Supporting Information for:-

Solvent free one-pot multi-component synthesis of β-azaarene substituted ketones via Sn-catalyzed C(sp^3)-H functionalization of 2-alkylazaarenes†

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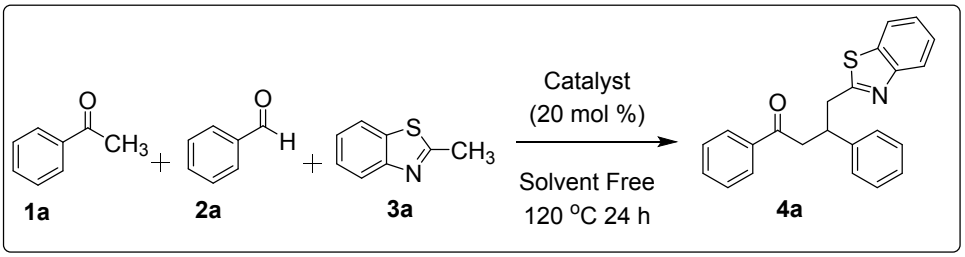
1. General Information

All reactions were carried out with the open atmosphere in flame-dried glassware. All reactions were carried out with the open atmosphere in flame-dried glassware. All solvent was used LR grade and all reagents and substrates were purchased from commercial suppliers and Sigma Aldrich, Alfa easer, Avra synthesis. All these commercially available chemicals were used without further purification.

Analytical thin layer chromatography was performed on TLC Silica gel 60 F_{254}. And routine monitoring of reaction was performed by TLC using 0.25 mm E. Merck pre-coated silica gel TLC plates (60 F254) using UV light to visualize the course of the reactions or $KMnO_4$ staining solutions followed by heating. Column Chromatography was performed on silica gel (60-120 mesh) by standard techniques eluting with solvents as indicated.

All compounds were fully characterized by using ^{1}H and ^{13}C NMR, the spectra were recorded at 200, 400, 500 MHz and 50 MHz spectrometer using $CDCl_3$ as solvent at room temperature. The Chemical shifts (δ) values are reported in ppm with TMS as internal standard. Abbreviations for signal couplings are: s, singlet; d, doublet; t, triplet; m, multiplet. q, quartet etc.

2. General Procedures for the Optimization of the Reaction Conditions:-



To a 10 ml round bottom flask equipped with a magnetic stir bar was added **1a** acetophenone (1 mmol), **2a** benzaldehyde (1 mmol), **3a** 2-methyl benzothiazole (1 mmol) and catalysts (20 mol

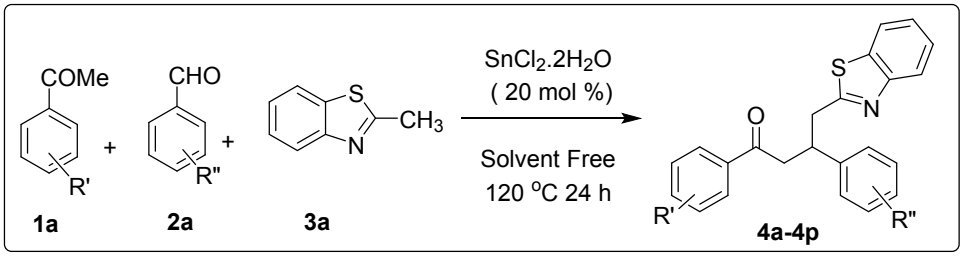
%) were taken, later RBF was capped with condenser. The reaction mixture was reflux at oil bath 120 ^{o}C, and the progress of the reaction was monitored by TLC with reaction time as shown in reaction optimization condition (**Table 1**). After the completion of the reaction, the reaction mixture was diluted with 10 mL ethyl acetate and 10 mL water, stirred for 10 minutes. The organic layer and aqueous layer were separated. The organic layer was dried over anhydrous Na_2SO_4. The solvent was evaporated and the crude residue was purified by column chromatography on silica gel to afford the corresponding desired compound (**4a**) in moderate to good yield.

Table 1 Optimization of the Reaction condition [a, b]

Entry	Catalyst	Solvent	Temp. (^{o}C)	Time (h)	Yield (%)[b]
1	$ZnCl_2$	DMF	120	24	N.R[d]
2	$Cu(OAc)_2$	DMF	120	24	N.R[d]
3	$FeCl_3$	DMF	120	24	N.R[d]
4	$AlCl_3$	DMF	120	24	N.R[d]
5	$CuCl_2$	DMF	120	24	N.R[d]
6	$InCl_3$	DMF	120	24	25
7	$SnCl_2.2H_2O$	DMF	120	24	38
8	DTP/SiO_2	DMF	120	24	16
9	$SnCl_22H_2O$	1,4, Dioxane	110	24	N.R[d]
10	$SnCl_22H_2O$	Toluene	110	24	N.R[d]
11	$SnCl_22H_2O$	DCE	100	24	N.R[d]
12	$SnCl_22H_2O$	DMSO	120	24	N.R[d]
13	$SnCl_22H_2O$	NMP	120	24	N.R[d]
14	$ZnCl_2$	-	120	24	41
15	$Cu(OAc)_2$	-	120	24	N.R[d]
16	$FeCl_3$	-	120	24	N.R[d]
17	$AlCl_3$	-	120	24	N.R[d]
18	$CuCl_2$	-	120	24	N.R[d]

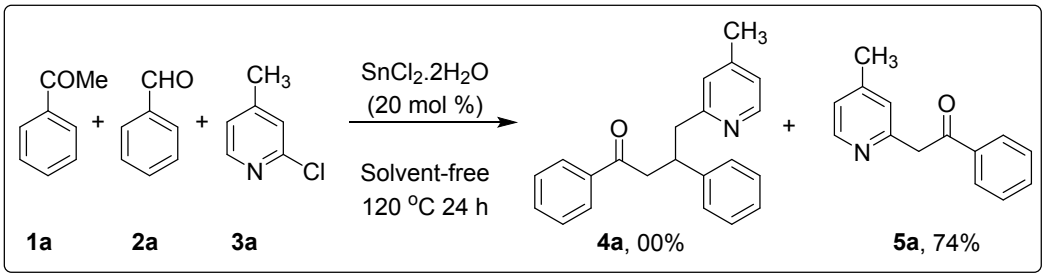
19	$InCl_3$	-	120	24	65
20	$SnCl_2.2H_2O$	-	120	24	72
21	DTP/SiO_2	-	120	24	40
[a]Reaction conditions: acetophenone **1a** (1 mmol), benzaldehyde **2a** (1.2 mmol), 2-methyl benziimidazole **3a** (1 mmol), Catalyst (20 mol %), Solvent (5 mL). 120 ^{0}C for 24 h. [b] Isolated yield. [c] DTP/SiO_2 100 mg catalyst was used, [d]No reaction.					

3. General Experimental Procedures for the Synthesis of Compound 4a to 4p:-



To a 10 ml round bottom flask equipped with a magnetic stir bar was added acetophenone **1a** (1 mmol), aldehydes **2a** (1 mmol), 2-methyl benzothiazole **3a** (1 mmol), $SnCl_2.2H_2O$ (20 mol %) were taken and RBF was capped with condenser. The resultant reaction solution was kept stirring at 120 ^{0}C in oil bath. The completion of the reaction was monitored by TLC. After the completion of the reaction, the reaction mixture was diluted with 10 mL ethyl acetate and 10 mL water and it was stirred for 10 minutes. Thereafter the organic layer and aqueous layer were separated. The organic layer was dried over anhydrous Na_2SO_4. The solvent was evaporated and the crude residue was purified by column chromatography on silica gel in 15-25% solution of ethyl acetate in pet ether to afford the corresponding desired compounds derivative (**4a-4p**) in moderate to good yields.

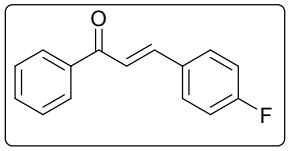
4. General Procedure for the Synthesis of Compound 5a:-



The general experimental procedure was used for the synthesis of compound **5a:-** The resultant solution containing RBF equipped with condenser was kept for stirring at 120 ^{0}C in oil bath for 16 h. The isolated compound was found oily liquid in 74 yield of **5a.**

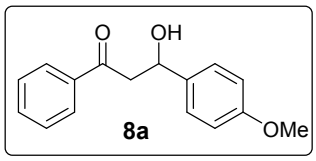
Experimental procedure for the synthesis of **6a** and **8a** was carried out from literature procedure.[1, 2]

(E)-3-(4-fluorophenyl)-1-phenylprop-2-en-1-one: (6a)



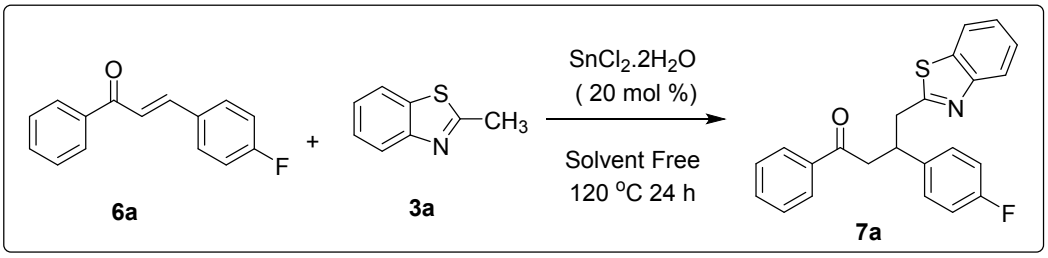
Yellow solid, ^{1}H NMR ($CDCl_3$, 200MHz): δ = 7.92 - 8.03 (m, 2 H), 7.41 - 7.81 (m, 2 H), 7.06 - 7.14 ppm (m, 2 H); **^{13}C NMR** ($CDCl_3$, 50MHz): δ = 189.5, 166.5, 161.5, 143.3, 138.6, 138.2, 133.1, 132.7, 131.7, 131.6, 131.3, 131.2, 130.4, 130.2, 128.9, 128.6, 128.5, 126.1, 121.7, 121.7, 116.4, 115.9, 115.5, 115.0.

3-hydroxy-3-(4-methoxyphenyl)-1-phenylpropan-1-one: (8a),

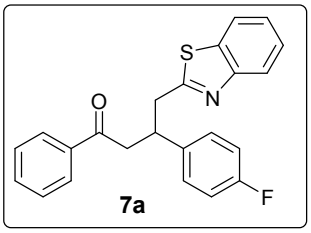


White solid, **^{1}H NMR** ($CDCl_3$, 200MHz): δ = 7.94 - 7.09 (m, 2 H), 7.27 - 7.64 (m, 5 H), 6.88 - 6.96 (m, 2 H), 5.27 - 5.33 (m, 1 H), 3.82 (s, 3 H), 3.56 (d, *J*=2.5 Hz, 1 H), 3.36 - 3.39 ppm (m, 2 H); **^{13}C NMR** ($CDCl_3$, 50MHz): δ = 200.9, 159.7, 137.2, 135.8, 134.2, 129.3, 128.8, 127.6, 114.5, 5.9, 47.9

5) Control Experimental Procedures for the Synthesis of Compound 7a:-

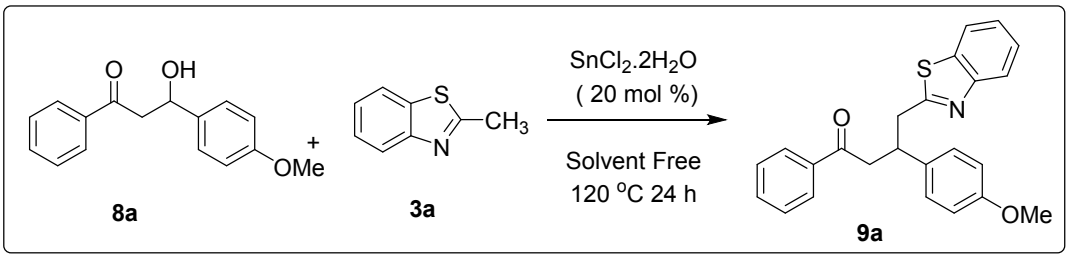


To a 10 ml round bottom flask equipped with a magnetic stir bar was added enone **6a** (1 mmol), benzothiazole **3a** (1 mmol), $SnCl_2.2H_2O$ (20 mol %) were taken and RBF was capped with condenser. Same general procedure followed for compound. **4-(benzo[d]thiazol-2-yl)-3-(4-fluorophenyl)-1-phenylbutan-1-one: 7a**

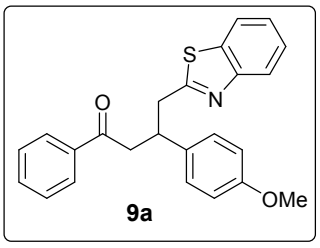


Yield: 88 %; Brown solid, mp 104-107 °C; **^{1}H NMR** ($CDCl_3$, 200MHz): d = 7.79 - 7.95 (m, 3 H), 7.41 - 7.60 (m, 4 H), 7.24 - 7.40 (m, 4 H), 6.91- 7.00 (t, *J*=8.7 Hz, 2 H), 3.97 - 4.20 (m, 1 H), 3.36 - 3.64 (m, 4 H); **^{13}C NMR** ($CDCl_3$, 50MHz): d = 197.6, 173.6, 155.4, 148.6, 134.3, 129.2, 128.6, 128.0, 125.9, 122.7, 121.5, 115.7, 115.3, 77.6, 76.4, 62.8, 44.5, 40.8 .

Control Experimental Procedures for the Synthesis of Compound 9a:-



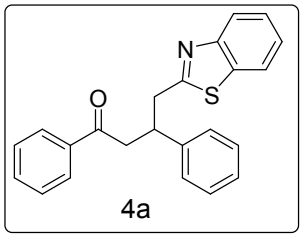
To a 10 ml round bottom flask equipped with a magnetic stir bar was added aldol product **8a** (1 mmol), benzothiazole **3a** (1 mmol), $SnCl_2.2H_2O$ (20 mol %) were taken and RBF was capped with condenser. Same general procedure followed for compound. **4-(benzo[d]thiazol-2-yl)-3-(4-methoxyphenyl)-1-phenylbutan-1-one: (9a)**



Yield: 62 %; Brown solid, mp 132-133 °C; **^{1}H NMR** ($CDCl_3$, 200MHz): d = 7.92 - 7.96 (m, 2 H), 7.73 - 7.78 (dd, *J*=7.8, 0.9 Hz, 2 H), 7.16 - 7.45 (m, 7 H), 6.76 - 6.80 (m, 2 H), 3.79 - 3.89 (m, 1 H), 3.73 (s, 3 H), 3.43 - 3.67 (m, 4 H); **^{13}C NMR** ($CDCl_3$, 50MHz): d = 204.4, 169.9, 159.2, 153.6, 135.9, 134.2, 129.4, 126.4, 125.3, 123.2, 122.0, 114.7, 55.7, 46.1, 41.5

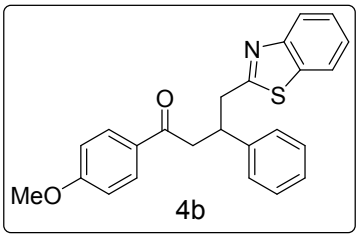
6. Spectral Data of Compounds 4a to 4p and 5a:-

4-(benzo[d]thiazol-2-yl)-1,3-diphenylbutan-1-one (4a)



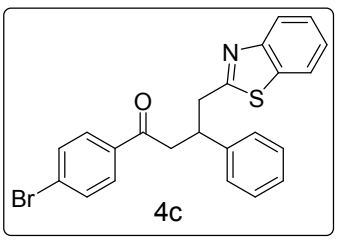
Yield: 72%; Yellow solid, mp 108-110 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm 8.19 (d, J=7.02 Hz, 1 H) 8.05 (d, J=7.93 Hz, 2 H) 8.83 (d, J=7.63 Hz, 2 H) 7.50 - 7.68 (m, 2 H) 7.43 - 7.42 (m, 6 H) 7.27 (d, J=6.10 Hz, 1 H) 4.06 (d, J=6.10 Hz, 1 H) 3.17 - 3.82 (m, 2 H) 3.66 - 3.71 (m, 2 H)
^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 197.6, 170.5, 169.8, 152.2, 141.6, 135.0, 133.5, 130.4, 129.1, 128.6, 128.0, 127.7, 126.4, 125.3, 122.7, 121.7, 46.4, 40.53

4-(benzo[d]thiazol-2-yl)-1-(4-methoxyphenyl)-3-phenylbutan-1-one (4b)



Yield: 75%; Yellow solid, mp 84-86 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm 8.17 (d, *J*=7.93 Hz, 8 H) 7.96 (d, *J*=7.93 Hz, 8 H) 7.63 (t, *J*=7.63 Hz, 10 H) 7.37 - 7.55 (m, 34 H) 4.13 - 4.25 (m, 5 H) 4.01 (s, 3 H) 3.85 - 3.93 (m, 7 H) 3.73 - 3.82 (m, 9 H)
^{13}C NMR (126 MHz, $CDCl_3$) δ ppm 199.9, 169.8, 161.8, 152.7, 142.6, 141.7, 135.2, 133.3, 133.1, 131.2, 130.3, 129.0, 128.9, 128.5, 128.0, 127.9, 127.6, 127.2, 126.3, 126.2, 125.2, 125.1, 122.8, 122.7, 121.7, 121.6, 121.0, 119.4, 113.2, 55.7, 48.3, 46.3, 42.2.

4-(benzo[d]thiazol-2-yl)-1-(4-bromophenyl)-3-phenylbutan-1-one (4c)

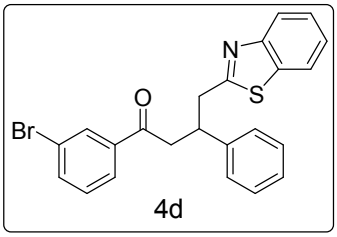


Yield: 80%; Grey solid, mp 54-155 °C; **^{1}H NMR** (200 MHz, $CDCl_3$) δ ppm 8.03 (d, *J*=7.83 Hz,

2 H) 7.81 (d, *J*=7.71 Hz, 2 H) 7.34 - 7.52 (m, 5 H) 7.20 - 7.30 (m, 4 H) 4.56 (br. s., 2 H) 4.10 (m, 1 H) 3.56 - 3.81 (m, 2 H)

^{13}C NMR (101 MHz, $CDCl_3$) δ ppm 196.7, 171.5, 170.7, 142.4, 135.4, 134.4, 133.5, 131.8, 130.2, 129.8, 129.6, 128.8, 128.4, 128.3, 127.5, 127.1, 126.4, 125.3, 125.2, 122.2, 122.0, 121.5, 44.3, 41.5, 40.0.

4-(benzo[d]thiazol-2-yl)-1-(3-bromophenyl)-3-phenylbutan-1-one (4d)

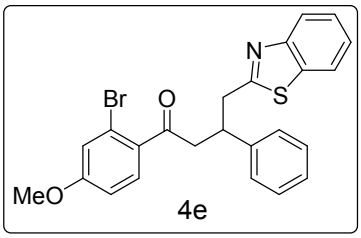


4d

Yield: 73%; Yellow solid, mp 90-91 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm 8.21 (d, *J*=7.58 Hz, 1 H) 8.06 - 8.12 (m, 2 H) 7.82 - 7.90 (m, 2 H) 7.40 - 7.67 (m, 2 H) 7.27 - 7.43 (m, 6 H) 4.06 - 4.12 (m, 1 H) 3.79 - 3.85 (m, 2 H) 3.68 - 3.73 (m, 2 H);

^{13}C NMR (101 MHz, $CDCl_3$) δ ppm 199.4, 161.3, 152.2, 142.1, 141.2, 132.8, 130.7, 129.8, 128.4, 128.0, 127.5, 127.4, 127.0, 126.7, 125.8, 125.7, 124.7, 124.6, 122.3, 122.2, 121.2, 121.1, 120.5, 118.9, 112.7, 47.8, 45.8, 41.7.

4-(benzo[d]thiazol-2-yl)-1-(2-bromo-4-methoxyphenyl)-3-phenylbutan-1-one (4e)

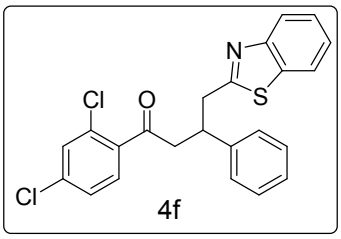


4e

Yield: 82%; Brown solid, mp 83-84 °C; **^{1}H NMR** (500 MHz, $CDCl_3$) δ ppm 8.21 (d, *J*=7.93 Hz, 1 H) 8.07 (d, *J*=7.93 Hz, 1 H) 7.83 (d, *J*=7.93 Hz, 1 H) 7.66 - 7.69 (m, 1 H) 7.50 - 7.57 (m, 3 H) 7.32 - 7.43 (m, 3 H) 7.28 (m, 2 H) 4.06 - 4.09 (m, 2 H) 3.81 (s, 3 H) 3.78 (d, *J*=6.41 Hz, 2 H) 3.66 - 3.70 (m, 2 H)

^{13}C NMR (126 MHz, $CDCl_3$ *d*) δ ppm 199.1, 170.5, 169.8, 152.3, 141.6, 135.1, 133.4, 130.4, 130.3, 129.1, 128.6, 128.0, 127.6, 126.4, 125.3, 122.7, 121.7, 46.4, 40.5, 32.2.

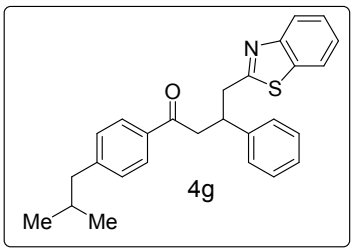
4-(benzo[d]thiazol-2-yl)-1-(2,4-dichlorophenyl)-3-phenylbutan-1-one (4f)



Yield: 80%; Brown solid, mp 60-62 °C; **^{1}H NMR** (200 MHz, $CDCl_3$) δ ppm 7.72 – 8.09 (m, 4 H) 7.21 - 7.42 (m, 8H) 3.94 - 4.02 (m, 1 H) 3.52 - 3.69 (m, 4 H)

^{13}C NMR (126MHz , $CDCl_3$) δ ppm = 199.0, 168.4, 153.1, 152.3, 149.1, 147.5, 144.0, 134.9, 130.0, 129.0, 126.7, 125.7, 124.3, 122.9, 121.8, 96.5, 77.5, 77.3, 45.9, 40.0, 32.3

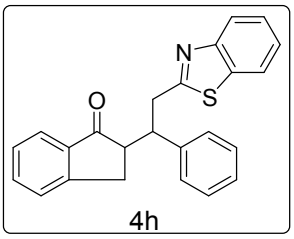
4-(benzo[d]thiazol-2-yl)-1-(4-isobutylphenyl)-3-phenylbutan-1-one (4g)



Yield: 74%; Grey solid, mp 138-139 °C; **^{13}C NMR** (126MHz , $CDCl_3$) δ ppm = 201.8, 171.2, 170.1, 151.2, 141.1, 134.5, 133.5, 130.3, 129.7, 128.9, 128.4, 128.3, 127.8, 127.6, 126.7, 126.4, 125.3, 122.3, 121.6, 96.2, 46.2, 40.1, 36.7, 29.8, 22.8

^{1}H NMR (500MHz , $CDCl_3$) δ ppm = 8.21 (m, 2 H), 8.09 (d, *J* = 7.6 Hz, 2 H), 7.84 (d, *J* = 7.6 Hz, 2 H), 7.68 (t, *J* = 6.7 Hz, 2 H), 7.52 - 7.57 (m, 3 H), 7.44 - 7.35 (m, 2 H), 4.11 (m, 1 H), 3.86 - 3.82 (m, 2 H), 3.75 - 3.70 (m, 2 H), 2.40 (m, 2 H), 2.10 – 1.98 (m, 1 H) 0.99 - 0.93 (m, 6 H)

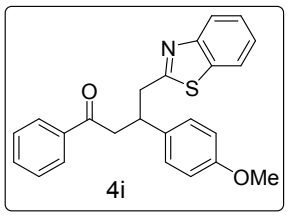
2-(2-(benzo[d]thiazol-2-yl)-1-phenylethyl)-2,3-dihydro-1H-inden-1-one (4h)



Yield: 64%; Brown solid, mp 81-83 °C; **^{1}H NMR** (400 MHz, $CDCl_3$) δ ppm =8.11 (d, *J*=7.34 Hz, 1 H), 8.00 - 8.08 (m, 1 H), 7.66 - 7.81 (m, 2 H), 7.41 - 7.61 (m, 4 H), 7.11 - 7.31 (m, 5 H), 3.99 - 4.12 (m, 1 H), 3.85 - 3.99 (m, 1 H), 3.56 - 3.84 (m, 2 H), 2.98 - 3.28 (m, 2 H), 2.87 - 2.98 (m, 1 H)

^{13}C NMR (101 MHz , $CDCl_3$) δ ppm =207.0, 170.7, 170.3, 153.4, 150.8, 141.0, 139.9, 139.7, 137.3, 136.8, 134.8, 134.7, 134.3, 134.2, 133.3, 130.1, 129.9, 128.9, 128.7, 128.6, 128.5, 128.3, 127.8, 127.5, 127.3, 127.2, 126.7, 126.5, 126.4, 126.4, 126.3, 125.6, 125.4, 124.0, 123.7, 122.1, 122.0, 121.6, 121.6, 121.5, 96.2, 51.4, 51.2, 39.9, 37.5, 30.0.

4-(benzo[d]thiazol-2-yl)-3-(4-methoxyphenyl)-1-phenylbutan-1-one (4i)

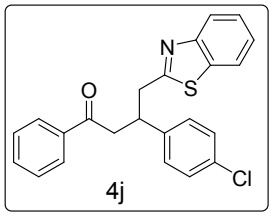


4i

Yield: 76%; Brown solid, mp 132-133 ^{o}C; **^{1}H NMR** (400MHz , $CDCl_3$) δ ppm = 8.00 (d, *J* = 8.1 Hz, 2 H), 7.76 (d, *J* = 7.8 Hz, 2 H), 7.45 (t, *J* = 7.6 Hz, 3 H), 7.40 - 7.30 (m, 2 H), 7.30 - 7.16 (m, *J* = 8.3 Hz, 2 H), 6.77 (d, *J* = 8.6 Hz, 2 H), 3.99 (m, *J* = 6.6 Hz, 1 H), 3.73 (s, 3 H) 3.87 - 3.71 (m, 2 H), 3.65 - 3.50 (m, 2 H)

^{1}H NMR (500MHz , $CDCl_3$) δ ppm =195.5, 170.5, 158.8, 150.5, 134.2, 132.7, 128.8, 126.6, 125.5, 122.0, 121.6, 114.3, 96.2, 77.3, 55.0, 45.3, 40.1, 29.7

4-(benzo[d]thiazol-2-yl)-3-(4-chlorophenyl)-1-phenylbutan-1-one (4j)

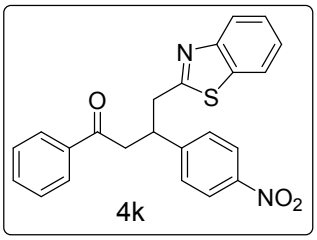


4j

Yield: 82%; Yellow solid, mp 97-98 ^{o}C; **^{1}H NMR** (500MHz , $CDCl_3$) δ ppm = 8.09 (d, *J* = 8.2 Hz, 2 H), 7.85 (d, *J* = 7.9 Hz, 2 H), 7.55 (t, *J* = 7.5 Hz, 2 H), 7.45 (t, *J* = 7.5 Hz, 2 H), 7.35 - 7.29 (m, 5 H), 4.23 (m, 1 H), 3.85 (dd, *J* = 6.1, 14.6 Hz, 2 H), 3.74 (dd, *J* = 8.5, 14.6 Hz, 2 H)

^{13}C NMR (126MHz , $CDCl_3$) δ ppm =197.1, 170.1, 149.3, 142.4, 138.8, 133.5, 133.3, 129.0, 128.9, 126.8, 125.7, 121.6, 121.5, 96.0, 76.7, 76.5, 45.1, 39.2, 34.5

4-(benzo[d]thiazol-2-yl)-3-(4-nitrophenyl)-1-phenylbutan-1-one (4k)

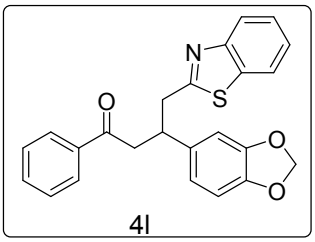


4k

Yield: 80%; Yellow solid, mp 158-160 °C; **^{1}H NMR** (500MHz , $CDCl_3$) δ ppm = 8.09 - 8.13 (m, 2 H), 7.96 (d, *J* = 8.2 Hz, 2 H), 7.78 (d, *J* = 7.9 Hz, 2 H), 7.56 - 7.42 (m, 5 H), 7.42 - 7.33 (m, 2 H), 4.32 - 4.21 (m, 1 H), 3.75 (dd, *J* = 6.4, 15.0 Hz, 2 H), 3.62 (dd, *J* = 8.5, 15.0 Hz, 2 H)

^{13}C NMR (126MHz , $CDCl_3$) δ ppm = 198.7, 168.1, 152.1, 148.9, 147.3, 134.6, 128.8, 126.5, 125.4, 124.0, 122.6, 121.6, 96.2, 45.7, 39.7, 32.0

3-(benzo[d][1,3]dioxol-5-yl)-4-(benzo[d]thiazol-2-yl)-1-phenylbutan-1-one (4l)

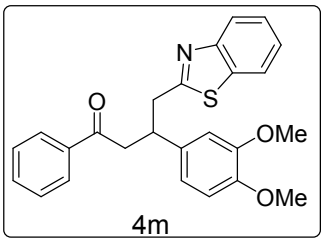


4l

Yield: 70%; Yellow solid, mp 102-104 °C; **^{1}H NMR** (200 MHz , $CDCl_3$) δ ppm = 8.00 (d, *J* = 7.2 Hz, 2 H), 7.89 - 7.69 (m, 2 H), 7.60 - 7.15 (m, 5 H), 6.97 - 6.55 (m, 2 H), 5.92 (s, 1 H), 4.09 - 3.80 (m, 1 H), 3.90 - 3.50 (m, 4 H);

^{13}C NMR (126 MHz, $CDCl_3$) δ ppm = 199.9, 170.4, 151.3, 149.4, 148.5, 134.7, 133.6, 128.8, 128.4, 126.7, 125.6, 122.4, 121.8, 119.9, 96.4, 45.9, 40.4, 30.0

4-(benzo[d]thiazol-2-yl)-3-(3,4-dimethoxyphenyl)-1-phenylbutan-1-one (4m)



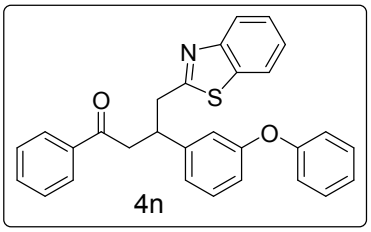
4m

Yield: 71%; Yellow solid, mp 107-109 °C; **^{1}H NMR** (500MHz , $CDCl_3$) δ ppm = 7.99 (d, *J* = 7.9 Hz, 2 H), 7.84 - 7.73 (m, 2 H), 7.56 - 7.32 (m, 5 H), 6.93 - 6.79 (m, 1 H), 6.79 - 6.69 (m, 2 H), 3.96 (d, *J* = 6.1 Hz, 1 H), 3.80 (s, 4 H), 3.76 - 3.58 (m, 7 H)

^{13}C NMR (126MHz , $CDCl_3$) δ ppm = 199.3, 170.1, 151.1, 149.1, 148.2, 134.4, 133.4, 128.5,

128.1, 126.4, 125.3, 122.2, 121.5, 119.6, 111.3, 111.1, 96.2, 77.2, 77.0, 76.7, 55.8, 55.6, 45.7, 40.1, 29.7

4-(benzo[d]thiazol-2-yl)-3-(3-phenoxyphenyl)-1-phenylbutan-1-one (4n)

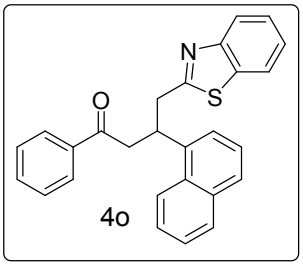


4n

Yield: 77%; Brown solid, mp 52-54 ^{o}C; **^{1}H NMR** (500MHz , $CDCl_3$) δ ppm= 8.15 - 8.08 (m, 2 H), 8.15 - 7.91 (m, 2 H), 7.64 - 7.45 (m, 6 H), 7.25 (s, 1 H), 7.29 (s, 1 H), 7.23 - 7.15 (m, 2 H), 7.08 - 6.88 (m, 4 H), 4.19 - 4.03 (m, 1 H), 3.87 - 3.63 (m, 3 H), 3.59 (t, *J* = 5.8 Hz, 1 H)

^{13}C NMR (126MHz , $CDCl_3$) δ ppm= 197.2, 168.9, 157.1, 156.8, 156.8, 151.8, 143.1, 134.6, 132.8, 130.0, 129.8, 129.6, 129.5, 129.5, 129.4, 129.3, 128.3, 127.9, 126.1, 126.0, 125.9, 124.9, 124.9, 123.0, 122.8, 122.3, 122.1, 121.8, 121.3, 121.2, 121.2, 118.8, 118.7, 118.4, 118.4, 118.3, 118.0, 117.9, 117.6, 117.3, 95.9, 76.7, 76.5, 45.8, 41.1, 39.9

4-(benzo[d]thiazol-2-yl)-3-(naphthalen-1-yl)-1-phenylbutan-1-one (4o)

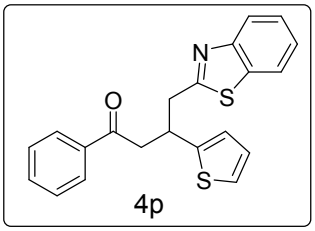


4o

Yield: 80%; Yellow solid, mp 86-87 ^{o}C; **^{1}H NMR** (200MHz , $CDCl_3$) δ ppm= 8.22 - 8.07 (m, 1 H), 7.85 - 7.71 (m, 2 H), 7.55 - 7.12 (m, 13 H), 4.85 (t, *J* = 6.6 Hz, 1 H), 3.69 (d, *J* = 7.2 Hz, 4 H)

^{13}C NMR (126MHz , $CDCl_3$) δ ppm= 199.9, 169.5, 161.8, 152.7, 141.8, 135.2, 133.3, 131.3, 130.3, 129.0, 128.9, 128.0, 127.6, 126.3, 125.2, 122.8, 121.7, 119.5, 96.4, 48.3, 42.2, 40.7

4-(benzo[d]thiazol-2-yl)-1-phenyl-3-(thiophen-2-yl)butan-1-one (4r)

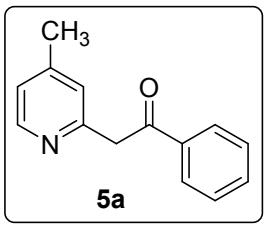


4p

Yield: 81%; Brown solid, mp 61-63 ^{o}C; **^{1}H NMR** (200MHz , $CDCl_3$) δ ppm =8.03 - 7.99 (m, 2 H), 7.81 - 7.77 (m, 2 H), 7.64 - 7.22 (m, 5 H), 7.16 (dd, *J* = 1.3, 4.9 Hz, 1 H), 6.90 - 6.85 (m, 2 H), 4.43 - 4.13 (m, 2 H), 3.82 - 3.56 (m, 3 H)

^{13}C NMR (50MHz , $CDCl_3$) δ ppm= 199.8, 168.8, 160.9, 152.2, 143.8, 135.0, 126.9, 126.2, 125.5, 125.1, 124.2, 122.6, 121.5, 96.2, 77.6, 76.4, 46.2, 41.3, 29.8

2-(4-methylpyridin-2-yl)-1-phenylethan-1-one (5a)



5a

Yield: 74%; Colorless oil; **^{1}H NMR** (200MHz , $CDCl_3$) δ ppm= 8.06 - 8.02 (m, 2 H), 7.67 - 7.48 (m, 3 H), 7.10 (d, *J* = 6.9 Hz, 1 H), 6.42 (s, 1 H), 6.08 (dd, *J* = 1.9, 6.9 Hz, 1 H), 5.34 (s, 2 H), 2.24 (s, 3 H)

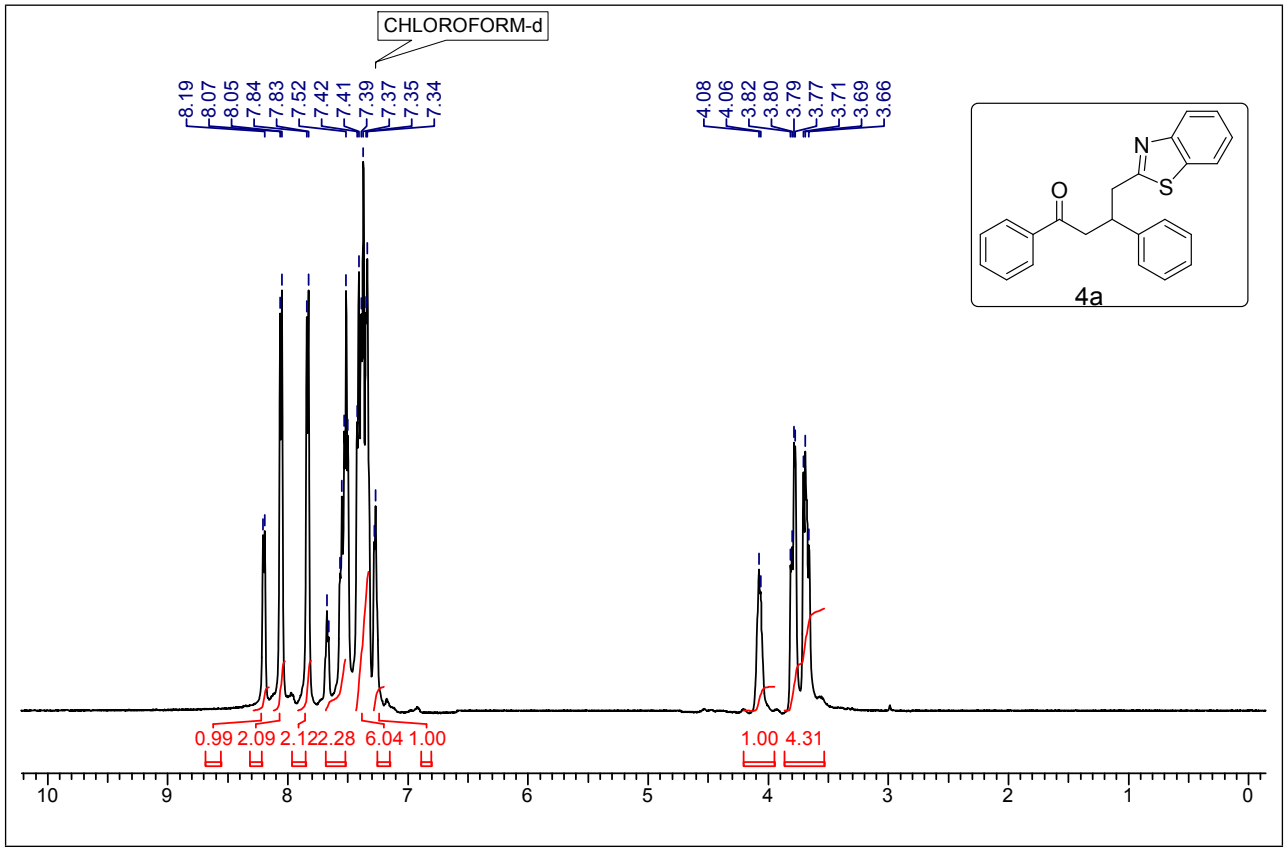
^{13}C NMR (101MHz , $CDCl_3$) δ ppm= 192.3, 162.2, 151.6, 137.0, 134.9, 134.0, 128.9, 128.3, 119.3, 108.6, 96.2, 77.3, 76.7, 53.6, 21.5

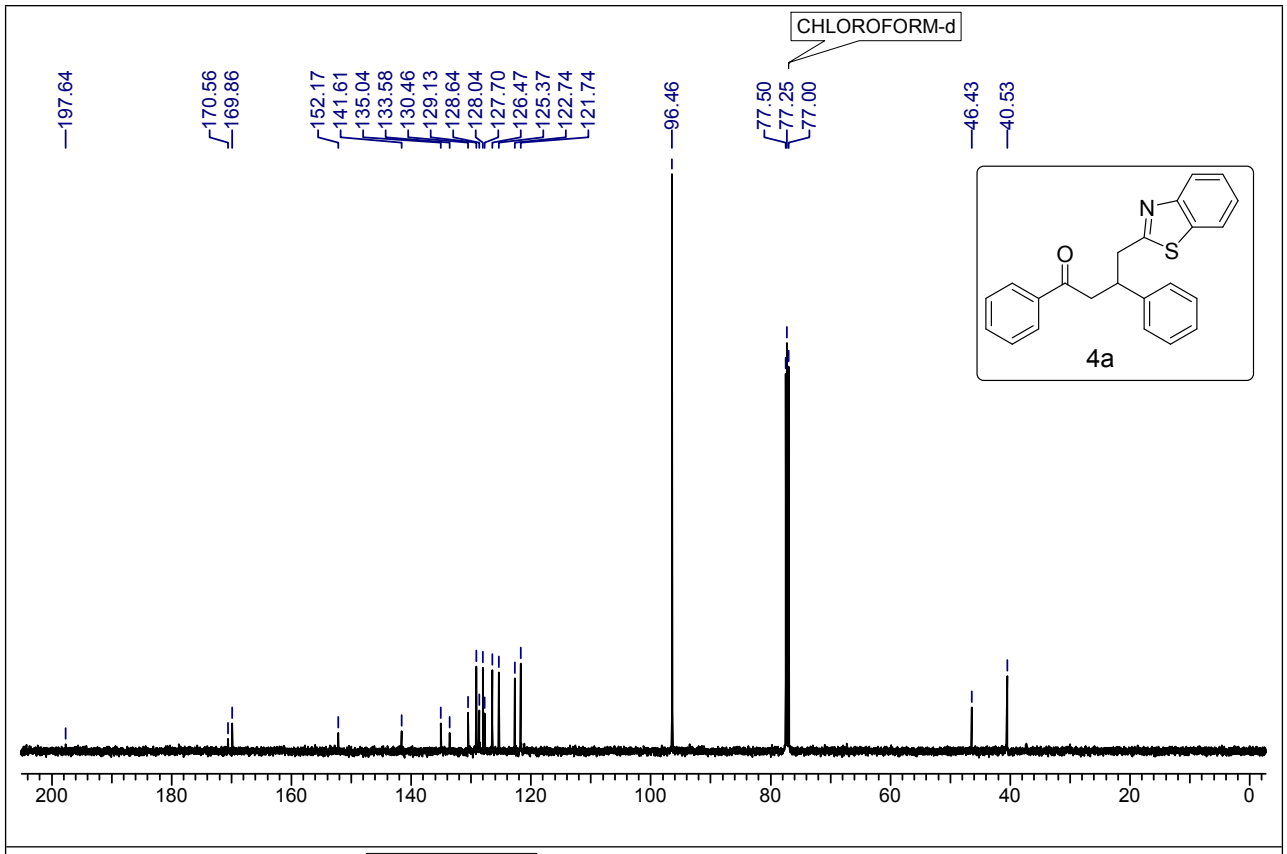
References:-

1) Y. Qian, G.-Y. Ma, Y. Yang, K. Cheng, Q.-Z. Zheng, W.-J. Mao, L. Shi, J. Zhao, H.-L. Zhu. *Bioorg. Med. Chem.* 2010, **18**, 4310–4316.

2) P. Singh, A. Bhardwaj. *J. Med. Chem*. 2010, **53**, 3707–3717.

7. ^{1}H NMR and ^{13}C NMR Spectra of Product:-

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129.13
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128.04
127.70
126.47
125.37
122.74
121.74
96.46
77.50
77.25
77.00
46.43
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S
O
4a
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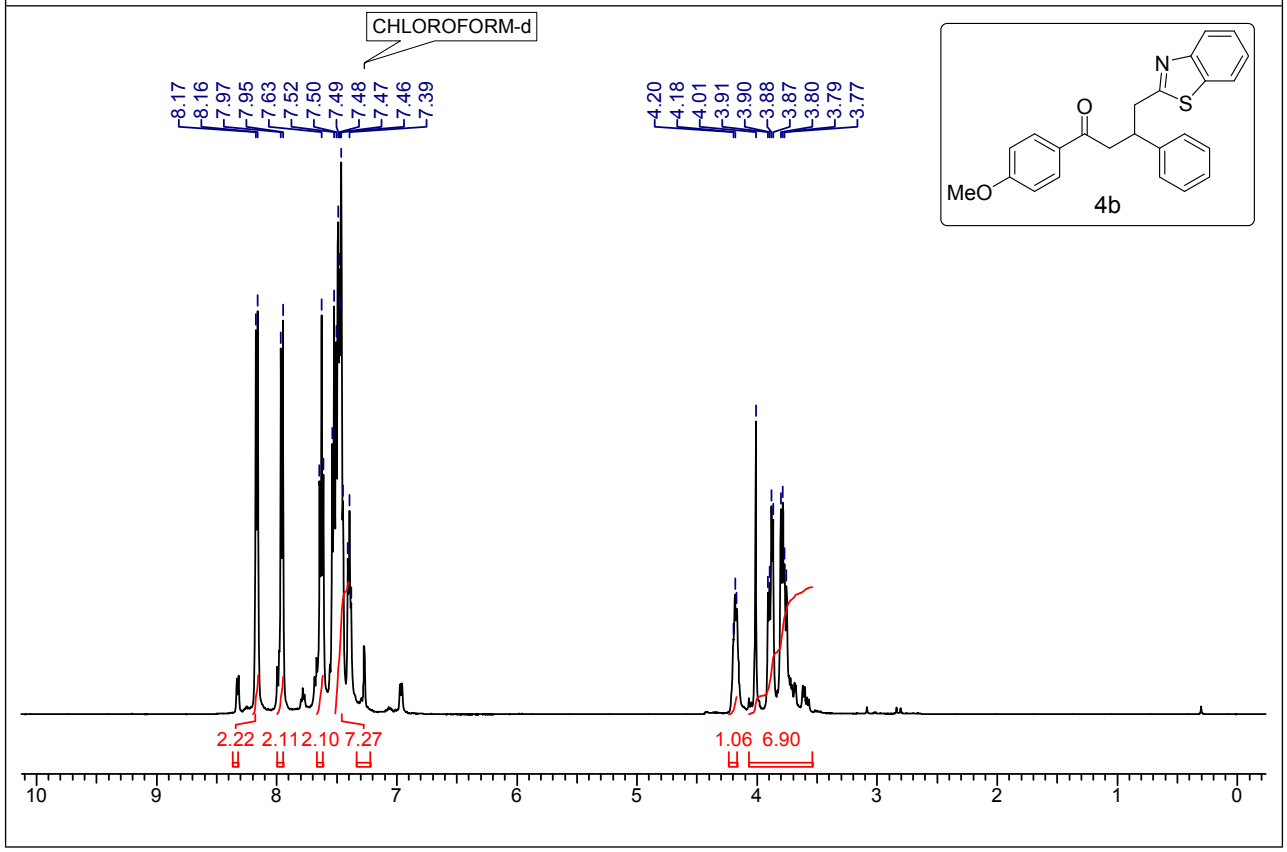
140
120
100
80
60
40
20
0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7.46
7.39
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4.18
4.01
3.91
3.90
3.88
3.87
3.80
3.79
3.77
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S
O
MeO
4b
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7
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3
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1
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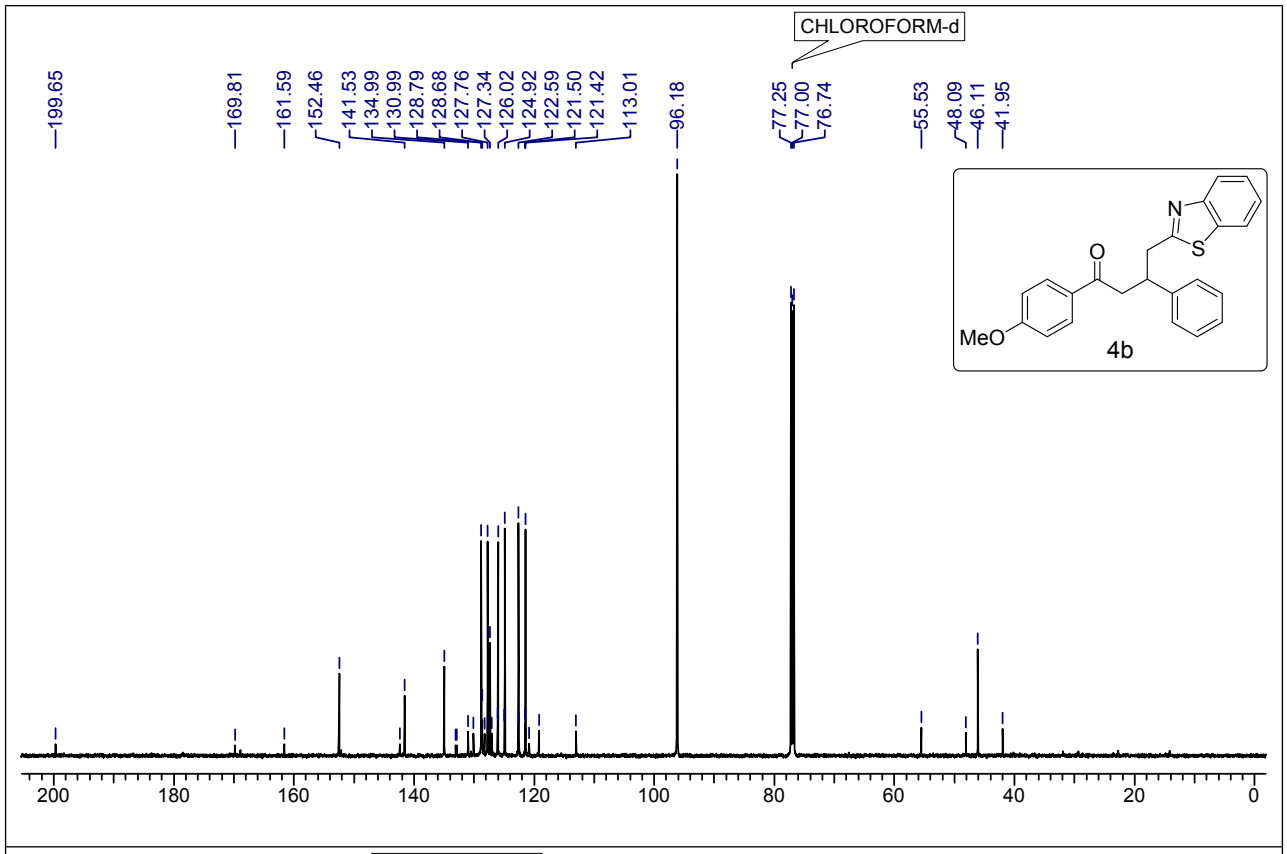
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124.92
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121.50
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77.00
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55.53
48.09
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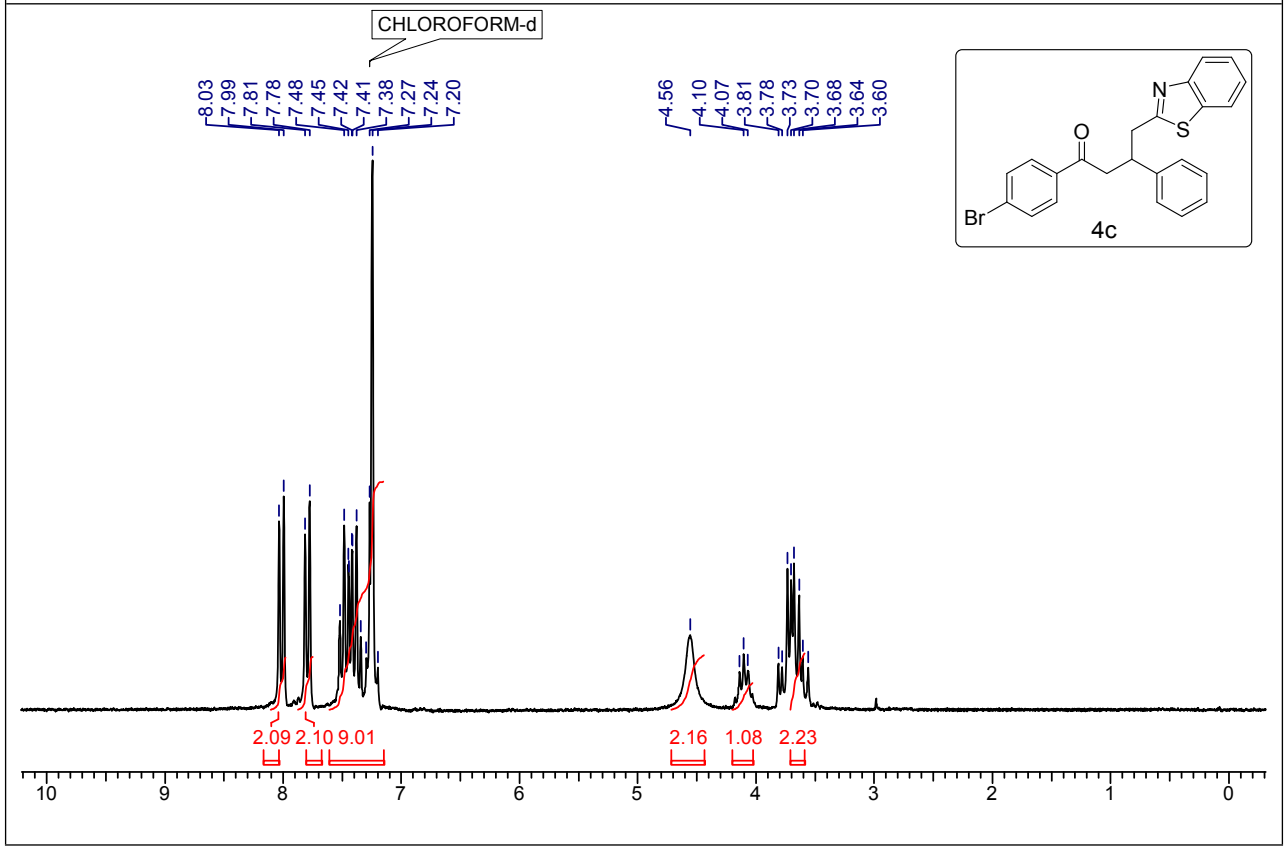
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7.24
7.20
4.56
4.10
4.07
3.81
3.78
3.73
3.70
3.68
3.64
3.60
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S
O
Br
4c
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9.01
2.16
1.08
2.23
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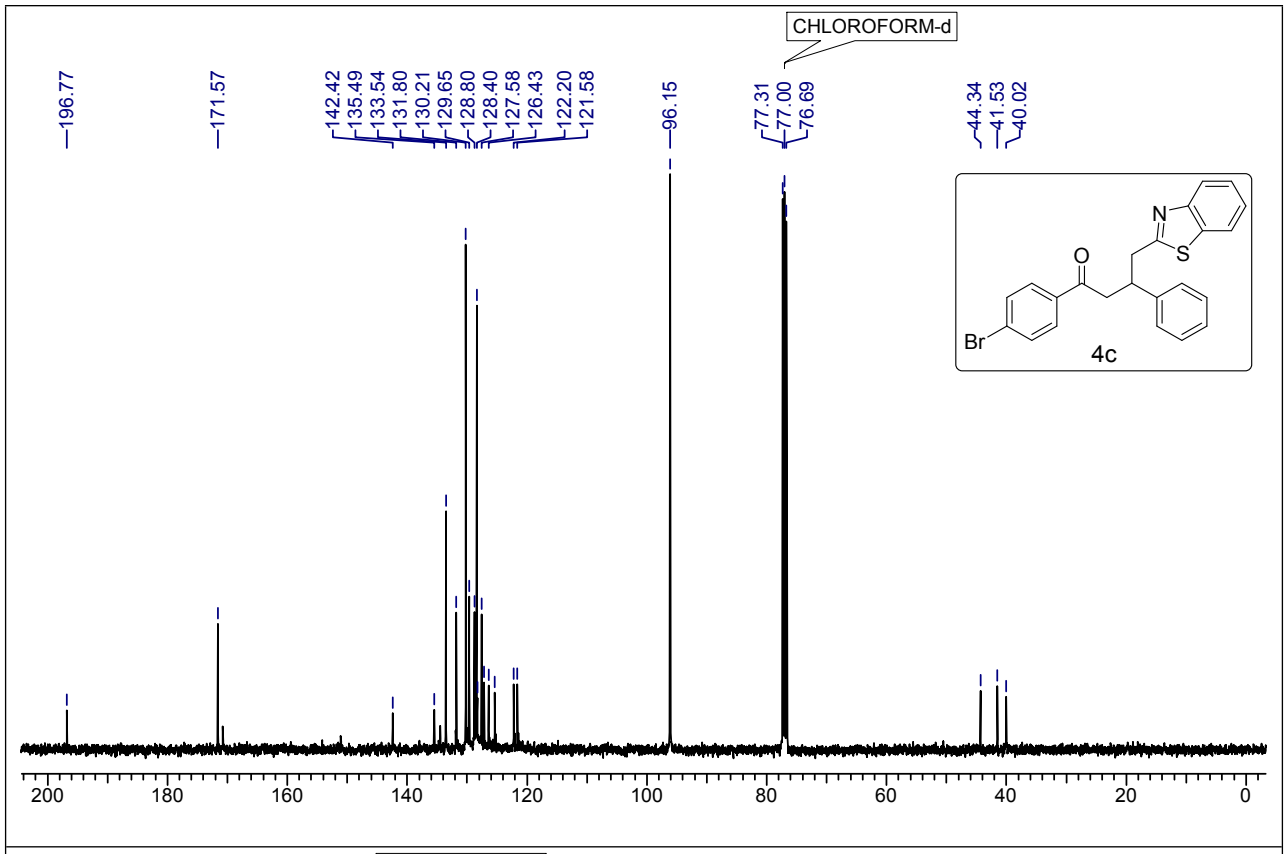
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121.58
96.15
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77.00
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S
O
Br
4c
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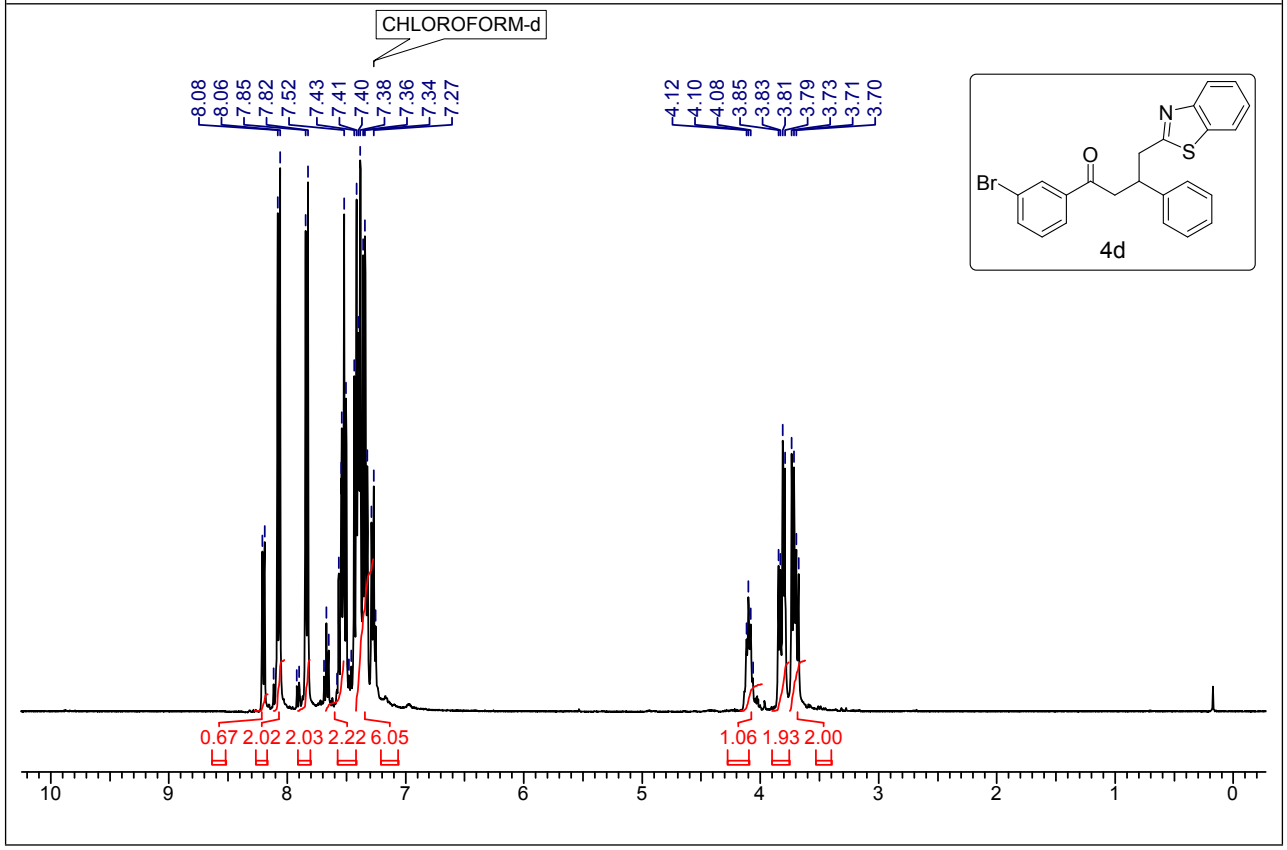
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7.38
7.36
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7.27
4.12
4.10
4.08
3.85
3.83
3.81
3.79
3.73
3.71
3.70
N
S
O
Br
4d
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1.06
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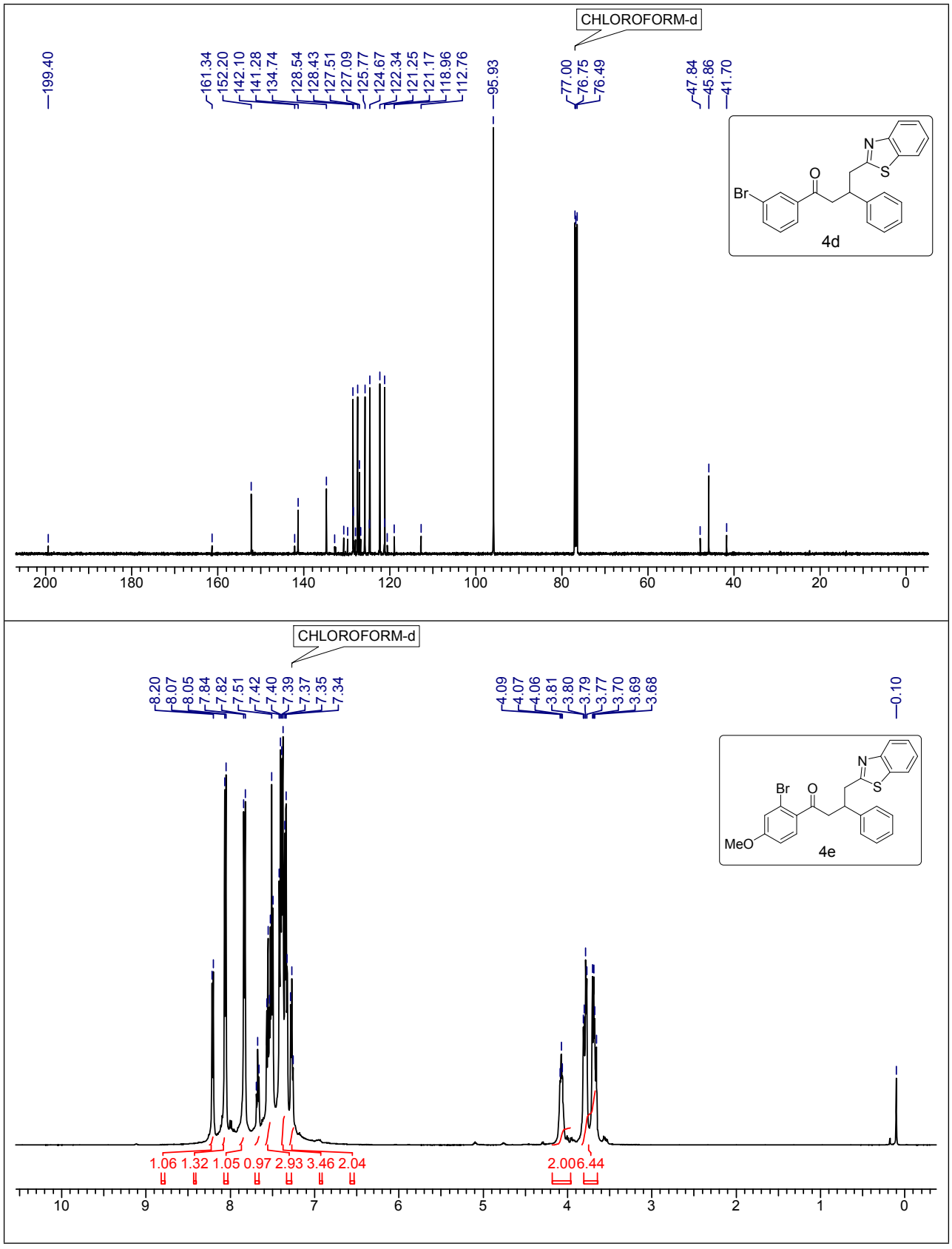
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S
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40
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7.40
7.39
7.37
7.35
7.34
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4.06
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MeO
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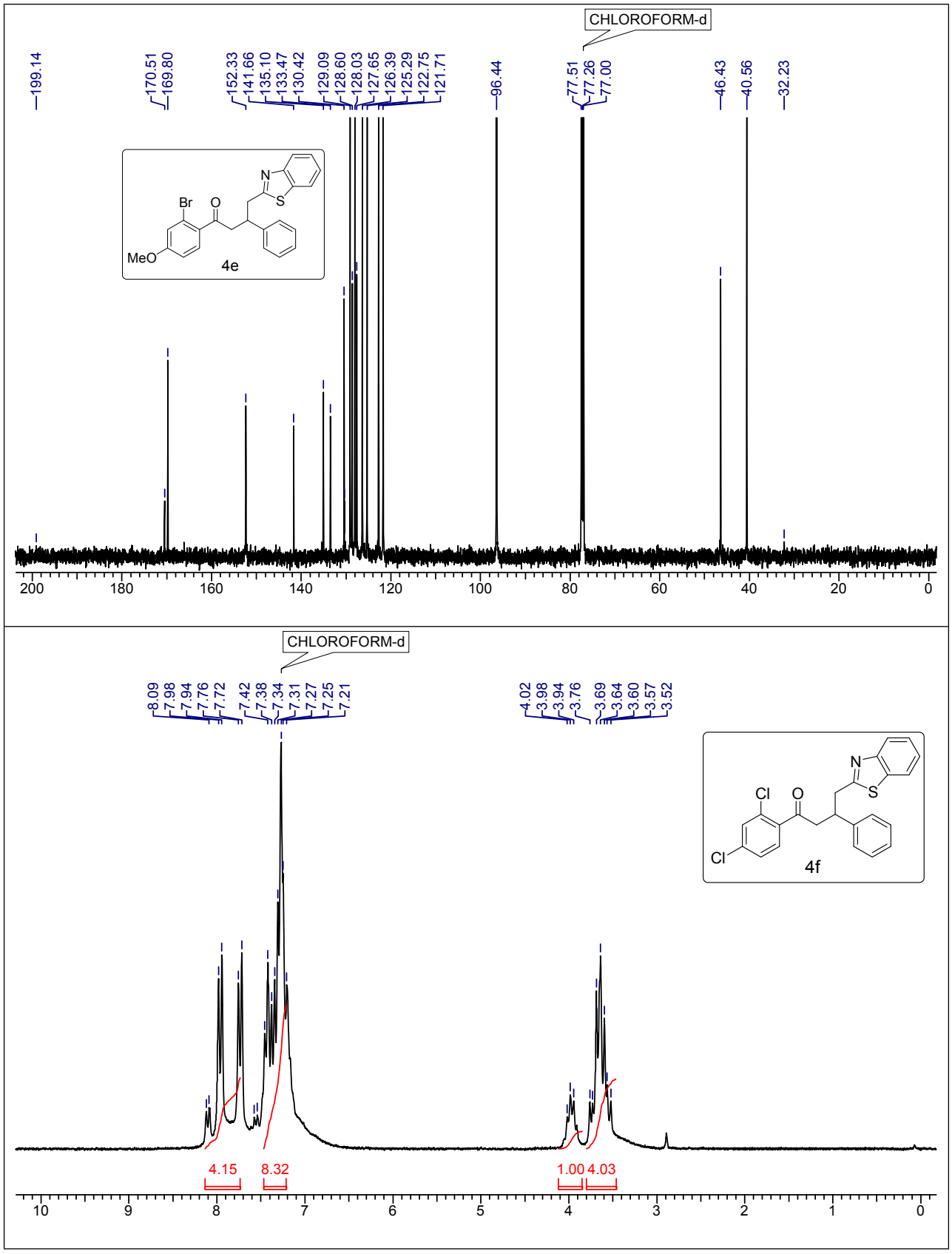
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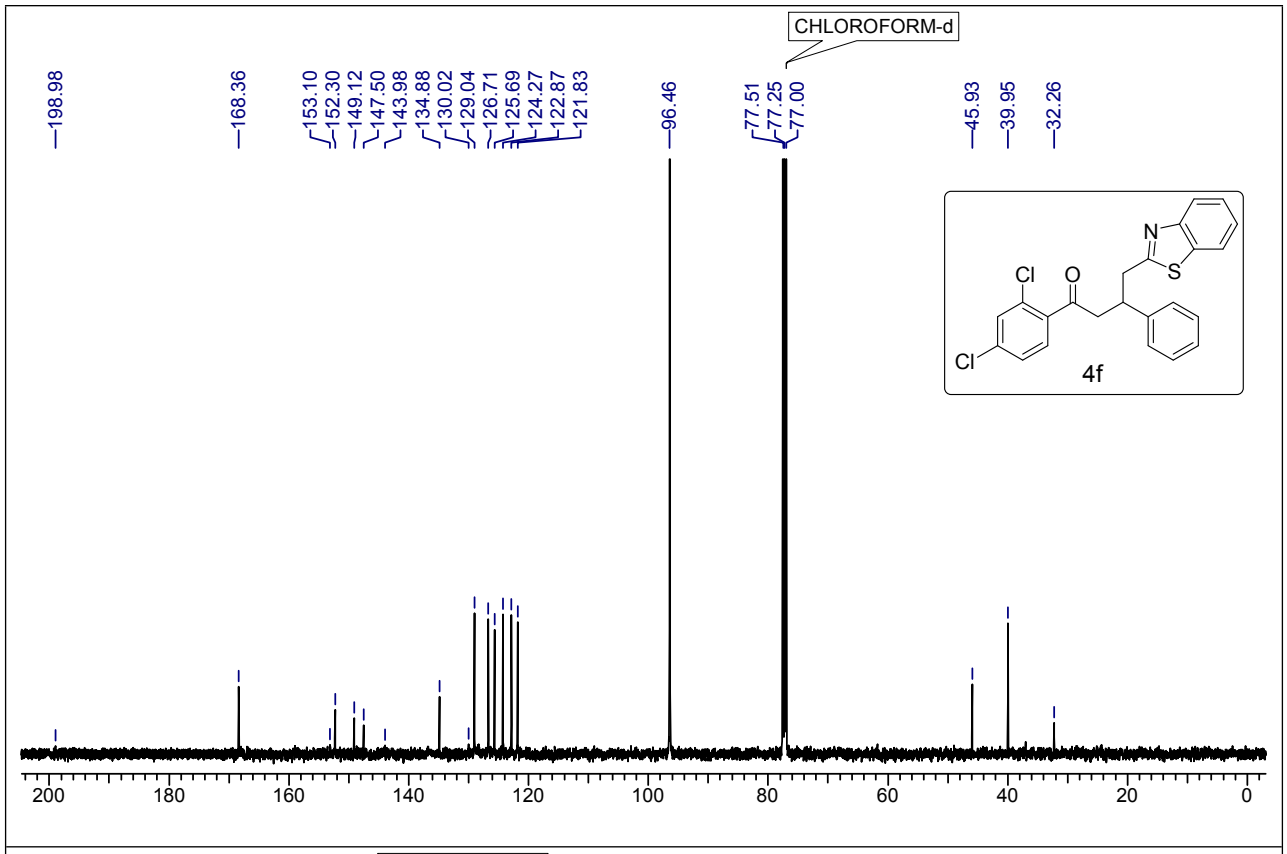
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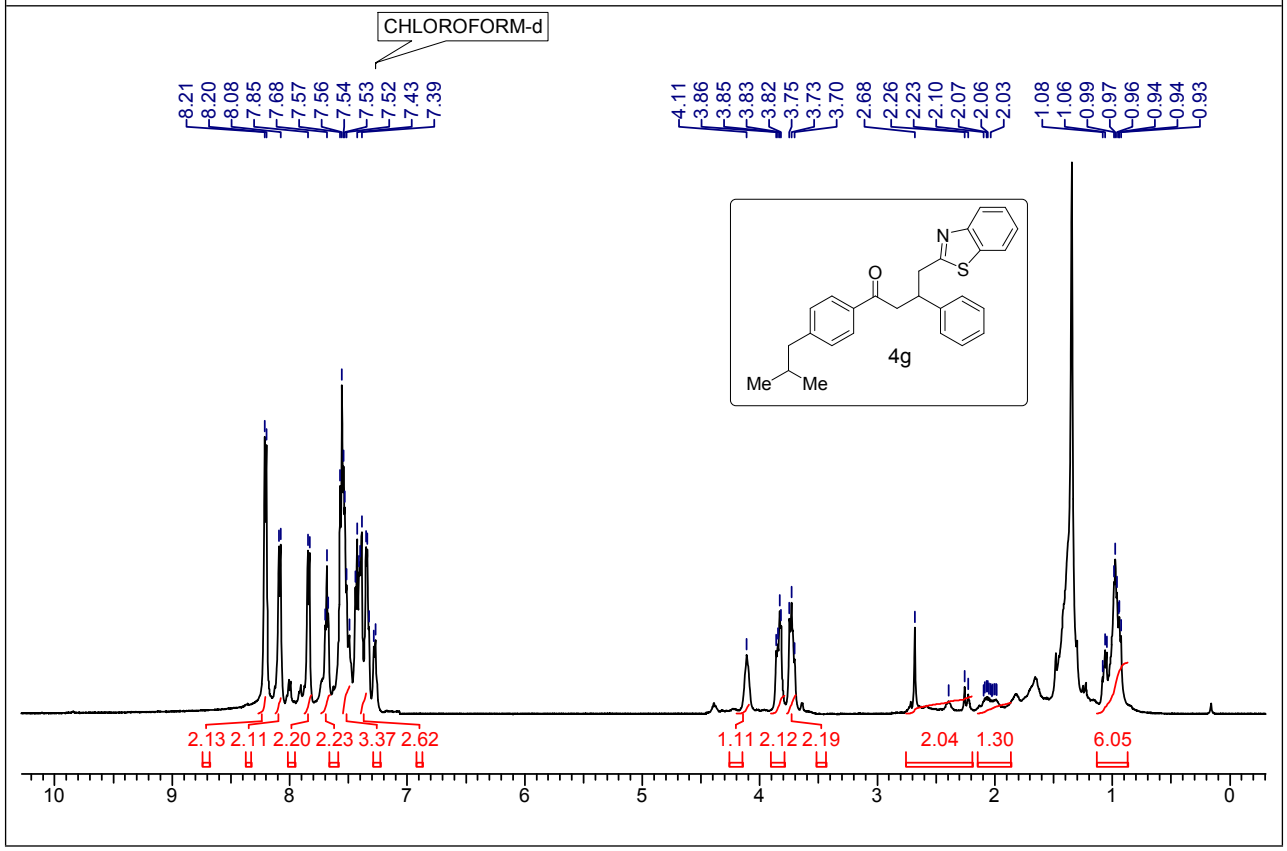
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2.06
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1.08
1.06
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0.97
0.96
0.94
0.94
0.93
N
S
O
4g
Me
Me
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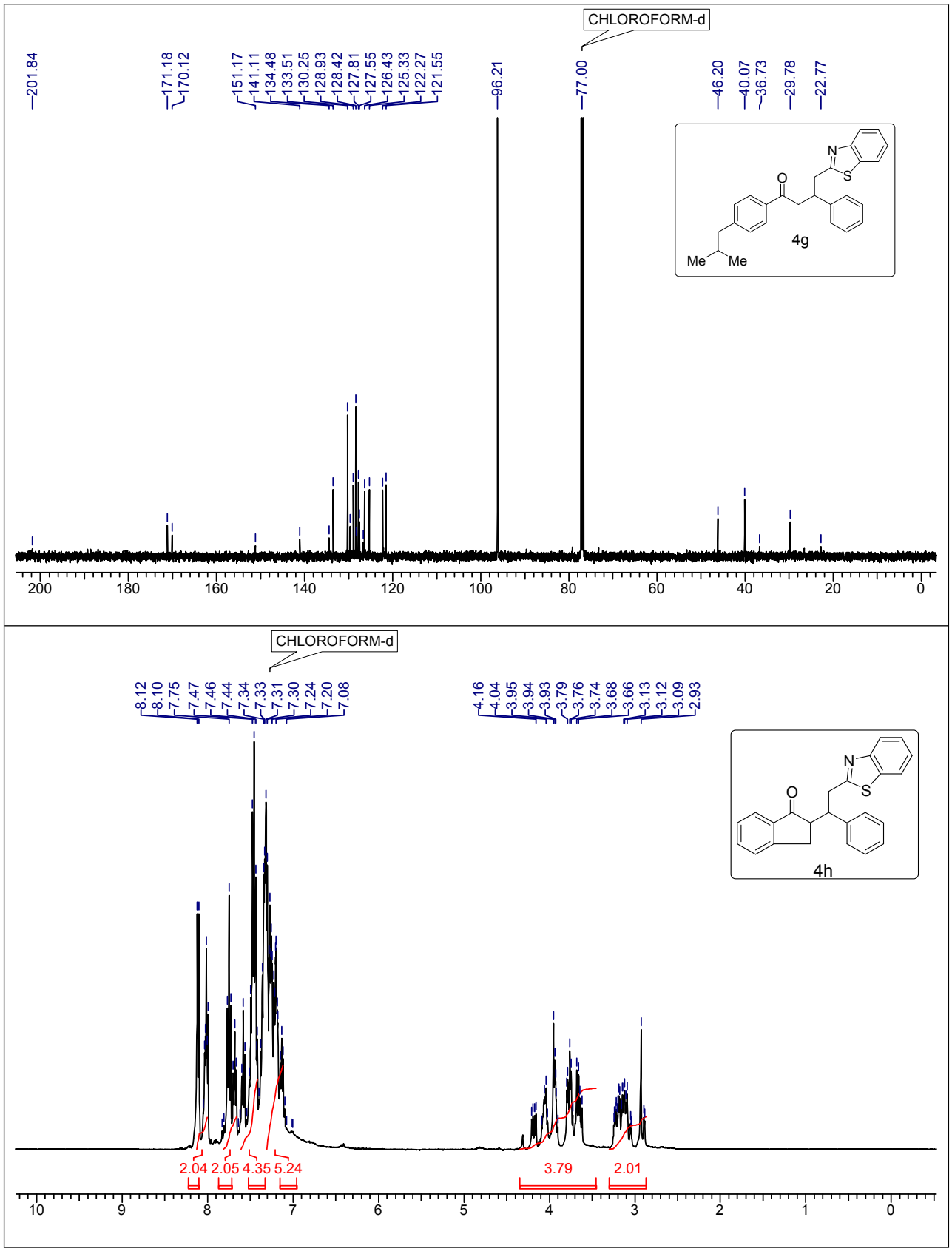
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Me
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120
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80
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3.12
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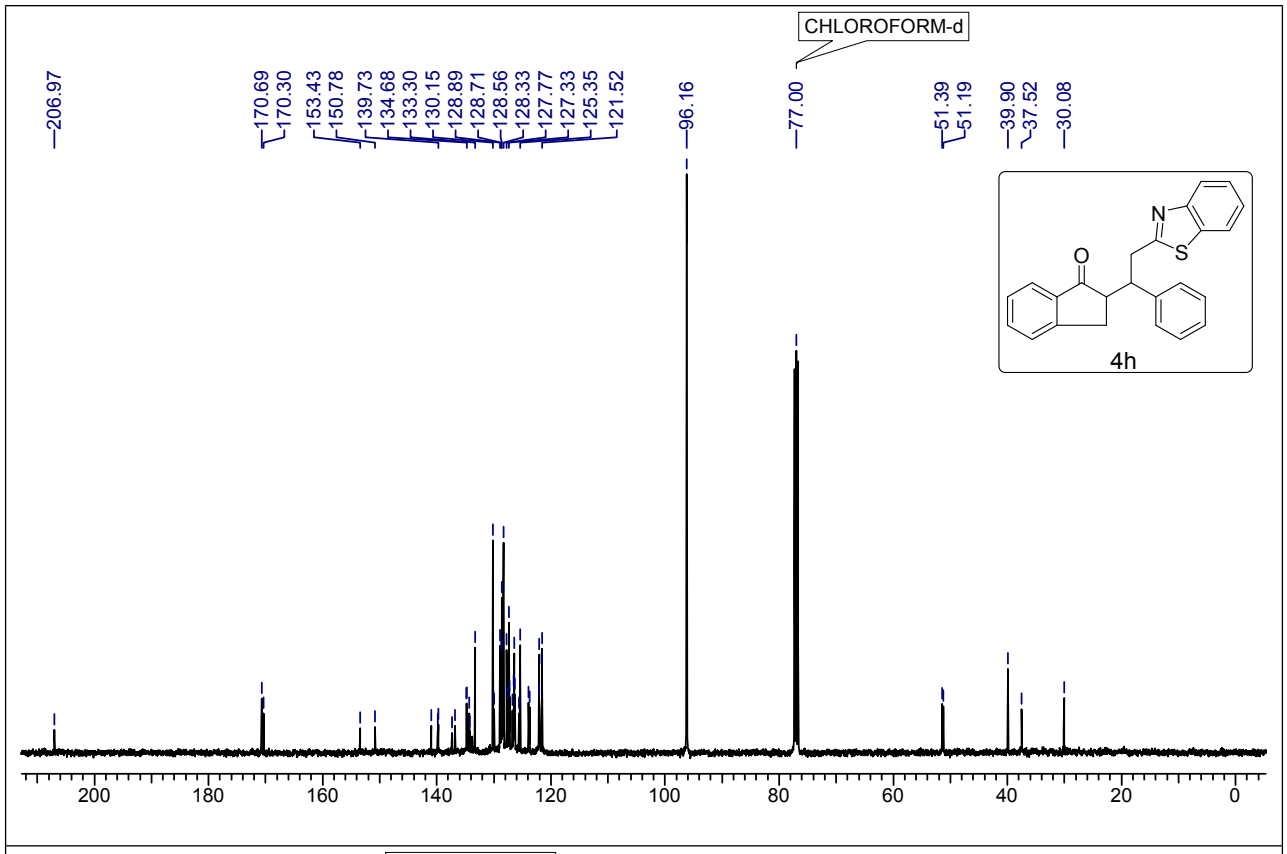
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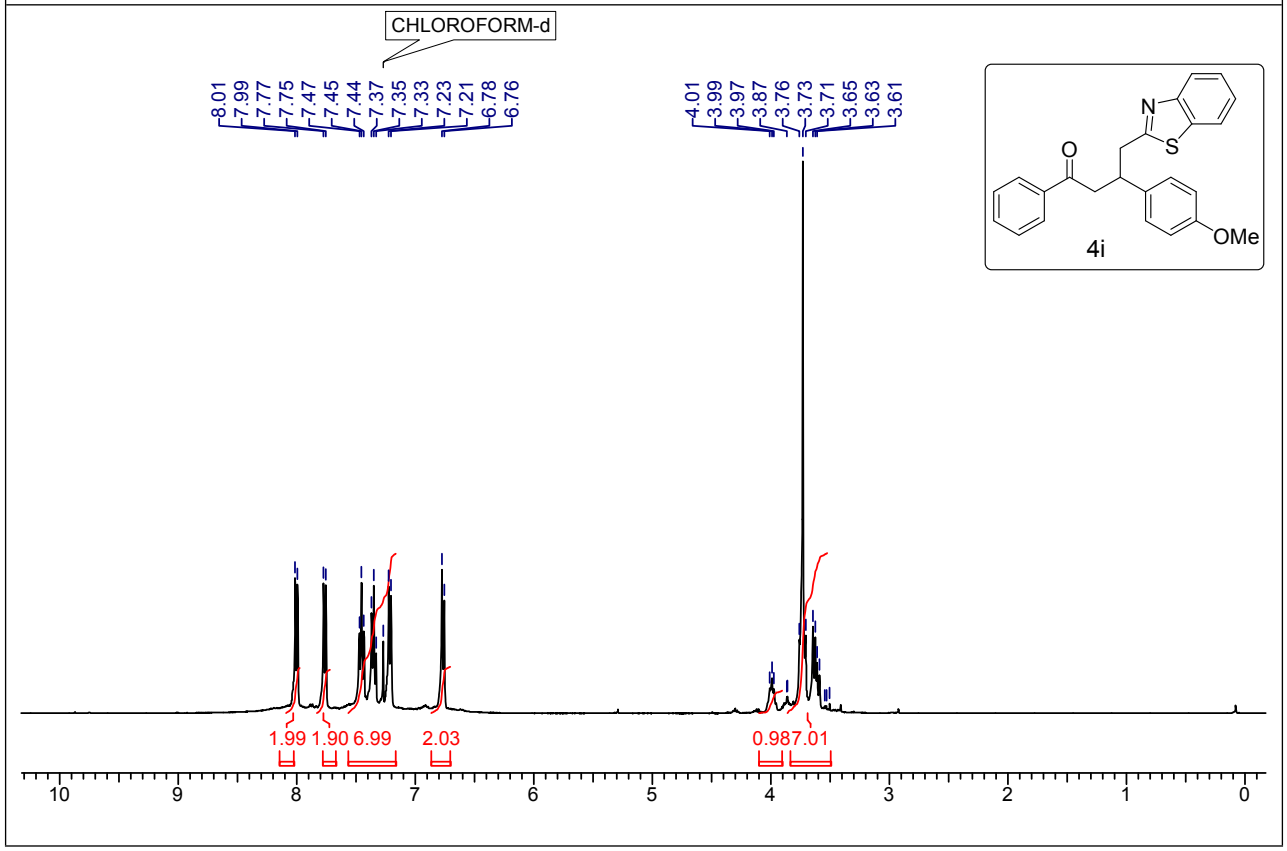
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OMe
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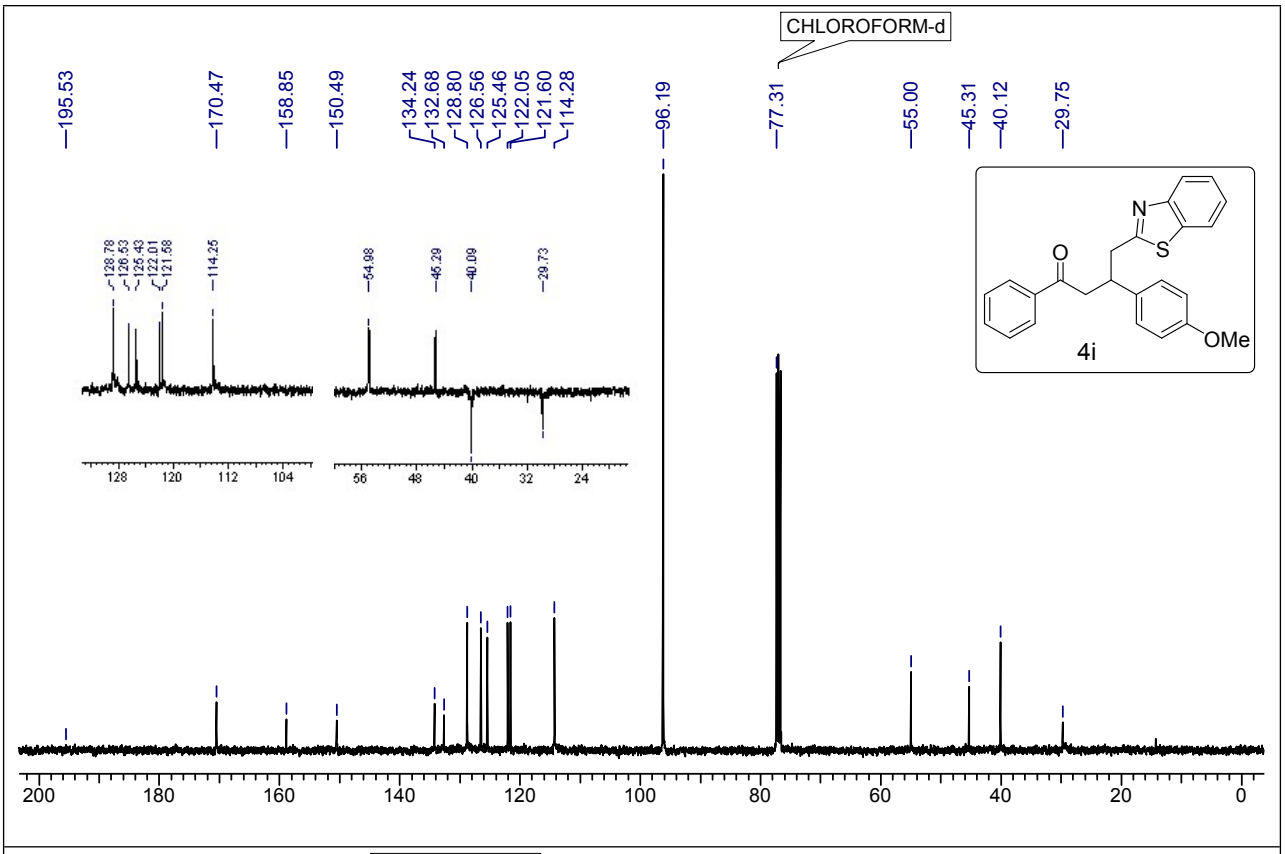
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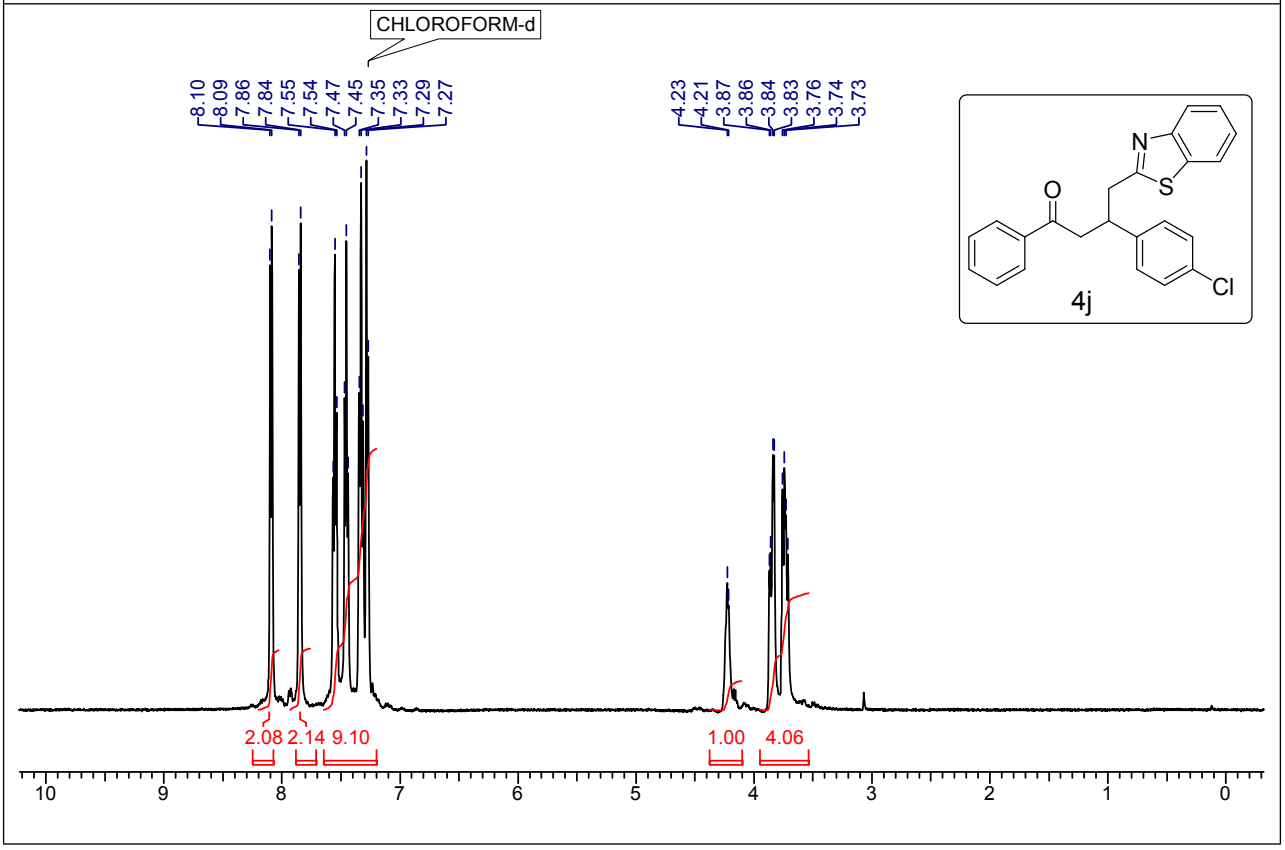
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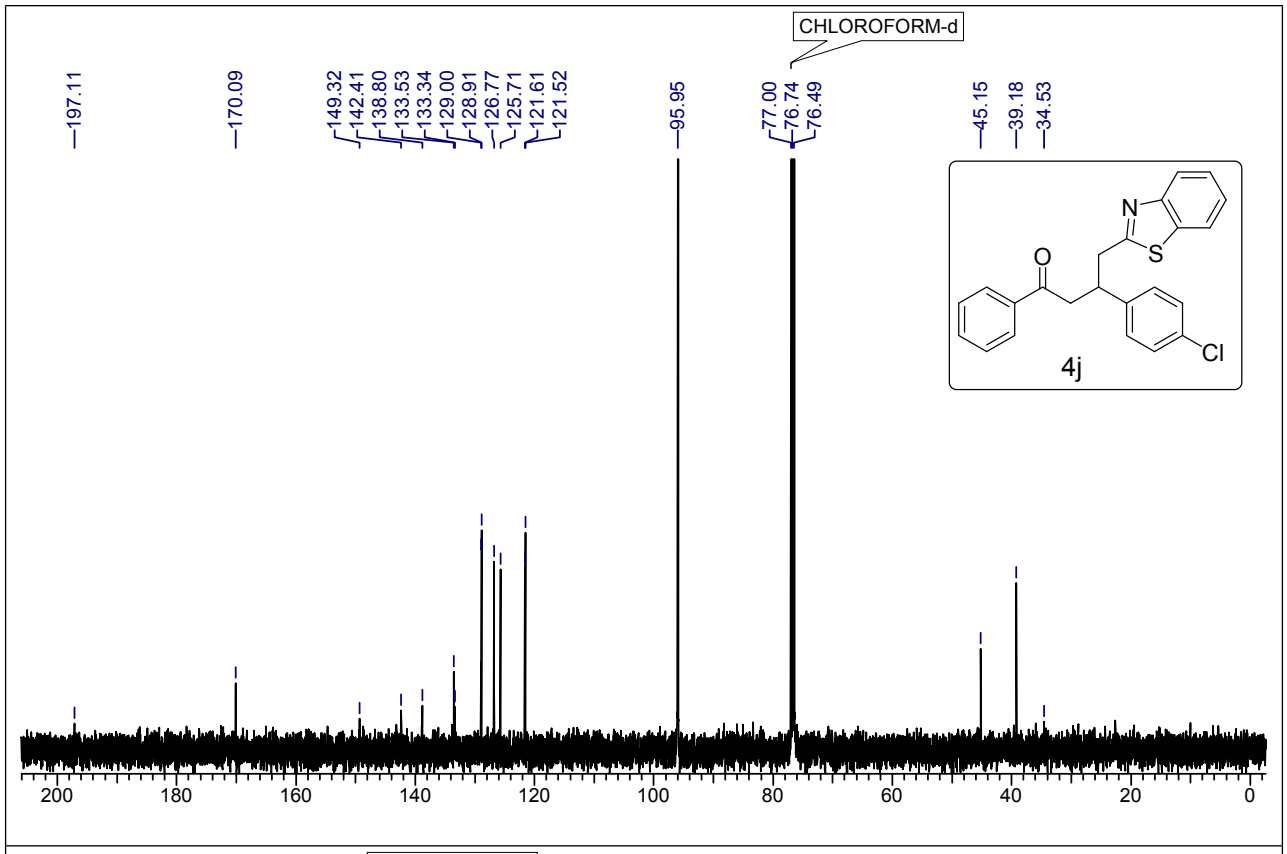
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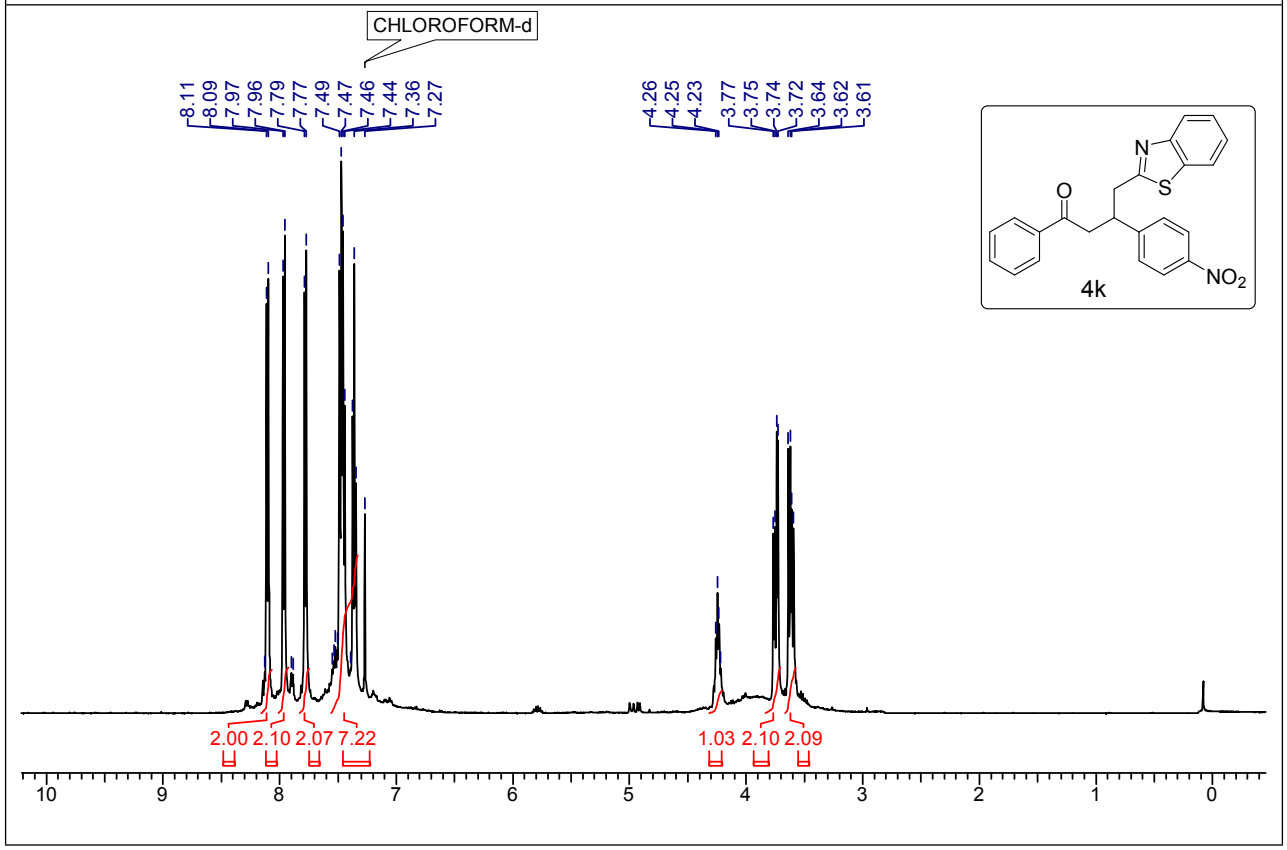
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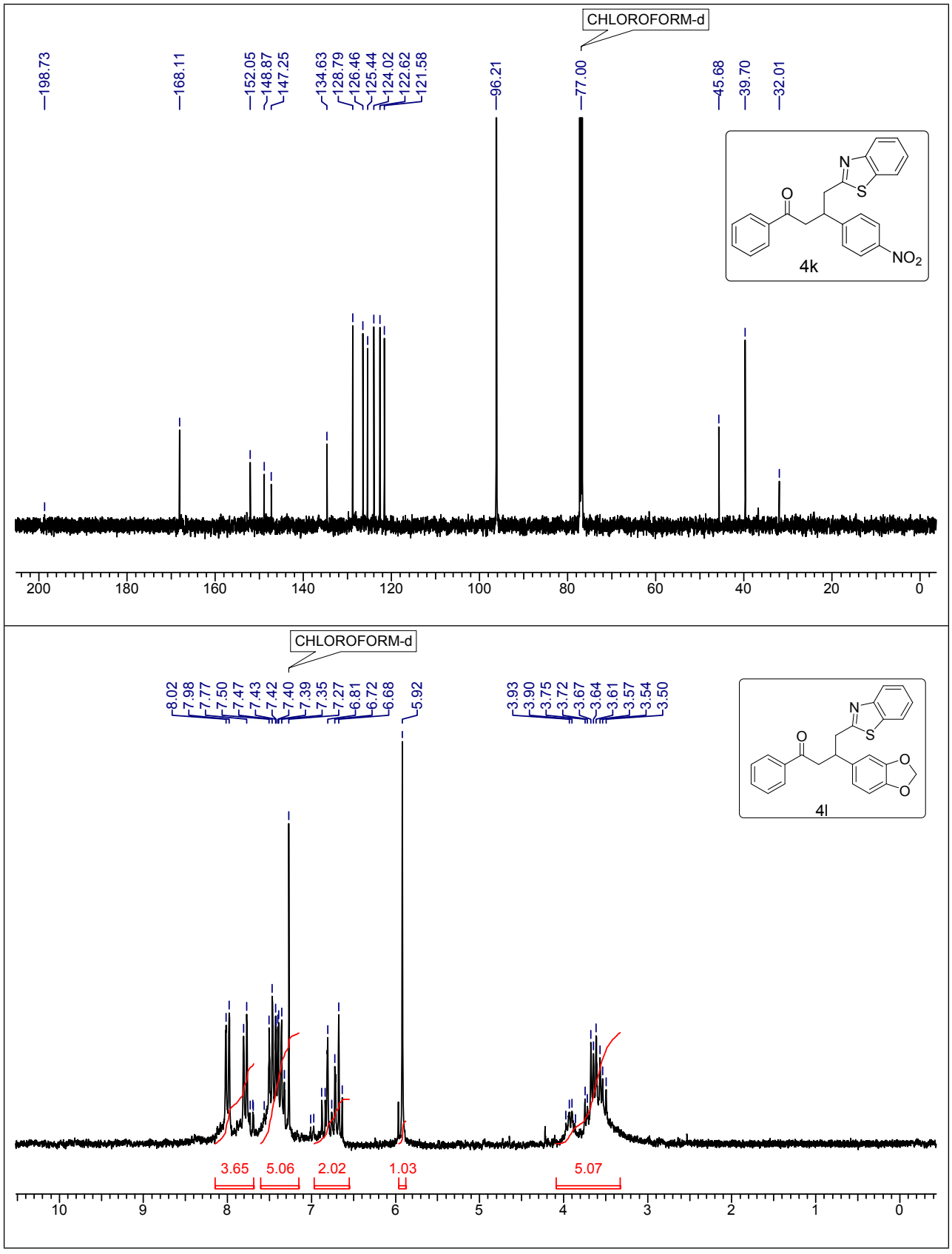
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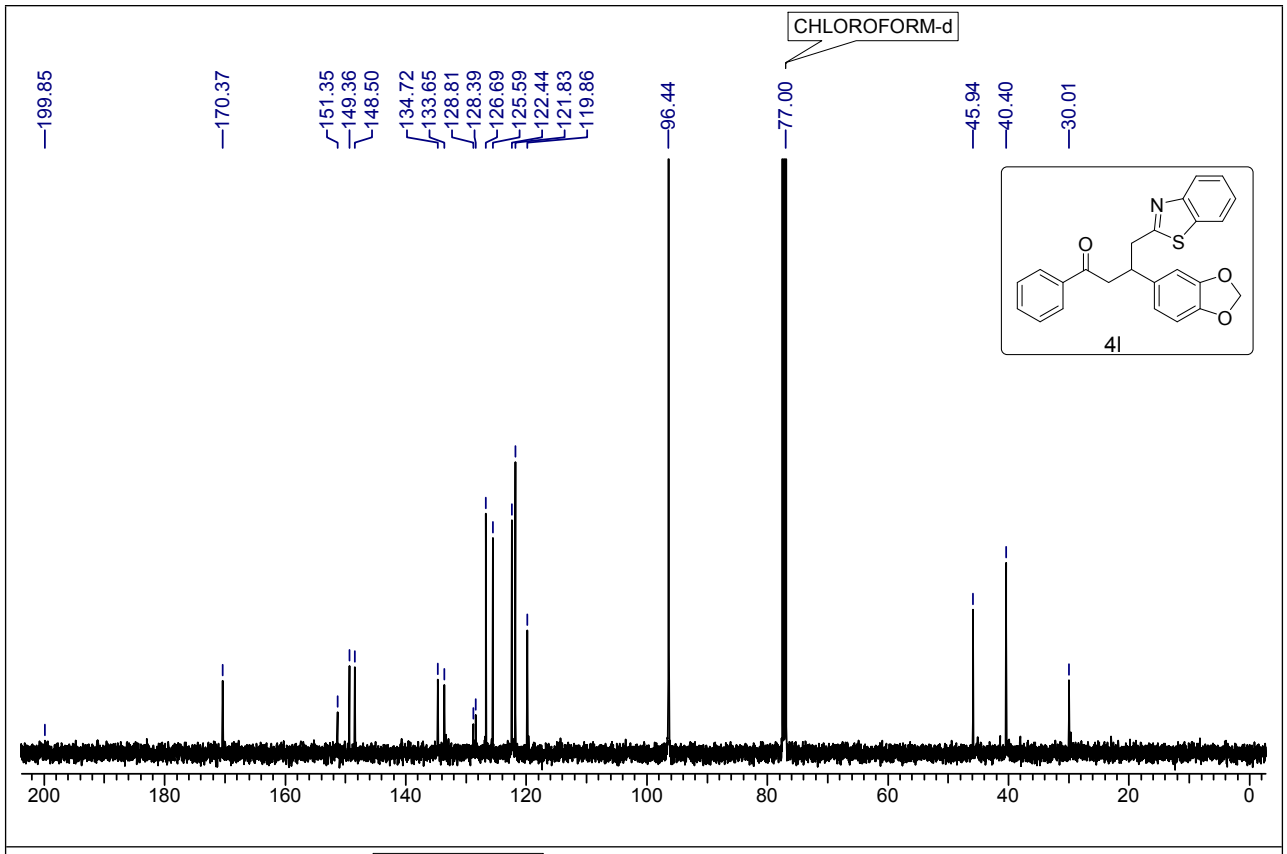
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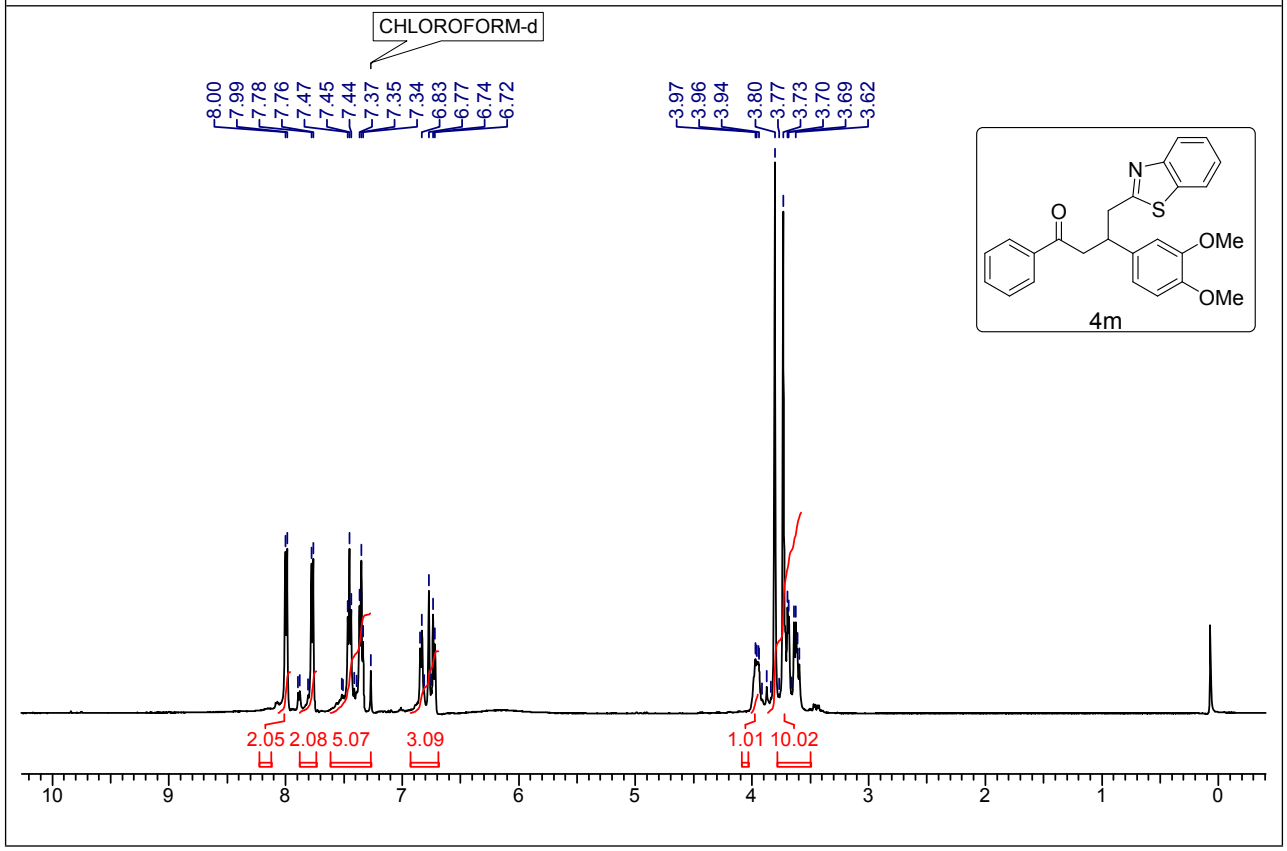
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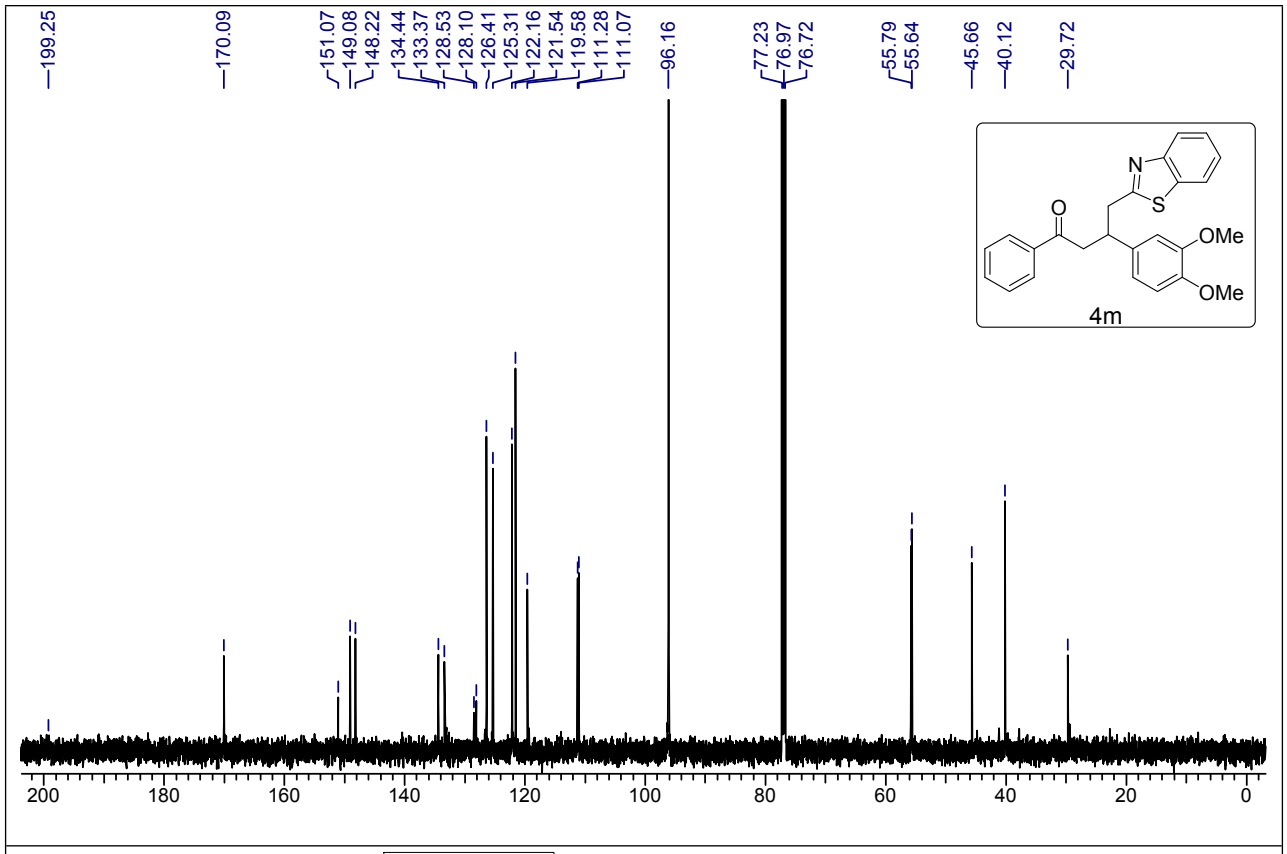
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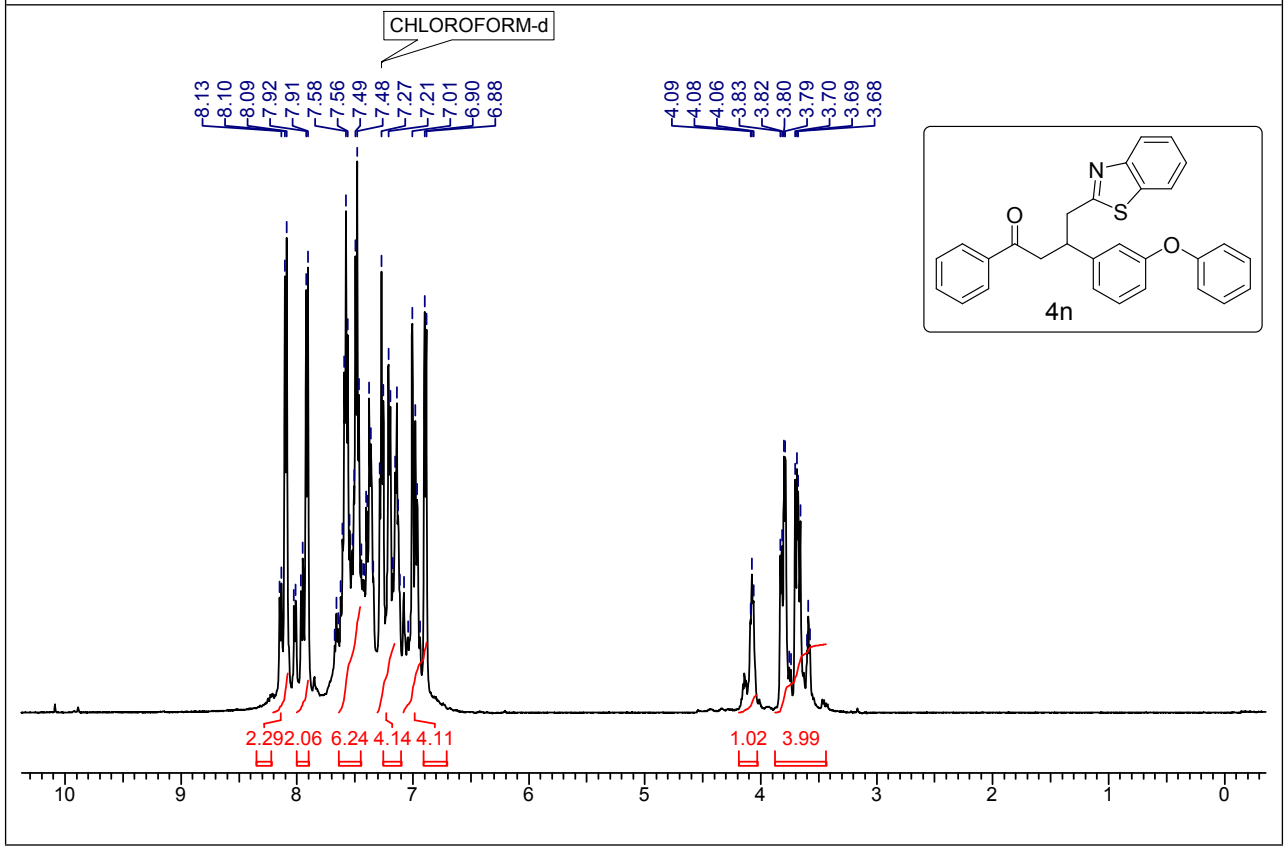
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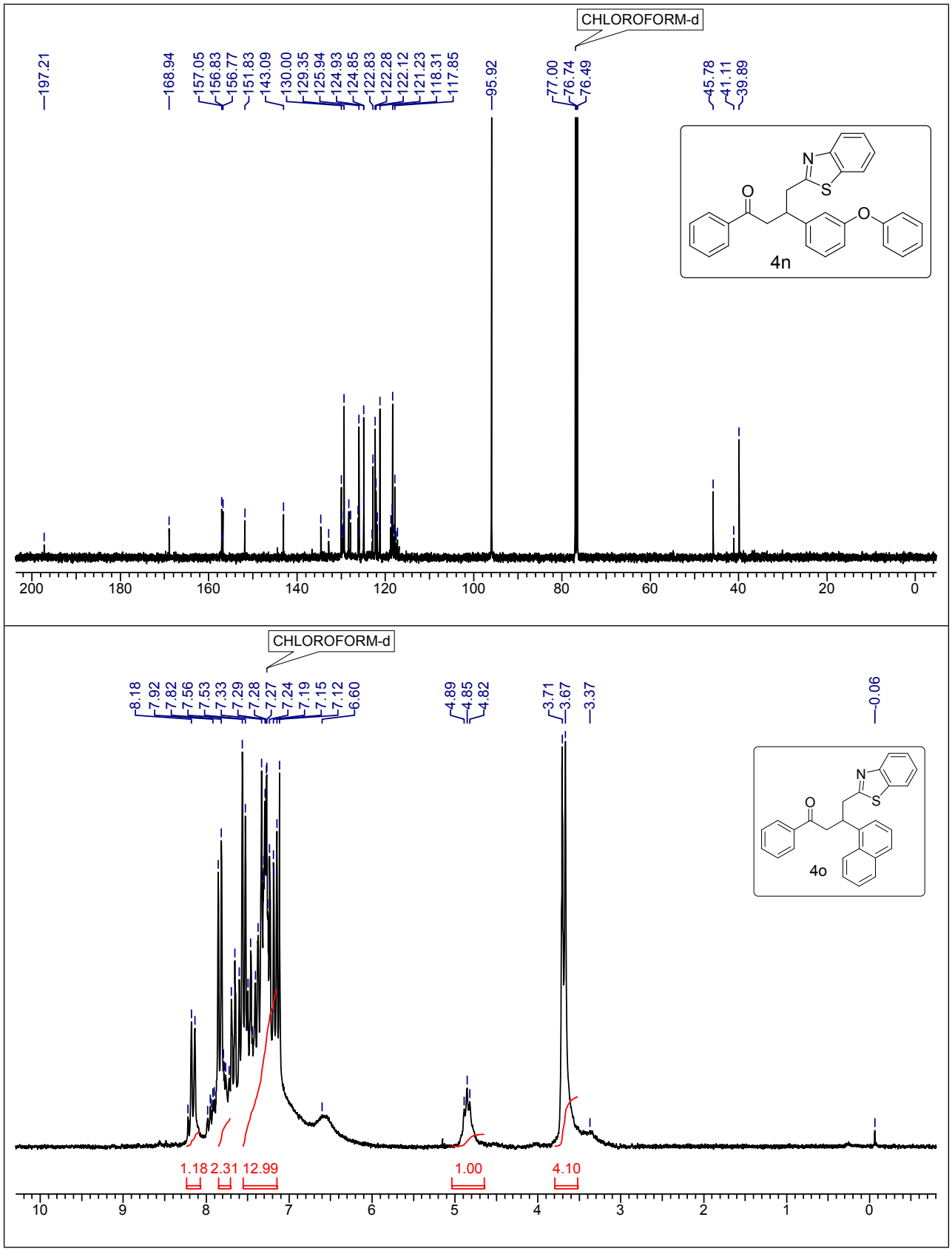
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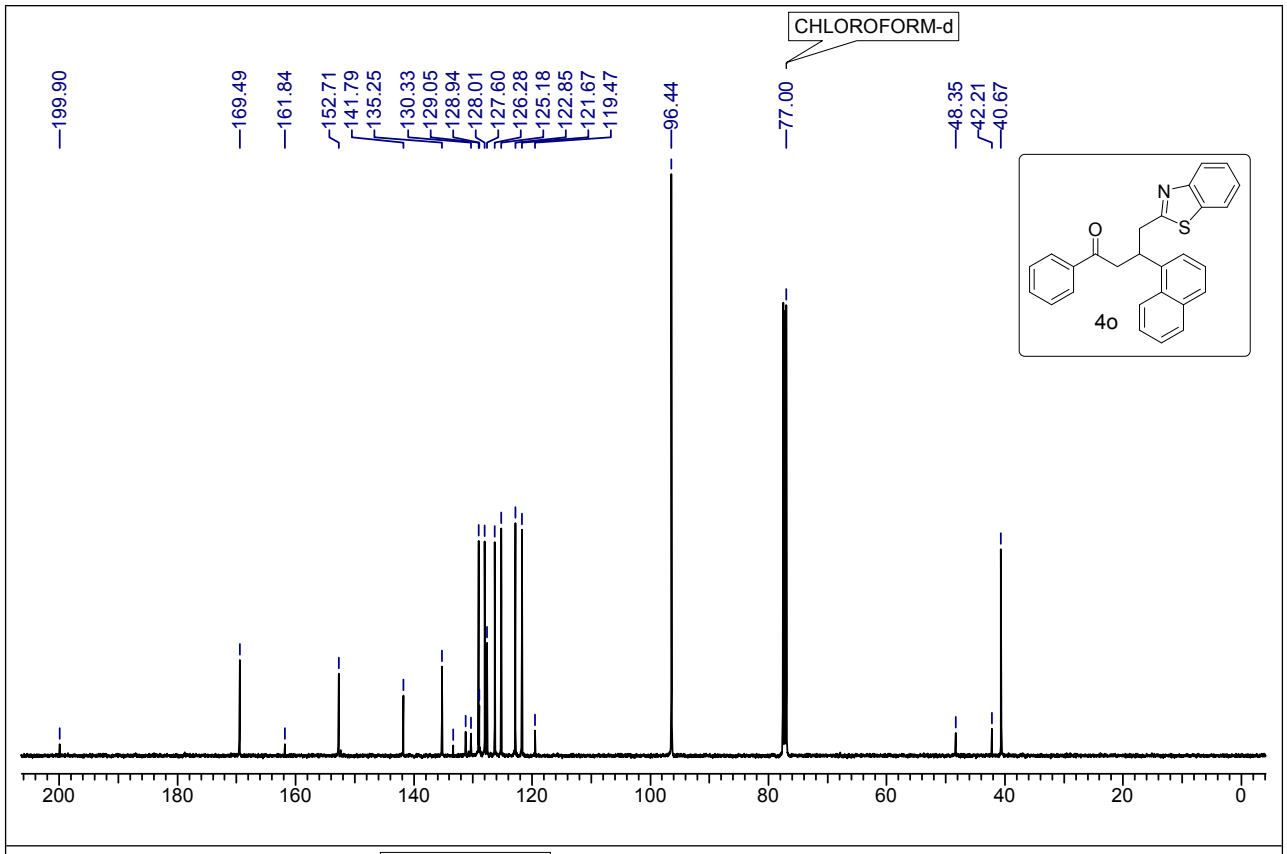
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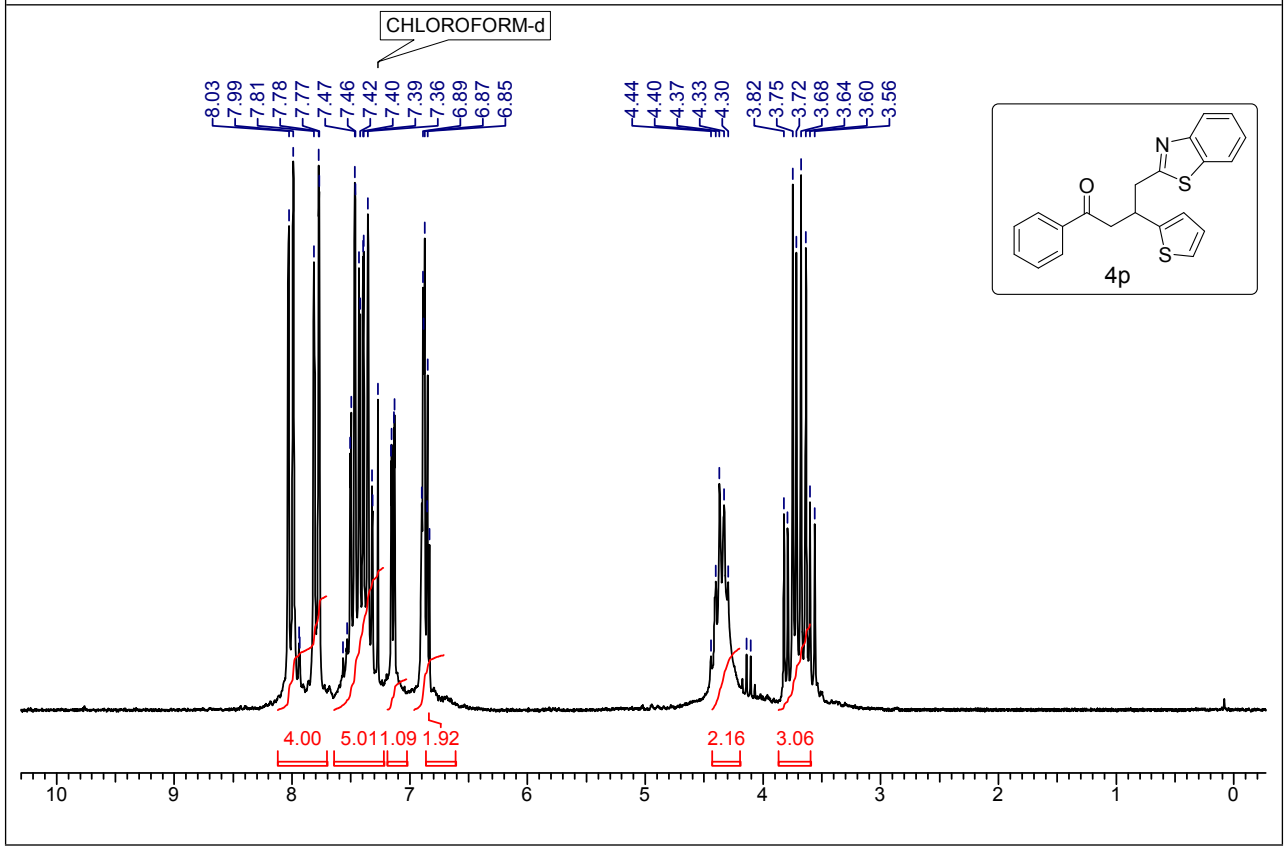
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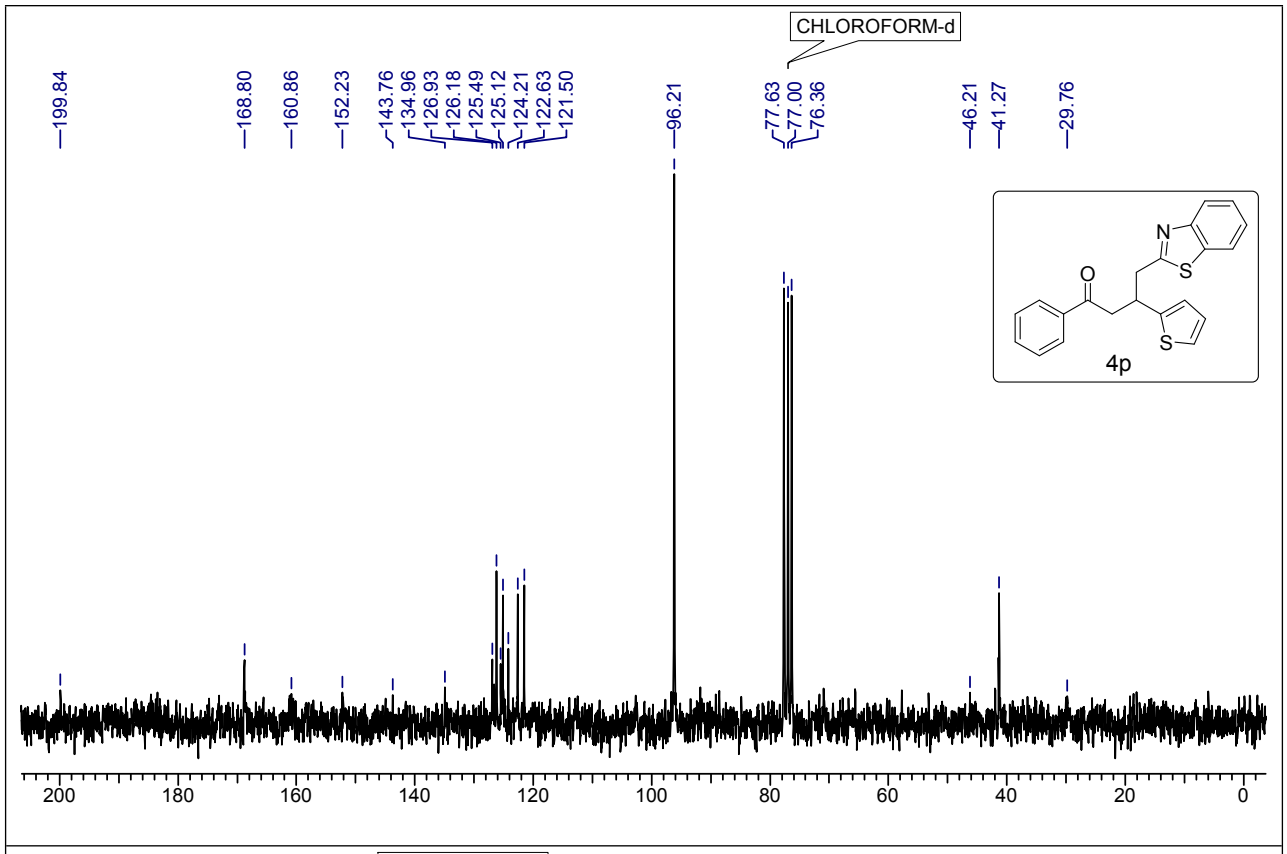
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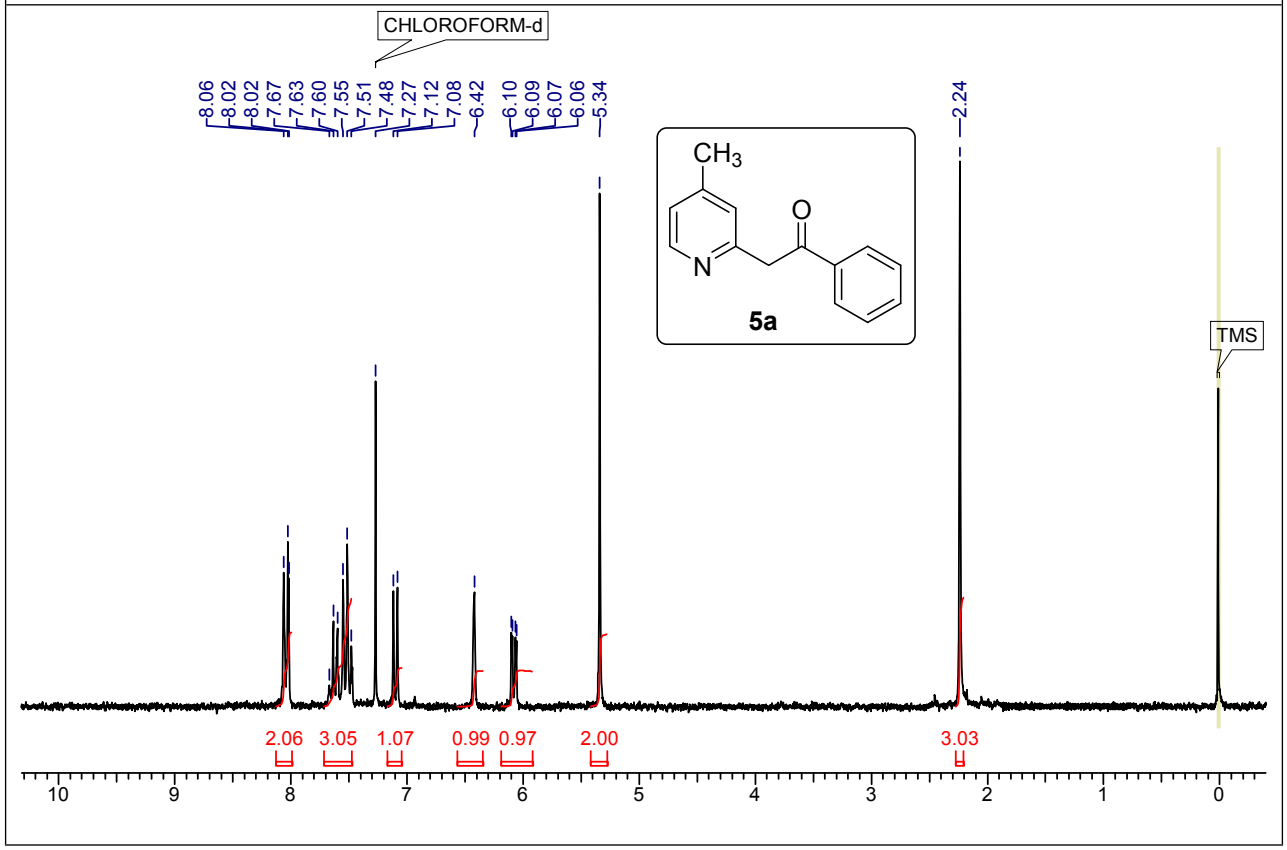
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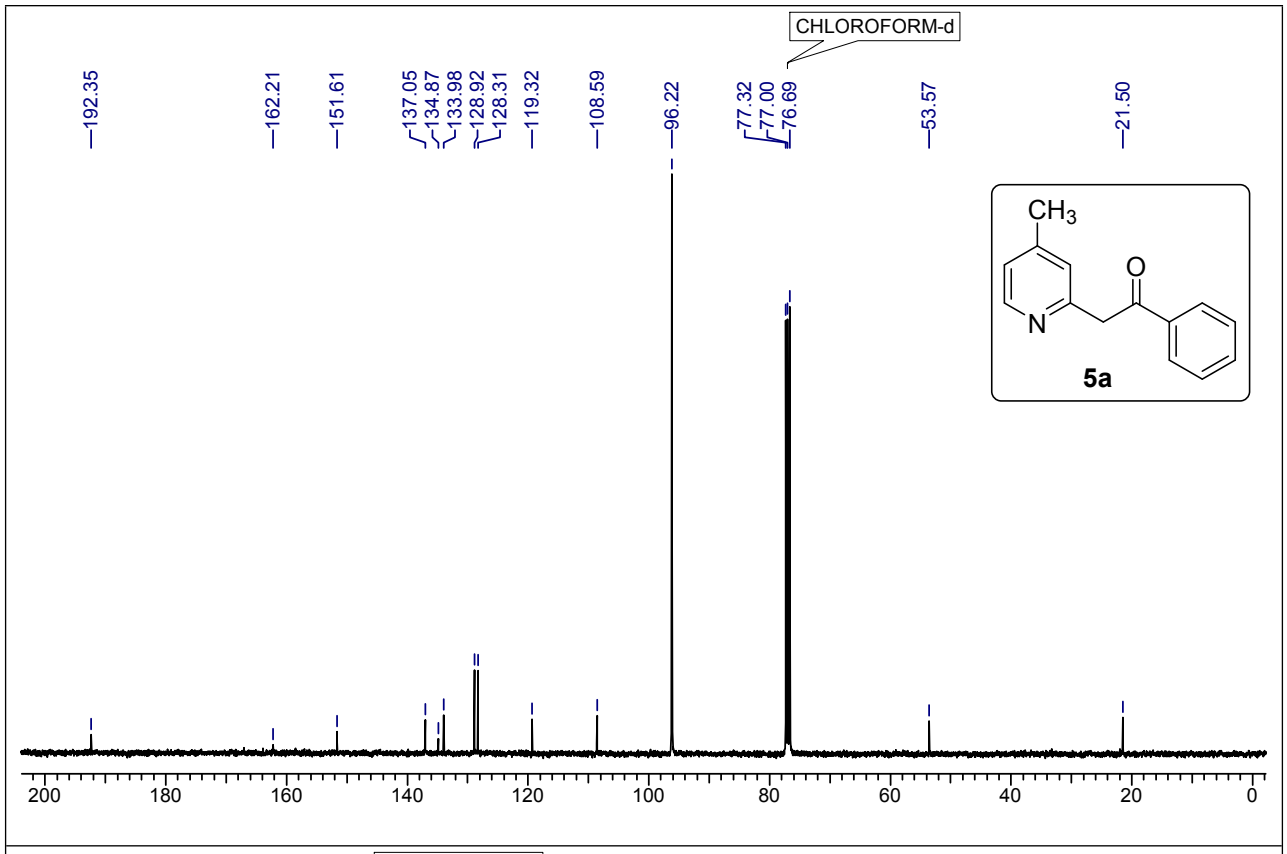
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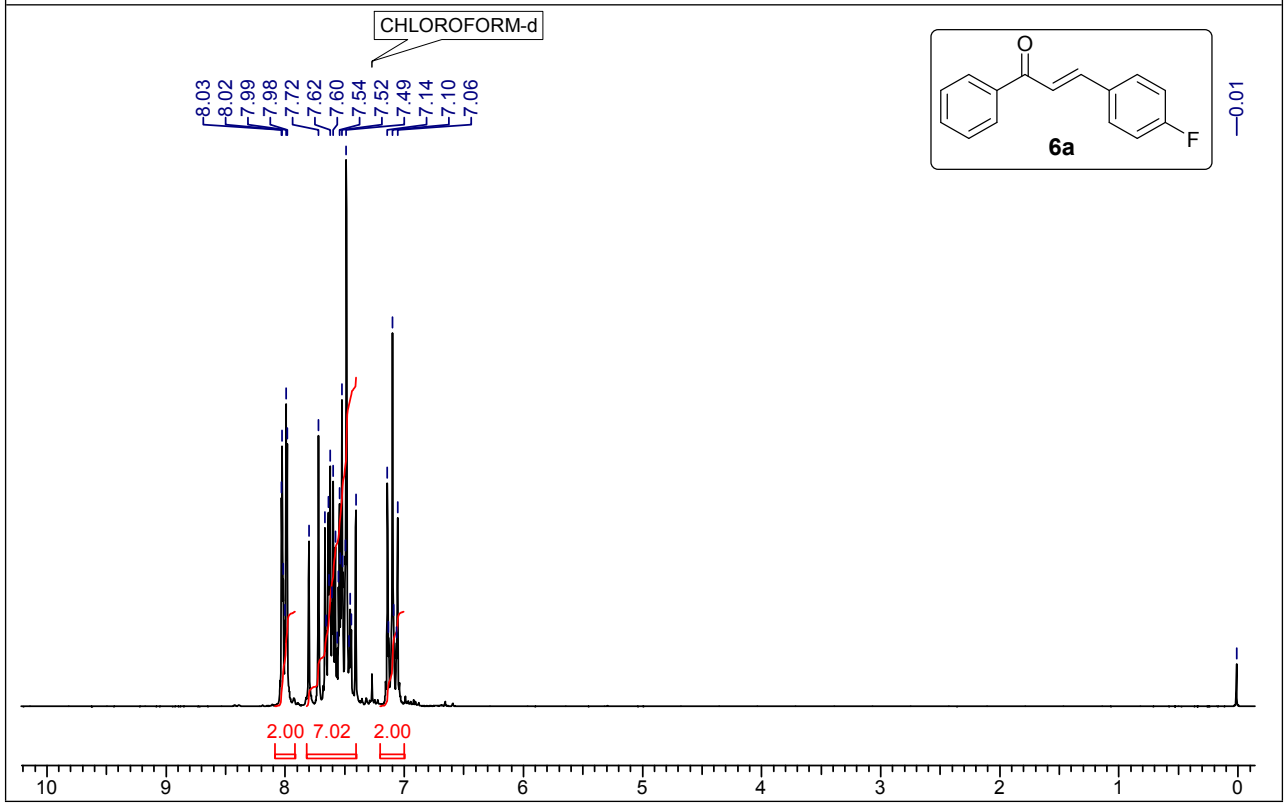
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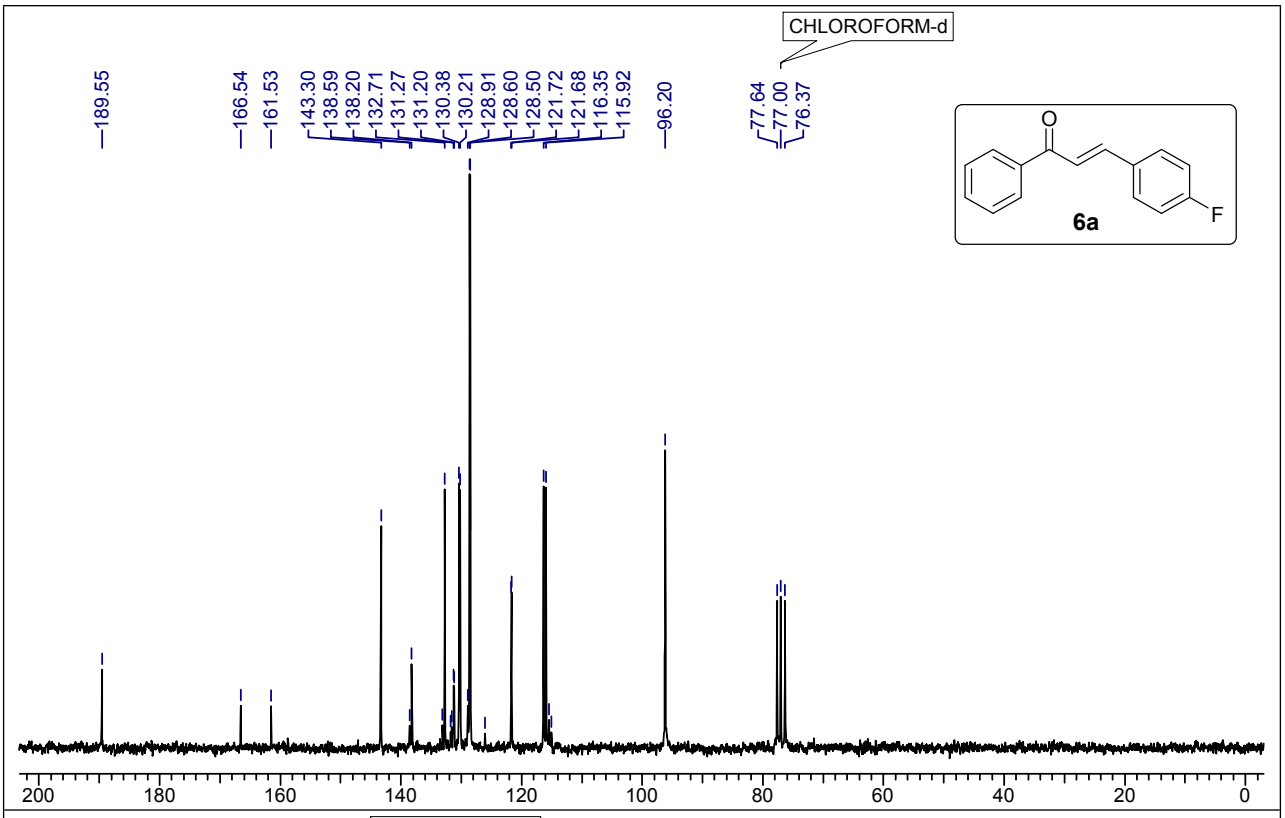
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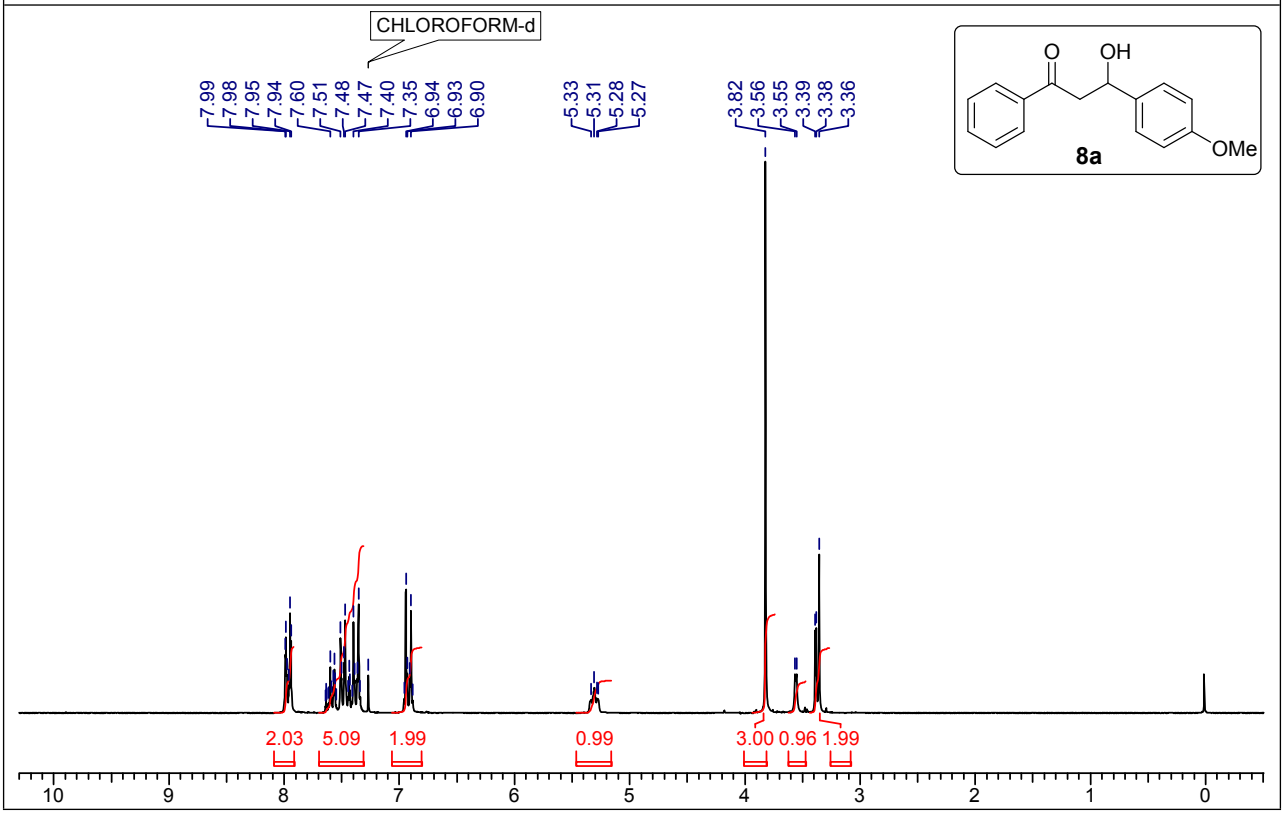
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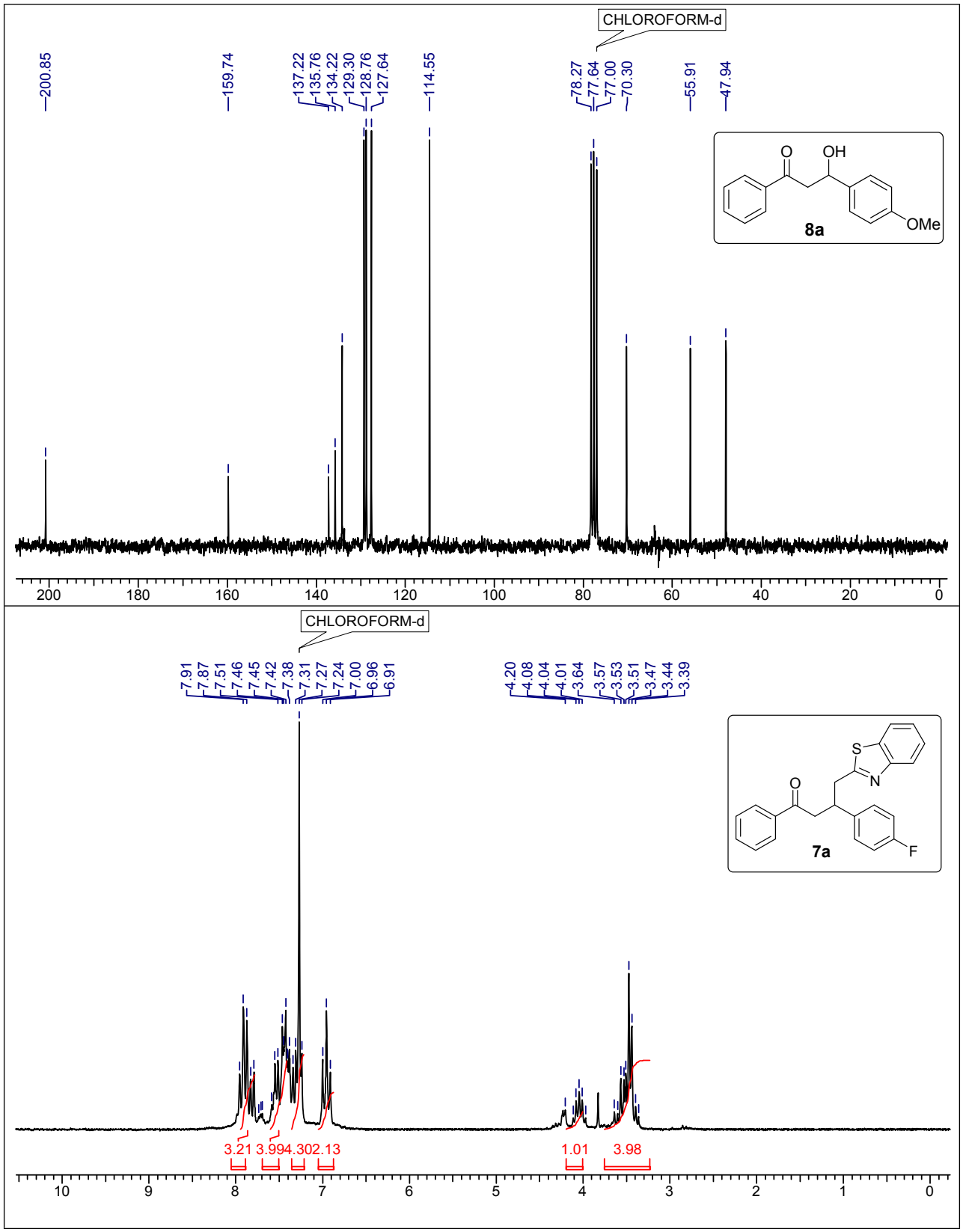
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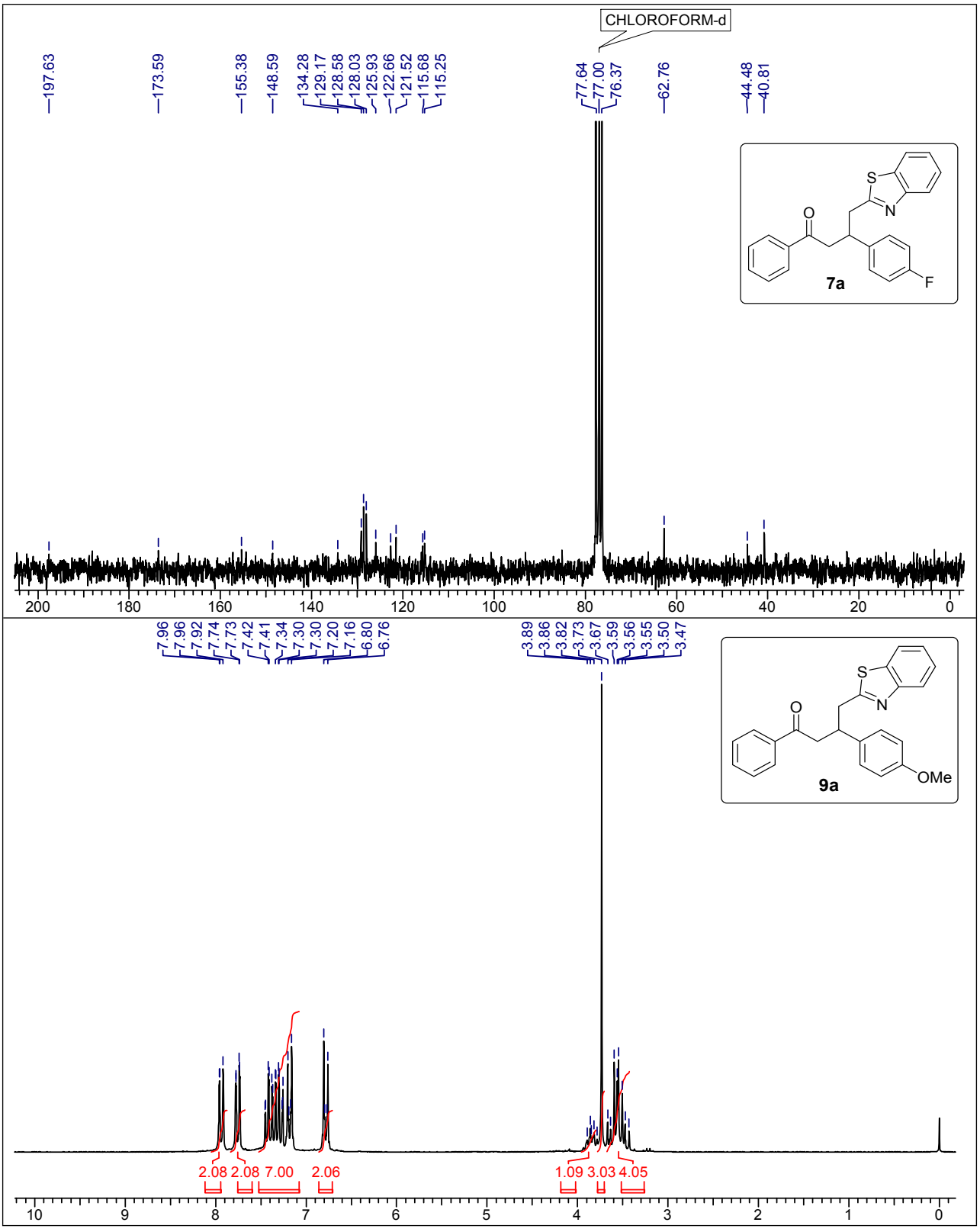
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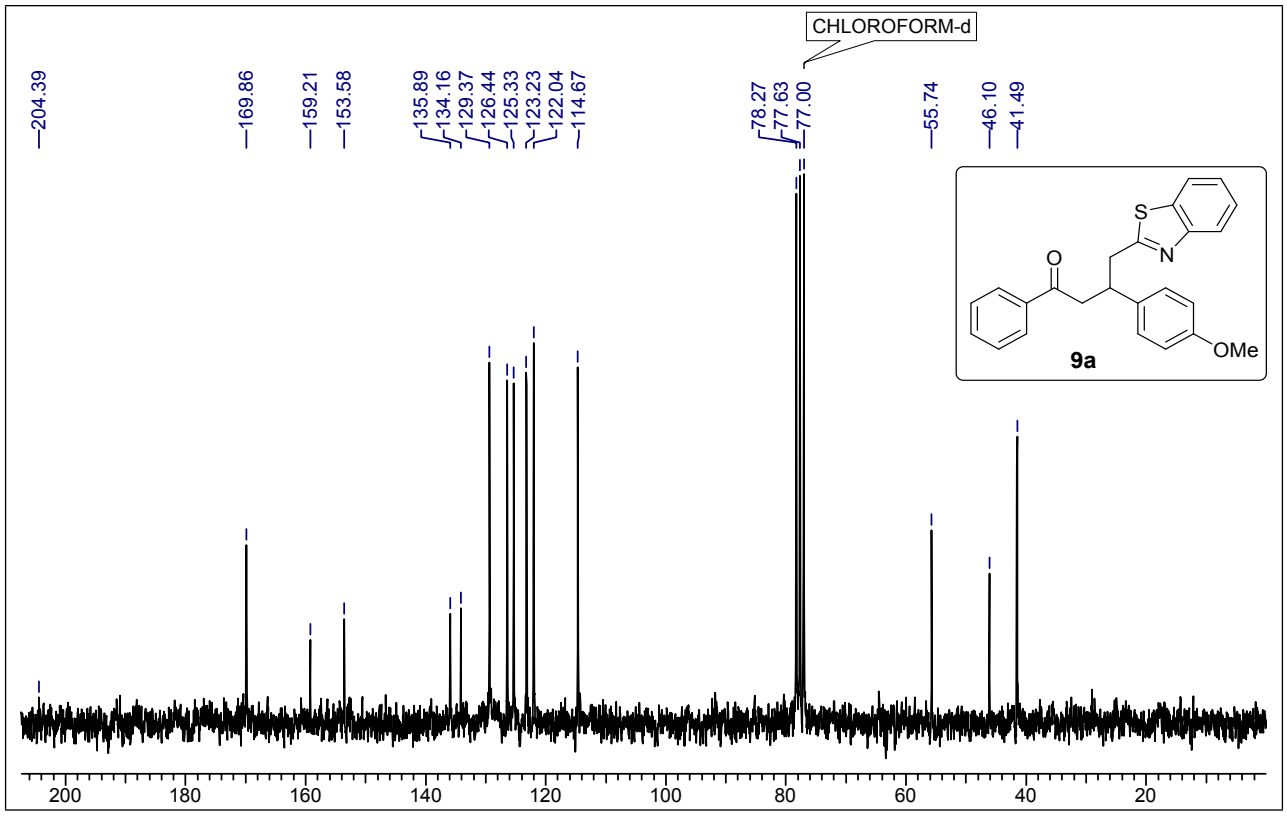
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