Supporting Information

Deep eutectic solvent as a green catalyst for one-pot multicomponent synthesis of 2-substituted benzothiazole derivatives†

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Section S1. Chemicals, supplies and instruments

S1.1. Chemicals and supplies

Choline chloride (98%), imidazole (assay 99%), 2-fluorobenzaldehyde (assay 97%), 2-chlorobenzaldehyde (assay 99%), 4-fluorobenzaldehyde (assay 98%), 4-bromobenzaldehyde (grade reagent, assay 99%), 4-(dimethylamino)benzaldehyde (grade ACS reagent, assay 99%), methyl 4-formylbenzoate (assay 99%), 4-hydroxy-3-methoxybenzaldehyde (assay 98%), 3,4-dihydroxybenzaldehyde (assay 97%), 2-hydroxy-5-methylbenzaldehyde (assay 98%), furfural (assay 99%), 1*H*-pyrrole-2-carboxaldehyde (assay 98%), 4-imidazolecarboxaldehyde (assay 98%), 4-pyridinecarboxaldehyde (assay 98%), cyclohexanecarboxaldehyde (assay 97%), acetophenone (grade reagentPlus, assay 99%), 2-hydroxyacetophenone (assay 98%), 3-methylacetophenone (assay 98%), 4-methylacetophenone (assay 95%), 4-methoxyacetophenone (assay 99%), phenol (grade reagentPlus, assay 99%) were obtained from Sigma-Aldrich. Urea (purity 98%), glycerol (for analysis), zinc chloride (for analysis), benzaldehyde (for synthesis), 4-methoxybenzaldehyde (for synthesis), TLC (silica gel 60 F254) were obtained from Merck. 1-Fluoro-2-nitrobenzene (98%), 1-chloro-2-nitrobenzene (98%), 1-bromo-2-nitrobenzene (98%), and 1-iodo-2-nitrobenzene (98%) were obtained from Across. Ethyl acetate (purity 99.5%), and *n*-hexane (purity 99.5%) were obtained from Xilong Chemical Co., Ltd (China).

S1.2. Analytical techniques

The ^{1}H and ^{13}C NMR spectra were recorded on a Bruker Advance 500 instruments using $CDCl_3$ and $(CD_3)_2O$ as solvent and solvent peaks or TMS as internal standards. HRMS (ESI) data were collected using Bruker micrOTOF-QII MS at 80 eV. FT-IR spectra were recorded in the form of KBr pellets by a Bruker Vertex 70. Analytical thin-layer chromatography (TLC) was acquired on F-254 silica gel coated aluminum plates from Merck. Silica gel column chromatography was carried out with silica

gel (60, 230-400 mesh) from Merck. Thermal gravimetric analysis (TGA) was obtained using a TA Q500 thermal analysis system with the sample held in a platinum pan in a continuous airflow.

S2. FTIR spectra and assessment of green metrics

S2.1. FTIR spectra

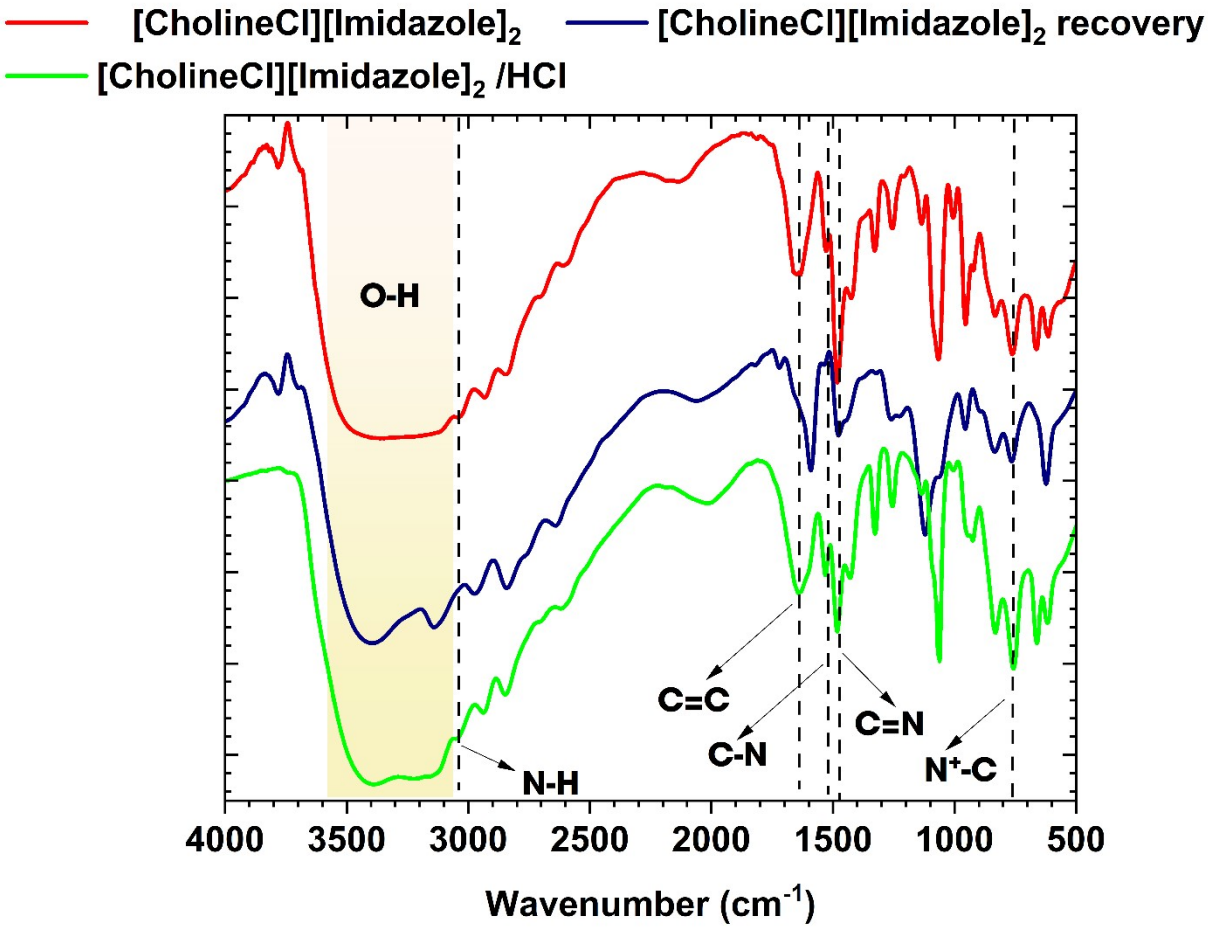
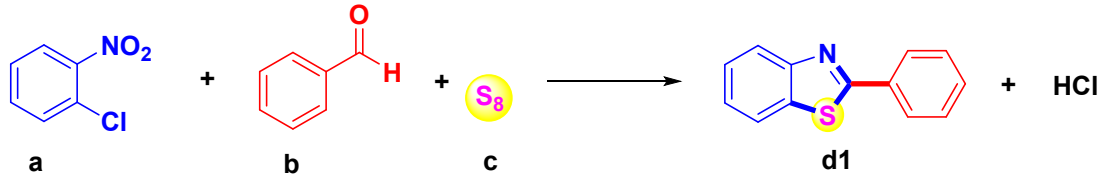


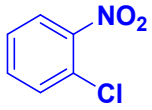
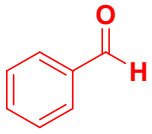
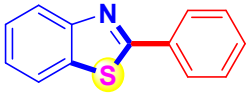
Figure S1. FTIR spectra of [CholineCl][Imidazole]$_2$; [CholineCl][Imidazole]$_2$ recovery; and [CholineCl][Imidazole]$_2$/HCl.

S2.2. Assessment of green metrics

The green chemistry matrix has been computed for the synthesis of 2-phenylbenzo[*d*]thiazole using the specified parameters:[1-4]

Scheme S1. Model reaction for green matrix calculation



Compound name	M.W. (g/mol)	In present work M.W. (mg)
	156.99	156.99
	106.04	106.04
S_8	63.94	63.94
	211.05	211.05
HCl	36.45	36.45

The total mass of reactants = 326.97

Obtained product = 0.16461g = 164.61 mg

S2.2.1. Environmental factor(E-factor)

$$\text{E-Factor} = \frac{Mass\ of\ waste}{Mass\ of\ product}$$

In which, the mass of waste is included sulfur, HCl

$$\text{E-Factor} = \frac{63.94 + 36.45}{164.61} = 0.61$$

(Ideal valve of E-factor is considered zero)

S2.2.2. Atom-economy (AE)

The optimal value of the AE factor is 100%, indicating that all initial material is fully transformed into the final output.

$$\text{AE} = \frac{MW\ of\ product}{\sum MW\ of\ stoichiometric\ reactants} 100$$

$$\text{AE} = \frac{211.05}{156.99 + 106.04 + 63.94} 100 = 64.54\%$$

S2.2.3. Process mass intensity (PMI)

$$\text{PMI} = \frac{\sum (Mass\ of\ stoichiometric\ reactants\ +\ solvent)}{Mass\ of\ product}$$

$$PMI = \frac{326.97}{164.61} = 1.98$$

Ideal value of PMI = E-Factor + 1 = 0.61 + 1 = 1.61

The variation in value between both findings is rather small.

S2.2.4. Reaction mass efficiency (RME)

$$RME = \frac{Mass\ of\ product}{\sum(mass\ of\ stoichiometric\ reactants)}100$$

$$RME = \frac{164.61}{326.97}100 = 50.34\%$$

S2.2.5. Eco-score (E-score)

Ideal reactions Eco-score value is 100.

Eco-scale from 0 to 100 using the following scores: > 75, excellent; > 50, acceptable; and < 50, inadequate.

E-score has been calculated for the reaction based on the following 6 parameters below.

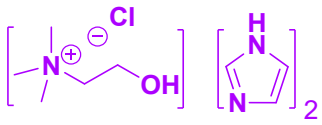
Entry	Parameter	Values	Penalty points
1	Yield	(100-78)/2	11
2	Price of the reaction component	Inexpensive	0.0
3	Safety (Reactant)	T(Toxic) = 4+4+4 = 12	12.0
4	Technical setup	Common setup	0.0
5	Temperature /time	120 °C/ 6 h	5.0
6	Workup and purification	Crystallization	1.0
	Total penalty points		29.0
	Based on the hazard warning symbols		

Eco-Score = 100 – The sum of individual penalties = 100 – 29.0 = 71.0 (> 50, acceptable synthesis)

As per the above results, it was concluded that the reaction has a low Environment-factor (E-factor = 0.61), high atom economy (AE = 64.54%), high process mass intensity (PMI = 1.98), and medium reaction mass efficiency (RME = 50.34%), with acceptable eco-score (71.0%). These values clearly indicated the eco-friendliness of the present synthesis.

S3. Spectra data

[CholineCl][Imidazole]$_2$

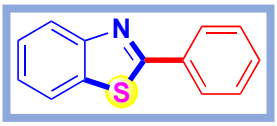


White solid, m.p = 58 °C

^{1}H NMR (500 MHz, D_2O-d_2) δ = 7.76 (s, 2H), 7.13 (s, 4H), 4.05 – 4.02 (m, 2H), 3.49 – 3.47 (m, 2H), 3.17 (s, 9H).

^{13}C NMR (125 MHz, D_2O-d_2) δ = 136.1, 121.8, 67.5, 55.6, 53.9.

2-Phenylbenzo[*d*]thiazole[5] (d1)

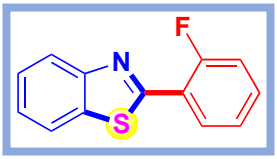


White solid, m.p = 110-111 °C

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.11 – 8.08 (m, 3H), 7.91 (d, J = 8.0 Hz, 1H), 7.51 – 7.48 (m, 4H), 7.39 (t, J = 7.6 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 168.1, 154.2, 135.1, 133.7, 131.0, 129.0, 127.6, 126.3, 125.2, 123.3, 121.6.

2-(2-Fluorophenyl)benzo[*d*]thiazole[6] (d2)

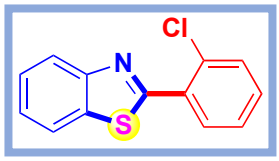


White solid, m.p = 90-91°C

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.37 (td, J = 7.7, 1.7 Hz, 1H), 8.07 (d, J = 8.2 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.47 (t, J = 7.7 Hz, 1H), 7.44 – 7.39 (m, 1H), 7.36 (t, J = 7.6 Hz, 1H), 7.26 (t, J = 7.4 Hz, 1H), 7.20 – 7.16 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 161.6, 161.1, 159.6, 152.6, 135.8, 132.2, 132.1, 129.8, 129.8, 126.3, 125.3, 124.7 (d, J = 3.4 Hz), 1H, 123.3, 121.5, 116.5, 116.3.

2-(2-Chlorophenyl)benzo[*d*]thiazole[6] (d3)

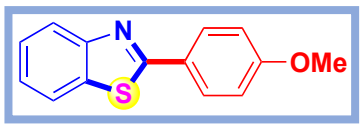


White solid, m.p = 98-99 °C

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.24 – 8.20 (m, 1H), 8.14 (d, *J* = 8.2 Hz, 1H), 7.95 (d, *J* = 8.4 Hz, 1H), 7.55 – 7.51 (m, 2H), 7.45 – 7.40 (m, 3H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 164.2, 152.4, 136.1, 132.8, 132.2, 131.8, 131.2, 130.8, 127.1, 126.3, 125.5, 123.5, 121.4.

2-(4-Methoxyphenyl)benzo[*d*]thiazole[7] (d4)

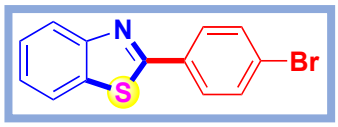


Brown solid, m.p = 123-124 °C

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.05 – 8.02 (m, 3H), 7.88 (d, *J* = 7.9 Hz, 1H), 7.47 (ddd, *J* = 8.3, 7.3, 1.2 Hz, 1H), 7.37 – 7.33 (m, 1H), 7.02 – 6.99 (m, 2H), 3.89 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 167.9, 162.0, 154.2, 134.9, 129.1, 126.4, 126.2, 124.8, 122.8, 121.5, 114.4, 55.5.

2-(4-Bromophenyl)benzo[*d*]thiazole[6] (d5)

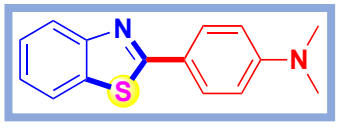


Orange solid, m.p = 131-132 °C

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.07 (d, *J* = 8.2 Hz, 1H), 7.97 (d, *J* = 8.5 Hz, 2H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.63 (d, *J* = 8.5 Hz, 2H), 7.50 (t, *J* = 8.1 Hz, 1H), 7.40 (t, *J* = 7.6 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 166.7, 154.1, 145.1, 135.1, 132.6, 132.2, 128.9, 126.5, 125.5, 123.3, 121.7.

4-(Benzo[*d*]thiazol-2-yl)-*N*,*N*-dimethylaniline[8] (d6)

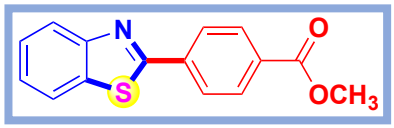


Yellow solid, m.p = 171-172 °C

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 7.97 (t, *J* = 9.3 Hz, 3H), 7.84 (d, *J* = 7.9 Hz, 1H), 7.43 (t, *J* = 7.7 Hz, 1H), 7.30 (t, *J* = 7.6 Hz, 1H), 6.75 (d, *J* = 9.0 Hz, 2H), 3.06 (s, 6H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 168.8, 154.3, 152.2, 134.5, 128.9, 126.0, 124.2, 122.3, 121.3, 111.7, 40.2.

Methyl 4-(benzo[d]thiazol-2-yl)benzoate[9] (d7)

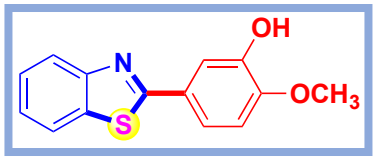


White solid, m.p = 210-211 °C

^{1}H NMR (500 MHz, $CDCl_3$-d) δ = 8.16 (s, 4H), 8.10 (dt, *J* = 8.2, 0.9 Hz, 1H), 7.92 (dt, *J* = 8.0, 0.9 Hz, 1H), 7.52 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H), 7.42 (ddd, *J* = 8.2, 7.1, 1.2 Hz, 1H), 3.96 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 166.7, 166.4, 153.9, 137.3, 135.2, 132.1, 130.3, 127.5, 126.7, 125.8, 123.6, 121.7, 52.3.

4-(Benzo[*d*]thiazol-2-yl)-2-methoxyphenol[9] (d8)

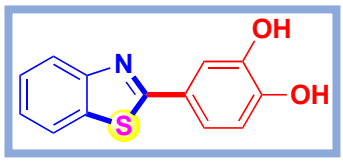


White solid, m.p = 168-169 °C

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.03 (d, *J* = 8.2 Hz, 1H), 7.87 (d, *J* = 7.9 Hz, 1H), 7.72 (s, 1H), 7.54 (s, 1H), 7.50 – 7.43 (m, 1H), 7.35 (d, *J* = 15.8 Hz, 1H), 7.01 (d, *J* = 8.2 Hz, 1H), 6.10 (s, 1H), 4.01 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 168.1, 154.1, 148.6, 147.0, 134.9, 126.2, 124.8, 122.8, 122.0, 121.5, 114.8, 109.4, 56.2.

4-(Benzo[*d*]thiazol-2-yl)benzene-1,2-diol[10] (d9)

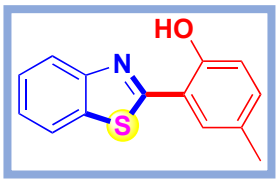


White solid, m.p = 153-154 °C

^{1}H NMR (500 MHz, $(CD_3)_2CO$-d_6) δ = 8.45 (s, 2H), 8.00 (ddd, J = 8.0, 1.3, 0.7 Hz, 1H), 7.95 (dt, J = 8.2, 0.9 Hz, 1H), 7.66 (d, J = 2.2 Hz, 1H), 7.54 – 7.43 (m, 2H), 7.38 (ddd, J = 8.2, 7.2, 1.2 Hz, 1H), 6.97 (d, J = 8.3 Hz, 1H).

^{13}C NMR (125 MHz, $(CD_3)_2CO$-d_6) δ = 167.6, 154.4, 134.8, 126.2, 125.8, 124.8, 122.5, 121.7, 120.1, 115.7, 114.1.

2-(Benzo[*d*]thiazol-2-yl)-4-methylphenol[9] (d10)

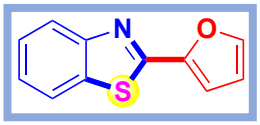


White solid, m.p = 127-128 ºC.

^{1}H NMR (500 MHz, $CDCl_3$-d) δ = 12.30 (s, 1H), 7.95 (d, J = 8.1 Hz, 1H), 7.86 (d, J = 10.3 Hz, 1H), 7.47 (dd, J = 17.4, 9.3 Hz, 2H), 7.38 (q, J = 5.8 Hz, 1H), 7.17 (d, J = 8.0 Hz, 1H), 7.01 (d, J = 9.0 Hz, 1H), 2.34 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$-d) δ = 169.4, 155.9, 151.9, 133.7, 132.6, 128.7, 128.3, 126.6, 125.4, 122.1, 121.5, 117.7, 116.4, 29.8, 20.5.

2-(Furan-2-yl)benzo[*d*]thiazole[11] (d11)

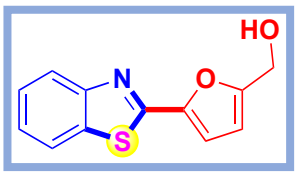


Pink solid, m.p = 101-102 ºC

^{1}H NMR (500 MHz, $CDCl_3$-d) δ = 8.05 (d, J = 8.2 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.60 (s, 1H), 7.49 (t, J = 7.7 Hz, 1H), 7.38 (t, J = 7.6 Hz, 1H), 7.19 (d, J = 3.6 Hz, 1H), 6.60 (dd, J = 3.2, 1.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$-d) δ = 157.6, 153.8, 148.8, 144.7, 134.3, 126.5, 125.2, 123.1, 121.6, 112.5, 111.4.

(5-(benzo*[d]*thiazol-2-yl)furan-2-yl)methanol (d12)

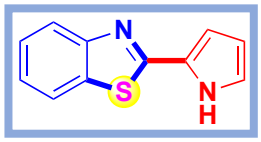


Yellow solid, m.p = 113-115 ºC

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.08 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.0 Hz, 1H), 7.52 – 7.49 (m, 1H), 7.41 – 7.38 (m, 1H), 7.24 (d, *J* = 3.5 Hz, 1H), 6.50 (d, *J* = 3.5 Hz, 1H), 4.74 (s, 2H), 2.81 (s, 1H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 157.7, 157.5, 152.7, 147.9, 133.8, 127.0, 125.6, 122.9, 121.8, 113.7, 110.7, 57.6.

2-(1*H*-Pyrrol-2-yl)benzo[*d*]thiazole[12] (d13)

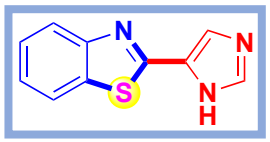


White solid, m.p = 155–156 °C

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 10.10 (s, 1H), 7.89 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 7.9 Hz, 1H), 7.45 – 7.41 (m, 1H), 7.34 – 7.30 (m, 1H), 6.97 (td, *J* = 2.6, 1.4 Hz, 1H), 6.86 (ddd, *J* = 3.7, 2.5, 1.4 Hz, 1H), 6.34 – 6.31 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 160.3, 153.5, 134.0, 126.4, 126.2, 124.5, 122.0, 121.9, 121.5, 112.4, 110.7.

2-(1*H*-Imidazol-5-yl)benzo[*d*]thiazole[12] (d14)

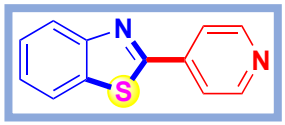


White solid

^{1}H NMR (500 MHz, $(CD_3)_2CO$-d_6) δ = 8.02 (d, *J* = 6.3 Hz, 1H), 7.93 – 7.91 (m, 2H), 7.84 (s, 1H), 7.47 (ddd, *J* = 8.3, 7.2, 1.3 Hz, 1H), 7.37 (ddd, *J* = 8.3, 7.2, 1.2 Hz, 1H).

^{13}C NMR (125 MHz, $(CD_3)_2CO$-d_6) δ = 165.1, 155.4, 137.7, 137.1, 135.6, 127.0, 125.5, 123.2, 122.8, 117.5.

2-(Pyridin-4-yl)benzo[*d*]thiazole[13] (d15)

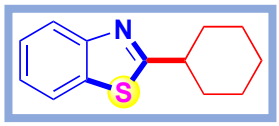


White solid, m.p = 125–126 °C

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.80 – 8.74 (m, 2H), 8.13 (d, *J* = 8.2 Hz, 1H), 7.98 – 7.88 (m, 3H), 7.57 – 7.53 (m, 1H), 7.49 – 7.43 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 166.1, 165.3, 154.2, 150.9, 140.7, 135.4, 134.5, 129.63, 127.0, 126.3, 124.1, 122.0, 121.4.

2-Cyclohexylbenzo[*d*]thiazole[13] (d16)

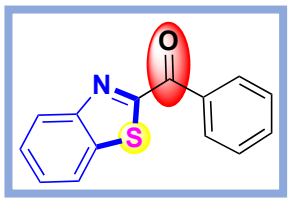


Light yellow oil

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.01 – 7.94 (m, 1H), 7.84 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.44 (ddd, *J* = 8.3, 7.1, 1.2 Hz, 1H), 7.37 – 7.31 (m, 1H), 3.23 – 3.01 (m, 1H), 2.34 – 2.18 (m, 2H), 1.98 – 1.88 (m, 2H), 1.80 – 1.73 (m, 1H), 1.66 – 1.59 (m, 2H), 1.51 – 1.43 (m, 2H), 1.32 (dt, *J* = 12.5, 3.5 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 177.9, 125.9, 125.9, 124.6, 124.6, 122.5, 121.6, 43.4, 33.4, 29.7, 26.0, 25.8.

Benzo[*d*]thiazol-2-yl(phenyl)methanone[14] (f1)

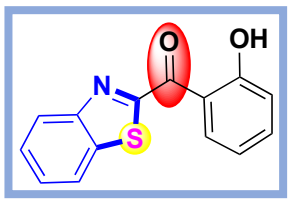


Yellow solid, M.p = 102-103 ^{o}C

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.56 (d, *J* = 9.2 Hz, 2H), 8.25 (d, *J* = 8.6 Hz, 1H), 8.02 (d, *J* = 7.6 Hz, 1H), 7.70 – 7.65 (m, 1H), 7.61 – 7.54 (m, 4H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 185.4, 167.2, 153.9, 137.1, 135.0, 133.9, 131.3, 128.5, 127.6, 126.9, 125.8, 122.2.

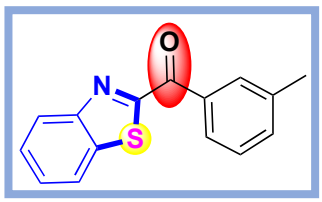
Benzo[*d*]thiazol-2-yl(2-hydroxyphenyl)methanone[14] (f2)



White solid

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 11.53 (s, 1H), 8.26 (dd, *J* = 8.0, 1.5 Hz, 1H), 8.21 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.52 – 7.43 (m, 2H), 7.34 (d, *J* = 7.6 Hz, 1H), 7.20 – 7.15 (m, 1H), 7.07 – 7.06 (m, 1H), 6.94 (t, *J* = 7.7 Hz, 1H).

Benzo[*d*]thiazol-2-yl(3-methylphenyl)methanone[14] (f3)

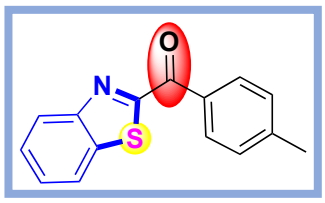


White solid

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.49 – 8.47 (d, J = 8.5 Hz, 2H), 8.25 – 8.23 (d, J = 8.5 Hz, 1H), 8.02 – 8.01 (d, J = 8.0 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.37 – 7.36 (d, J = 8.0 Hz, 2H), 2.47 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ = 185.7, 167.3, 153.9, 138.3, 137.0, 135.0, 134.7, 131.5, 128.7, 128.4, 127.6, 126.9, 125.8, 122.2, 21.4.

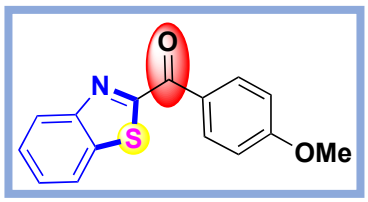
Benzo[*d*]thiazol-2-yl(4-methylphenyl)methanone[14] (f4)



White solid, m.p = 110-111 °C.

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.48 (d, *J* = 8.5 Hz, 2H), 8.24 (d, *J* = 8.5 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.52 (m, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 2.27 (s, 3H).

Benzo[*d*]thiazol-2-yl(4-methoxyphenyl)methanone[14] (f5)



White solid, m.p = 116-117 °C.

^{1}H NMR (500 MHz, $CDCl_3$-*d*) δ = 8.65 (d, *J* = 8.9 Hz, 2H), 8.23 (d, *J* = 8.1 Hz, 1H), 8.01 (d, *J* = 7.9 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 1H), 7.04 (d, *J* = 8.9 Hz, 2H), 3.92 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$-*d*) δ =164.44, 133.87, 127.37, 126.79, 125.55, 122.13, 113.91, 55.57.

Section S4. ^{1}H, ^{13}C NMR spectroscopy

[CholineCl][Imidazole]$_2$

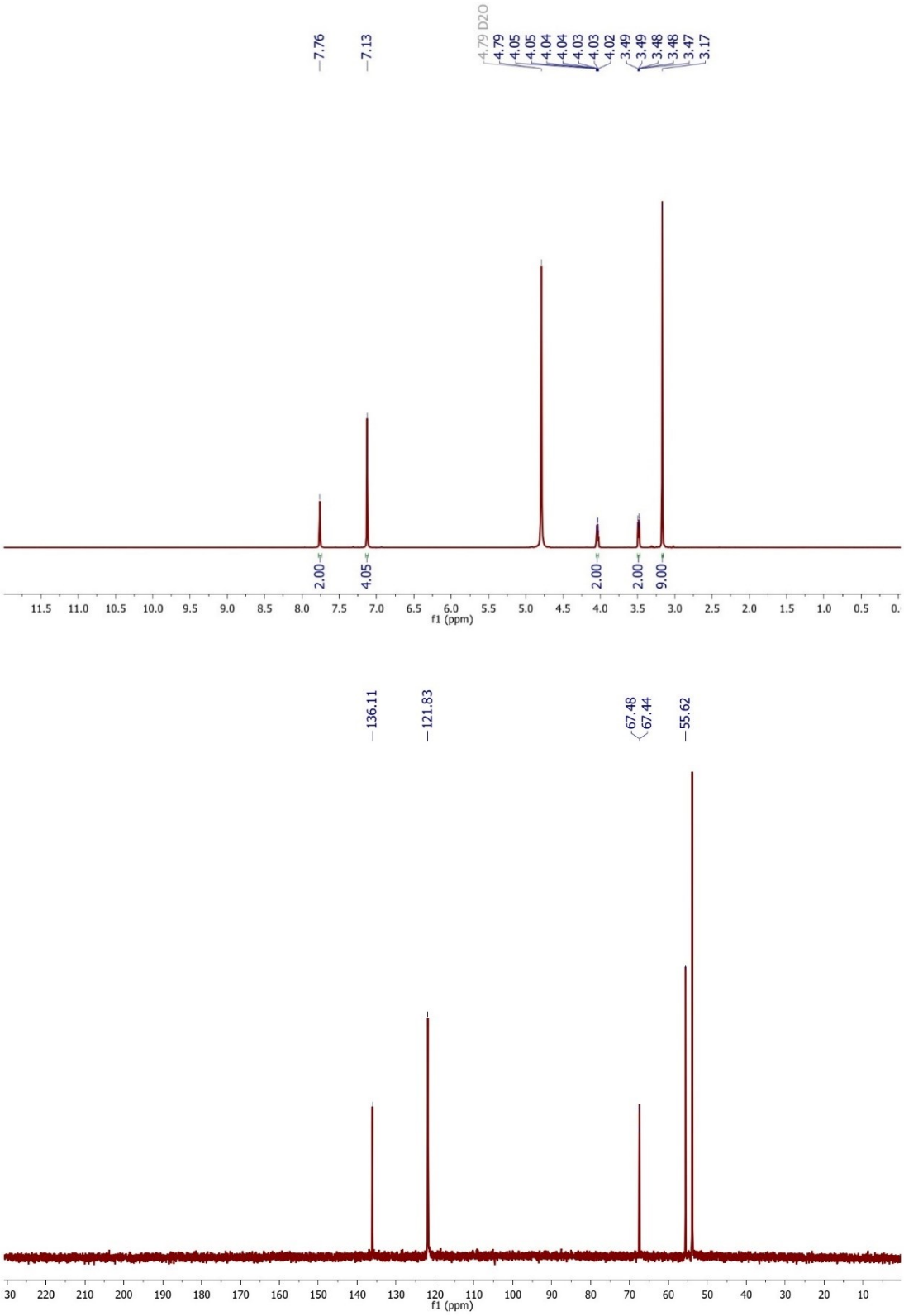


Figure S2. ^{1}H and ^{13}C NMR spectra of DES [CholineCl][Imidazole]$_2$

2-Phenylbenzo[*d*]thiazole (d1)

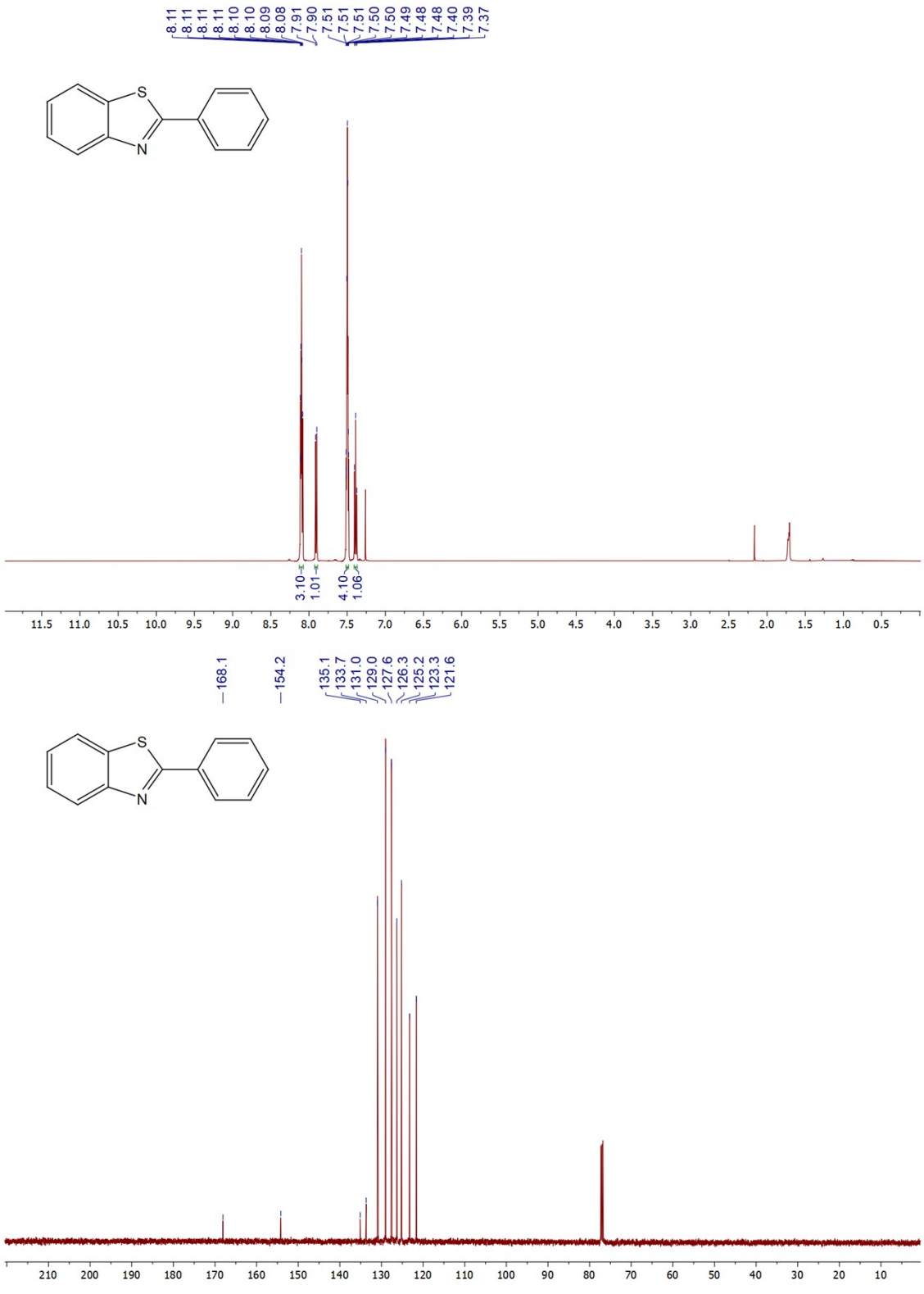


Figure S3. ^{1}H and ^{13}C NMR spectra of 2-phenylbenzo[*d*]thiazole (d1)

2-(2-Fluorophenyl)benzo[*d*]thiazole (d2)

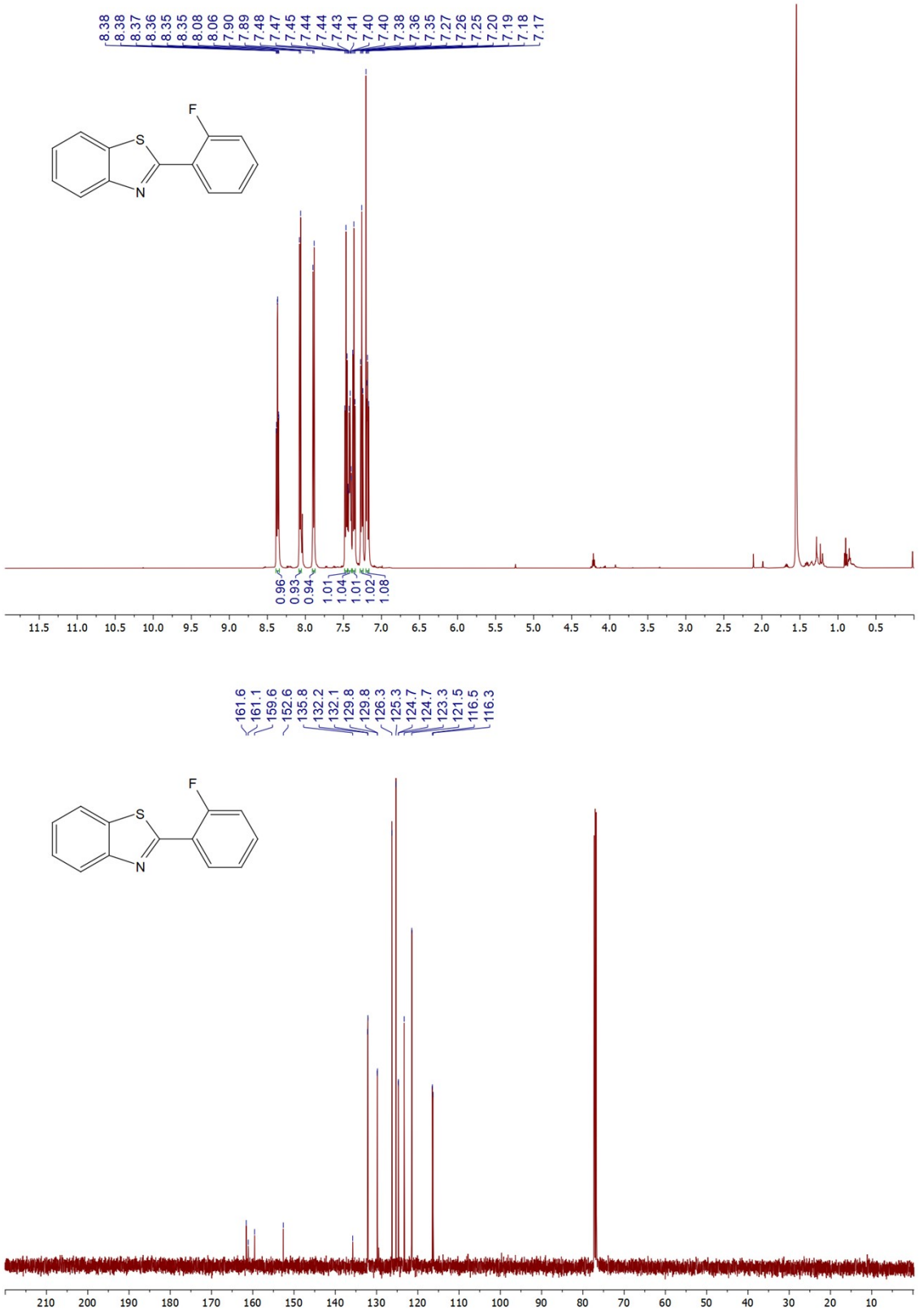


Figure S4. ^{1}H and ^{13}C NMR spectra of 2-(2-fluorophenyl)benzo[*d*]thiazole (d2)

2-(2-Chlorophenyl)benzo[*d*]thiazole (d3)

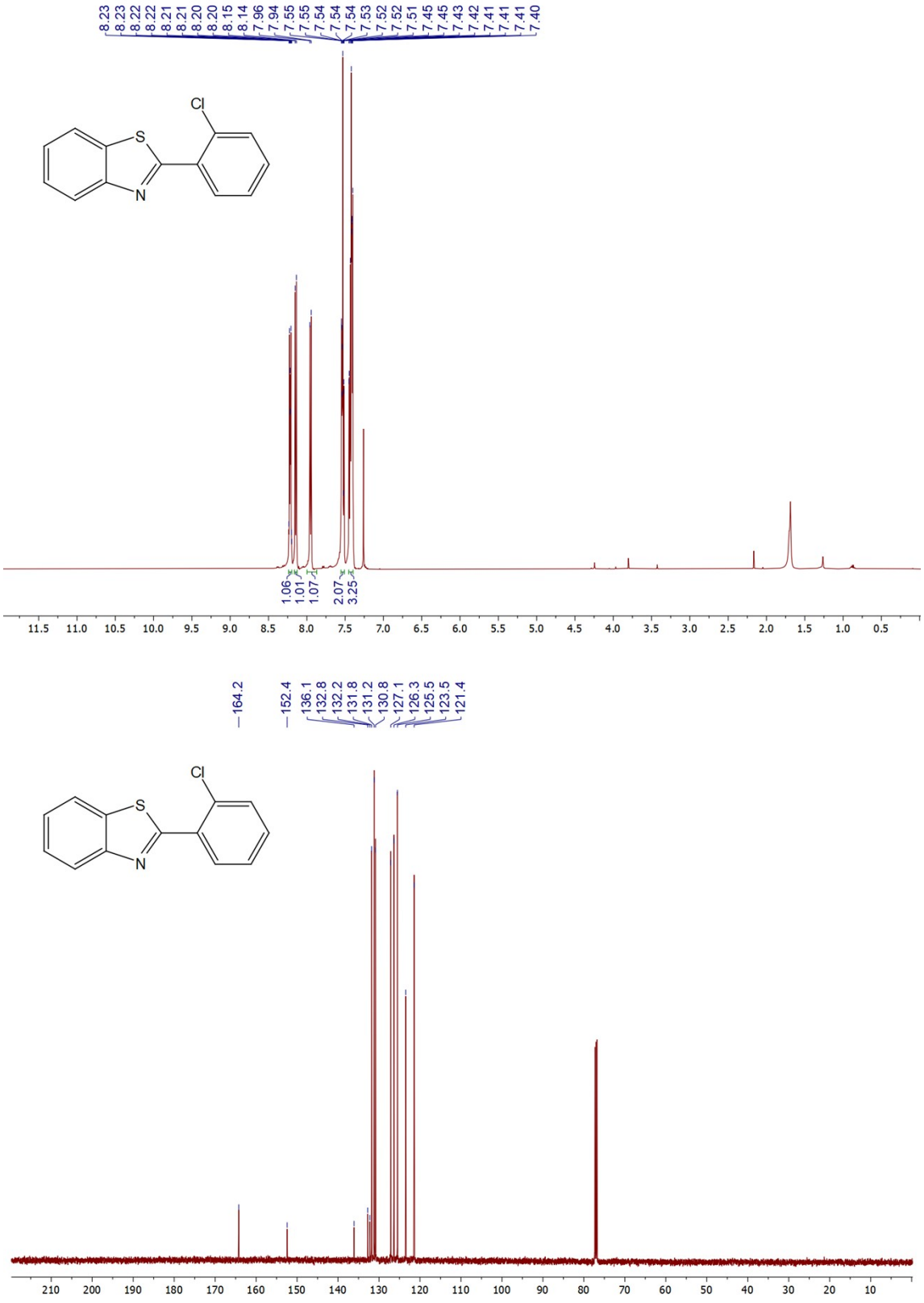


Figure S5. ^{1}H and ^{13}C NMR spectra of 2-(2-chlorophenyl)benzo[d]thiazole (d3)

2-(4-Methoxyphenyl)benzo[*d*]thiazole (d4)

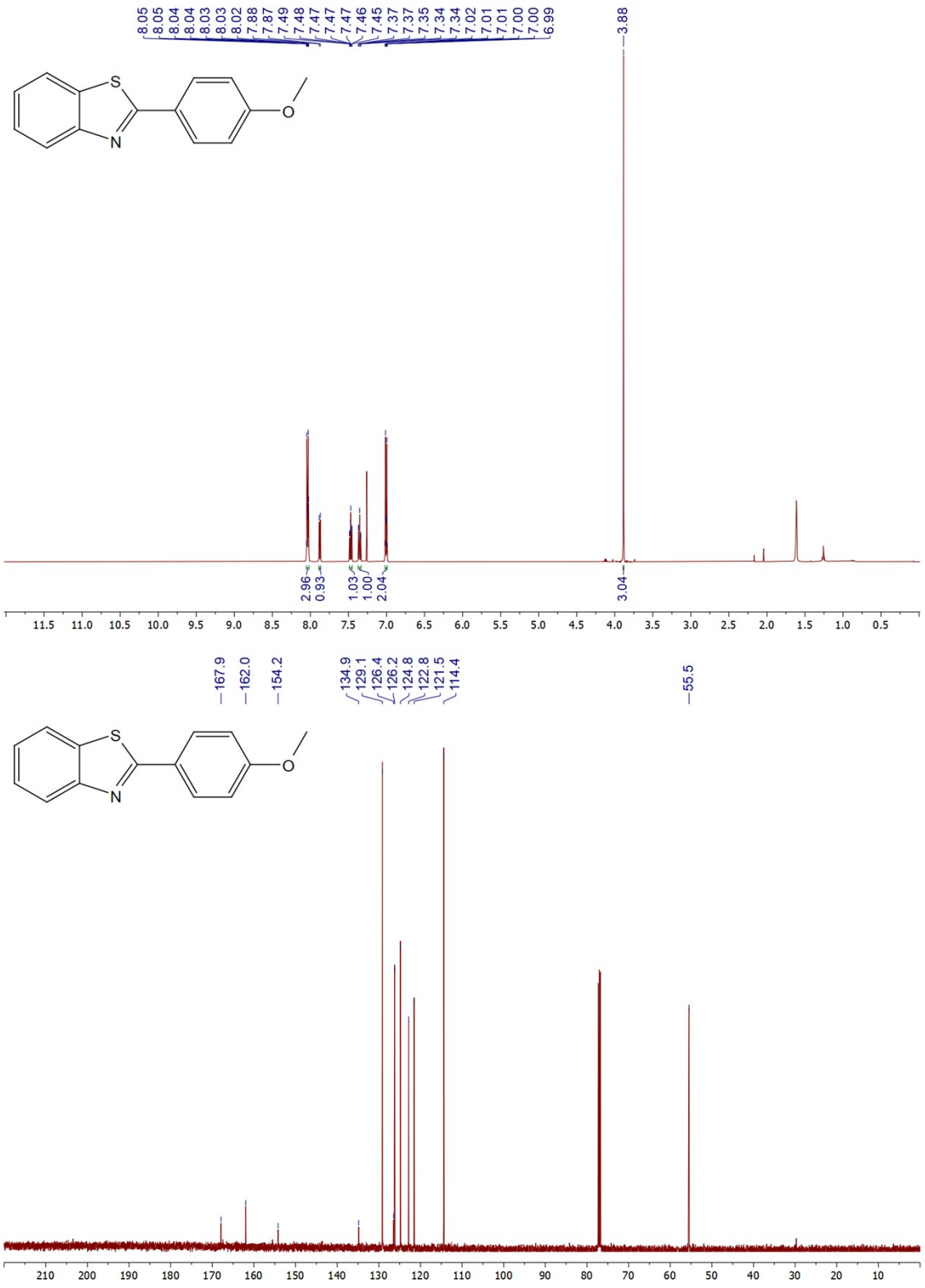


Figure S6. ^{1}H and ^{13}C NMR spectra of 2-(4-methoxyphenyl)benzo[*d*]thiazole (d4)

2-(4-Bromophenyl)benzo[*d*]thiazole (d5)

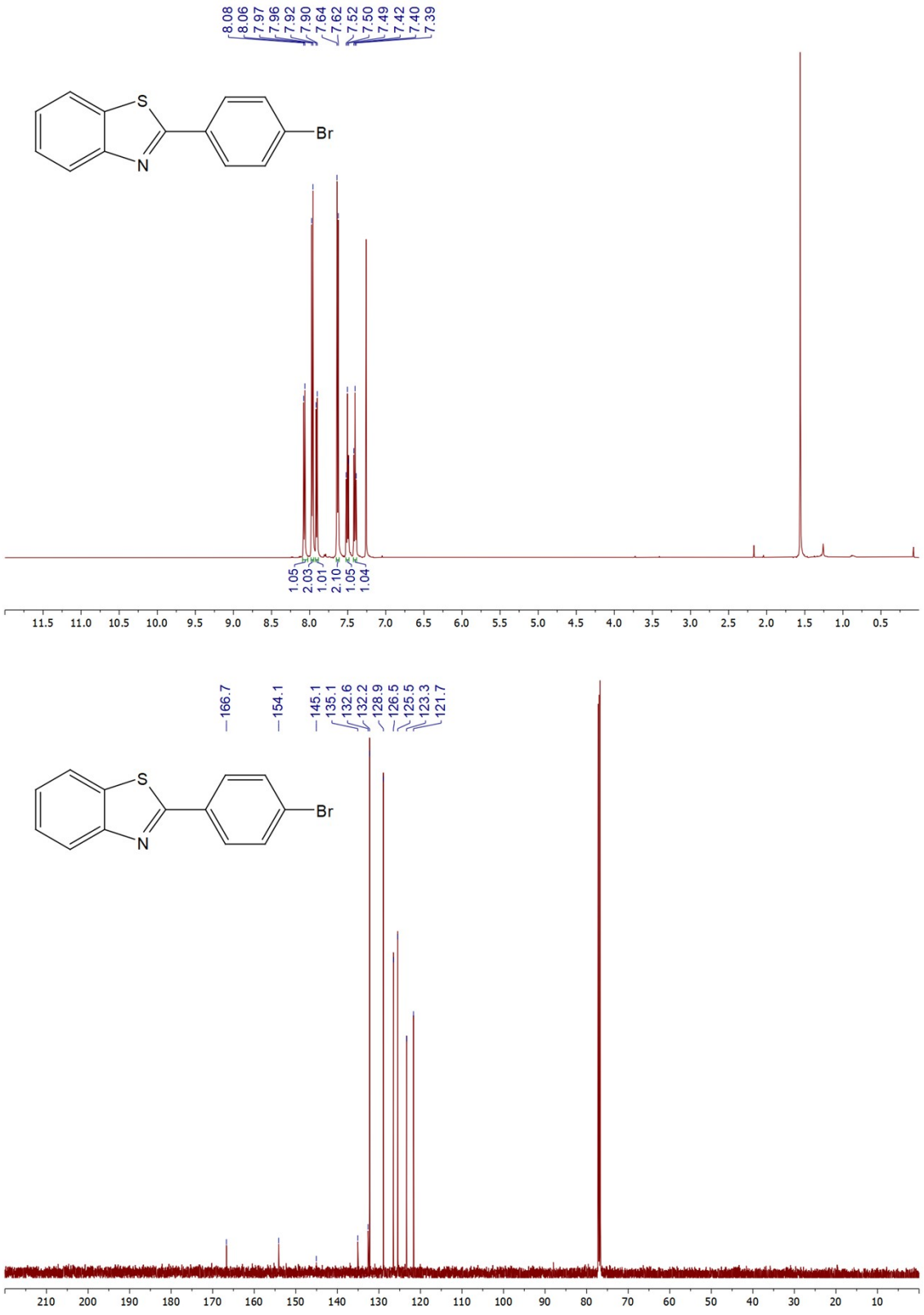


Figure S7. ^{1}H and ^{13}C NMR spectra of 2-(4-bromophenyl)benzo[*d*]thiazole (d5)

2-(Benzo[*d*]thiazol-2-yl)-*N,N*-dimethylaniline (d6)

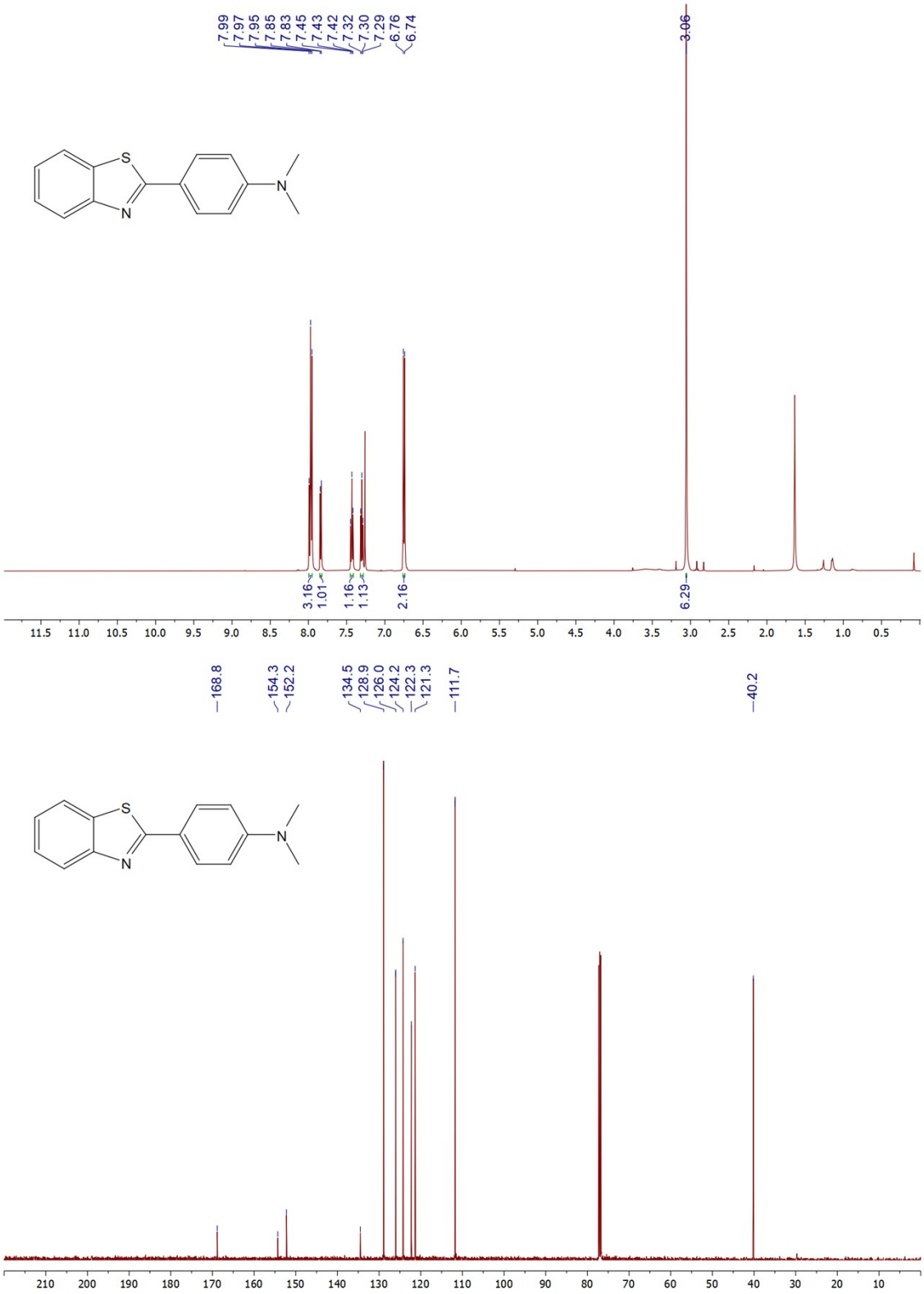


Figure S8. ^{1}H and ^{13}C NMR spectra of 2-(benzo[*d*]thiazol-2-yl)-*N,N*-dimethylaniline (d6)

Methyl 4-(benzo[*d*]thiazol-2-yl)benzoate (d7)

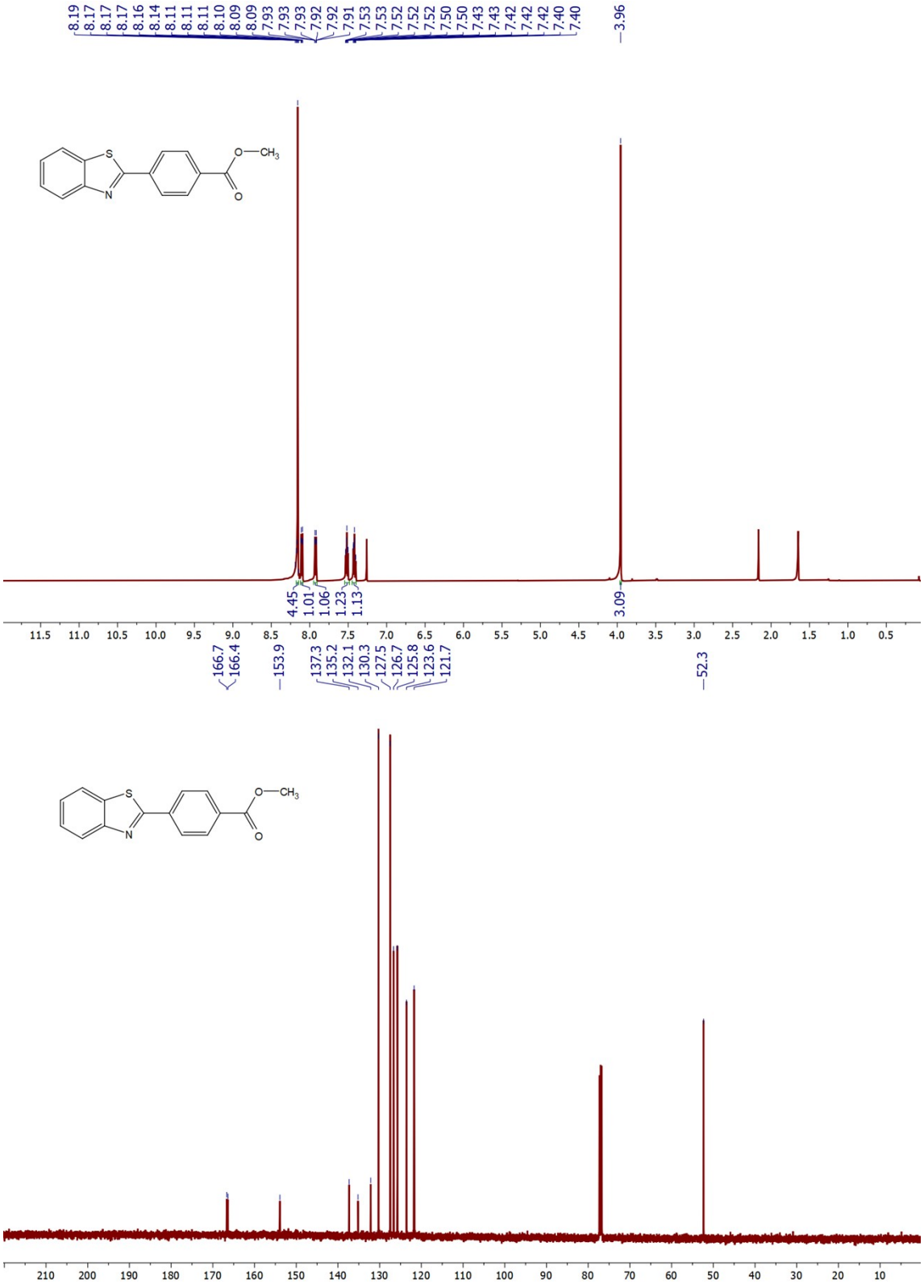


Figure S9. ^{1}H and ^{13}C NMR spectra of Methyl 4-(benzo[*d*]thiazol-2-yl)benzoate (d7)

4-(Benzo[*d*]thiazol-2-yl)-2-methoxyphenol (d8)

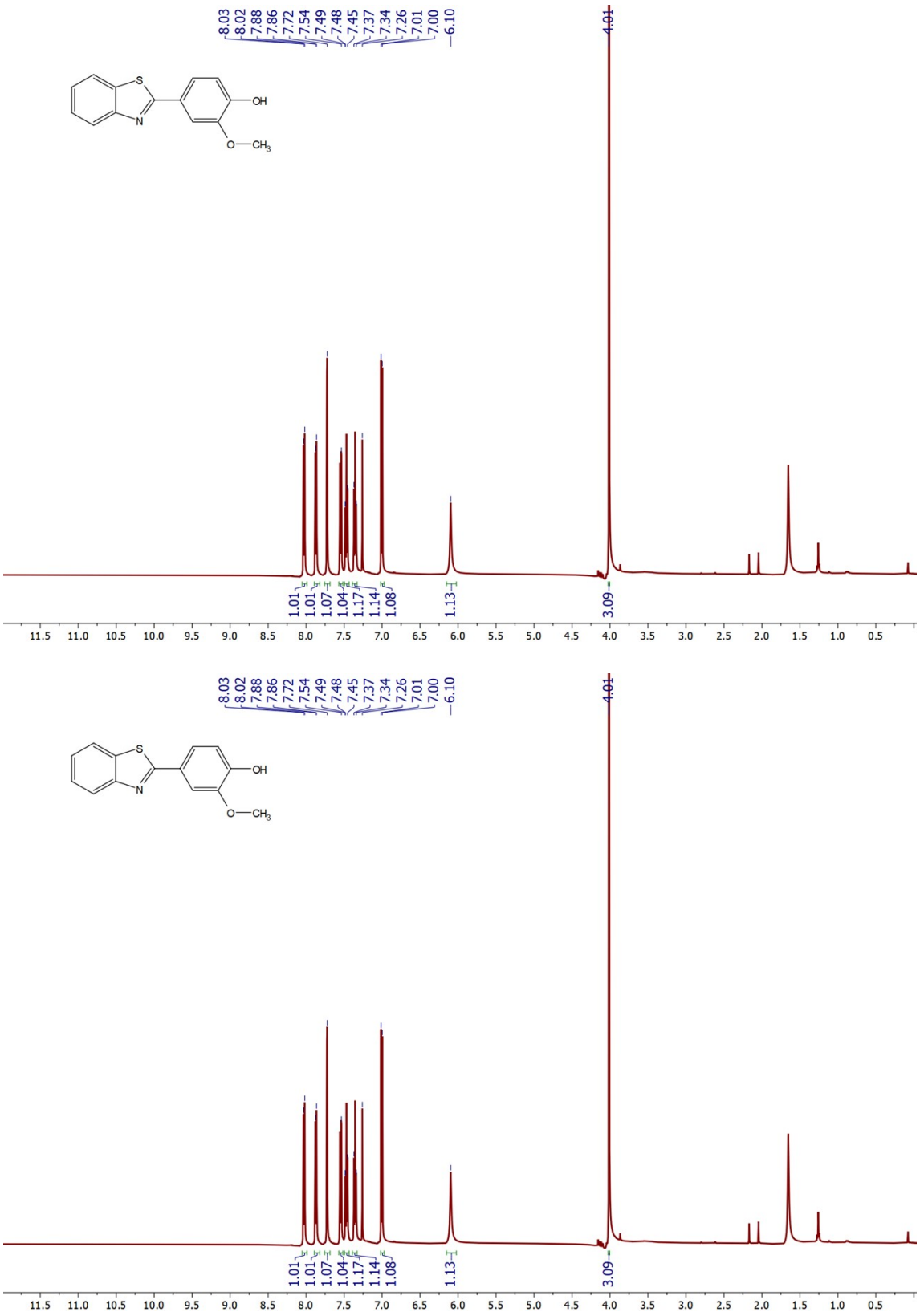


Figure S10. ^{1}H and ^{13}C NMR spectra of 4-(Benzo[*d*]thiazol-2-yl)-2-methoxyphenol (d8)

4-(Benzo[*d*]thiazol-2-yl)benzene-1,2-diol (d9)

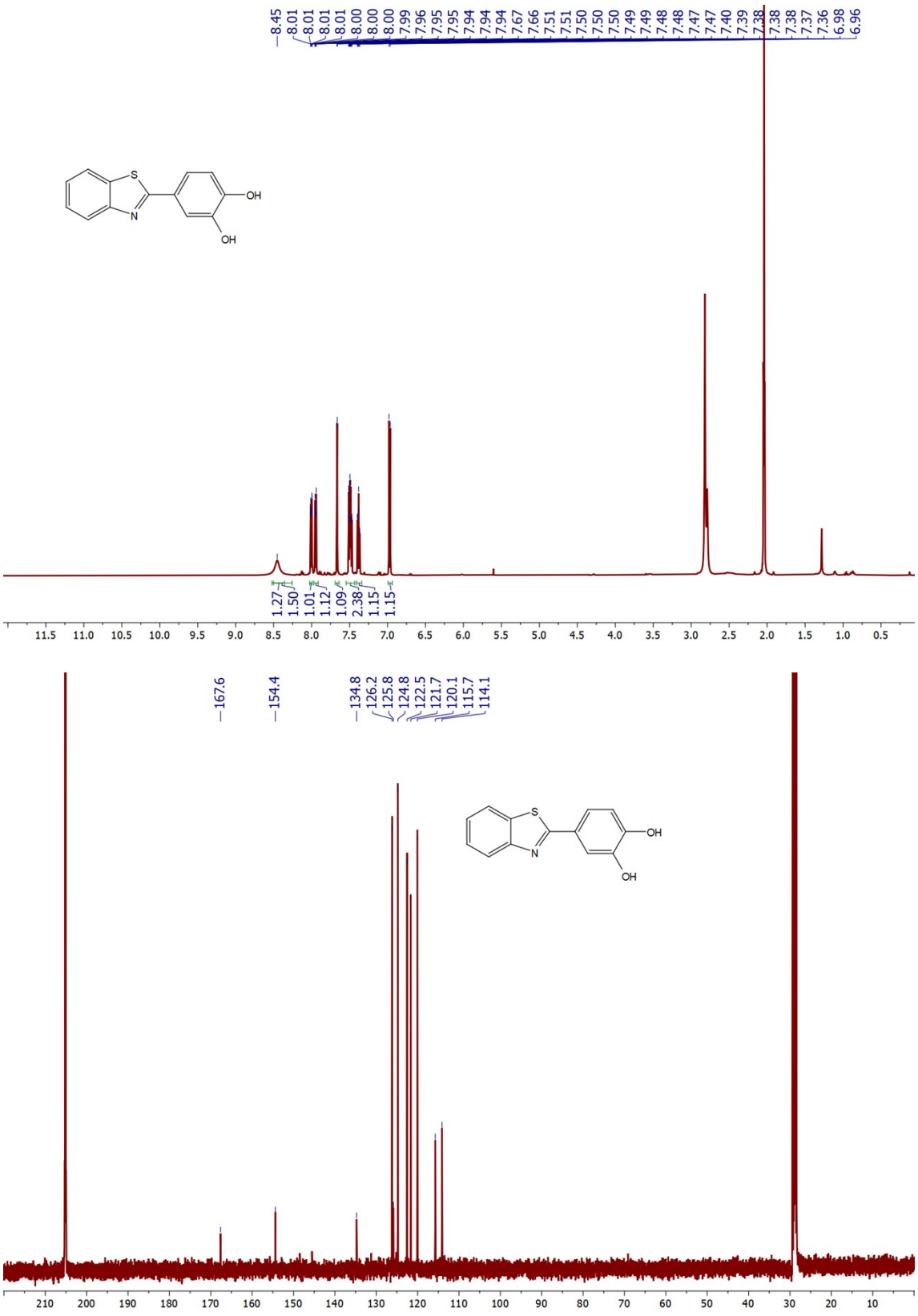


Figure S11. ^{1}H and ^{13}C NMR spectra of 4-(Benzo[*d*]thiazol-2-yl)benzene-1,2-diol (d9)

2-(Benzo[*d*]thiazol-2-yl)-4-methylphenol (d10)

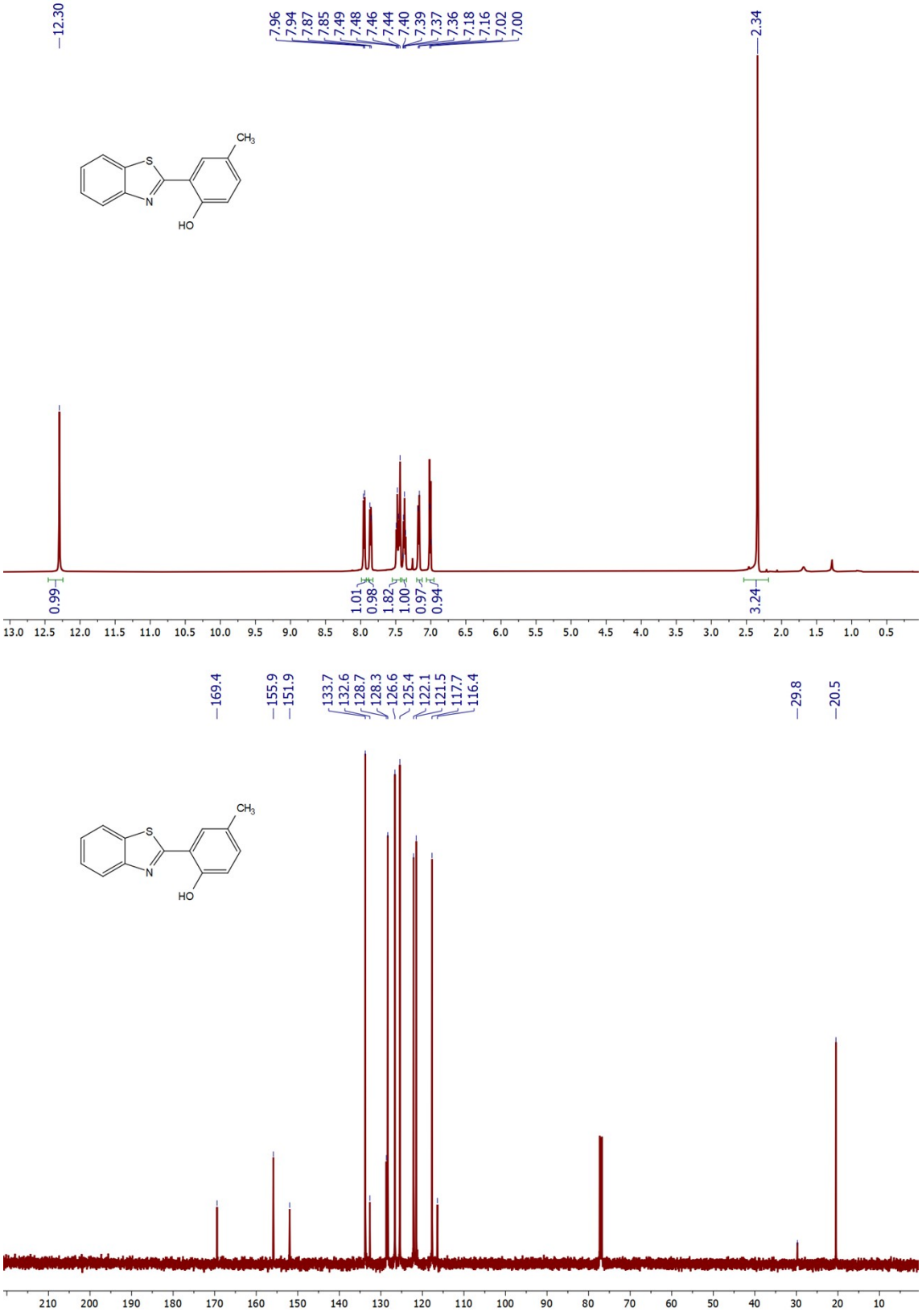


Figure S12. ^{1}H and ^{13}C NMR spectra of 2-(Benzo[*d*]thiazol-2-yl)-4-methylphenol (d10)

2-(Furan-2-yl)benzo[*d*]thiazole (d11)

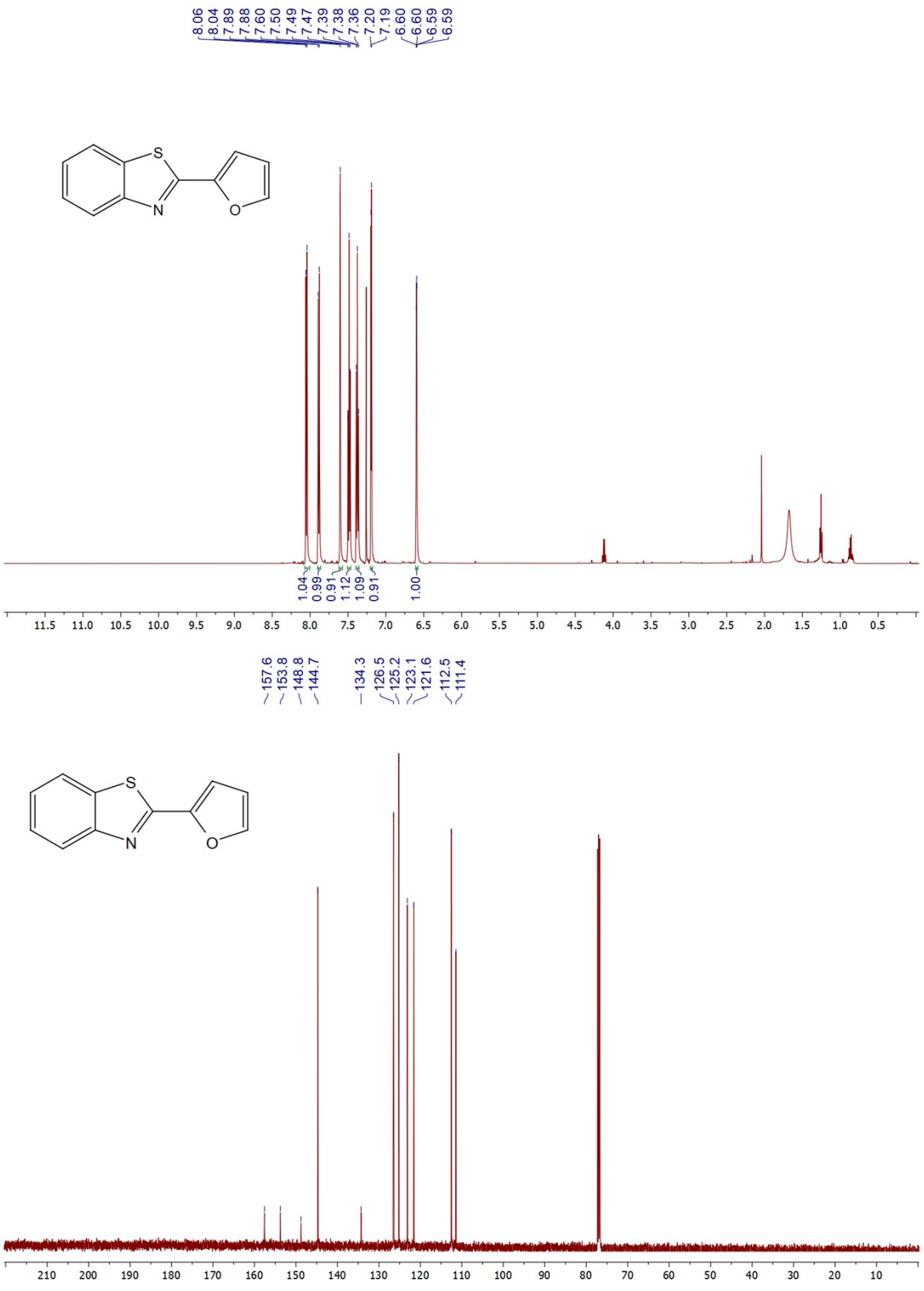


Figure S13. ^{1}H and ^{13}C NMR spectra of 2-(Furan-2-yl)benzo[*d*]thiazole (d11)

(5-(Benzo[*d*]thiazol-2-yl)furan-2-yl)methanol (d12)

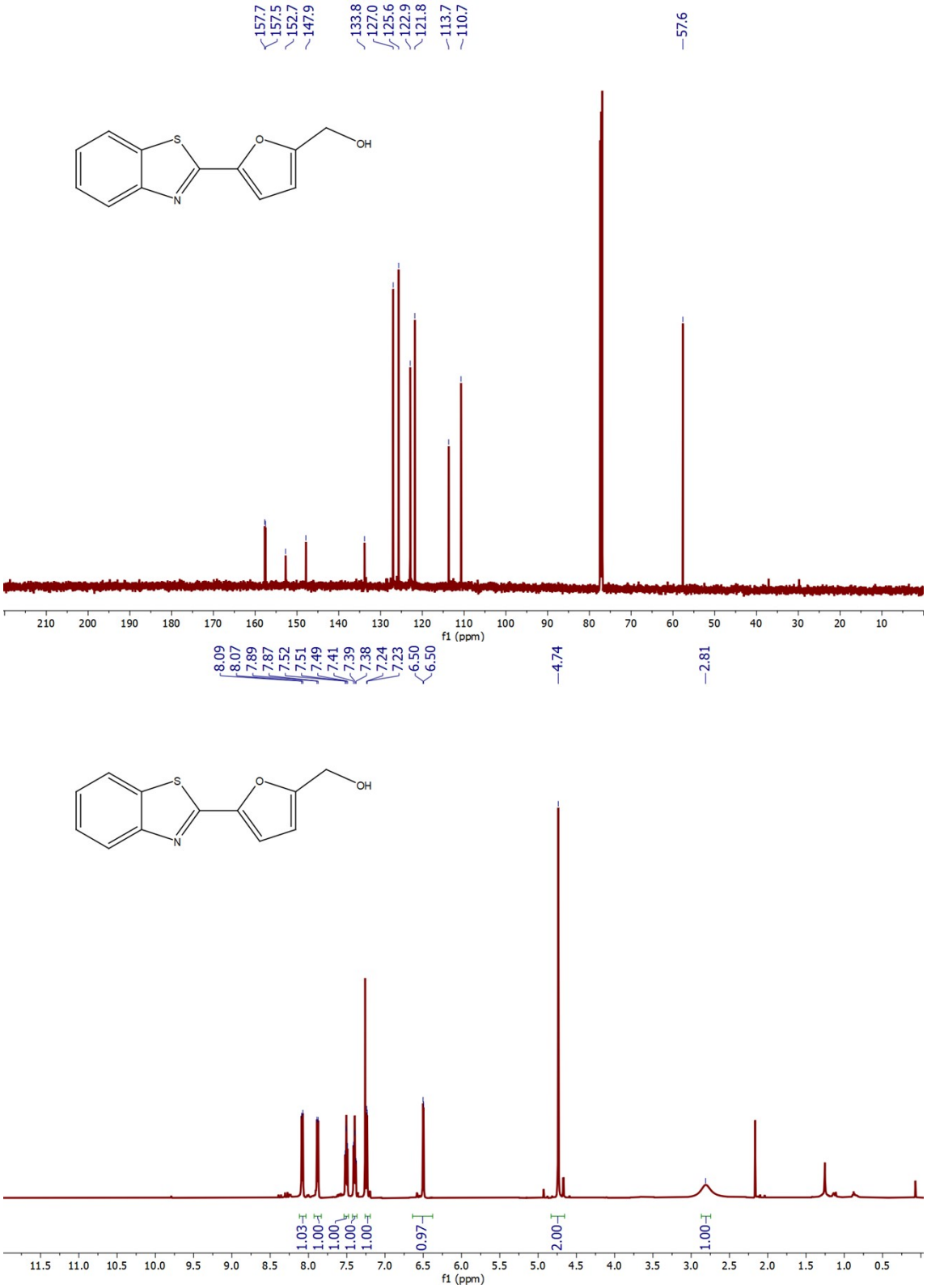


Figure S14. ^{1}H and ^{13}C NMR spectra of (5-(benzo[*d*]thiazol-2-yl)furan-2-yl)methanol (d12)

2-(1*H*-Pyrrol-2-yl)benzo[*d*]thiazole (d13)

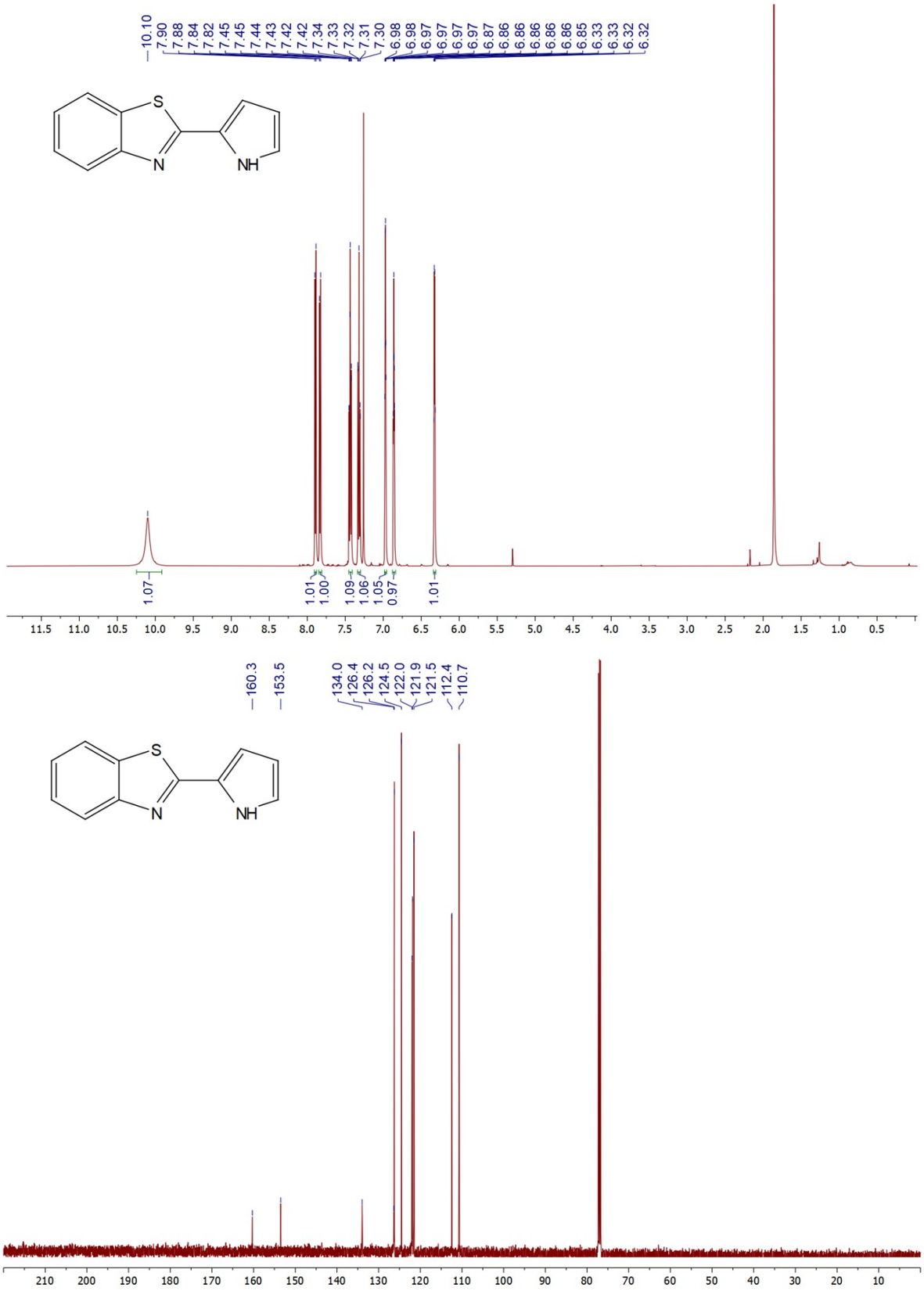


Figure S15. ^{1}H and ^{13}C NMR spectra of 2-(1*H*-Pyrrol-2-yl)benzo[*d*]thiazole (d13)

2-(1*H*-Imidazol-5-yl)benzo[*d*]thiazole (d14)

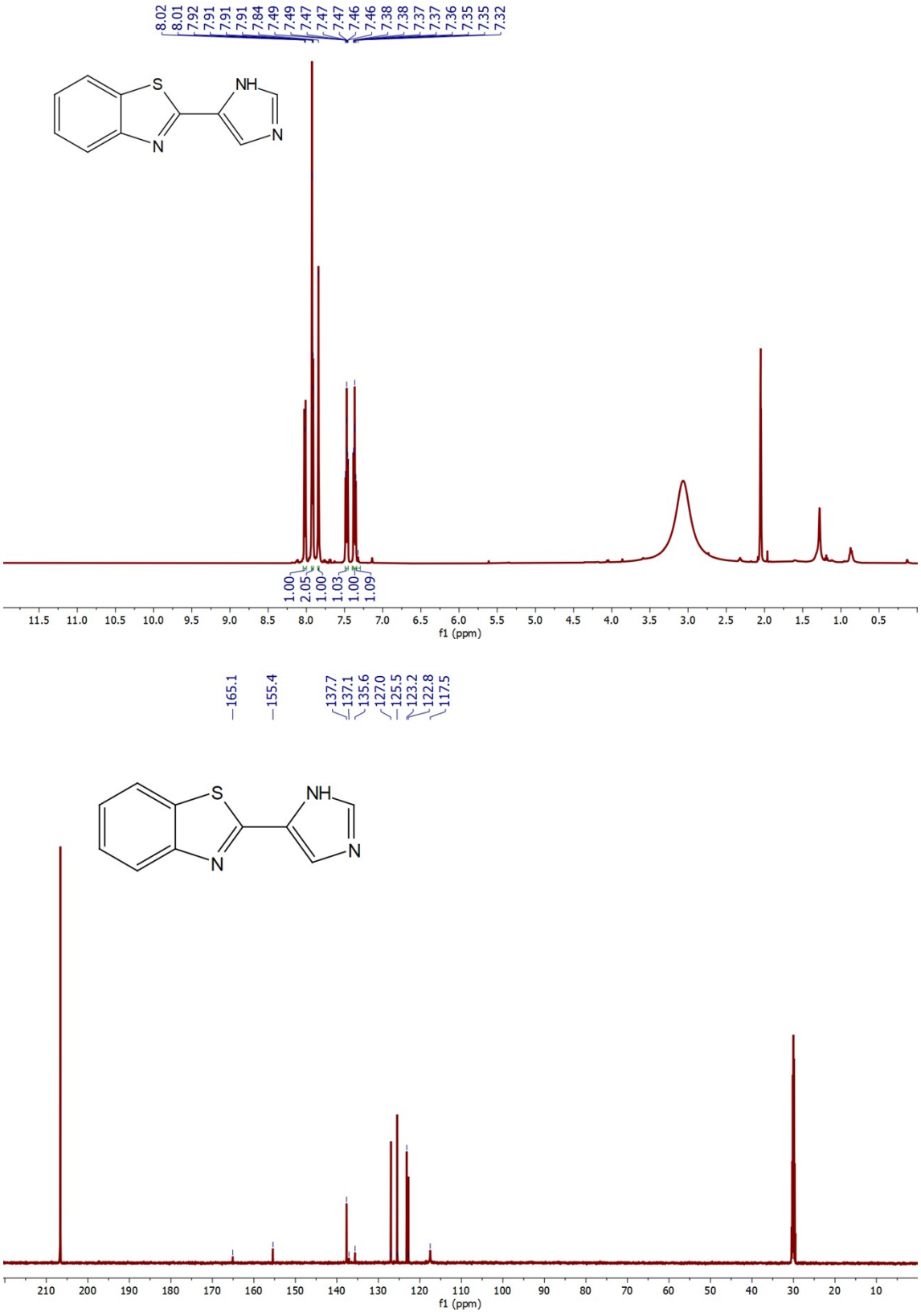


Figure S16. ^{1}H and ^{13}C NMR spectra of 2-(1*H*-Imidazol-5-yl)benzo[*d*]thiazole (d14)

2-(Pyridin-4-yl)benzo[*d*]thiazole (d15)

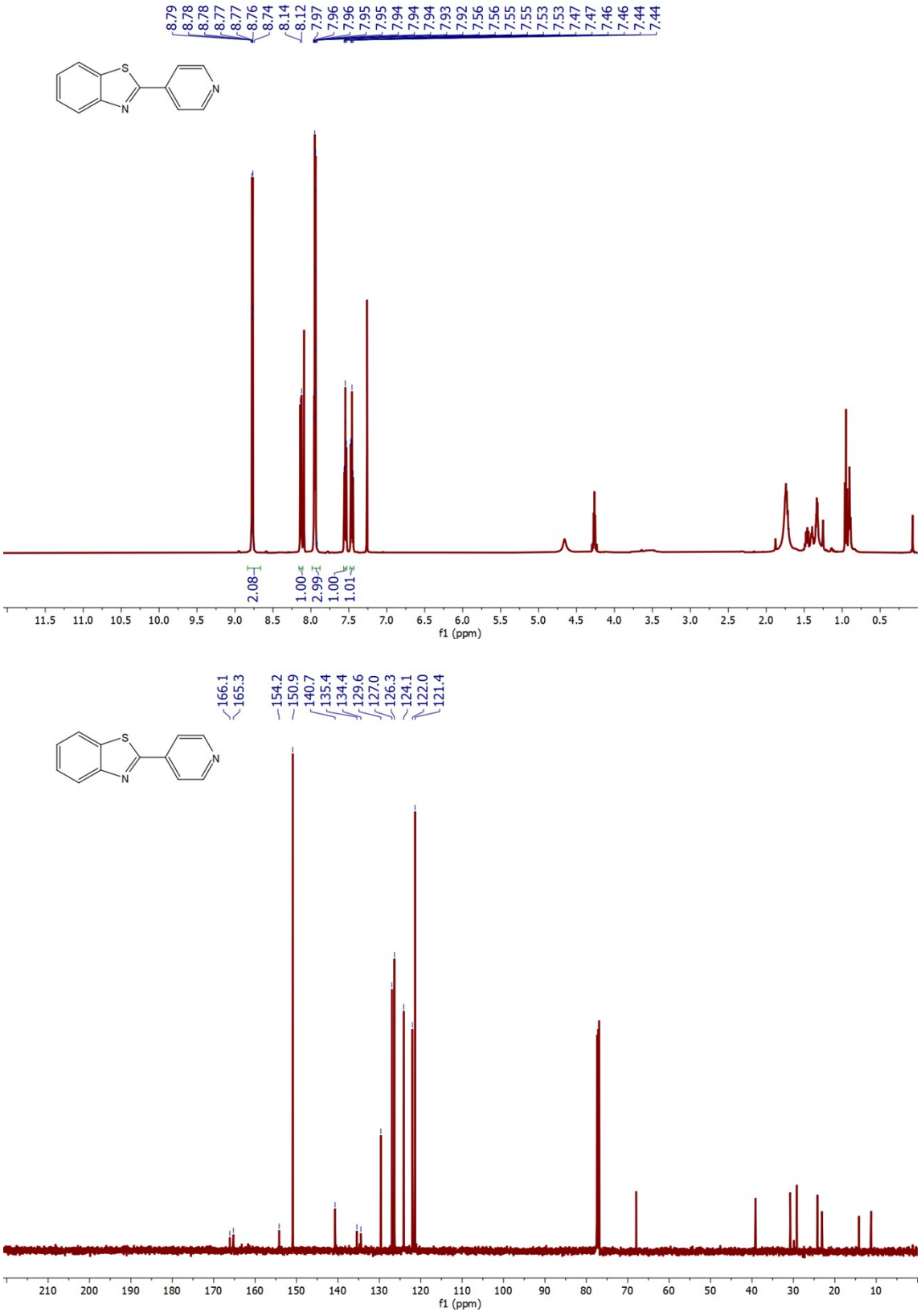


Figure S17. ^{1}H and ^{13}C NMR spectra of 2-(Pyridin-4-yl)benzo[*d*]thiazole (d15)

2-Cyclohexylbenzo[*d*]thiazole (d16)

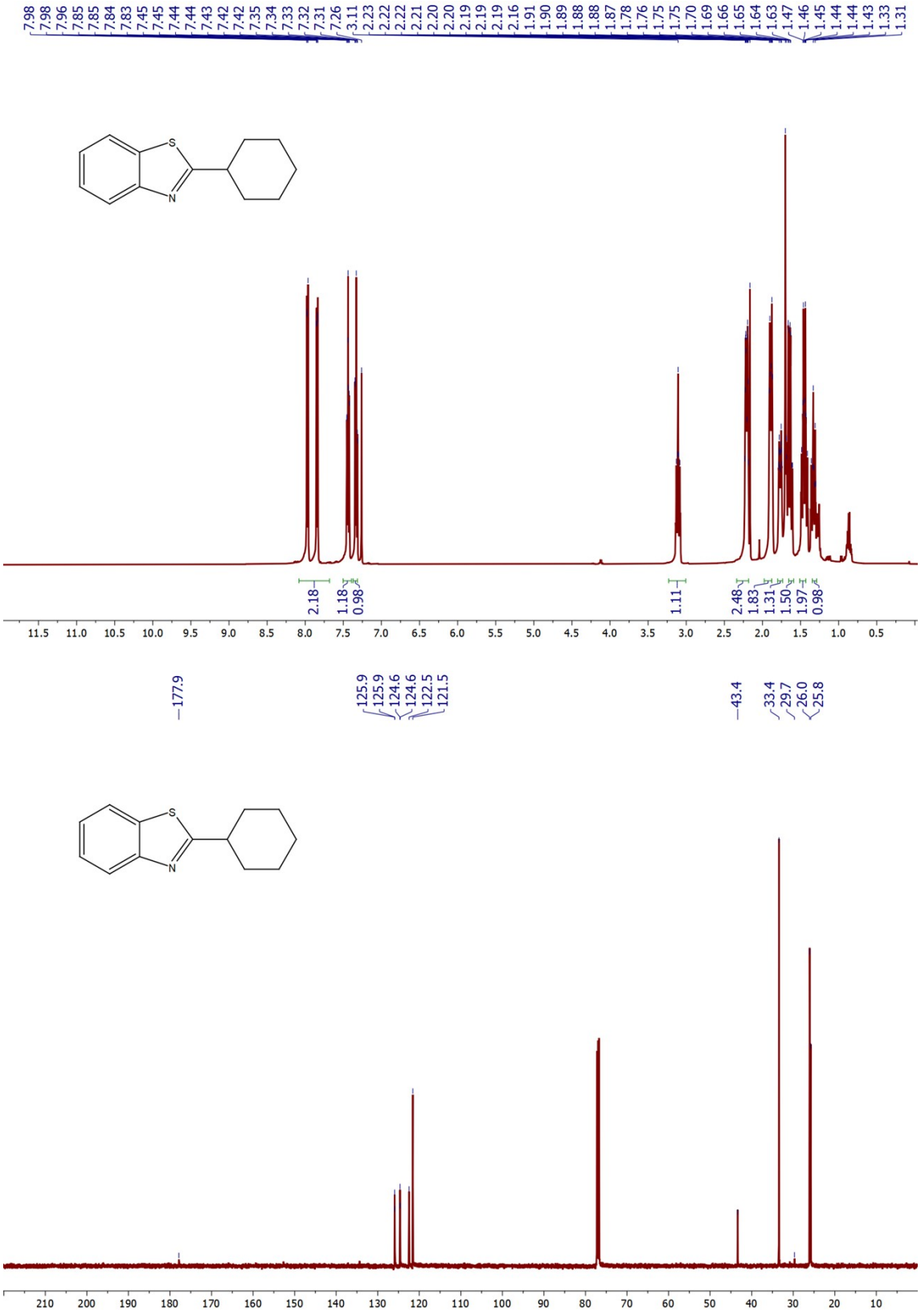


Figure S18. ^{1}H and ^{13}C NMR spectra of 2-Cyclohexylbenzo[*d*]thiazole (d16)

Benzo[*d*]thiazol-2-yl(phenyl)methanone (f1)

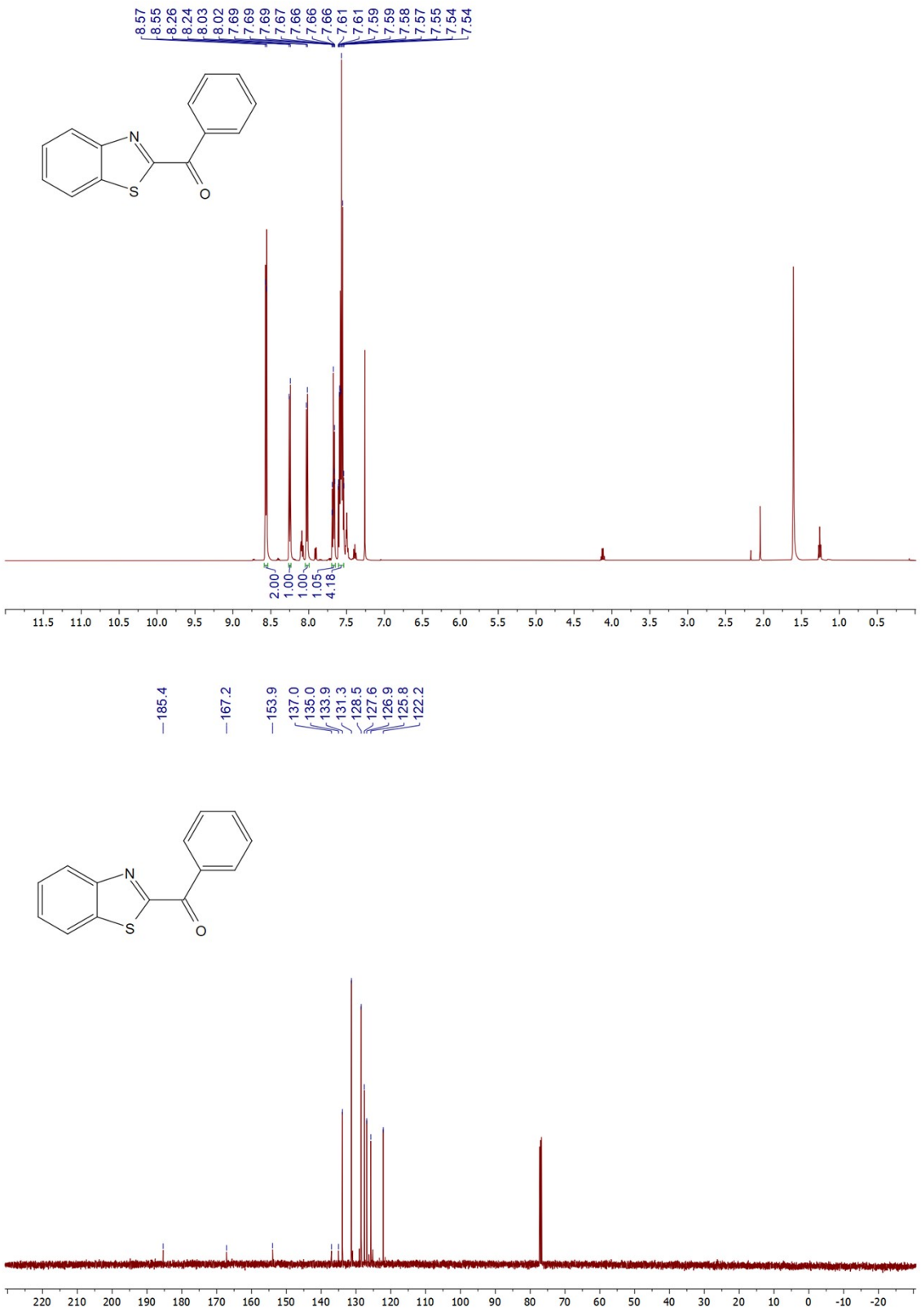


Figure S19. ^{1}H and ^{13}C NMR spectra of benzo[*d*]thiazol-2-yl(phenyl)methanone (f1)

Benzo[*d*]thiazol-2-yl(2-hydroxyphenyl)methanone (f2)

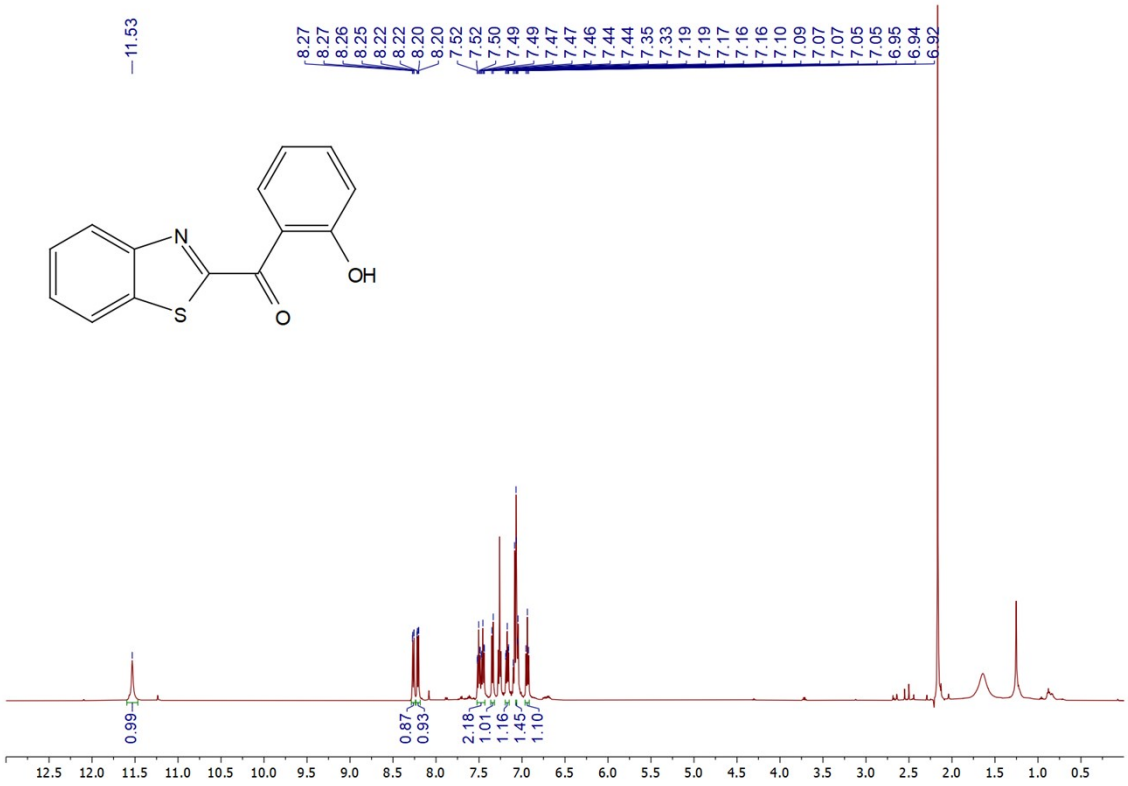


Figure S20. ^{1}H NMR spectra of benzo[*d*]thiazol-2-yl(2-hydroxyphenyl)methanone (f2)

Benzo[*d*]thiazol-2-yl(3-methylphenyl)methanone (f3)

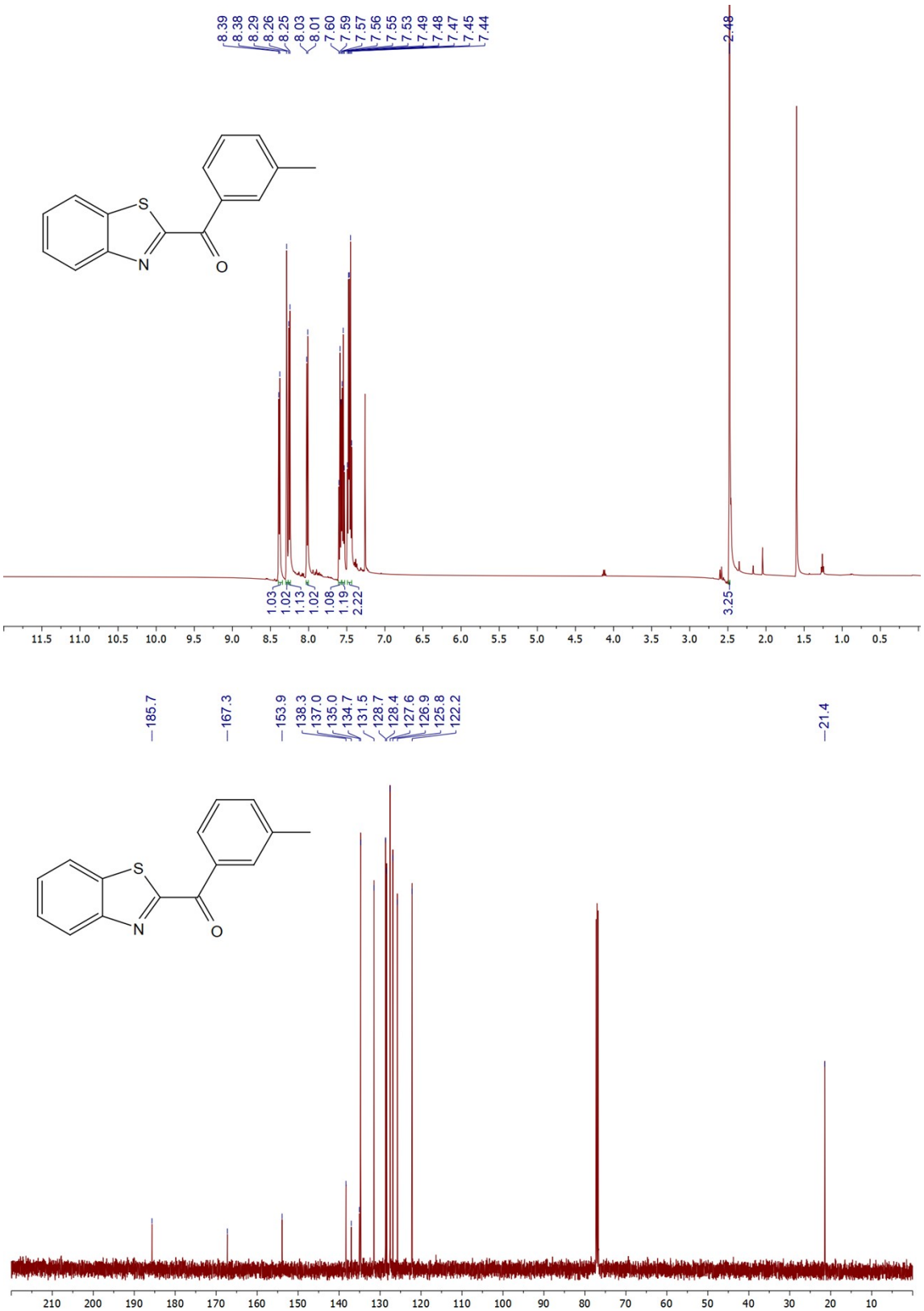


Figure S21. ^{1}H and ^{13}C NMR spectra of benzo[*d*]thiazol-2-yl(3-methylphenyl)methanone (f3)

Benzo[*d*]thiazol-2-yl(4-methylphenyl)methanone (f4)

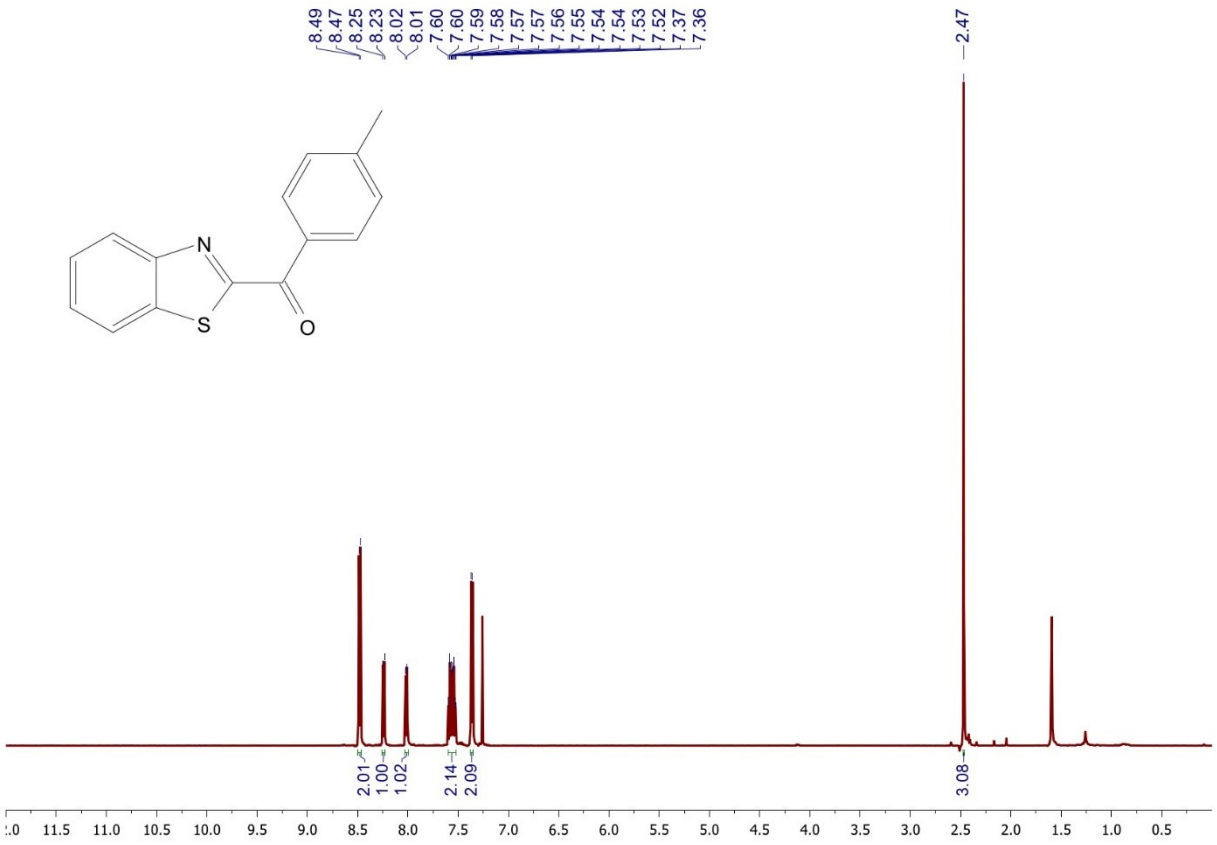


Figure S22. ^{1}H NMR spectra of benzo[*d*]thiazol-2-yl(4-methylphenyl)methanone (f4)

Benzo[*d*]thiazol-2-yl(4-methoxyphenyl)methanone (f5)

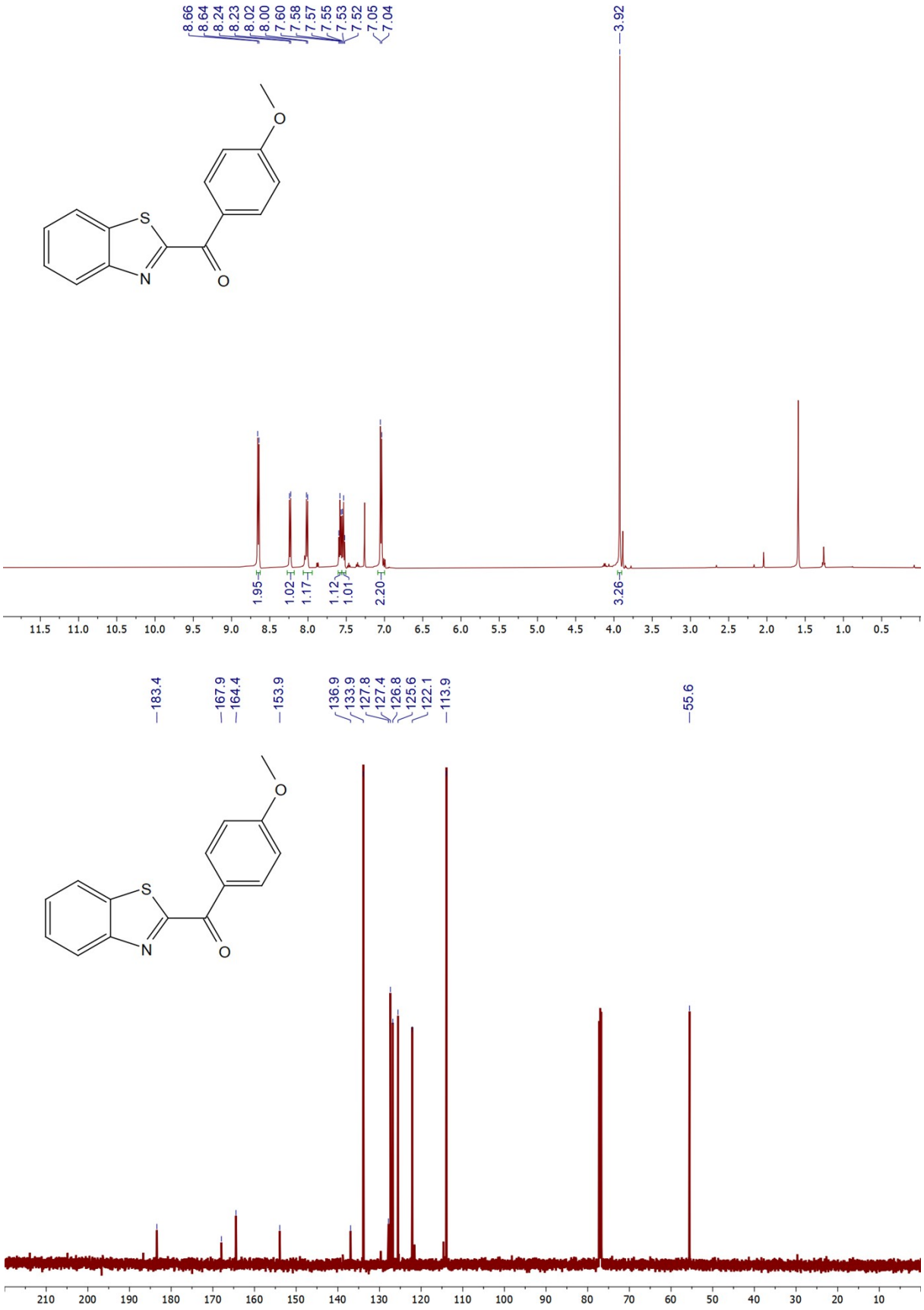


Figure S23. ^{1}H and ^{13}C NMR spectra of benzo[*d*]thiazol-2-yl(4-methoxyphenyl)methanone (f5)

Section S5. References

1. R. A. Sheldon, *ACS Sustainable Chem. Eng.*, 2018, **6**, 32-48.
2. D. J. C. Constable, A. D. Curzons and V. L. Cunningham, *Green Chem.*, 2002, **4**, 521-527.
3. K. Van Aken, L. Strekowski and L. Patiny, *Beilstein J. Org. Chem.*, 2006, **2**, 3.
4. N. Sahiba, A. Sethiya, J. Soni and S. Agarwal, *ChemistrySelect*, 2020, **5**, 13076-13080.
5. R. R. Putta, S. Chun, S. B. Lee, D.-C. Oh and S. Hong, *Front. Chem.*, 2020, **8**, 429.
6. G. Bolakatti, M. Palkar, M. Katagi, G. Hampannavar, R. V. Karpoormath, S. Ninganagouda and A. Badiger, *J. Mol. Struct.*, 2021, **1227**, 129413.
7. Y. M. Ha, Y. Uehara, D. Park, H. O. Jeong, J. Y. Park, Y. J. Park, J. Y. Lee, H. J. Lee, Y. M. Song, H. R. Moon and H. Y. Chung, *Appl Biochem Biotechnol*, 2012, **168**, 1416-1433.
8. M. B. Yadav, S. S. Vagh and Y. T. Jeong, *Res Chem Intermed*, 2020, **46**, 3801-3815.
9. S. Agrawal, R. Kumari, T. Sophronea, N. Kumari and P. M. Luthra, *Biomed. Pharmacother.*, 2022, **156**, 113838.
10. M.-Q. Hu, H. Li, Y. Lin, Y. Zhang, J. Tang, J.-P. Zuo, L.-F. Yu, X.-K. Tong, W. Tang and F. Yang, *RSC Adv.*, 2020, **10**, 43299-43311.
11. A. A. Aleksandrov, M. M. Elchaninov, D. A. Tishina, Y. E. Tarakanova and M. L. Shmanovsky, *Russ J Org Chem* 2021, **57**, 664-667.
12. T. T. Thanh, H. L. Xuan and T. N. Quoc, *RSC Adv.*, 2021, **11**, 28797-28808.
13. Z. M. Nofal, E. A. Soliman, S. S. Abd El-Karim, M. I. El-Zahar, A. M. Srour, S. Sethumadhavan and T. J. Maher, *J. Heterocyclic Chem.*, 2014, **51**, 1797-1806.
14. S. Agrawal, R. Kumari, T. Sophronea, N. Kumari and P. M. Luthra, *Biomed. Pharmacother.*, 2022, **156**, 113838.