Electronic Supplementary Information

for

Regioselective deoxygenative chalcogenation of 7-azindole *N*-oxides promoted by I_2/PEG-200

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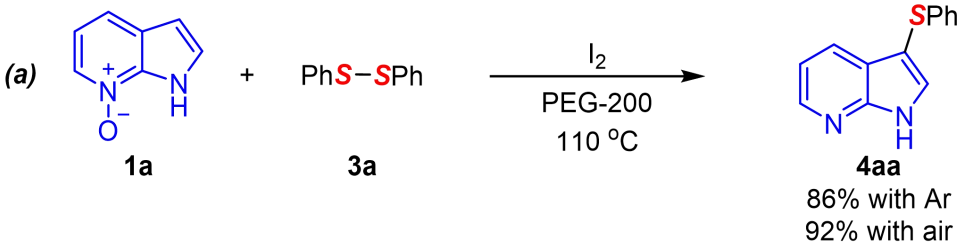
1 Mechanistic Studies

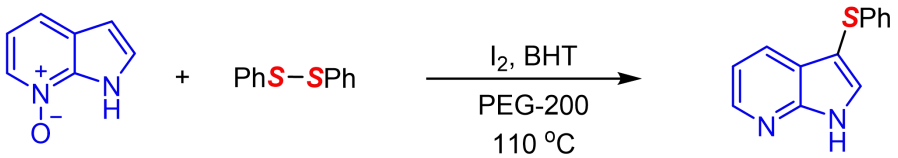
1.1 The Effect of *N*-Oxides and Air on the Reaction



1a **3a** **4aa**
86% with Ar
92% with air

Two parallel experiments were carried out according to reaction ***a*** as follows: 1*H*-pyrrolo[2,3-*b*]pyridine 7-oxide (**1a**, 33.5 mg, 0.25 mmol, 1.00 equiv), 1,2-diphenyldisulfane (**3a**, 32.7 mg, 0.15 mmol, 0.60 equiv), I_2 (0.025 mmol, 10 mol%), and PEG-200 (0.6 mL) were added to two vails. Purification by flash column chromatography on silica gel affords the analytically pure product **4aa** (48.6 mg, 86%) and (52 mg, 92%) under argon and air, respectively.

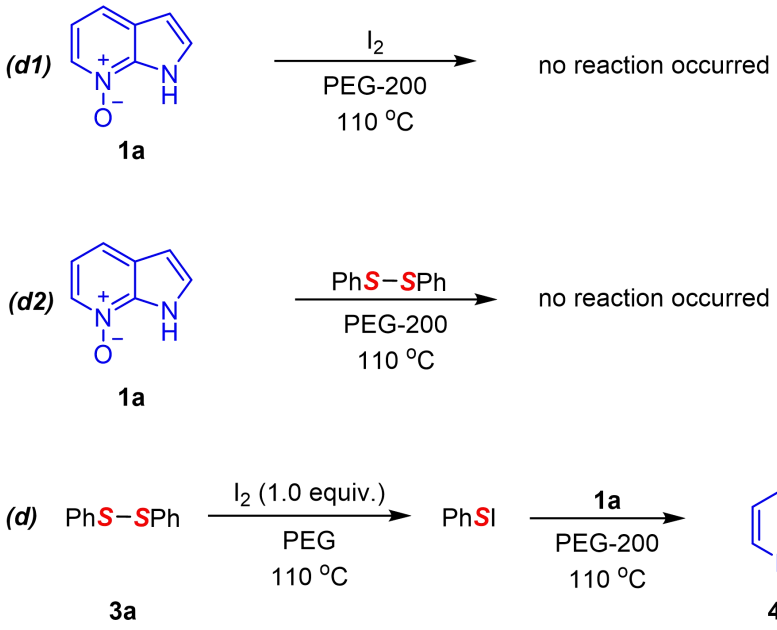
1.2 The Effect of Radical Scavenger



1a **3a** **4aa** (85%)

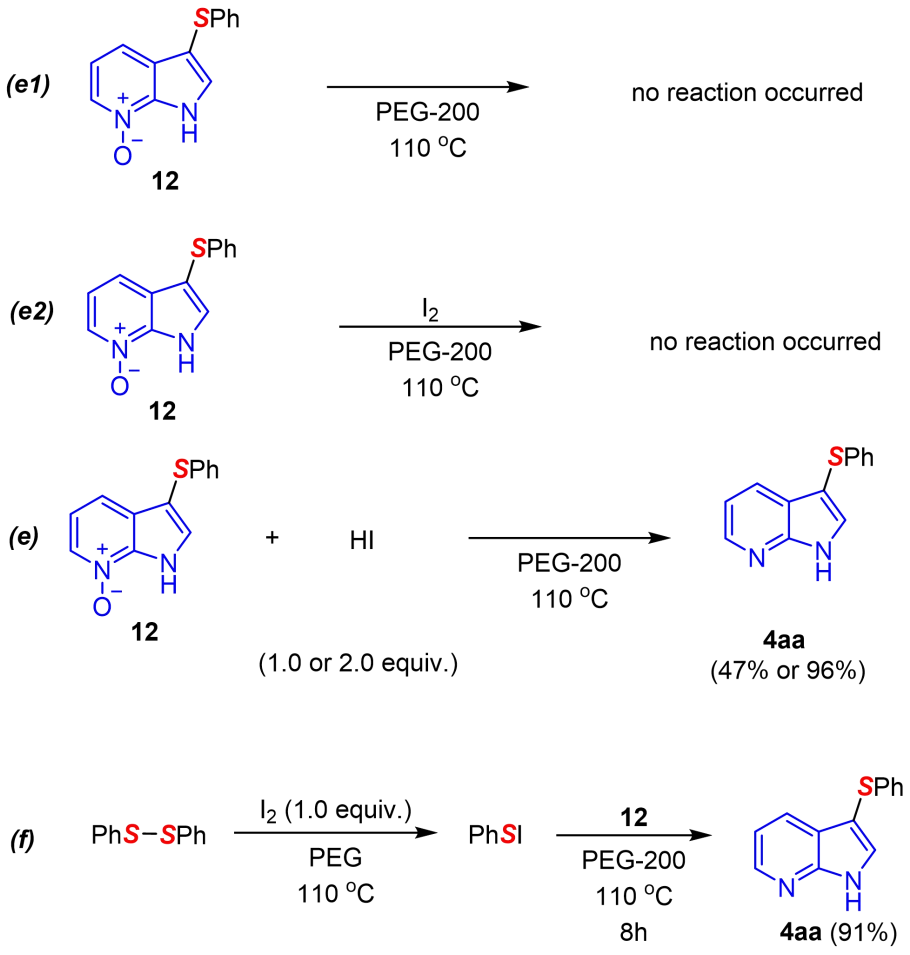
According to the **GP2,** 1*H*-pyrrolo[2,3-*b*]pyridine 7-oxide derivative (**1a**, 33.5 mg, 0.25 mmol, 1.0 equiv),1,2-diphenyldisulfane (**3a**, 32.7 mg, 0.15 mmol, 0.60 equiv), I_2 (6.4 mg, 0.025 mmol, 10 mol%), PEG-200 (0.6 mL), and BHT (110 mg, 0.5 mmol, 2 equiv.) was added. Purification by flash column chromatography on silica gel afforded the analytically pure product (48 mg, 85%).

1.3 Control Experiments



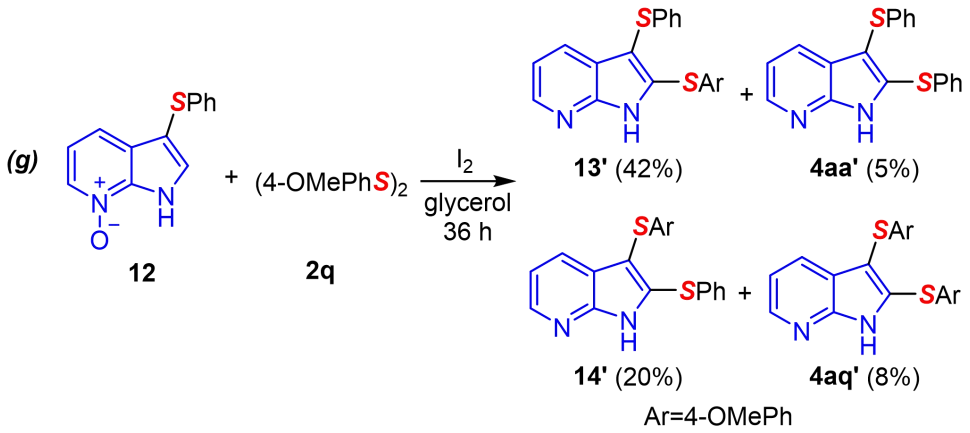
1a (33.5 mg, 0.25 mmol, 1.0 equiv) was subjected to the iodine (64 mg, 0.25 mmol, 1 equiv), and disulfides (**3a**, 32.7 mg, 0.15 mmol, 0.60 equiv) for 20 hours, respectively, no reaction ouccured. However, Heating the I_2 (38.1 mg, 0.15 mmol, 0.6 equiv), and **3a** (32.7 mg, 0.15 mmol, 0.6 equiv) to generate the in *situ* formed PhSI, then **1a** (33.5 mg, 0.25 mmol, 1equiv) was added into the above solution for 12 hours, **4aa** was delivered the in 54.8 mg and 97% yield. This observation shows that the reaction would start from the formation of an electrophilic sulfur species.

1.4 Control Experiments for the Deoxygenation Step



To elucidate the deoxygenation step, **12** (60.5 mg, 0.25 mmol) was subjected to the PEG (0.6 mL) and I_2 (63 mg, 0.25 mmol, 1equiv), no reaction occurred after 20 hours. However, the desired product **4aa** was formed in the addition of HI and PhSI. When 1 equiv. of HI solution (50% wt, 64 mg, 0.25 mmol) was used, deoxygenative product was obtained in 47% yield (26.6 mg) after 20 hours, while 2 equiv. of HI solution (50 wt%, 128 mg, 0.5 mmol) was used, the product was obtained in 96% yield (54.2 mg). PhSI was prepare from I_2 (63.5 mg, 0.25 mmol, 1 equiv), and **3a** (54.5 mg, 0.25 mmol, 1 equiv) in situ, then **12** (60.5 mg, 0.25 mmol) was added to the mixture for 8 hours to delivery the product in 91% yield (51.4 mg).

1.5 Experimental Details for the Mixed Disulfenylation



2 X-Ray Crystal Data of Compound 4aa

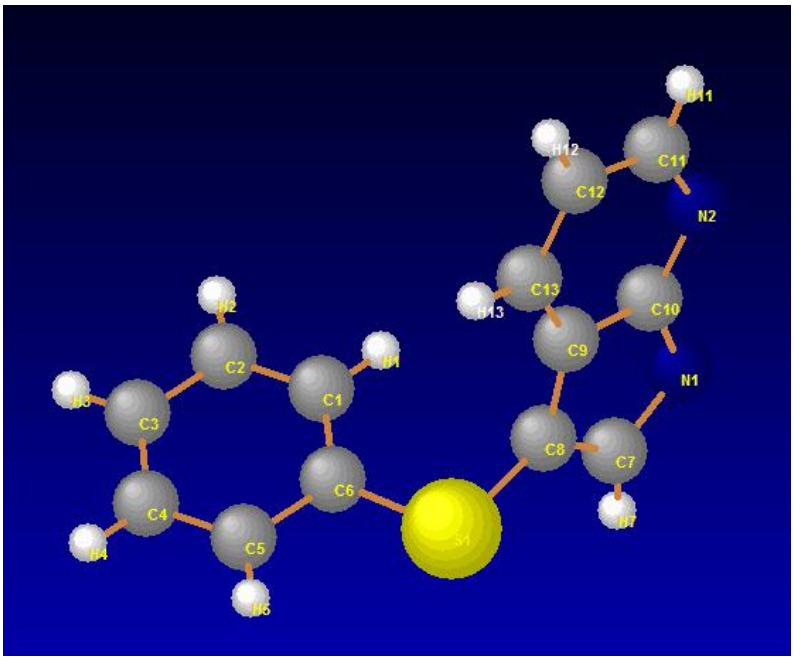


Figure S1. Crystal Structure of Compound **4aa**

Table S1. Crystal data and structure refinement for compound **4aa**

Identification code	SUST_1788_0m
Empirical formula	$C_{13}N_2SH_{10}$
Formula weight	226.29
Temperature/K	273.15
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	5.8840(6)
b/Å	8.0198(7)
c/Å	24.297(3)
α/°	90
β/°	95.847(7)
γ/°	90
Volume/Å^3	1140.6(2)
Z	4
ρ_{calc}g/cm^3	1.318
μ/mm^{-1}	0.255
F(000)	472.0

Crystal size/mm^3	0.15 × 0.14 × 0.13
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	5.352 to 56.54
Index ranges	-7 ≤ h ≤ 5, -10 ≤ k ≤ 10, -32 ≤ l ≤ 24
Reflections collected	11367
Independent reflections	2722 [R_{int} = 0.0666, R_{sigma} = 0.0828]
Data/restraints/parameters	2722/0/145
Goodness-of-fit on F^2	1.074
Final R indexes [I>=2σ (I)]	R_1 = 0.0660, wR_2 = 0.1480
Final R indexes [all data]	R_1 = 0.1487, wR_2 = 0.1717
Largest diff. peak/hole / e Å^{-3}	0.23/-0.26

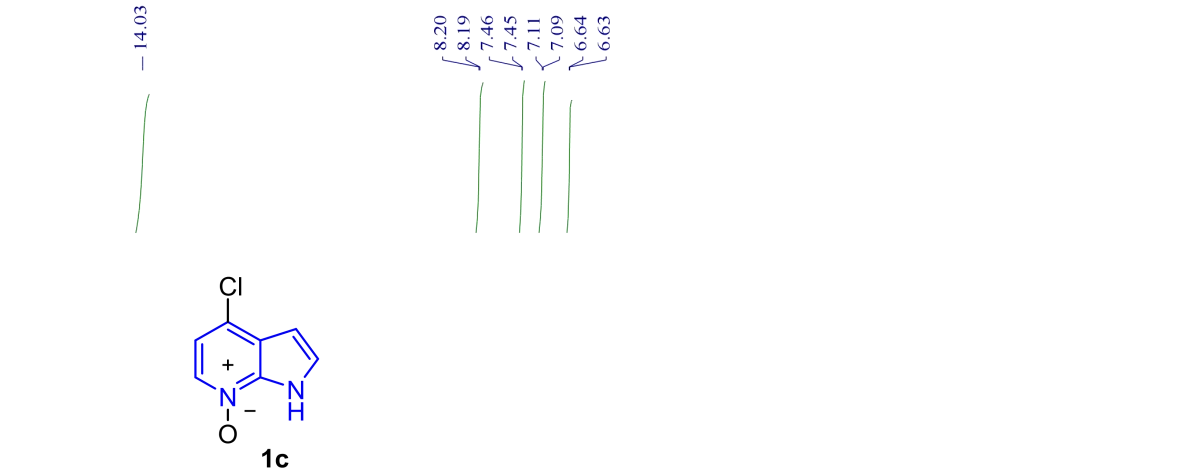
Table S2. Bond lengths [Å].

Atom	Atom	Length/Å	Atom	Atom	Length/Å
C1	C2	1.380(4)	C8	C9	1.436(5)
C1	C6	1.374(4)	C8	S1	1.739(4)
C2	C3	1.362(5)	C9	C10	1.409(5)
C3	C4	1.364(6)	C9	C13	1.378(5)
C4	C5	1.381(5)	C10	N1	1.364(4)
C5	C6	1.377(5)	C10	N2	1.341(4)
C6	S1	1.776(3)	C11	C12	1.377(6)
C7	C8	1.360(5)	C11	N2	1.338(4)
C7	N1	1.351(4)	C12	C13	1.386(6)

Table S3. Bond angles [°].

Atom	Atom	Atom	Angle/˚	Atom	Atom	Atom	Angle/˚
C6	C1	C2	119.6(4)	C10	C9	C8	105.7(3)
C3	C2	C1	121.3(3)	C13	C9	C8	137.0(4)
C2	C3	C4	119.4(4)	C13	C9	C10	117.3(3)
C3	C4	C5	120.1(4)	N1	C10	C9	108.8(3)
C6	C5	C4	120.6(4)	N2	C10	C9	126.5(3)
C1	C6	C5	119.0(3)	N2	C10	N1	124.7(4)
C1	C6	S1	124.1(3)	N2	C11	C12	124.3(4)
C5	C6	S1	116.9(3)	C11	C12	C13	120.8(4)
N1	C7	C8	111.5(3)	C9	C13	C12	117.3(4)
C7	C8	C9	106.1(3)	C7	N1	C10	107.9(3)
C7	C8	S1	126.3(3)	C11	N2	C10	113.9(4)
C9	C8	S1	127.5(3)	C8	S1	C6	104.04(16)

3 ^{1}H, ^{13}C, and ^{19}F Spectra



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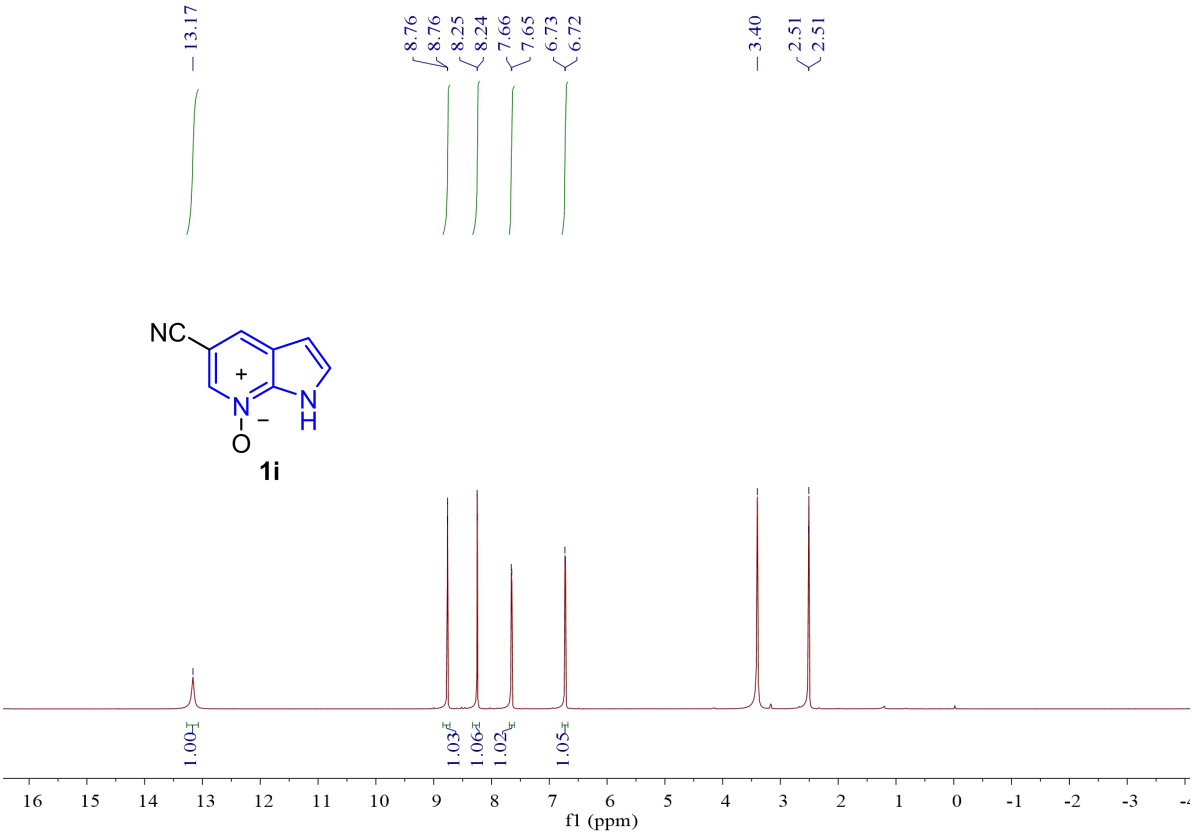

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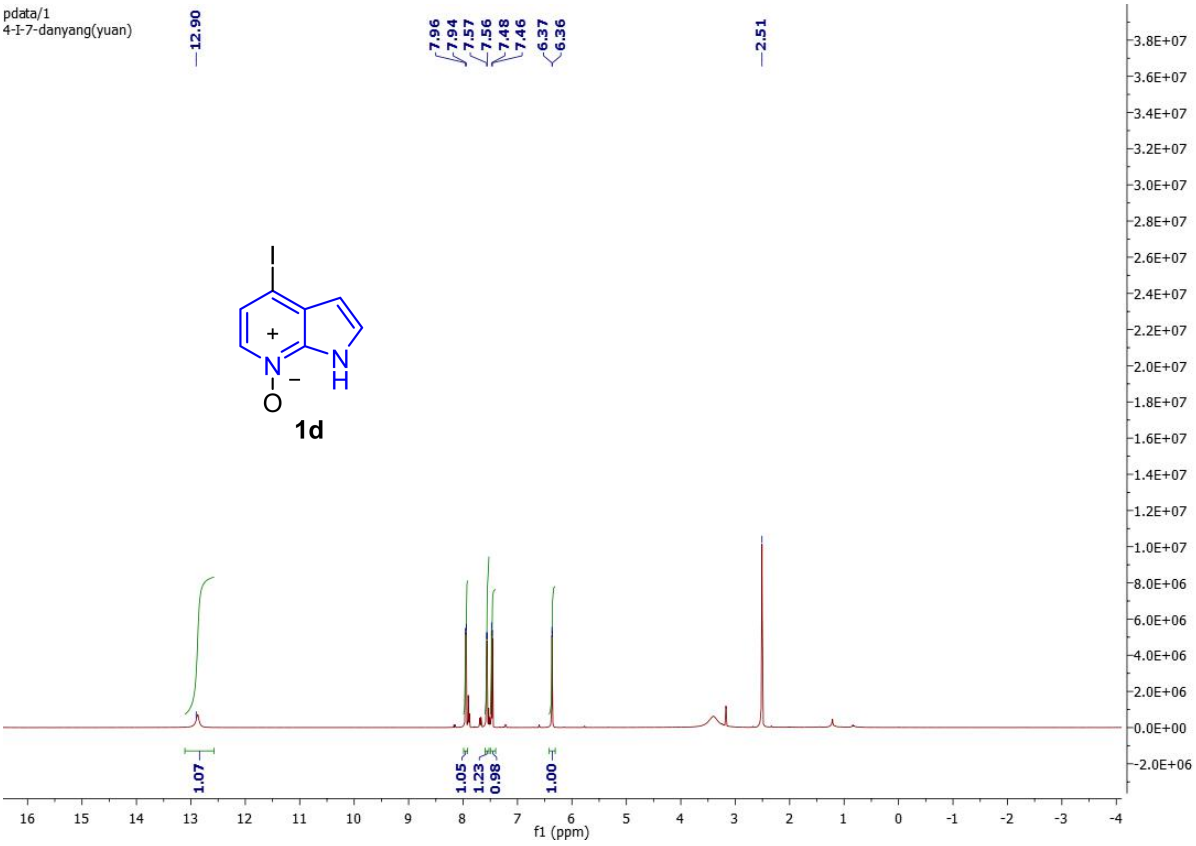
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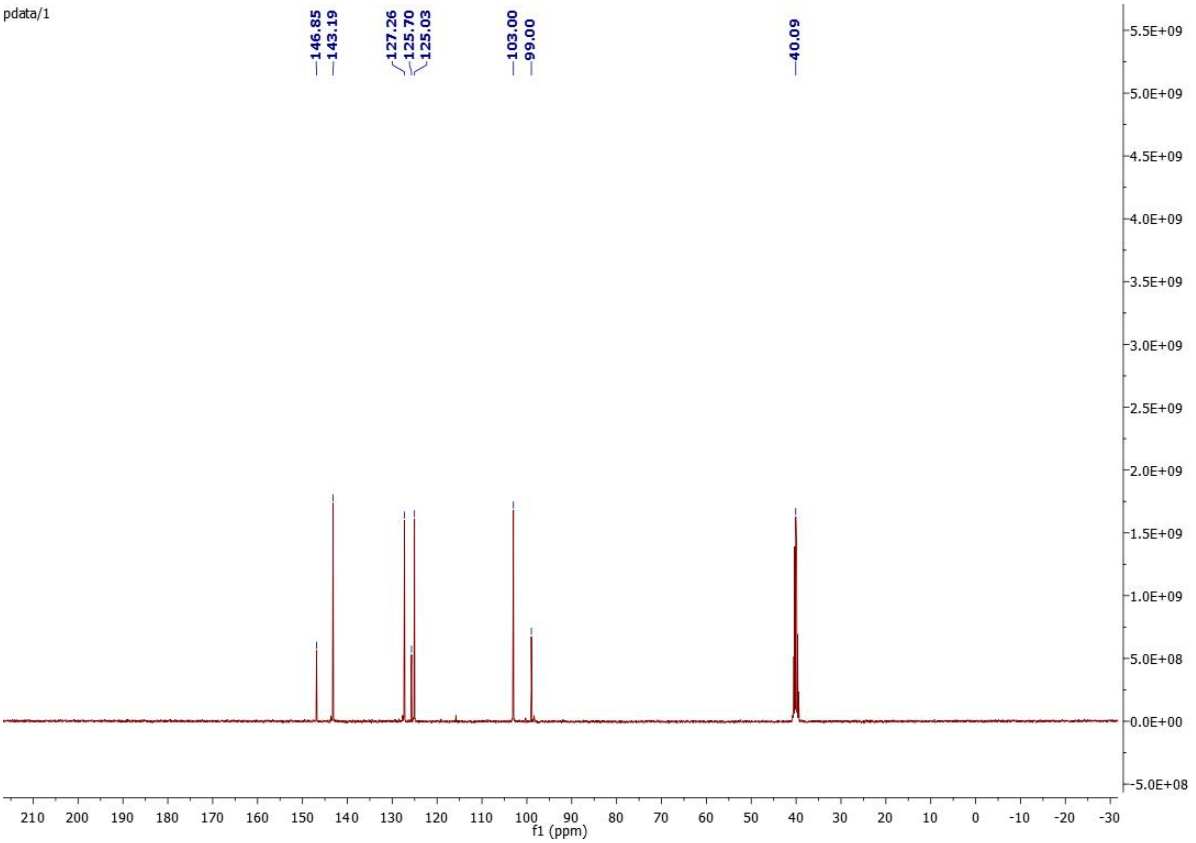
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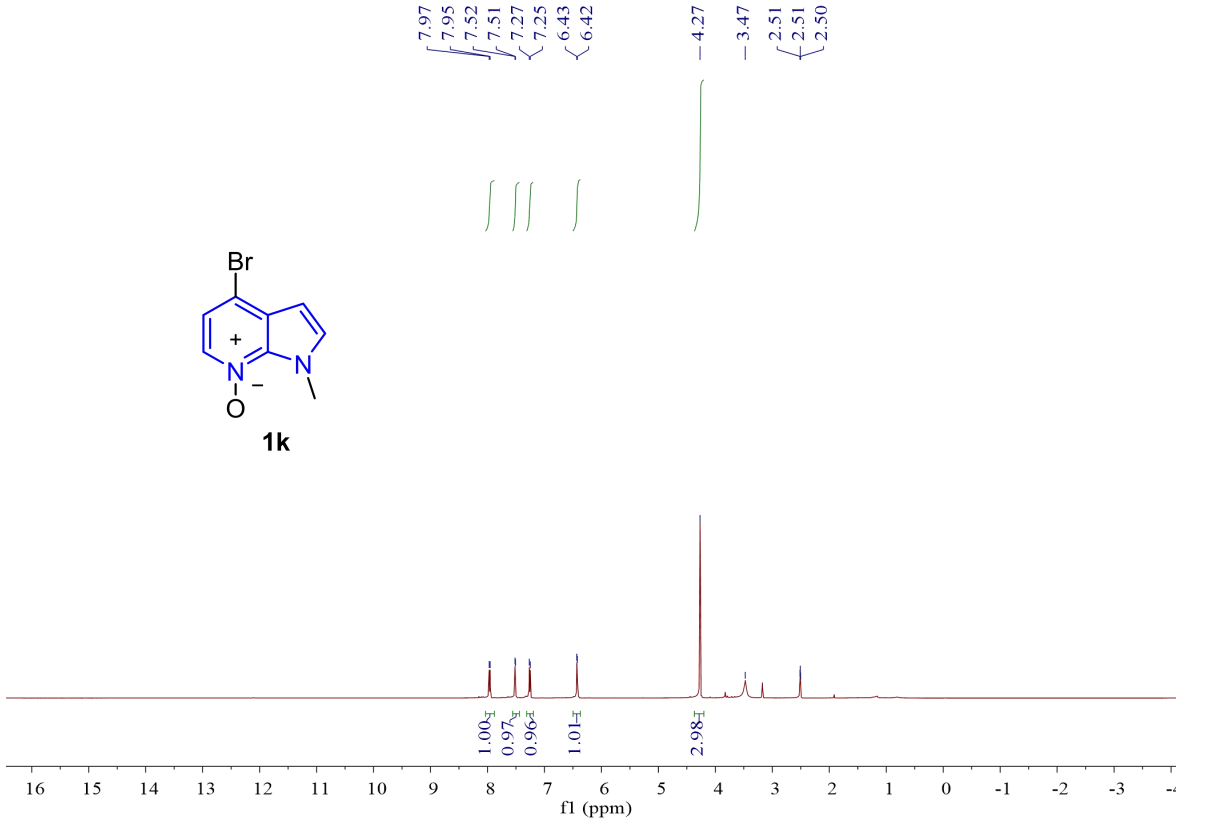
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N
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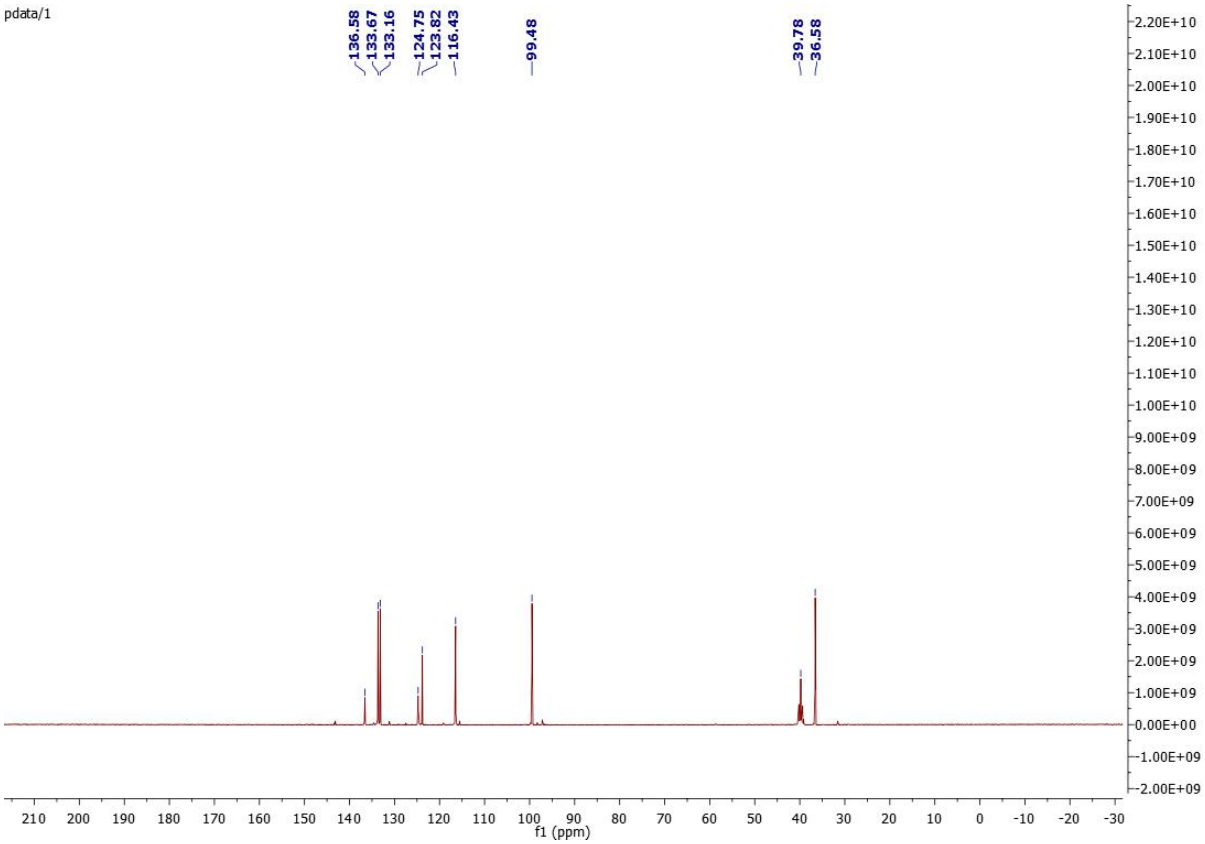
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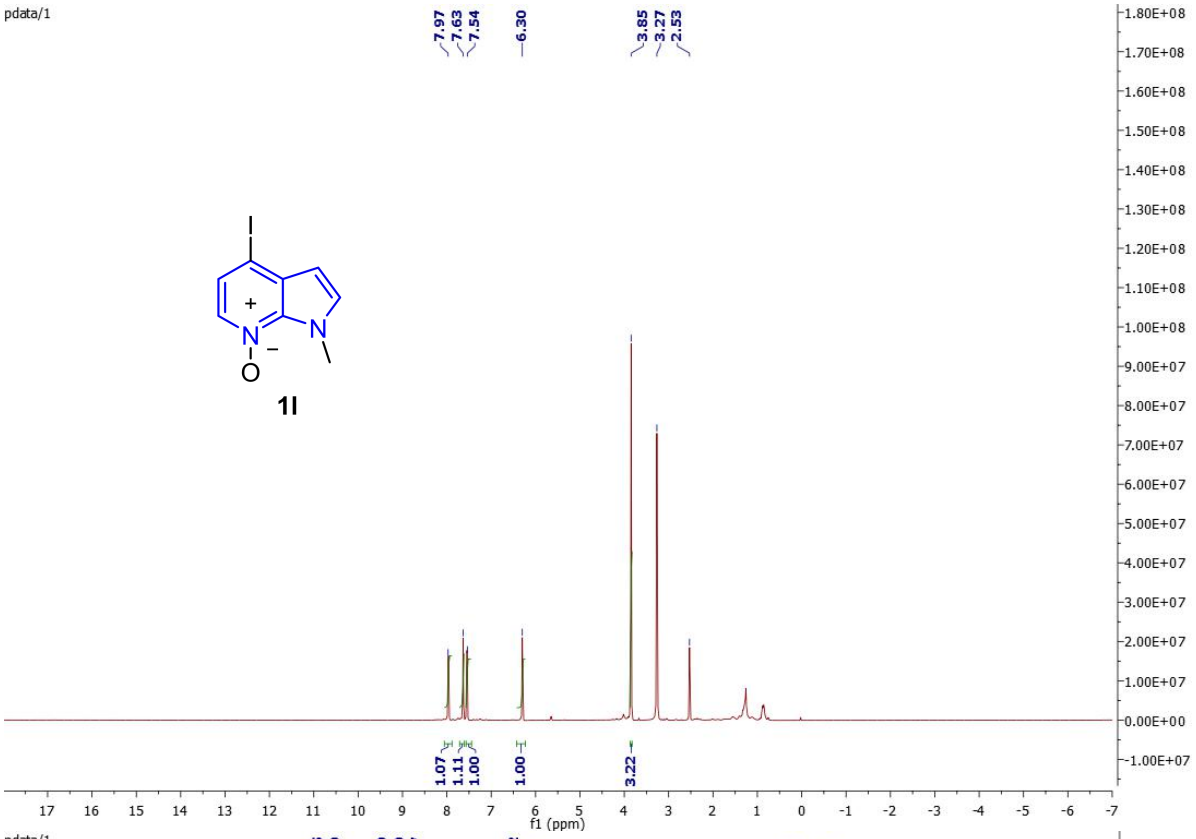
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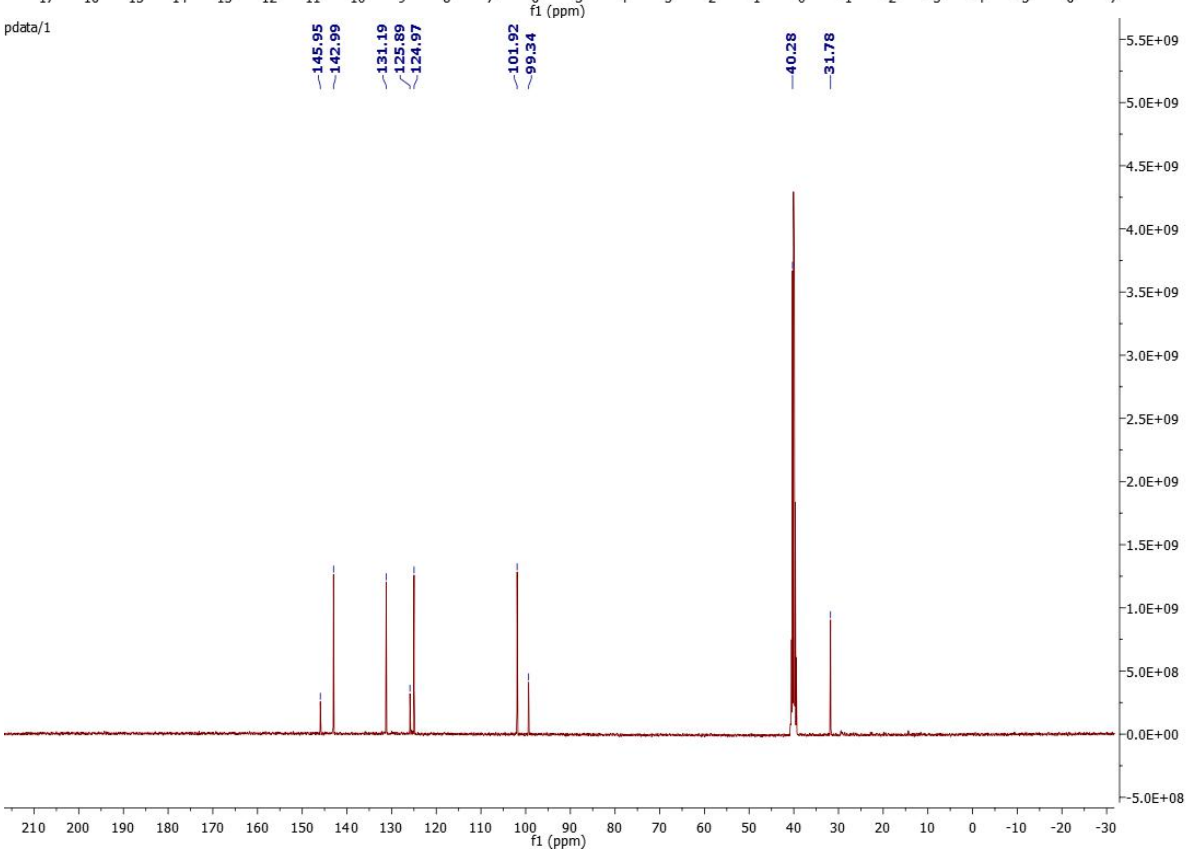
1l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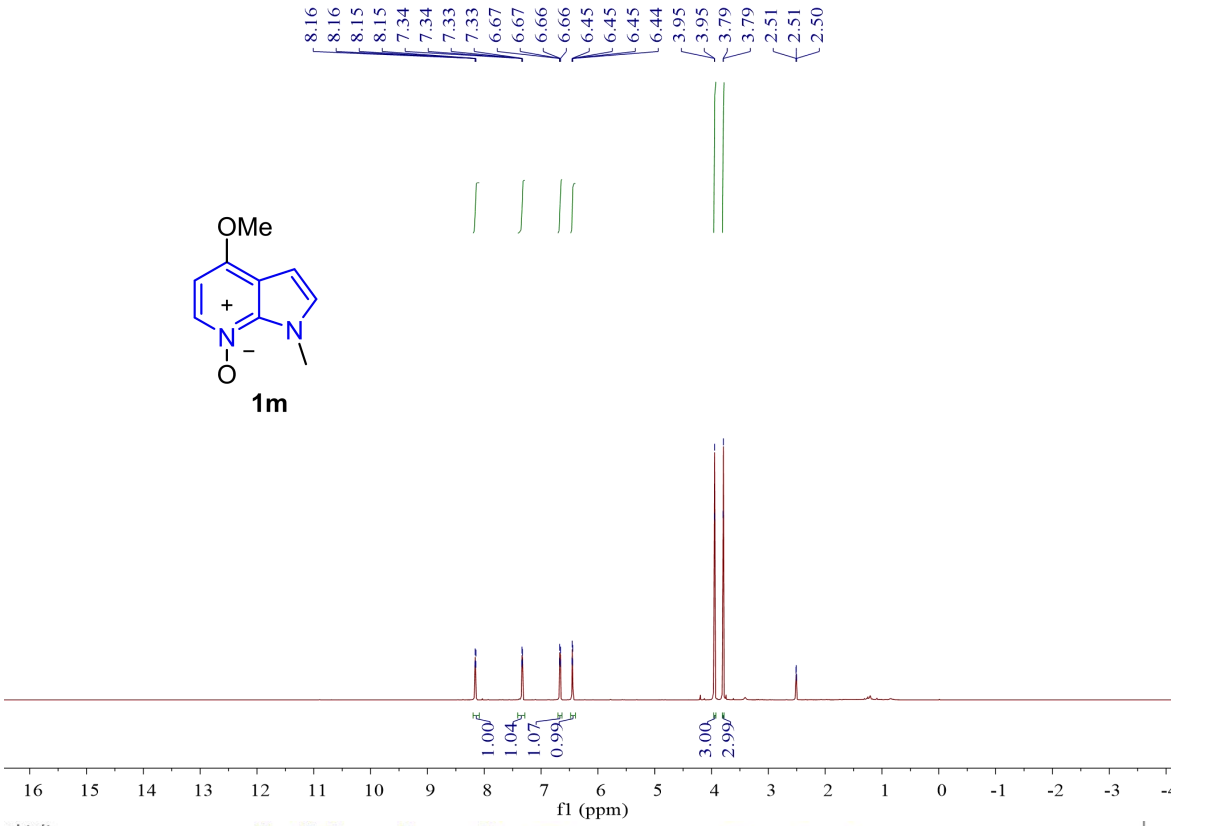
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6.67
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6.45
6.44
3.95
3.95
3.79
3.79
2.51
2.51
2.50
OMe
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N
N
−
O
1m
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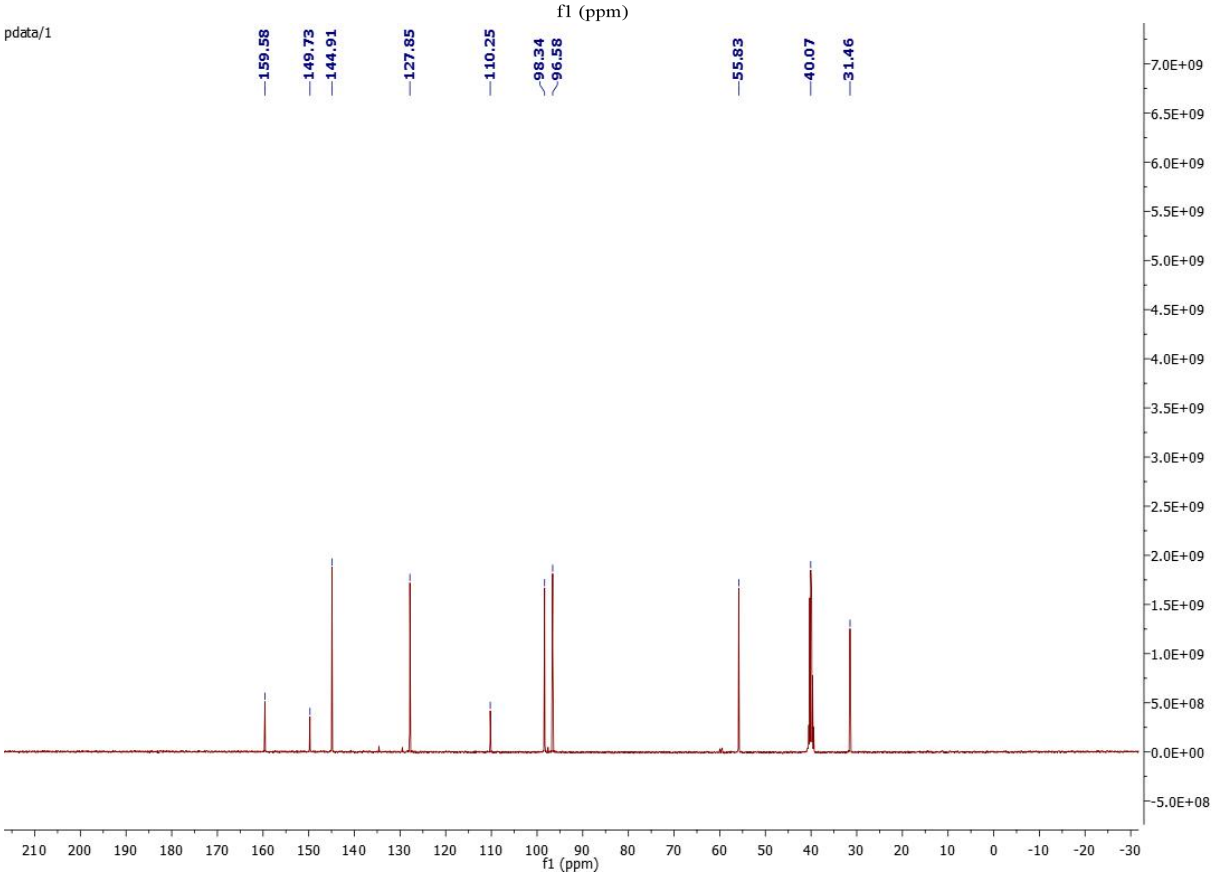
1.07
0.99
3.00
2.99
f1 (ppm)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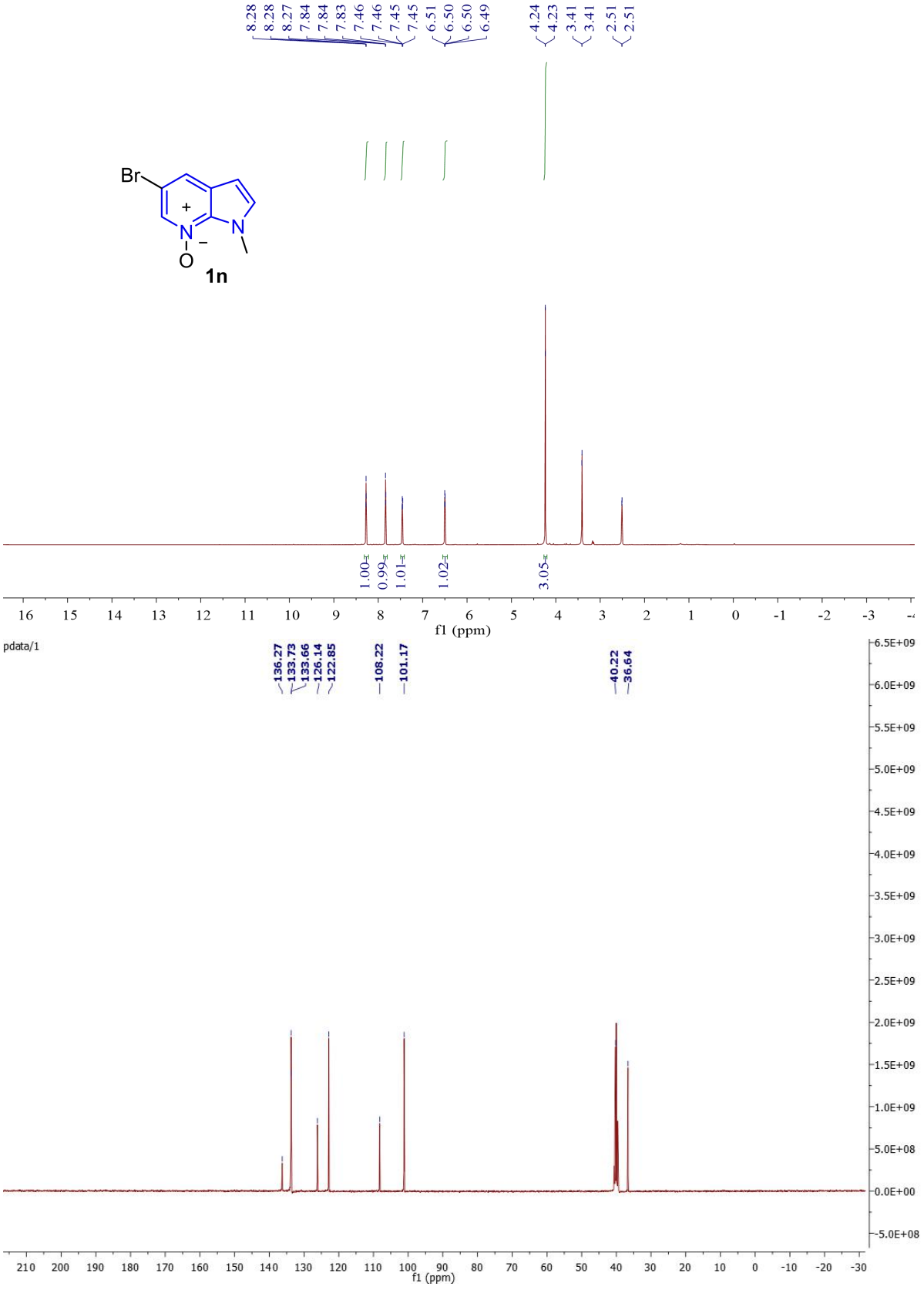
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6.49
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4.23
3.41
3.41
2.51
2.51
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N
N
−
O
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0.99
1.01
1.02
3.05
f1 (ppm)
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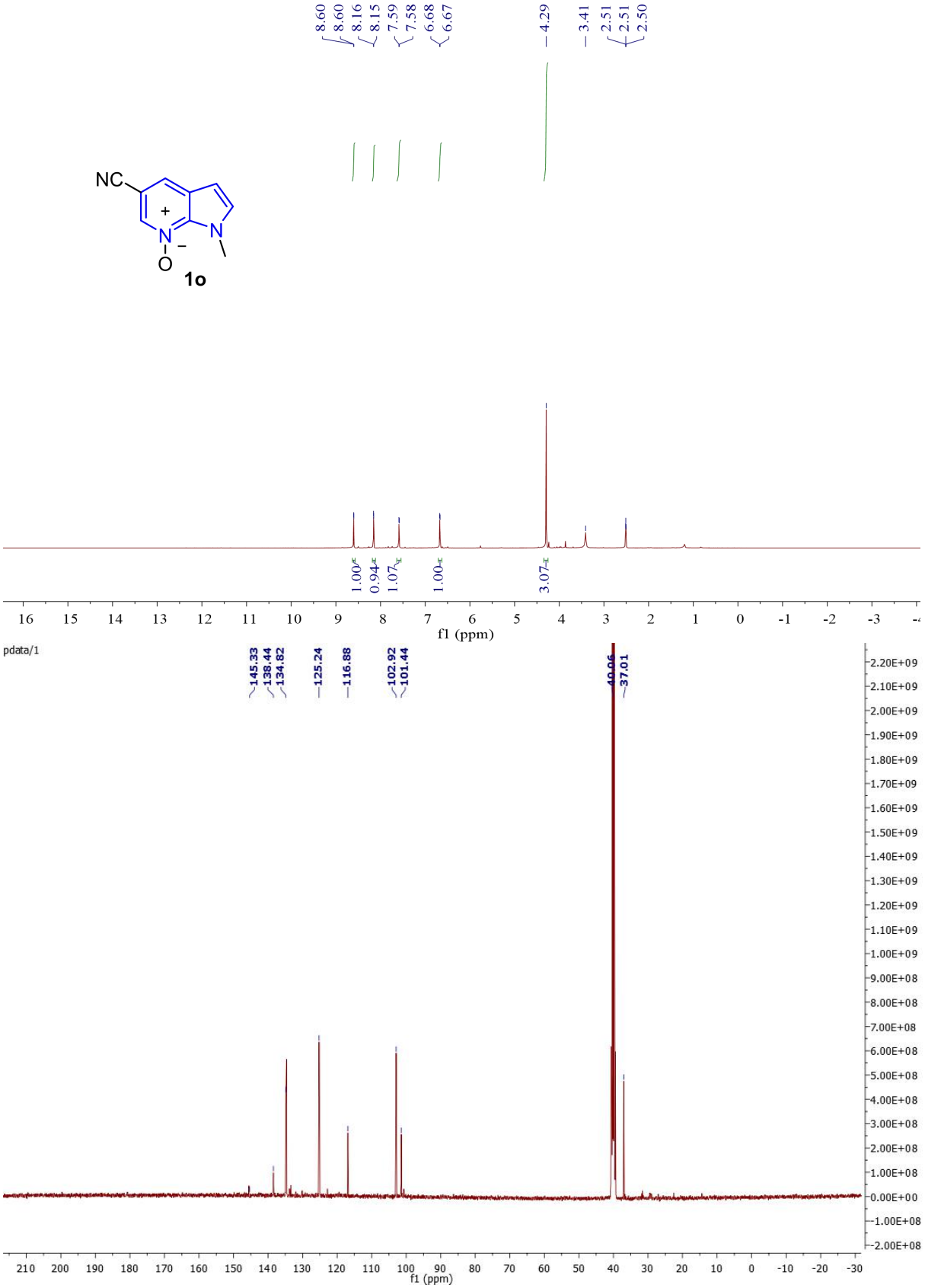
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N
N
−
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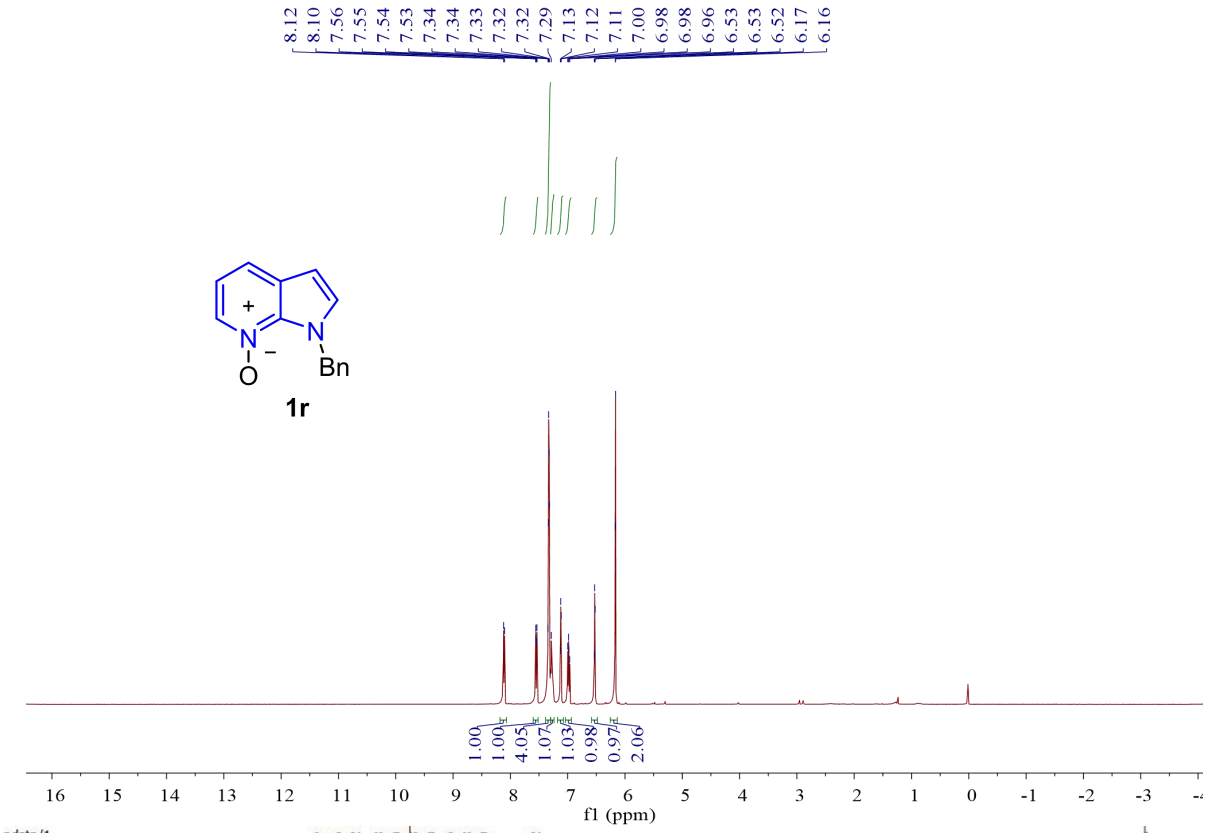
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6.53
6.53
6.52
6.17
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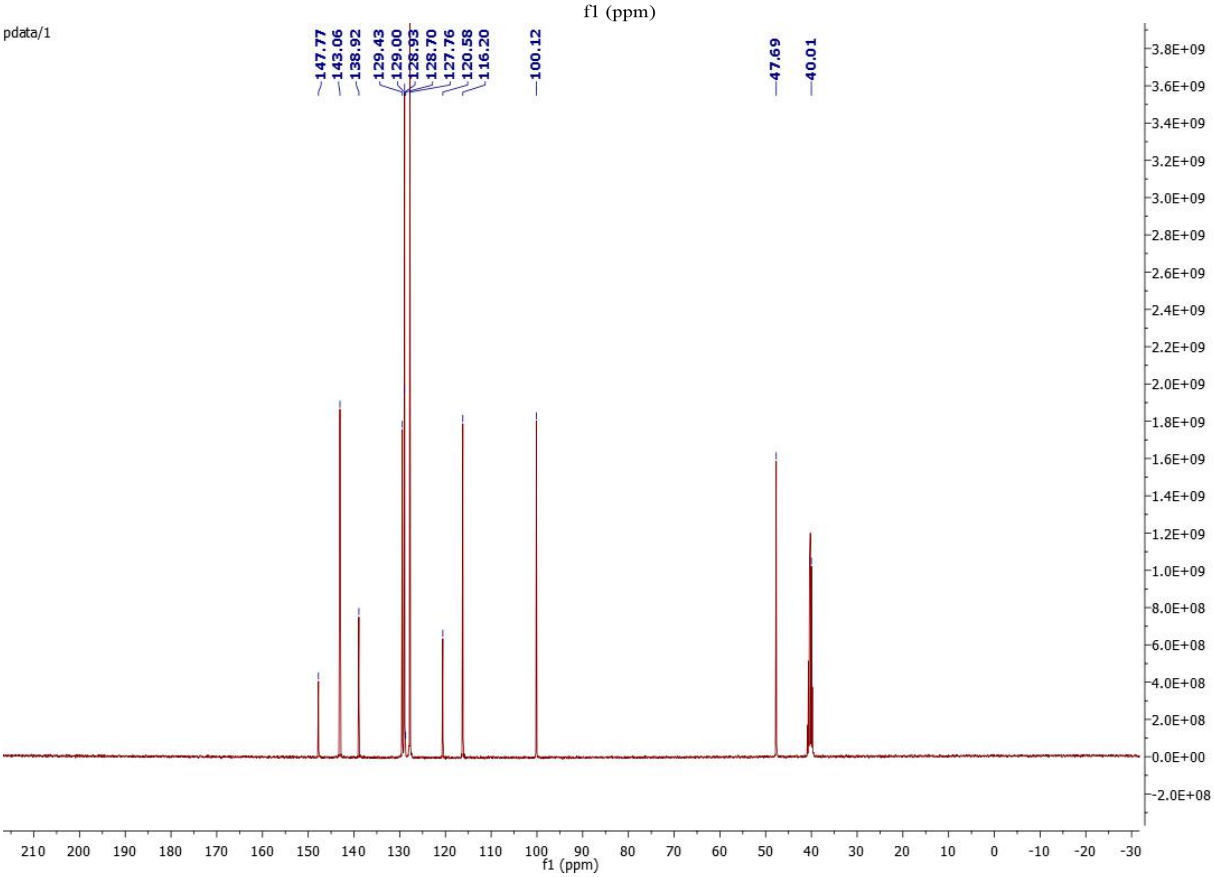
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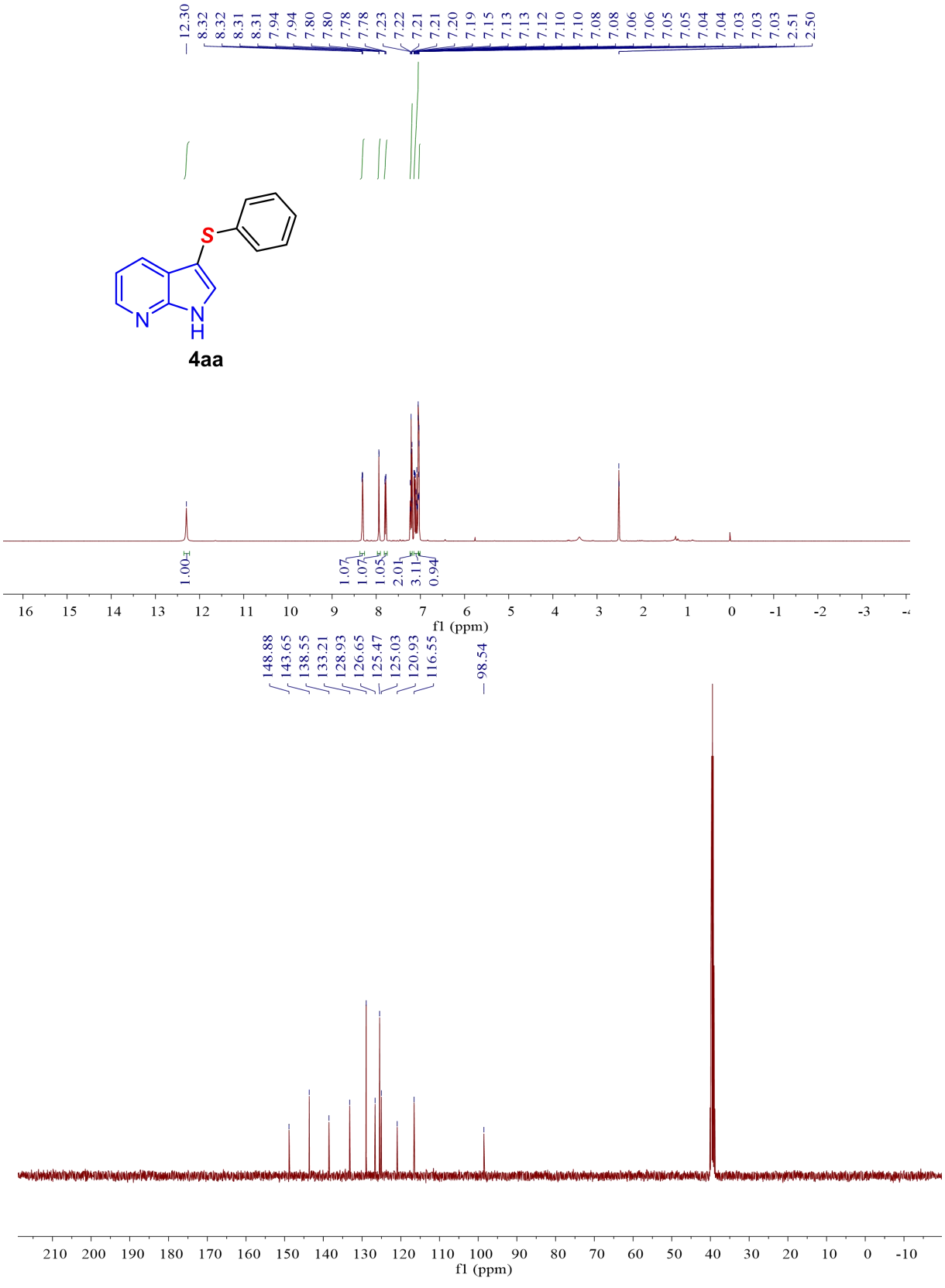
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7.13
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N
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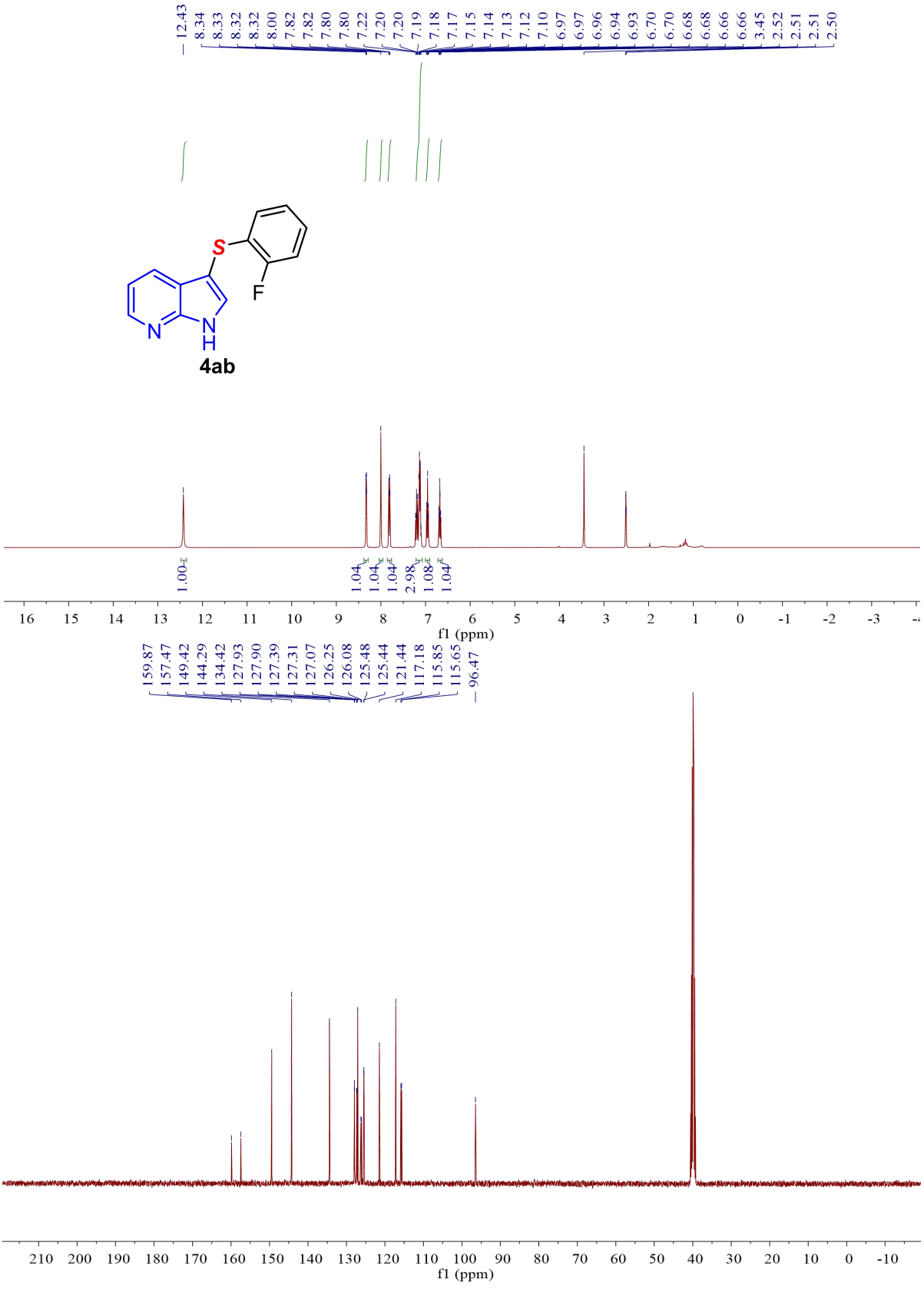
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7.17
7.15
7.14
7.13
7.12
7.10
6.97
6.97
6.96
6.94
6.93
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F
N
N
H
4ab
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1.04
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1.08
1.04
f1 (ppm)
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157.47
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127.90
127.39
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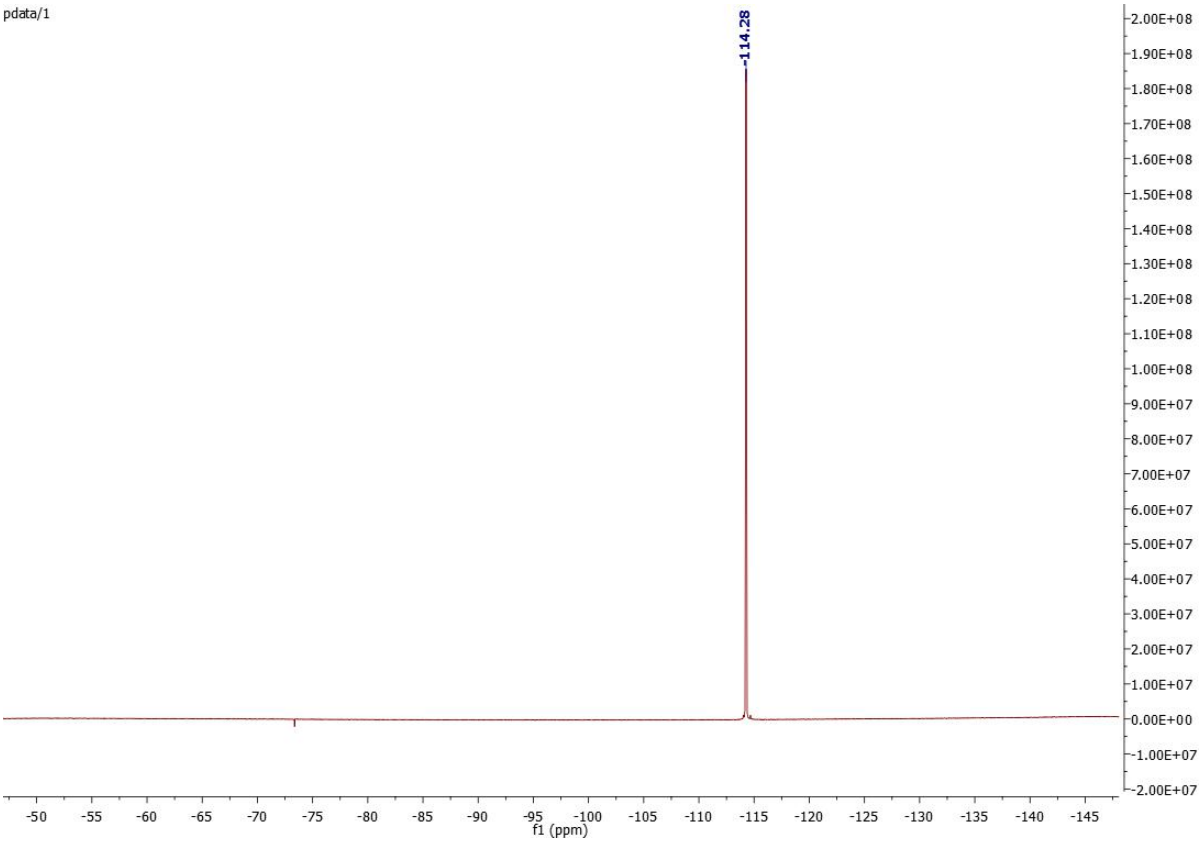
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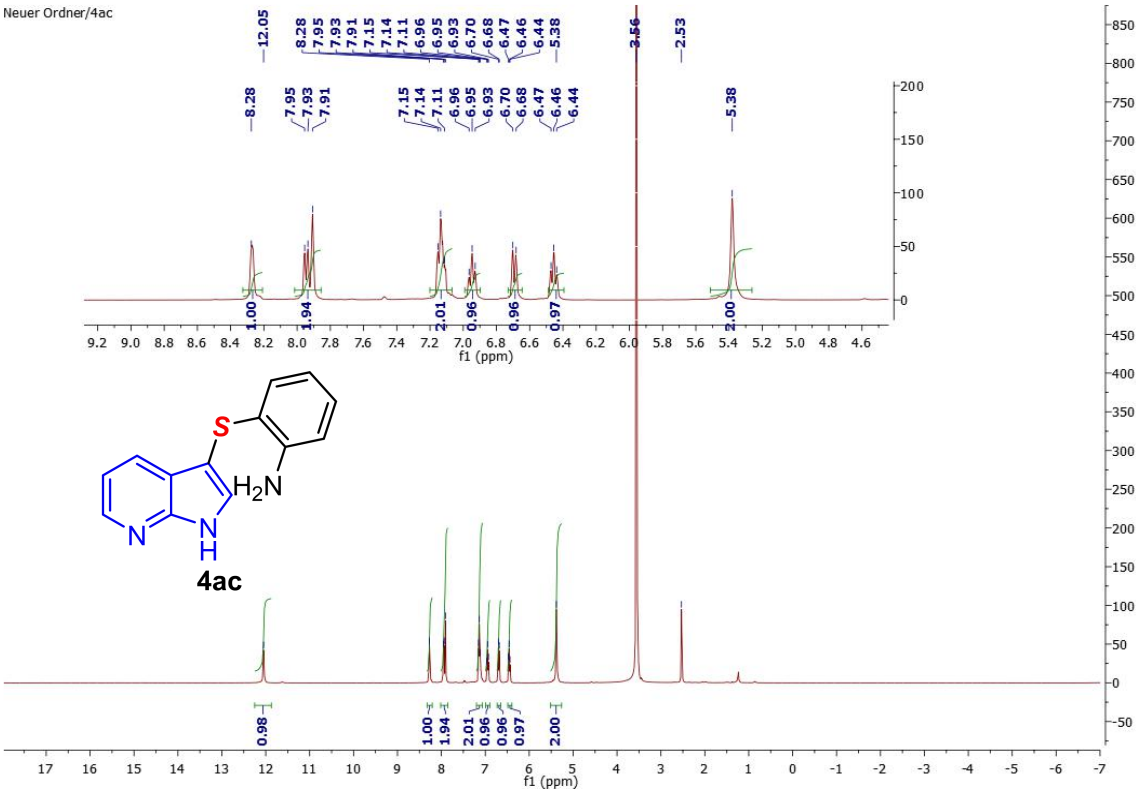
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7.14
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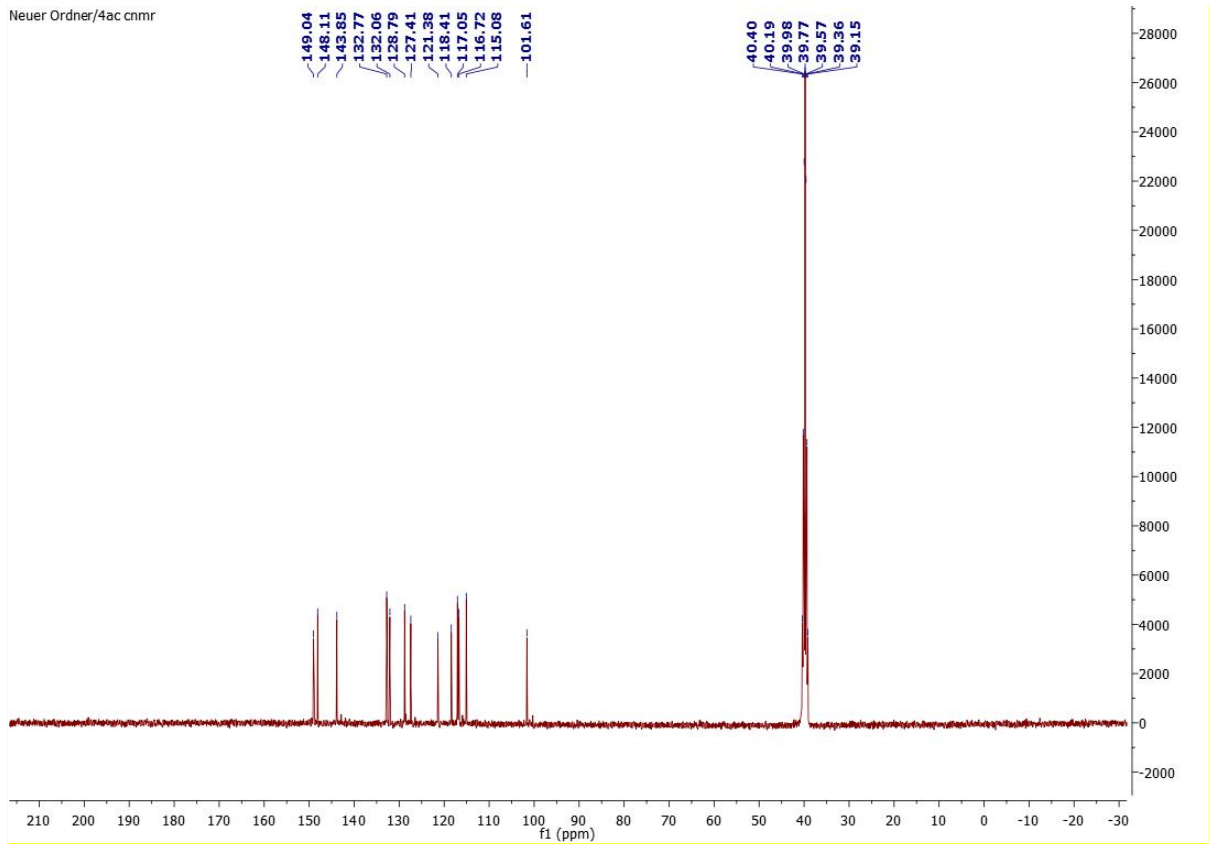
6.70
6.68
6.47
6.46
6.44
5.38
3.56
2.53
1.00
1.94
2.01
0.96
0.96
0.97
2.00
f1 (ppm)
S
H2N
N
H
4ac


Neuer Ordner/4ac cnmr
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148.11
143.85
132.77
132.06
128.79
127.41
121.38
118.41
117.05
116.72
115.08
101.61
40.40
40.19
39.98
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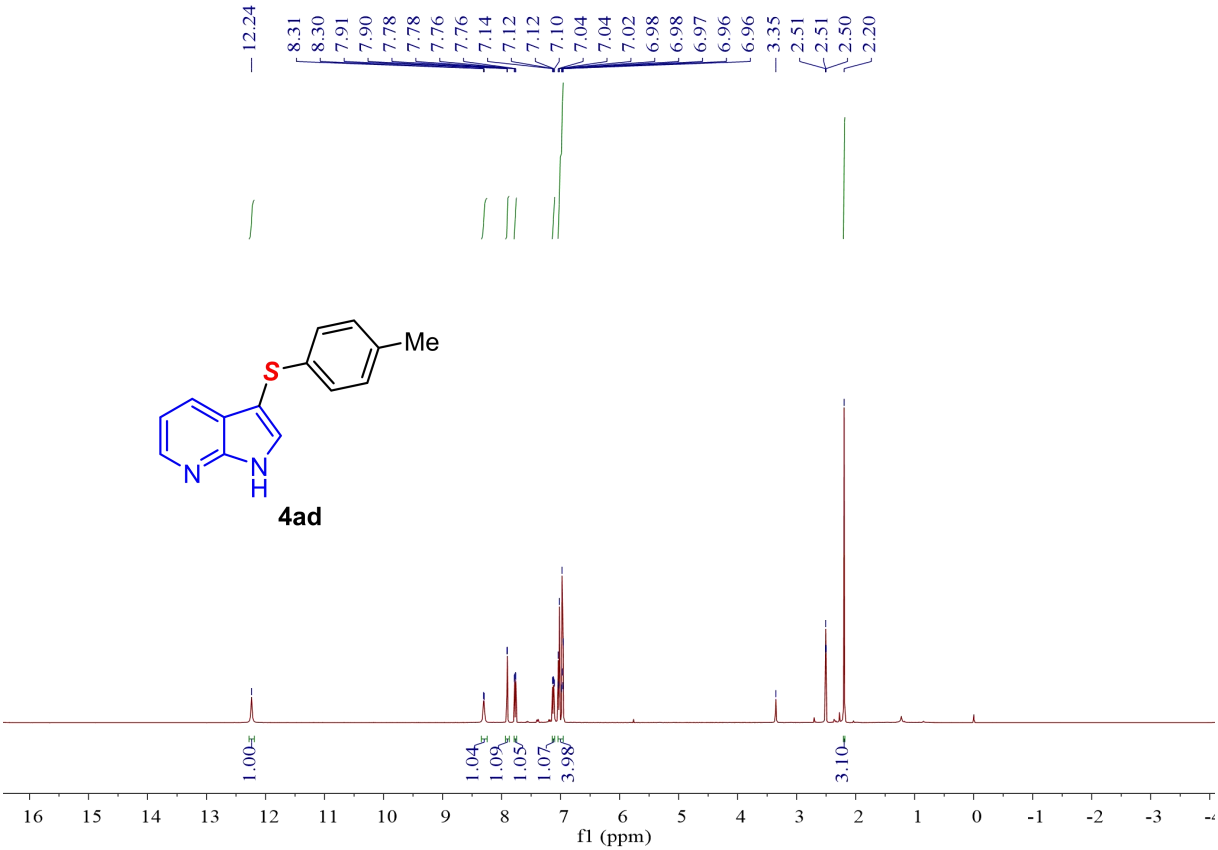
39.57
39.36
39.15
f1 (ppm)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8.31
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7.90
7.78
7.78
7.76
7.76
7.14
7.12
7.12
7.10
7.04
7.04
7.02
6.98
6.98
6.97
6.96
6.96
3.35
2.51
2.51
2.50
2.20
Me
S
N
H
4ad
1.00
1.04
1.09
1.05
1.07
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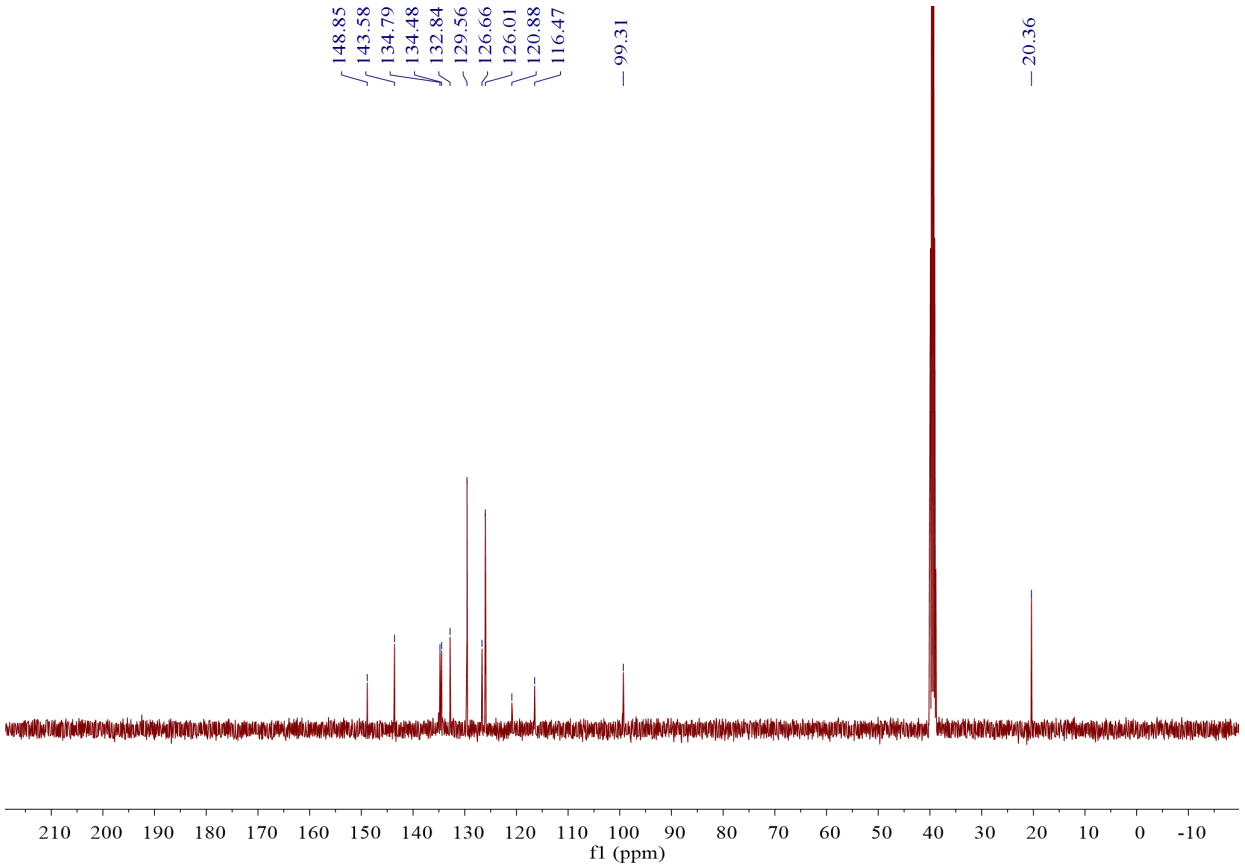
3.10
f1 (ppm)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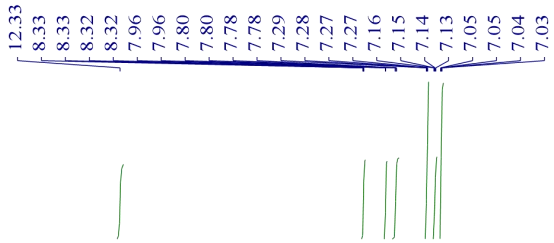
129.56
126.66
126.01
120.88
116.47
99.31
20.36
f1 (ppm)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8.33
8.32
8.32
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7.80
7.80
7.78
7.78
7.29
7.28
7.27
7.27
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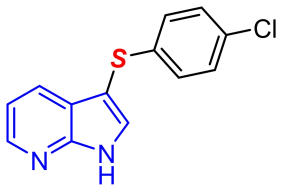
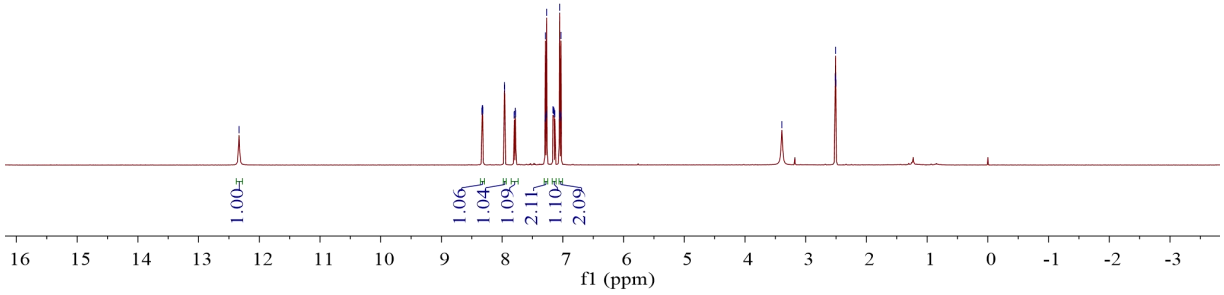
7.13
7.05
7.05
7.04
7.03
3.39
2.51
2.51
2.50


Cl
S
N
H

4ae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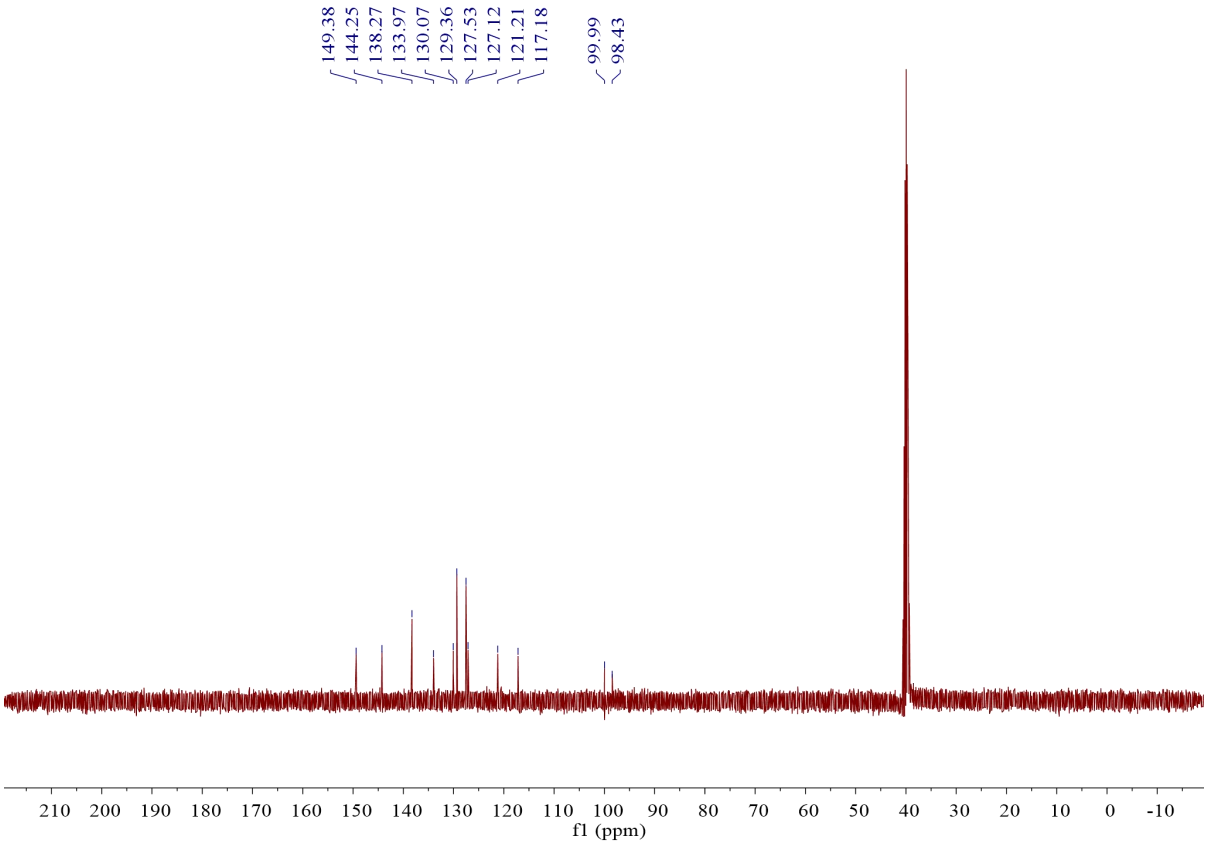
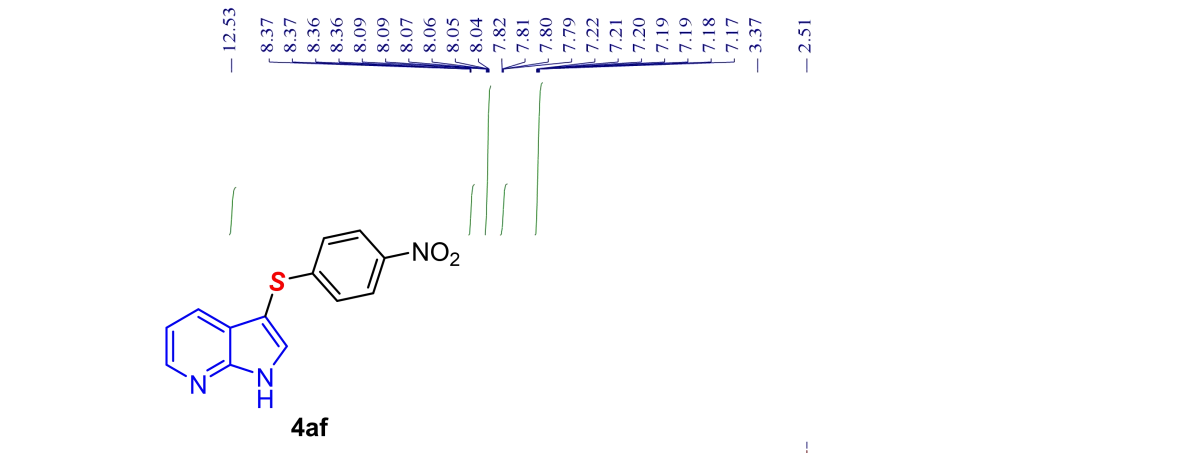
1.06
1.04
1.09
2.11
1.10
2.09
f1 (ppm)


149.38
144.25
138.27
133.97
130.07
129.36
127.53
127.12
121.21
117.18
99.99
98.43
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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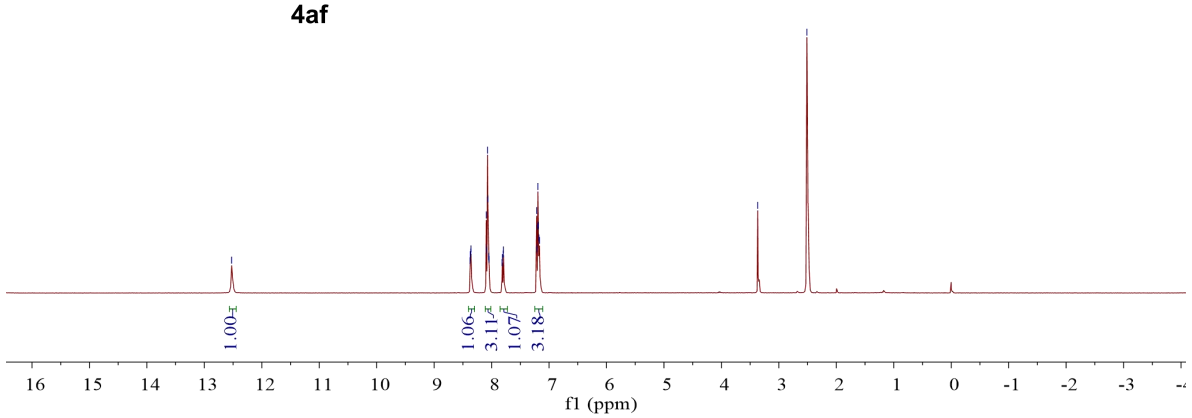
8.37
8.37
8.36
8.36
8.09
8.09
8.07
8.06
8.05
8.04
7.82
7.81
7.80
7.79
7.22
7.21
7.20
7.19
7.19
7.18
7.17
3.37
2.51
NO2
S
N
H

4af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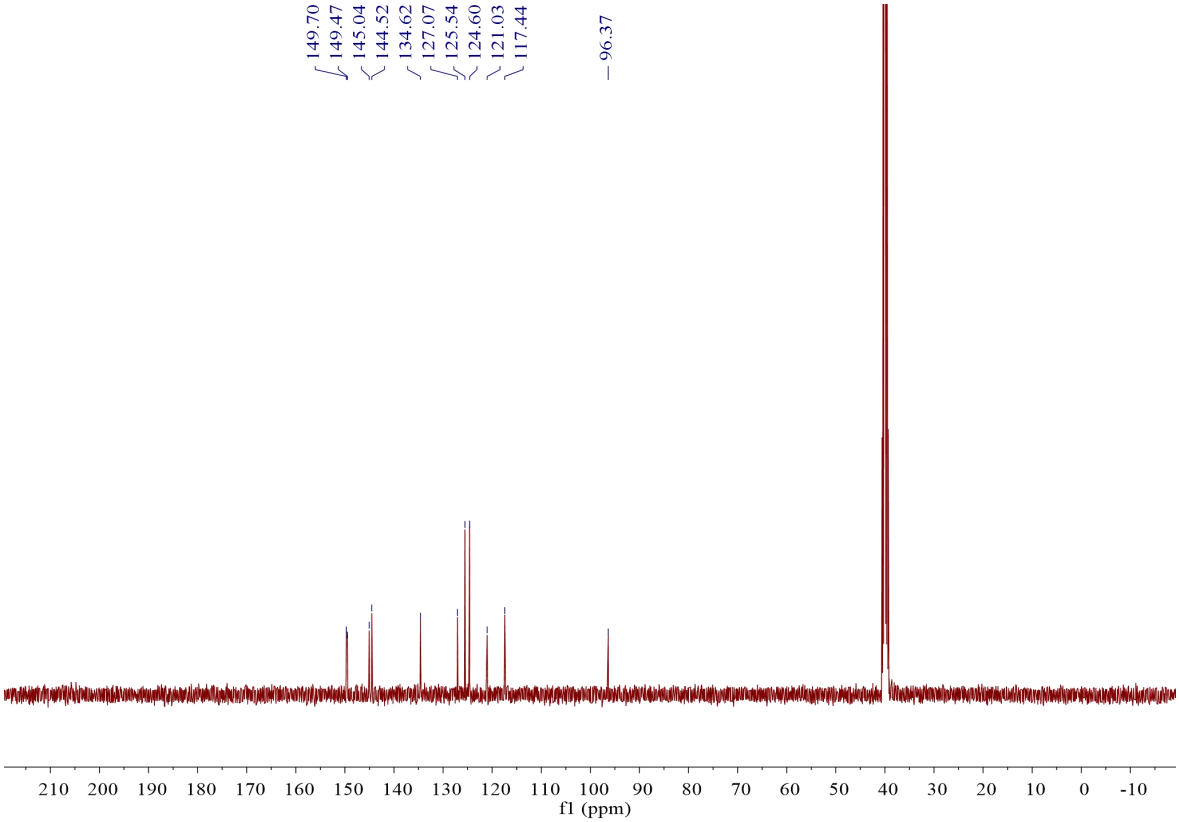
1.06
3.11
1.07
3.18
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)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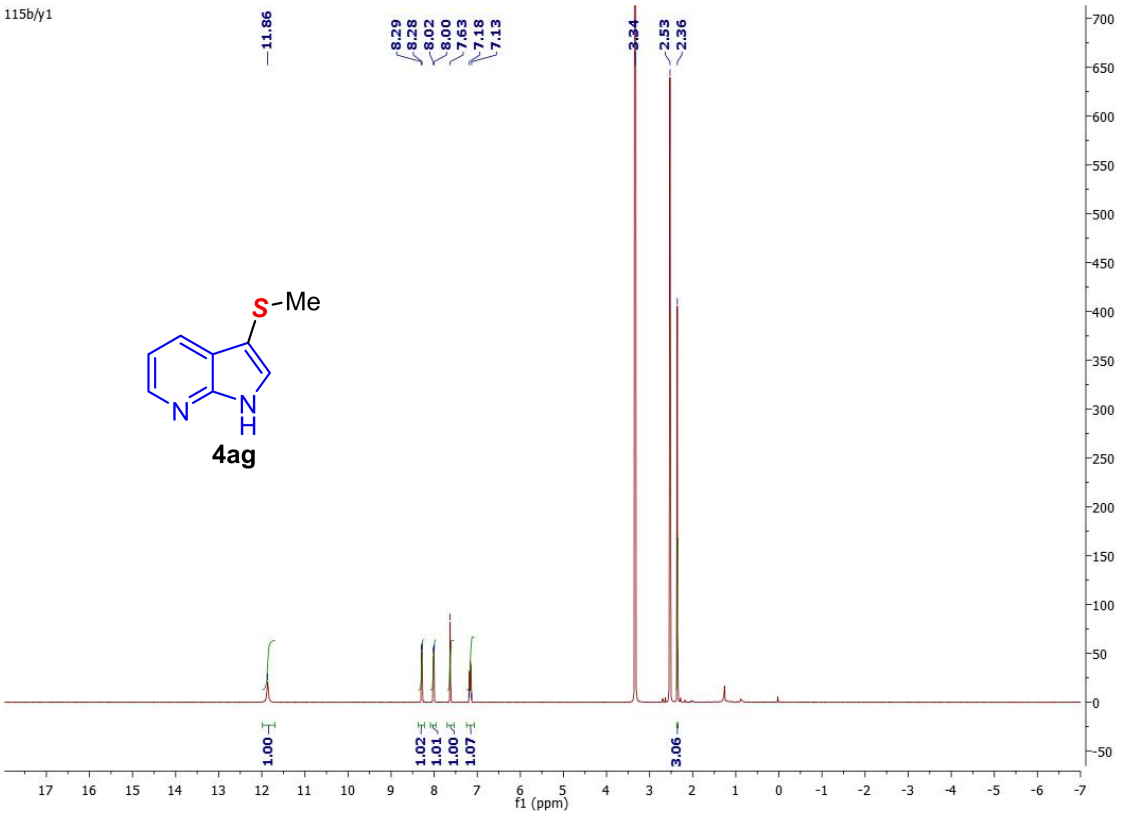
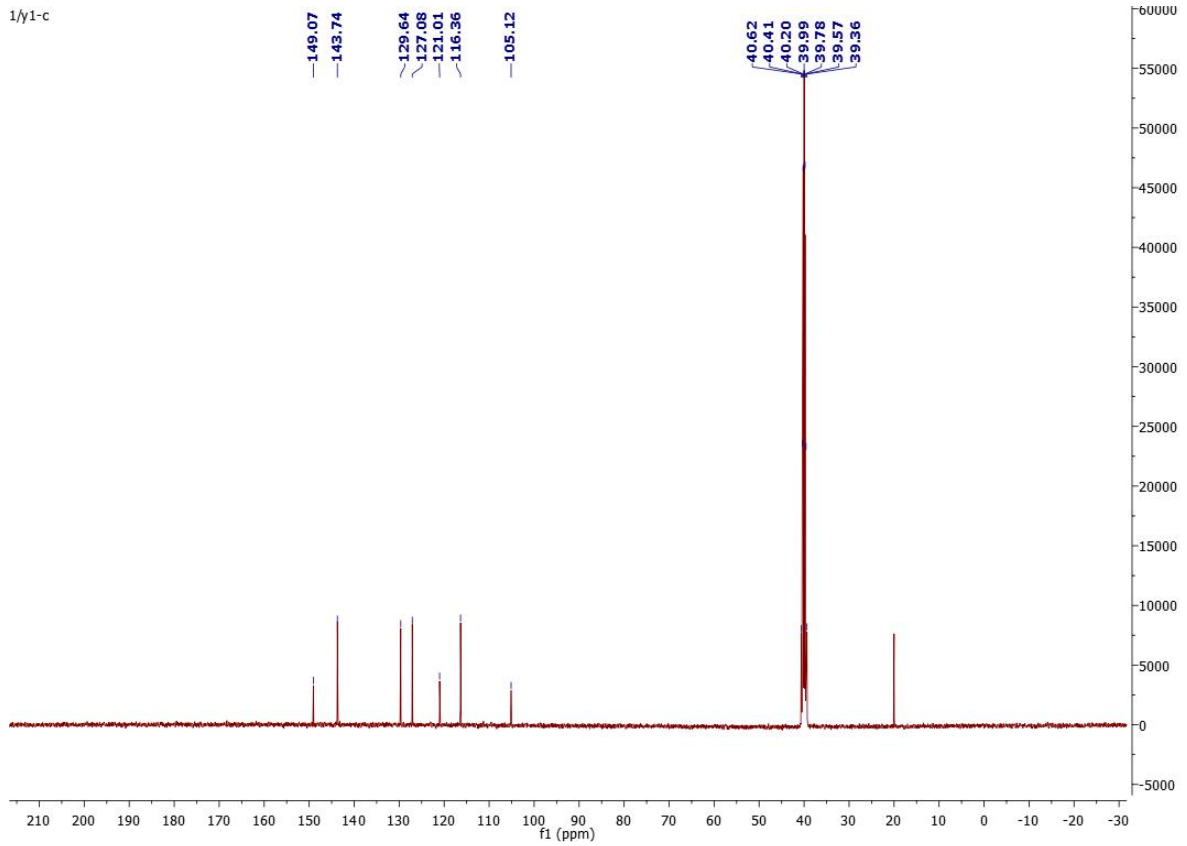
149.47
145.04
144.52
134.62
127.07
125.54
124.60
121.03
117.44
96.37
f1 (ppm)


115b/y1
11.86
8.29
8.28
8.02
8.00
7.63
7.18
7.13
3.24
2.53
2.36
S-Me
N
N
H
4ag
1.00
1.02
1.01
1.00
1.07
3.06
f1 (ppm)


1/y1-c
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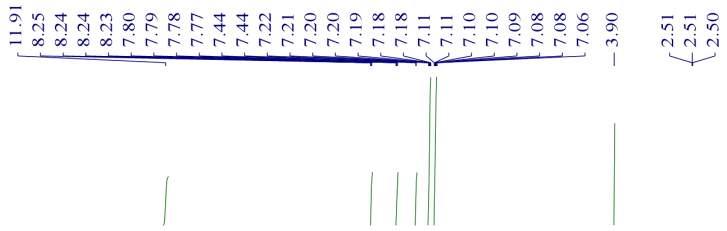
143.74
129.64
127.08
121.01
116.36
105.12
40.62
40.41
40.20
39.99
39.78
39.57
39.36
f1 (ppm)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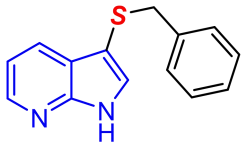
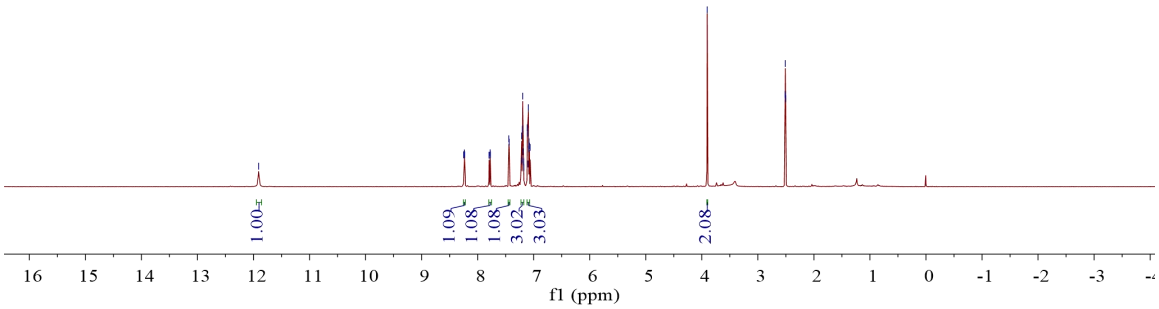
8.24
8.24
8.23
7.80
7.79
7.78
7.77
7.44
7.44
7.22
7.21
7.20
7.20
7.19
7.18
7.18
7.11
7.11
7.10
7.10
7.09
7.08
7.08
7.06
3.90
2.51
2.51
2.50


S
N
H

4ah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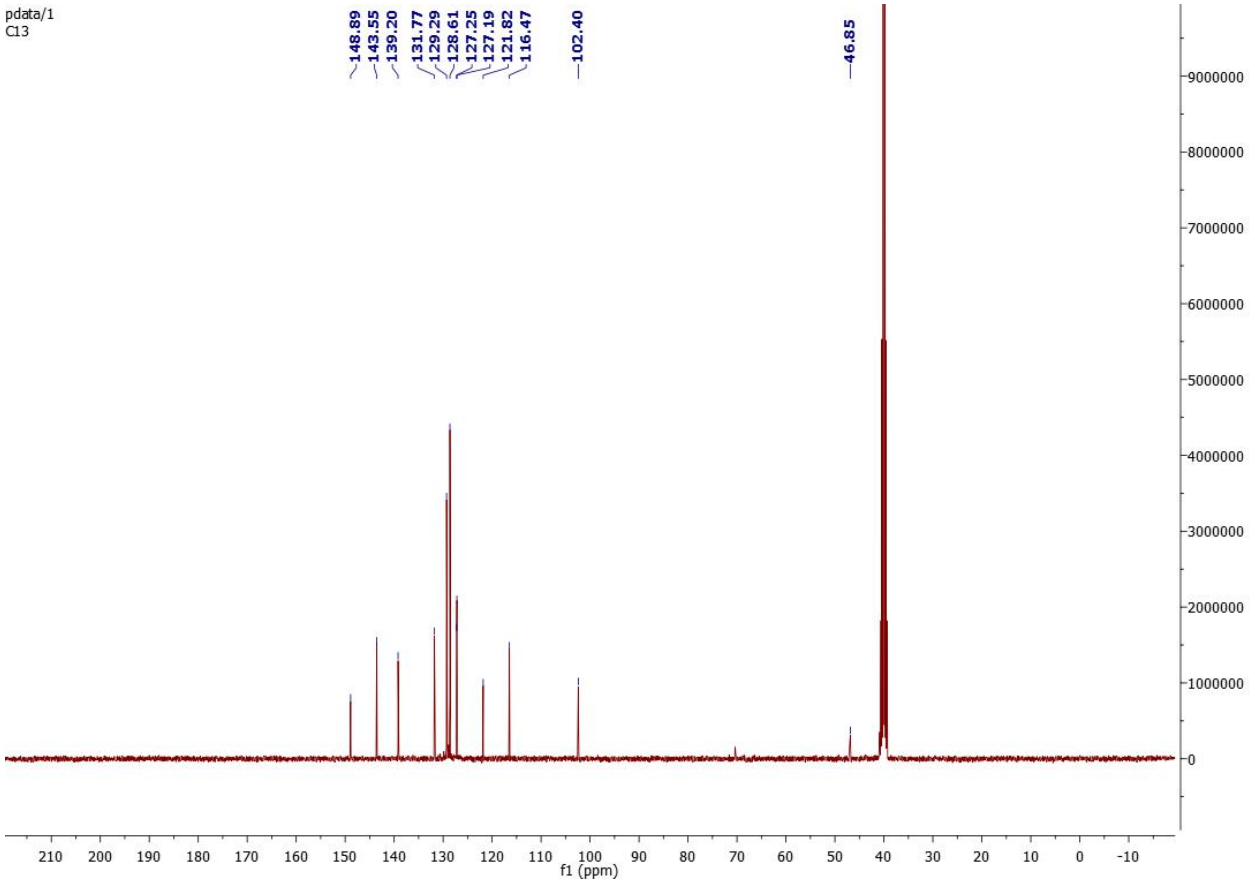
1.09
1.08
1.08
3.02
3.03
2.08
f1 (ppm)


pdata/1
C13
148.89
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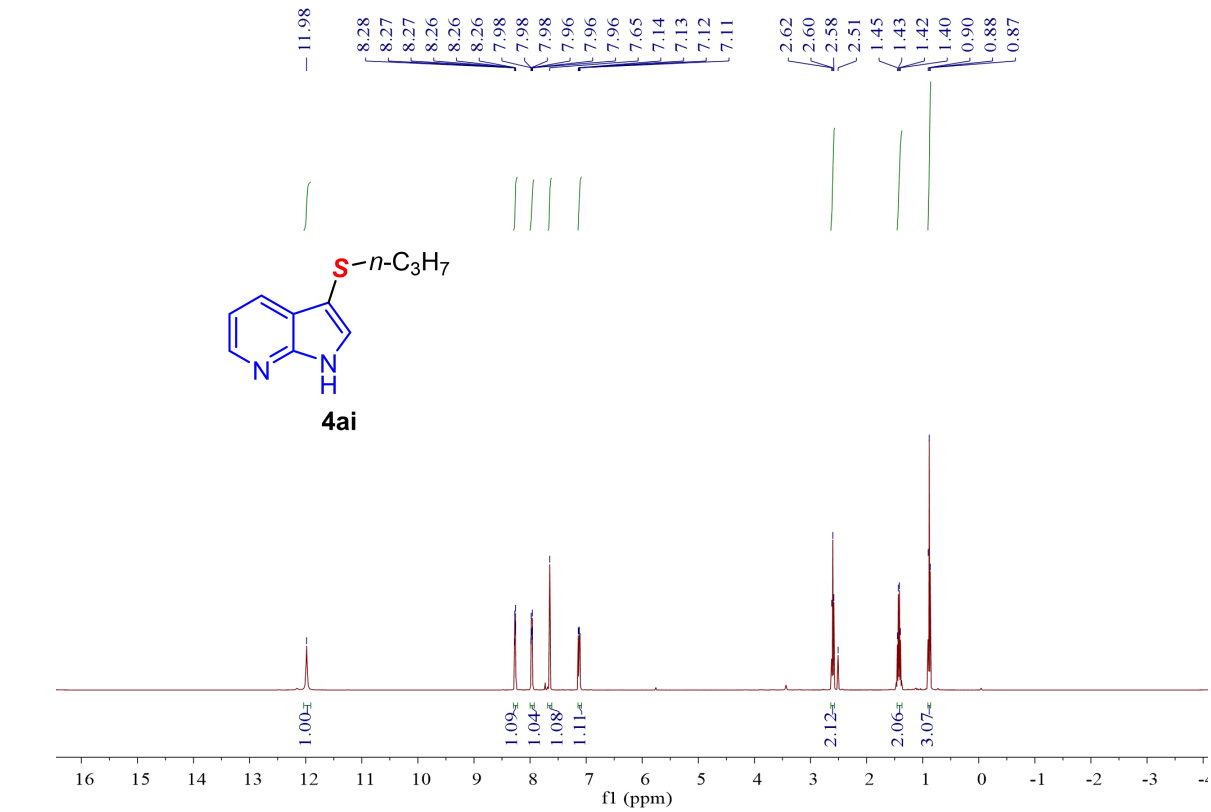
129.29
128.61
127.25
127.19
121.82
116.47
102.40
46.85
f1 (ppm)


11.98
8.28
8.27
8.27
8.26
8.26
8.26
7.98
7.98
7.98
7.96
7.96
7.96
7.65
7.14
7.13
7.12
7.11
2.62
2.60
2.58
2.51
1.45
1.43
1.42
1.40
0.90
0.88
0.87
S–n-C3H7
N
H
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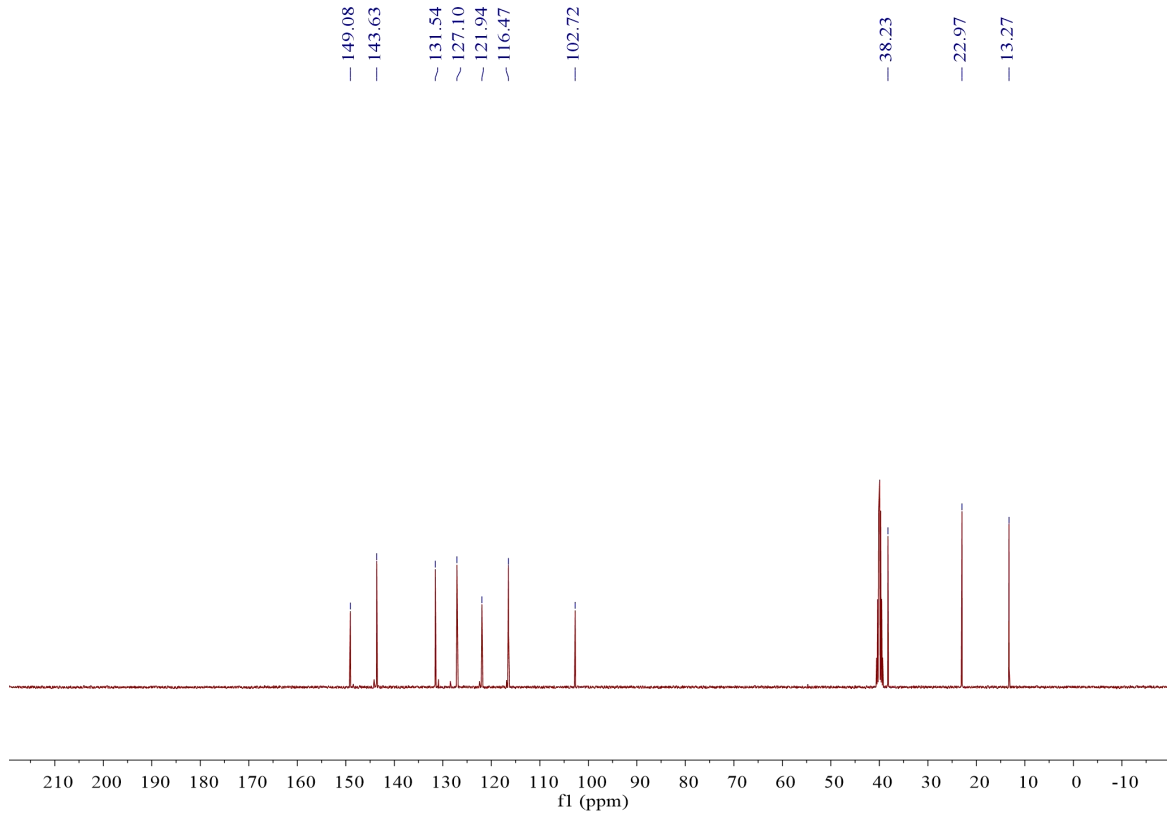
1.09
1.04
1.08
1.11
2.12
2.06
3.07
f1 (ppm)

4ai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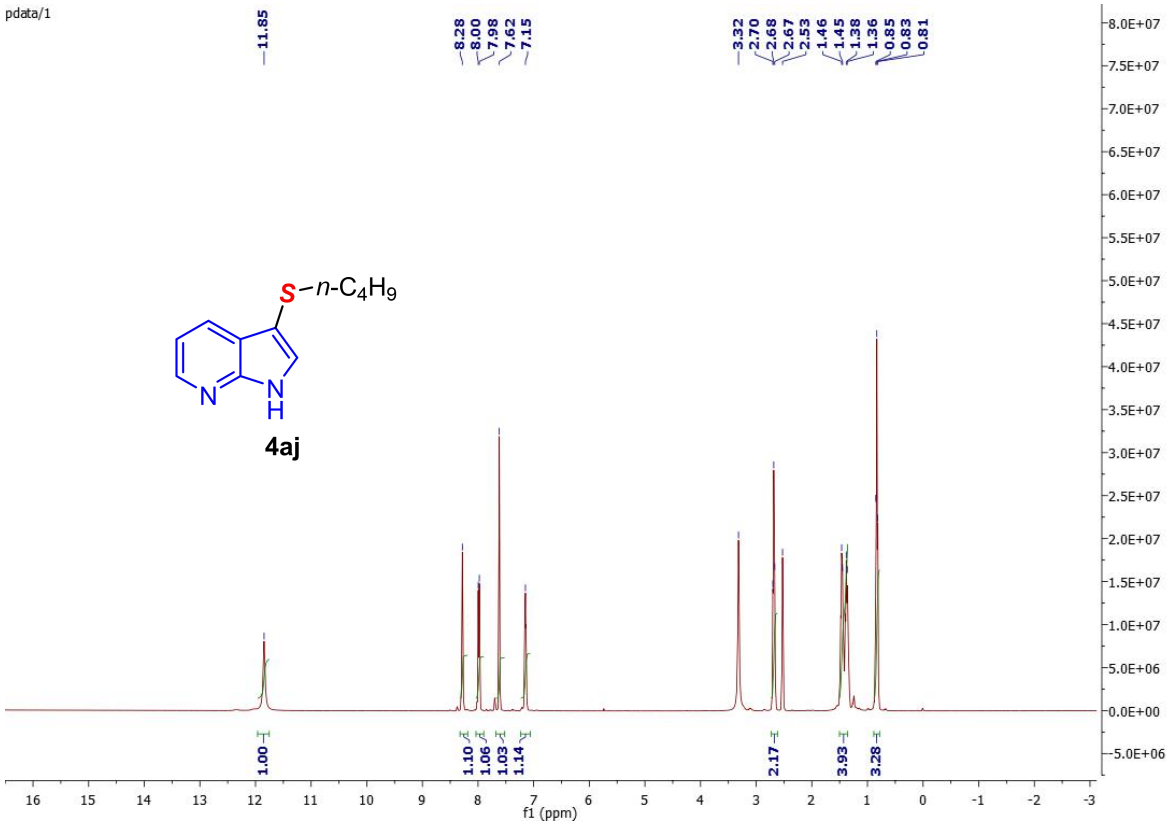
143.63
131.54
127.10
121.94
116.47
102.72
38.23
22.97
13.27
f1 (ppm)


pdata/1
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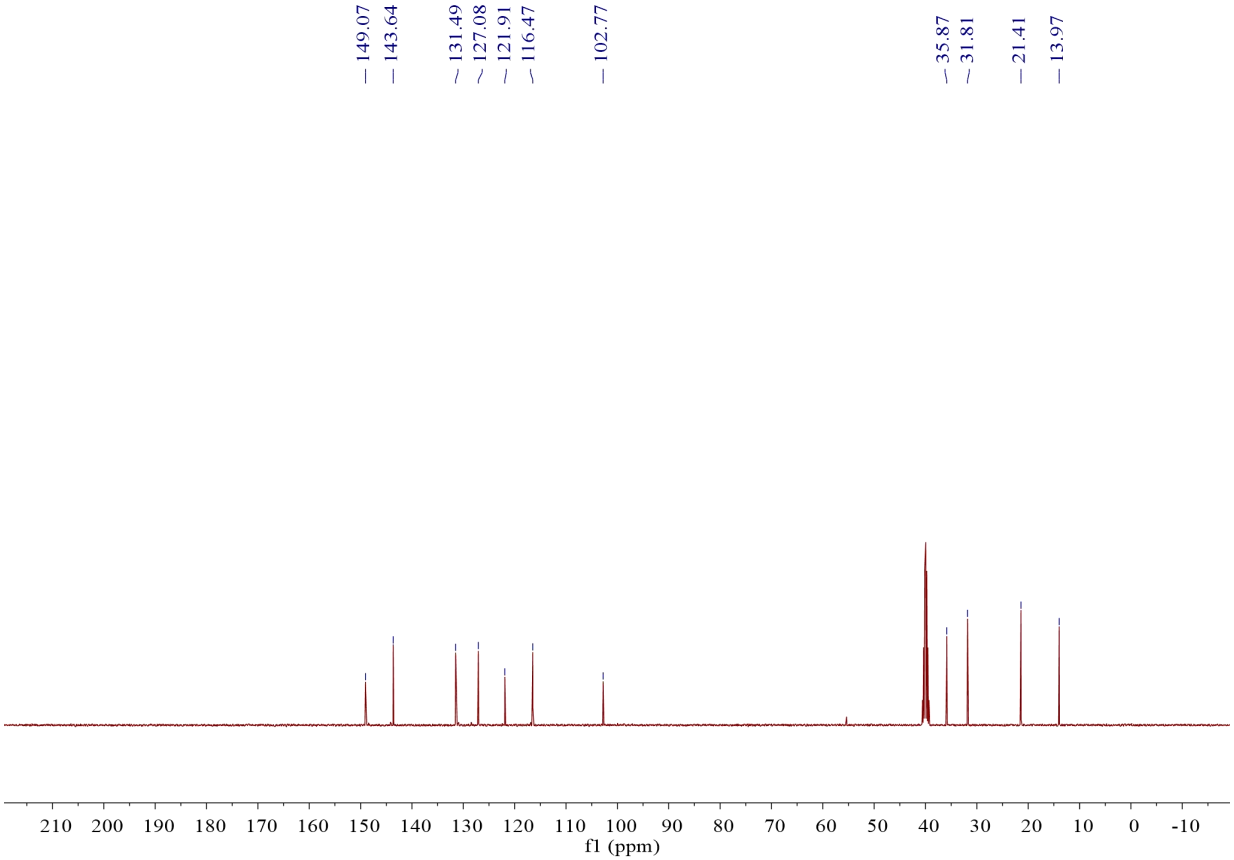
8.28
8.00
7.98
7.62
7.15
3.32
2.70
2.68
2.67
2.53
1.46
1.45
1.38
1.36
0.85
0.83
0.81
S–n-C4H9
N
H
4aj
1.00
1.10
1.06
1.03
1.14
2.17
3.93
3.28
f1 (ppm)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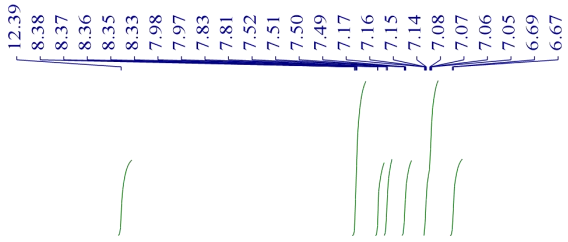
127.08
121.91
116.47
102.77
35.87
31.81
21.41
13.97
fl (ppm)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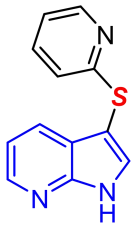
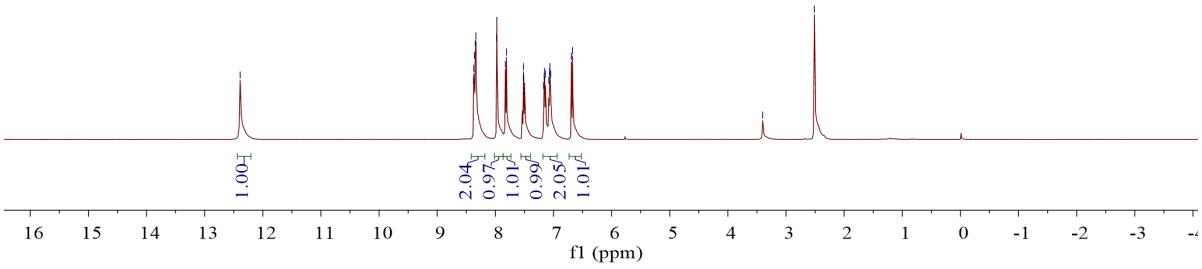
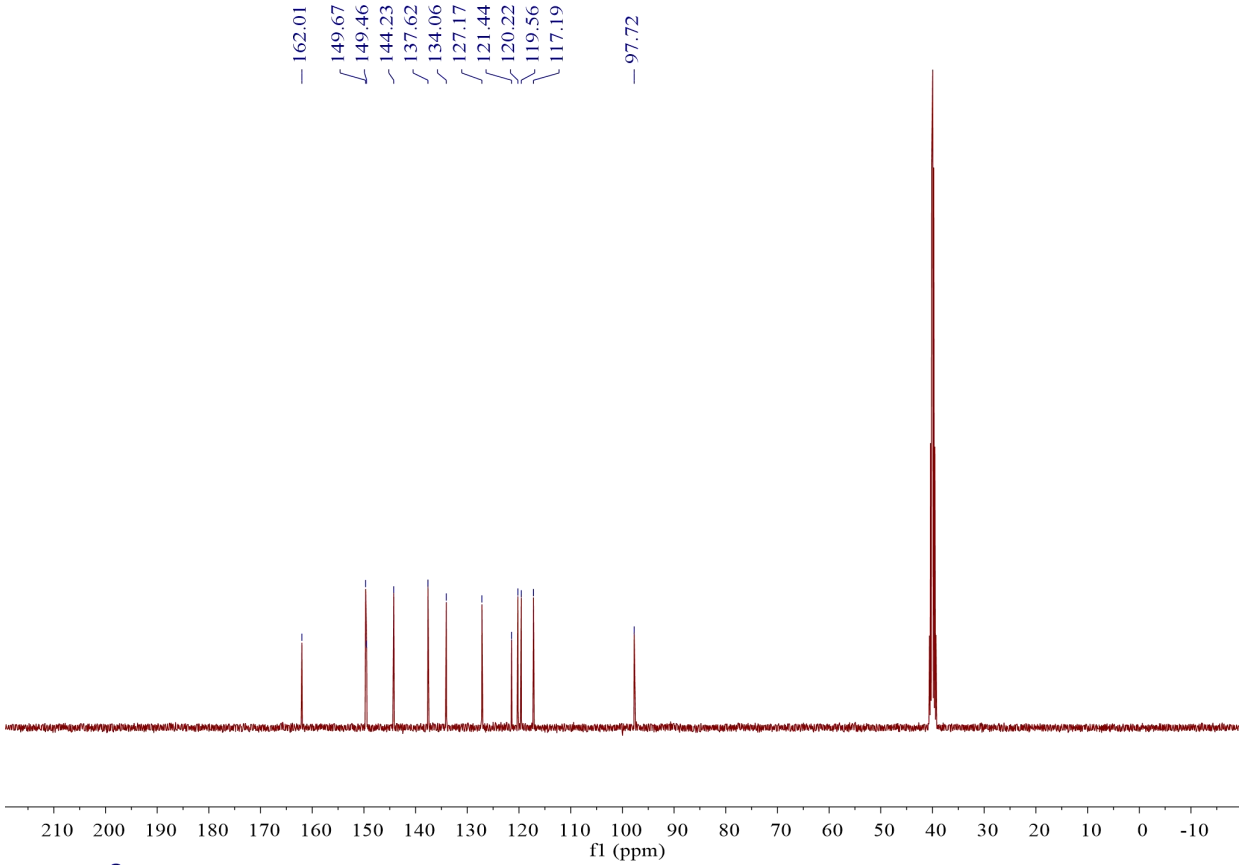
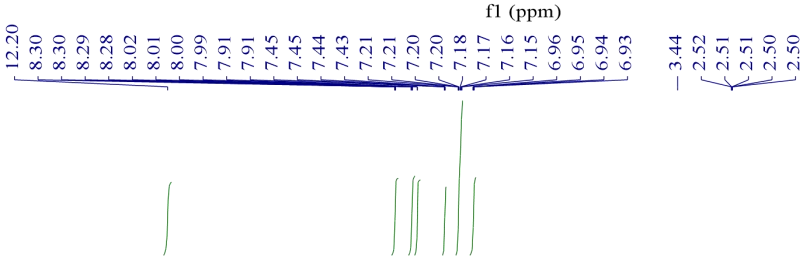
8.38
8.37
8.36
8.35
8.33
7.98
7.97
7.83
7.81
7.52
7.51
7.50
7.49
7.17
7.16
7.15
7.14
7.08
7.07
7.06
7.05
6.69
6.67
3.40
2.51


N
S
N
H

4ak


1.00
2.04
0.97
1.01
0.99
2.05
1.01
fl (ppm)


162.01
149.67
149.46
144.23
137.62
134.06
127.17
121.44
120.22
119.56
117.19
97.72
f1 (ppm)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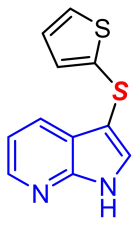
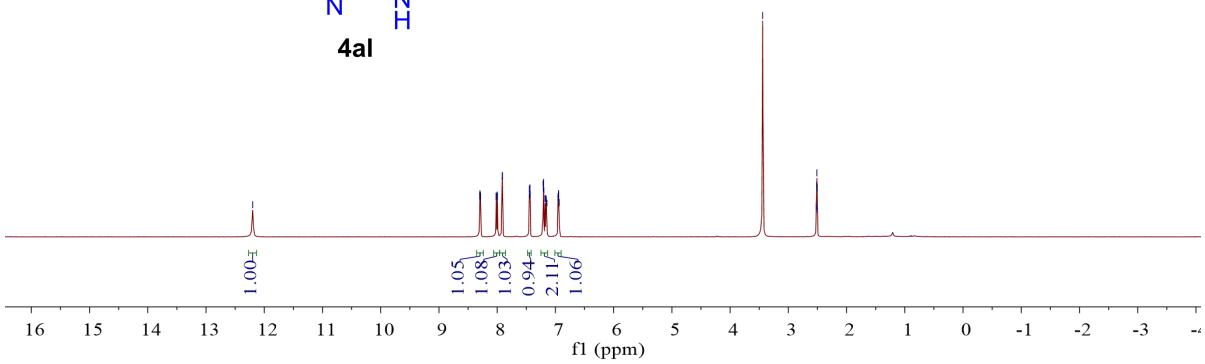
8.28
8.02
8.01
8.00
7.99
7.91
7.91
7.91
7.45
7.44
7.43
7.21
7.21
7.20
7.20
7.18
7.17
7.16
7.15
6.96
6.95
6.94
6.93
3.44
2.52
2.51
2.51
2.50
2.50


S
S
N
N
H

4al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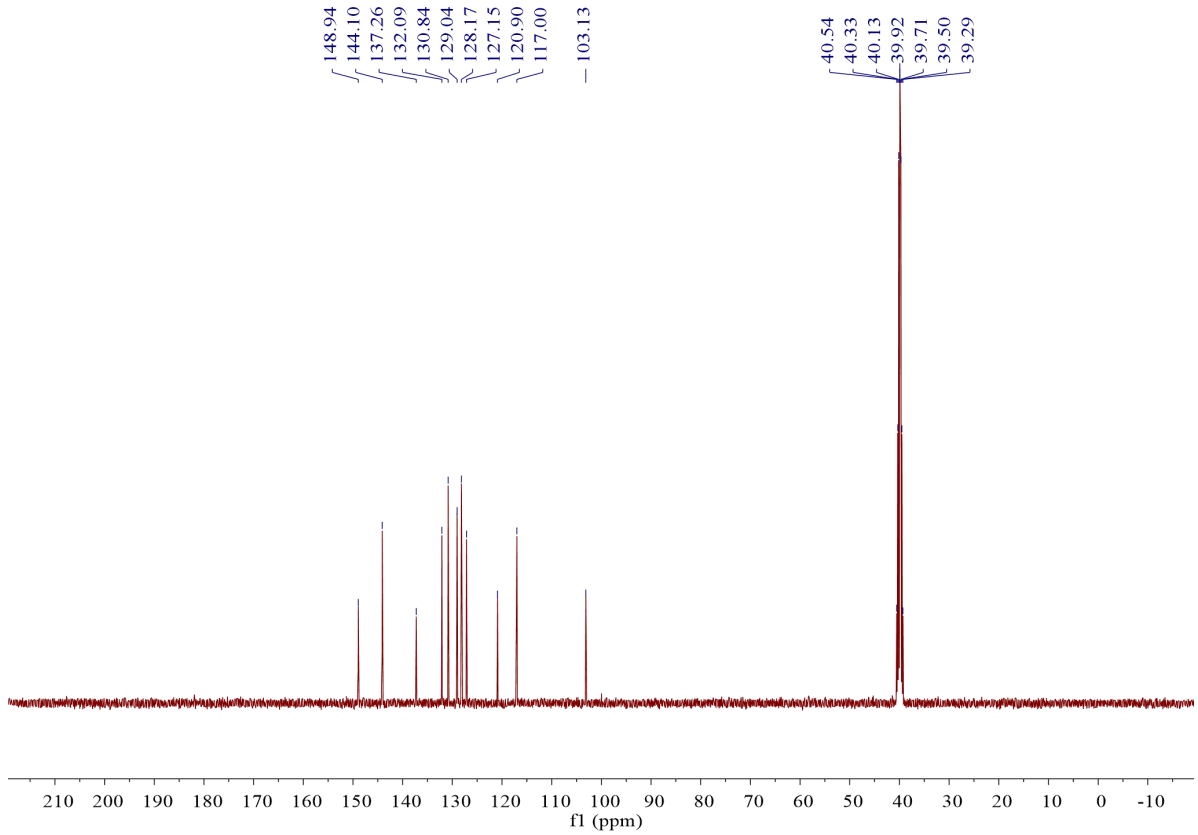
1.08
1.03
0.94
2.11
1.06
f1 (ppm)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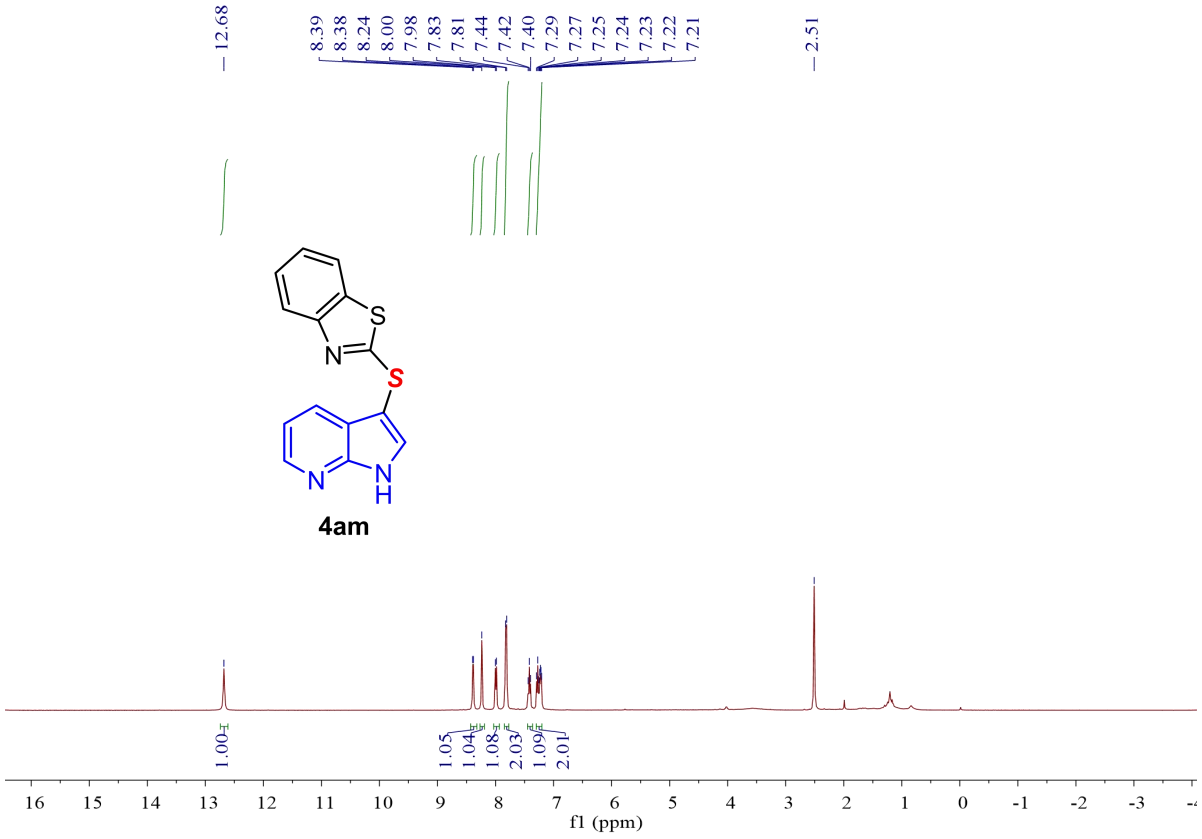
144.10
137.26
132.09
130.84
129.04
128.17
127.15
120.90
117.00
103.13
40.54
40.33
40.13
39.92
39.71
39.50
39.29
f1 (ppm)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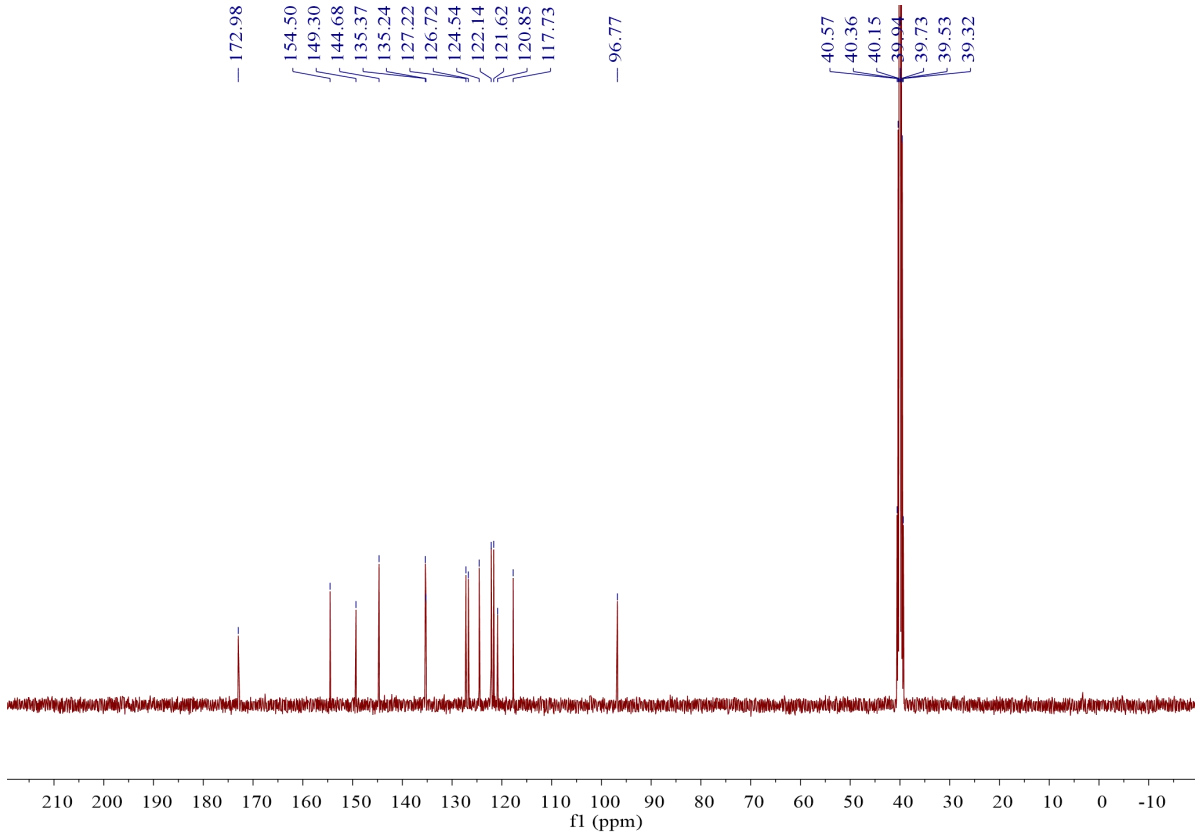
7.83
7.81
7.44
7.42
7.40
7.29
7.27
7.25
7.24
7.23
7.22
7.21
2.51
S
N
S
N
N
H
4am
1.00
1.05
1.04
1.08
2.03
1.09
2.01
f1 (ppm)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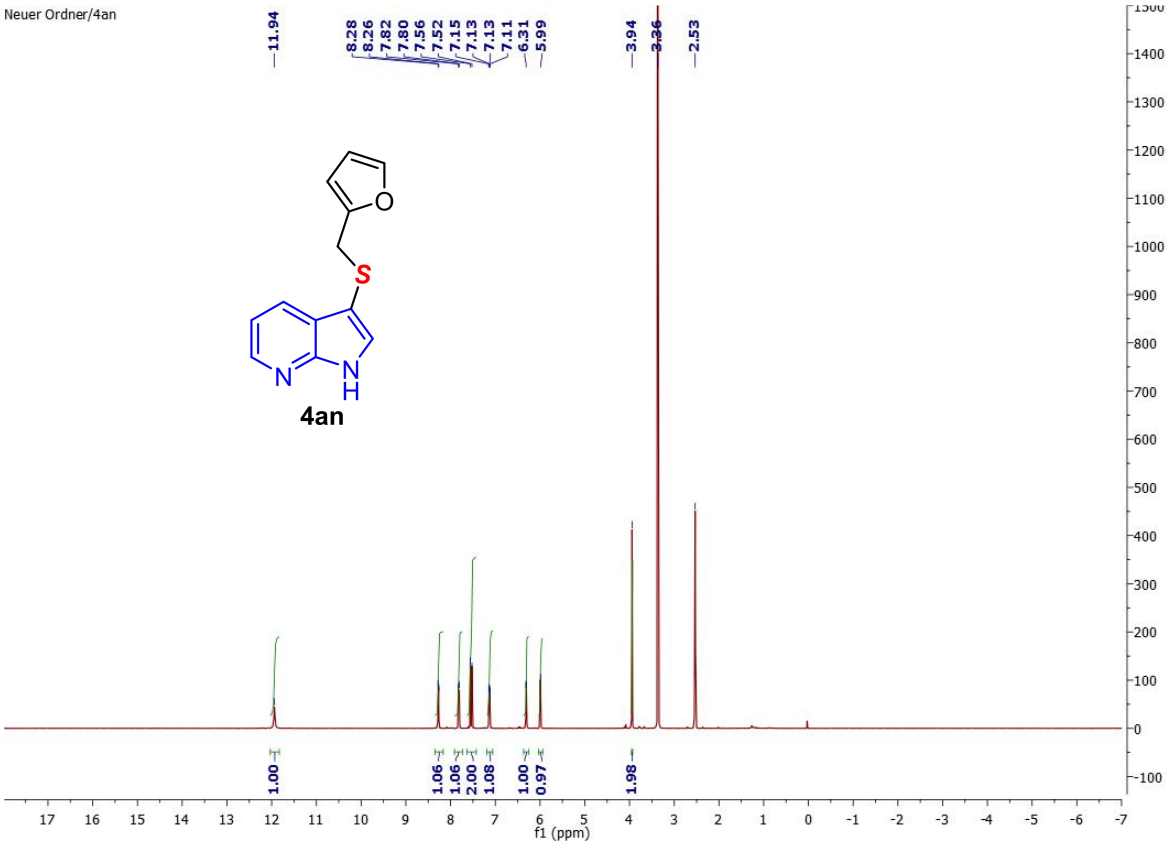
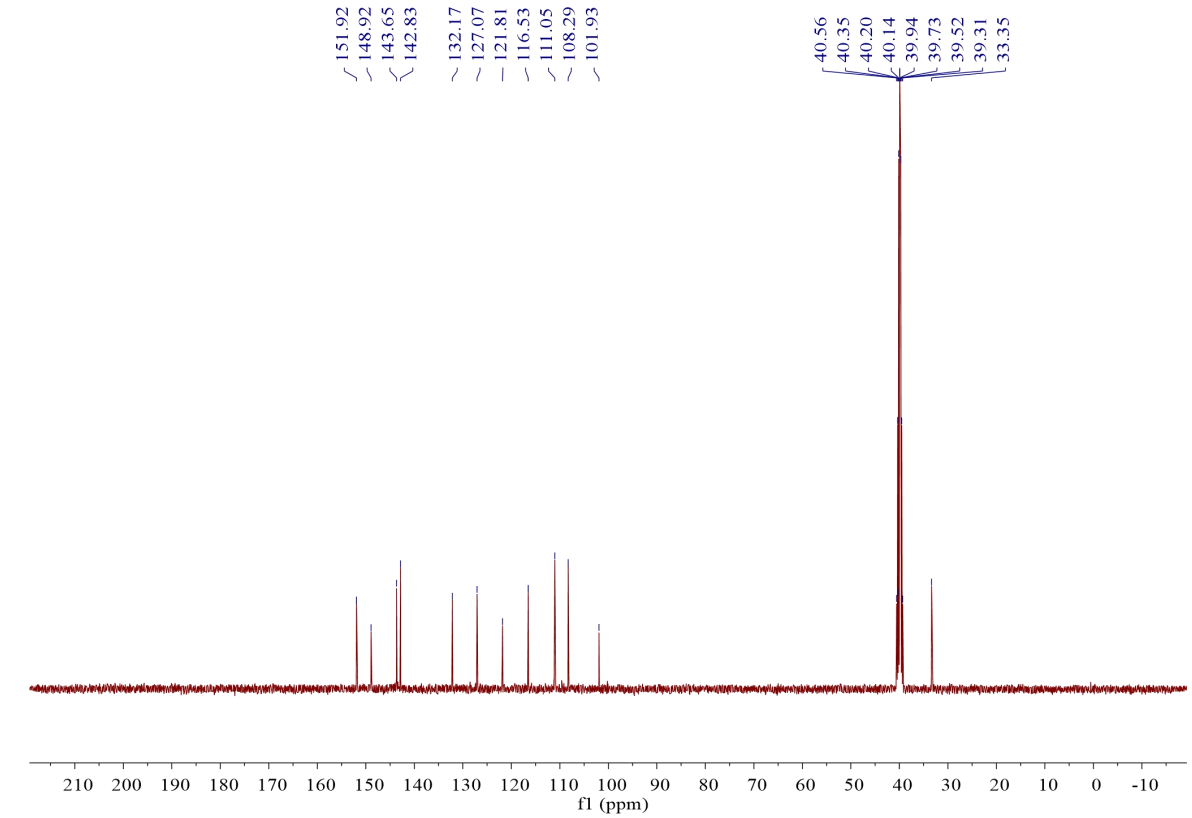
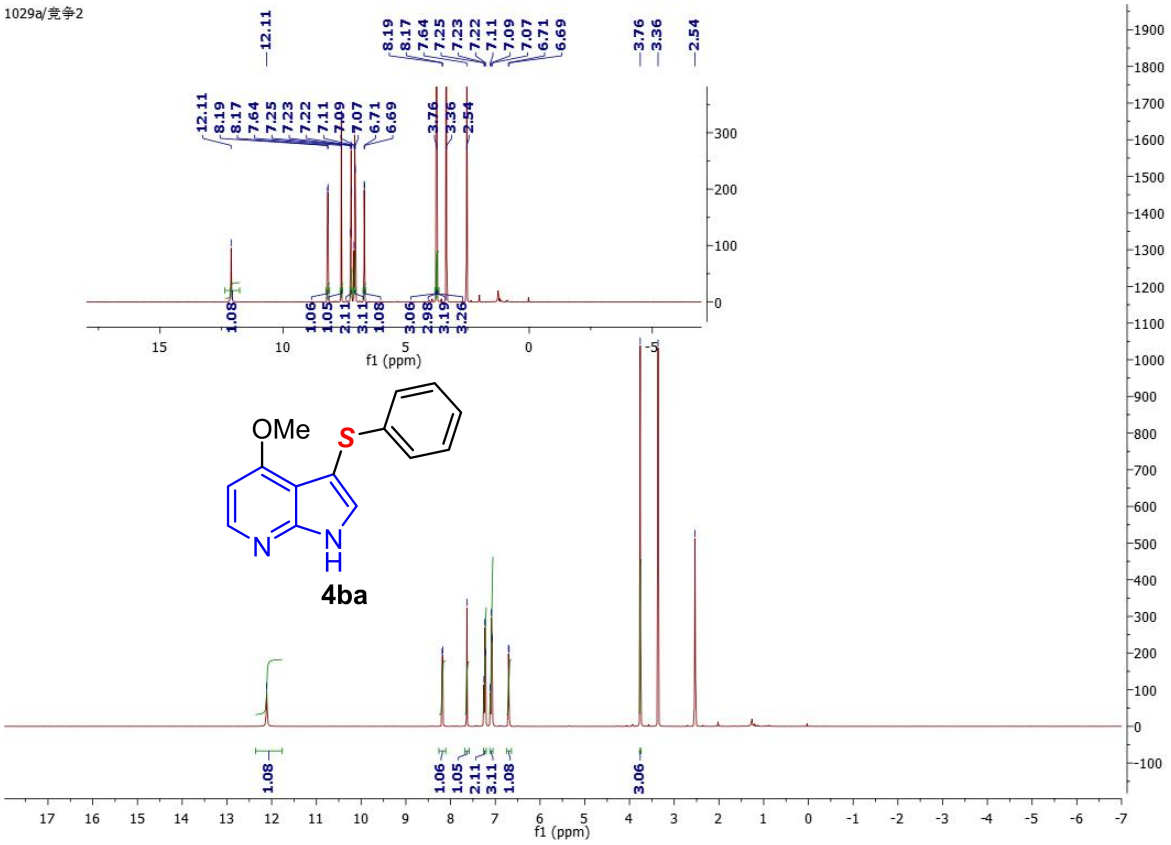
154.50
149.30
144.68
135.37
135.24
127.22
126.72
124.54
122.14
121.62
120.85
117.73
96.77
40.57
40.36
40.15
39.94
39.73
39.53
39.32
f1 (ppm)


Neuer Ordner/4an
11.94
8.28
8.26
7.82
7.80
7.56
7.52
7.15
7.13
7.13
7.11
6.31
5.99
3.94
3.26
2.53
O
S
N
N
H
4an
1.00
1.06
1.06
2.00
1.08
1.00
0.97
1.98
f1 (ppm)


151.92
148.92
143.65
142.83
132.17
127.07
121.81
116.53
111.05
108.29
101.93
40.56
40.35
40.20
40.14
39.94
39.73
39.52
39.31
33.35
f1 (ppm)


1029a/竞争2
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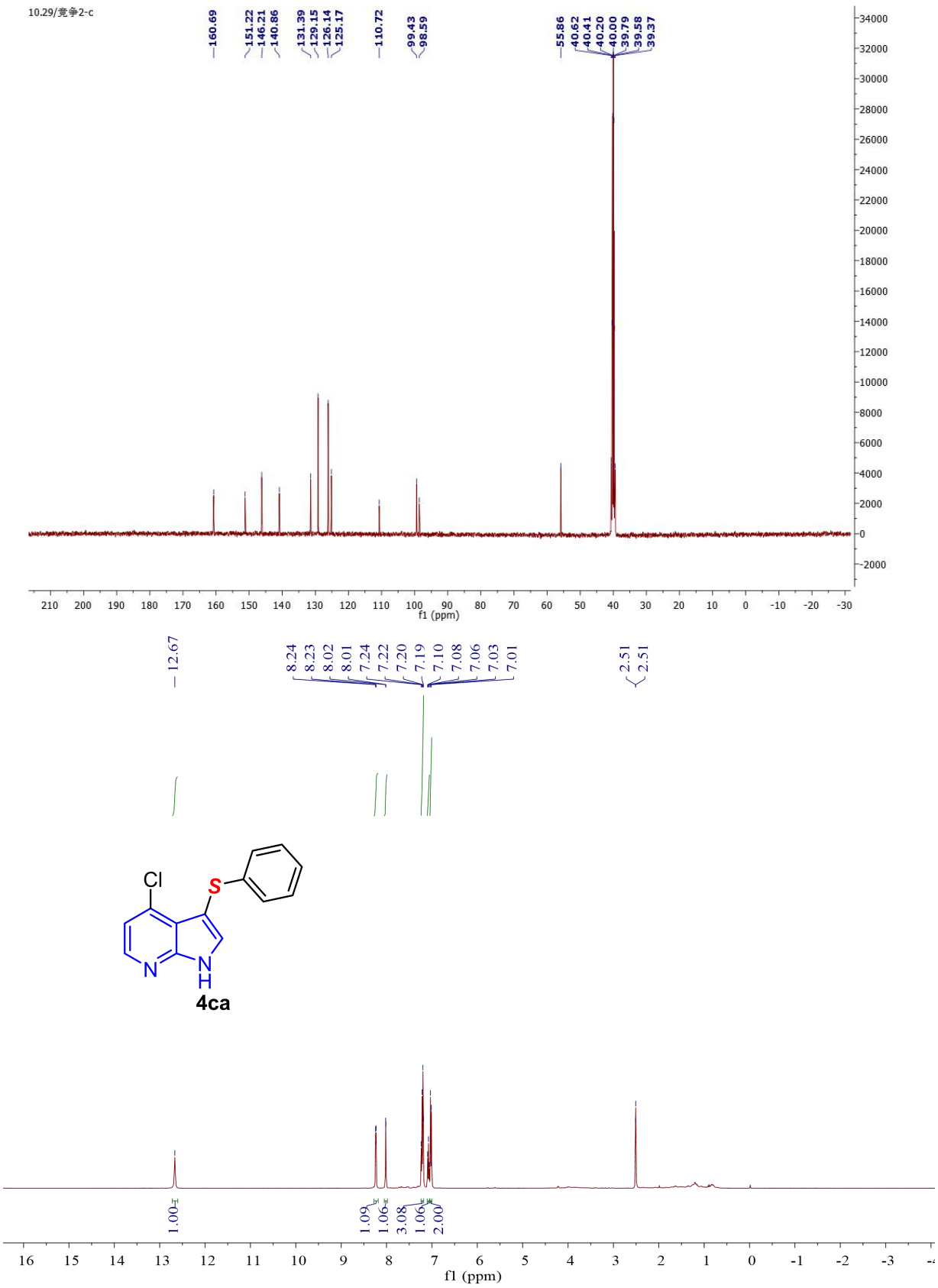
8.19
8.17
7.64
7.25
7.23
7.22
7.11
7.09
7.07
6.71
6.69
3.76
3.36
2.54
f1 (ppm)
OMe
S
N
N
H
4ba


10.29/竞争2-c
160.69
151.22
146.21
140.86
131.39
129.15
126.14
125.17
110.72
99.43
98.59
55.86
40.62
40.41
40.20
40.00
39.79
39.58
39.37
f1 (ppm)
12.67
8.24
8.23
8.02
8.01
7.24
7.22
7.20
7.19
7.10
7.08
7.06
7.03
7.01
2.51
2.51
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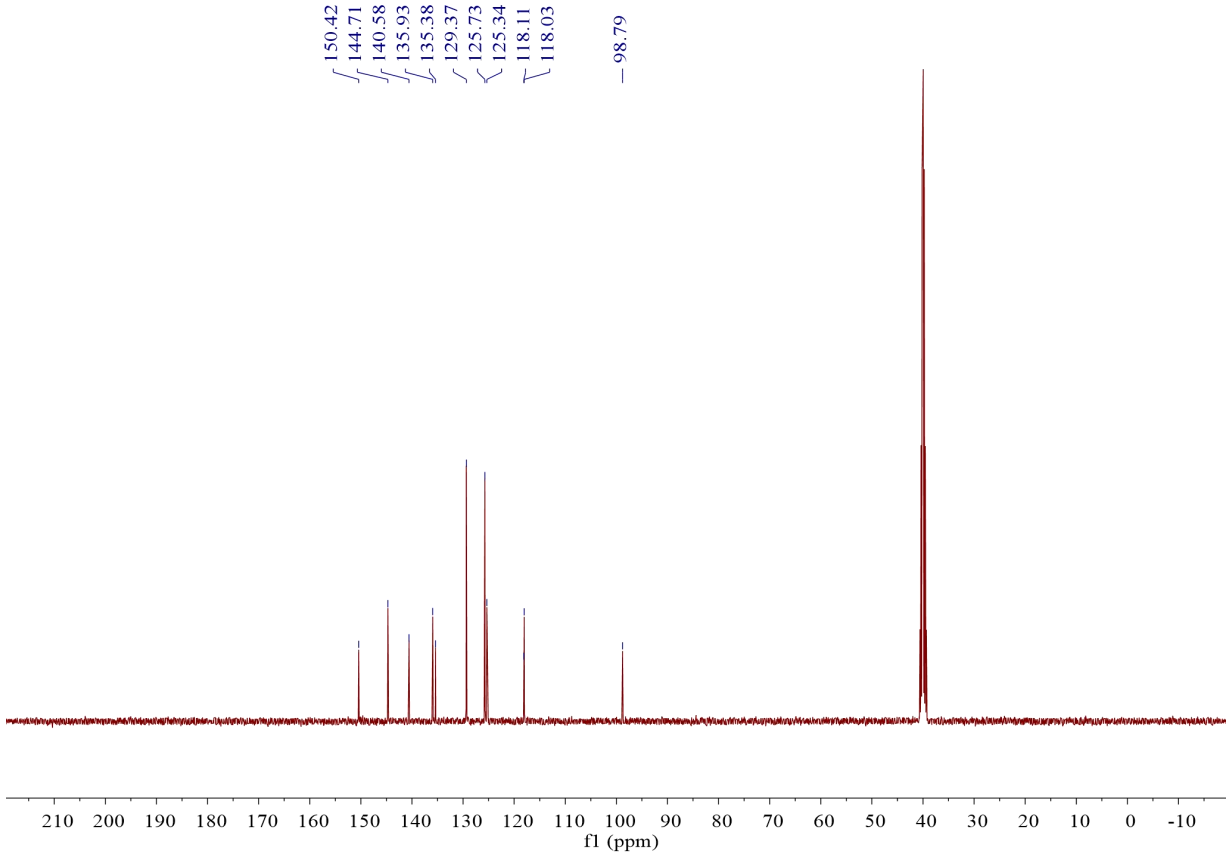
S
N
H
4ca
1.00
1.09
1.06
3.08
1.06
2.00
f1 (ppm)


150.42
144.71
140.58
135.93
135.38
129.37
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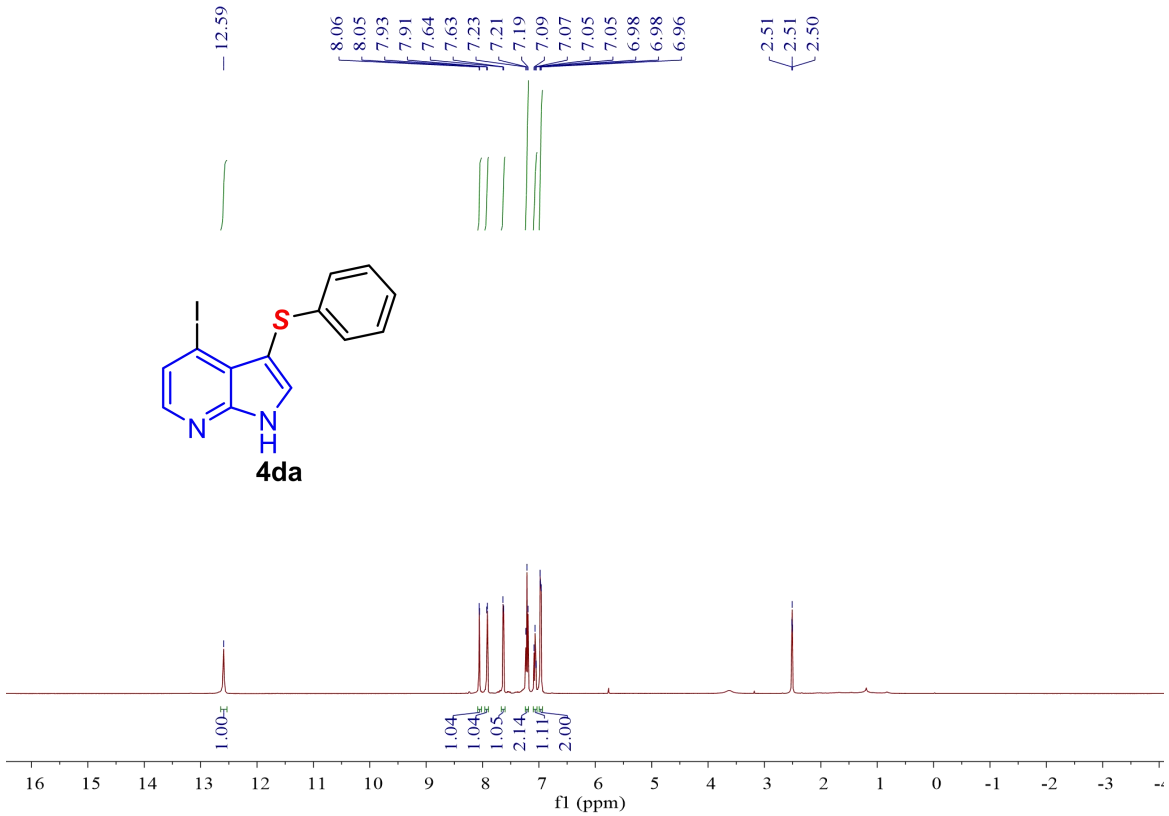
125.34
118.11
118.03
98.79
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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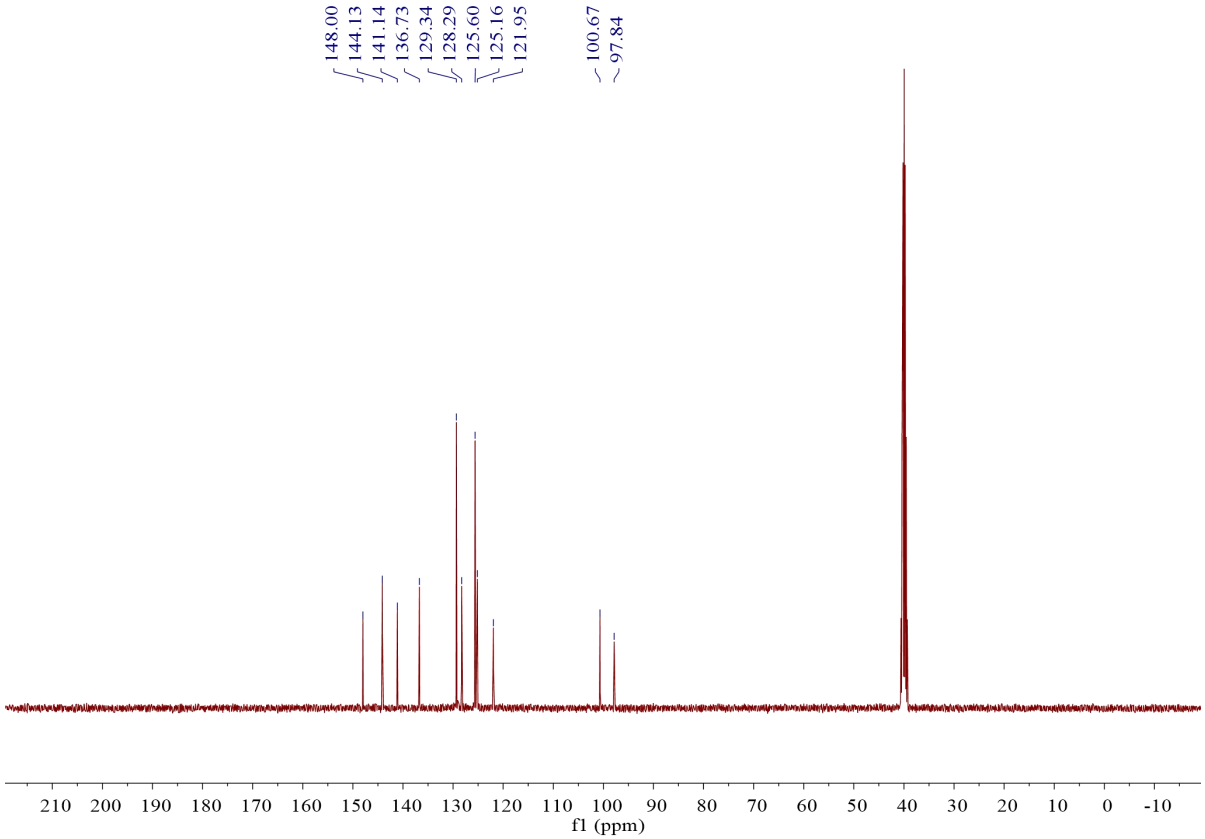
8.06
8.05
7.93
7.91
7.64
7.63
7.23
7.21
7.19
7.09
7.07
7.05
7.05
6.98
6.98
6.96
2.51
2.51
2.50
I
S
N
N
H
4da
1.00
1.04
1.04
1.05
2.14
1.11
2.00
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)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144.13
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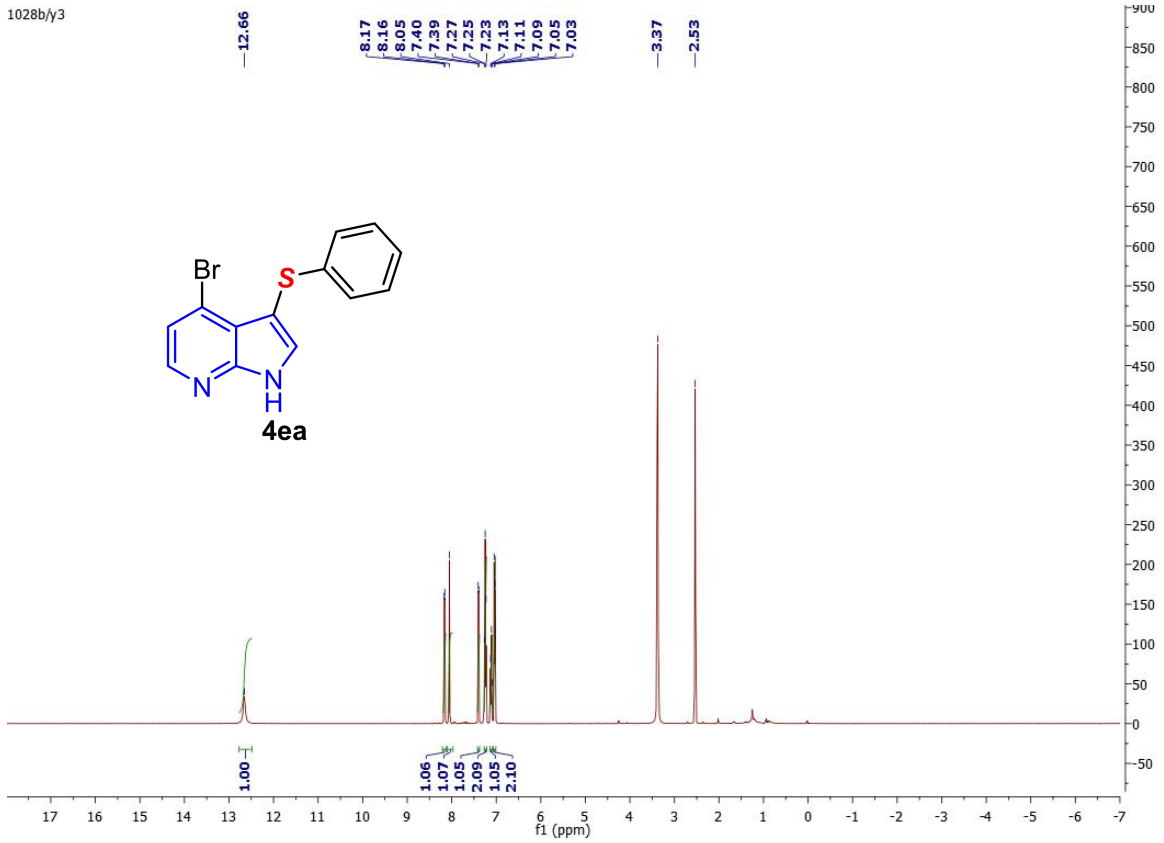
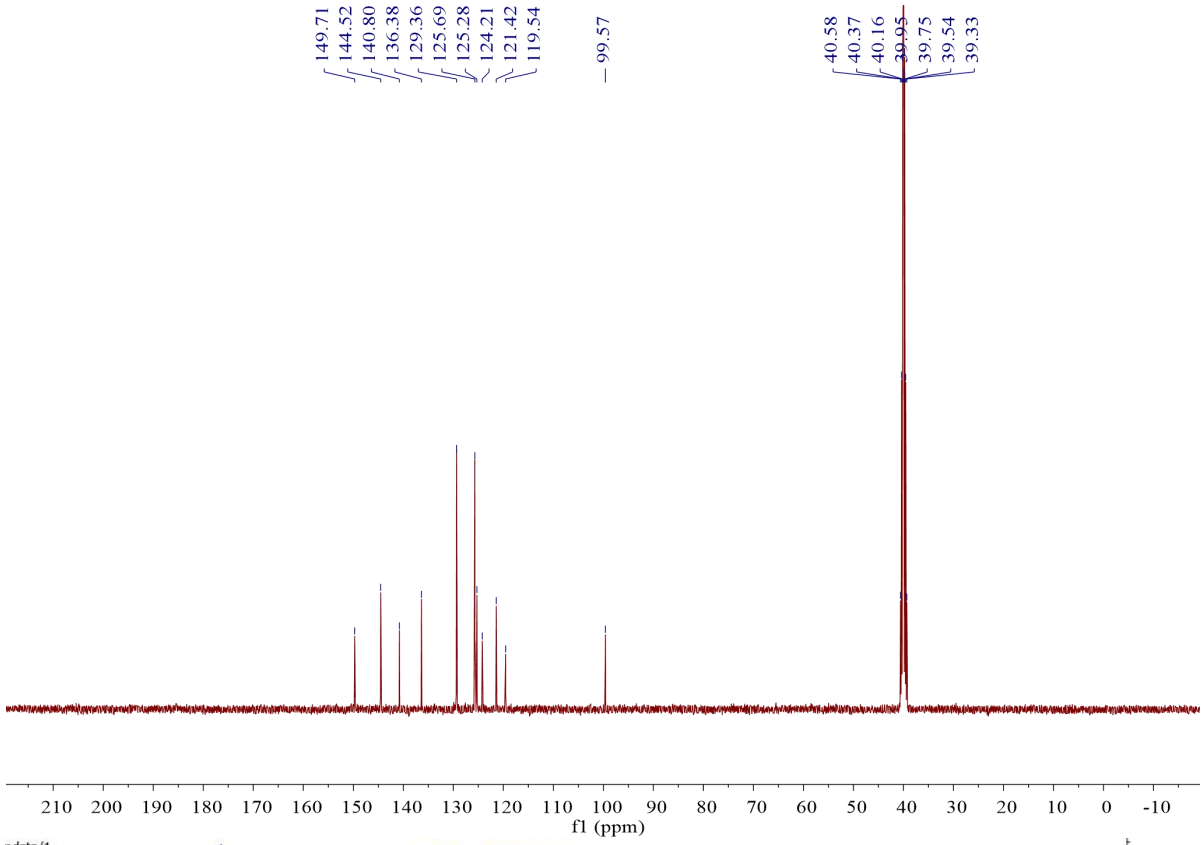
136.73
129.34
128.29
125.60
125.16
121.95
100.67
97.84
f1 (ppm)


1028b/y3
12.66
8.17
8.16
8.05
7.40
7.39
7.27
7.25
7.23
7.13
7.11
7.09
7.05
7.03
3.37
2.53
Br
S
N
N
H
4ea
1.00
1.06
1.07
1.05
2.09
1.05
2.10
f1 (ppm)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136.38
129.36
125.69
125.28
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121.42
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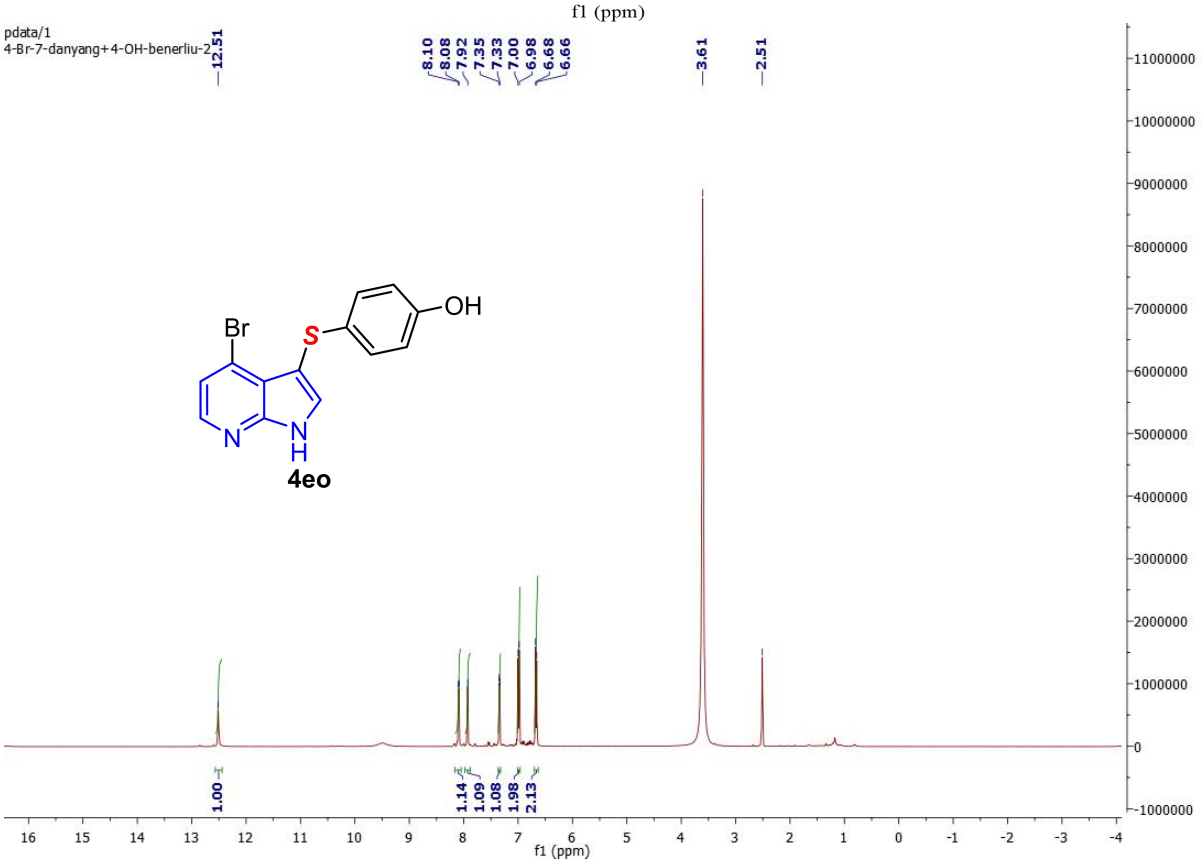
99.57
40.58
40.37
40.16
39.95
39.75
39.54
39.33
f1 (ppm)


pdata/1
4-Br-7-danyang+4-OH-benerliu-2
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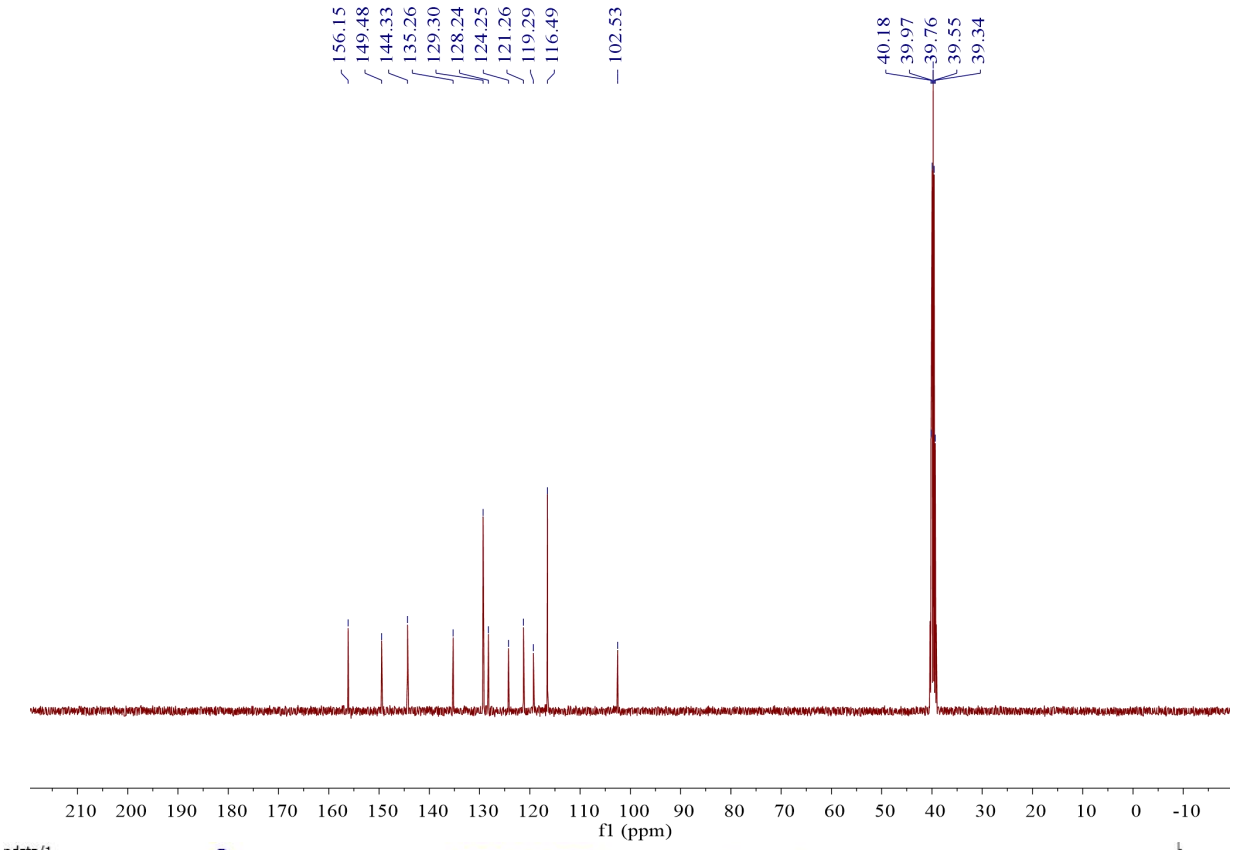
8.10
8.08
7.92
7.35
7.33
7.00
6.98
6.68
6.66
3.61
2.51
Br
S
OH
N
H
4eo
1.00
1.14
1.09
1.08
1.98
2.13
f1 (ppm)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149.48
144.33
135.26
129.30
128.24
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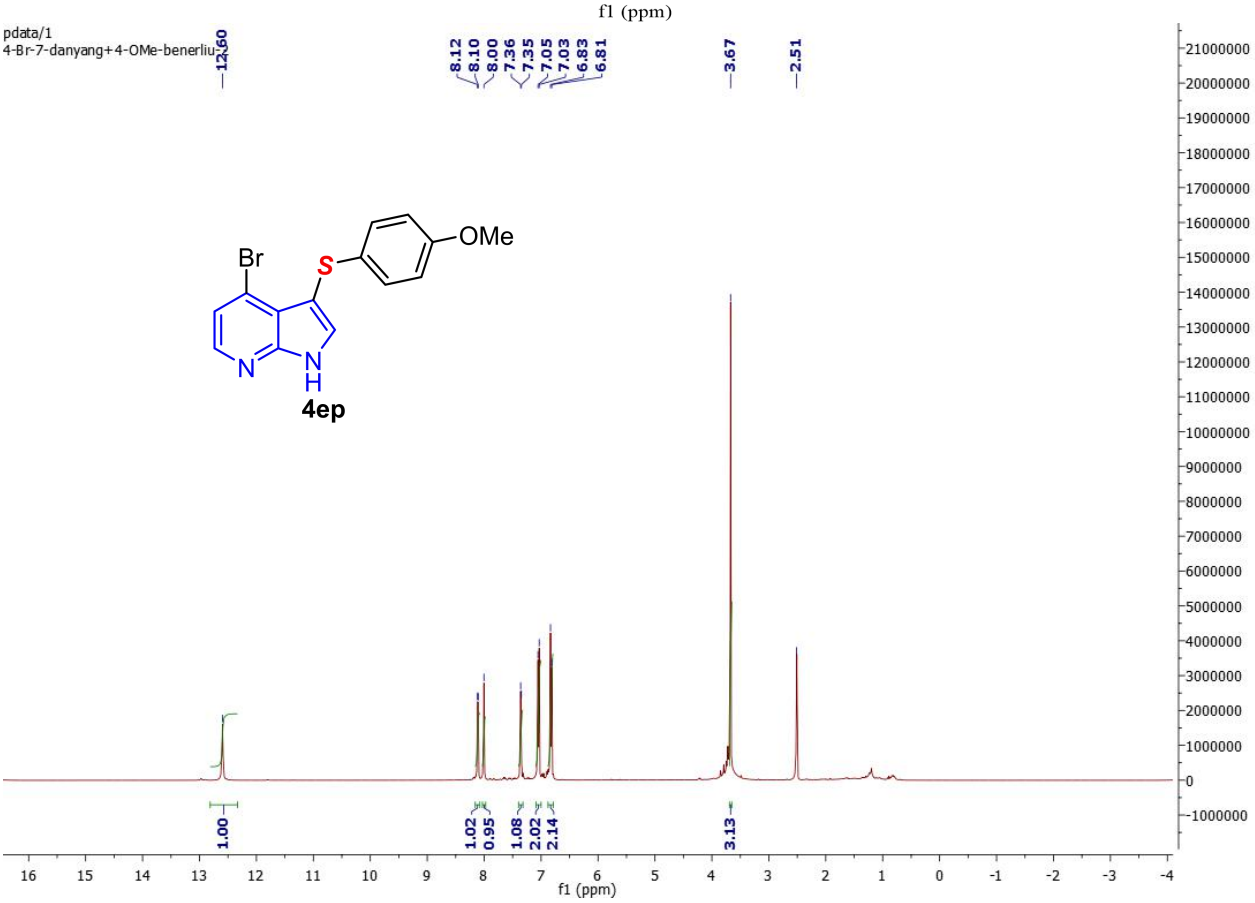
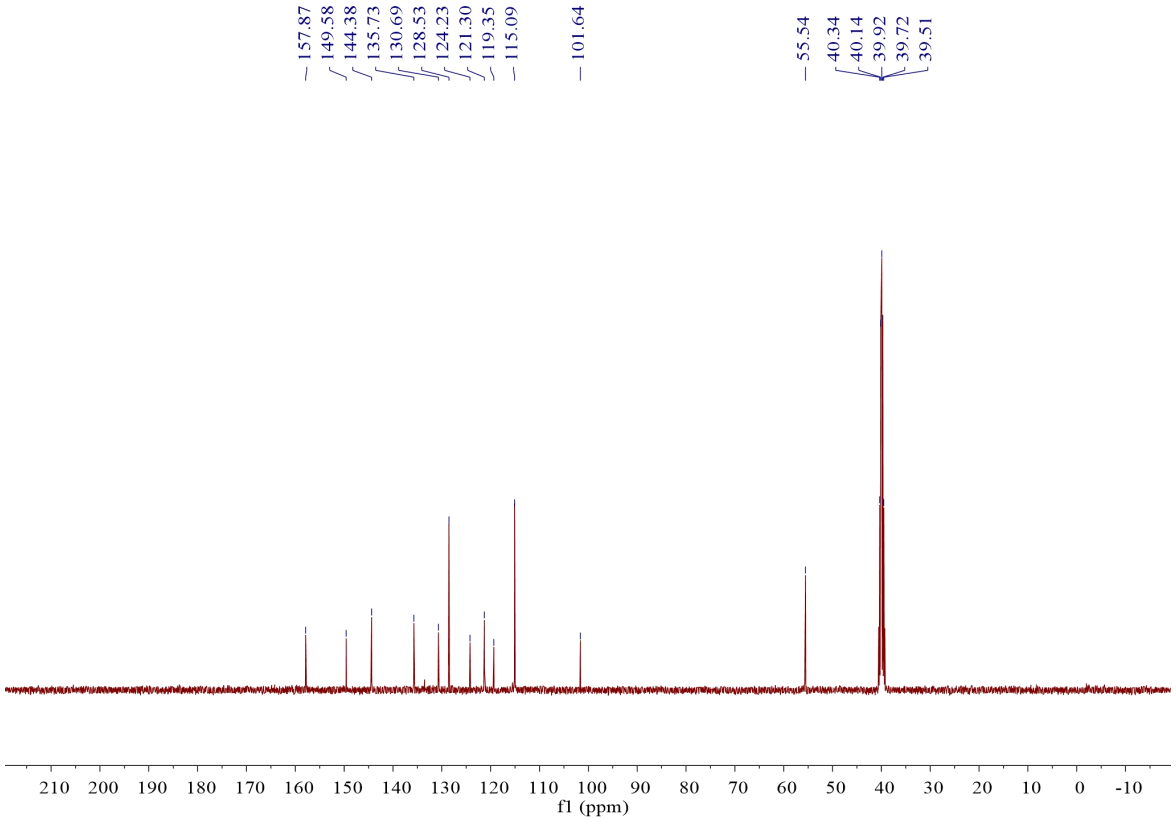
121.26
119.29
116.49
102.53
40.18
39.97
39.76
39.55
39.34
f1 (ppm)


pdata/1
4-Br-7-danyang+4-OMe-benerliu
12.60
8.12
8.10
8.00
7.36
7.35
7.05
7.03
6.83
6.81
3.67
2.51
Br
S
OMe
N
N
H
4ep
1.00
1.02
0.95
1.08
2.02
2.14
3.13
f1 (ppm)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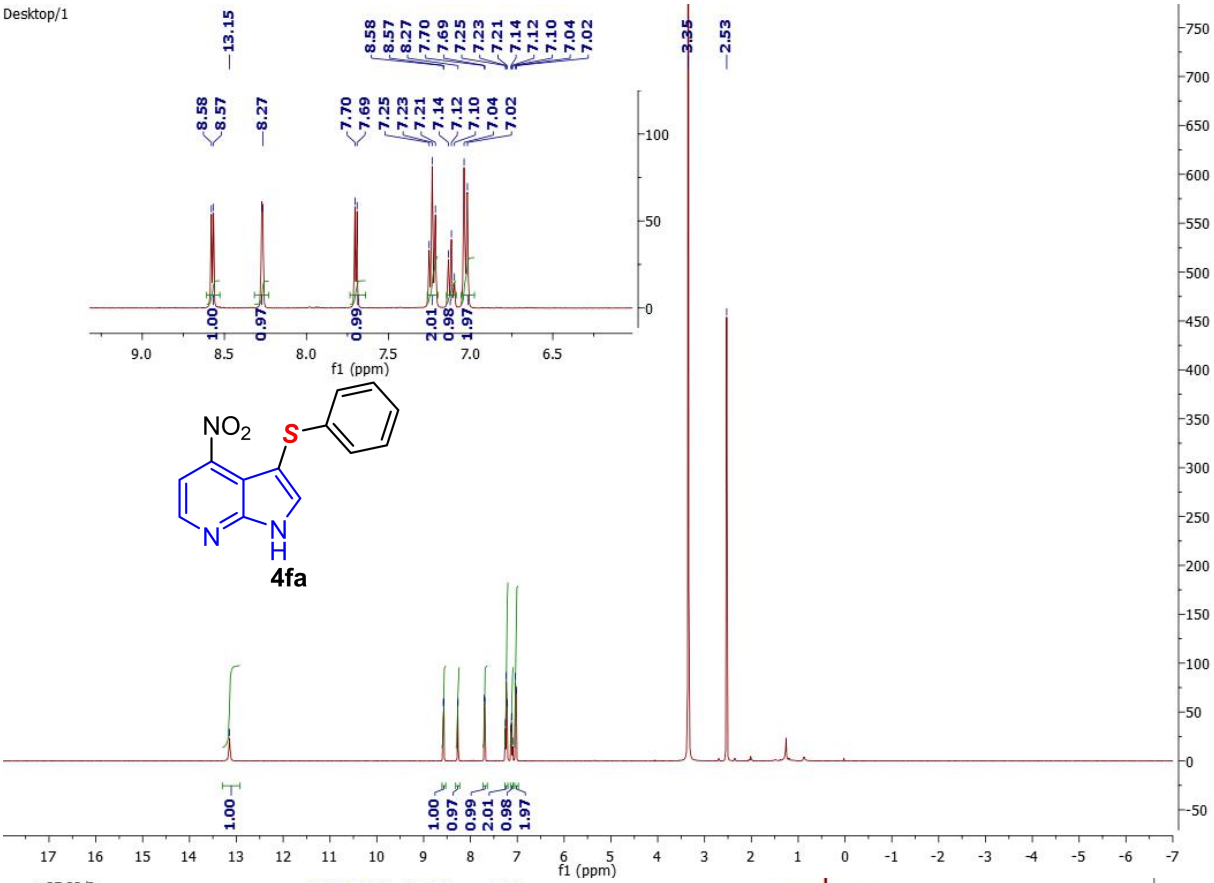
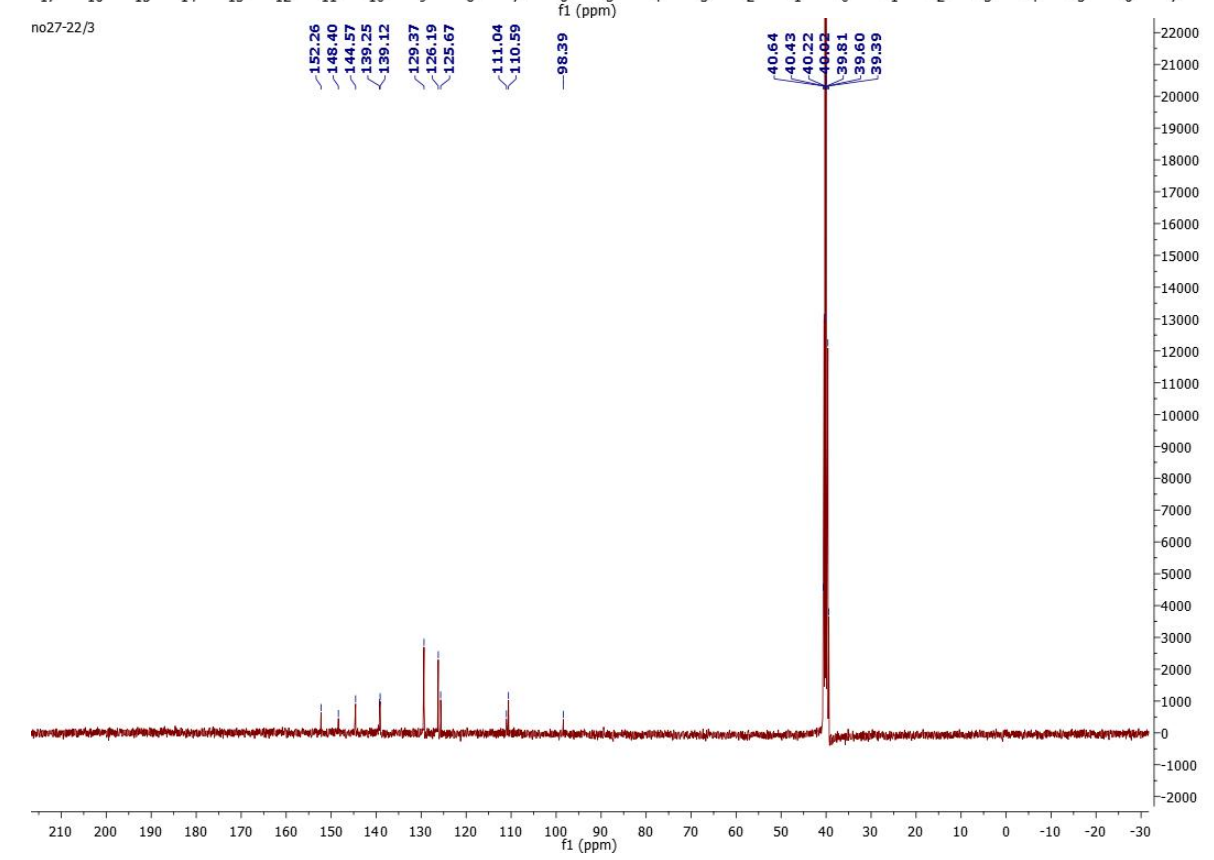
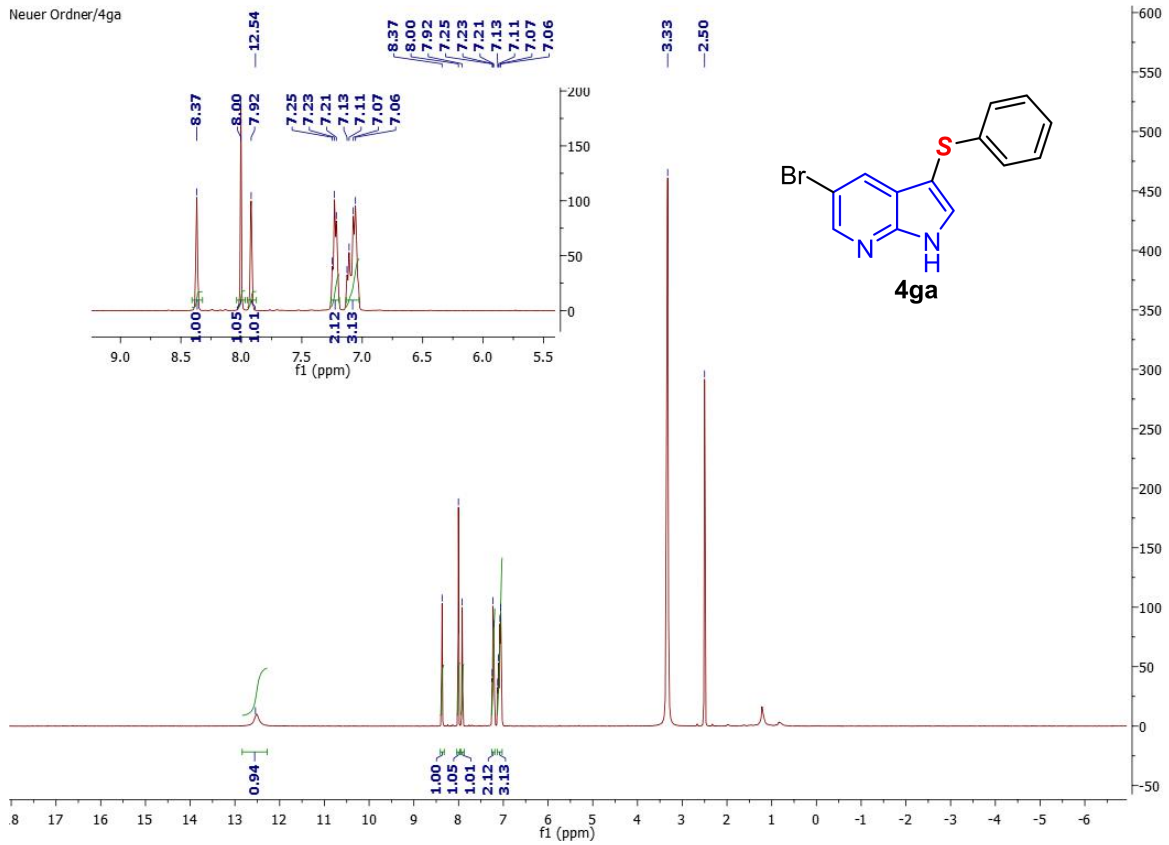
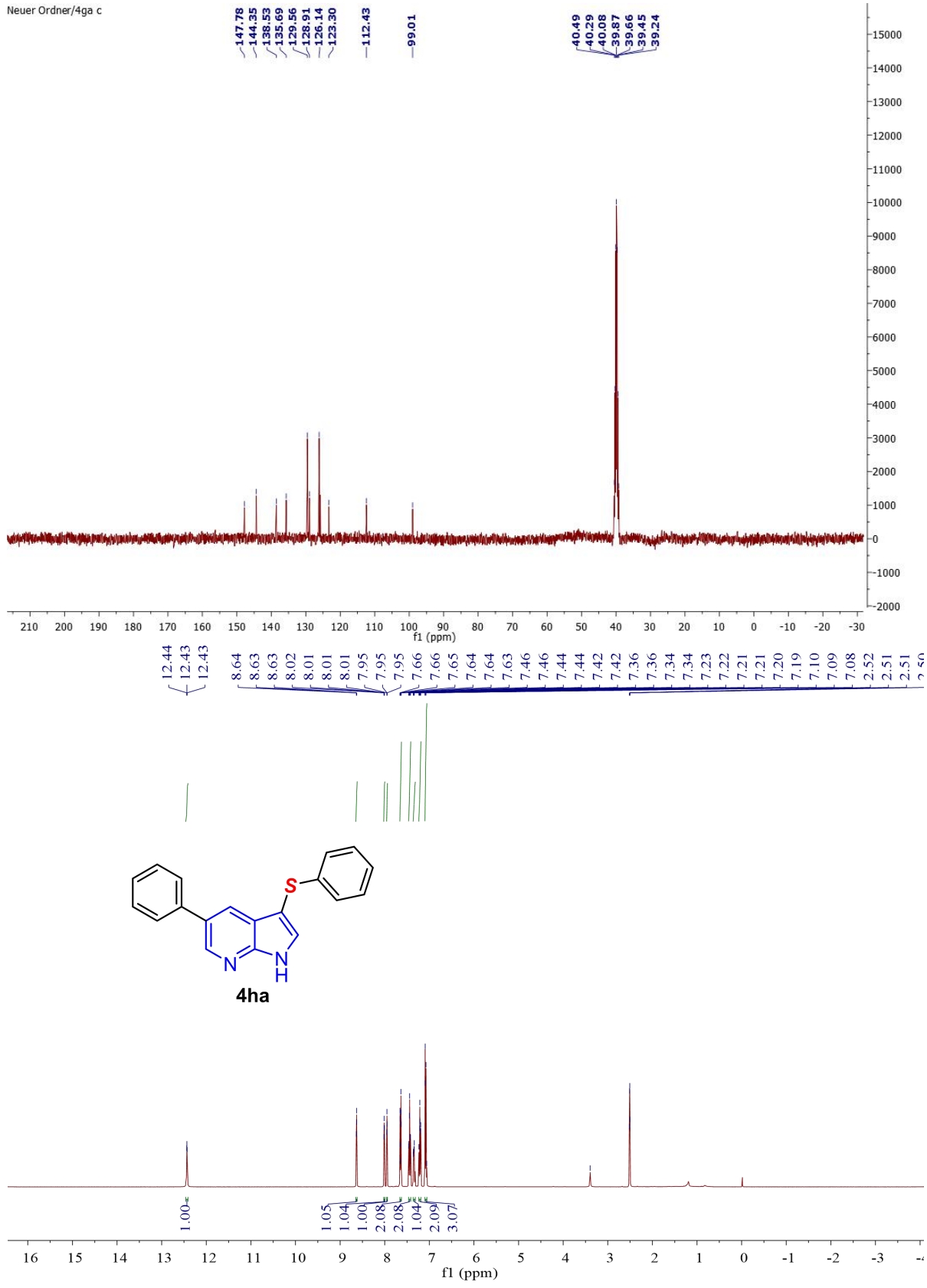
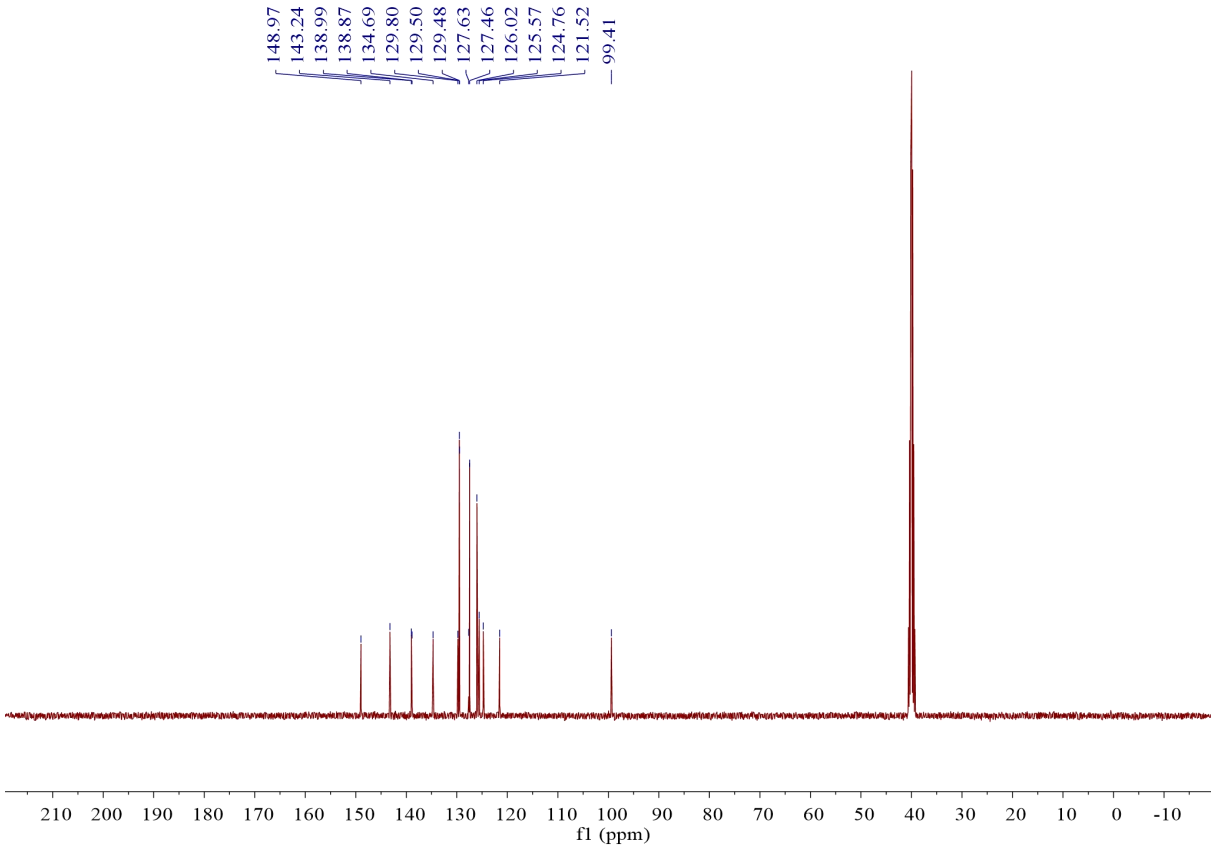
149.58
144.38
135.73
130.69
128.53
124.23
121.30
119.35
115.09
101.64
55.54
40.34
40.14
39.92
39.72
39.51
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Desktop/1
13.15
8.58
8.57
8.27
7.70
7.69
7.25
7.23
7.21
7.14
7.12
7.10
7.04
7.02
3.35
2.53
1.00
0.97
0.99
2.01
0.98
1.97
f1 (ppm)
NO2
S
N
H
4fa


no27-22/3
152.26
148.40
144.57
139.25
139.12
129.37
126.19
125.67
111.04
110.59
98.39
40.64
40.43
40.22
40.02
39.81
39.60
39.39
f1 (ppm)


Neuer Ordner/4ga
12.54
8.37
8.00
7.92
7.25
7.23
7.21
7.13
7.11
7.07
7.06
3.33
2.50
1.00
1.05
1.01
2.12
3.13
0.94
f1 (ppm)
Br
S
N
H
4ga


Neuer Ordner/4ga c
147.78
144.35
138.53
135.69
129.56
128.91
126.14
123.30
112.43
99.01
40.49
40.29
40.08
39.87
39.66
39.45
39.24
f1 (ppm)
12.44
12.43
12.43
8.64
8.63
8.63
8.02
8.01
8.01
8.01
7.95
7.95
7.95
7.66
7.66
7.65
7.64
7.64
7.63
7.46
7.46
7.44
7.44
7.42
7.42
7.36
7.36
7.34
7.34
7.23
7.22
7.21
7.21
7.20
7.19
7.10
7.09
7.08
2.52
2.51
2.51
S
N
H
4ha
1.00
1.05
1.04
1.00
2.08
2.08
1.04
2.09
3.07
f1 (ppm)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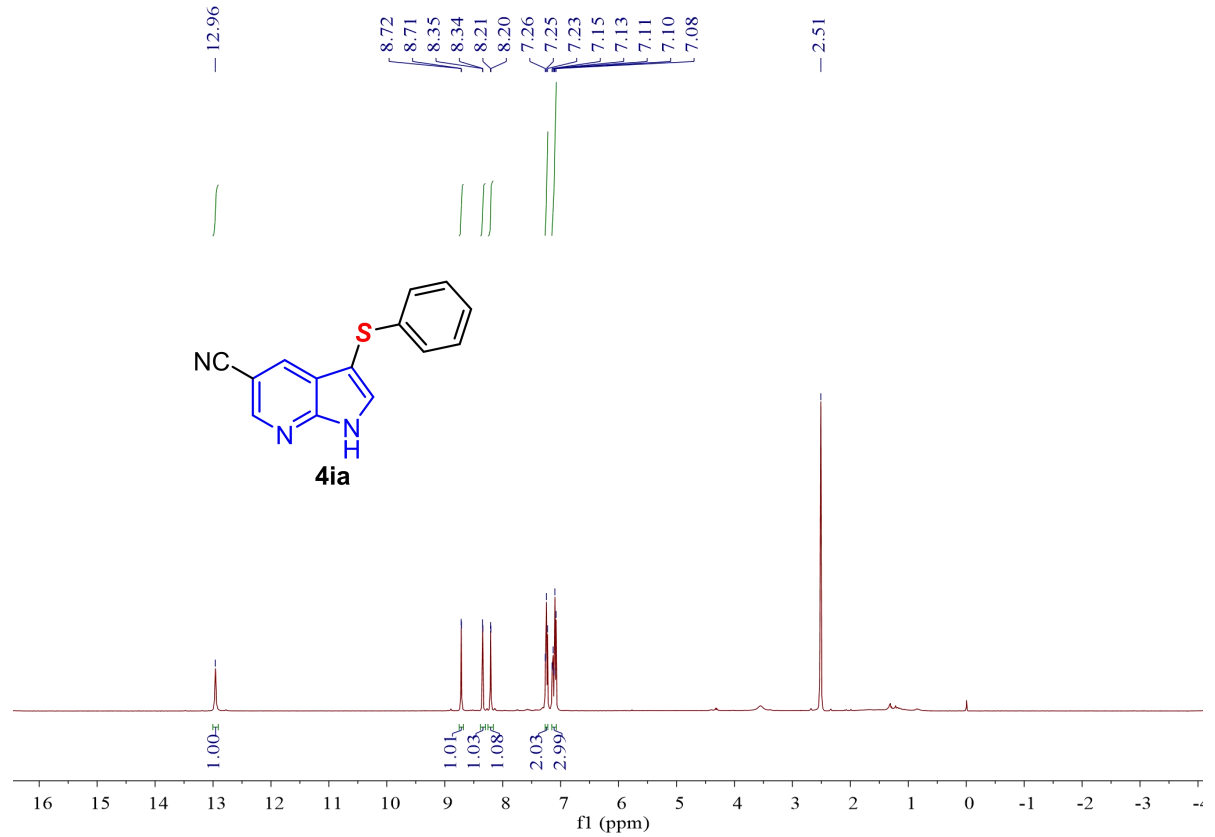
143.24
138.99
138.87
134.69
129.80
129.50
129.48
127.63
127.46
126.02
125.57
124.76
121.52
99.41
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.71
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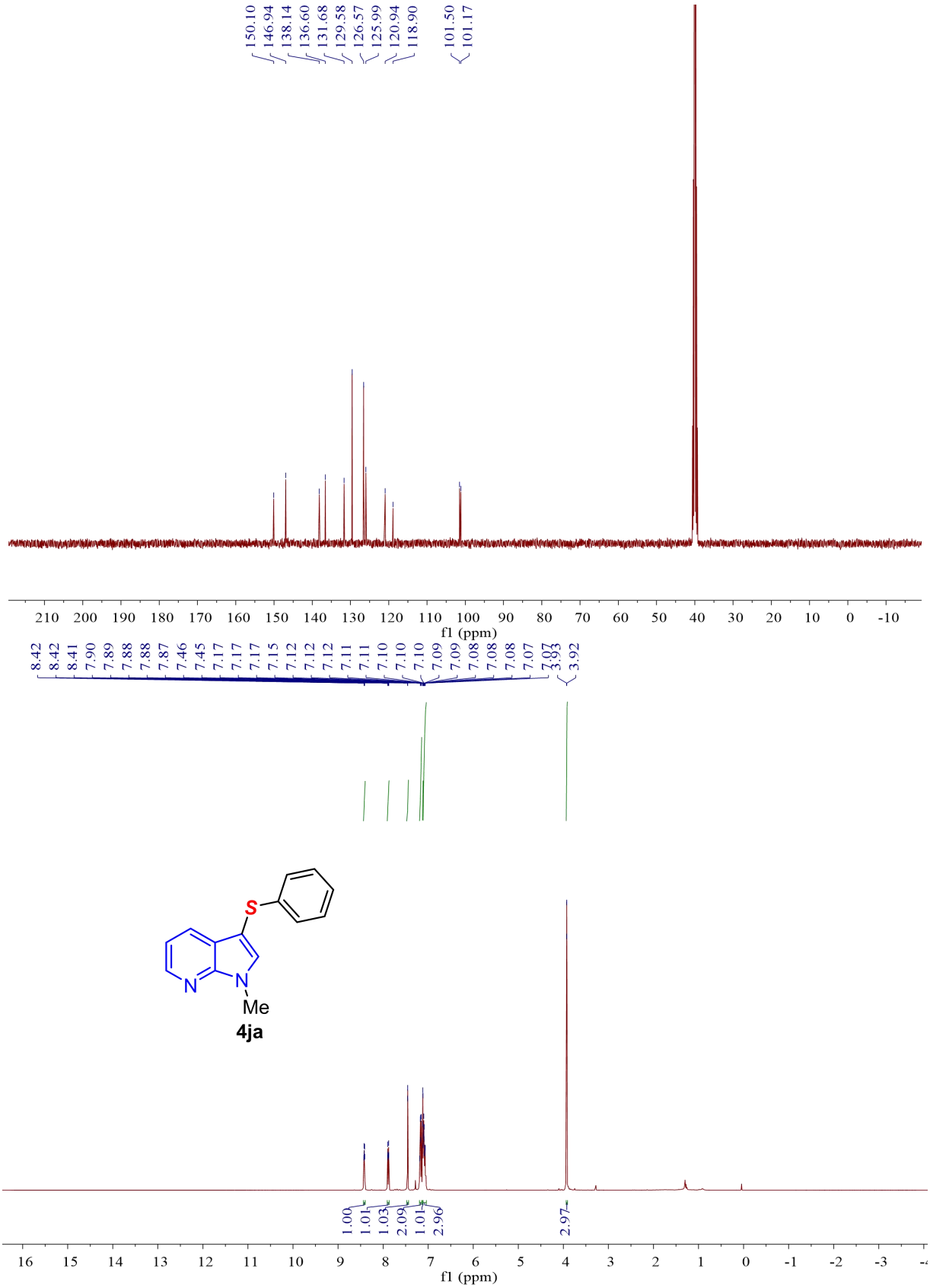
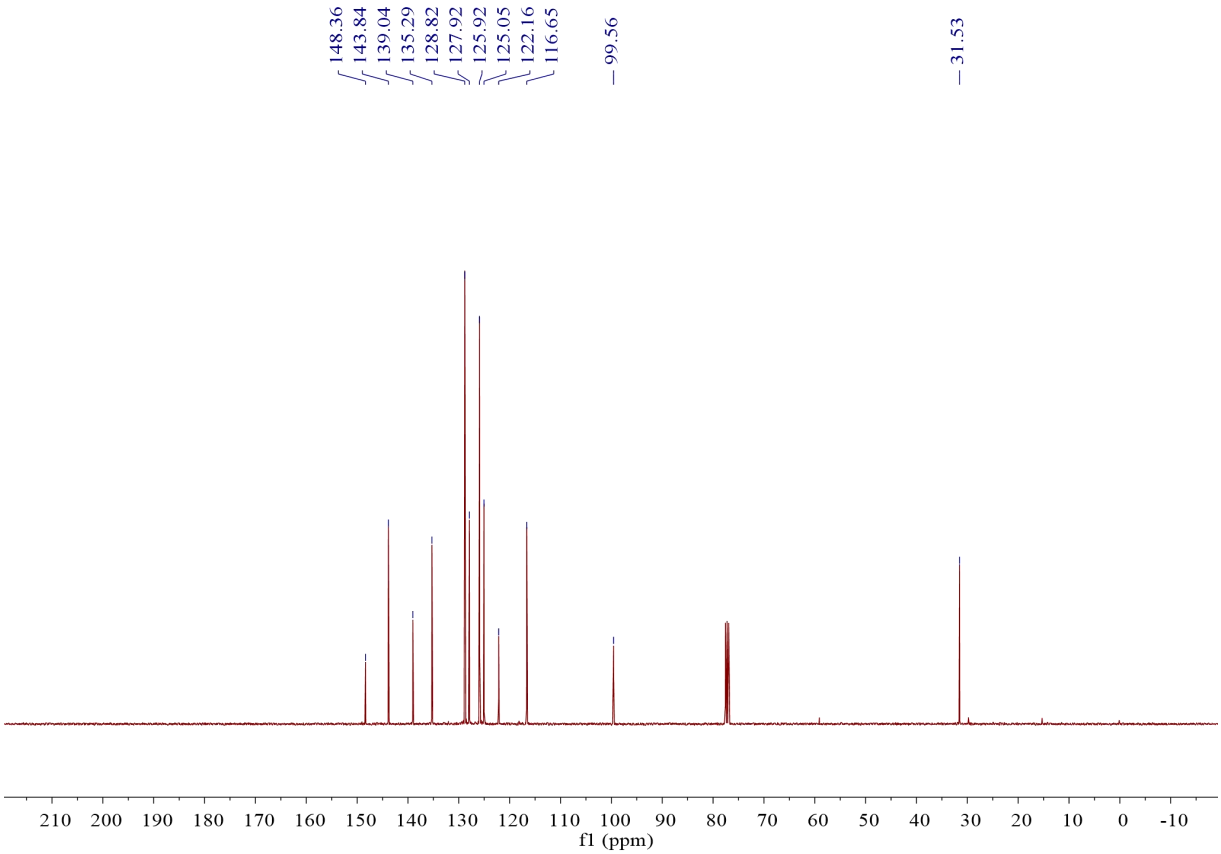
8.21
8.20
7.26
7.25
7.23
7.15
7.13
7.11
7.10
7.08
2.51
NC
S
N
N
H
4ia
1.00
1.01
1.03
1.08
2.03
2.99
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


150.10
146.94
138.14
136.60
131.68
129.58
126.57
125.99
120.94
118.90
101.50
101.17
f1 (ppm)
8.42
8.42
8.41
7.90
7.89
7.88
7.88
7.87
7.46
7.45
7.17
7.17
7.17
7.15
7.12
7.12
7.12
7.11
7.11
7.10
7.10
7.10
7.09
7.09
7.08
7.08
7.08
7.07
7.07
3.93
3.92
S
N
N
Me
4ja
1.00
1.01
1.03
2.09
1.01
2.96
2.97
f1 (ppm)


148.36
143.84
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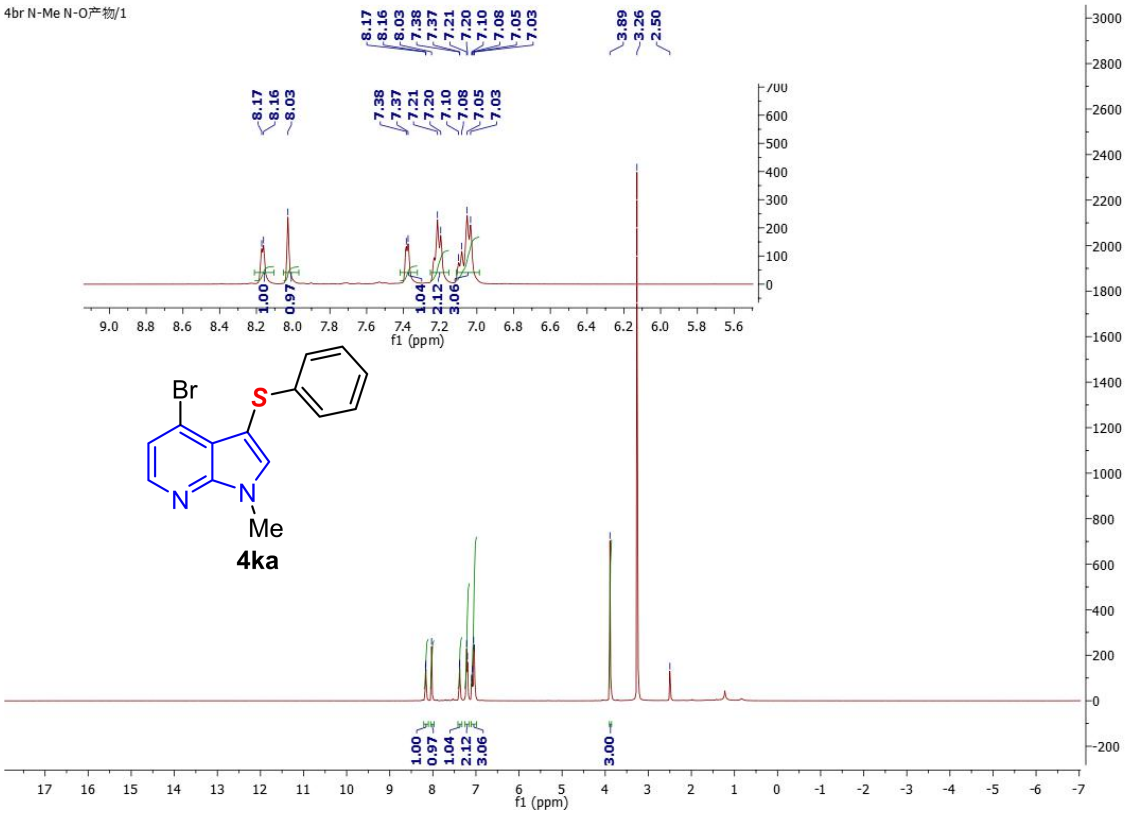
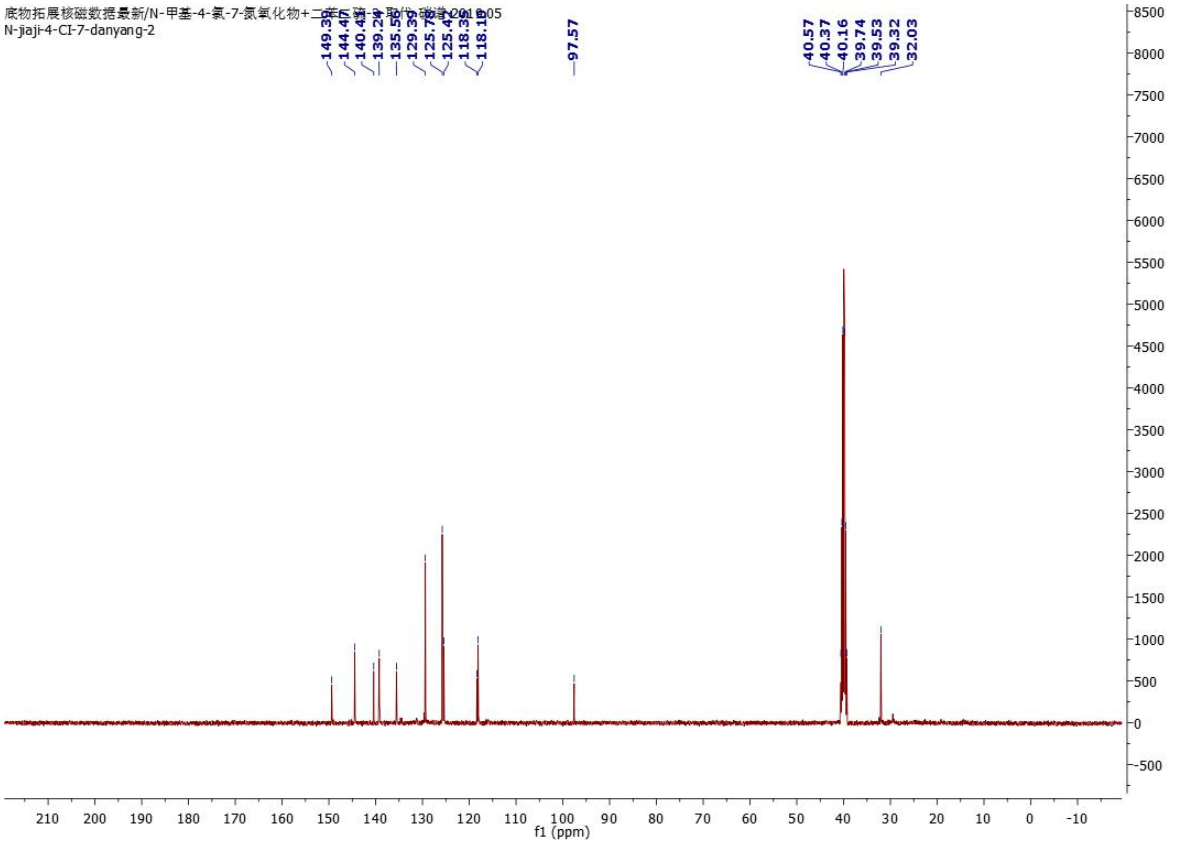
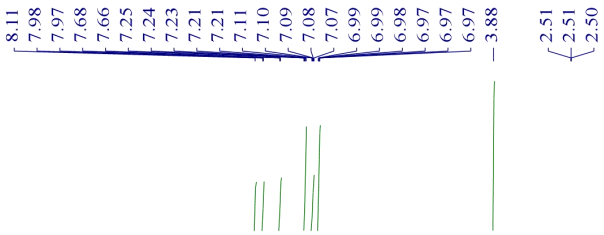
128.82
127.92
125.92
125.05
122.16
116.65
99.56
31.53
f1 (ppm)


4br N-Me N-O产物/1
8.17
8.16
8.03
7.38
7.37
7.21
7.20
7.10
7.08
7.05
7.03
3.89
3.26
2.50
1.00
0.97
1.04
2.12
3.06
3.00
f1 (ppm)
Br
S
N
N
Me
4ka


N-jiaji-4-Cl-7-danyang-2
149.38
144.47
140.48
139.24
135.56
129.39
125.76
125.44
118.36
118.18
97.57
40.57
40.37
40.16
39.74
39.53
39.32
32.03
f1 (ppm)


8.11
7.98
7.97
7.68
7.66
7.25
7.24
7.23
7.21
7.21
7.11
7.10
7.09
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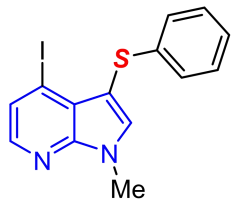
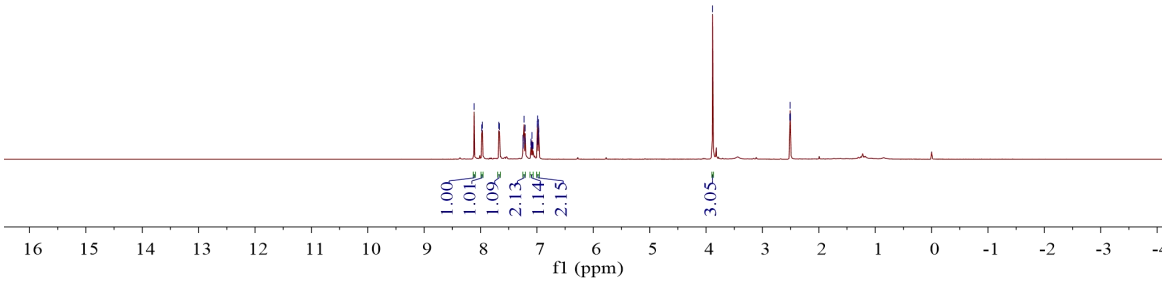
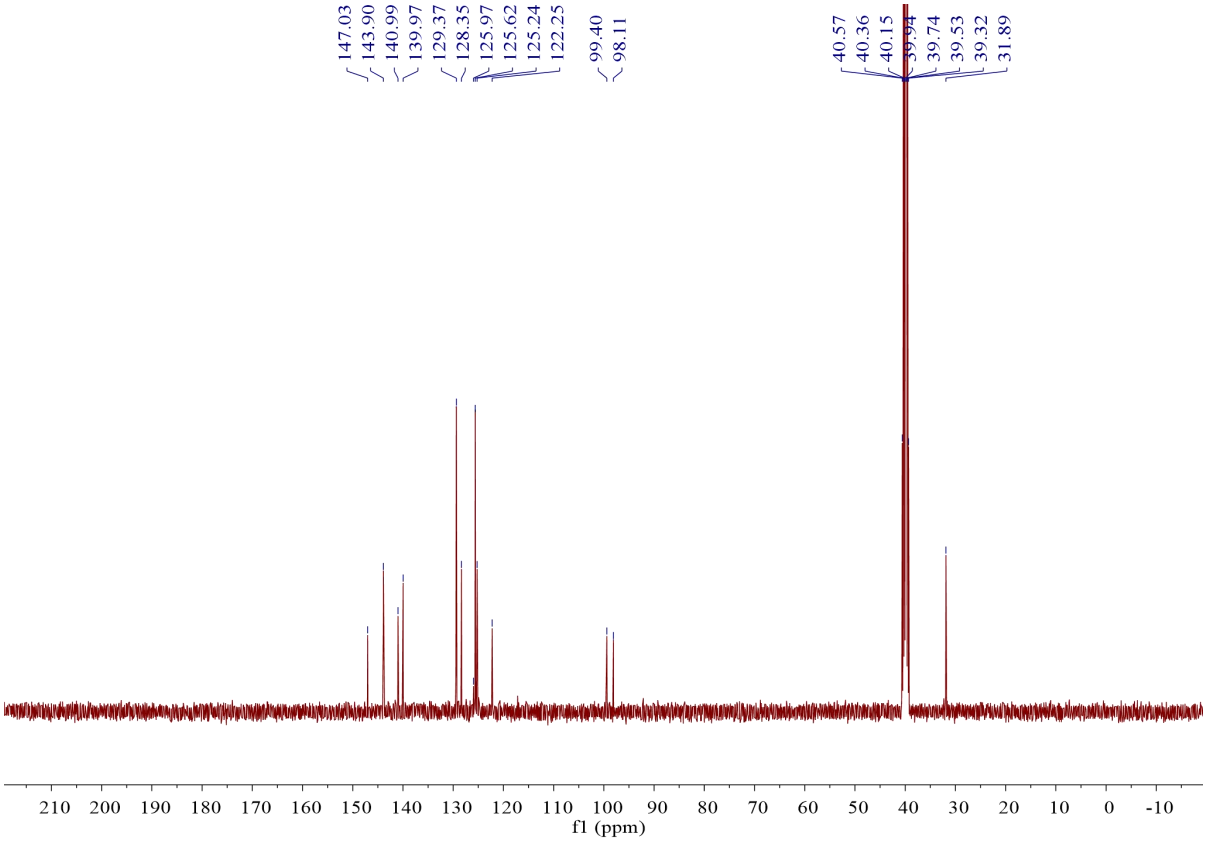
6.97
6.97
3.88
2.51
2.51
2.50


S
N
N
Me

4la


1.00
1.01
1.09
2.13
1.14
2.15
3.05
f1 (ppm)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143.90
140.99
139.97
129.37
128.35
125.97
125.62
125.24
122.25
99.40
98.11
40.57
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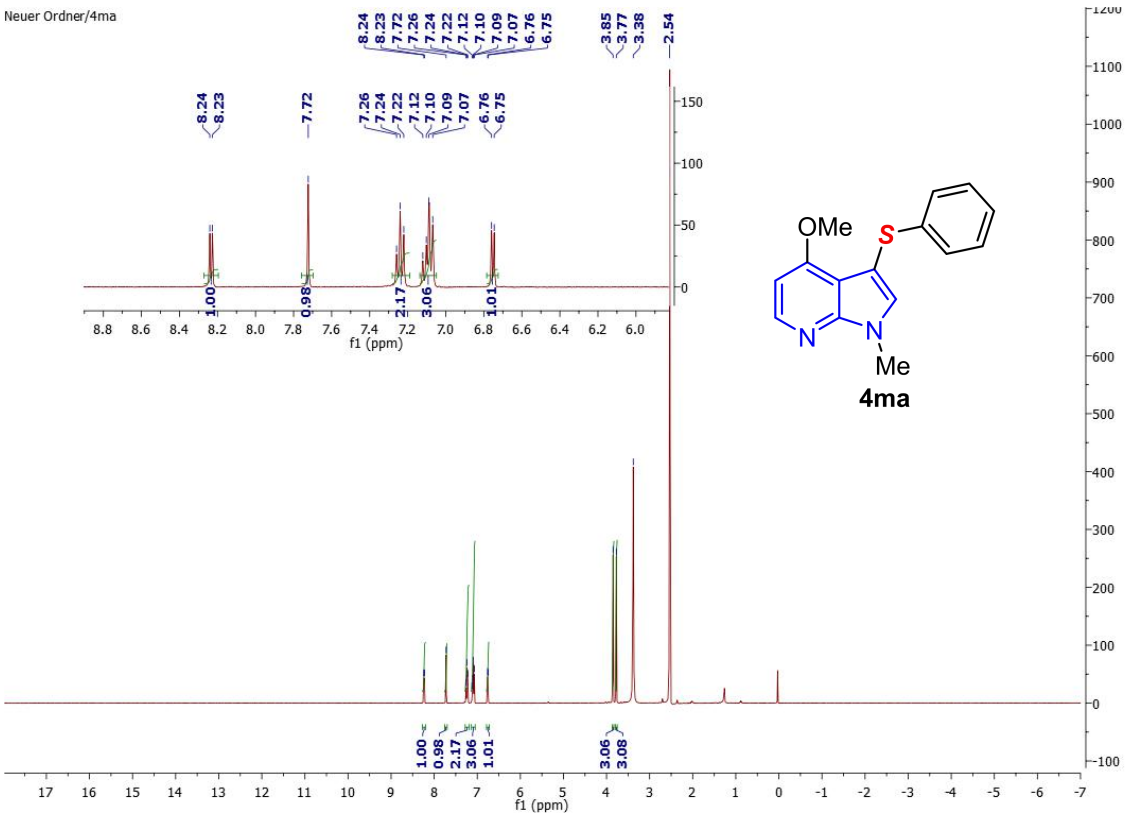
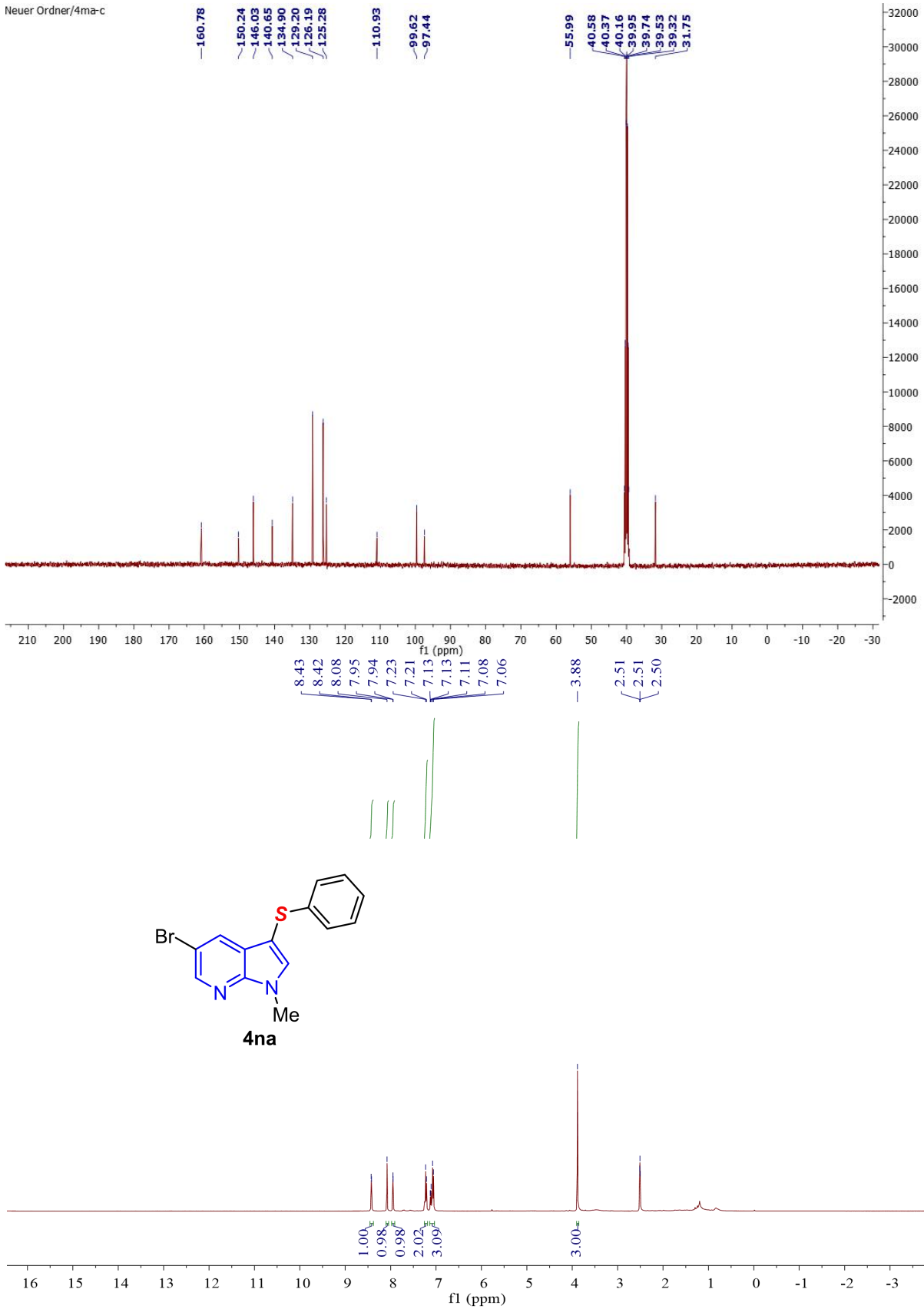
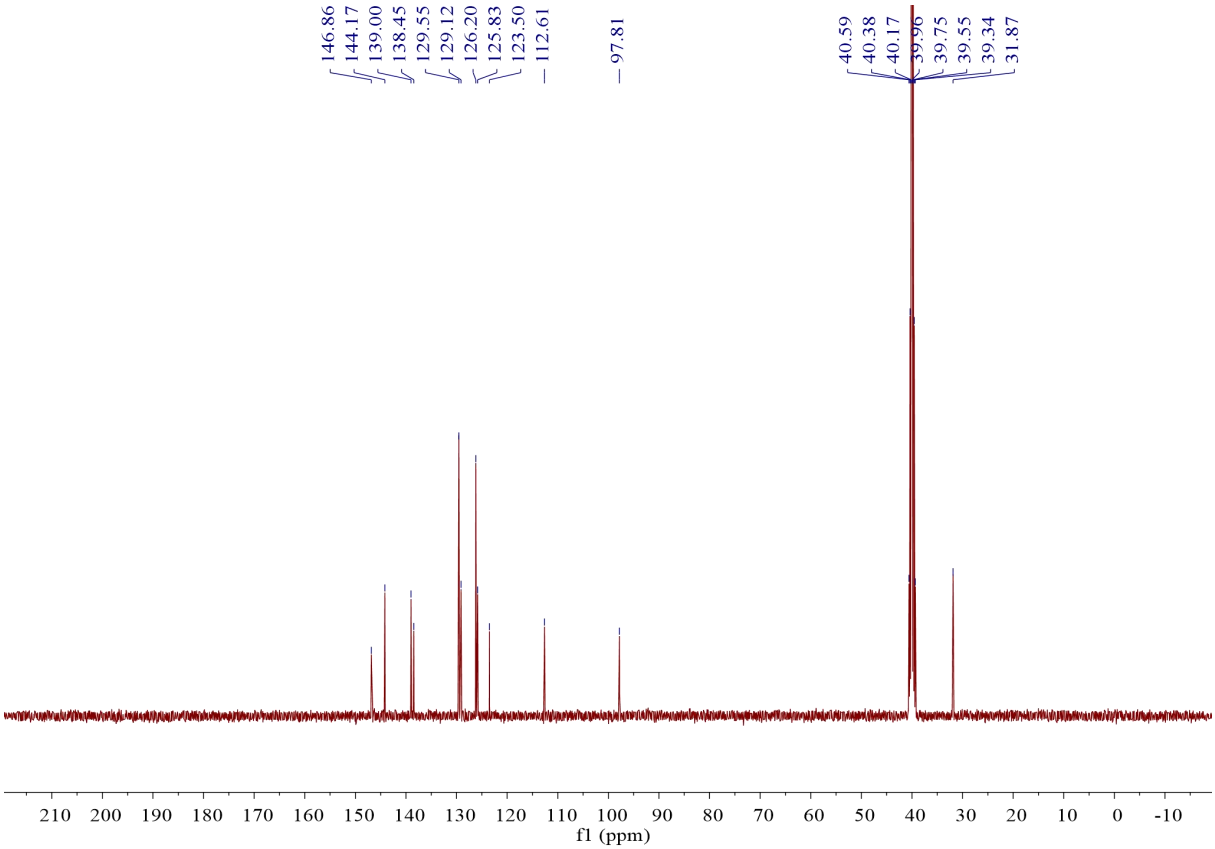
39.74
39.53
39.32
31.89
f1 (ppm)


Neuer Ordner/4ma
8.24
8.23
7.72
7.26
7.24
7.22
7.12
7.10
7.09
7.07
6.76
6.75
3.85
3.77
3.38
2.54
1.00
0.98
2.17
3.06
1.01
3.06
3.08
f1 (ppm)
OMe
S
N
N
Me
4ma


Neuer Ordner/4ma-c
160.78
150.24
146.03
140.65
134.90
129.20
126.19
125.28
110.93
99.62
97.44
55.99
40.58
40.37
40.16
39.95
39.74
39.53
39.32
31.75
f1 (ppm)
8.43
8.42
8.08
7.95
7.94
7.23
7.21
7.13
7.13
7.11
7.08
7.06
3.88
2.51
2.51
2.50
Br
S
N
N
Me
4na
1.00
0.98
0.98
2.02
3.09
3.00
f1 (ppm)


146.86
144.17
139.00
138.45
129.55
129.12
126.20
125.83
123.50
112.61
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40.59
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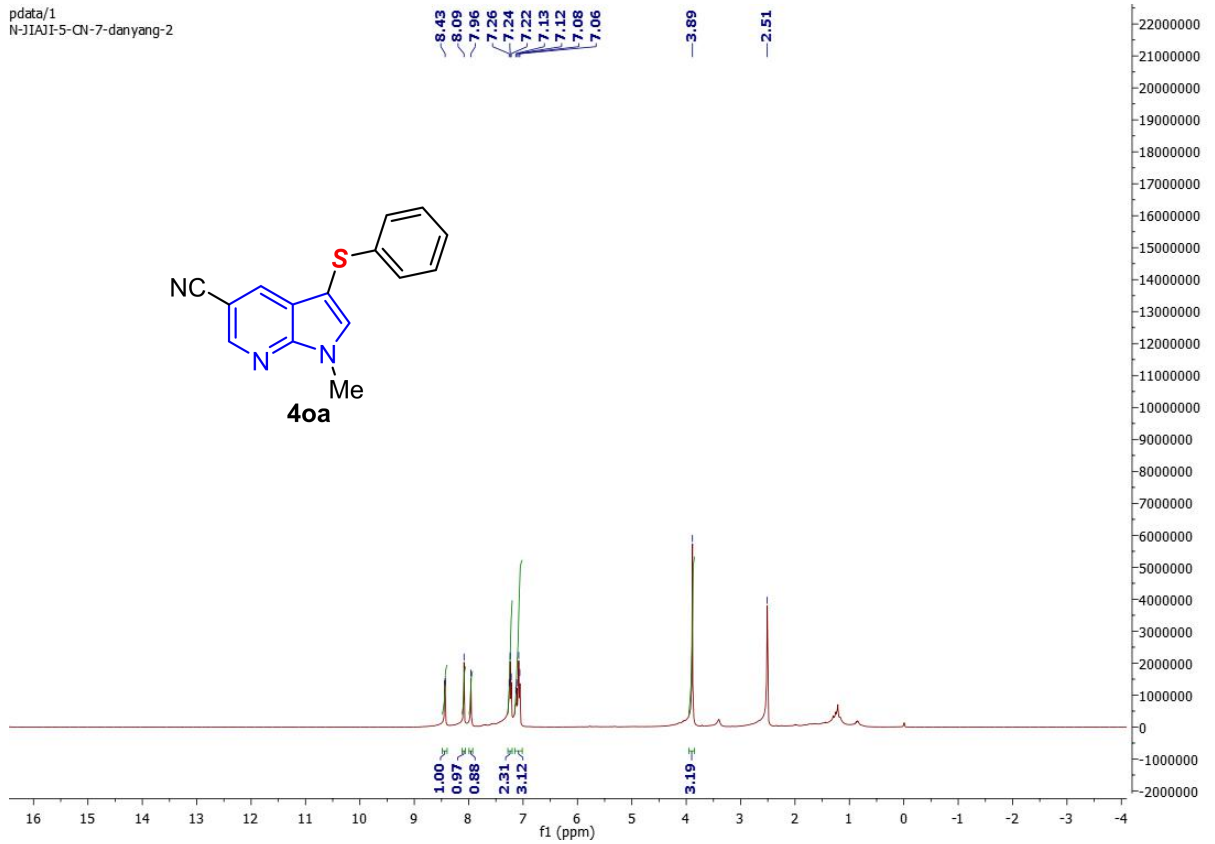
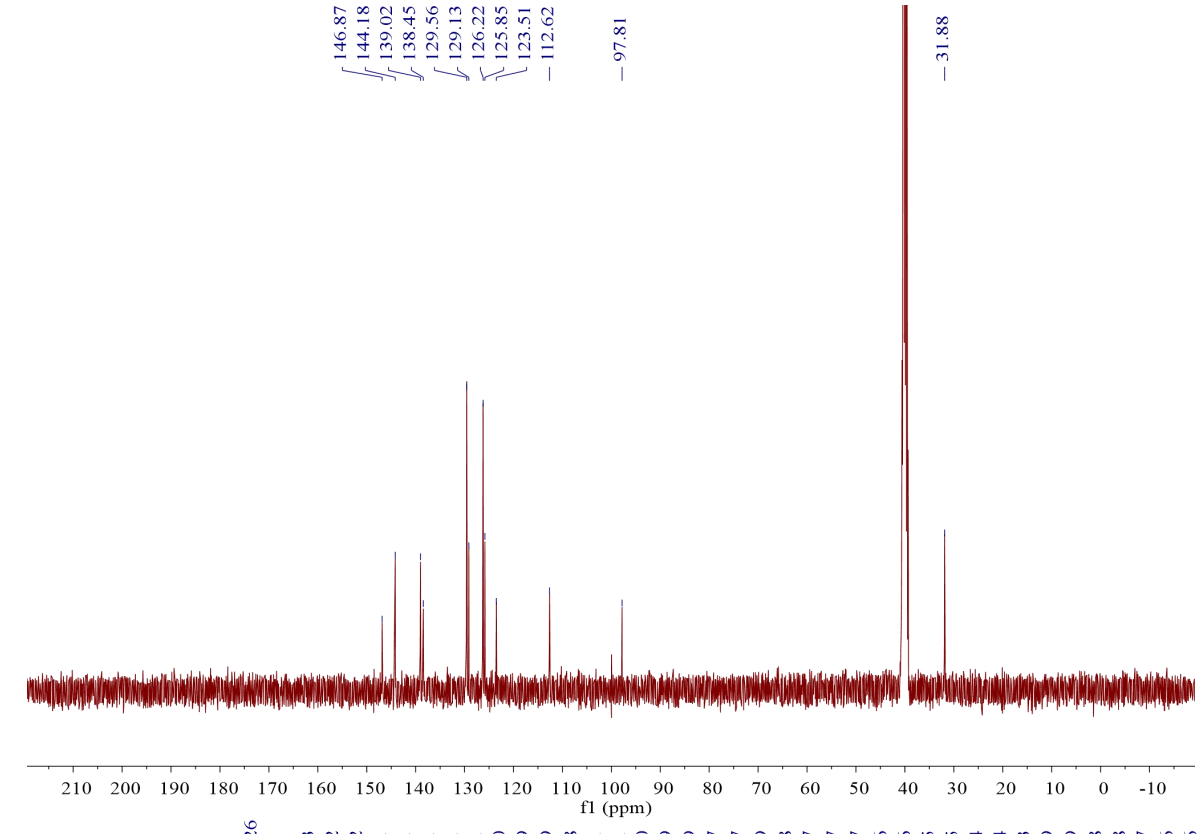
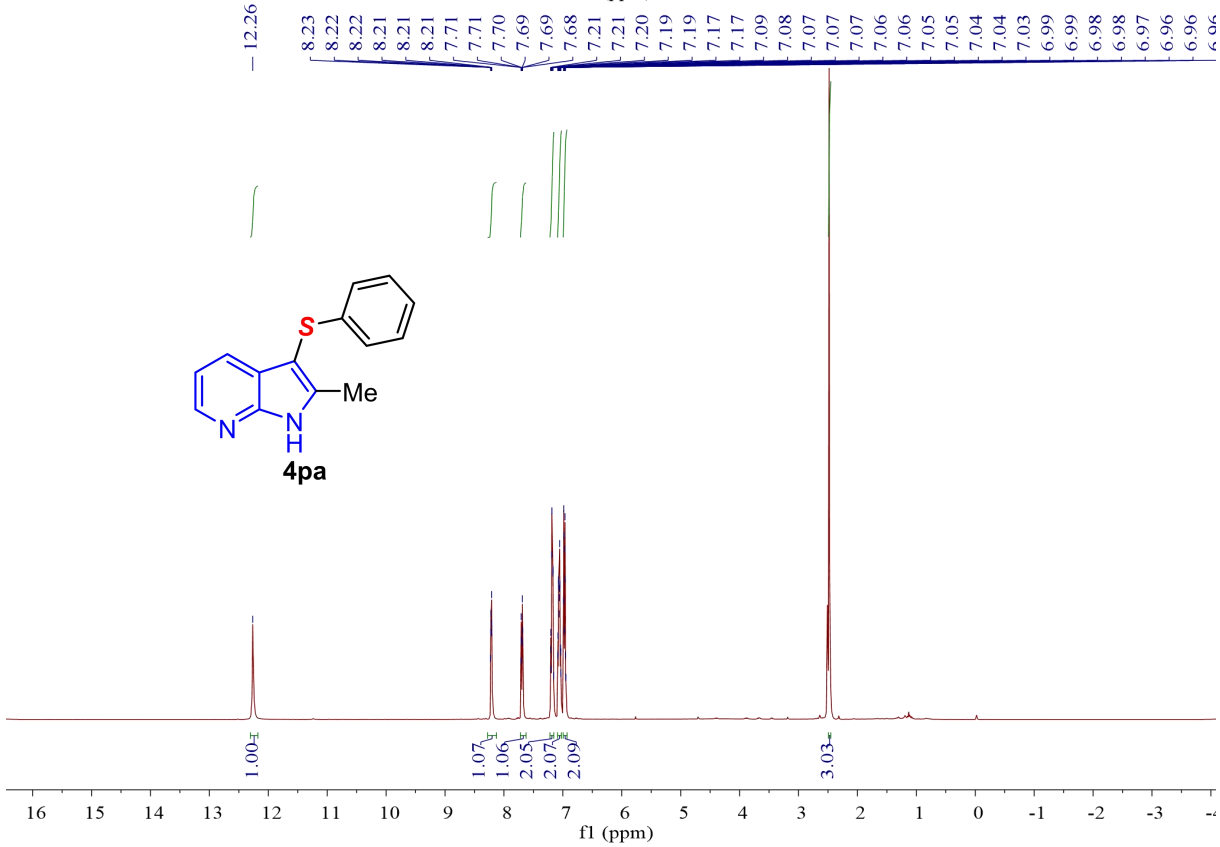
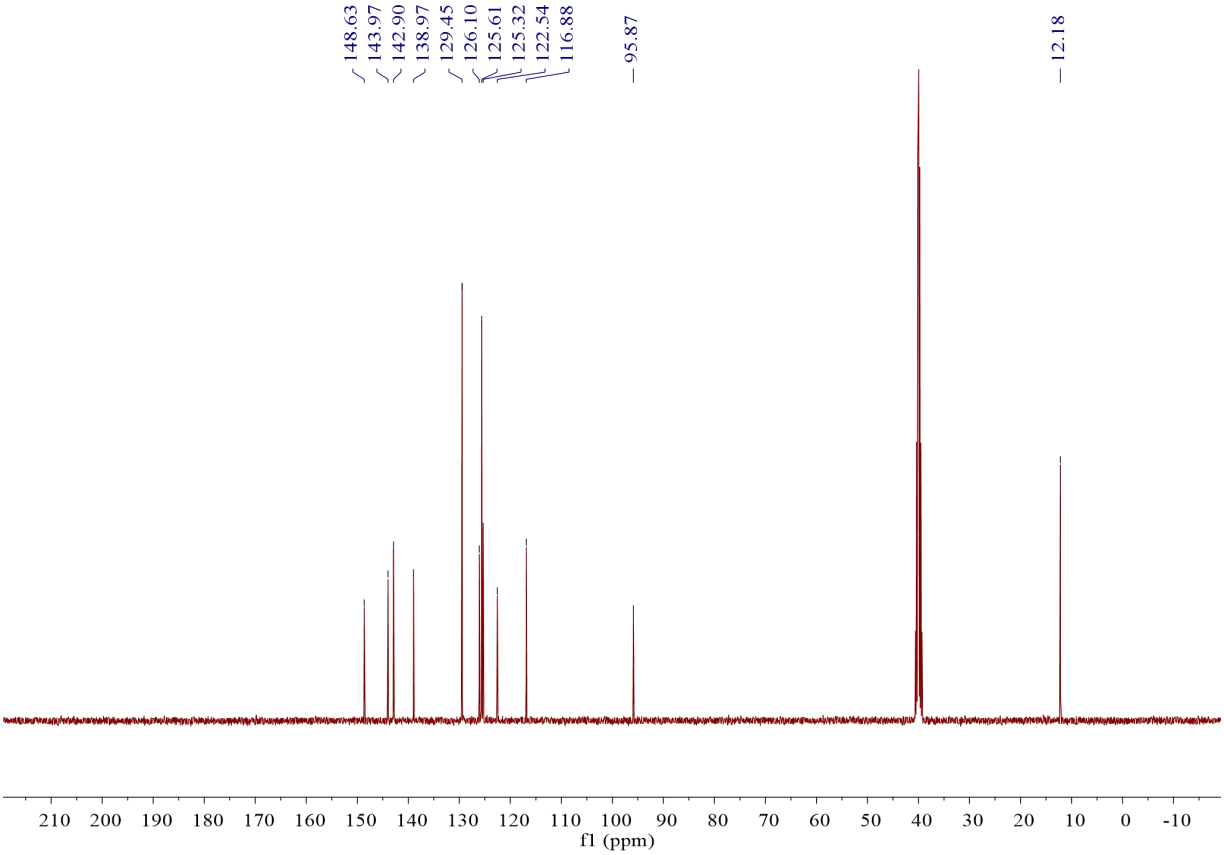
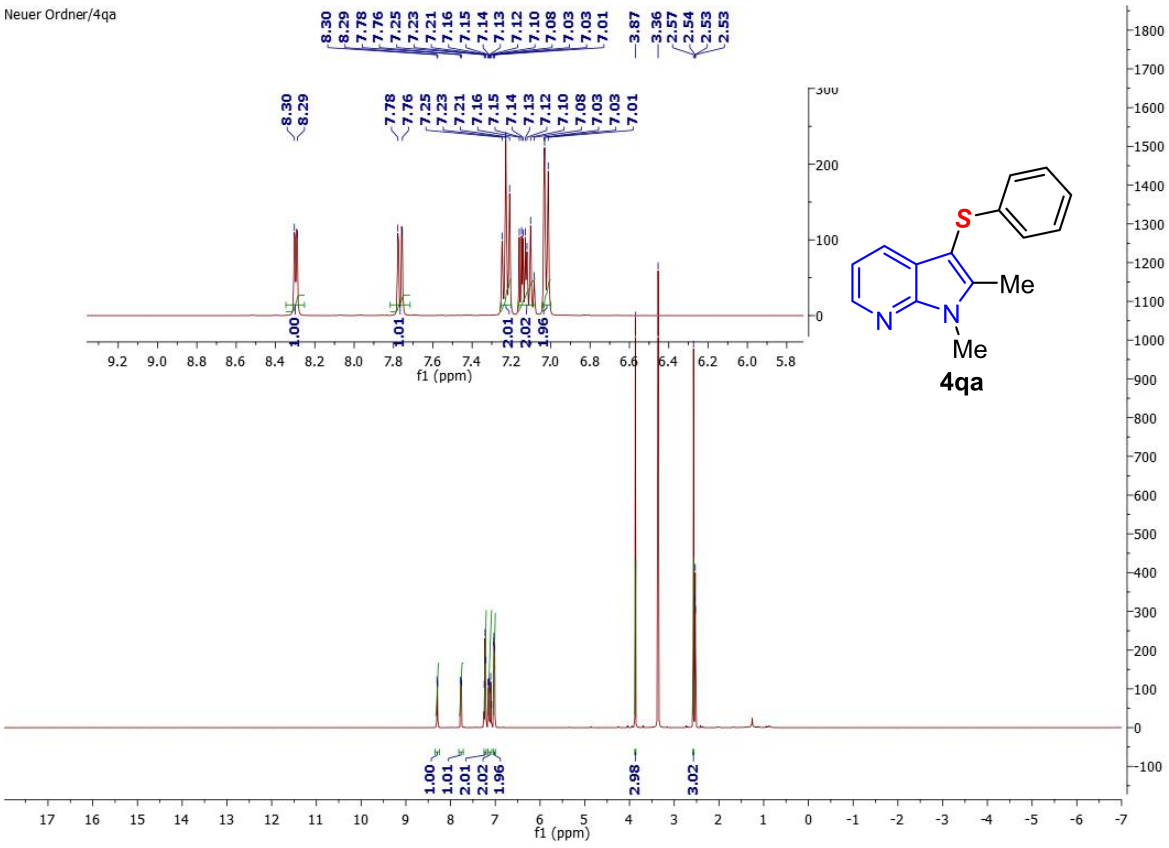
39.75
39.55
39.34
31.87
f1 (ppm)

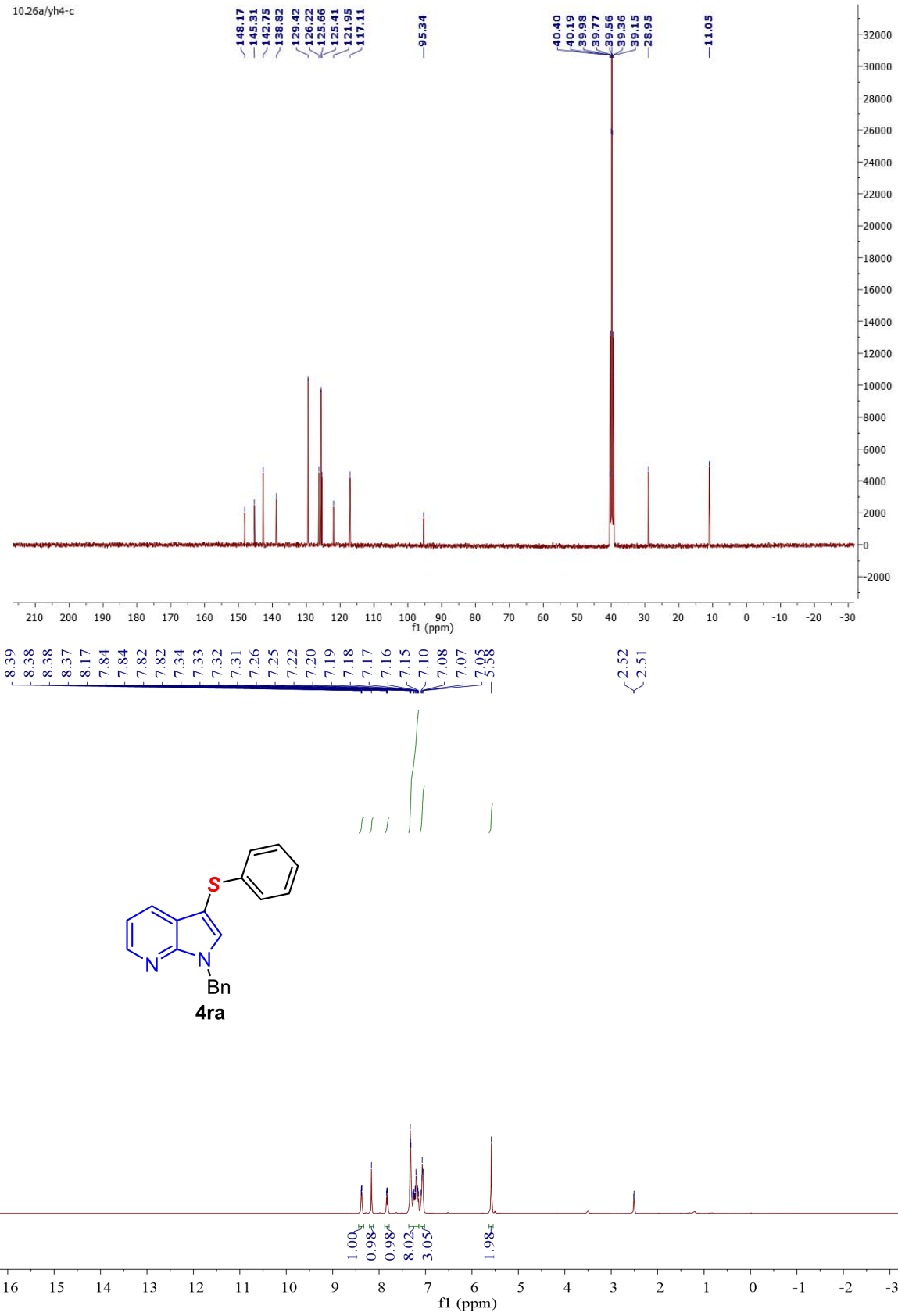

pdata/1
N-JIAJI-5-CN-7-danyang-2
8.43
8.09
7.96
7.26
7.24
7.22
7.13
7.12
7.08
7.06
3.89
2.51
NC
S
N
N
Me
4oa
1.00
0.97
0.88
2.31
3.12
3.19
f1 (ppm)

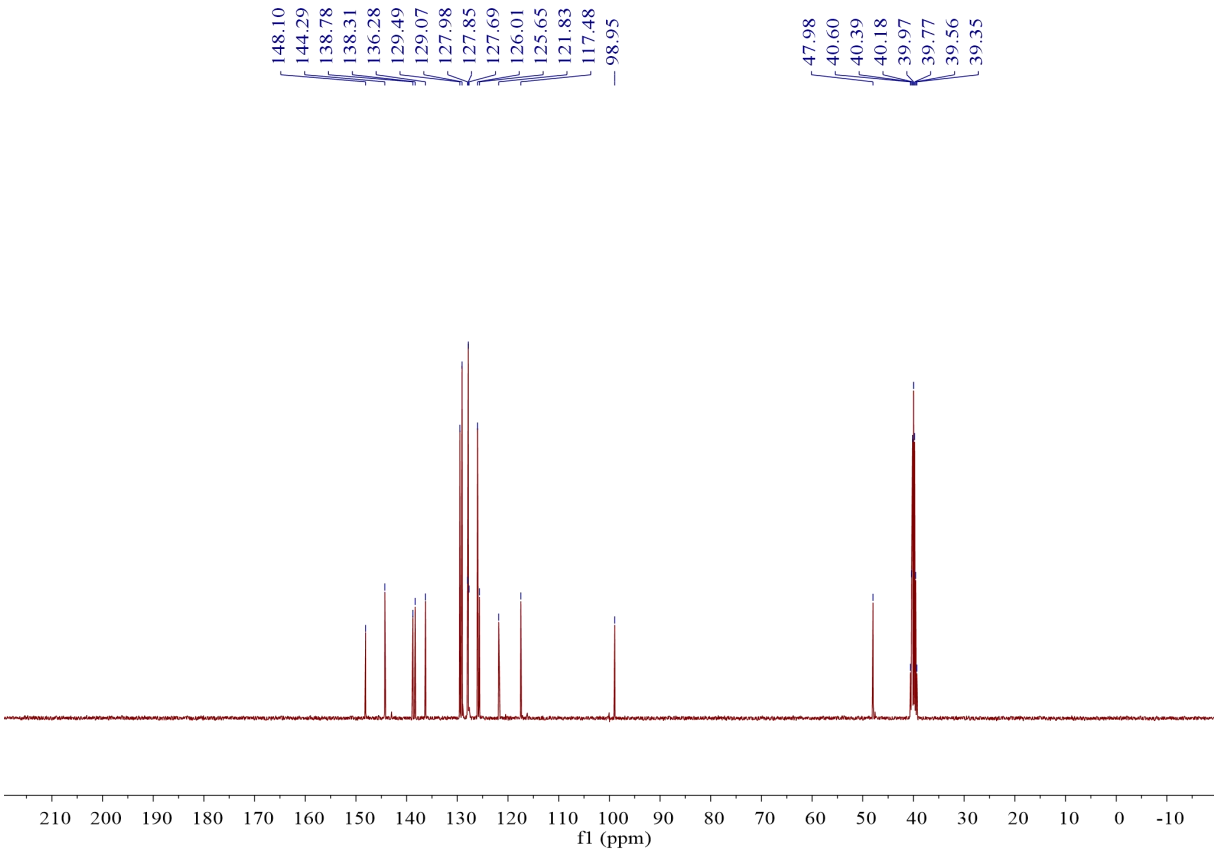

146.87
144.18
139.02
138.45
129.56
129.13
126.22
125.85
123.51
112.62
97.81
31.88
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


12.26
8.23
8.22
8.22
8.21
8.21
8.21
7.71
7.71
7.70
7.69
7.69
7.68
7.21
7.21
7.20
7.19
7.19
7.17
7.17
7.09
7.08
7.07
7.07
7.07
7.06
7.06
7.05
7.05
7.04
7.04
7.03
6.99
6.99
6.98
6.98
6.97
6.96
6.96
S
Me
N
H
4pa
1.00
1.07
1.06
2.05
2.07
2.09
3.03
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)


148.63
143.97
142.90
138.97
129.45
126.10
125.61
125.32
122.54
116.88
95.87
12.18
f1 (ppm)


Neuer Ordner/4qa
8.30
8.29
7.78
7.76
7.25
7.23
7.21
7.16
7.15
7.14
7.13
7.12
7.10
7.08
7.03
7.03
7.01
3.87
3.36
2.57
2.54
2.53
2.53
1.00
1.01
2.01
2.02
1.96
2.98
3.02
f1 (ppm)
S
Me
N
Me
4qa


10.26a/yh4-c
148.17
145.31
142.75
138.82
129.42
126.22
125.66
125.41
121.95
117.11
95.34
40.40
40.19
39.98
39.77
39.56
39.36
39.15
28.95
11.05
f1 (ppm)
8.39
8.38
8.38
8.37
8.17
7.84
7.84
7.82
7.82
7.34
7.33
7.32
7.31
7.26
7.25
7.22
7.20
7.19
7.18
7.17
7.16
7.15
7.10
7.08
7.07
7.05
5.58
2.52
2.51
S
N
N
Bn
4ra
1.00
0.98
0.98
8.02
3.05
1.98
f1 (ppm)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138.78
138.31
136.28
129.49
129.07
127.98
127.85
127.69
126.01
125.65
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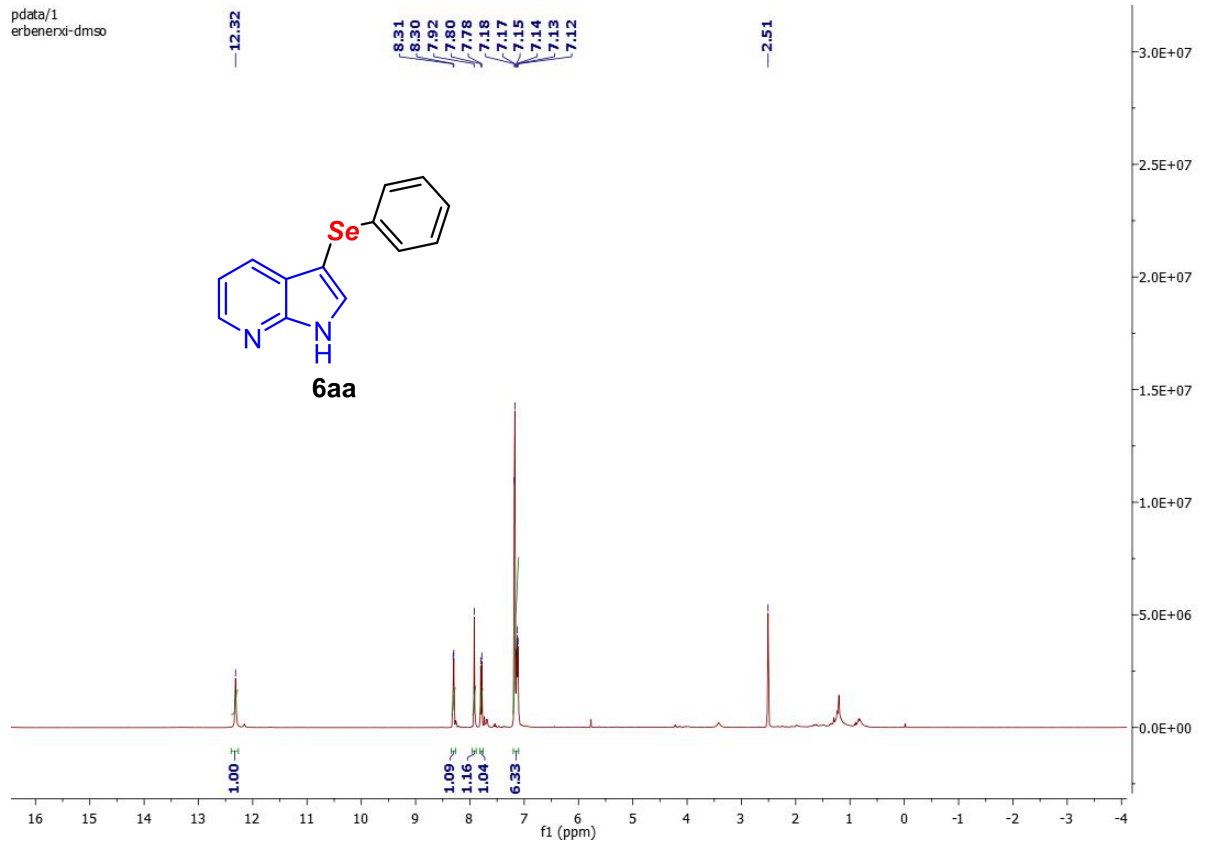
47.98
40.60
40.39
40.18
39.97
39.77
39.56
39.35
f1 (ppm)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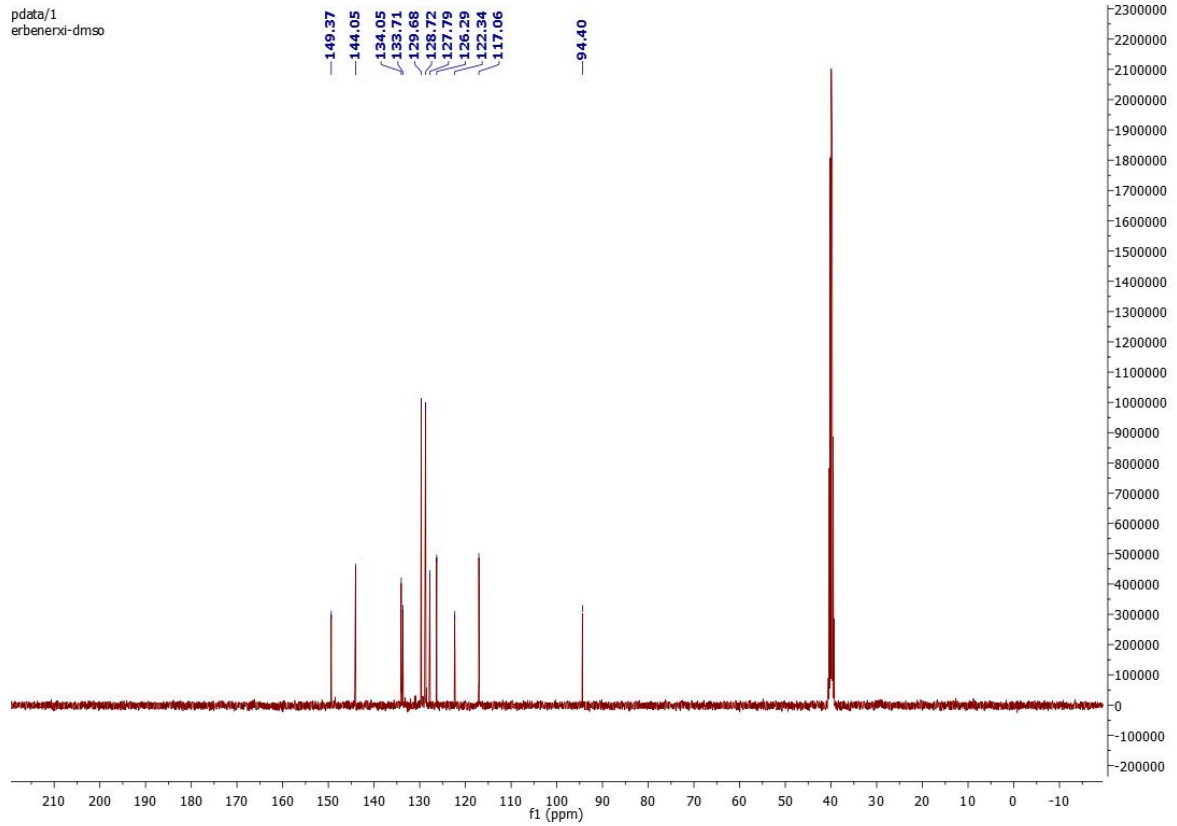
erbenerxi-dmso
12.32
8.31
8.30
7.92
7.80
7.78
7.18
7.17
7.15
7.14
7.13
7.12
2.51
Se
N
H
6aa
1.00
1.09
1.16
1.04
6.33
f1 (ppm)


pdata/1
erbenerxi-dmso
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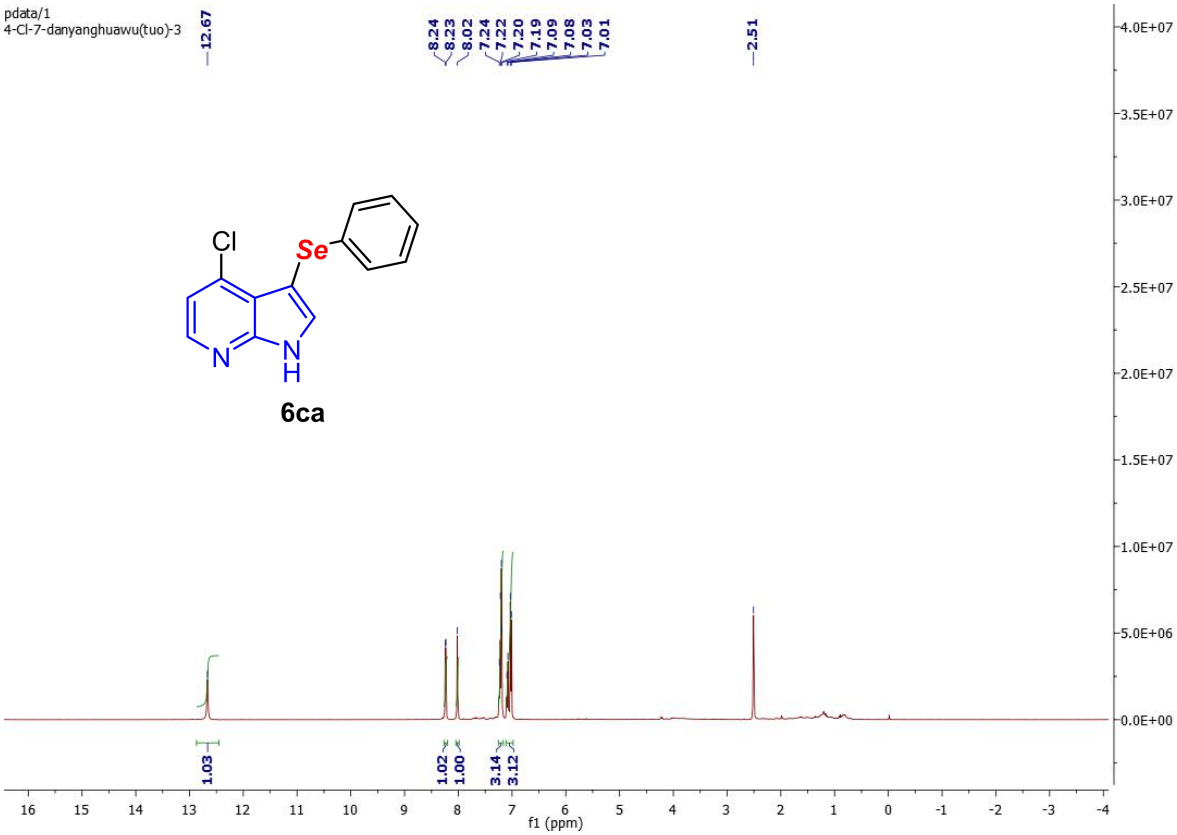
144.05
134.05
133.71
129.68
128.72
127.79
126.29
122.34
117.06
94.40
f1 (ppm)


pdata/1
4-Cl-7-danyanghuawu(tuo)-3
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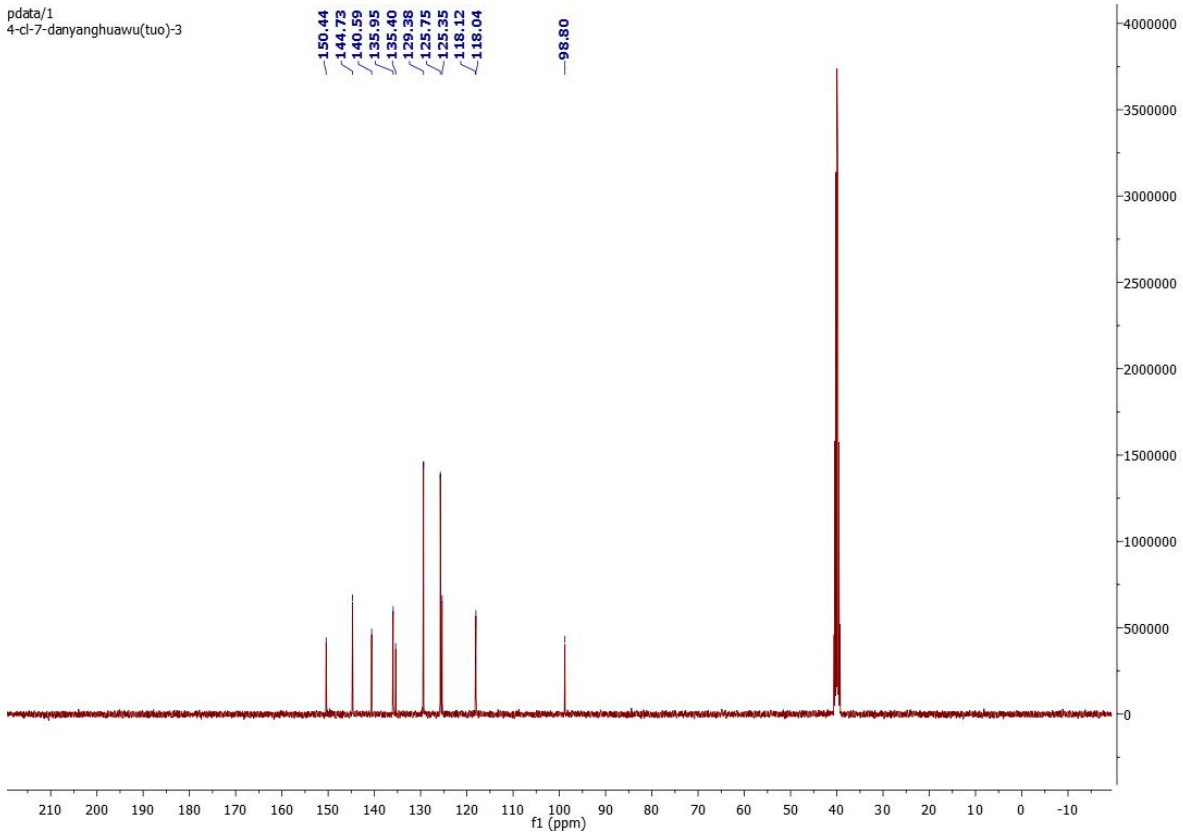
8.24
8.23
8.02
7.24
7.22
7.20
7.19
7.09
7.08
7.03
7.01
2.51
1.03
1.02
1.00
3.14
3.12
f1 (ppm)

Cl
Se
N
H

6ca


pdata/1
4-cl-7-danyanghuawu(tuo)-3
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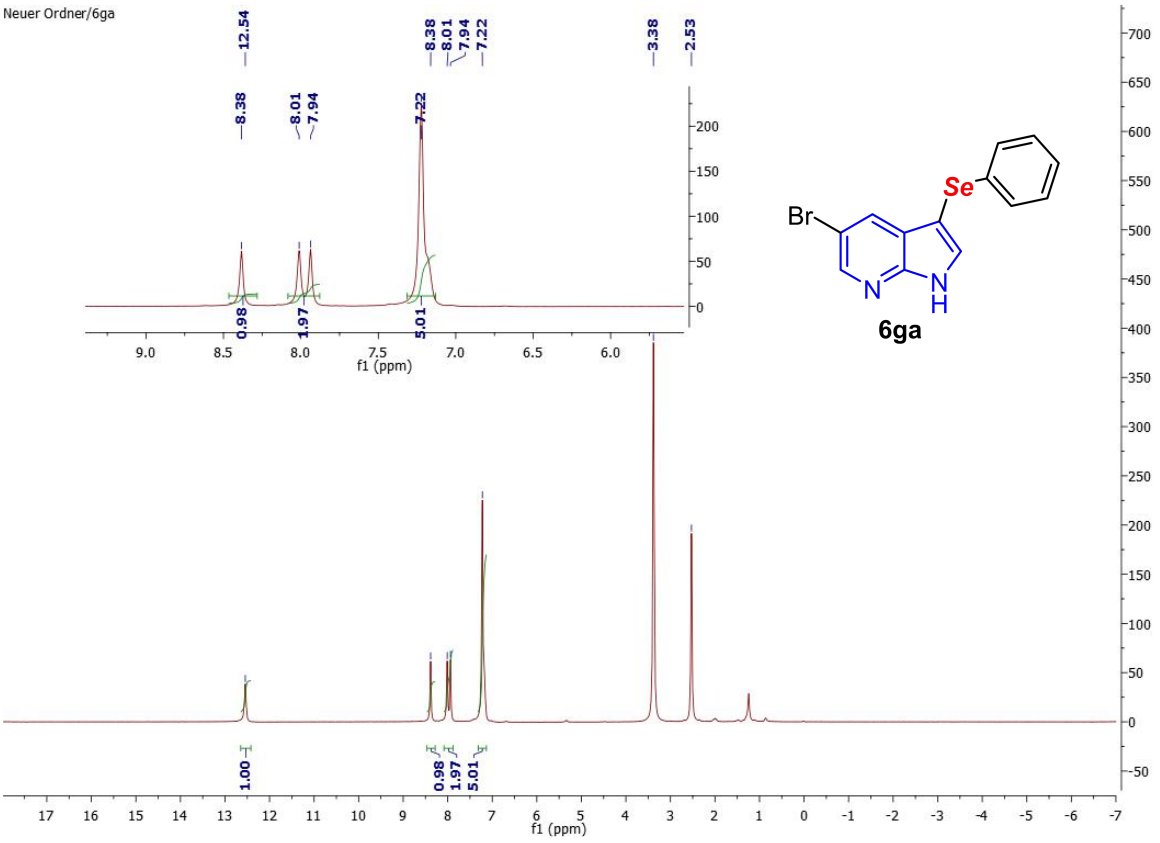
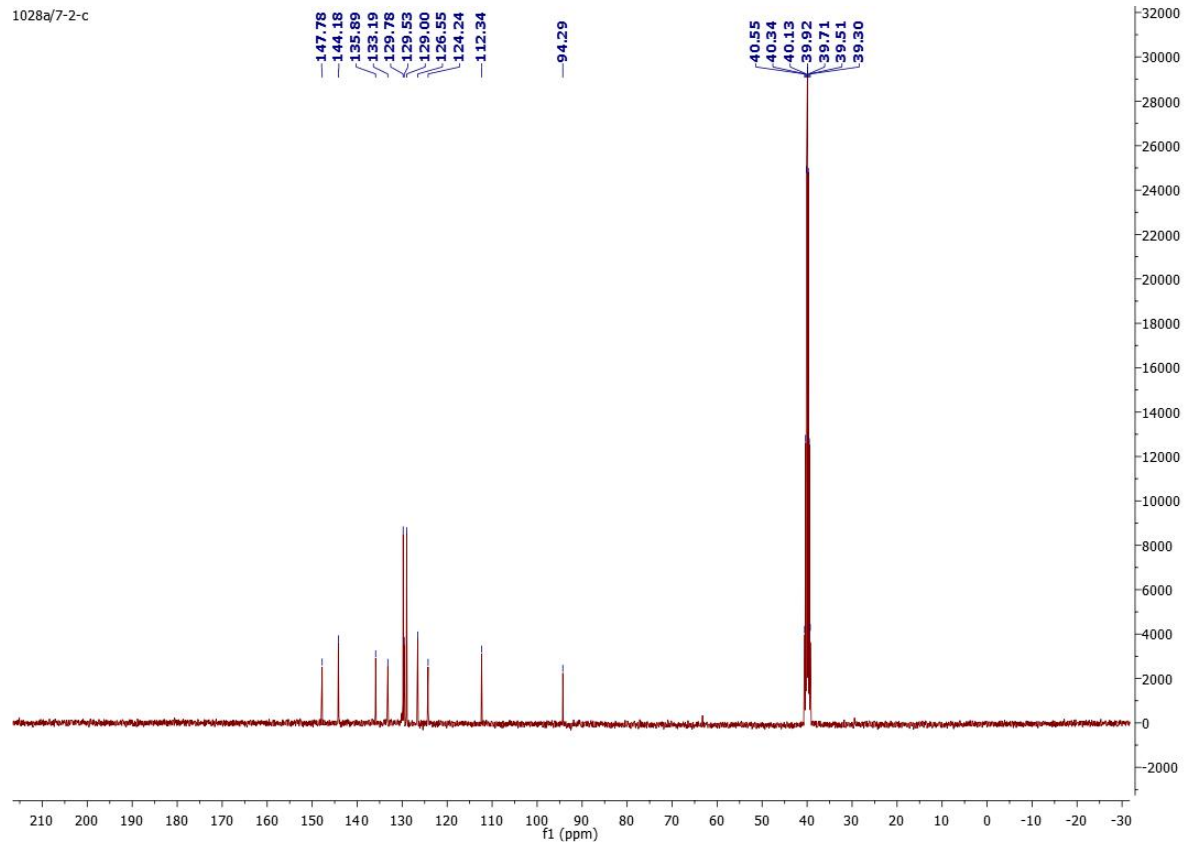
144.73
140.59
135.95
135.40
129.38
125.75
125.35
118.12
118.04
98.80
f1 (ppm)


Neuer Ordner/6ga
12.54
8.38
8.01
7.94
7.22
3.38
2.53
0.98
1.97
5.01
1.00
f1 (ppm)

Br
Se
N
N
H

6ga


1028a/7-2-c
147.78
144.18
135.89
133.19
129.78
129.53
129.00
126.55
124.24
112.34
94.29
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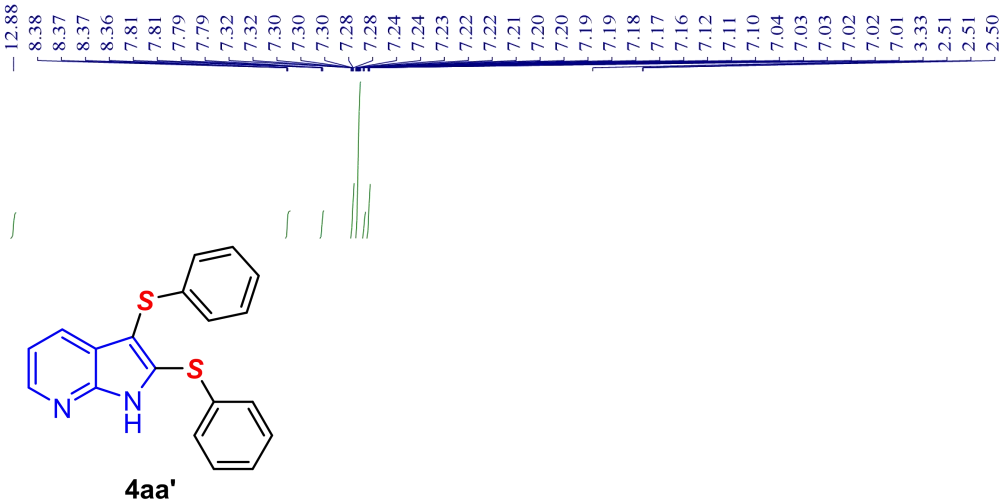
40.13
39.92
39.71
39.51
39.30
f1 (ppm)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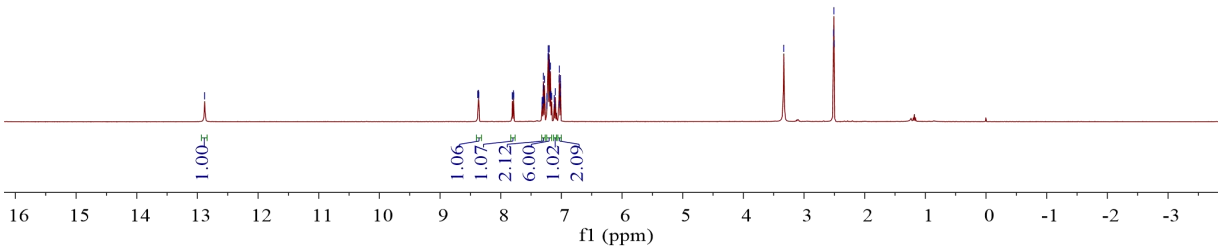
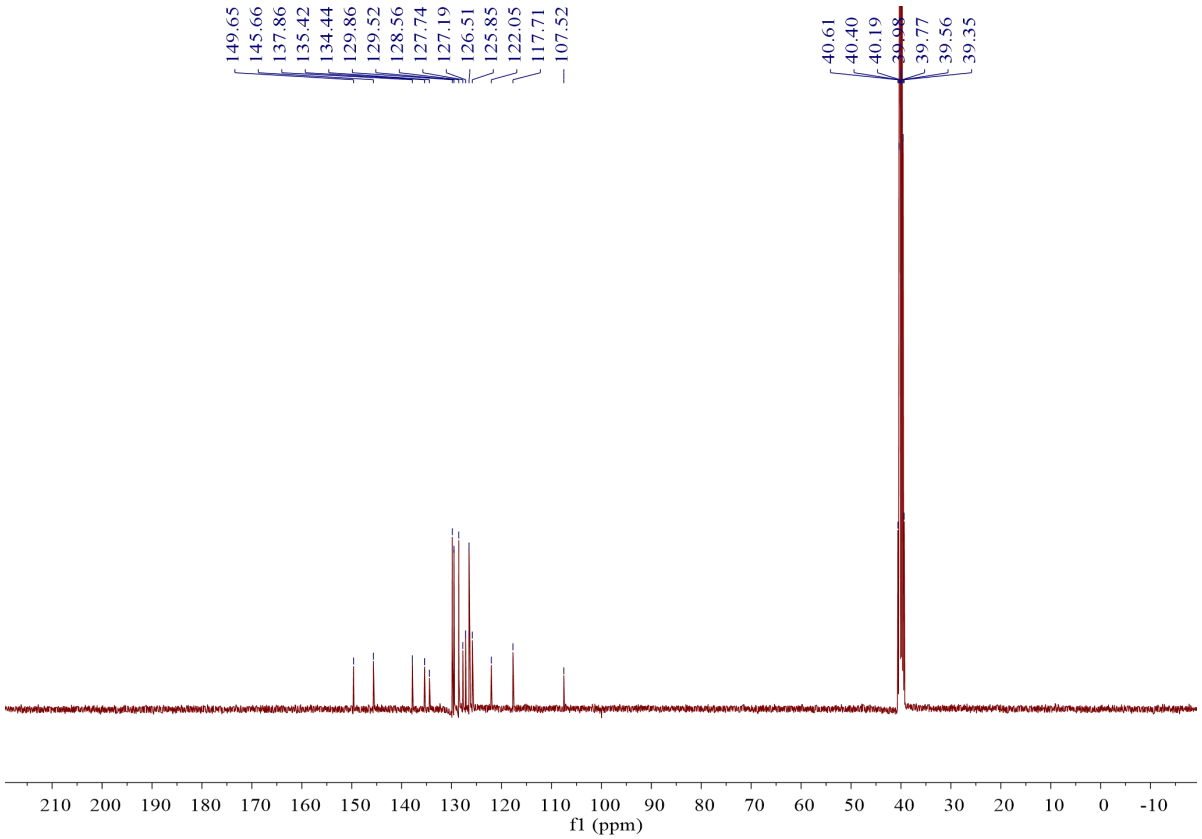
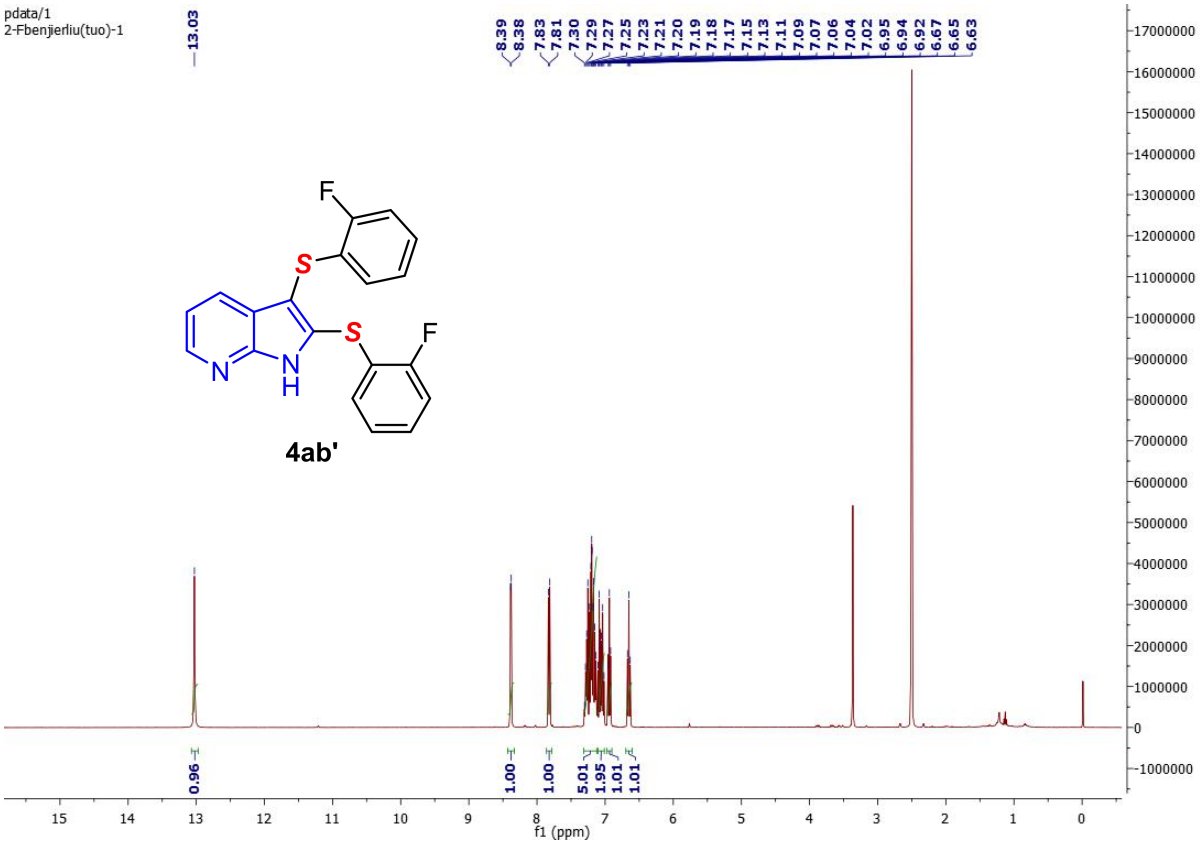
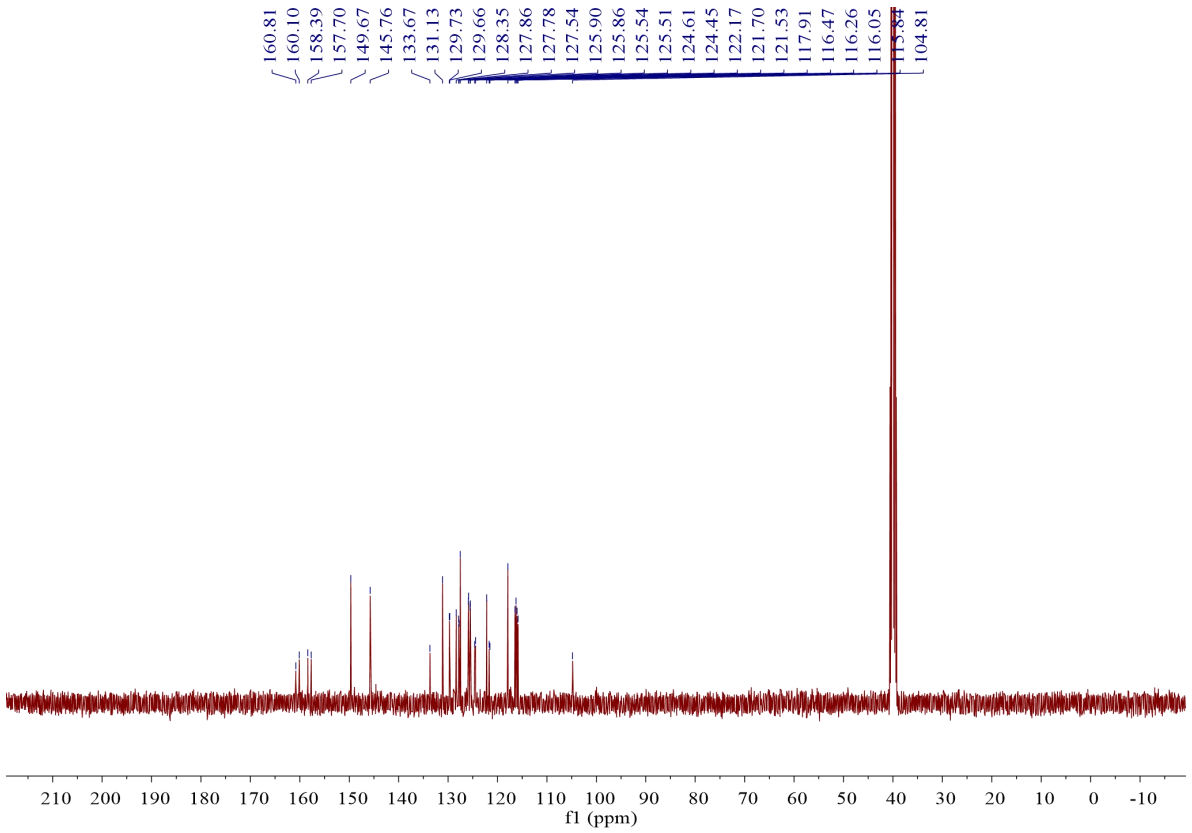
8.38
8.37
8.37
8.36
7.81
7.81
7.79
7.79
7.32
7.32
7.30
7.30
7.30
7.28
7.28
7.24
7.24
7.23
7.22
7.22
7.21
7.20
7.20
7.19
7.19
7.18
7.17
7.16
7.12
7.11
7.10
7.04
7.03
7.03
7.02
7.02
7.01
3.33
2.51
2.51
2.50

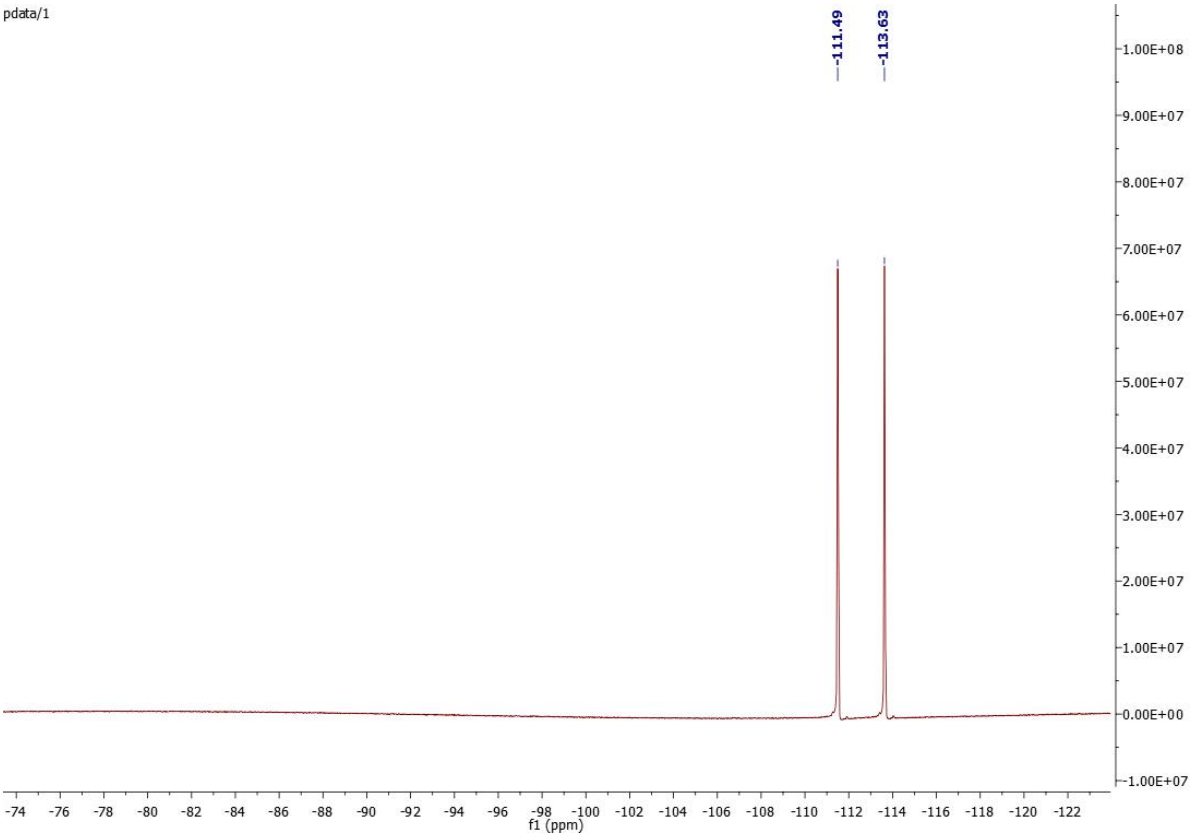
4aa'

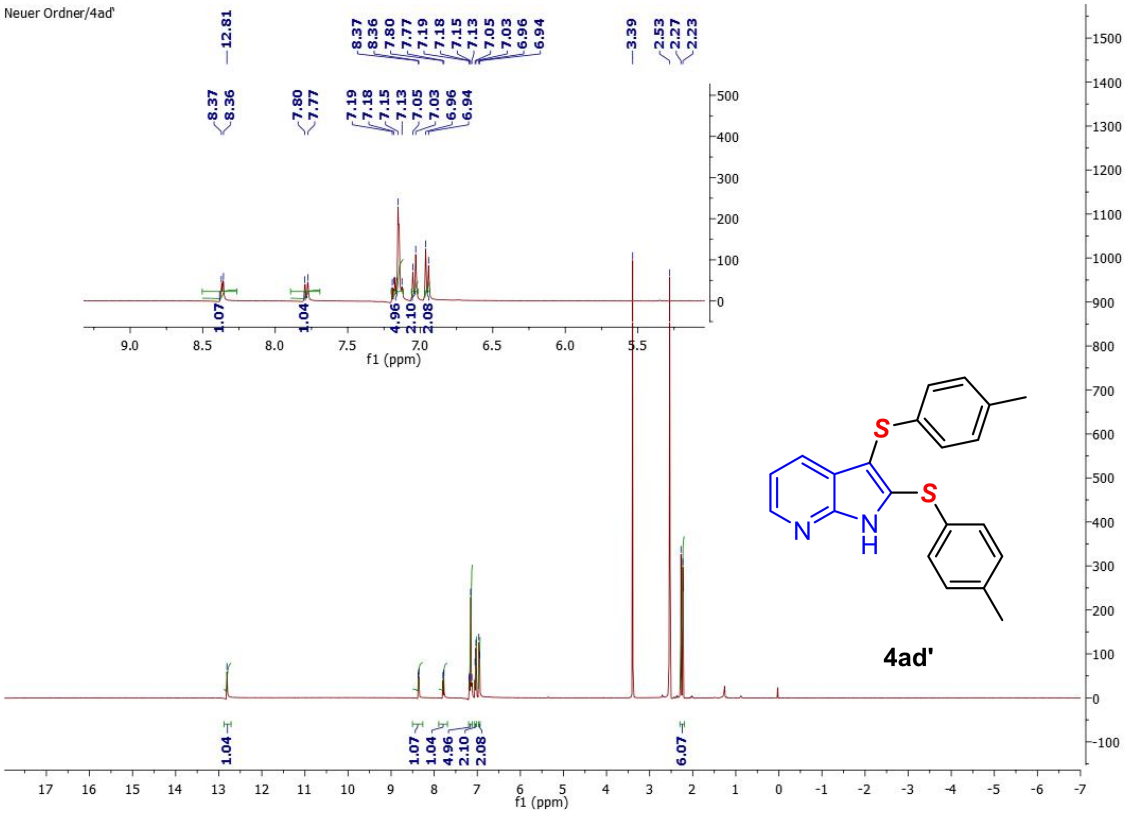

1.00
1.06
1.07
2.12
6.00
1.02
2.09
f1 (ppm)

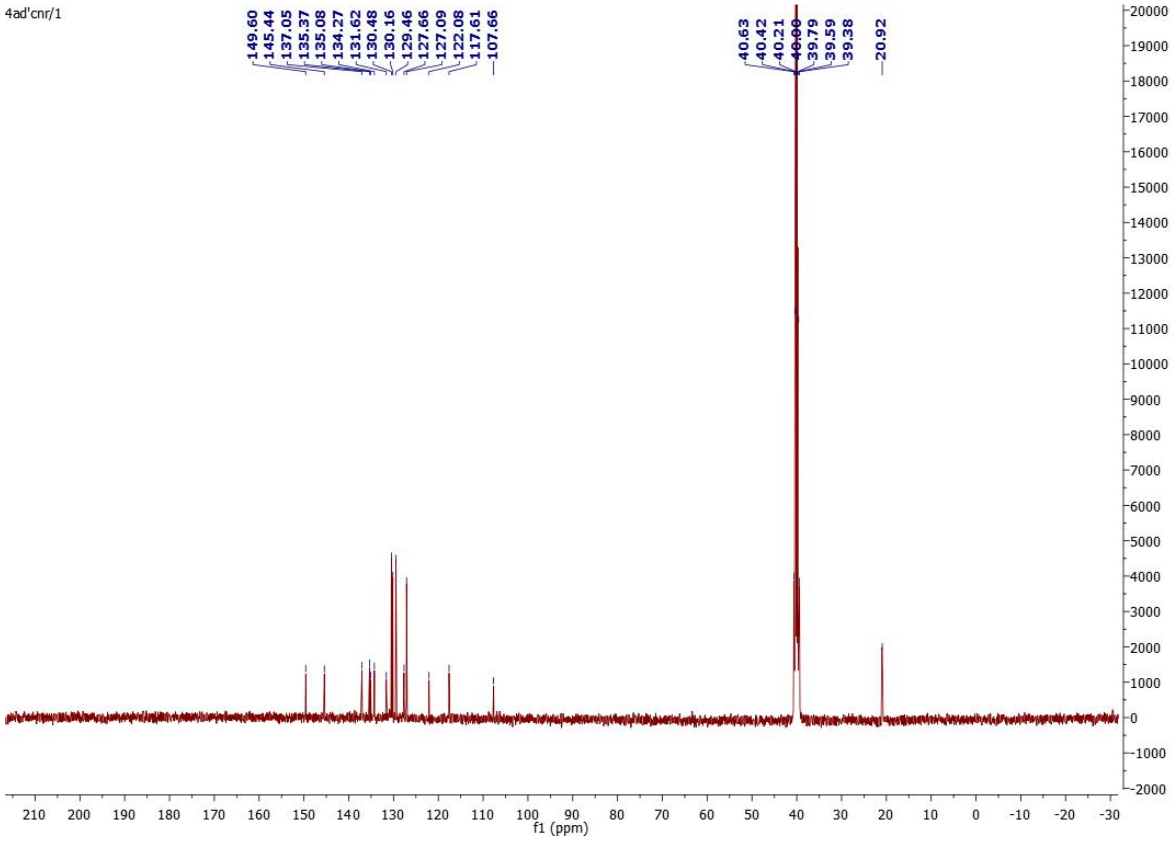

149.65
145.66
137.86
135.42
134.44
129.86
129.52
128.56
127.74
127.19
126.51
125.85
122.05
117.71
107.52
40.61
40.40
40.19
39.98
39.77
39.56
39.35
f1 (ppm)


pdata/1
2-Fbenjierliu(tuo)-1
13.03
8.39
8.38
7.83
7.81
7.30
7.29
7.27
7.25
7.23
7.21
7.20
7.19
7.18
7.17
7.15
7.13
7.11
7.09
7.07
7.06
7.04
7.02
6.95
6.94
6.92
6.67
6.65
6.63
F
S
S
F
N
H
4ab'
0.96
1.00
1.00
5.01
1.95
1.01
1.01
f1 (ppm)


160.81
160.10
158.39
157.70
149.67
145.76
133.67
131.13
129.73
129.66
128.35
127.86
127.78
127.54
125.90
125.86
125.54
125.51
124.61
124.45
122.17
121.70
121.53
117.91
116.47
116.26
116.05
115.84
104.81
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


pdata/1
-111.49
-113.63
1.00E+08
9.00E+07
8.00E+07
7.00E+07
6.00E+07
5.00E+07
4.00E+07
3.00E+07
2.00E+07
1.00E+07
0.00E+00
-1.00E+07
-74 -76 -78 -80 -82 -84 -86 -88 -90 -92 -94 -96 -98 -100 -102 -104 -106 -108 -110 -112 -114 -116 -118 -120 -122
f1 (ppm)


Neuer Ordner/4ad'
12.81
8.37
8.36
7.80
7.77
7.19
7.18
7.15
7.13
7.05
7.03
6.96
6.94
3.39
2.53
2.27
2.23
1.07
1.04
4.96
2.10
2.08
6.07
f1 (ppm)
S
S
N
H
4ad'


4ad'cnr/1
149.60
145.44
137.05
135.37
135.08
134.27
131.62
130.48
130.16
129.46
127.66
127.09
122.08
117.61
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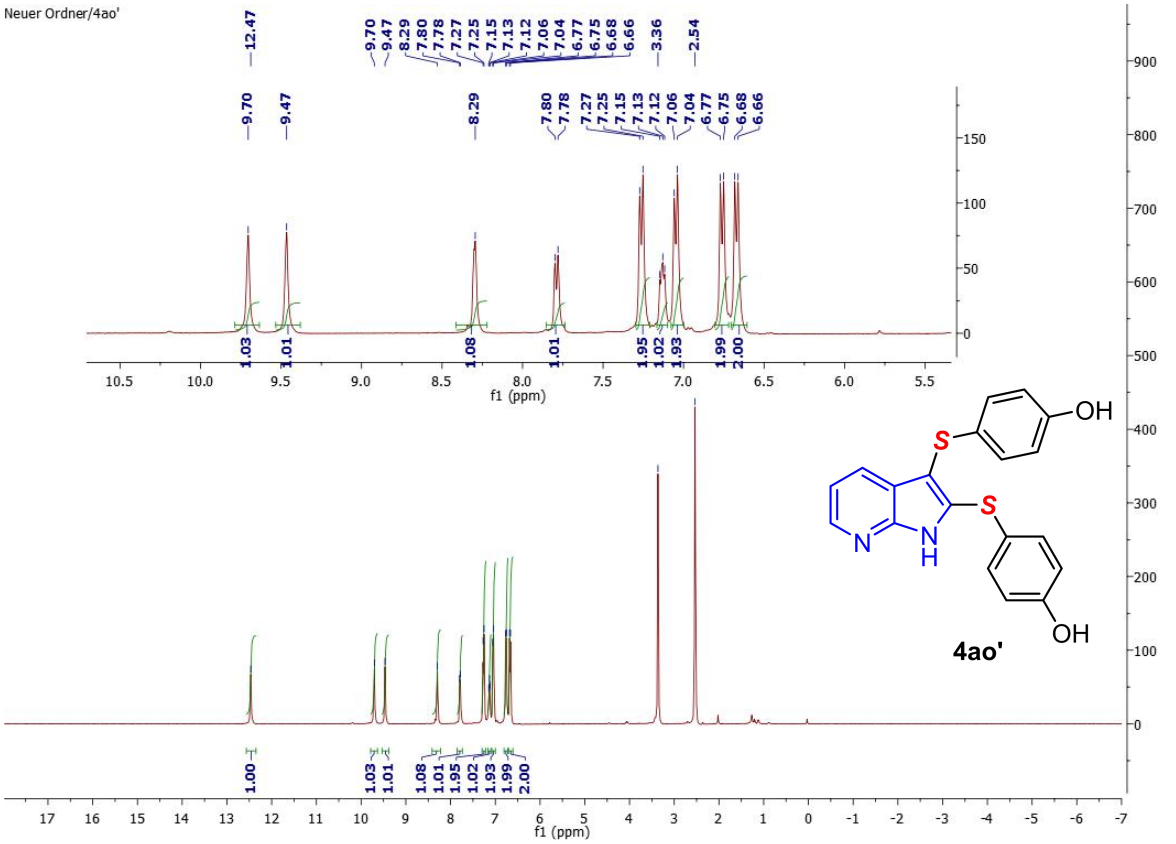
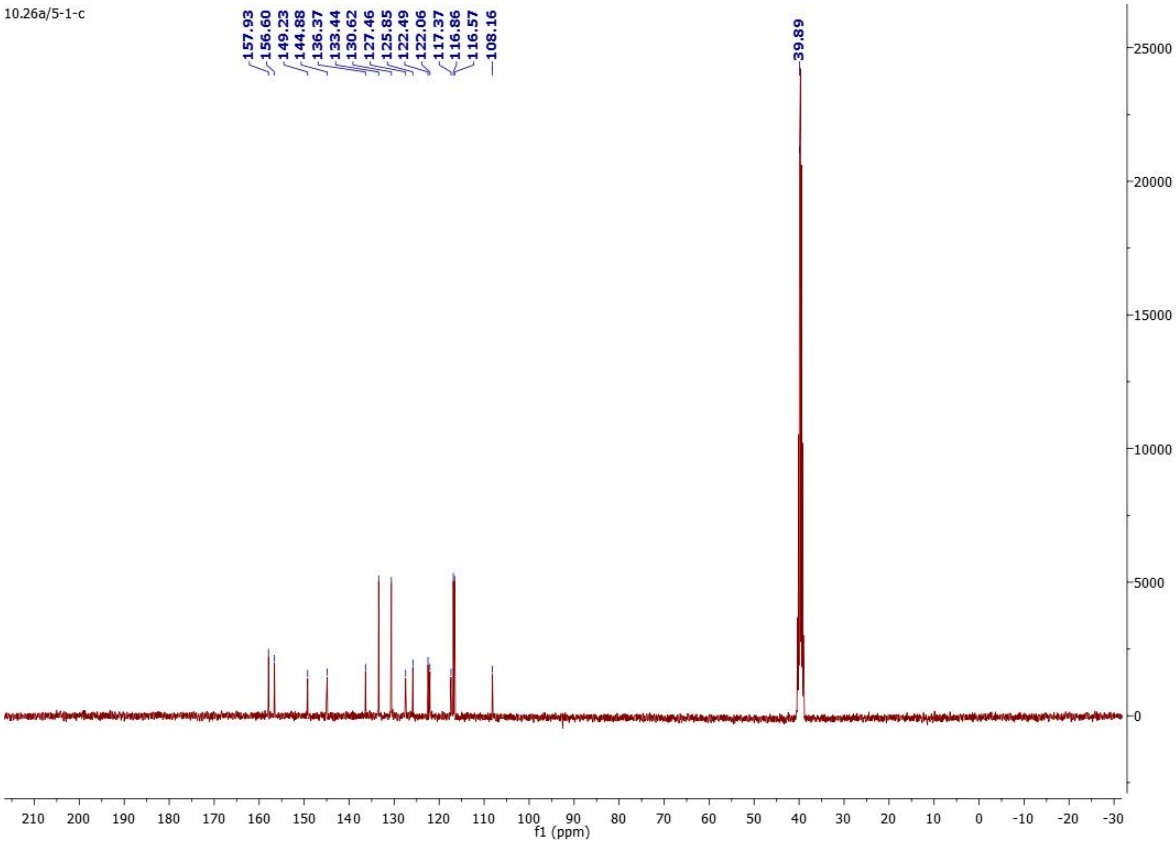
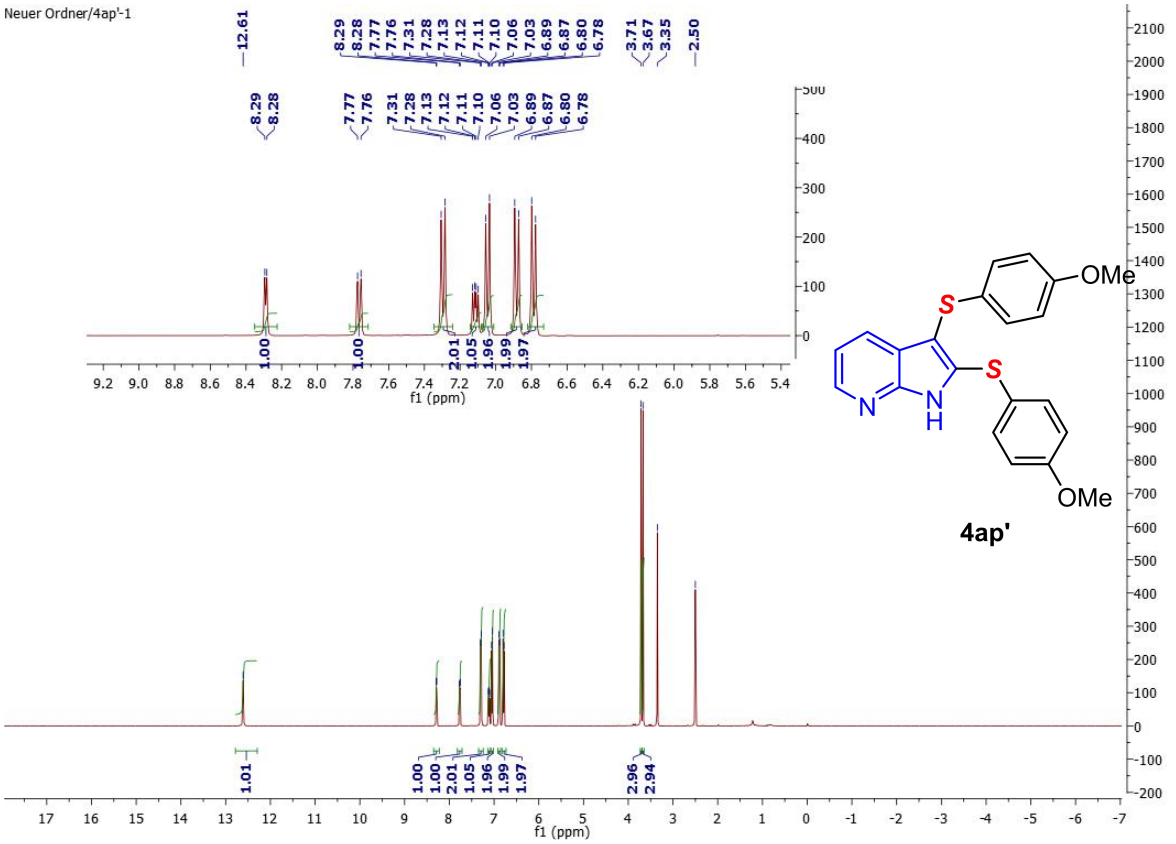
40.63
40.42
40.21
40.00
39.79
39.59
39.38
20.92
f1 (ppm)


Neuer Ordner/4ao'
12.47
9.70
9.47
8.29
7.80
7.78
7.27
7.25
7.15
7.13
7.12
7.06
7.04
6.77
6.75
6.68
6.66
3.36
2.54
1.03
1.01
1.08
1.01
1.95
1.02
1.93
1.99
2.00
f1 (ppm)
1.00
1.03
1.01
1.08
1.01
1.95
1.02
1.93
1.99
2.00
f1 (ppm)
OH
S
S
N
H
OH
4ao'


10.26a/5-1-c
157.93
156.60
149.23
144.88
136.37
133.44
130.62
127.46
125.85
122.49
122.06
117.37
116.86
116.57
108.16
39.89
f1 (ppm)


Neuer Ordner/4ap'-1
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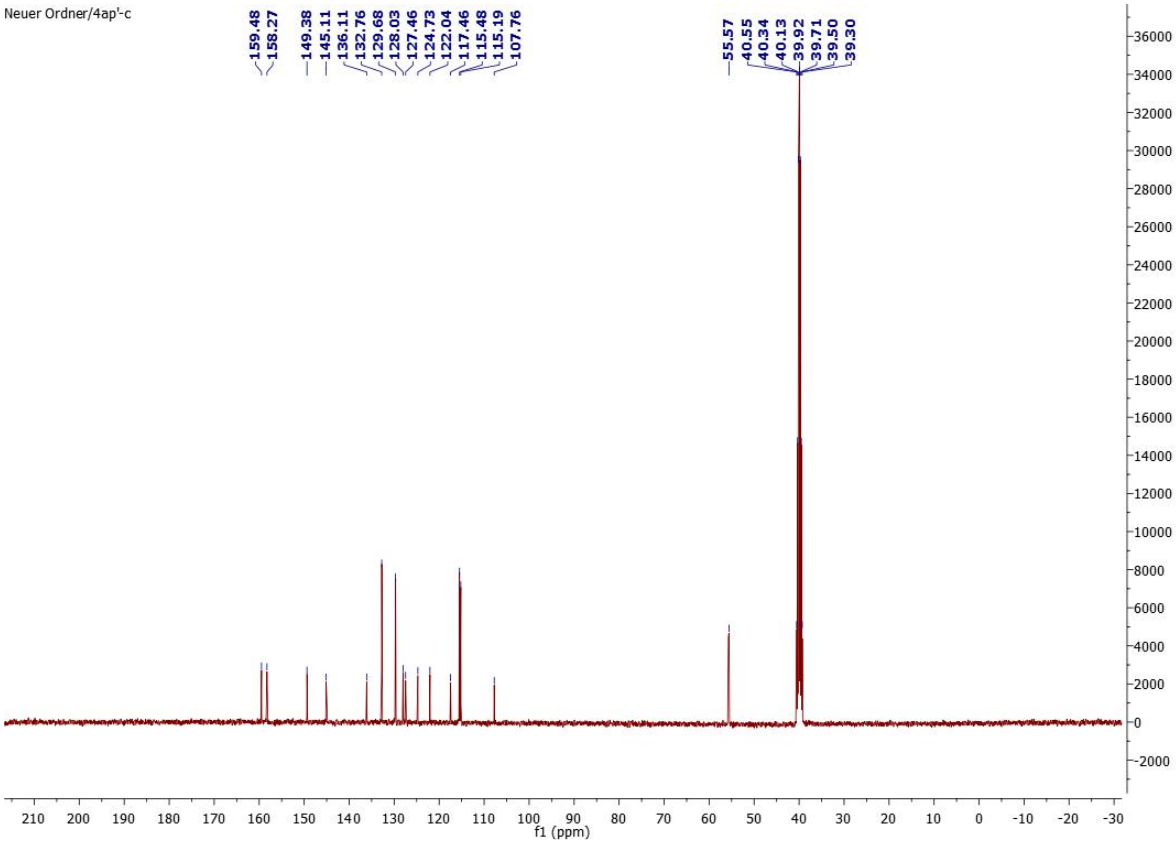
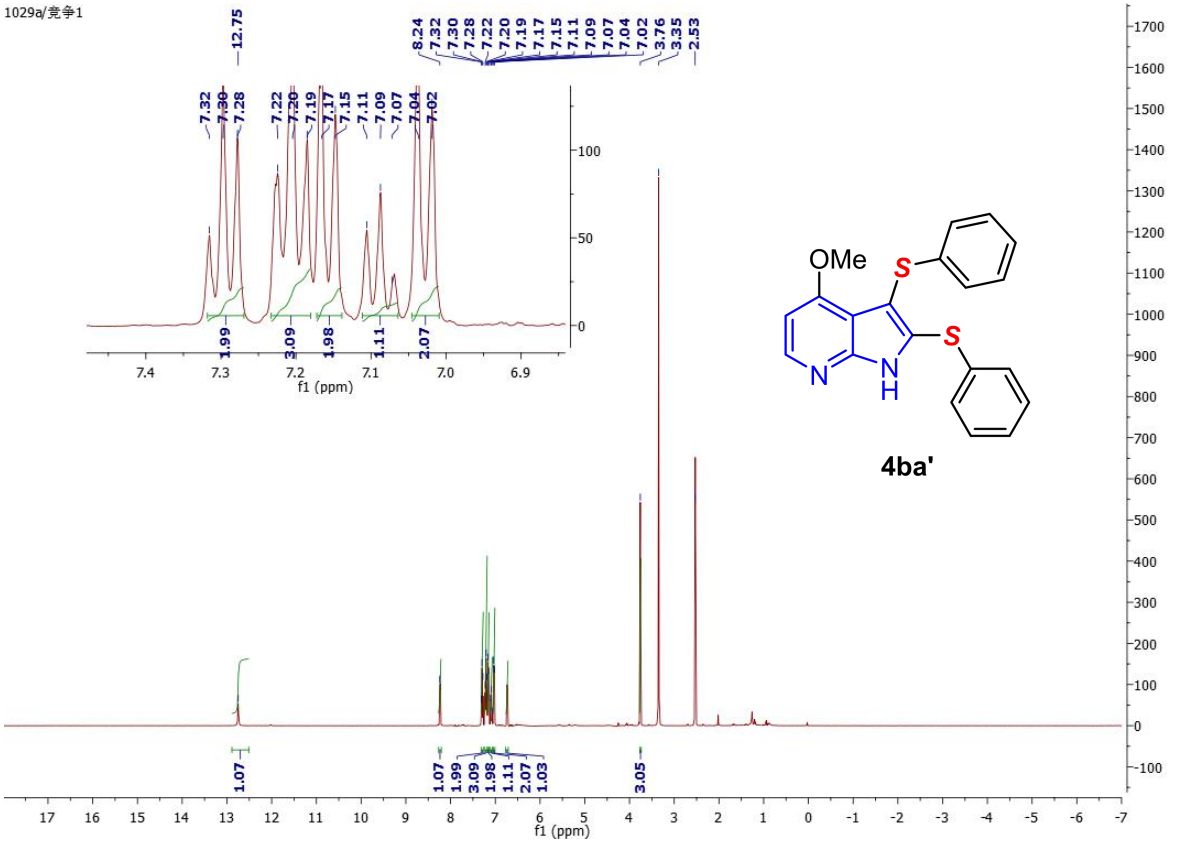
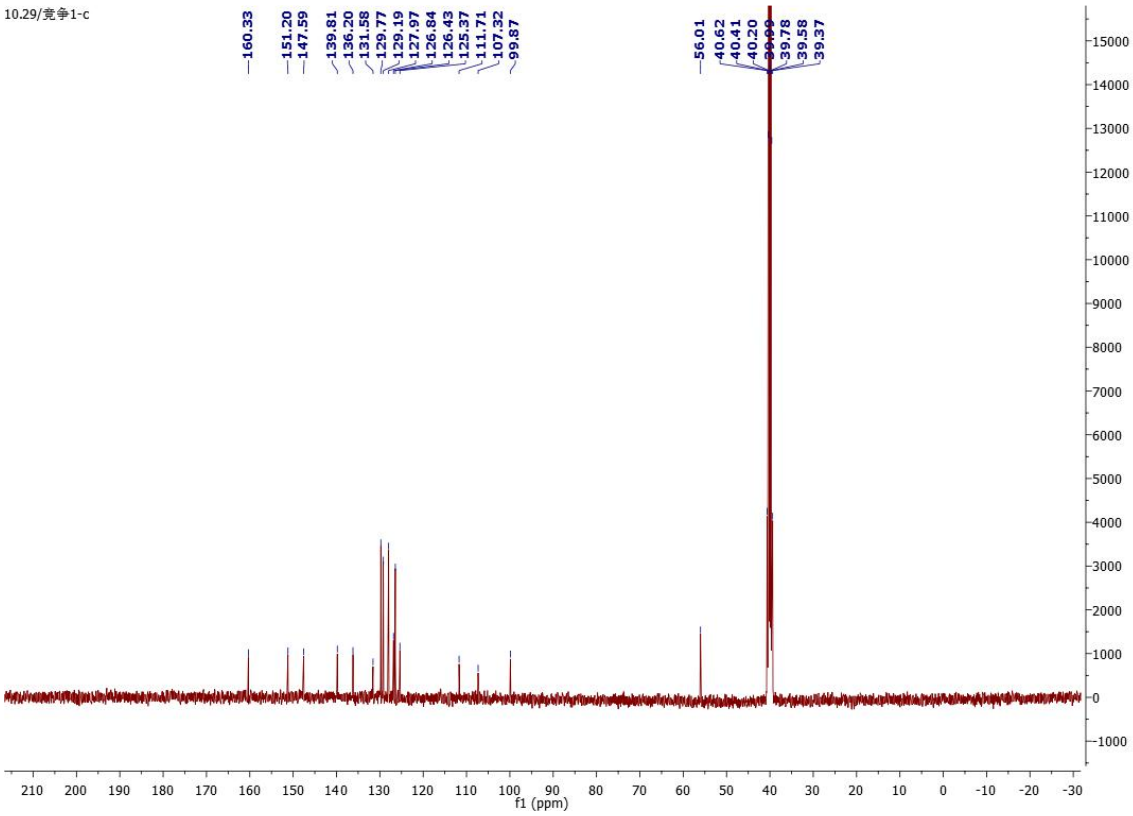
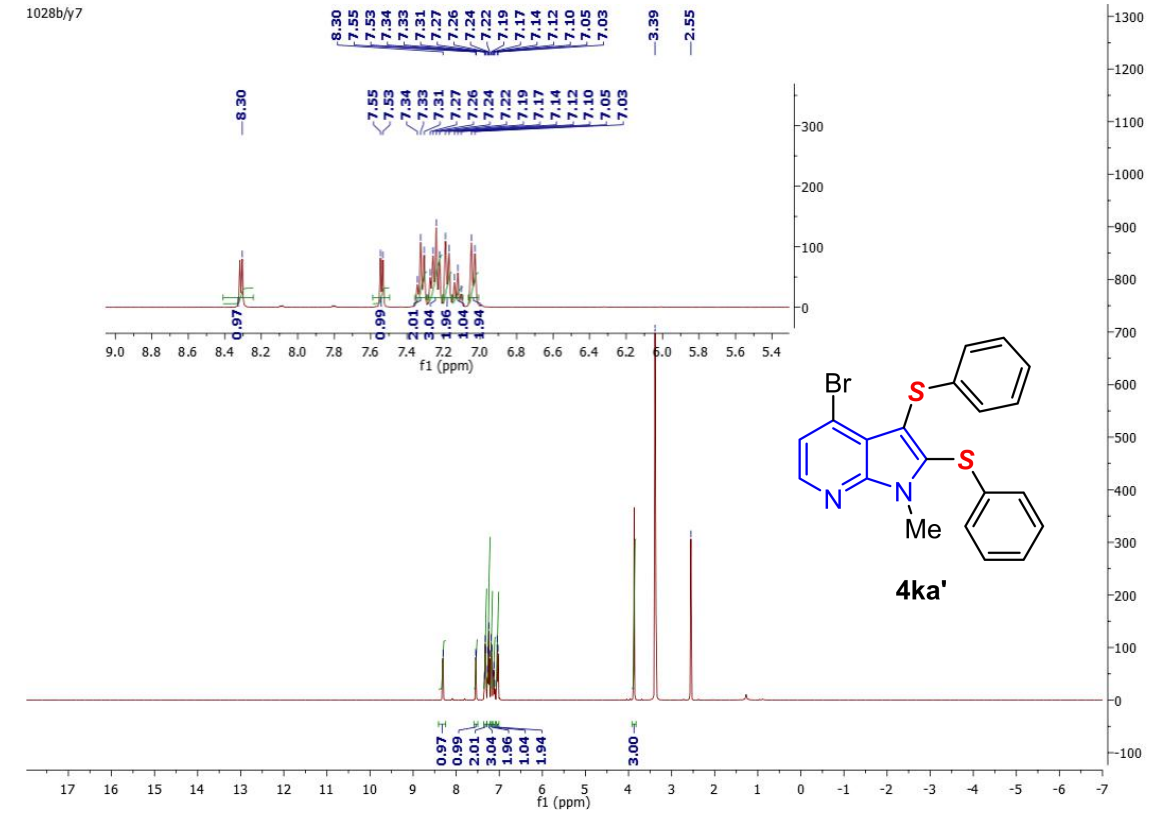
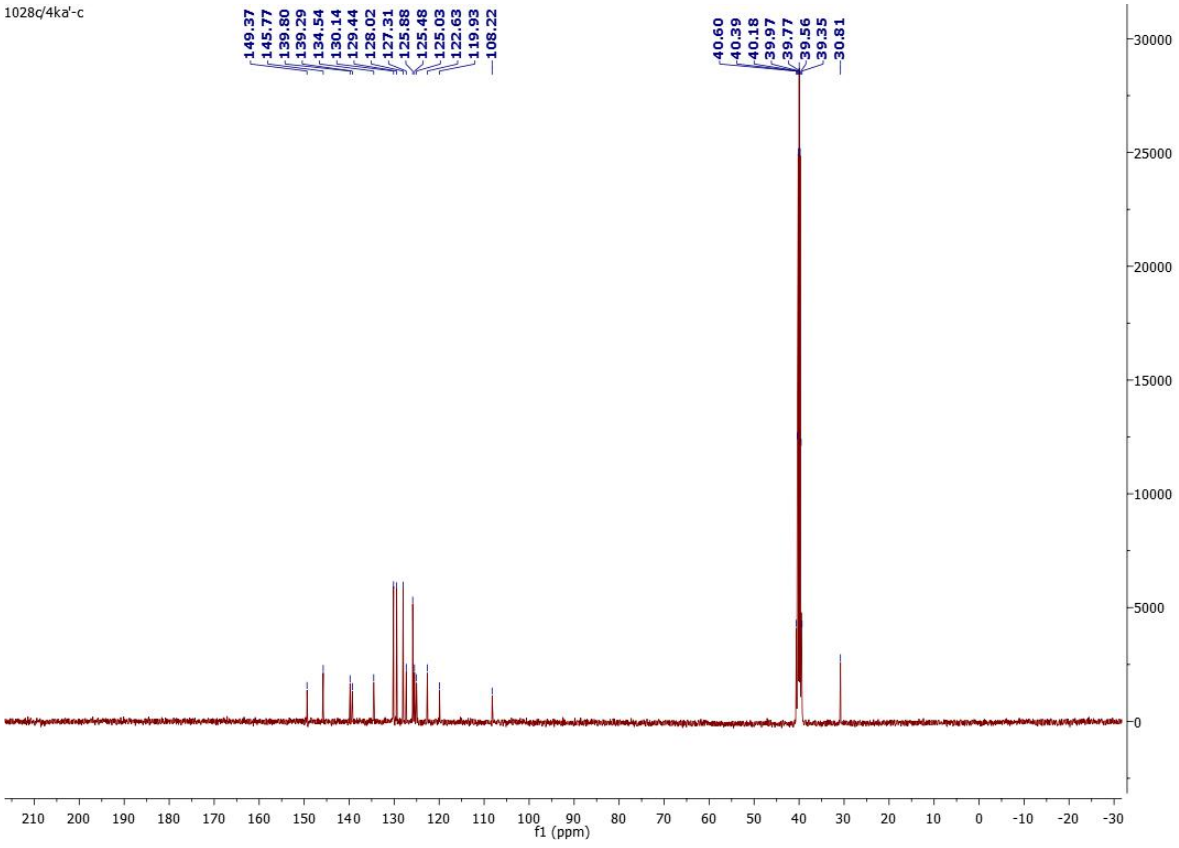
8.29
8.28
7.77
7.76
7.31
7.28
7.13
7.12
7.11
7.10
7.06
7.03
6.89
6.87
6.80
6.78
3.71
3.67
3.35
2.50
1.00
1.00
2.01
1.05
1.96
1.99
1.97
1.01
2.96
2.94
f1 (ppm)
OMe
S
S
N
H
OMe
4ap'


Neuer Ordner/4ap'-c
159.48
158.27
149.38
145.11
136.11
132.76
129.68
128.03
127.46
124.73
122.04
117.46
115.48
115.19
107.76
55.57
40.55
40.34
40.13
39.92
39.71
39.50
39.30
f1 (ppm)


1029a/竞争1
12.75
8.24
7.32
7.30
7.28
7.22
7.20
7.19
7.17
7.15
7.11
7.09
7.07
7.04
7.02
3.76
3.35
2.53
1.99
3.09
1.98
1.11
2.07
1.07
1.99
3.09
1.98
1.11
2.07
1.03
3.05
f1 (ppm)
OMe
S
S
N
H
4ba'


10.29/竞争1-c
160.33
151.20
147.59
139.81
136.20
131.58
129.77
129.19
127.97
126.84
126.43
125.37
111.71
107.32
99.87
56.01
40.62
40.41
40.20
39.78
39.58
39.37
f1 (ppm)


1028b/y7
8.30
7.55
7.53
7.34
7.33
7.31
7.27
7.26
7.24
7.22
7.19
7.17
7.14
7.12
7.10
7.05
7.03
3.39
2.55
0.97
0.99
2.01
3.04
1.96
1.04
1.94
3.00
f1 (ppm)
Br
S
S
N
N
Me
4ka'


1028c/4ka'-c
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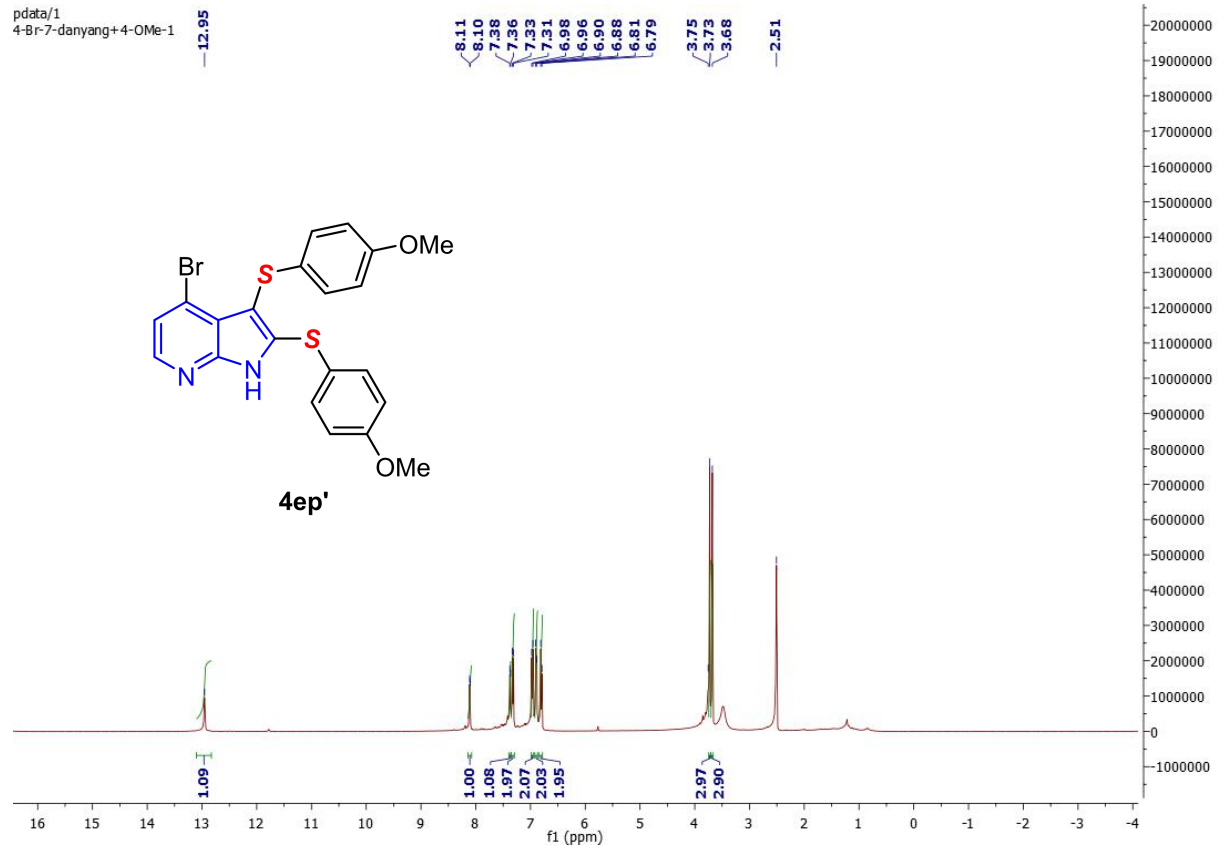
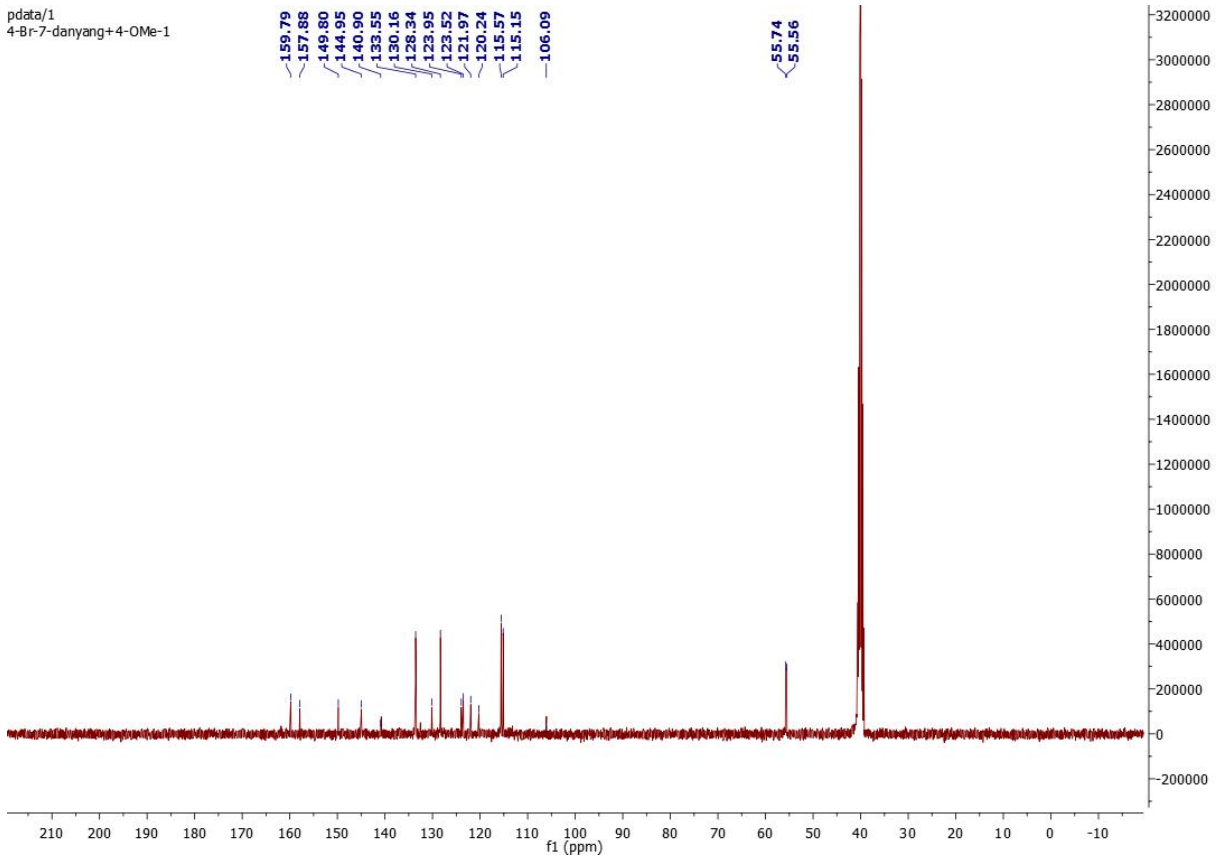
145.77
139.80
139.29
134.54
130.14
129.44
128.02
127.31
125.88
125.48
125.03
122.63
119.93
108.22
40.60
40.39
40.18
39.97
39.77
39.56
39.35
30.81
f1 (ppm)


pdata/1
4-Br-7-danyang+4-OMe-1
12.95
8.11
8.10
7.38
7.36
7.33
7.31
6.98
6.96
6.90
6.88
6.81
6.79
3.75
3.73
3.68
2.51
Br
S
S
N
H
OMe
OMe
4ep'
1.09
1.00
1.08
1.97
2.07
2.03
1.95
2.97
2.90
f1 (ppm)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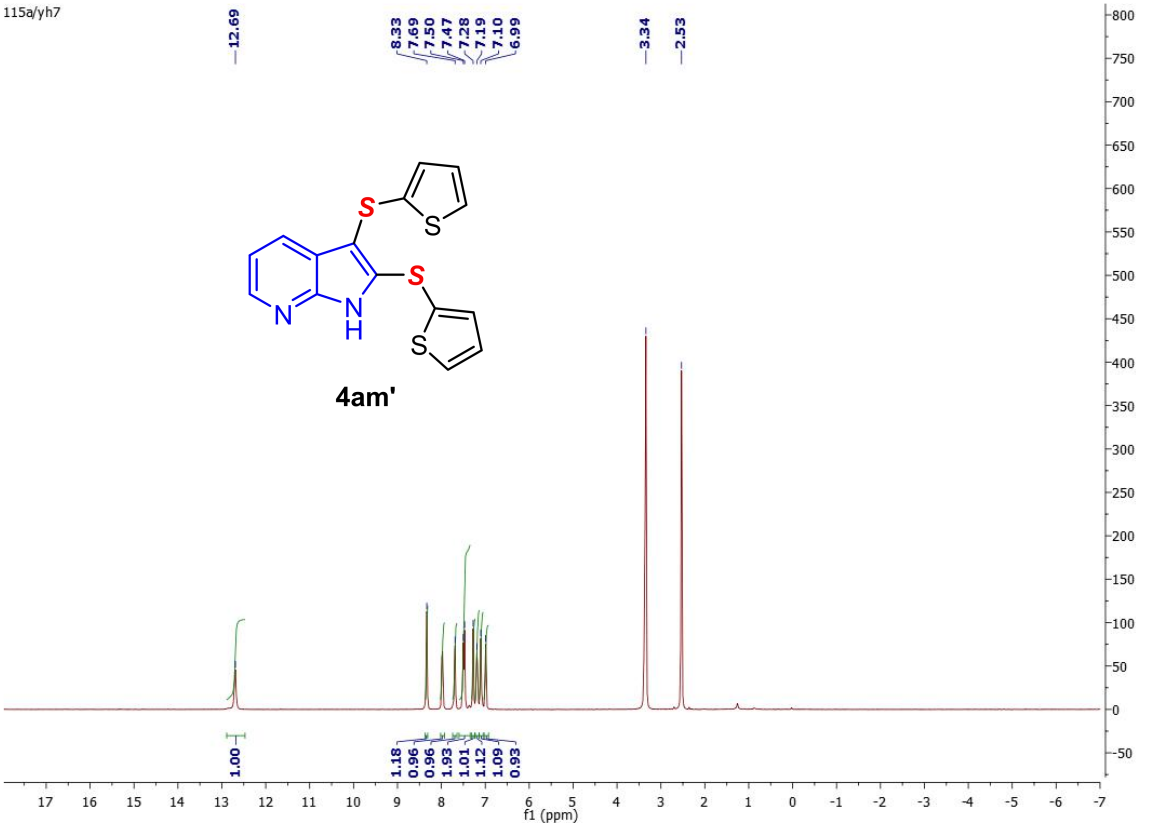
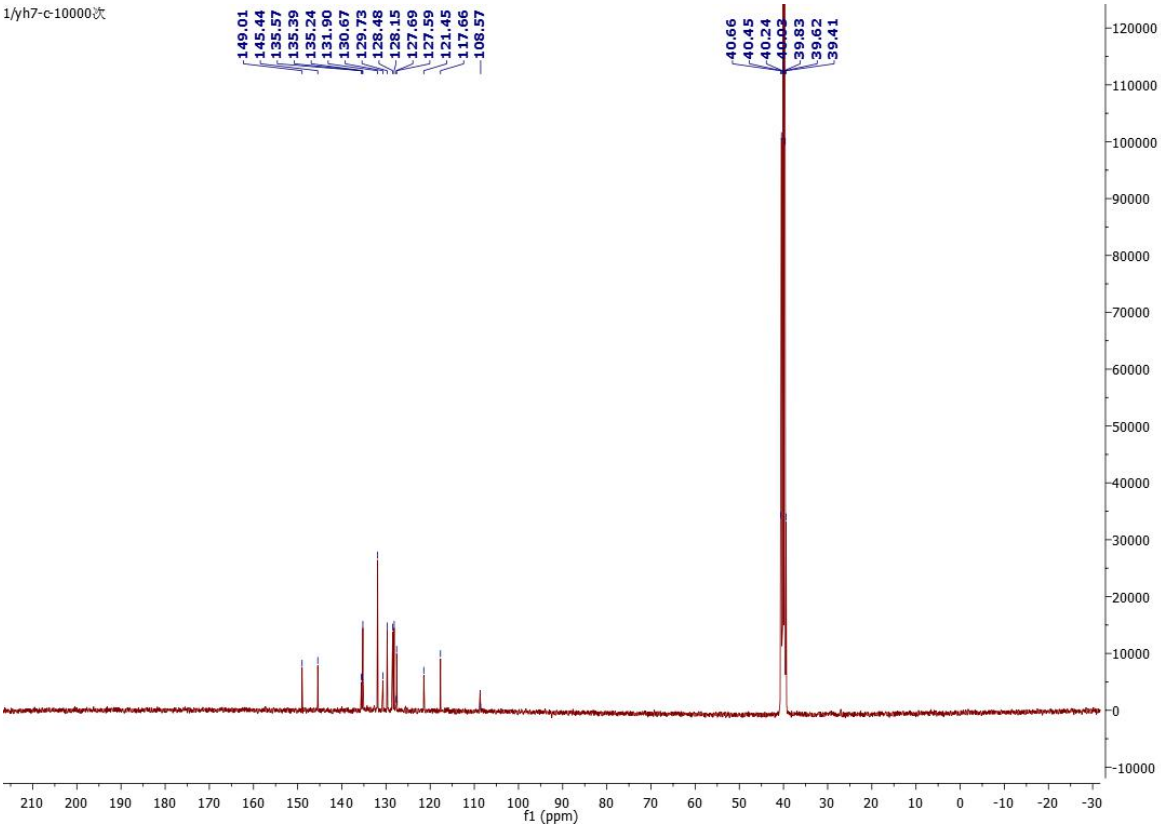
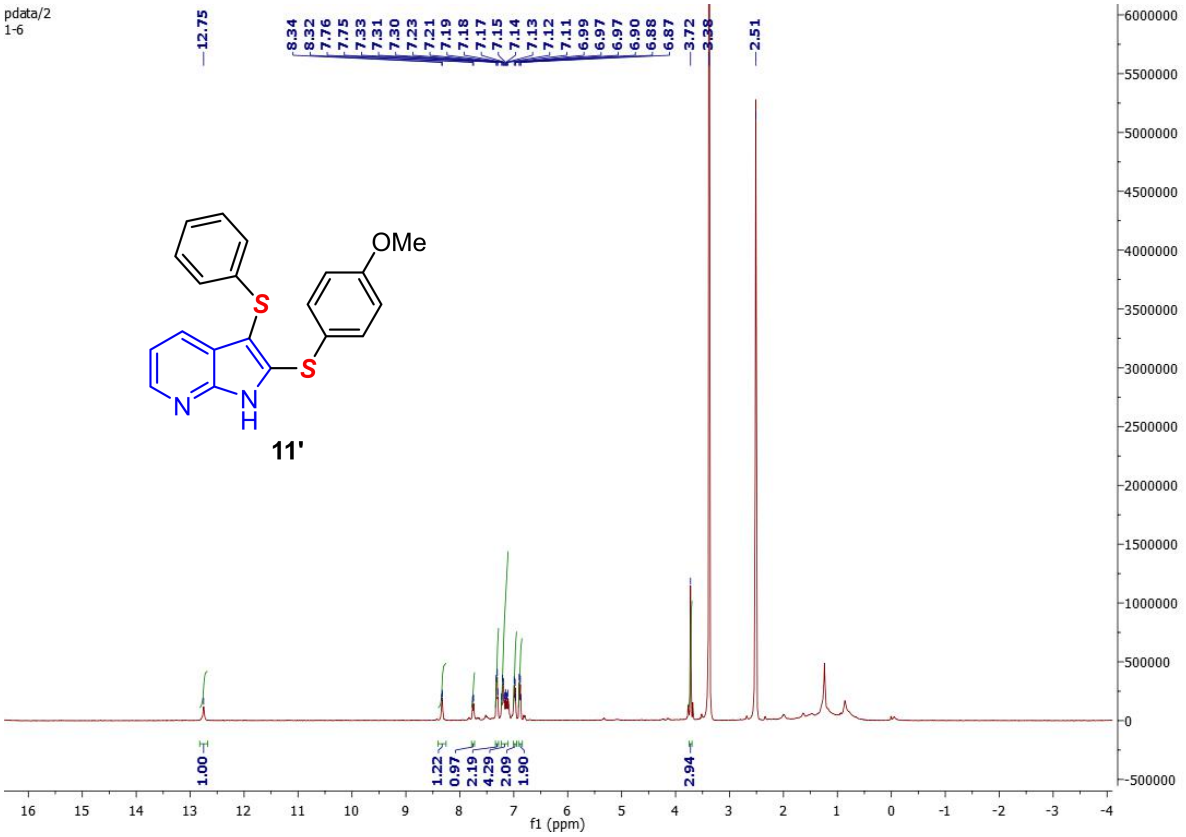
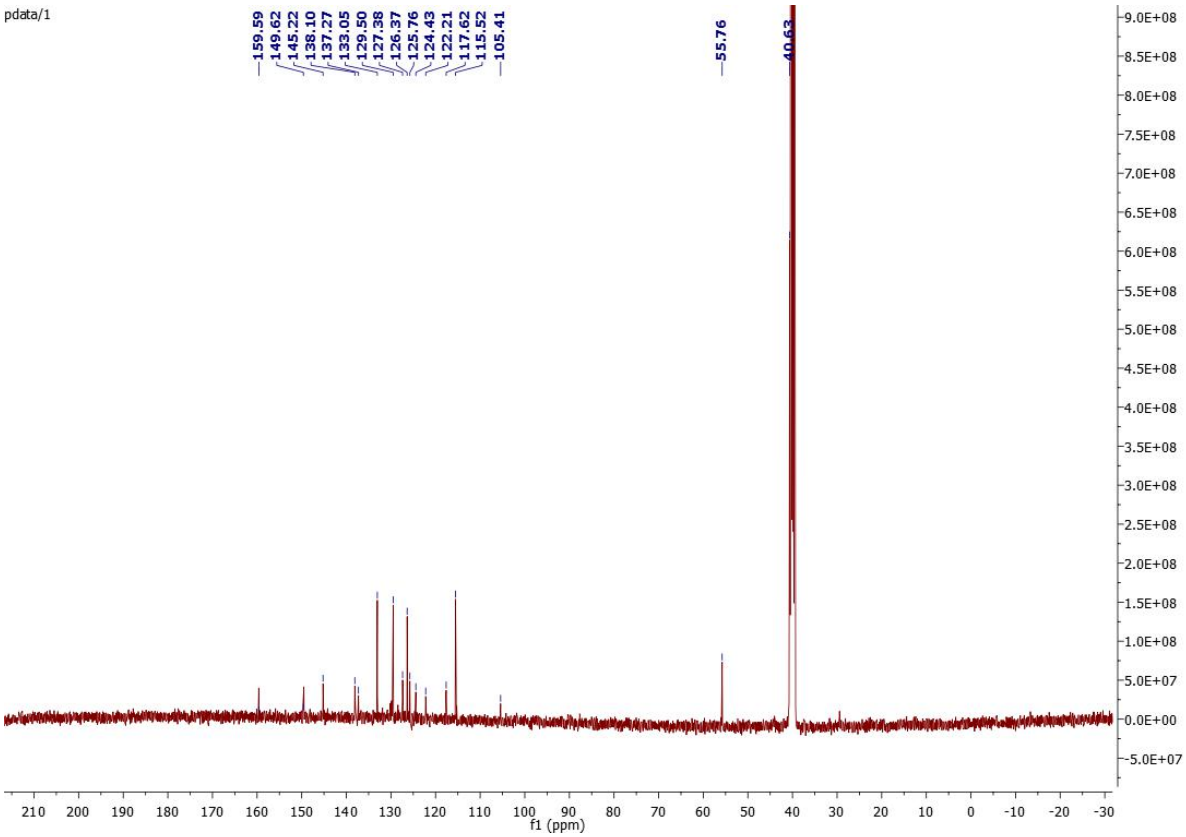
4-Br-7-danyang+4-OMe-1
159.79
157.88
149.80
144.95
140.90
133.55
130.16
128.34
123.95
123.52
121.97
120.24
115.57
115.15
106.09
55.74
55.56
f1 (ppm)

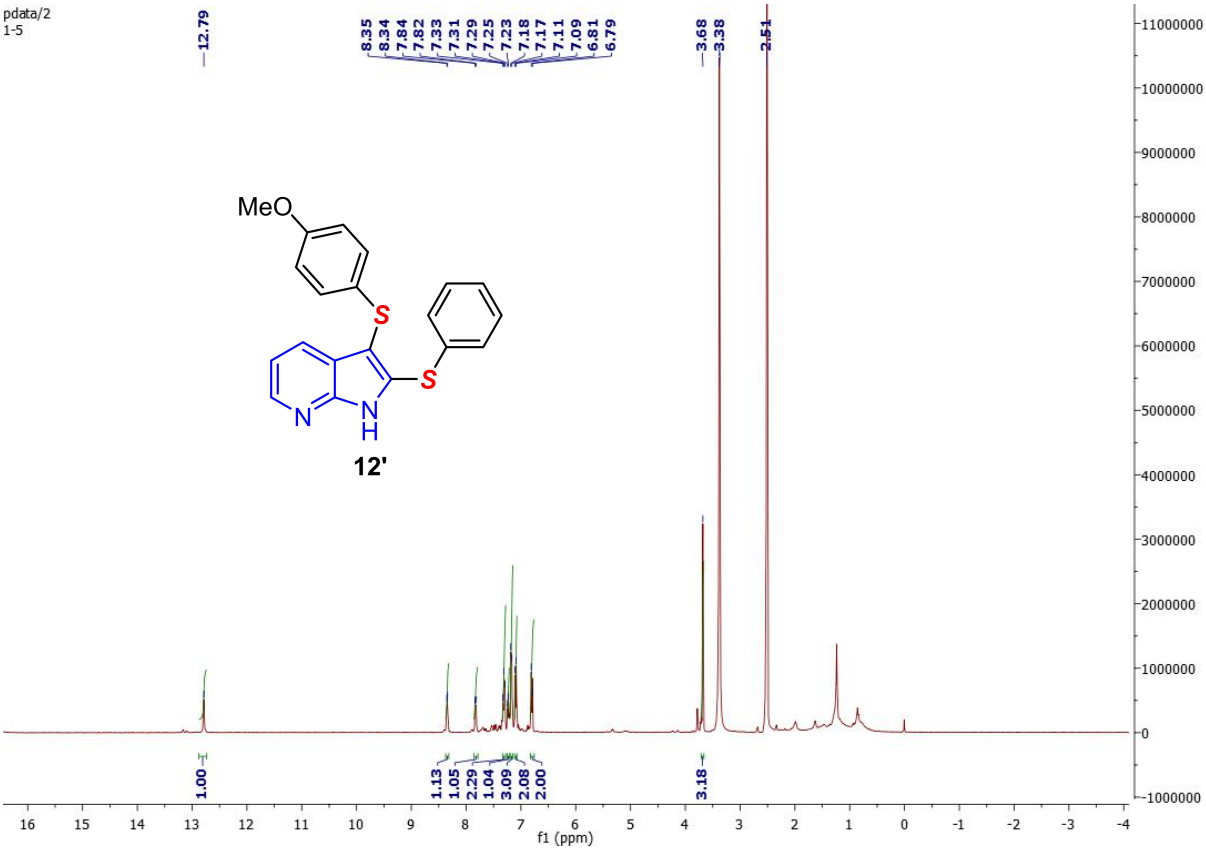

115a/yh7
12.69
8.33
7.69
7.50
7.47
7.28
7.19
7.10
6.99
3.34
2.53
1.00
1.18
0.96
0.96
1.93
1.01
1.12
1.09
0.93
f1 (ppm)

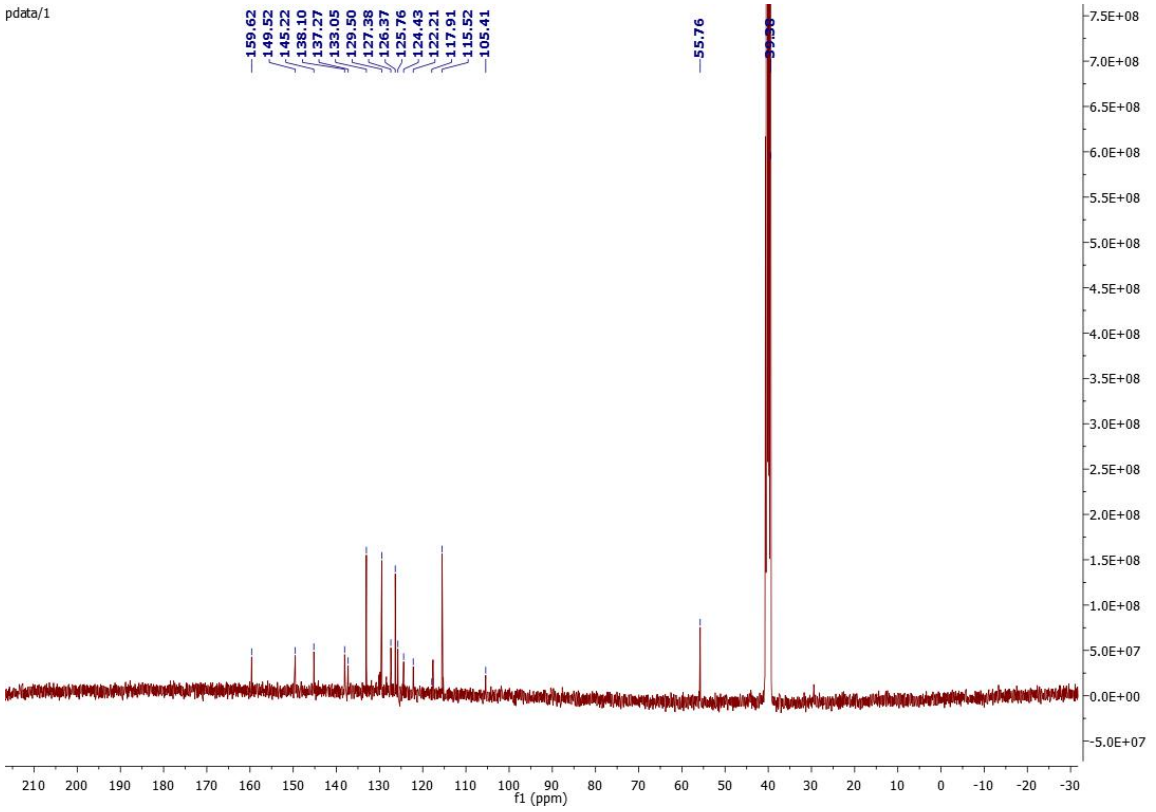
4am'

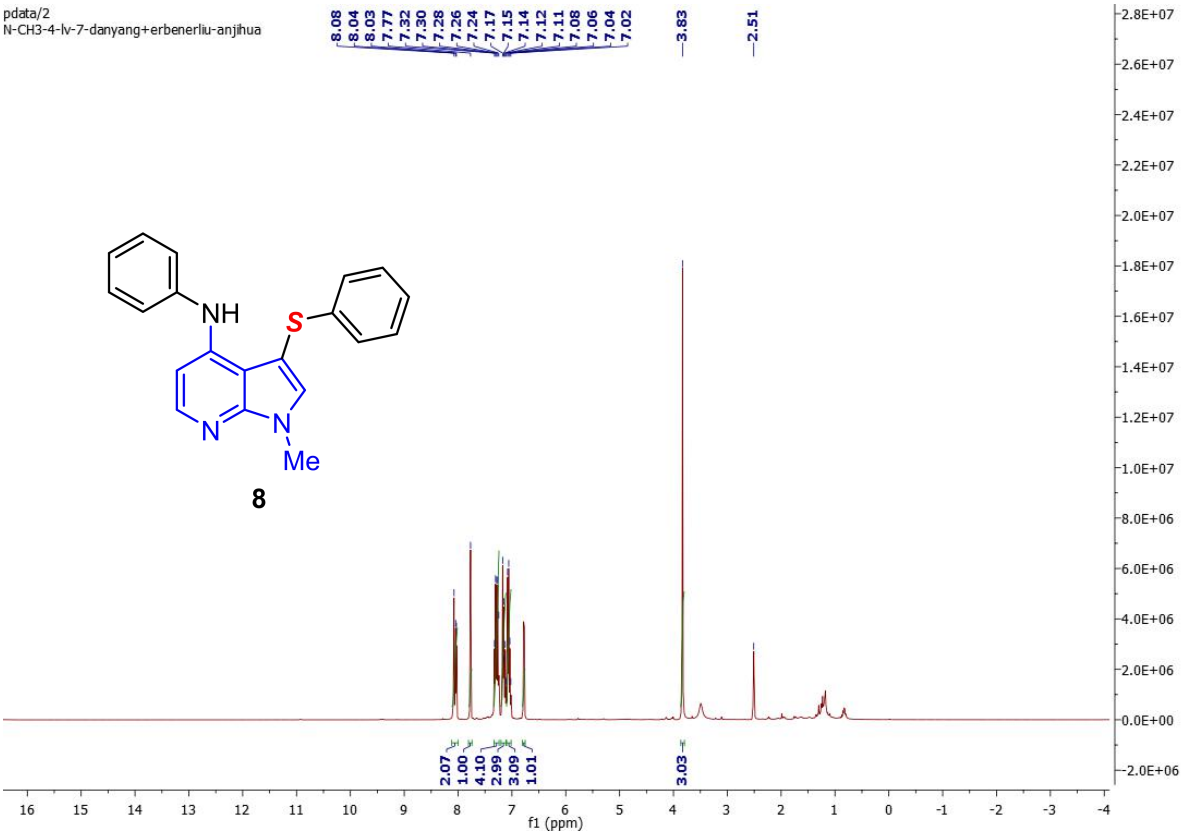

1/yh7-c-10000次
149.01
145.44
135.57
135.39
135.24
131.90
130.67
129.73
128.48
128.15
127.69
127.59
121.45
117.66
108.57
40.66
40.45
40.24
40.03
39.83
39.62
39.41
f1 (ppm)

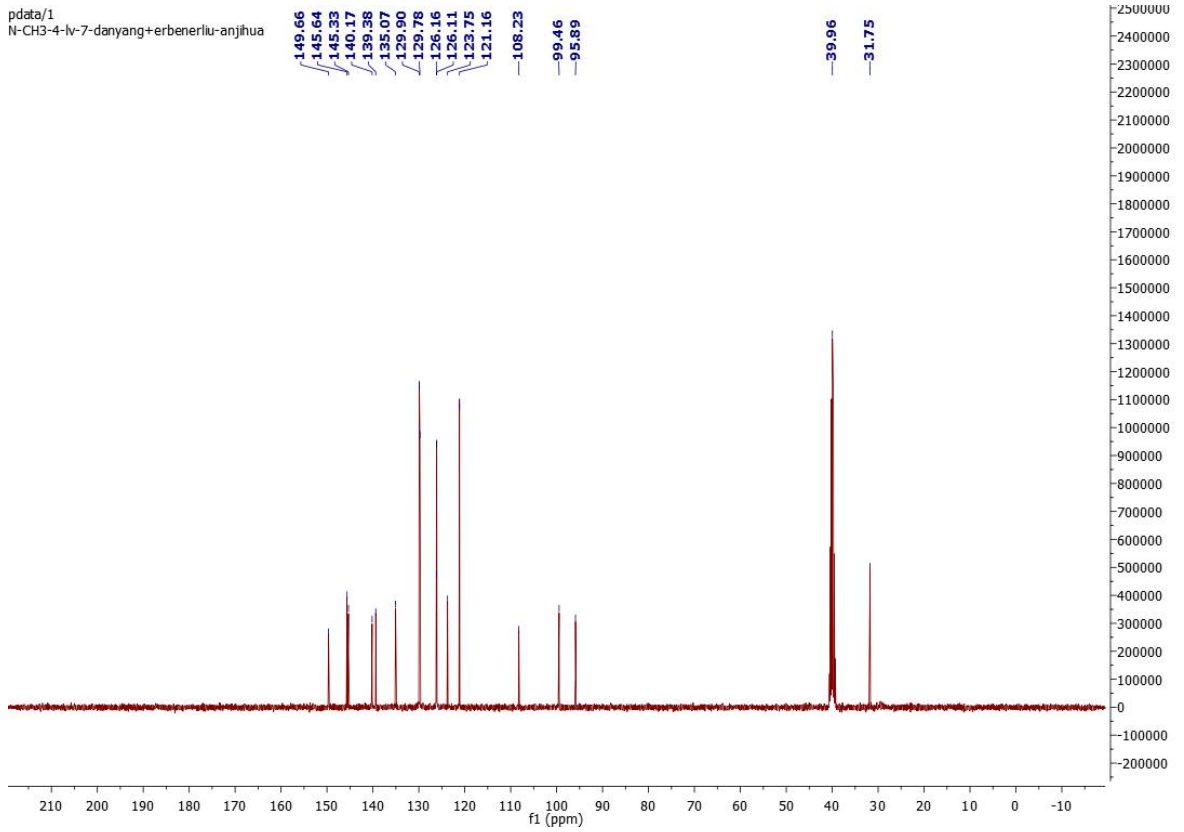

pdata/2
1-6
12.75
8.34
8.32
7.76
7.75
7.33
7.31
7.30
7.23
7.21
7.19
7.18
7.17
7.15
7.14
7.13
7.12
7.11
6.99
6.97
6.97
6.90
6.88
6.87
3.72
3.38
2.51
OMe
S
S
N
H
11'
1.00
1.22
0.97
2.19
4.29
2.09
1.90
2.94
f1 (ppm)

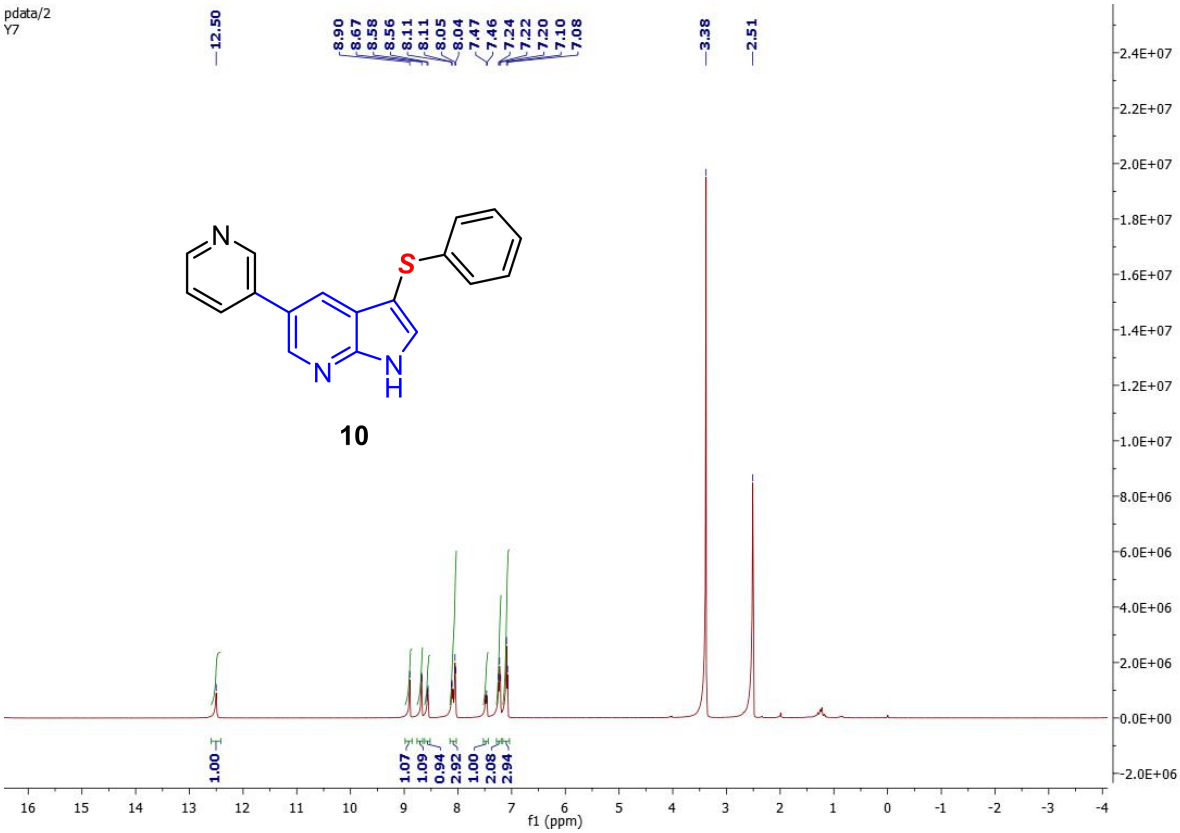

pdata/1
159.59
149.62
145.22
138.10
137.27
133.05
129.50
127.38
126.37
125.76
124.43
122.21
117.62
115.52
105.41
55.76
40.63
f1 (ppm)


pdata/2
1-5
12.79
8.35
8.34
7.84
7.82
7.33
7.31
7.29
7.25
7.23
7.18
7.17
7.11
7.09
6.81
6.79
3.68
3.38
2.51
MeO
S
S
N
H
12'
1.00
1.13
1.05
2.29
1.04
3.09
2.08
2.00
3.18
f1 (ppm)

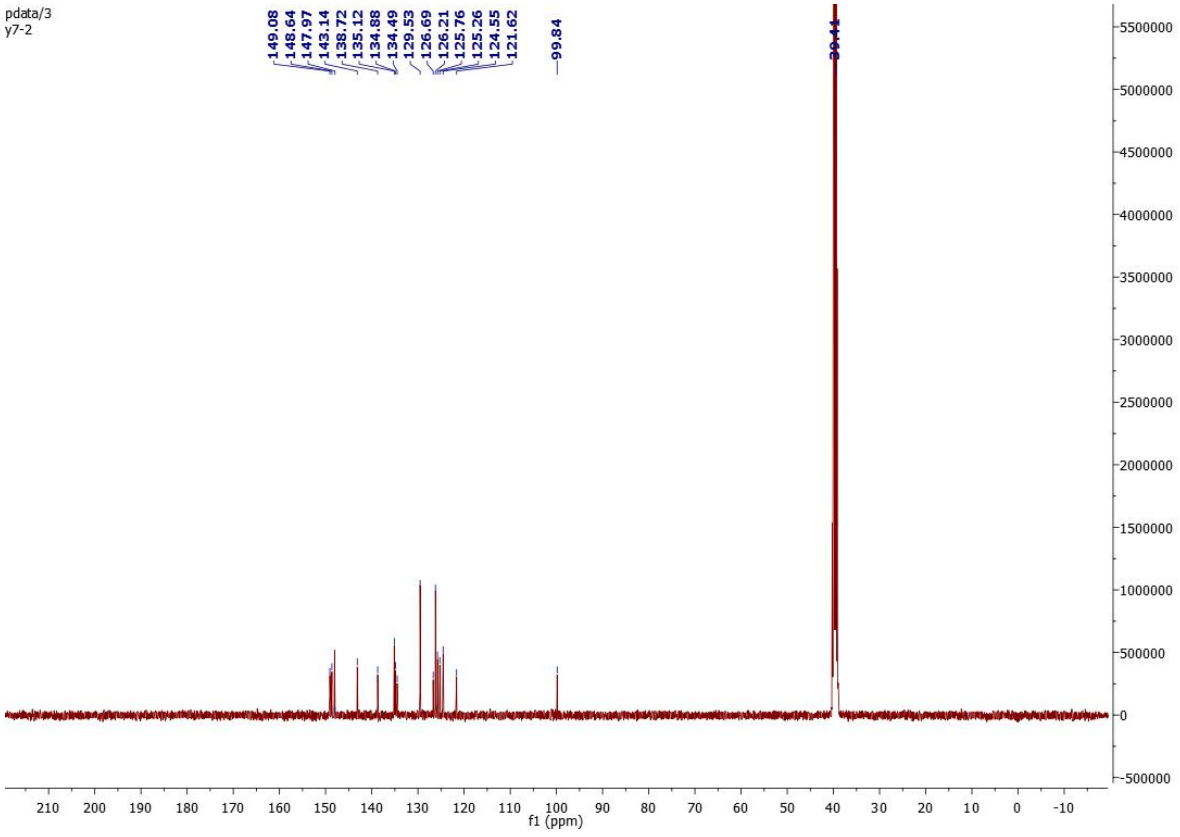

pdata/1
159.62
149.52
145.22
138.10
137.27
133.05
129.50
127.38
126.37
125.76
124.43
122.21
117.91
115.52
105.41
55.76
39.36
f1 (ppm)

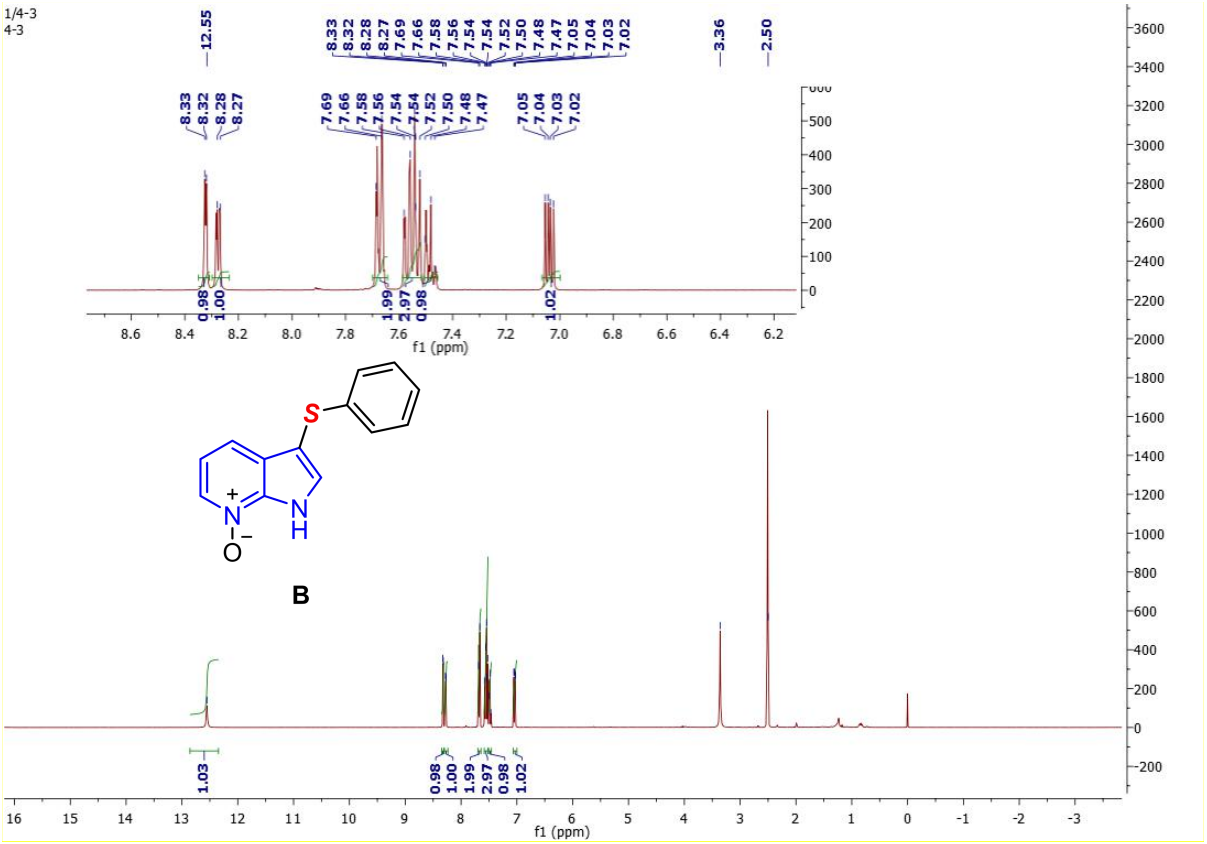

pdata/2
N-CH3-4-lv-7-danyang+erbenerliu-anjihua
8.08
8.04
8.03
7.77
7.32
7.30
7.28
7.26
7.24
7.17
7.15
7.14
7.12
7.11
7.08
7.06
7.04
7.02
3.83
2.51
NH
S
N
N
Me
8
2.07
1.00
4.10
2.99
3.09
1.01
3.03
f1 (ppm)

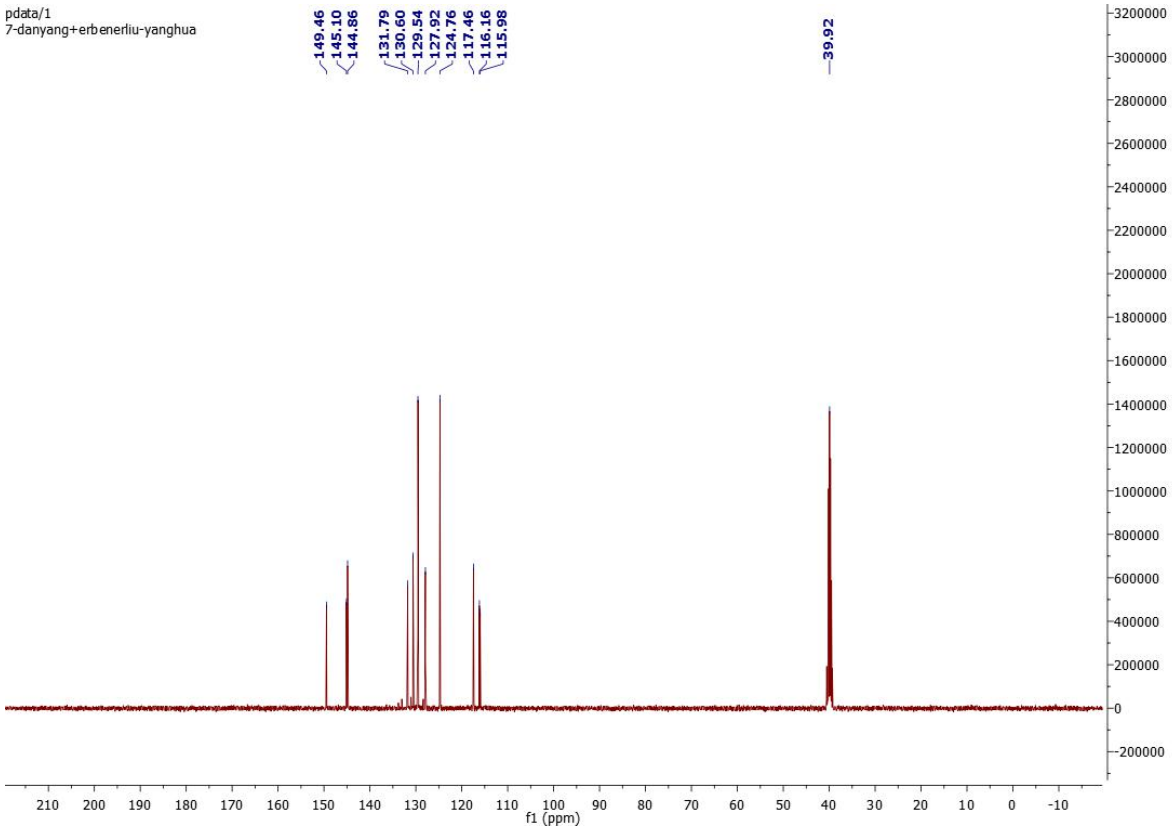

pdata/1
N-CH3-4-lv-7-danyang+erbenerliu-anjihua
149.66
145.64
145.33
140.17
139.38
135.07
129.90
129.78
126.16
126.11
123.75
121.16
108.23
99.46
95.89
39.96
31.75
f1 (ppm)


pdata/2
Y7
12.50
8.90
8.67
8.58
8.56
8.11
8.11
8.05
8.04
7.47
7.46
7.24
7.22
7.20
7.10
7.08
3.38
2.51
1.00
1.07
1.09
0.94
2.92
1.00
2.08
2.94
f1 (ppm)

10


pdata/3
y7-2
149.08
148.64
147.97
143.14
138.72
135.12
134.88
134.49
129.53
126.69
126.21
125.76
125.26
124.55
121.62
99.84
99.41
f1 (ppm)


1/4-3
4-3
12.55
8.33
8.32
8.28
8.27
7.69
7.66
7.58
7.56
7.54
7.52
7.50
7.48
7.47
7.05
7.04
7.03
7.02
3.36
2.50
0.98
1.00
1.99
2.97
0.98
1.02
f1 (ppm)
S
N
H
O
B
1.03
0.98
1.00
1.99
2.97
0.98
1.02
f1 (ppm)


pdata/1
7-danyang+erbenerliu-yanghua
149.46
145.10
144.86
131.79
130.60
129.54
127.92
124.76
117.46
116.16
115.98
39.92
f1 (ppm)