Electronic Supporting Information

Axial, Helical, and Planar Chirality in Directly Linked Basket-Handle Porphyrin Arrays

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Contents:

1. ALIE surfaces of a Zn-BHP with different meso-substituents and different metalation

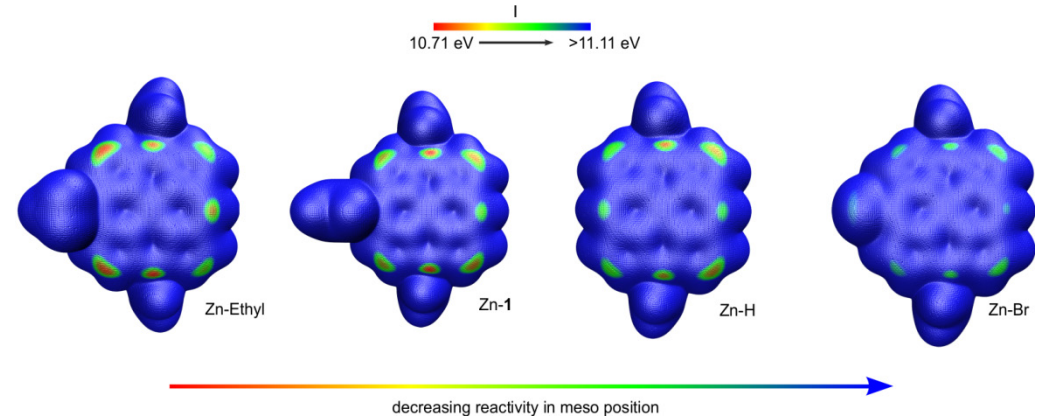


Figure S1. ALIE surfaces of **1** with Zn as central metal and different substituents in *meso* position. Instead of relative *I* values absolute ones were used for the color of the surfaces allowing a comparison of the reactivities in the free meso position. The nucleophilicity clearly decreases from ethyl to phenyl or hydrogen and with bromine the reactivity in the free *meso* position nearly vanishes.

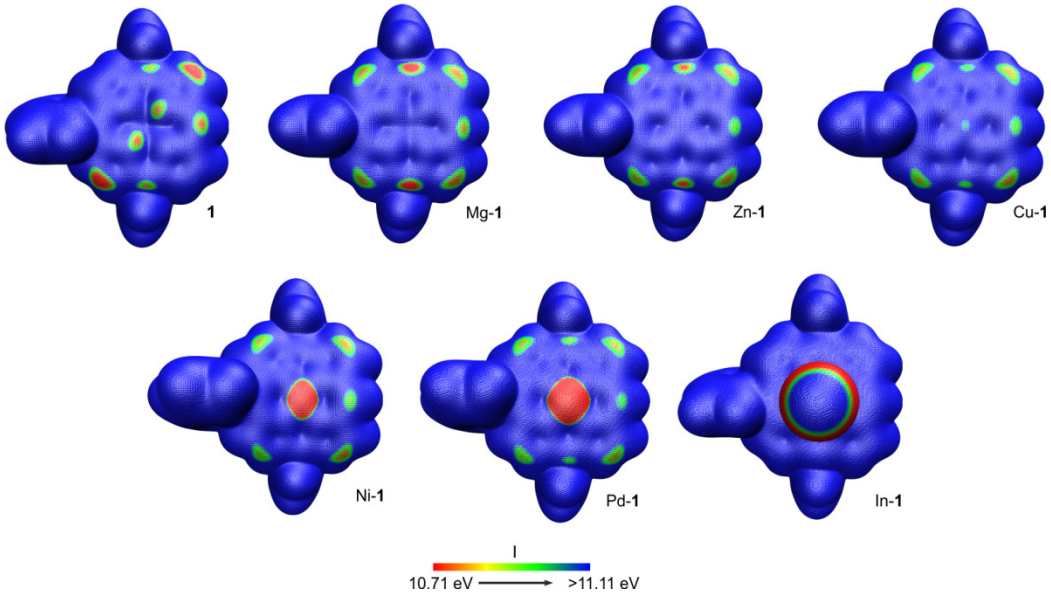


Figure S2. ALIE surfaces of **1** with different central atoms and constant *I* values were used for the color of the surfaces allowing a comparison of the reactivities in the free *meso* position. The nucleophilicity significantly depends on the central metals and with In(III) inside no reactivity is observable in the *meso* position.

2. Comparison of exptl and calcd ECD and UV spectra on **Ni-2a** and **Ni-3**

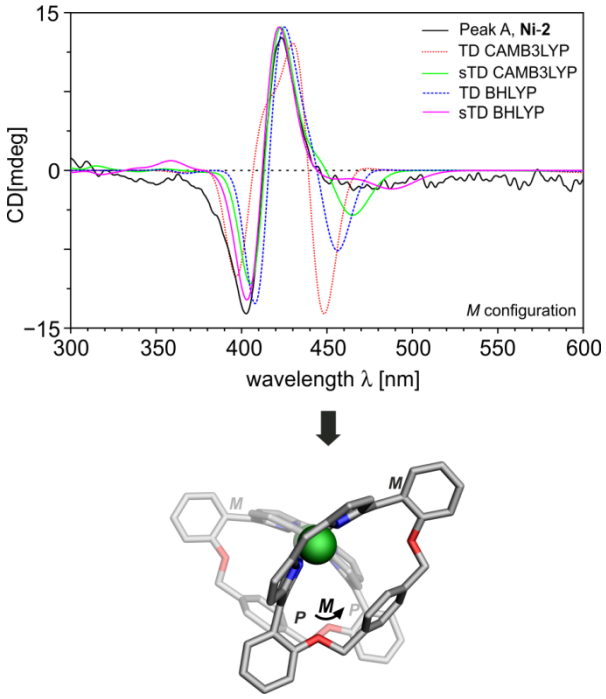


Figure S3. Comparison of experimental and calculated ECD spectra of **Ni-2a** (arbitrarily only results for the *M* configuration at the central axis are shown). All methods determined the same absolute configuration for Peak A, Δ_{ESI} values vary from 67% for TD CAMB3LYP to 97% for sTD BHLYP (sTD CAMB3LYP: 92%; TD BHLYP: 77%).

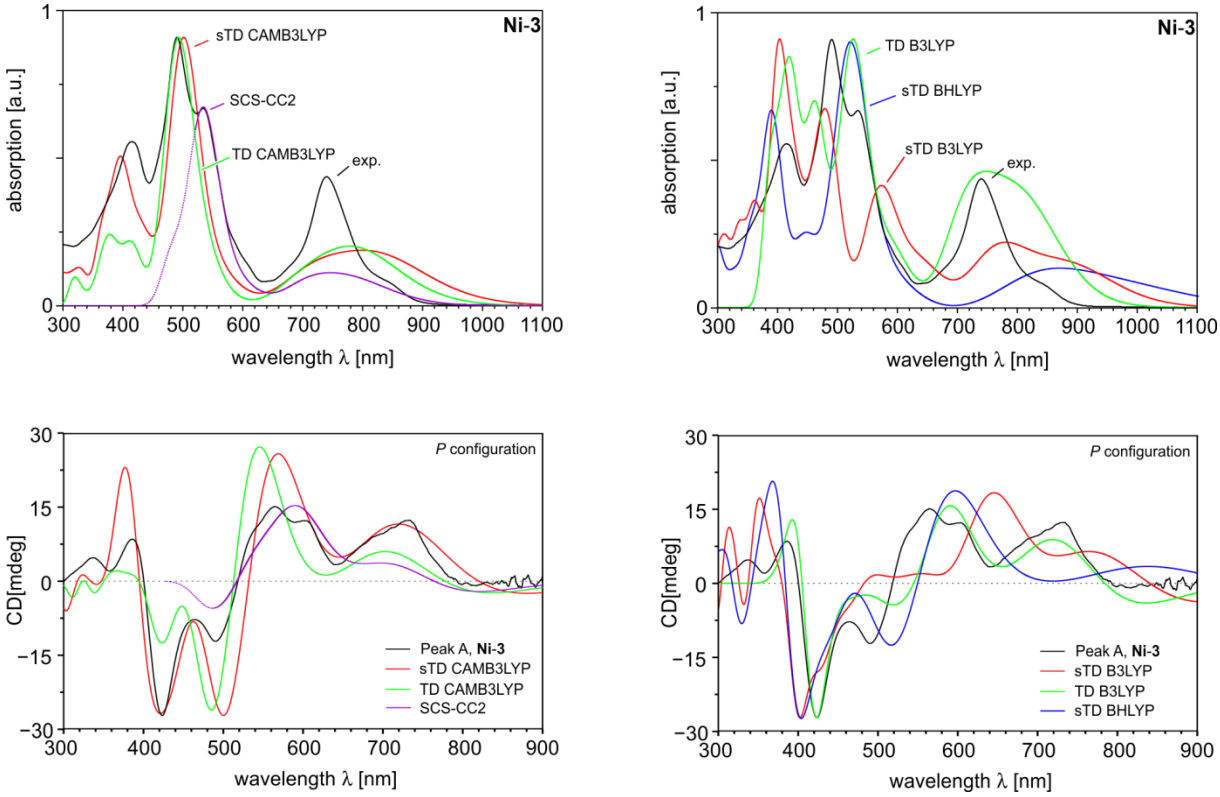


Figure S4. Comparison of experimental and calculated UV and ECD spectra of **Ni-3** (arbitrarily only results for the *P* configuration are shown). All methods determined the same absolute configuration, however, the comparison of the UV spectra reveals that B3LYP is unsuited to predict the excited states of **Ni-3**. Δ_{ESI} values: TD CAMB3LYP, 76%; sTD CAMB3LYP, 90%; sTD BHLYP, 58%; TD B3LYP, 87%; sTD B3LYP, 57%.

3. VT NMR investigations of **7a**

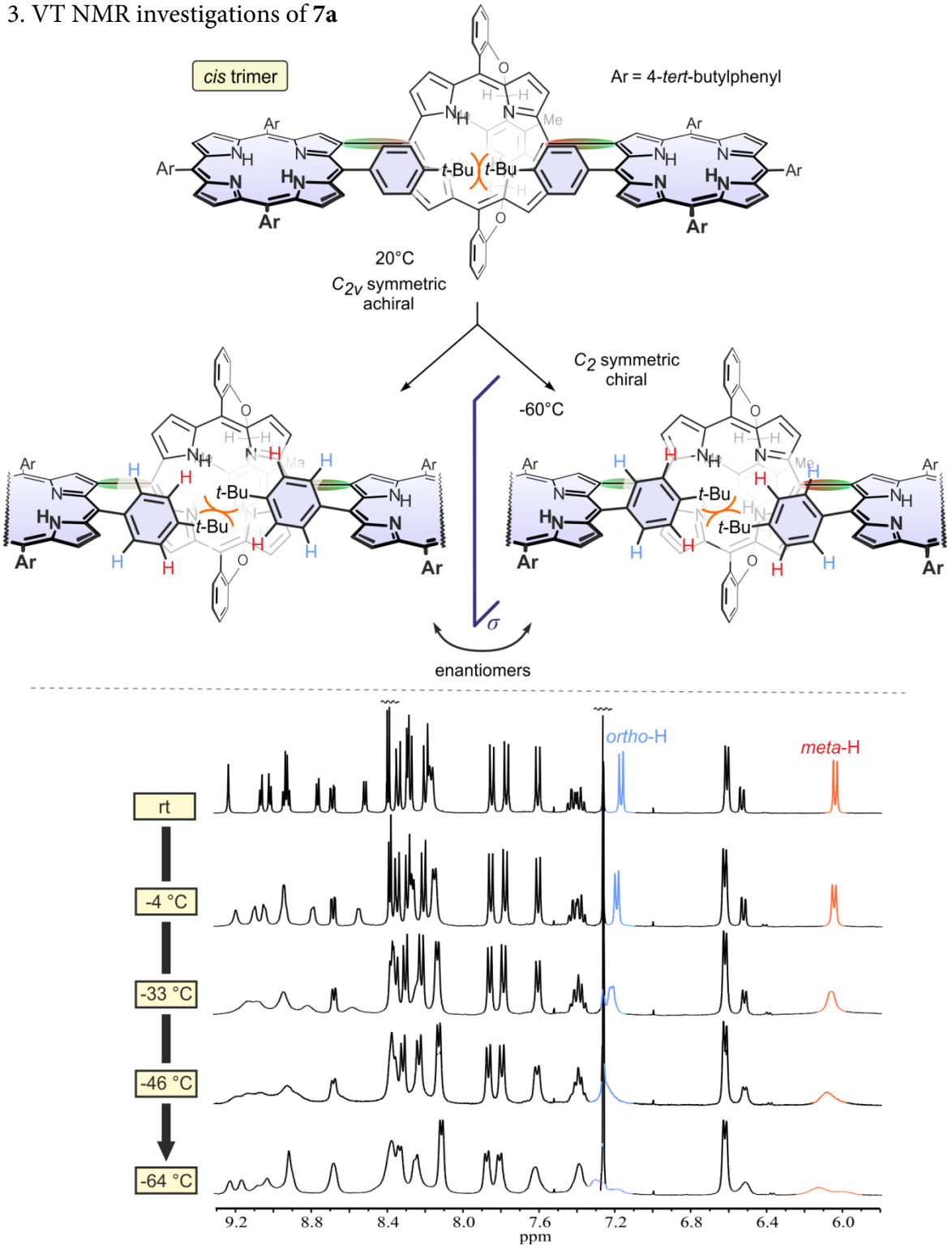


Figure S5. VT NMR of trimer **7a**. The signal splitting caused by the transition from an achiral to a chiral conformation begins at -30°C and is fully present at -60°C. Compared to previous examples, the t-Bu groups do not increase the stability of these conformations.

4. Conformations and comparison of exptl and calcd ECD and UV spectra of *M*-**6b**

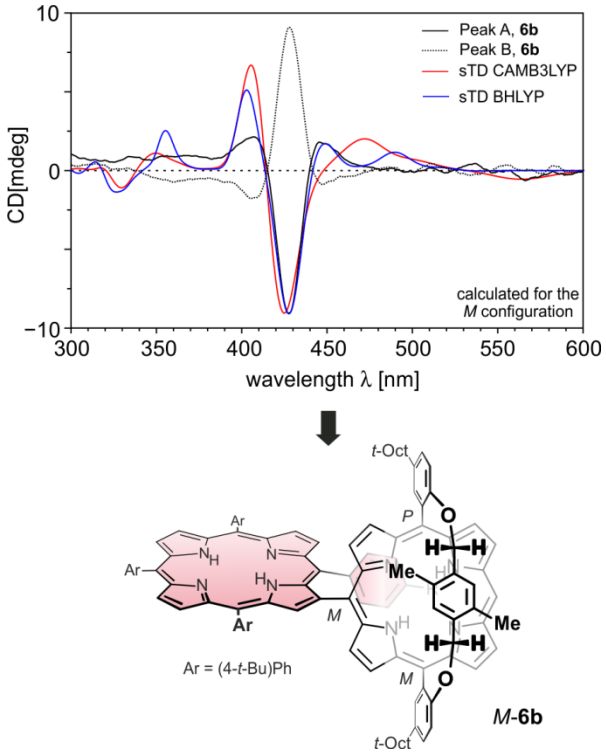


Figure S6. Comparison of experimental and calculated ECD spectra of **6b** (arbitrarily only the calculated results for the *M* configuration at the central axis are shown). Both methods determined the same absolute configuration for Peak A (sTD CAMB3LYP: Δ_{ESI} = 80%; TD BHLYP: Δ_{ESI} = 86%).

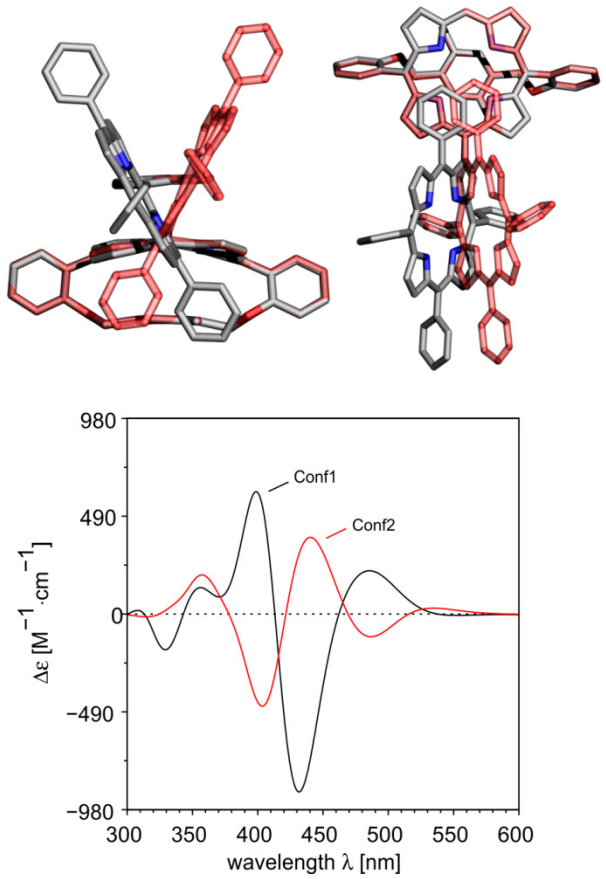


Figure S7. Side and above view of the overlay plots of the two possible conformations of *P*-**6b** (Conf2 is shown in translucent red, top). Conf1 is the slightly preferred conformation and has in addition a higher ECD intensity than Conf2 (sTD BHLYP results, bottom) and is thus clearly dominating the ECD spectrum.

5. Comparison of exptl and calcd ECD and UV spectra on **7b** and **8**

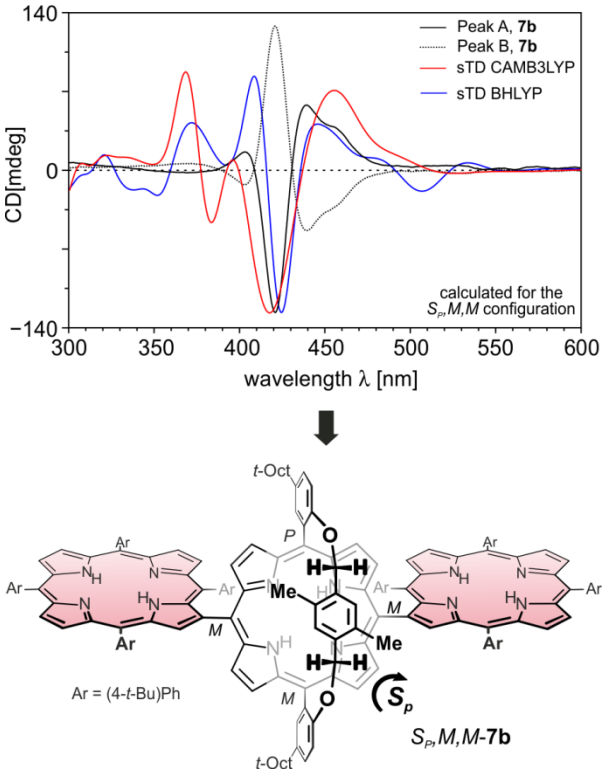


Figure S8. Comparison of experimental and calculated ECD spectra of **7b** (arbitrarily only the calculated results for the S_P,*M*,*M* configuration are shown, determination of the descriptors of the inner axes is possible only due to the arrested tautomerism of free-base BHPs). Both methods used determined the same absolute configuration for Peak A (sTD CAMB3LYP: Δ_{ESI} = 68%; sTD BHLYP: Δ_{ESI} = 56%).

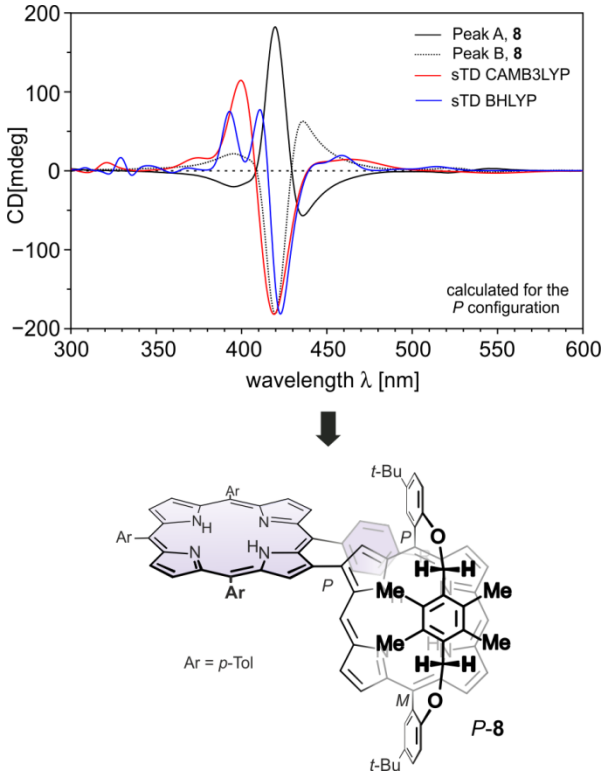


Figure S9. Determination of the absolute configuration of **8** by comparison of experimental and calculated ECD spectra (arbitrarily only the calculated results for the *P* configuration at the central axis are shown). Both TD methods determined the same absolute configuration for Peak A (sTD CAMB3LYP: Δ_{ESI} = 68%; sTD BHLYP: Δ_{ESI} = 53%).

6. Elucidation of the absolute configuration of **11**

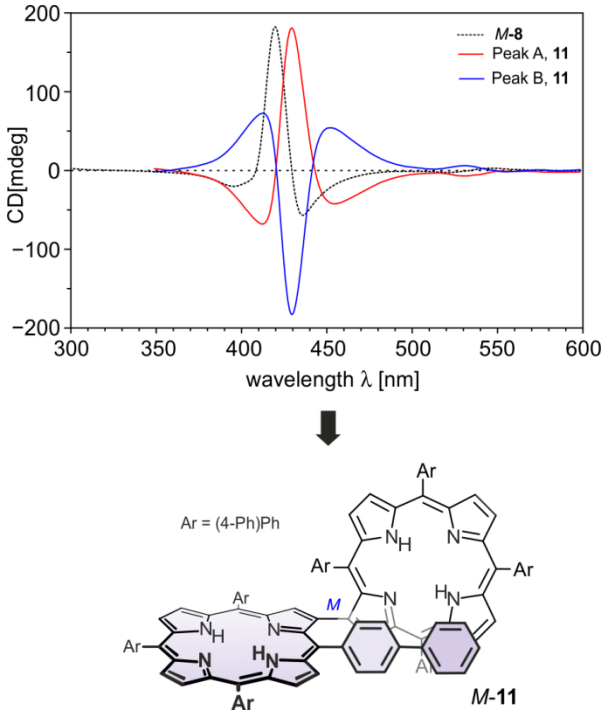


Figure S10. Determination of the absolute configuration of **11** by comparison of experimental ECD spectra of *M*-**8** with that measured for the enantiomers of **11**. The curve measured for the more rapid eluting enantiomer matches with that of *M*-**8** (although a clear red shift is observable), thus this enantiomer is *M*-configured while the slower eluting one is *P*-configured.

7. Comformations and absolute stereostucture of **14a**

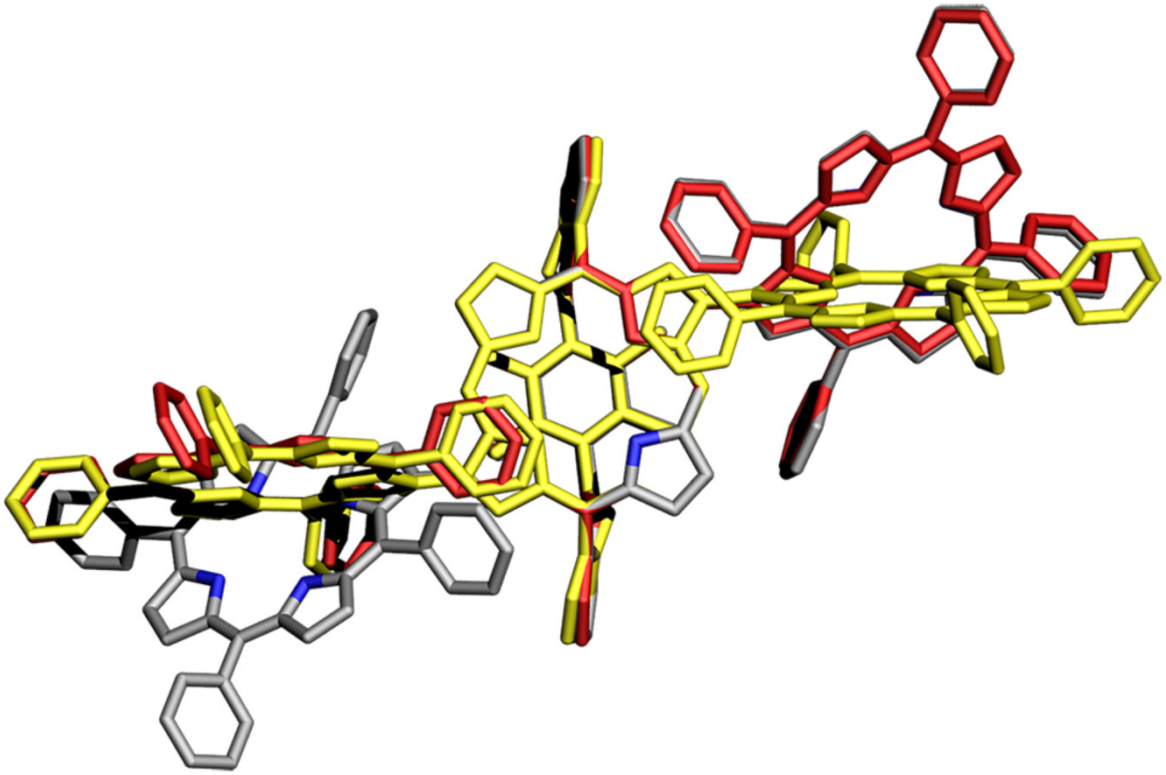


Figure S11. Overlay plot of the three conformations of *M*,*M*-**14a** (hydrogens and *t*-Bu groups omitted for clarity), the main conformer (>90% populated) and conformer 2 (yellow) are C_2 symmetric while conformer 3 (red) has C_1 symmetry.

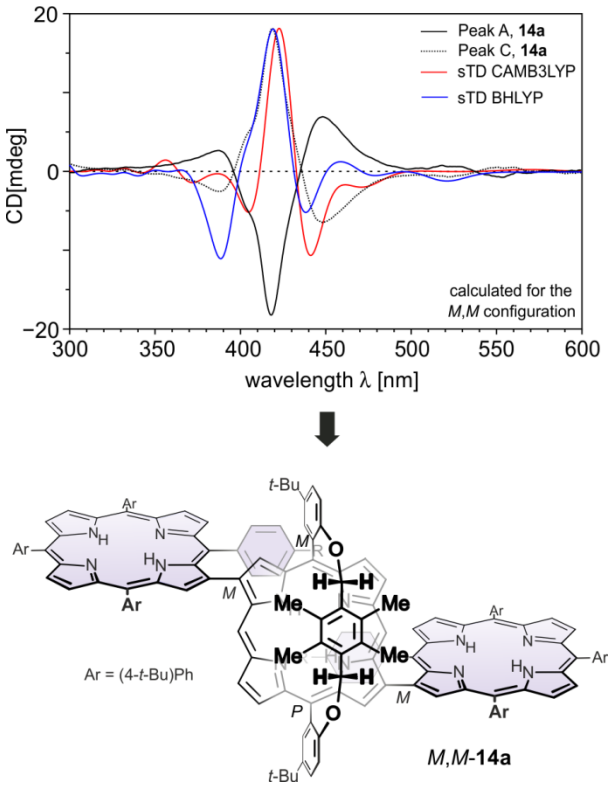
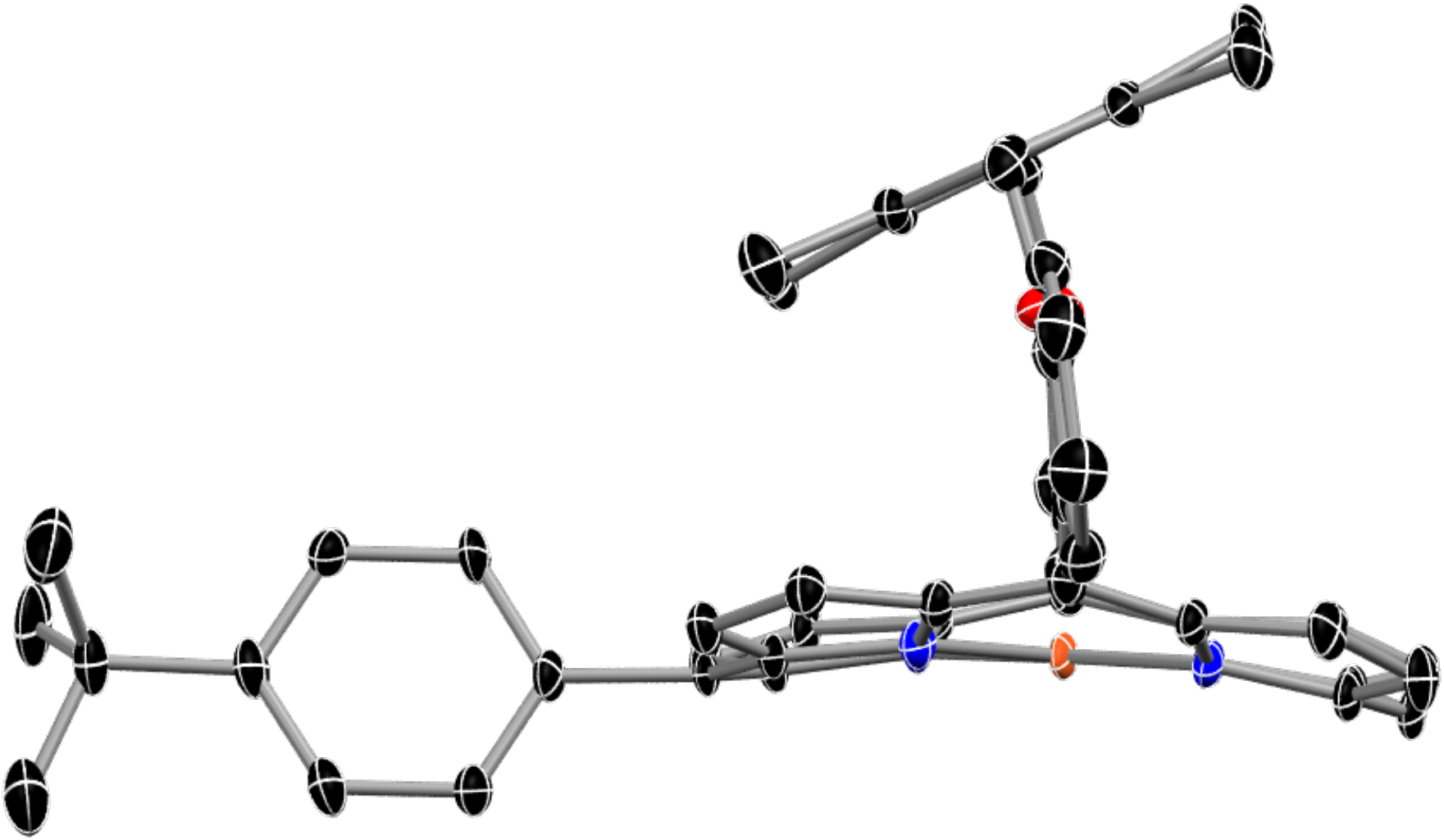


Figure S12. Determination of the absolute configuration of **14a** by comparison of experimental and calculated ECD spectra (arbitrarily only the calculated results for the *M*,*M* configuration at the outer axes are shown). Both TD methods determined the same absolute configuration for Peak A (sTD CAMB3LYP: Δ_{ESI} = 64%; sTD BHLYP: Δ_{ESI} = 76%).

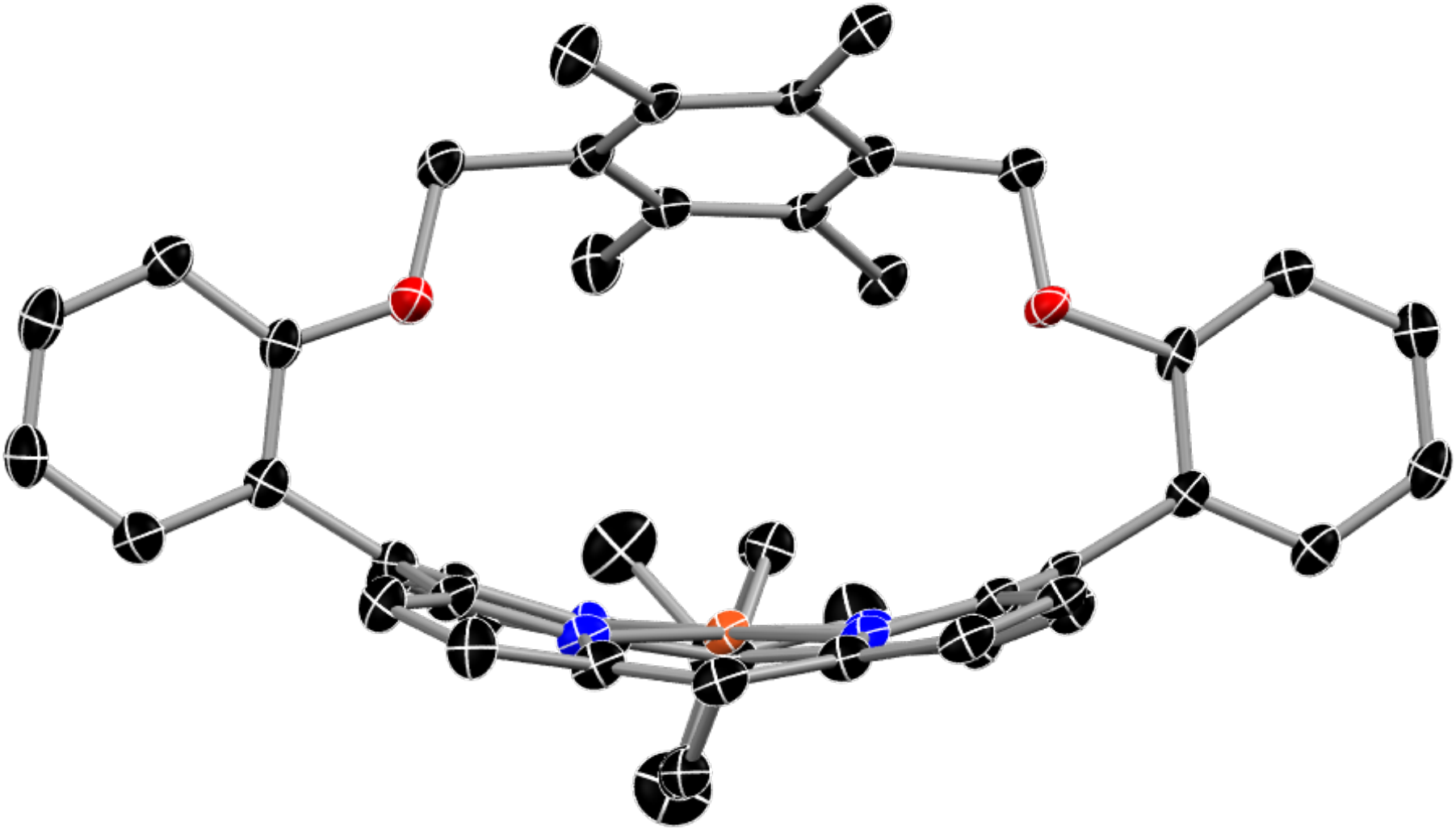
8. X-Ray crystallographic details and ORTEP plot of **Cu-1c**

Crystal data collection and processing parameters are given below. Crystals were immersed in a film of perfluoropolyether oil on a glass fiber and transferred to a Bruker X8 Apex-2 diffractometer with CCD area detector and mirror-monochromated Mo-Kα radiation equipped with an Cryosystems low-temperature device. Data were collected at 100 K. The images were processed with the Bruker software packages and equivalent reflections were merged. Corrections for Lorentz-polarization effects and absorption were performed if necessary and the structure were solved by direct methods. Subsequent difference Fourier syntheses revealed the positions of all other non-hydrogen atoms, and hydrogen atoms were included in calculated positions and refined using a riding model. Extinction corrections were applied as required. Crystallographic calculations were performed using the SHELXTL software package. All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were assigned to idealized positions and were included in structure factors calculations. Crystallographic data (excluding structure factors) for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC 1437573. Copies of the data can be obtained free of charge on application to CCDC.

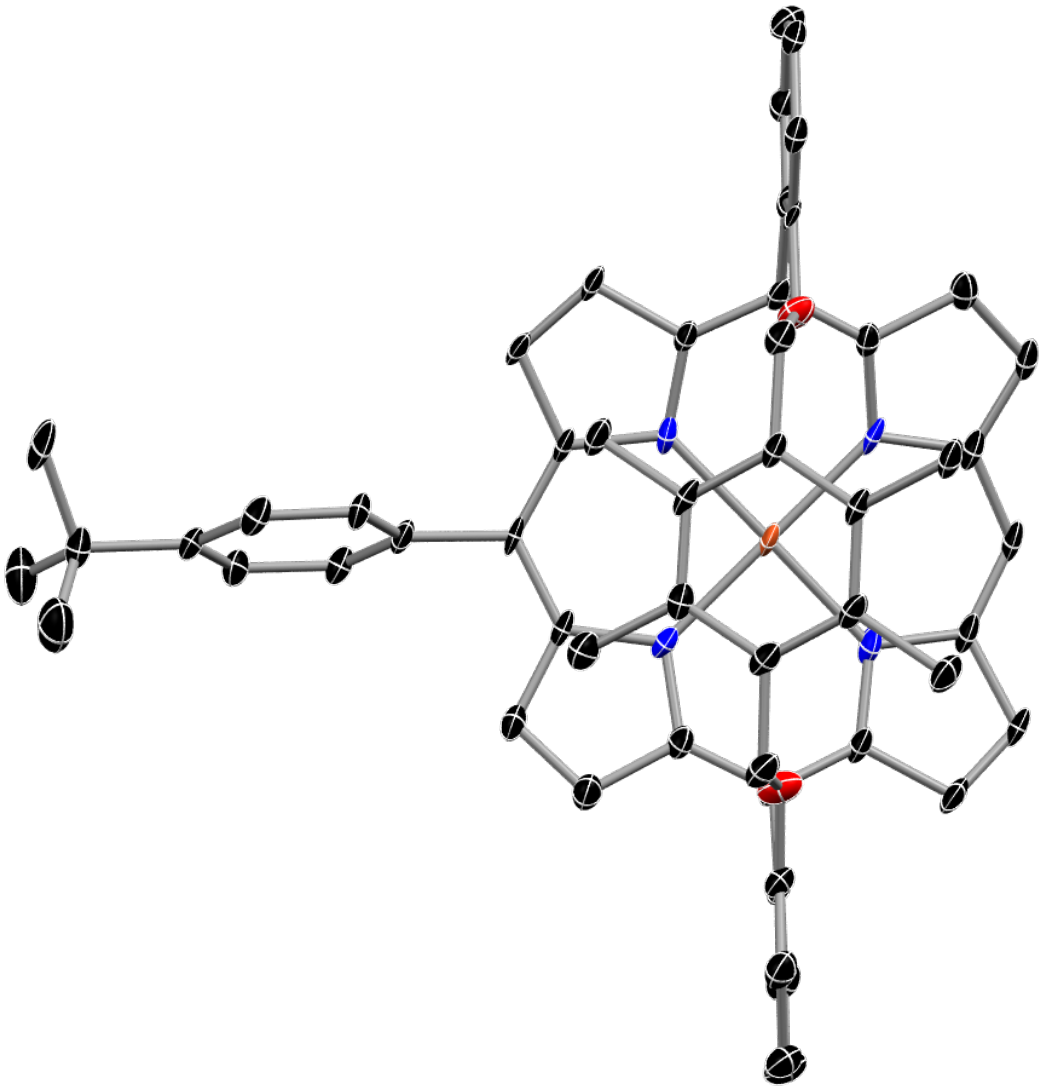
Crystal Structure Determination of Cu-1c: $C_{54}H_4N_4CuO_2 \cdot CHCl_3$, M_r = 965.85, red block, 0.45 × 0.35 × 0.05 mm, monoclinic, space group $P2_1/c$, a = 17.844(3) Å, b = 16.028(3) Å, c = 16.127(3), β = 93.772(5)°, V = 4602.2(14) Å^3, T = 100 K, Z = 4, $\rho_{calcd.}$ = 1.394 g·cm^{-3}, μ = 0.697 mm^{-1}, F(000) = 2004, 35388 reflections in h(–18/22), k(–19/19), l(–19/19) measured in the range 1.793° < θ < 26.136°, completeness 100 %, 9100 independent reflections, 5691 observed reflections ($I > 2\sigma(I)$), 603 parameters, 0 restraints; *all data:* R_1 = 0.1174 and wR_2 = 0.1889, $I > 2\sigma(I)$: R_1 = 0.0632 and wR_2 = 0.1541, *Goof* 1.026, largest difference peak/hole 1.133/–1.661 e·Å^{-3}



Side view of the thermal ellipsoid plot of **Cu-1c**, set at 50% probability level; hydrogen atoms and solvent molecules omitted for clarity



Side view of the thermal ellipsoid plot of **Cu-1c**, set at 50% probability level; hydrogen atoms and solvent molecules omitted for clarity



Top view of the thermal ellipsoid plot of **Cu-1c**, set at 50% probability level; hydrogen atoms and solvent molecules omitted for clarity

9. Chromatographic conditions for the enantiomeric resolution of **M-2, Ni-3, 6b/c, 7b/c, 8, 11, 14a**

Resolution of chiral BHPs on Chiralpakk IA column

compound	solvent A (%)[a]	solvent B (%)[b]	flow (mL/min)	rt peak A[c]	rt peak B[d]	CD @ XX nm[e]	peak A[f]	peak B[f]
Ni-2a	DCM (13)	*n* -hexane (87)	1.5	6:49	7:12	420	+	-
Ni-2b	DCM (20)	*n* -hexane (80)	1.0	8:25	8:42	420	+	-
Ni-2c	DCM (20)	*n* -hexane (80)	0.5	15:15	15:54	420	+	-
Ni-2d	DCM (30)	*n* -hexane (70)	1.0	7:55	8:24	420	+	-
Pd-2e	DCM (10)	*n* -hexane (90)	1.5	3:34	5:03	420	-	+
Cu-2c	DCM (15)	*n* -hexane (85)	1.2	7:26	7:40	420	-	+
Ni-3	DCM (20)	*n* -hexane (80)	1.5	3:31	3:45	420	-	+
6b	DCM (10)	*n* -hexane (90)	1.5	4:00	5:12	420	-	+
7b	DCM (13)	*n* -hexane (87)	1.5	2:58	3:30	420	-	+
6c	DCM (10)	*n* -hexane (90)	1.0	9:23	10:53	420	-	+
7c	DCM (10)	*n* -hexane (90)	1.5	5:36	6:07	420	-	+
8	DCM (50)	*n* -hexane (50)	1.5	4:27	5:13	430	+	-
11	*i* -propanol (5)	*n* -hexane (95)	1.5	4:42	5:09	420	-	+
14a/b	*i* -propanol (14)	*n* -hexane (86)	1.5	4:11	4:33	420	-	+

[a] DCM = dichloromethane; b with 0.1% HNEt2, [c] rt peak A = retention time (rt) of faster eluting enantiomer; [d] rt peak B = rt of slower-eluting enantionmer; [e] wavelength at which CD trace was measured for the HPLC chromatogram; [f] amplitude of the CD trace (- = negative amplitude, + = positive amplitude);

10. UV/Vis absorption spectra of the di- and trimeric porphyrins

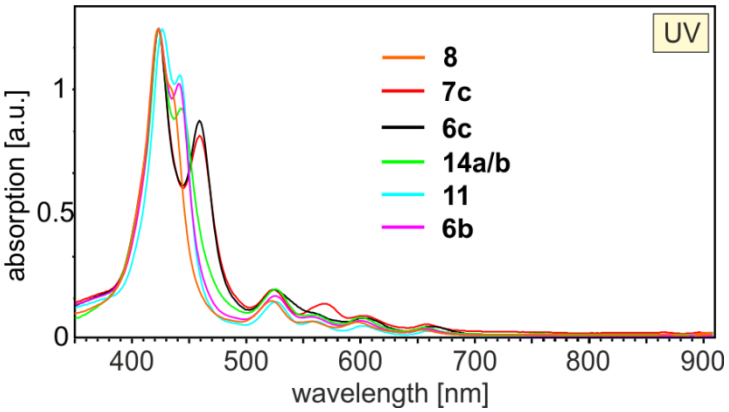


Figure S13. UV/Vis spectra of di- and trimeric porphyrins in dichloromethane/*n*-hexane (1/9) solution.

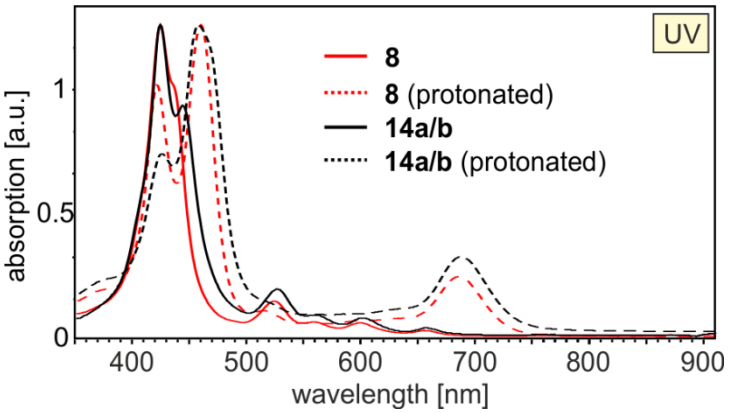
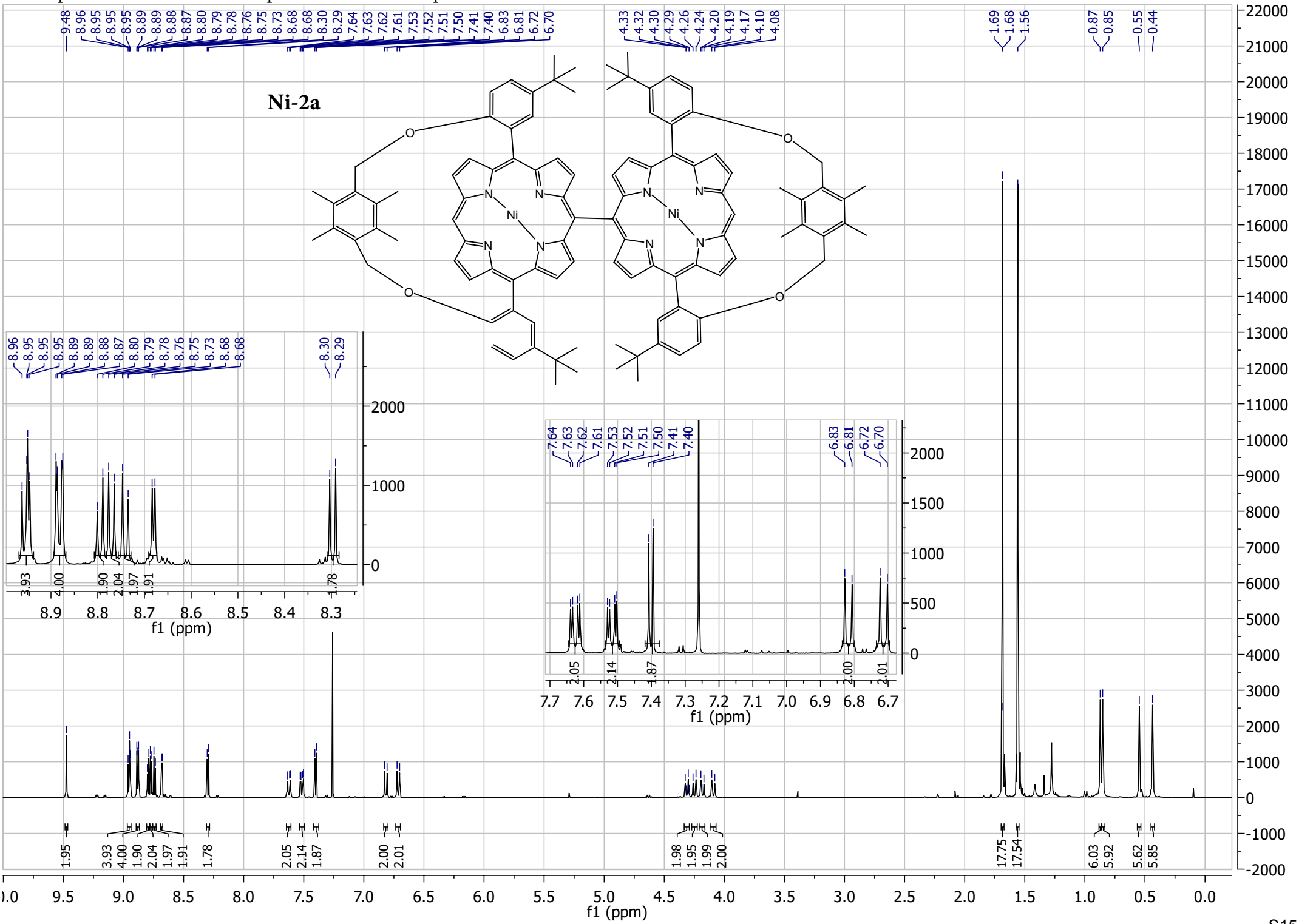


Figure S14. UV/Vis spectra of di- and trimeric *β*-*β*-linked porphyrins in dichloromethane/*n*-hexane (1/9) solution with (solid curve) and without (broken curve; resulting in a protonated species) the addition of $HNEt_2$.


Ni-2a
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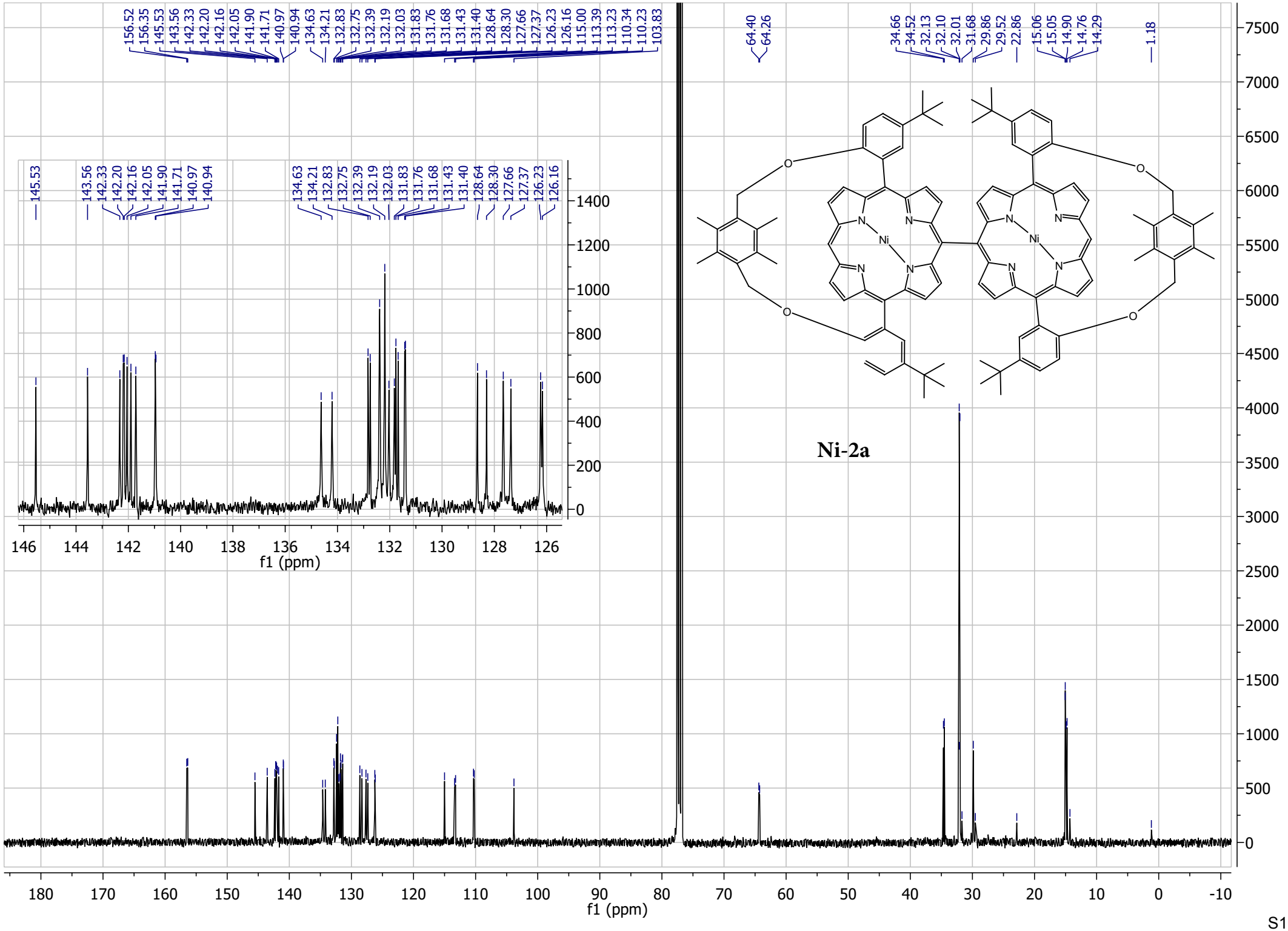
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134.21
132.83
132.75
132.39
132.19
132.03
131.83
131.76
131.68
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131.40
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128.30
127.66
127.37
126.23
126.16
115.00
113.39
113.23
110.34
110.23
103.83
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64.26
34.66
34.52
32.13
32.10
32.01
31.68
29.86
29.52
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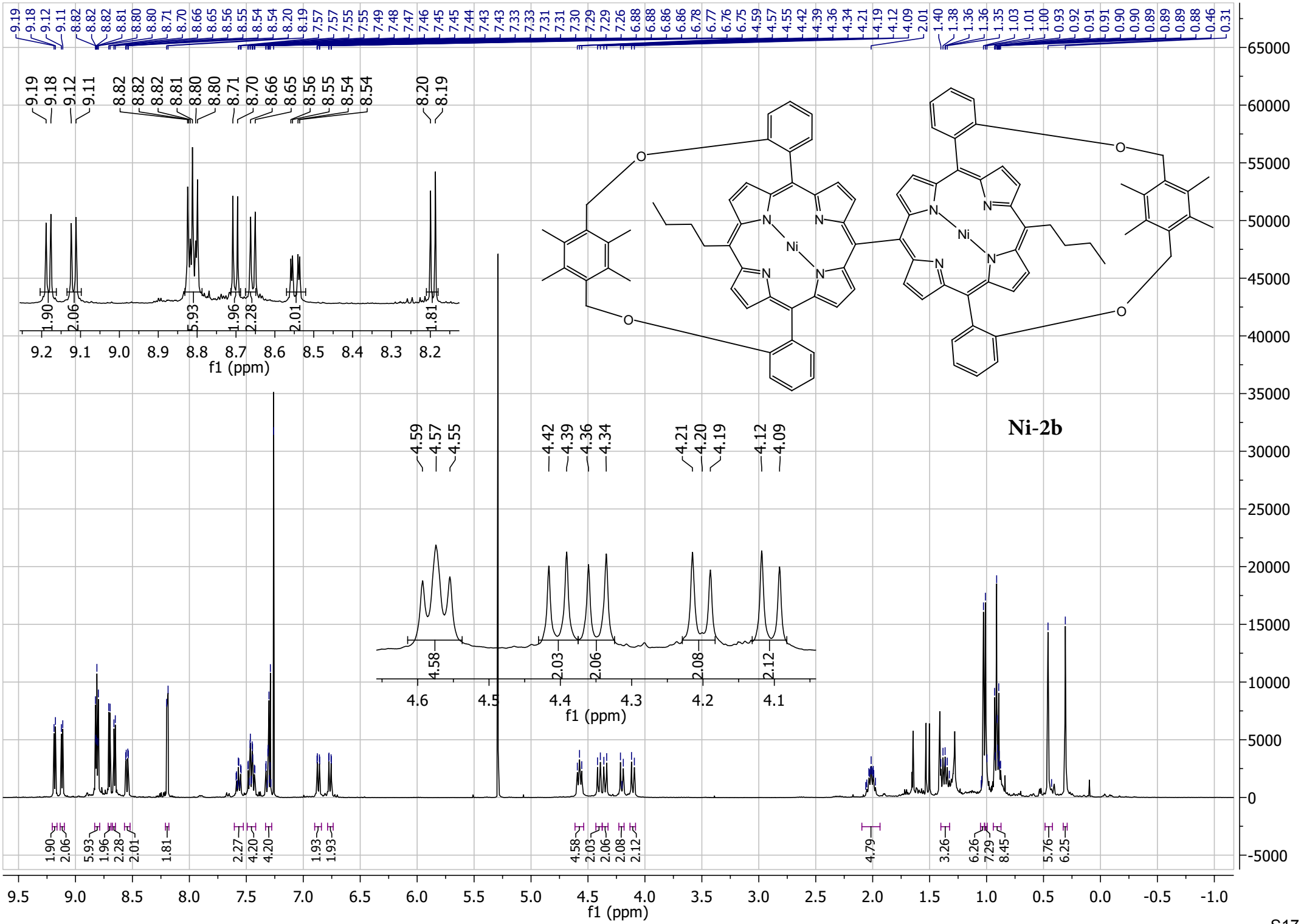
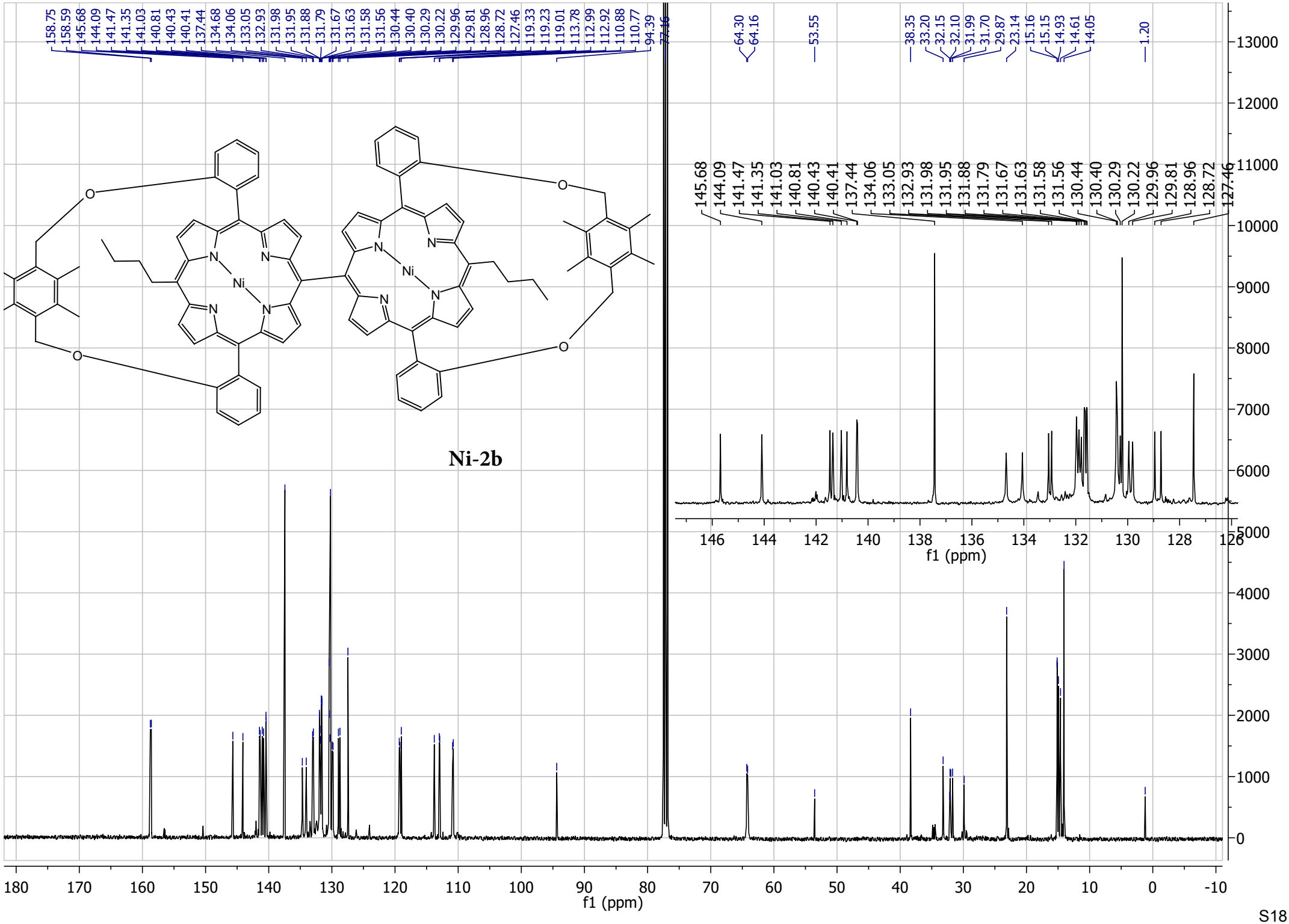
14.29
1.18
Ni-2a
f1 (ppm)
f1 (ppm)


Ni-2b
f1 (ppm)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119.23
119.01
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112.92
110.88
110.77
94.39
77.16
64.30
64.16
53.55
38.35
33.20
32.15
32.10
31.99
31.70
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15.15
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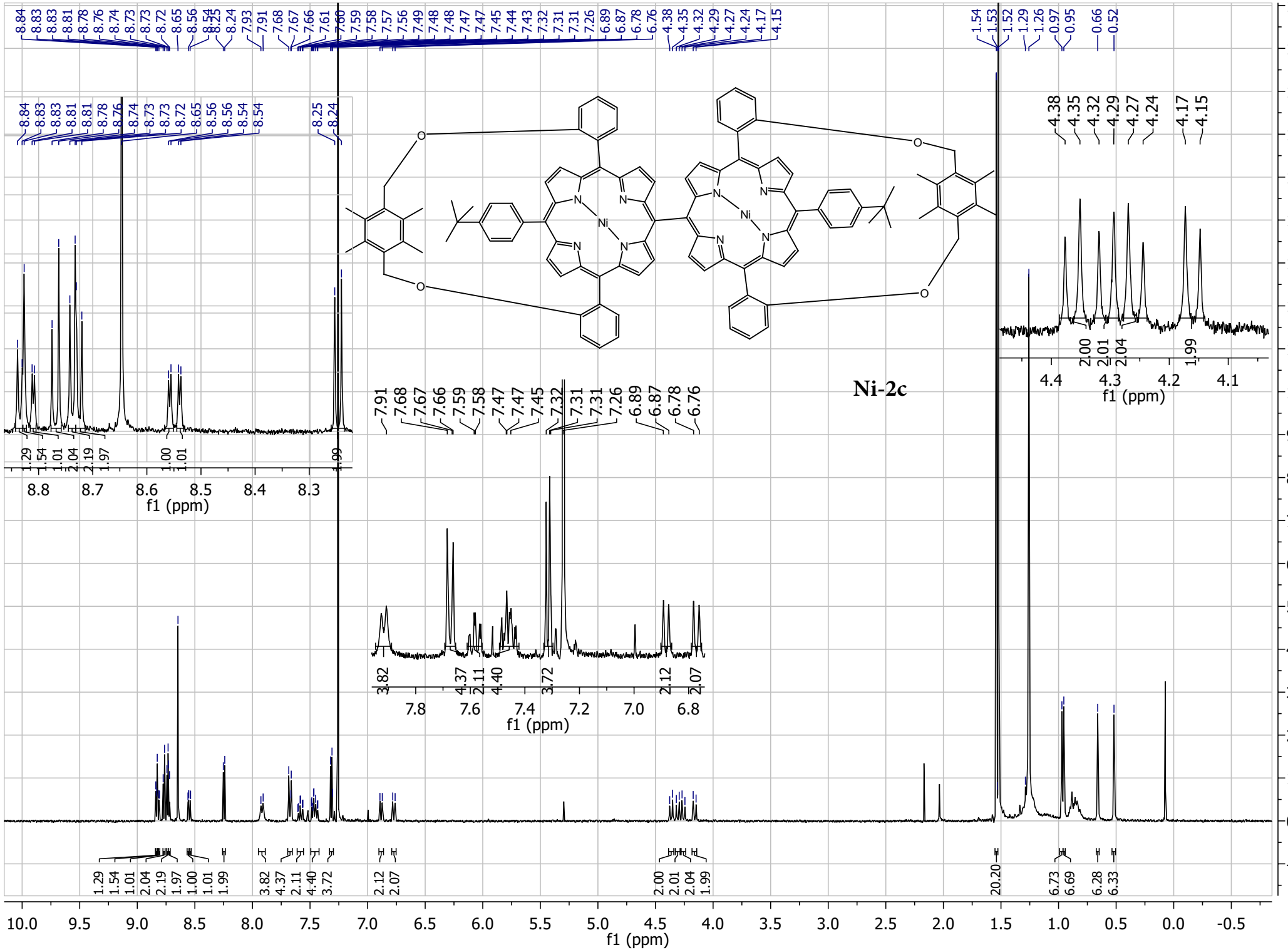
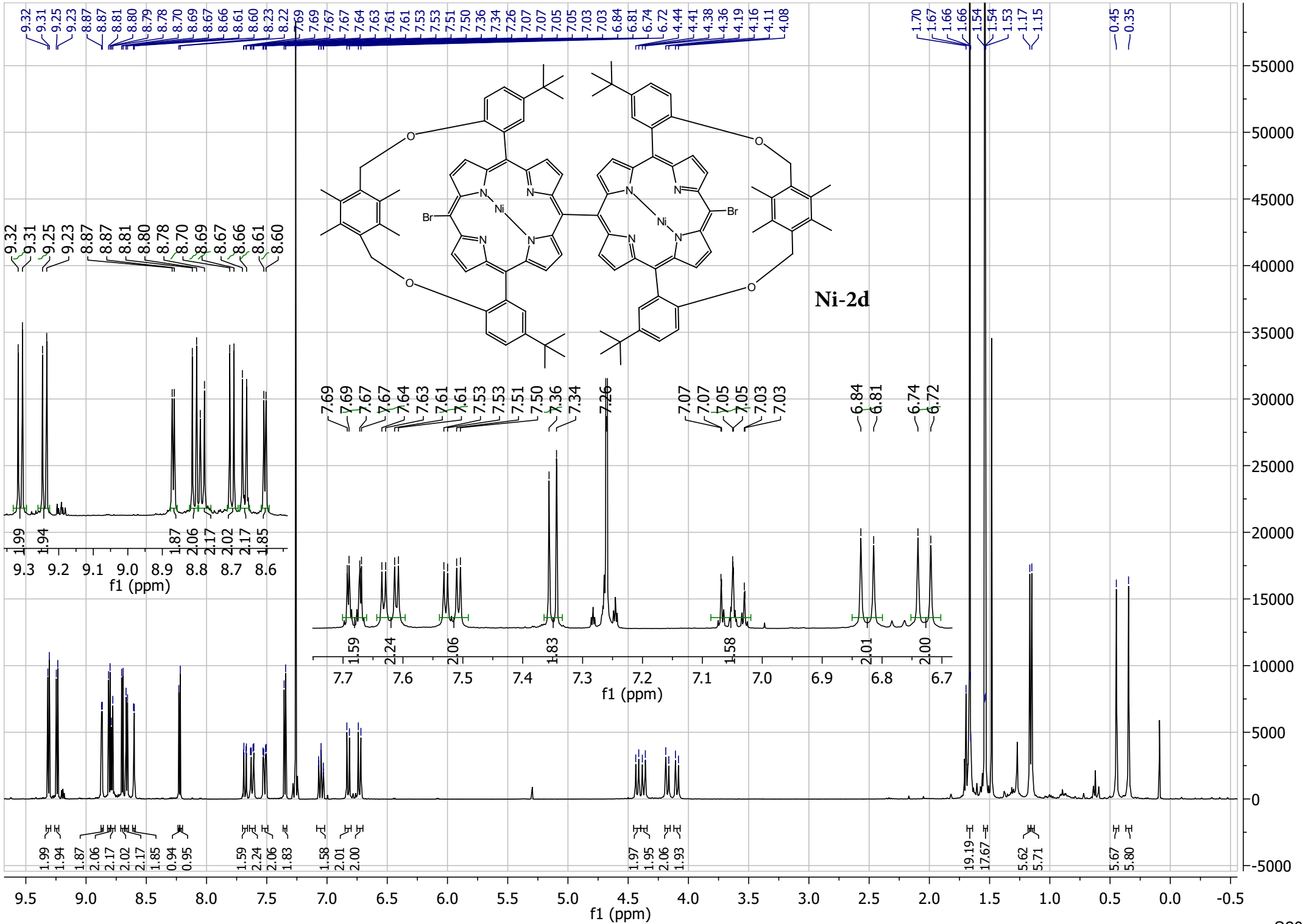
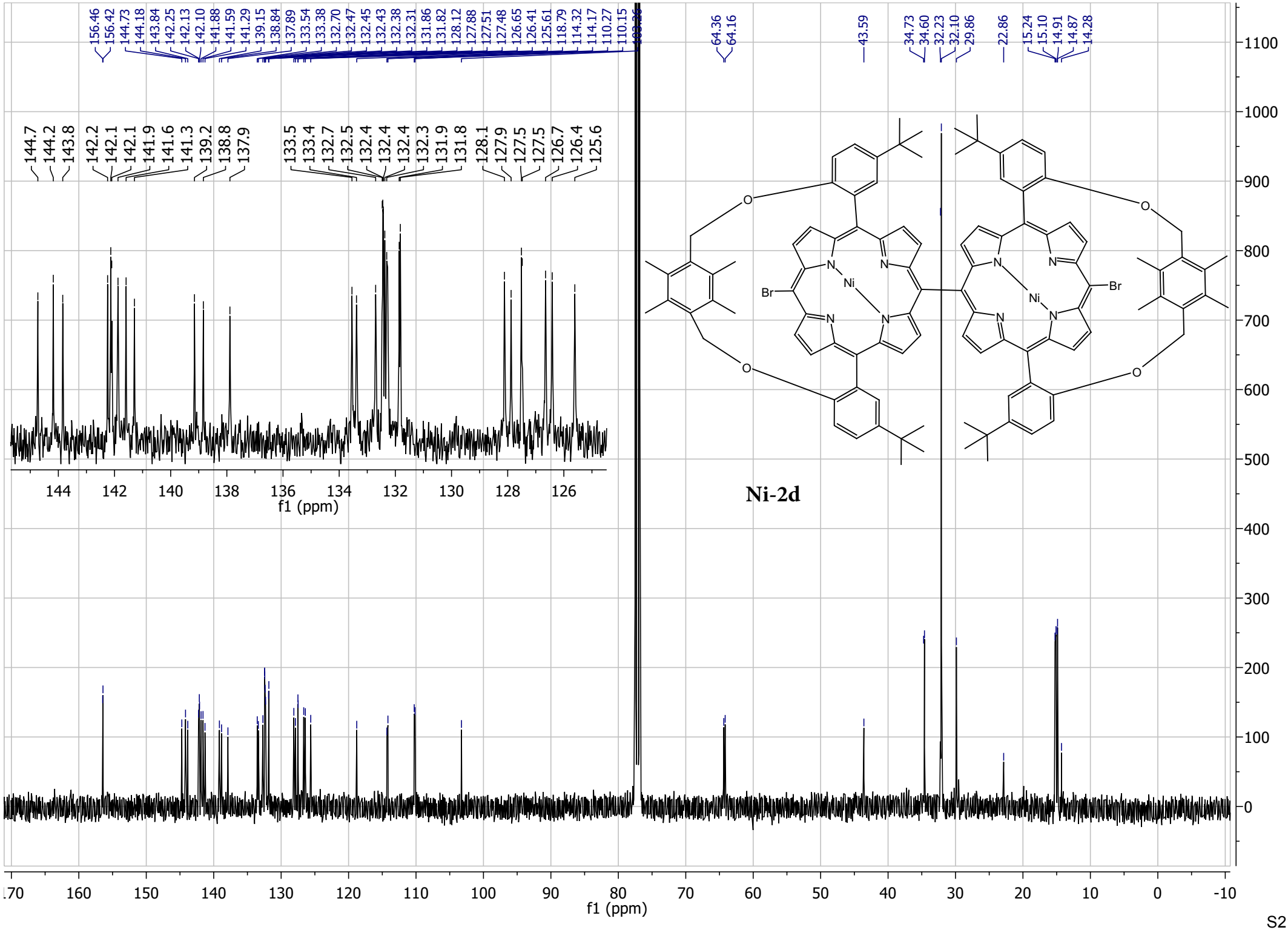
14.61
14.05
1.20
O
N
Ni
f1 (ppm)

Ni-2b


Ni-2c
f1 (ppm)


Ni-2d
f1 (ppm)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133.38
132.70
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132.45
132.43
132.38
132.31
131.86
131.82
128.12
127.88
127.51
127.48
126.65
126.41
125.61
118.79
114.32
114.17
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110.15
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64.16
43.59
34.73
34.60
32.23
32.10
29.86
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15.24
15.10
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14.87
14.28
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143.8
142.2
142.1
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131.9
131.8
128.1
127.9
127.5
127.5
126.7
126.4
125.6
144
142
140
138
136
134
132
130
128
126
f1 (ppm)
Br
Ni
N
O
Br
Ni
N
O
Ni-2d
1100
1000
900
800
700
600
500
400
300
200
100
0
170
160
150
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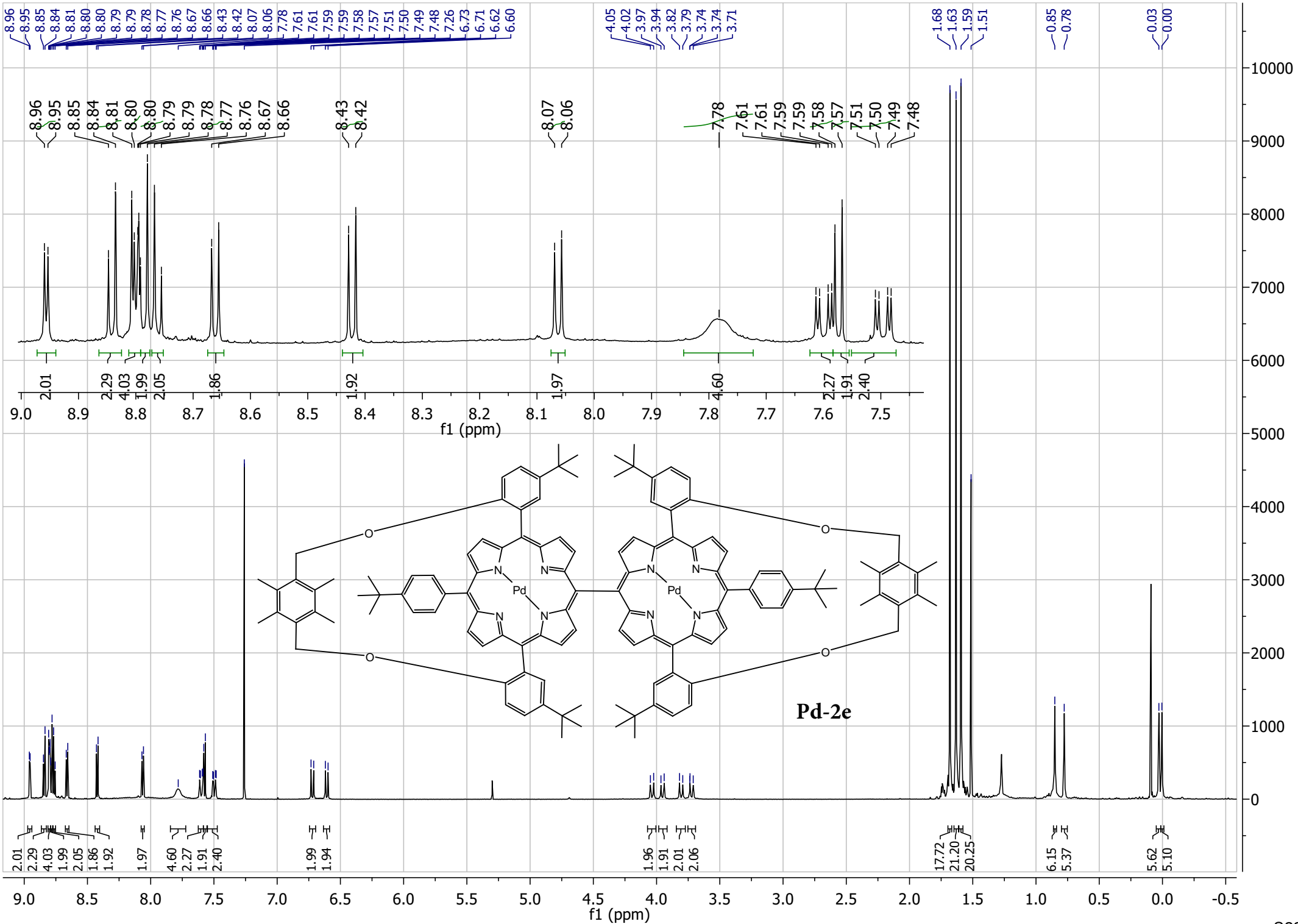
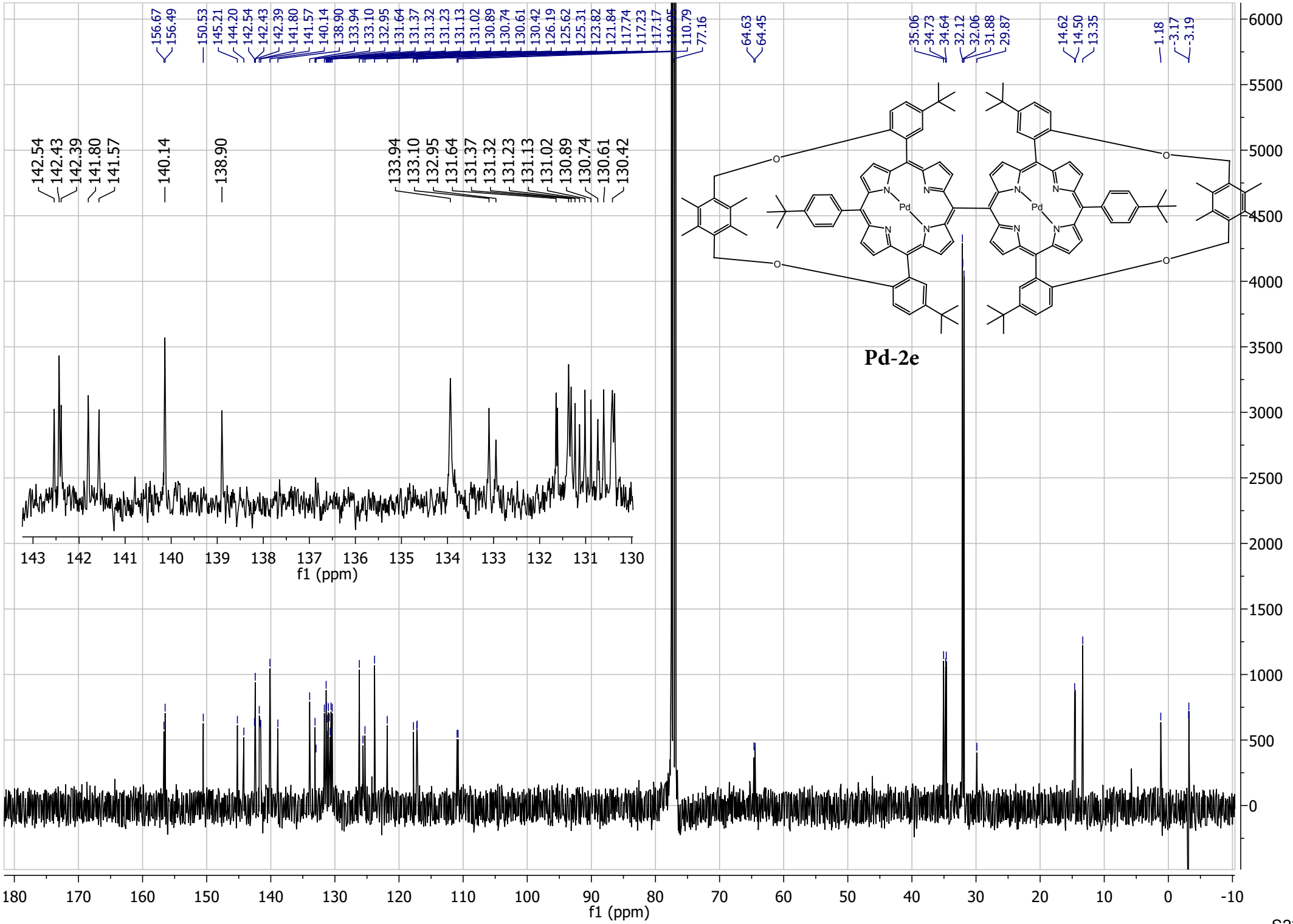
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Pd-2e
f1 (ppm)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117.23
117.17
110.79
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64.63
64.45
35.06
34.73
34.64
32.12
32.06
31.88
29.87
14.62
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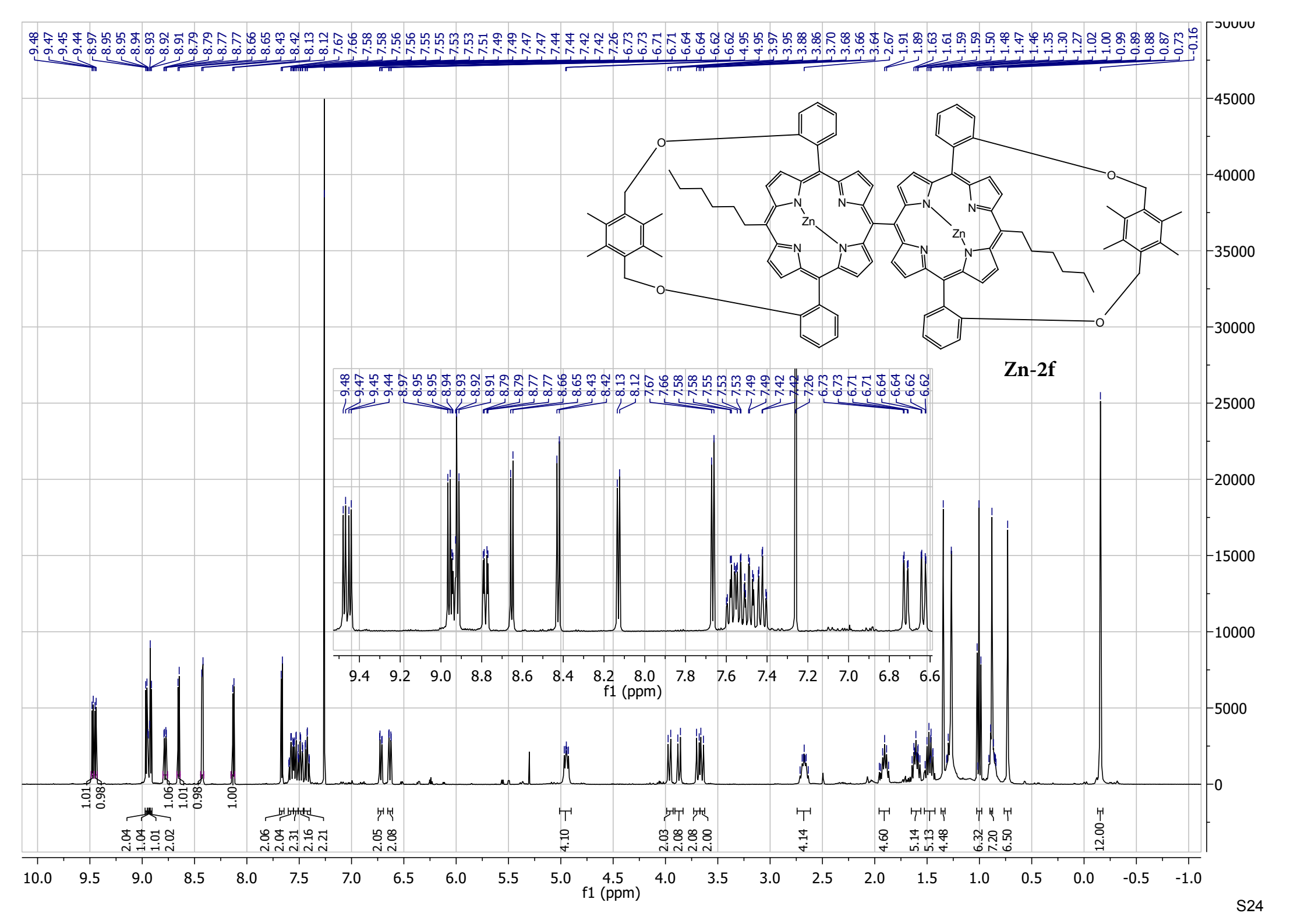
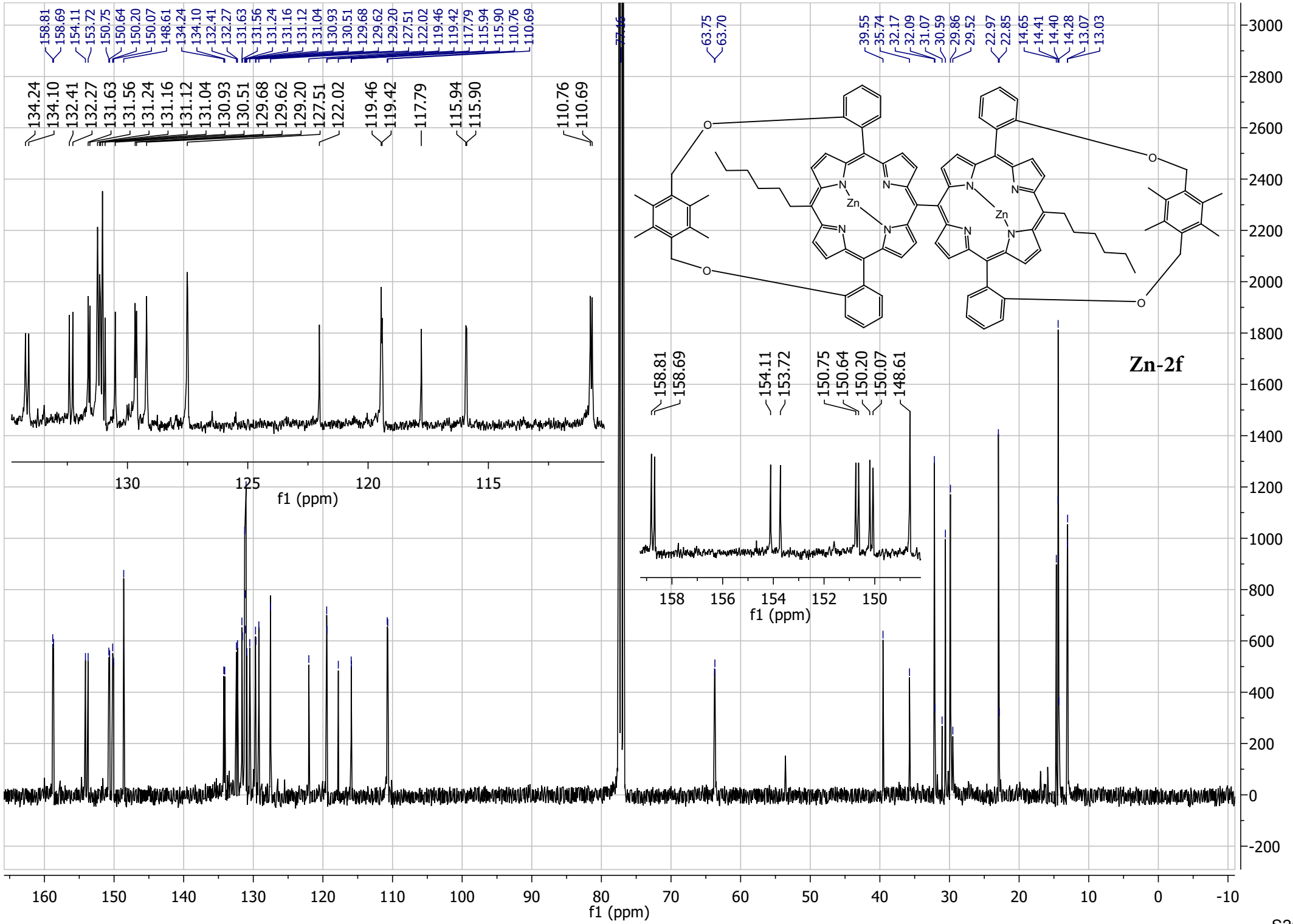
Pd
Pd
f1 (ppm)
f1 (ppm)

Pd-2e


Zn-2f
f1 (ppm)
f1 (ppm)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154.11
153.72
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150.64
150.20
150.07
148.61
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134.10
132.41
132.27
131.63
131.56
131.24
131.16
131.12
131.04
130.93
130.51
129.68
129.62
129.20
127.51
122.02
119.46
119.42
117.79
115.94
115.90
110.76
110.69
77.46
63.75
63.70
39.55
35.74
32.17
32.09
31.07
30.59
29.86
29.52
22.97
22.85
14.65
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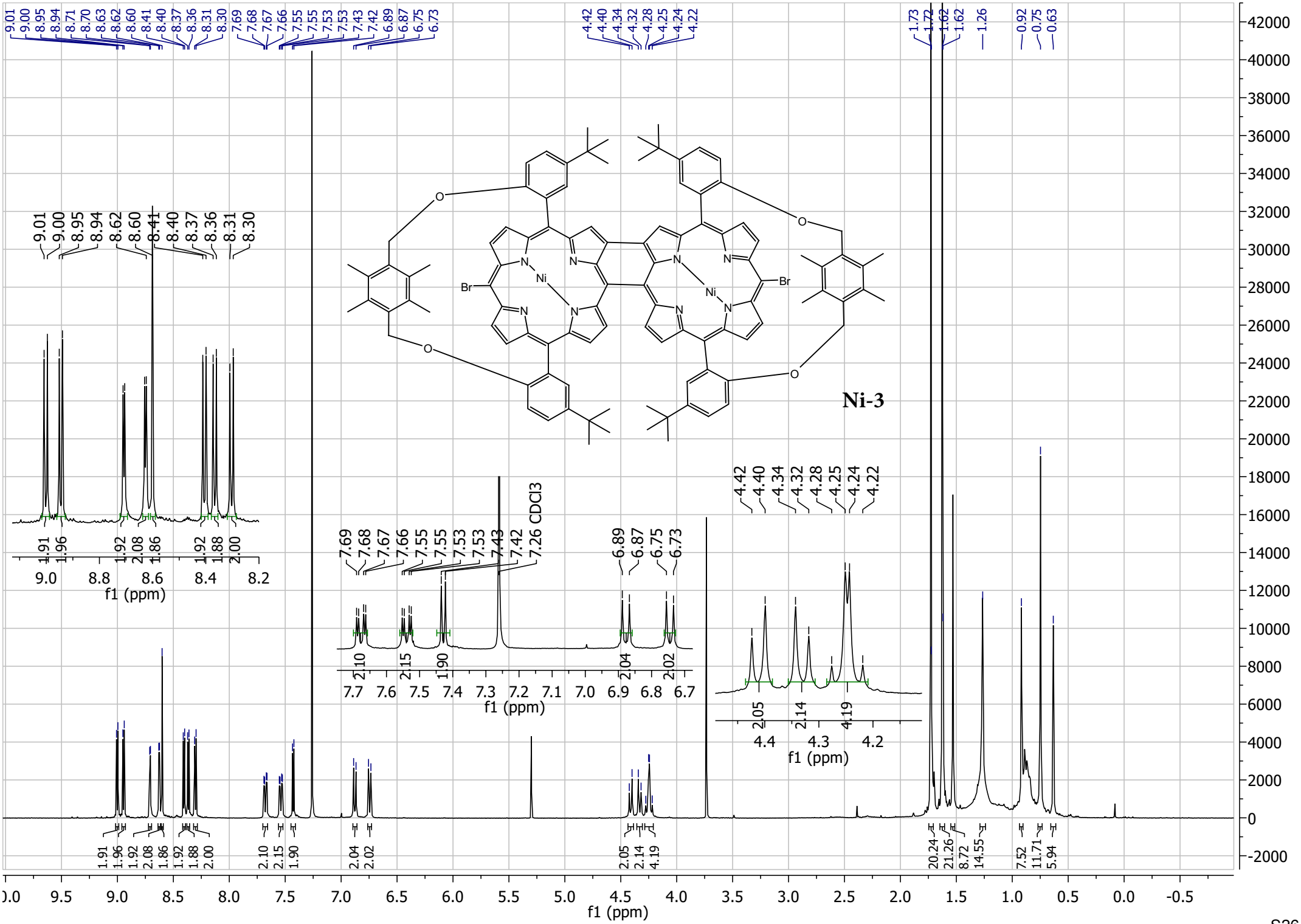
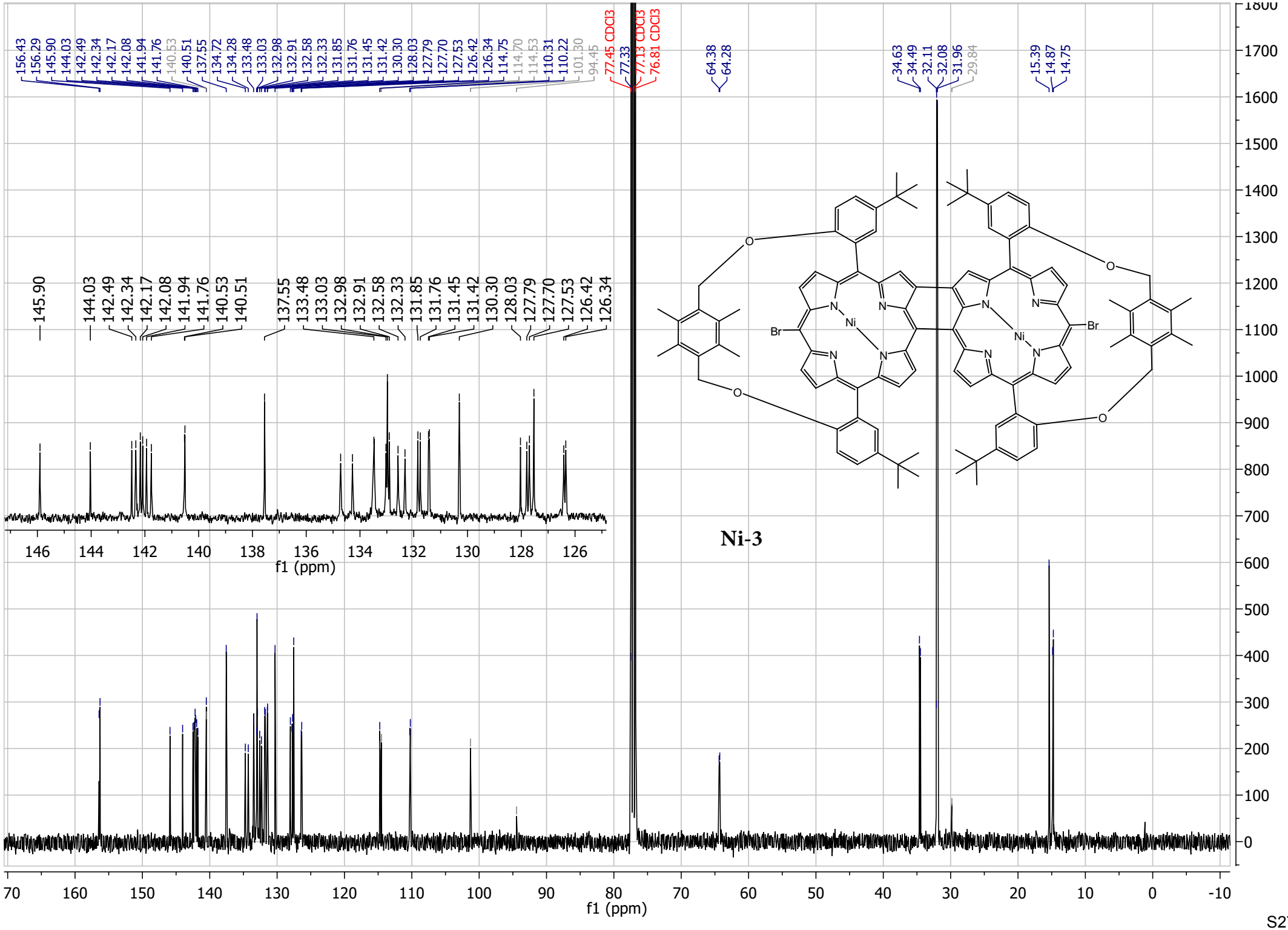
14.40
14.28
13.07
13.03
Zn-2f
f1 (ppm)
f1 (ppm)
f1 (ppm)


Ni-3
f1 (ppm)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156.29
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140.53
140.51
137.55
134.72
134.28
133.48
133.03
132.98
132.91
132.58
132.33
131.85
131.76
131.45
131.42
130.30
128.03
127.79
127.70
127.53
126.42
126.34
114.75
114.70
114.53
110.31
110.22
101.30
94.45
77.45 CDCl3
77.33
77.13 CDCl3
76.81 CDCl3
64.38
64.28
34.63
34.49
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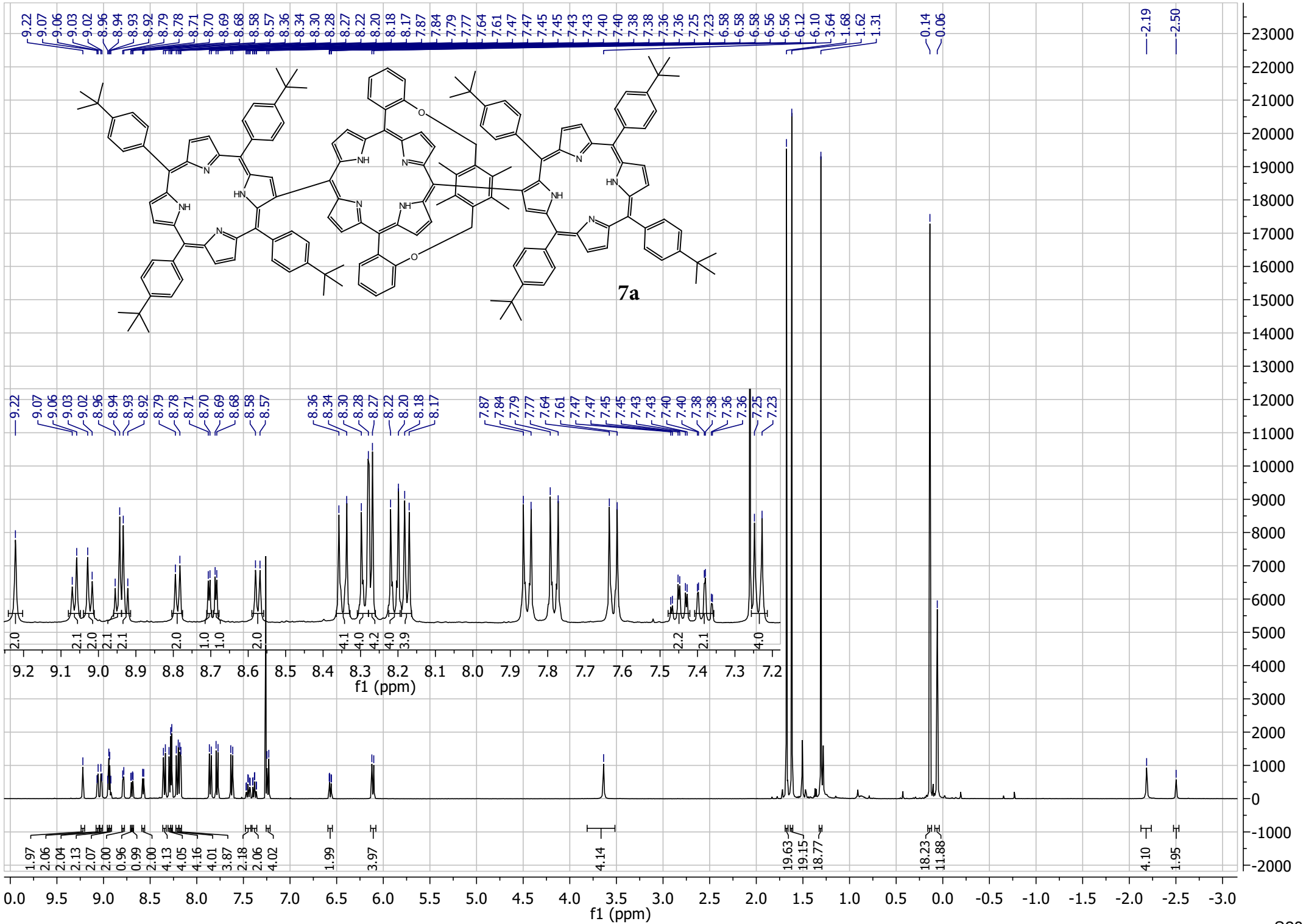
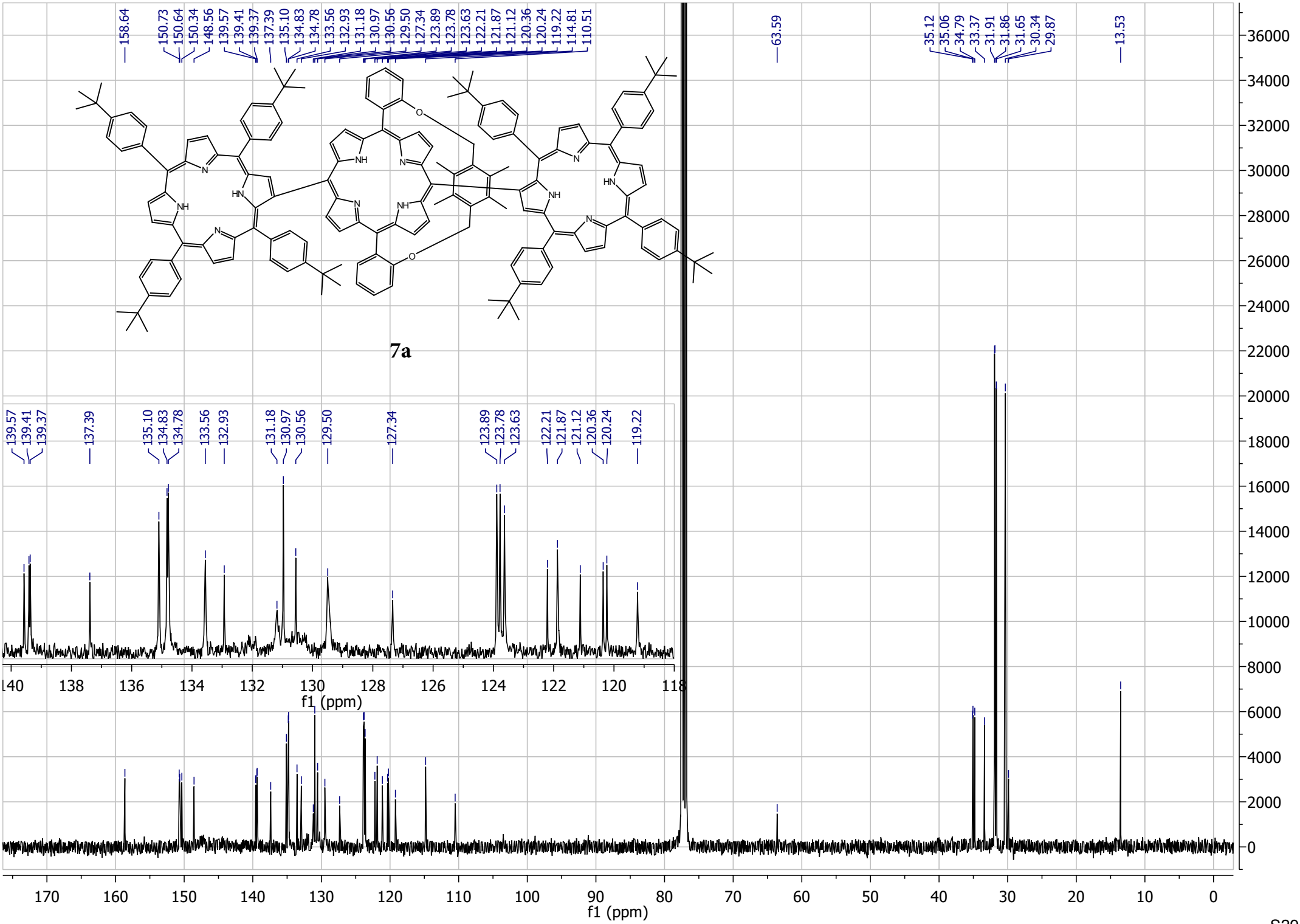
32.08
31.96
29.84
15.39
14.87
14.75
Ni-3
f1 (ppm)
f1 (ppm)


9.22 9.07 9.06 9.03 9.02 8.96 8.94 8.93 8.92 8.79 8.78 8.71 8.70 8.69 8.68 8.58 8.57 8.36 8.34 8.30 8.28 8.27 8.22 8.20 8.18 8.17 7.87 7.84 7.79 7.77 7.64 7.61 7.47 7.47 7.45 7.45 7.43 7.43 7.40 7.40 7.38 7.38 7.36 7.36 7.25 7.23 6.58 6.58 6.58 6.56 6.56 6.12 6.10 3.64 1.68 1.62 1.31 0.14 0.06 2.19 2.50
7a
f1 (ppm)
f1 (ppm)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150.64
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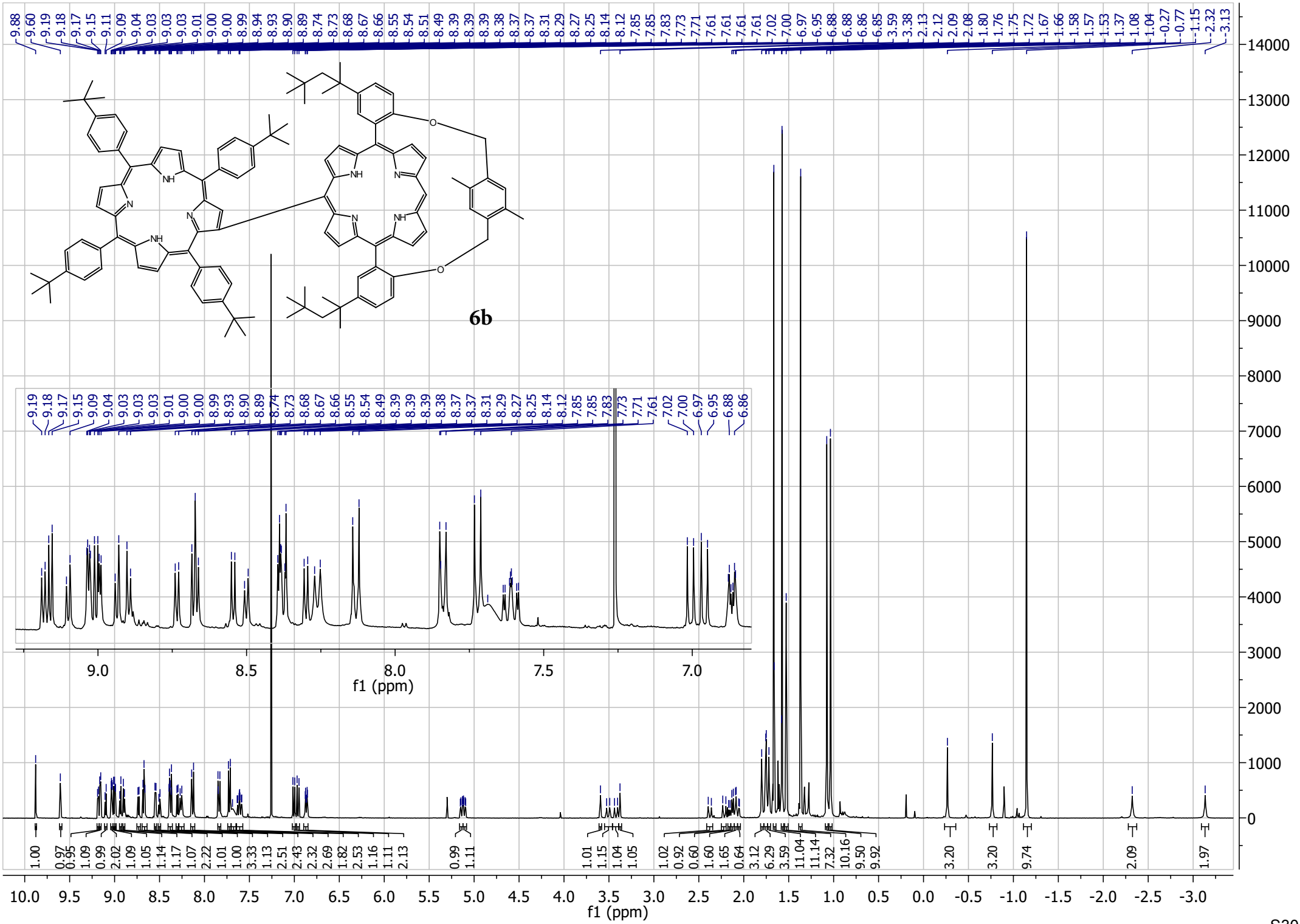
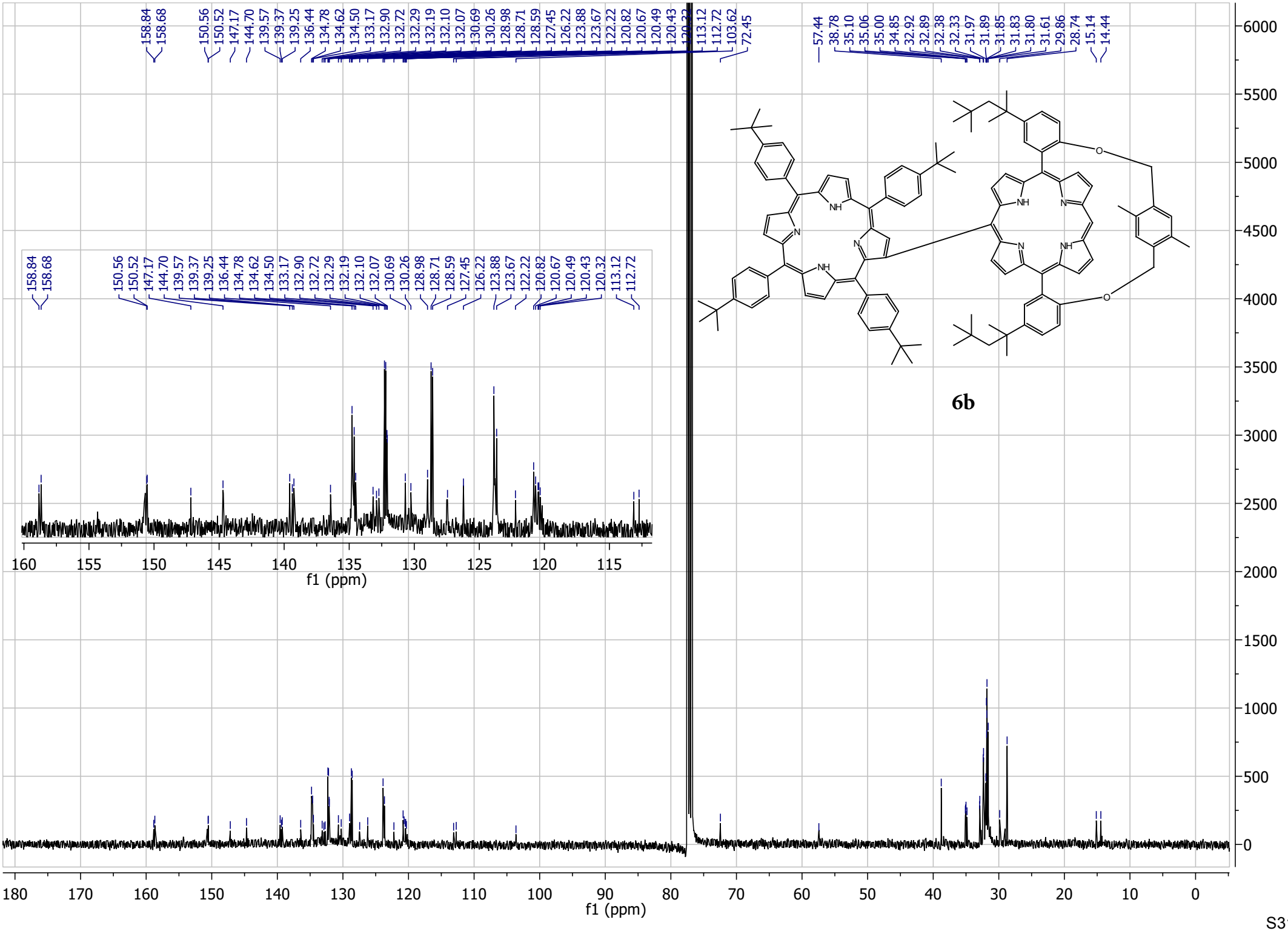
139.57
139.41
139.37
137.39
135.10
134.83
134.78
133.56
132.93
131.18
130.97
130.56
129.50
127.34
123.89
123.78
123.63
122.21
121.87
121.12
120.36
120.24
119.22
114.81
110.51
63.59
35.12
35.06
34.79
33.37
31.91
31.86
31.65
30.34
29.87
13.53
f1 (ppm)
f1 (ppm)

7a


6b
f1 (ppm)
f1 (ppm)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134.50
133.17
132.90
132.72
132.29
132.19
132.10
132.07
130.69
130.26
128.98
128.71
128.59
127.45
126.22
123.88
123.67
122.22
120.82
120.67
120.49
120.43
120.32
113.12
112.72
103.62
72.45
57.44
38.78
35.10
35.06
35.00
34.85
32.92
32.89
32.38
32.33
31.97
31.89
31.85
31.83
31.80
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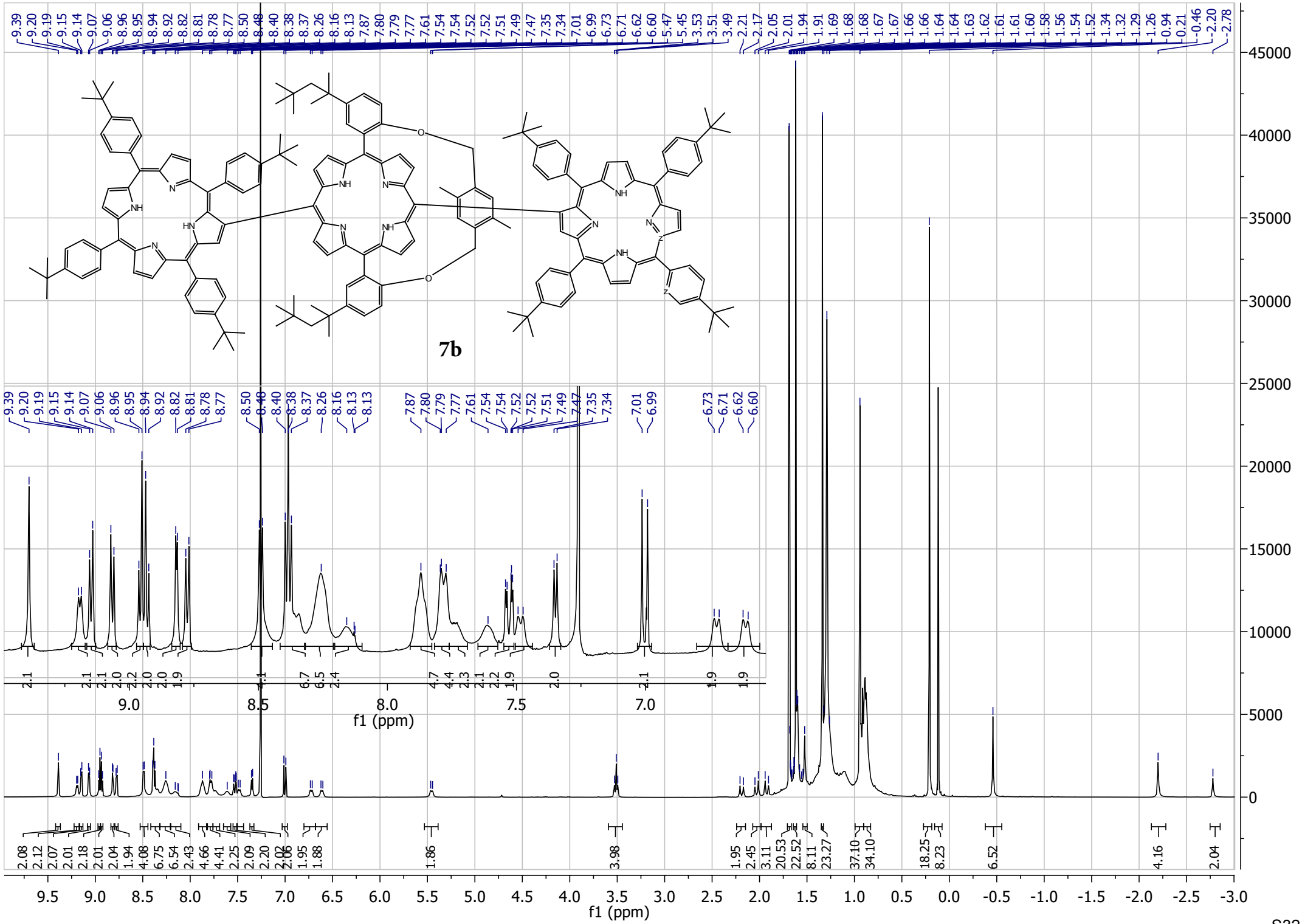
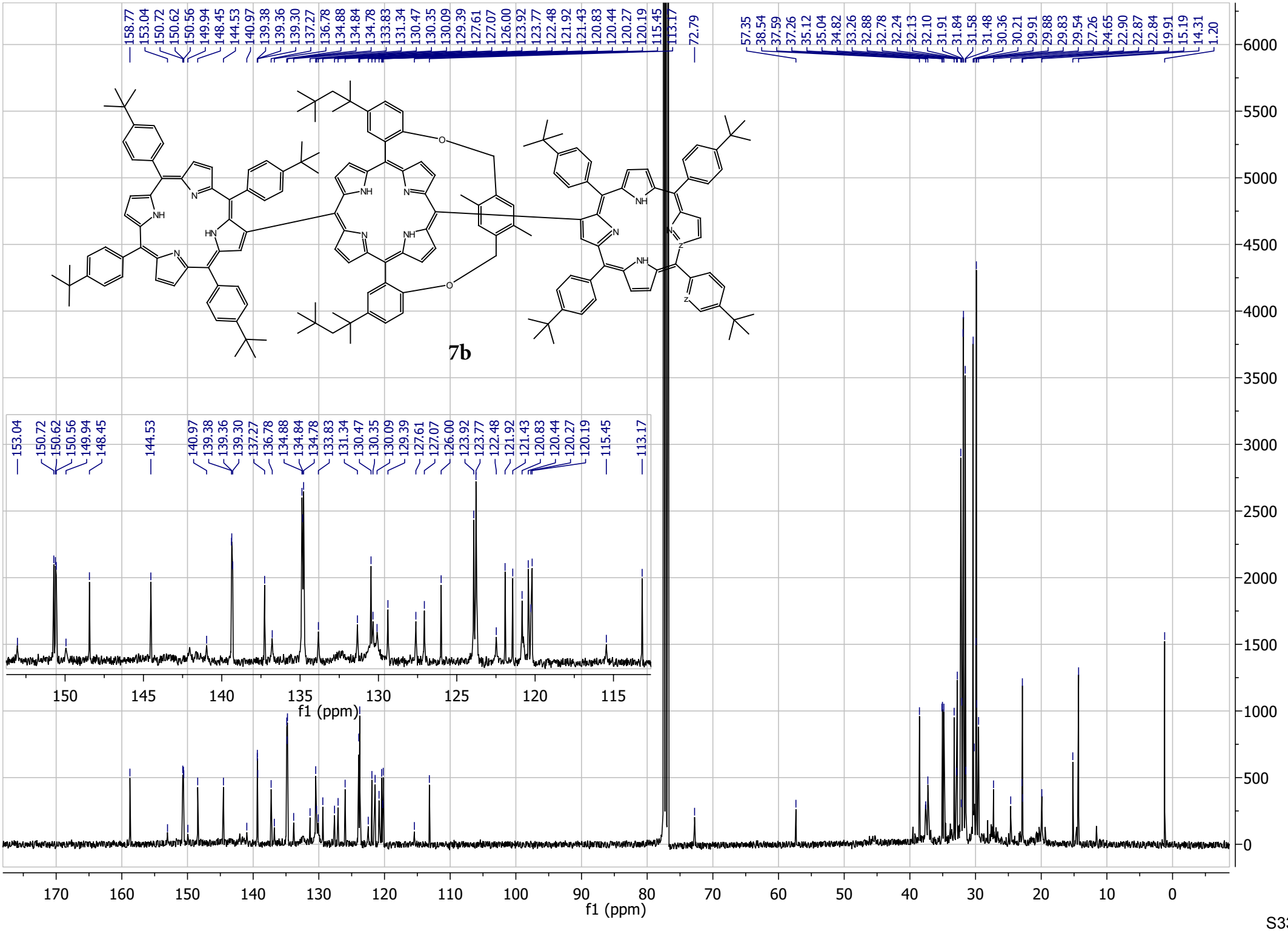
29.86
28.74
15.14
14.44
NH
N
O
6b
f1 (ppm)
f1 (ppm)


7b
f1 (ppm)
f1 (ppm)


158.77
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136.78
134.88
134.84
134.78
133.83
131.34
130.47
130.35
130.09
129.39
127.61
127.07
126.00
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123.77
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120.44
120.27
120.19
115.45
113.17
72.79
57.35
38.54
37.59
37.26
35.12
35.04
34.82
33.26
32.88
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29.54
27.26
24.65
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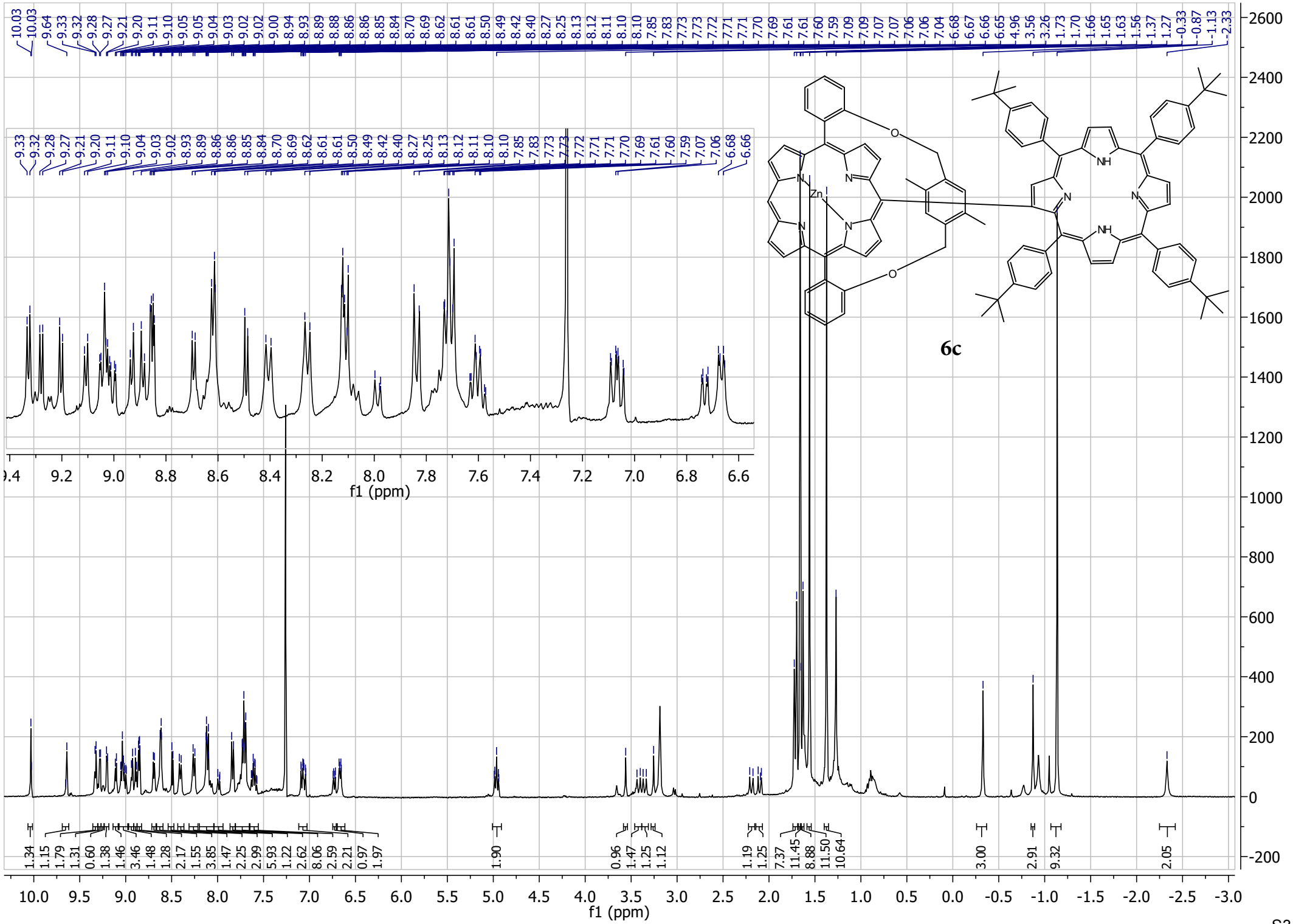
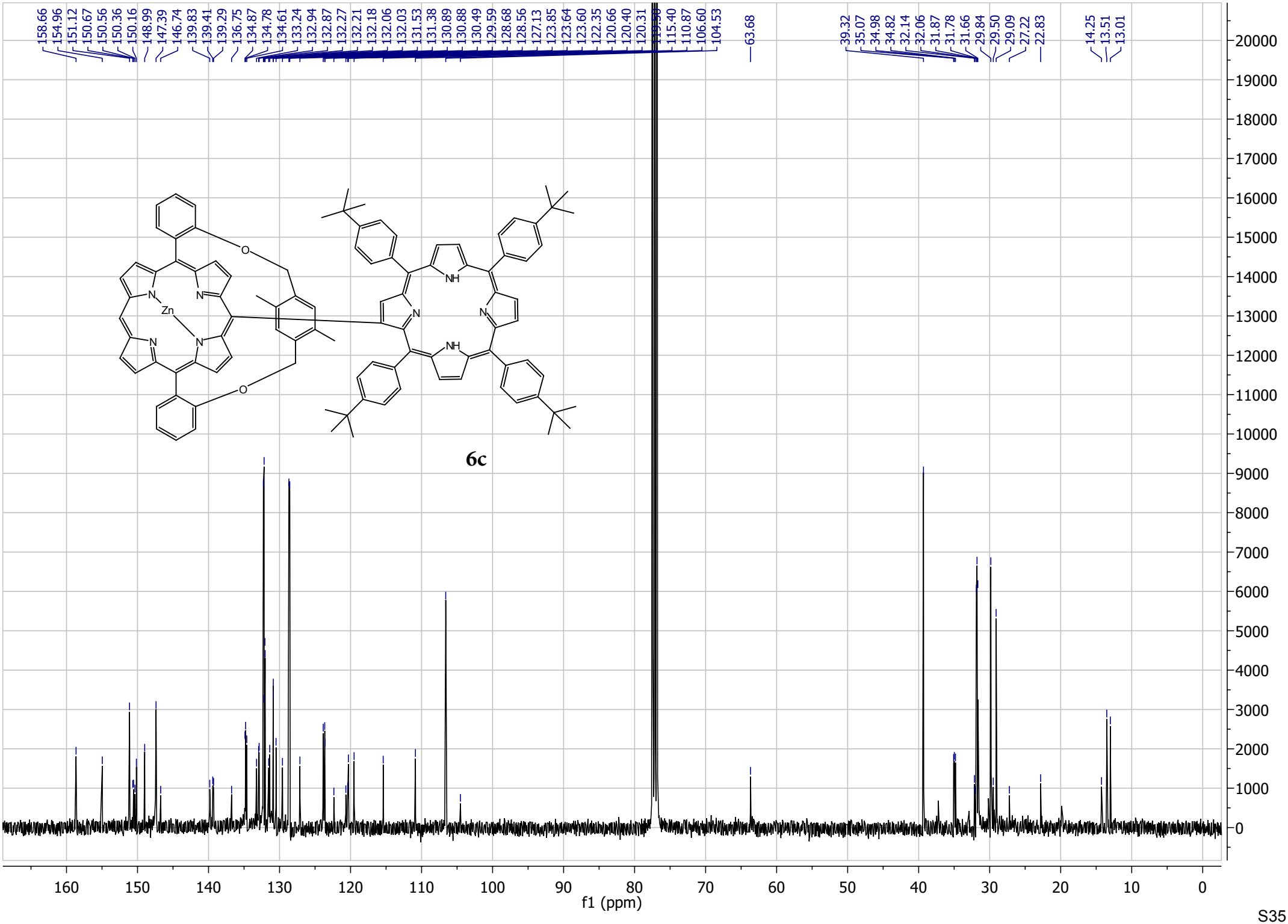
22.87
22.84
19.91
15.19
14.31
1.20
7b
f1 (ppm)
f1 (ppm)


6c
f1 (ppm)
f1 (ppm)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150.16
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147.39
146.74
139.83
139.41
139.29
136.75
134.87
134.78
134.61
133.24
132.94
132.87
132.27
132.21
132.18
132.06
132.03
131.53
131.38
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130.49
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128.68
128.56
127.13
123.85
123.64
123.60
122.35
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120.40
120.31
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110.87
106.60
104.53
63.68
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34.98
34.82
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32.06
31.87
31.78
31.66
29.84
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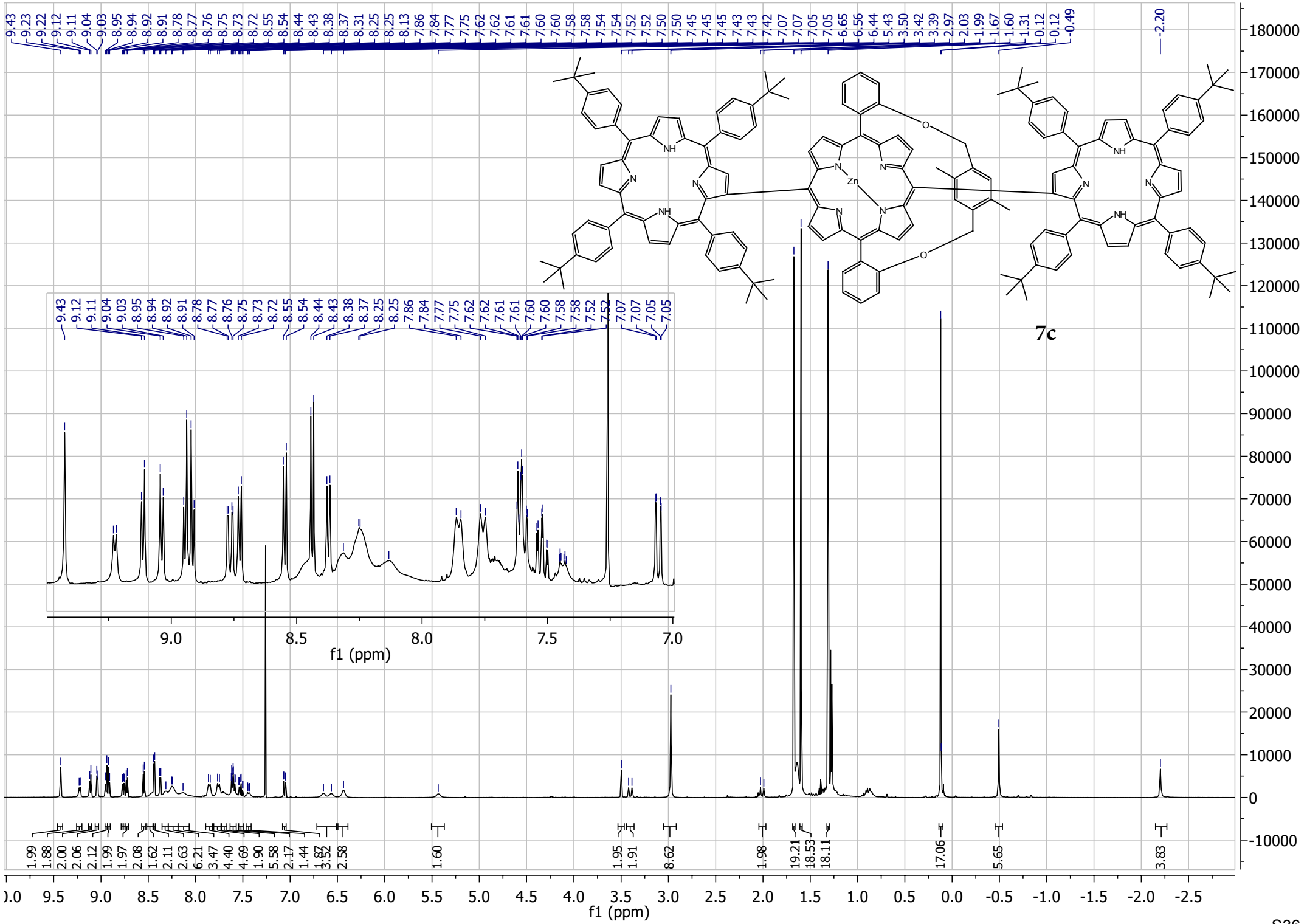
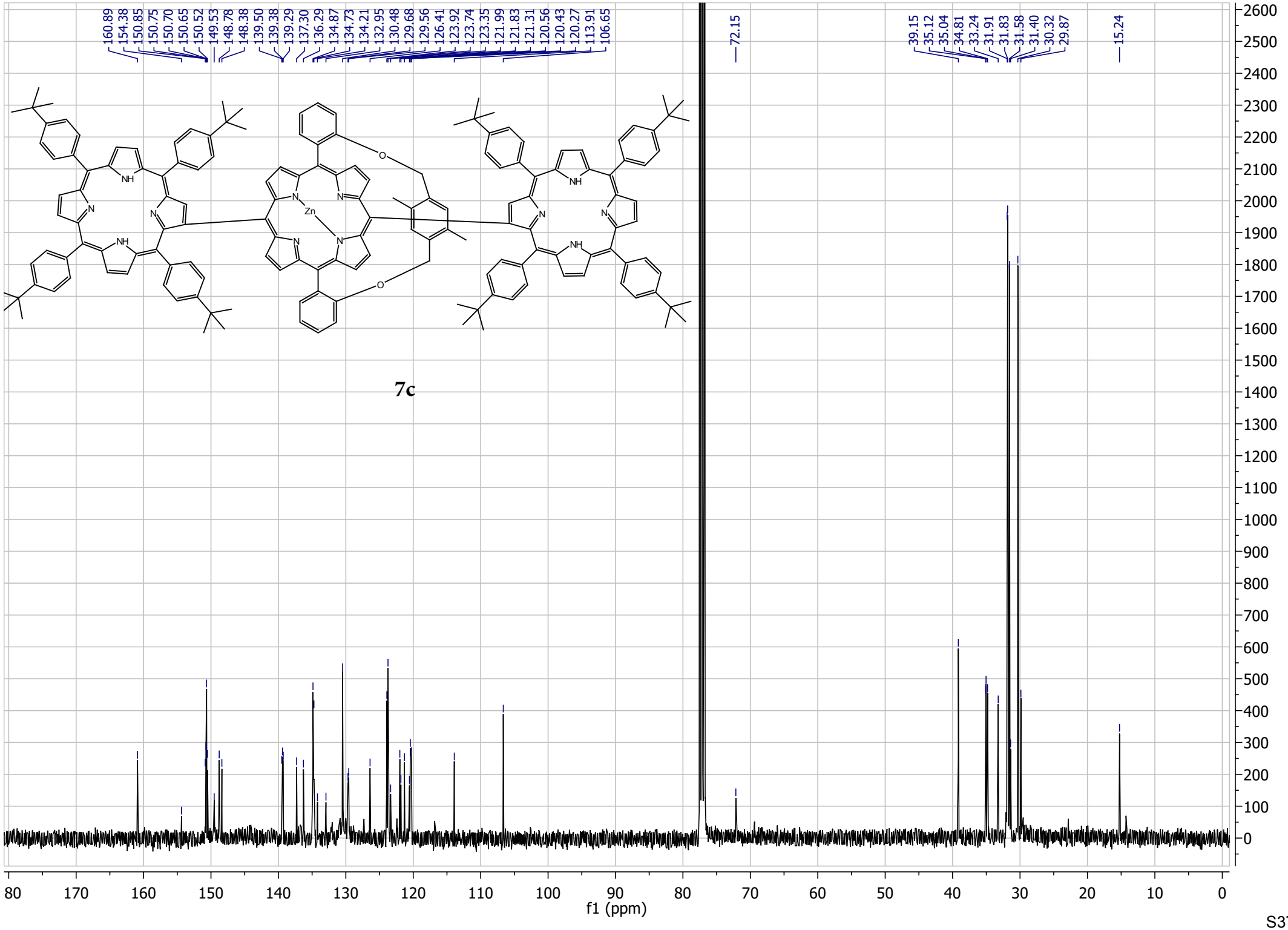
27.22
22.83
14.25
13.51
13.01
Zn
N
NH
O
6c
f1 (ppm)


9.43 9.23 9.22 9.12 9.11 9.04 9.03 8.95 8.94 8.92 8.91 8.78 8.77 8.76 8.75 8.73 8.72 8.55 8.54 8.44 8.43 8.38 8.37 8.31 8.25 8.25 8.13 7.86 7.84 7.77 7.75 7.62 7.62 7.61 7.61 7.60 7.60 7.58 7.58 7.54 7.54 7.52 7.52 7.50 7.50 7.45 7.45 7.45 7.43 7.43 7.42 7.07 7.07 7.05 7.05 6.65 6.56 6.44 5.43 3.50 3.42 3.39 2.97 2.03 1.99 1.67 1.60 1.31 0.12 0.12 -0.49 -2.20
7c
f1 (ppm)
1.99 1.88 2.00 2.06 2.12 1.99 1.97 2.08 1.62 2.11 2.63 6.21 3.47 4.40 4.69 1.90 5.58 2.17 1.44 1.87 3.52 2.58 1.60 1.95 1.91 8.62 1.98 19.21 18.53 18.11 17.06 5.65 3.83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148.38
139.50
139.38
139.29
137.30
136.29
134.87
134.73
134.21
132.95
130.48
129.68
129.56
126.41
123.92
123.74
123.35
121.99
121.83
121.31
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120.43
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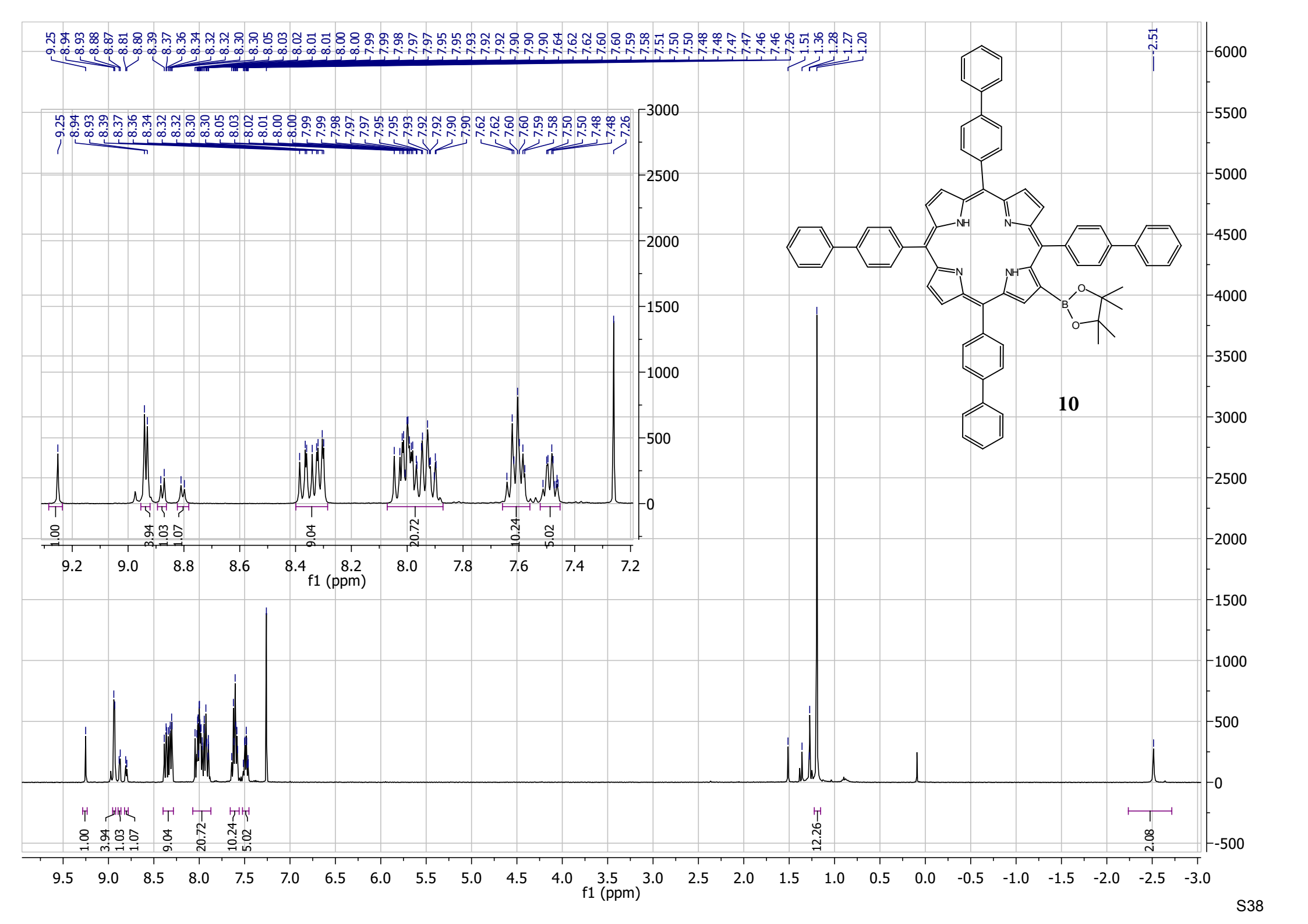
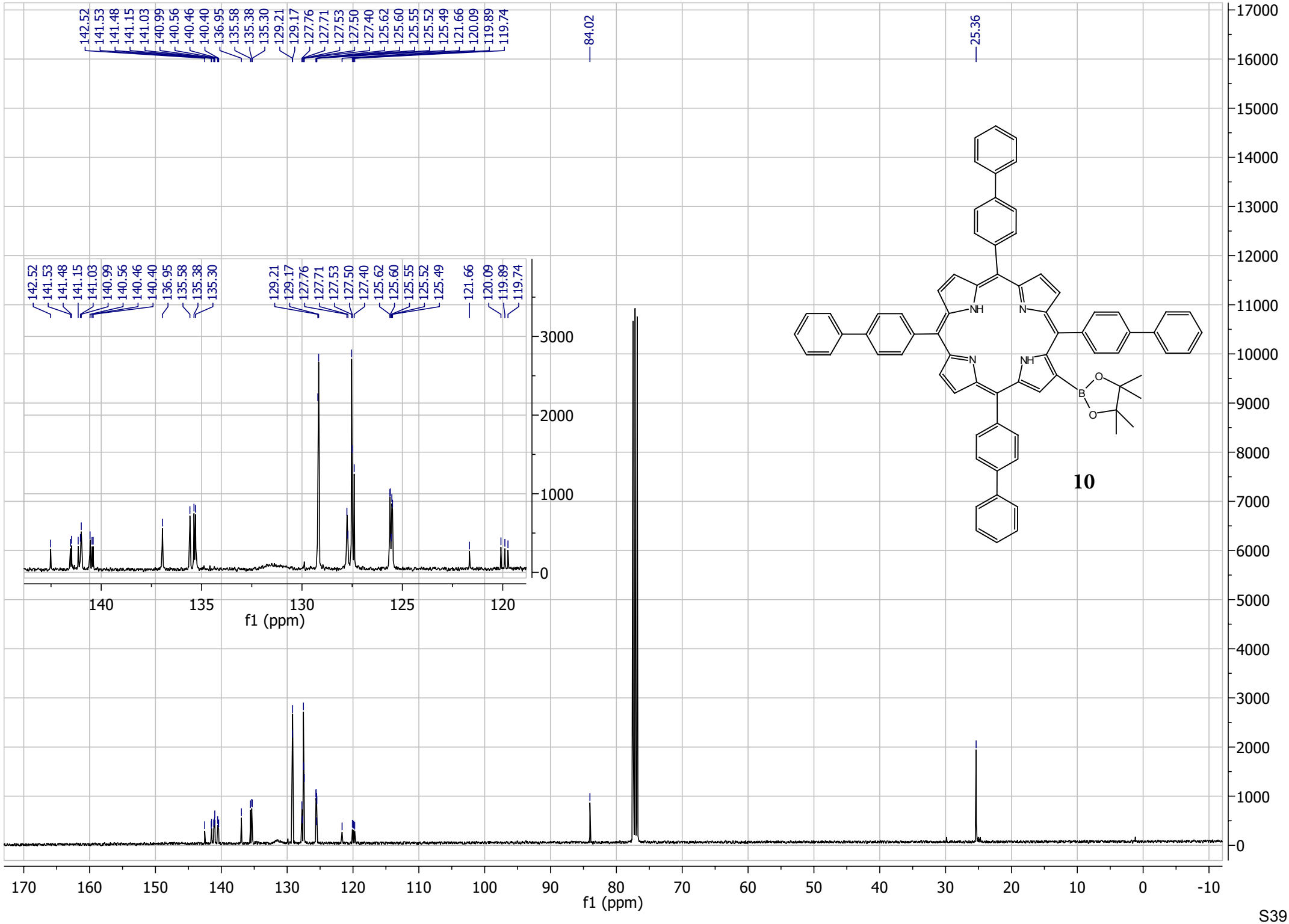
113.91
106.65
72.15
39.15
35.12
35.04
34.81
33.24
31.91
31.83
31.58
31.40
30.32
29.87
15.24
NH
N
Zn
O
f1 (ppm)

7c


9.25 8.94 8.93 8.88 8.87 8.81 8.80 8.39 8.37 8.36 8.34 8.32 8.32 8.30 8.30 8.05 8.03 8.02 8.01 8.01 8.00 8.00 7.99 7.99 7.98 7.97 7.97 7.95 7.95 7.93 7.92 7.92 7.90 7.90 7.90 7.64 7.62 7.62 7.60 7.60 7.59 7.58 7.51 7.50 7.50 7.48 7.48 7.47 7.47 7.46 7.46 7.26 1.51 1.36 1.28 1.27 1.20
2.51
NH
N
N
NH
B
O
O
10
1.00 3.94 1.03 1.07 9.04 20.72 10.24 5.02
f1 (ppm)
12.26
2.08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141.03
140.99
140.56
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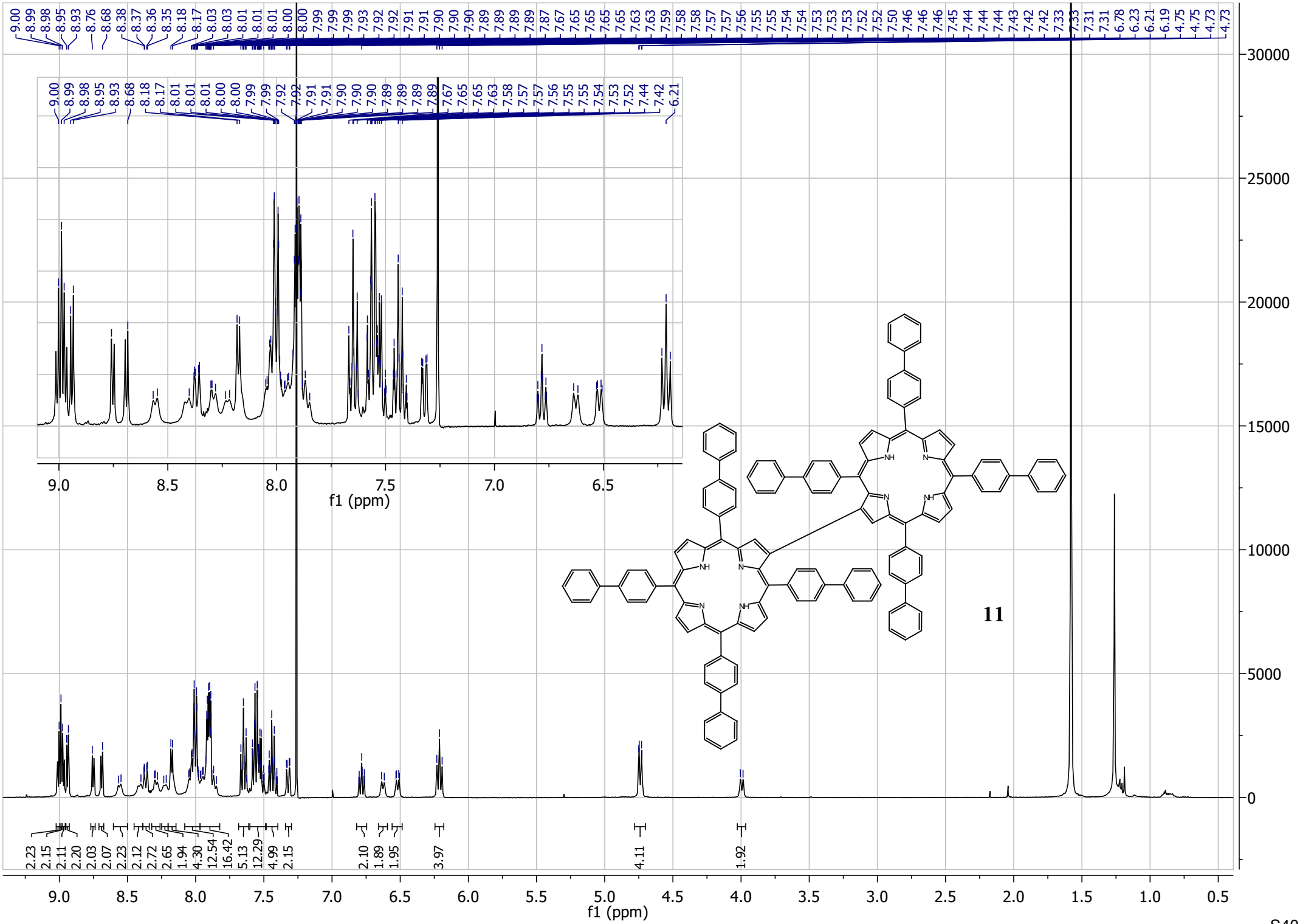
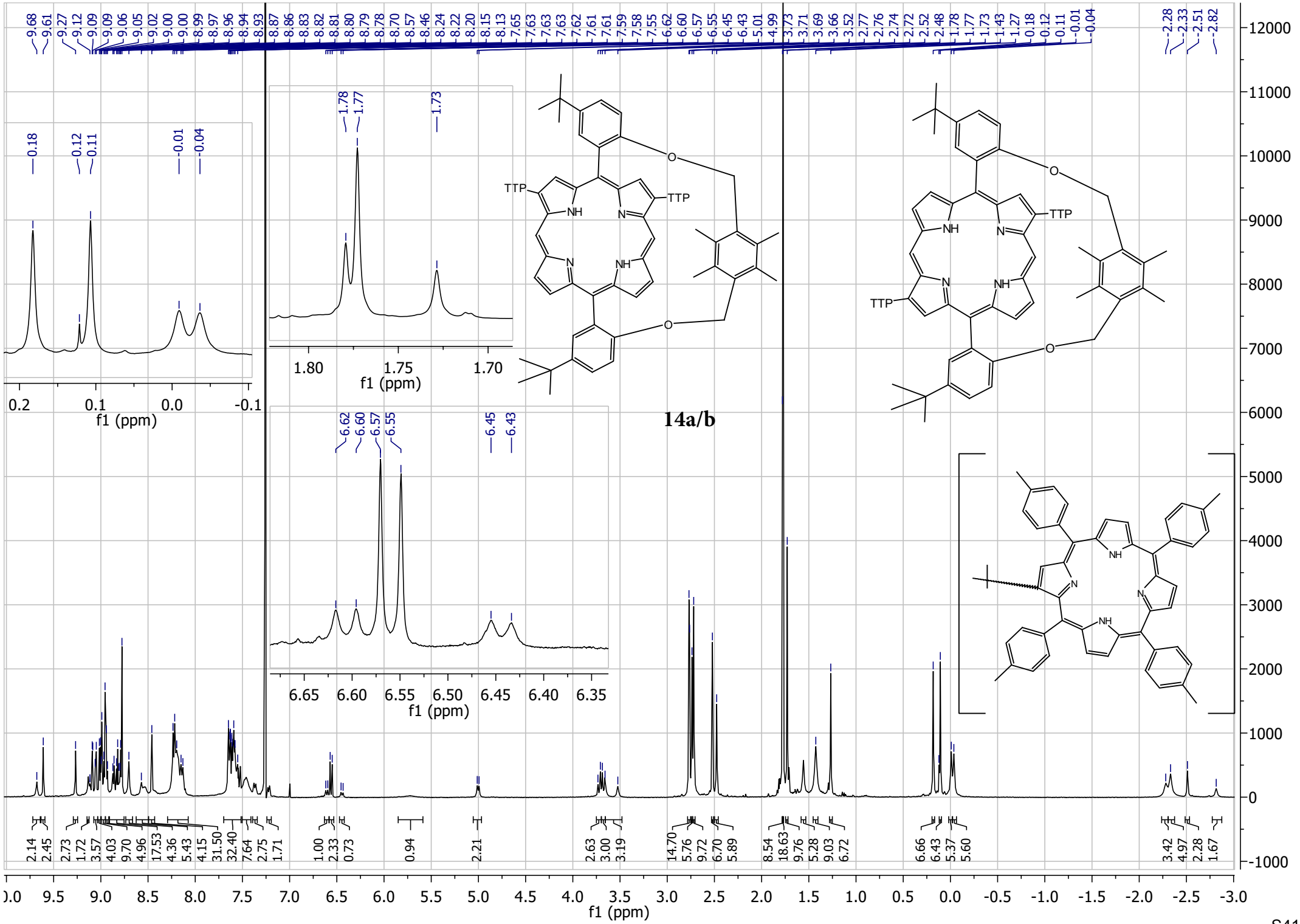
140.40
136.95
135.58
135.38
135.30
129.21
129.17
127.76
127.71
127.53
127.50
127.40
125.62
125.60
125.55
125.52
125.49
121.66
120.09
119.89
119.74
84.02
25.36
f1 (ppm)
10


f1 (ppm)
11


14a/b
f1 (ppm)
TTP
NH
N
O

12. Computational details

Cartesian coordinates and energies of the calculated structures

If not stated otherwise B97-D3/def2-TZVP energies are shown, no imaginary frequencies were found

Cu-1
energy: -3961.491191801866 Hartrees

C	-0.974243	-0.851673	2.749338
C	-2.170187	-0.399188	3.420261
C	-3.173862	-0.398411	2.494711
C	-2.585843	-0.784862	1.232817
C	-3.238913	-0.696152	-0.000001
C	-2.585837	-0.784824	-1.232820
C	-3.173857	-0.398376	-2.494715
C	-2.170180	-0.399138	-3.420262
C	-0.974233	-0.851618	-2.749339
C	0.264957	-1.042958	-3.369324
C	0.495382	-0.354487	-4.672241
C	1.131688	0.906472	-4.587450
C	1.283085	1.704396	-5.723348
C	0.828603	1.230632	-6.957298
C	0.231343	-0.024469	-7.061057
C	0.063820	-0.809430	-5.915440
N	-1.251417	-1.081402	1.419355
N	-1.251408	-1.081352	-1.419357
C	1.346402	-1.671342	-2.749242
C	2.558474	-2.074880	-3.423282
C	3.344955	-2.690966	-2.492572
C	2.643430	-2.613173	-1.232520
C	3.191184	-2.945149	-0.000013
H	4.179944	-3.394178	-0.000015
C	2.643429	-2.613188	1.232499
C	3.344954	-2.690994	2.492550
C	2.558472	-2.074921	3.423267
C	1.346397	-1.671381	2.749231
C	0.264948	-1.043009	3.369320
C	0.495370	-0.354537	4.672236
C	0.063831	-0.809492	5.915438
C	0.231346	-0.024527	7.061053
C	0.828574	1.230588	6.957290
C	1.283031	1.704366	5.723335
C	1.131641	0.906439	4.587438
N	1.418728	-2.014095	-1.420618
N	1.418726	-2.014115	1.420603
H	-2.229317	-0.133294	4.466134
H	-4.210267	-0.125491	2.636001
H	-4.210267	-0.125479	-2.636012
H	-2.229312	-0.133247	-4.466136
H	1.758253	2.677466	-5.649651
H	0.950758	1.849601	-7.842562
H	-0.112862	-0.388269	-8.024598
H	-0.425657	-1.777634	-5.977430
H	2.757582	-1.917526	-4.474741
H	4.324749	-3.130983	-2.627912
H	4.324749	-3.131011	2.627886
H	2.757578	-1.917579	4.474728
H	-0.425622	-1.777707	5.977431
H	-0.112840	-0.388336	8.024598
H	0.950723	1.849560	7.842553
H	1.758173	2.677448	5.649635
Cu	0.084288	-1.546052	-0.000005
C	4.164923	2.218815	1.421395
C	1.638729	2.609949	2.909503
C	1.638310	2.574260	1.401406
C	2.853937	2.441160	0.704800
C	1.638823	2.609969	-2.909517
C	0.413751	2.575353	0.704709
C	0.413775	2.575362	-0.704764
C	1.638358	2.574274	-1.401421
C	2.853961	2.441166	-0.704775
H	4.065187	2.202188	2.505704
O	1.574951	1.235209	3.343033
H	2.540801	3.088990	-3.304980
H	0.777705	3.156241	-3.306358
C	-0.912555	2.536226	1.424628
C	-0.912507	2.536238	-1.424727
O	1.575018	1.235231	-3.343050
C	4.164970	2.218825	-1.421328
H	-1.519931	1.702965	-1.058631
H	-0.817284	2.390422	-2.498924
H	-1.494422	3.451838	-1.252307
H	4.908804	2.980279	1.156344
H	4.588538	1.249036	1.131696
H	2.540684	3.088992	3.304991
H	0.777587	3.156200	3.306322
H	-1.494458	3.451833	1.252205
H	-0.817368	2.390390	2.498825
H	-1.519974	1.702965	1.058497
H	4.065272	2.202213	-2.505640
H	4.588573	1.249042	-1.131626
H	4.908844	2.980285	-1.156243
C	-4.688500	-0.332410	0.000012
C	-5.082630	1.011392	-0.000223
C	-5.671359	-1.327833	0.000281
H	-4.319238	1.784927	-0.000421
H	-5.367799	-2.371776	0.000475
C	-6.434694	1.353530	-0.000202
C	-7.025291	-0.987056	0.000304
H	-6.727926	2.400492	-0.000386
H	-7.778931	-1.770251	0.000511
C	-7.409391	0.354519	0.000060
H	-8.463329	0.620860	0.000075

In-1
energy: -8700.148674265598 Hartrees

C	8.596310	11.612234	7.998569
C	8.705374	12.991870	7.775696
C	7.624493	13.843884	7.336896
H	6.627355	13.502156	7.097457
C	8.109300	15.121641	7.295457
H	7.579372	16.024928	7.021234
C	9.477517	15.070484	7.749892
C	10.273033	16.183137	8.019600
C	11.489221	16.190528	8.701524
C	12.157961	17.369962	9.195715
H	11.836917	18.387856	9.014440
C	13.213013	16.944941	9.954648
H	13.920034	17.545847	10.509389
C	13.222664	15.501408	9.900458
C	14.130762	14.680598	10.580956

C	14.149270	13.275702	10.541349
C	15.116113	12.454477	11.228375
H	15.944441	12.828762	11.812771
C	14.790832	11.149829	10.979550
H	15.310680	10.267175	11.321464
C	13.588520	11.154034	10.179955
C	12.847135	10.013818	9.823836
C	11.578894	10.036375	9.215997
C	10.699331	8.895163	9.111121
H	10.952364	7.886017	9.402012
C	9.498733	9.351556	8.643593
H	8.594903	8.784072	8.472674
C	9.637653	10.769937	8.421556
C	7.212859	11.079824	8.195392
C	6.410172	10.458147	7.247996
H	6.786810	10.337618	6.235579
C	5.137808	9.985961	7.596335
H	4.516281	9.499239	6.850449
C	4.676241	10.138864	8.901875
H	3.690805	9.770666	9.175744
C	5.464616	10.765443	9.874480
H	5.096527	10.884118	10.888705
C	6.727446	11.236897	9.517100
C	7.392252	12.031446	11.745899
H	7.205931	11.055144	12.207173
H	6.511003	12.658077	11.926429
C	8.650200	12.676247	12.277910
C	9.723318	11.871815	12.713228
C	10.850720	12.483117	13.294837
C	10.906452	13.887933	13.393712
C	9.897852	14.689665	12.829583
C	8.764517	14.077597	12.259484
C	12.019744	11.647560	13.769850
H	12.915778	11.847220	13.169841
H	11.811387	10.580612	13.705171
H	12.270230	11.857591	14.815675
C	7.730307	14.945838	11.580128
H	7.041493	14.373089	10.960341
H	8.221882	15.664983	10.916969
H	7.143067	15.528282	12.302927
C	12.135580	14.549406	13.970768
H	11.882007	15.420111	14.589309
H	12.730229	13.865338	14.581807
C	14.200318	15.366755	12.925460
C	14.825806	15.830443	14.083065
H	14.286902	15.865811	15.024859
C	16.156907	16.255963	14.010334
H	16.646702	16.621267	14.909406
C	16.853373	16.221326	12.803727
H	17.885123	16.557495	12.758397
C	16.222668	15.738161	11.650476
H	16.760903	15.680957	10.707899
C	14.904162	15.301449	11.699798
N	9.821124	13.761962	8.001428
N	13.245150	12.460401	9.900452
N	10.915097	11.153185	8.756933
N	12.176213	15.074207	9.118328
O	12.907533	14.959618	12.828841
O	7.604713	11.875469	10.335405
In	11.786469	13.075181	8.465389
Cl	12.886805	12.902722	6.412634
H	9.850703	17.152367	7.770918
C	10.028115	16.192219	12.756044
H	9.097232	16.691578	13.043902
H	10.828030	16.581706	13.384787
H	10.259135	16.502820	11.728724
C	9.704441	10.373667	12.499140
H	10.632669	10.047070	12.021548
H	9.605840	9.818126	13.440857
H	8.902405	10.058787	11.833557
C	13.385190	8.678210	10.211371
C	13.489391	8.300930	11.557095
C	13.777511	7.766730	9.221759
C	13.977461	7.042507	11.906914
C	14.267708	6.508628	9.571013
C	14.368833	6.142549	10.914169
H	13.180065	9.001411	12.327171
H	13.699794	8.055774	8.177237
H	14.046650	6.762832	12.955139
H	14.574556	5.815086	8.792341
H	14.749451	5.161543	11.185973

Mg-1

energy: -2499.320309100221 Hartrees

C	-0.990495	-0.941586	2.800125
C	-2.187676	-0.475202	3.465564
C	-3.175139	-0.405267	2.520675
C	-2.580680	-0.778114	1.255108
C	-3.208986	-0.653681	0.000013
C	-2.580691	-0.778103	-1.255089
C	-3.175162	-0.405254	-2.520645
C	-2.187718	-0.475208	-3.465553
C	-0.990518	-0.941558	-2.800120
C	0.263929	-1.133883	-3.416244
C	0.468962	-0.429878	-4.718578
C	1.074201	0.846321	-4.617624
C	1.204894	1.664690	-5.740476
C	0.756868	1.198704	-6.980301
C	0.187888	-0.067840	-7.100682
C	0.042949	-0.874740	-5.966737
N	-1.261137	-1.125500	1.461107
N	-1.261148	-1.125488	-1.461100
C	1.409997	-1.674600	-2.802278
C	2.662374	-1.953420	-3.472431
C	3.534867	-2.405934	-2.520260
C	2.835241	-2.369756	-1.254485
C	3.413514	-2.594444	-0.000022
H	4.457944	-2.895637	-0.000027
C	2.835252	-2.369767	1.254448
C	3.534887	-2.405959	2.520219
C	2.662398	-1.953465	3.472403
C	1.410017	-1.674639	2.802260
C	0.263950	-1.133946	3.416244
C	0.468981	-0.429947	4.718580
C	0.042974	-0.874815	5.966739
C	0.187862	-0.067901	7.100677
C	0.756803	1.198660	6.980298
C	1.204843	1.664646	5.740479
C	1.074179	0.846273	4.617626
N	1.540119	-1.952587	-1.463074
N	1.540128	-1.952609	1.463052
H	-2.264224	-0.235221	4.516945
H	-4.201896	-0.096498	2.660204

H	-4.201922	-0.096493	-2.660164
H	-2.264284	-0.235245	-4.516937
H	1.657945	2.647254	-5.653677
H	0.861784	1.833308	-7.856660
H	-0.151700	-0.424474	-8.068584
H	-0.424385	-1.852839	-6.042242
H	2.842013	-1.820905	-4.531101
H	4.564643	-2.712860	-2.655287
H	4.564666	-2.712882	2.655236
H	2.842042	-1.820966	4.531075
H	-0.424330	-1.852929	6.042245
H	-0.151735	-0.424537	8.068575
H	0.861683	1.833273	7.856654
H	1.657870	2.647221	5.653681
Mg	0.146093	-1.521787	-0.000004
C	4.078170	1.979839	1.423785
C	1.583516	2.528682	2.910483
C	1.575166	2.465516	1.401907
C	2.782621	2.270182	0.704854
C	1.583587	2.528710	-2.910473
C	0.350785	2.505773	0.705350
C	0.350808	2.505810	-0.705370
C	1.575199	2.465545	-1.401901
C	2.782635	2.270193	-0.704815
H	3.976363	1.978270	2.507955
O	1.509742	1.164646	3.366871
H	2.494759	3.005049	-3.289612
H	0.731455	3.093276	-3.301092
C	-0.974781	2.510123	1.427627
C	-0.974737	2.510242	-1.427683
O	1.509774	1.164678	-3.366868
C	4.078186	1.979849	-1.423730
H	-1.613388	1.702000	-1.057921
H	-0.881379	2.351446	-2.500331
H	-1.523755	3.447784	-1.264600
H	4.864528	2.694347	1.151815
H	4.442587	0.983616	1.144202
H	2.494660	3.005053	3.289646
H	0.731356	3.093216	3.301085
H	-1.523795	3.447682	1.264635
H	-0.881454	2.351201	2.500258
H	-1.613426	1.701925	1.057753
H	3.976394	1.978314	-2.507904
H	4.442582	0.983612	-1.144170
H	4.864551	2.694337	-1.151730
C	-4.644727	-0.230619	0.000022
C	-4.987259	1.127367	-0.000313
C	-5.666795	-1.186145	0.000356
H	-4.195505	1.871630	-0.000575
H	-5.404349	-2.241281	0.000621
C	-6.325132	1.522224	-0.000326
C	-7.006401	-0.793195	0.000344
H	-6.577055	2.579998	-0.000591
H	-7.790154	-1.546301	0.000600
C	-7.338113	0.562271	0.000002
H	-8.380796	0.869534	-0.000012

Ni-1

energy: -3826.314886245016 Hartrees

C	0.995621	0.782926	2.678416
C	2.161119	0.269790	3.349491
C	3.185104	0.290441	2.448174
C	2.636774	0.743847	1.193739
C	3.305261	0.650644	-0.027001
C	2.628634	0.724524	-1.243534
C	3.175211	0.310424	-2.511993
C	2.141633	0.275439	-3.401785
C	0.972973	0.756952	-2.713090
C	-0.256418	1.000635	-3.321692
C	-0.556647	0.321949	-4.613271
C	-1.240120	-0.912359	-4.518985
C	-1.473965	-1.683337	-5.660610
C	-1.050626	-1.209271	-6.905356
C	-0.402395	0.019418	-7.015938
C	-0.156111	0.777541	-5.866654
N	1.299779	1.061013	1.357970
N	1.284549	1.026228	-1.393496
C	-1.232875	1.773212	-2.704605
C	-2.373712	2.340737	-3.377893
C	-2.999618	3.155543	-2.479982
C	-2.292609	3.026197	-1.230564
C	-2.757862	3.495657	-0.014493
H	-3.640705	4.127557	-0.014353
C	-2.278977	3.044471	1.203337
C	-2.970891	3.192688	2.458936
C	-2.336590	2.387964	3.360315
C	-1.205565	1.807995	2.681584
C	-0.226966	1.035292	3.296033
C	-0.520023	0.367814	4.594908
C	-0.102017	0.830106	5.840128
C	-0.344323	0.085004	6.998688
C	-1.005817	-1.137980	6.905561
C	-1.445623	-1.619095	5.669312
C	-1.215522	-0.861055	4.518211
N	-1.200427	2.197396	-1.392085
N	-1.187066	2.215204	1.363427
H	2.185510	-0.041038	4.384050
H	4.210588	-0.017758	2.593485
H	4.209412	0.048923	-2.681806
H	2.164460	-0.012469	-4.443014
H	-1.987780	-2.636019	-5.583294
H	-1.236660	-1.808176	-7.793232
H	-0.080847	0.383364	-7.987161
H	0.369771	1.726186	-5.933990
H	-2.624147	2.156111	-4.413376
H	-3.885565	3.761102	-2.622892
H	-3.853620	3.802413	2.604102
H	-2.575744	2.217366	4.400933
H	0.433632	1.774188	5.893793
H	-0.009694	0.454490	7.963358
H	-1.189351	-1.726922	7.800588
H	-1.968913	-2.567620	5.605777
Ni	0.052844	1.628576	-0.016334
C	-4.357902	-2.442163	1.517558
C	-1.846350	-2.585452	2.914269
C	-1.850055	-2.630178	1.406390
C	-3.079281	-2.560422	0.713939
C	-1.840317	-2.624555	-2.889516
C	-0.626093	-2.631747	0.719389
C	-0.624112	-2.638617	-0.690914
C	-1.846111	-2.648270	-1.381209
C	-3.077396	-2.571747	-0.693036
H	-4.256172	-1.692027	2.307520

O	-1.626899	-1.202107	3.267019
H	-2.780762	-2.989878	-3.310959
H	-1.030054	-3.232659	-3.306721
C	0.699102	-2.580017	1.438383
C	0.703257	-2.588141	-1.406317
O	-1.637732	-1.243729	-3.260727
C	-4.353791	-2.469893	-1.502463
H	1.280405	-1.719408	-1.073392
H	0.610228	-2.500842	-2.487059
H	1.311269	-3.475117	-1.183518
H	-4.625333	-3.394413	1.994347
H	-5.209952	-2.145594	0.908232
H	-2.791478	-2.932905	3.340136
H	-1.044069	-3.197805	3.340589
H	1.307883	-3.466820	1.217689
H	0.603140	-2.493196	2.518828
H	1.278815	-1.711915	1.108394
H	-4.255610	-1.723380	-2.296482
H	-5.211531	-2.178835	-0.898587
H	-4.609888	-3.427394	-1.974858
C	4.754249	0.303813	-0.012172
C	5.194152	-0.976522	-0.374646
C	5.700101	1.253350	0.394920
H	4.461455	-1.720466	-0.674531
H	5.361900	2.244756	0.683379
C	6.550840	-1.296715	-0.341209
C	7.057854	0.934879	0.426923
H	6.877002	-2.294966	-0.621232
H	7.780769	1.684451	0.738474
C	7.486916	-0.340919	0.057662
H	8.544631	-0.590395	0.083671

Pd-1

energy: -7390.041018284742 Hartrees

C	-2.875290	1.031661	-0.696871
C	-3.545011	2.248402	-0.308358
C	-2.609164	3.240142	-0.307505
C	-1.336804	2.626351	-0.608617
C	-0.104593	3.272101	-0.484119
C	1.121530	2.603265	-0.470286
C	2.387639	3.220195	-0.158582
C	3.316544	2.224559	-0.093443
C	2.644382	0.988995	-0.420196
C	3.265654	-0.259114	-0.515027
C	4.663426	-0.411151	-0.034609
C	4.928104	-1.276171	1.048933
C	6.234048	-1.435950	1.520542
C	7.290168	-0.755575	0.917063
C	7.044676	0.086596	-0.168131
C	5.741944	0.251165	-0.635385
N	-1.531614	1.286594	-0.865801
N	1.308488	1.246813	-0.639288
C	2.643518	-1.395454	-1.033075
C	3.331587	-2.620350	-1.371727
C	2.405622	-3.464132	-1.907280
C	1.139695	-2.776535	-1.872611
C	-0.065732	-3.319880	-2.281041
H	-0.048653	-4.327566	-2.683840
C	-1.297977	-2.709748	-2.137777
C	-2.570083	-3.335566	-2.399601
C	-3.532260	-2.469453	-1.971841
C	-2.853286	-1.293130	-1.485426
C	-3.496144	-0.202201	-0.897772
C	-4.763811	-0.488344	-0.176830
C	-6.000965	0.117262	-0.402806
C	-7.077012	-0.109109	0.457822
C	-6.916597	-0.943336	1.564627
C	-5.698424	-1.585211	1.796058
C	-4.630666	-1.380197	0.919593
N	1.312466	-1.518642	-1.338655
N	-1.502261	-1.451904	-1.613869
H	-4.597402	2.330454	-0.079992
H	-2.747145	4.282858	-0.059719
H	2.535626	4.276603	0.012273
H	4.363171	2.313664	0.155986
H	6.402711	-2.111710	2.354396
H	8.302913	-0.891810	1.287370
H	7.864925	0.603496	-0.657889
H	5.547586	0.886468	-1.495041
H	4.388046	-2.791785	-1.225300
H	2.549305	-4.469504	-2.281292
H	-2.693279	-4.321097	-2.829543
H	-4.605991	-2.599648	-1.970478
H	-6.112954	0.779441	-1.257243
H	-8.033364	0.369754	0.268662
H	-7.748887	-1.114348	2.242822
H	-5.577364	-2.258214	2.640444
Pd	-0.100320	-0.097846	-1.144908
C	-0.984692	-4.313914	1.442388
C	-2.707600	-2.080730	2.276164
C	-1.227647	-1.865361	2.038836
C	-0.391700	-2.972660	1.809808
C	3.023659	-1.431938	2.543743
C	-0.676175	-0.579948	2.162508
C	0.722723	-0.421728	2.255203
C	1.555530	-1.557229	2.189227
C	1.001891	-2.830317	1.940026
H	-2.001345	-4.210939	1.059781
O	-3.439518	-2.035931	1.025741
H	3.203268	-1.938655	3.503659
H	3.317841	-0.391315	2.669284
C	-1.587767	0.615565	2.287204
C	1.269944	0.951931	2.556853
O	3.937605	-2.054140	1.595858
C	1.877159	-4.058327	1.855579
H	0.659637	1.726518	2.094191
H	2.283731	1.101974	2.187154
H	1.275319	1.147128	3.637983
H	-1.004390	-5.013578	2.289572
H	-0.391880	-4.782305	0.650935
H	-2.877315	-3.059239	2.739547
H	-3.106896	-1.317827	2.950864
H	-1.713481	0.935710	3.330802
H	-2.576921	0.416097	1.879989
H	-1.210456	1.479128	1.740303
H	2.184988	-4.252907	0.821784
H	1.352601	-4.944024	2.222812
H	2.793974	-3.946481	2.435274
C	-0.117812	4.741194	-0.226342
C	0.205842	5.249562	1.038608
C	-0.477771	5.635066	-1.242538
H	0.476783	4.558042	1.831402
H	-0.733780	5.243801	-2.223321

C	0.176446	6.622305	1.280761
C	-0.505302	7.008880	-1.002484
H	0.425688	7.001720	2.268361
H	-0.780111	7.691137	-1.802779
C	-0.178064	7.506230	0.260098
H	-0.201063	8.576653	0.448548

Zn-1

energy: -4103.724875770310 Hartrees

C	-0.981313	-0.919036	2.784107
C	-2.177672	-0.454949	3.450665
C	-3.168728	-0.402316	2.510760
C	-2.575696	-0.779133	1.246463
C	-3.211354	-0.665366	-0.000002
C	-2.575695	-0.779125	-1.246466
C	-3.168727	-0.402311	-2.510764
C	-2.177671	-0.454940	-3.450668
C	-0.981310	-0.919024	-2.784109
C	0.265573	-1.112992	-3.402256
C	0.477537	-0.414013	-4.705166
C	1.086157	0.860505	-4.607486
C	1.222731	1.672723	-5.734447
C	0.778178	1.201487	-6.973438
C	0.206482	-0.064215	-7.089840
C	0.055080	-0.864774	-5.952319
N	-1.253518	-1.115188	1.448216
N	-1.253515	-1.115176	-1.448219
C	1.391491	-1.678099	-2.786046
C	2.634721	-1.990730	-3.456258
C	3.485089	-2.489572	-2.509447
C	2.783289	-2.443446	-1.246183
C	3.354232	-2.700095	-0.000003
H	4.385417	-3.042608	-0.000003
C	2.783289	-2.443450	1.246178
C	3.485088	-2.489579	2.509442
C	2.634719	-1.990740	3.456254
C	1.391490	-1.678109	2.786042
C	0.265570	-1.113004	3.402253
C	0.477534	-0.414027	4.705164
C	0.055079	-0.864791	5.952316
C	0.206479	-0.064233	7.089839
C	0.778172	1.201470	6.973439
C	1.222723	1.672710	5.734448
C	1.086150	0.860494	4.607486
N	1.505637	-1.976049	-1.450342
N	1.505637	-1.976054	1.450337
H	-2.248948	-0.207854	4.500619
H	-4.197950	-0.102045	2.649724
H	-4.197951	-0.102047	-2.649729
H	-2.248947	-0.207848	-4.500622
H	1.677688	2.654630	-5.650964
H	0.887853	1.831406	-7.852598
H	-0.130327	-0.424854	-8.057212
H	-0.414622	-1.841998	-6.024355
H	2.819738	-1.849339	-4.512726
H	4.503146	-2.833356	-2.642992
H	4.503145	-2.833363	2.642987
H	2.819736	-1.849352	4.512723
H	-0.414621	-1.842016	6.024351
H	-0.130328	-0.424874	8.057211
H	0.887846	1.831388	7.852599
H	1.677677	2.654618	5.650966
Zn	0.130962	-1.533891	-0.000002
C	4.094386	2.047685	1.422939
C	1.590876	2.552067	2.910333
C	1.584634	2.500211	1.401748
C	2.794404	2.320955	0.704727
C	1.590884	2.552074	-2.910330
C	0.360368	2.534479	0.705136
C	0.360370	2.534481	-0.705136
C	1.584638	2.500215	-1.401745
C	2.794406	2.320957	-0.704722
H	3.993290	2.042761	2.507201
O	1.518106	1.183747	3.357340
H	2.500103	3.026819	-3.295503
H	0.736991	3.111461	-3.304348
C	-0.965347	2.532035	1.427095
C	-0.965343	2.532038	-1.427098
O	1.518115	1.183756	-3.357340
C	4.094389	2.047688	-1.422930
H	-1.600914	1.722276	-1.055743
H	-0.872030	2.371792	-2.499523
H	-1.518023	3.467759	-1.265702
H	4.870505	2.773996	1.152632
H	4.473592	1.057608	1.141054
H	2.500094	3.026811	3.295511
H	0.736982	3.111452	3.304350
H	-1.518025	3.467757	1.265701
H	-0.872036	2.371784	2.499520
H	-1.600918	1.722276	1.055735
H	3.993297	2.042771	-2.507194
H	4.473592	1.057609	-1.141050
H	4.870509	2.773996	-1.152617
C	-4.650453	-0.256585	-0.000000
C	-5.004795	1.098221	-0.000088
C	-5.662813	-1.222140	0.000092
H	-4.219319	1.849165	-0.000159
H	-5.390309	-2.274683	0.000162
C	-6.346311	1.480367	-0.000087
C	-7.006046	-0.841584	0.000094
H	-6.608313	2.535653	-0.000157
H	-7.782728	-1.601954	0.000165
C	-7.350193	0.510818	0.000004
H	-8.395704	0.808340	0.000004

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energy: -2298.192388439009 Hartrees

C	-0.942303	-0.872417	2.802683
C	-2.126960	-0.414947	3.468345
C	-3.147621	-0.377505	2.547812
C	-2.607892	-0.746183	1.269970
C	-3.238362	-0.660145	0.019050
C	-2.587674	-0.809270	-1.224312
C	-3.178778	-0.369491	-2.486415
C	-2.188567	-0.434834	-3.416854
C	-1.013897	-0.966104	-2.735155
C	0.218569	-1.182963	-3.382044
C	0.447502	-0.465074	-4.672624
C	1.016254	0.826645	-4.549993
C	1.209586	1.627205	-5.678161
C	0.849096	1.133293	-6.936164
C	0.304643	-0.141937	-7.072553

C	0.105336	-0.934900	-5.936228
N	-1.287476	-1.073143	1.486698
N	-1.284033	-1.190202	-1.410819
C	1.334836	-1.805898	-2.813623
C	2.568466	-2.142547	-3.464331
C	3.405112	-2.700270	-2.526064
C	2.728114	-2.675529	-1.261561
C	3.273943	-2.924107	-0.004336
H	4.293280	-3.299904	0.004575
C	2.710647	-2.589881	1.231040
C	3.467039	-2.596239	2.480637
C	2.667528	-2.011457	3.412401
C	1.410279	-1.698951	2.735650
C	0.321513	-1.082434	3.374305
C	0.558690	-0.387701	4.675688
C	0.183874	-0.871444	5.926432
C	0.347422	-0.088095	7.074098
C	0.883435	1.194052	6.963995
C	1.279467	1.697762	5.721518
C	1.131728	0.902552	4.582703
N	1.470320	-2.176316	-1.498470
N	1.459727	-2.070710	1.421912
H	-2.179859	-0.171599	4.519549
H	-4.175927	-0.097014	2.720281
H	-4.191153	-0.013960	-2.619106
H	-2.238129	-0.155861	-4.460539
H	1.639997	2.618652	-5.583157
H	1.000974	1.756457	-7.813944
H	0.028846	-0.517493	-8.053548
H	-0.336395	-1.923914	-6.024158
H	2.764718	-1.975541	-4.514119
H	4.413874	-3.062866	-2.671621
H	4.477509	-2.967538	2.602159
H	2.884550	-1.810961	4.453324
H	-0.258166	-1.861976	5.993160
H	0.047491	-0.474399	8.043837
H	1.002627	1.811440	7.850870
H	1.706978	2.692332	5.643898
C	4.083047	2.282087	1.470515
C	1.531219	2.642155	2.913034
C	1.556583	2.620623	1.404489
C	2.781654	2.470892	0.725402
C	1.605140	2.539245	-2.904074
C	0.341179	2.634525	0.693277
C	0.356632	2.639828	-0.715394
C	1.588130	2.567330	-1.395244
C	2.791717	2.410904	-0.682276
H	4.013856	2.552365	2.523579
O	1.521887	1.260581	3.328756
H	2.570717	2.858164	-3.309433
H	0.837075	3.191816	-3.334346
C	-0.991010	2.601035	1.407354
C	-0.960823	2.649157	-1.452356
O	1.341485	1.173312	-3.276134
C	4.092919	2.121954	-1.398855
H	-1.490732	1.702543	-1.296402
H	-0.851529	2.765397	-2.529663
H	-1.618354	3.449676	-1.092630
H	4.891259	2.872223	1.027283
H	4.390859	1.228740	1.437624
H	2.405064	3.155860	3.328972
H	0.640043	3.143118	3.303003
H	-1.458145	3.594974	1.448363
H	-0.913842	2.218729	2.424643
H	-1.687856	1.942295	0.882938
H	3.931754	1.699444	-2.391007
H	4.685475	1.391466	-0.841156
H	4.714115	3.022114	-1.506859
C	-4.676471	-0.263844	0.004980
C	-5.081966	1.014278	0.414868
C	-5.649332	-1.167660	-0.443700
H	-4.331558	1.726398	0.746033
H	-5.339263	-2.157416	-0.767172
C	-6.428340	1.377062	0.383970
C	-6.996353	-0.807019	-0.472529
H	-6.725954	2.374102	0.698306
H	-7.738937	-1.522076	-0.817486
C	-7.389989	0.466437	-0.057768
H	-8.439444	0.748949	-0.082267
H	-0.635905	-1.334475	0.753819
H	0.791129	-1.972184	-0.772741

Ni-2

Energy: -7606.2793018050

C	-4.7286025	3.0395774	-0.6506594
C	-5.7841964	3.9560328	-1.0164853
C	-6.7411781	3.8734853	-0.0355869
C	-6.3249888	2.8259148	0.8728446
C	-7.1495741	2.2556956	1.8539196
C	-6.8413220	1.0188102	2.4419396
C	-7.8259834	0.1790279	3.0923051
C	-7.2431241	-1.0494993	3.2787791
C	-5.8746365	-0.9376741	2.8258740
C	-4.8968207	-1.9295220	2.9782184
C	-5.3033863	-3.3395525	3.2403677
C	-5.1624916	-4.2471964	2.1524772
C	-5.6232060	-5.5702590	2.2660945
C	-6.1962864	-6.0035940	3.4728905
C	-6.3074838	-5.1305370	4.5638938
C	-5.8627663	-3.8034042	4.4402356
N	-5.0762200	2.3499881	0.4994023
N	-5.6503332	0.3257606	2.3009633
C	-3.5390239	-1.6445507	2.7919717
C	-2.4675231	-2.5029087	3.2485568
C	-1.2922597	-1.8527389	2.9740394
C	-1.6452489	-0.6273362	2.2875229
C	-0.7268374	0.1827063	1.6163719
C	-1.1322992	1.1591477	0.6977762
C	-0.2454632	1.7658245	-0.2774182
C	-1.0443145	2.4375961	-1.1648094
C	-2.4061153	2.2973422	-0.7013158
C	-3.4939598	2.9350605	-1.3062357
C	-3.3323742	3.4185935	-2.7068510
C	-3.3508256	4.7651026	-3.0990487
C	-3.2516885	5.1257567	-4.4538305
C	-3.1316906	4.1271125	-5.4296168
C	-3.0927868	2.7712603	-5.0642745
C	-3.1788059	2.4146589	-3.7070453
N	-3.0239586	-0.4992185	2.2194502
N	-2.4440784	1.5211772	0.4394605
H	-5.7697526	4.6055932	-1.8915397
H	-7.6671634	4.4416041	0.0503497
H	-8.8471129	0.4856370	3.3205431
H	-7.6851799	-1.9496627	3.7055878

H	-5.5246122	-6.2608535	1.4223252
H	-6.5480824	-7.0387352	3.5592346
H	-6.7430668	-5.4776314	5.5076041
H	-5.9543381	-3.1070889	5.2816352
H	-2.6181607	-3.4643511	3.7412319
H	-0.2697736	-2.1736112	3.1762683
H	0.8389948	1.6526995	-0.2927921
H	-0.7589113	3.0008889	-2.0520850
H	-3.4450898	5.5365006	-2.3262951
H	-3.2681467	6.1826084	-4.7429255
H	-3.0579864	4.3998399	-6.4892966
H	-2.9830124	1.9969982	-5.8304066
Ni	-4.0437845	0.9281060	1.3707167
C	-1.6939124	-2.2387498	-3.7143841
C	-3.5224258	0.0239792	-4.0452258
C	-3.8680027	-1.0962938	-3.0855976
C	-2.9735949	-2.1829634	-2.8994197
C	-4.8973784	-4.2076616	-0.2688766
C	-5.0449413	-0.9782050	-2.3114178
C	-5.3760300	-1.9979430	-1.3843185
C	-4.5192988	-3.1125213	-1.2436653
C	-3.2881228	-3.1841481	-1.9463553
H	-1.0102527	-1.4102710	-3.4503434
O	-3.1134716	1.1417942	-3.2437315
H	-4.3679122	-5.1523060	-0.4821145
H	-5.9812354	-4.4233337	-0.3140282
C	-5.9625967	0.2192722	-2.4130704
C	-6.6163063	-1.8227024	-0.5369274
O	-4.5622792	-3.7387443	1.0455284
C	-2.3243752	-4.3134941	-1.6290624
H	-6.5405224	-0.8912404	0.0507743
H	-6.7767797	-2.6326659	0.1861277
H	-7.5260864	-1.7335654	-1.1591524
H	-1.8999105	-2.1637331	-4.7969853
H	-1.1421273	-3.1770936	-3.5712651
H	-2.7124916	-0.2502245	-4.7407715
H	-4.3989081	0.3139947	-4.6563243
H	-5.6612093	0.9479145	-3.1765144
H	-5.9845670	0.7610412	-1.4513289
H	-7.0021772	-0.0886190	-2.6281271
H	-2.3179428	-4.5340589	-0.5494839
H	-1.2886418	-4.0639740	-1.8936082
H	-2.5814325	-5.2490759	-2.1636462
C	-8.4733958	2.8727670	2.1690494
C	-9.5175870	2.8924279	1.2215555
C	-8.7086513	3.4152038	3.4488025
H	-9.3484090	2.4498309	0.2334285
H	-7.9025435	3.3939103	4.1910661
C	-10.7619654	3.4531141	1.5417859
C	-9.9532274	3.9759651	3.7693539
H	-11.5657344	3.4562228	0.7956614
H	-10.1190648	4.3978668	4.7679116
C	-10.9826284	3.9988207	2.8159940
H	-11.9559928	4.4372813	3.0663734
C	4.7286025	-3.0395774	-0.6506594
C	5.7841964	-3.9560328	-1.0164853
C	6.7411781	-3.8734853	-0.0355869
C	6.3249888	-2.8259148	0.8728446
C	7.1495741	-2.2556956	1.8539196
C	6.8413220	-1.0188102	2.4419396
C	7.8259834	-0.1790279	3.0923051
C	7.2431241	1.0494993	3.2787791
C	5.8746365	0.9376741	2.8258740
C	4.8968207	1.9295220	2.9782184
C	5.3033863	3.3395525	3.2403677
C	5.1624916	4.2471964	2.1524772
C	5.6232060	5.5702590	2.2660945
C	6.1962864	6.0035940	3.4728905
C	6.3074838	5.1305370	4.5638938
C	5.8627663	3.8034042	4.4402356
N	5.0762200	-2.3499881	0.4994023
N	5.6503332	-0.3257606	2.3009633
C	3.5390239	1.6445507	2.7919717
C	2.4675231	2.5029087	3.2485568
C	1.2922597	1.8527389	2.9740394
C	1.6452489	0.6273362	2.2875229
C	0.7268374	-0.1827063	1.6163719
C	1.1322992	-1.1591477	0.6977762
C	0.2454632	-1.7658245	-0.2774182
C	1.0443145	-2.4375961	-1.1648094
C	2.4061153	-2.2973422	-0.7013158
C	3.4939598	-2.9350605	-1.3062357
C	3.3323742	-3.4185935	-2.7068510
C	3.3508256	-4.7651026	-3.0990487
C	3.2516885	-5.1257567	-4.4538305
C	3.1316906	-4.1271125	-5.4296168
C	3.0927868	-2.7712603	-5.0642745
C	3.1788059	-2.4146589	-3.7070453
N	3.0239586	0.4992185	2.2194502
N	2.4440784	-1.5211772	0.4394605
H	5.7697526	-4.6055932	-1.8915397
H	7.6671634	-4.4416041	0.0503497
H	8.8471129	-0.4856370	3.3205431
H	7.6851799	1.9496627	3.7055878
H	5.5246122	6.2608535	1.4223252
H	6.5480824	7.0387352	3.5592346
H	6.7430668	5.4776314	5.5076041
H	5.9543381	3.1070889	5.2816352
H	2.6181607	3.4643511	3.7412319
H	0.2697736	2.1736112	3.1762683
H	-0.8389948	-1.6526995	-0.2927921
H	0.7589113	-3.0008889	-2.0520850
H	3.4450898	-5.5365006	-2.3262951
H	3.2681467	-6.1826084	-4.7429255
H	3.0579864	-4.3998399	-6.4892966
H	2.9830124	-1.9969982	-5.8304066
Ni	4.0437845	-0.9281060	1.3707167
C	1.6939124	2.2387498	-3.7143841
C	3.5224258	-0.0239792	-4.0452258
C	3.8680027	1.0962938	-3.0855976
C	2.9735949	2.1829634	-2.8994197
C	4.8973784	4.2076616	-0.2688766
C	5.0449413	0.9782050	-2.3114178
C	5.3760300	1.9979430	-1.3843185
C	4.5192988	3.1125213	-1.2436653
C	3.2881228	3.1841481	-1.9463553
H	1.0102527	1.4102710	-3.4503434
O	3.1134716	-1.1417942	-3.2437315
H	4.3679122	5.1523060	-0.4821145
H	5.9812354	4.4233337	-0.3140282
C	5.9625967	-0.2192722	-2.4130704
C	6.6163063	1.8227024	-0.5369274
O	4.5622792	3.7387443	1.0455284
C	2.3243752	4.3134941	-1.6290624

H	6.5405224	0.8912404	0.0507743
H	6.7767797	2.6326659	0.1861277
H	7.5260864	1.7335654	-1.1591524
H	1.8999105	2.1637331	-4.7969853
H	1.1421273	3.1770936	-3.5712651
H	2.7124916	0.2502245	-4.7407715
H	4.3989081	-0.3139947	-4.6563243
H	5.6612093	-0.9479145	-3.1765144
H	5.9845670	-0.7610412	-1.4513289
H	7.0021772	0.0886190	-2.6281271
H	2.3179428	4.5340589	-0.5494839
H	1.2886418	4.0639740	-1.8936082
H	2.5814325	5.2490759	-2.1636462
C	8.4733958	-2.8727670	2.1690494
C	9.5175870	-2.8924279	1.2215555
C	8.7086513	-3.4152038	3.4488025
H	9.3484090	-2.4498309	0.2334285
H	7.9025435	-3.3939103	4.1910661
C	10.7619654	-3.4531141	1.5417859
C	9.9532274	-3.9759651	3.7693539
H	11.5657344	-3.4562228	0.7956614
H	10.1190648	-4.3978668	4.7679116
C	10.9826284	-3.9988207	2.8159940
H	11.9559928	-4.4372813	3.0663734

Ni-3

energy: -12293.34759189 Hartrees

C	0.000000	-5.523192	-0.239985
C	0.000000	-6.739944	0.032572
C	0.000000	-7.422525	0.996843
C	0.000000	-6.665478	1.253793
C	0.000000	-7.112116	1.970035
C	0.000000	-6.554982	1.846346
C	0.000000	-7.201994	2.197011
C	0.000000	-6.432220	1.673956
C	0.000000	-5.270630	1.077595
C	0.000000	-4.169502	0.564371
C	0.000000	-4.323982	0.236895
C	0.000000	-4.578216	-1.127189
C	0.000000	-4.850683	-1.517974
C	0.000000	-4.836754	-0.553972
C	0.000000	-4.555165	0.788968
C	0.000000	-4.303704	1.178278
N	0.000000	-5.494779	0.507277
N	0.000000	-5.366653	1.180505
C	0.000000	-2.952124	0.298515
C	0.000000	-1.695641	0.113394
C	0.000000	-0.713969	0.083881
C	0.000000	-1.409051	0.179747
C	0.000000	-0.736367	-0.009926
C	0.000000	-1.484313	-0.432346
C	0.000000	-0.964433	-1.237147
C	0.000000	-2.043071	-1.651042
C	0.000000	-3.215474	-1.049304
C	0.000000	-4.491623	-1.078503
C	0.000000	-4.797135	-2.076440
C	0.000000	-4.838493	-1.793559
C	0.000000	-5.217733	-2.781302
C	0.000000	-5.563629	-4.060442
C	0.000000	-5.520711	-4.372252
C	0.000000	-5.125137	-3.385512
N	0.000000	-2.759262	0.312214
N	0.000000	-2.856867	-0.336520
H	0.000000	-7.014809	-0.439262
H	0.000000	-8.378055	1.459678
H	0.000000	-8.148727	2.730548
H	0.000000	-6.613912	1.709763
H	0.000000	-5.059510	-2.567002
H	0.000000	-5.043202	-0.863131
H	0.000000	-4.538765	1.534023
H	0.000000	-4.103450	2.227873
H	0.000000	-1.579230	0.042278
H	0.000000	0.086055	-1.488628
H	0.000000	-2.055427	-2.283703
H	0.000000	-4.582256	-0.782503
H	0.000000	-5.248398	-2.548162
H	0.000000	-5.868049	-4.833930
H	0.000000	-5.783686	-5.377471
Ni	0.000000	-4.118227	0.434379
C	0.000000	-3.715792	-5.960924
C	0.000000	-5.692643	-4.638281
C	0.000000	-5.627832	-4.310755
C	0.000000	-4.638558	-4.919451
C	0.000000	-5.317484	-3.172390
C	0.000000	-6.467266	-3.293951
C	0.000000	-6.372534	-2.932240
C	0.000000	-5.422778	-3.576772
C	0.000000	-4.507709	-4.518962
H	0.000000	-3.078284	-5.522123
O	0.000000	-5.015067	-3.567213
H	0.000000	-4.845923	-3.959466
H	0.000000	-6.312526	-2.969436
C	0.000000	-7.433770	-2.531192
C	0.000000	-7.257616	-1.816343
O	0.000000	-4.528179	-1.972390
C	0.000000	-3.372492	-5.042265
H	0.000000	-7.095216	-0.903102
H	0.000000	-7.067654	-1.540787
H	0.000000	-8.329716	-2.070500
H	0.000000	-4.287015	-6.785415
H	0.000000	-3.052061	-6.421994
H	0.000000	-5.206936	-5.598645
H	0.000000	-6.736506	-4.697438
H	0.000000	-7.465282	-2.887004
H	0.000000	-7.143948	-1.466626
H	0.000000	-8.462160	-2.564225
H	0.000000	-3.062981	-4.299434
H	0.000000	-2.476487	-5.258686
H	0.000000	-3.639589	-5.975493
Br	0.000000	-8.701714	3.024852
C	0.000000	5.523192	0.239985
C	0.000000	6.739944	-0.032572
C	0.000000	7.422525	-0.996843
C	0.000000	6.665478	-1.253793
C	0.000000	7.112116	-1.970035
C	0.000000	6.554982	-1.846346
C	0.000000	7.201994	-2.197011
C	0.000000	6.432220	-1.673956
C	0.000000	5.270630	-1.077595
C	0.000000	4.169502	-0.564371
C	0.000000	4.323982	-0.236895
C	0.000000	4.578216	1.127189
C	0.000000	4.850683	1.517974

C	0.000000	4.836754	0.553972
C	0.000000	4.555165	-0.788968
C	0.000000	4.303704	-1.178278
N	0.000000	5.494779	-0.507277
N	0.000000	5.366653	-1.180505
C	0.000000	2.952124	-0.298515
C	0.000000	1.695641	-0.113394
C	0.000000	0.713969	-0.083881
C	0.000000	1.409051	-0.179747
C	0.000000	0.736367	0.009926
C	0.000000	1.484313	0.432346
C	0.000000	0.964433	1.237147
C	0.000000	2.043071	1.651042
C	0.000000	3.215474	1.049304
C	0.000000	4.491623	1.078503
C	0.000000	4.797135	2.076440
C	0.000000	4.838493	1.793559
C	0.000000	5.217733	2.781302
C	0.000000	5.563629	4.060442
C	0.000000	5.520711	4.372252
C	0.000000	5.125137	3.385512
N	0.000000	2.759262	-0.312214
N	0.000000	2.856867	0.336520
H	0.000000	7.014809	0.439262
H	0.000000	8.378055	-1.459678
H	0.000000	8.148727	-2.730548
H	0.000000	6.613912	-1.709763
H	0.000000	5.059510	2.567002
H	0.000000	5.043202	0.863131
H	0.000000	4.538765	-1.534023
H	0.000000	4.103450	-2.227873
H	0.000000	1.579230	-0.042278
H	0.000000	-0.086055	1.488628
H	0.000000	2.055427	2.283703
H	0.000000	4.582256	0.782503
H	0.000000	5.248398	2.548162
H	0.000000	5.868049	4.833930
H	0.000000	5.783686	5.377471
Ni	0.000000	4.118227	-0.434379
C	0.000000	3.715792	5.960924
C	0.000000	5.692643	4.638281
C	0.000000	5.627832	4.310755
C	0.000000	4.638558	4.919451
C	0.000000	5.317484	3.172390
C	0.000000	6.467266	3.293951
C	0.000000	6.372534	2.932240
C	0.000000	5.422778	3.576772
C	0.000000	4.507709	4.518962
H	0.000000	3.078284	5.522123
O	0.000000	5.015067	3.567213
H	0.000000	4.845923	3.959466
H	0.000000	6.312526	2.969436
C	0.000000	7.433770	2.531192
C	0.000000	7.257616	1.816343
O	0.000000	4.528179	1.972390
C	0.000000	3.372492	5.042265
H	0.000000	7.095216	0.903102
H	0.000000	7.067654	1.540787
H	0.000000	8.329716	2.070500
H	0.000000	4.287015	6.785415
H	0.000000	3.052061	6.421994
H	0.000000	5.206936	5.598645
H	0.000000	6.736506	4.697438
H	0.000000	7.465282	2.887004
H	0.000000	7.143948	1.466626
H	0.000000	8.462160	2.564225
H	0.000000	3.062981	4.299434
H	0.000000	2.476487	5.258686
H	0.000000	3.639589	5.975493
Br	0.000000	8.701714	-3.024852

6b_conf1

energy (B3LYP-D3): -3899.93276336114 Hartrees

C	2.706440	-2.326565	1.405916
C	1.498422	-2.255805	2.189336
C	0.689590	-1.285042	1.625870
C	1.402800	-0.713036	0.515378
C	0.983157	0.349955	-0.310966
C	1.846124	1.083667	-1.154427
C	1.459310	2.319868	-1.840867
C	2.614073	2.842029	-2.357041
C	3.676371	1.881451	-2.038650
C	5.024323	2.075800	-2.439187
C	5.416226	3.469803	-2.790044
C	5.396180	4.433480	-1.748211
C	5.696776	5.777596	-2.022962
C	6.027391	6.172030	-3.327556
C	6.067706	5.223897	-4.361576
C	5.760534	3.882328	-4.089840
N	2.605353	-1.365598	0.430772
N	3.180644	0.821064	-1.337613
C	6.018785	1.083707	-2.444885
C	7.365307	1.180493	-2.955777
C	7.958445	-0.061414	-2.821235
C	7.011924	-0.934161	-2.175979
C	7.228778	-2.233979	-1.706802
H	8.193137	-2.686716	-1.961515
C	6.399142	-2.942619	-0.820353
C	6.822528	-4.171465	-0.143805
C	5.888488	-4.409895	0.827060
C	4.884554	-3.346876	0.696926
C	3.774117	-3.228004	1.563997
C	3.806939	-4.019582	2.828702
C	3.043512	-5.177927	3.050001
C	3.148515	-5.886015	4.257270
C	4.026797	-5.436213	5.255303
C	4.788467	-4.275561	5.054259
C	4.679550	-3.563739	3.848446
N	5.858611	-0.205816	-1.992092
N	5.203434	-2.494376	-0.323980
H	1.285608	-2.889362	3.050432
H	-0.305317	-0.973363	1.943447
H	0.452850	2.737036	-1.887538
H	2.744400	3.769241	-2.917190
H	5.664326	6.498062	-1.198371
H	6.258094	7.223700	-3.535618
H	6.324376	5.530755	-5.382111
H	5.760399	3.138720	-4.895380
H	7.798169	2.085311	-3.382677
H	8.969410	-0.354179	-3.111105
H	7.732603	-4.735807	-0.362741
H	5.865444	-5.214078	1.564399
H	2.373278	-5.527482	2.255807

H	2.552031	-6.792112	4.414346
H	4.118032	-5.989282	6.197828
H	5.479270	-3.905187	5.819652
C	7.454735	-1.063862	2.109378
C	4.828196	-1.166058	3.771611
C	5.101692	-0.175579	2.651866
C	6.328397	-0.069818	1.954183
C	6.032526	3.347504	0.293146
C	4.112607	0.802301	2.429221
C	4.308589	1.945520	1.632925
C	5.556266	2.078565	0.976512
C	6.501457	1.045686	1.112066
H	7.169183	-2.061152	1.740210
O	5.458630	-2.454949	3.642062
H	6.394297	4.049994	1.075202
H	6.898140	3.110325	-0.351329
H	3.147112	0.694795	2.941070
C	3.219551	2.987139	1.533286
O	5.048187	4.071425	-0.473025
H	7.454264	1.135667	0.573611
H	2.372913	2.734526	2.194437
H	2.840982	3.078114	0.502602
H	3.590391	3.990137	1.813351
H	7.734534	-1.197387	3.169799
H	8.347158	-0.729628	1.553427
H	3.736713	-1.297272	3.883516
H	5.199185	-0.726477	4.723251
N	-5.389976	1.837446	0.674105
C	-4.567593	2.864042	1.059098
C	-5.341537	3.956223	1.661950
C	-6.649376	3.563398	1.625094
C	-6.659388	2.230190	1.012420
C	-3.157483	2.901248	0.946653
C	-2.443770	4.120458	1.450428
C	-2.492497	5.328497	0.727275
C	-1.807262	6.462833	1.186053
C	-1.061838	6.404030	2.373463
C	-1.008407	5.205715	3.101960
C	-1.695993	4.072809	2.643930
C	-7.846161	1.485766	0.793580
C	-9.146521	2.060536	1.256880
C	-9.405351	2.232082	2.632788
C	-10.624679	2.768334	3.069360
C	-11.605804	3.140817	2.137550
C	-11.359522	2.974033	0.766116
C	-10.139676	2.438374	0.329528
C	-7.894706	0.226913	0.158705
N	-6.812237	-0.468720	-0.337737
C	-7.217191	-1.656295	-0.909478
C	-8.650639	-1.717210	-0.763218
C	-9.061167	-0.578116	-0.099903
C	-6.397655	-2.620248	-1.531496
C	-4.986984	-2.568294	-1.652344
N	-4.154424	-1.587412	-1.174296
C	-2.881996	-1.987764	-1.497298
C	-2.905867	-3.263978	-2.222794
C	-4.217936	-3.631134	-2.309043
C	-1.674206	-1.298062	-1.206039
C	-1.608749	-0.045855	-0.551120
N	-2.710772	0.688660	-0.151137
C	-2.331180	1.890141	0.410652
C	-0.896324	1.926186	0.363995
C	-0.437852	0.743442	-0.193578
C	-7.105641	-3.806481	-2.114670
C	-7.254662	-3.935236	-3.509899
C	-7.920679	-5.041113	-4.057141
C	-8.448268	-6.033255	-3.216280
C	-8.305075	-5.913854	-1.825397
C	-7.638413	-4.807718	-1.278696
C	-0.394455	-1.946588	-1.635834
C	0.046573	-3.134502	-1.015761
C	1.271153	-3.713766	-1.371134
C	2.075880	-3.113858	-2.351833
C	1.633358	-1.948375	-2.993946
C	0.403089	-1.374294	-2.645119
H	-4.930293	4.886797	2.054666
H	-7.525828	4.113569	1.969132
H	-3.070559	5.368810	-0.203088
H	-1.851589	7.395090	0.610277
H	-0.523220	7.289892	2.730326
H	-0.430642	5.152663	4.032537
H	-1.657797	3.135601	3.211124
H	-8.640576	1.934576	3.359099
H	-10.811214	2.891251	4.143035
H	-12.559482	3.560395	2.479240
H	-12.118469	3.268331	0.031213
H	-9.941919	2.316971	-0.741597
H	-9.270610	-2.538326	-1.121820
H	-10.075686	-0.305225	0.188800
H	-2.035062	-3.793669	-2.609121
H	-4.634845	-4.528024	-2.768154
H	-0.275399	2.735872	0.743712
H	-6.842672	-3.157360	-4.162899
H	-8.030549	-5.126775	-5.144905
H	-8.969081	-6.898181	-3.644085
H	-8.710676	-6.687469	-1.162275
H	-7.520901	-4.712918	-0.193006
H	-0.566452	-3.580561	-0.225675
H	1.616019	-4.618420	-0.857303
H	3.053656	-3.542065	-2.598127
H	2.258884	-1.468657	-3.755122
H	0.068187	-0.453259	-3.134129
H	-3.670271	0.357006	-0.281044
H	-5.849524	-0.129519	-0.274536
H	3.343122	-1.129298	-0.235084
H	5.046482	-0.540590	-1.468182

6b_conf2

energy (B3LYP-D3): -3899.93216146609 Hartrees

C	-3.725699	1.827545	-1.971590
C	-2.766918	2.893626	-2.121140
C	-1.592141	2.494354	-1.506184
C	-1.829312	1.210049	-0.902219
C	-0.953726	0.437322	-0.111916
C	-1.359705	-0.679620	0.653090
C	-0.512093	-1.288356	1.681238
C	-1.296505	-2.206684	2.322867
C	-2.595854	-2.183072	1.639928
C	-3.656909	-3.054498	1.992967
C	-3.570713	-3.700097	3.333131
C	-3.662395	-2.860235	4.473490
C	-3.523083	-3.401539	5.762110
C	-3.301421	-4.776202	5.927888

C	-3.227909	-5.618515	4.807661
C	-3.360080	-5.078115	3.520000
N	-3.117169	0.851782	-1.219130
N	-2.602508	-1.256009	0.637400
C	-4.802099	-3.295369	1.214934
C	-5.851873	-4.255273	1.455732
C	-6.742793	-4.180960	0.399715
C	-6.290411	-3.138841	-0.484555
C	-6.961962	-2.600832	-1.589011
H	-7.882311	-3.110715	-1.893494
C	-6.654798	-1.389345	-2.230447
C	-7.563621	-0.734943	-3.175877
C	-7.060183	0.520835	-3.376661
C	-5.822353	0.594956	-2.588218
C	-5.010227	1.752076	-2.543011
C	-5.606391	3.022745	-3.050779
C	-5.273893	3.607851	-4.284513
C	-5.904889	4.785164	-4.714829
C	-6.884769	5.385563	-3.909260
C	-7.223619	4.819274	-2.671763
C	-6.587029	3.644996	-2.237303
N	-5.110788	-2.658193	0.034930
N	-5.591240	-0.579433	-1.928983
H	-2.954453	3.818715	-2.666431
H	-0.649757	3.038652	-1.452930
H	0.522945	-1.017006	1.893153
H	-1.032496	-2.851498	3.162214
H	-3.590452	-2.725012	6.621014
H	-3.190264	-5.191091	6.936849
H	-3.053814	-6.693164	4.935314
H	-3.274375	-5.721447	2.636401
H	-5.895575	-4.916273	2.321489
H	-7.652877	-4.765238	0.250802
H	-8.476921	-1.173380	-3.586167
H	-7.467638	1.324877	-3.991611
H	-4.523544	3.116608	-4.915102
H	-5.639848	5.226001	-5.682785
H	-7.387147	6.301131	-4.243764
H	-7.985268	5.269681	-2.025877
C	-8.028653	0.799510	0.322296
C	-6.064106	3.214589	0.067983
C	-5.787170	1.947430	0.860892
C	-6.704070	0.884893	1.042371
C	-5.152882	-1.059441	3.928961
C	-4.580004	1.927559	1.586012
C	-4.268197	0.964016	2.562322
C	-5.202292	-0.079452	2.770417
C	-6.359539	-0.115758	1.972270
H	-7.892376	0.695417	-0.764838
O	-6.962410	3.076610	-1.047946
H	-5.599211	-0.567253	4.820281
H	-5.787120	-1.933373	3.693866
H	-3.856392	2.736153	1.415634
C	-2.991078	1.089199	3.357351
O	-3.844637	-1.509731	4.333525
H	-7.066120	-0.944113	2.116653
H	-2.467691	2.029627	3.113875
H	-2.306271	0.250283	3.156132
H	-3.186961	1.071778	4.444692
H	-8.630899	1.713539	0.470862
H	-8.611542	-0.064555	0.683787
H	-5.105611	3.642482	-0.278724
H	-6.520684	3.962909	0.752193
N	5.439417	1.896268	0.568636
C	4.663133	2.966710	0.929517
C	5.496793	4.090470	1.373227
C	6.790951	3.658663	1.298856
C	6.734631	2.278743	0.803811
C	3.247731	3.020195	0.907675
C	2.575806	4.241027	1.451965
C	2.690568	4.579997	2.816129
C	2.043082	5.712945	3.328379
C	1.270908	6.526416	2.484790
C	1.151290	6.200808	1.124843
C	1.797991	5.067246	0.613576
C	7.890595	1.482782	0.597712
C	9.212474	2.024178	1.035750
C	10.238940	2.274879	0.100808
C	11.477477	2.782893	0.516696
C	11.711210	3.047233	1.875047
C	10.697731	2.801830	2.814447
C	9.459070	2.295082	2.398409
C	7.889026	0.201520	0.006144
N	6.792206	-0.447375	-0.521772
C	7.152944	-1.673419	-1.039808
C	8.567870	-1.819676	-0.805547
C	9.015329	-0.679477	-0.168190
C	6.301881	-2.603363	-1.674437
C	4.895999	-2.476131	-1.816706
N	4.103785	-1.492911	-1.280257
C	2.818805	-1.807997	-1.645957
C	2.795946	-3.013922	-2.481926
C	4.091763	-3.431541	-2.587146
C	1.635970	-1.107718	-1.287673
C	1.612856	0.106313	-0.561808
N	2.734163	0.840192	-0.218416
C	2.387237	2.007924	0.426738
C	0.955105	2.004694	0.532468
C	0.466550	0.849515	-0.057053
C	6.954681	-3.829677	-2.229564
C	6.653762	-5.102308	-1.700802
C	7.265289	-6.253569	-2.215656
C	8.187598	-6.151548	-3.268703
C	8.494506	-4.890740	-3.803146
C	7.883794	-3.739240	-3.286905
C	0.331898	-1.704159	-1.717872
C	-0.483545	-1.053043	-2.663620
C	-1.733758	-1.581713	-3.013084
C	-2.182368	-2.774514	-2.428078
C	-1.363126	-3.448295	-1.510040
C	-0.113942	-2.920702	-1.161419
H	5.134668	5.073042	1.677699
H	7.698580	4.217421	1.529881
H	3.286701	3.938311	3.474493
H	2.136907	5.957915	4.393163
H	0.763692	7.411888	2.886020
H	0.555101	6.834939	0.457704
H	1.711888	4.815436	-0.449833
H	10.051382	2.078927	-0.960994
H	12.261407	2.979546	-0.224556
H	12.680050	3.444484	2.200432
H	10.873997	3.001472	3.878274
H	8.668449	2.096681	3.130692
H	9.150228	-2.698286	-1.080660

H	10.027789	-0.460790	0.169730
H	1.908660	-3.458225	-2.933278
H	4.477310	-4.285960	-3.144336
H	0.365072	2.766261	1.040167
H	5.936823	-5.178418	-0.875673
H	7.023482	-7.234688	-1.789536
H	8.665247	-7.052288	-3.672294
H	9.208786	-4.803292	-4.630706
H	8.115548	-2.755019	-3.709677
H	-0.143149	-0.109022	-3.103361
H	-2.372492	-1.047249	-3.725393
H	-3.175657	-3.166014	-2.674771
H	-1.711708	-4.374167	-1.037908
H	0.511166	-3.425846	-0.418026
H	3.688025	0.521995	-0.404313
H	5.838734	-0.081670	-0.478154
H	-4.604024	-1.852546	-0.340409
H	-3.561187	-0.008152	-0.888541

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energy (B3LYP-D3): -5813.39782573965 Hartrees

C	3.352571	-2.062681	2.266211
C	2.403361	-1.726075	3.299158
C	1.334460	-1.088313	2.695070
C	1.628047	-0.979857	1.291065
C	0.843927	-0.378900	0.286747
C	1.344922	-0.023460	-0.987778
C	0.611525	0.799366	-1.955004
C	1.519500	1.147867	-2.917992
C	2.773223	0.476786	-2.561778
C	3.967320	0.642759	-3.306250
C	4.034159	1.842510	-4.189090
C	4.109896	3.105941	-3.550519
C	4.127543	4.283459	-4.315463
C	4.080017	4.211298	-5.715492
C	4.025896	2.964211	-6.356923
C	4.002881	1.787582	-5.592803
N	2.852726	-1.561807	1.090186
N	2.627663	-0.253101	-1.416344
C	5.129667	-0.134021	-3.182342
C	6.356593	0.000439	-3.928260
C	7.208632	-1.010648	-3.524343
C	6.535383	-1.770067	-2.505038
C	7.041999	-2.855764	-1.762996
C	6.462063	-3.315483	-0.554937
C	7.087824	-4.313927	0.317969
C	6.419168	-4.245823	1.509689
C	5.360051	-3.248419	1.330037
C	4.516287	-2.837371	2.391725
C	4.992429	-3.143839	3.771694
C	4.424200	-4.123698	4.602857
C	4.960850	-4.385460	5.872804
C	6.077856	-3.663471	6.320203
C	6.648853	-2.672207	5.508631
C	6.109115	-2.406679	4.239935
N	5.295632	-1.205175	-2.335829
N	5.374794	-2.744479	0.058638
H	2.522836	-1.978965	4.352899
H	0.422266	-0.717082	3.162773
H	-0.435770	1.094421	-1.880437
H	1.365392	1.781664	-3.792741
H	4.177364	5.245649	-3.793855
H	4.090819	5.134082	-6.307830
H	3.991800	2.907308	-7.450994
H	3.942047	0.807369	-6.080524
H	6.538014	0.766542	-4.682322
H	8.215130	-1.222178	-3.885122
H	7.937905	-4.946453	0.059927
H	6.609378	-4.811054	2.423408
H	3.563296	-4.694011	4.233968
H	4.513335	-5.159293	6.507210
H	6.505344	-3.869320	7.308891
H	7.517975	-2.093001	5.839592
C	8.020198	-0.484303	1.021864
C	6.021243	-0.179975	3.354305
C	5.785215	0.363848	1.956791
C	6.742713	0.314472	0.915978
C	5.397372	2.901205	-1.540352
C	4.609076	1.110681	1.756699
C	4.373466	1.905214	0.619710
C	5.363962	1.910235	-0.391196
C	6.487182	1.075875	-0.239568
H	7.810893	-1.562979	1.103748
O	6.690050	-1.456797	3.439147
H	5.772490	3.872730	-1.151686
H	6.123312	2.553834	-2.296804
H	3.847799	1.108748	2.548012
C	3.113739	2.733589	0.528787
O	4.134588	3.182580	-2.181750
H	7.229790	1.046179	-1.047829
H	2.526636	2.659233	1.459649
H	2.479037	2.404345	-0.309830
H	3.338206	3.800296	0.343425
H	8.598915	-0.215998	1.925021
H	8.660886	-0.317832	0.139973
H	5.056569	-0.235279	3.889113
H	6.658857	0.543362	3.907764
N	-5.380189	1.099360	2.033735
C	-4.631295	2.225075	1.808979
C	-5.421235	3.436994	2.058017
C	-6.665860	3.013002	2.427398
C	-6.618870	1.546660	2.416779
C	-3.272885	2.270150	1.413500
C	-2.640962	3.616527	1.221289
C	-2.981980	4.414819	0.111394
C	-2.371599	5.661587	-0.084940
C	-1.409968	6.127071	0.824621
C	-1.065475	5.341088	1.934692
C	-1.677863	4.095530	2.131711
C	-7.733078	0.731858	2.741972
C	-9.004631	1.394450	3.165800
C	-9.064155	2.128806	4.368428
C	-10.254578	2.751553	4.767970
C	-11.405753	2.649046	3.971998
C	-11.358743	1.919645	2.774260
C	-10.167861	1.297631	2.374190
C	-7.732536	-0.678040	2.693647
N	-6.664801	-1.471043	2.328870
C	-7.007327	-2.805298	2.385527
C	-8.383233	-2.860195	2.813996
C	-8.820300	-1.566155	3.014549
C	-6.184612	-3.906124	2.071063
C	-4.829312	-3.850479	1.661214

N	-4.056950	-2.725047	1.514123
C	-2.817864	-3.171242	1.127063
C	-2.804504	-4.634423	1.009683
C	-4.054995	-5.058188	1.355415
C	-1.673038	-2.375243	0.850675
C	-1.648857	-0.962428	0.915144
N	-2.742956	-0.177867	1.235421
C	-2.431369	1.164074	1.165961
C	-1.051846	1.241258	0.774638
C	-0.552645	-0.043650	0.637546
C	-6.823807	-5.257653	2.189678
C	-7.169425	-5.991306	1.037555
C	-7.767582	-7.254493	1.149106
C	-8.030088	-7.801314	2.414649
C	-7.690994	-7.077739	3.568025
C	-7.092336	-5.814674	3.455696
C	-0.420028	-3.099910	0.462543
C	0.270676	-3.881134	1.412107
C	1.463514	-4.531774	1.072402
C	1.992855	-4.399121	-0.219476
C	1.303858	-3.639899	-1.175887
C	0.099206	-3.006370	-0.842161
H	-5.062653	4.462086	1.959476
H	-7.535052	3.622421	2.676935
H	-3.728752	4.045738	-0.601179
H	-2.643459	6.269480	-0.956324
H	-0.929037	7.099921	0.668153
H	-0.317071	5.699117	2.651849
H	-1.411663	3.478834	2.998109
H	-8.165502	2.202018	4.991062
H	-10.284000	3.315974	5.707792
H	-12.336919	3.136675	4.284100
H	-12.252528	1.839862	2.143869
H	-10.127009	0.737071	1.433309
H	-8.948663	-3.781738	2.948942
H	-9.803796	-1.240791	3.352125
H	-1.952658	-5.240887	0.702253
H	-4.428023	-6.081630	1.399903
H	-0.489193	2.162350	0.631634
H	-6.963621	-5.561017	0.050853
H	-8.032138	-7.813129	0.243225
H	-8.497624	-8.789350	2.501249
H	-7.889327	-7.499804	4.560574
H	-6.821813	-5.248421	4.354253
H	-0.126144	-3.952199	2.430155
H	2.000396	-5.117255	1.827343
H	2.952739	-4.862918	-0.470047
H	1.720410	-3.515227	-2.179540
H	-0.430269	-2.404158	-1.587821
H	-3.655878	-0.578298	1.468831
H	-5.752464	-1.093991	2.061298
H	3.339782	-1.555029	0.191154
H	4.651960	-1.474326	-1.588213
N	13.068197	-4.777463	-3.717387
C	13.085551	-4.231124	-2.460483
C	14.456709	-4.155116	-1.941956
C	15.262082	-4.677899	-2.913452
C	14.376488	-5.052478	-4.022030
C	11.966847	-3.762402	-1.732049
C	12.198338	-3.185646	-0.367623
C	12.545423	-4.017581	0.715206
C	12.719256	-3.482126	1.999437
C	12.545484	-2.107462	2.220067
C	12.205011	-1.269258	1.147458
C	12.035902	-1.804504	-0.136857
C	14.844885	-5.639334	-5.224965
C	16.316462	-5.843211	-5.394833
C	17.186268	-4.737662	-5.494022
C	18.565571	-4.925711	-5.656733
C	19.097655	-6.222496	-5.723327
C	18.241415	-7.329938	-5.625732
C	16.861843	-7.141703	-5.463042
C	14.017665	-6.051463	-6.290753
N	12.643032	-5.946890	-6.333506
C	12.152521	-6.450008	-7.519822
C	13.292212	-6.905934	-8.277034
C	14.428115	-6.649765	-7.535399
C	10.800961	-6.519207	-7.916253
C	9.686981	-6.050684	-7.176229
N	9.713621	-5.428755	-5.952708
C	8.407139	-5.129579	-5.657328
C	7.512695	-5.592076	-6.725270
C	8.312202	-6.155785	-7.677587
C	7.926404	-4.474869	-4.490839
C	8.739938	-4.050319	-3.417524
N	10.109619	-4.240671	-3.354738
C	10.622516	-3.770311	-2.163793
C	9.510431	-3.256138	-1.418137
C	8.357647	-3.391009	-2.177067
C	10.539358	-7.147967	-9.251959
C	9.959348	-8.429261	-9.340399
C	9.716141	-9.018351	-10.589287
C	10.051152	-8.334794	-11.768236
C	10.629824	-7.058763	-11.690872
C	10.872004	-6.469788	-10.441512
C	6.450709	-4.233557	-4.410133
C	5.843285	-3.288020	-5.260987
C	4.466071	-3.046288	-5.193401
C	3.672805	-3.758734	-4.282583
C	4.264615	-4.711251	-3.439903
C	5.645432	-4.945217	-3.501425
H	14.748894	-3.755717	-0.970167
H	16.344900	-4.805504	-2.890012
H	12.668860	-5.092725	0.541762
H	12.982419	-4.143833	2.833316
H	12.673838	-1.690387	3.225843
H	12.068779	-0.193496	1.310842
H	11.768556	-1.151668	-0.975788
H	16.767248	-3.726344	-5.447195
H	19.227263	-4.054946	-5.736797
H	20.176825	-6.369906	-5.850294
H	18.650118	-8.346632	-5.670161
H	16.193130	-8.005572	-5.376131
H	13.231331	-7.364409	-9.263578
H	15.462480	-6.852284	-7.811427
H	6.427063	-5.495694	-6.732682
H	8.012535	-6.600858	-8.626813
H	9.571261	-2.799459	-0.432956
H	9.700480	-8.960637	-8.417456
H	9.265522	-10.016738	-10.641175
H	9.860947	-8.795024	-12.745137
H	10.889823	-6.516377	-12.607887
H	11.319301	-5.471265	-10.378040
H	6.467076	-2.728883	-5.965640

H	4.011230	-2.292691	-5.846537
H	2.594137	-3.571208	-4.235214
H	3.648891	-5.277198	-2.732191
H	6.110195	-5.680432	-2.835411
H	10.638864	-4.686970	-4.108580
H	12.085273	-5.543911	-5.576941

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C	3.465155	-2.202462	1.777010
C	2.537420	-2.193602	2.881313
C	1.390101	-1.537734	2.467827
C	1.621152	-1.057218	1.132410
C	0.790982	-0.248644	0.327963
C	1.243688	0.388245	-0.849396
C	0.495015	1.442831	-1.534990
C	1.310182	1.895164	-2.535894
C	2.526431	1.072010	-2.477921
C	3.564975	1.185667	-3.432538
C	3.562267	2.427102	-4.261399
C	3.853981	3.653174	-3.611880
C	3.801910	4.860893	-4.327812
C	3.468851	4.858338	-5.689862
C	3.193126	3.648355	-6.345583
C	3.238085	2.443189	-5.629533
N	2.870900	-1.494411	0.759134
N	2.459555	0.181592	-1.446364
C	4.625305	0.281635	-3.632579
C	5.611757	0.340451	-4.682676
C	6.464362	-0.736825	-4.528924
C	6.055266	-1.455522	-3.351111
C	6.723926	-2.523629	-2.713798
C	6.362382	-3.016248	-1.435890
C	7.213495	-3.922521	-0.658983
C	6.673624	-3.969180	0.593899
C	5.485601	-3.105206	0.563889
C	4.703985	-2.871527	1.719525
C	5.314065	-3.287237	3.018107
C	4.872599	-4.383188	3.779001
C	5.527006	-4.746299	4.965666
C	6.641952	-4.013597	5.399367
C	7.094233	-2.914267	4.655772
C	6.435887	-2.546254	3.471594
N	4.923390	-0.830560	-2.874011
N	5.304709	-2.572393	-0.683939
H	2.722022	-2.666085	3.845756
H	0.475143	-1.373038	3.036471
H	-0.501009	1.793882	-1.260874
H	1.112506	2.686906	-3.259762
H	4.022724	5.792123	-3.794781
H	3.427721	5.805337	-6.241249
H	2.930128	3.643826	-7.409584
H	2.998222	1.494156	-6.123203
H	5.641435	1.106275	-5.457475
H	7.314116	-1.007538	-5.154774
H	8.113412	-4.420629	-1.020657
H	7.037003	-4.519417	1.462379
H	4.018644	-4.967324	3.415702
H	5.174887	-5.609384	5.542586
H	7.163395	-4.298433	6.321102
H	7.964645	-2.328983	4.972316
C	8.090523	-0.409763	0.304385
C	6.197004	-0.262360	2.778282
C	5.935460	0.416118	1.444481
C	6.825224	0.414619	0.343401
C	5.428910	3.200694	-1.852016
C	4.796113	1.240065	1.389076
C	4.530835	2.143291	0.343505
C	5.431844	2.157810	-0.748050
C	6.518188	1.263302	-0.737584
H	7.876067	-1.489301	0.309486
O	6.925242	-1.503266	2.727239
H	5.989744	4.090633	-1.492779
H	5.977555	2.804795	-2.726218
H	4.095586	1.218116	2.235036
C	3.340676	3.067082	0.443601
O	4.138442	3.684776	-2.272332
H	7.200577	1.262523	-1.598500
H	2.832740	2.943352	1.415181
H	2.609446	2.875970	-0.356460
H	3.640759	4.126085	0.341677
H	8.723941	-0.217310	1.189143
H	8.680973	-0.177325	-0.597737
H	5.233259	-0.421307	3.296068
H	6.792965	0.429444	3.413319
N	-5.502418	0.761988	2.115209
C	-4.635407	1.201937	3.080822
C	-5.367152	1.730111	4.238926
C	-6.694493	1.616096	3.936549
C	-6.759725	1.020687	2.597320
C	-3.220511	1.173925	3.018055
C	-2.455554	1.801823	4.141285
C	-2.503546	3.194591	4.353692
C	-1.776941	3.783510	5.397922
C	-0.992083	2.988587	6.247283
C	-0.938929	1.600597	6.047255
C	-1.664695	1.012699	5.002126
C	-7.980341	0.755617	1.925284
C	-9.256630	1.209034	2.555565
C	-10.241506	0.275786	2.942491
C	-11.439565	0.701833	3.532058
C	-11.674315	2.069185	3.742675
C	-10.702692	3.007045	3.360671
C	-9.503904	2.580838	2.772862
C	-8.084317	0.091228	0.684526
N	-7.042428	-0.473649	-0.020946
C	-7.499859	-1.055230	-1.184642
C	-8.922273	-0.824197	-1.229275
C	-9.277765	-0.127658	-0.091440
C	-6.727177	-1.746754	-2.141456
C	-5.317480	-1.901558	-2.114108
N	-4.445288	-1.324475	-1.225655
C	-3.193440	-1.731333	-1.614255
C	-3.274016	-2.633619	-2.768794
C	-4.598828	-2.737855	-3.081965
C	-1.952911	-1.358221	-1.030600
C	-1.817721	-0.555255	0.125723
N	-2.880008	-0.115463	0.895784
C	-2.441754	0.599584	1.989470
C	-1.008978	0.645783	1.896771
C	-0.609190	-0.050646	0.767436
C	-7.478391	-2.366362	-3.277691
C	-7.287250	-1.908413	-4.597740

C	-7.990201	-2.486809	-5.663516
C	-8.894363	-3.533828	-5.426971
C	-9.091808	-3.998477	-4.117636
C	-8.390570	-3.417839	-3.051639
C	-0.711006	-1.827589	-1.721152
C	0.152131	-2.764420	-1.122248
C	1.359681	-3.113780	-1.740935
C	1.710643	-2.539608	-2.970721
C	0.832290	-1.648770	-3.601742
C	-0.371332	-1.295453	-2.981732
H	-4.918633	2.110553	5.157290
H	-7.549586	1.883554	4.558364
H	-3.112918	3.813037	3.685110
H	-1.819525	4.869329	5.545434
H	-0.423776	3.449891	7.063625
H	-0.333019	0.971873	6.710705
H	-1.631853	-0.072257	4.848641
H	-10.052404	-0.792296	2.786302
H	-12.190384	-0.038230	3.833908
H	-12.611637	2.403241	4.203203
H	-10.881142	4.077840	3.516562
H	-8.747200	3.312083	2.467761
H	-9.573094	-1.142269	-2.043221
H	-10.269638	0.225358	0.189373
H	-2.428832	-3.124675	-3.251542
H	-5.055879	-3.335343	-3.871499
H	-0.354508	1.169787	2.591728
H	-6.582271	-1.089401	-4.778980
H	-7.833762	-2.115623	-6.683518
H	-9.442741	-3.987088	-6.261349
H	-9.791374	-4.820791	-3.925346
H	-8.537403	-3.783493	-2.029099
H	-0.111771	-3.186360	-0.146287
H	2.051649	-3.805129	-1.247670
H	2.680299	-2.770401	-3.419126
H	1.107952	-1.190626	-4.558593
H	-1.040641	-0.565639	-3.448875
H	-3.856526	-0.287000	0.642224
H	-6.064156	-0.418073	0.271059
H	3.287786	-1.235204	-0.140644
H	4.491962	-1.093321	-1.982678
N	12.807031	-4.368343	-4.501876
C	12.706655	-3.005352	-4.398718
C	13.991196	-2.362430	-4.699984
C	14.871046	-3.373057	-4.965811
C	14.115370	-4.622654	-4.822996
C	11.545948	-2.273343	-4.049392
C	11.664292	-0.792831	-3.866595
C	12.442560	-0.259050	-2.818926
C	12.519009	1.126479	-2.620073
C	11.819936	2.000718	-3.466400
C	11.046596	1.481204	-4.515915
C	10.969975	0.095874	-4.713755
C	14.693760	-5.904804	-5.007640
C	16.165580	-5.995021	-5.246959
C	16.670026	-6.515367	-6.457316
C	18.051344	-6.598398	-6.680010
C	18.951540	-6.163929	-5.695089
C	18.461471	-5.645649	-4.486493
C	17.080413	-5.561548	-4.264350
C	13.976479	-7.119888	-4.978200
N	12.610784	-7.250238	-4.837292
C	12.241411	-8.578616	-4.869149
C	13.456033	-9.340542	-5.019800
C	14.511774	-8.453182	-5.085246
C	10.930999	-9.093361	-4.779176
C	9.752310	-8.334039	-4.565309
N	9.677873	-6.988543	-4.307801
C	8.342355	-6.711160	-4.154570
C	7.532963	-7.918463	-4.357415
C	8.413119	-8.931643	-4.608838
C	7.769369	-5.450023	-3.838363
C	8.495086	-4.247524	-3.712881
N	9.840149	-4.112638	-4.007883
C	10.257420	-2.810822	-3.833951
C	9.114662	-2.078692	-3.370769
C	8.028448	-2.938952	-3.284971
C	10.789118	-10.575757	-4.929461
C	10.356587	-11.367667	-3.846053
C	10.218337	-12.755354	-3.986075
C	10.508413	-13.372906	-5.212437
C	10.939782	-12.594430	-6.297353
C	11.080773	-11.206905	-6.156039
C	6.284288	-5.399751	-3.680341
C	5.494618	-4.747309	-4.646556
C	4.097399	-4.766538	-4.552668
C	3.471829	-5.423510	-3.481992
C	4.251691	-6.052482	-2.500715
C	5.648444	-6.048130	-2.603822
H	14.176575	-1.287857	-4.724199
H	15.920018	-3.290904	-5.252595
H	12.978182	-0.944148	-2.152052
H	13.121409	1.524813	-1.794856
H	11.878211	3.084184	-3.308791
H	10.502104	2.157623	-5.185723
H	10.368347	-0.312220	-5.533983
H	15.965437	-6.843224	-7.229819
H	18.426346	-6.997796	-7.629984
H	20.032246	-6.228441	-5.869085
H	19.158850	-5.309188	-3.709978
H	16.695457	-5.163731	-3.318767
H	13.499136	-10.428563	-5.057005
H	15.571432	-8.686791	-5.183411
H	6.444469	-7.968629	-4.327534
H	8.187661	-9.976189	-4.826188
H	9.120327	-1.029290	-3.082598
H	10.131851	-10.882536	-2.889471
H	9.884910	-13.357738	-3.132565
H	10.397491	-14.458214	-5.322803
H	11.162239	-13.068769	-7.260827
H	11.409955	-10.595619	-7.004066
H	5.986684	-4.237993	-5.482720
H	3.492700	-4.269856	-5.320540
H	2.379377	-5.432163	-3.407510
H	3.769879	-6.550487	-1.650976
H	6.260195	-6.543244	-1.843248
H	10.427760	-4.902113	-4.286522
H	11.981440	-6.460111	-4.679392

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C	-2.778723	1.109368	-2.289990
C	-1.463882	1.680912	-2.228528
C	-0.655178	0.825373	-1.490347
C	-1.497262	-0.258283	-1.022304
C	-1.143275	-1.223166	-0.078255
H	-0.099594	-1.190327	0.250650
C	-1.979231	-2.147987	0.565308
C	-1.531142	-2.951640	1.706562
C	-2.649895	-3.564993	2.200893
C	-3.756298	-3.154193	1.329370
C	-5.104167	-3.520282	1.568161
C	-5.451308	-3.952135	2.958737
C	-5.501196	-2.884136	3.902907
C	-5.826564	-3.131758	5.245753
C	-6.108438	-4.449790	5.649058
C	-6.068204	-5.507212	4.731267
C	-5.739480	-5.251571	3.385990
N	-2.742673	-0.060991	-1.569213
N	-3.318045	-2.322865	0.336640
C	-6.178997	-3.189625	0.722520
C	-7.565890	-3.549115	0.872838
C	-8.263748	-2.978558	-0.175397
C	-7.331500	-2.214052	-0.966763
C	-7.654230	-1.325670	-2.000423
H	-8.710575	-1.314852	-2.292457
C	-6.832376	-0.349600	-2.593969
C	-7.372214	0.716175	-3.446223
C	-6.343261	1.593397	-3.657102
C	-5.178676	1.024470	-2.971268
C	-3.915649	1.656571	-2.917640
C	-3.823776	3.118265	-3.226454
C	-3.597911	3.691481	-4.481276
C	-3.495477	5.088738	-4.622680
C	-3.616018	5.911069	-3.495020
C	-3.847720	5.361303	-2.220998
C	-3.960123	3.968090	-2.089876
N	-6.087578	-2.408078	-0.408522
N	-5.500498	-0.154997	-2.351799
H	-1.161078	2.602841	-2.725256
H	-0.505590	-3.000923	2.081881
H	-2.737345	-4.230404	3.061863
H	-5.862239	-2.312310	5.970704
H	-6.362035	-4.644684	6.698178
H	-6.288969	-6.529802	5.057396
H	-5.700835	-6.069215	2.656685
H	-7.953520	-4.168157	1.682591
H	-9.335046	-3.038781	-0.377506
H	-8.406331	0.787698	-3.793747
H	-6.351610	2.530688	-4.216521
H	-3.492395	3.033715	-5.352048
H	-3.315723	5.528766	-5.610001
H	-3.530831	6.999548	-3.599743
H	-3.944019	6.013110	-1.346823
C	-6.923811	2.739781	0.574121
C	-4.226791	3.907716	0.352567
C	-4.479484	2.775679	1.327234
C	-5.785888	2.246163	1.440242
C	-5.247817	-0.449650	4.103823
C	-3.387316	2.158055	1.984869
C	-3.626085	1.084098	2.878742
C	-4.959222	0.654947	3.106933
C	-6.024533	1.169470	2.329566
H	-6.683696	3.656085	0.017571
O	-4.201603	3.297256	-0.939085
H	-6.239593	-0.315261	4.575678
H	-4.501949	-0.477487	4.918928
C	-1.976179	2.621655	1.676531
C	-2.452007	0.369493	3.518745
O	-5.217876	-1.672886	3.367078
C	-7.405844	0.550473	2.358039
H	-1.742549	0.035507	2.741585
H	-2.747821	-0.538751	4.060418
H	-1.893506	1.020660	4.217513
H	-7.837633	2.930674	1.164264
H	-7.181964	1.974213	-0.182108
H	-5.027989	4.670719	0.398829
H	-3.269088	4.423692	0.541261
H	-1.778178	3.640690	2.060574
H	-1.803845	2.638358	0.586226
H	-1.211063	1.964101	2.109702
H	-7.472905	-0.339462	2.997785
H	-7.691992	0.224579	1.341178
H	-8.178037	1.271370	2.687381
H	-5.217863	-1.946541	-0.687653
H	-3.577649	-0.620744	-1.381145
N	5.492872	1.693182	0.716667
C	4.734994	2.824385	0.871642
C	5.507322	3.884649	1.530679
C	6.740182	3.355065	1.788835
C	6.708043	1.978072	1.283425
C	3.386305	2.990970	0.476180
C	2.688904	4.263508	0.845779
C	2.427217	4.569278	2.197272
C	1.734853	5.737853	2.545001
C	1.294263	6.620210	1.546220
C	1.553748	6.328590	0.198037
C	2.245051	5.159364	-0.148733
C	7.810355	1.090062	1.375377
C	9.024071	1.533435	2.124828
C	10.266054	1.672916	1.469919
C	11.404320	2.089152	2.174098
C	11.320494	2.371603	3.546199
C	10.090558	2.236376	4.208702
C	8.952154	1.821374	3.504232
C	7.848291	-0.199067	0.802065
N	6.866963	-0.763569	0.014146
C	7.238140	-2.026205	-0.398053
C	8.529800	-2.286914	0.187468
C	8.900380	-1.175695	0.918403
C	6.502870	-2.894366	-1.233776
C	5.193388	-2.662127	-1.727883
N	4.362478	-1.622234	-1.393767
C	3.194571	-1.841567	-2.080364
C	3.301288	-3.040522	-2.919073
C	4.547118	-3.554105	-2.696803
C	2.013383	-1.051898	-2.021200
C	1.908627	0.175963	-1.325359
N	2.975539	0.822822	-0.725523
C	2.595104	2.045207	-0.214228
C	1.194246	2.179831	-0.485408
C	0.749408	1.040178	-1.141910

C	7.178860	-4.172631	-1.617801
C	6.651347	-5.414143	-1.205449
C	7.283648	-6.613379	-1.561079
C	8.453558	-6.591394	-2.336162
C	8.986679	-5.362215	-2.753774
C	8.355007	-4.162888	-2.396322
C	0.811763	-1.549858	-2.756078
C	0.231393	-0.789578	-3.790886
C	-0.945296	-1.217812	-4.418385
C	-1.558314	-2.416631	-4.024266
C	-0.972745	-3.198093	-3.017093
C	0.205901	-2.770507	-2.393066
H	5.152847	4.894147	1.742400
H	7.597460	3.845138	2.251725
H	2.763361	3.873168	2.974011
H	1.533377	5.957069	3.600465
H	0.751849	7.533625	1.818042
H	1.218031	7.015596	-0.588069
H	2.447462	4.929606	-1.201029
H	10.328091	1.463357	0.396032
H	12.359674	2.199655	1.647073
H	12.210678	2.697292	4.097370
H	10.017779	2.450481	5.281796
H	7.992778	1.708052	4.021365
H	9.083299	-3.217781	0.068454
H	9.809515	-1.036995	1.502699
H	2.533407	-3.414564	-3.596292
H	5.000218	-4.432517	-3.157069
H	0.573688	3.016906	-0.171738
H	5.740393	-5.428338	-0.596707
H	6.862793	-7.569603	-1.227740
H	8.947463	-7.529747	-2.615257
H	9.895985	-5.336598	-3.366262
H	8.765281	-3.202623	-2.728970
H	0.700578	0.154754	-4.086639
H	-1.397065	-0.602053	-5.204693
H	-2.495491	-2.735682	-4.494889
H	-1.452129	-4.128772	-2.692780
H	0.642821	-3.361075	-1.580934
H	3.906522	0.403563	-0.660658
H	5.973736	-0.307842	-0.184722

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C	2.224297	-2.472106	0.336203
C	0.853718	-2.150856	0.606725
C	0.489086	-1.091012	-0.208650
C	1.666792	-0.717999	-0.975937
C	1.788154	0.386898	-1.822451
H	0.864762	0.950780	-1.989363
C	2.967654	0.943579	-2.345247
C	2.999081	2.276116	-2.957188
C	4.321644	2.590009	-3.112534
C	5.073323	1.425501	-2.634441
C	6.488286	1.388406	-2.575247
C	7.216908	2.693766	-2.568634
C	7.063103	3.458565	-1.374758
C	7.780032	4.652988	-1.196251
C	8.638608	5.099416	-2.216293
C	8.785511	4.366691	-3.401477
C	8.076045	3.163146	-3.569101
N	2.662596	-1.602282	-0.633985
N	4.231666	0.438685	-2.203260
C	7.233739	0.247745	-2.220375
C	8.665193	0.088606	-2.192992
C	8.936833	-1.198754	-1.767383
C	7.682478	-1.843705	-1.469325
C	7.517784	-3.072136	-0.816397
H	8.442485	-3.634281	-0.642944
C	6.353958	-3.588494	-0.217467
C	6.392330	-4.719697	0.714736
C	5.149933	-4.787348	1.285240
C	4.353458	-3.731918	0.651083
C	3.008814	-3.444246	0.985873
C	2.463264	-3.959608	2.278193
C	2.035500	-5.268882	2.525208
C	1.606631	-5.655717	3.808252
C	1.612311	-4.721315	4.852375
C	2.030626	-3.397017	4.631659
C	2.447771	-3.014313	3.346710
N	6.690428	-0.946109	-1.796520
N	5.103731	-3.033676	-0.260526
H	0.230728	-2.666119	1.334959
H	2.122220	2.885862	-3.191246
H	4.763294	3.506360	-3.508940
H	7.666957	5.233929	-0.275184
H	9.194305	6.034742	-2.077444
H	9.453474	4.724766	-4.192977
H	8.193716	2.570851	-4.484126
H	9.375510	0.867714	-2.470486
H	9.914636	-1.663085	-1.624946
H	7.268910	-5.337843	0.926109
H	4.794639	-5.473100	2.055914
H	2.049352	-5.990692	1.700735
H	1.273731	-6.683937	3.989251
H	1.282811	-5.018015	5.855489
H	2.024843	-2.671202	5.451341
C	6.000797	-1.307707	3.033823
C	3.241702	-0.762362	3.928658
C	3.993587	0.280668	3.125963
C	5.326920	0.012893	2.735776
C	6.208059	3.262586	0.912729
C	3.318584	1.436095	2.657142
C	4.024840	2.389318	1.882150
C	5.408083	2.196754	1.634748
C	6.040237	0.980438	1.984610
H	5.414510	-1.964599	3.690114
O	2.855118	-1.772259	2.992217
H	7.252349	3.291228	1.276610
H	5.781082	4.269916	1.069785
C	1.840839	1.612442	2.955480
C	3.290852	3.568687	1.275317
O	6.193590	2.929442	-0.478693
C	7.439337	0.644289	1.516720
H	2.339122	3.247216	0.822229
H	3.862300	4.043399	0.465165
H	3.037392	4.344704	2.022315
H	6.994409	-1.166118	3.495585
H	6.160713	-1.865996	2.093193
H	3.880228	-1.206966	4.715748
H	2.347421	-0.347746	4.425080
H	1.648015	1.665842	4.043270
H	1.254258	0.761144	2.563938

H	1.423477	2.530167	2.518863
H	7.876734	1.408385	0.860846
H	7.424325	-0.294055	0.934858
H	8.131440	0.478235	2.363830
H	5.684341	-1.061711	-1.645360
H	3.637798	-1.567562	-0.940782
N	-5.163172	2.255243	0.280092
C	-4.076894	3.065717	0.483669
C	-4.499054	4.420899	0.858242
C	-5.864402	4.398174	0.898651
C	-6.263057	3.037543	0.520188
C	-2.717975	2.687141	0.368636
C	-1.661442	3.711238	0.650504
C	-0.809243	4.158739	-0.380801
C	0.200012	5.095896	-0.121004
C	0.372506	5.602580	1.176212
C	-0.464232	5.159661	2.211838
C	-1.473239	4.220836	1.951285
C	-7.615300	2.620350	0.429861
C	-8.694045	3.617456	0.709060
C	-9.561576	3.448284	1.808184
C	-10.578517	4.378076	2.066823
C	-10.745521	5.491532	1.229218
C	-9.889539	5.668860	0.131190
C	-8.873047	4.739002	-0.127435
C	-8.034420	1.324069	0.061995
N	-7.214214	0.250416	-0.217069
C	-7.958821	-0.838611	-0.620746
C	-9.341498	-0.431503	-0.580415
C	-9.387442	0.883800	-0.164629
C	-7.470745	-2.091032	-1.048334
C	-6.106979	-2.456571	-1.171532
N	-5.019615	-1.669696	-0.887366
C	-3.918793	-2.451166	-1.132412
C	-4.318401	-3.780343	-1.607859
C	-5.683960	-3.788624	-1.618529
C	-2.559799	-2.076527	-0.961024
C	-2.125201	-0.801476	-0.534304
N	-2.957075	0.286765	-0.336597
C	-2.236718	1.401663	0.034941
C	-0.861812	0.999608	0.084837
C	-0.773190	-0.347383	-0.240892
C	-8.506937	-3.107321	-1.419651
C	-8.692486	-3.484948	-2.765000
C	-9.664827	-4.433184	-3.112666
C	-10.466643	-5.017630	-2.119991
C	-10.290909	-4.647570	-0.777823
C	-9.318928	-3.698358	-0.430725
C	-1.507468	-3.098562	-1.248047
C	-1.381944	-4.245303	-0.439199
C	-0.326359	-5.145046	-0.637640
C	0.615082	-4.913910	-1.652076
C	0.477930	-3.794258	-2.485934
C	-0.578824	-2.896696	-2.288482
H	-3.837306	5.263512	1.061353
H	-6.540555	5.213235	1.158655
H	-0.947674	3.763135	-1.393587
H	0.856404	5.428702	-0.933755
H	1.162966	6.333889	1.380655
H	-0.327588	5.542134	3.230460
H	-2.121857	3.866985	2.760532
H	-9.424860	2.581817	2.465276
H	-11.239949	4.234786	2.929773
H	-11.540771	6.218875	1.431336
H	-10.017473	6.533058	-0.531725
H	-8.209717	4.870653	-0.989630
H	-10.178304	-1.069864	-0.862285
H	-10.268464	1.513987	-0.047401
H	-3.640718	-4.585629	-1.891854
H	-6.346079	-4.608917	-1.897073
H	-0.035173	1.635679	0.394249
H	-8.066935	-3.024132	-3.537889
H	-9.799281	-4.714147	-4.164152
H	-11.226633	-5.759805	-2.391899
H	-10.910623	-5.102961	0.004023
H	-9.175650	-3.410822	0.617225
H	-2.096351	-4.403733	0.376606
H	-0.225224	-6.016951	0.019132
H	1.458341	-5.600737	-1.788673
H	1.209291	-3.606987	-3.280383
H	-0.672425	-2.008224	-2.922507
H	-3.972203	0.235856	-0.452227
H	-6.193828	0.288447	-0.165719

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energy (B3LYP-D3): -5892.01149813957 Hartrees

C	0.267137	-3.138284	1.604750
C	1.301608	-4.138207	1.541592
C	2.513961	-3.501019	1.728405
C	2.254763	-2.089280	1.870824
C	3.210562	-1.068986	1.814866
C	2.998463	0.310038	1.646849
C	4.076843	1.230449	1.208451
C	3.471044	2.455474	1.062634
C	2.068464	2.274629	1.422869
C	1.105466	3.307866	1.342299
C	1.483356	4.538590	0.579538
C	1.252052	4.451263	-0.824148
C	1.619145	5.507890	-1.672869
C	2.211508	6.657275	-1.119120
C	2.433527	6.758933	0.260324
C	2.067630	5.694015	1.104915
N	0.887015	-1.933762	1.851005
N	1.812964	0.972628	1.773010
C	-0.267137	3.138284	1.604750
C	-1.301608	4.138207	1.541592
C	-2.513961	3.501019	1.728405
C	-2.254763	2.089280	1.870824
C	-3.210562	1.068986	1.814866
C	-2.998463	-0.310038	1.646849
C	-4.076843	-1.230449	1.208451
C	-3.471044	-2.455474	1.062634
C	-2.068464	-2.274629	1.422869
C	-1.105466	-3.307866	1.342299
C	-1.483356	-4.538590	0.579538
C	-2.067630	-5.694015	1.104915
C	-2.433527	-6.758933	0.260324
C	-2.211508	-6.657275	-1.119120
C	-1.619145	-5.507890	-1.672869
C	-1.252052	-4.451263	-0.824148
N	-0.887015	1.933762	1.851005
N	-1.812964	-0.972628	1.773010
H	1.117148	-5.198376	1.363284

H	3.512533	-3.942931	1.723658
H	3.926420	3.382947	0.717855
H	1.443105	5.442752	-2.751420
H	2.498568	7.482104	-1.782486
H	2.894854	7.659840	0.680395
H	2.249013	5.747644	2.183419
H	-1.117148	5.198376	1.363284
H	-3.512533	3.942931	1.723658
H	-3.926420	-3.382947	0.717855
H	-2.249013	-5.747644	2.183419
H	-2.894854	-7.659840	0.680395
H	-2.498568	-7.482104	-1.782486
H	-1.443105	-5.442752	-2.751420
C	-2.787106	-0.883757	-2.326516
C	-0.588826	-2.862835	-2.575463
C	-0.284087	-1.379891	-2.542945
C	-1.347922	-0.446098	-2.475747
C	0.588826	2.862835	-2.575463
C	1.059460	-0.941717	-2.445030
C	1.347922	0.446098	-2.475747
C	0.284087	1.379891	-2.542945
C	-1.059460	0.941717	-2.445030
H	-3.117448	-0.730727	-1.283794
O	-0.670247	-3.290521	-1.211839
H	1.541683	3.070127	-3.094022
H	-0.198995	3.432825	-3.102429
C	2.787106	0.883757	-2.326516
O	0.670247	3.290521	-1.211839
H	3.469563	0.300798	-2.967828
H	3.117448	0.730727	-1.283794
H	2.951860	1.948186	-2.543750
H	-2.951860	-1.948186	-2.543750
H	-3.469563	-0.300798	-2.967828
H	0.198995	-3.432825	-3.102429
H	-1.541683	-3.070127	-3.094022
N	9.976563	-0.352509	-1.230625
C	9.018084	-1.249387	-1.624767
C	9.575180	-2.227680	-2.567224
C	10.879889	-1.871712	-2.760978
C	11.114989	-0.698908	-1.911593
C	7.658161	-1.243022	-1.230804
C	6.730184	-2.259996	-1.819055
C	6.449960	-2.273870	-3.201295
C	5.548786	-3.203433	-3.739382
C	4.908543	-4.131535	-2.904221
C	5.175732	-4.125656	-1.527003
C	6.080322	-3.199675	-0.990730
C	12.355458	-0.015393	-1.856950
C	13.479662	-0.501493	-2.716065
C	14.102941	-1.738771	-2.455419
C	15.159950	-2.188980	-3.258372
C	15.611385	-1.408396	-4.333402
C	14.998987	-0.174707	-4.600672
C	13.941381	0.275002	-3.798135
C	12.624401	1.100395	-1.036872
N	11.746440	1.685489	-0.148173
C	12.362757	2.705639	0.546459
C	13.709913	2.793204	0.038994
C	13.872665	1.808850	-0.914978
C	11.799216	3.486488	1.577922
C	10.468823	3.390878	2.061335
N	9.462436	2.615226	1.544562
C	8.358225	2.870043	2.318488
C	8.684806	3.808709	3.397261
C	10.000230	4.138494	3.233155
C	7.055792	2.331269	2.132436
C	6.729738	1.343537	1.176034
N	7.661858	0.647877	0.425374
C	7.056633	-0.325789	-0.338598
C	5.651128	-0.223857	-0.086176
C	5.422319	0.804600	0.823112
C	12.701068	4.494834	2.218253
C	12.435258	5.873783	2.089493
C	13.274542	6.822803	2.689132
C	14.392391	6.408261	3.429371
C	14.665476	5.038615	3.566185
C	13.826951	4.089778	2.964545
C	5.959498	2.816236	3.021389
C	5.254814	1.911894	3.841712
C	4.172883	2.342970	4.617391
C	3.785660	3.691158	4.596120
C	4.498517	4.605967	3.806581
C	5.576426	4.172171	3.023961
H	9.036237	-3.063118	-3.015191
H	11.615104	-2.346970	-3.411219
H	6.938271	-1.537820	-3.849719
H	5.336734	-3.194763	-4.815248
H	4.195876	-4.851191	-3.323701
H	4.674585	-4.843873	-0.867279
H	6.292640	-3.195405	0.084551
H	13.753262	-2.343520	-1.610787
H	15.636922	-3.152073	-3.039814
H	16.438704	-1.760494	-4.961120
H	15.342669	0.439097	-5.442123
H	13.456819	1.235197	-4.009561
H	14.449838	3.517805	0.377018
H	14.771419	1.576688	-1.485611
H	8.003156	4.144456	4.178940
H	10.607267	4.799713	3.852409
H	4.889393	-0.814706	-0.588531
H	11.562719	6.194350	1.509195
H	13.056073	7.891417	2.575064
H	15.048175	7.150591	3.899655
H	15.532667	4.706243	4.149468
H	14.033866	3.019462	3.077793
H	5.549303	0.856933	3.847333
H	3.621051	1.621509	5.230754
H	2.929349	4.027285	5.192595
H	4.206717	5.662678	3.789923
H	6.111161	4.878856	2.379636
H	8.661668	0.860716	0.448016
H	10.773753	1.390661	-0.037959
H	0.376013	-1.047369	1.860813
H	-0.376013	1.047369	1.860813
N	-9.976563	0.352509	-1.230625
C	-9.018084	1.249387	-1.624767
C	-9.575180	2.227680	-2.567224
C	-10.879889	1.871712	-2.760978
C	-11.114989	0.698908	-1.911593
C	-7.658161	1.243022	-1.230804
C	-6.730184	2.259996	-1.819055
C	-6.449960	2.273870	-3.201295
C	-5.548786	3.203433	-3.739382
C	-4.908543	4.131535	-2.904221

C	-5.175732	4.125656	-1.527003
C	-6.080322	3.199675	-0.990730
C	-12.355458	0.015393	-1.856950
C	-13.479662	0.501493	-2.716065
C	-14.102941	1.738771	-2.455419
C	-15.159950	2.188980	-3.258372
C	-15.611385	1.408396	-4.333402
C	-14.998987	0.174707	-4.600672
C	-13.941381	-0.275002	-3.798135
C	-12.624401	-1.100395	-1.036872
N	-11.746440	-1.685489	-0.148173
C	-12.362757	-2.705639	0.546459
C	-13.709913	-2.793204	0.038994
C	-13.872665	-1.808850	-0.914978
C	-11.799216	-3.486488	1.577922
C	-10.468823	-3.390878	2.061335
N	-9.462436	-2.615226	1.544562
C	-8.358225	-2.870043	2.318488
C	-8.684806	-3.808709	3.397261
C	-10.000230	-4.138494	3.233155
C	-7.055792	-2.331269	2.132436
C	-6.729738	-1.343537	1.176034
N	-7.661858	-0.647877	0.425374
C	-7.056633	0.325789	-0.338598
C	-5.651128	0.223857	-0.086176
C	-5.422319	-0.804600	0.823112
C	-12.701068	-4.494834	2.218253
C	-12.435258	-5.873783	2.089493
C	-13.274542	-6.822803	2.689132
C	-14.392391	-6.408261	3.429371
C	-14.665476	-5.038615	3.566185
C	-13.826951	-4.089778	2.964545
C	-5.959498	-2.816236	3.021389
C	-5.254814	-1.911894	3.841712
C	-4.172883	-2.342970	4.617391
C	-3.785660	-3.691158	4.596120
C	-4.498517	-4.605967	3.806581
C	-5.576426	-4.172171	3.023961
H	-9.036237	3.063118	-3.015191
H	-11.615104	2.346970	-3.411219
H	-6.938271	1.537820	-3.849719
H	-5.336734	3.194763	-4.815248
H	-4.195876	4.851191	-3.323701
H	-4.674585	4.843873	-0.867279
H	-6.292640	3.195405	0.084551
H	-13.753262	2.343520	-1.610787
H	-15.636922	3.152073	-3.039814
H	-16.438704	1.760494	-4.961120
H	-15.342669	-0.439097	-5.442123
H	-13.456819	-1.235197	-4.009561
H	-14.449838	-3.517805	0.377018
H	-14.771419	-1.576688	-1.485611
H	-8.003156	-4.144456	4.178940
H	-10.607267	-4.799713	3.852409
H	-4.889393	0.814706	-0.588531
H	-11.562719	-6.194350	1.509195
H	-13.056073	-7.891417	2.575064
H	-15.048175	-7.150591	3.899655
H	-15.532667	-4.706243	4.149468
H	-14.033866	-3.019462	3.077793
H	-5.549303	-0.856933	3.847333
H	-3.621051	-1.621509	5.230754
H	-2.929349	-4.027285	5.192595
H	-4.206717	-5.662678	3.789923
H	-6.111161	-4.878856	2.379636
H	-8.661668	-0.860716	0.448016
H	-10.773753	-1.390661	-0.037959
C	2.198182	-1.910825	-2.214654
H	1.876459	-2.958522	-2.152626
H	2.983578	-1.842101	-2.988257
H	2.691056	-1.686169	-1.250282
C	-2.198182	1.910825	-2.214654
H	-2.691056	1.686169	-1.250282
H	-1.876459	2.958522	-2.152626
H	-2.983578	1.842101	-2.988257
H	4.248915	-1.409752	1.761207
H	-4.248915	1.409752	1.761207

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energy (B3LYP-D3): -5892.00729024176 Hartrees

C	1.725296	2.619509	0.328643
C	3.106766	3.023011	0.358879
C	3.879026	1.893714	0.162353
C	2.988053	0.767795	0.039629
C	3.339062	-0.583419	0.019072
C	2.485618	-1.692380	0.111121
C	3.007571	-3.054972	0.327404
C	1.910612	-3.829453	0.616419
C	0.742363	-2.963980	0.459881
C	-0.593150	-3.417052	0.576799
C	-0.817295	-4.708242	1.292577
C	-1.140910	-4.580403	2.671611
C	-1.199634	-5.716317	3.496239
C	-0.972136	-6.986050	2.941326
C	-0.693011	-7.127467	1.573992
C	-0.611148	-5.987205	0.756913
N	1.705964	1.265702	0.091306
N	1.122099	-1.679711	0.166023
C	-1.725296	-2.619509	0.328643
C	-3.106766	-3.023011	0.358879
C	-3.879026	-1.893714	0.162353
C	-2.988053	-0.767795	0.039629
C	-3.339062	0.583419	0.019072
C	-2.485618	1.692380	0.111121
C	-3.007571	3.054972	0.327404
C	-1.910612	3.829453	0.616419
C	-0.742363	2.963980	0.459881
C	0.593150	3.417052	0.576799
C	0.817295	4.708242	1.292577
C	0.611148	5.987205	0.756913
C	0.693011	7.127467	1.573992
C	0.972136	6.986050	2.941326
C	1.199634	5.716317	3.496239
C	1.140910	4.580403	2.671611
N	-1.705964	-1.265702	0.091306
N	-1.122099	1.679711	0.166023
H	3.440607	4.048541	0.520166
H	4.967970	1.820621	0.135441
H	1.900327	-4.894678	0.849013
H	-1.437224	-5.604920	4.560006
H	-1.025770	-7.872662	3.584463
H	-0.527303	-8.122396	1.145371
H	-0.358729	-6.080843	-0.305796

H	-3.440607	-4.048541	0.520166
H	-4.967970	-1.820621	0.135441
H	-1.900327	4.894678	0.849013
H	0.358729	6.080843	-0.305796
H	0.527303	8.122396	1.145371
H	1.025770	7.872662	3.584463
H	1.437224	5.604920	4.560006
C	-2.057668	2.076793	3.817293
C	0.817300	2.794173	4.310845
C	0.388675	1.355292	4.094883
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Energy (B3LYP-D3): -5892.00915948034 Hartrees

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C	-5.150110	-1.608204	3.040811
C	-4.045727	-2.050878	3.777537
C	-3.623965	-3.385013	3.678487
C	-4.325674	-4.275610	2.852042
C	-5.426536	-3.829909	2.109018
H	-9.085042	3.558627	-3.599352
H	-11.651024	2.800724	-4.006305
H	-6.947660	2.098561	-4.493560
H	-5.361014	3.800468	-5.404404
H	-4.239535	5.421604	-3.859809
H	-4.725339	5.335899	-1.406012
H	-6.328533	3.642852	-0.509363
H	-13.783777	2.684480	-2.192685
H	-15.692511	3.499667	-3.584353
H	-16.467757	2.162044	-5.554185
H	-15.320267	0.009629	-6.121148
H	-13.410273	-0.793495	-4.725113
H	-14.337320	-3.260720	-0.426372
H	-14.710233	-1.254461	-2.208787
H	-7.846650	-3.908981	3.299320
H	-10.438437	-4.609021	2.964306
H	-4.876020	1.312099	-1.273870
H	-11.384409	-5.919975	0.574919
H	-12.831287	-7.692797	1.579717
H	-14.829440	-7.052440	2.946918
H	-15.365790	-4.632036	3.301978
H	-13.912573	-2.868997	2.292180
H	-5.470624	-0.562809	3.105980
H	-3.502707	-1.348134	4.419785
H	-2.749485	-3.729524	4.242883
H	-4.007024	-5.321949	2.775633
H	-5.953194	-4.515190	1.435687
H	-8.610376	-0.473773	-0.281665
H	-10.709186	-1.042113	-0.773284
C	2.385640	-1.127213	-2.962474
H	2.049995	-2.172914	-2.959876
H	3.148097	-1.010437	-3.755981
H	2.904689	-0.964109	-1.999790
C	-1.993336	2.719190	-2.726349
H	-2.519586	2.431038	-1.797255
H	-1.665623	3.756705	-2.580279
H	-2.753850	2.711144	-3.528018
H	4.311260	-0.768942	1.014922
H	-4.263635	1.806947	1.149288

Zn-Br

energy: -6494.796695366117 Hartrees

C	-1.051374	-0.903707	2.784105
C	-2.241484	-0.461604	3.472027
C	-3.252742	-0.429071	2.553594
C	-2.678168	-0.791290	1.279045
C	-3.302508	-0.707783	0.025967
C	-2.700118	-0.778051	-1.238596
C	-3.297659	-0.405081	-2.499356
C	-2.303305	-0.429162	-3.436224
C	-1.100389	-0.875968	-2.773801
C	0.144126	-1.058262	-3.401652
C	0.339014	-0.362985	-4.709084
C	0.960790	0.905661	-4.628004
C	1.077086	1.713884	-5.760482
C	0.602416	1.243449	-6.988395
C	0.021612	-0.019859	-7.089431
C	-0.111296	-0.815372	-5.946530
N	-1.342769	-1.099958	1.451695
N	-1.367708	-1.083670	-1.437920
C	1.276034	-1.626793	-2.801256
C	2.510549	-1.941542	-3.486461
C	3.368053	-2.448304	-2.550654
C	2.679497	-2.404756	-1.279831
C	3.261834	-2.669568	-0.040858
C	2.701551	-2.417630	1.211023
C	3.413906	-2.469017	2.468352
C	2.573080	-1.970670	3.423747
C	1.325025	-1.654652	2.764134
C	0.203751	-1.091250	3.388606
C	0.423596	-0.396359	4.692536
C	0.019377	-0.856694	5.942343
C	0.177355	-0.060161	7.081722
C	0.736598	1.211205	6.963875
C	1.164210	1.690869	5.721993
C	1.022579	0.882218	4.592943
N	1.401829	-1.931209	-1.468519
N	1.426492	-1.949274	1.427005
H	-2.299764	-0.218675	4.523468
H	-4.283334	-0.151232	2.717897
H	-4.331136	-0.126381	-2.642729
H	-2.381076	-0.176252	-4.484003
H	1.540448	2.693412	-5.688734
H	0.697690	1.870456	-7.871250
H	-0.336076	-0.382432	-8.048810
H	-0.587915	-1.790443	-6.006384
H	2.684511	-1.797597	-4.544156
H	4.382988	-2.796985	-2.696004
H	4.432214	-2.816284	2.591905
H	2.766337	-1.833564	4.479010
H	-0.441125	-1.838545	6.015718
H	-0.144518	-0.428538	8.051508
H	0.851183	1.838533	7.844209
H	1.609566	2.677618	5.637630
Zn	0.037261	-1.503923	-0.006995
C	3.996503	2.087061	1.392268
C	1.497935	2.579667	2.890126

C	1.483486	2.526003	1.381313
C	2.691457	2.352071	0.679305
C	1.476201	2.595319	-2.930540
C	0.255979	2.560581	0.689715
C	0.250733	2.563604	-0.721070
C	1.472938	2.532912	-1.422020
C	2.686240	2.356243	-0.729964
H	3.898217	2.072717	2.476323
O	1.441230	1.210375	3.339722
H	2.376285	3.089873	-3.312798
H	0.611922	3.140551	-3.320647
C	-1.067108	2.561387	1.417260
C	-1.077448	2.567758	-1.439174
O	1.430378	1.228170	-3.391111
C	3.986180	2.096621	-1.454143
H	-1.726774	1.779600	-1.049130
H	-0.988067	2.385678	-2.508613
H	-1.612835	3.515660	-1.295720
H	4.762921	2.825367	1.126350
H	4.387616	1.104651	1.100814
H	2.405172	3.063368	3.269278
H	0.641314	3.130779	3.289489
H	-1.610320	3.503983	1.269205
H	-0.969553	2.388825	2.487516
H	-1.713203	1.764994	1.038311
H	3.881005	2.094651	-2.537633
H	4.377082	1.110179	-1.176183
H	4.755671	2.830407	-1.184739
H	4.292202	-3.015275	-0.051722
Br	-5.187460	-0.313170	0.044776

Zn-Ethyl

energy: -3951.249829816408 Hartrees

C	-1.086344	-0.918542	2.794594
C	-2.295715	-0.490247	3.465605
C	-3.290715	-0.478830	2.528270
C	-2.688039	-0.841480	1.266274
C	-3.319898	-0.751926	0.026474
C	-2.707280	-0.822619	-1.224152
C	-3.329932	-0.443202	-2.471303
C	-2.350738	-0.444471	-3.425094
C	-1.130668	-0.882285	-2.779587
C	0.115614	-1.036246	-3.402517
C	0.303006	-0.343589	-4.711572
C	0.964312	0.906739	-4.644277
C	1.066478	1.719595	-5.774630
C	0.539862	1.272461	-6.989924
C	-0.078789	0.026271	-7.079864
C	-0.198319	-0.772969	-5.938258
N	-1.356503	-1.129160	1.460646
N	-1.379265	-1.108096	-1.443806
C	1.265900	-1.568015	-2.792018
C	2.485732	-1.876267	-3.496691
C	3.382042	-2.324383	-2.568486
C	2.733189	-2.257907	-1.274806
C	3.358684	-2.495204	-0.036585
C	2.754212	-2.273279	1.214943
C	3.425666	-2.347425	2.496562
C	2.544143	-1.908871	3.443587
C	1.310787	-1.601478	2.762502
C	0.169693	-1.076698	3.395805
C	0.382120	-0.380552	4.699694
C	-0.065120	-0.816769	5.943765
C	0.084008	-0.013093	7.079416
C	0.677585	1.242848	6.964566
C	1.148595	1.698979	5.729377
C	1.016158	0.882683	4.605063
N	1.433162	-1.825735	-1.454277
N	1.455958	-1.847983	1.420216
H	-2.369452	-0.240279	4.514584
H	-4.332006	-0.215029	2.666340
H	-4.372856	-0.175915	-2.588819
H	-2.442102	-0.180370	-4.469129
H	1.560216	2.684880	-5.710114
H	0.625286	1.902637	-7.871579
H	-0.475529	-0.320085	-8.029922
H	-0.703134	-1.734248	-5.989983
H	2.630770	-1.769237	-4.563096
H	4.393141	-2.654032	-2.760482
H	4.441417	-2.673954	2.668469
H	2.707191	-1.808579	4.508056
H	-0.550581	-1.786680	6.015374
H	-0.270501	-0.364278	8.044266
H	0.786007	1.875605	7.841841
H	1.620939	2.673346	5.646255
Zn	0.043655	-1.458724	-0.004392
C	4.036174	1.954879	1.390364
C	1.555395	2.547576	2.885833
C	1.538415	2.468058	1.377673
C	2.741139	2.260192	0.676018
C	1.536092	2.565865	-2.932309
C	0.311323	2.515704	0.686415
C	0.305906	2.518375	-0.724323
C	1.527811	2.474974	-1.424773
C	2.735844	2.264656	-0.733013
H	3.937599	1.954764	2.474594
O	1.474682	1.189661	3.361027
H	2.441268	3.063012	-3.299848
H	0.676563	3.125188	-3.312888
C	-1.010772	2.527704	1.415721
C	-1.021582	2.532890	-1.443736
O	1.485836	1.210484	-3.423763
C	4.025725	1.966243	-1.459515
H	-1.673510	1.744506	-1.057404
H	-0.930858	2.354233	-2.513825
H	-1.553206	3.482643	-1.297804
H	4.830173	2.660368	1.116692
H	4.388208	0.954544	1.109072
H	2.472209	3.021585	3.254767
H	0.709384	3.123089	3.273947
H	-1.552267	3.470247	1.260666
H	-0.910687	2.364172	2.487268
H	-1.657916	1.727709	1.044915
H	3.918084	1.972256	-2.542830
H	4.381789	0.964900	-1.187029
H	4.820555	2.671618	-1.187762
H	-4.374431	-0.489685	0.036685
C	4.787566	-3.006351	-0.051970
H	5.314135	-2.612900	-0.924772
H	5.329876	-2.621336	0.814948
C	4.857898	-4.542182	-0.060292
H	4.351291	-4.947653	-0.942482
H	4.368319	-4.956810	0.827257

H	5.898969	-4.885324	-0.072037

Zn-H

energy: -3872.594866227726 Hartrees

C	-1.072865	-0.922321	2.797045
C	-2.277951	-0.480769	3.466874
C	-3.273053	-0.457548	2.529022
C	-2.674460	-0.827414	1.267510
C	-3.303025	-0.731093	0.025674
C	-2.694622	-0.810683	-1.227348
C	-3.314044	-0.425935	-2.474150
C	-2.335303	-0.439808	-3.429165
C	-1.119123	-0.889772	-2.785099
C	0.126845	-1.052331	-3.413935
C	0.316597	-0.350104	-4.717711
C	0.958715	0.909081	-4.638421
C	1.066398	1.724877	-5.766305
C	0.562825	1.272476	-6.989424
C	-0.038393	0.018700	-7.089970
C	-0.162414	-0.784223	-5.951341
N	-1.346349	-1.130466	1.463753
N	-1.370163	-1.111694	-1.449481
C	1.268785	-1.599501	-2.806711
C	2.510160	-1.891581	-3.489281
C	3.381219	-2.368287	-2.549759
C	2.692271	-2.332842	-1.279407
C	3.279402	-2.579561	-0.038418
C	2.713613	-2.347240	1.215244
C	3.424125	-2.393315	2.473255
C	2.568869	-1.925335	3.431727
C	1.315413	-1.630154	2.773007
C	0.183203	-1.089064	3.403593
C	0.398139	-0.385654	4.703155
C	-0.029241	-0.827545	5.952065
C	0.123509	-0.022294	7.086107
C	0.701220	1.240314	6.964351
C	1.151775	1.702366	5.723790
C	1.014827	0.885101	4.600496
N	1.402963	-1.892108	-1.471896
N	1.427188	-1.910307	1.433675
H	-2.349329	-0.230403	4.515979
H	-4.310993	-0.181081	2.667416
H	-4.353719	-0.146309	-2.591601
H	-2.424973	-0.176764	-4.473686
H	1.546035	2.696602	-5.694303
H	0.652125	1.905309	-7.868784
H	-0.417956	-0.330952	-8.045795
H	-0.653637	-1.752047	-6.011028
H	2.680450	-1.752713	-4.548336
H	4.404410	-2.692902	-2.693283
H	4.450051	-2.717744	2.596330
H	2.756923	-1.794804	4.488845
H	-0.502428	-1.803107	6.028759
H	-0.215741	-0.377567	8.054915
H	0.812825	1.874233	7.840382
H	1.611486	2.682262	5.636075
Zn	0.033851	-1.498156	-0.006146
C	4.025669	2.024961	1.390647
C	1.532240	2.561262	2.887814
C	1.518808	2.494847	1.379237
C	2.724713	2.307413	0.677344
C	1.511377	2.578217	-2.931922
C	0.291491	2.532648	0.687707
C	0.285975	2.534787	-0.722814
C	1.507938	2.501326	-1.423835
C	2.719351	2.311936	-0.732019
H	3.927643	2.018855	2.474866
O	1.453007	1.198270	3.350348
H	2.415226	3.070429	-3.308610
H	0.651023	3.134697	-3.315062
C	-1.030789	2.535186	1.416609
C	-1.041761	2.538487	-1.441687
O	1.456075	1.217496	-3.408816
C	4.015383	2.037463	-1.457314
H	-1.688368	1.746779	-1.053660
H	-0.950772	2.358590	-2.511436
H	-1.579397	3.485034	-1.296848
H	4.804905	2.747832	1.119819
H	4.398221	1.033562	1.105075
H	2.446424	3.034181	3.264009
H	0.683724	3.130680	3.279487
H	-1.577168	3.475123	1.262687
H	-0.930573	2.370521	2.487881
H	-1.673535	1.732579	1.044279
H	3.908343	2.036637	-2.540661
H	4.393724	1.045987	-1.179913
H	4.794239	2.761671	-1.188738
H	-4.354572	-0.456665	0.036061
H	4.318043	-2.899958	-0.049263