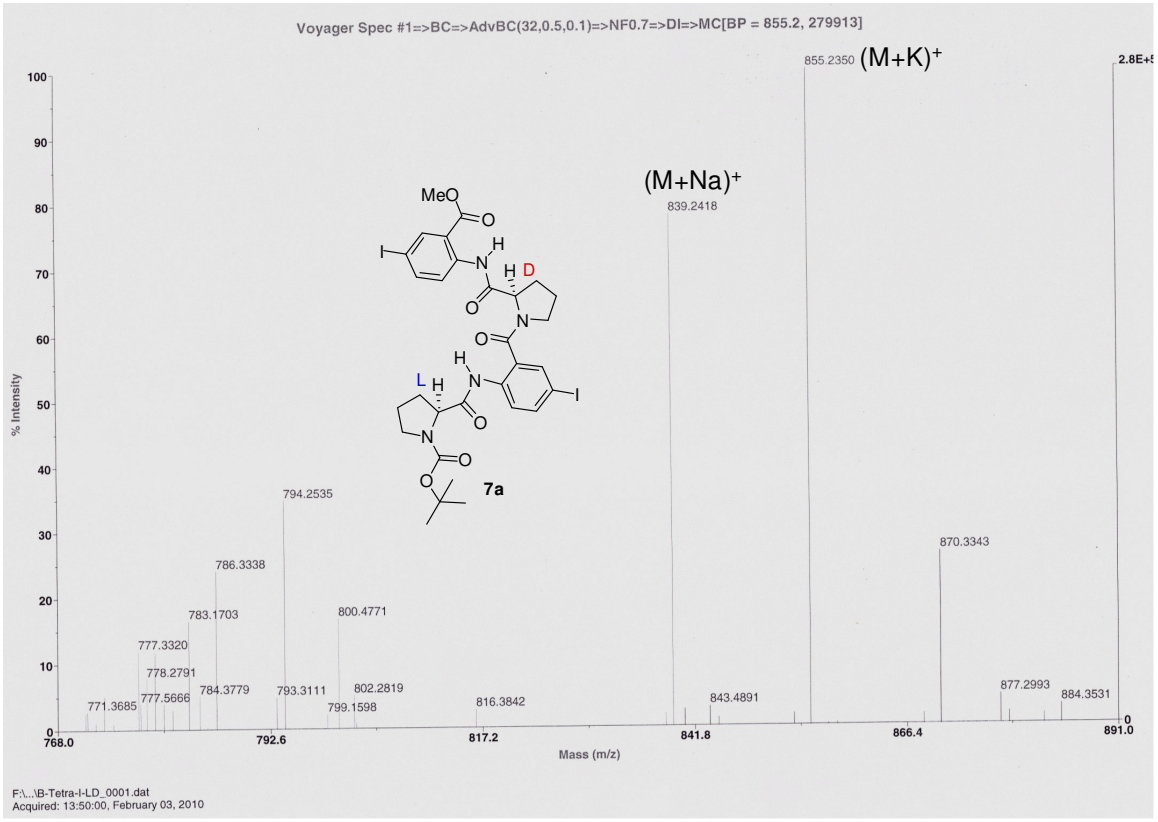
Max. 511.7 cour
(M+Na)+ 497.3570
OMe
D
6a
375.2520
475.3762
(M+K)+
513.3534
Intensity, counts
m/z, amu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855.2350 (M+K)+
(M+Na)+
839.2418
MeO
O
I
H
N
H D
O
N
O
H
N
L H
I
O
N
O
O
7a
794.2535
786.3338
783.1703
800.4771
777.3320
778.2791
777.5666
784.3779
793.3111
802.2819
771.3685
799.1598
816.3842
843.4891
870.3343
877.2993
884.3531
% Intensity
Mass (m/z)
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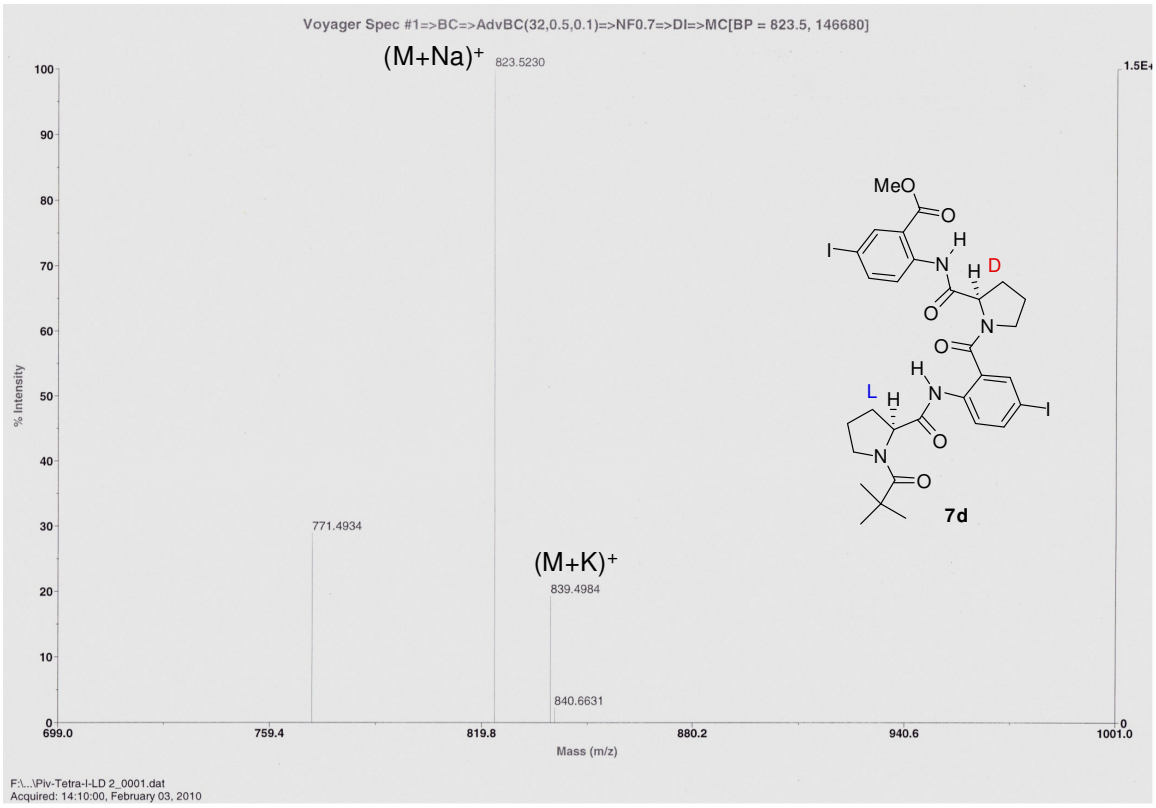
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(M+Na)+
823.5230
MeO
O
I
H
N
H D
O
N
O
H
N
L H
I
O
N
O
O
7d
771.4934
(M+K)+
839.4984
840.6631
% Intensity
Mass (m/z)
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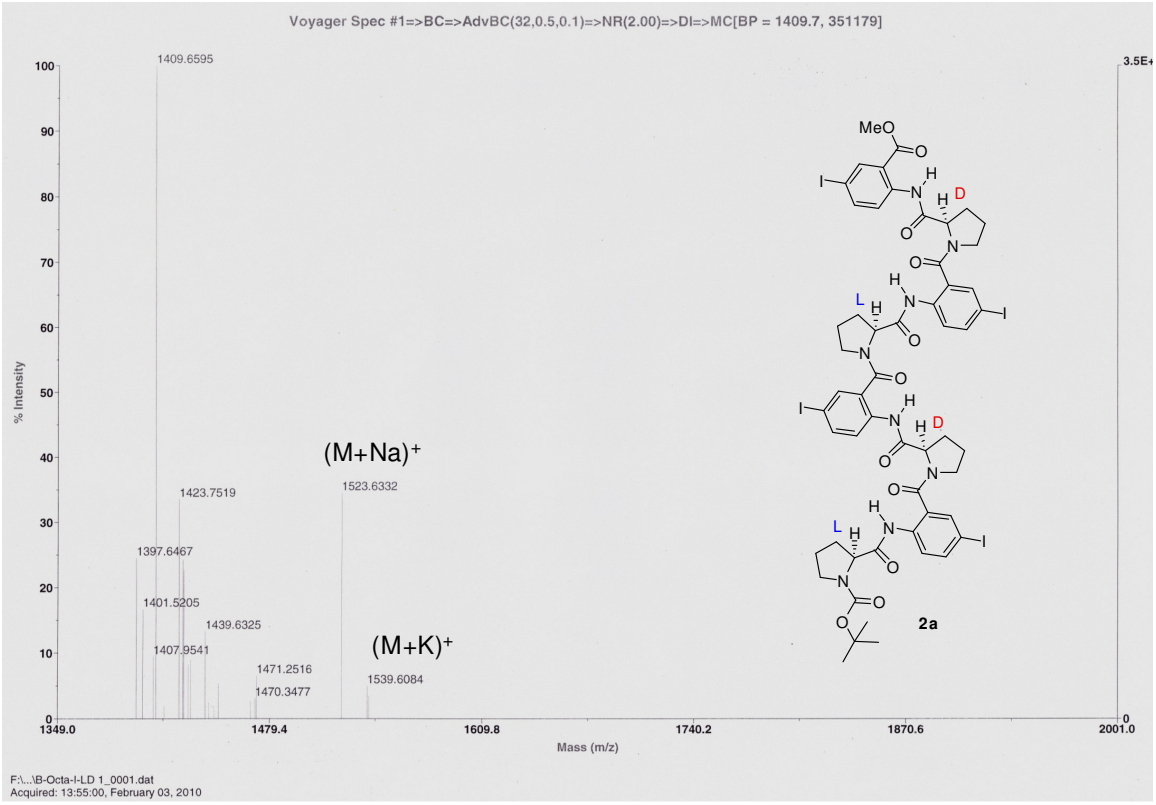
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(M+Na)+
1523.6332
1423.7519
1397.6467
1401.5205
1439.6325
1407.9541
(M+K)+
1471.2516
1470.3477
1539.6084
% Intensity
Mass (m/z)
1349.0
1479.4
1609.8
1740.2
1870.6
2001.0
2a
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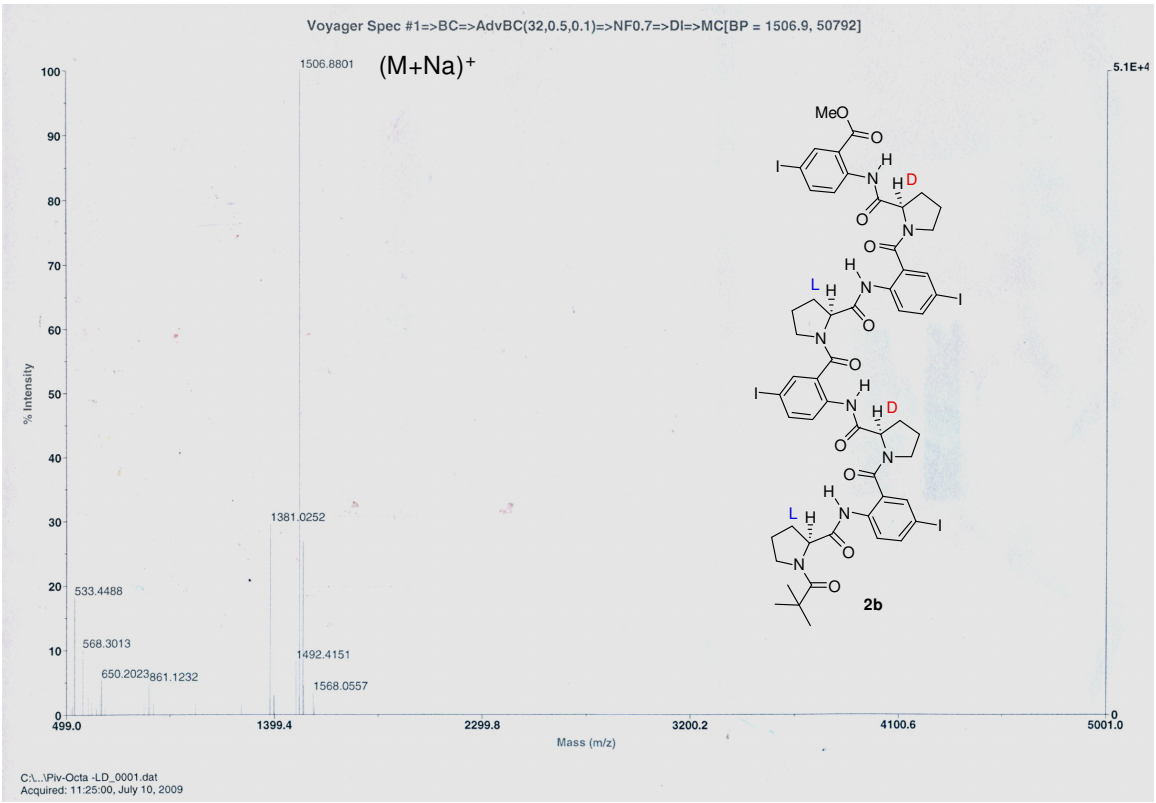
Voyager Spec #1=>BC=>AdvBC(32,0.5,0.1)=>NF0.7=>DI=>MC[BP = 1506.9, 50792]
1506.8801
(M+Na)+
1381.0252
533.4488
568.3013
650.2023
861.1232
1492.4151
1568.0557
% Intensity
Mass (m/z)
499.0
1399.4
2299.8
3200.2
4100.6
5001.0
2b
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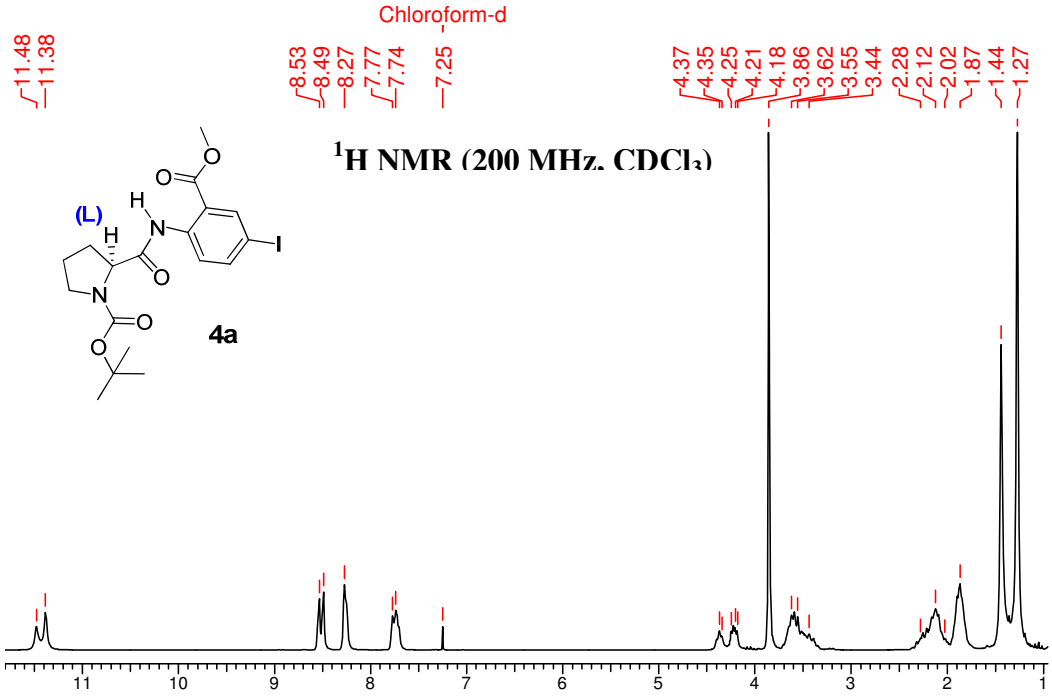
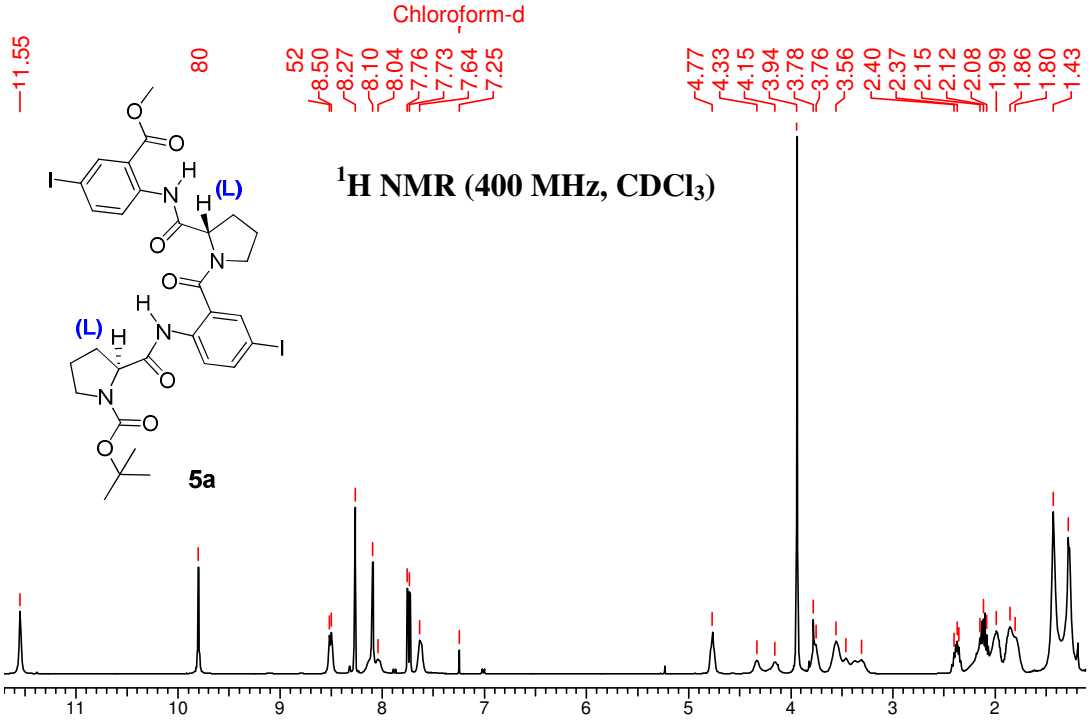
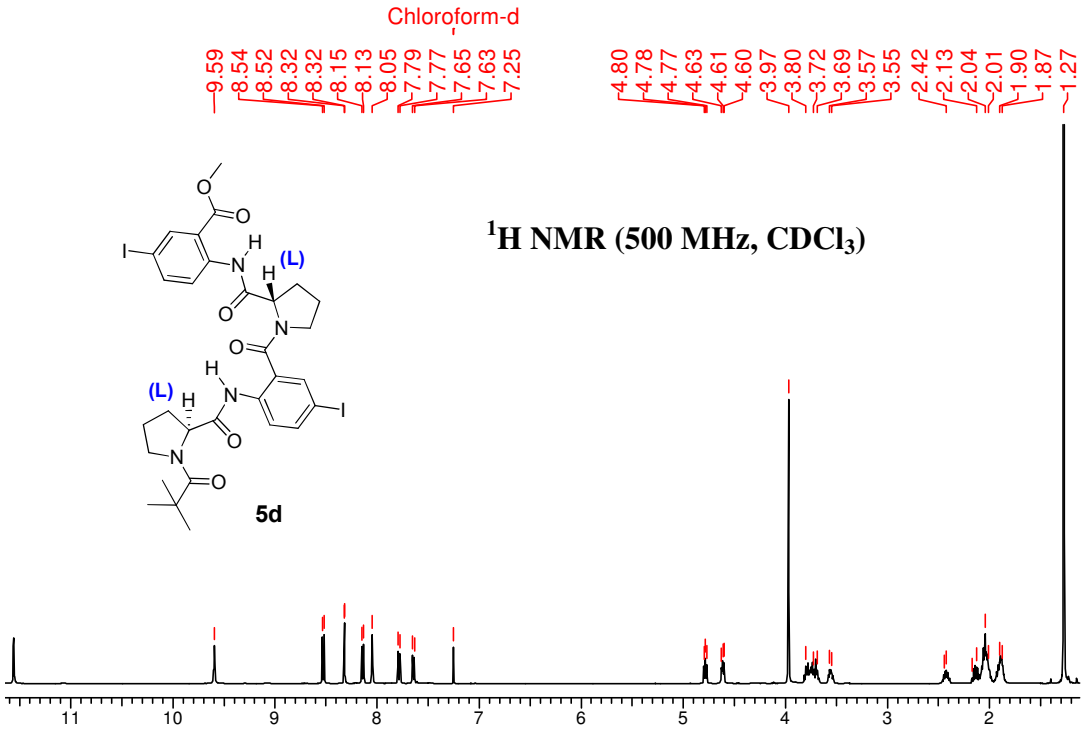
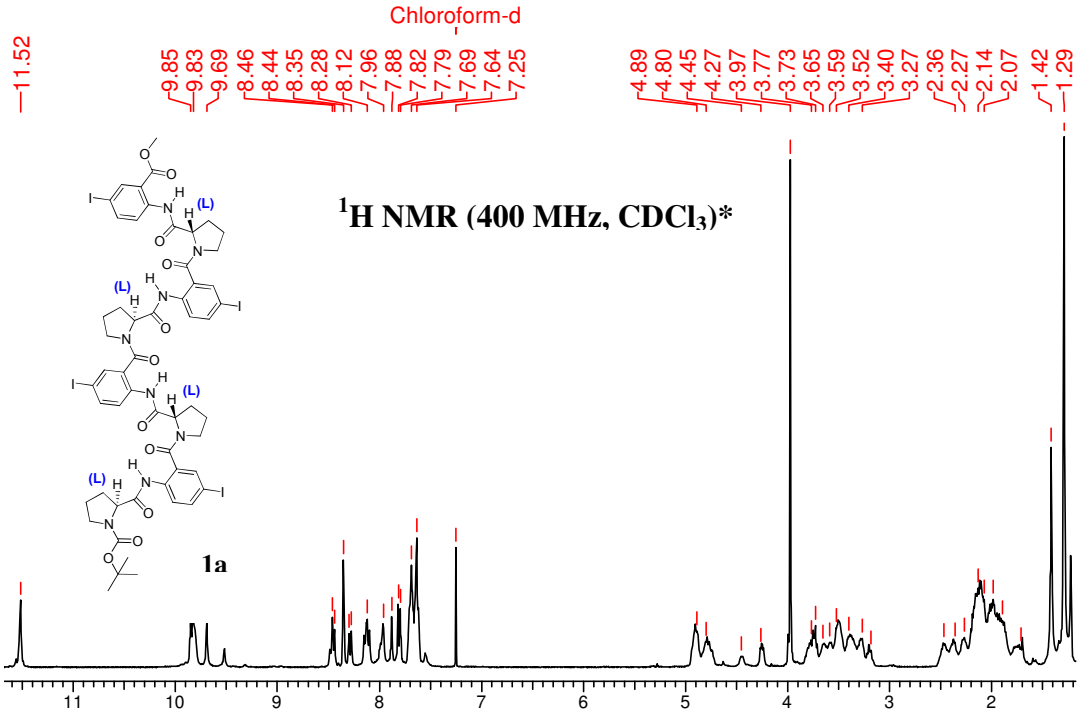




NOTE: Signal broadening and / or multiple set of signals seen are due to rotamer formation at the N-terminus (N^{t}BOC Pro effect: *Chem. Eur. J.* **2008**, 14, 6192)

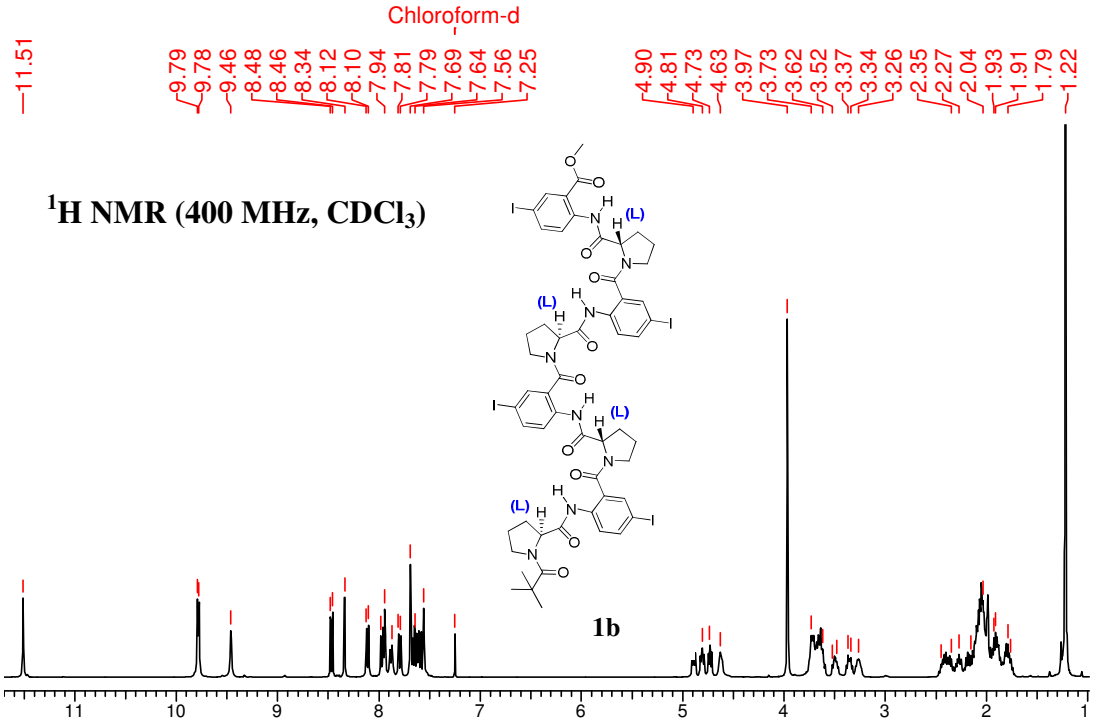


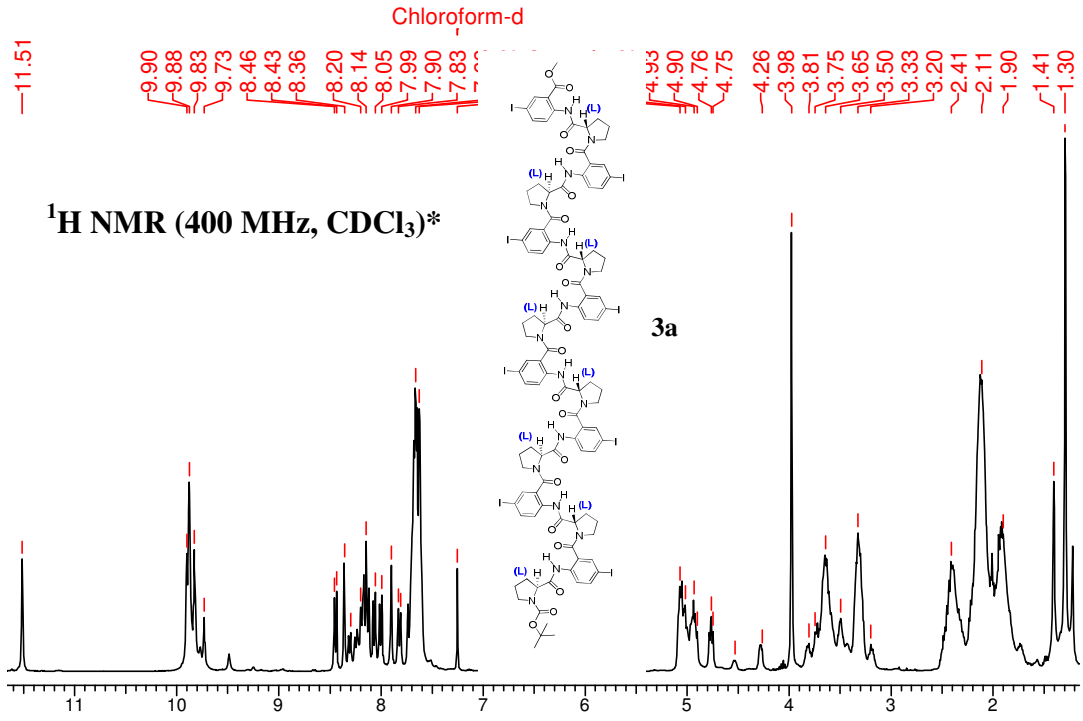
^{1}H NMR (500 MHz, $CDCl_3$)



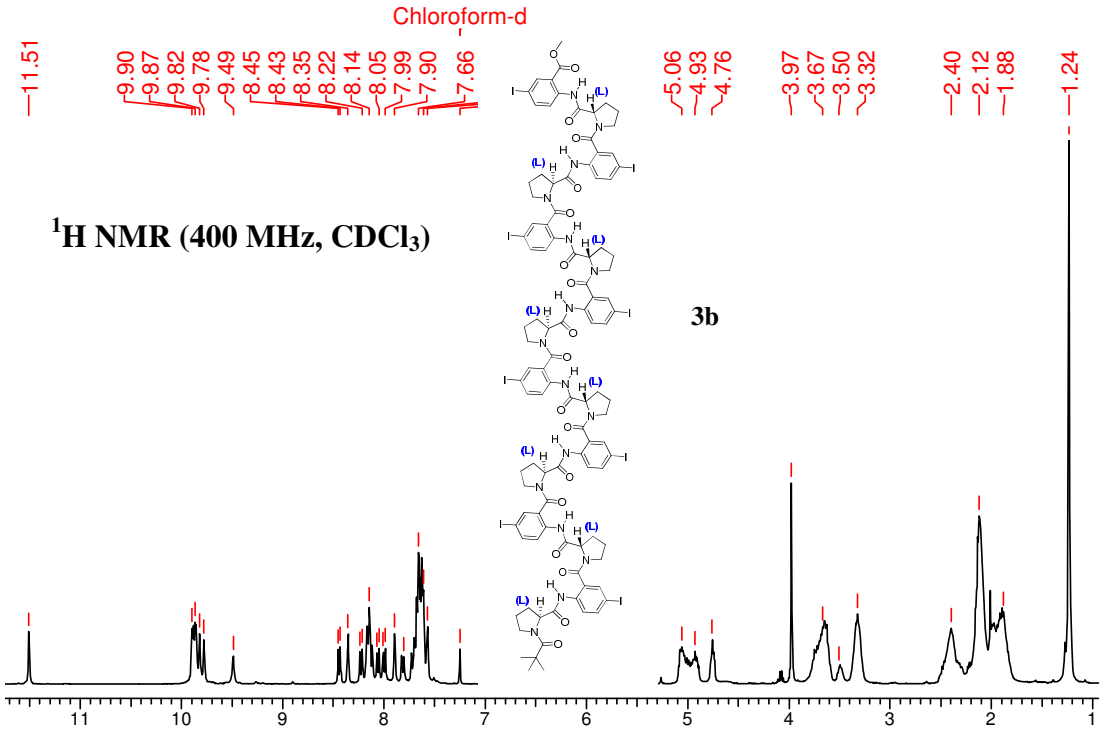
^{1}H NMR (400 MHz, $CDCl_3$)*

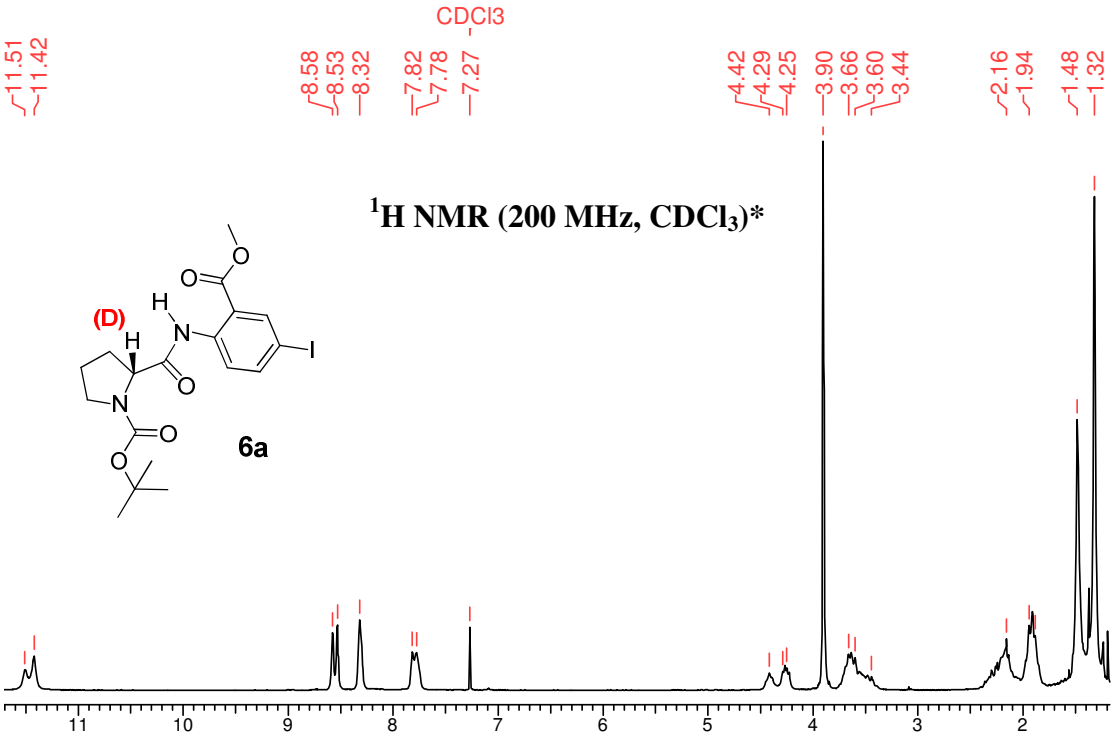
* Signal broadening and / or multiple set of signals seen are due to rotamer formation at the N-terminus (N^{t}BOC Pro effect: *Chem. Eur. J.* **2008**, 14, 6192)





***** Signal broadening and / or multiple set of signals seen are due to rotamer formation at the N-terminus (N^{t}BOC Pro effect: *Chem. Eur. J.* **2008**, 14, 6192)





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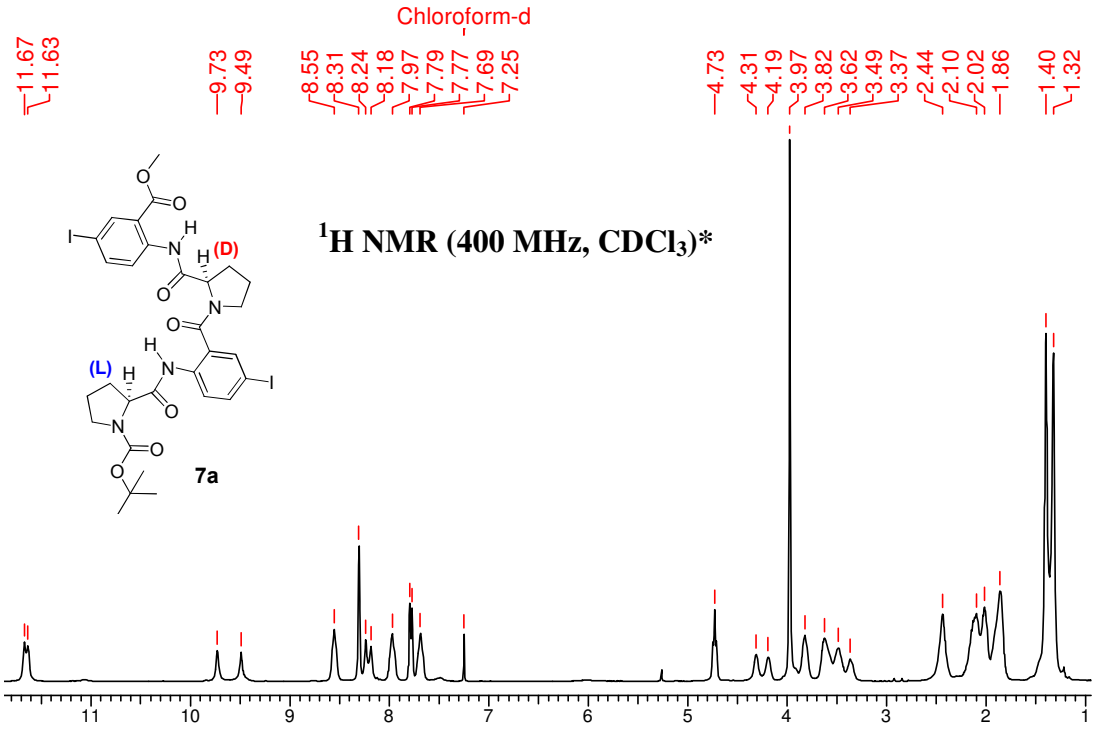

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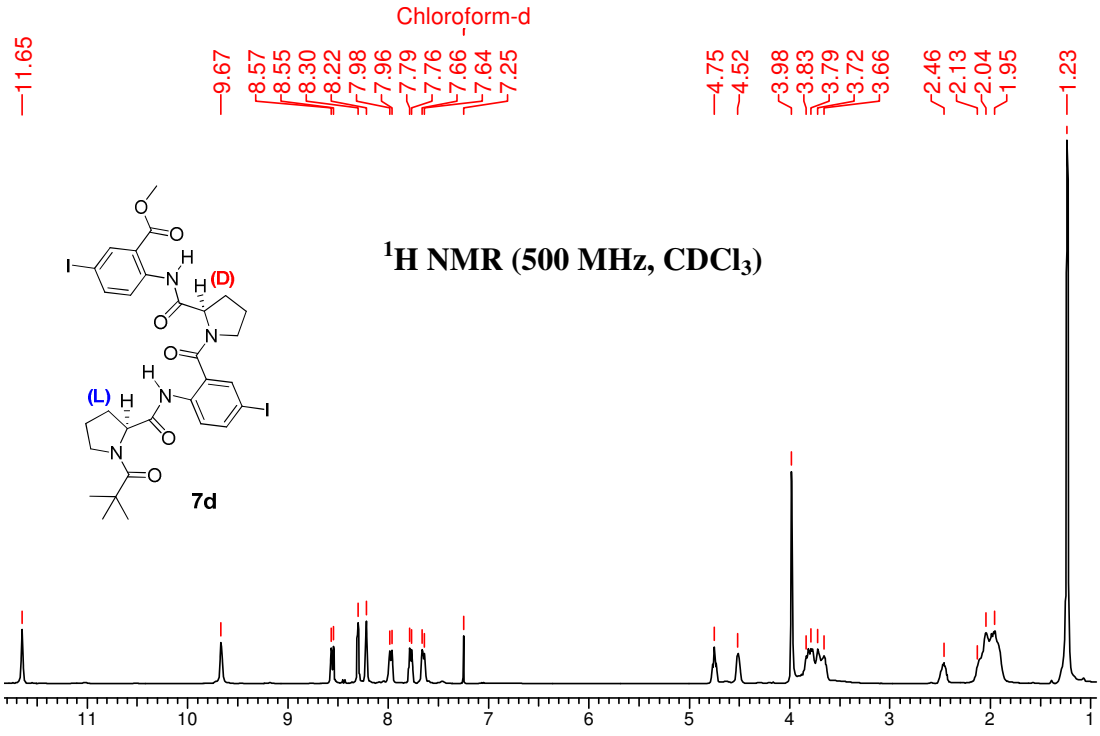

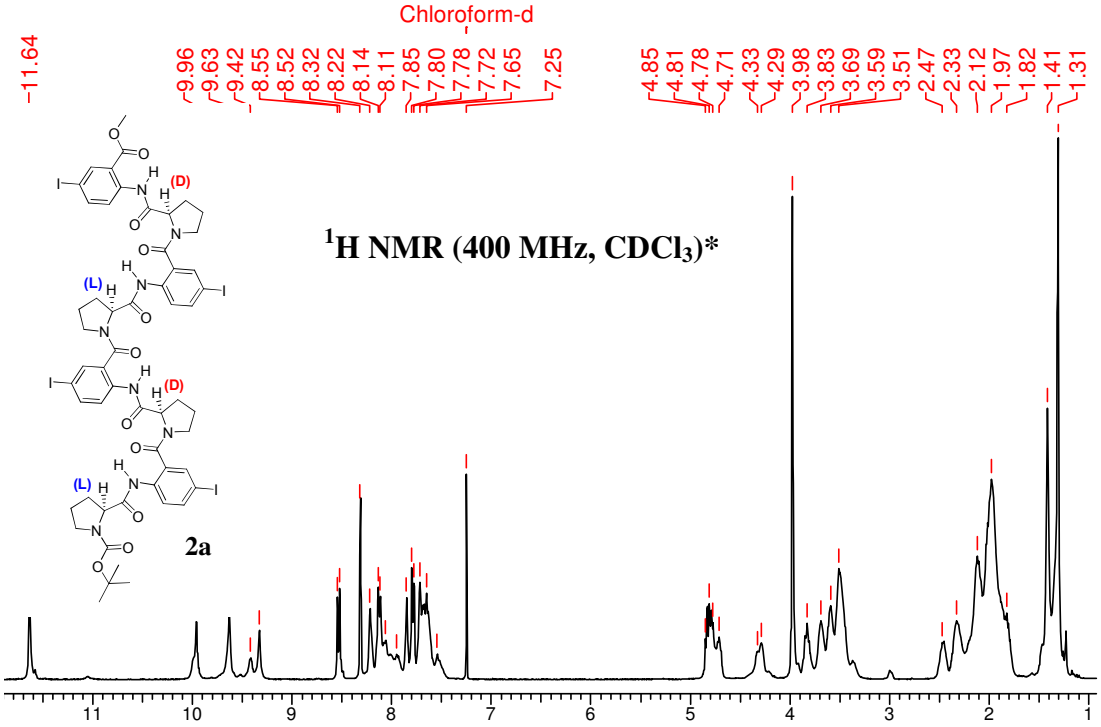

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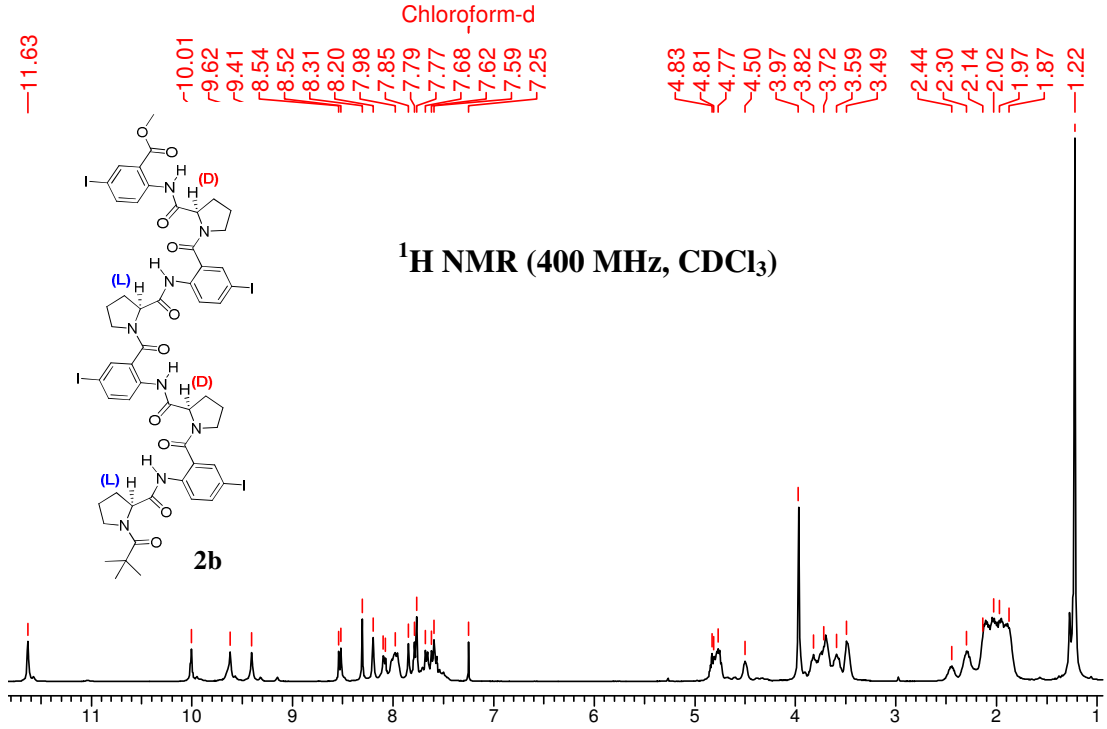
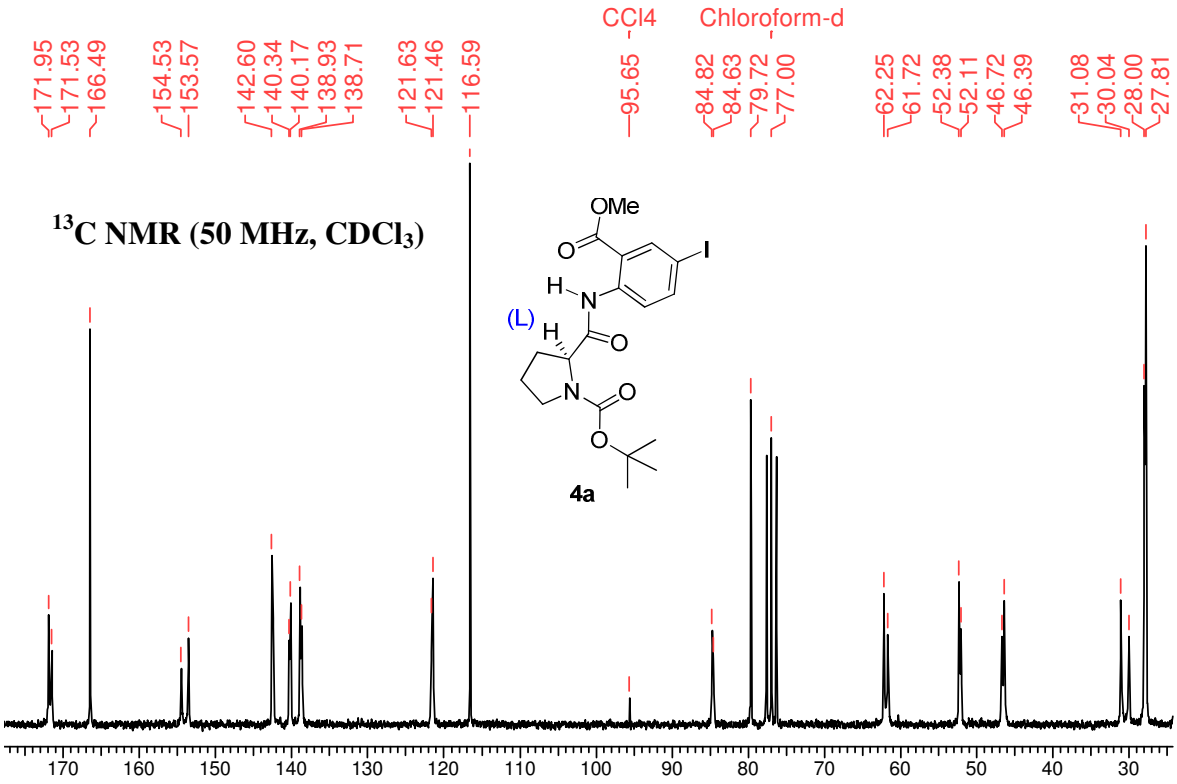
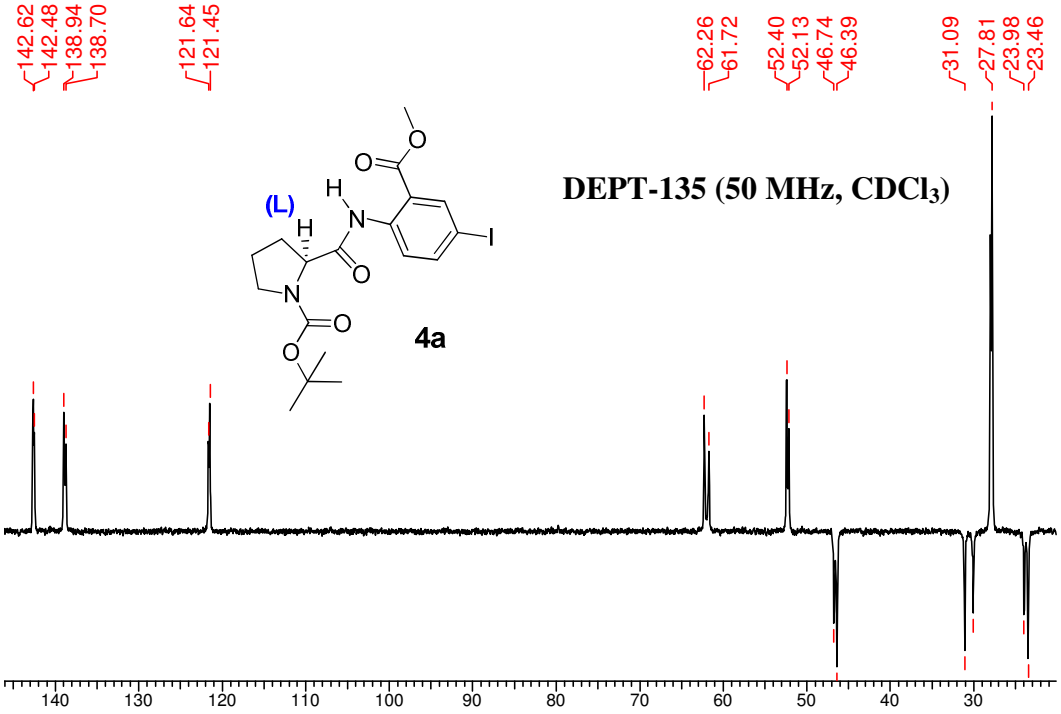
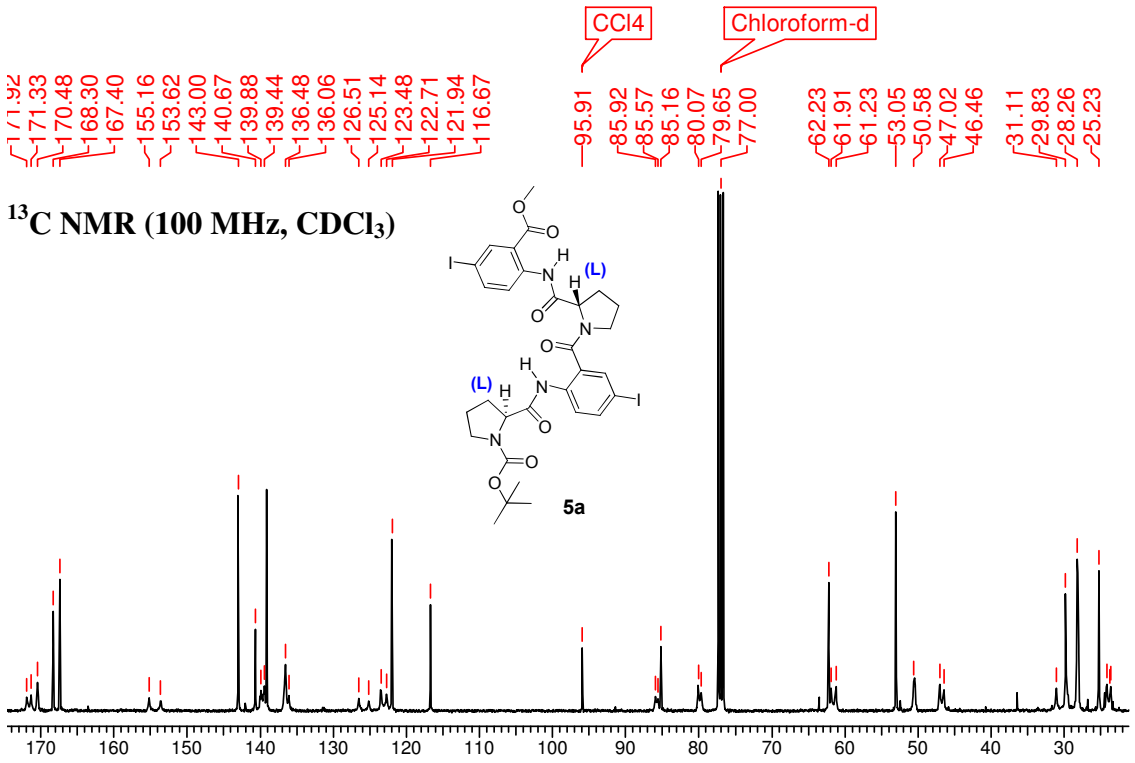
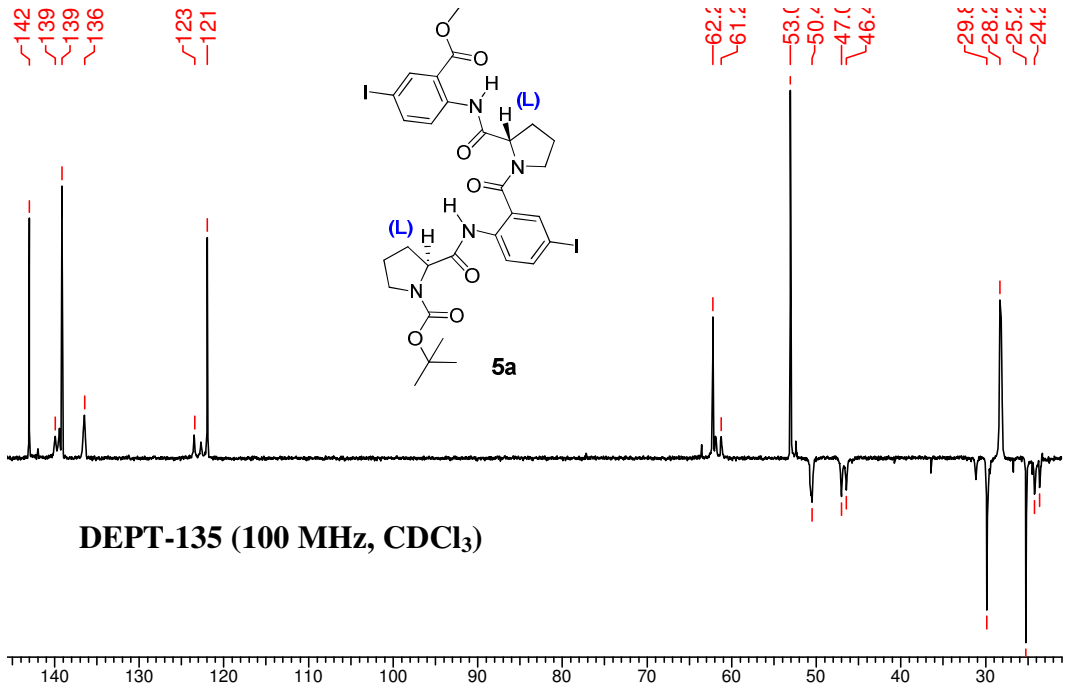




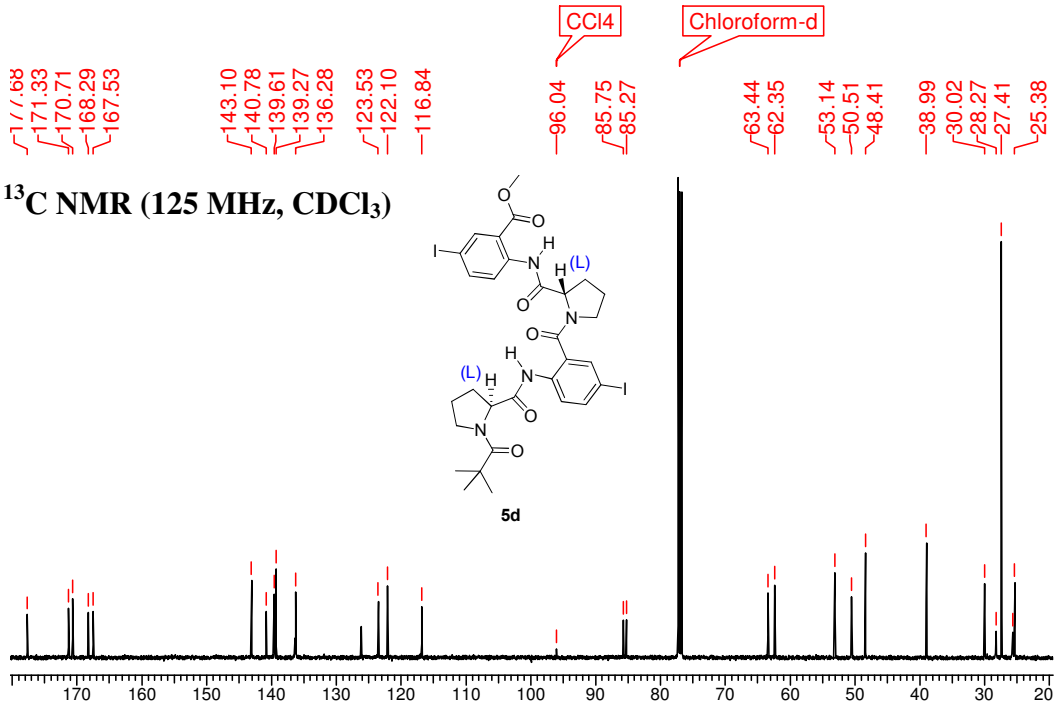


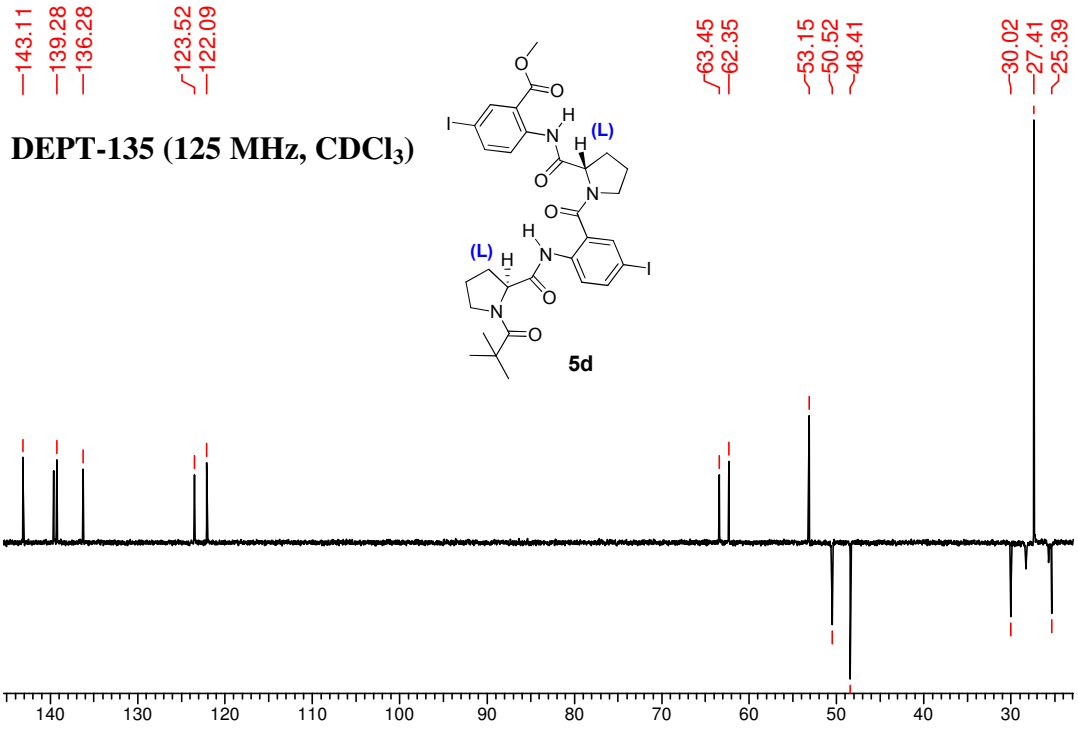
NOTE: Signal broadening and / or multiple set of signals seen are due to rotamer formation at the N-terminus (N^{t}BOC Pro effect: *Chem. Eur. J.* **2008**, 14, 6192)

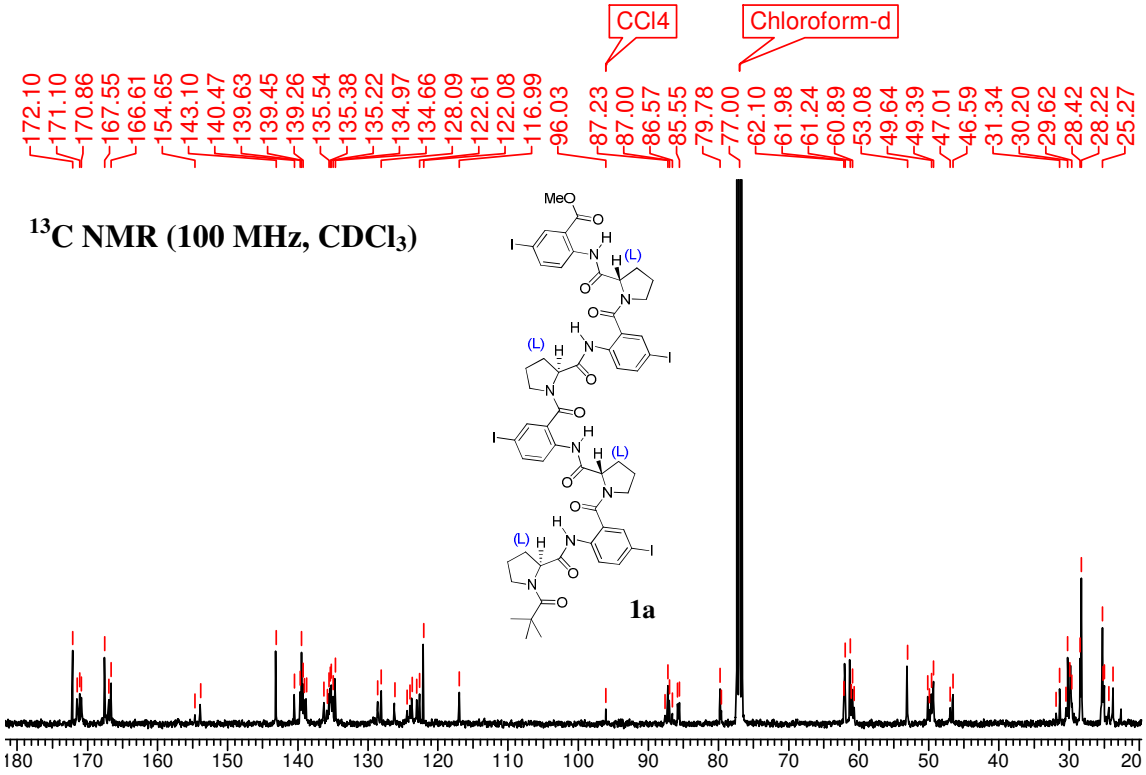


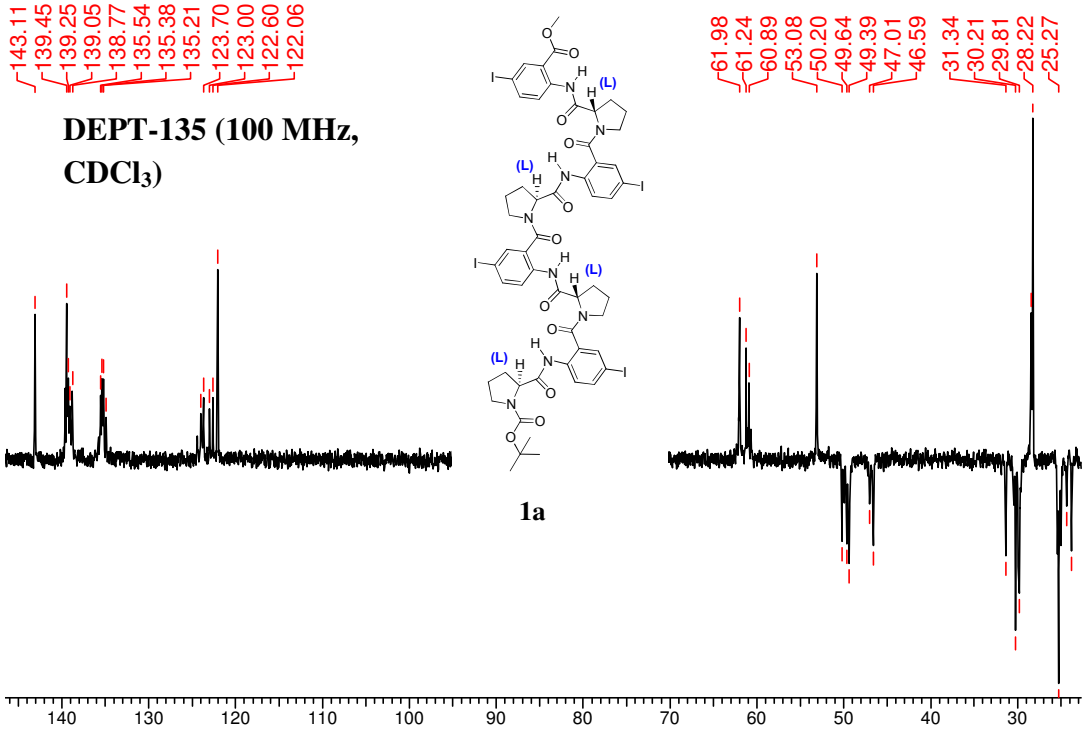


NOTE: Signal broadening and / or multiple set of signals seen are due to rotamer formation at the N-terminus (N^{t}BOC Pro effect: *Chem. Eur. J.* **2008**, 14, 6192)









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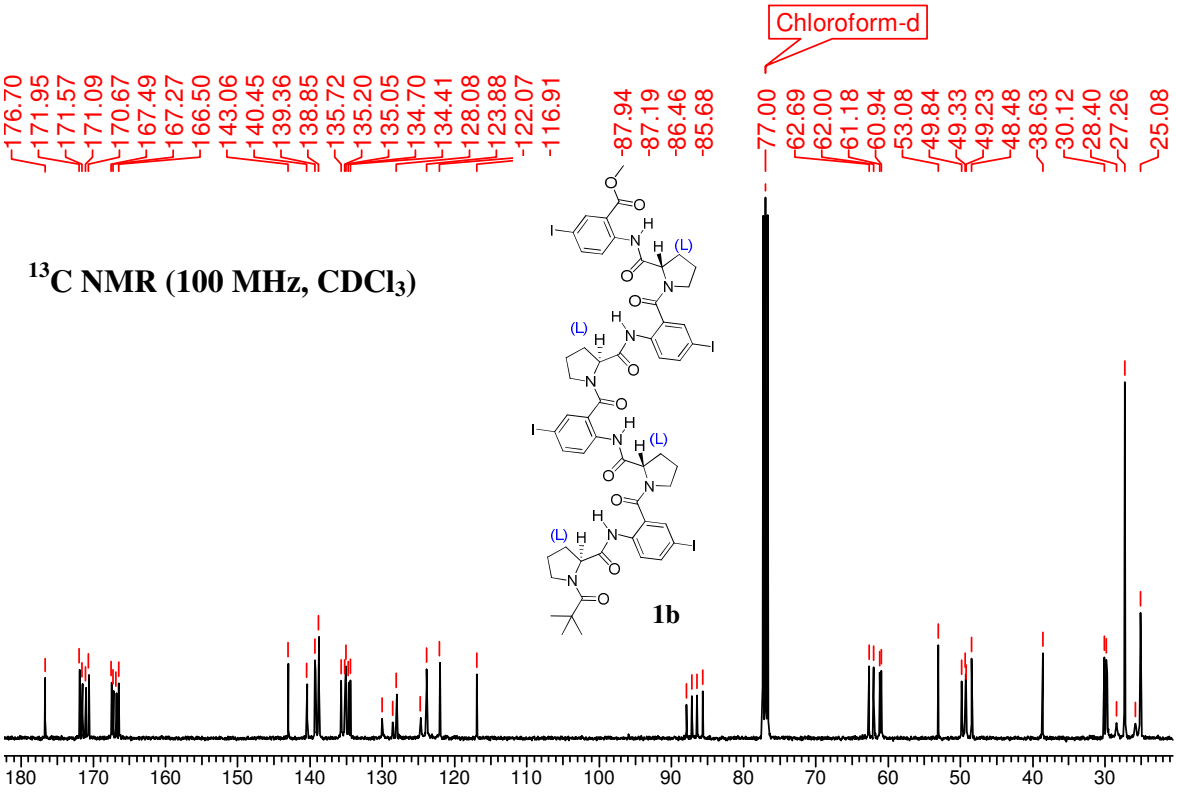

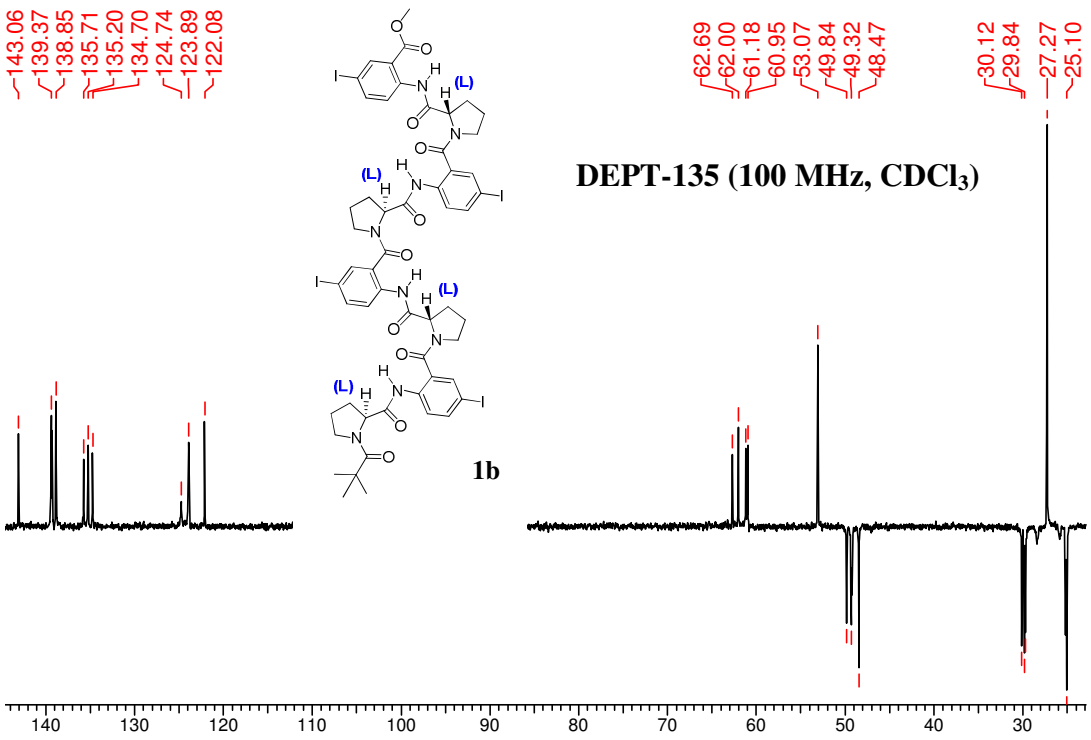

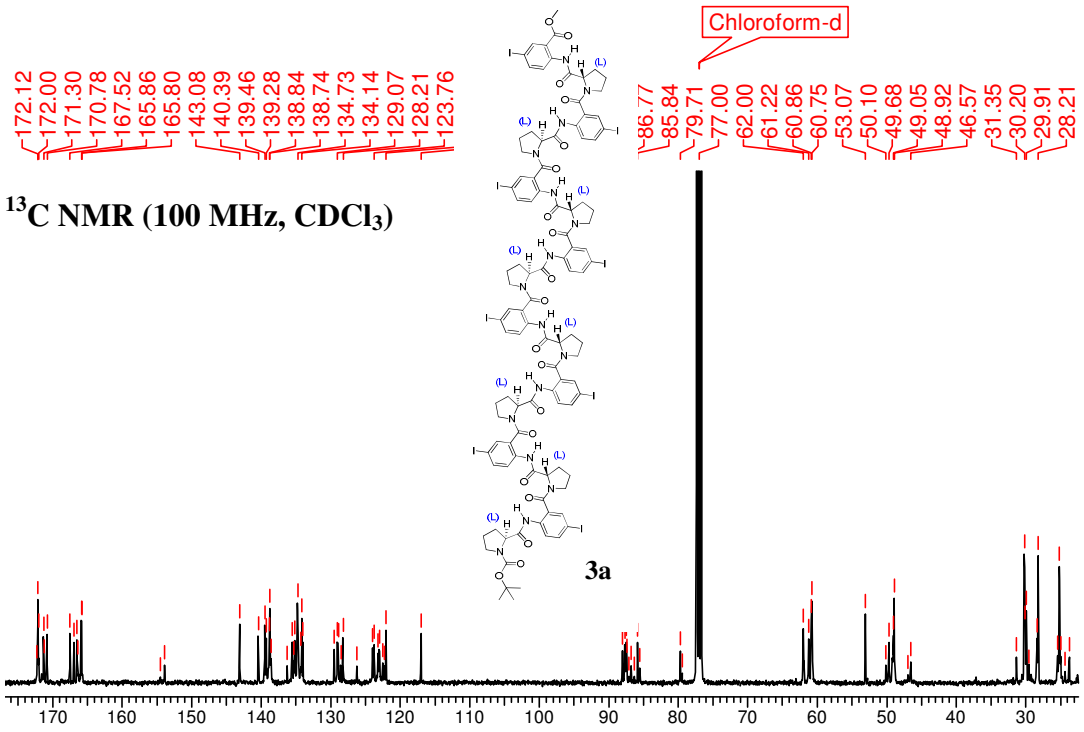

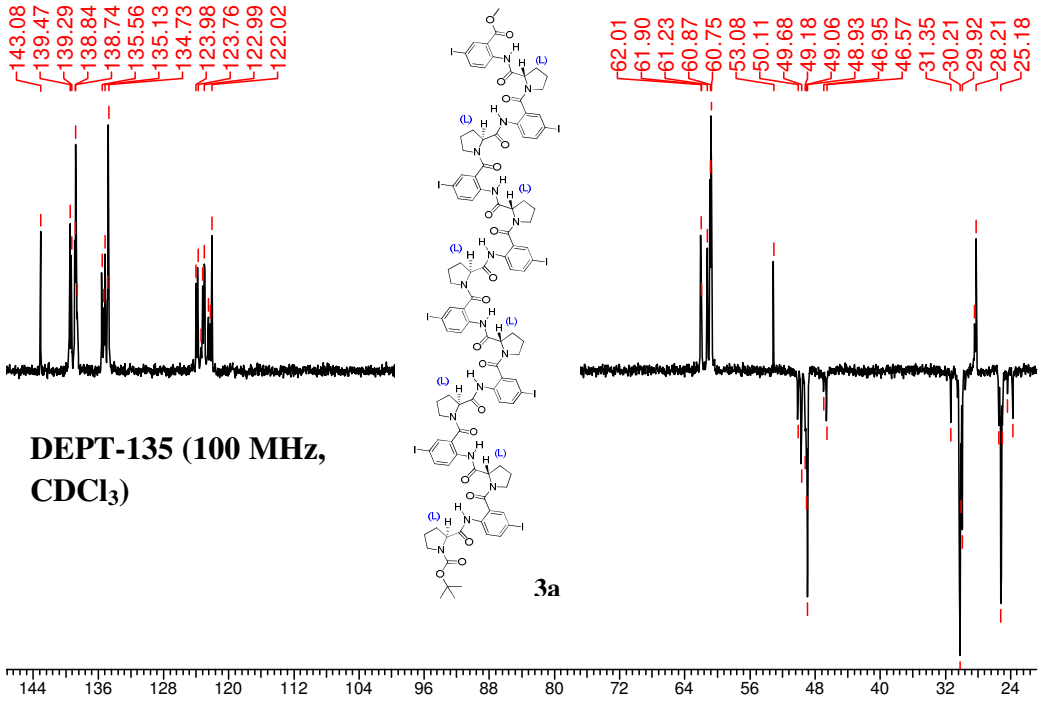

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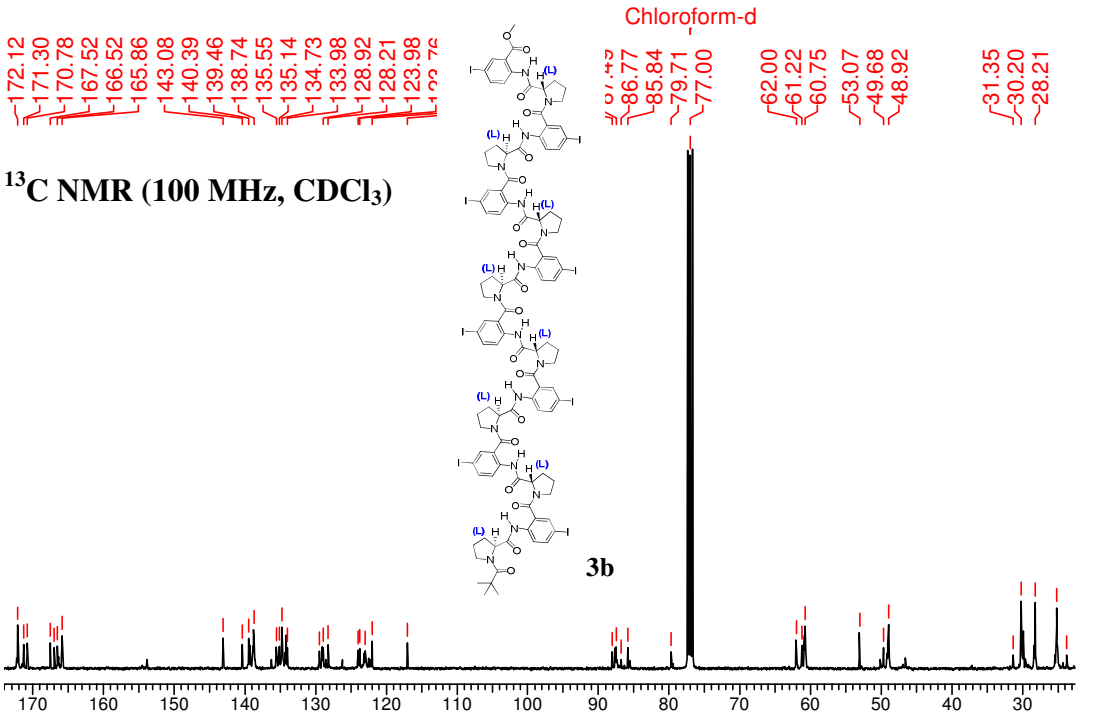

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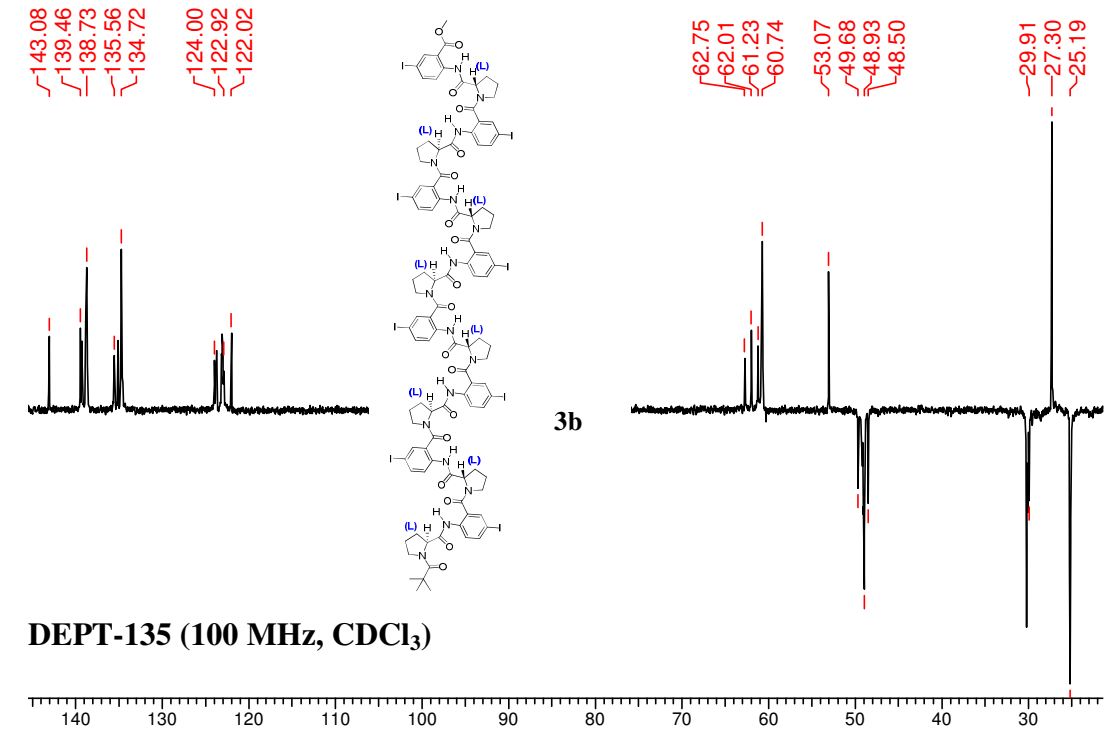
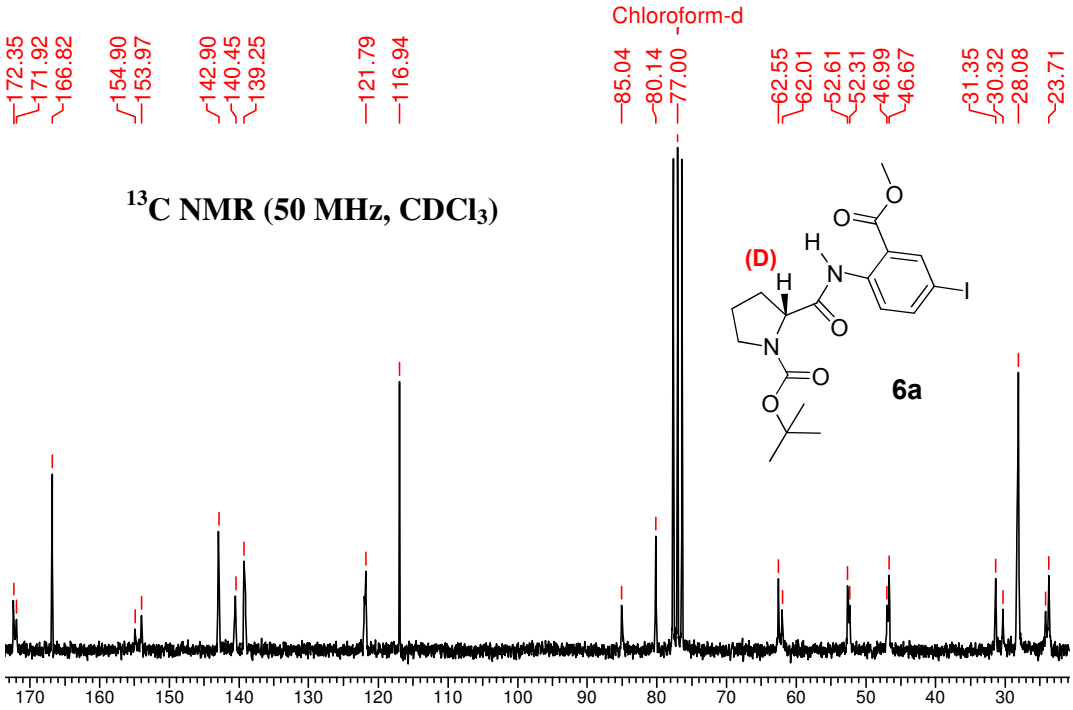
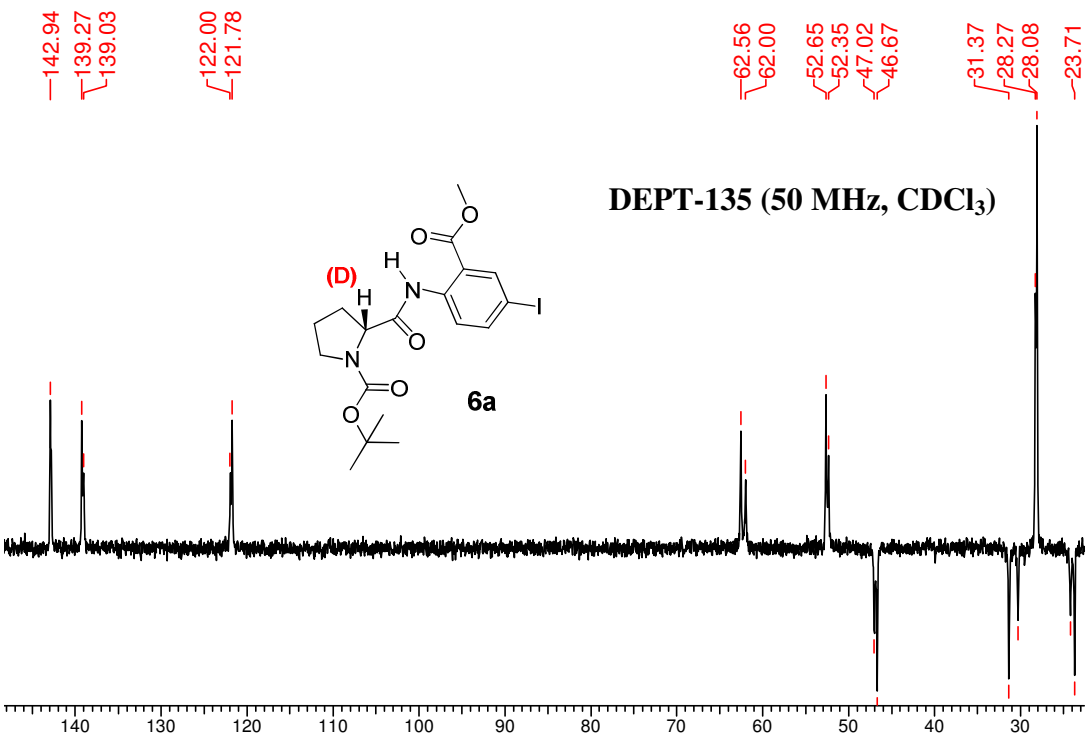
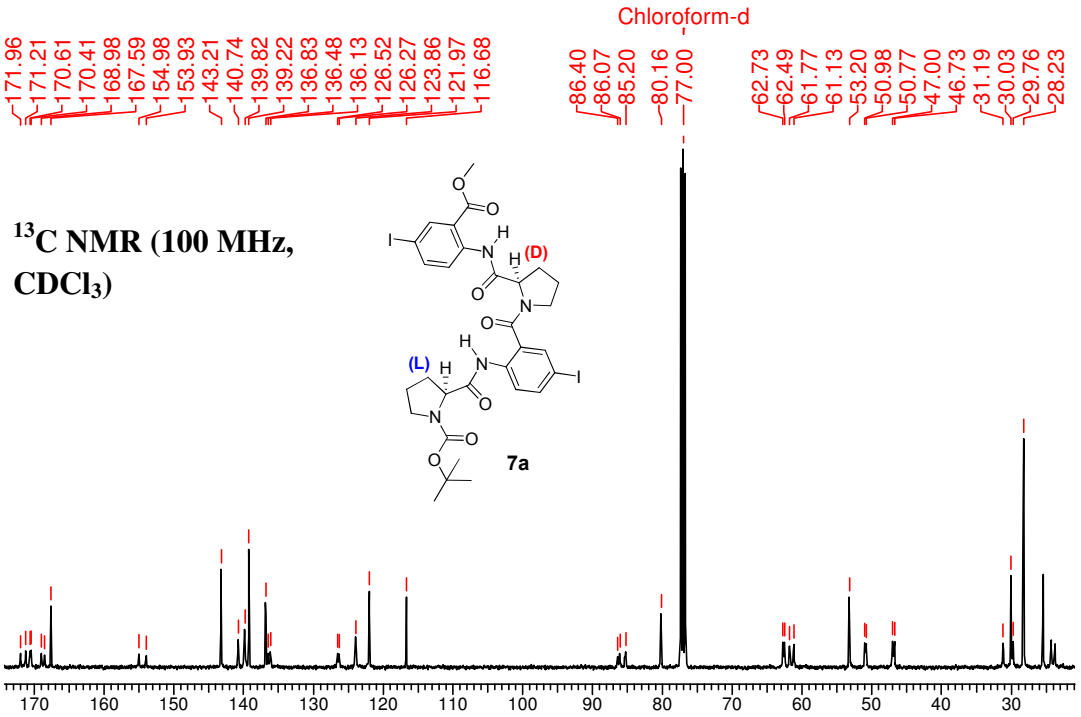


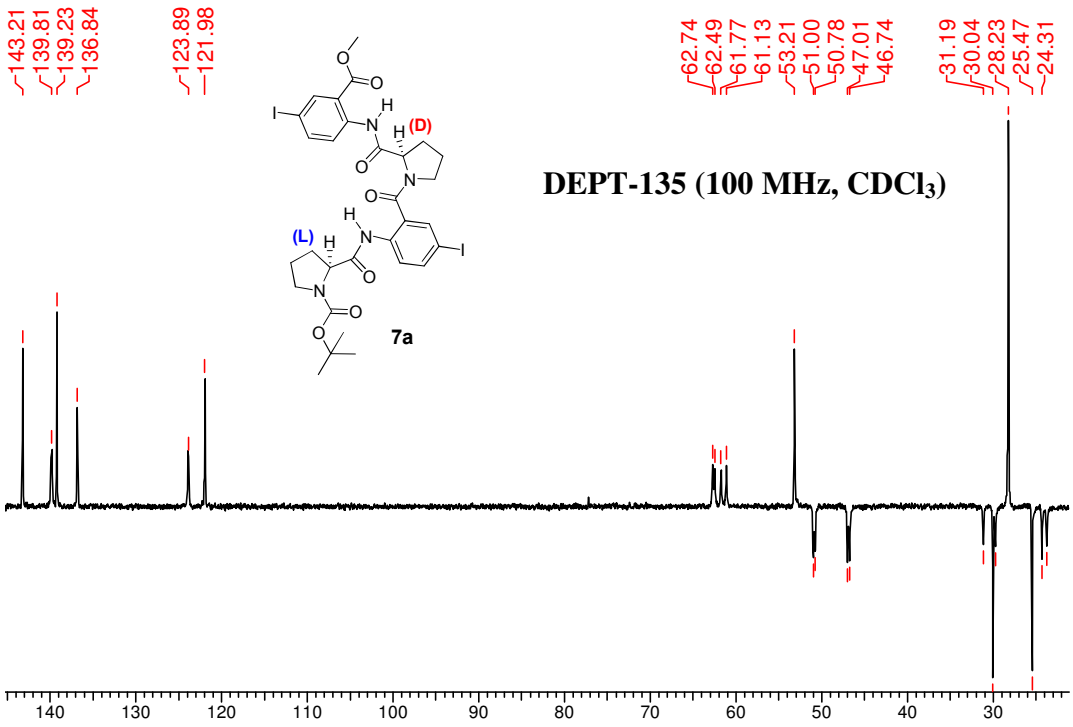
DEPT-135 (100 MHz, $CDCl_3$)





NOTE: Signal broadening and / or multiple set of signals seen are due to rotamer formation at the N-terminus (N^{t}BOC Pro effect: *Chem. Eur. J.* **2008**, 14, 6192).





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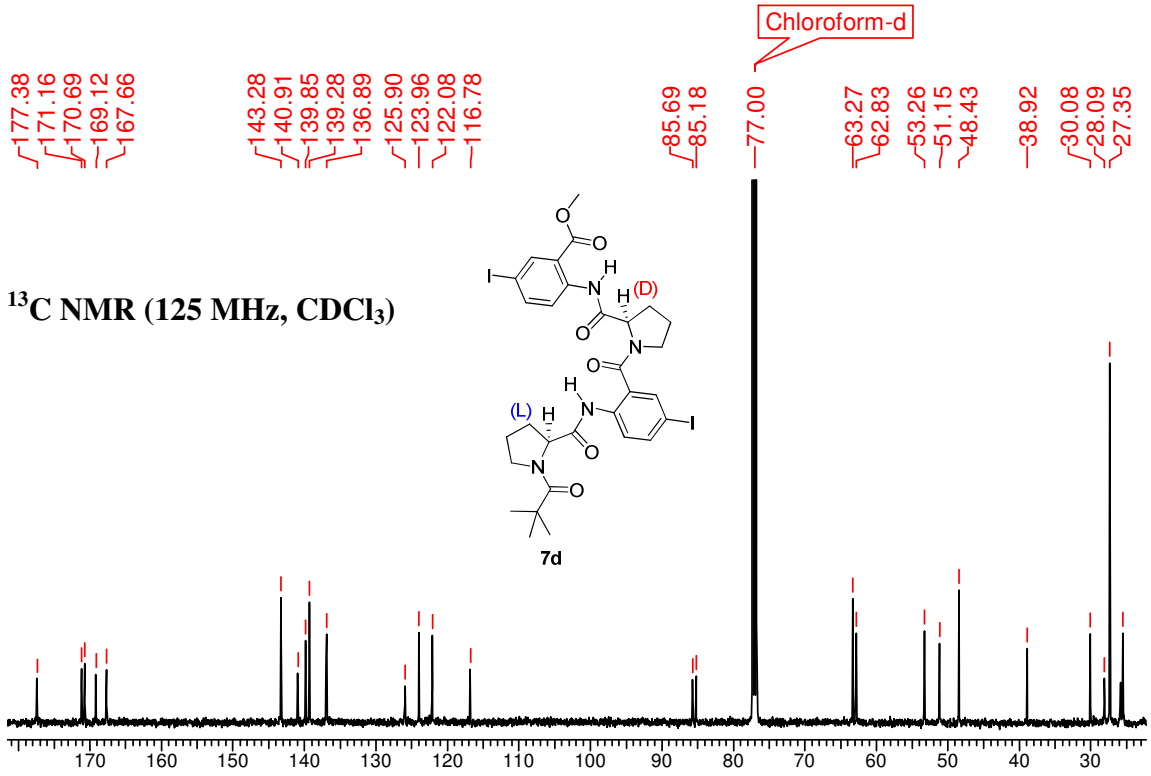
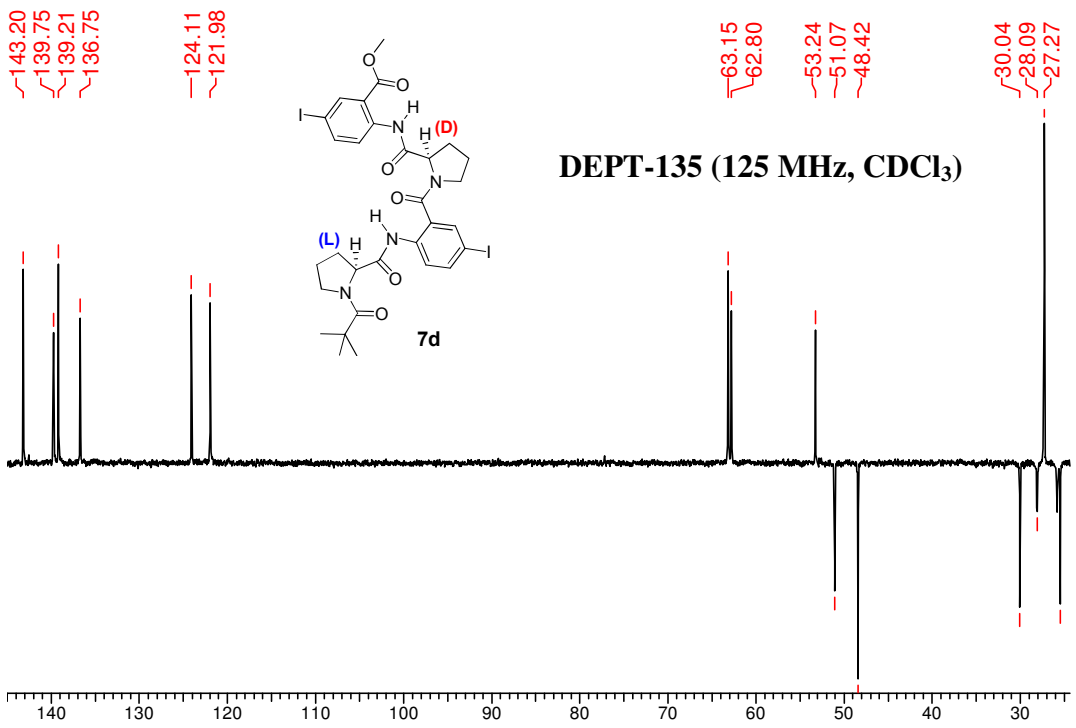


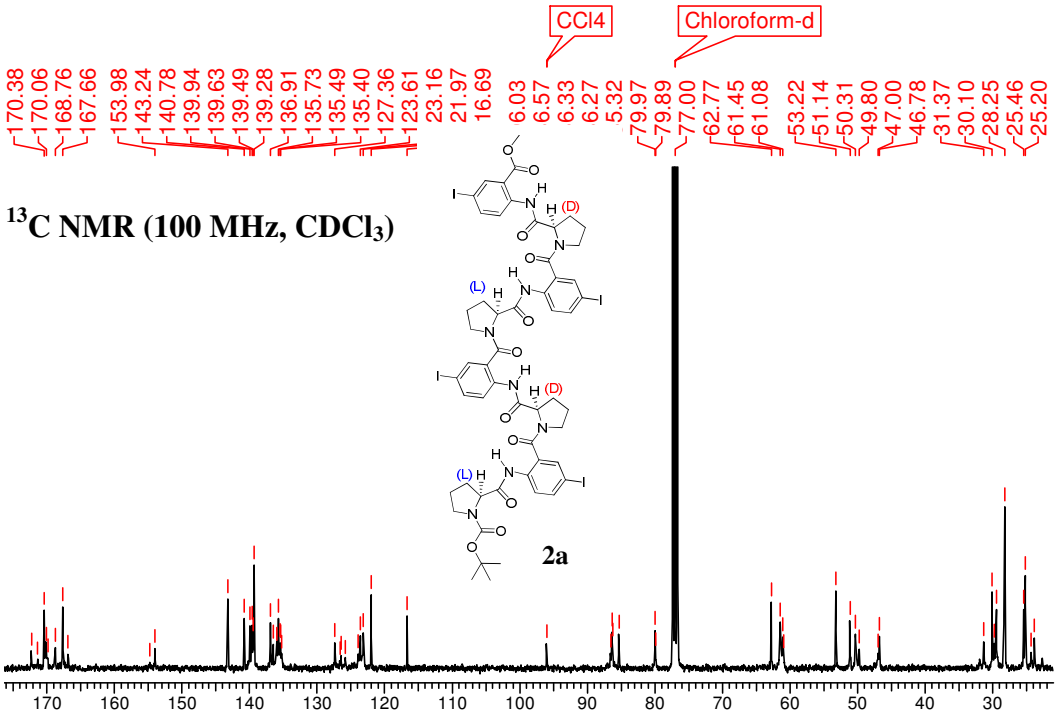
^{13}C NMR (125 MHz, $CDCl_3$)

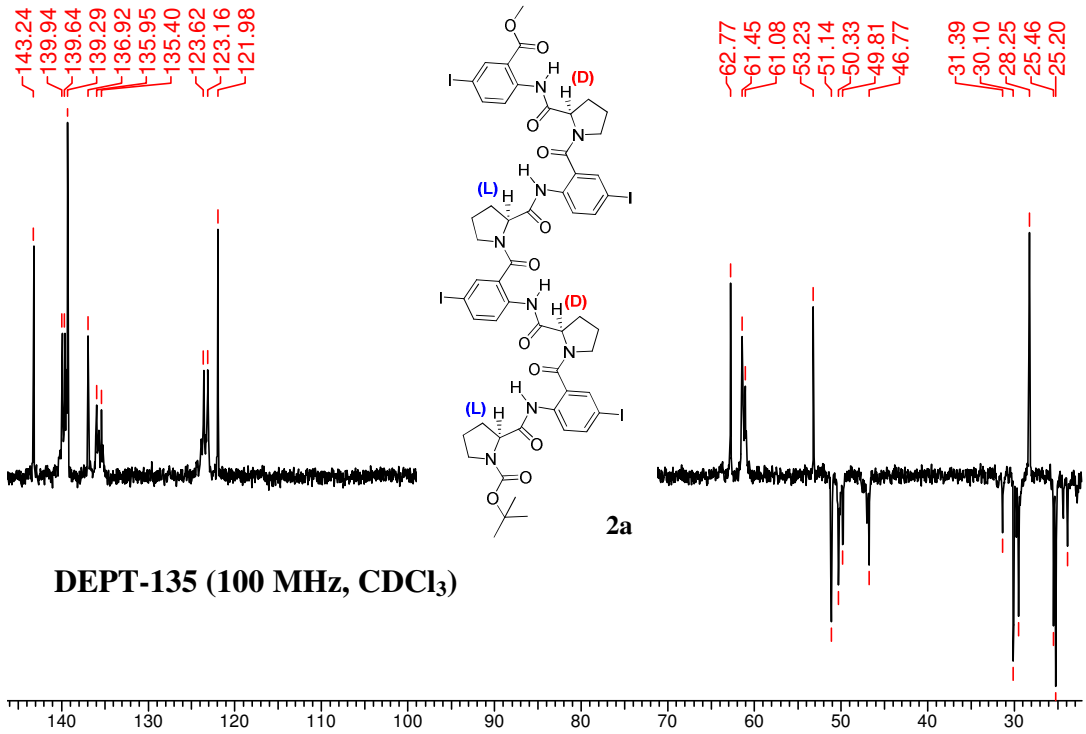
7d



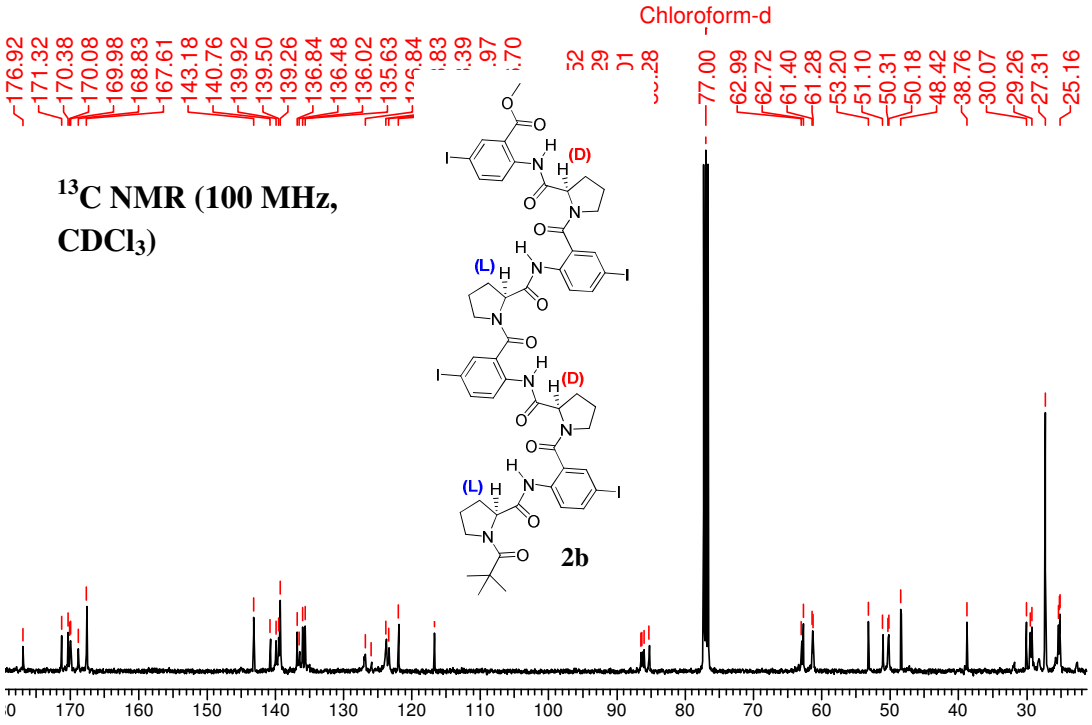
7d

DEPT-135 (125 MHz, $CDCl_3$)





NOTE: Signal broadening and / or multiple set of signals seen are due to rotamer formation at the N-terminus (N^{t}BOC Pro effect: *Chem. Eur. J.* **2008**, 14, 6192).


Chloroform-d
176.92
171.32
170.38
170.08
169.98
168.83
167.61
143.18
140.76
139.92
139.50
139.26
136.84
136.48
136.02
135.63
77.00
62.99
62.72
61.40
61.28
53.20
51.10
50.31
50.18
48.42
38.76
30.07
29.26
27.31
25.16
13C NMR (100 MHz, CDCl3)
(D)
(L)
2b

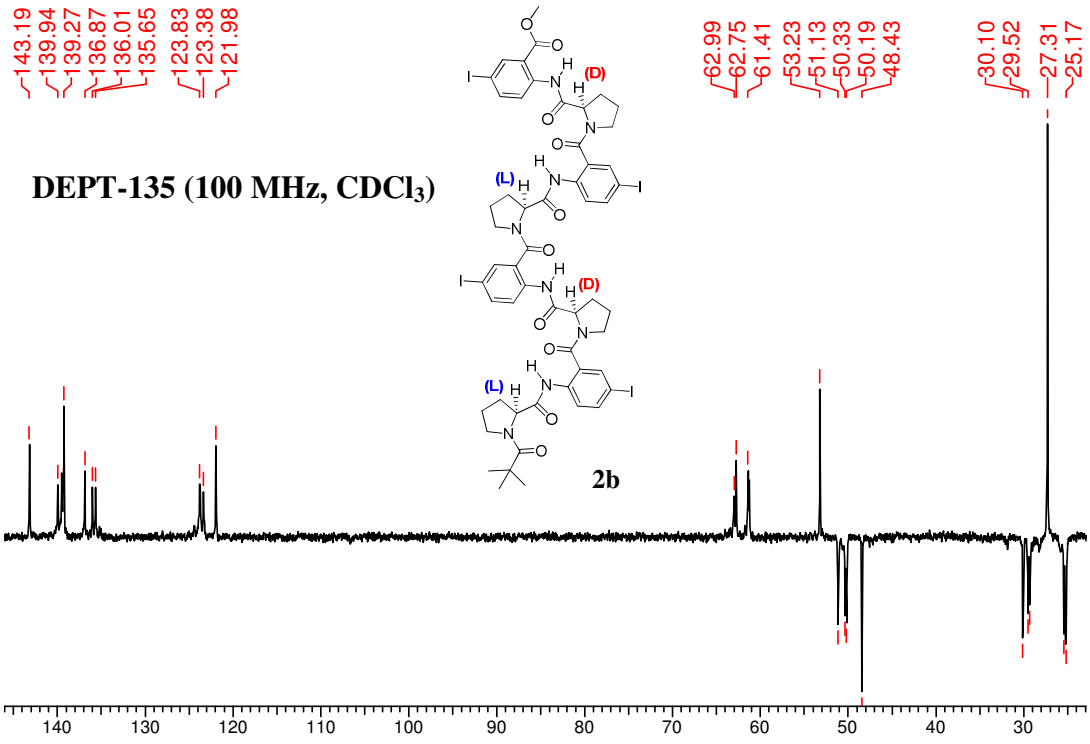
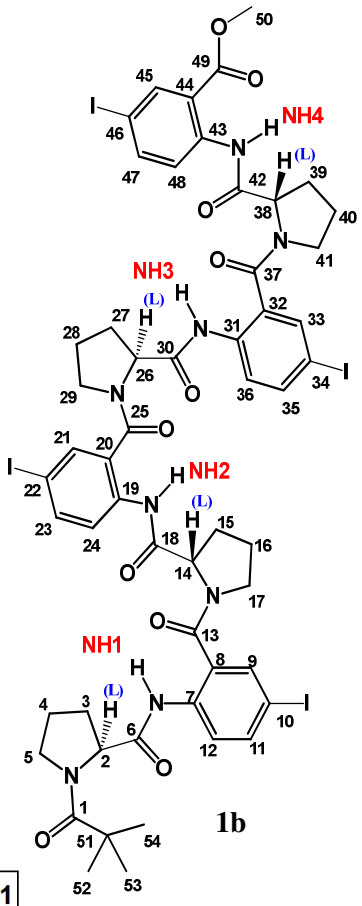

143.19
139.94
139.27
136.87
136.01
135.65
123.83
123.38
121.98
62.99
62.75
61.41
53.23
51.13
50.33
50.19
48.43
30.10
29.52
27.31
25.17
DEPT-135 (100 MHz, CDCl3)
(D)
(L)
2b

Table S1. Titration Study of octamer 1b in $CDCl_3$ (10 mmol) with DMSO-d6 (volume of DMSO-d6 added at each addition = 5 μl)

No	$V_{DMSO-d6}$ (in μ lit)	NH4	NH3	NH2	NH1
1	0	11.53	9.80	9.79	9.47
2	5	11.50	9.79	9.77	9.45
3	10	11.49	9.78	9.75	9.44
4	15	11.47	9.76	9.73	9.42
5	20	11.45	9.75	9.71	9.40
6	25	11.43	9.74	9.69	9.38
7	30	11.41	9.72	9.67	9.36
8	35	11.38	9.71	9.65	9.34
9	40	11.36	9.69	9.63	9.32
10	45	11.34	9.68	9.61	9.30
11	50	11.32	9.66	9.59	9.28



1b

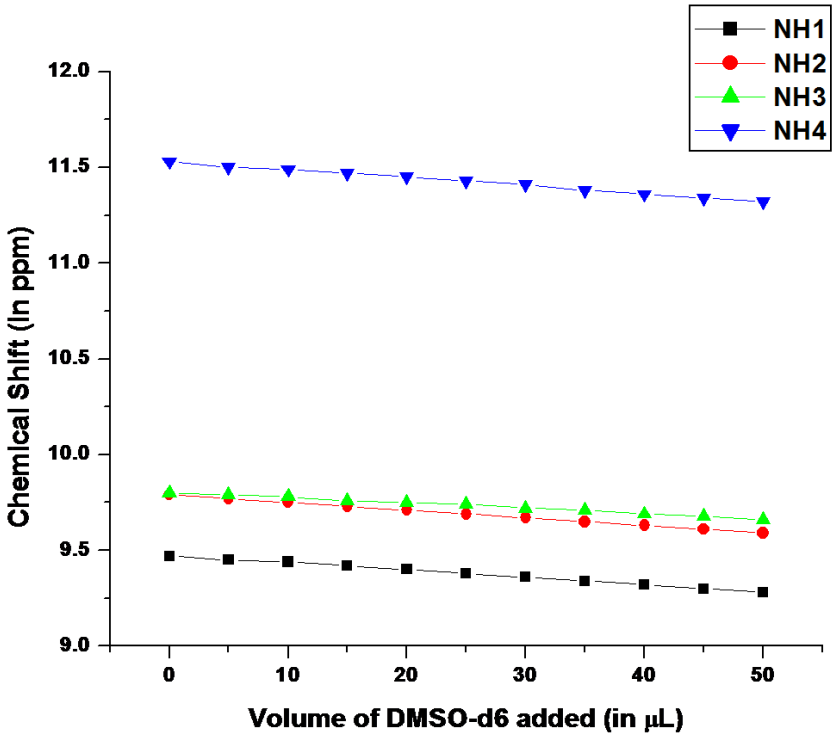
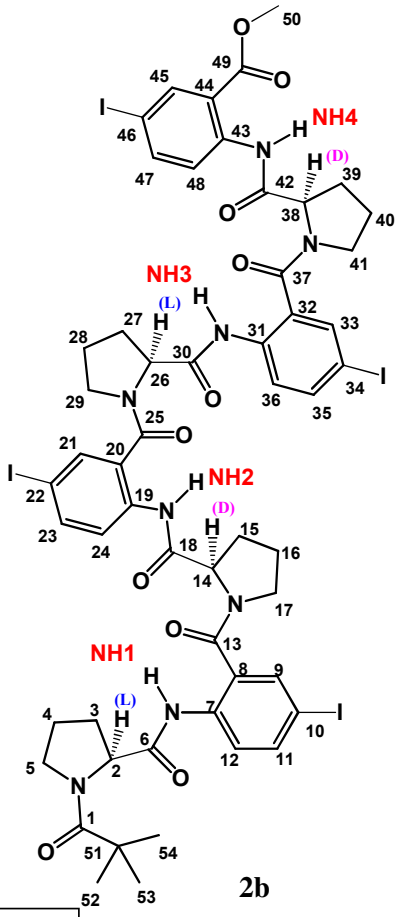
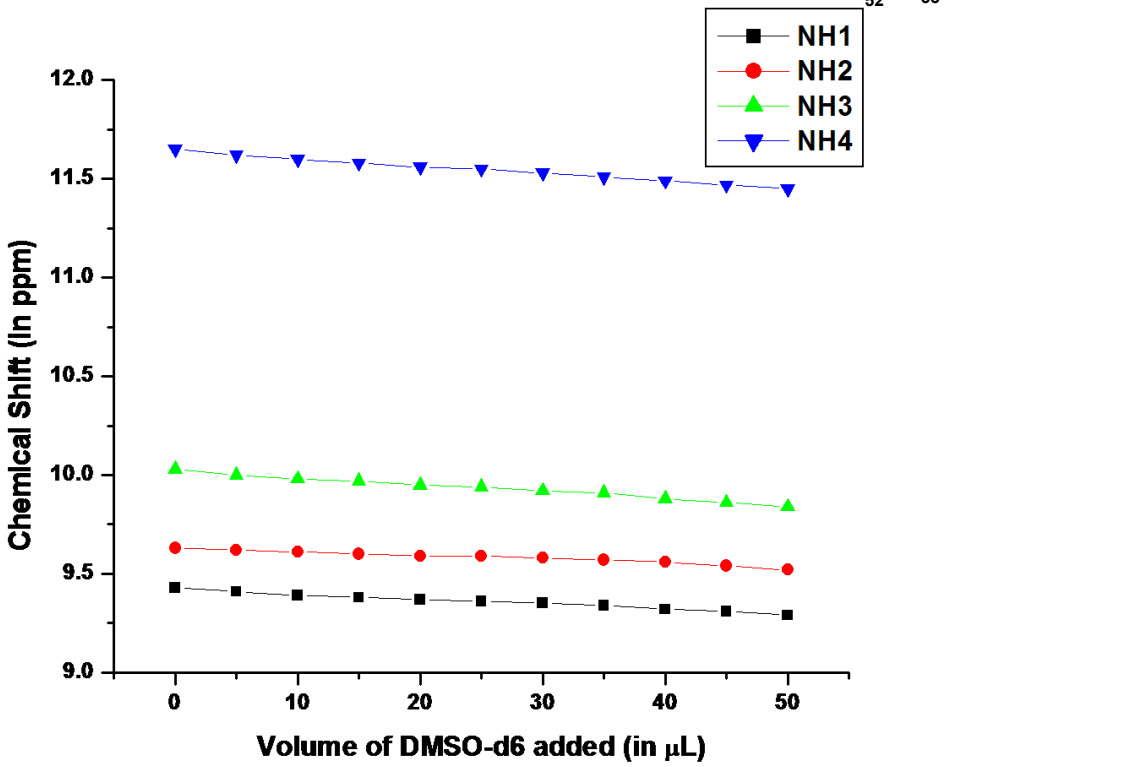


Table S2. Titration Study of octamer 2b in $CDCl_3$ (10 mmol) with DMSO-d6 (volume of DMSO-d6 added at each addition = 5 μl)

No	$V_{DMSO-d6}$ (in μ lit)	NH4	NH3	NH2	NH1
1	0	11.65	10.03	9.63	9.43
2	5	11.62	10.00	9.62	9.41
3	10	11.60	9.98	9.61	9.39
4	15	11.58	9.97	9.60	9.38
5	20	11.56	9.95	9.59	9.37
6	25	11.55	9.94	9.59	9.36
7	30	11.53	9.92	9.58	9.35
8	35	11.51	9.91	9.57	9.34
9	40	11.49	9.88	9.56	9.32
10	45	11.47	9.86	9.54	9.31
11	50	11.45	9.84	9.52	9.29



2b



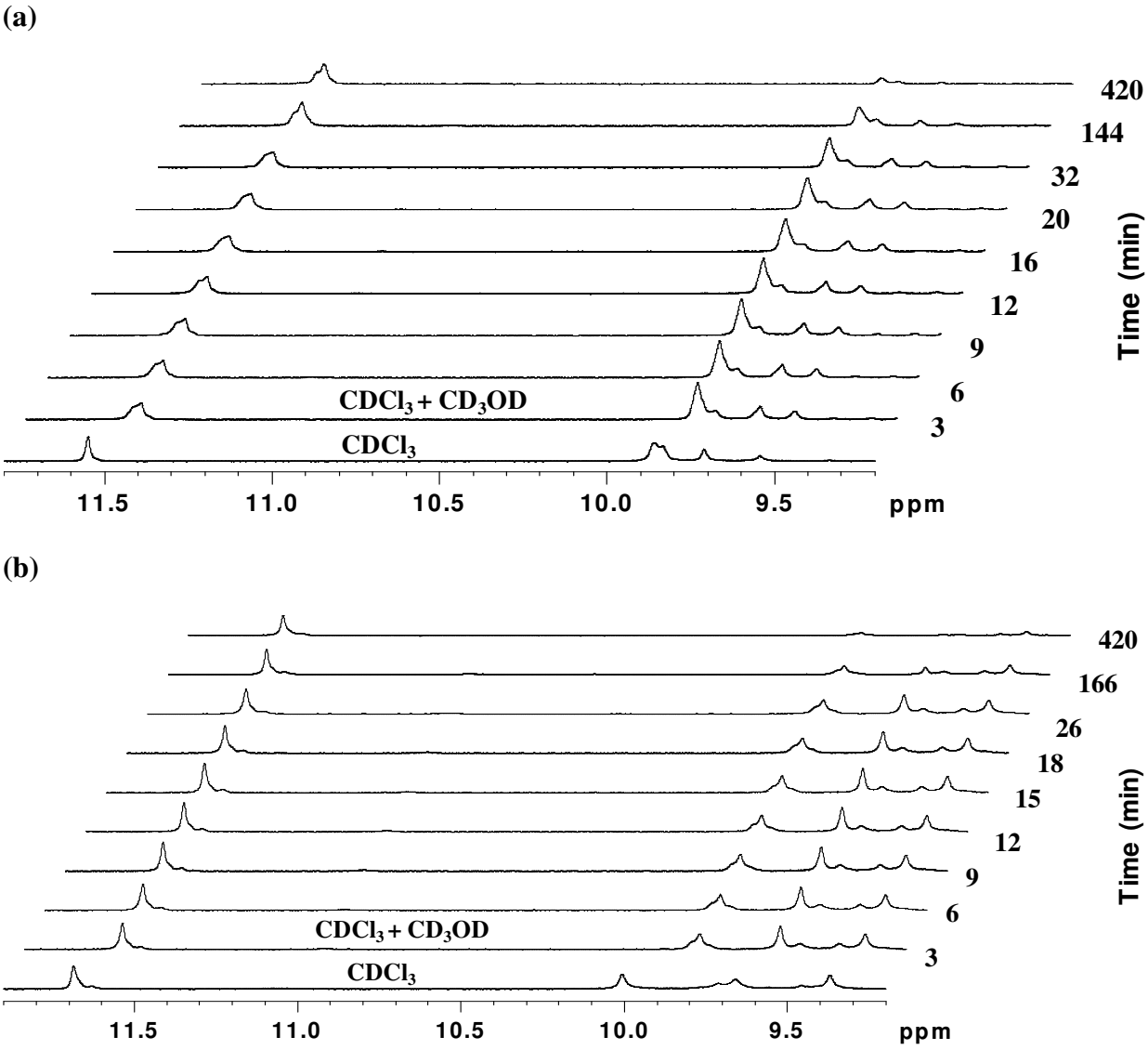


Figure S1. H/D Exchange experiment of **(a)** octamer **1a** and **(b)** octamer **2a** (400MHz) (NH region).

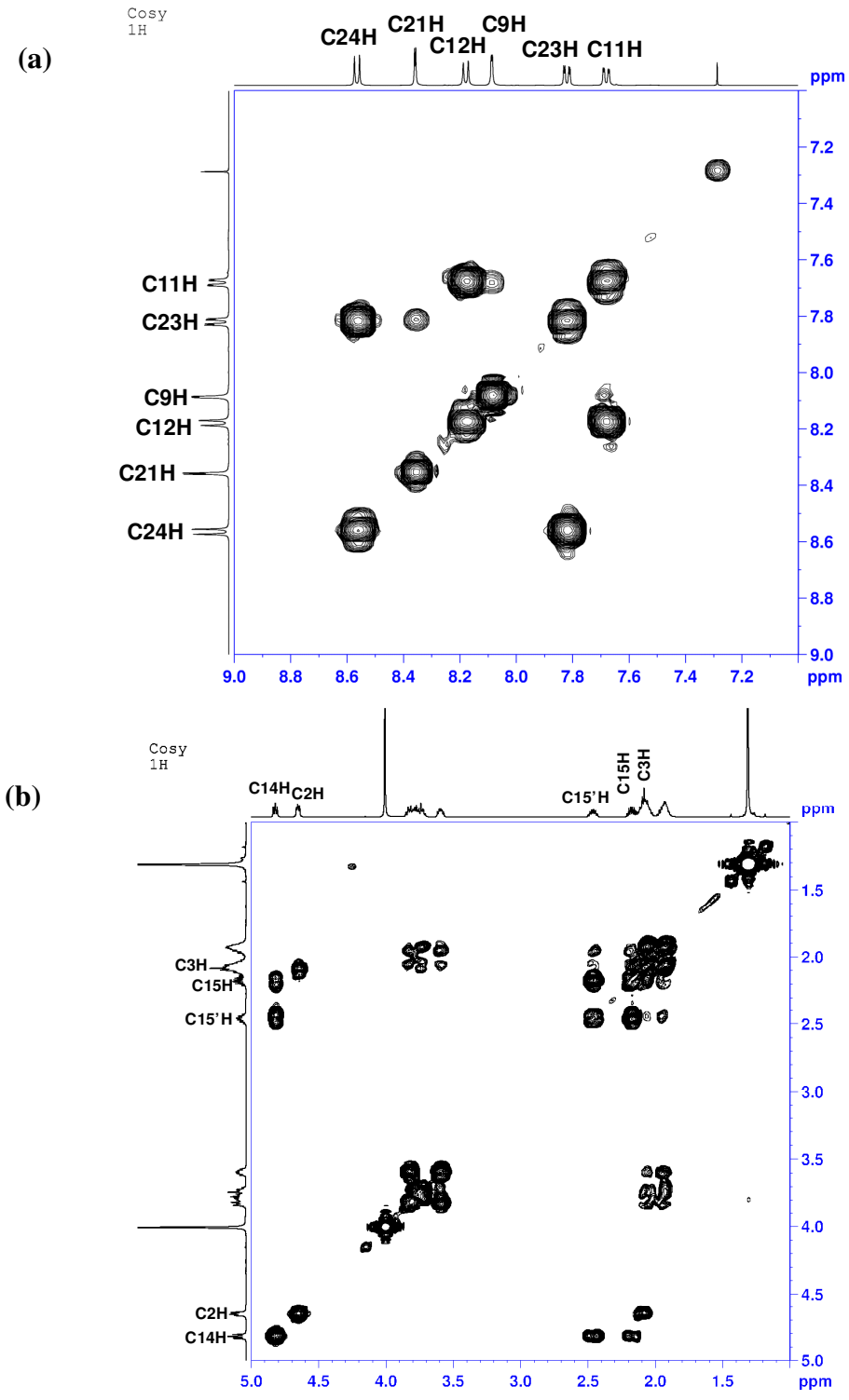


Figure S2. Partial COSY spectra of **5d** (500MHz, $CDCl_3$): Aromatic **(a)** and aliphatic regions **(b)**.

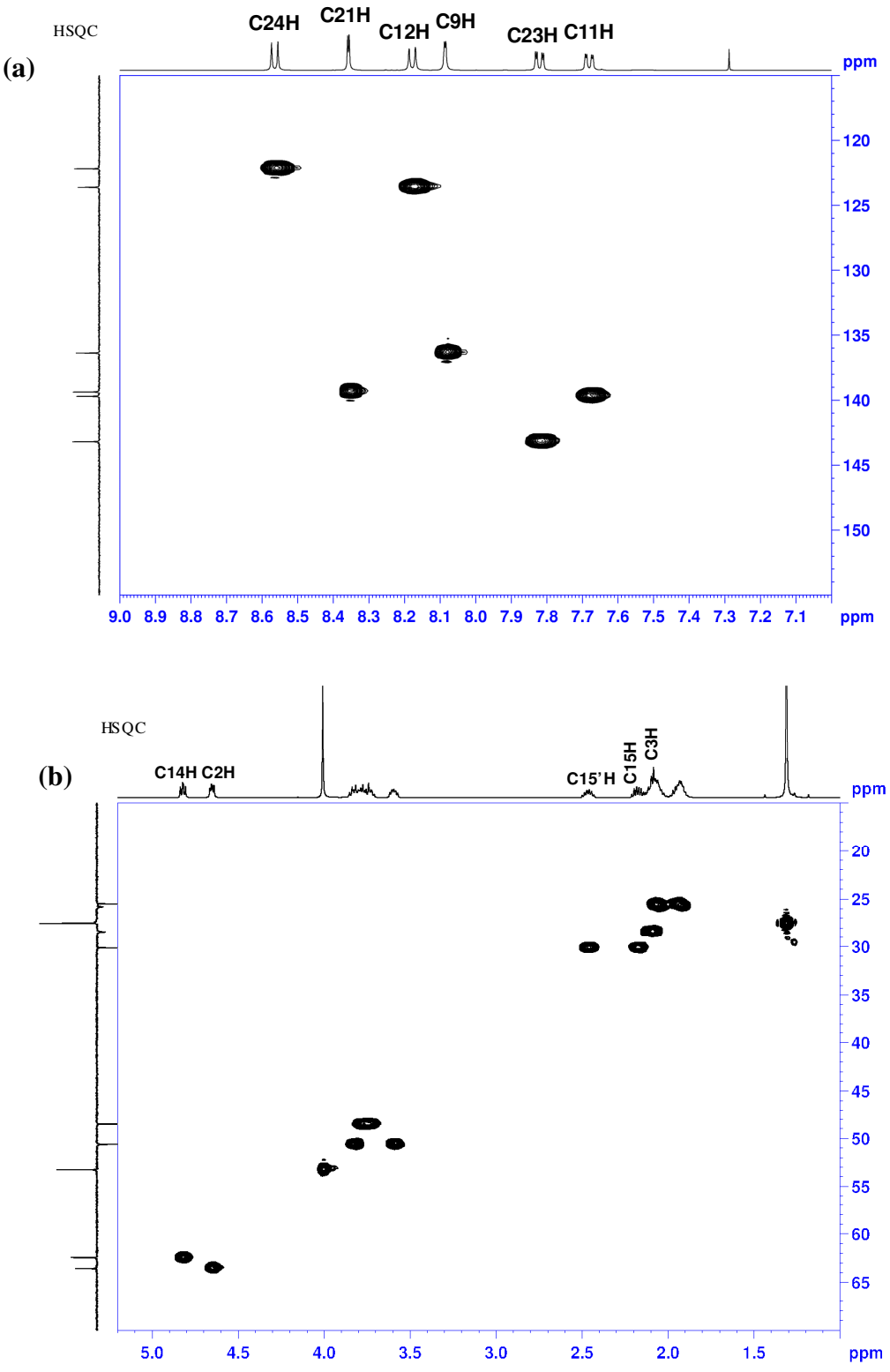


Figure S3. Partial HSQC spectra of **5d** (500MHz, $CDCl_3$): Aromatic **(a)** and aliphatic regions **(b)**.

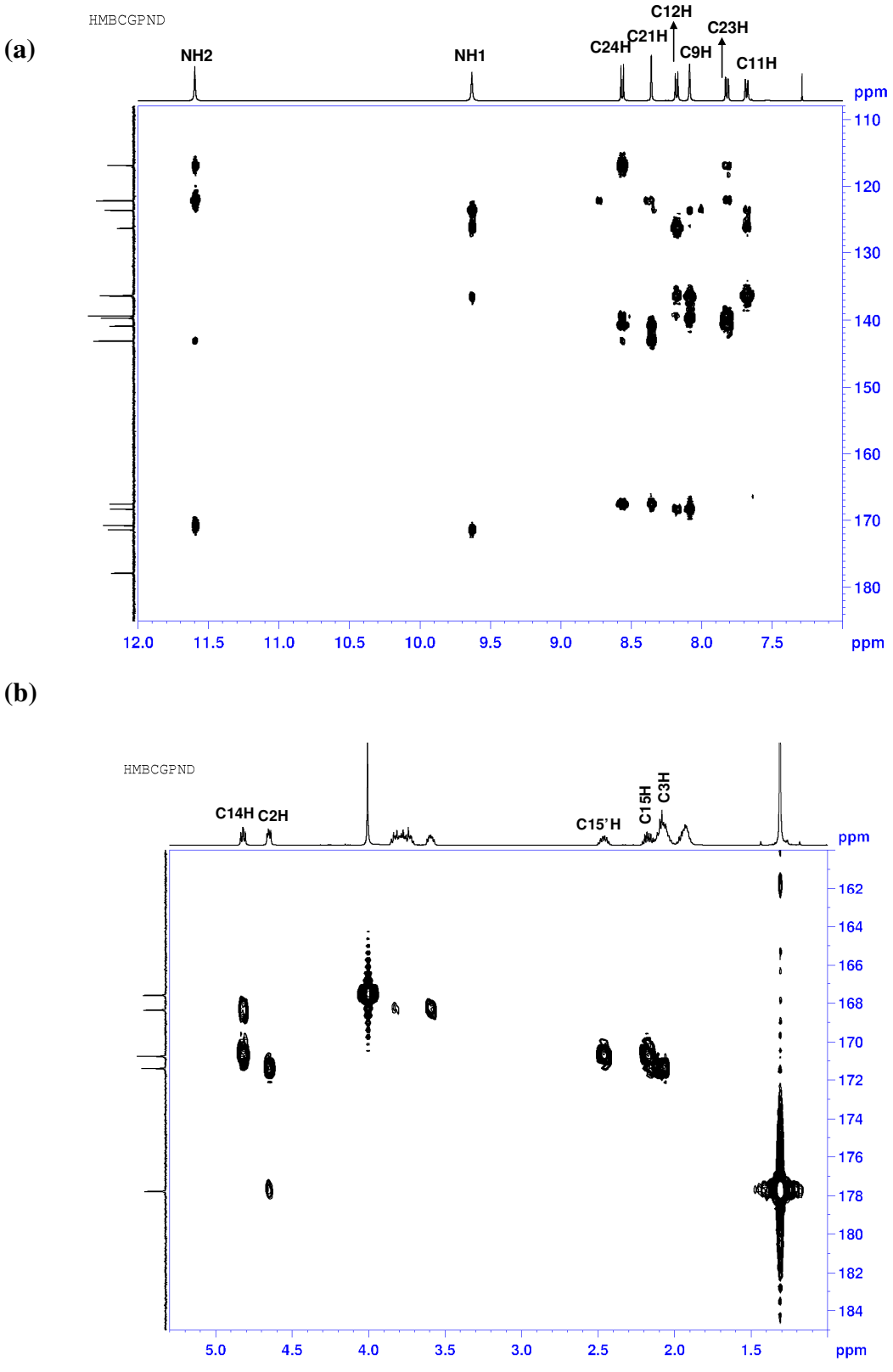


Figure S4. Partial HMBC (^{1}H-^{13}C) spectra of **5d** (500MHz, $CDCl_3$).

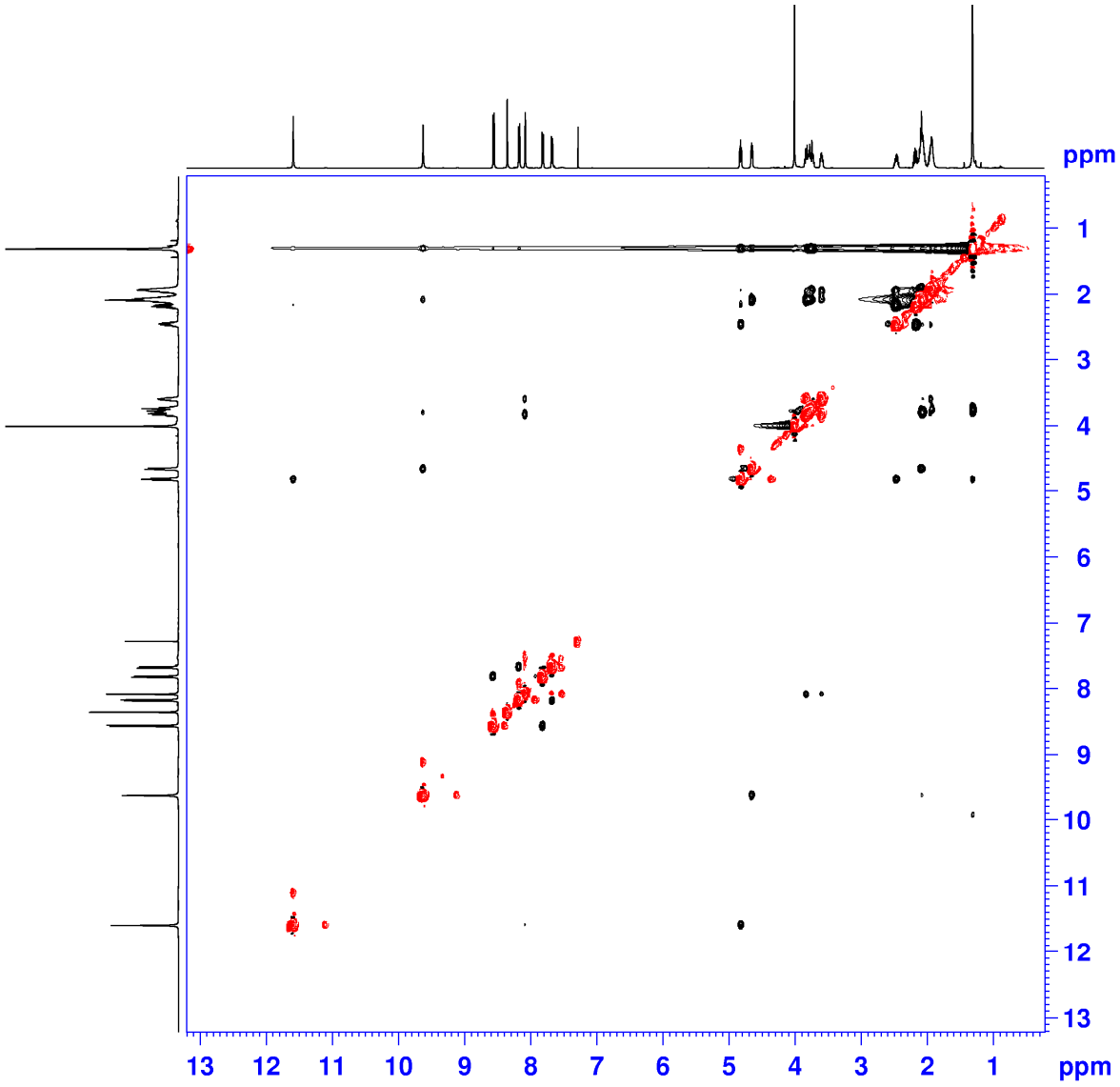


Figure S5. 2D NOESY spectrum of **5d** (400 MHz, $CDCl_3$).

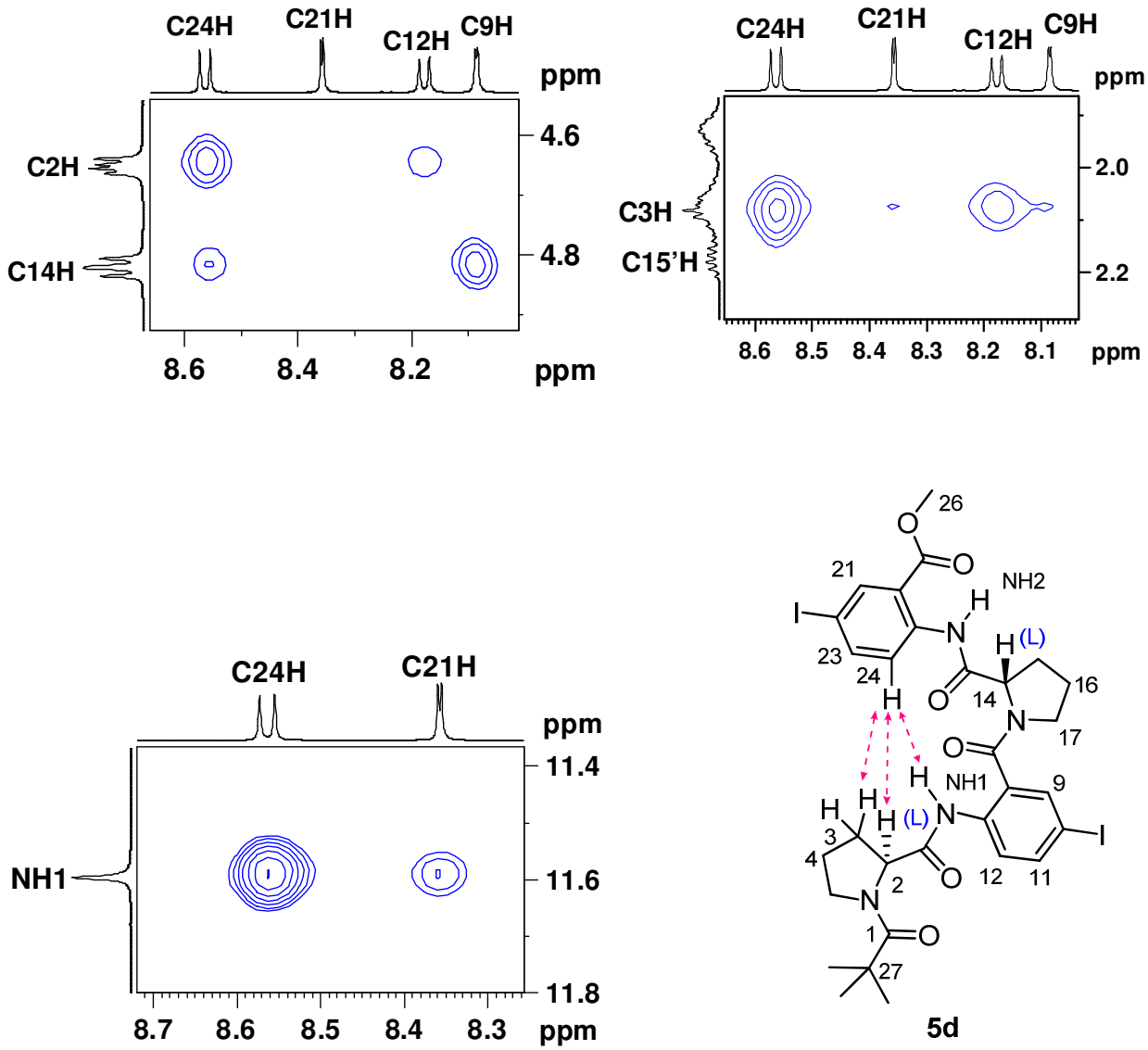


Figure S6. 2D NOESY Extracts of **5d** (500 MHz, $CDCl_3$).

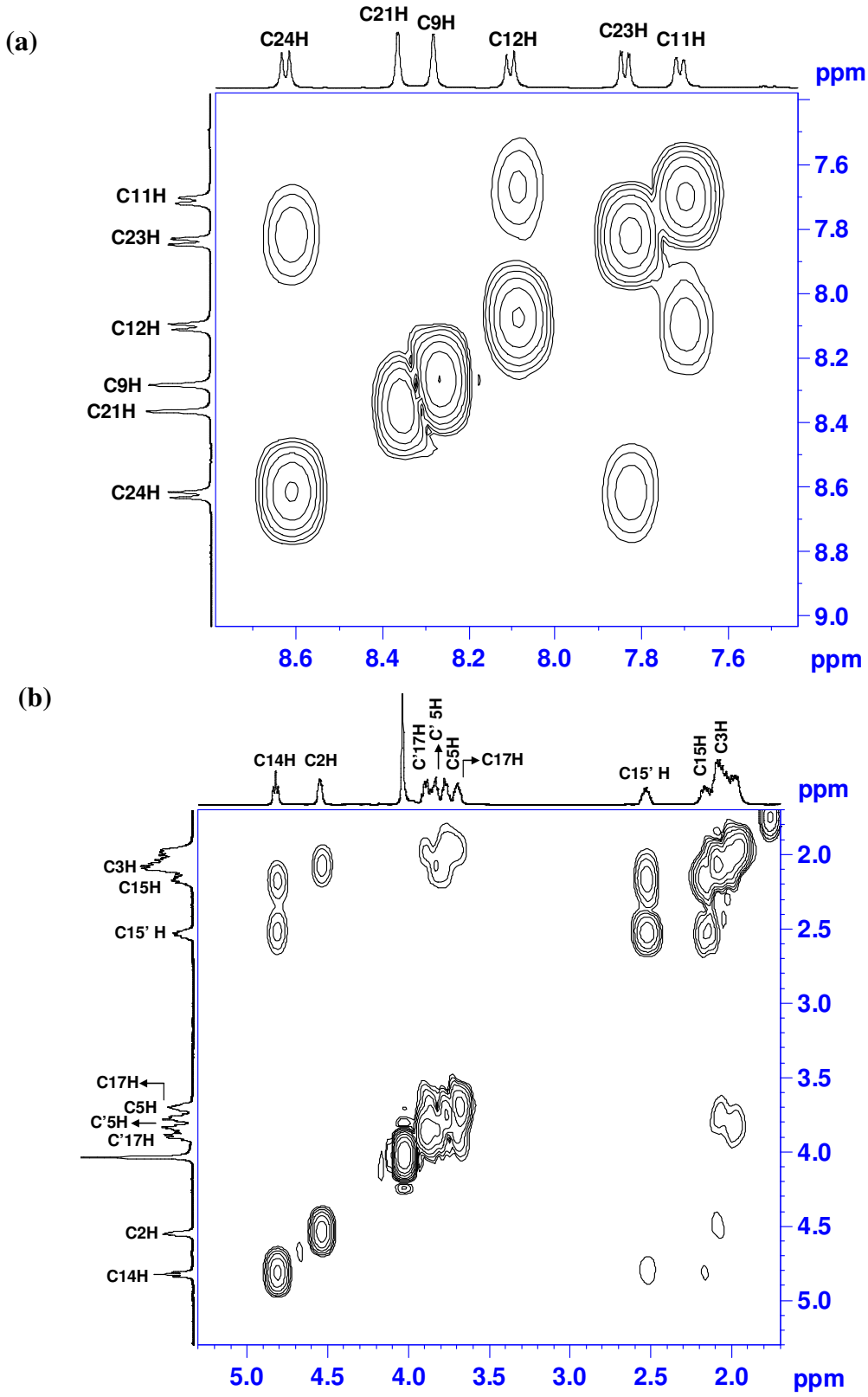


Figure S7. Partial COSY spectra of **7d** (500MHz, $CDCl_3$): Aromatic **(a)** and aliphatic regions **(b)**.

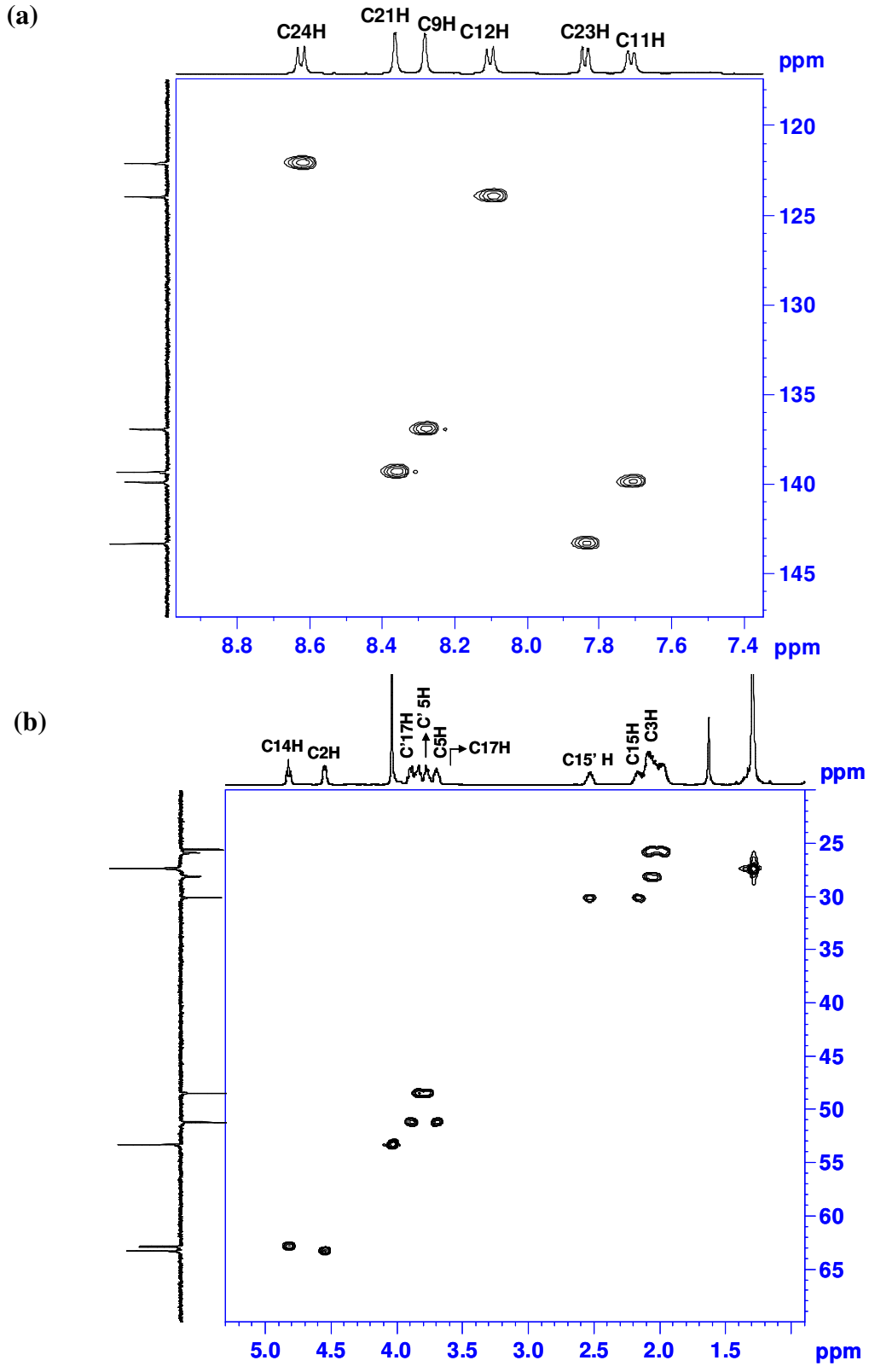


Figure S8. Partial HSQC spectra of **7d** (500MHz, $CDCl_3$): Aromatic **(a)** and aliphatic regions **(b)**.

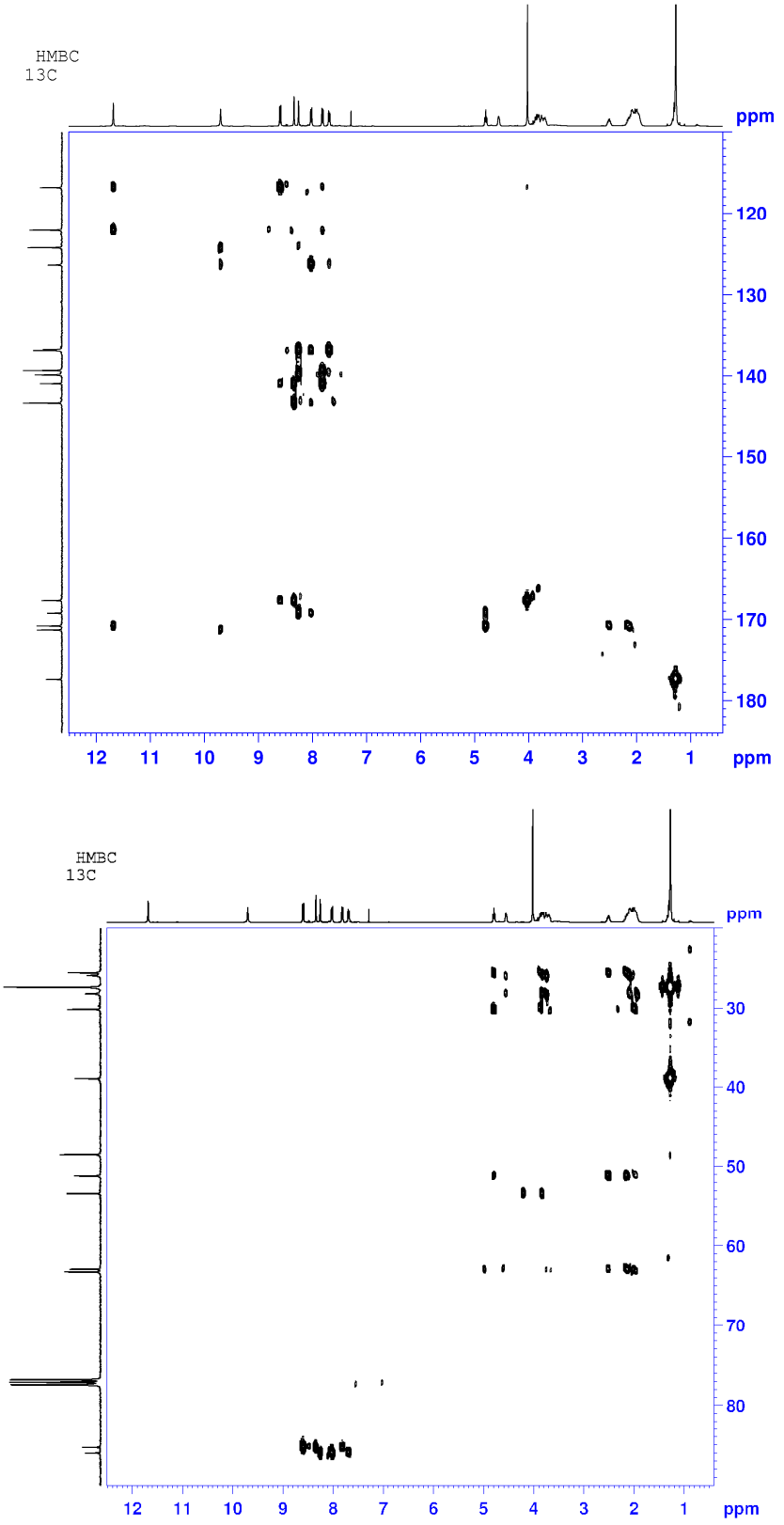


Figure S9. Partial HMBC (^{1}H-^{13}C) spectra of **7d** (500MHz, $CDCl_3$.

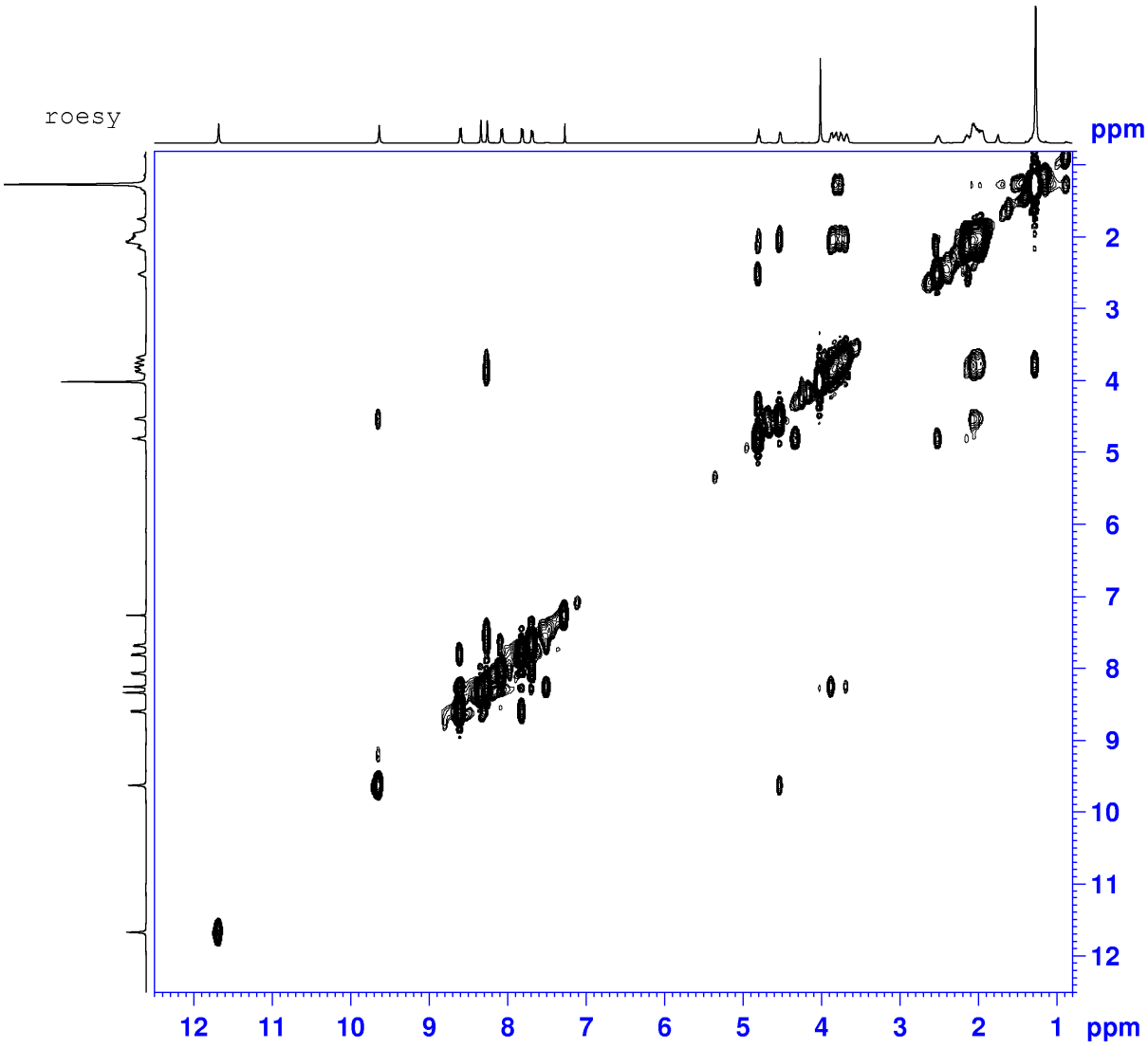


Figure S10. 2D ROESY spectrum of **7d** (500 MHz, $CDCl_3$).

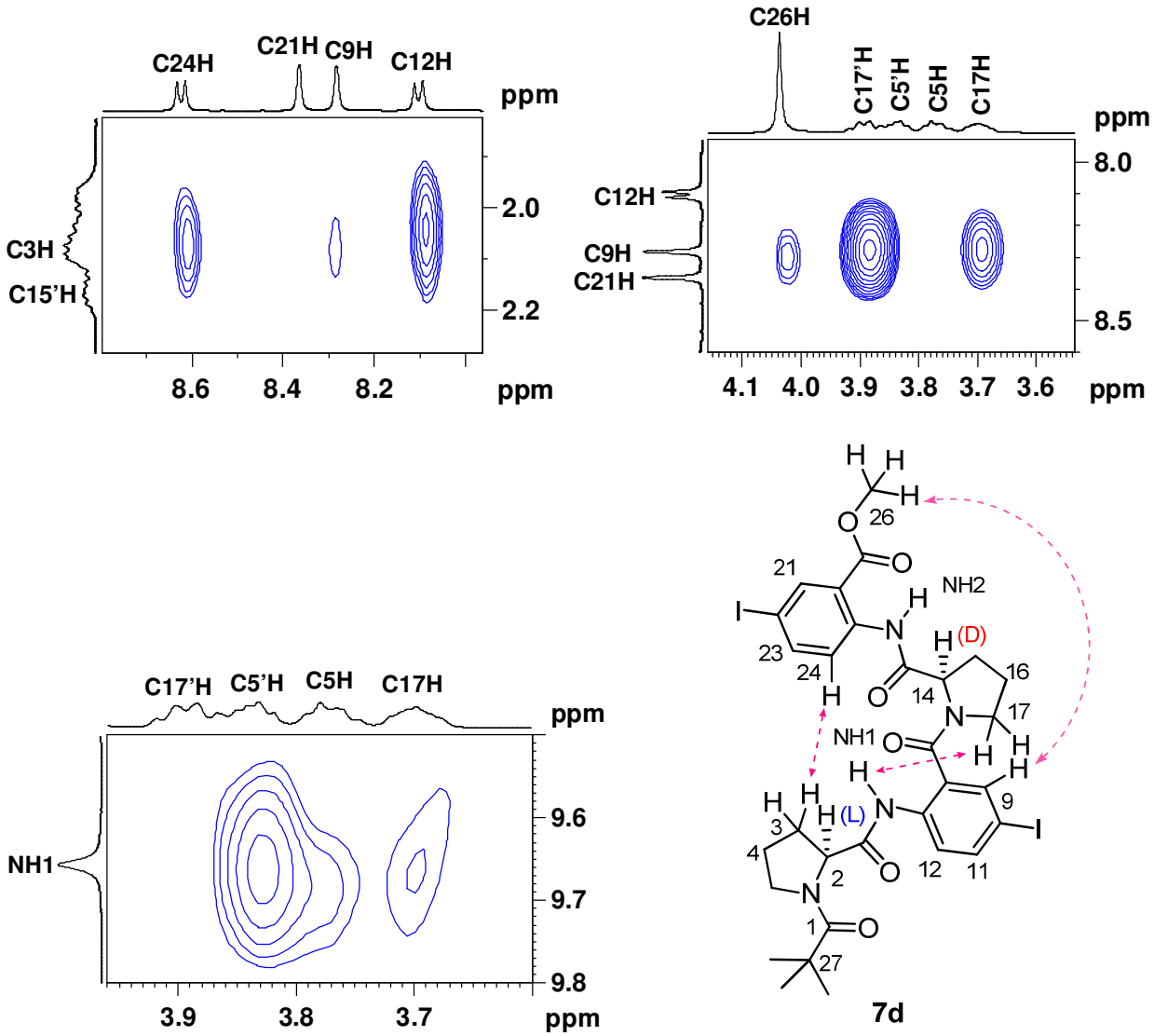


Figure S11. 2D ROESY Extracts of **7d** (500 MHz, $CDCl_3$).

Table S3. Comparison of experimental inter-residual distances (NOE) and theoretical inter-residual distances of **5d**. The reference distance between two aromatic protons was considered as 2.44 Å. Distances of 2.0 ± 0.5 Å, 3.0 ± 1.0 Å and 4.0 ± 1.5 Å were incorporated for strong, medium and weak NOE intensities, respectively. [a]Theoretical distance (in Å) were taken from the global minimum energy conformer obtained from DFT calculation studies.

Chemical Shift of Proton 1 [ppm]	Chemical Shift of Proton 2 [ppm]	NOE between	NOE Intensity	Theoretical distance[a]
8.5654	7.8124	C24H &C23H	Strong	2.5
8.1851	7.6664	C12H & C11H	Strong	2.5
11.5895	9.6279	NH2 & NH1	Weak	5.5
11.5831	8.5488	NH2 & C24H	Medium	3.73
11.5895	8.0854	NH2 & C9H	Medium	6.7
11.5958	4.8099	NH2 & C14H	Strong	2.36
11.5958	4.0037	NH2 & C26H	Medium	4.44
11.5895	2.4485	NH2 & C15aH	Medium	3.57
11.5895	2.1564	NH2 & C15bH	Medium	2.75
11.5958	1.3058	NH2 &C28H, C29H, C30H	Medium	7.83
9.6305	1.3058	NH1 & C28H, C29H, C30H	Medium	5.76
9.6368	2.0803	NH1 & C3aH/C3bH	Medium	3.58
9.6242	1.9216	NH1 & C4H/C16H	Weak	5.14/3.8
8.5591	2.0993	C24H & C3aH/ C3bH	Medium	3.38
8.5591	1.9216	C24H & C4H/C16H	Weak	4.4/4.9
8.1724	2.0676	C12H & C3aH/ C4H or C16H	Weak	4.3/6.3

11.5958	3.8069	NH2 & C17aH	Medium	5.62
11.5831	3.5974	NH2 & C17bH	Weak	5.68
9.6495	3.5784	NH1 & C17bH	Medium	3.8
9.6305	3.8006	NH1 & C5H	Medium	5.3
8.0963	3.5847	C9H & C17bH	Medium	4.2
8.0773	3.826	C9H & C17aH	Strong	3.8
7.821	2.099	C23H & C3H/4H	Weak	4.4/4.8
8.3626	3.9973	C21H & C26H	Medium	3.86
9.6305	4.6448	NH1 & C2H	Strong	2.13
8.5591	4.6385	C24 & C2H	Medium	3.24
8.1787	4.6385	C12H & C2H	Weak	4.8
8.5528	4.8162	C24H & C14H	Weak	4.81
8.0836	4.8099	C9H & C14H	Weak	4.71
9.6305	4.8226	NH1 & C14H	Medium	4.1
9.6242	8.1552	NH1 & C12H	Medium	3.75
4.8187	1.3058	C14H & C28H, C29H, C30H	Weak	7.45
4.6475	1.2995	C2H & C28H, C29H, C30H	Medium	4.54
4.8124	1.9279	C14H & C4H/C16H	Medium	4.2
4.8124	2.1755	C14H & C15bH	Strong	2.4
4.6412	1.8898	C2H & C4H/C16H	Medium	3.2
4.8124	3.5784	C14H & C17bH	Medium	3.7

Table S4. Comparison of experimental inter-residual distances (NOE) and theoretical inter-residual distances of **7d**. The reference distance between two aromatic protons was considered as 2.44 Å. Distances of 2.0 ± 0.5 Å, 3.0 ± 1.0 Å and 4.0 ± 1.5 Å were incorporated for strong, medium and weak NOE intensities, respectively. [a]Theoretical distance (in Å) were taken from the global minimum energy conformer obtained from DFT calculation studies.

Chemical Shift of Proton 1 [ppm]	Chemical Shift of Proton 2 [ppm]	NOE between	NOE Intensity	Theoretical distance[a]
8.6125	7.812	C23H & C24H	Strong	2.5
8.1066	7.6622	C12 & C11H	Strong	2.49
9.6543	8.1015	NH1 & C12H	Medium	3.73
11.6945	8.6272	NH2 & C24H	Medium	3.73
11.6945	8.2712	NH2 & C9H	Medium	6.29
11.6979	3.8888	NH2 & C17aH	Weak	5.58
11.6945	4.8038	NH2 & C14H	Strong	2.19
9.6509	4.8304	NH1 & C14H	Medium	4.36
9.6543	4.5277	NH1 & C2H	Medium	3.63
9.6543	3.8056	NH1 & C5aH	Medium	3.24
9.6543	2.0453	NH1 & C3aH/ C4H/C16H	Medium	3.88
8.6158	4.8205	C24H & C14H	Weak	4.84
8.2763	4.7972	C9H & C14H	Weak	4.54
8.0999	3.8056	C12H & C5aH	Weak	6.61
8.2664	3.8822	C9H & C17H	Medium	3.67
8.3629	4.0551	C21H & C26H	Medium	4.45
8.6125	2.0686	C24H & C3aH/ C3bH	Medium	3.19

8.0833	2.0353	C12H & C4H/ C16H	Weak	7.0
8.2897	2.052	C9H & C3H/ C4H/C16aH	Weak	5.08/6.0
4.8149	2.5311	C14H & C15aH	Strong	2.44
4.8082	2.0253	C14H & C4H/ C16aH	Medium	3.01
4.5386	2.032	C2H & C3H/ C4H/ C16H	Strong	2.44
4.542	1.2833	C2H & C28H, C29H, C30H	Medium	4.25
4.8182	1.2933	C14H & C28H, C29H, C30H	Weak	5.16
3.843	1.2866	C5aH & C28H, C29H, C30H	Medium	4.2
3.7265	1.2833	C17bH & C28H, C29H, C30H	Medium	2.6

Quantum chemical calculations: Monte-Carlo conformational search

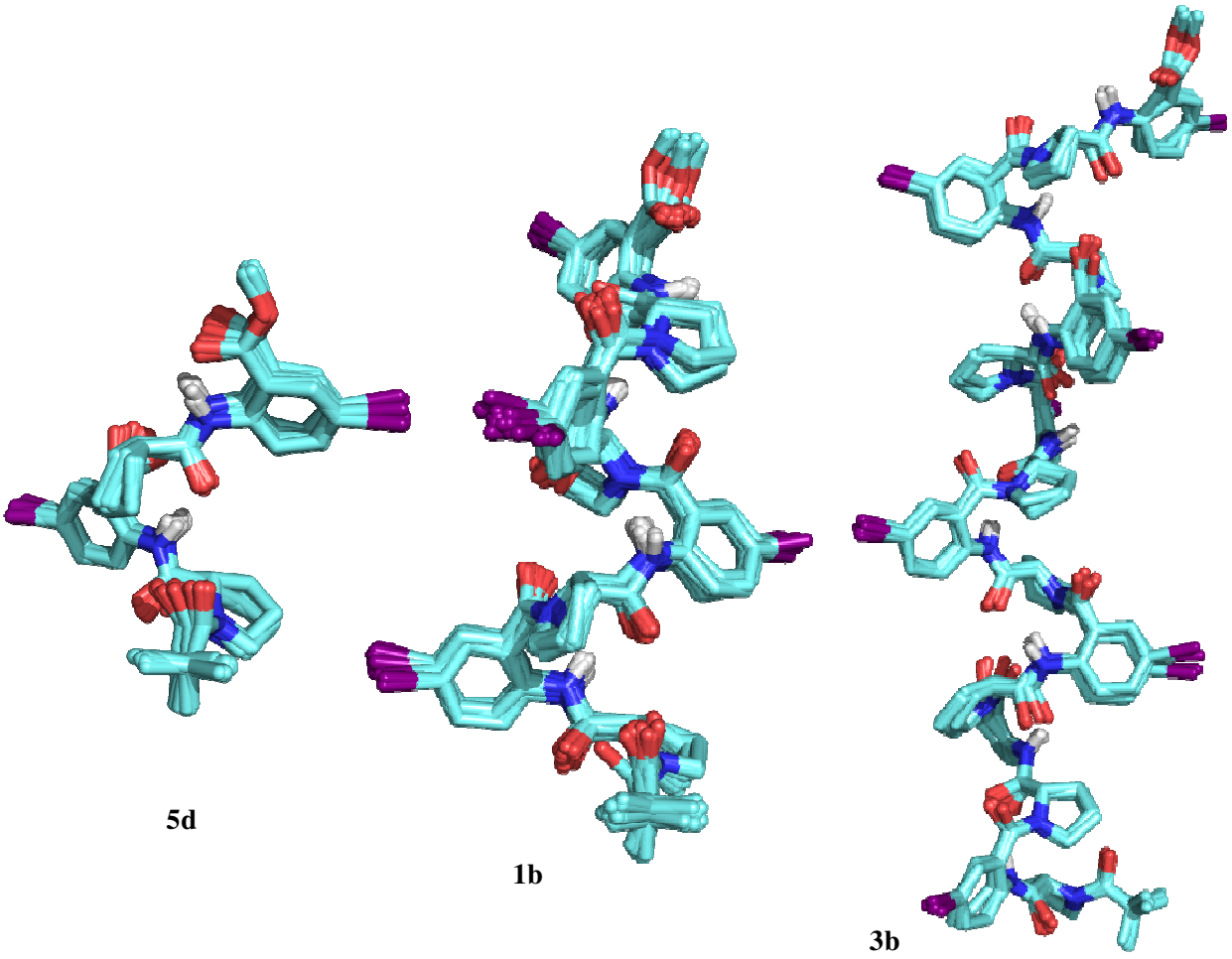


Figure S12. View of lowest energy conformations of *Ant-Pro* oligomers (**5d**, **1b** and **3b**) according to Monte-Carlo conformational search within the range of 5 Kcal/mole of the global minima (number of conformers obtained are 42, 29 and 5, for **5d**, **1b** and **3b**, respectively).

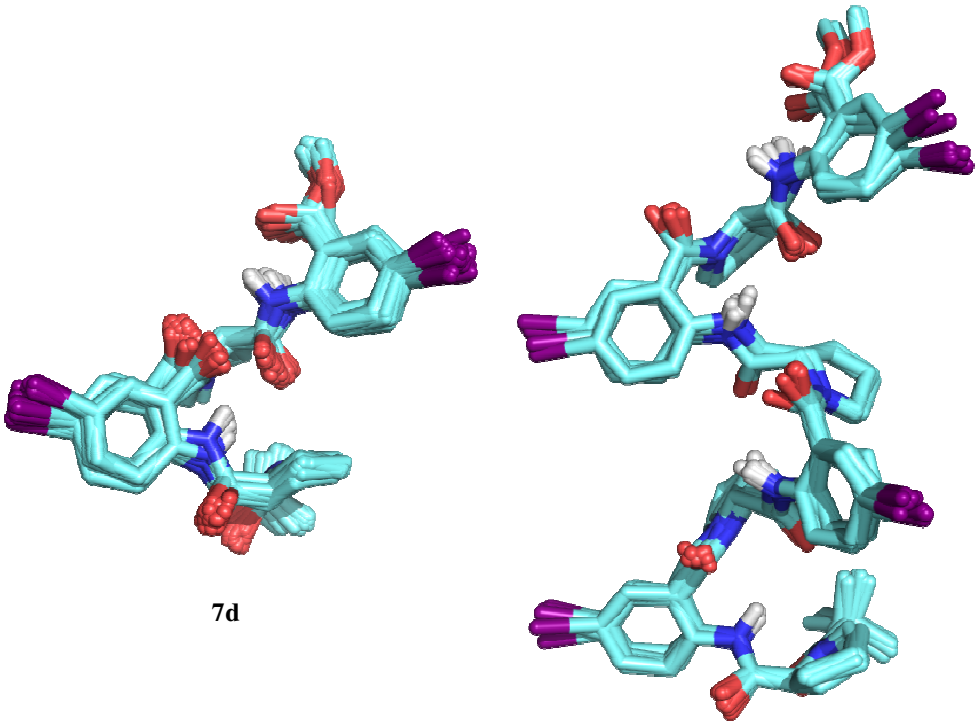


Figure S13. View of lowest energy conformations of *Ant-Pro* oligomers (**7d** and **2b**) according to Monte-Carlo conformational search within the range of 5 Kcal/mole of the global minima (number of conformers obtained are 114 and 17 for **7d** and **2b**, respectively).

Table S5. Monte-Carlo conformations of **5d**. Total energies and RMSD values of all conformers. RMSD values of each conformer were calculated w. r. t. global minimum energy conformer.

Sr. No.	Energy of Conformers (kcal/mol)	RMSD Value	Sr. No.	Energy of Conformers (kcal/mol)	RMSD Value
1	146.9342	---	23	150.7336	0.478
2	147.1276	0.463	24	150.874	0.514
3	147.2771	0.105	25	150.8776	0.501
4	147.7805	0.001	26	150.9135	0.467
5	148.0063	0.003	27	151.1287	0.504
6	148.0922	0.460	28	151.2967	0.495
7	148.5326	0.525	29	151.3093	0.326
8	148.6007	0.463	30	151.4407	0.417
9	148.6931	0.484	31	151.4520	0.472
10	149.3140	0.527	32	151.4566	0.472
11	149.4737	0.459	33	151.4596	0.488
12	149.5321	0.454	34	151.5221	0.502
13	149.7847	0.495	35	151.5809	0.472
14	150.1346	0.504	36	151.6692	0.489
15	150.2033	0.496	37	151.6845	0.500
16	150.2679	0.505	38	151.6948	0.491
17	150.3085	0.473	39	151.7438	0.471
18	150.4788	0.493	40	151.7912	0.103
19	150.4829	0.044	41	151.8503	0.498
20	150.5755	0.488	42	151.9140	0.502
21	150.6214	0.470	43	151.9143	0.535
22	150.6663	0.493			

Table S6. Monte-Carlo conformations of **1b**. Total energies and RMSD values of all conformers. RMSD values of each conformer were calculated w. r. t. global minimum energy conformer.

Sr. No.	Energy of Conformers (kcal/mol)	RMSD Value	Sr. No.	Energy of Conformers (kcal/mol)	RMSD Value
1	281.6411	---	16	285.6788	0.269
2	281.6854	0.234	17	285.7157	0.232
3	283.1891	0.040	18	285.7364	0.385
4	283.2275	0.314	19	285.8012	0.288
5	283.6169	0.220	20	285.8311	0.388
6	283.8819	0.181	21	285.8668	0.213
7	284.1992	0.185	22	285.8813	0.273
8	284.7424	0.235	23	285.8898	0.380
9	284.8415	0.137	24	286.1710	0.377
10	284.9128	0.381	25	286.2325	0.424
11	284.9533	0.381	26	286.2372	0.435
12	285.1925	0.419	27	286.3506	0.234
13	285.2920	0.227	28	286.3827	0.452
14	285.5359	0.393	29	286.5491	0.218
15	285.5467	0.383	30	286.6033	0.454

Table S7. Monte-Carlo conformations of **3b**. Total energies and RMSD values of all conformers. RMSD values of each conformer were calculated w. r. t. global minimum energy conformer.

Sr. No.	Energy of Conformers (kcal/mol)	RMSD Value
1	528.7645	---
2	529.2117	0.383
3	532.0802	0.514
4	532.1024	0.481
5	532.6039	0.469
6	533.5323	0.520

Table S8. Monte-Carlo conformations of **7d**. Total energies and RMSD values of all conformers. RMSD values of each conformer were calculated w. r. t. global minimum energy conformer.

Sr. No.	Energy of Conformers (kcal/mol)	RMSD Value	Sr. No.	Energy of Conformers (kcal/mol)	RMSD Value
1	149.6405	----	38	152.6440	0.202
2	150.1099	0.602	39	152.6831	0.202
3	150.4557	0.219	40	152.7944	0.495
4	150.4825	0.197	41	152.8060	0.563
5	150.5389	0.252	42	152.8090	0.243
6	150.7751	0.517	43	152.9087	0.618
7	150.9399	0.258	44	152.9361	0.641
8	150.9594	0.377	45	152.9794	0.491
9	150.9854	0.639	46	152.9953	0.405
10	151.1953	0.639	47	153.0688	0.030
11	151.2252	0.408	48	153.0774	0.604
12	151.2354	0.549	49	153.1518	0.111
13	151.4183	0.610	50	153.1554	0.565
14	151.4830	0.102	51	153.1564	0.563
15	151.5864	0.092	52	153.1643	0.603
16	151.6083	0.639	53	153.2785	0.247
17	151.6828	0.249	54	153.3099	0.441
18	151.7083	0.470	55	153.3415	0.211
19	151.7867	0.370	56	153.3417	0.108
20	151.9209	0.200	57	153.3909	0.368
21	151.9295	0.487	58	153.4023	0.396
22	151.9907	0.516	59	153.4160	0.559
23	152.0415	0.371	60	153.4561	0.072
24	152.0958	0.462	61	153.5014	0.194
25	152.1115	0.364	62	153.5414	0.383
26	152.1299	0.491	63	153.5513	0.640
27	152.1935	0.495	64	153.6000	0.562
28	152.2449	0.468	65	153.6727	0.189
29	152.3416	0.517	66	153.6850	0.096
30	152.3530	0.461	67	153.6922	0.616
31	152.3992	0.253	68	153.7173	0.460
32	152.4301	0.445	69	153.7247	0.439
33	152.4587	0.062	70	153.7276	0.640
34	152.5425	0.583	71	153.7480	0.515
35	152.5647	0.192	72	153.7538	0.616
36	152.6077	0.351	73	153.7615	0.474
37	152.6260	0.191	74	153.7659	0.617

75	153.8066	0.259	96	154.2870	0.562
76	153.8418	0.507	97	154.3339	0.209
77	153.8826	0.393	98	154.3666	0.227
78	153.8919	0.573	99	154.4285	0.209
79	153.8942	0.561	100	154.4442	0.227
80	153.9390	0.608	101	154.4605	0.444
81	153.9623	0.124	102	154.4633	0.575
82	153.9765	0.490	103	154.5189	0.538
83	154.0103	0.259	104	154.5245	0.407
84	154.0146	0.441	105	154.5337	0.190
85	154.0304	0.129	106	154.5388	0.657
86	154.0395	0.463	107	154.5451	0.456
87	154.0630	0.223	108	154.5490	0.464
88	154.0665	0.434	109	154.5632	0.465
89	154.1172	0.260	110	154.5719	0.477
90	154.1260	0.206	111	154.6034	0.357
91	154.1528	0.465	112	154.6065	0.497
92	154.2316	0.439	113	154.6066	0.482
93	154.2419	0.186	114	154.6364	0.352
94	154.2428	0.639	115	154.6364	0.535
95	154.2566	0.611			

Table S9. Monte-Carlo conformations of **2b**. Total energies and RMSD values of all conformers. RMSD values of each conformer were calculated w. r. t. global minimum energy conformer.

Sr. No.	Energy of Conformers (kcal/mol)	RMSD Value	Sr. No.	Energy of Conformers (kcal/mol)	RMSD Value
1	149.6405	---	10	151.1953	0.312
2	150.1099	0.319	11	151.2252	0.438
3	150.4557	0.321	12	151.2354	0.299
4	150.4825	0.437	13	151.4183	0.437
5	150.5389	0.316	14	151.483	0.316
6	150.7751	0.310	15	151.5864	0.315
7	150.9399	0.305	16	151.6083	0.317
8	150.9594	0.272	17	151.6828	0.376
9	150.9854	0.326	18	151.7083	0.366

Details of the quantum chemical calculations

All quantum chemical calculations were performed at the HF/CEP-31G, and DFT/B3LYP/CEP-31G levels of *ab initio* MO theory employing the Gaussian03 software package.[1] The geometries of the molecules were completely optimized.

The backbone torsion angles and total energies for the derivatives **1b-3b**, **5d** and **7d** are given in the following tables.

Table S10. Backbone Torsion Angles[a], calculated minimum energy[b] of tetrapeptide **5d** according to the HF/CEP-31G and B3LYP/CEP-31G levels of *ab initio* MO theory.

Pro1		Ant1			Pro2		Ant2		
ϕ	ψ	ϕ	θ	ψ	ϕ	ψ	ϕ	θ	ψ
-63.7	142.3	166.5	0.2	-64.1	-71.8	166.0	-177.8	-0.2	-
-64.7	134.8	171.9	0.3	-62.5	-73.0	165.0	-179.8	- 0.2	-

[a] In degrees, first line HF/CEP-31G, second line B3LYP/CEP-31G data. [c]E_T (HF/CEP-31G) = -540.015846 x 10^{-3} kcal/mol; E_T(B3LYP/CEP-31G) = -554.110355 x 10^{-3} kcal/mol.

Table S11. Backbone Torsion Angles[a] and calculated minimum energy[b] for **1b** according to the HF/CEP-31G and B3LYP/CEP-31G levels of *ab initio* MO theory.

Pro1		Ant1			Pro2		Ant2		
ϕ	ψ	ϕ	θ	ψ	ϕ	ψ	ϕ	θ	ψ
-63.4	142.1	167.8	0.7	-65.8	-68.4	156.6	156.5	1.2	-65.3
-63.4	135.6	173.0	0.8	-63.7	-68.8	153.6	161.7	0.8	-62.4
Pro3		Ant3			Pro4		Ant4		
ϕ	ψ	ϕ	θ	ψ	ϕ	ψ	ϕ	θ	ψ
-66.9	157.2	155.1	0.9	-64.1	-69.9	166.0	-177.0	-0.1	-
-65.8	153.5	159.4	0.0	-61.7	-69.5	165.8	-178.1	-0.2	-

[a] In degrees, first line HF/CEP-31G, second line B3LYP/CEP-31G data. [b]E_T (HF/CEP-31G) = -966.7196489 x 10^{-3} kcal/mol; E_T(B3LYP/CEP-31G) = -991.984863 x 10^{-3} kcal/mol.

Table S12. Backbone Torsion Angles[a] and calculated minimum energy[b] for **3a** according to the HF/6-31G and B3LYP/6-31G levels of *ab initio* MO theory.

Pro1		Ant1			Pro2		Ant2		
ϕ	ψ	ϕ	θ	ψ	ϕ	ψ	ϕ	θ	ψ
-65.0	142.6	161.4	-1.8	-60.5	-58.0	149.8	159.9	1.1	-65.9
-66.5	134.8	168.0	-1.1	-59.1	-56.8	144.9	164.6	0.7	-63.6
Pro3		Ant3			Pro4		Ant4		
ϕ	ψ	ϕ	θ	ψ	ϕ	ψ	ϕ	θ	ψ
-67.0	155.6	147.3	-0.4	-61.2	-57.9	150.1	151.9	-1.0	-61.2
-65.1	151.0	153.3	-0.3	-59.3	-56.9	145.4	157.1	-1.4	-58.9
Pro1		Ant1			Pro2		Ant2		
ϕ	ψ	ϕ	θ	ψ	ϕ	ψ	ϕ	θ	ψ
-57.4	150.3	159.8	1.2	-65.8	-67.2	157.1	156.5	1.2	-65.6
-56.2	146.2	164.5	0.4	-62.8	-66.6	154.6	162.0	0.7	-62.6
Pro3		Ant3			Pro4		Ant4		
ϕ	ψ	ϕ	θ	ψ	ϕ	ψ	ϕ	θ	ψ
-66.9	156.9	155.5	0.9	-64.2	-69.9	166.1	-176.8	-0.1	-
-65.0	153.0	160.1	-0.1	-61.9	-69.8	166.0	-178.3	-0.0	-

[a] In degrees, first line HF/CEP-31G, second line B3LYP/CEP-31G data.[c] E_T (HF/CEP-31G) = -1820.133887 x 10^{-3} kcal/mol; E_T(B3LYP/CEP-31G) = -1867.741303 x 10^{-3} kcal/mol.

Table S13. Backbone Torsion Angles[a], and calculated minimum energy[b] of tetrapeptide **7d** according to the HF/CEP-31G and B3LYP/CEP-31G levels of *ab initio* MO theory.

Pro1		Ant1			Pro2		Ant2		
ϕ	ψ	ϕ	θ	ψ	ϕ	ψ	ϕ	θ	ψ
-59.6	-37.5	151.6	0.5	76.3	61.7	-146.5	178.2	0.3	-
-57.2	-46.5	164.2	-0.2	65.3	64.4	-147.9	178.1	0.2	-

[a] In degrees, first line HF/CEP-31G, second line B3LYP/CEP-31G data. [c]E_T (HF/CEP-31G) = -533.992974 x 10^{-3} kcal/mol; E_T(B3LYP/CEP-31G) = -554.088142 x 10^{-3} kcal/mol.

Table S14. Backbone Torsion Angles[a] for **2b**[b] according to the HF/CEP-31G and B3LYP/CEP-31G levels of *ab initio* MO theory.

Pro1		Ant1			Pro2		Ant2		
ϕ	ψ	ϕ	θ	ψ	ϕ	ψ	ϕ	θ	ψ
-58.9	-38.2	153.5	0.6	77.8	61.6	-150.2	165.5	-0.2	-66.4
-56.8	-47.0	164.3	0.0	65.8	66.4	-152.2	174.5	0.4	-69.5
Pro3		Ant3			Pro4		Ant4		
ϕ	ψ	ϕ	θ	ψ	ϕ	ψ	ϕ	θ	ψ
-61.5	154.3	-168.1	0.4	66.9	61.6	-155.7	174.5	0.4	-
-62.5	153.4	-174.3	0.4	65.2	61.5	-154.0	177.4	0.3	-

[a] In degrees, first line HF/CEP-31G, second line B3LYP/CEP-31G data.[b] E_T (HF/CEP-31G) = -966.678266 x 10^{-3} kcal/mol; E_T(B3LYP/CEP-31G) = -991.944321 x 10^{-3} kcal/mol.

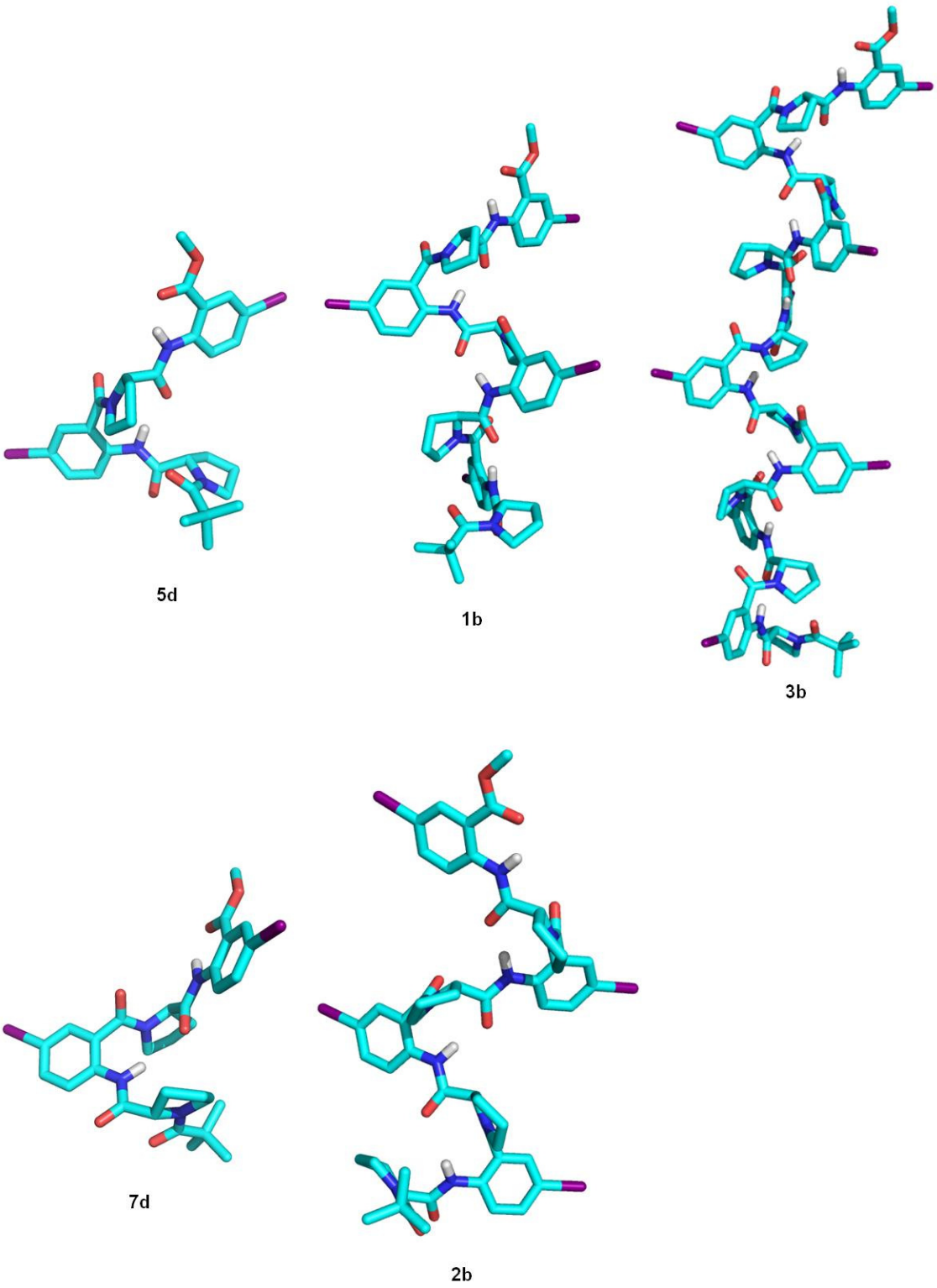


Figure S14. Possible minimum energy conformations of Ant-Pro oligomers according to B3LYP/CEP-31G.

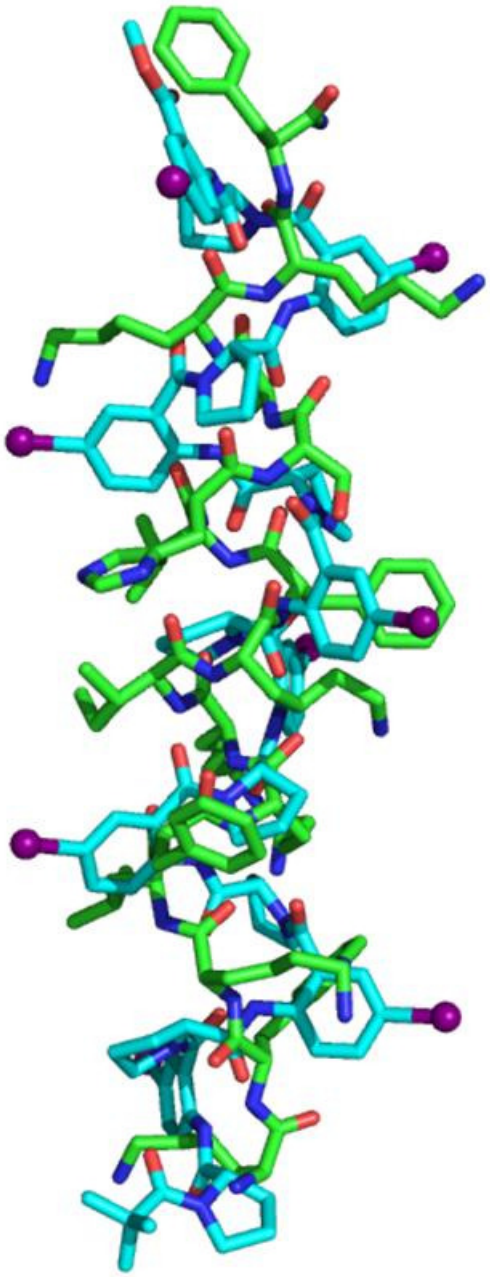


Figure S15. Superimposed 3D structure of AMP Magainin-II (green) with *Ant-Pro* hexadecamer **3b** (cyan).

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