Supporting Information
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Thieme

Supporting Information

Peri-Selective Direct Acylmethylation and Amidation of Naphthalene Derivatives Using Iridium and Rhodium Catalysts

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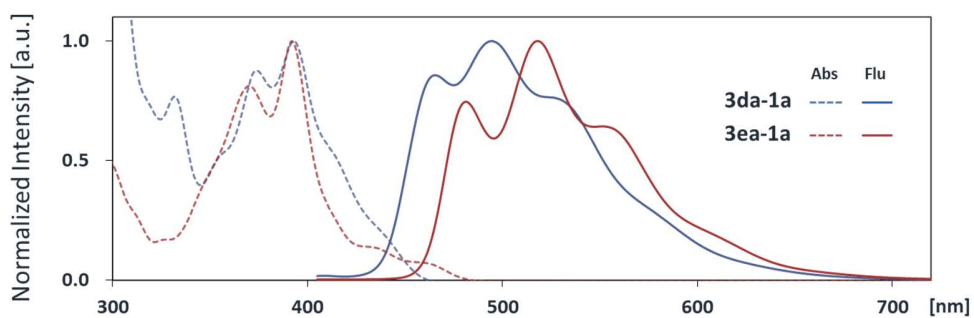
Contents:

1. Optical properties

Figure S1. Normalized absorption and fluorescence spectra of **3da-1** (blue) and **3ea-1** (red) as 1.0×10^{-5} MCHCl$_3$ solutions.

Table S1. Summary of the optical properties (excited at 390 nm).

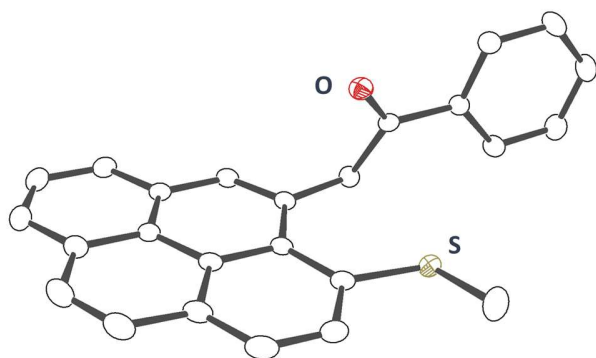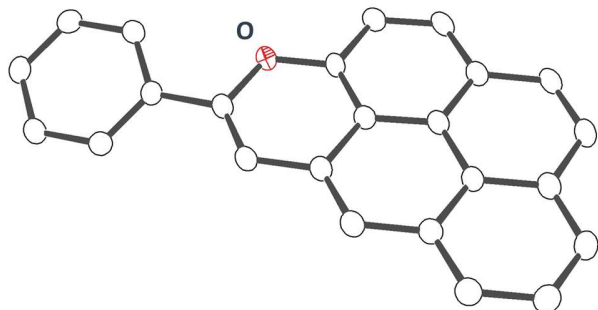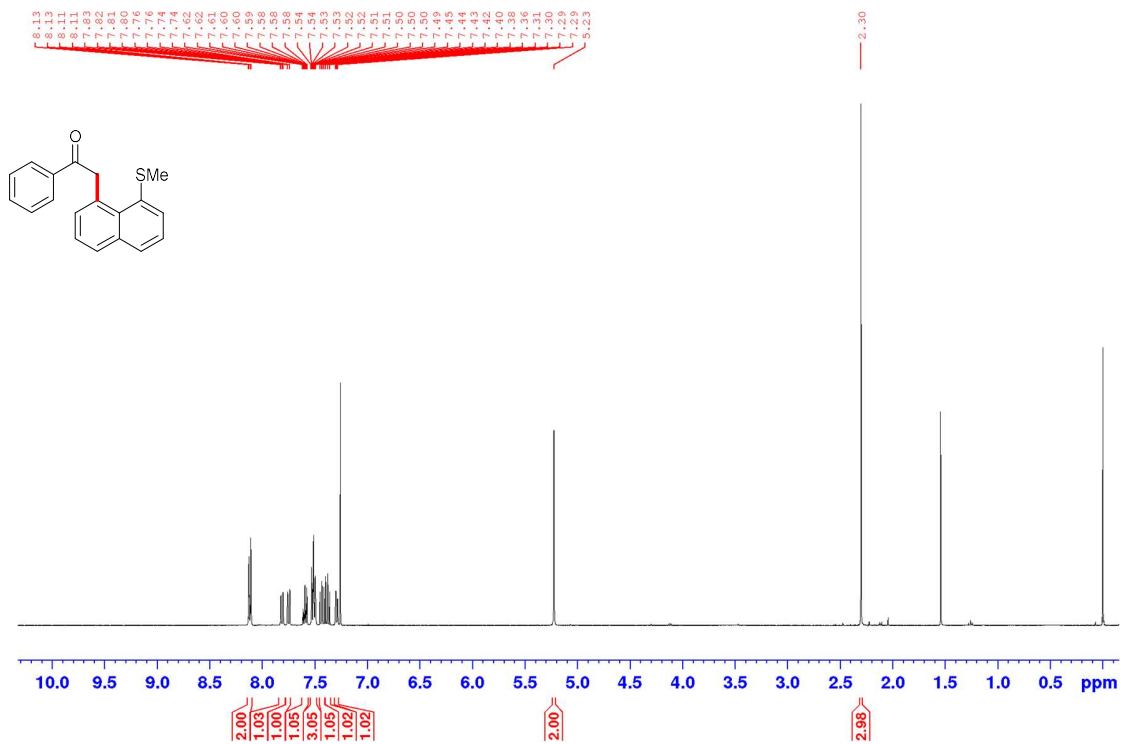| conc.	λ_{abs} [nm] (ε [10^3M^{-1}cm^{-1}])	λ_{abs}^{onset} [nm]	E_g [eV]	λ_{Fl} [nm]	Φ (%)
3da-1	370 (18), 392 (22), 430 (3.0)	481	2.58	481, 518, 551	24
3ea-1	332 (5.8), 374 (6.6), 393 (7.6)	460	2.70	465, 494, 525	22

2. ORTEP drawings

Figure S2. ORTEP drawing for **3ea** with 40% thermal ellipsoid. Hydrogen atoms are omitted for clarity.

Table S2. Crystal data for **3aa**

CCDC number	2027648
Crystal system	orthorhombic
Space group	$P\,2_12_12_1$ (No. 19)
Unit cell parameter [Å]	$a = 8.6647(3)$
	$b = 11.9879(3)$
	$c = 17.1653(5)$
Cell volume [Å^3]	1782.99(9)
Z	4
R factor ($I > 2.0\sigma(I)$)	$R1 = 0.0345, wR2 = 0.0867$
R factor (all data)	$R1 = 0.0387, wR2 = 0.0896$
Rint	0.0354
Goodness of fit	1.071

Figure S3. ORTEP drawing for **3ea-1** with 40% thermal ellipsoid. Hydrogen atoms are omitted for clarity.

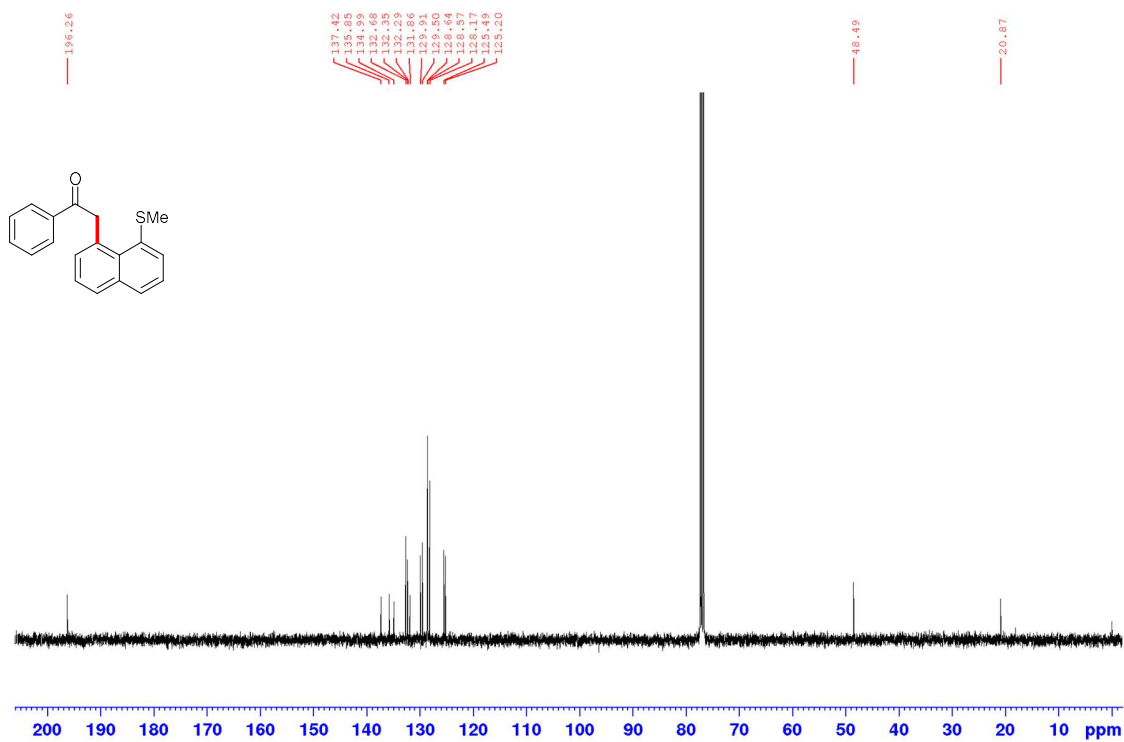**Table S3.** Crystal data for **3ab-dimer**

CCDC number	2027649
Crystal system	monoclinic
Space group	$P\,2_1/c$ (No. 14)
Unit cell parameter [Å, deg]	$a = 14.8770(11)$
	$b = 4.8413(3),\ \beta = 108.486(8)$
	$c = 21.7040(17)$
Cell volume [Å^3]	1482.5(2)
Z	4
R factor ($I > 2.0\sigma(I)$)	$R1 = 0.0512,\ wR2 = 0.1388$
R factor (all data)	$R1 = 0.0835,\ wR2 = 0.1542$
Rint	0.0437
Goodness of fit	1.050

3. Copy of NMR spectra

¹H NMR of **3aa** (400 MHz, CDCl₃)

¹³C NMR of **3aa** (100 MHz, CDCl₃)

¹H NMR of **3ba** (400 MHz, CDCl₃)
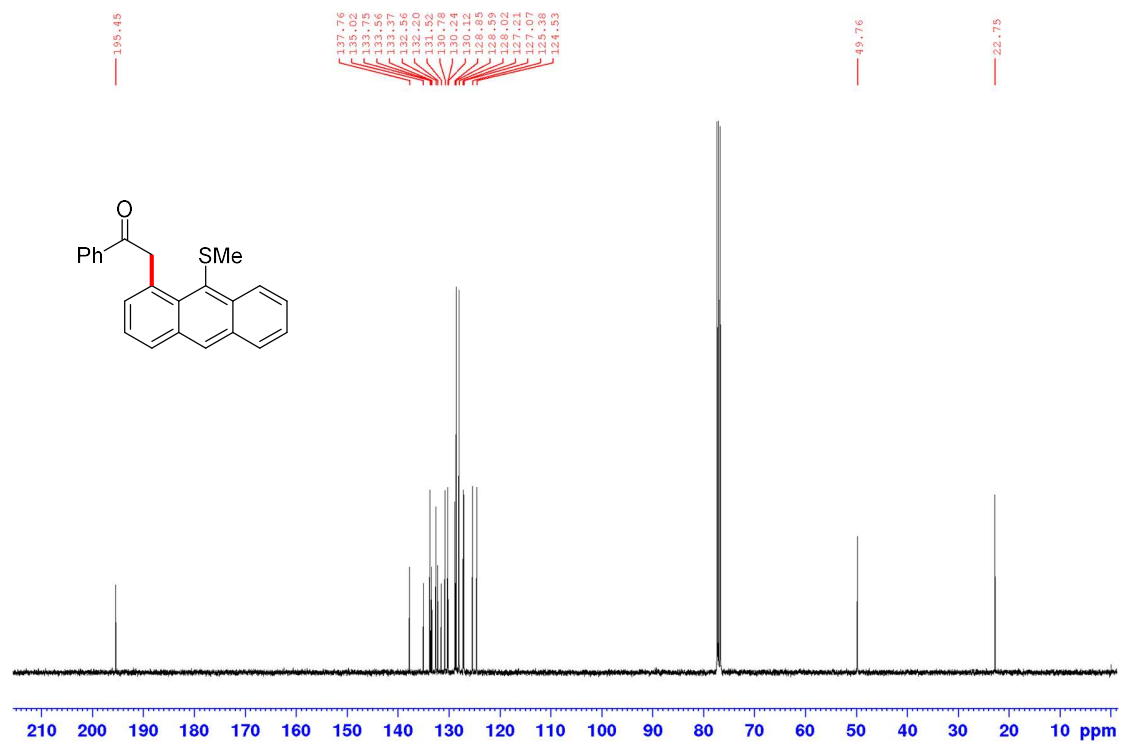

¹³C NMR of **3ba** (100 MHz, CDCl₃)

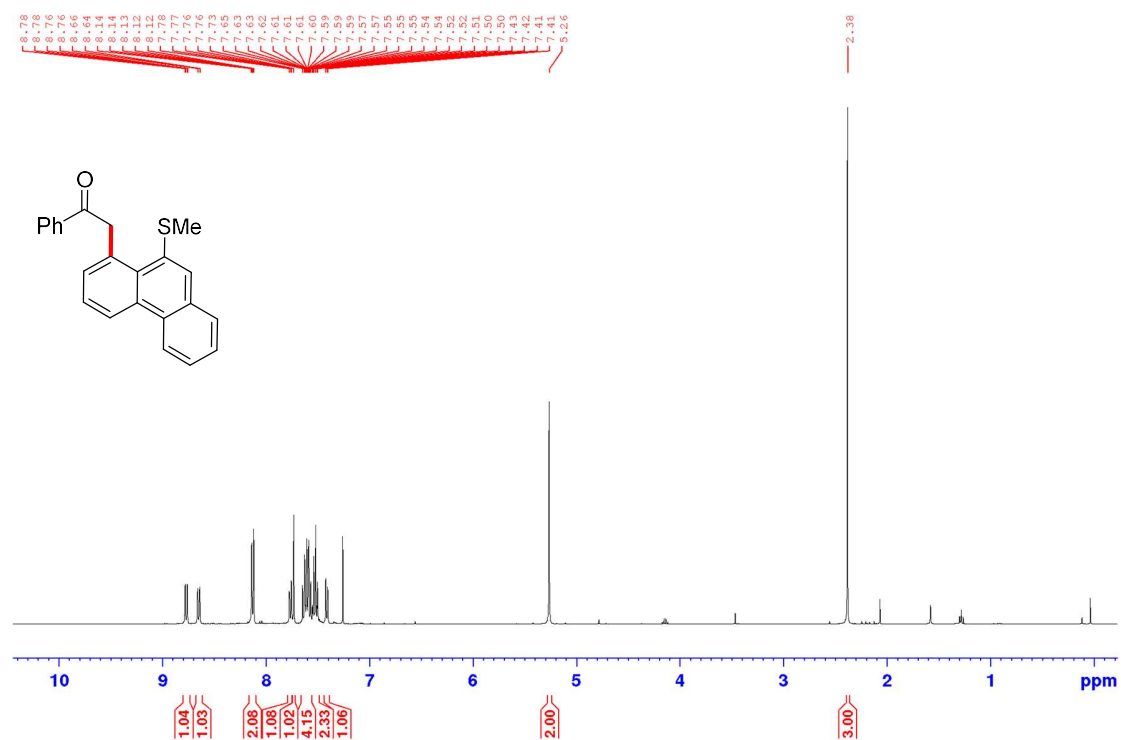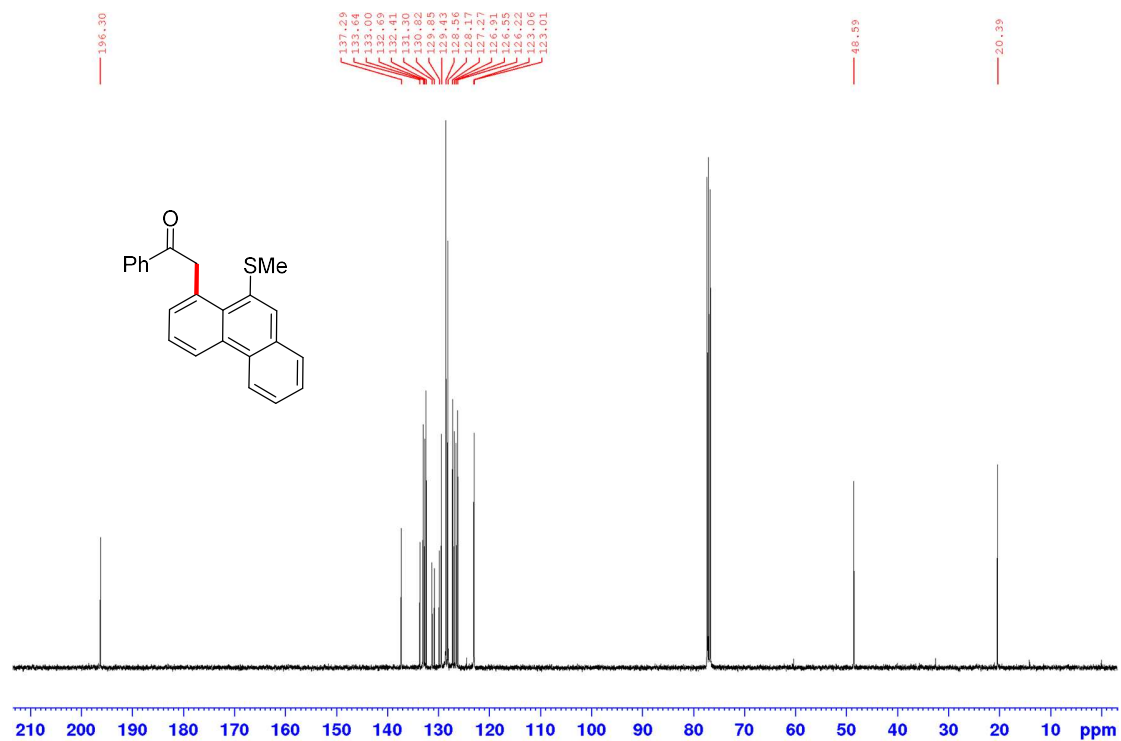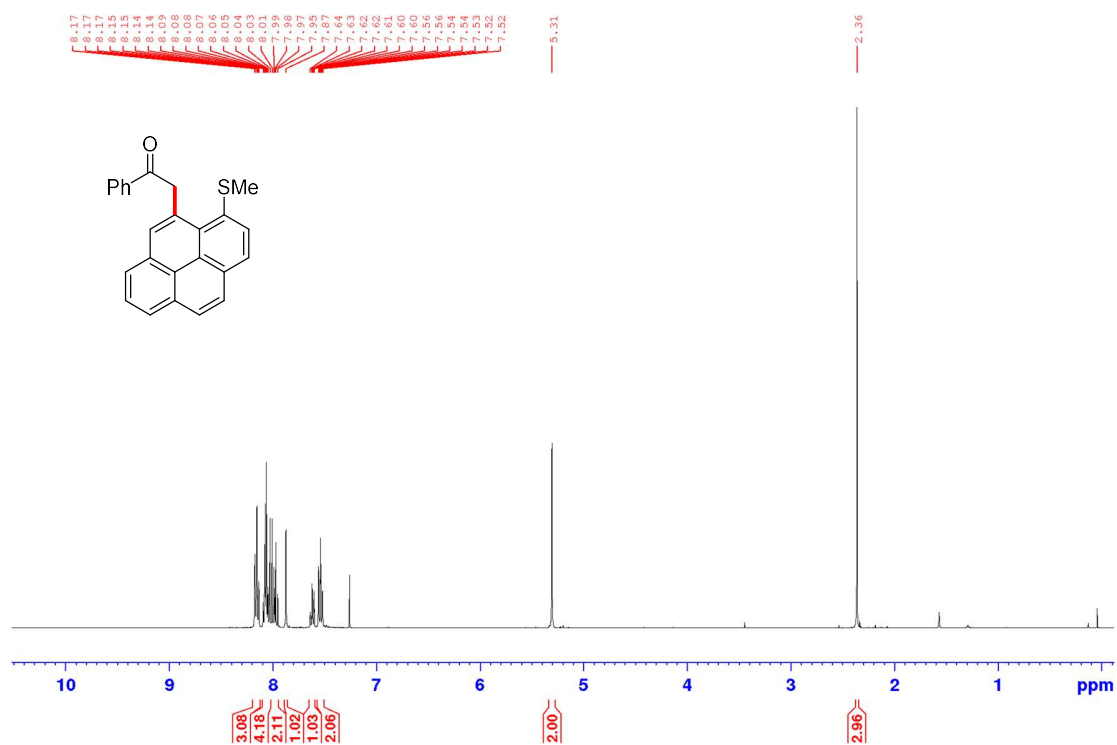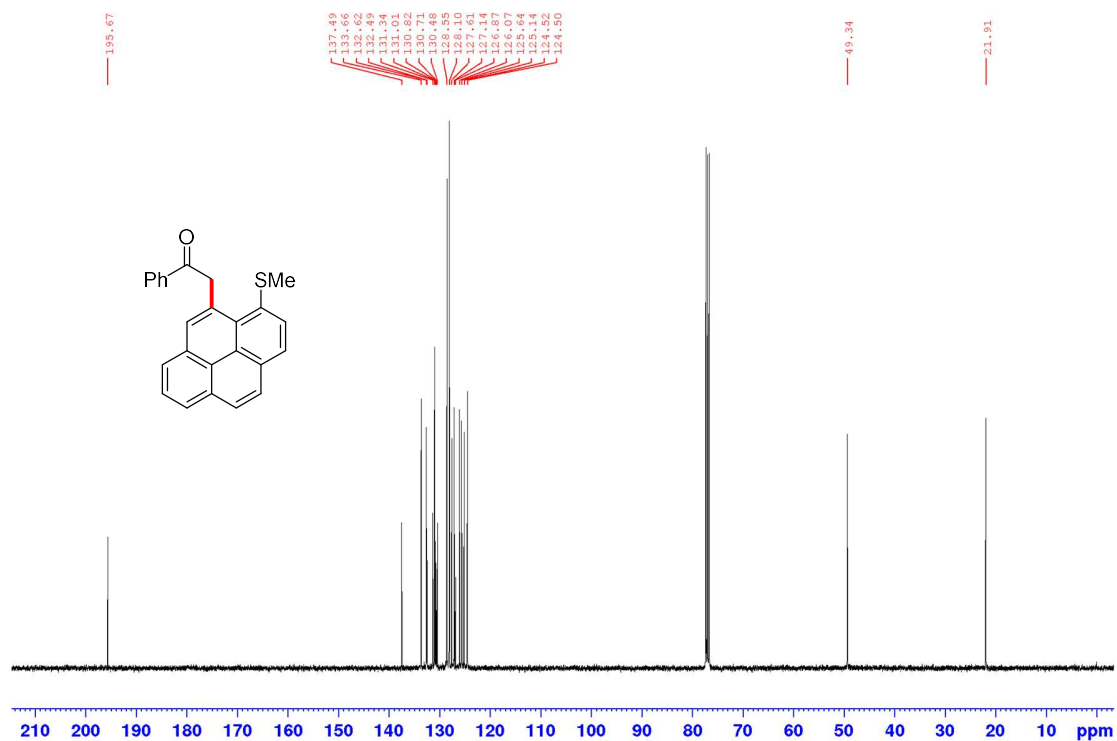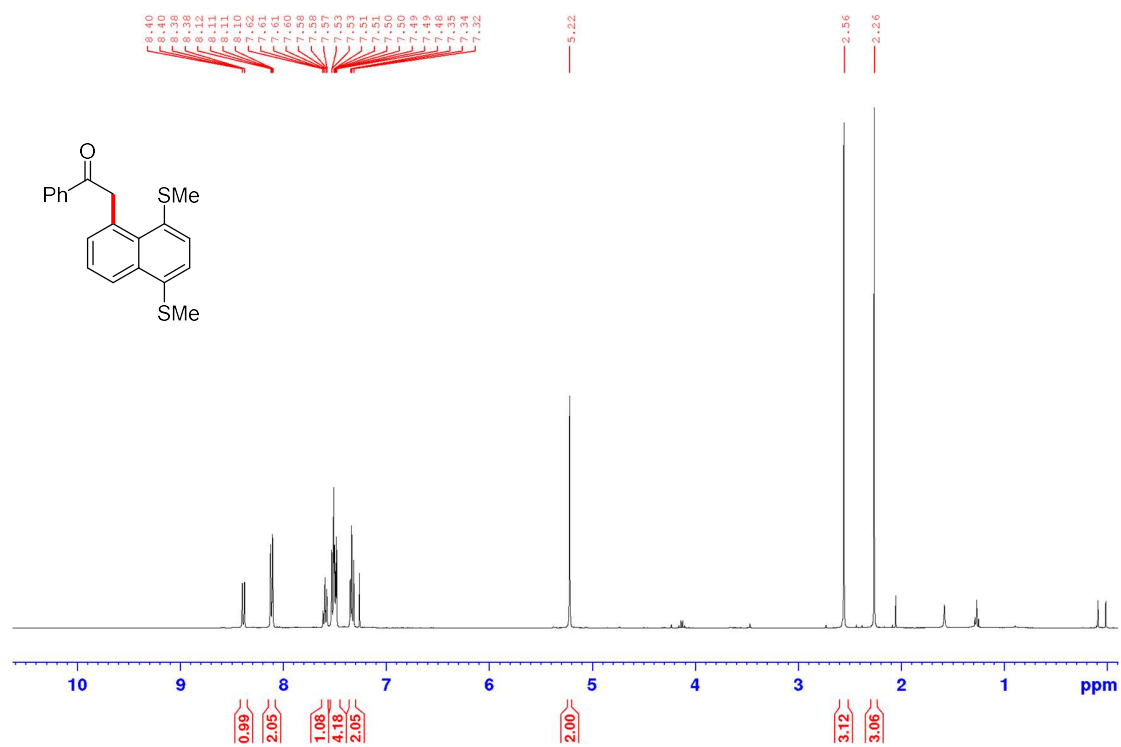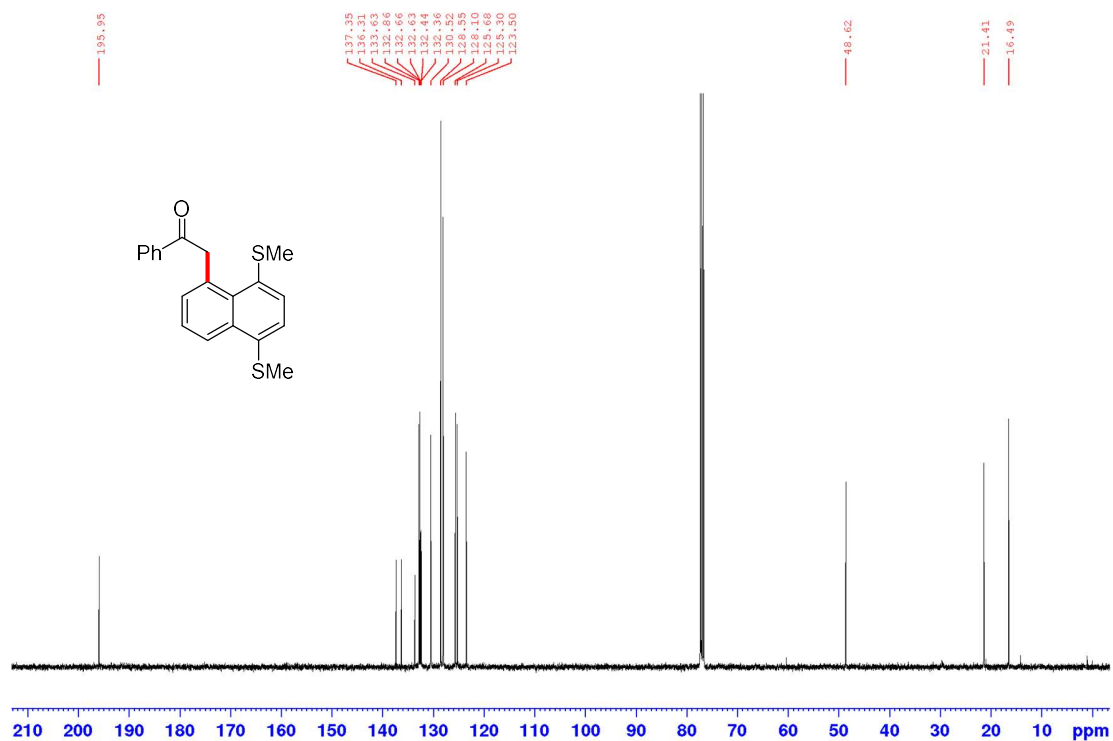¹H NMR of **3ca** (400 MHz, CDCl₃)

¹³C NMR of **3ca** (100 MHz, CDCl₃)

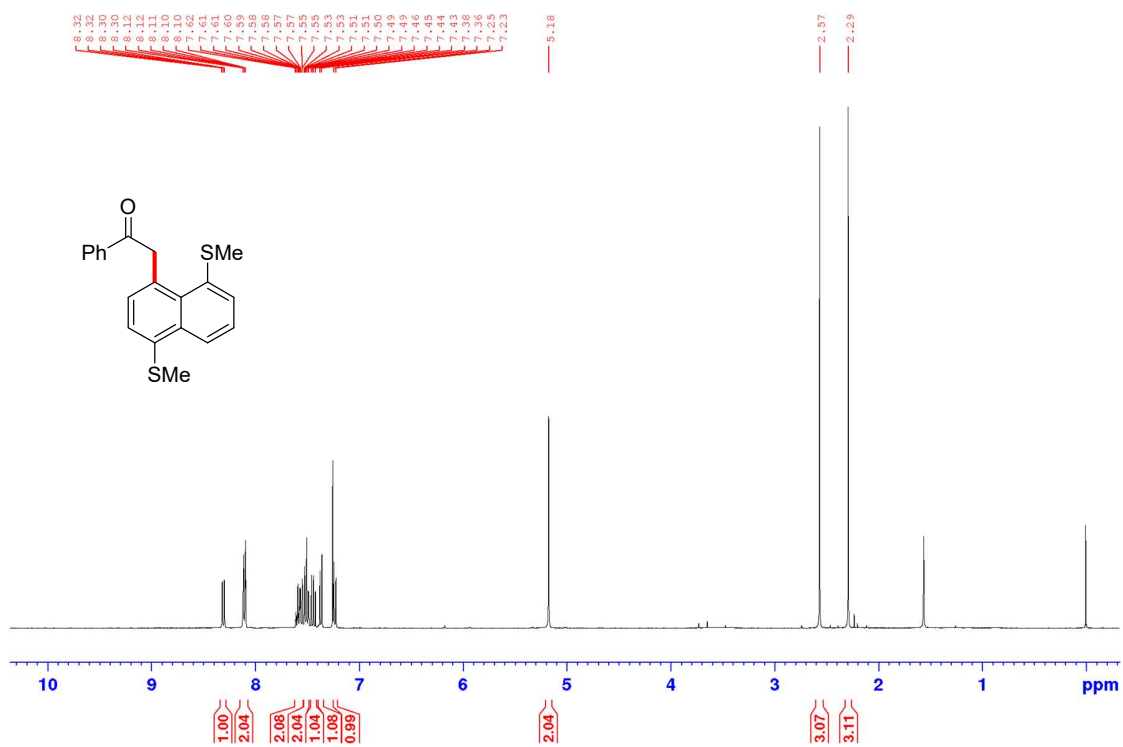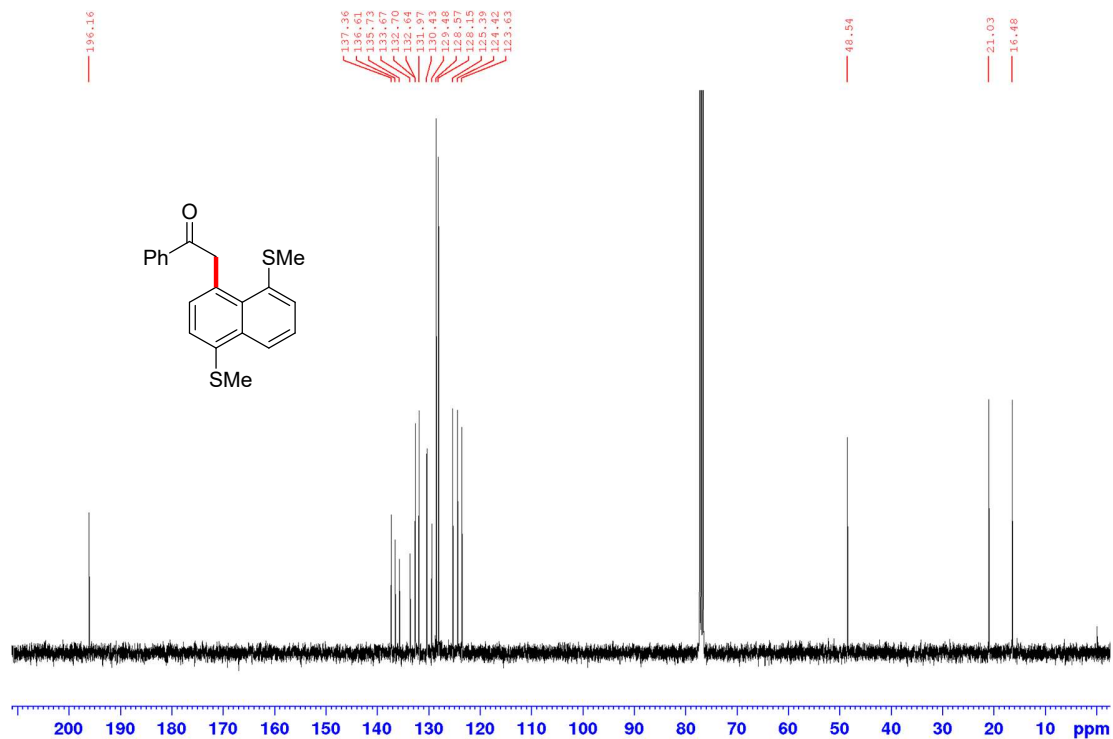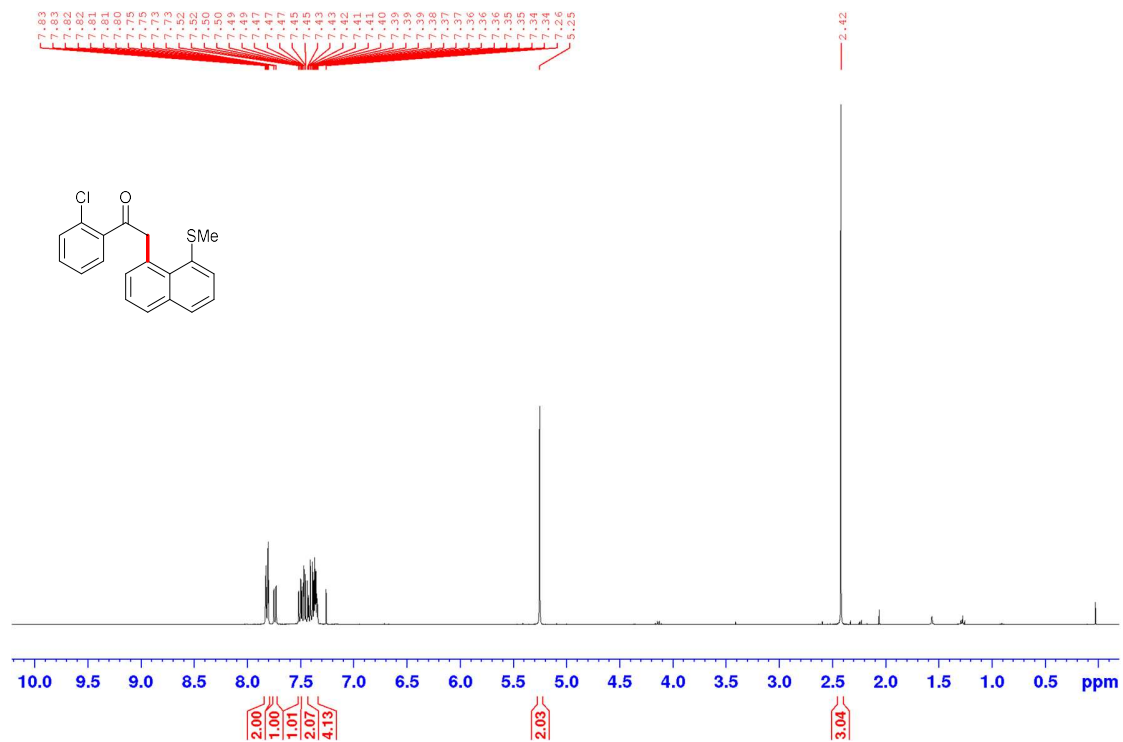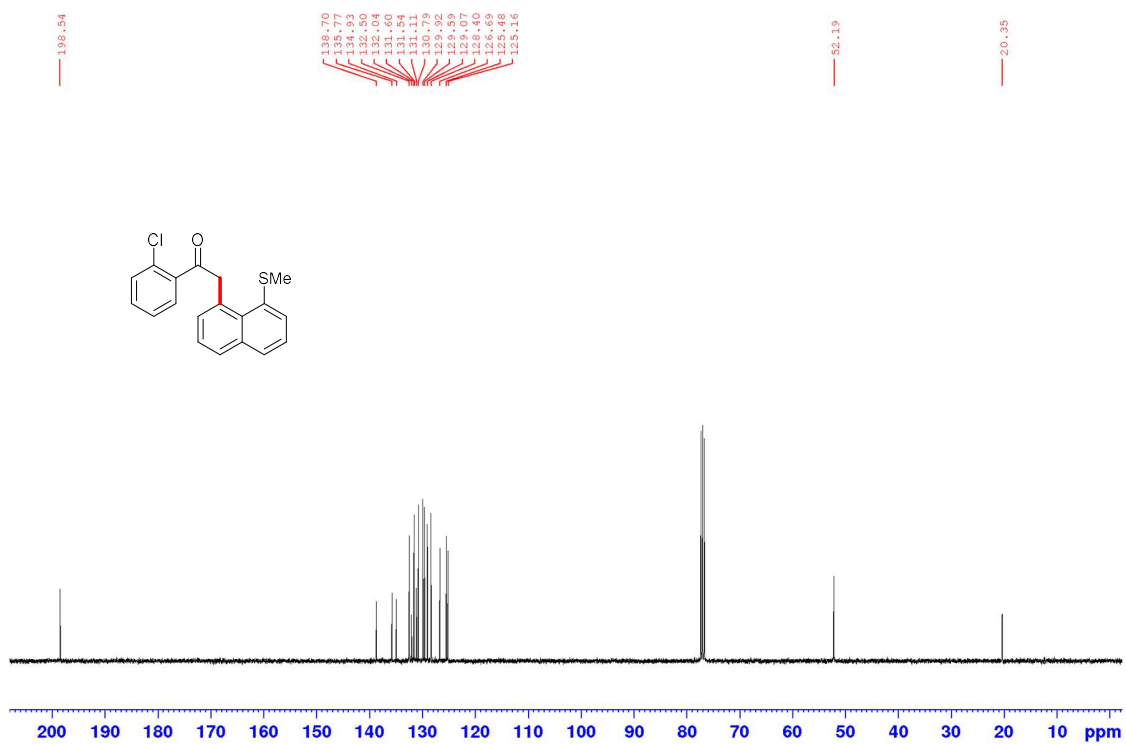¹H NMR of **3da** (400 MHz, CDCl₃)

¹³C NMR of **3da** (100 MHz, CDCl₃)

¹H NMR of **3ea** (400 MHz, CDCl₃)

¹³C NMR of **3ea** (100 MHz, CDCl₃)
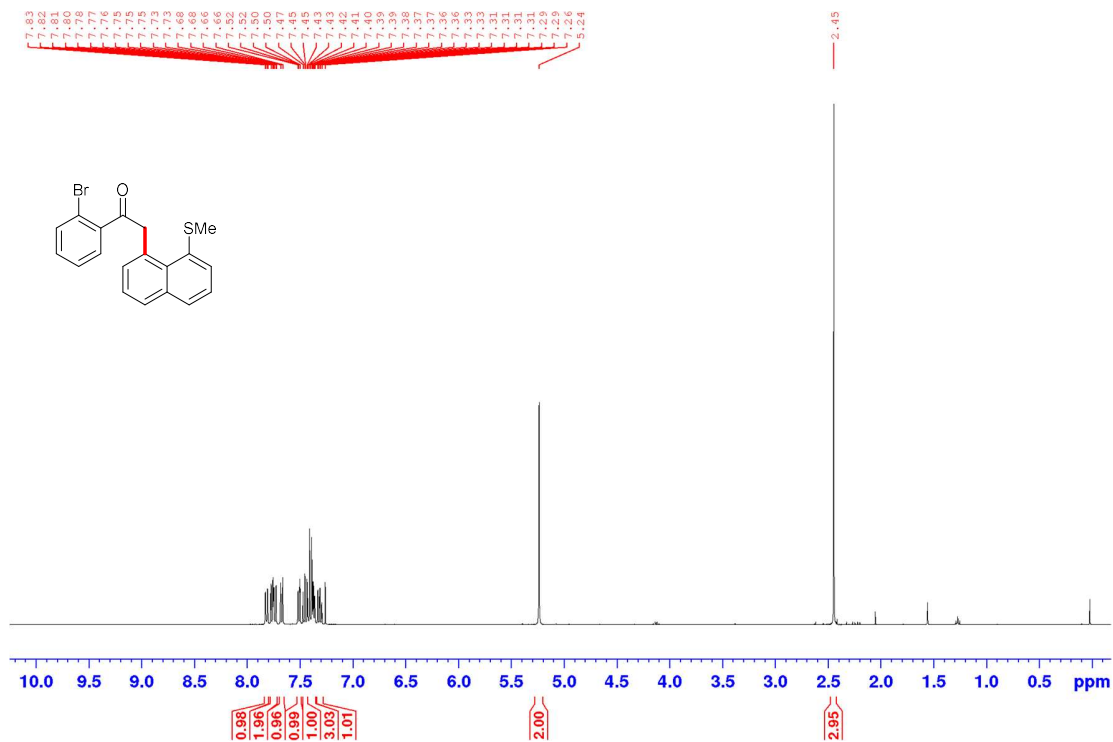
¹H NMR of **3fa** (400 MHz, CDCl₃)
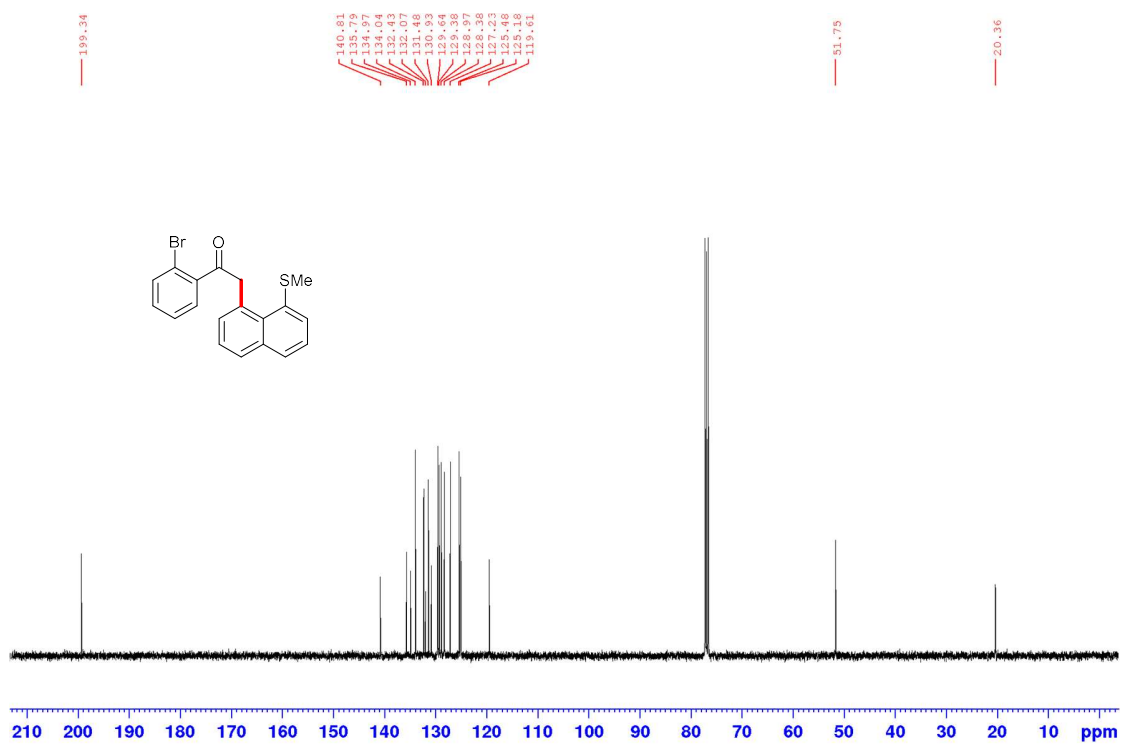

¹³C NMR of **3fa** (100 MHz, CDCl₃)
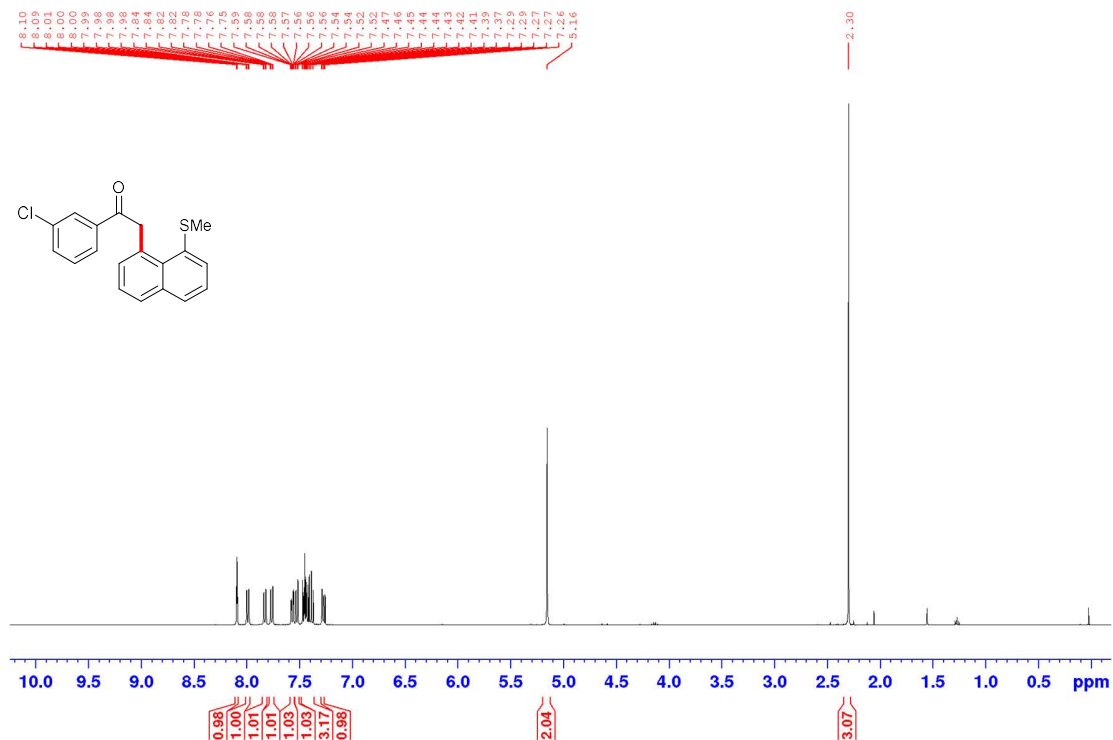
¹H NMR of **3ga** (400 MHz, CDCl₃)

¹³C NMR of **3ga** (100 MHz, CDCl₃)

¹H NMR of **3ab** (400 MHz, CDCl₃)

¹³C NMR of **3ab** (100 MHz, CDCl₃)

¹H NMR of **3ac** (400 MHz, CDCl₃)
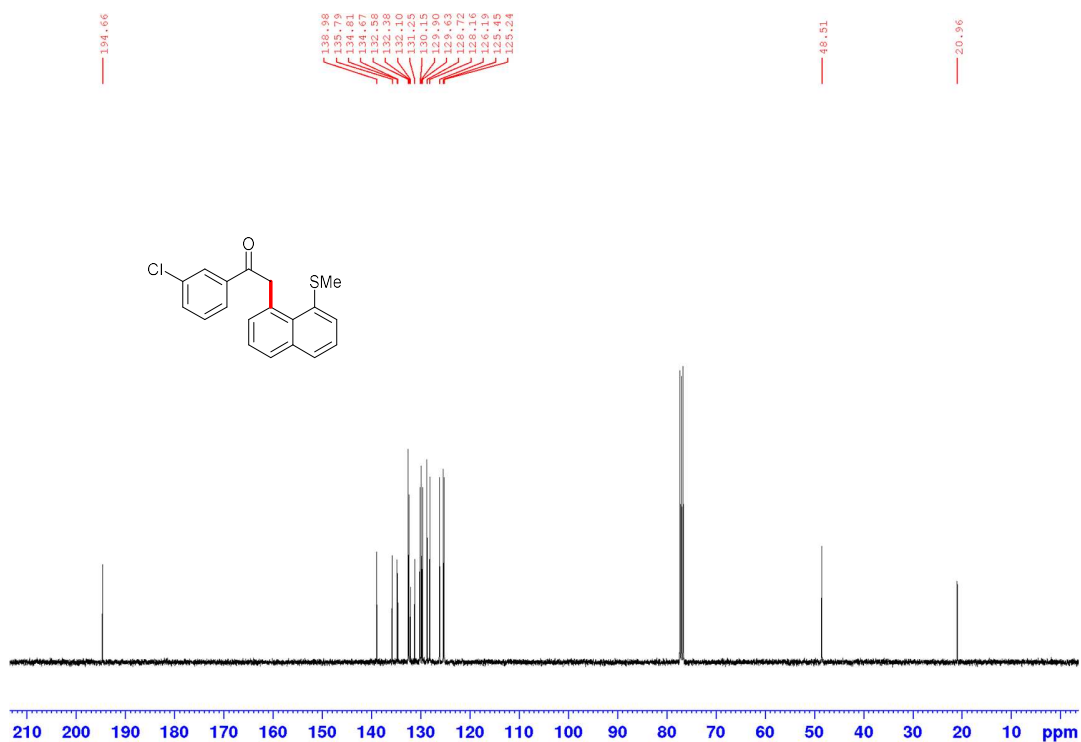

¹³C NMR of **3ac** (100 MHz, CDCl₃)

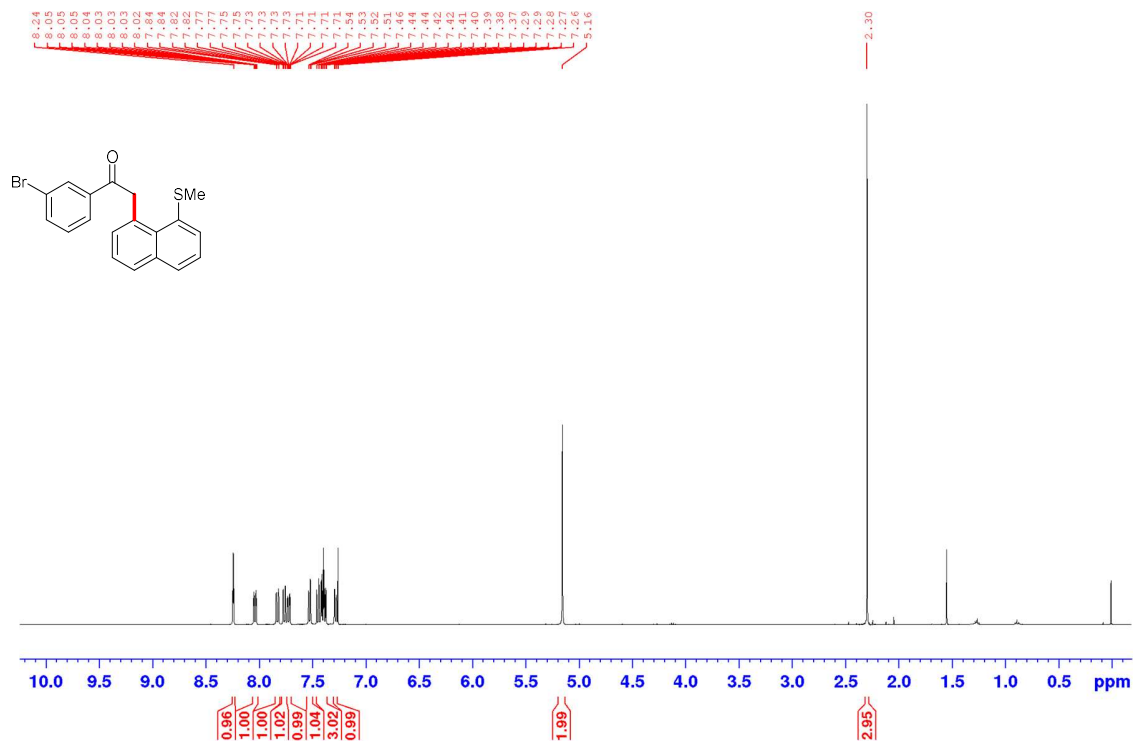¹H NMR of **3ad** (400 MHz, CDCl₃)

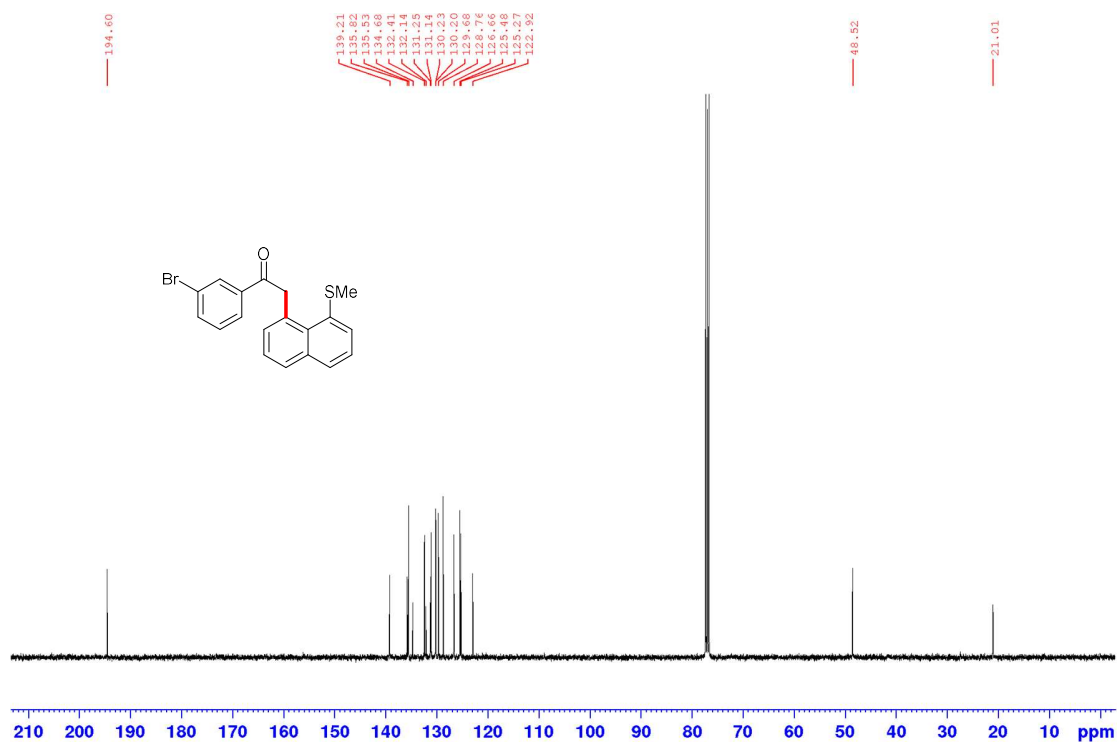¹³C NMR of **3ad** (100 MHz, CDCl₃)
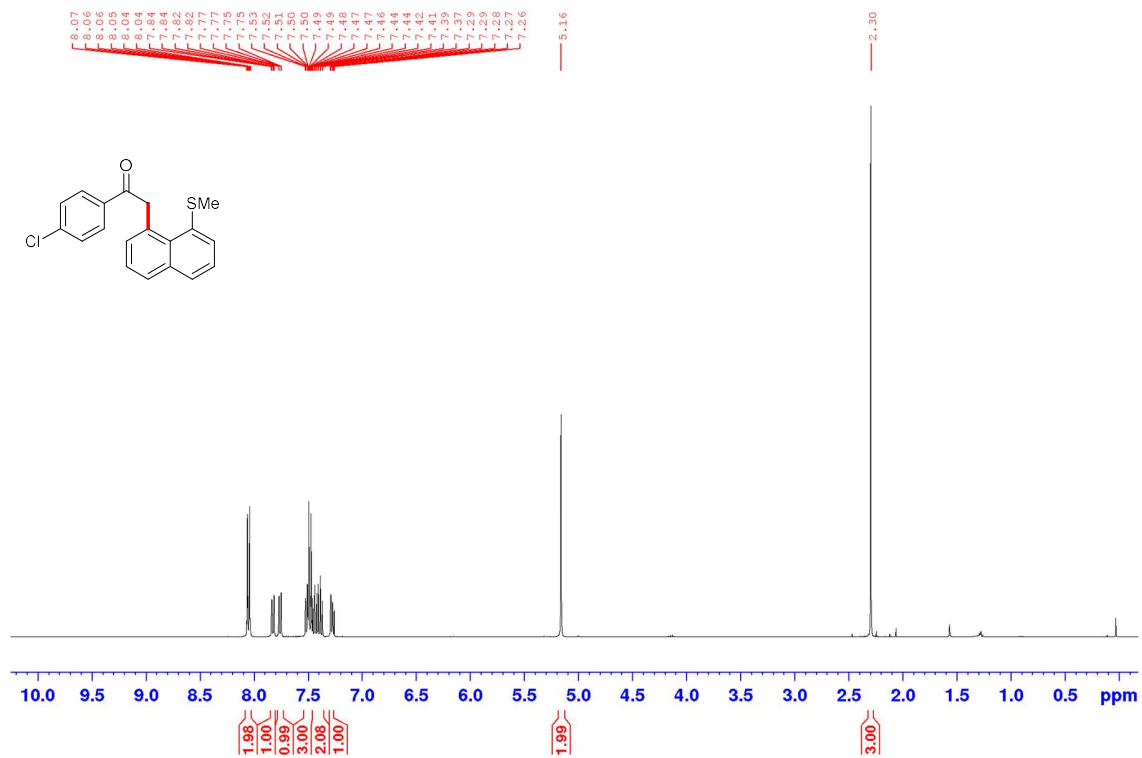
¹H NMR of **3ae** (400 MHz, CDCl₃)
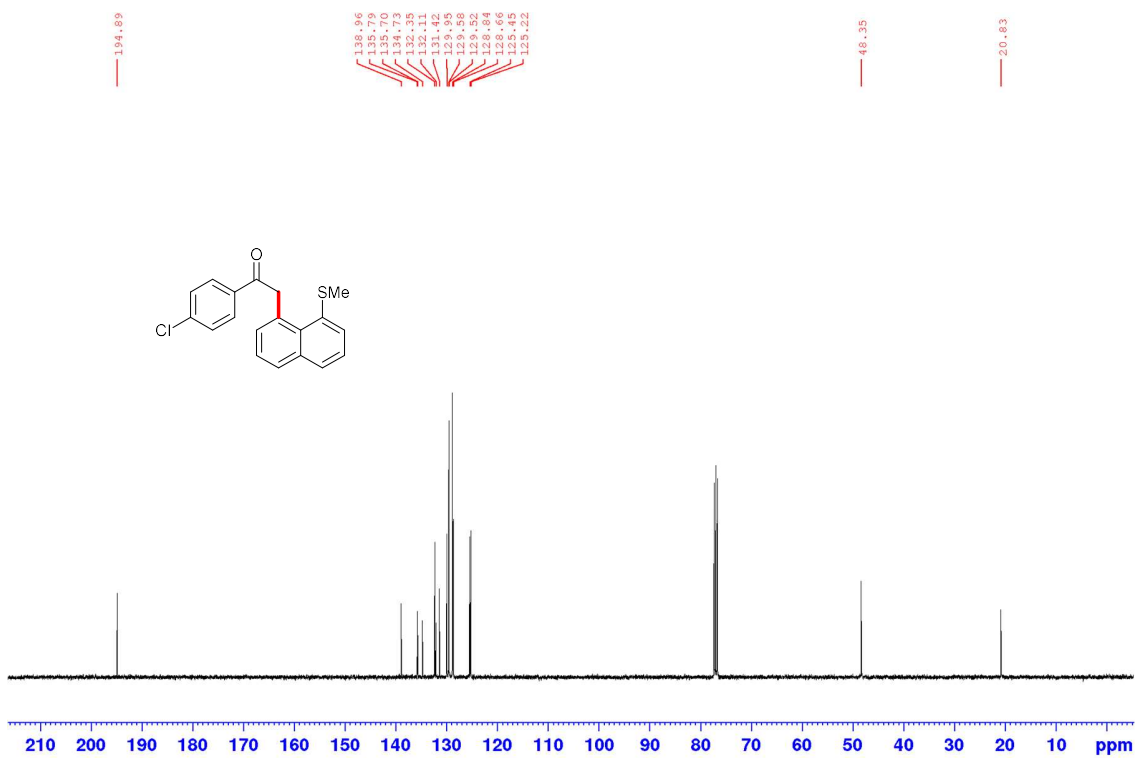

¹³C NMR of **3ae** (100 MHz, CDCl₃)
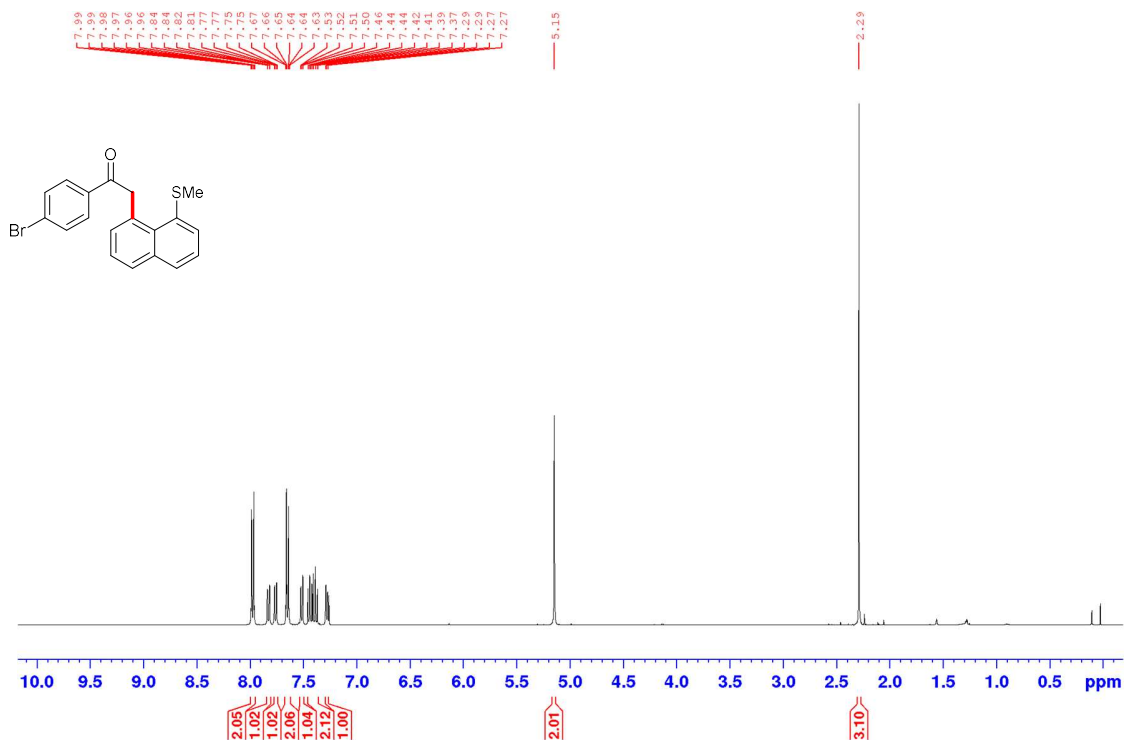
¹H NMR of **3af** (400 MHz, CDCl₃)
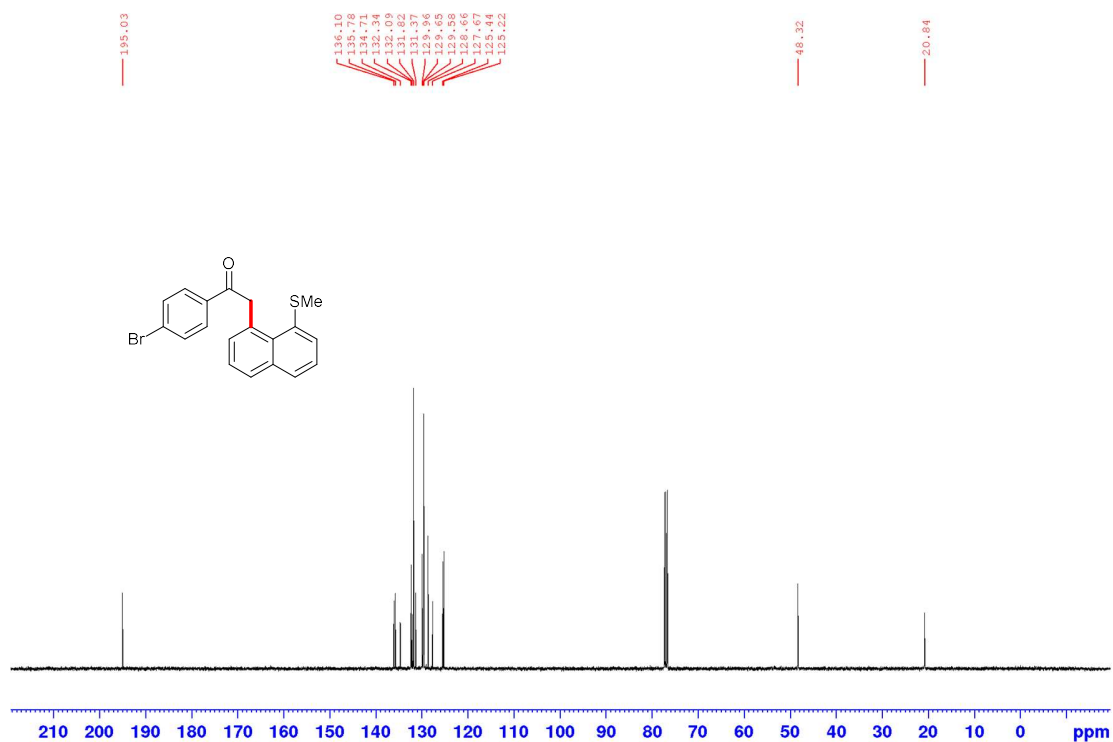

¹³C NMR of **3af** (100 MHz, CDCl₃)

¹H NMR of **3ag** (400 MHz, CDCl₃)

¹³C NMR of **3ag** (100 MHz, CDCl₃)

¹H NMR of **3ah** (400 MHz, CDCl₃)

¹³C NMR of **3ah** (100 MHz, CDCl₃)

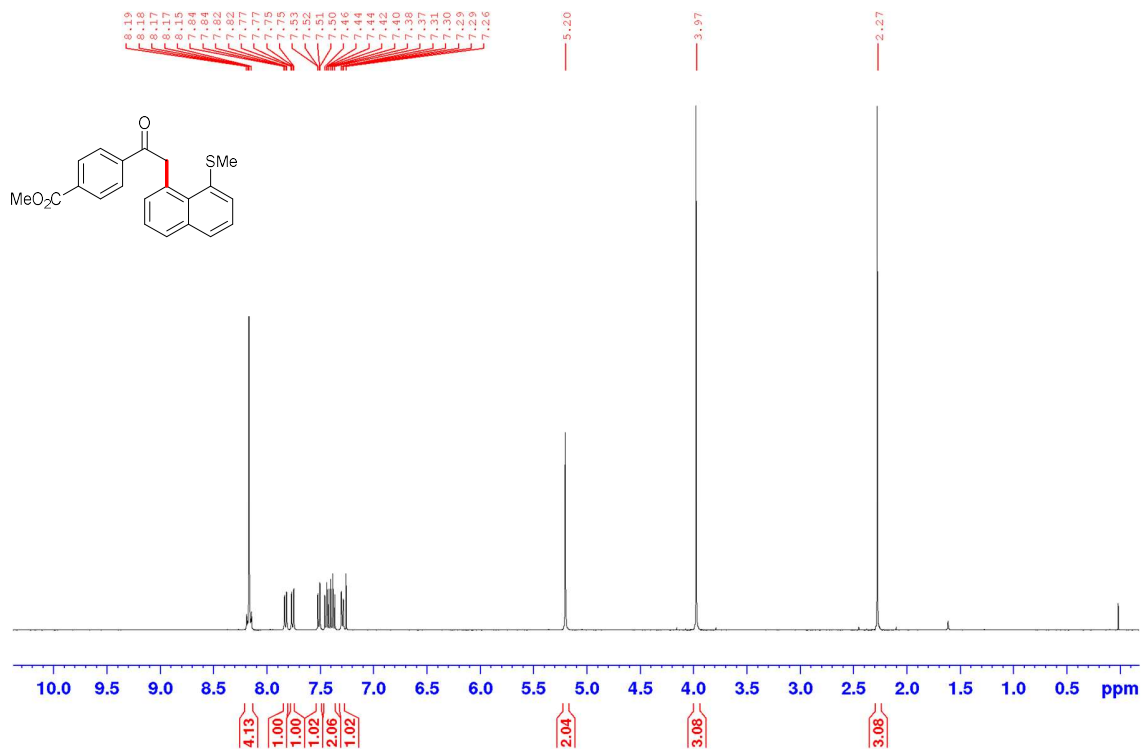¹H NMR of **3ai** (400 MHz, CDCl₃)

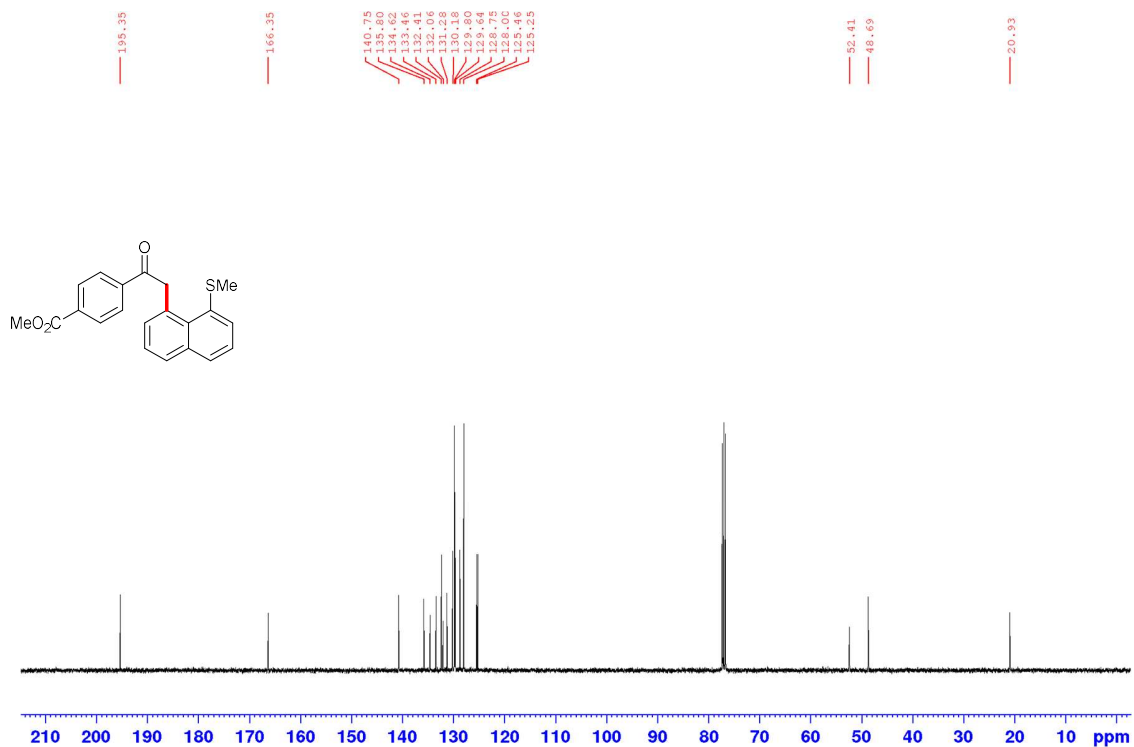¹³C NMR of **3ai** (100 MHz, CDCl₃)
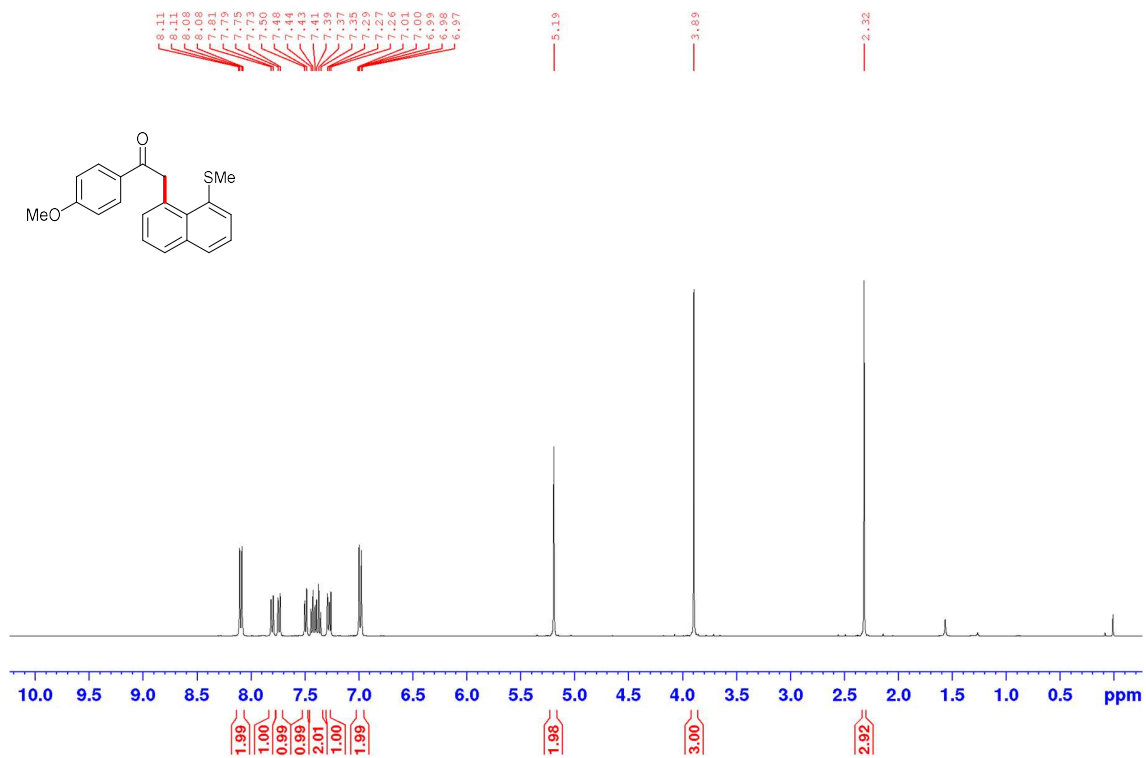
¹H NMR of **3aj** (400 MHz, CDCl₃)
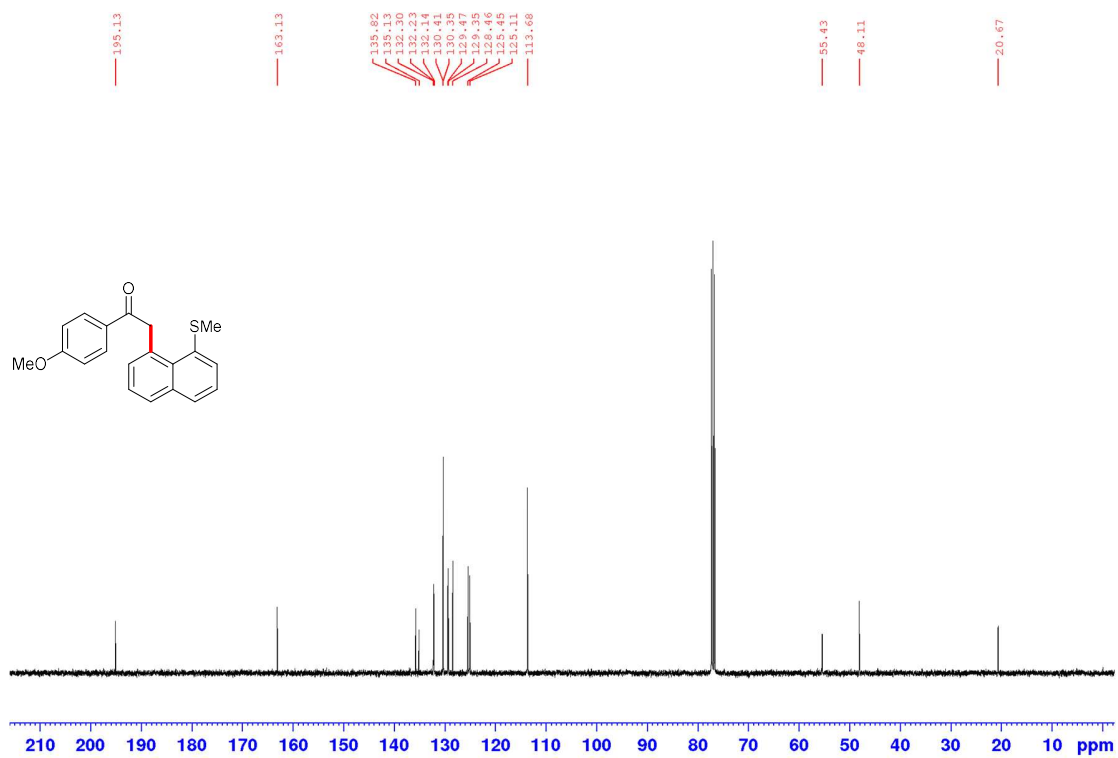

¹³C NMR of **3aj** (100 MHz, CDCl₃)

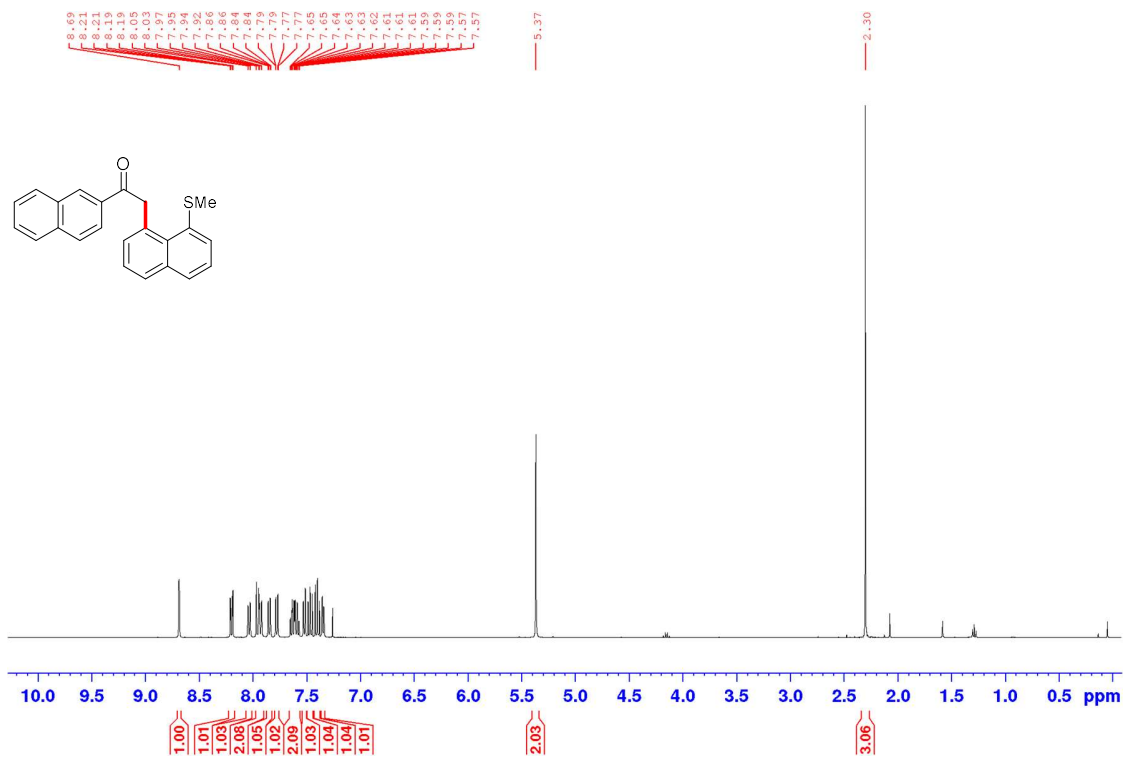¹H NMR of **3ak** (400 MHz, CDCl₃)
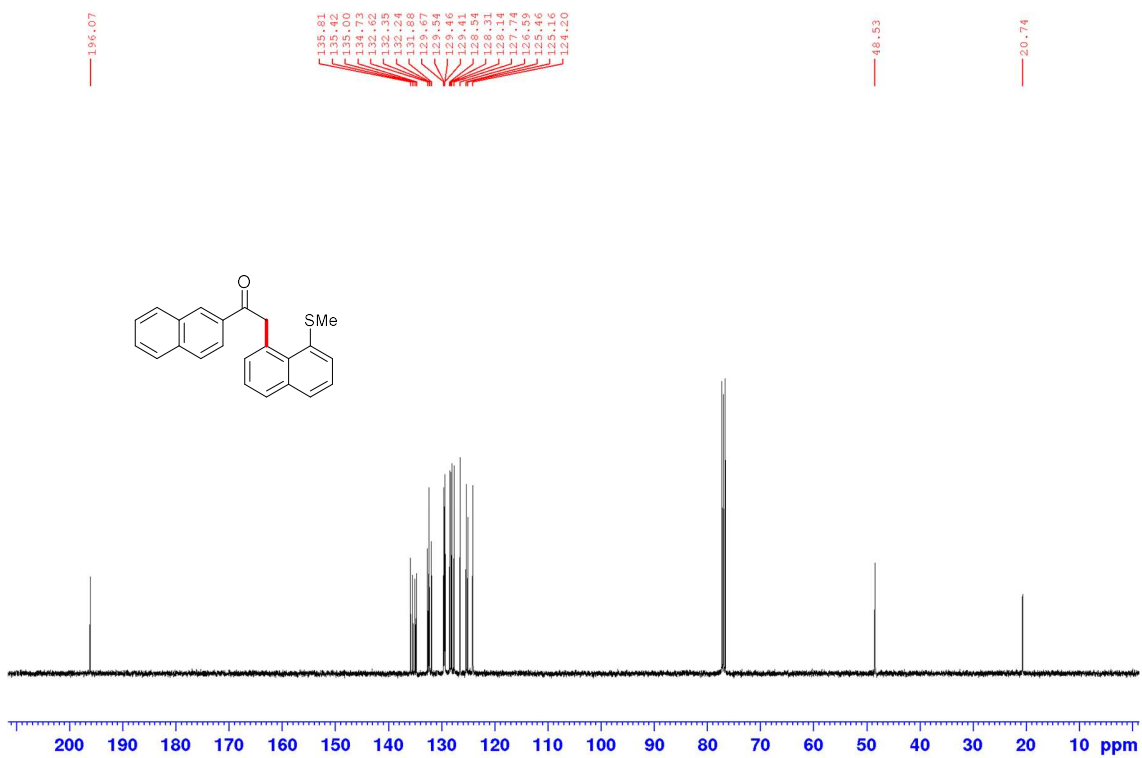

¹³C NMR of **3ak** (100 MHz, CDCl₃)
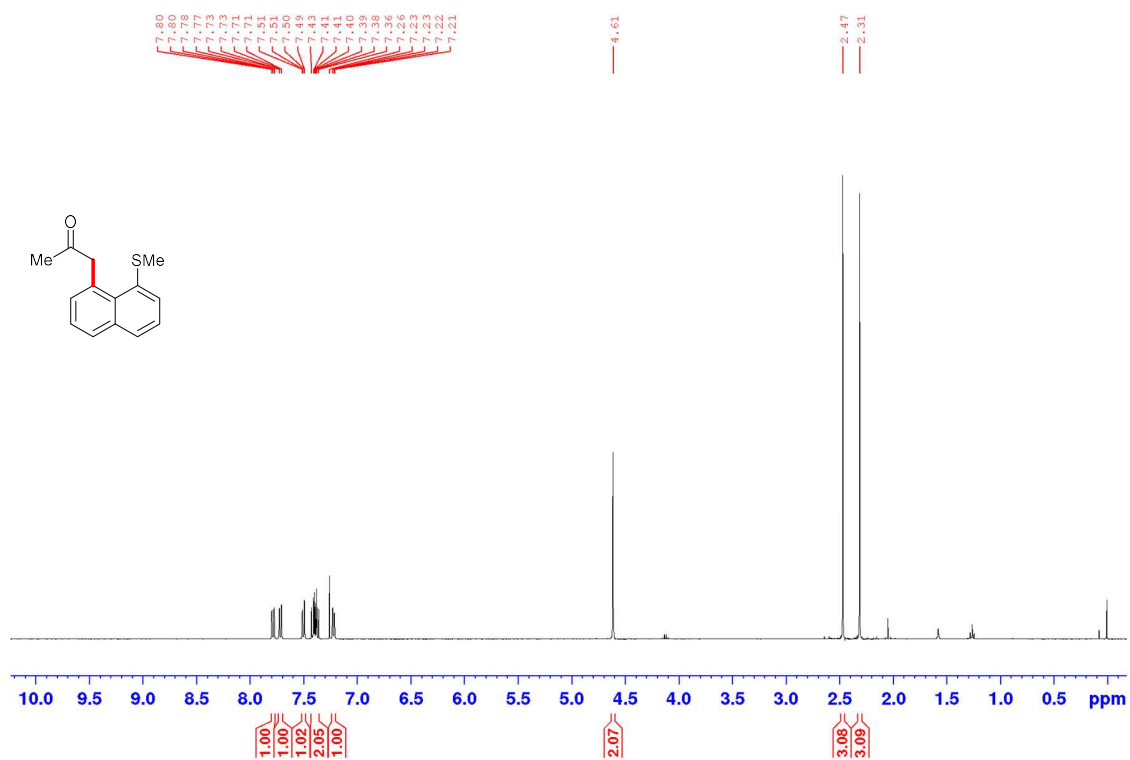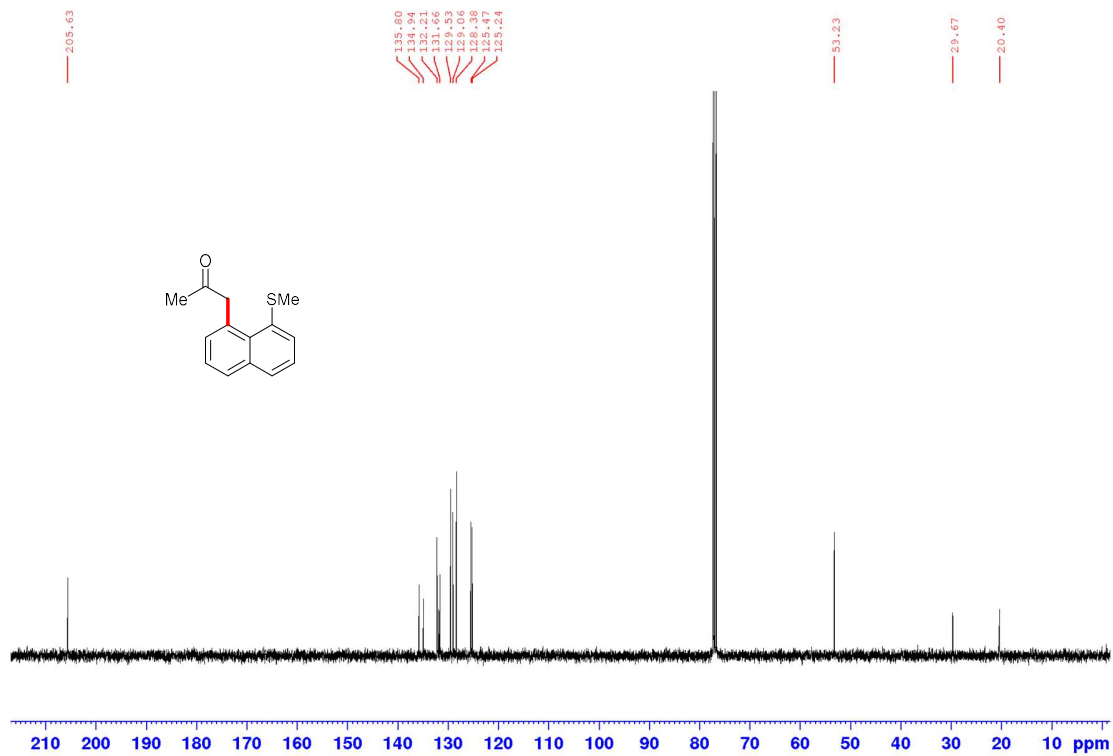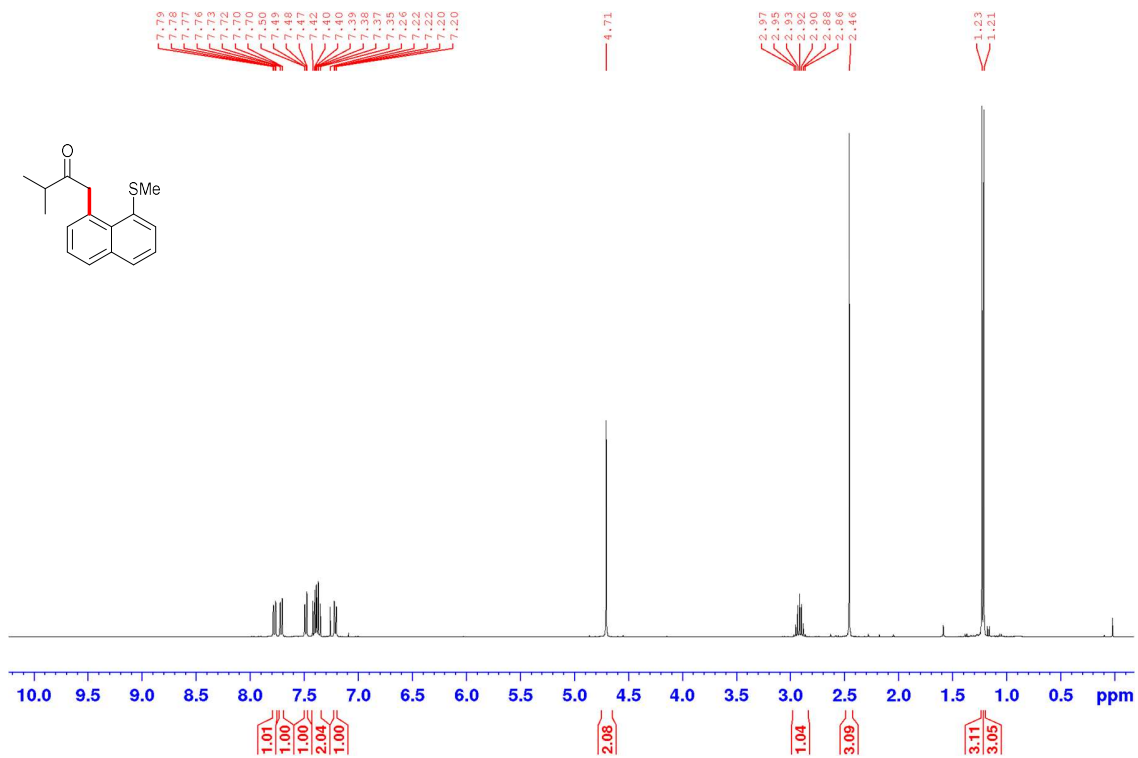
¹H NMR of **3al** (400 MHz, CDCl₃)

¹³C NMR of **3al** (100 MHz, CDCl₃)

¹H NMR of **3am** (400 MHz, CDCl₃)

7.78
7.78
7.76
7.76
7.72
7.72
7.70
7.70
7.49
7.47
7.41
7.39
7.38
7.37
7.36
7.34
7.20
7.26
7.20
7.19
7.18

4.70
2.69
2.68
2.67
2.66
2.65
2.63
2.62
2.45
2.04
2.03
2.02
2.00
1.86
1.85
1.84
1.83
1.82
1.81
1.80
1.72
1.71
1.71
1.70
1.69
1.69
1.68
1.68
1.67
1.53
1.50
1.47
1.44
1.43
1.37

1.01
1.00
1.00
2.03
1.00

2.03

1.04
3.04

2.09
2.13
1.13
2.14
3.60

¹³C NMR of **3am** (100 MHz, CDCl₃)

210.46

135.74
135.01
132.14
132.01
131.90
129.22
128.87
128.29
125.36
125.07

50.48
50.34

28.93
25.93
25.80
20.30

¹H NMR of **3an** (400 MHz, CDCl₃)

¹³C NMR of **3an** (100 MHz, CDCl₃)

S24

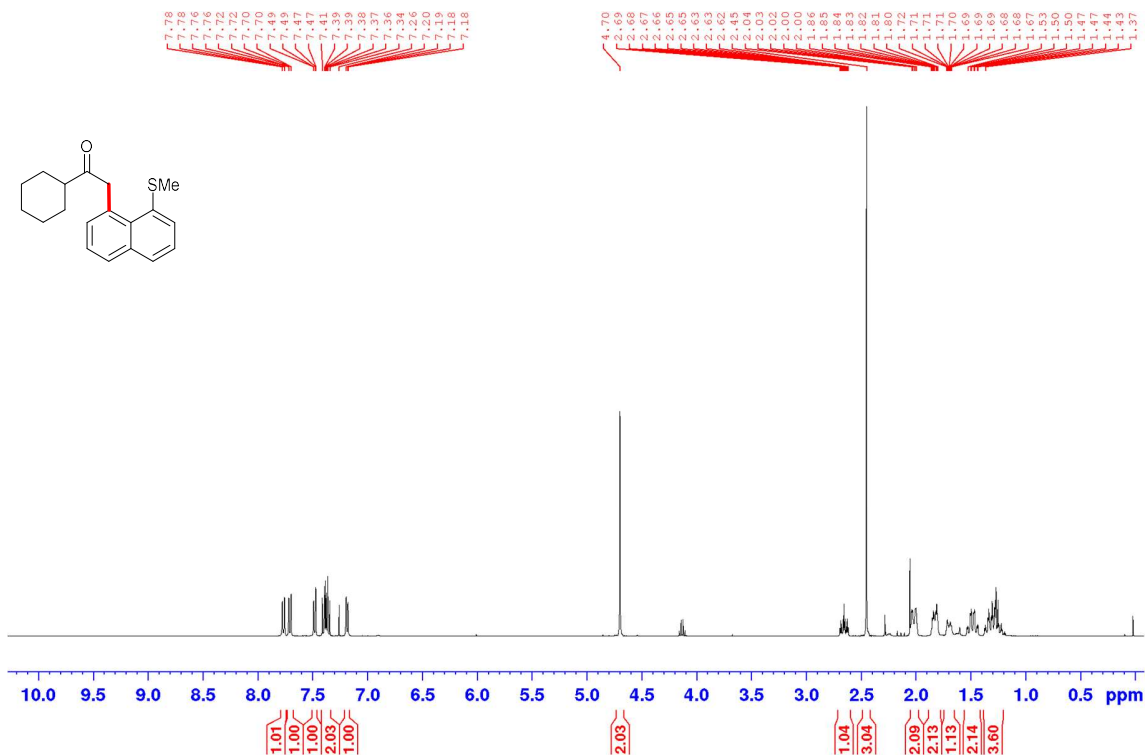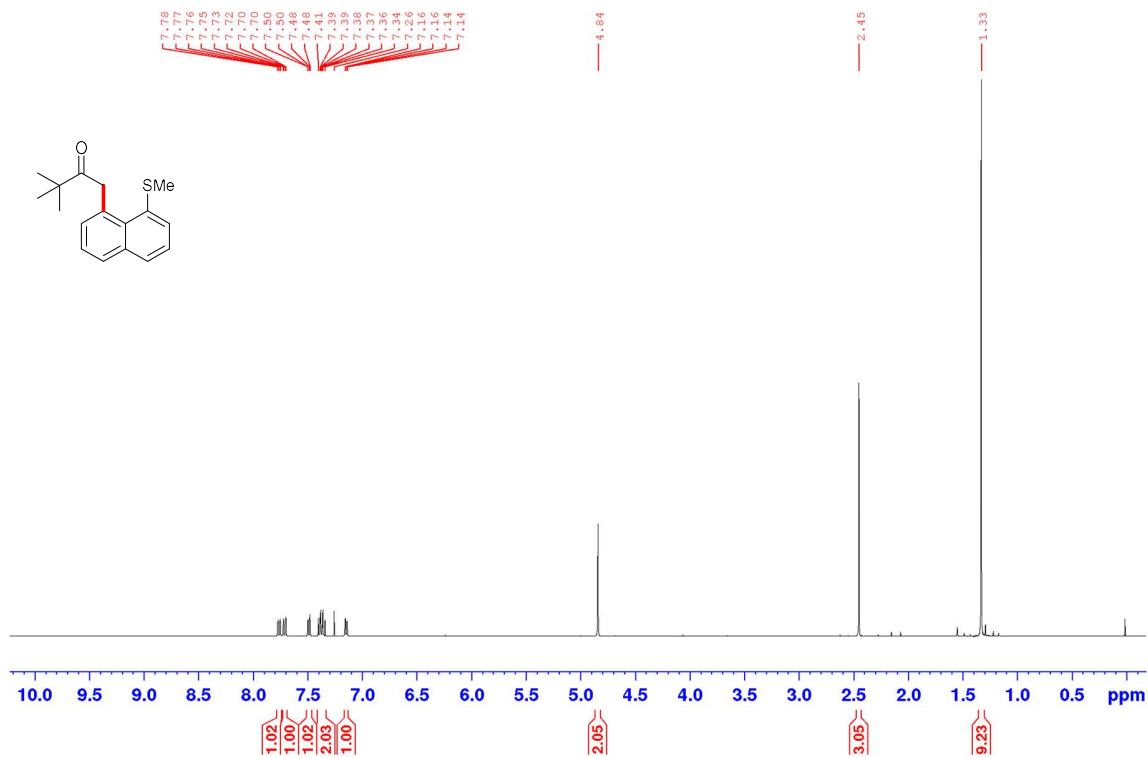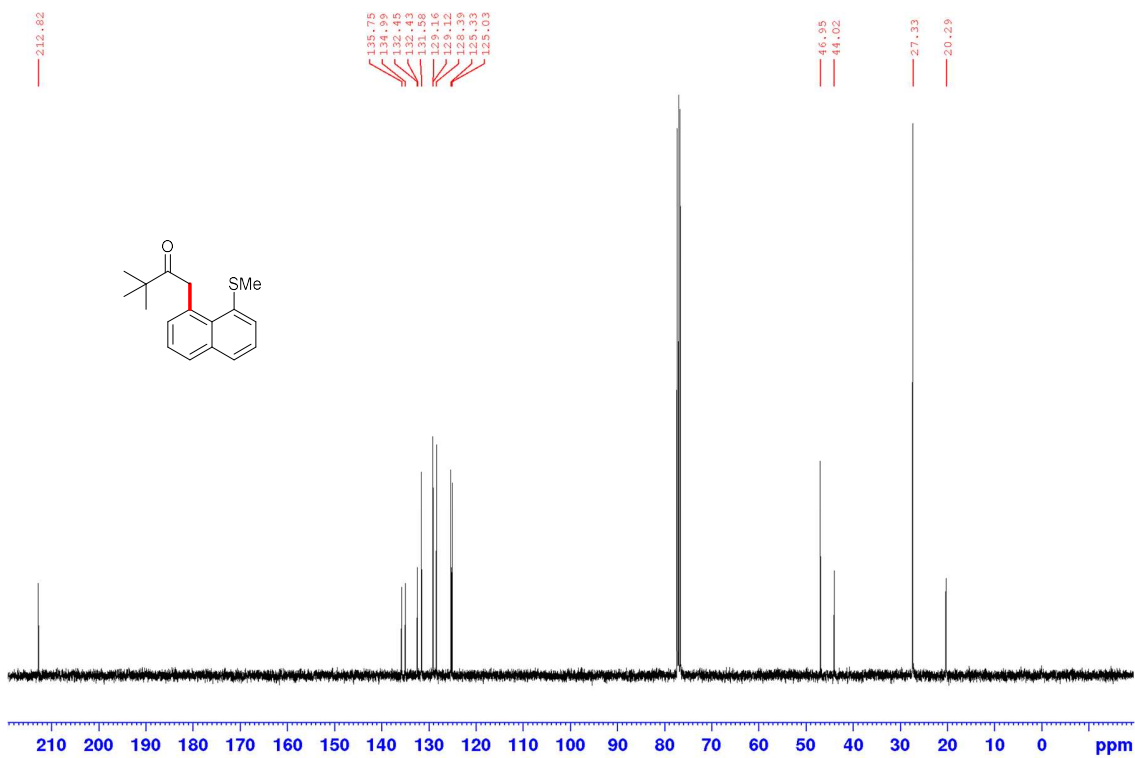¹H NMR of **3ap** (400 MHz, CDCl₃)

¹³C NMR of **3ap** (100 MHz, CDCl₃)

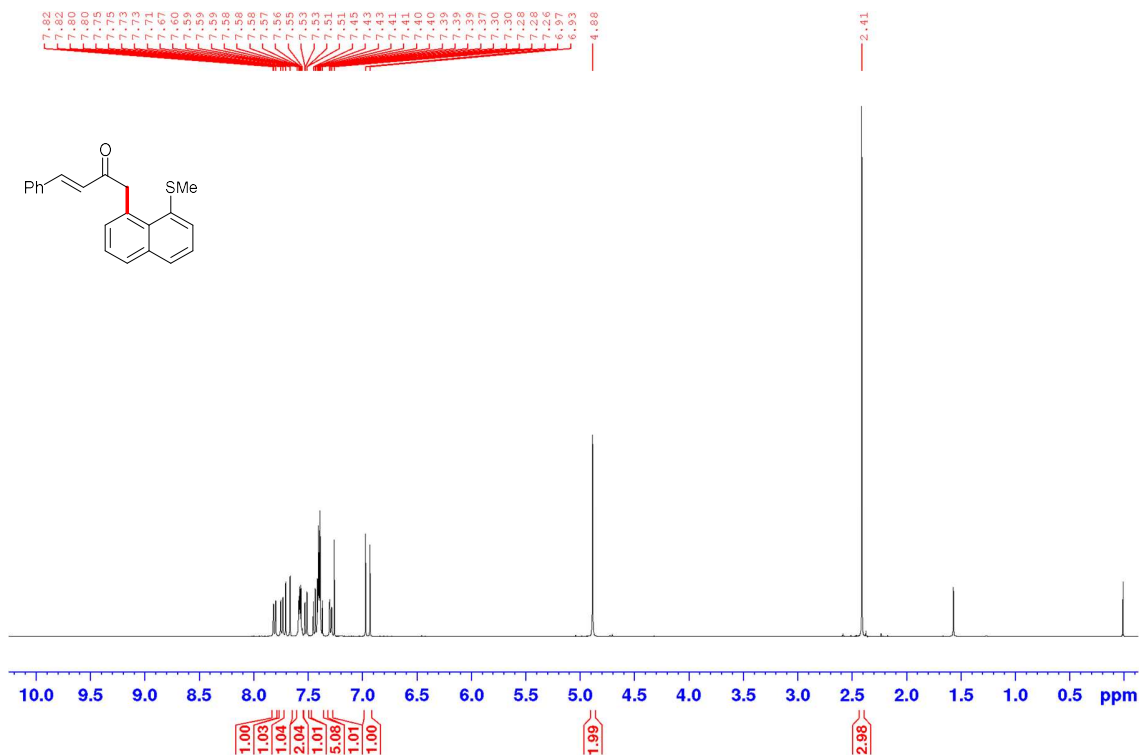¹H NMR of **3aa-1** (400 MHz, CDCl₃)
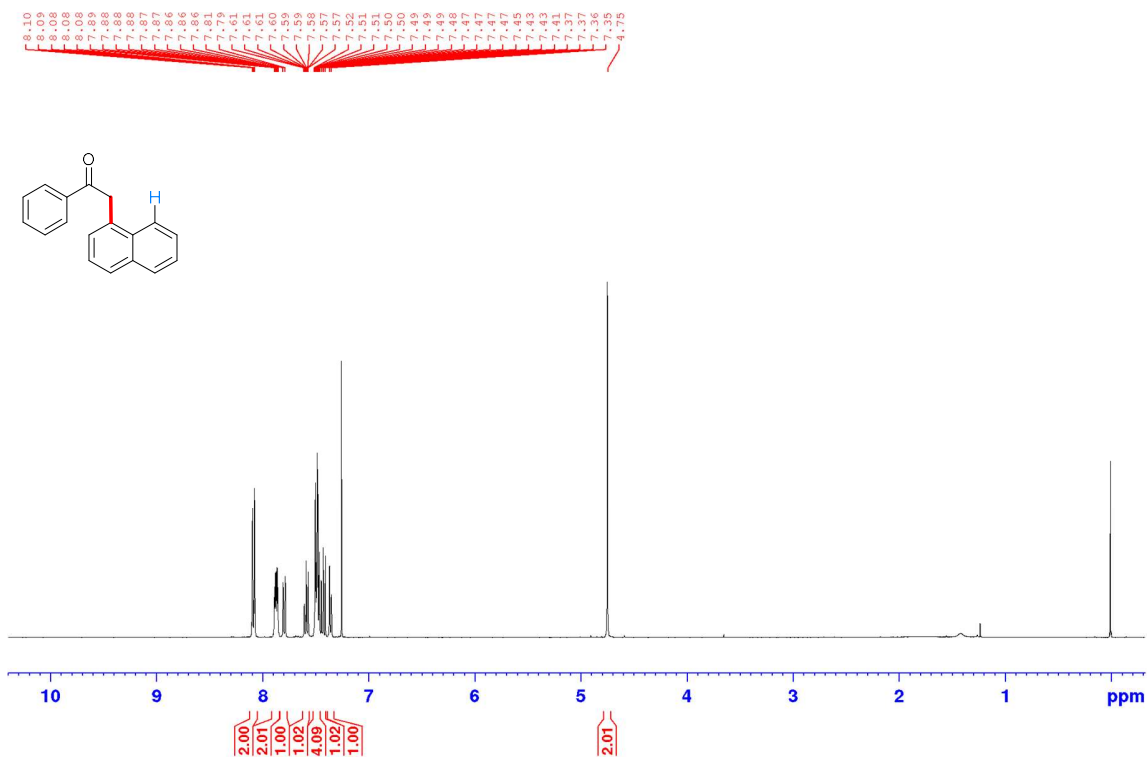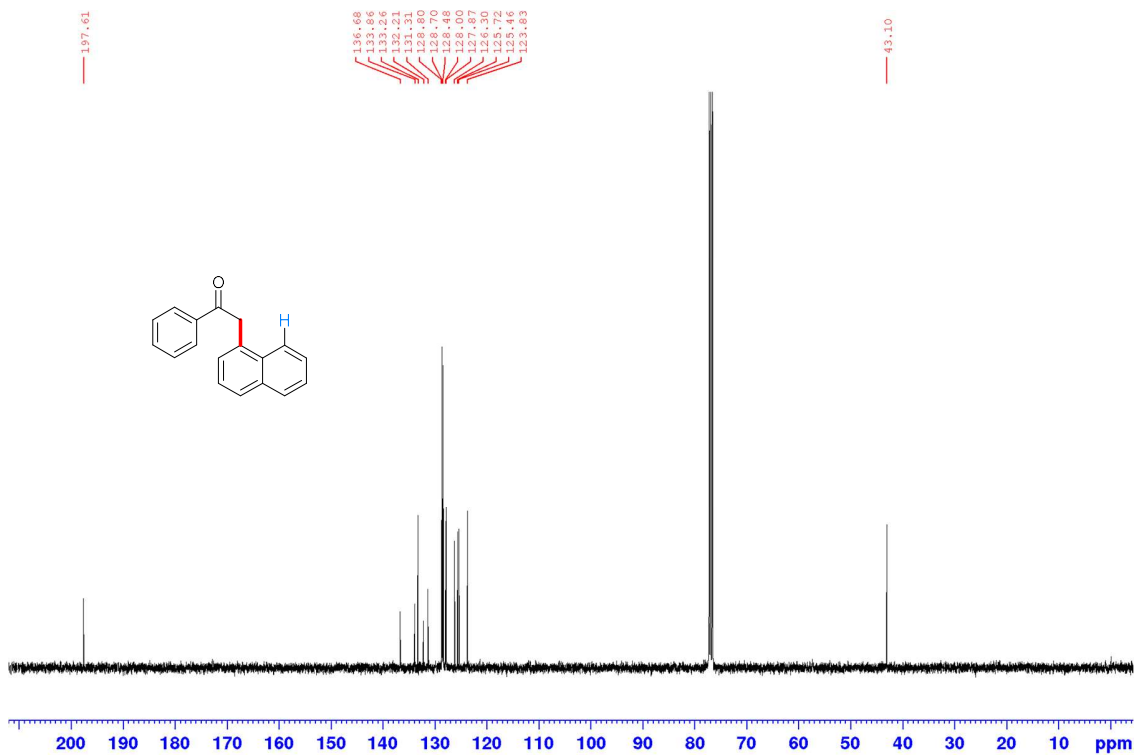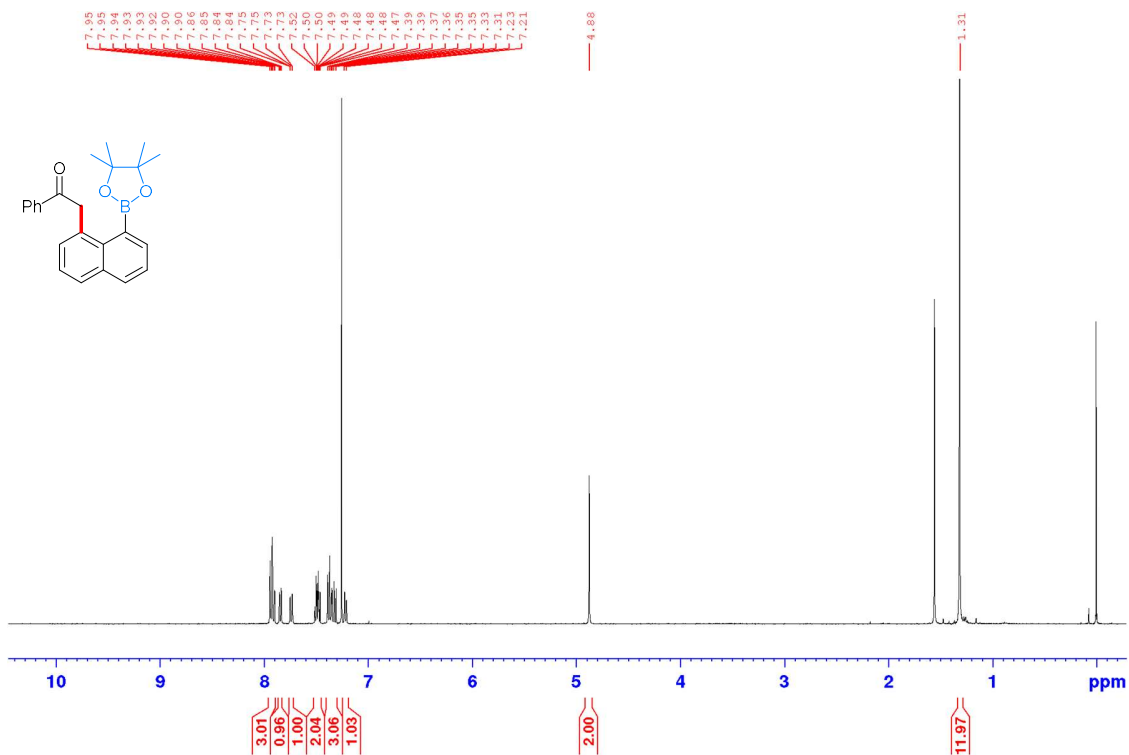

¹³C NMR of **3aa-1** (100 MHz, CDCl₃)

¹H NMR of **3aa-2** (400 MHz, CDCl₃)

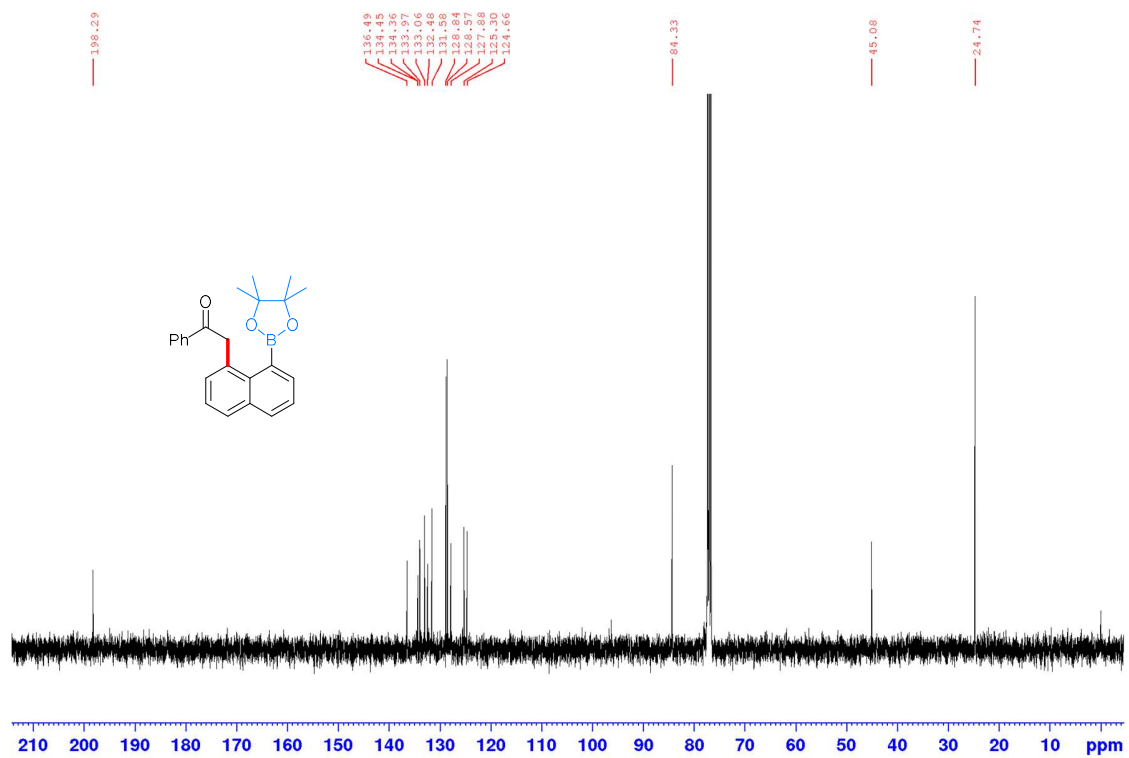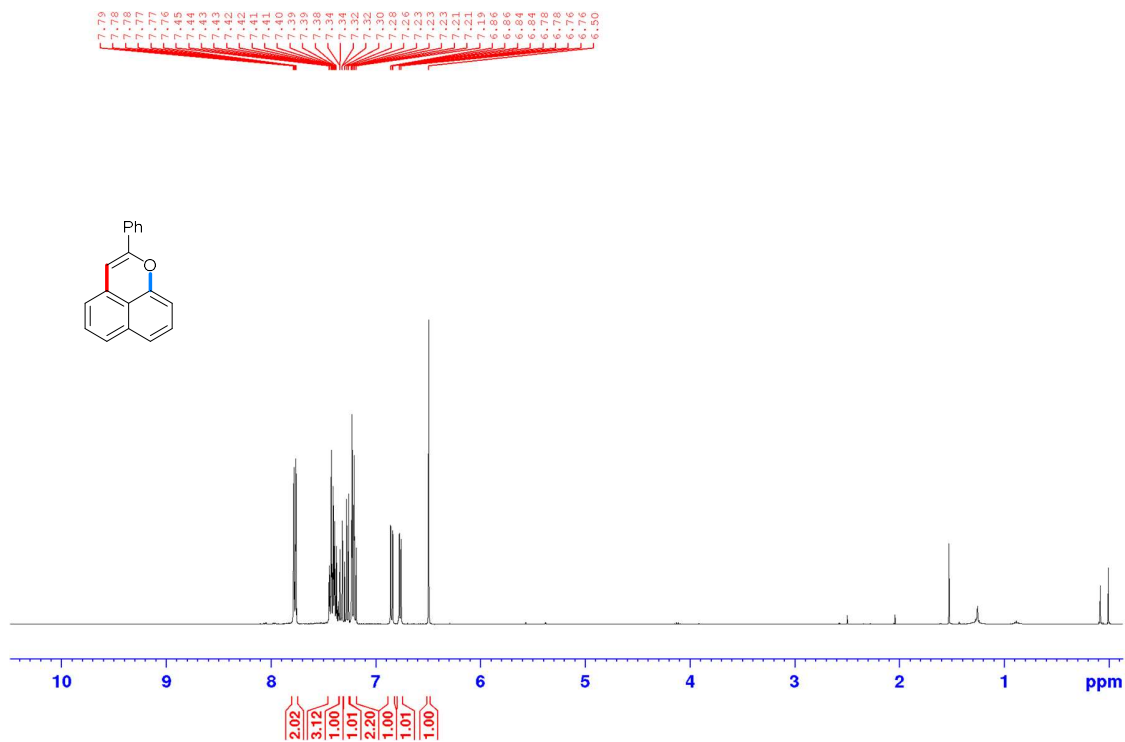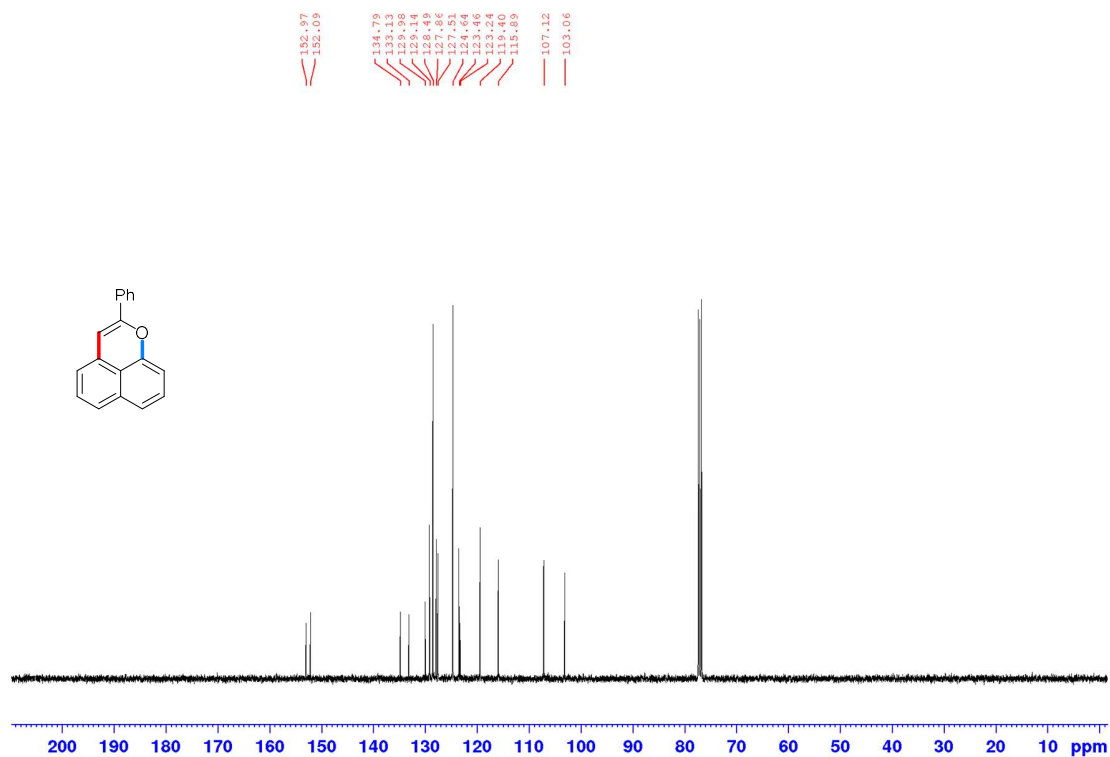

¹³C NMR of **3aa-2** (100 MHz, CDCl₃)

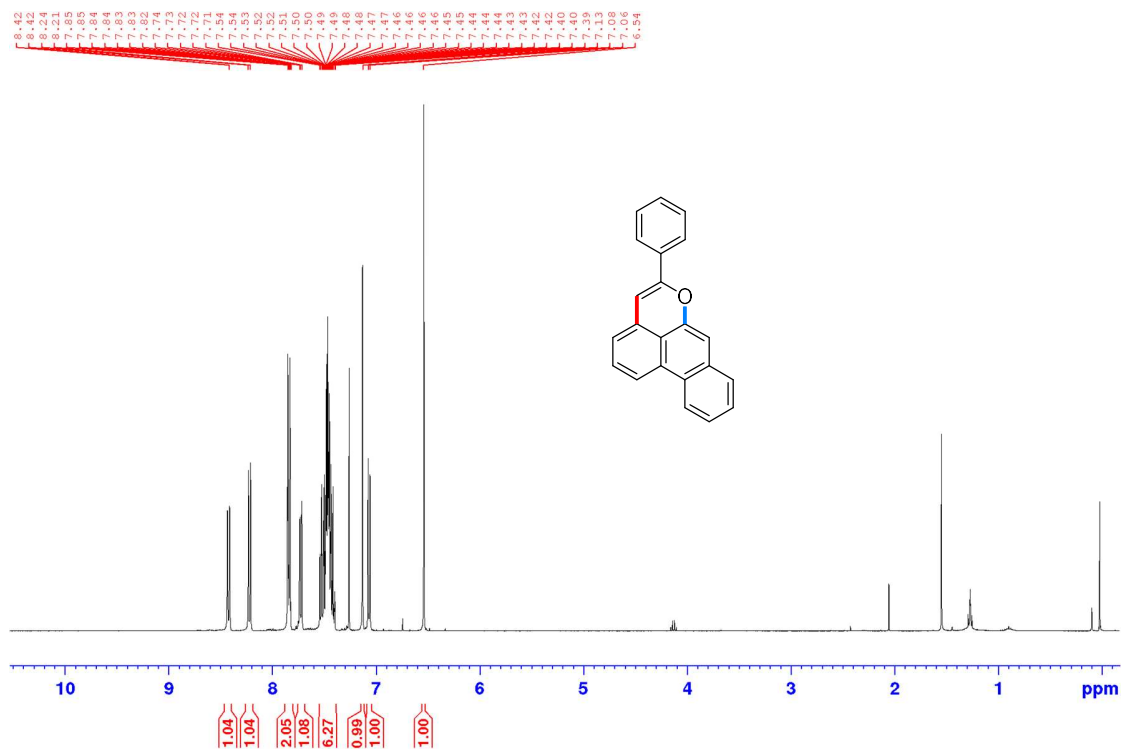¹H NMR of **3aa-3** (400 MHz, CDCl₃)
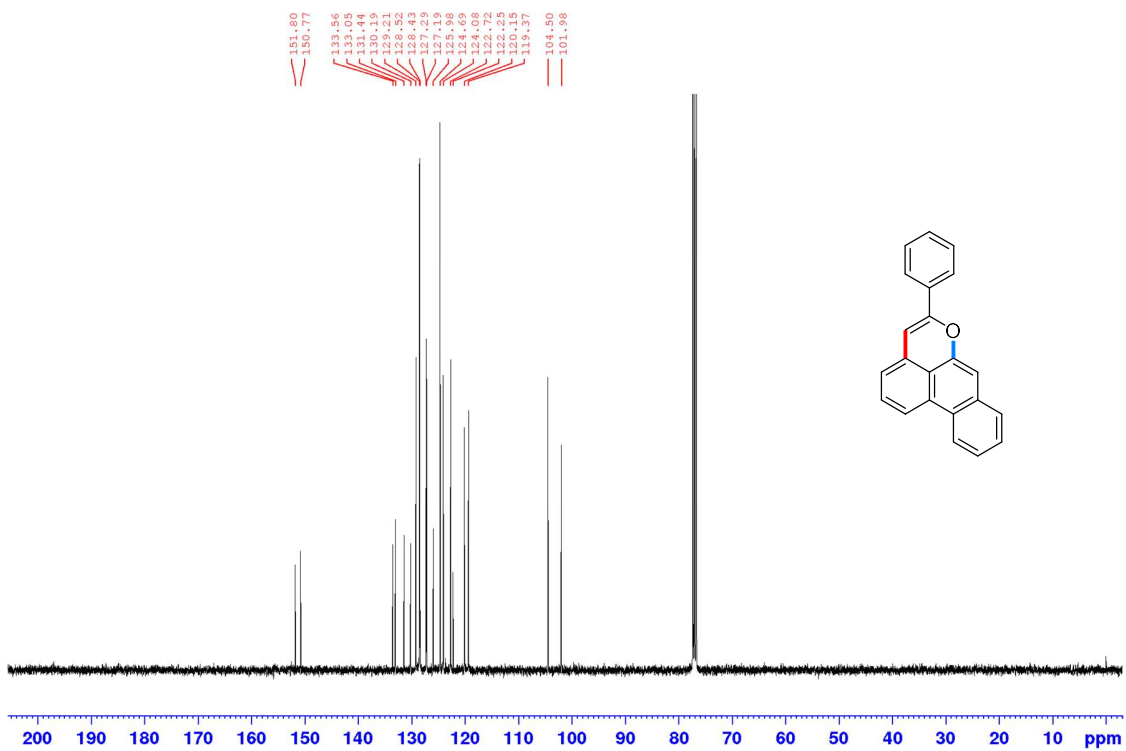

¹³C NMR of **3aa-3** (100 MHz, CDCl₃)
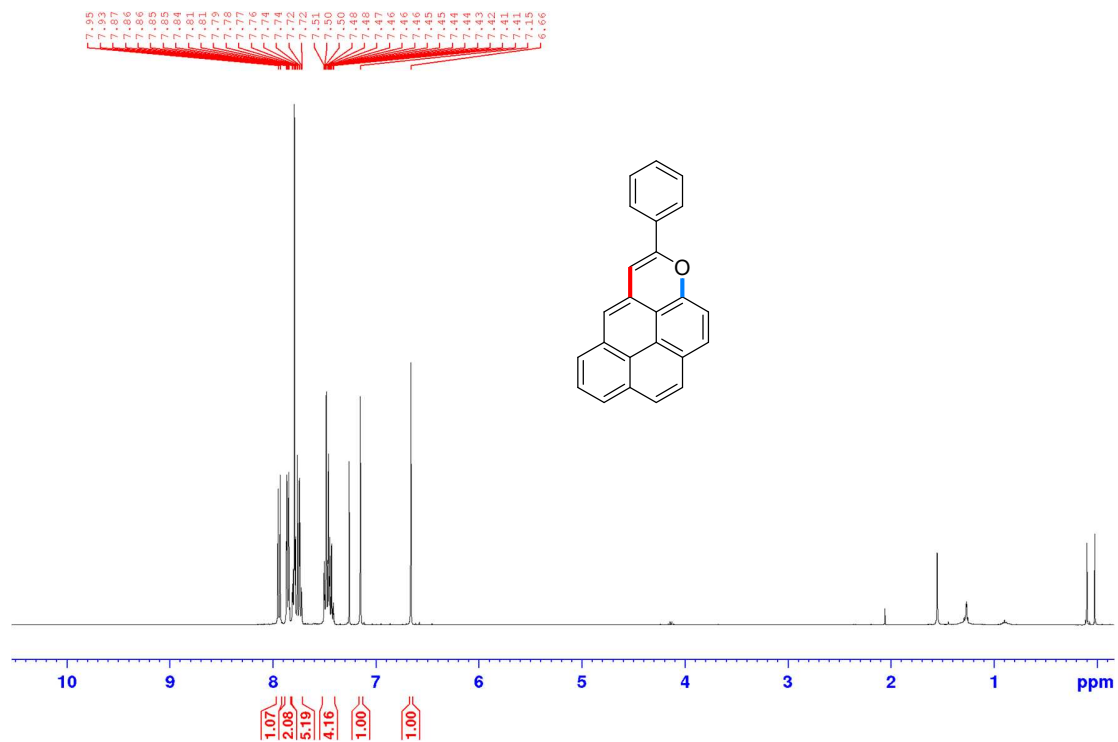
¹H NMR of **3da-1** (400 MHz, CDCl₃)

¹³C NMR of **3da-1** (100 MHz, CDCl₃)

¹H NMR of **3ea-1** (400 MHz, CDCl₃)

The peak list reads (ppm): 7.95, 7.93, 7.87, 7.86, 7.85, 7.84, 7.81, 7.79, 7.78, 7.77, 7.76, 7.74, 7.72, 7.51, 7.50, 7.48, 7.47, 7.46, 7.46, 7.45, 7.44, 7.43, 7.42, 7.41, 7.15, 6.66

Integration values: 1.07, 2.08, 5.19, 4.16, 1.00, 1.00

¹³C NMR of **3ea-1** (100 MHz, CDCl₃)

The peak list reads (ppm): 152.42, 150.30, 133.82, 133.15, 132.30, 129.25, 128.55, 126.76, 126.51, 126.47, 125.97, 125.91, 125.64, 125.14, 124.72, 122.16, 122.03, 118.40, 114.62, 112.26, 104.00

S30

¹H NMR of **3aa-4** (400 MHz, CDCl₃)

8.49
8.49
8.47
8.10
8.09
8.07
8.07
8.06
8.05
8.04
8.03
7.92
7.92
7.90
7.70
7.68
7.66
7.66
7.65
7.64
7.63
7.63
7.62
7.61
7.55
7.54
7.53
7.52
7.51
7.51
7.49
7.37
7.37
7.35

5.21
5.17

4.72
4.68

2.52

| 10 | 9 | 8 | 7 | 6 | 5 | 4 | 3 | 2 | 1 | ppm |

0.98
1.96
1.00
1.00
1.00
1.03
3.03
1.01

1.00

1.00

3.02

¹³C NMR of **3aa-4** (100 MHz, CDCl₃)

197.13

144.02
136.33
135.18
133.53
133.22
132.88
129.45
129.33
129.04
128.85
128.13
126.02
125.36
123.74

47.89
45.53

| 210 | 200 | 190 | 180 | 170 | 160 | 150 | 140 | 130 | 120 | 110 | 100 | 90 | 80 | 70 | 60 | 50 | 40 | 30 | 20 | 10 | ppm |

¹H NMR of **3aa-5** (400 MHz, CDCl₃)
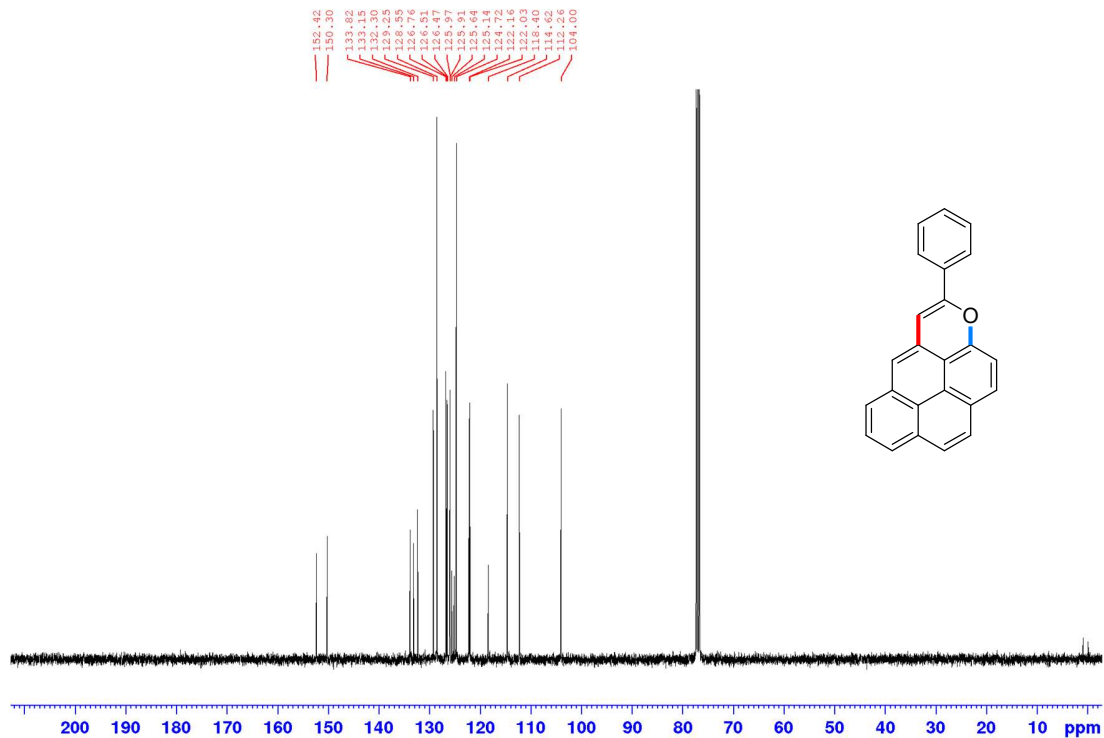

¹³C NMR of **3aa-5** (100 MHz, CDCl₃)
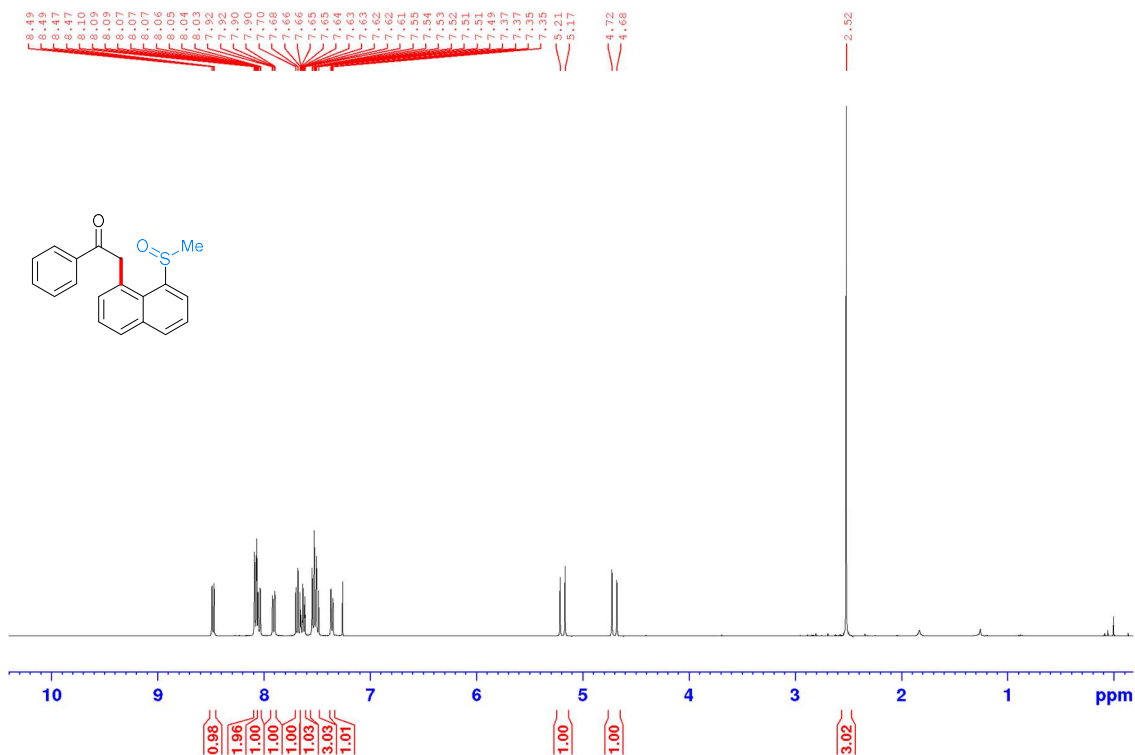
¹H NMR of **3ba-1** (400 MHz, CDCl₃)
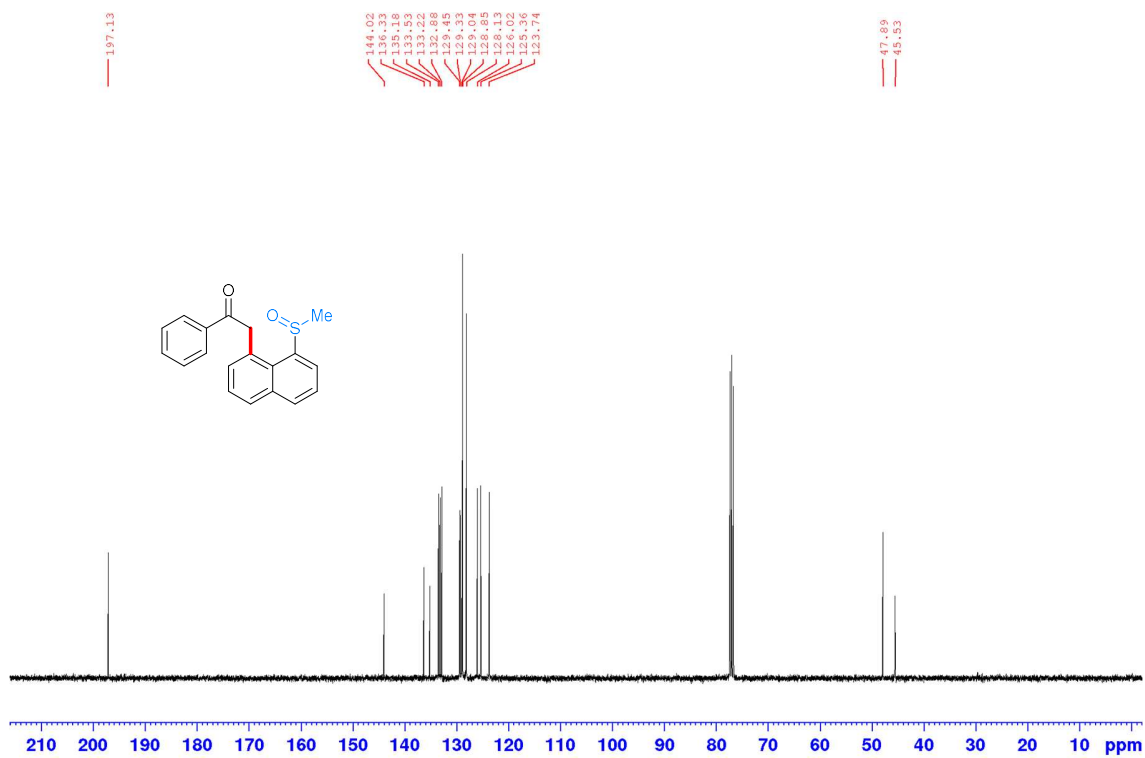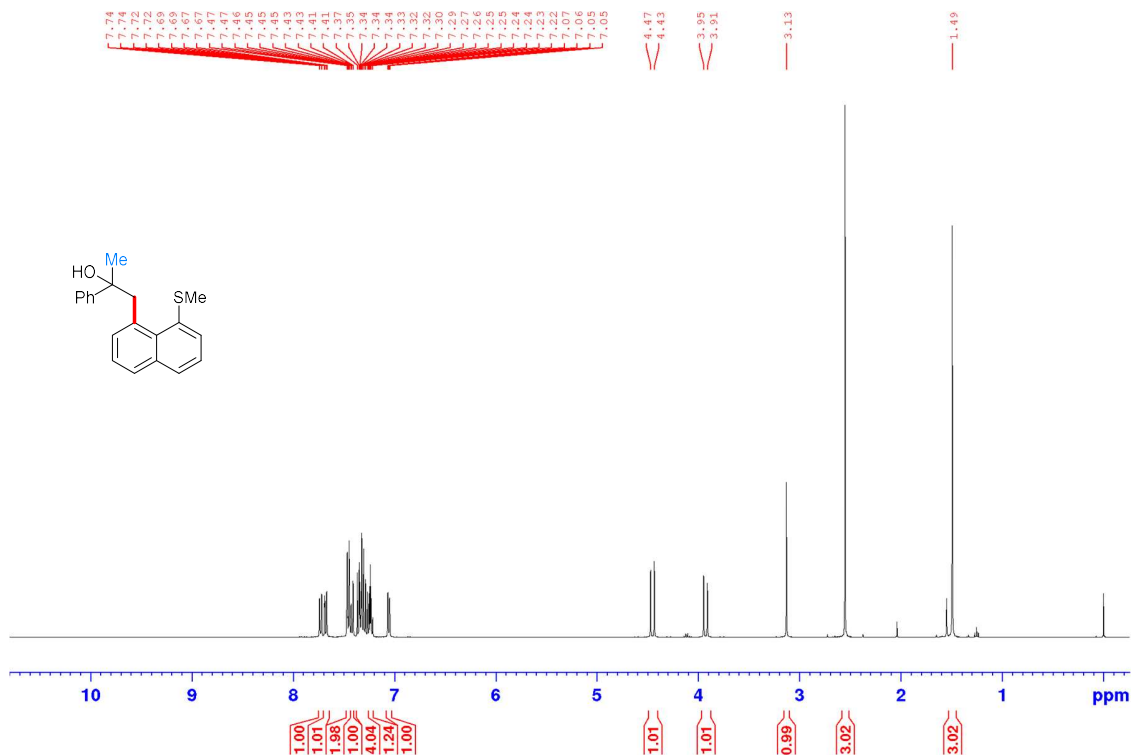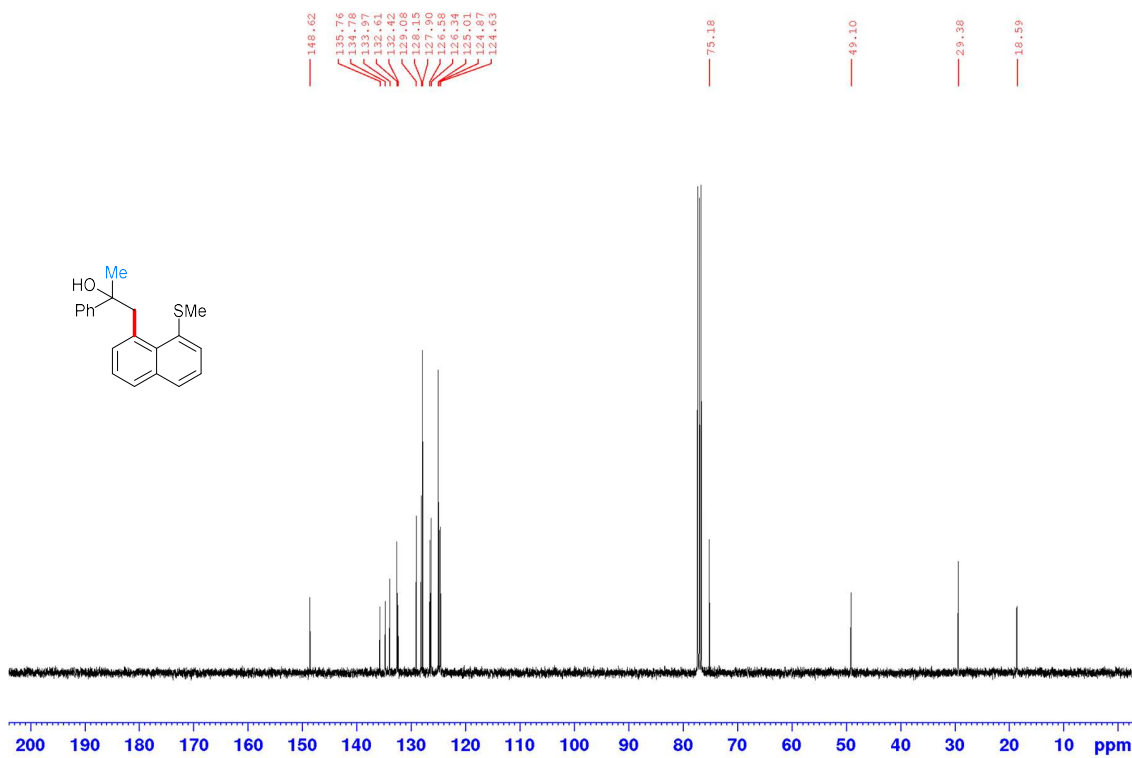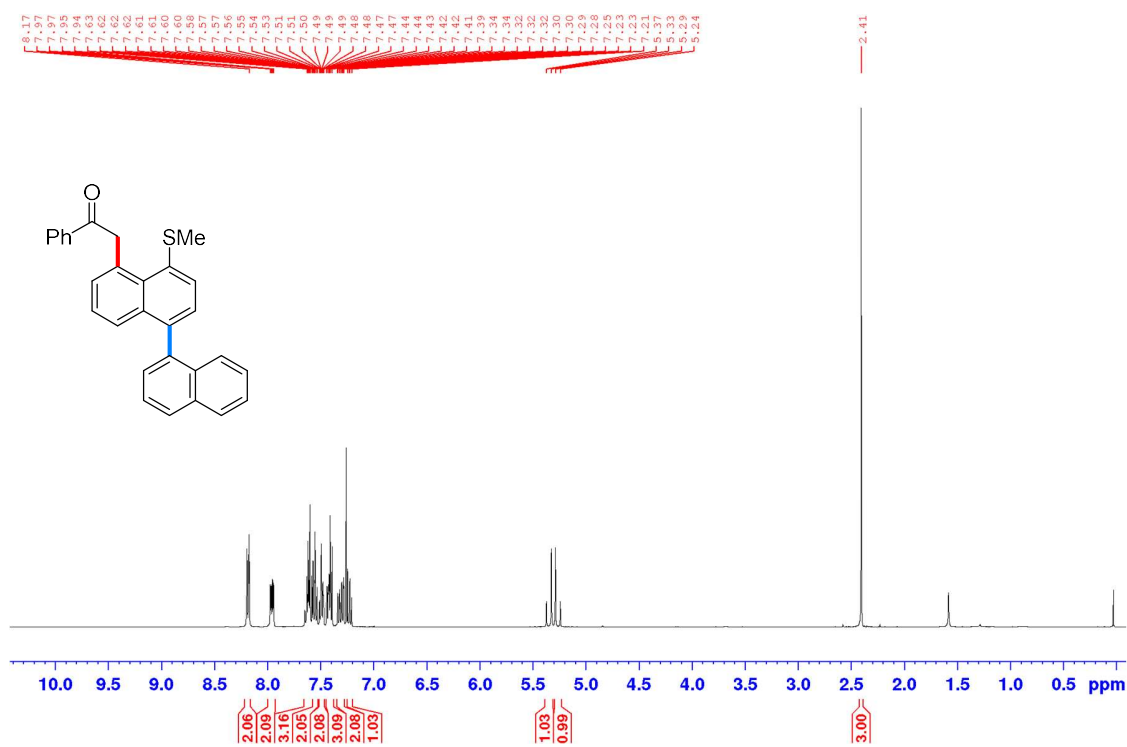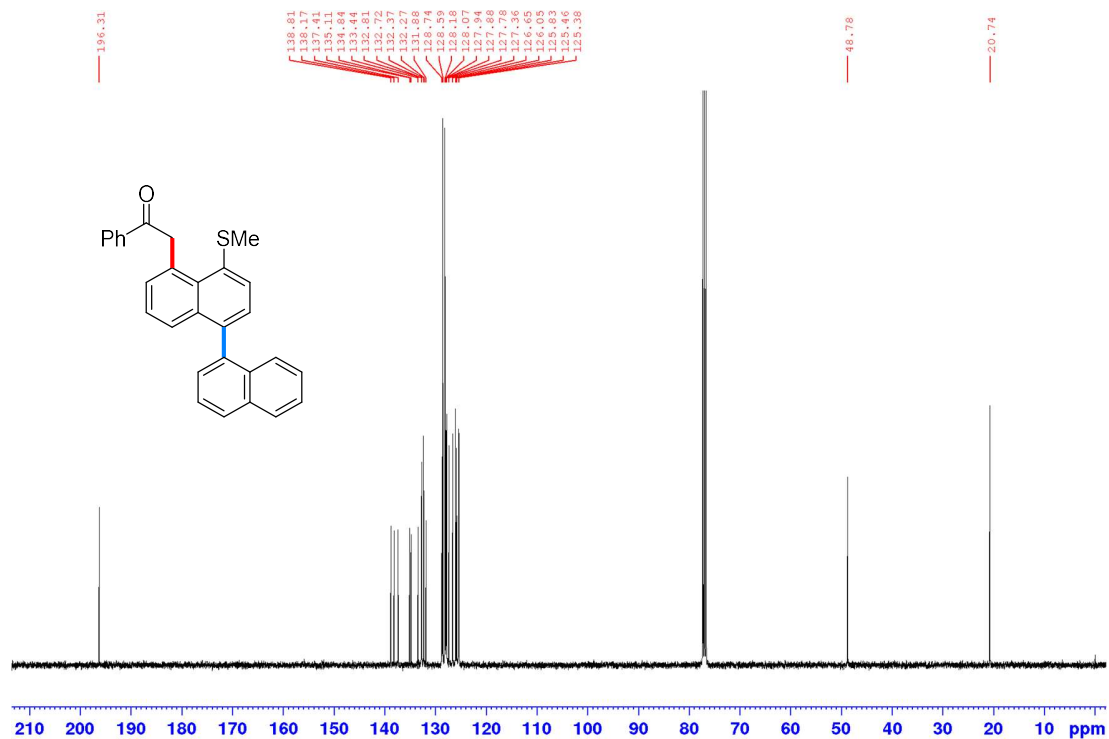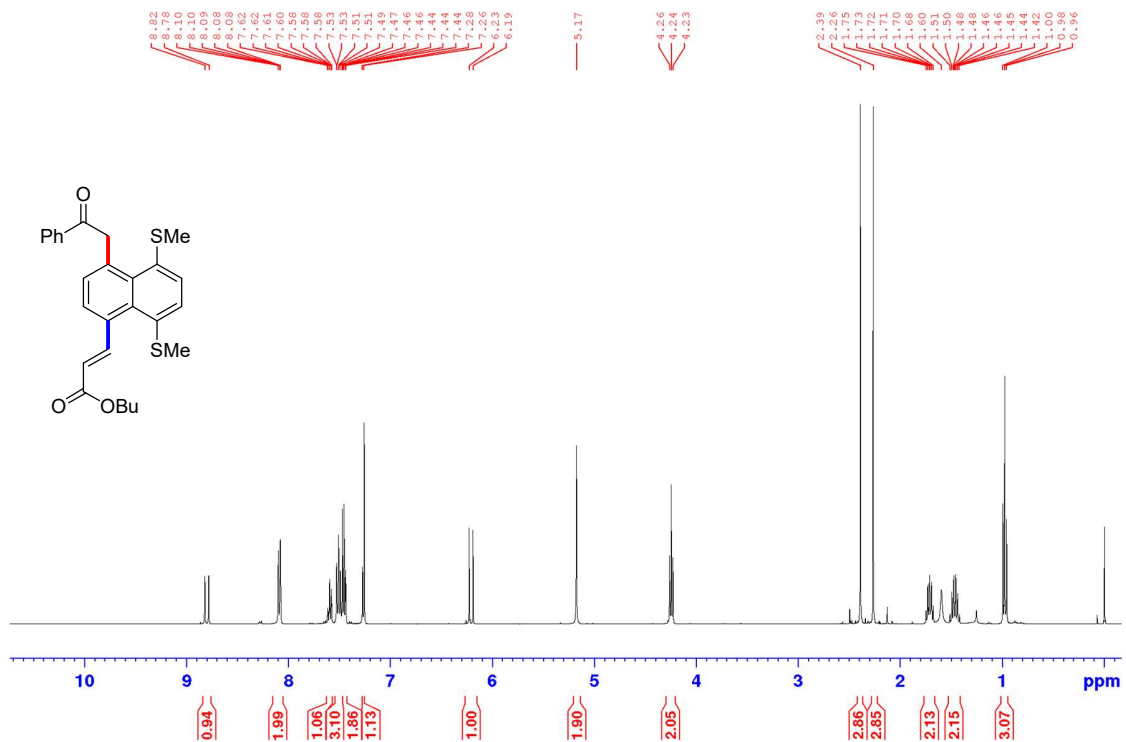

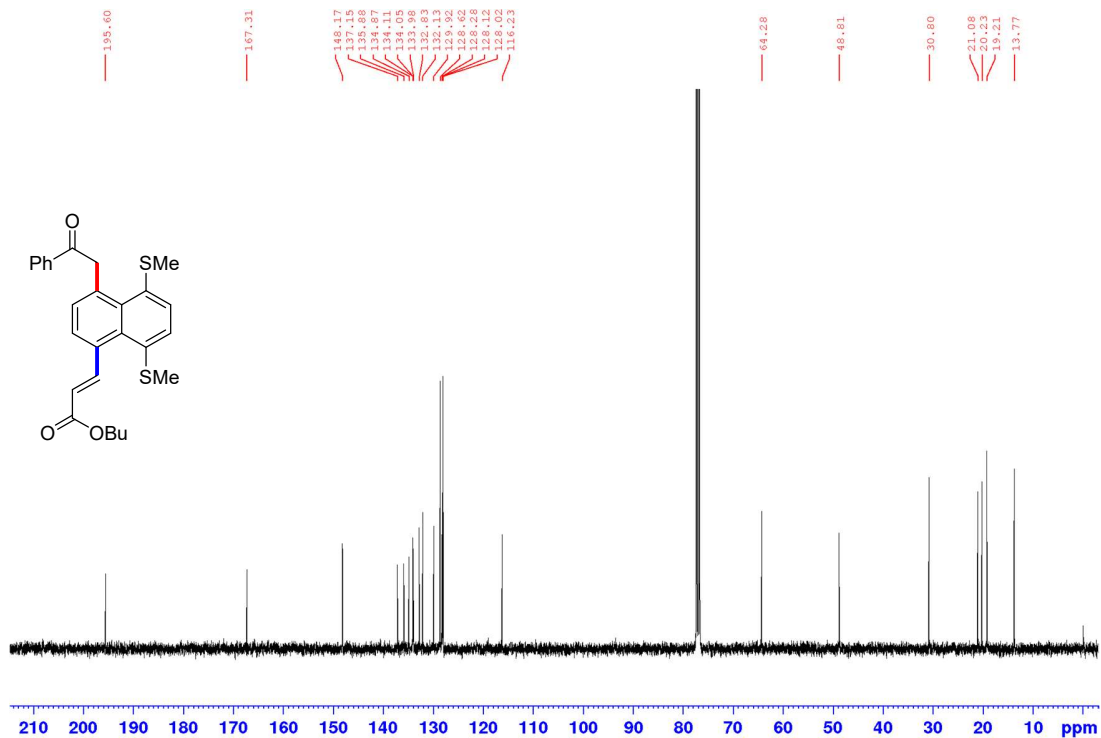¹³C NMR of **3ba-1** (100 MHz, CDCl₃)
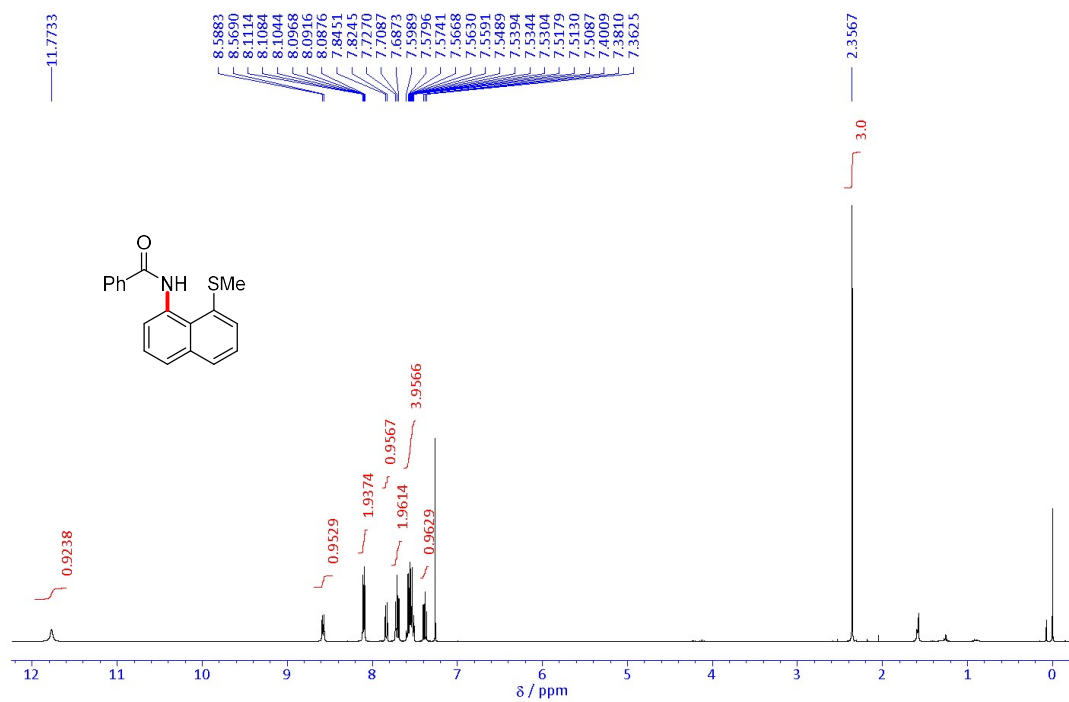
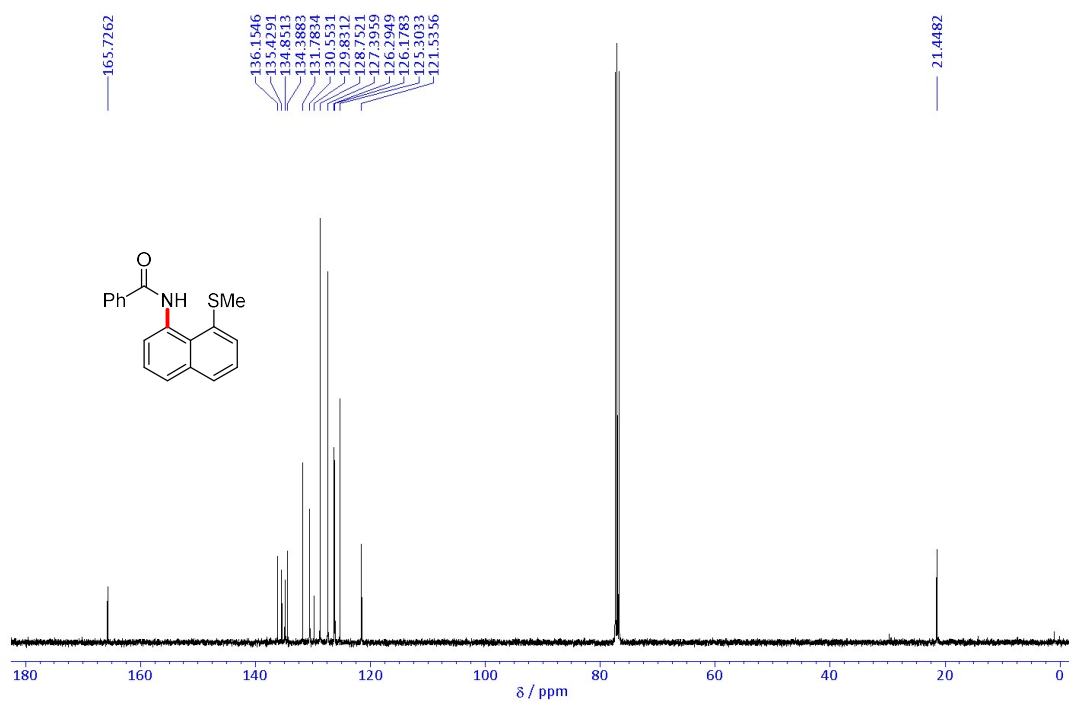¹H NMR of **3fa-1** (400 MHz, CDCl₃)

¹³C NMR of **3fa-1** (100 MHz, CDCl₃)

¹H NMR of **5aa** (400 MHz, CDCl₃)

11.7733

8.5883
8.5690
8.1114
8.1084
8.1044
8.0968
8.0916
8.0876
7.8451
7.8245
7.7770
7.7087
7.6873
7.5989
7.5796
7.5741
7.5668
7.5630
7.5591
7.5489
7.5394
7.5344
7.5304
7.5179
7.5130
7.5087
7.4009
7.3810
7.3625

2.3567

3.0

0.9238

0.9529
1.9374
0.9567
3.9566
1.9614
0.9629

12   11   10   9   8   7   6   5   4   3   2   1   0
δ / ppm

¹³C NMR of **5aa** (100 MHz, CDCl₃)

165.7262

136.1546
135.4291
134.8513
134.3883
131.7834
130.5531
129.8312
128.7521
127.3959
126.2949
126.1783
125.3033
121.5356

21.4482

180   160   140   120   100   80   60   40   20   0
δ / ppm

S35

¹H NMR of **5da** (400 MHz, CDCl₃)

¹³C NMR of **5da** (100 MHz, CDCl₃)

¹H NMR of **5ea** (400 MHz, CDCl₃)
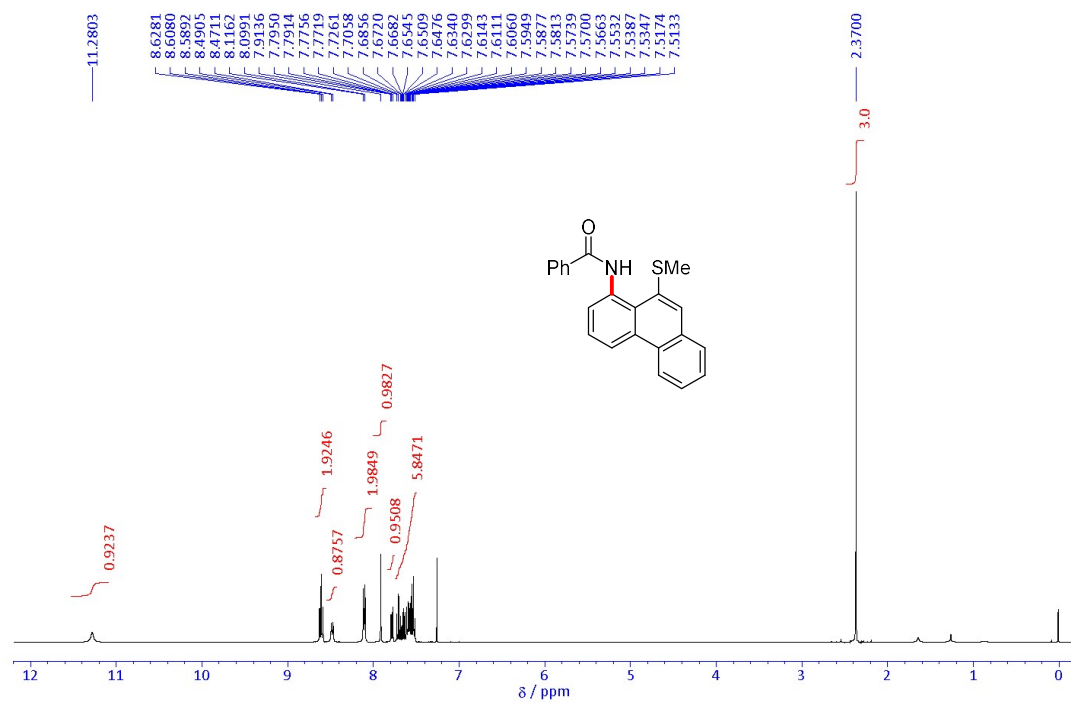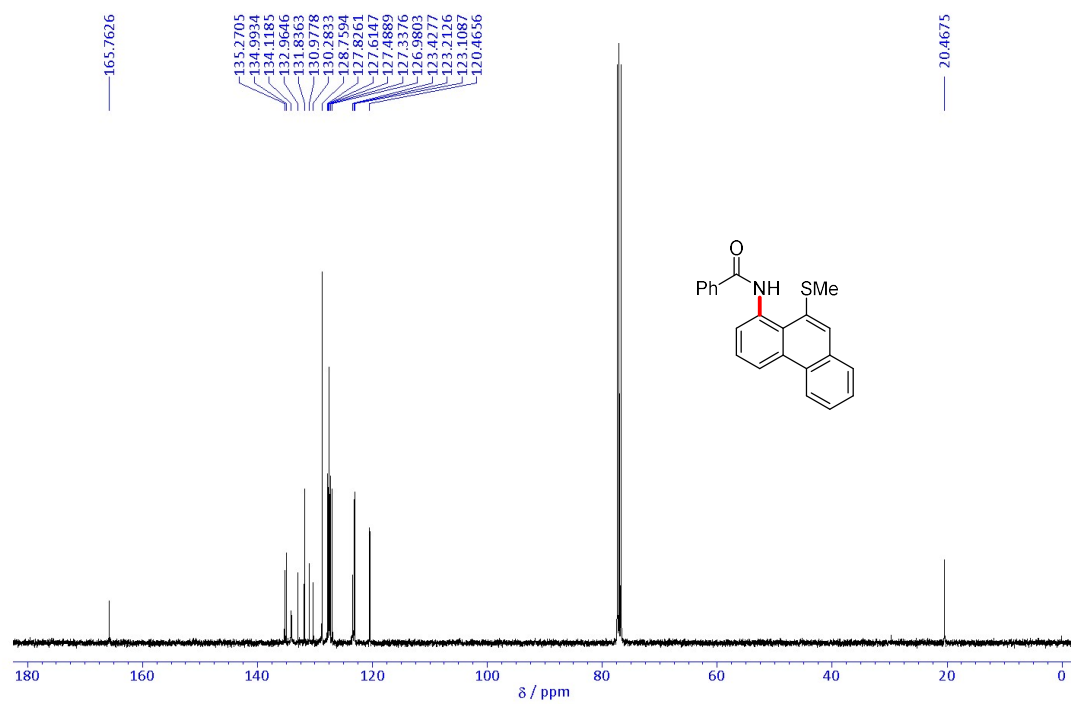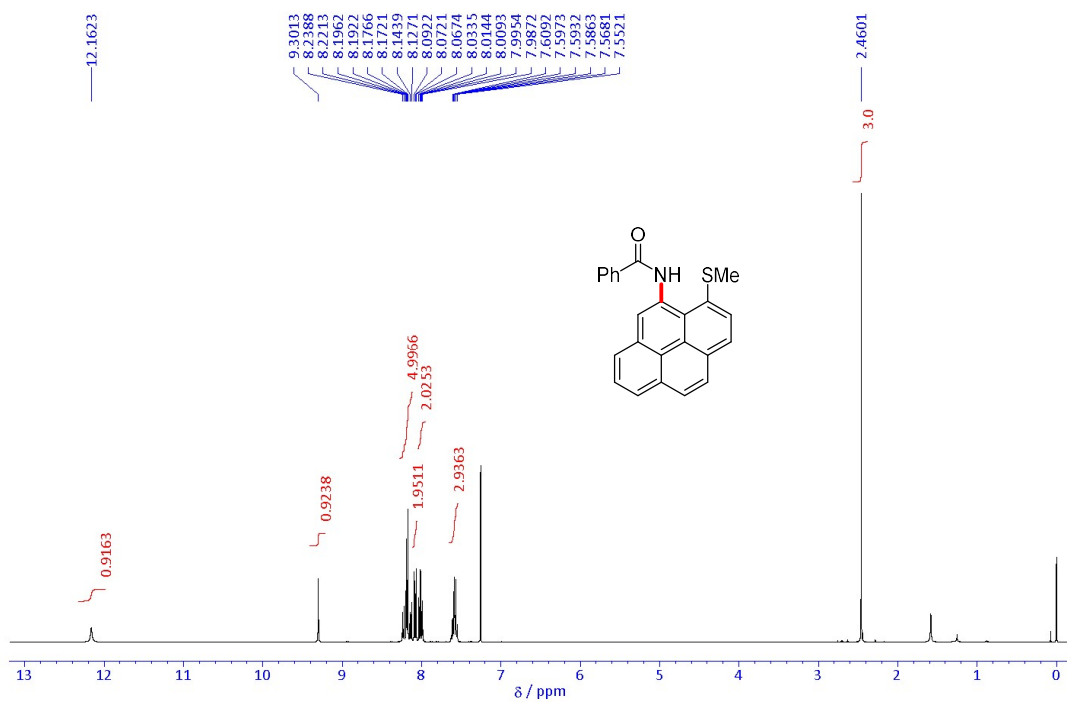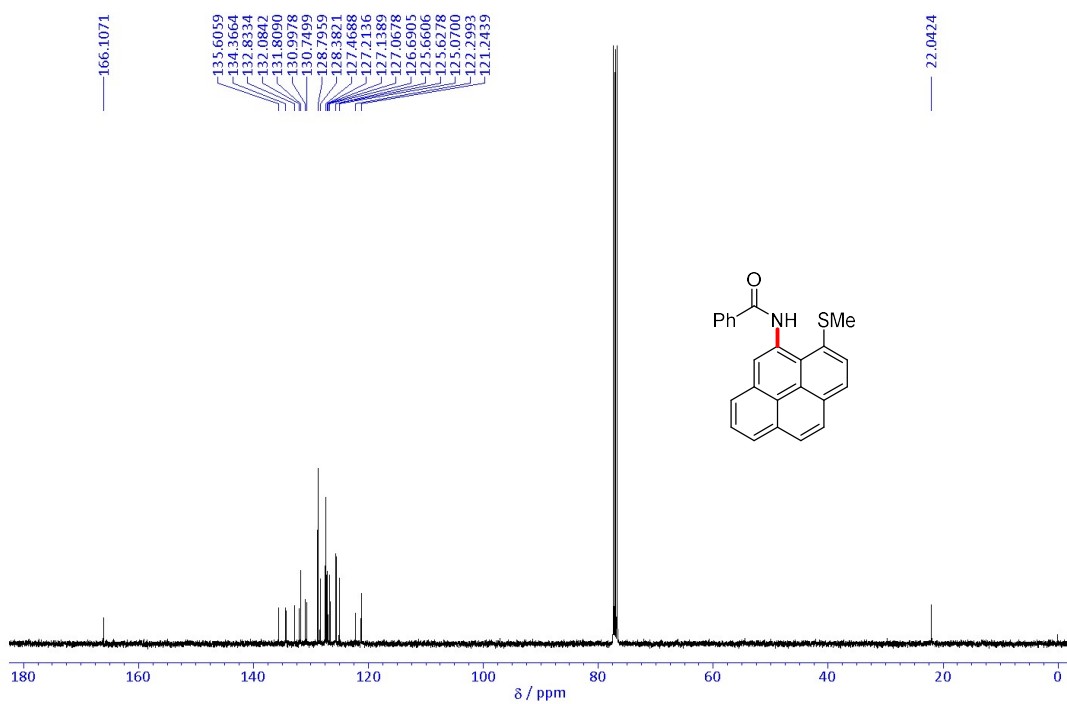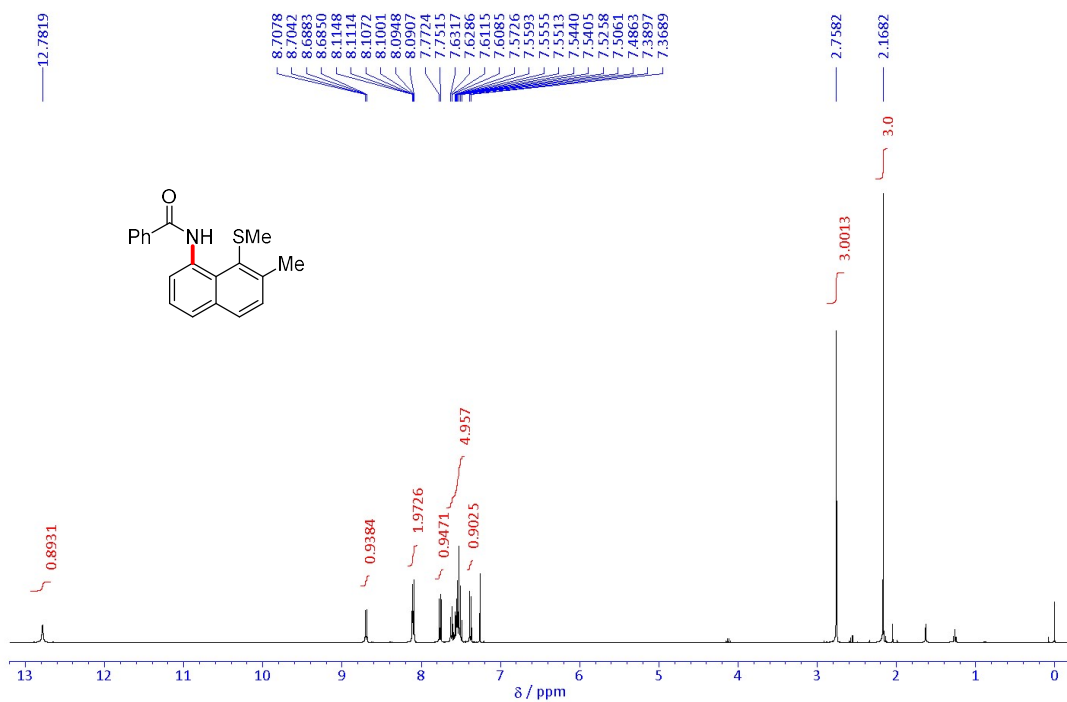
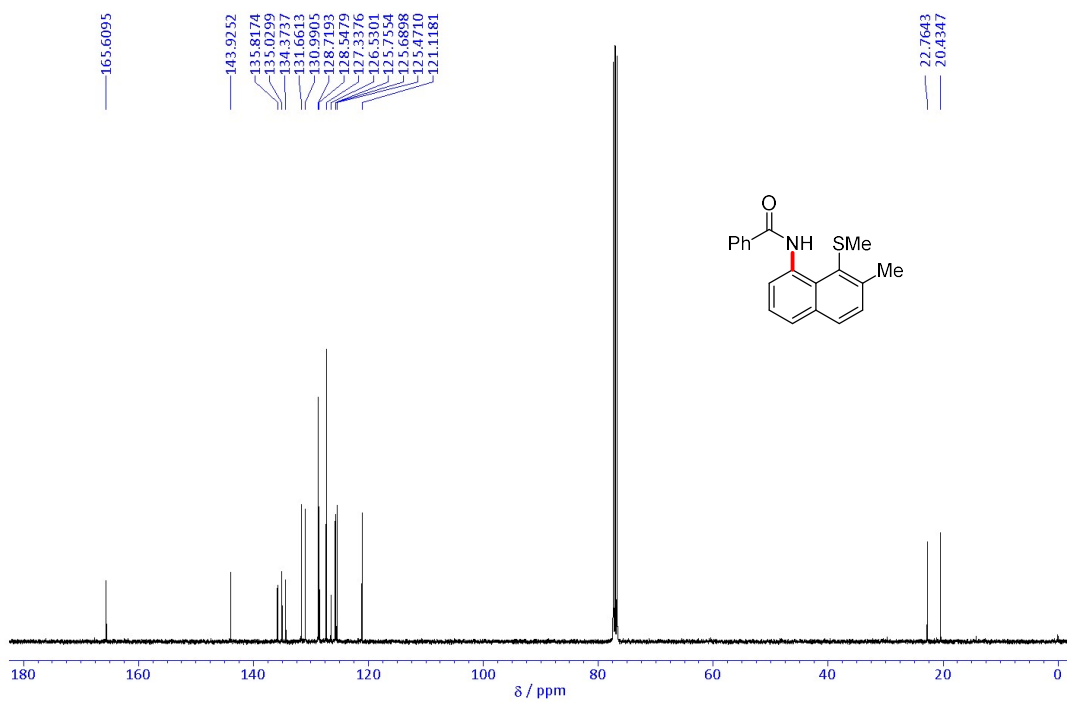^{1}H NMR of **5ea** (400 MHz, CDCl$_3$)

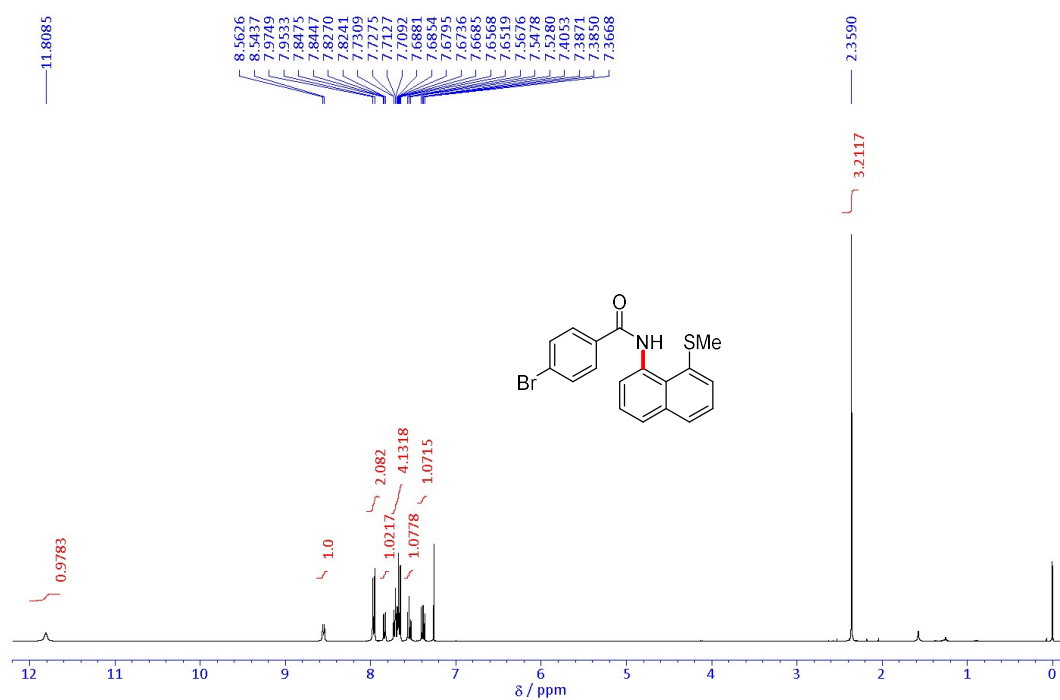^{13}C NMR of **5ea** (100 MHz, CDCl$_3$)

¹H NMR of **5ha** (400 MHz, CDCl₃)
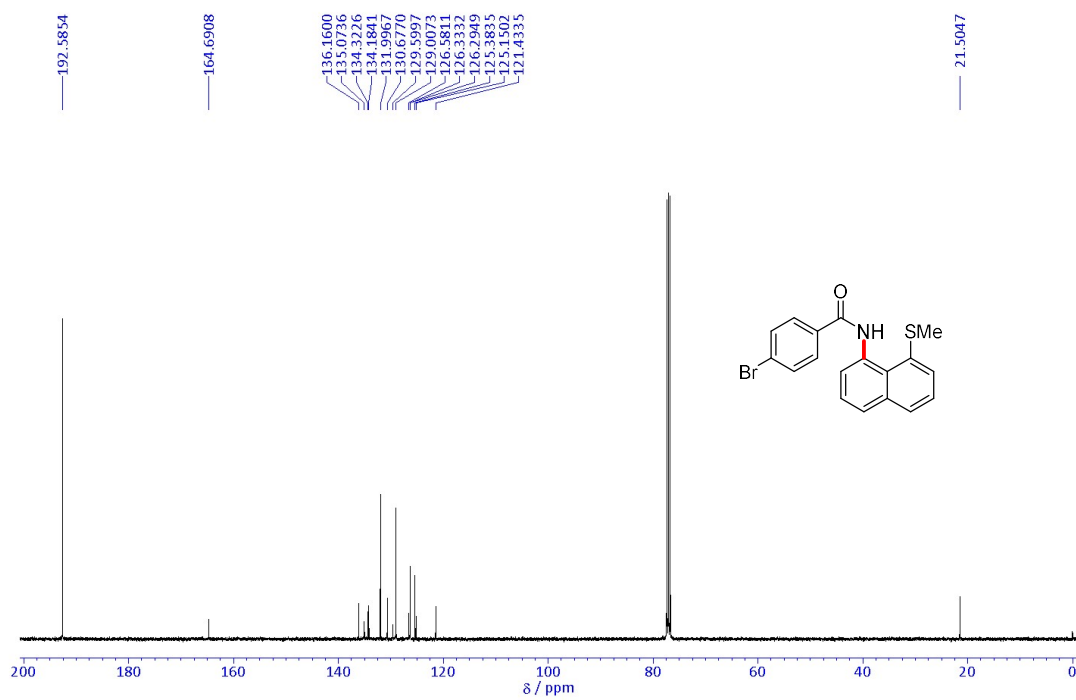

¹³C NMR of **5ha** (100 MHz, CDCl₃)

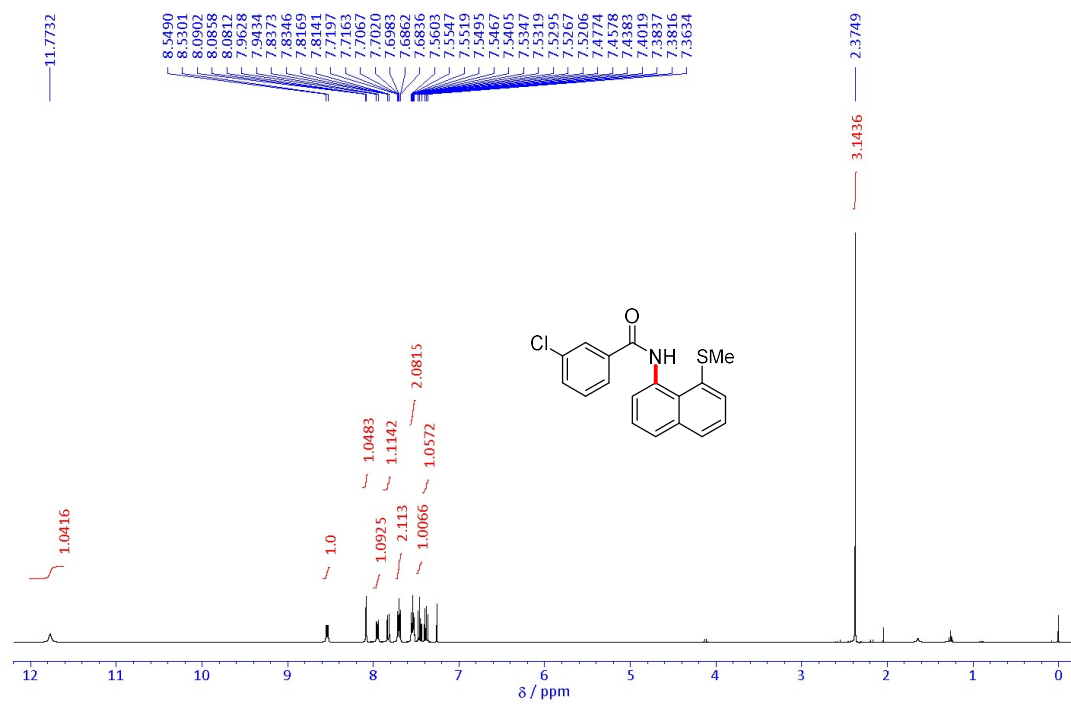¹H NMR of **5ab** (400 MHz, CDCl₃ and CS₂)

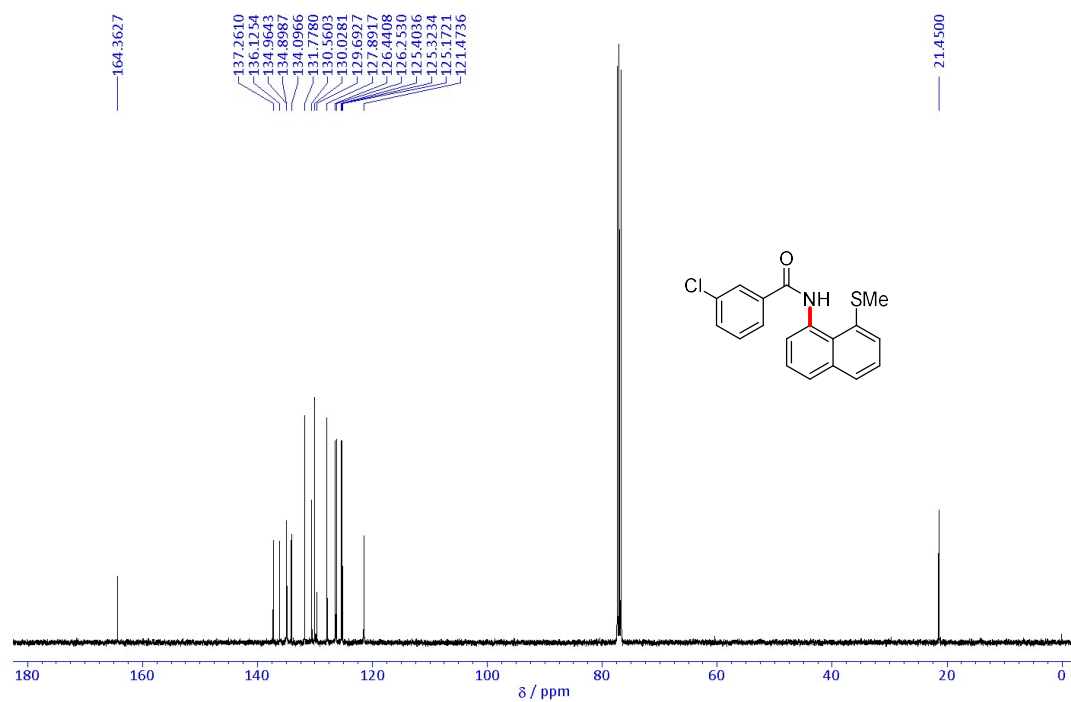

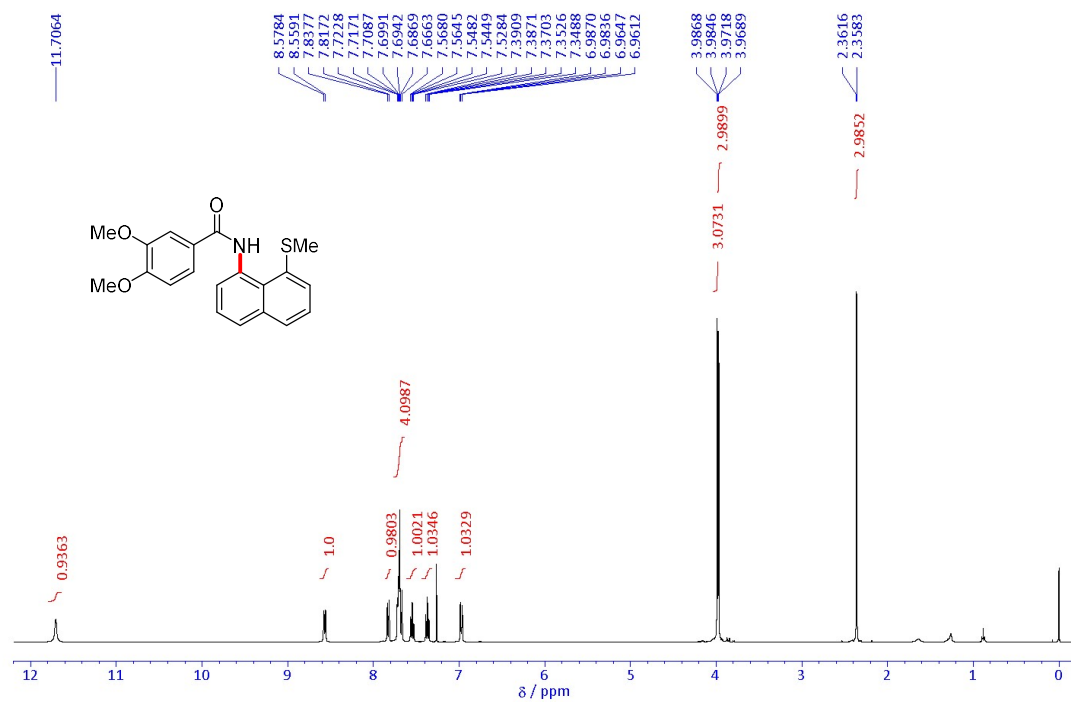¹³C NMR of **5ab** (100 MHz, CDCl₃ and CS₂)

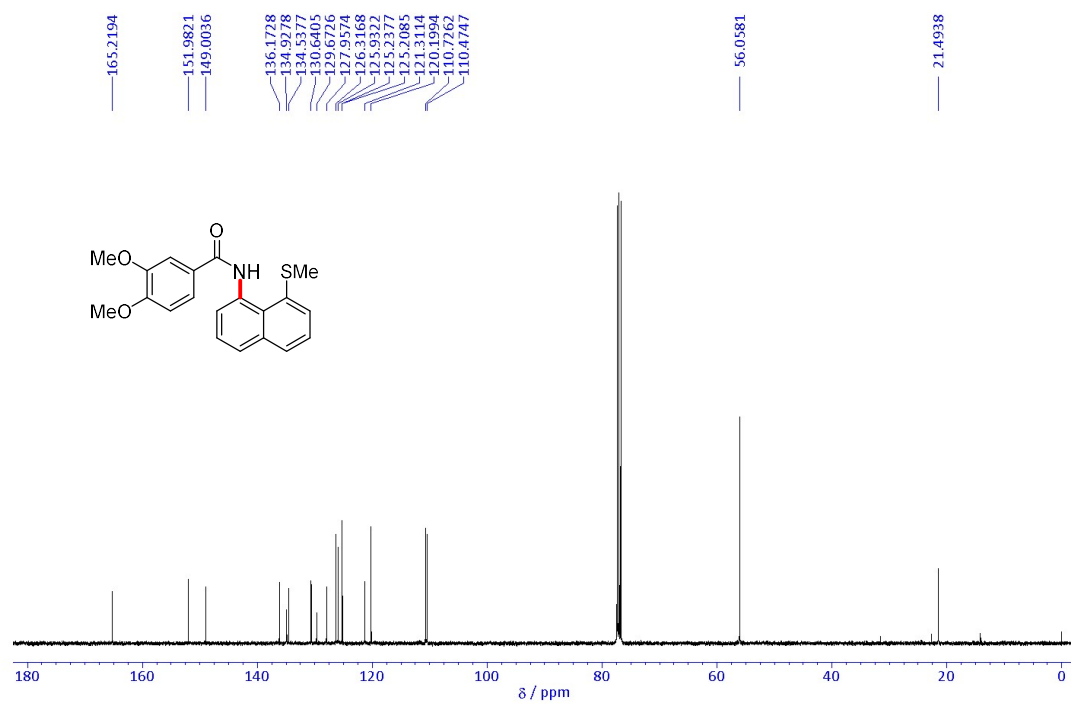¹H NMR of **5ac** (400 MHz, CDCl₃)

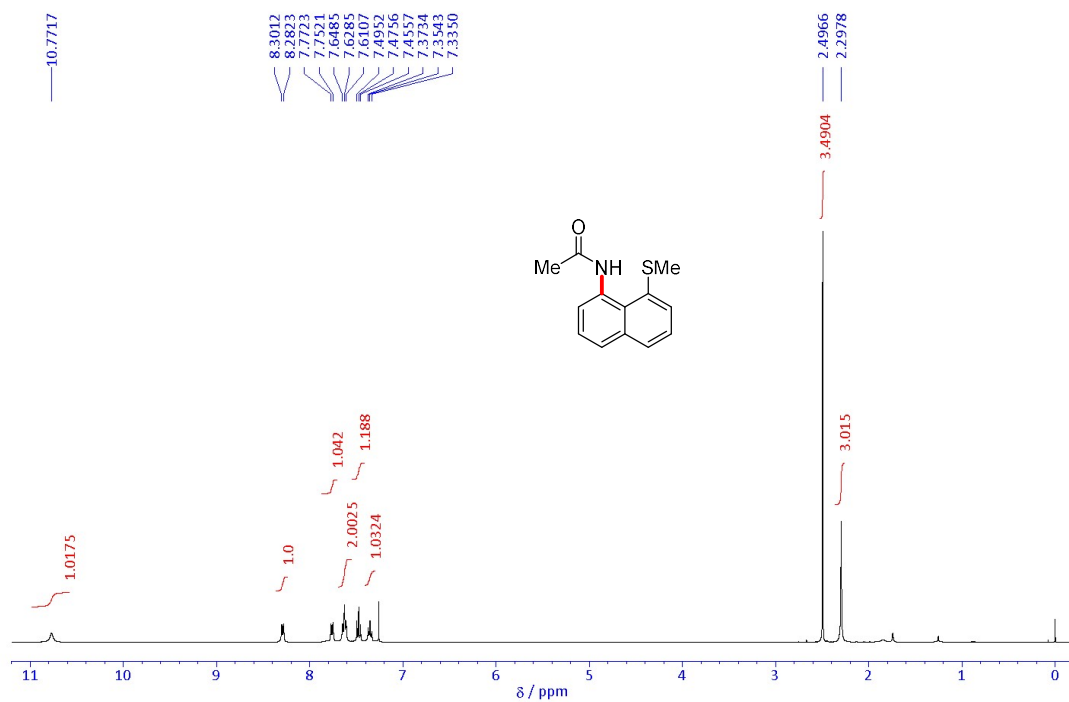¹³C NMR of **5ac** (100 MHz, CDCl₃)

^{1}H NMR of **5ad** (400 MHz, CDCl$_3$)
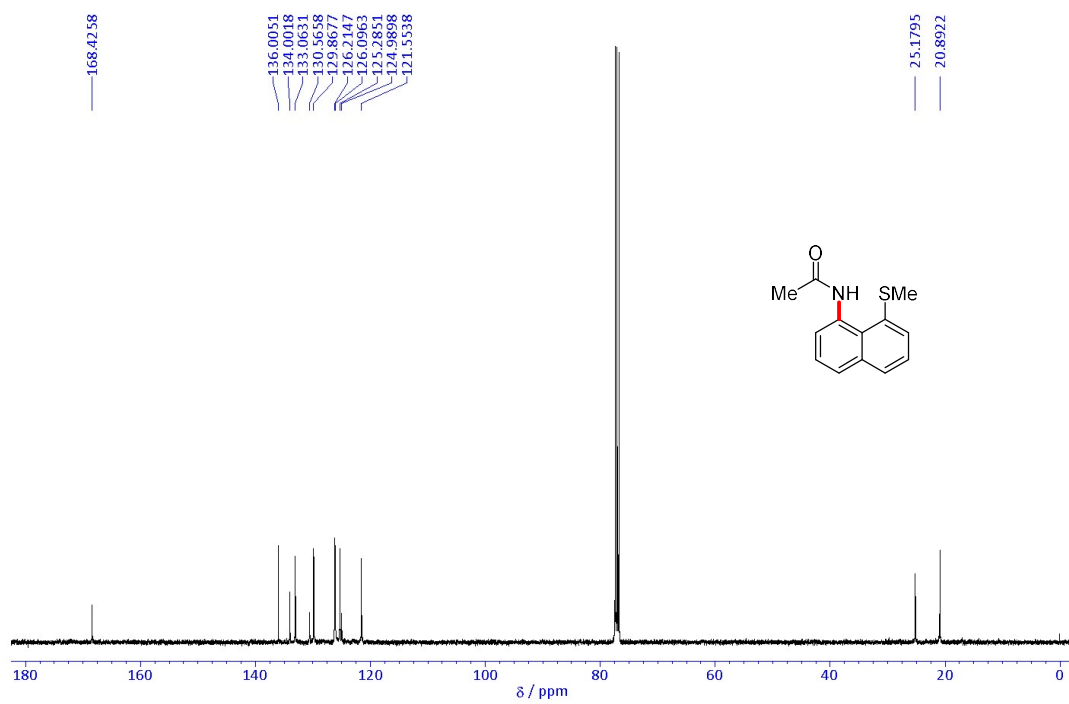

^{13}C NMR of **5ad** (100 MHz, CDCl$_3$)

¹H NMR of **5ae** (400 MHz, CDCl₃)

¹³C NMR of **5ae** (100 MHz, CDCl₃)

¹H NMR of **5af** (400 MHz, CDCl₃)

¹³C NMR of **5af** (100 MHz, CDCl₃)

¹H NMR of **5ag** (400 MHz, CDCl₃)

¹³C NMR of **5ag** (100 MHz, CDCl₃)

¹H NMR of **5ah** (400 MHz, CDCl₃)

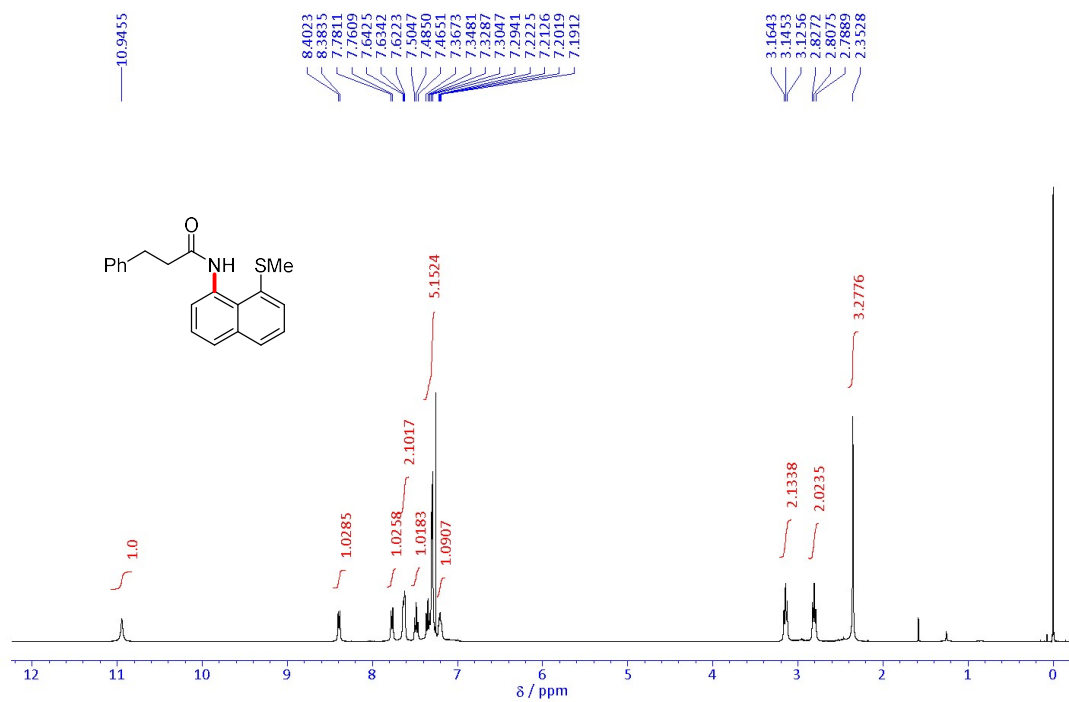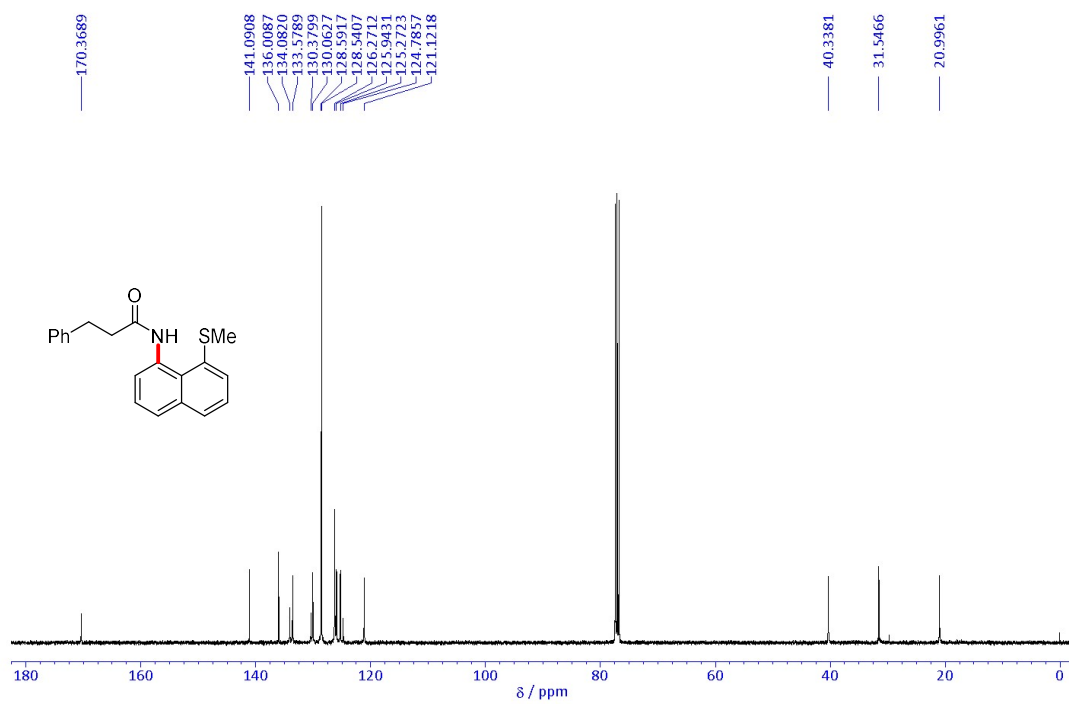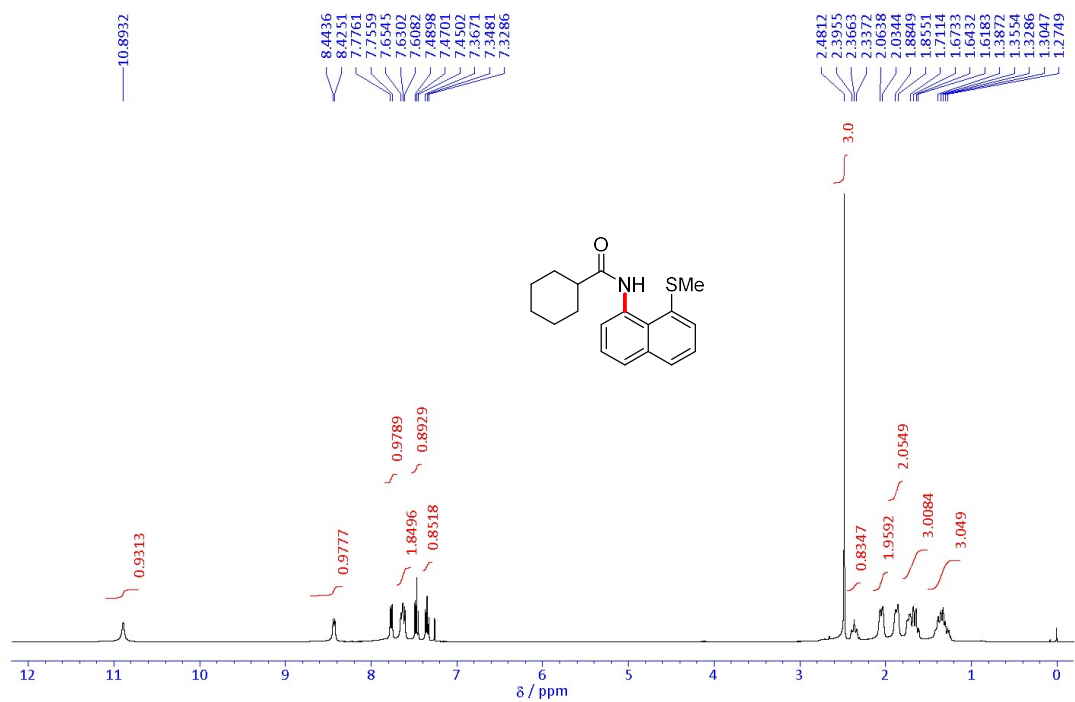¹³C NMR of **5ah** (100 MHz, CDCl₃)