Supporting Information

Synergism in semiconducting nanocomposite: Visible light photocatalysis towards formation of C-S and C-N bonds

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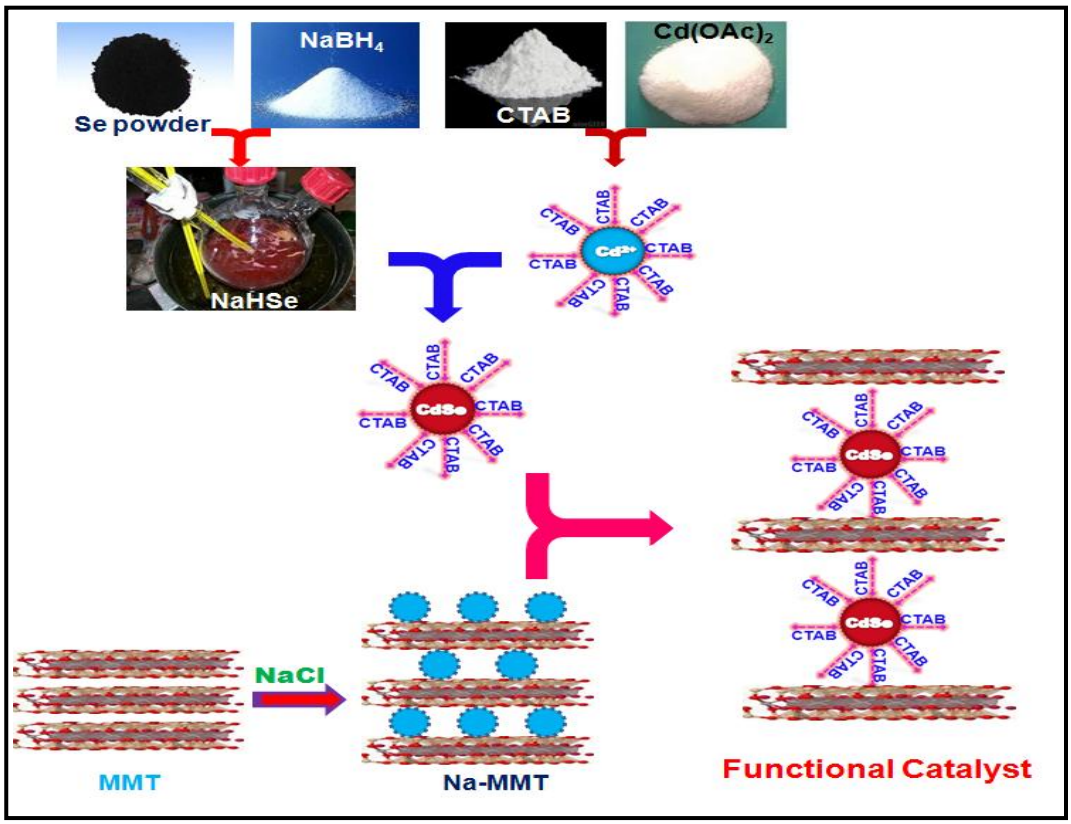


Figure S1: Schematic representation for synthesis of CdSe/MMT nanocomposite

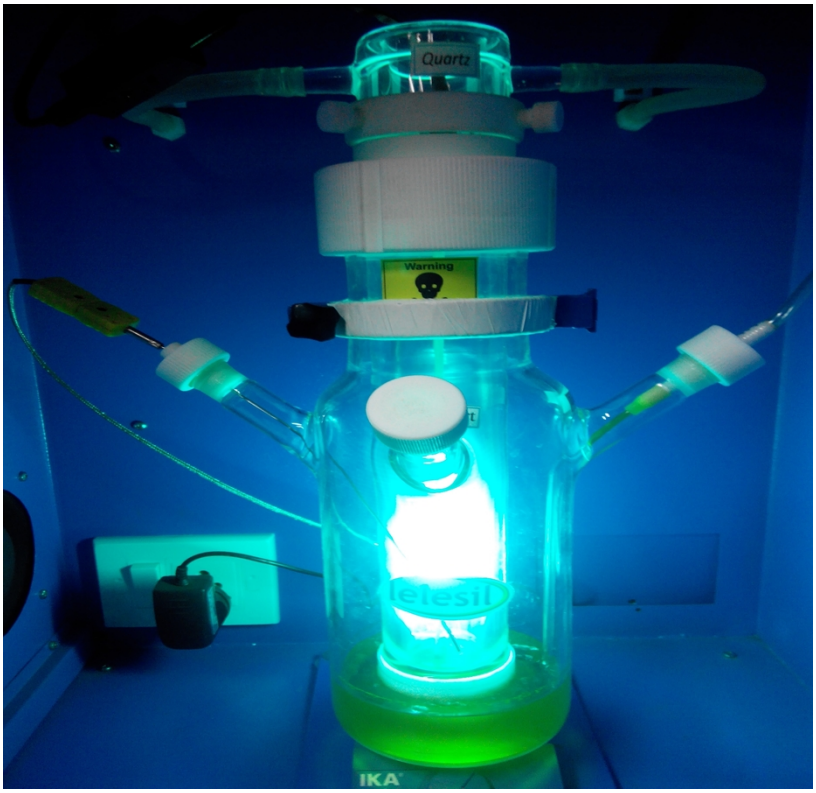


Figure S2: Set-up of photochemical reactor used in the synthesis of benzothiazoles and benzimidazoles

Quantum yield of photochemical synthesis of 2-substituted benzazoles

These values are calculated from ferrioxalate actinometry [1, 2]. The photon flux of light source absorbed is correlated with time required for the conversion of Fe(III) to Fe(II) using ferrioxalate in the photochemical reactor. Under the identical experimental conditions, the time required for maximum conversion to 2-substituted benzazoles is obtained. Thus, % quantum yield can estimates as

% Quantum yield = time required for complete reduction of Fe(III) to Fe(II)/time required for maximum conversion to product X 100

Reference:

1. D. Dulin and T. Mill, *Environ. Sci. Technol.*, 1982, **16**, 815–820.

2. B. D . Kocara and W. P . I nskeep, *Environ. Sci. Technol*. 2003, **37**, 1581-1588.

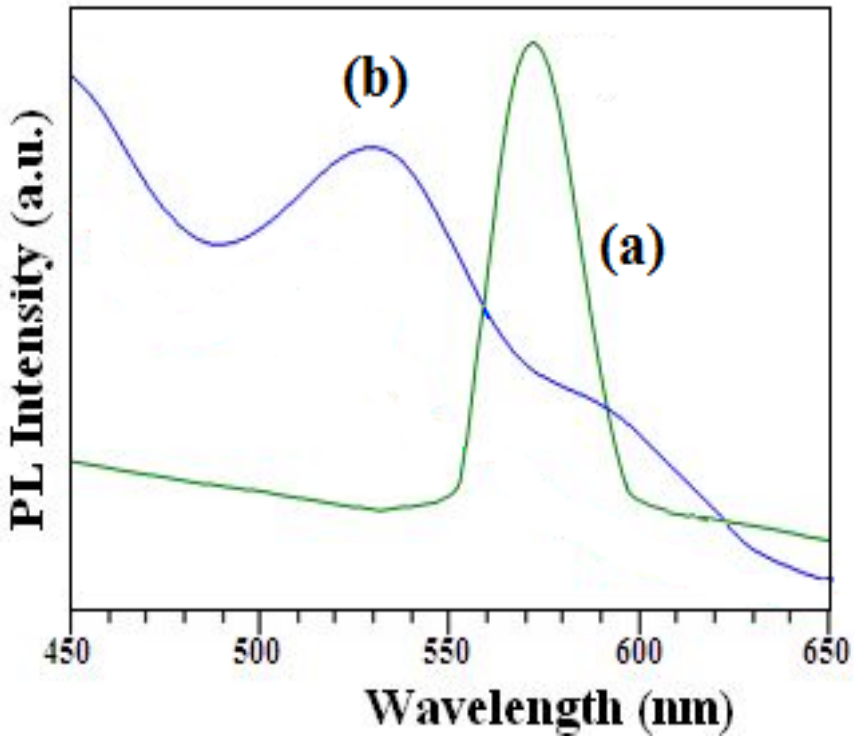
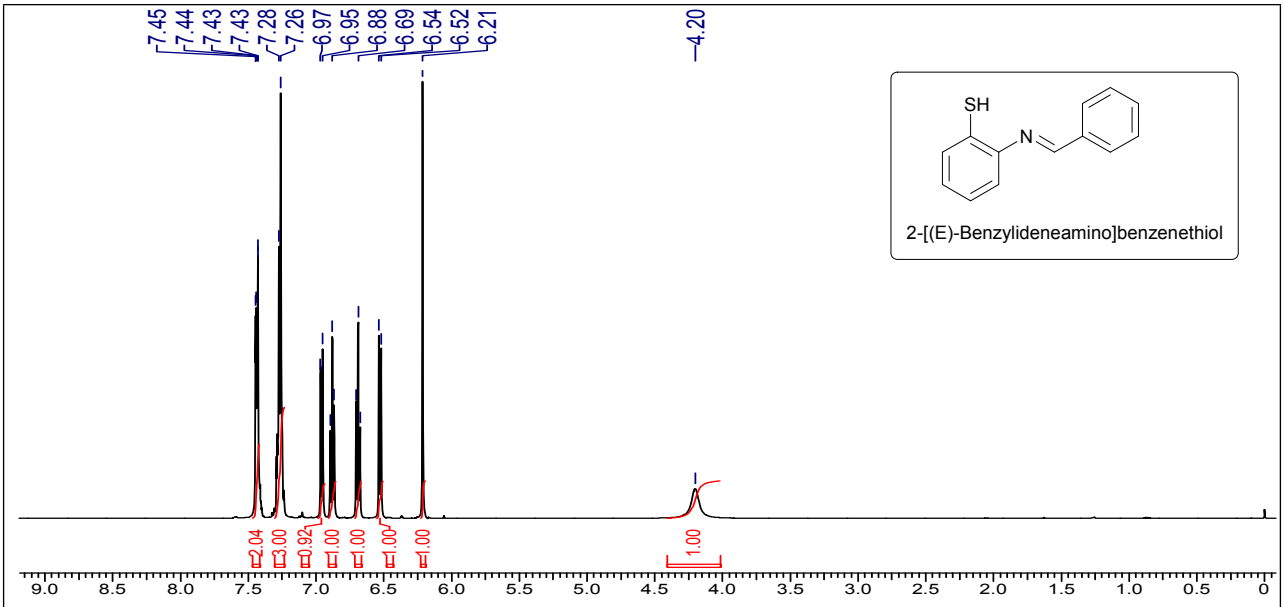
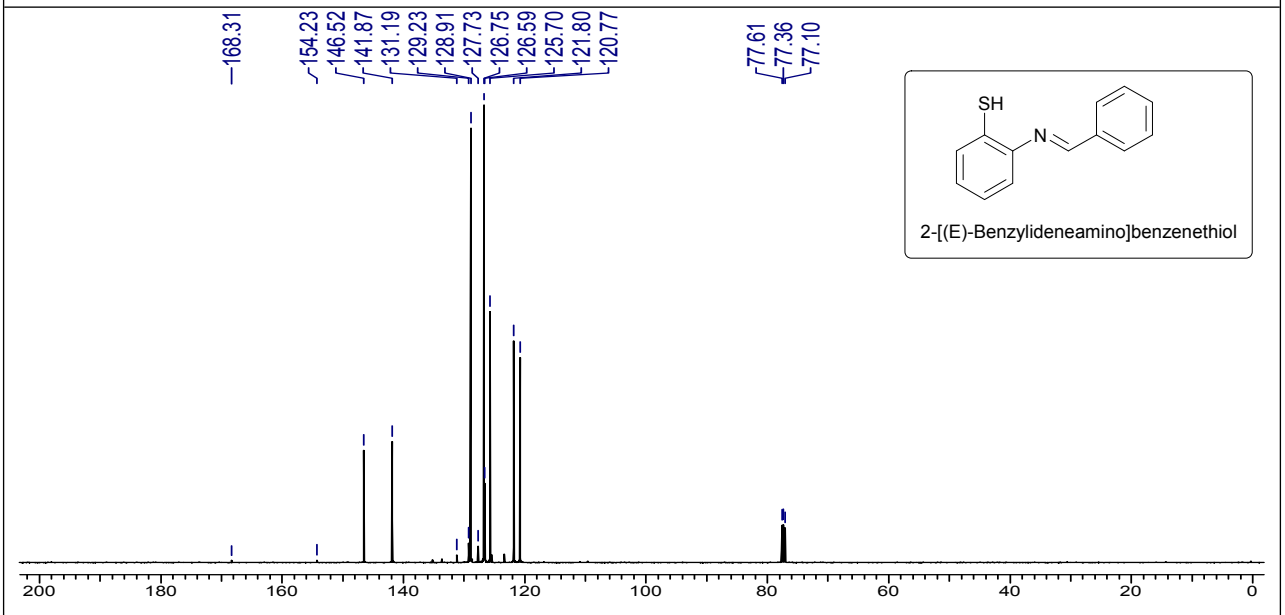


Figure S3: Photoluminescence spectra of (a) CdSe NP's and (b) 10% CdSe/MMT



^{1}H NMR (500 MHz, $CDCl_3$): (δ ppm) 7.45-7.43 (dd, *J* = 7.63, 1.83 Hz, 2 H), 7.28-7.26 (m, 3 H), 6.97-6.95 (d, *J* = 8.39 Hz, 1 H), 6.88 (t, *J* = 7.71 Hz, 1 H), 6.69 (t, *J* = 8.09 Hz, 1 H), 6.54-6.52 (d, *J* = 8.39 Hz, 1 H), 6.21 (s, 1 H), 4.20 (br. s., 1 H).



^{13}C NMR (125 MHz, $CDCl_3$): (δ ppm) 168.3, 154.2, 146.5, 141.8, 131.1, 129.2, 128.9, 127.7, 126.7, 126.5, 125.7, 121.8, 120.7.

Figure S4: ^{1}H and ^{13}C spectra of imine intermediate of **3a** in presence of MMT

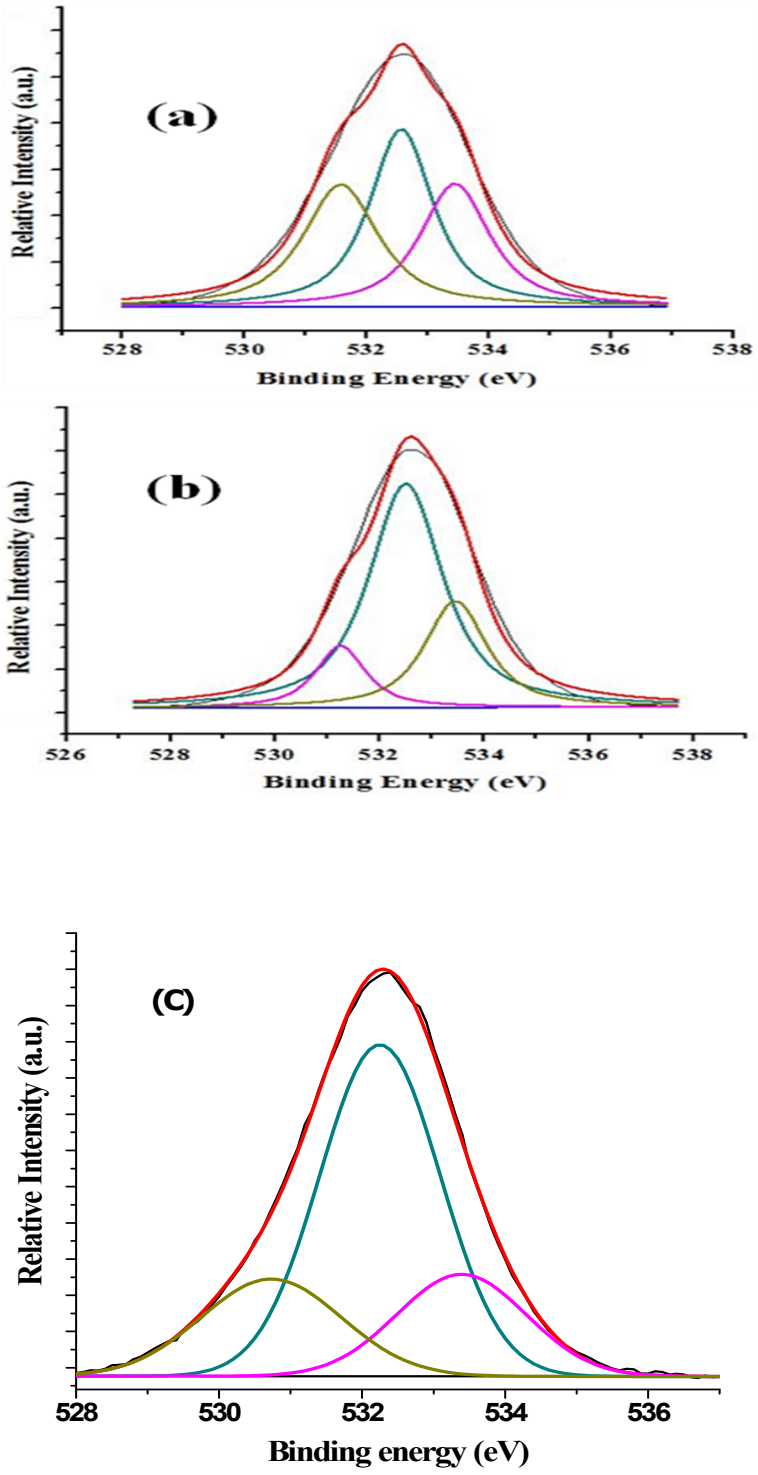
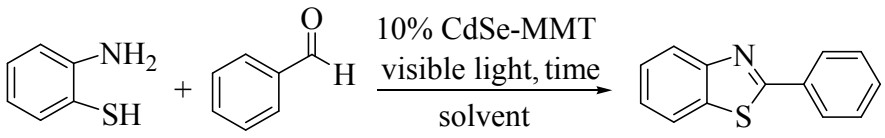


Figure S5: XPS spectra of oxygen region for 10% CdSe/MMT (a) fresh, (b) reused and (c) calcined catalyst

Table T1: Solvent dependent synthesis of 2-phenylbenzothiazole under optimized conditions[a]



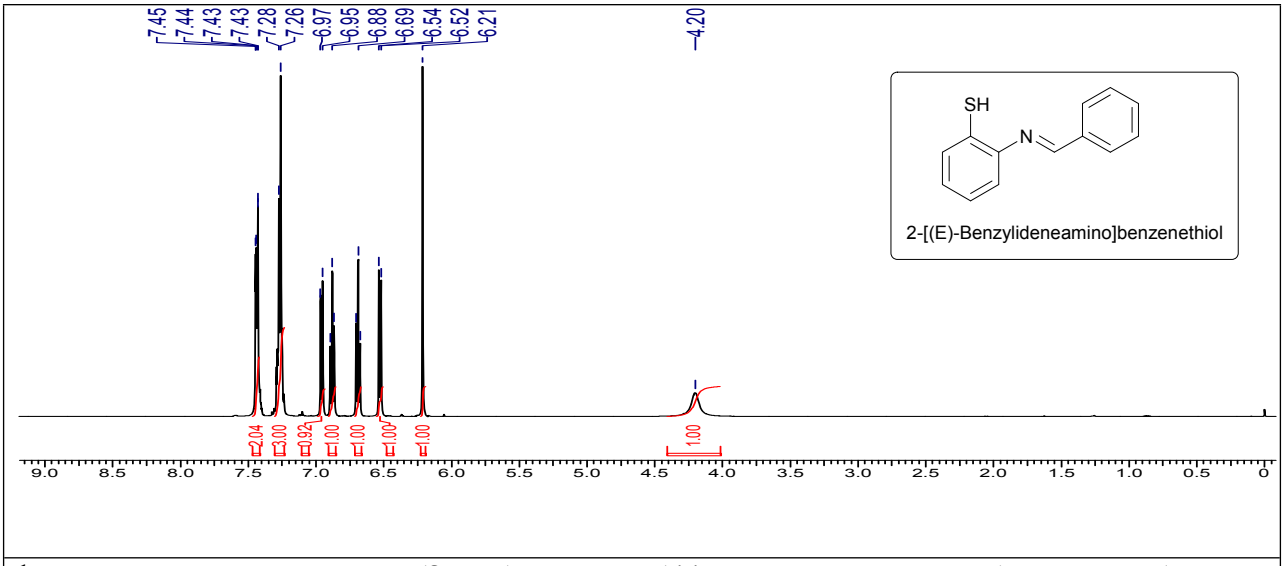
1 **2a** **3a**

entry	Solvent	Reaction time (h)	Isolated yield (%)
1	MeOH	0.5	86
2	EtOH	0.5	93
3	MeCN	0.5	82
4	MeCl	1	40
5	DCM	1	58
6	CTC	1	33
7	THF	1	38
8	DMSO	1	60
9	DMF	1	45

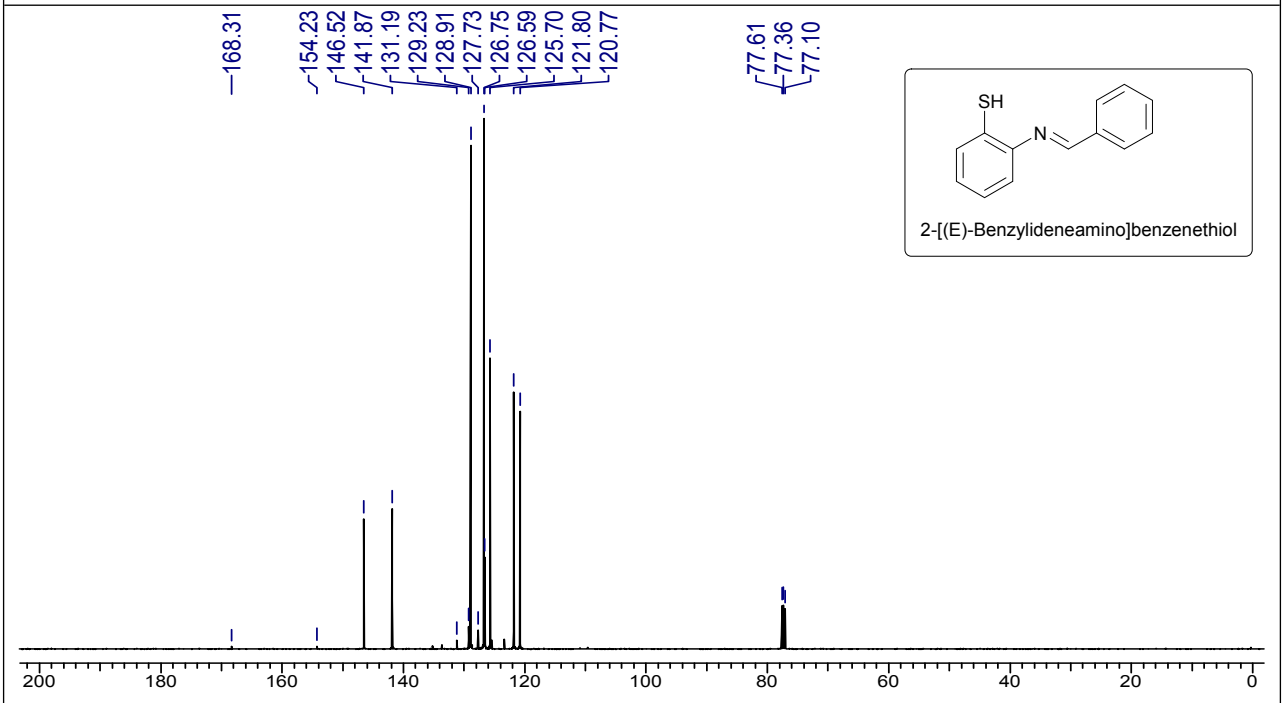
[a]Reaction conditions: 10 mmol of 2-aminothioohenol, 10 mmol of benzaldehyde, 5 mg of 10% CdSe/MMT, 30 mL solvent and 35 W tungsten lamp as light source.

Table T2: Composition analysis of 10% CdSe/MMT nanocomposite from XPS

Catalyst	Cd bound to Se (Cd_a)	Cd bound to other atoms (Cd_b)	Cd_b/Cd_a	Cd/Se ratio
Fresh	0.67	0.33	0.49	1.05:1
Used	0.31	0.69	2.2	1.89:1



^{1}H NMR (500 MHz, $CDCl_3$): (δ ppm) 7.45-7.43 (dd, *J* = 7.63, 1.83 Hz, 2 H), 7.28-7.26 (m, 3 H), 6.97-6.95 (d, *J* = 8.39 Hz, 1 H), 6.88 (t, *J* = 7.71 Hz, 1 H), 6.69 (t, *J* = 8.09 Hz, 1 H), 6.54-6.52 (d, *J* = 8.39 Hz, 1 H), 6.21 (s, 1 H), 4.20 (br. s., 1 H).



^{13}C NMR (125 MHz, $CDCl_3$): (δ ppm) 168.3, 154.2, 146.5, 141.8, 131.1, 129.2, 128.9, 127.7, 126.7, 126.5, 125.7, 121.8, 120.7.

Figure S6: ^{1}H and ^{13}C 2-Phenylbenzothiazole imine under oxygen free condition.

NMR Spectral Data

2-Phenylbenzo[d]thiazole (3a): mp 111-113 °C; **^{1}H NMR (500 MHz, $CDCl_3$):** (δ ppm) 8.03-8.00 (d, *J* = 6.06 Hz, 3 H), 7.85-7.81 (d, *J* = 7.58 Hz, 1 H), 7.42-7.31 (m, 5 H); **^{13}C NMR (100 MHz, $CDCl_3$):** (δ ppm) 168.0, 154.0, 135.0, 133.5, 130.9, 128.9, 127.5, 126.2, 125.1, 123.1, 121.5.

(4-Benzothiazol-2-yl-phenyl)-dimethyl-amine (3b): mp 174-176 °C; **^{1}H NMR (500 MHz, DMSO-d_6)**: (δ ppm) 8.05-8.03 (d, *J* = 7.48 Hz, 1 H), 7.94-7.89 (m, 3 H), 7.48 (s, 1 H), 7.38-7.35 (m, 1 H), 6.83-6.82 (d, *J* = 9.00 Hz, 2 H), 3.02 (s, 6 H); **^{13}C NMR (125 MHz, DMSO-d_6):** (δ ppm) 168.3, 154.3, 152.6, 134.2, 128.9, 126.7, 124.9, 122.4, 122.3, 120.5, 112.2, 40.1.

4-(Benzo[d]thiazol-2-yl)phenol (3c): mp 230-231 °C; **^{1}H NMR (500 MHz, DMSO-d_6)**: (δ ppm) 10.21 (br. s., 1 H), 8.06-7.92 (m, 4 H), 7.51-7.39 (m, 2 H), 6.95-6.93 (d, *J* = 8.54 Hz, 2 H); ^{13}C NMR (125 MHz, DMSO-d_6) δ ppm 167.4, 160.4, 153.7, 134.0, 129.0, 126.3, 124.8, 124.0, 122.2, 122.0, 116.0.

2-(4-Methoxyphenyl)benzo[d]thiazole (3d): mp 119-121 °C; **^{1}H NMR (400 MHz, $CDCl_3$)**: (δ ppm) 7.96-7.93 (d, *J* = 8.70 Hz, 3 H), 7.79-7.77 (d, *J* = 7.79 Hz, 1 H), 7.40-7.36 (m, 1 H), 7.28 (m, 1 H), 7.17-6.89 (d, *J* = 8.70 Hz, 2 H), 3.78 (s, 3 H); **^{13}C NMR (100 MHz, $CDCl_3$)**: (δ ppm) 167.8, 161.8, 154.1, 134.8, 129.0, 126.3, 126.1, 124.7, 122.7, 121.4, 114.3, 55.4.

2-p-Tolyl-benzothiazole (3e): mp 84-85 °C; **^{1}H NMR (400 MHz, $CDCl_3$)**: (δ ppm) 8.10-8.09 (d, *J* = 7.82 Hz, 1 H) 7.96-7.89 (m, 4 H) 7.51-7.49 (m, 1 H) 7.41-7.33 (m, 3 H) 2.47 (s, 3 H); **^{13}C NMR (100 MHz, $CDCl_3$)** (δ ppm) 167.3, 153.0, 137.8, 132.4, 130.7, 127.8, 126.9, 125.2, 124.0, 123.8, 122.1, 120.5, 20.3.

2-(3-Nitrophenyl)benzo[d]thiazole (3f): mp 182-184 °C; **^{1}H NMR (500 MHz, DMSO-d_6)** (δ ppm) 8.82 (br. s., 1 H) 8.50- 8.41 (d, 7.81, 2 H) 8.22-8.16 (d, *J* = 7.79 Hz, 2 H) 7.88 (s, 1 H), 7.60-7.54 (d, *J* = 7.82 Hz, 2 H); **^{13}C NMR (125 MHz, DMSO-d_6)**: (δ ppm) 164.8, 153.2, 148.4, 134.7, 134.1, 133.4, 131.2, 127.0, 126.2, 125.6, 123.3, 122.6, 121.1.

2-(4-Chlorophenyl)benzo[d]thiazole (3g): mp 111-113 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** (δ ppm) 8.09 - 8.02 (m, 3 H) 7.92-7.90 (d, *J* = 7.33 Hz, 1 H) 7.51 - 7.46 (m, 3 H) 7.41 (m, 1 H); **^{13}C NMR (100 MHz, $CDCl_3$):** (δ ppm) 165.5, 153.0, 135.9, 134.0, 131.0, 128.2, 127.6, 125.4, 124.3, 122.2, 120.6.

2-(4-Fluorophenyl)benzo[d]thiazole (3h): mp 97-99 °C; **^{1}H NMR (500 MHz, $CDCl_3$):** (δ ppm) 8.11-8.06 (m, 3 H), 7.91-7.90 (d, *J* = 7.93 Hz, 1 H), 7.51-7.49 (t, *J* = 7.63 Hz, 1 H), 7.41-7.40 (t, *J* = 7.63 Hz, 1 H), 7.21-7.17 (t, *J* = 8.54 Hz, 2 H); **^{13}C NMR (125 MHz, $CDCl_3$):** (δ ppm) 166.7, 165.4, 163.4, 154.0, 135.0, 129.9, 129.5, 126.3, 125.2, 123.1, 121.5, 116.2.

2-(3-Bromophenyl)benzo[d]thiazole (3i): mp 92-94 °C; **^{1}H NMR (400 MHz, $CDCl_3$):** (δ ppm) 8.29 (s, 1 H), 8.11-8.09 (d, *J* = 8.07 Hz, 1 H), 8.01-7.99 (d, *J* = 7.82 Hz, 1 H), 7.93-7.91 (d, *J* = 7.82 Hz, 1 H), 7.52 (d, *J* = 8.07 Hz, 1 H), 7.42 (t, *J* = 8.31 Hz, 1 H), 7.39-7.37 (m, 2 H); **^{13}C NMR (100 MHz, $CDCl_3$):** (δ ppm) 166.1, 153.9, 135.4, 135.0, 133.7, 130.4, 130.2, 126.5, 126.1, 125.5, 123.4, 123.1, 121.6.

2-(Pyridin-2-yl)benzo[d]thiazole (3j): mp 134-136 °C; **^{1}H NMR (500 MHz, DMSO-d_6):** (δ ppm) 8.71 (br. s., 1 H), 8.30 (br. s., 1 H), 8.13-7.97 (m, 3 H), 7.55-7.47 (m, 3 H); **^{13}C NMR (125 MHz, DMSO-d_6):** (δ ppm) 168.9, 153.6, 150.3, 149.8, 137.7, 135.3, 126.4, 125.9, 125.8, 123.2, 122.4, 120.2.

2-(Thiophen-2-yl)benzo[d]thiazole (3k): mp 98-100 °C; **^{1}H NMR (500 MHz, DMSO-d_6):** (δ ppm) 8.04-7.99 (m, 2 H), 7.84-7.77 (m, 2 H) 7.51-7.48 (m, 1 H), 7.42-7.38 (m, 1

H), 7.21-7.19 (dd, J = 4.96, 3.74 Hz, 1 H); **^{13}C NMR (125 MHz, DMSO-d_6):** (δ ppm) 161.8, 153.0, 136.3, 134.2, 130.7, 129.6, 129.5, 128.6, 126.6, 125.4, 122.4, 122.1.

2-Methylbenzo[d]thiazole (3l): bp 236-237 °C; **^{1}H NMR (500 MHz, DMSO-d_6):** (δ ppm) 8.26 (br. s., 1 H), 7.95 (br. s., 1 H), 7.54 (br. s., 1 H), 7.41 (br. s., 1 H), 2.80 (br. s., 3 H); **^{13}C NMR (125 MHz, DMSO-d_6):** (δ ppm) 166.0, 153.3, 135.6, 125.5, 124.2, 122.1, 121.2, 19.4.

Benzo[d]thiazole (3m): bp 227-228 °C; **^{1}H NMR (500 MHz, DMSO-d_6):** (δ ppm) 8.63 (br. s., 1 H), 7.87 (br. s., 1 H), 7.55 (br. s., 1 H), 7.13-7.05 (m, 2 H); **^{13}C NMR (125 MHz, DMSO-d_6):** (δ ppm) 149.2, 148.4, 128.9, 121.3, 120.7, 118.8, 117.1.

2-Phenyl-1H-benzo[d]imidazole (4a): mp 293-295 °C; **^{1}H NMR (500 MHz, DMSO-d_6):** (δ ppm) 12.93 (br. s., 1 H), 8.21-8.20 (d, J = 8.55 Hz, 2 H), 7.61-7.47 (m, 5 H), 7.22-7.20 (d, J = 9.16 Hz, 2 H); **^{13}C NMR (125 MHz, DMSO-d_6)**: (δ ppm) 151.2, 144.0, 135.5, 130.1, 129.7, 128.9, 126.4, 126.1, 122.0, 118.6, 111.3.

2-(3-Nitrophenyl)-1H-benzo[d]imidazole (4f): mp 278-280 °C; **^{1}H NMR (500 MHz, DMSO-d_6):** (δ ppm) 13.29 (br. s., 1 H), 9.00 (br. s., 1 H), 8.59-8.58 (t, J = 6.26 Hz, 1 H), 8.30-8.27 (t, J = 8.62 Hz, 1 H), 7.82-7.80 (m, 1 H), 7.70 (s, 1 H), 7.57 (s, 1 H), 7.24 (m, 2 H); **^{13}C NMR (125 MHz, DMSO-d_6):** (δ ppm) 149.0, 148.3, 143.6, 135.1, 132.4, 131.7, 130.6, 124.2, 123.2, 122.1, 120.8, 119.2, 111.7.

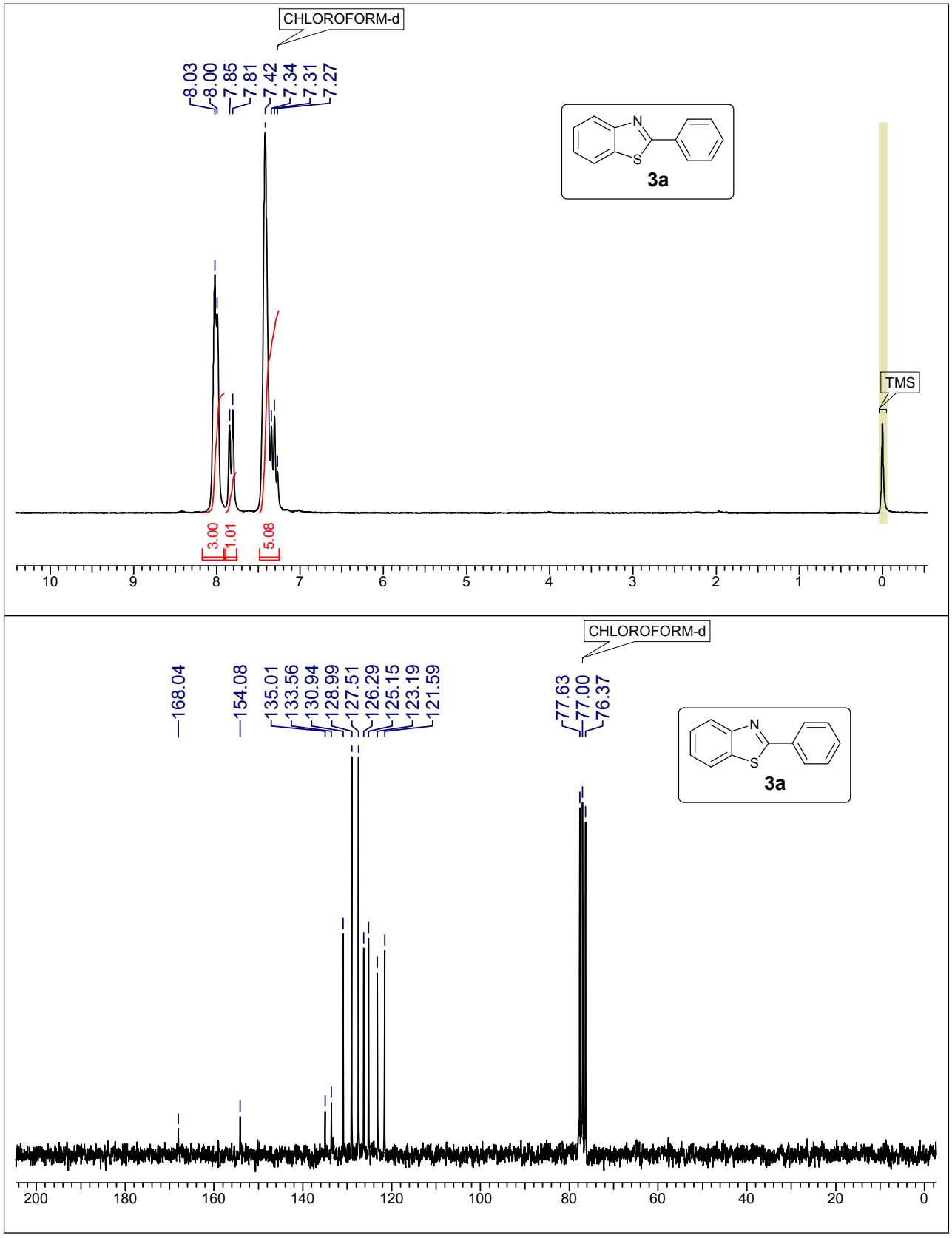
2-(Pyridin-2-yl)-1H-benzo[d]imidazole (4j): mp 218-220 °C; ^{1}H **NMR (500 MHz, DMSO-d_6):** (δ ppm) 13.13 (br. s., 1 H) 8.73- 8.72 (m, 1H) 8.35-8.33 (d, J = 7.93 Hz, 1 H) 8.01-7.99 (td, J = 7.71, 1.68 Hz, 1 H) 7.72 (d, J = 7.48 Hz, 1 H) 7.52 - 7.50 (m, 2 H) 7.25- 7.21 (m, 2 H); **^{13}C NMR (125 MHz, DMSO-d_6):** (δ ppm) 150.7, 149.3, 148.5, 143.8, 137.5, 134.9, 124.7, 123.1, 121.9, 121.4, 119.3, 112.0.

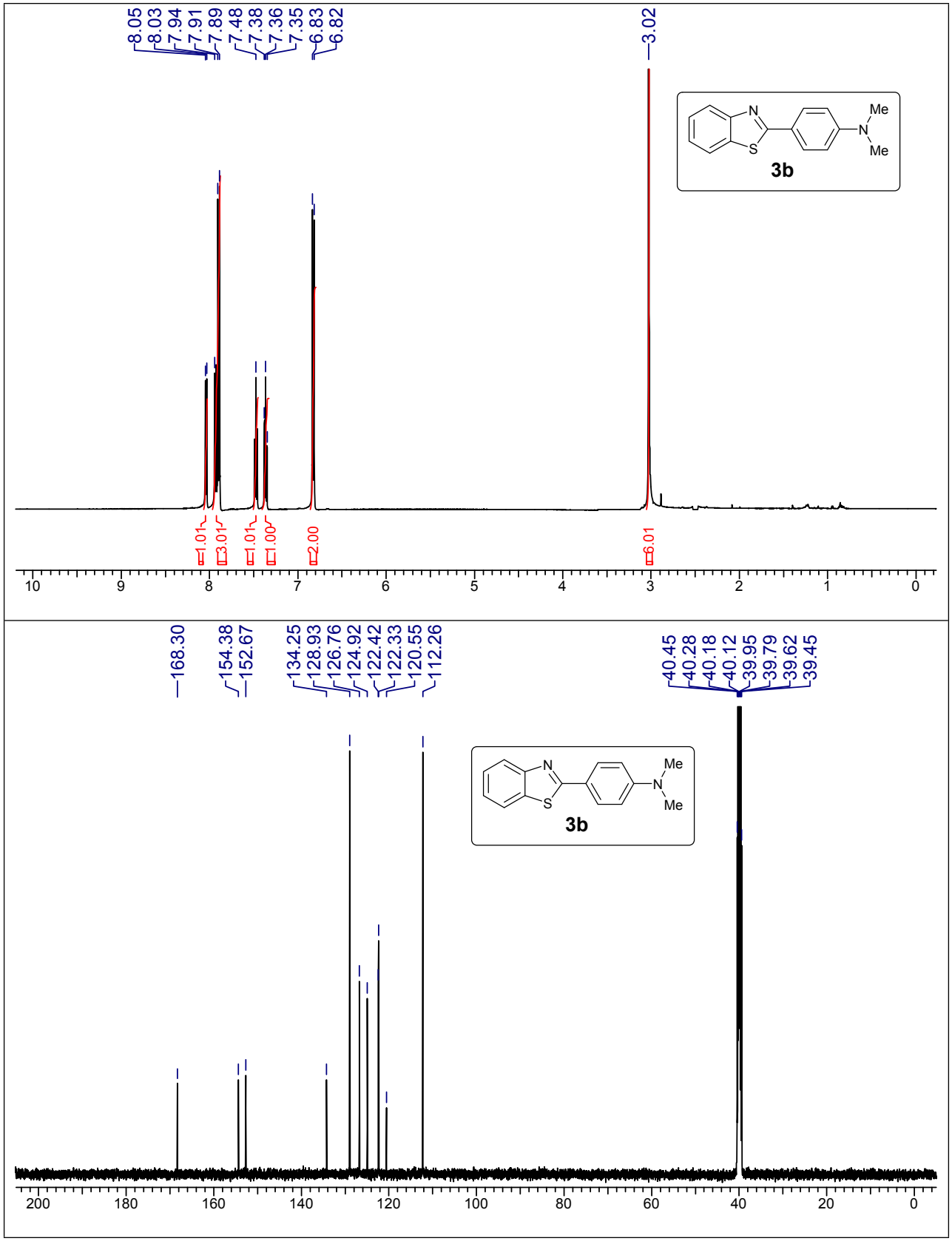
2-(Thiophen-2-yl)-1H-benzo[d]imidazole (4k): mp 286-288 °C; **^{1}H NMR (500 MHz, DMSO-d_6):** (δ ppm) 7.82-7.81 (d, *J* = 5.95 Hz, 1 H), 7.74-7.73 (d, *J* = 4.58 Hz, 1 H), 7.71-7.69 (m, 2 H), 7.30-7.24 (m, 3 H); **^{13}C NMR (125 MHz, DMSO-d_6):** (δ ppm) 146.7, 132.0, 128.4, 127.8, 127.0, 126.1, 122.6.

2-Methyl-1H-benzo[d]imidazole (4l): mp 174-176 °C; **^{1}H NMR (500 MHz, DMSO-d_6):** (δ ppm) 12.38 (br. s., 1 H) 7.50-7.49 (dd, *J* = 5.49, 3.20 Hz, 2 H) 7.13-7.11 (dd, *J* = 5.49, 3.20 Hz, 2 H) 2.53 (s, 3 H); **^{13}C NMR (125 MHz, DMSO-d_6):** (δ ppm) 151.3, 121.1, 14.6.

1H-Benzo[d]imidazole (4m): mp 171-173 °C; **^{1}H NMR (500 MHz, DMSO-d_6):** (δ ppm) 12.63 (br. s., 1 H) 8.30 (s, 1 H) 7.65-7.63 (dd, *J* = 5.95, 3.05 Hz, 2 H) 7.21-7.19 (dd, *J* = 5.95, 3.05 Hz, 2 H); **^{13}C NMR (125 MHz, DMSO-d_6):** (δ ppm) 142.2, 138.1, 121.8, 115.4.

^{1}H-NMR & ^{13}C- NMR spectra

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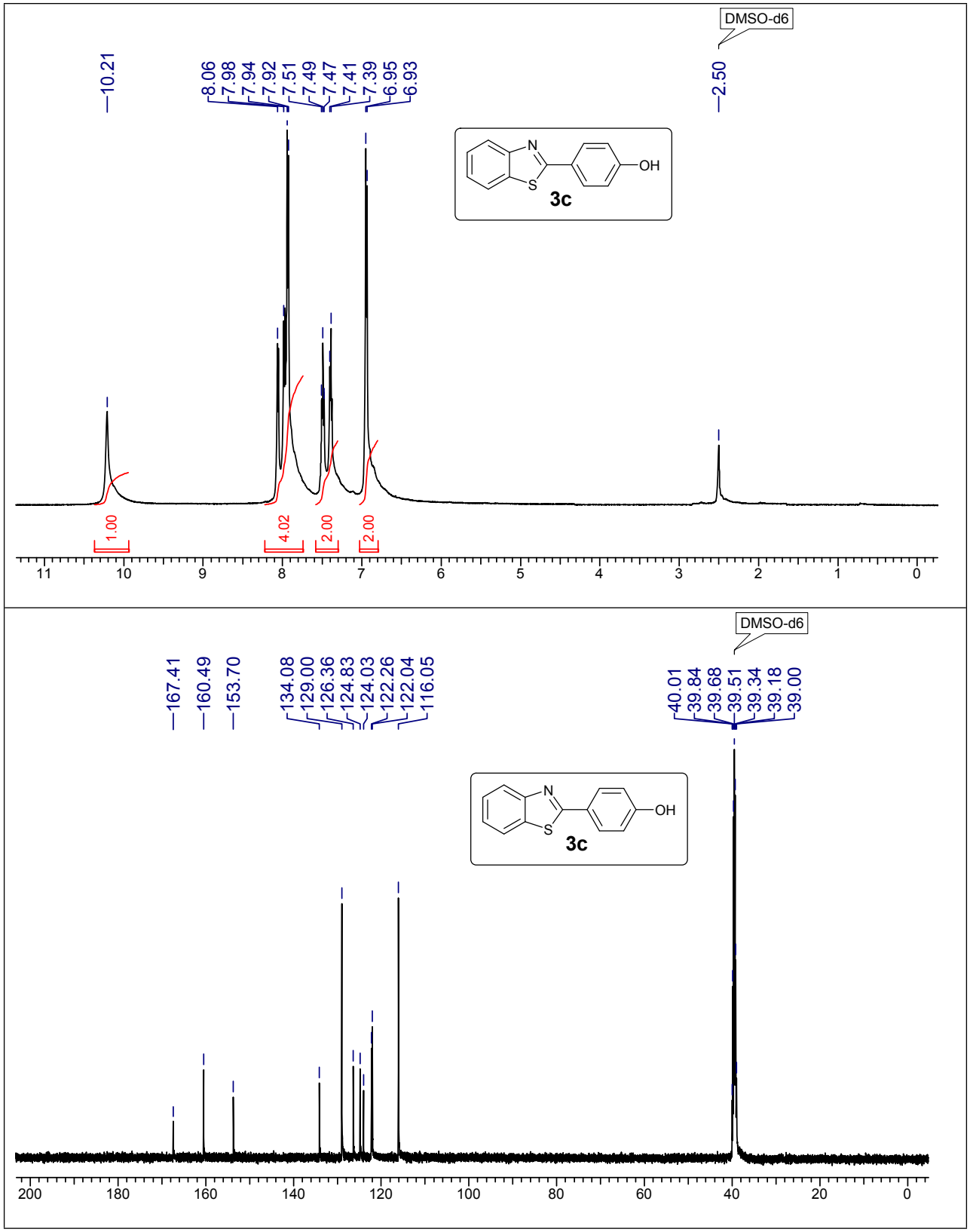
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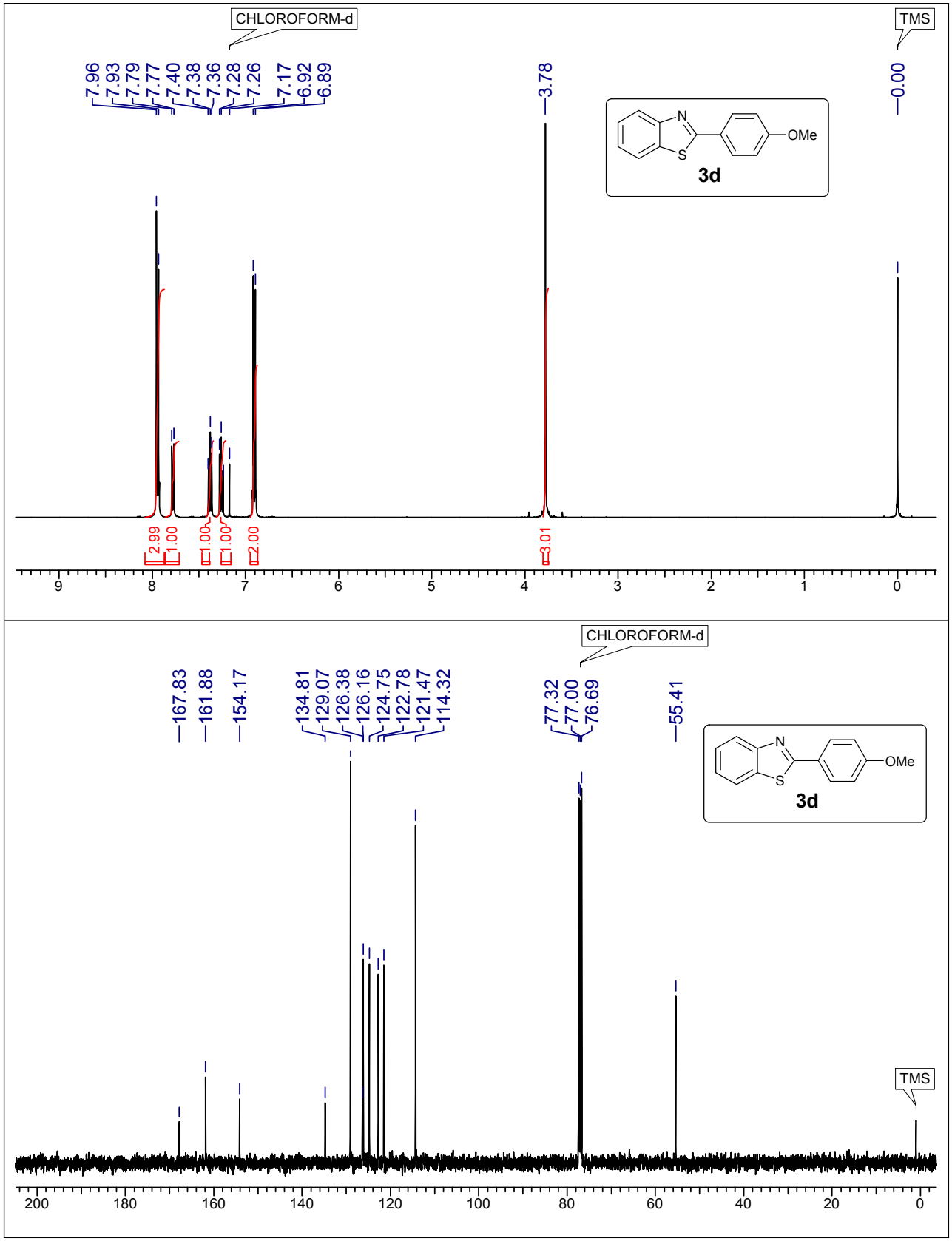
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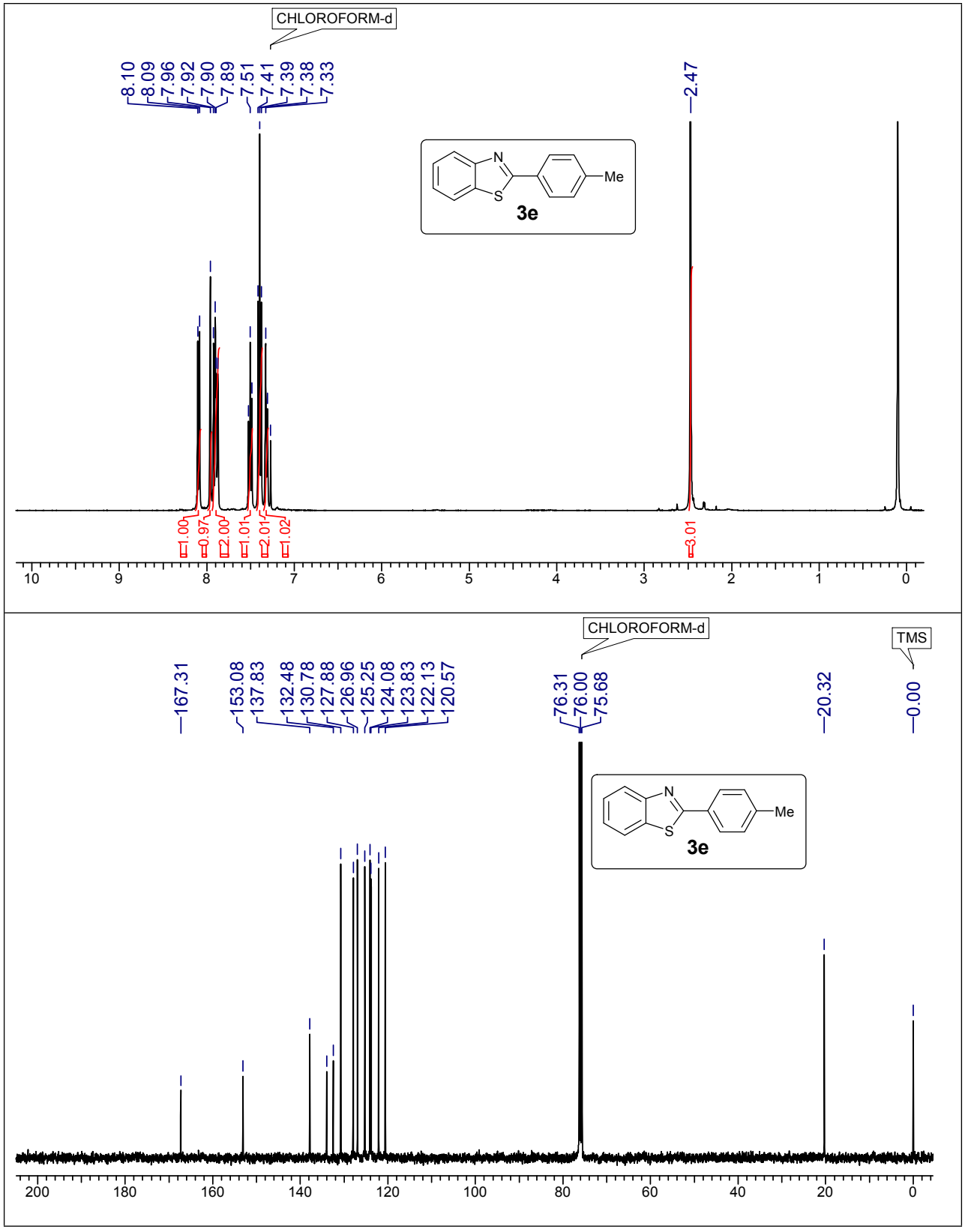
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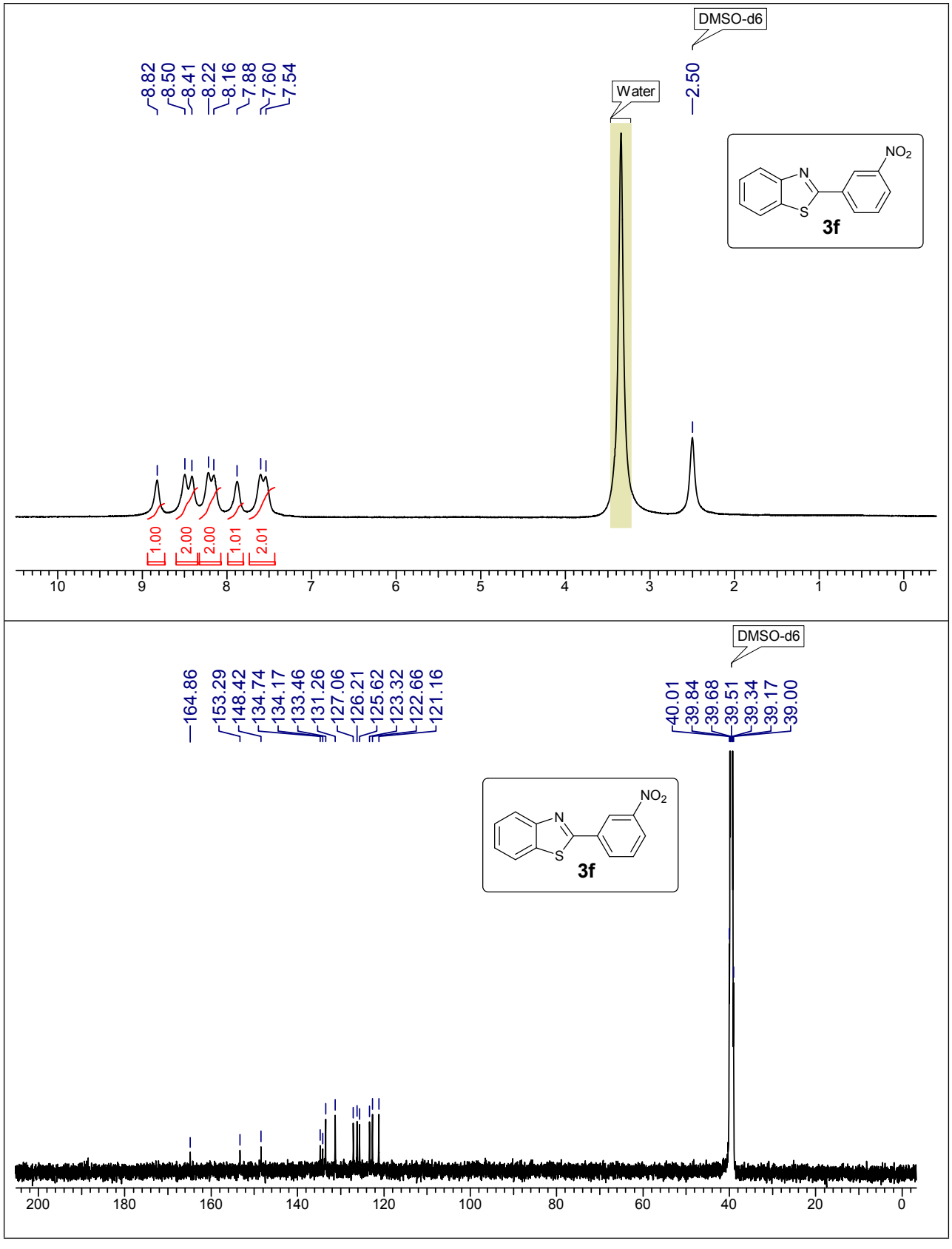
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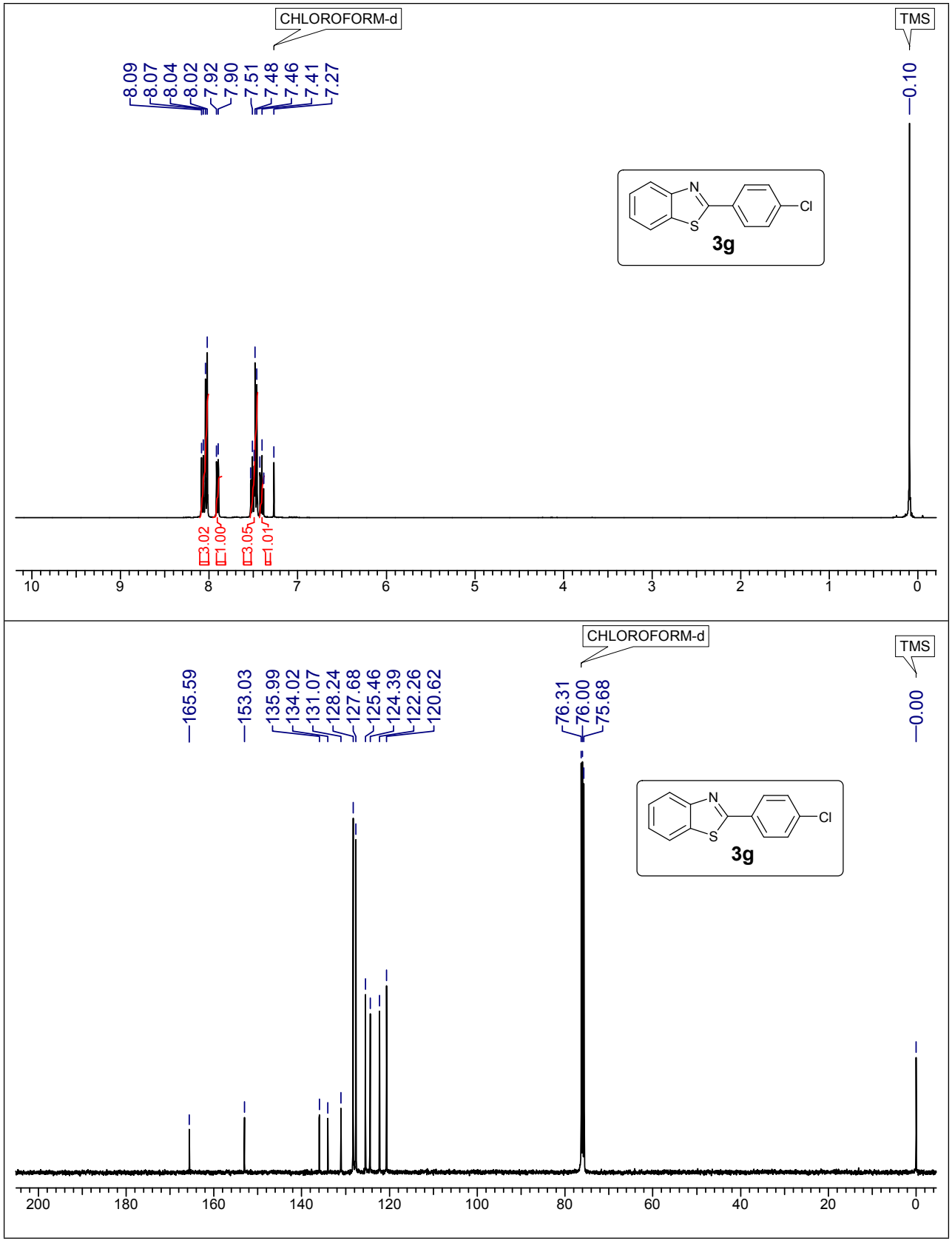
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8.02
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7.41
7.27
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N
S
Cl
3g
3.02
1.00
3.05
1.01
10
9
8
7
6
5
4
3
2
1
0
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TMS
165.59
153.03
135.99
134.02
131.07
128.24
127.68
125.46
124.39
122.26
120.62
76.31
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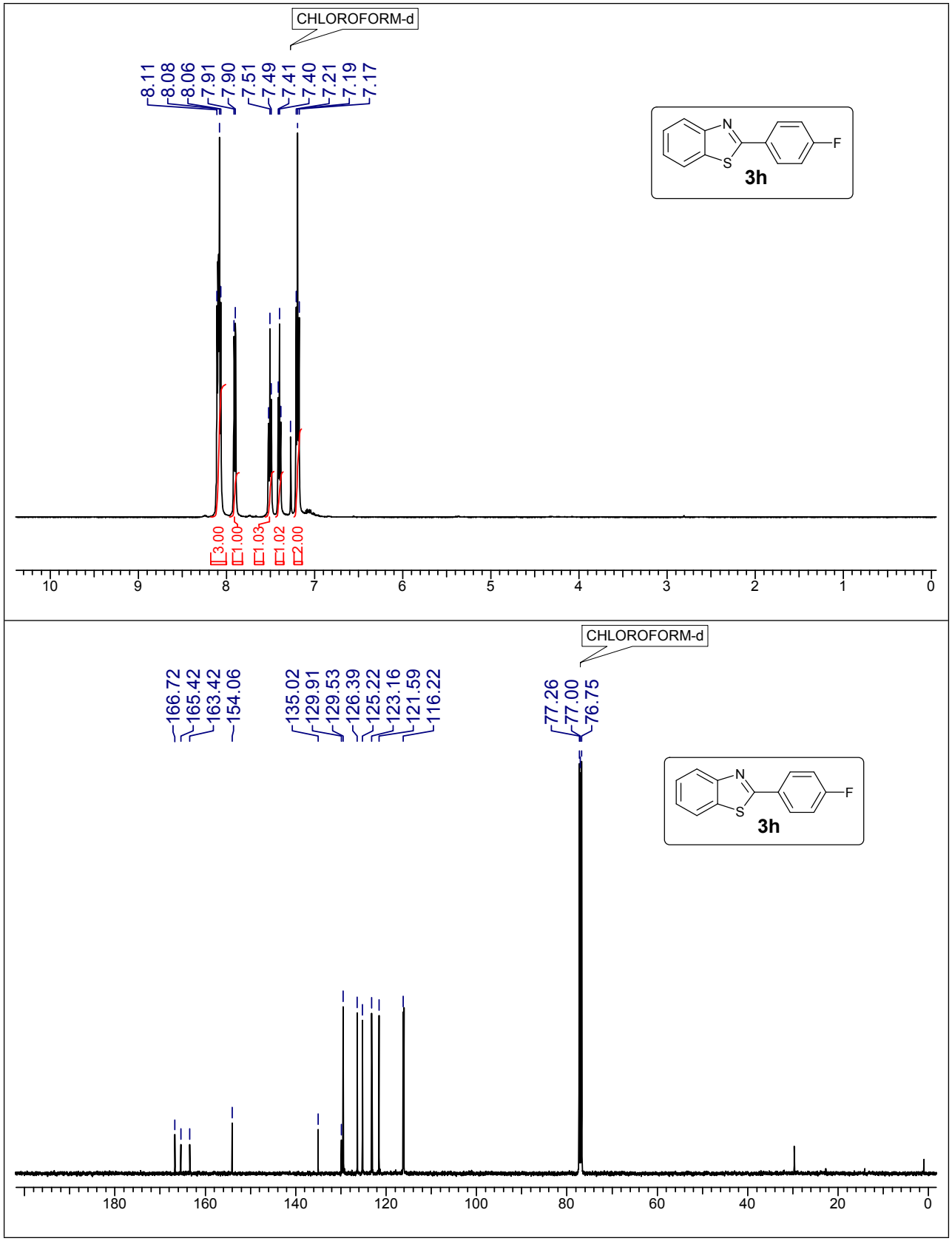
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7.21
7.19
7.17
3.00
1.00
1.03
1.02
2.00
10
9
8
7
6
5
4
3
2
1
0
N
S
F
3h
CHLOROFORM-d
166.72
165.42
163.42
154.06
135.02
129.91
129.53
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125.22
123.16
121.59
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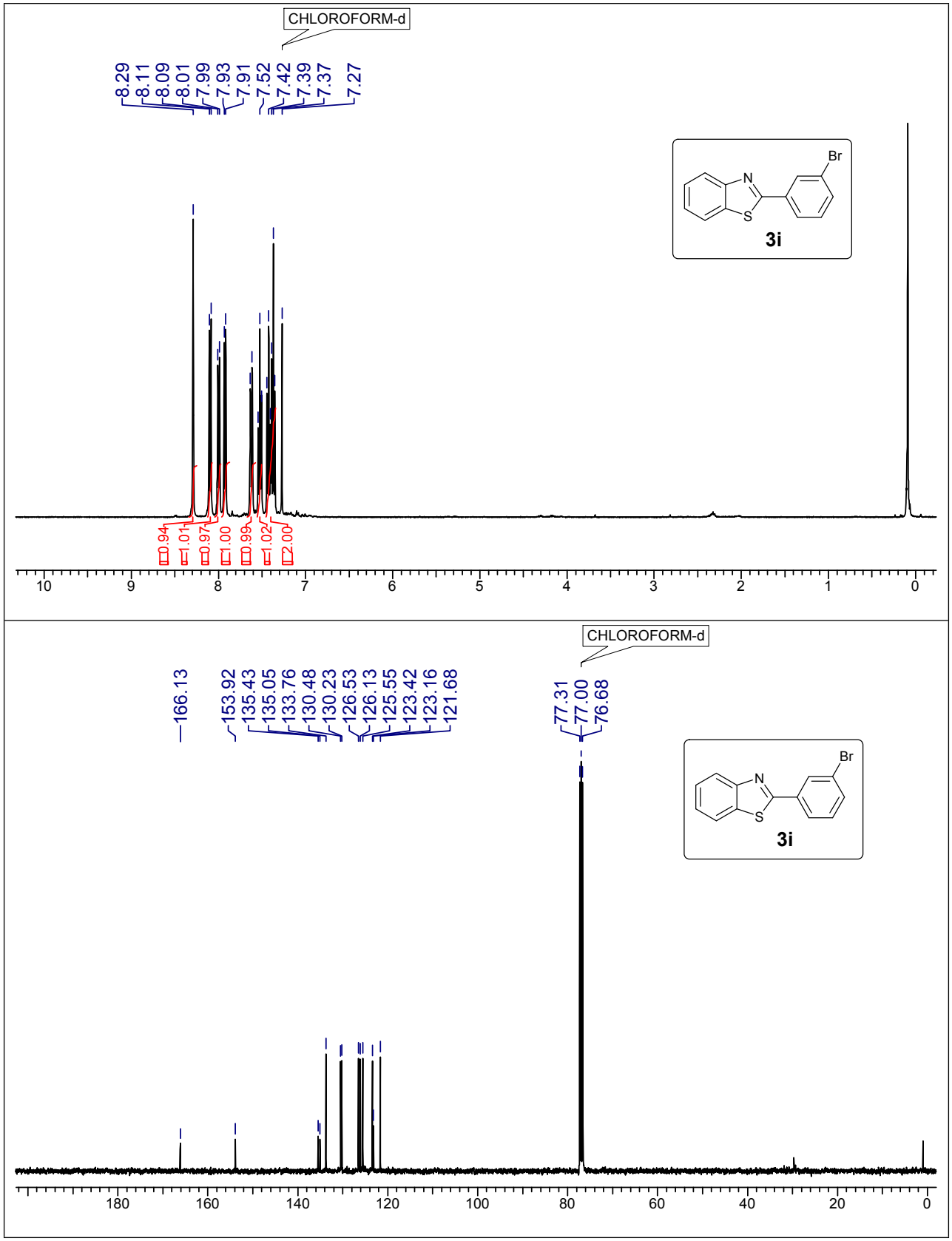
S
F
3h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7.39
7.37
7.27
Br
N
S
3i
0.94
1.01
0.97
1.00
0.99
1.02
2.00
10
9
8
7
6
5
4
3
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0
CHLOROFORM-d
166.13
153.92
135.43
135.05
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130.48
130.23
126.53
126.13
125.55
123.42
123.16
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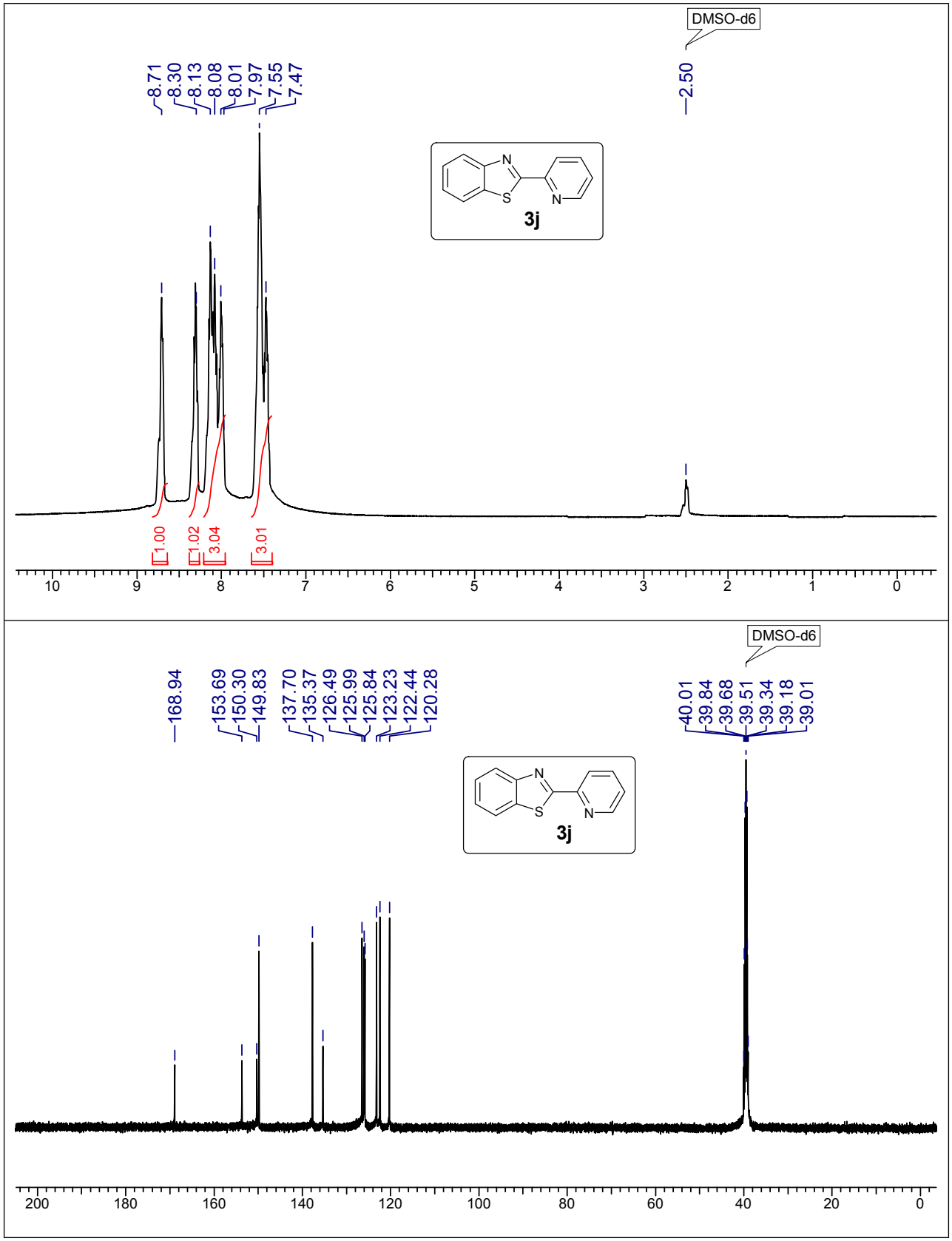
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7.55
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1.02
3.04
3.01
10
9
8
7
6
5
4
3
2
1
0
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168.94
153.69
150.30
149.83
137.70
135.37
126.49
125.99
125.84
123.23
122.44
120.28
40.01
39.84
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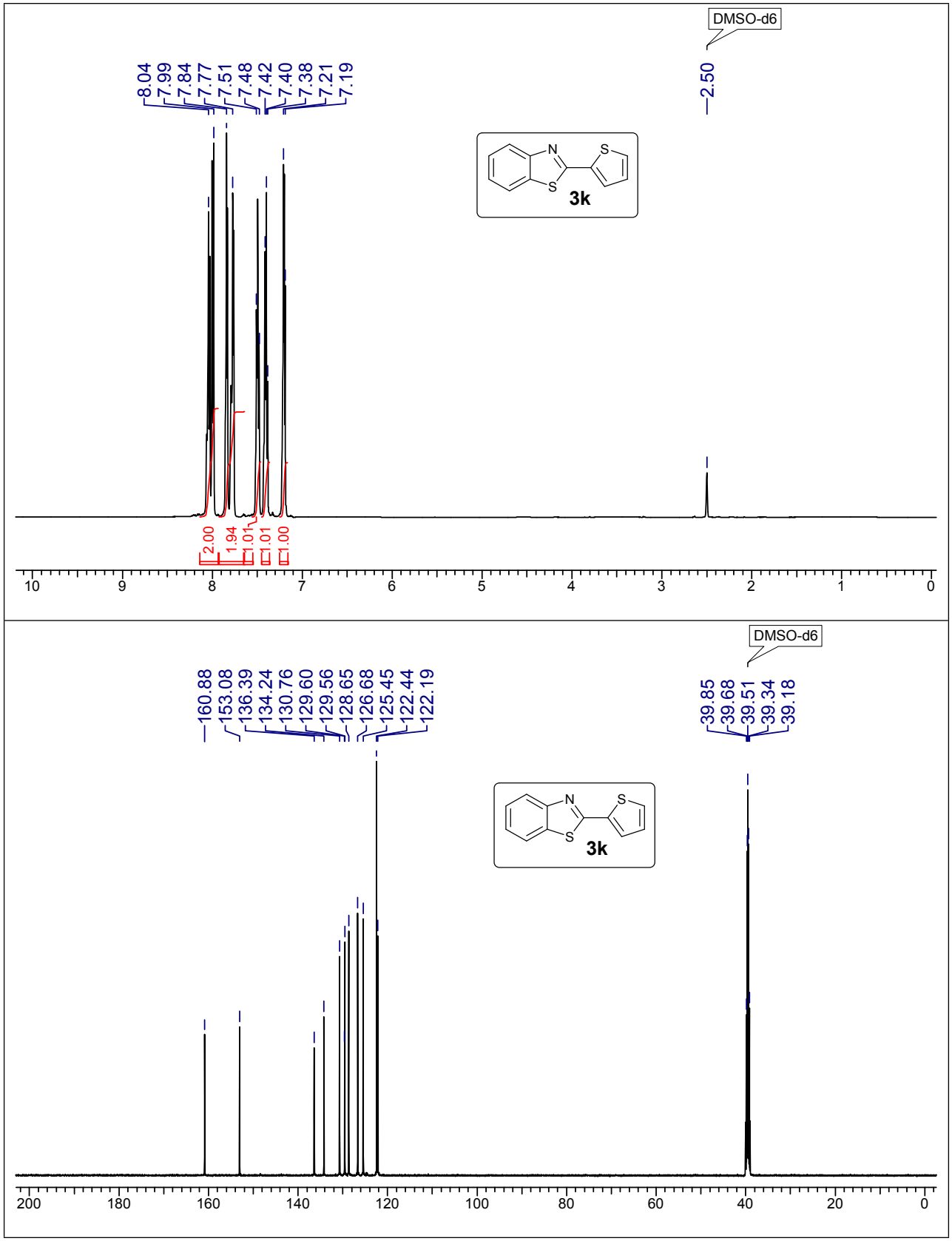
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2.50
N
S
S
3k
2.00
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1.01
1.01
1.00
10
9
8
7
6
5
4
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2
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153.08
136.39
134.24
130.76
129.60
129.56
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126.68
125.45
122.44
122.19
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39.68
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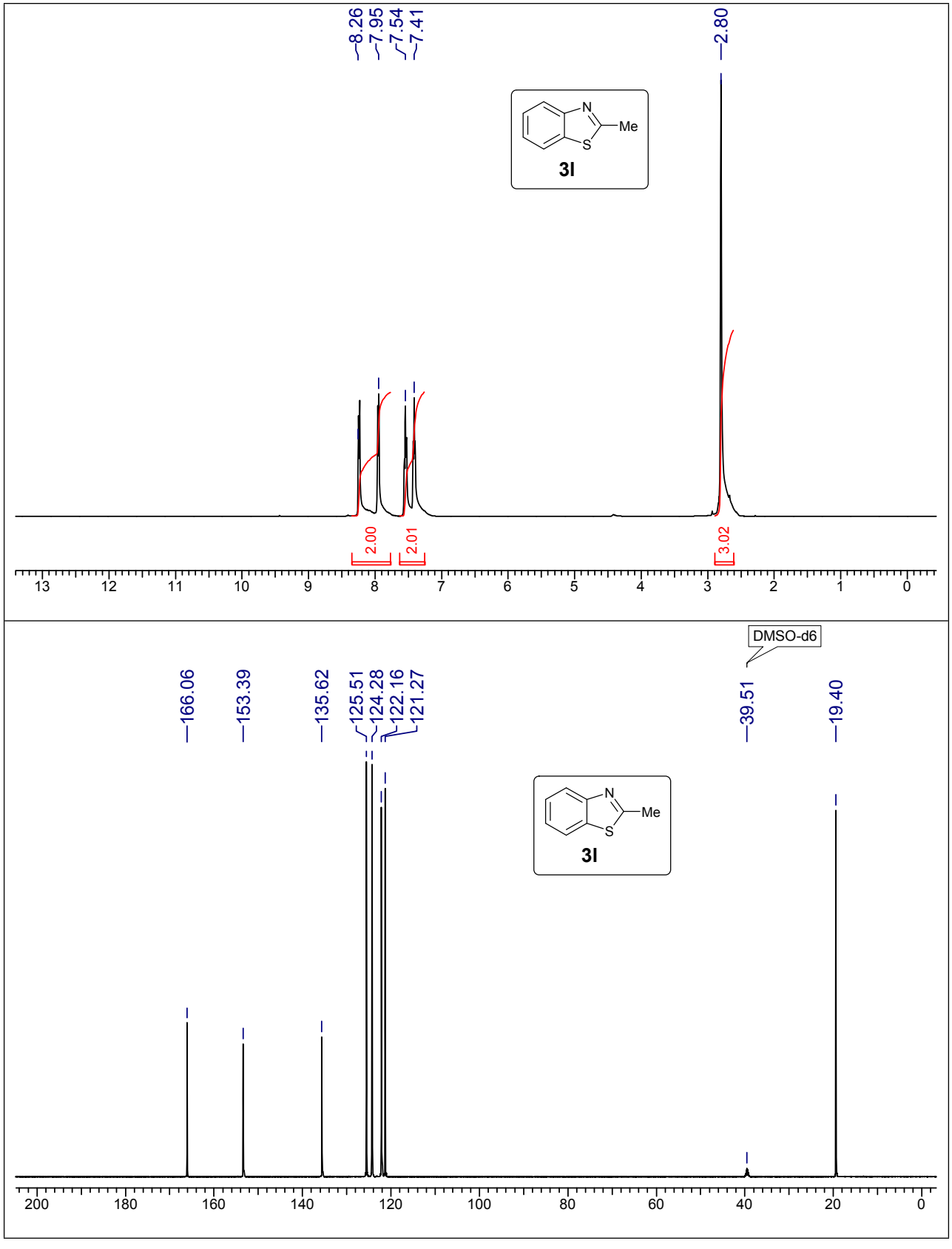
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7.54
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3.02
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11
10
9
8
7
6
5
4
3
2
1
0
DMSO-d6
166.06
153.39
135.62
125.51
124.28
122.16
121.27
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19.40
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Me
S
3l
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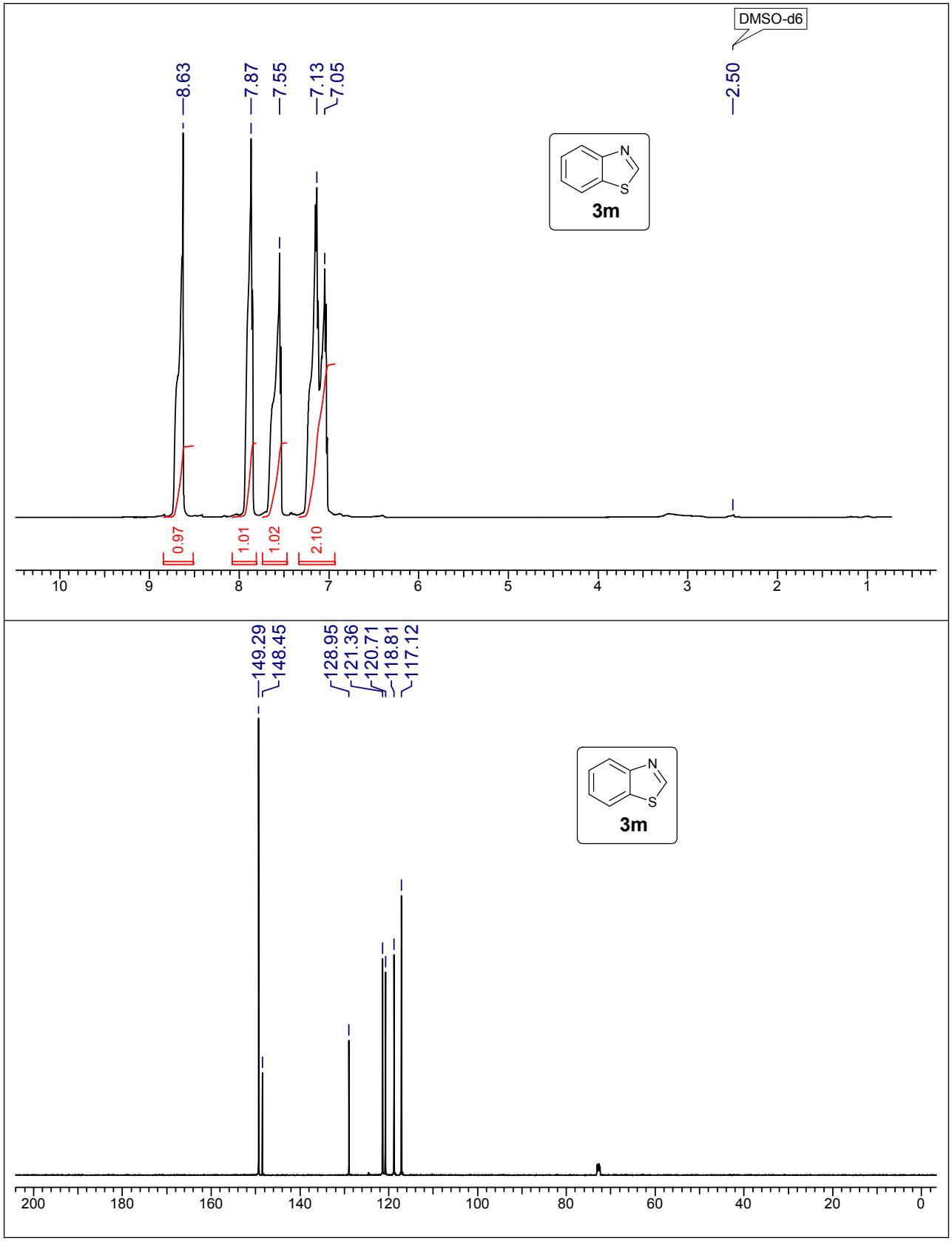
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5
4
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148.45
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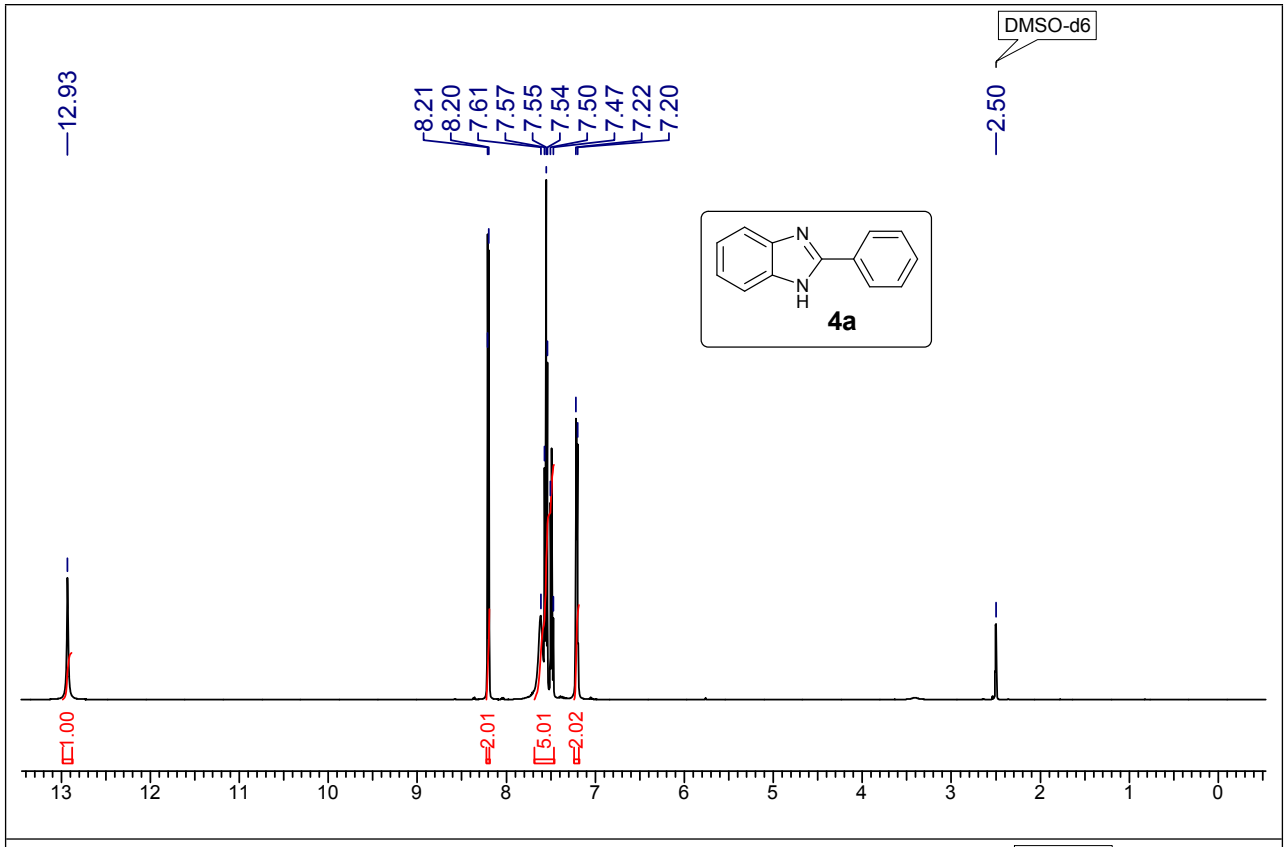
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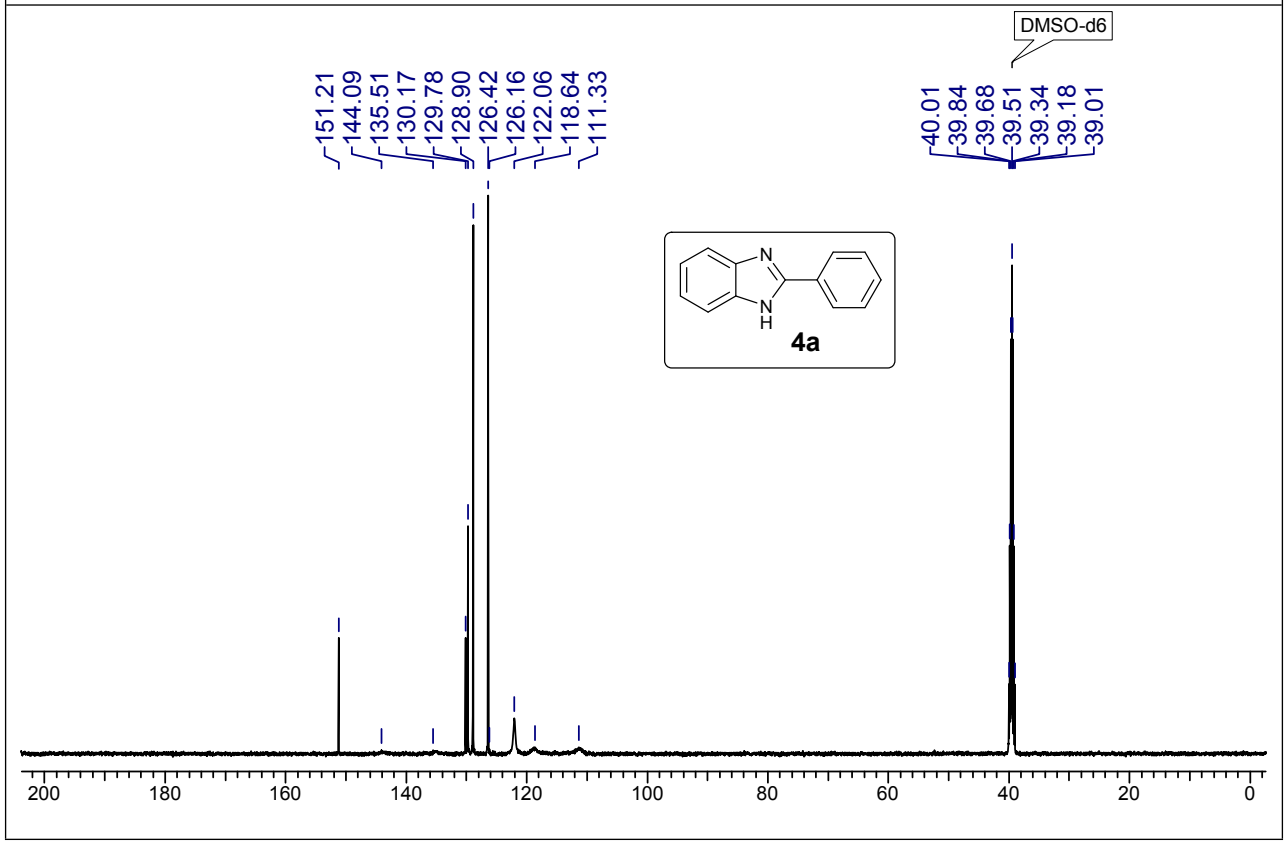
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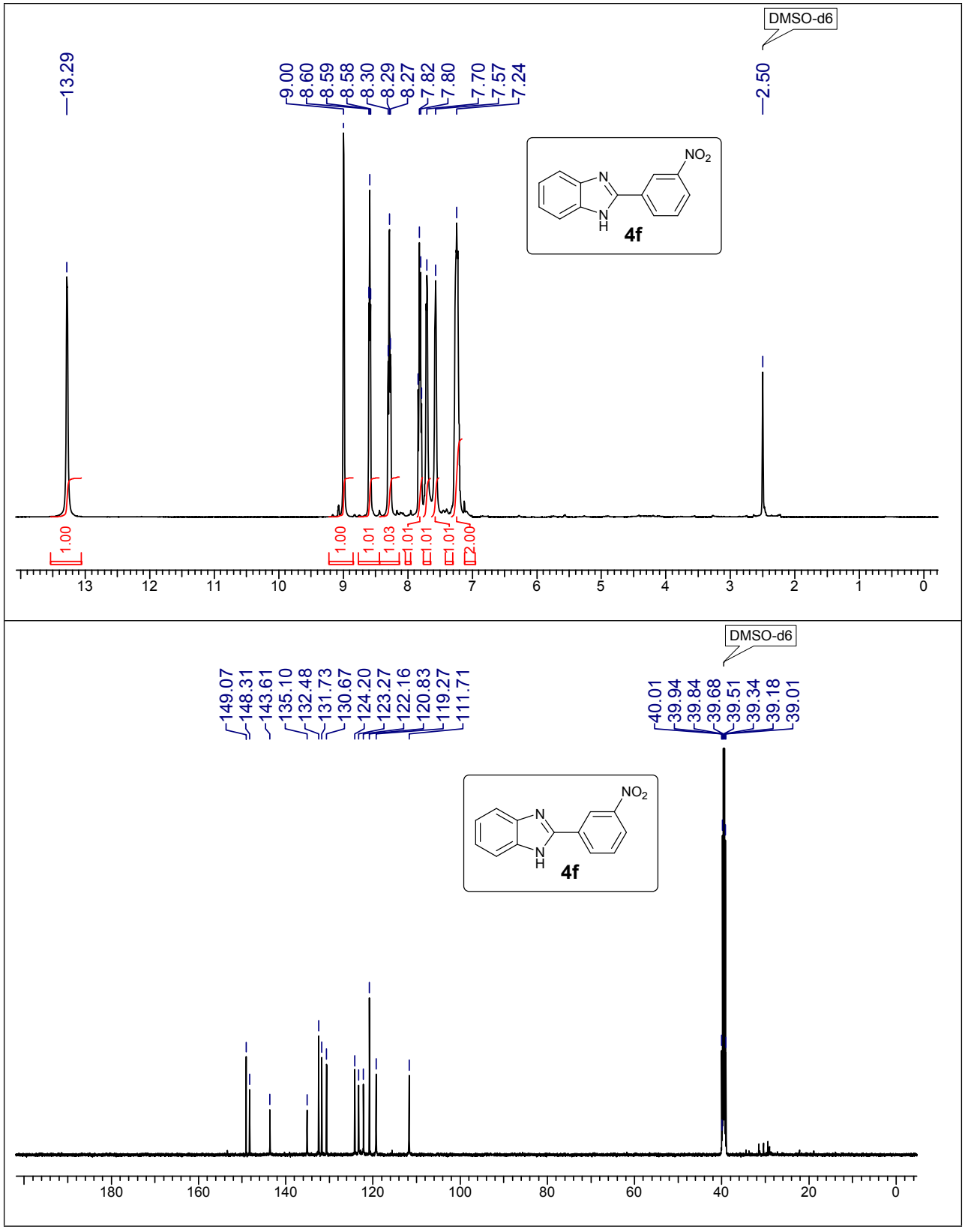
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7.70
7.57
7.24
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N
H
4f
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1.00
1.01
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1.01
1.01
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2.00
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12
11
10
9
8
7
6
5
4
3
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148.31
143.61
135.10
132.48
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123.27
122.16
120.83
119.27
111.71
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39.94
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39.68
39.51
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NO2
N
N
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4f
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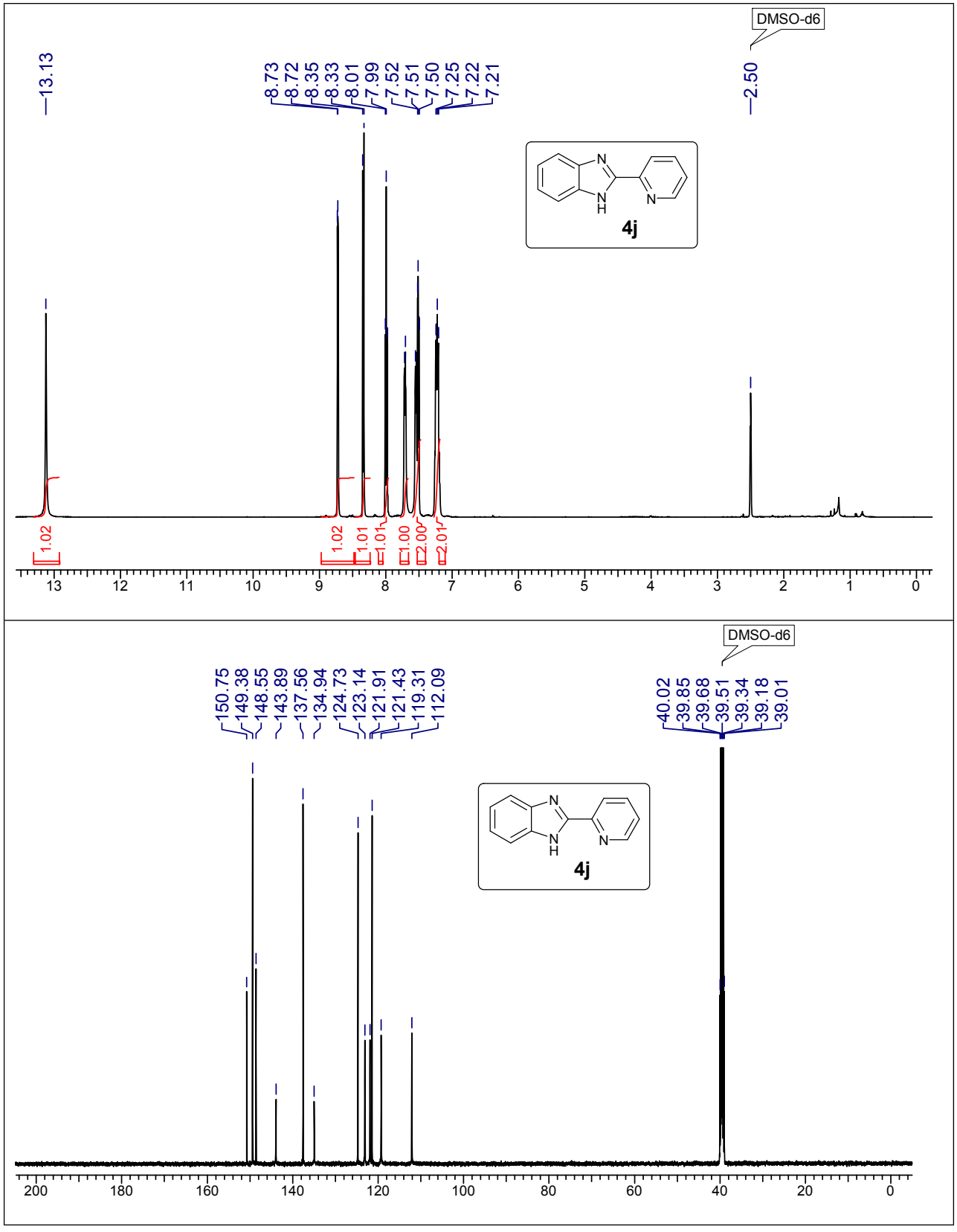
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7.21
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1.02
1.01
1.01
1.00
2.00
2.01
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12
11
10
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8
7
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5
4
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40.02
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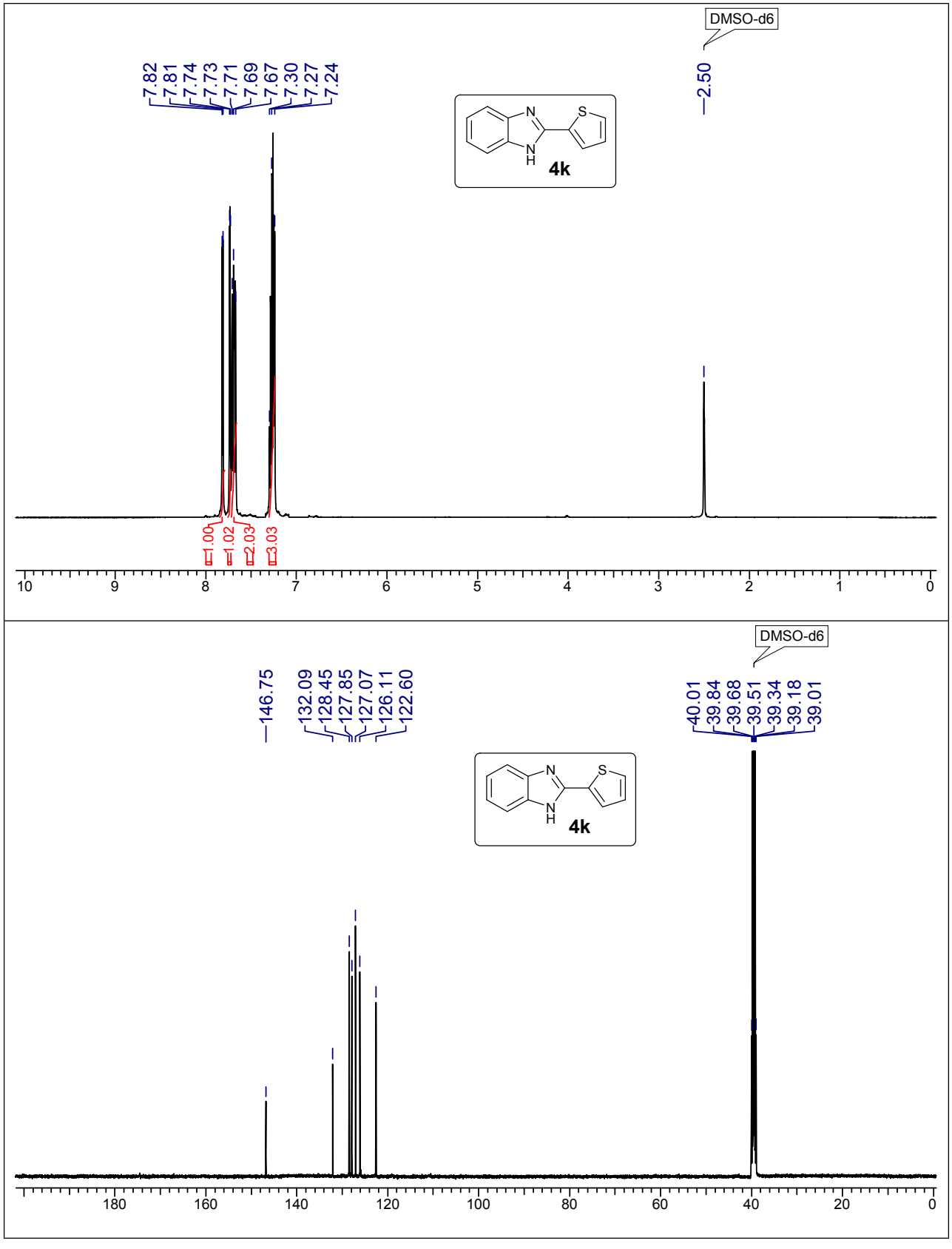
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1.02
2.03
3.03
10
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7
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4
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0
DMSO-d6
146.75
132.09
128.45
127.85
127.07
126.11
122.60
40.01
39.84
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39.34
39.18
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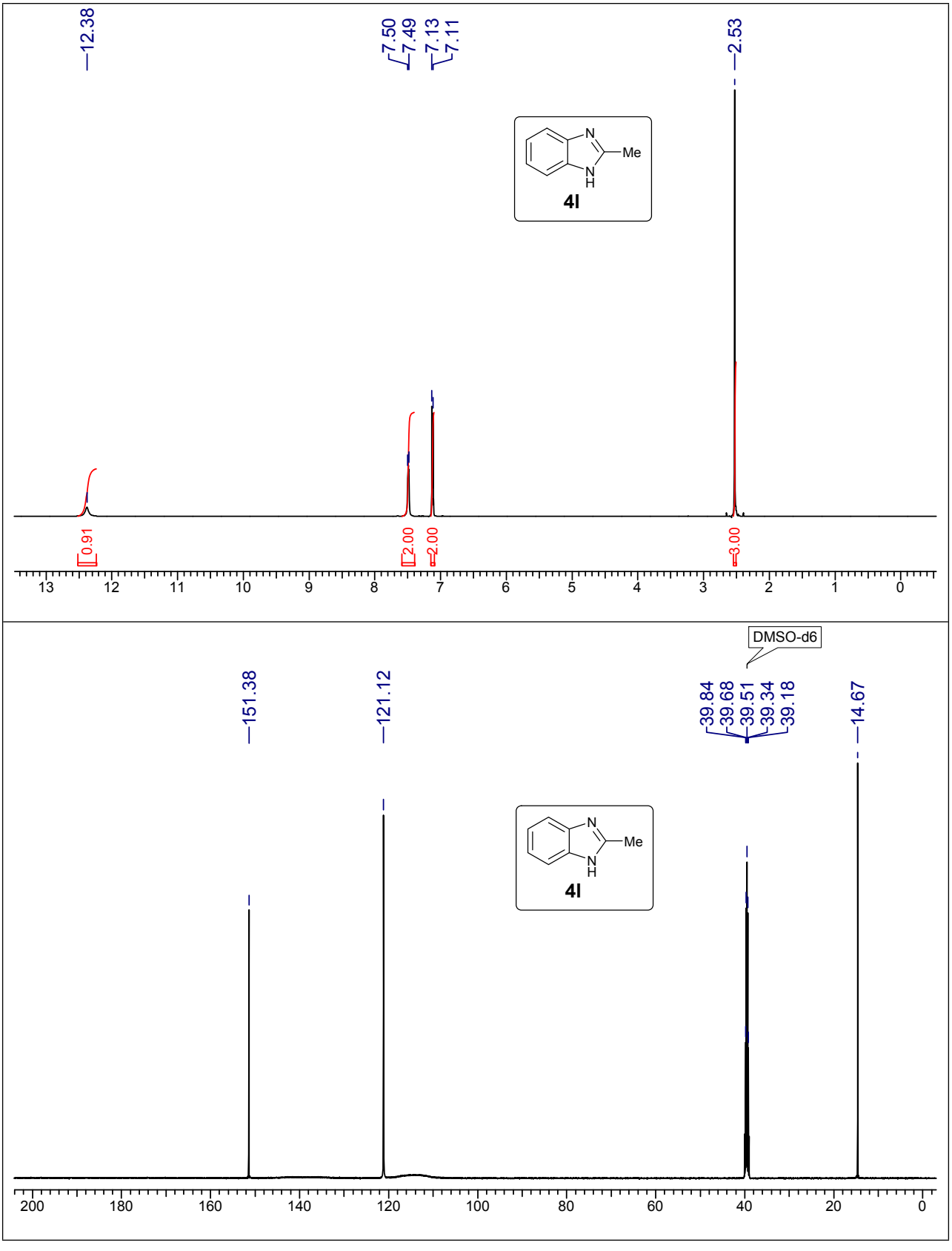
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2.00
3.00
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12
11
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DMSO-d6
151.38
121.12
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39.68
39.51
39.34
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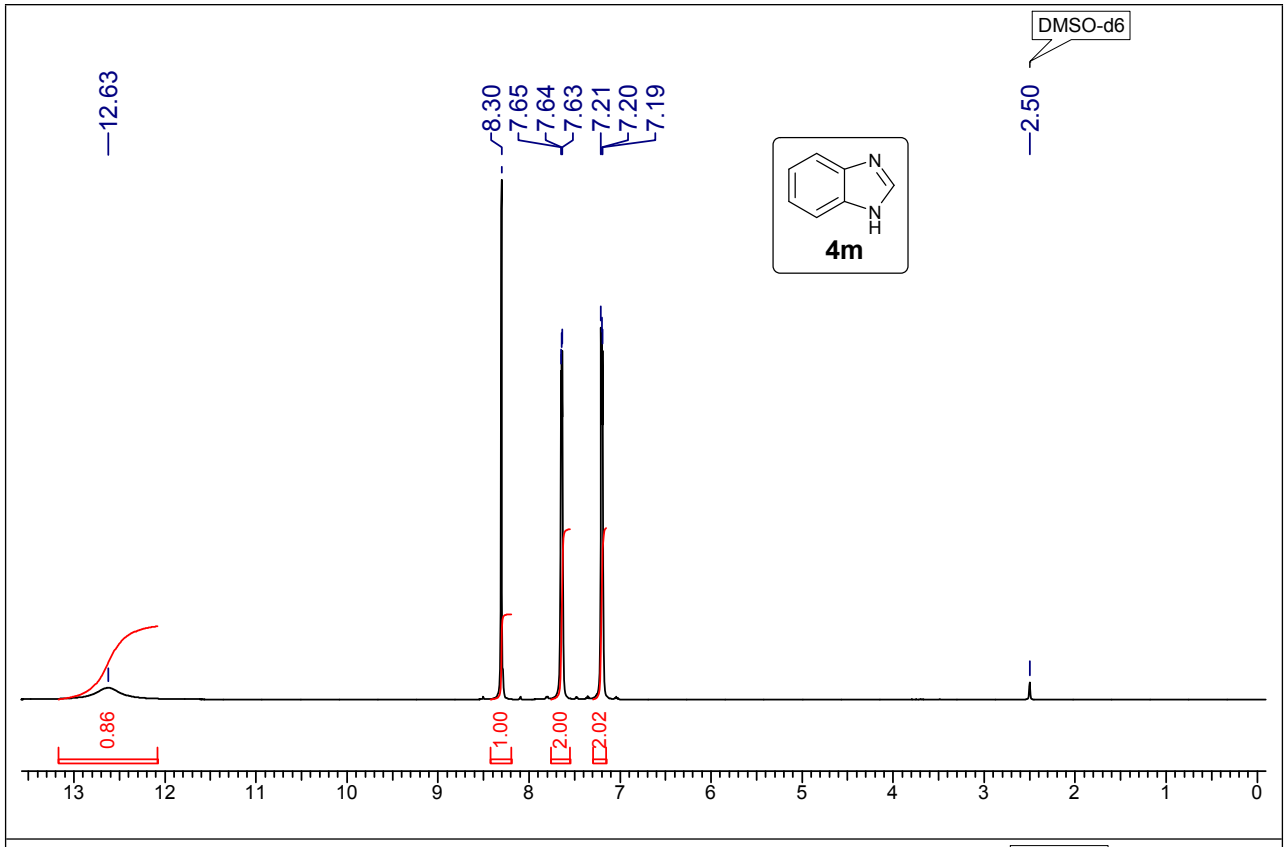
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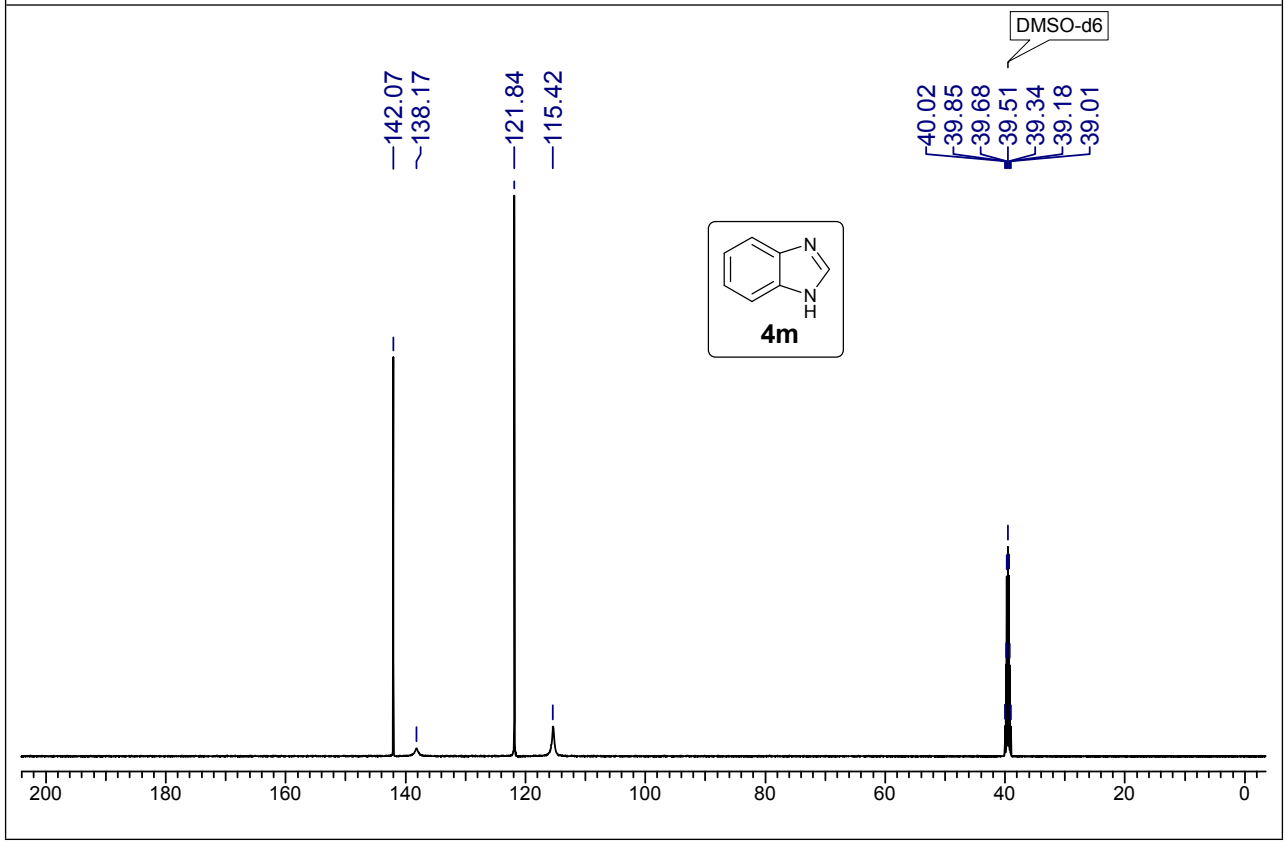
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