

Supporting Information

SUPRAMOLECULAR CHIROGENESIS IN AMIDE-LINKED BIS(ZINC PORPHYRIN): APPLICATION FOR ABSOLUTE CONFIGURATIONAL ASSIGNMENT OF CHIRAL CARBOXYLIC ACIDS AND CHIRAL

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1. Comparison of ^1H NMR Spectra of Bis(zinc porphyrin) BP2 with those of the Monomeric Counterparts Zn-5 and Zn-8 derivative.

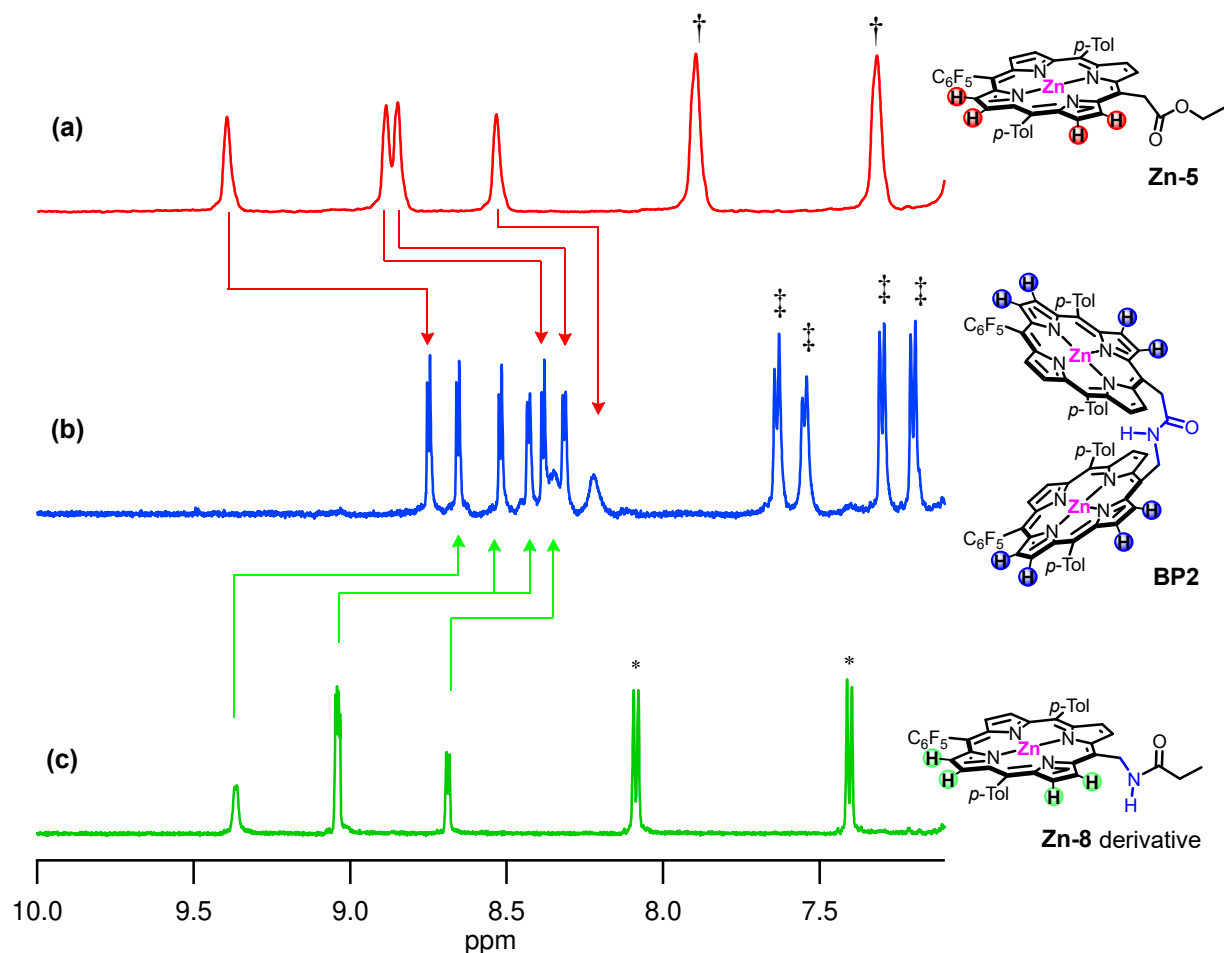


Figure S1. ^1H NMR spectra ($\text{C}_6\text{D}_5\text{CD}_3$, 80°C) of (a) **Zn-5** (\dagger = proton on the *p*-tolyl ring in **Zn-5**), (b) **BP2** (\ddagger = proton on the *p*-tolyl ring in **BP2**), and (c) **Zn-8** derivative (* = proton on the *p*-tolyl ring in **Zn-8** derivative). The cofacial arrangement of porphyrin rings in **BP2** was identified by ^1H NMR spectroscopy. The proton signals of the β -pyrrolic positions of the porphyrin units in **BP2** exhibited significant upfield shifts compared with those of its monomeric counterparts **Zn-5** and **Zn-8** derivative.

2. Comparison of UV-Vis Spectra of Bis(zinc porphyrin) BP2 with those of the Monomeric Counterparts Zn-5 and Zn-7.

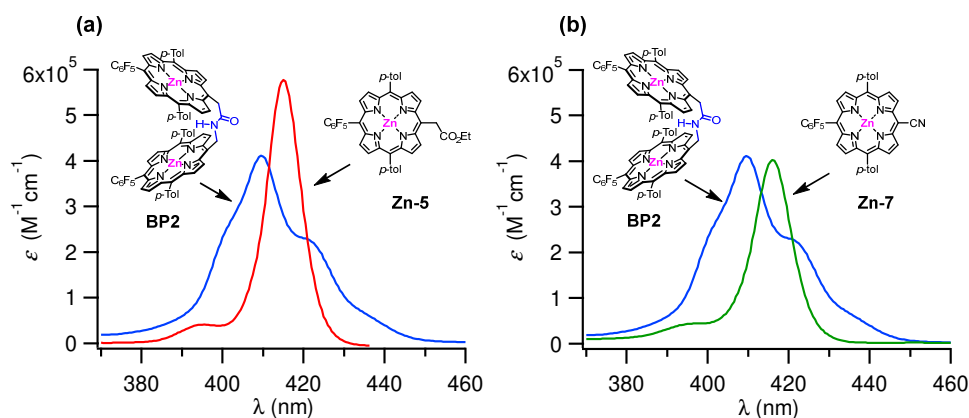


Figure S2. UV-Vis spectra of (a) **BP2** (blue-line) and **Zn-5** (red-line) (b) **BP2** (blue-line) and **Zn-7** (green-line) in 1% $\text{CH}_2\text{Cl}_2/n$ -hexane at 25 °C.

3. Job's Continuous Plot Analysis to Determine Complex Stoichiometry

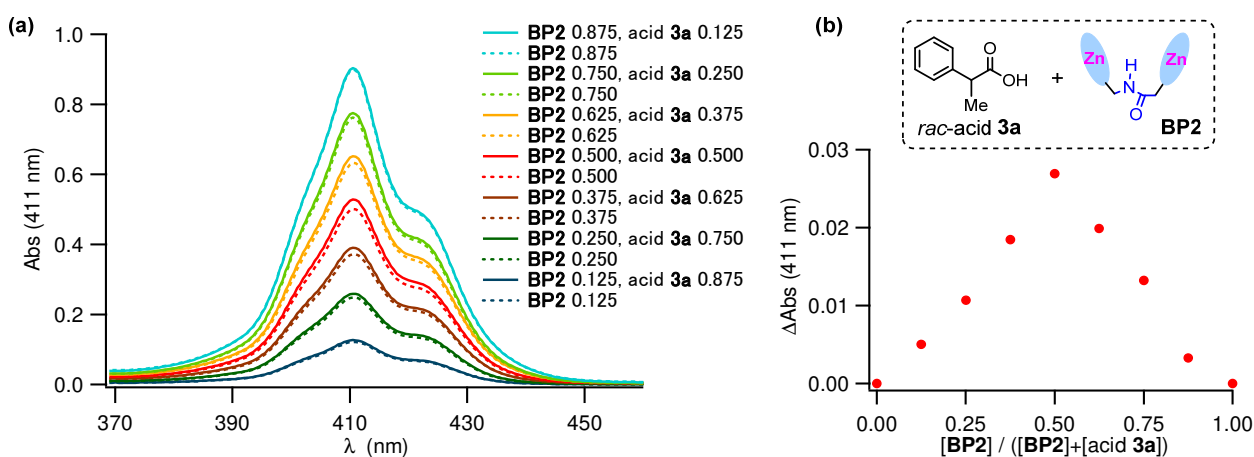


Figure S3. (a) Spectral changes of host molecule **BP2** and carboxylic acid **3a** (guest molecule) in 15% $\text{CH}_2\text{Cl}_2/n$ -hexane were prepared with a fixed total concentration of host and guest molecules (2.0×10^{-6} M). The UV-vis spectra were recorded at 25 °C and ΔAbs was monitored at 411 nm. (b) Job's plot of **BP2** and carboxylic acid **3a**. The peak at a mole fraction of 0.5 corresponds to a 1:1 **BP2**/carboxylic acid **3a** complex.

4. Spectroscopic Titrations for Evaluation of Association Constants

The association constants K_{assoc} for host-guest complexes were determined through titration of the host molecules **BP1** or **BP2** with carboxylic acid **3a** as the guest molecule. K_{assoc} values were evaluated from the following equation by applying a nonlinear curve-fitting method to the changes in absorbance (Δ_{Abs}) upon titration of host molecule **BP1** or **BP2** with guest molecule:

$$\Delta_{\text{Abs}} = \frac{L[\alpha] - \sqrt{\alpha^2 L^2 - 4K_{\text{assoc}}^2 \cdot A \cdot X \cdot L^2}}{2K_{\text{assoc}} \cdot A}$$

$$\alpha = K_{\text{assoc}} \cdot X + K_{\text{assoc}} \cdot A + 1$$

where X and A represent $[\text{Guest}]_{\text{total}}$ and $[\text{Host}]_{\text{total}}$, respectively; L denotes Δ_{Abs} at 100% complexation; L and K_{assoc} are parameters.¹ IGOR Pro (ver 6.22) software was used for curve-fitting analysis.

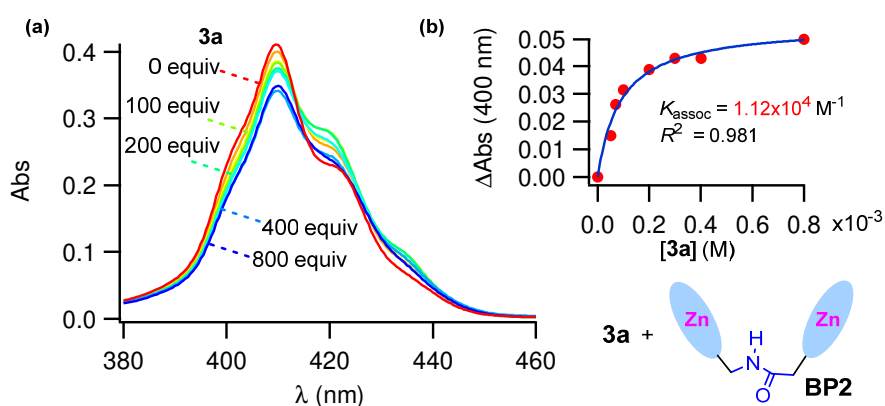


Figure S4 (a) Spectral changes on titrating **BP2** in 5% CH₂Cl₂/n-hexane at 25 °C with carboxylic acid **3a**. (b) Changes in Δ_{Abs} at 400 nm for evaluating K_{assoc} ($[\text{BP2}] = 1.0 \times 10^{-6} \text{ M}$; $[\text{3a}]/[\text{BP2}] = 0\text{--}800$).

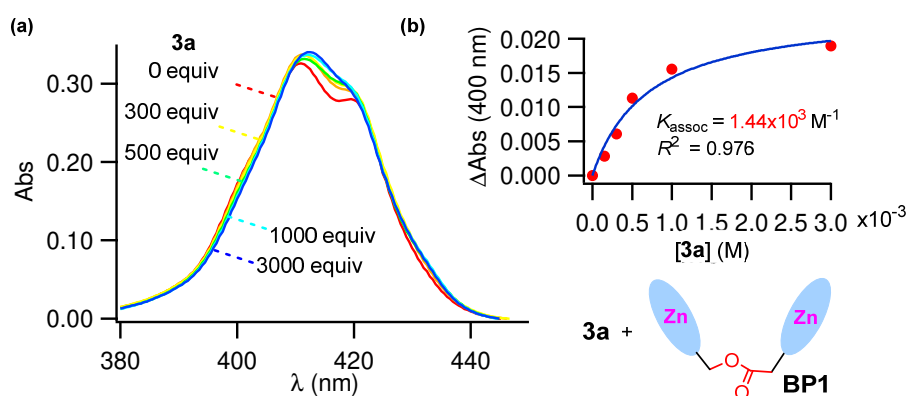


Figure S5 (a) Spectral changes on titrating **BP1** in 5% CH₂Cl₂/n-hexane at 25 °C with carboxylic acid **3a**. (b) Changes in Δ_{Abs} at 400 nm for evaluating K_{assoc} ($[\text{BP1}] = 1.0 \times 10^{-6} \text{ M}$; $[\text{3a}]/[\text{BP1}] = 0\text{--}3,000$).

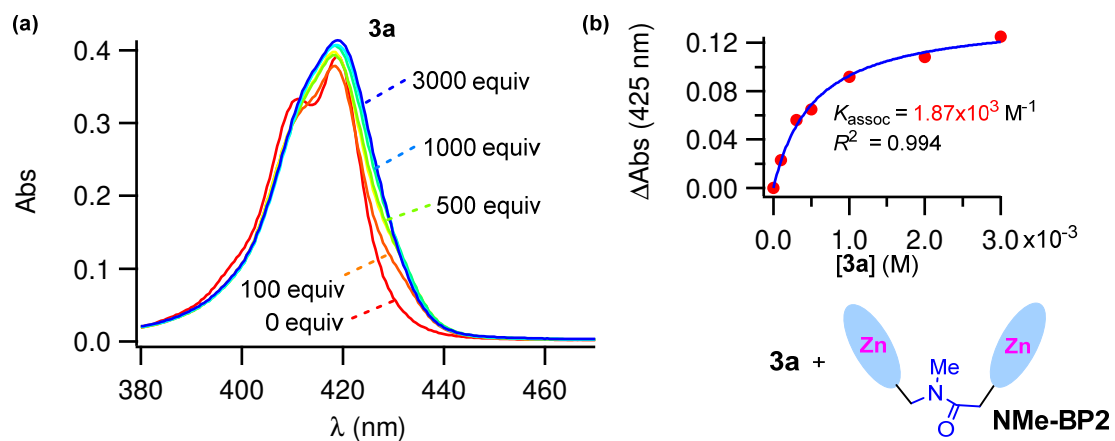
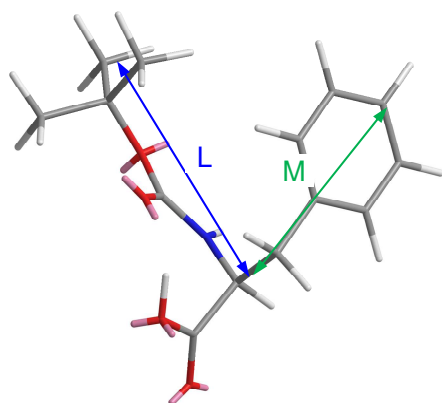


Figure S6 (a) Spectral changes on titrating **NMe-BP2** in 5% $\text{CH}_2\text{Cl}_2/n$ -hexane at 25 °C with carboxylic acid **3a**. (b) Changes in Δ Abs at 425 nm for evaluating K_{assoc} ($[\text{NMe-BP2}] = 1.0 \times 10^{-6} \text{ M}$; $[\mathbf{3a}]/[\text{NMe-BP2}] = 0\text{--}3,000$).

5. MM2 Optimized Structure and Length of the Substituents of N-protected Amino Acid Derivatives 10

The MM2-optimized structures of N-protected amino acid derivatives **10** were used to obtain the length of the substituents and determine the priority of the larger (L) and medium (M) groups by the length of the substituents as in the method reported by Borhan and coworkers.³ These calculations were performed using the Chem3D Ultra 16.0 (Perkin Elmer) software package

MM2 optimized structure of (S)-10a



4.2089 kcal/mol

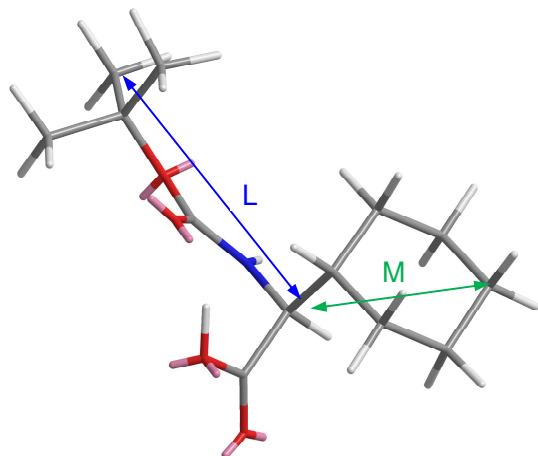
L (BocNH): 5.99 Å,

M (Bn): 4.96 Å

Cartesian Coordinates for (S)-10a

Atom	X (Å)	Y (Å)	Z (Å)
C(1)	4.465	-1.963	-1.616
C(2)	2.957	-1.791	-1.816
O(3)	2.239	-2.882	-1.477
O(4)	2.465	-0.752	-2.202
N(5)	4.926	-2.150	-0.232
C(6)	5.086	-2.996	-2.575
O(7)	5.298	-3.333	1.707
C(8)	5.312	-4.489	2.489
C(9)	3.929	-4.760	3.096
C(10)	5.828	-5.701	1.703
C(11)	6.298	-4.202	3.634
C(12)	4.639	-3.252	0.522
O(13)	3.864	-4.079	0.111
C(14)	6.546	-3.225	-2.240
C(15)	7.459	-2.266	-2.472
C(16)	8.751	-2.452	-2.162
C(17)	9.149	-3.609	-1.611
C(18)	8.249	-4.575	-1.375
C(19)	6.959	-4.381	-1.689
H(20)	4.871	-0.960	-1.904
H(21)	2.763	-3.695	-1.446
H(22)	5.611	-1.505	0.155
H(23)	5.001	-2.654	-3.634
H(24)	4.515	-3.950	-2.515
H(25)	3.538	-3.861	3.625
H(26)	3.978	-5.590	3.836
H(27)	3.171	-5.060	2.342
H(28)	6.805	-5.479	1.219
H(29)	5.983	-6.572	2.379
H(30)	5.129	-6.049	0.912
H(31)	6.380	-5.065	4.333
H(32)	5.977	-3.318	4.232
H(33)	7.319	-3.987	3.245
H(34)	7.147	-1.308	-2.921
H(35)	9.487	-1.654	-2.357
H(36)	10.210	-3.764	-1.352
H(37)	8.570	-5.527	-0.921
H(38)	6.234	-5.186	-1.482
Lp(39)	1.798	-2.981	-1.872
Lp(40)	2.057	-2.815	-0.910
Lp(41)	1.867	-0.723	-2.254
Lp(42)	2.840	-0.300	-2.324
Lp(43)	5.863	-3.276	1.513
Lp(44)	4.981	-2.935	2.023
Lp(45)	3.751	-4.555	0.452
Lp(46)	3.600	-3.975	-0.417

MM2 optimized structure of (S)-10b



14.4637 kcal/mol

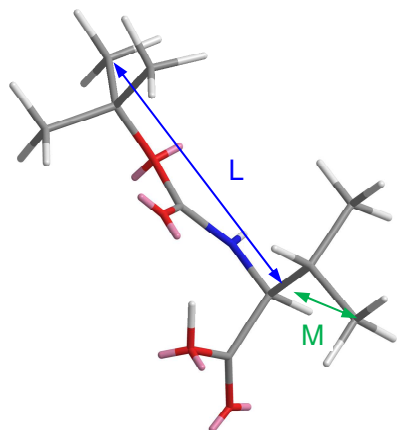
L (BocNH): 5.98 Å,

M (cyclohexyl): 3.82 Å

Cartesian Coordinates for (S)-10b

Atom	X (Å)	Y (Å)	Z (Å)
C(1)	-0.920	1.516	-0.958
C(2)	-2.428	1.727	-1.108
O(3)	-3.112	0.566	-1.184
O(4)	-2.945	2.823	-1.162
N(5)	-0.534	1.294	0.443
C(6)	-0.289	0.527	-1.966
O(7)	-0.301	0.114	2.404
C(8)	-0.179	-1.076	3.123
C(9)	-1.547	-1.544	3.633
C(10)	0.520	-2.171	2.306
C(11)	0.705	-0.740	4.336
C(12)	-0.825	0.164	1.151
O(13)	-1.465	-0.726	0.649
C(14)	1.234	0.372	-1.783
C(15)	2.017	1.609	-2.248
C(16)	1.694	1.941	-3.712
C(17)	0.184	2.124	-3.917
C(18)	-0.591	0.889	-3.435
H(19)	-0.742	-0.479	-1.783
H(20)	-0.485	2.518	-1.193
H(21)	-2.563	-0.218	-1.040
H(22)	0.017	2.000	0.927
H(23)	1.582	-0.506	-2.378
H(24)	1.481	0.141	-0.720
H(25)	-2.062	-0.740	4.207
H(26)	-1.439	-2.422	4.310
H(27)	-2.232	-1.858	2.816
H(28)	1.460	-1.791	1.844
H(29)	0.792	-3.034	2.955
H(30)	-0.110	-2.593	1.494
H(31)	0.849	-1.623	4.999
H(32)	0.255	0.071	4.953
H(33)	1.715	-0.394	4.017
H(34)	3.112	1.425	-2.138
H(35)	1.775	2.483	-1.600
H(36)	2.057	1.113	-4.367
H(37)	2.236	2.866	-4.022
H(38)	-0.028	2.304	-4.999
H(39)	-0.163	3.034	-3.374
H(40)	-1.685	1.044	-3.585
H(41)	-0.308	0.025	-4.084
Lp(42)	-3.545	0.573	-0.768
Lp(43)	-3.332	0.527	-1.741
Lp(44)	-3.540	2.871	-1.221
Lp(45)	-2.518	3.242	-1.122
Lp(46)	-0.640	0.478	2.740
Lp(47)	0.274	0.255	2.302
Lp(48)	-1.590	-1.221	0.965
Lp(49)	-1.606	-0.572	0.087

MM2 optimized structure of (S)-10c



7.8268 kcal/mol

L (BocNH): 5.98 Å,

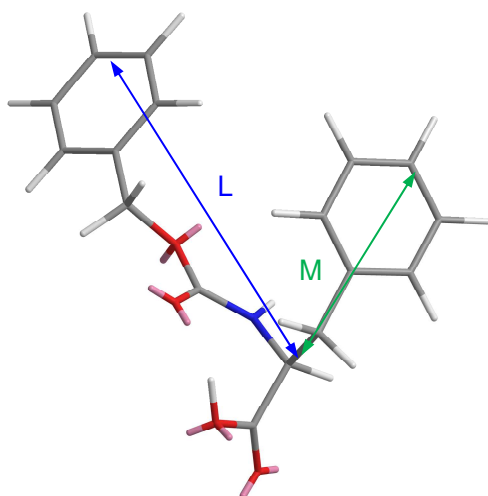
M (isopropyl): 2.55 Å

Cartesian Coordinates for (S)-10c

Atom	X (Å)	Y (Å)	Z (Å)
C(1)	-0.239	1.622	-1.403
C(2)	-1.748	1.836	-1.551
O(3)	-2.434	0.676	-1.626
O(4)	-2.262	2.933	-1.606
N(5)	0.147	1.400	-0.002
C(6)	0.389	0.631	-2.411
O(7)	0.381	0.219	1.958
C(8)	0.500	-0.971	2.677
C(9)	-0.870	-1.437	3.187
C(10)	1.197	-2.068	1.860
C(11)	1.384	-0.638	3.891
C(12)	-0.145	0.269	0.706
O(13)	-0.787	-0.619	0.205
C(14)	1.912	0.475	-2.229
H(15)	2.434	1.393	-2.582
H(16)	0.621	1.928	-4.160
C(17)	0.086	0.993	-3.880
H(18)	-0.065	-0.374	-2.226
H(19)	0.197	2.623	-1.639
H(20)	-1.885	-0.108	-1.483
H(21)	0.699	2.105	0.482
H(22)	2.279	-0.401	-2.818
H(23)	2.154	0.316	-1.153
H(24)	-1.383	-0.632	3.759
H(25)	-0.762	-2.314	3.865
H(26)	-1.553	-1.752	2.370
H(27)	2.140	-1.691	1.402
H(28)	1.465	-2.933	2.510
H(29)	0.568	-2.487	1.046
H(30)	1.525	-1.521	4.554
H(31)	0.935	0.174	4.508
H(32)	2.395	-0.293	3.573
H(33)	-1.010	1.147	-4.016
H(34)	0.423	0.169	-4.554
Lp(35)	-2.865	0.684	-1.209
Lp(36)	-2.655	0.638	-2.183
Lp(37)	-2.857	2.982	-1.664
Lp(38)	-1.834	3.351	-1.566
Lp(39)	0.044	0.583	2.295
Lp(40)	0.956	0.357	1.855
Lp(41)	-0.912	-1.114	0.521
Lp(42)	-0.929	-0.465	-0.357

MM2 optimized structure of (S)-10d

1.1547 kcal/mol



1.1547 kcal/mol

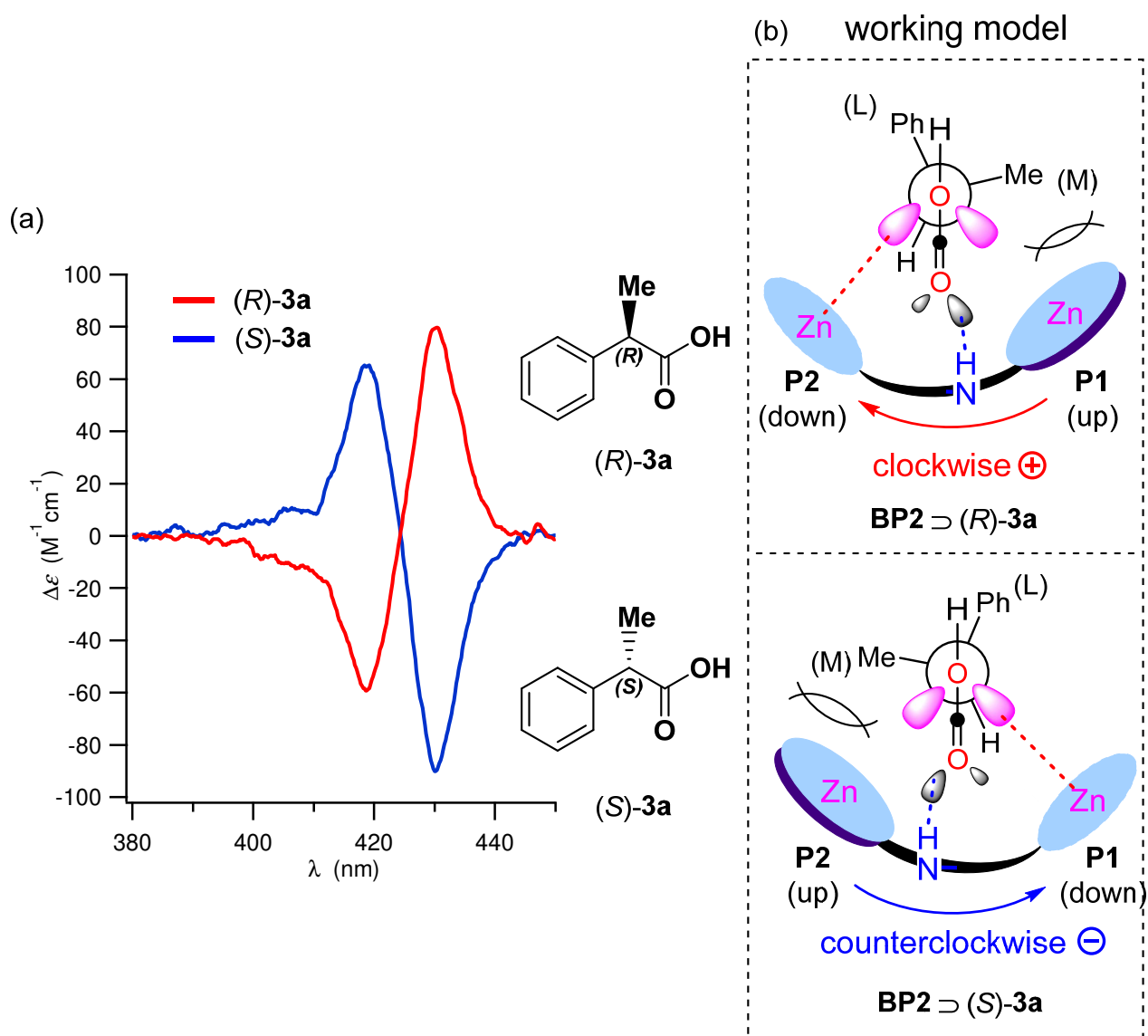
L (CbzNH): 8.44 Å,

M (Bn): 4.95 Å

Cartesian Coordinates for (S)-10d

Atom	X (Å)	Y (Å)	Z (Å)
C(1)	-1.795	0.878	-3.394
C(2)	-3.302	1.114	-3.507
O(3)	-4.010	-0.035	-3.515
O(4)	-3.797	2.217	-3.601
N(5)	-1.327	0.818	-2.002
C(6)	-1.231	-0.267	-4.255
O(7)	-1.023	-0.164	0.066
C(8)	-1.136	-1.308	0.887
H(9)	-2.192	-1.406	1.228
H(10)	-0.867	-2.217	0.301
C(11)	-0.192	-1.182	2.064
C(12)	-1.662	-0.179	-1.134
O(13)	-2.438	-1.045	-1.457
C(14)	0.261	-0.398	-4.026
C(15)	1.124	0.426	-4.648
C(16)	2.446	0.328	-4.437
C(17)	2.925	-0.600	-3.595
C(18)	2.076	-1.428	-2.968
C(19)	0.755	-1.326	-3.186
H(20)	-1.339	1.817	-3.800
H(21)	-3.485	-0.809	-3.263
H(22)	-0.631	1.486	-1.680
H(23)	-1.437	-0.073	-5.334
H(24)	-1.732	-1.233	-4.023
C(25)	-0.644	-0.889	3.297
C(26)	0.202	-0.780	4.332
C(27)	1.519	-0.961	4.146
C(28)	1.982	-1.252	2.922
C(29)	1.130	-1.361	1.891
H(30)	-1.722	-0.734	3.467
H(31)	-0.183	-0.539	5.337
H(32)	2.216	-0.871	4.996
H(33)	3.063	-1.401	2.762
H(34)	0.744	1.198	-5.337
H(35)	3.139	1.013	-4.954
H(36)	4.010	-0.681	-3.418
H(37)	2.463	-2.191	-2.272
H(38)	0.074	-2.013	-2.657
H(39)	1.523	-1.598	0.888
Lp(40)	-4.466	0.019	-3.129
Lp(41)	-4.200	-0.124	-4.077
Lp(42)	-4.393	2.276	-3.644
Lp(43)	-3.360	2.628	-3.595
Lp(44)	-1.239	0.302	0.377
Lp(45)	-0.441	-0.135	-0.073
Lp(46)	-2.581	-1.480	-1.069
Lp(47)	-2.620	-0.945	-2.020

6. CD Spectra, and Proposed Working Model of Chiral Mono-Carboxylic Acids with BP2



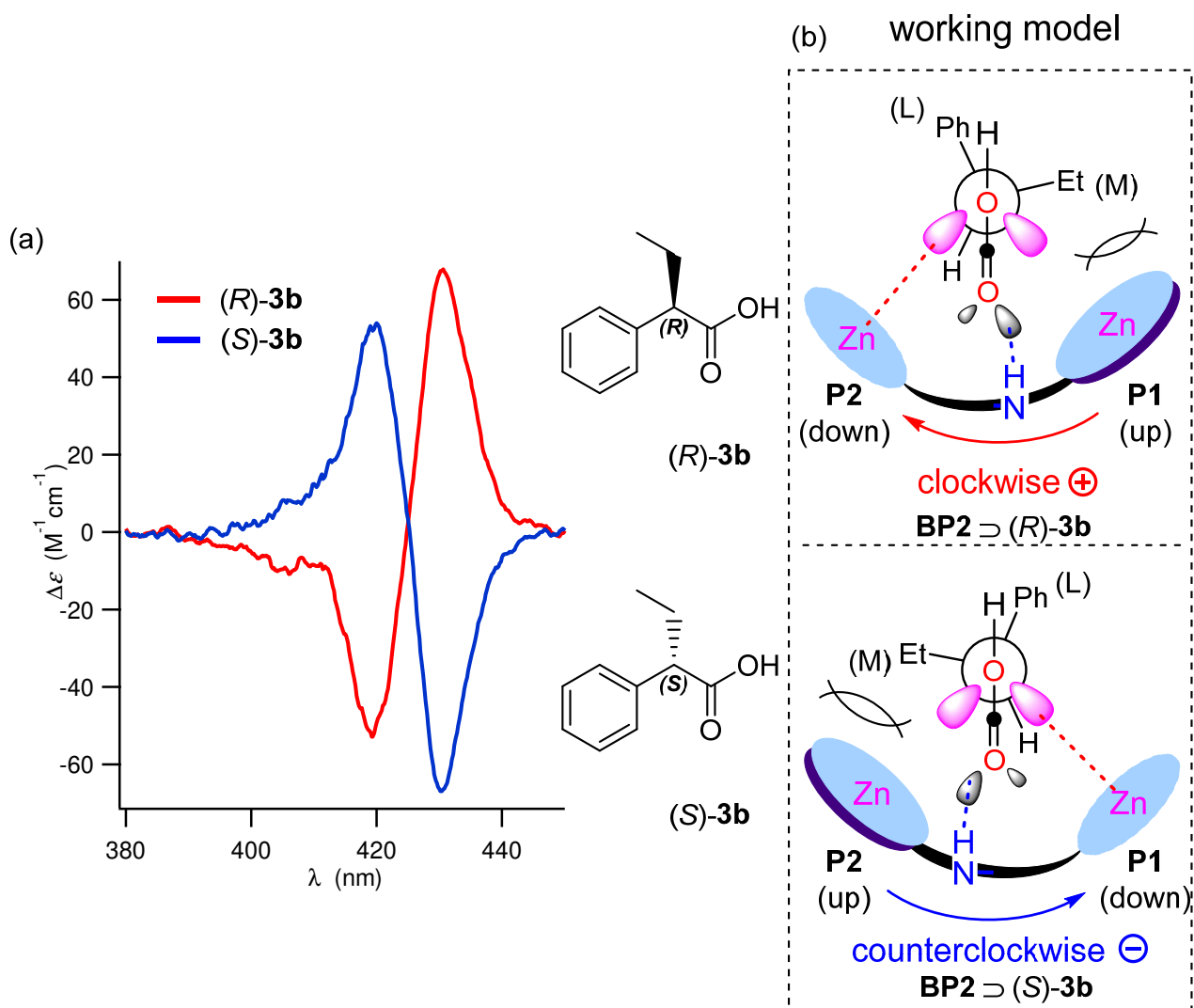


Figure S8. (a) ECCD spectrum of **3b** (2.0×10^{-4} M) in the presence of **BP2** (2.0×10^{-6} M) in 5% $\text{CH}_2\text{Cl}_2/n$ -hexane at 25 °C. (b) The proposed working model for assigning the absolute configuration of the chiral guest **3b** (dashed box). The priority of the substituents was determined by the A value:² H (S), 0.00 kJmol^{-1} ; Et (M), 7.49 kJmol^{-1} ; Ph (L), 11.71 kJmol^{-1} .

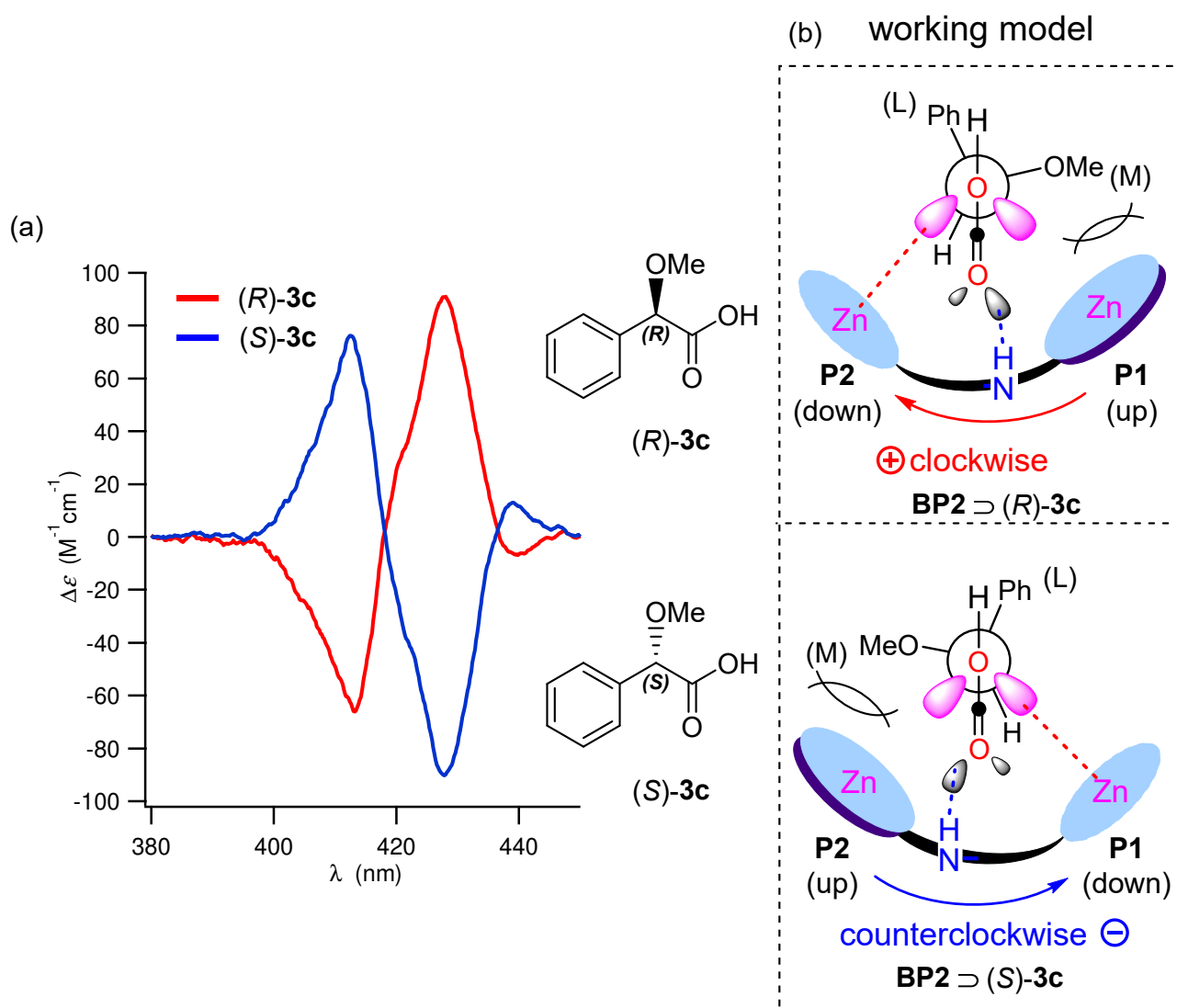


Figure S9. (a) ECCD spectrum of **3c** (2.0×10^{-4} M) in the presence of **BP2** (2.0×10^{-6} M) in 5% $\text{CH}_2\text{Cl}_2/n$ -hexane at 25 °C. (b) The proposed working model for assigning the absolute configuration of the chiral guest **3c** (dashed box). The priority of the substituents was determined by the A value:² H (S), 0.00 kJmol^{-1} ; MeO (M), 2.30–3.14 kJmol^{-1} ; Ph (L), 11.71 kJmol^{-1} .

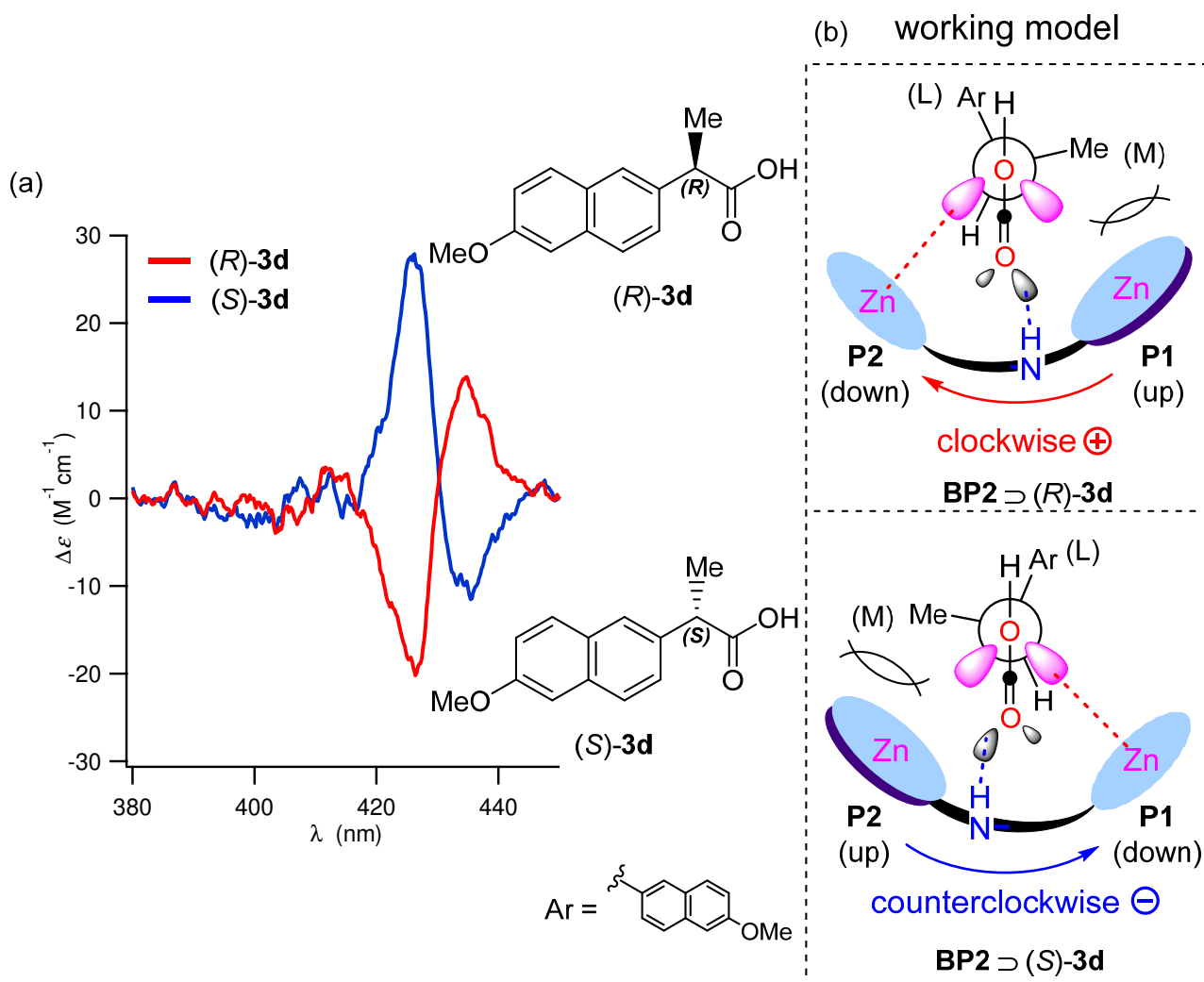
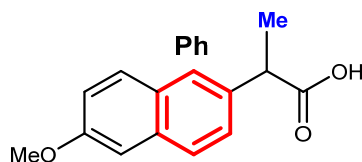


Figure S10. (a) ECCD spectrum of **3d** (2.0×10^{-4} M) in the presence of **BP2** (2.0×10^{-6} M) in 5% $\text{CH}_2\text{Cl}_2/n$ -hexane at 25 °C. (b) The proposed working model for assigning the absolute configuration of the chiral guest **3d** (dashed box). The conformational energy, A value (kJmol^{-1}), was not available for 6-methoxy-2-naphthyl substituent. As shown in the figure depicted below, the substrate **3d** consists of Me (blue) and Ph (red) moieties. The A value for Me and Ph are 7.28 kJmol^{-1} and 11.71 kJmol^{-1} , respectively.² Therefore, the blue colored Me and the red colored Ph moieties can be assigned to M and L groups, respectively.



7. CD spectra, and Proposed Working Model of Chiral N-Protected Amino Acid Derivatives with BP2

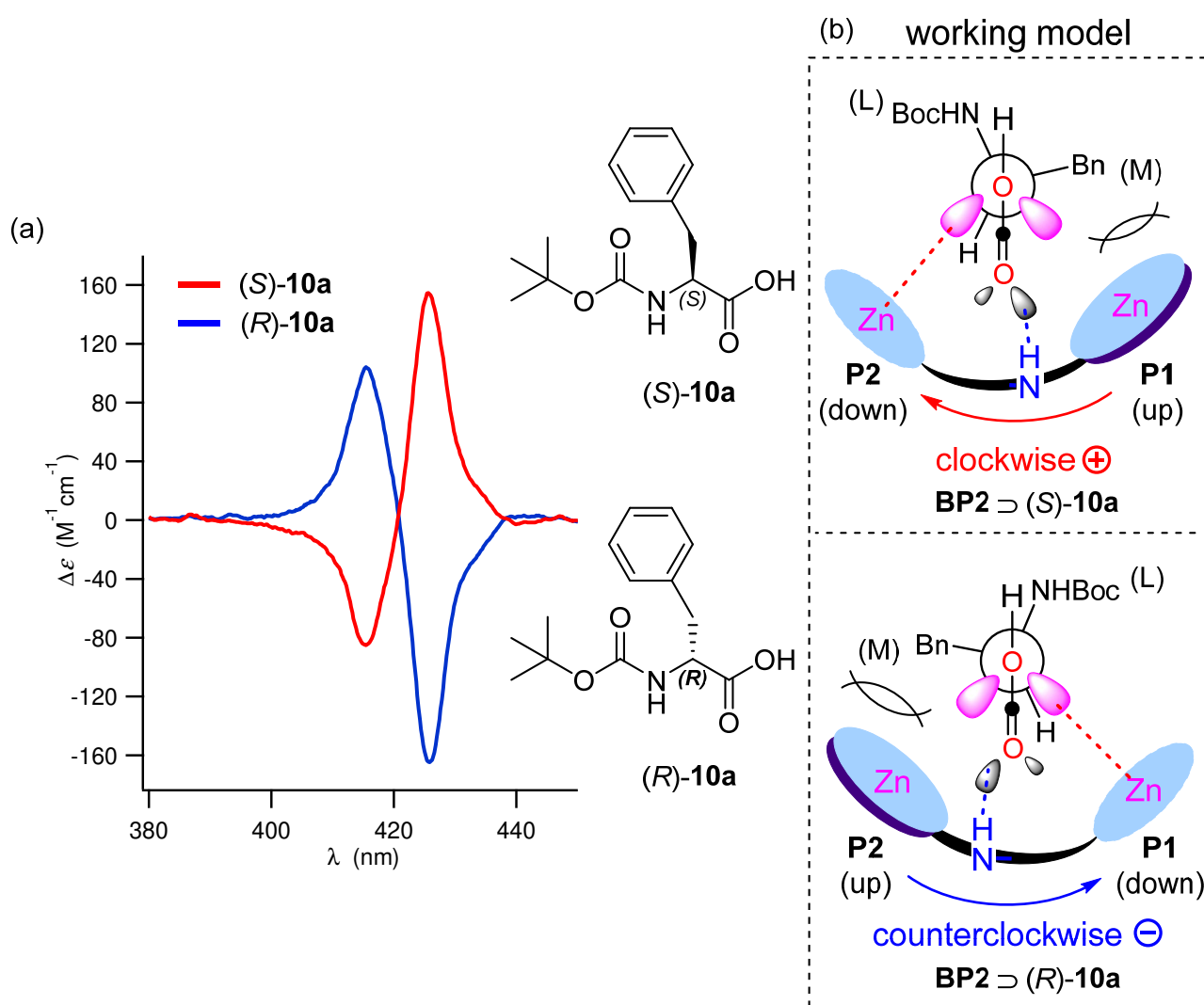


Figure S11. (a) ECCD spectrum of **10a** (2.0×10^{-4} M) in the presence of **BP2** (2.0×10^{-6} M) in 5% $\text{CH}_2\text{Cl}_2/n$ -hexane at 25 °C. (b) The proposed working model for assigning the absolute configuration of the chiral guest **10a** (dashed box). The priority of the substituents was determined by the length of the substituents:³ Bn (M), 4.96 Å; BocNH (L), 5.99 Å.

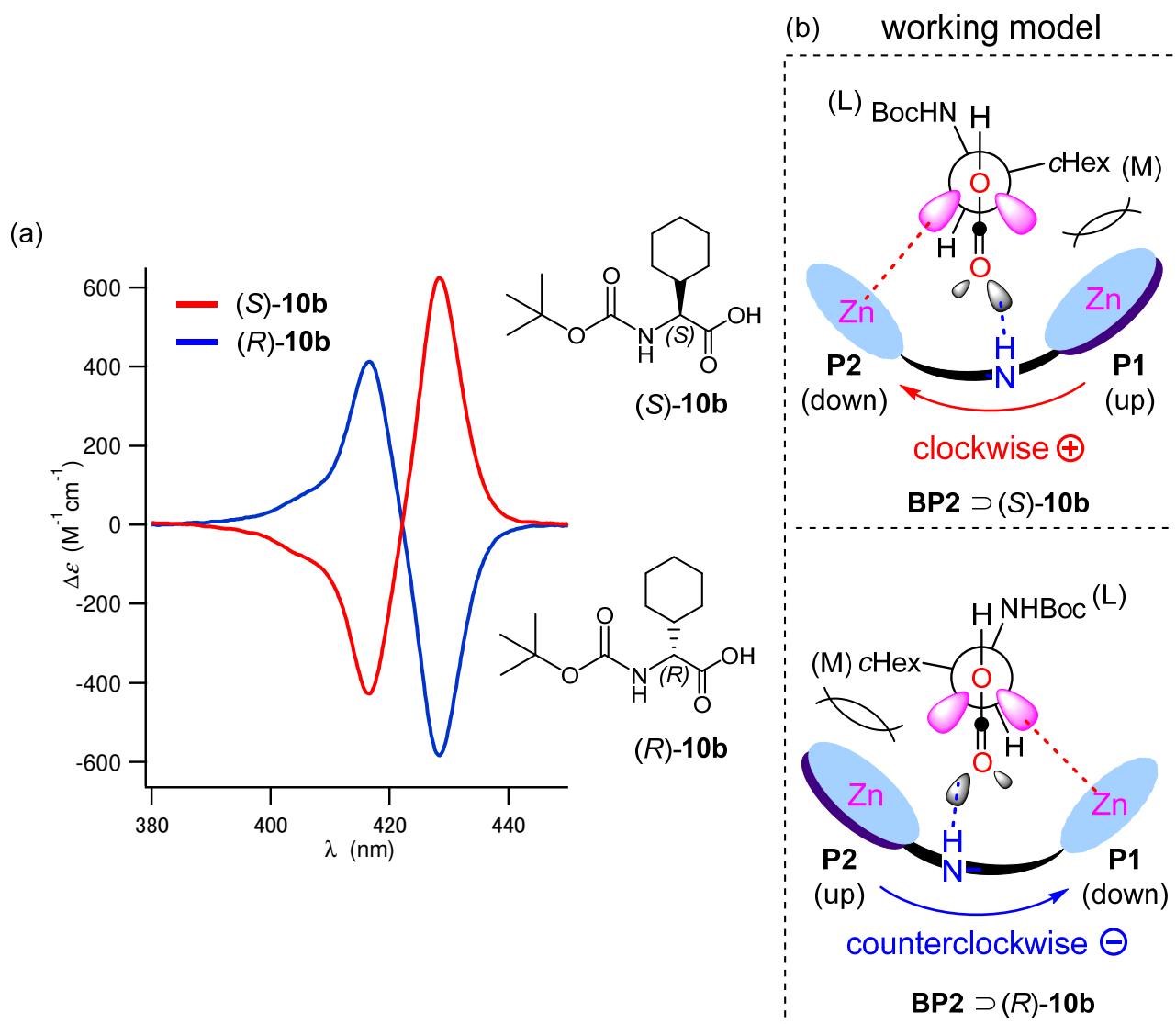


Figure S12. (a) ECCD spectrum of **10b** (2.0×10^{-4} M) in the presence of **BP2** (2.0×10^{-6} M) in 5% $\text{CH}_2\text{Cl}_2/n$ -hexane at 25 °C. (b) The proposed working model for assigning the absolute configuration of the chiral guest **10b** (dashed box). The priority of the substituents was determined by the length of the substituents:³ cyclohexyl (M), 3.82 Å; BocNH (L), 5.98 Å.

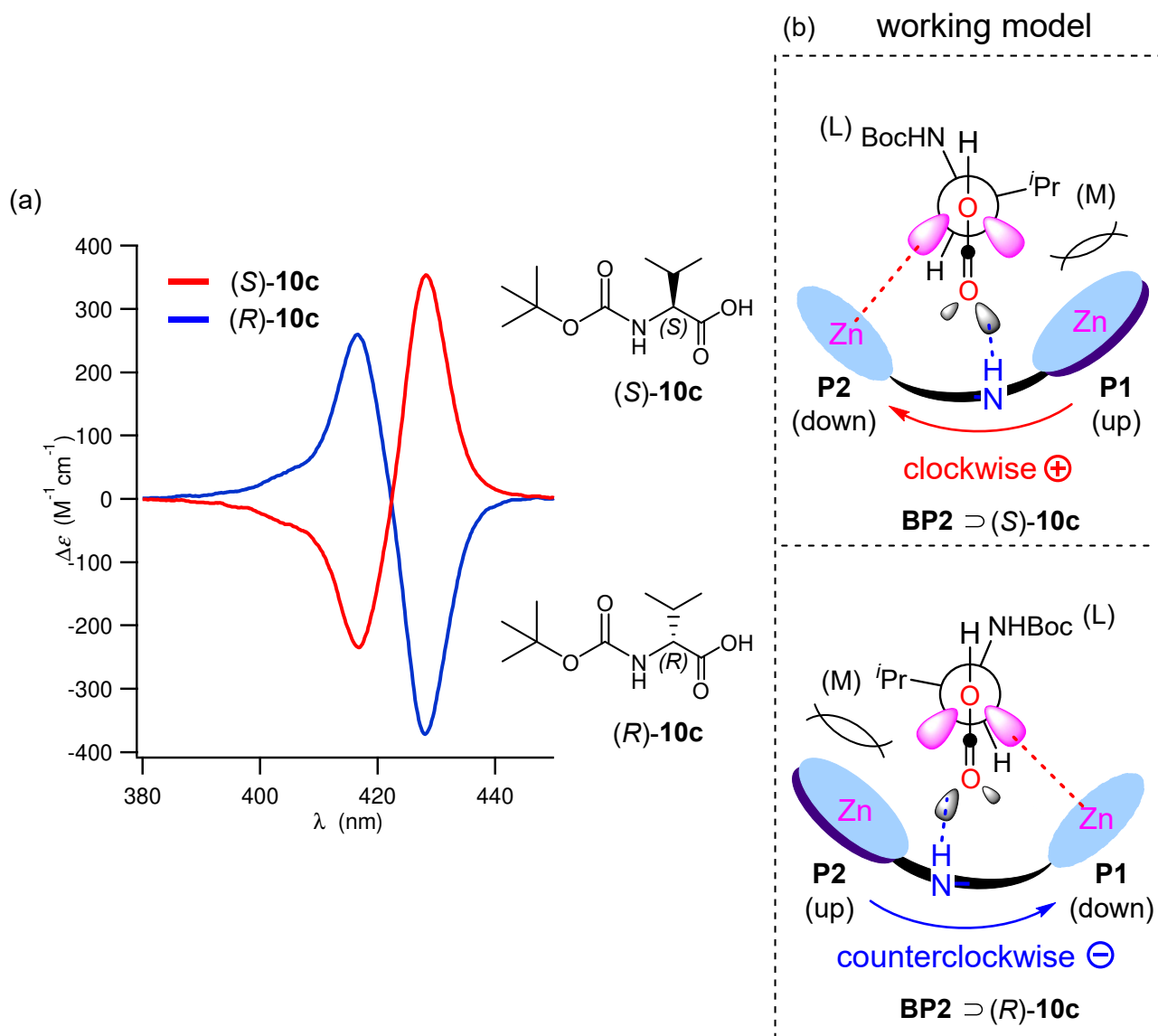


Figure S13. (a) ECCD spectrum of **10c** (2.0×10^{-4} M) in the presence of **BP2** (2.0×10^{-6} M) in 5% $\text{CH}_2\text{Cl}_2/n$ -hexane at 25 °C. (b) The proposed working model for assigning the absolute configuration of the chiral guest **10c** (dashed box). The priority of the substituents was determined by the length of the substituents:³ isopropyl (M), 2.55 Å; BocNH (L), 5.98 Å.

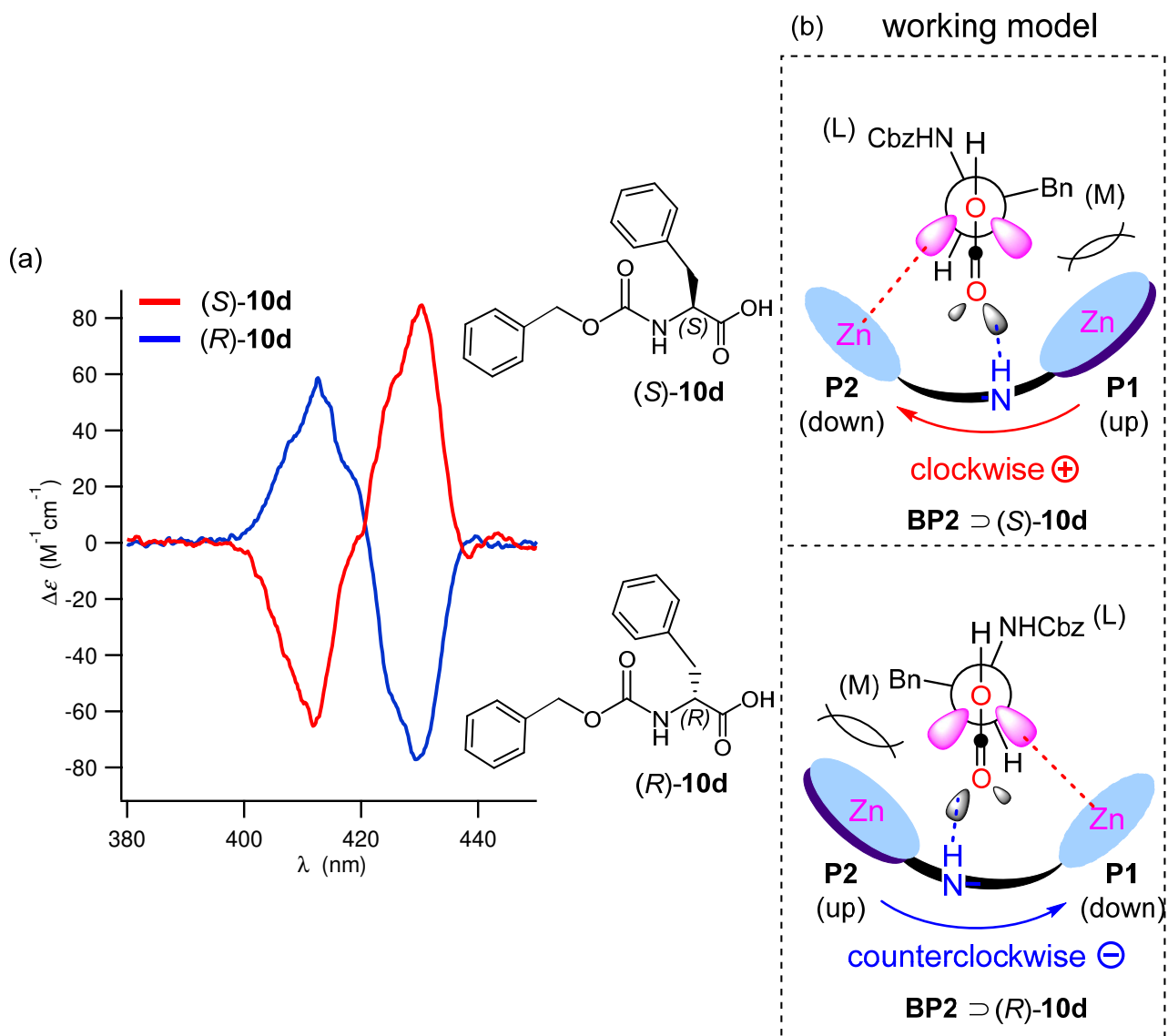


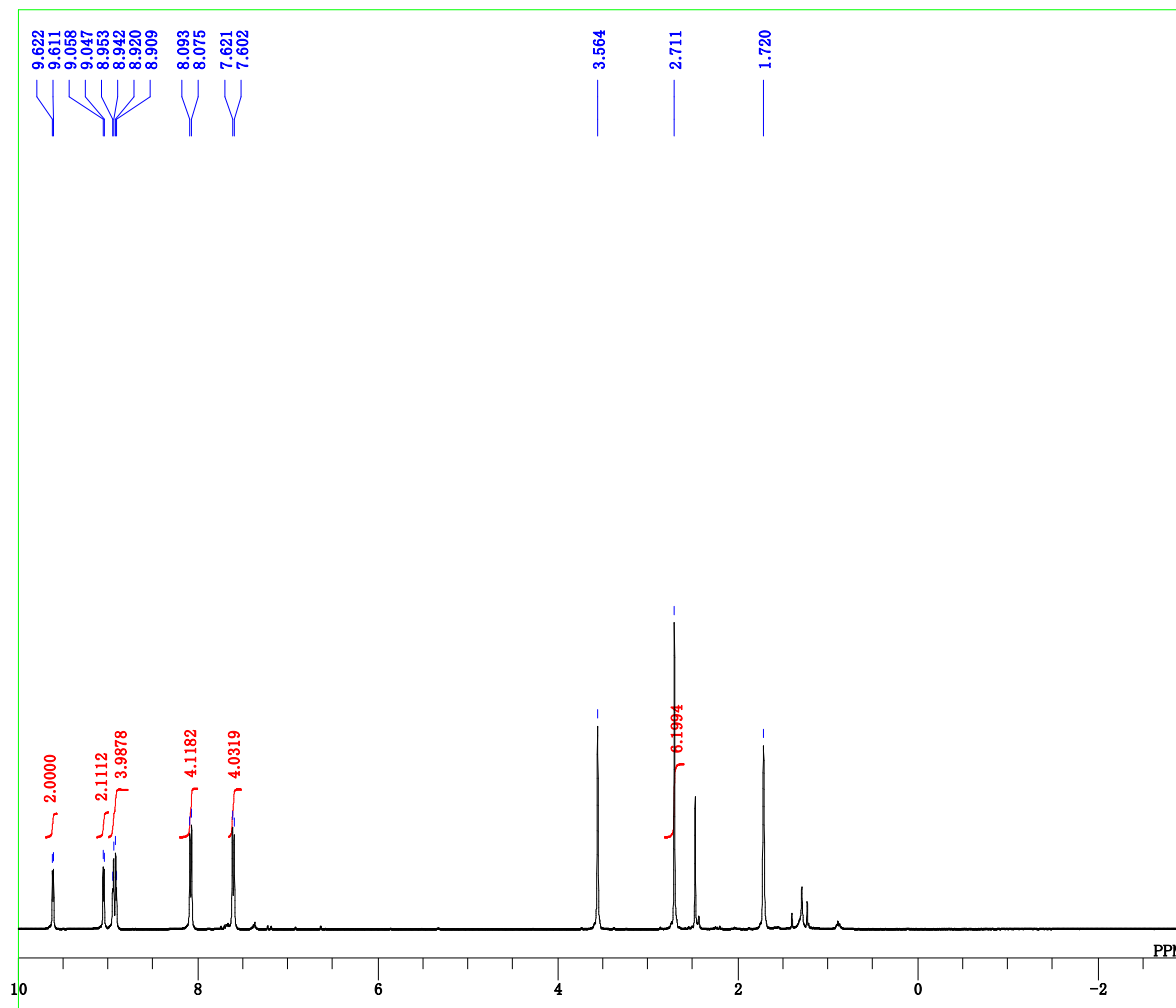
Figure S14. (a) ECCD spectrum of **10d** (2.0×10^{-4} M) in the presence of **BP2** (2.0×10^{-6} M) in 5% $\text{CH}_2\text{Cl}_2/n$ -hexane at 25 °C. (b) The proposed working model for assigning the absolute configuration of the chiral guest **10d** (dashed box). The priority of the substituents was determined by the length of the substituents:³ Bn (M), 4.95 Å; CbzNH (L), 8.44 Å.

8. References

- (1) Y. Shoji, K. Tashiro, and T. Aida, *J. Am. Chem. Soc.*, 2006, **128**, 10690.
- (2) (a) S. Winstein, and N. J. Holness, *J. Am. Chem. Soc.*, 1955, **77**, 5562; (b) E. L. Eliel, S. H. Wilen, and L. N. Mander, *Stereochemistry of Organic Compounds*, Wiley, New York, 1994, pp. 696-697, Table 11.7; (c) S. E. Boiadjev, and D. A. Lightner, *J. Am. Chem. Soc.*, 2000, **122**, 11328.
- (3) H. Gholami, J. Zhang, M. Anyika, and B. Borhan, *Org. Lett.*, 2017, **19**, 1722.

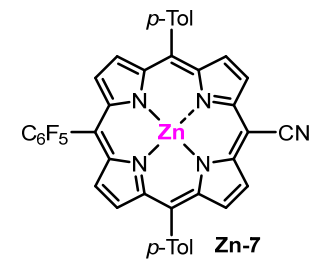
9. NMR Spectra of New Compounds

Zn-7 (¹H)

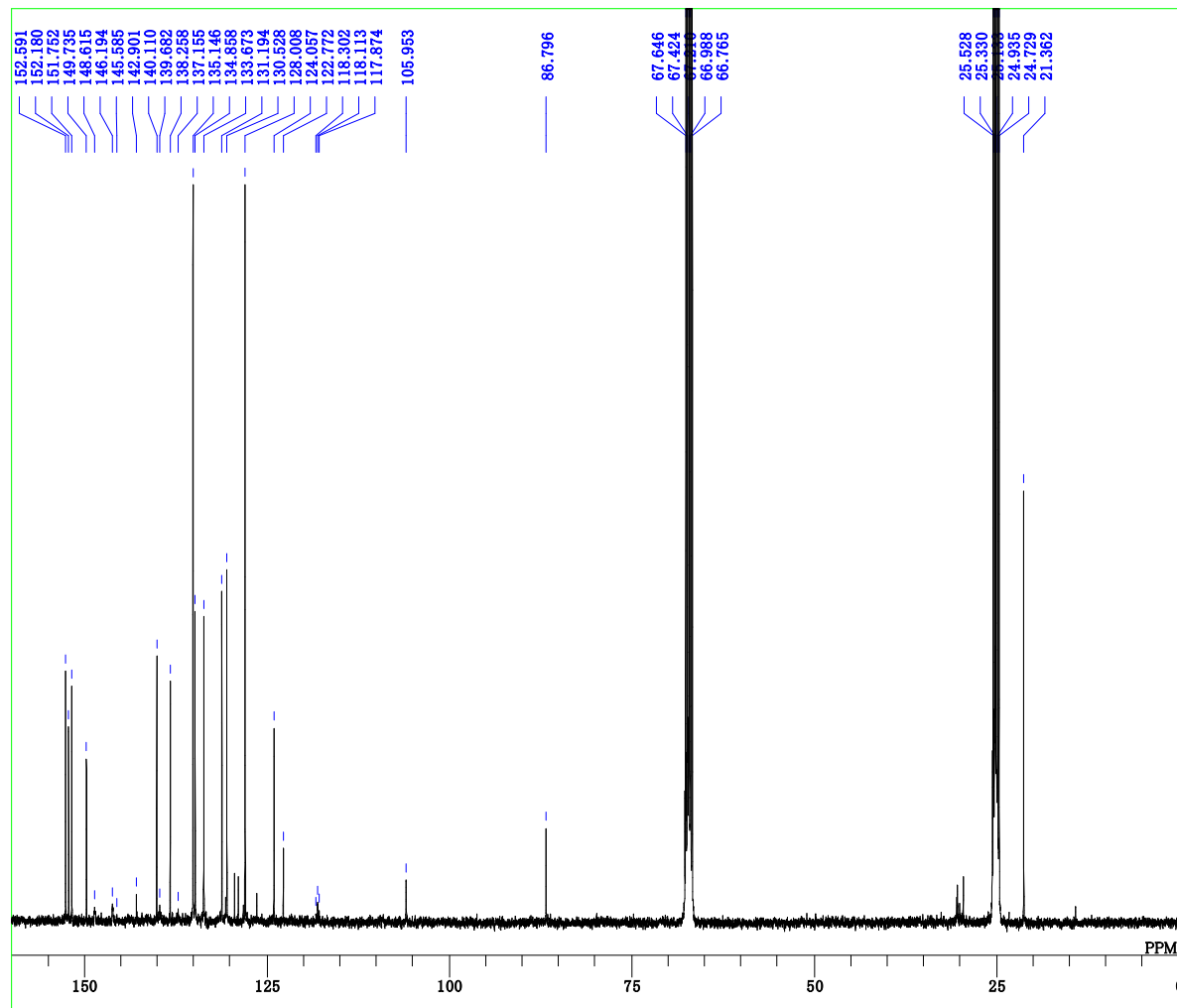


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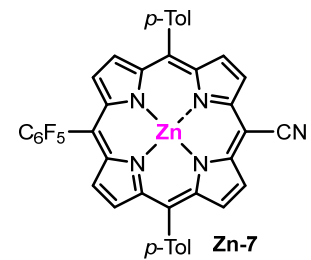
DFILE dSTpTol2C6F5(Zn)CN-B-2-1H解析.als
COMNT dSTpTol2C6F5(Zn)CN-B-2
DATIM Wed Nov 25 08:55:30 2020
1H
OBNUC
EXMOD NON
OBFREQ 399.65 MHz
OBSETE 124.00 KHz
OBFIN 10500.00 Hz
POINT 16384
FREQU 7992.01 Hz
SCANS 8
ACQTM 2.0500 sec
PD 4.9500 sec
PW1 6.20 usec
IRNUC
CTEMP 21.1 c
SLVNT C4D8O
EXREF 1.72 ppm
BF 1.20 Hz
RGAIN 17
    
```



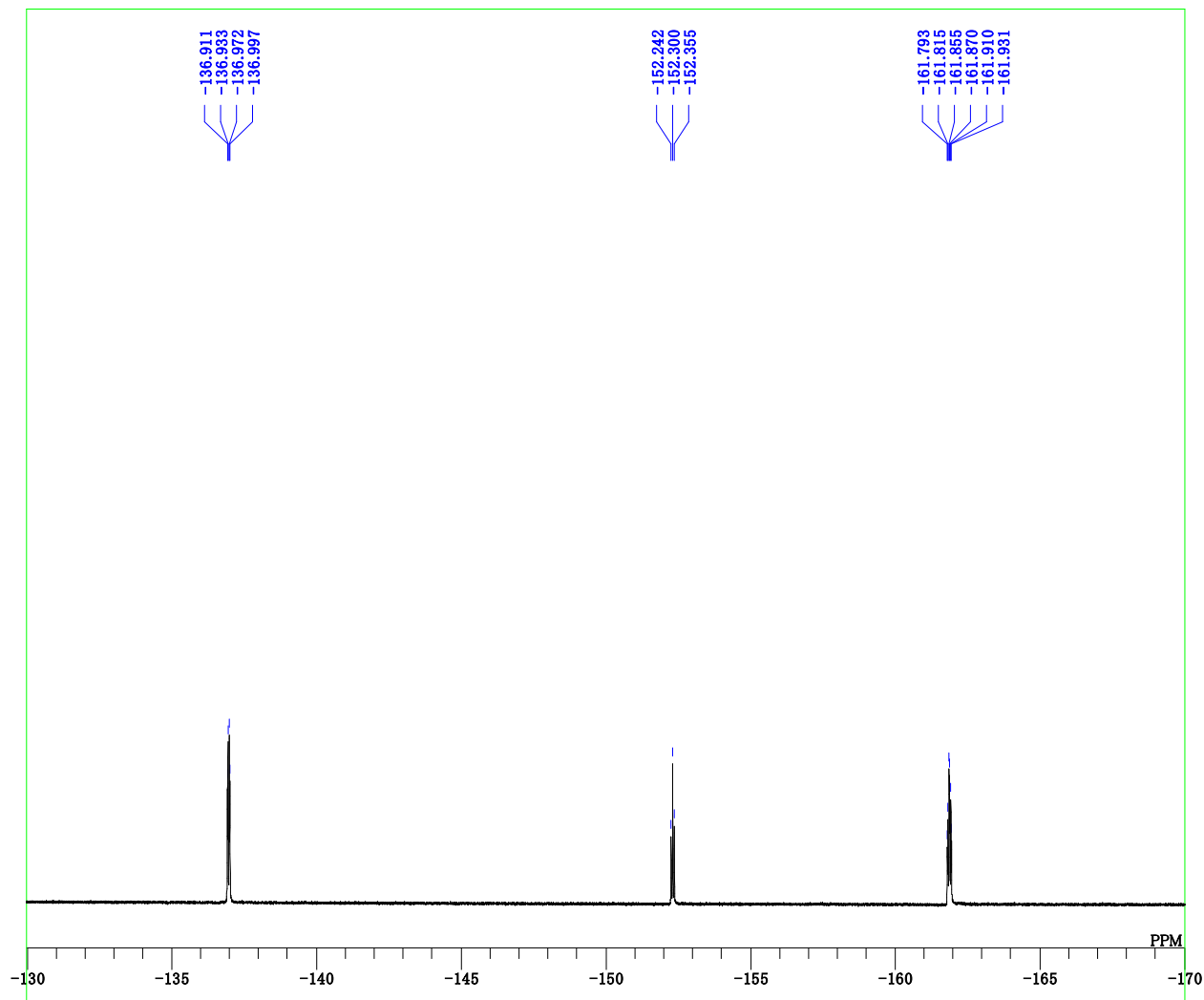
Zn-7 (¹³C)



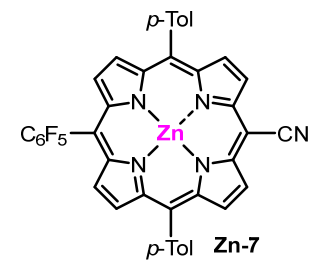
DFILE dStpTol2C6F5(Zn)CN-B-13C解析後.als
 COMNT dStpTol2C6F5(Zn)CN-B-13C
 DATIM Wed Nov 25 00:49:38 2020
 OBNUC 13C
 EXMOD BCM
 OBFRQ 100.40 MHz
 OBSET 125.00 KHz
 OBFIN 10500.00 Hz
 POINT 32768
 FREQU 27118.64 Hz
 SCANS 7680
 ACQTM 1.2083 sec
 PD 1.7920 sec
 PW1 6.20 usec
 IRNUC 1H
 CTEMP 22.6 c
 SLVNT C4D8O
 EXREF 67.21 ppm
 BF 1.20 Hz
 RGAIN 22



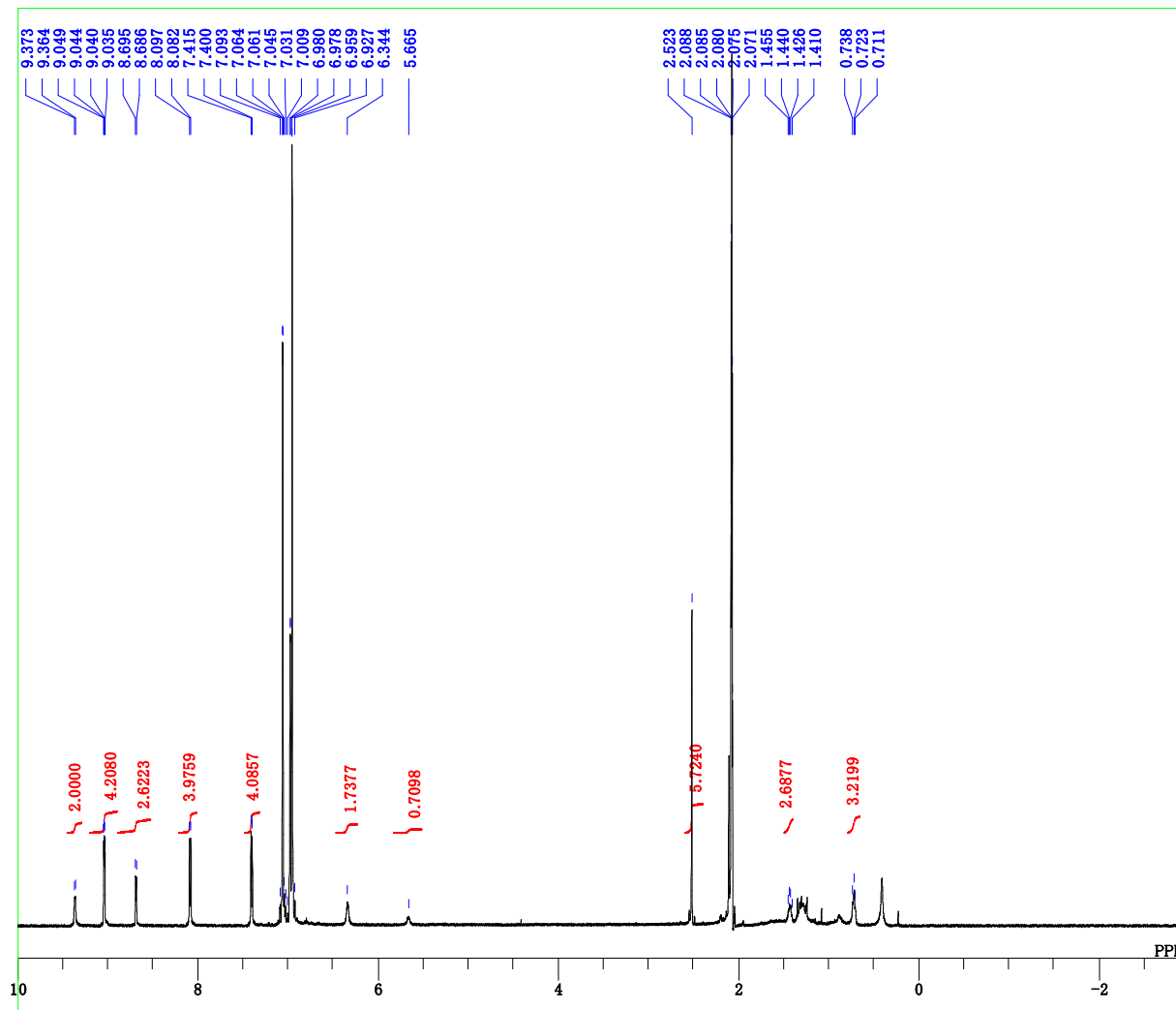
Zn-7 (¹⁹F)



DFILE 20190215pTol2C6F5ZnCN_E19F-1-1編集
COMNT single_pulse
DATIM 2019-02-15 17:37:41
OBNUC 19F
EXMOD single_pulse.jxp
OBFRQ 376.11 MHz
OBSET 4.62 KHz
OBFIN 8.27 Hz
POINT 13107
FREQU 15060.24 Hz
SCANS 16
ACQTM 0.8703 sec
PD 5.0000 sec
PW1 3.76 usec
IRNUC 19F
CTEMP 21.0 c
SLVNT CDCL3
EXREF -152.30 ppm
BF 0.12 Hz
RGAIN 48

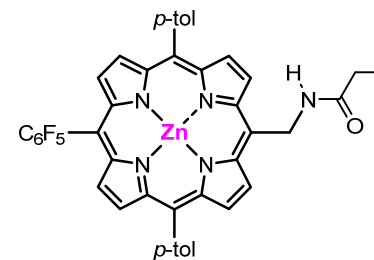


Zn-8 derivative; propionylamide derivative (¹H):

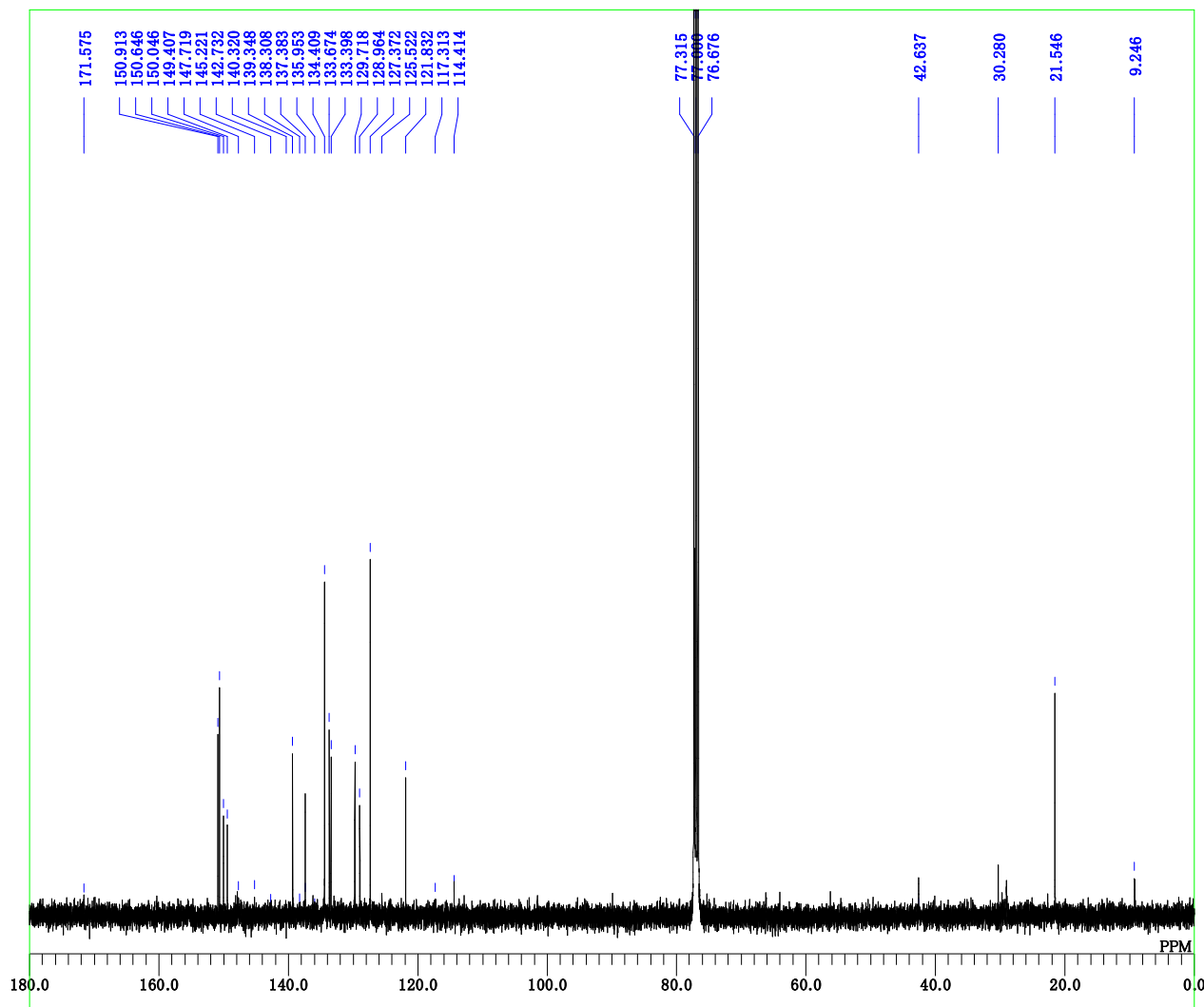


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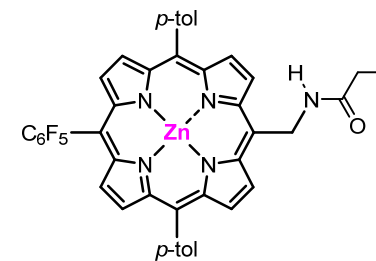
DFILE  武田編集NT-NHCOEt-80C_proton-1-1.al
COMNT  single_pulse
DATIM  2020-02-26 18:30:41
OBNUC  1H
EXMOD  proton.jxp
OBFRQ  500.16 MHz
OBSET  2.41 KHz
OBFIN  6.01 Hz
POINT  26214
FREQU  10000.00 Hz
SCANS  32
ACQTM  2.6214 sec
PD      5.0000 sec
PW1     3.00 usec
IRNUC  1H
CTEMP  80.0 c
SLVNT  C6D5CD3
EXREF  2.08 ppm
BF      0.02 Hz
RGAIN  66
    
```



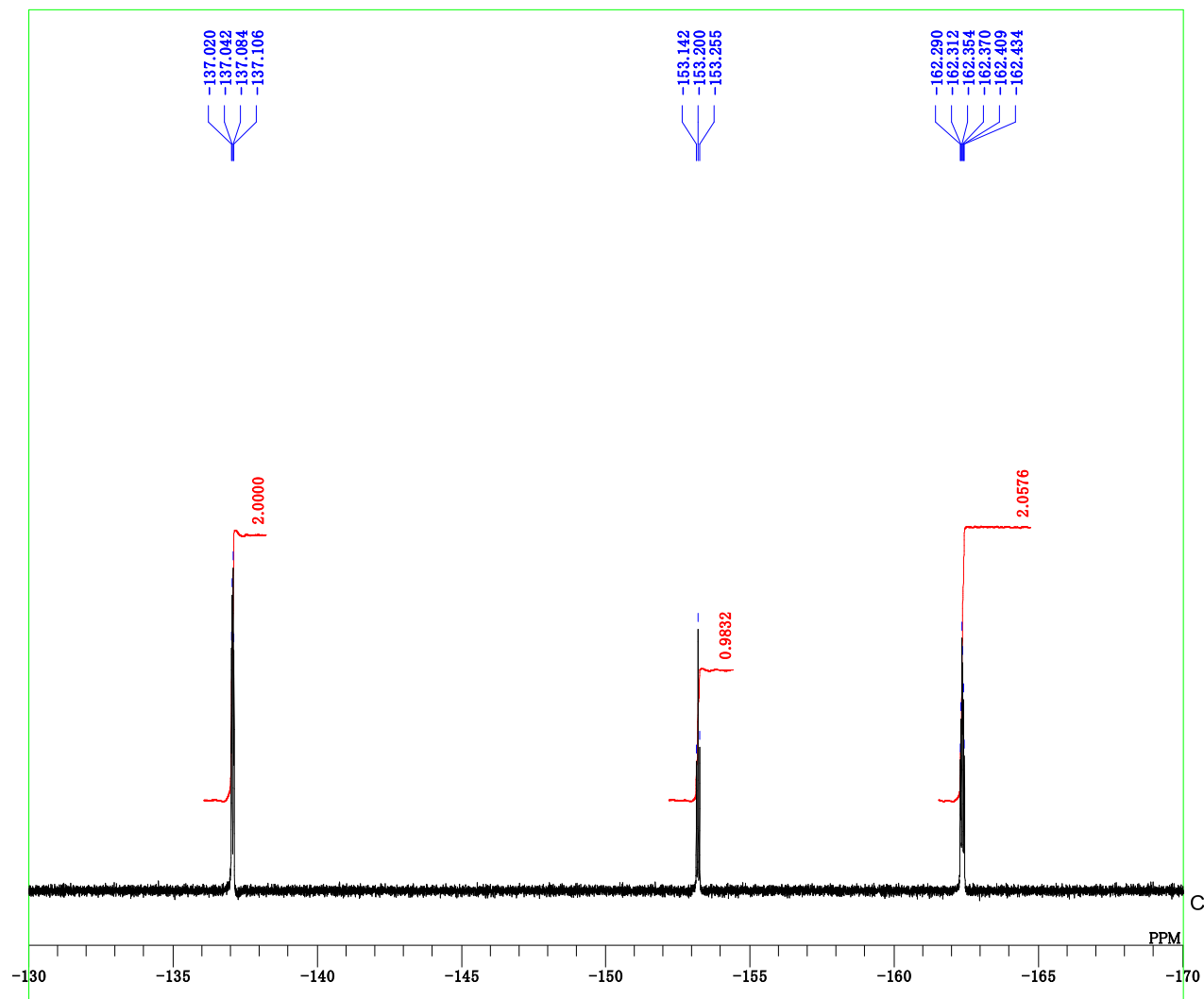
Zn-8 derivative; propionylamide derivative (¹³C)



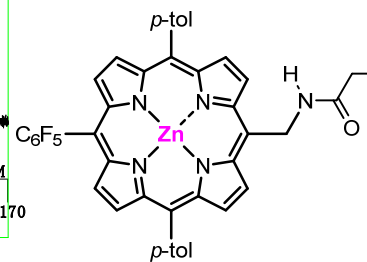
DFILE NT-NHCOEt_E13C-1-1.als 編集後.als
COMNT single pulse decoupled gated NOE
DATIM 2020-02-10 19:52:31
OBNUC 13C
EXMOD single_pulse_dec
OBFRQ 100.53 MHz
OBSET 5.35 KHz
OBFIN 5.86 Hz
POINT 26214
FREQU 25125.63 Hz
SCANS 45000
ACQTM 1.0433 sec
PD 2.0000 sec
PW1 3.60 usec
IRNUC 1H
CTEMP 21.2 c
SLVNT CDCL3
EXREF 77.00 ppm
BF 0.12 Hz
RGAIN 60



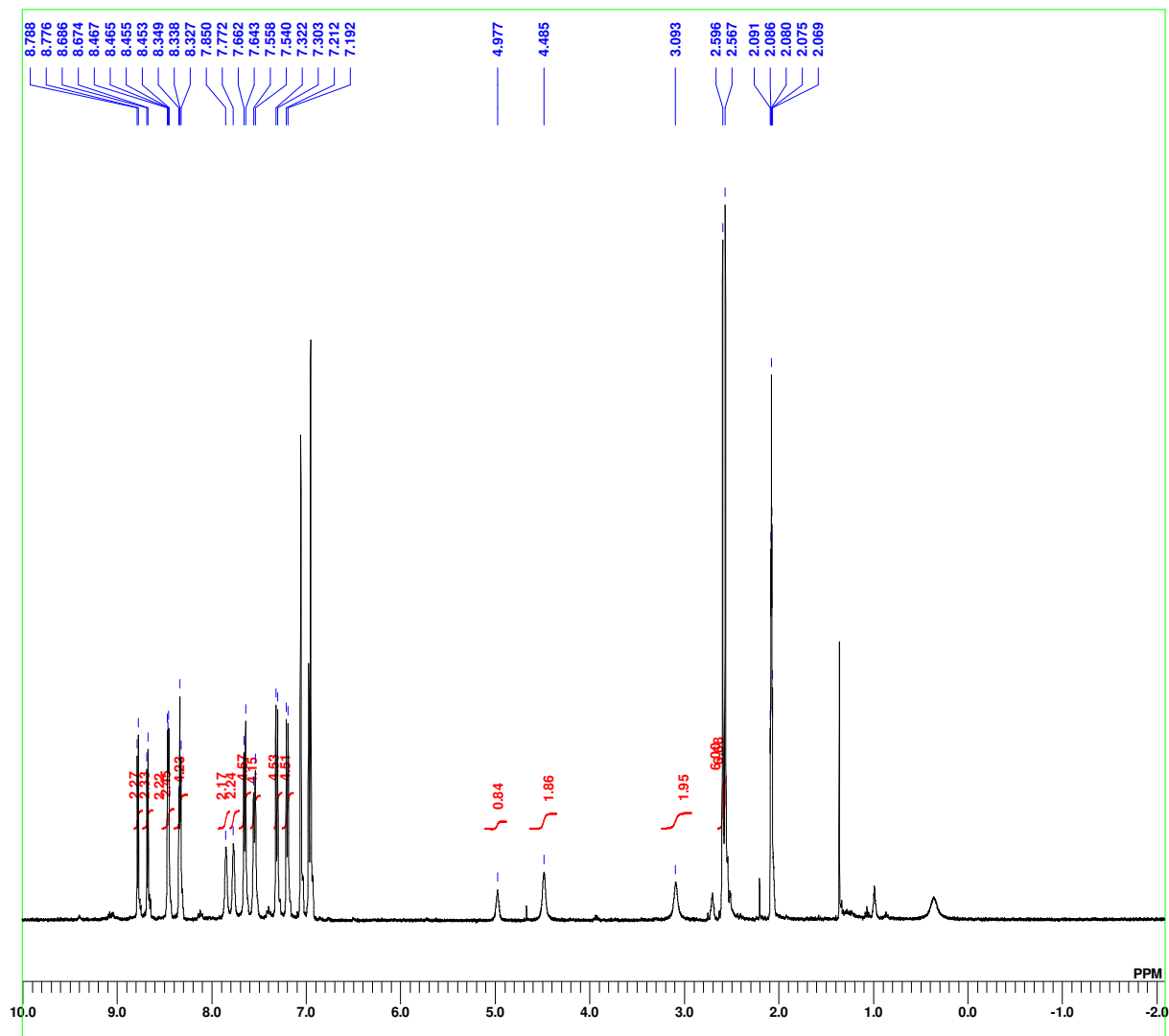
Zn-8 derivative; propionylamide derivative (¹⁹F)



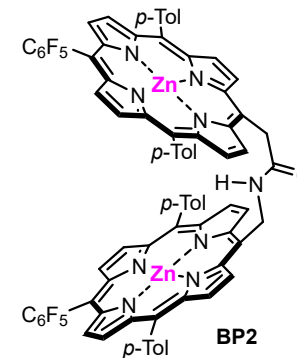
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COMNT single_pulse
DATIM 2020-02-10 19:45:37
OBNUC 19F
EXMOD single_pulse.jxp
OBFRQ 376.11 MHz
OBSET 4.62 KHz
OBFIN 8.27 Hz
POINT 13107
FREQU 15060.24 Hz
SCANS 16
ACQTM 0.8703 sec
PD 5.0000 sec
PW1 3.76 usec
IRNUC 19F
CTEMP 21.2 c
SLVNT CDCL3
EXREF -153.20 ppm
BF 0.12 Hz
RGAIN 48



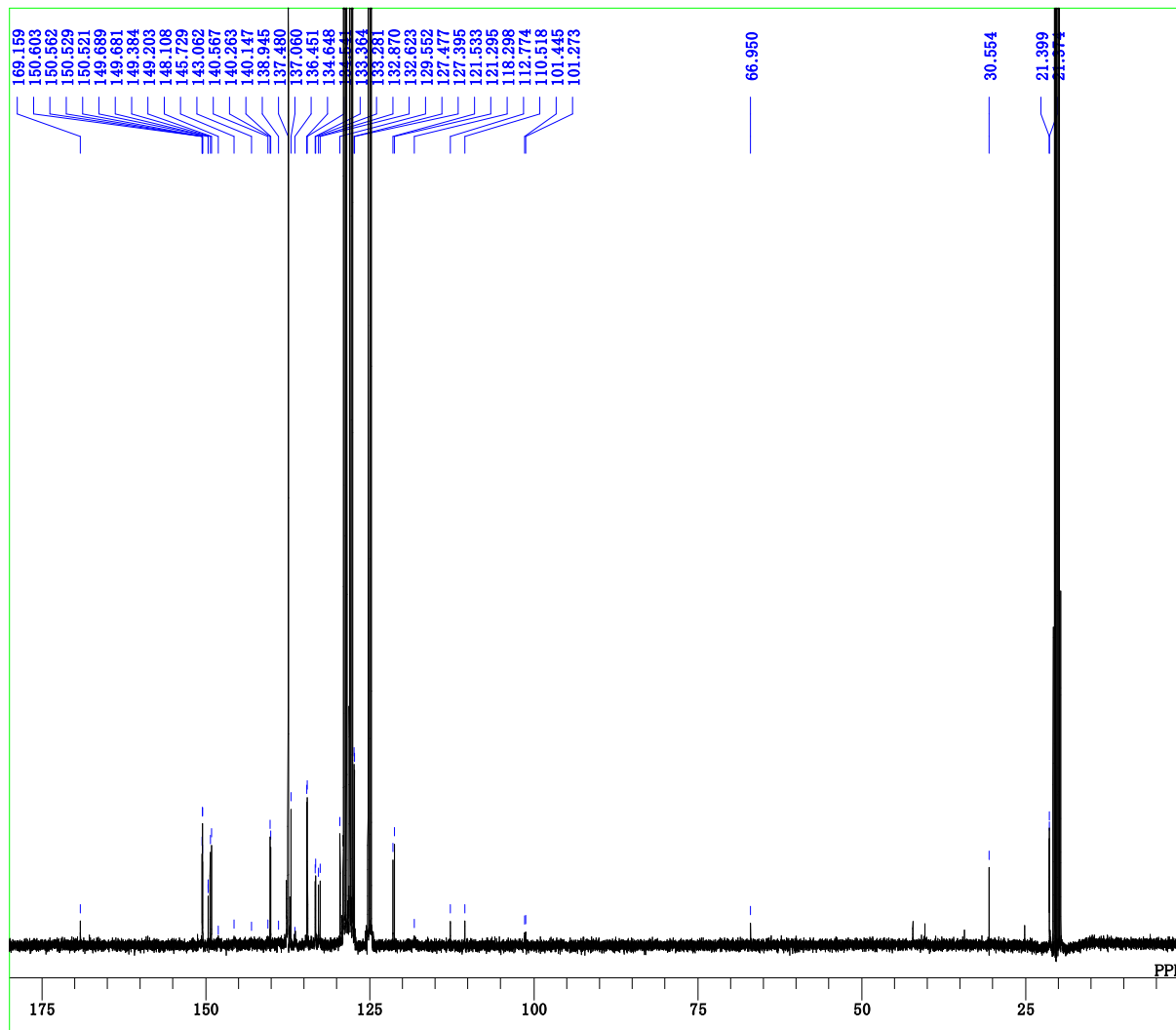
BP2 (¹H)



DFILE BP1Amide tol-d8 80C 1H.als%δ(CeSI-p.als
 COMNT BP1Amide tol-d8 80C 1H
 DATIM Sat Apr 20 18:52:55 2019
 OBNUC 1H
 EXMOD NON
 OBFRQ 399.65 MHz
 OBSSET 124.00 KHz
 OBFIN 10500.00 Hz
 POINT 16384
 FREQU 7992.01 Hz
 SCANS 16
 ACQTM 2.0500 sec
 PD 4.9500 sec
 PW1 5.80 usec
 IRNUC 1H
 CTEMP 80.2 c
 SLVNT C6D6
 EXREF 2.08 ppm
 BF 0.09 Hz
 RGAIN 21

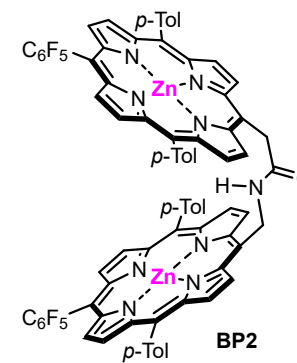


BP2 (¹³C)

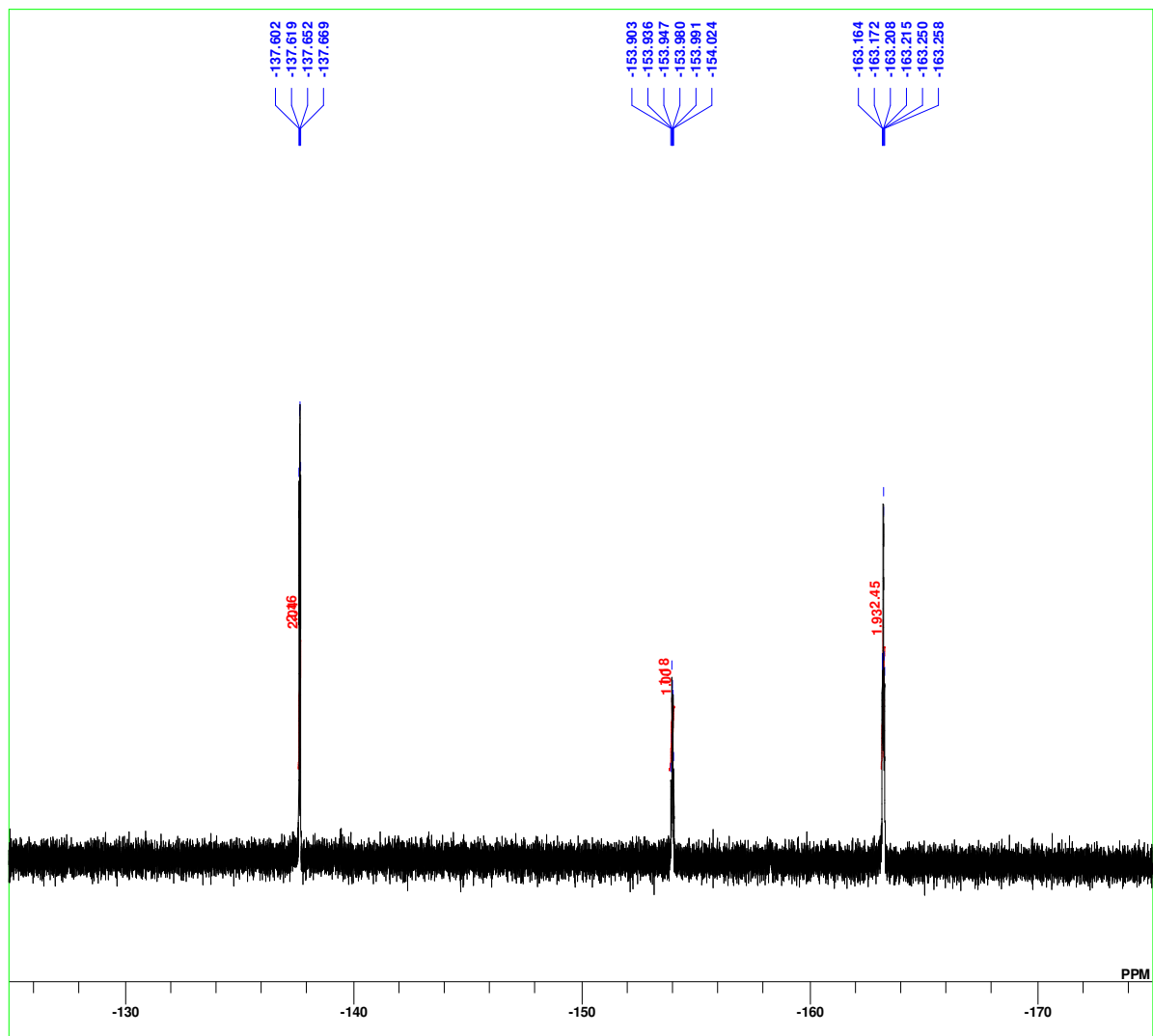


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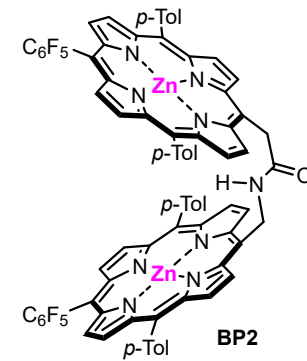
DFILE      BP1Amide tol-d8 80C 13C 編集後 .als
COMNT      BP1Amide tol-d8 80C 13C
DATIM      Mon Apr 22 10:41:33 2019
OBNUC      13C
EXMOD      BCM
OBFREQ     100.40 MHz
OBSET      125.00 KHz
OBFIN      10500.00 Hz
POINT      32768
FREQU      27118.64 Hz
SCANS      47488
ACQTM      1.2083 sec
PD         1.7920 sec
PW1        5.80 usec
IRNUC      1H
CTEMP      80.3 c
SLVNT      C6D6
EXREF      137.48 ppm
BF         1.20 Hz
RGAIN      23
    
```



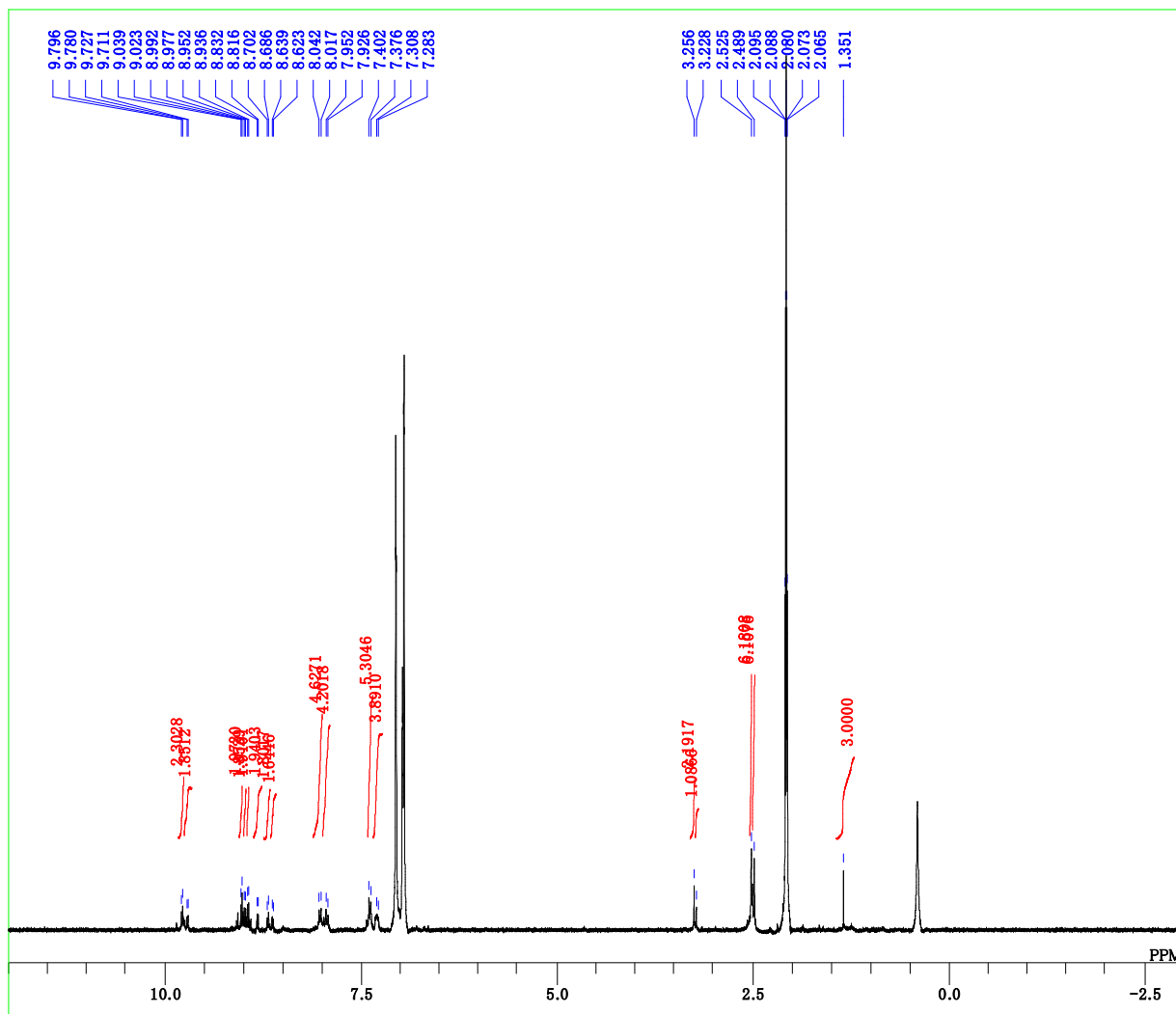
BP2 (¹⁹F)



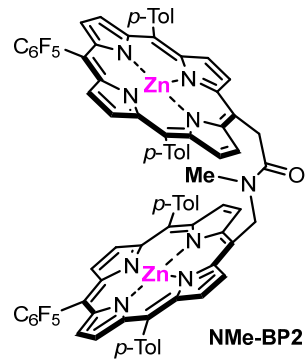
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 COMNT 19F told8 40C-2
 DATIM 2021-02-10 15:40:58
 OBNUC 19F
 EXMOD proton.jxp
 OBFREQ 470.54 MHz
 OBSSET 9.86 KHz
 OBFIN 7.77 Hz
 POINT 26214
 FREQU 23584.91 Hz
 SCANS 128
 ACQTM 1.1115 sec
 PD 5.0000 sec
 PW1 3.73 usec
 IRNUC 19F
 CTEMP 80.0 c
 SLVNT C6D5CD3
 EXREF -137.60 ppm
 BF -0.61 Hz
 RGAIN 50



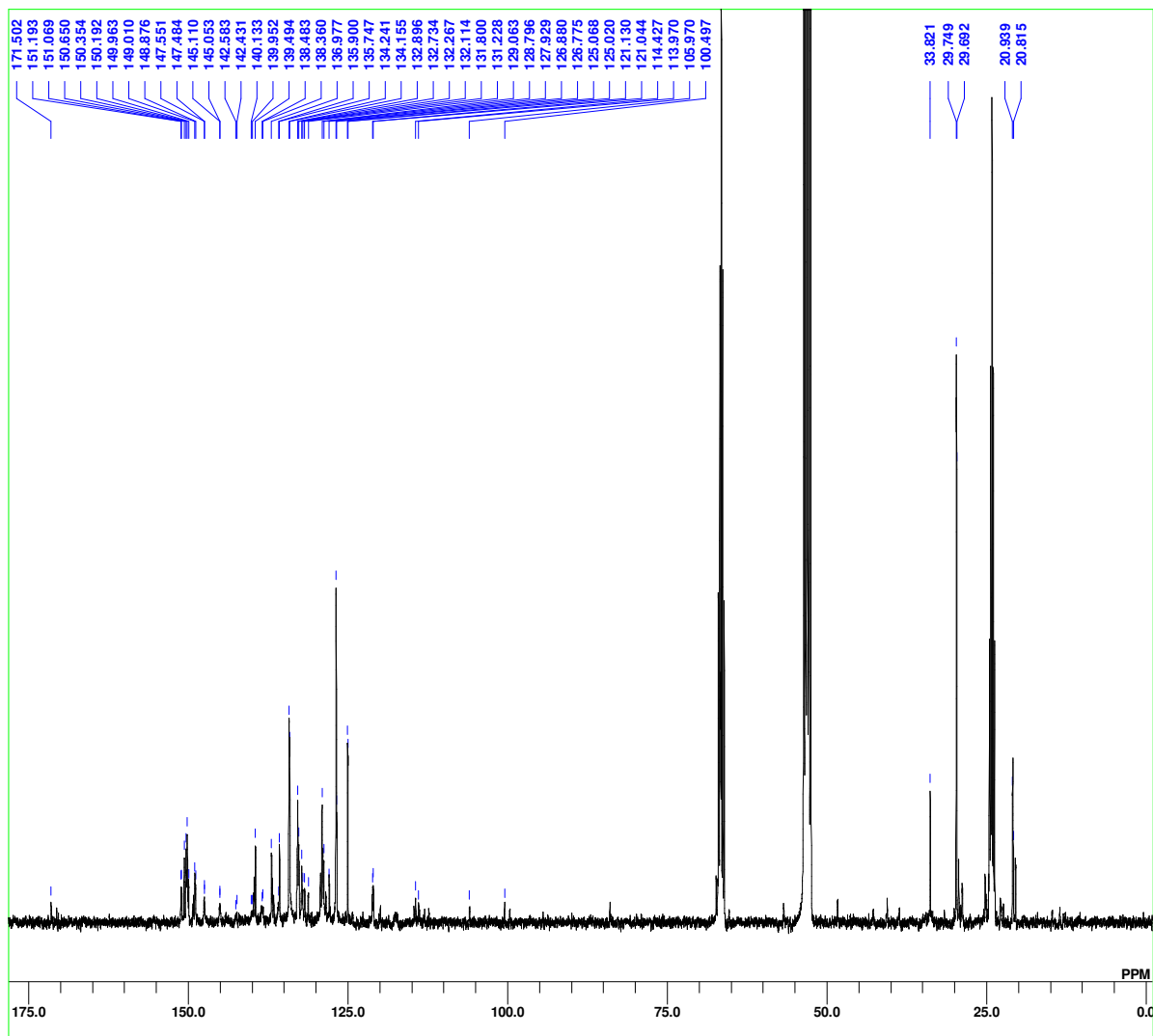
NMe-BP2 (¹H)



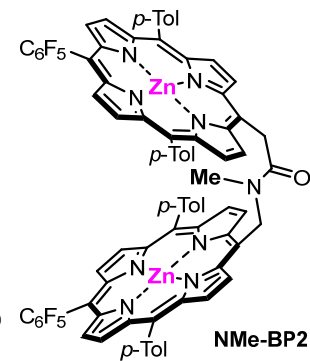
DFILE 武田編集NT6-56 N-MeAmide toluened8.a
 COMNT NT6-56 toluene-d8
 DATIM Tue Sep 24 10:41:21 2019
 OBNUC 1H
 EXMOD NON
 OBFREQ 300.40 MHz
 OBSET 130.00 KHz
 OBFIN 1150.00 Hz
 POINT 32768
 FREQU 6006.01 Hz
 SCANS 16
 ACQTM 5.4559 sec
 PD 1.5440 sec
 PW1 5.20 usec
 IRNUC 1H
 CTEMP 80.4 c
 SLVNT C6D5CD3
 EXREF 2.08 ppm
 BF 0.09 Hz
 RGAIN 21



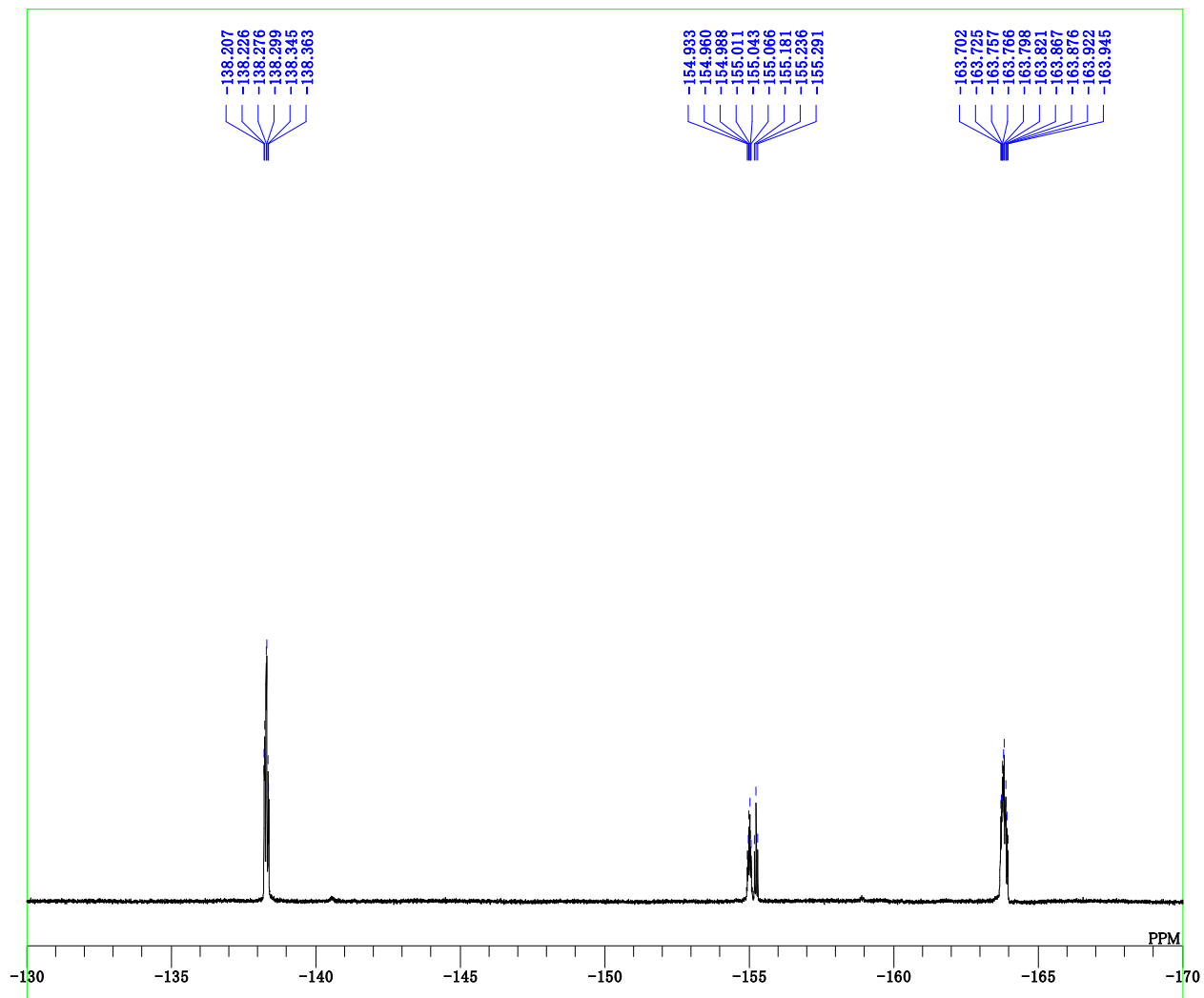
NMe-BP2 (¹³C)



DFILE NT-NMe_E13C-1-1%of.t.als
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 DATIM 2020-01-17 17:27:57
 OBNUC ¹³C
 EXMOD single_pulse_dec
 OBFRQ 100.53 MHz
 OBSET 5.35 KHz
 OBFIN 5.86 Hz
 POINT 26214
 FREQU 25125.63 Hz
 SCANS 76000
 ACQTM 1.0433 sec
 PD 2.0000 sec
 PW1 3.60 usec
 IRNUC ¹H
 CTEMP 22.0 c
 SLVNT CD2CL2
 EXREF 53.10 ppm
 BF 1.62 Hz
 RGAIN 60



NMe-BP2 (¹⁹F)



```

DFILE NT-NMe_E19F-3-2編集後.als
COMNT single_pulse
DATIM 2020-01-20 09:58:39
OBNUC 19F
EXMOD single_pulse.jxp
OBFRQ 376.11 MHz
OBSET 4.62 KHz
OBFIN 8.27 Hz
POINT 16384
FREQU 28280.54 Hz
SCANS 16
ACQTM 0.5793 sec
PD 5.0000 sec
PW1 3.76 usec
IRNUC 19F
CTEMP 23.0 c
SLVNT CD2CL2
EXREF -119.93 ppm
BF 0.12 Hz
RGAIN 44
    
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