Electronic Supplementary Material (ESI) for Chemical Communications


**Supplementary Information**

# $C_{aryl}$-$C_{alkyl}$ bond formation from $Cu(ClO_4)_2$-mediated oxidative cross coupling reaction between arenes and alkyllithium reagents through structurally well-defined Ar-Cu(III) intermediates

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## 1. General Information

Chemical shifts were reported in ppm versus tetramethylsilane with either tetramethylsilane or the residual solvent resonance as an internal standard. Melting points were uncorrected. All solvents were dried according to standard procedures prior to use. All other major chemicals were obtained from commercial sources and used without further purification.

## 2. Experimental details

The synthesis of aryl-copper(III) complexes follows our previous reported procedure (Yao, B.; Wang, D.-X.; Huang, Z.-T.; and Wang, M.-X. *Chem. Commun.***2009**, 2899).

**General procedure for the reaction between aryl-Cu(III) complexes 2 and alkyl lithium reagents 3:** Alkyllithium reagent **3** (1 mmol) in THF solution was added to the solution of aryl-copper(III) complex **2** (0.5 mmol) in THF (25 ml) at 0 ℃. The mixture was kept stirring at 0℃ for 10 minutes and then at room temperature for 45 minutes. The reaction was quenched by adding a saturated aqueous ammonium chloride solution (5 mL), followed by the addition of saturated aqueous EDTA solution (10 ml). The mixture was extracted with $CH_2Cl_2$ (3 × 20 mL). The combined organic layer was washed with brine (20 mL), dried with anhydrous $MgSO_4$, and concentrated under vacuum. The residue was chromatographed with a silica gel column using a mixture of petroleum ether, ethyl acetate, and dichloromethane (12:1:2) as mobile phase to afford pure product **4** and **1** (see Table 1). Compounds **4** were fully characterized by means of spectroscopic data and microanalysis. X-ray single crystal structure of **4f** was also obtained.

**General procedure for the reaction between aryl-Cu(III) complexes 2a and alkyl lithium reagent 3i:** To a cooled solution (-78 ℃) of dimethyl malonate (1.0 mmol) in THF (10 ml) was

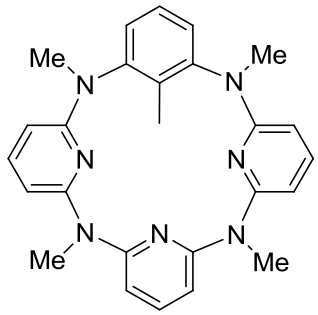
added *n*-BuLi (1.1mmol). After 0.5 h, the temperature of the reaction mixture was allowed to warm to room temperature. The resulting **3i** solution was then added to the solution of aryl-copper(III) complex **2a** (0.5 mmol) in THF (25 ml) at 0 ℃. The mixture was kept stirring at 0 $^{o}$C for 10 minutes and then at room temperature for 45 minutes. The reaction was quenched by adding a saturated aqueous ammonium chloride solution (5 mL), followed by the addition of saturated aqueous EDTA solution (10 ml). The mixture was extracted with $CH_2Cl_2$ (3 × 20 mL). The combined organic layer was washed with brine (20 mL), dried with anhydrous $MgSO_4$, and concentrated under vacuum. The residue was chromatographed with a silica gel column using a mixture of petroleum ether, ethyl acetate, and dichloromethane (12:1:2) as mobile phase to afford pure product **4i**.

**General procedure for the reaction between aryl-Cu(III) complexes 2b and ethyl cyanoacetate 3j:** To a cooled solution (0 ℃) of ethyl cyanoacetate (1.0 mmol) in THF (10 ml) was added NaH (1.2mmol). After 1.0 h, The resulting **3j** solution was then added to the solution of aryl-copper(III) complex **2b**(0.5 mmol) in THF (25 ml) at 0 ℃. The mixture was kept stirring at 0 C for 10 minutes and then at room temperature for 45 minutes. The reaction was quenched by adding a saturated aqueous ammonium chloride solution (5 mL), followed by the addition of saturated aqueous EDTA solution (10 ml). The mixture was extracted with $CH_2Cl_2$ (3 × 20 mL). The combined organic layer was washed with brine (20 mL), dried with anhydrous $MgSO_4$, and concentrated under vacuum. The residue was chromatographed with a silica gel column using a mixture of petroleum ether, ethyl acetate, and dichloromethane (12:1:2) as mobile phase to afford major product **4j**, then the major product **4j** was recrystallized from methanol to afford the pure product **4j**.

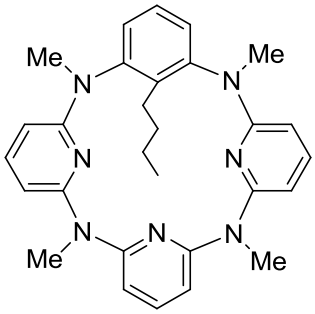
**Synthesis of 4b from a one-pot reaction of 1a:** Azacalix[1]arene[3]pyridine **1a** (211 mg, 0.5

mmol) and $Cu(ClO_4)_2 \cdot 6H_2O$ (278 mg, 0.75 mmol) were dissolved in a mixture of chloroform (5 mL) and methanol (5 mL). The solution turned dark blue immediately with precipitation of dark purple precipitates. After about 90 minutes, the solvent was removed under vacuum, and THF (25 ml) was then add to aryl-copper(III) complex. At 0℃, *n*-BuLi **3c**(1.0 mmol) was added under $N_2$ protection, and resulting mixture was kept stirring for 10 minutes and then at room temperature for 45 minutes. The reaction was quenched by adding a saturated aqueous ammonium chloride (5 mL) followed by the addition of a saturated aqueous EDTA solution (10 ml), and then was extracted with $CH_2Cl_2$ (3 × 20 mL). The combined organic layer was washed with brine (20 mL), dried with anhydrous $MgSO_4$ and concentrated under vacuum. The residue was chromatographed with a silica gel column using a mixture of petroleum ether, ethyl acetate and dichloromethane (12:1:2) as mobile phase to give pure **4b** (51%).

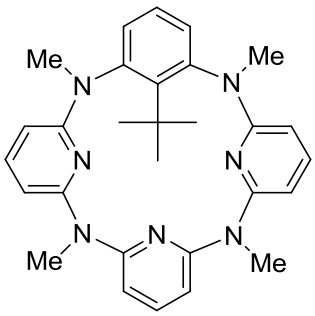
## 3. Characterization of Products



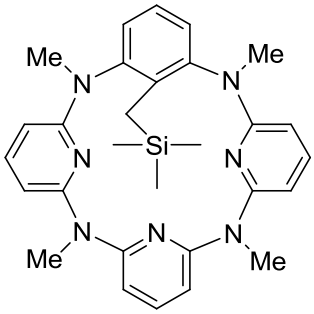

**4a:** 98mg, 45%; mp 230-232 °C; $^1$H NMR (400MHz, $CDCl_3$,) δ 7.39 (t, *J* = 8.0 Hz, 2H), 7.11 (t, *J* = 7.8 Hz, 1H), 6.96 (t, *J* = 7.8 Hz, 1H), 6.77 (d, *J* = 7.8 Hz, 2H), 6.55 (d, *J* = 7.8 Hz, 2H), 6.00 (d, *J* = 7.8 Hz, 2H), 5.97 (d, *J* = 7.8 Hz, 2H), 3.23 (s, 6H), 3.09 (s, 6H), 1.53 (s, 3H); $^{13}$C NMR (100MHz, CDCl3) δ 158.9, 158.7, 157.0, 147.3, 138.8, 137.3, 136.4, 126.6, 125.9, 120.8, 94.6, 93.9, 37.8, 36.1, 12.5; IR (KBr) ν 1576, 1413 $cm^{-1}$; MALDI-TOF *m/z* 438 $[M+H]^+$. HRMS(ESI) for $C_{26}H_{27}N_7$ $(M+H)^+$: 438.2401. Found: 438.2395.



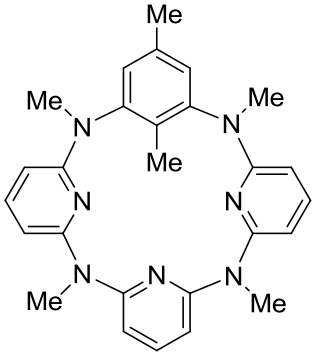

**4b:** 119mg, 50%; mp 182-184 °C; $^{1}$H NMR (400MHz, $CDCl_3$) δ 7.40 (t, *J* = 7.8 Hz, 2H), 7.08 (t, *J* = 7.8 Hz, 2H), 6.67 (t, *J* = 7. 8 Hz, 2H), 6.75 (d, *J* = 7.8 Hz, 2H ), 6.52 (d, *J* = 7.8 Hz, 2H), 6.01 (d, *J* = 7.8 Hz, 2H), 5.98 (d, *J* = 7.8 Hz, 2H), 3.24 (s, 6H), 3.13 (s, 6H), 1.96-1.91 (m, 2H), 1.18-1.03 (m, 4H), 0.67 (t, *J* = 7.3 Hz, 3H); $^{13}$C NMR (100MHz, $CDCl_3$) δ 158.8, 158.7, 157.1, 147.5, 141.5, 138.7, 137.2, 126.8, 126.3, 120.5, 94.8, 94.3, 39.1, 36.1, 31.7, 27.3, 23.2, 13.8; IR (KBr) ν 1581, 1419 $cm^{-1}$; MALDI-TOF *m/z* 480 $[M+H]^+$. Anal. Calcd. for $C_{29}H_{33}N_7$: C, 72.62; H, 6.94; N, 20.44. Found: C, 72.77; H, 7.10; N, 20.27.



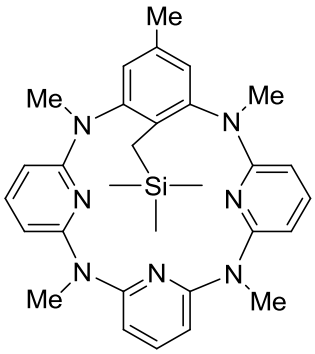

**4c:** 110mg, 46%; mp 236-237 °C; $^{1}$H NMR (300MHz, $CDCl_3$) δ 7.39 (t, *J* = 8.2 Hz, 2H), 7.09 (t, *J* = 7.8 Hz, 1H), 6.97 (t, *J* = 7.8 Hz, 1H), 6.75 (d, *J* = 7.8 Hz, 2H), 6.53 (d, *J* = 7.8 Hz, 2H), 6.01 (d, *J* = 7.8 Hz, 2H), 5.97 (d, *J* = 8.2 Hz, 2H), 3.23 (s, 6H), 3.13 (s, 6H), 0.63 (s, 9H); $^{13}$C NMR (100MHz, $CDCl_3$) δ 158.8, 158.6, 157.2, 147.4, 141.9, 138.7, 137.2, 126.9, 126.2, 120.5, 94.8, 94.4, 39.2, 36.1, 29.1, 22.9; IR (KBr) ν 1581, 1420 $cm^{-1}$; GC-MASS *m/z* 480$[M+H]^+$. HRMS(ESI) for $C_{29}H_{33}N_7$ $(M+H)^+$: 480.2876. Found: 480.2874.



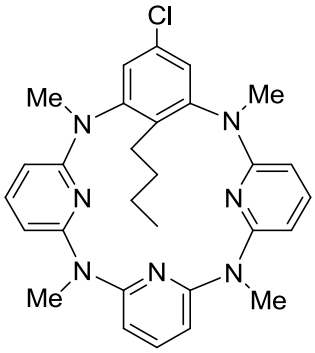

**4d:** 106mg, 42%; mp 260-262 C; $^{1}$H NMR (400MHz, $CDCl_3$) δ 7.40 (t, *J* = 8.2 Hz, 2H), 7.04 (t, *J* = 7.8 Hz, 1H), 6.88 (t, *J* = 7.6 Hz, 1H), 6.71 (d, *J* = 7.8 Hz, 2H), 6.51 (d, *J* = 7.8 Hz, 2H), 6.03 (d, *J* = 8.2 Hz, 2H), 5.99 (d, *J* = 7.8 hz, 2H), 3.26 (s, 6H), 3.12 (s, 6H), 1.55 (s, 2H), -0.27 (s, 9H); $^{13}$C NMR (100MHz, $CDCl_3$) δ 158.6, 158.5, 156.7, 146.7, 140.6, 138.6, 136.8, 124.8, 124.1, 120.4, 95.3, 94.9, 39.6, 35.9, 16.7, 0.95; IR (KBr) ν 1578, 1422 $cm^{-1}$; GC-MASS *m/z* 510$[M+H]^+$. HRMS(ESI) for $C_{29}H_{35}N_7Si$ $(M+H)^+$: 510.2796. Found:510.2804.




**4e:** 101mg, 45%; mp 151-152 $^{o}$C; $^{1}$H NMR (400MHz, $CDCl_3$,) δ 7.38 (t, *J* = 8.0 Hz, 2H), 7.14 (t, *J* = 7.8 Hz, 1H), 6.60-6.53 (m, 4H), 6.00 (d, *J* = 7.8 Hz, 2H), 6.95 (d, *J* = 7.8 Hz, 2H), 6.00 (d, *J* = 8.2 Hz, 2H), 3.24 (s, 6H), 3.08 (s, 6H), 2.23 (s, 3H), 1.49 (s, 3H); $^{13}$C NMR (100MHz, $CDCl_3$) δ 158.9, 158.8, 157.0, 147.0, 138.8, 136.5, 135.0, 132.9, 127.4, 120.7, 94.5, 93.9, 37.7, 36.1, 20.8, 12.2; IR (KBr) ν 1584, 1414 $cm^{-1}$; ESI-MS: *m/z* 452 $[M+H]^+$. HRMS(ESI) for $C_{27}H_{30}N_7$ $(M+H)^+$: 452.2557. Found: 452.2558.

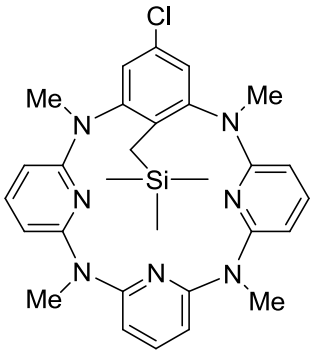



**4f:** 144mg, 55%; mp 245-246 C; $^{1}$H NMR (400MHz, $CDCl_3$) δ 7.39 (t, *J* = 8.0 Hz, 2H), 7.05 (t, *J* = 7.5 Hz, 1H), 6.54 (s, 2H), 6.53 (d, *J* = 8.7 Hz, 2H), 6.03 (d, *J* = 8.2 Hz, 2H), 5.98 (d, *J* = 8.2 Hz, 2H), 3.26 (s, 6H), 3.09 (s, 6H), 2.21 (s, 3H), 1.49 (s, 2H), -0.20 (s, 9H); $^{13}$C NMR (100MHz, $CDCl_3$) δ 158.8, 158.7, 157.0, 146.3, 138.8, 137.2, 136.4, 133.4, 125.7, 120.5, 95.4, 95.0, 39.6, 36.1, 20.7, 16.4, 0.19; IR (KBr) ν 1582, 1421 $cm^{-1}$; ESI-MS: *m/z* 524 $[M+H]^+$. HRMS(ESI) for $C_{30}H_{38}N_7Si$ $(M+H)^+$: 524.2952. Found: 524.2941. An X-ray-quality single crystal of **4f** was obtained by slow evaporation of the solution in a mixture of ethyl acetate and methanol at room temperature.

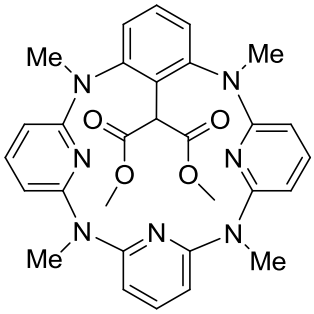



**4g:** 125mg, 49%; mp 120-121 $^{o}$C; $^{1}$H NMR (400MHz, $CDCl_3$) δ 7.40 (t, *J* = 8.0 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 1H), 6.76 (s, 2H), 6.58 (d, *J* = 7.8 Hz, 2H), 6.03 (d, *J* = 8.2 Hz, 2H), 5.98 (d, *J* = 8.2 Hz, 2H), 3.24 (s, 6H), 3.10 (s, 6H), 1.91 (t, *J* = 8.0 Hz, 2H), 1.15-1.01 (m, 4H), 0.65 (t, *J* = 7.1 Hz, 3H); $^{13}$C NMR (100MHz, $CDCl_3$) δ 158.7, 157.0, 148.5, 140.4, 138.9, 137.0, 127.4, 120.6, 95.4, 94.4, 38.7, 36.1, 31.4, 27.0, 23.2, 13.7; IR (KBr) ν 1569, 1420 $cm^{-1}$; ESI-MS: *m/z* 514(100%) $[M+H]^+$; 516 (43%) $[M+2+H]^+$. HRMS(ESI) for $C_{29}H_{33}ClN_7$ $(M+H)^+$: 514.2488. Found:

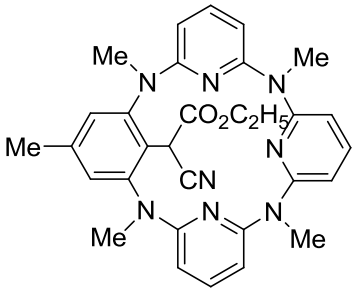
514.2480.




**4h**：144mg, 53%; mp 256-257 C; $^{1}$H NMR (400MHz, $CDCl_3$) δ 7.41 (t, *J* = 8.0 Hz, 2H), 7.25 (t, *J* = 7.8 Hz, 1H), 6.73 (s, 2H), 6.58 (d, *J* = 7.7 Hz, 2H), 6.06 (d, *J* = 8.2 Hz, 2H), 6.00 (d, *J* = 8.2 Hz, 2H), 3.26 (s, 6H), 3.09 (s, 6H), 1.51 (s, 2H), -0.18 (s, 9H); $^{13}$C NMR (100MHz, $CDCl_3$) δ 158.7, 158.6, 156.8, 147.5, 139.9, 139.0, 136.9, 128.3, 125.5, 120.6, 95.7, 95.7, 39.5, 36.0, 16.7, 0.14; IR (KBr) ν 1572, 1422 cm$^{-1}$; ESI-MS: *m/z* 544 (100%) $[M+H]^+$; 546 (42%) $[M+2+H]^+$. HRMS(ESI) for $C_{29}H_{35}N_7Si$ $(M+H)^+$: 544.2406. Found: 544.2409.

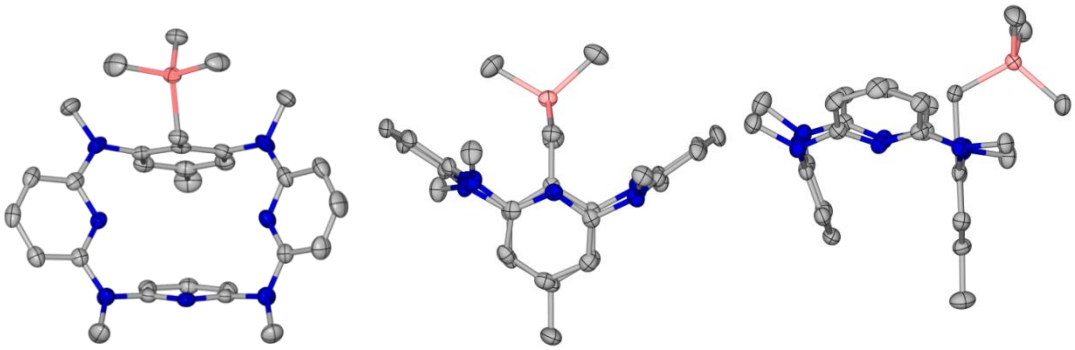



**4i:** 116mg, 42%; mp 182-183$^{o}$C; $^{1}$H NMR (400MHz, $CDCl_3$) δ 7.42 (t, *J* = 8.0 Hz, 2H), 7.09 (t, *J* = 6.6 Hz, 1H), 7.05 (t, *J* = 6.6 Hz, 1H), 6.79 (d, *J* = 7.7 Hz, 2H), 6.41 (d, *J* = 7.8 Hz, 2H), 6.15 (d, *J* = 7.8 Hz, 2H), 6.05 (d, *J* = 8.2 Hz, 2H), 4.37 (s, 1H), 3.26 (s, 6H), 3.22 (s, 6H), 3.01 (s, 6H); $^{13}$C NMR (100MHz, $CDCl_3$) δ 169.2, 159.3, 158.7, 156.9, 147.3, 138.9, 136.6, 133.3, 128.9, 127.6, 118.4, 97.7, 95.9, 51.5, 51.2, 37.8, 36.5; IR (KBr) ν 1750, 1727, 1574, 1422 cm$^{-1}$; ESI-MS: *m/z* 554$[M+H]^+$. HRMS(ESI) for $C_{30}H_{32}N_7O$ (M+H)+: 554.2510. Found: 554.2500.

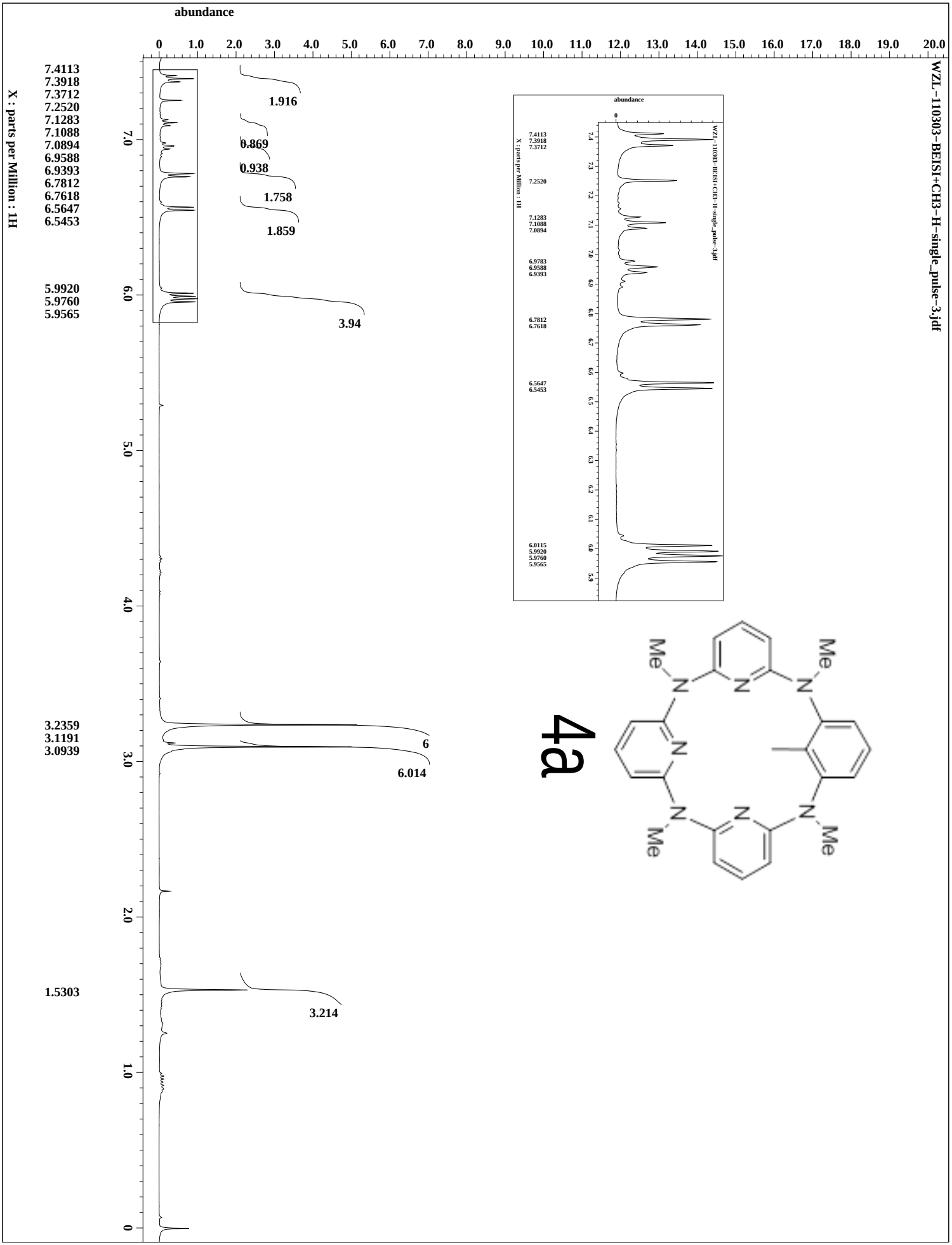



**4j:** 76mg, 35%; mp 180-181°C; $^{1}$H NMR (400MHz, $CDCl_3$) δ 7.47 (t, *J* = 8.3 Hz, 1H), 7.43 (t, *J* = 7.8 Hz, 1H), 7.12 (t, *J* = 7.3 Hz, 1H), 6.70 (s, 1H), 6.66 (s, 1H), 6.49 (d, *J* = 7.3 Hz, 1H), 6.44 (d, *J* = 7.8 Hz, 1H), 6.15 (d, *J* = 8.2 Hz, 1H), 6.12 (dd, *J* = 7.8, 1.4 Hz, 2H), 6.06 (d, *J* = 7.8 Hz, 1H), 4.61 (s, 1H), 3.85-3.80 (m, 1H), 3.69-3.65 (m, 1H), 3.23 (s, 3H), 3.22 (s, 3H), 3.11 (s, 6H), 2.27 (s, 3H), 1.04 (t, *J* = 7.1 Hz, 3H); $^{13}$C NMR (100MHz, $CDCl_3$) δ 165.3, 159.0, 158.9, 158.8, 158.6, 157.4, 157.1, 147.0, 139.8, 139.0, 135.9, 128.6, 128.4, 127.3, 119.5, 118.8, 115.5, 97.6, 97.0, 95.8, 95.5, 61.8, 38.3, 38.0, 36.5, 36.3, 36.1, 29.7, 21.2, 13.9; IR (KBr) ν 2247, 1734, 1577, 1421 $cm^{-1}$; GC-MS: *m/z* 548[M]$^{+}$. HRMS(ESI) for $C_{30}H_{32}N_7O$ $(M+H)^{+}$: 549.2721. Found: 549.2721.

## 4. X-ray structure of 4f



## 5. Copies of $^{1}$H and $^{13}$C NMR Spectra of Products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X : parts per Million : 1H
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7.4113
7.3918
7.3712
7.2520
7.1283
7.1088
7.0894
6.9588
6.9393
6.7812
6.7618
6.5647
6.5453
5.9920
5.9760
5.9565
3.2359
3.1191
3.0939
1.5303
1.916
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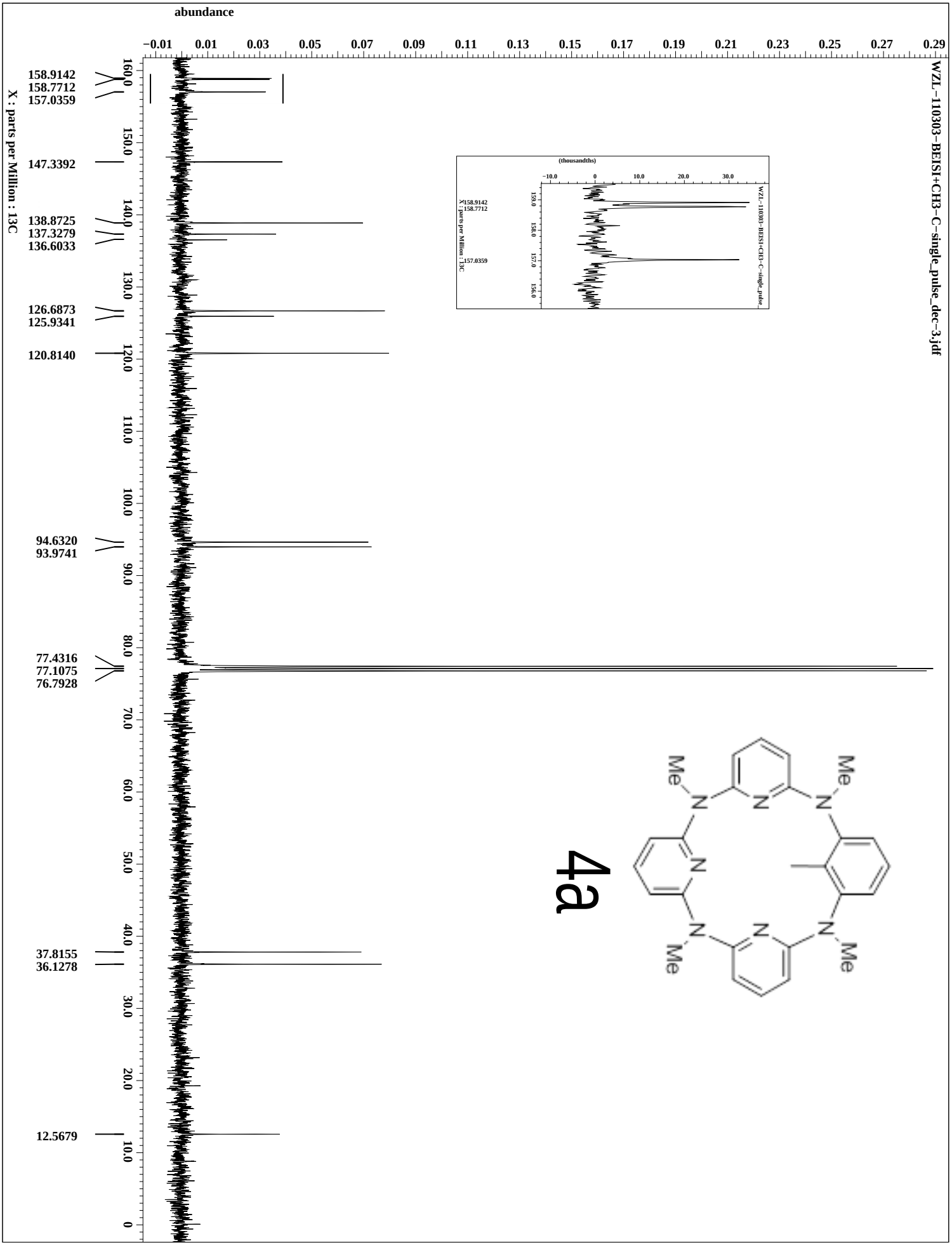
0.938
1.758
1.859
3.94
6
6.014
3.214
4a
Me
N


abundance
WZL-110303-BEISI+CH3-C-single_pulse_dec-3.jdf
X : parts per Million : 13C
158.9142
158.7712
157.0359
147.3392
138.8725
137.3279
136.6033
126.6873
125.9341
120.8140
94.6320
93.9741
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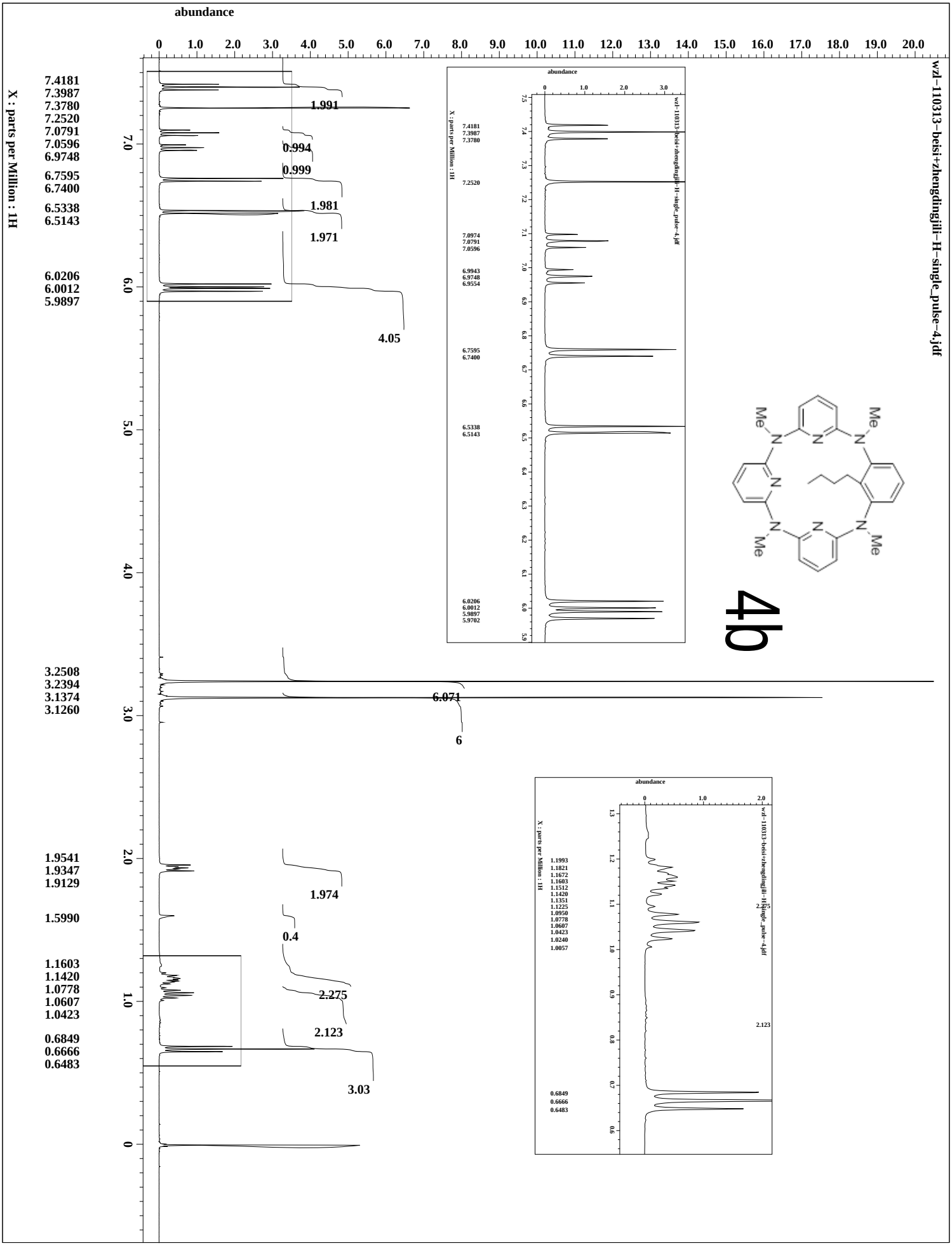
77.1075
76.7928
37.8155
36.1278
12.5679
(thousandths)
4a
Me
N


abundance
wzl-110313-beisi+zhengdingjili-H-single_pulse-4.jdf
X : parts per Million : 1H
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7.3987
7.3780
7.2520
7.0791
7.0596
6.9748
6.7595
6.7400
6.5338
6.5143
6.0206
6.0012
5.9897
3.2508
3.2394
3.1374
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1.9129
1.5990
1.1603
1.1420
1.0778
1.0607
1.0423
0.6849
0.6666
0.6483
1.991
0.994
0.999
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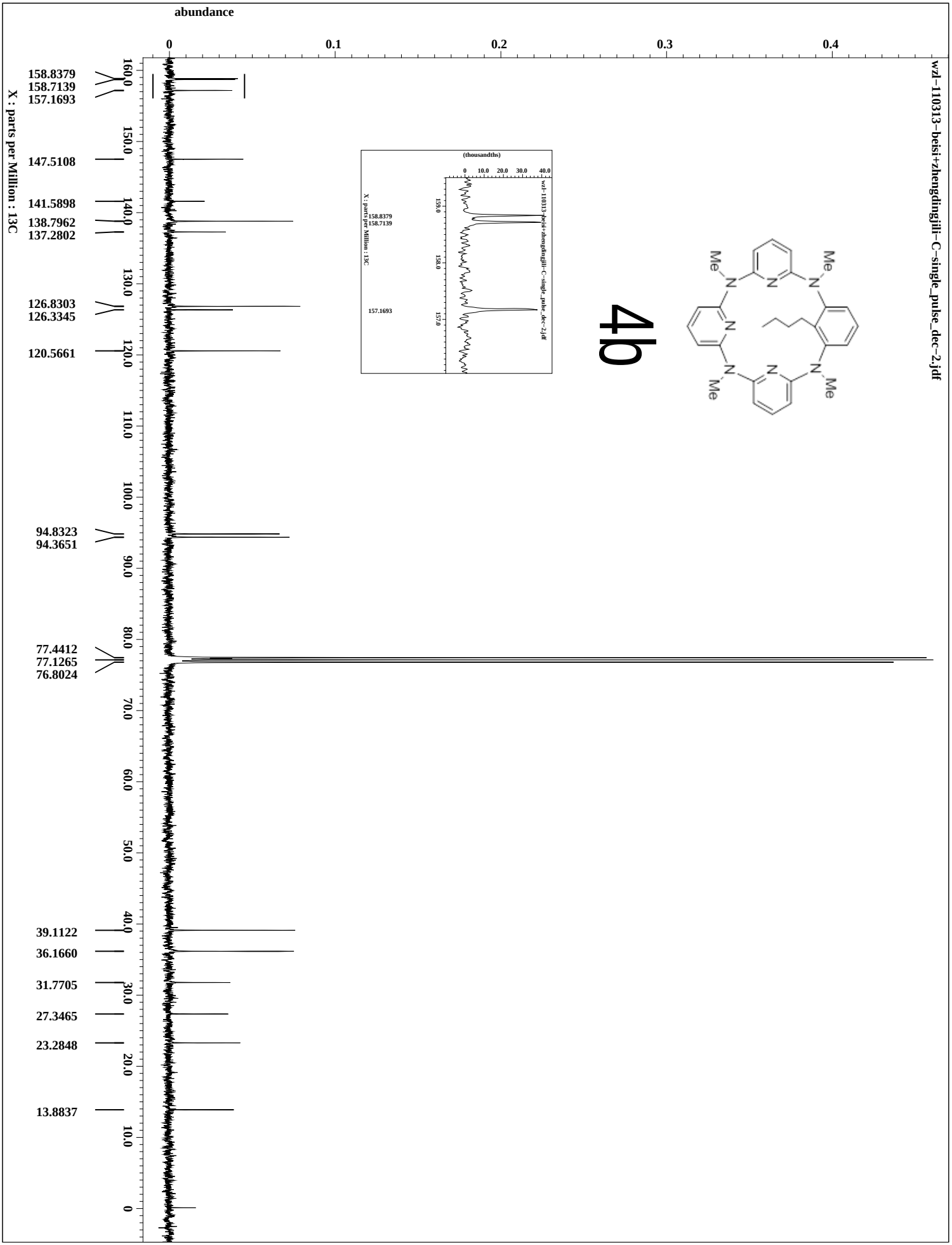
3.03
4b
Me
N


abundance
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0.1
0.2
0.3
0.4
wzl-110313-beisi+zhengdingjili-C-single_pulse_dec-2.jdf
X : parts per Million : 13C
158.8379
158.7139
157.1693
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141.5898
138.7962
137.2802
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120.5661
94.8323
94.3651
77.4412
77.1265
76.8024
39.1122
36.1660
31.7705
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23.2848
13.8837
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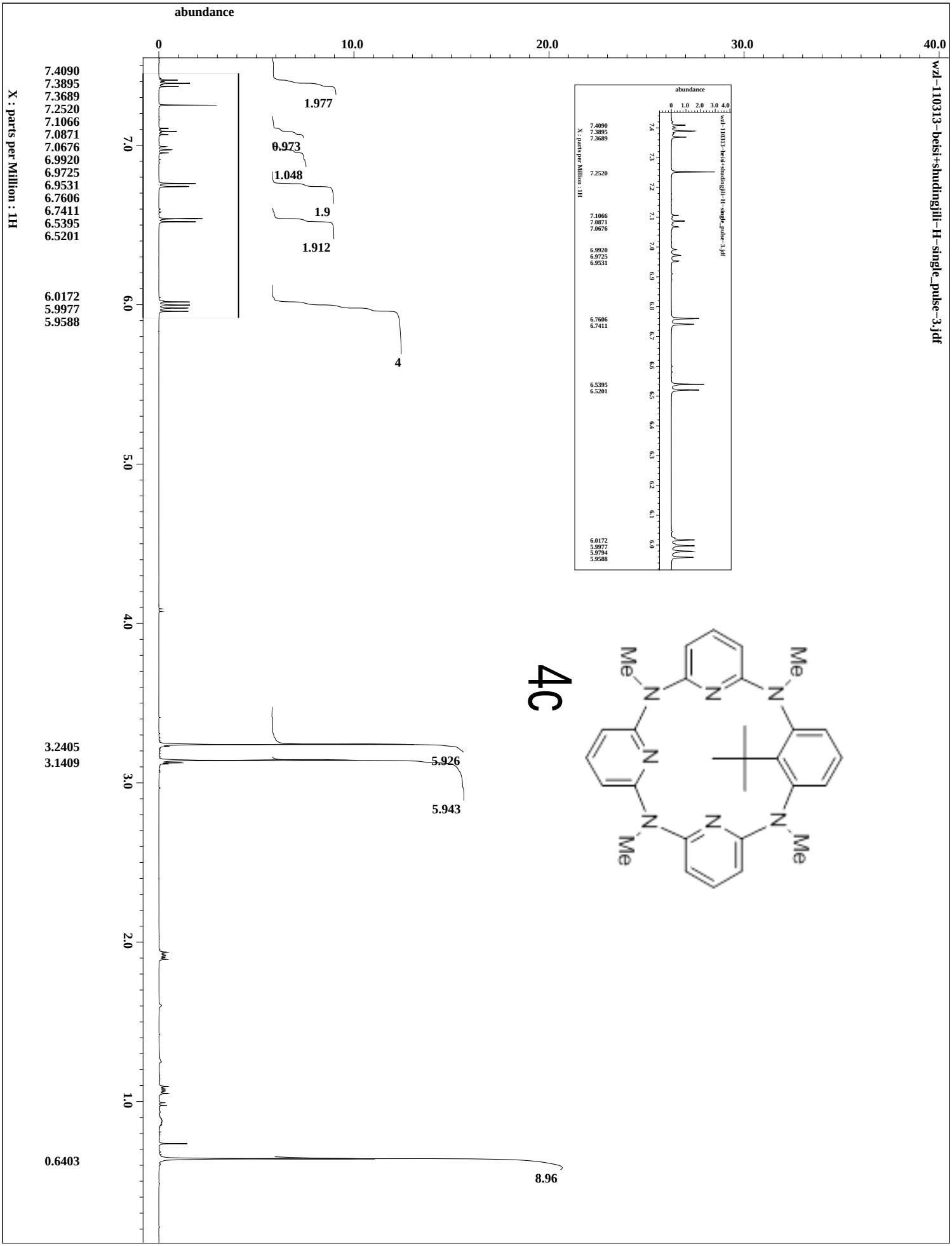
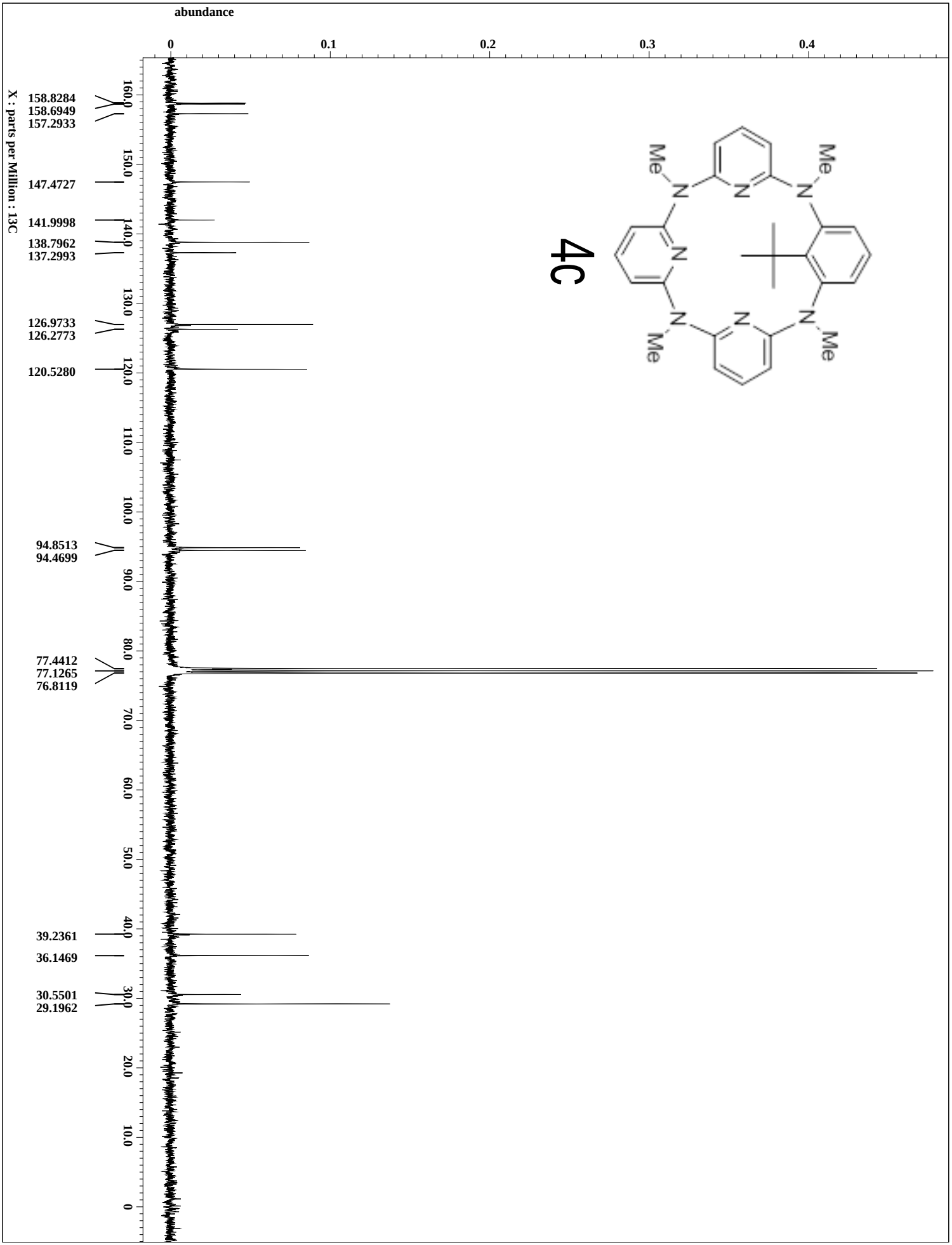
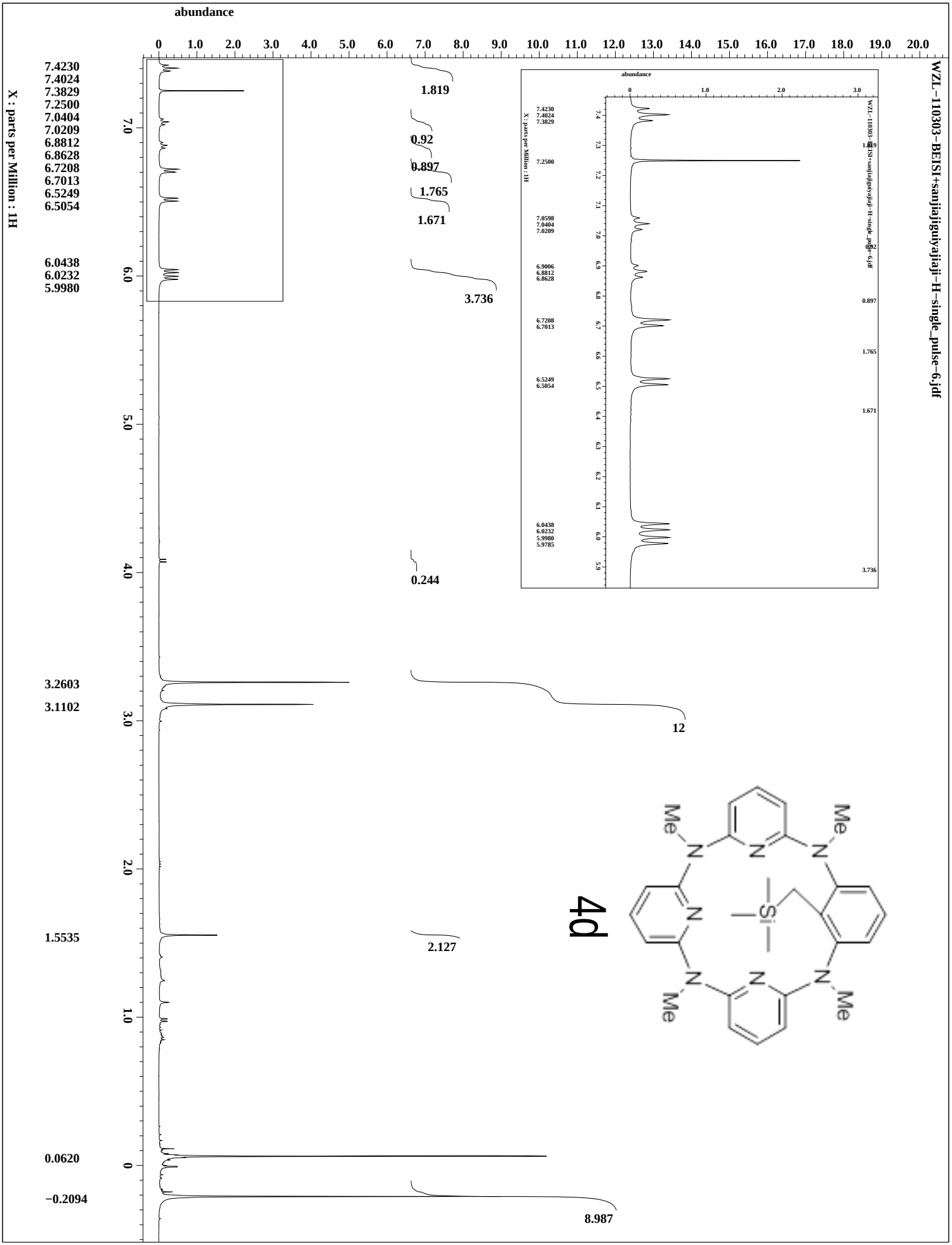
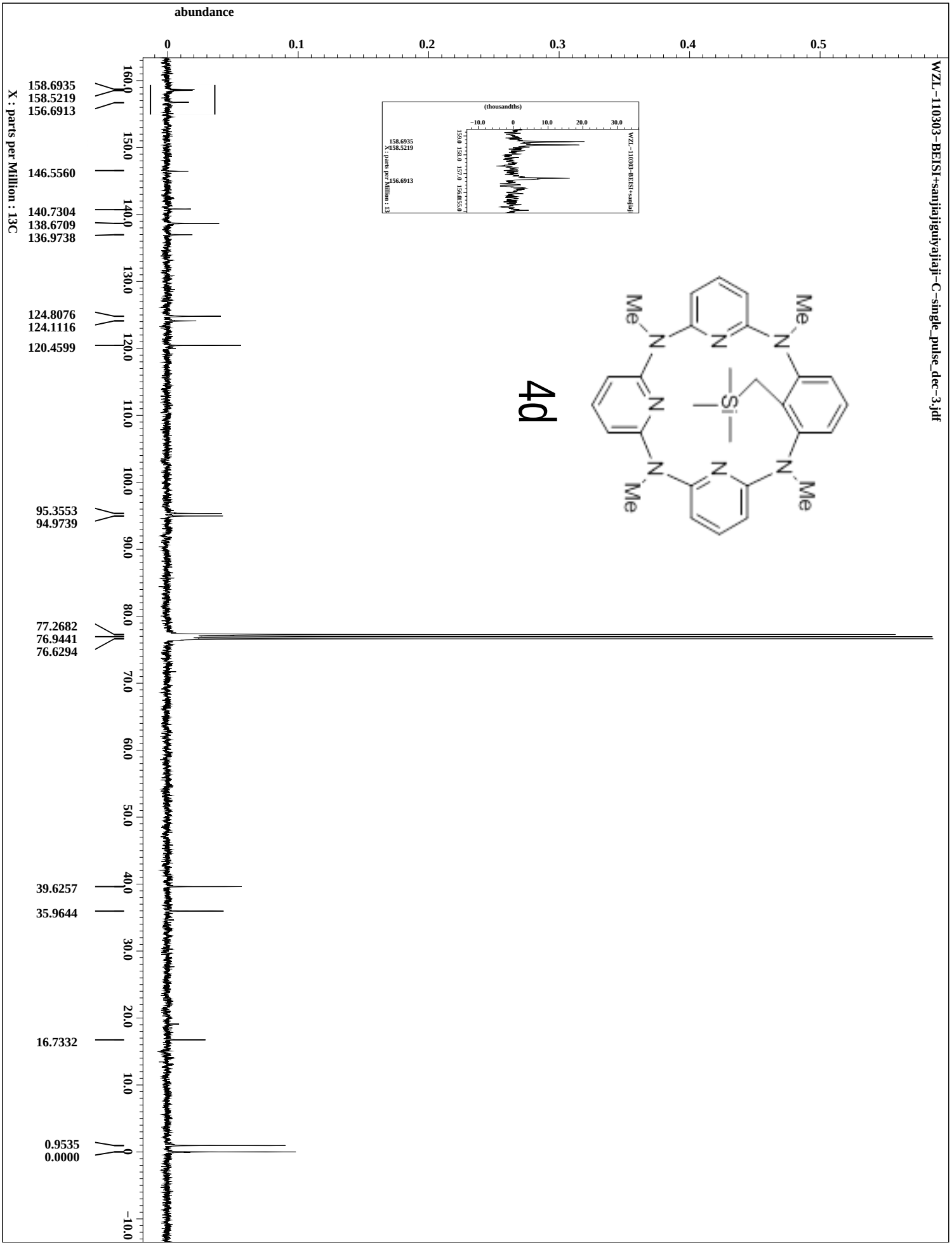
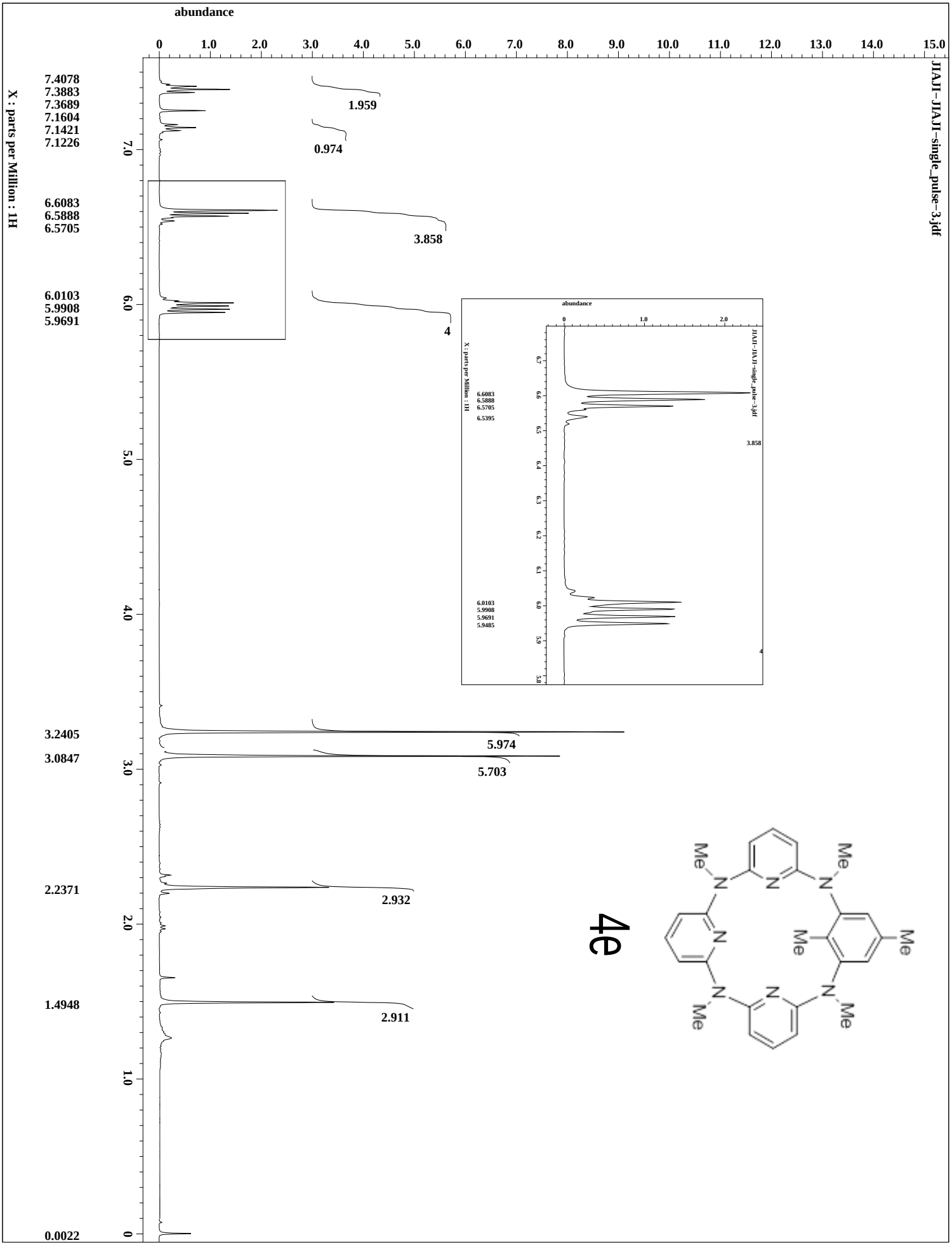
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
(thousandths)
0
10.0
20.0
30.0
40.0
4b
Me
N

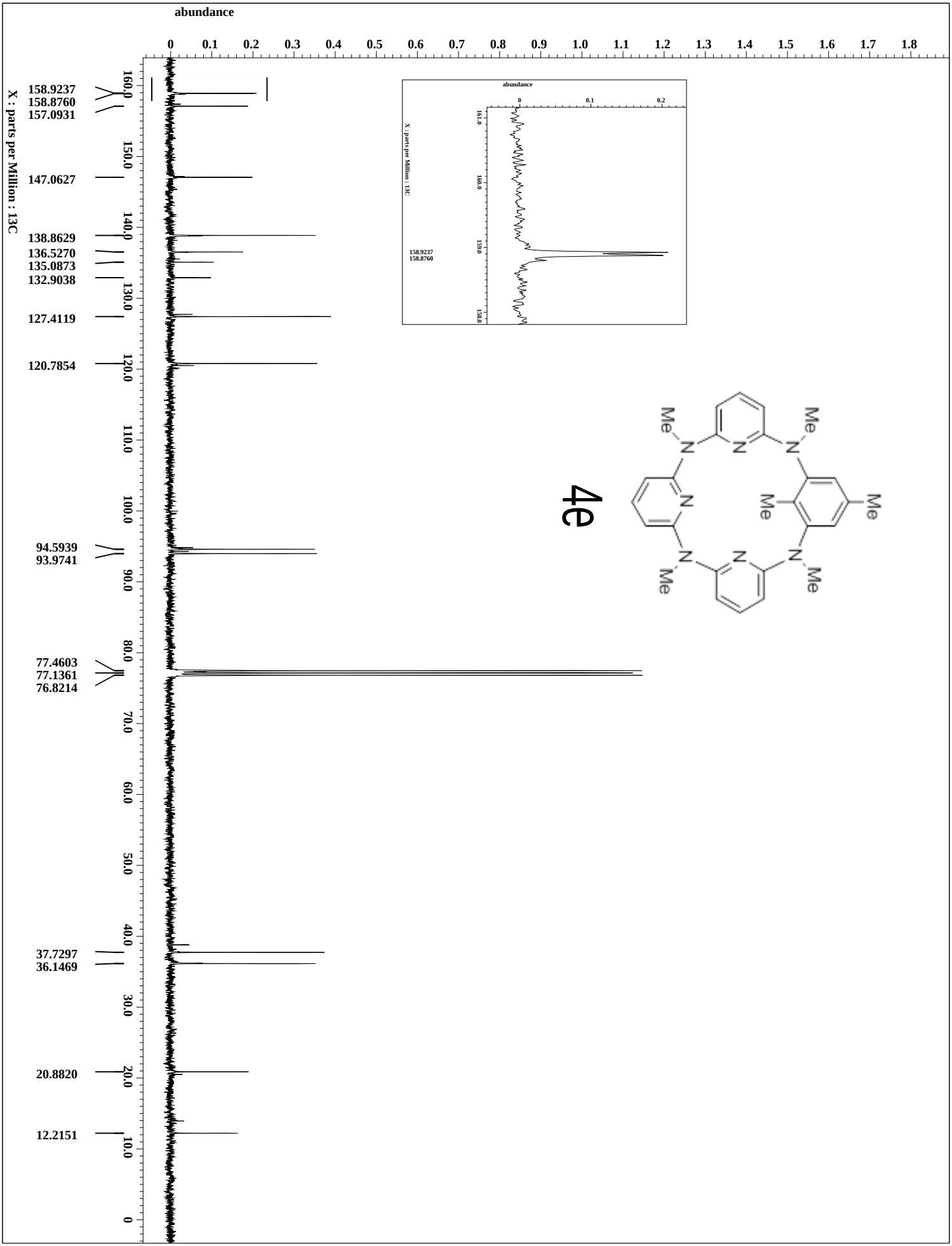

abundance
0
10.0
20.0
30.0
40.0
wzl-110313-beisi+shudingjili-H-single_pulse-3.jdf
X : parts per Million : 1H
7.4090
7.3895
7.3689
7.2520
7.1066
7.0871
7.0676
6.9920
6.9725
6.9531
6.7606
6.7411
6.5395
6.5201
6.0172
5.9977
5.9588
3.2405
3.1409
0.6403
1.977
0.973
1.048
1.9
1.912
4
5.926
5.943
8.96
7.0
6.0
5.0
4.0
3.0
2.0
1.0
4c
Me
N

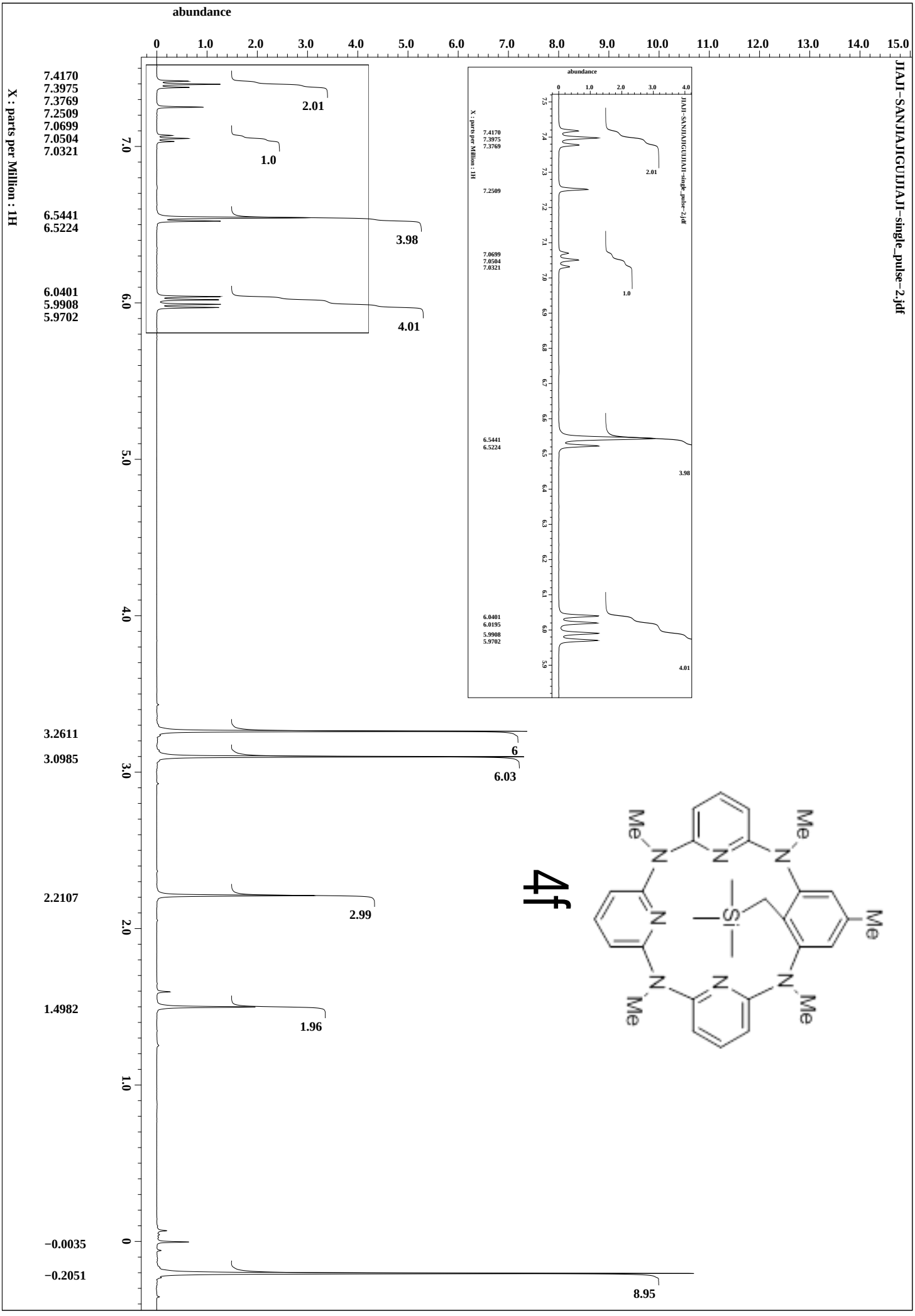


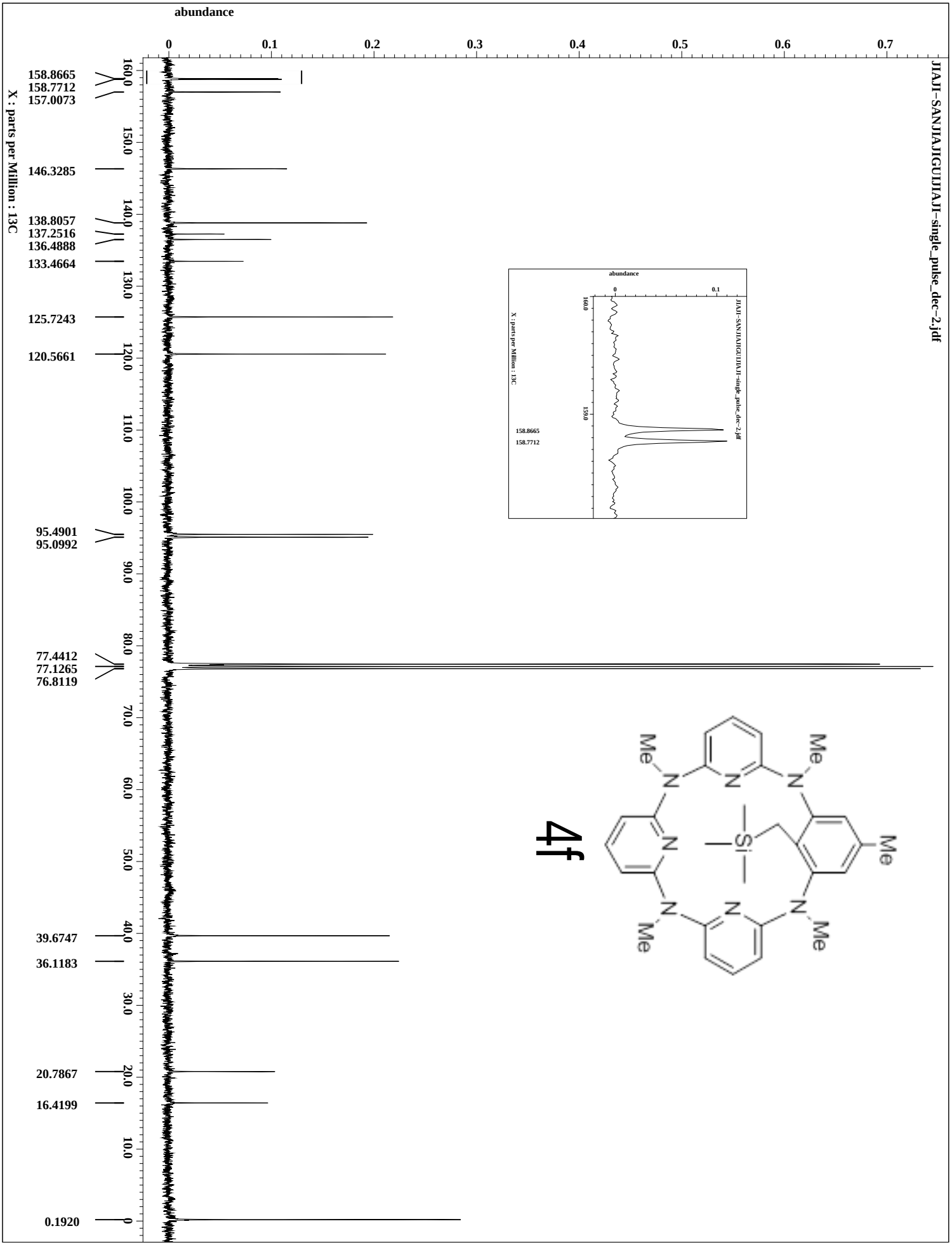

abundance
X : parts per Million : 1H
WZL−110303−BEISI+sanjiajiguiyajiaji−H−single_pulse−6.jdf
7.4230
7.4024
7.3829
7.2500
7.0404
7.0209
6.8812
6.8628
6.7208
6.7013
6.5249
6.5054
6.0438
6.0232
5.9980
3.2603
3.1102
1.5535
0.0620
−0.2094
1.819
0.92
0.897
1.765
1.671
3.736
0.244
12
2.127
8.987
4d
Me
N
Si

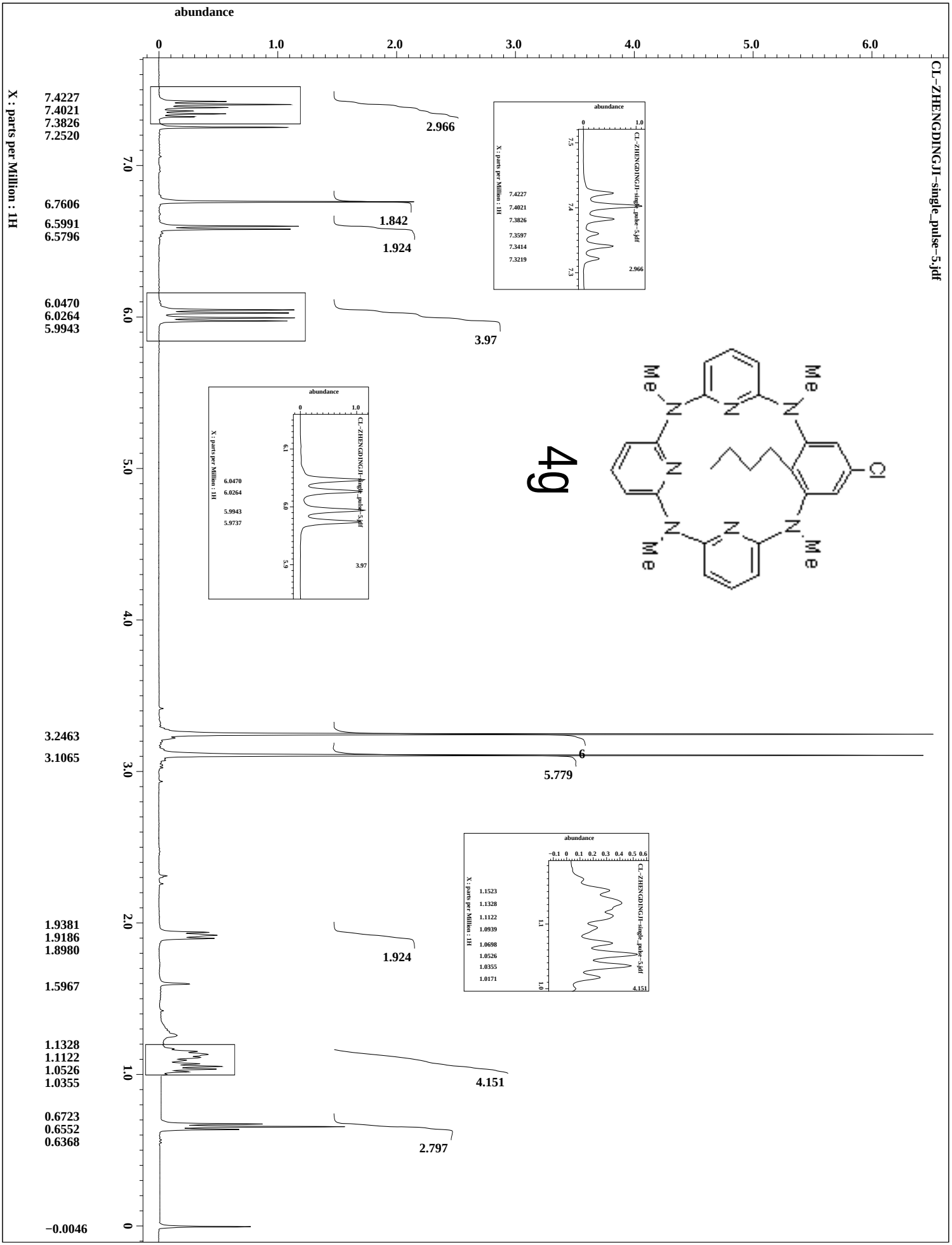

abundance
0
0.1
0.2
0.3
0.4
0.5
WZL-110303-BEISI+sanjiajiguiyajiaji-C-single_pulse_dec-3.jdf
X : parts per Million : 13C
158.6935
158.5219
156.6913
146.5560
140.7304
138.6709
136.9738
124.8076
124.1116
120.4599
95.3553
94.9739
77.2682
76.9441
76.6294
39.6257
35.9644
16.7332
0.9535
0.0000
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
-10.0
(thousandths)
-10.0
0
10.0
20.0
30.0
WZL-110303-BEISI+sanjia
4d
Me
N
Si

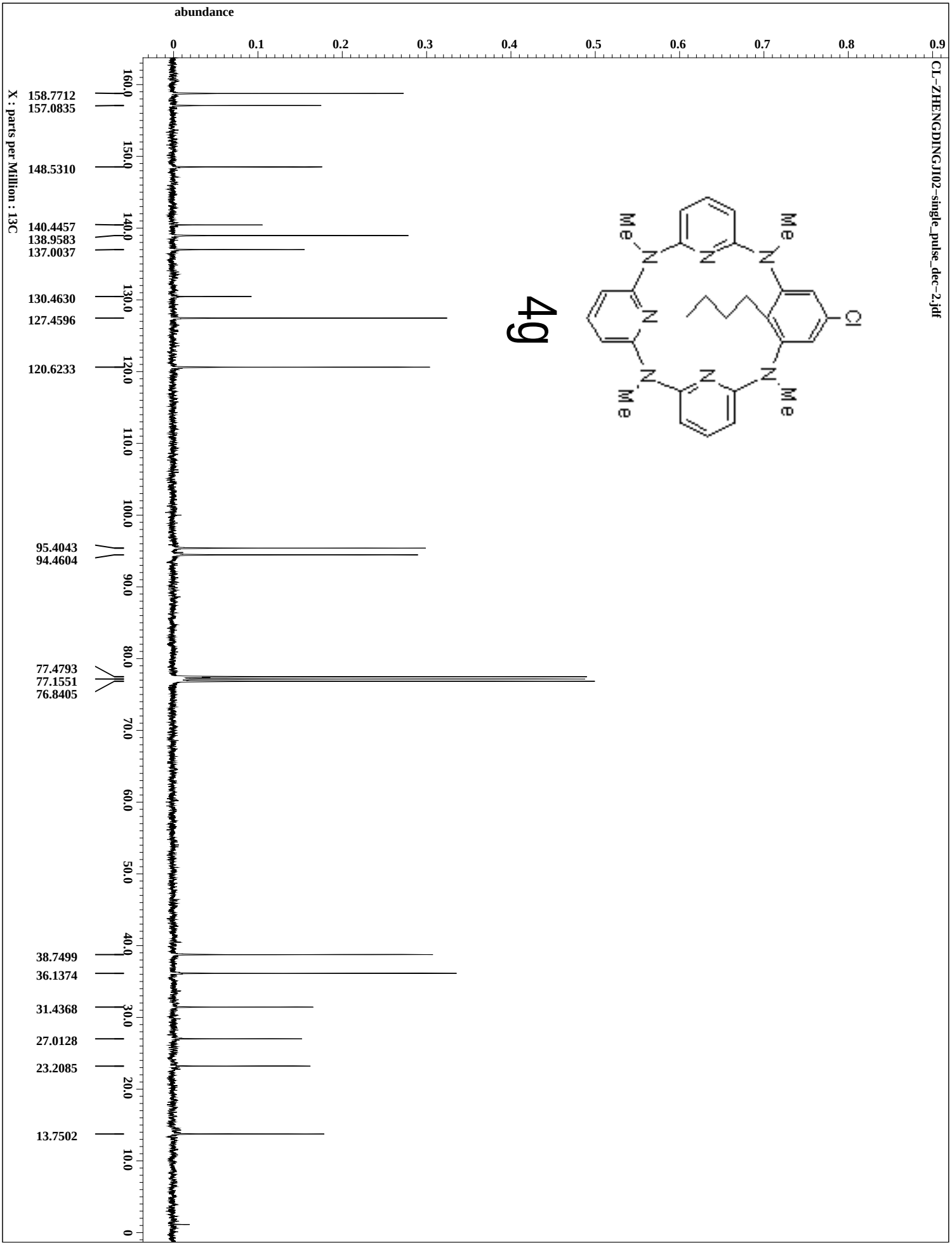

abundance
JIAJI-JIAJI-single_pulse-3.jdf
X : parts per Million : 1H
7.4078
7.3883
7.3689
7.1604
7.1421
7.1226
6.6083
6.5888
6.5705
6.0103
5.9908
5.9691
3.2405
3.0847
2.2371
1.4948
0.0022
1.959
0.974
3.858
4
5.974
5.703
2.932
2.911
6.5395
5.9485
4e
Me
N

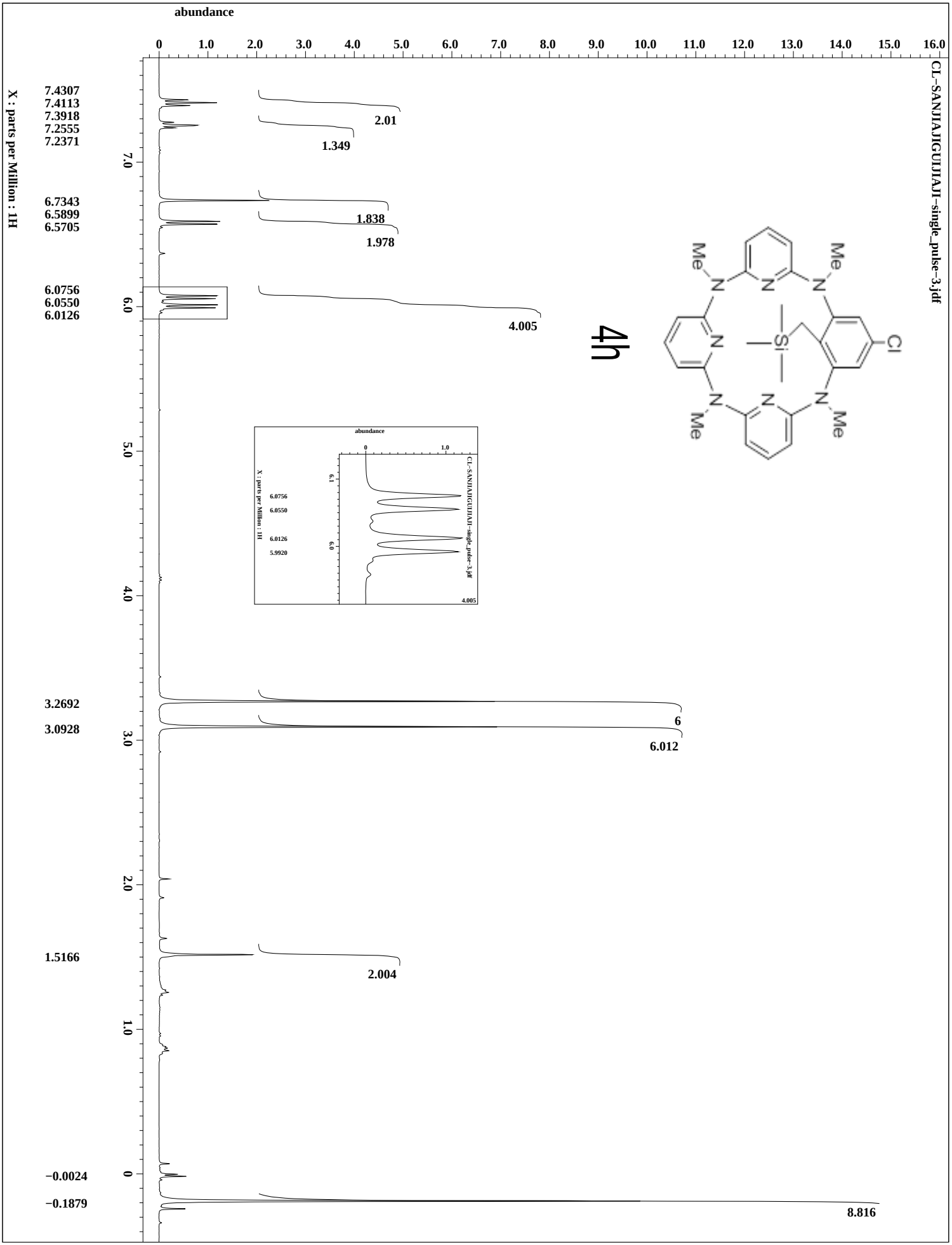


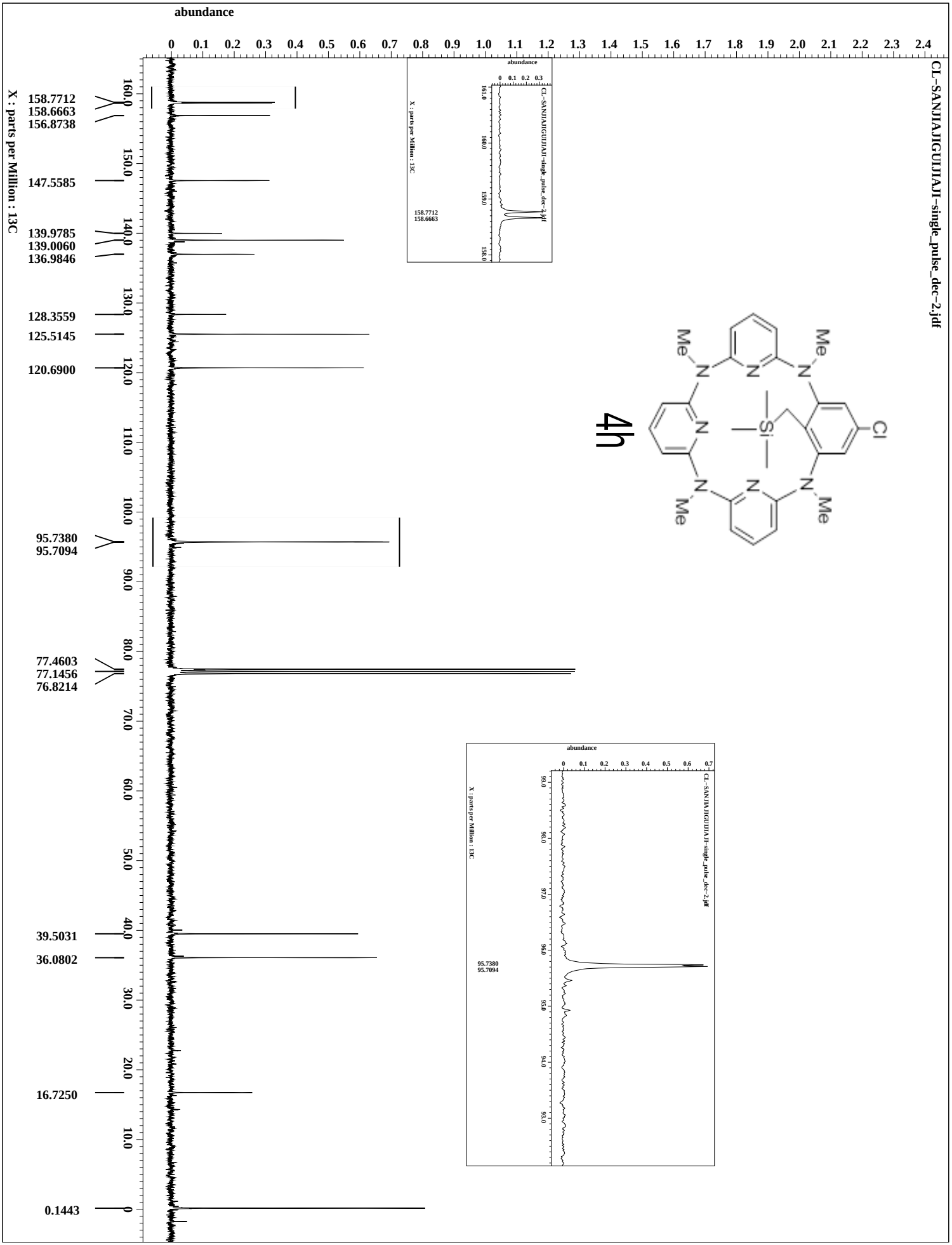


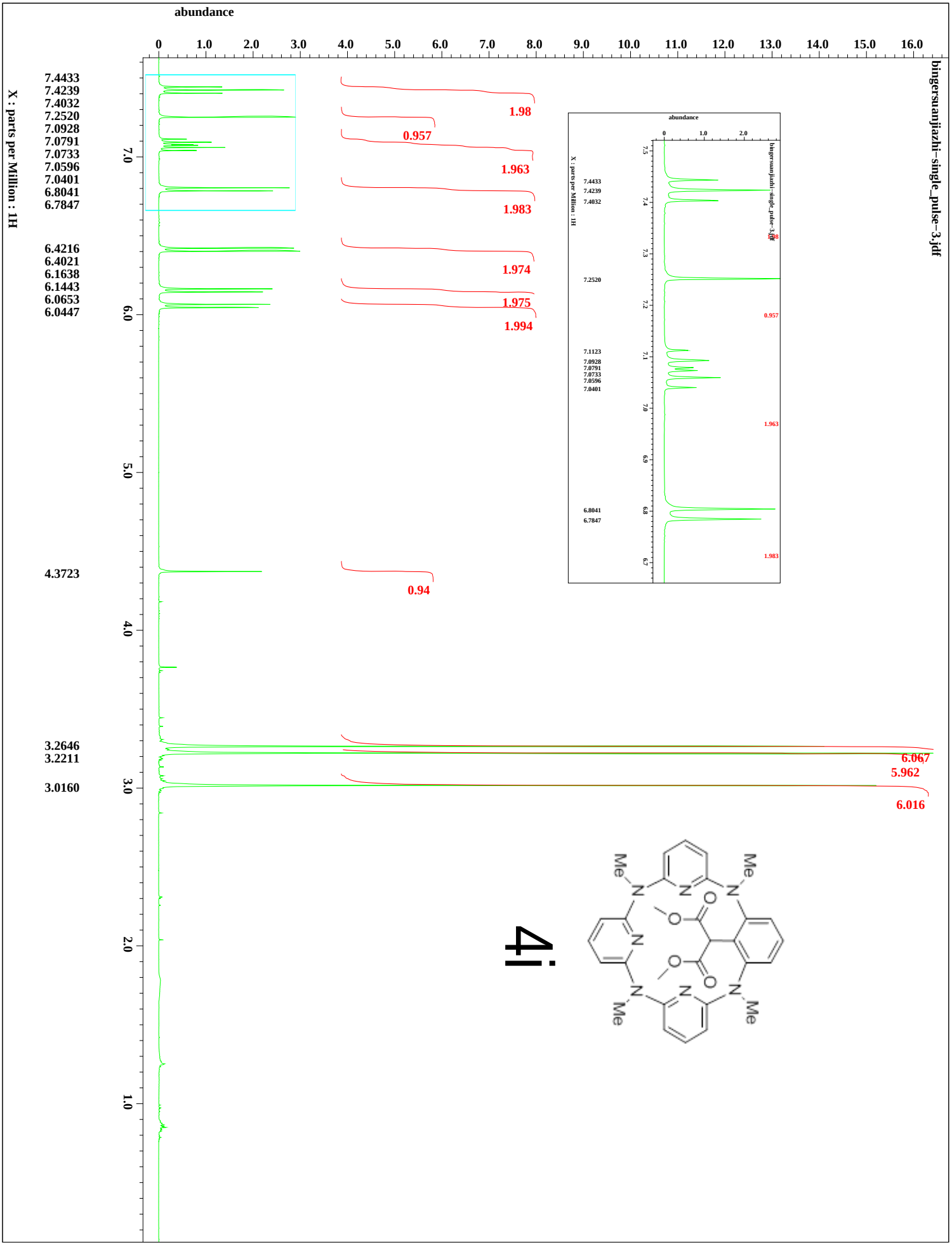

abundance
JIAJI-SANJIAJIGUIJIAJI-single_pulse_dec-2.jdf
X : parts per Million : 13C
158.8665
158.7712
157.0073
146.3285
138.8057
137.2516
136.4888
133.4664
125.7243
120.5661
95.4901
95.0992
77.4412
77.1265
76.8119
39.6747
36.1183
20.7867
16.4199
0.1920
4f
Me
N
Si


abundance
CL-ZHENGDINGJI-single_pulse-5.jdf
X : parts per Million : 1H
7.4227
7.4021
7.3826
7.2520
6.7606
6.5991
6.5796
6.0470
6.0264
5.9943
3.2463
3.1065
1.9381
1.9186
1.8980
1.5967
1.1328
1.1122
1.0526
1.0355
0.6723
0.6552
0.6368
−0.0046
2.966
1.842
1.924
3.97
6
5.779
1.924
4.151
2.797
49
Me
Me
Me
Me
Cl

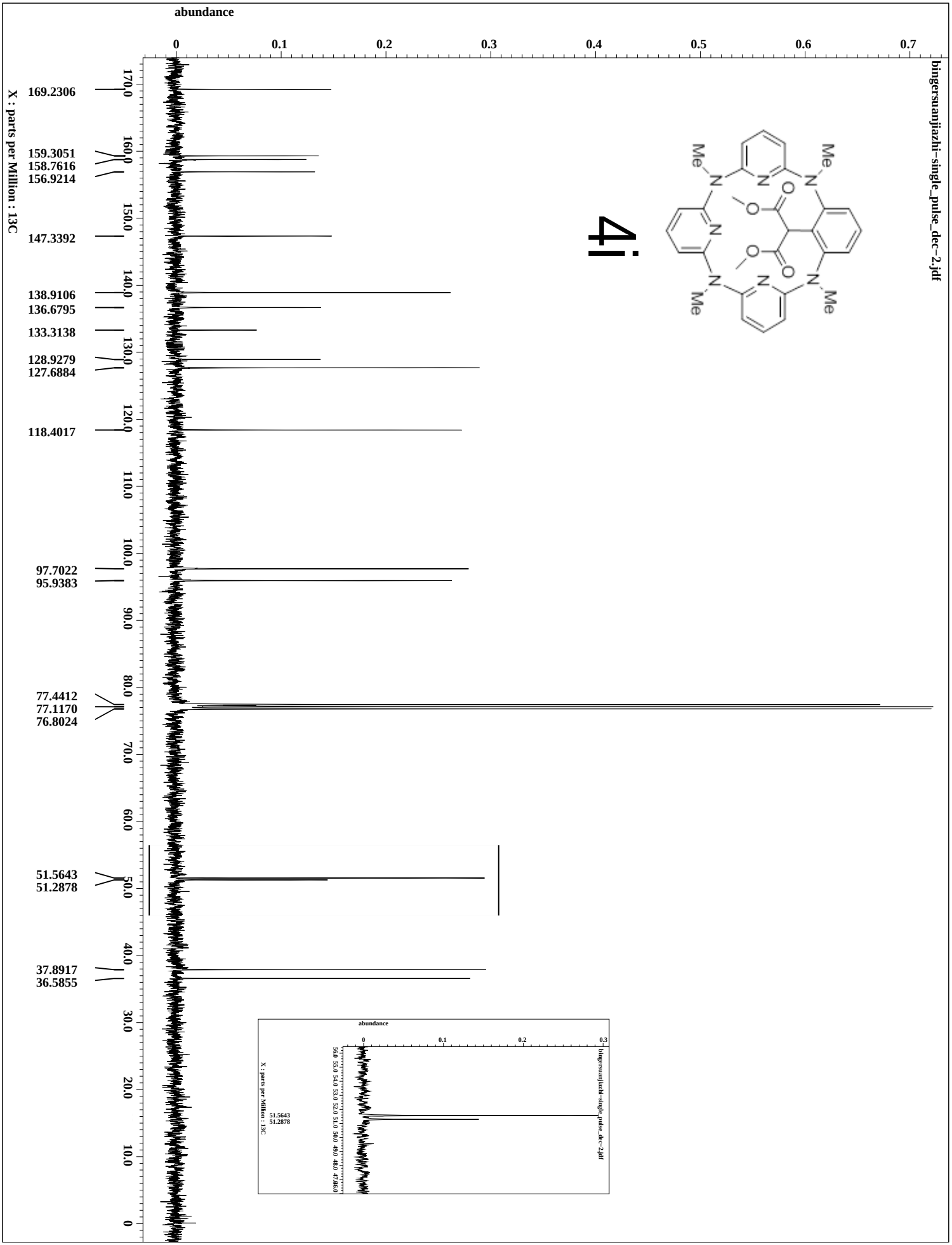





abundance
X : parts per Million : 13C
158.7712
158.6663
156.8738
147.5585
139.9785
139.0060
136.9846
128.3559
125.5145
120.6900
95.7380
95.7094
77.4603
77.1456
76.8214
39.5031
36.0802
16.7250
0.1443
CL-SANJIAJIGUJIAJI-single_pulse_dec-2.jdf
4h
Me
N
Si
Cl




4i


abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
bingersuanjiazhi-single_pulse_dec-2.jdf
X : parts per Million : 13C
169.2306
159.3051
158.7616
156.9214
147.3392
138.9106
136.6795
133.3138
128.9279
127.6884
118.4017
97.7022
95.9383
77.4412
77.1170
76.8024
51.5643
51.2878
37.8917
36.5855
4i
Me
N
O
abundance
X : parts per Million : 13C
51.5643
51.2878
bingersuanjiazhi-single_pulse_dec-2.jdf