Supporting Information

β-ketoenamine-linked covalent organic framework as heterogeneous photocatalyst for synthesis of 2-arylbenzothiazoles by cyclization reaction

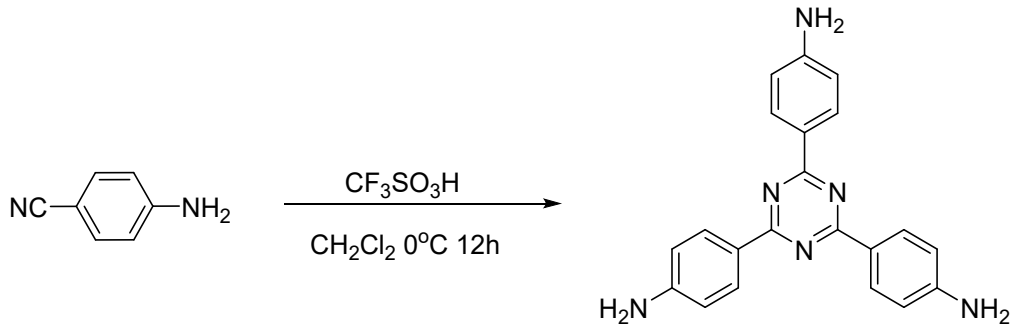
Ziqi Liu, Zhicheng Chen, Huixin Tong, Mengmeng Ji and Wenyi Chu*

School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, P. R. China.

(E-mail: wenyichu@hlju.edu.cn; Fax: +86-451-86609135; Tel: +86-451-86609135)

Contents of Supporting Information

1. Synthesis of 4,4',4''-(1,3,5-triazine-2,4,6-trial) trianiline (TAPT).



Scheme S1. Synthetic route approach to **TAPT**

TAPT was synthesized according to the procedures described in the literature. [1] *P*-aminophenonitrile (1.18 g, 10 mmol) was added into the round bottom flask under the N_2 atmosphere. CH_2Cl_2 (25 mL) as the solution was slowly dripped and followed with CF_3SO_3H (4 mL, 45 mmol) under an ice bath and then stirred for 12 h. After the reaction was completed, the yellow oil layer was separated and diluted by water (20mL) and the pH was adjusted to 9-11 with 0.5 M NaOH solution to precipitate the yellow solid under magneton agitation. The solid was repeatedly washed with collected water to get a yellow powder.

The pure product was obtained as a yellow solid (0.97 g, 82%); m.p. 381-382°C. ^{1}H NMR (400 MHz, DMSO) δ 8.35 (d, *J* = 8.4 Hz, 6H), 6.69 (d, *J* = 8.4 Hz, 6H), 5.90 (s, 6H) **(Figure S1)**. ^{13}C NMR (100 MHz, DMSO) δ 170.0, 153.4, 130.6, 123.4, 113.6 **(Figure S2)**. HRMS: $C_{21}H_{18}N_6$ for $[M+H]^+$: 355.1671. Found: 355.1665. Anal.calcd for: $C_{21}H_{18}N_6$: C 71.17, H 5.12, N 23.71; Found: C 71.18, H 5.12, N 23.70. FT-IR (KBr disc): v= 3454, 3325, 3210, 1633, 1606, 1577, 1498, 1433, 1367, 1309, 1296, 1180, 1149, 1130, 813 cm^{-1}

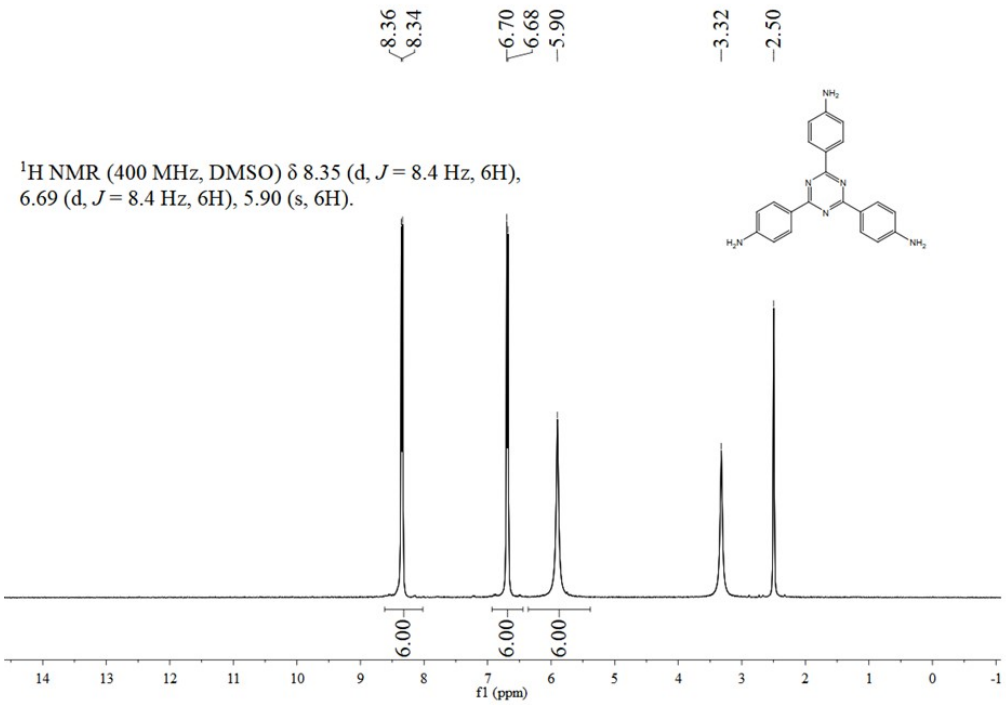


Figure S1. ^{1}H NMR of 4,4',4''-(1,3,5-triazine-2,4,6-triyl) trianiline **(TAPT)**

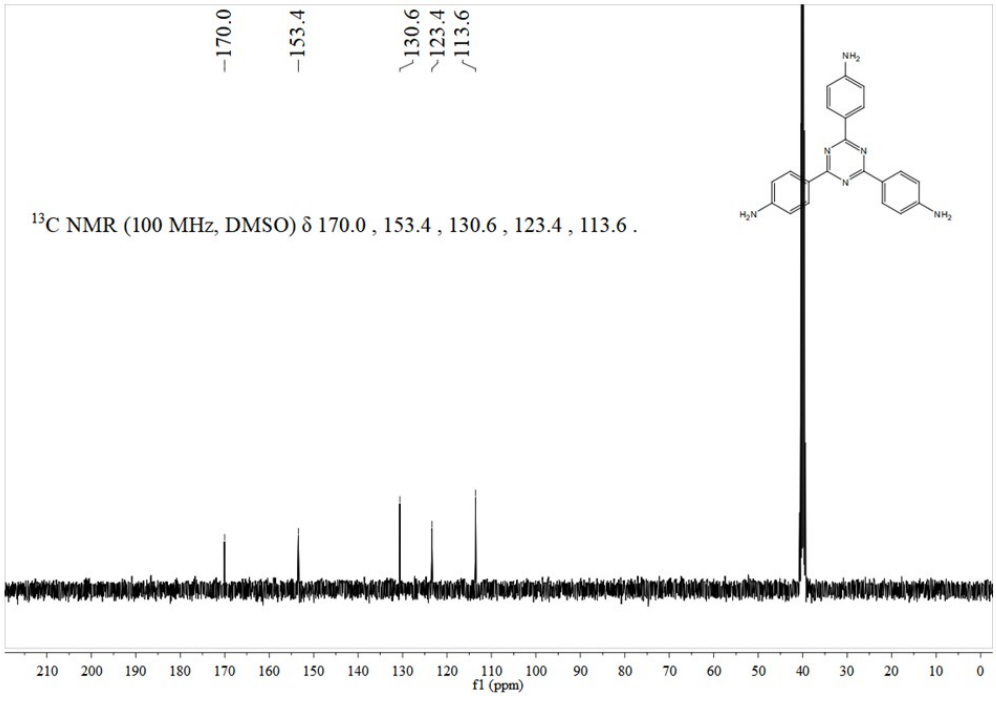
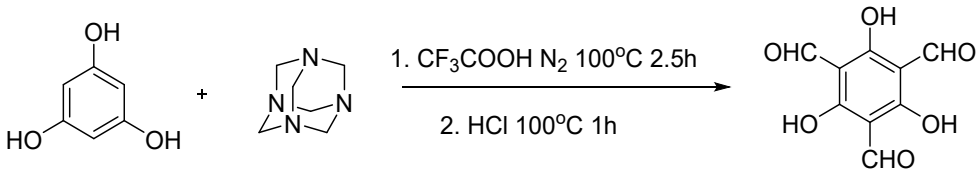


Figure S2. ^{13}C NMR of 4,4',4''-(1,3,5-triazine-2,4,6-triyl) trianiline **(TAPT)**

2. Synthesis of 2,4,6-trihydroxybenzene-1,3,5-tricarbaldehyde (TP)



Scheme S2. Synthetic route approach to TP

TP was synthesized according to the literature.[2] 1,3,5-trihydroxybenzene (3g, 23.8 mmol) and hexamethylenetetramine (8.34 g, 59.5 mmol) were added into the round bottom flask under the N_2 atmosphere. The solution was heated to 100°C and stirred for 2.5 h under the trifluoroacetic acid (47 mL) as a solution. Then, HCl (50 mL) was added and the mixture was kept at 100°C for another 1h. After cooling to room temperature, the filtrate was extracted with CH_2Cl_2 (3×100 mL) and the oil layer was separated and dried with anhydrous Na_2SO_4. The crude product was obtained by rotary evaporation of the solvent. The final product was collected in the form of light pink powder after recrystallization with hot ethanol.

The pure product was obtained as a white solid (540 mg, 18%); m.p. 199-200°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 14.11 (s, 3H), 10.15 (s, 3H) **(Figure S3)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 192.1, 173.6, 102.9, 77.4, 77.0, 76.7 **(Figure S4)**. HRMS: $C_9H_6O_6$ for $[M+H]^+$: 211.0243. Found: 211.0231. Anal.calcd for: $C_9H_6O_6$: C 51.44, H 2.88; Found: C 51.43, H 2.89. FT-IR (KBr disc): v= 2889, 1643, 1593, 1433, 1390, 1253, 1193, 968, 873, 817, 785, 607 cm^{-1}

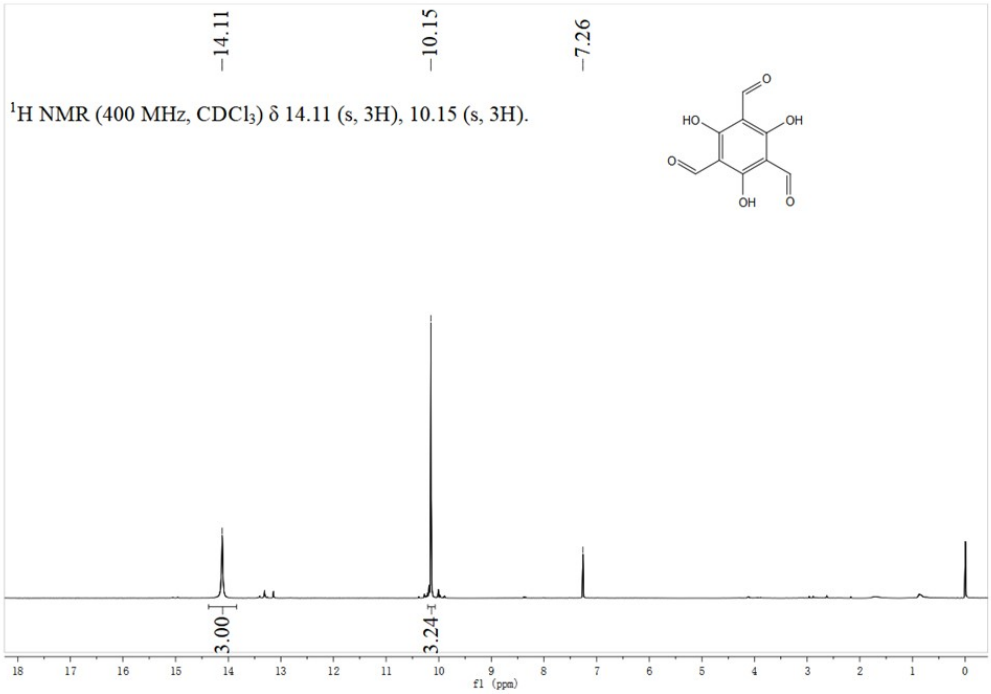


Figure S3. ^{1}H NMR of 2,4,6-trihydroxybenzene-1,3,5-tricarbaldehyde **(TP)**

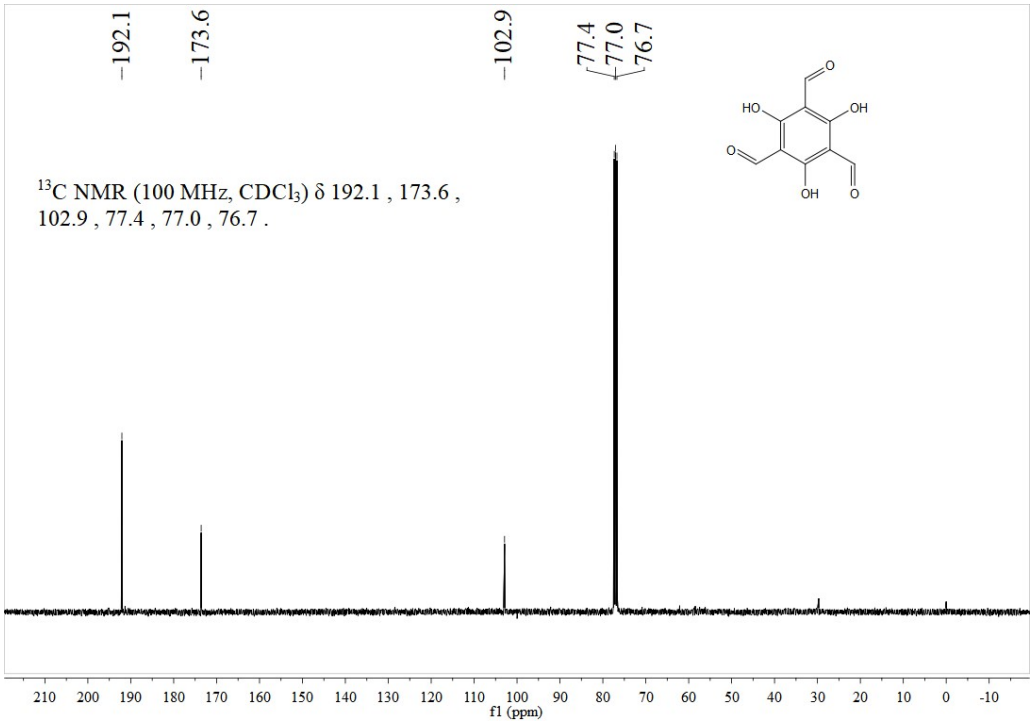


Figure S4. ^{13}C NMR of 2,4,6-trihydroxybenzene-1,3,5-tricarbaldehyde **(TP)**

3. The influence of the proportion of ethanol and water for reaction

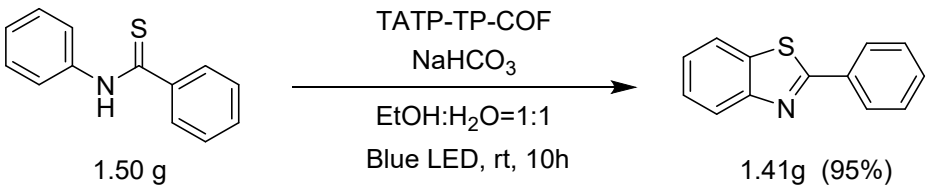
Table S1 The optimization of reaction solvents.

Entry	Photocatalyst (wt%)	Solvent (V:V)	Base (equiv.)	Yield (%)
1	TAPT-TP-COF (5)	EtOH:H_2O (1:1)	K_2CO_3	79
2	TAPT-TP-COF (5)	EtOH:H_2O (1:2)	K_2CO_3	63
3	TAPT-TP-COF (5)	EtOH:H_2O (1:3)	K_2CO_3	42
4	TAPT-TP-COF (5)	EtOH:H_2O (1:4)	K_2CO_3	25
5	TAPT-TP-COF (5)	H_2O	K_2CO_3	trace
6	TAPT-TP-COF (5)	EtOH:H_2O (2:1)	K_2CO_3	68
7	TAPT-TP-COF (5)	EtOH:H_2O (3:1)	K_2CO_3	57
8	TAPT-TP-COF (5)	EtOH:H_2O (4:1)	K_2CO_3	43
9	TAPT-TP-COF (5)	EtOH	K_2CO_3	34

Firstly, N-phenylbenzothioamide was chosen as the substrate by using TAPT-TP-COF as the photocatalyst and K_2CO_3 as the base in mixed solvents of EtOH/ H_2O (V: V= 1:1) under the irradiation of 10 W blue LED at room temperature for 10 hours. The yield of 2-phenylbenzothiazole was 79% (entry 1). Next, the proportion of water in the mixed solvent was gradually increased. As shown in entries 2-4, the yield of **2a** gradually decreased from 79% to 25%. When the water was used as the reaction solvent, the yield of the product decreased significantly (entry 5). From the experimental results, it can be seen that the reason for the gradually decreasing yield may be due to the increasing proportion of H_2O in the mixed solvent, which leads to a gradual decrease in the solubility of the substrate. Subsequently, on the basis of EtOH/ H_2O (V: V= 1:1), the proportion of EtOH in the mixed solvent was gradually increased, and the results were shown in entries 6-8. When the ratios of EtOH/ H_2O were V: V= 2:1, 3:1, 4:1, the yields of **2a** were 68%, 57%, 43%, respectively. A yield of 34% was obtained when anhydrous EtOH was selected as the solvent. This may be caused by a change in pH in the solvent due to a decrease in the solubility of the base

due to the increasing proportion of EtOH. Therefore, based on the above experiments results, EtOH/H_2O (V: V= 1:1) was selected as the solvent.

4. Photocatalytic gram-scale preparation of 2-phenylbenzothiazole



Scheme S3. Gram-scale preparation of 2-phenylbenzothiazole

To an ovendried 250 mL round bottomed flask containing a stirring bar, N-arylbenzothioamide (1.50 g, 0.7 mmol, 1.0 eq), TAPT-TP-COF (75 mg, wt%), $NaHCO_3$ (1.18 g, 2.0 eq) were added followed by 50 mL EtOH: H_2O (V:V=1:1,). The reaction was kept stirring at room temperature for 10 h under the irradiation of 10 W blue LED (monitored by TLC). After the reaction was completed, the reaction solution was filtered. Then the filtrate was concentrated under reduced pressure to obtain the crude product. The crude product was purified by column chromatography on silica gel with ethyl acetate: petroleum ether = 1:4 as the eluent. 1.41 g of the final product 2-phenylbenzothiazole was obtained with the yield of 95% by concentrated under reduced pressure.

5. Characterization of TAPT-TP-COF

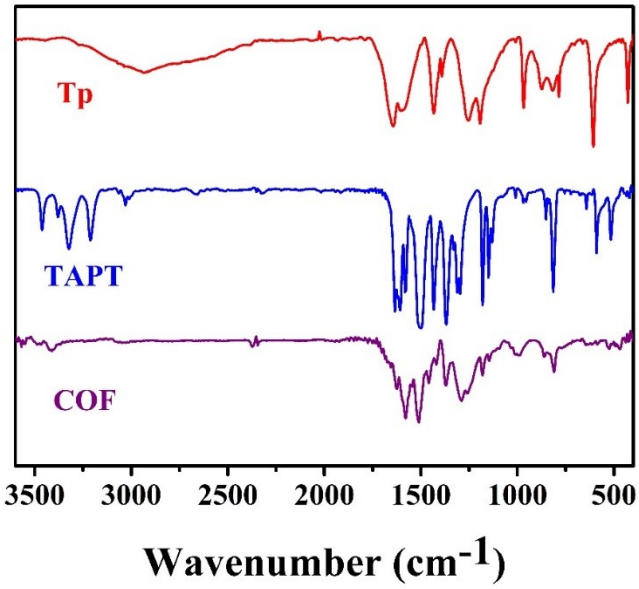


Figure S5. FT-IR spectra of (a) TP, (b) TAPT, and (c) TAPT-TP-COF

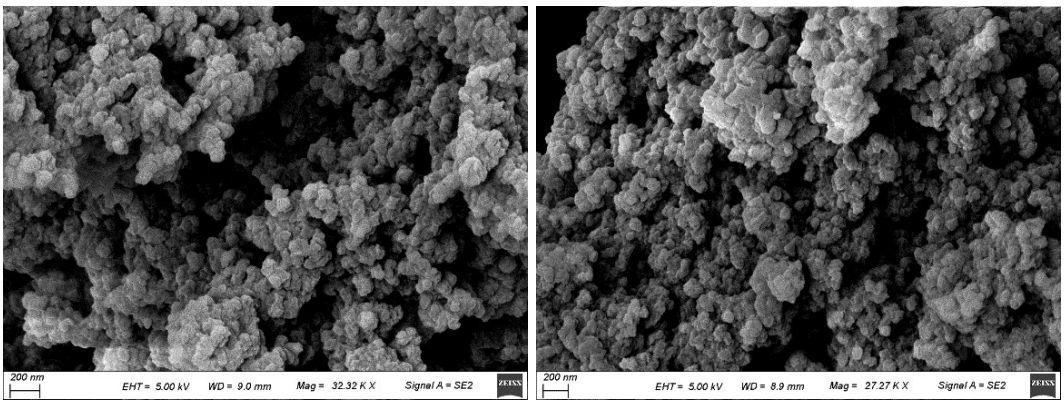


Figure S6. SEM images of TAPT-TP-COF

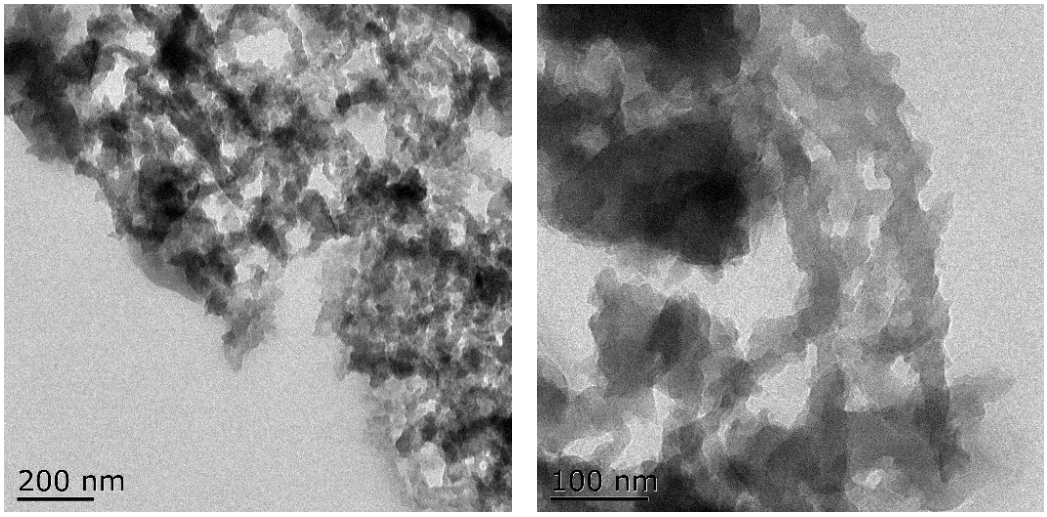


Figure S7 TEM images of TAPT-TP-COF

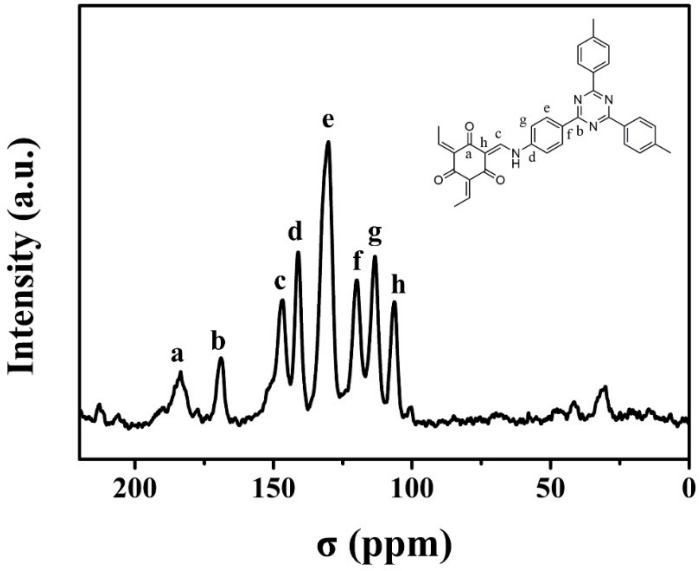


Figure S8 Solid-state ^{13}C CP-MAS NMR spectrum of TAPT-TP-COF

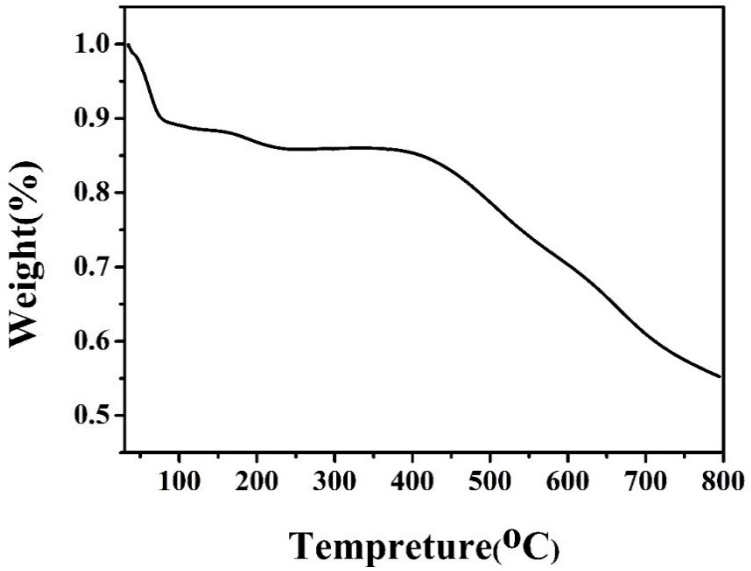


Figure S9 TGA spectrum of TAPT-TP-COF

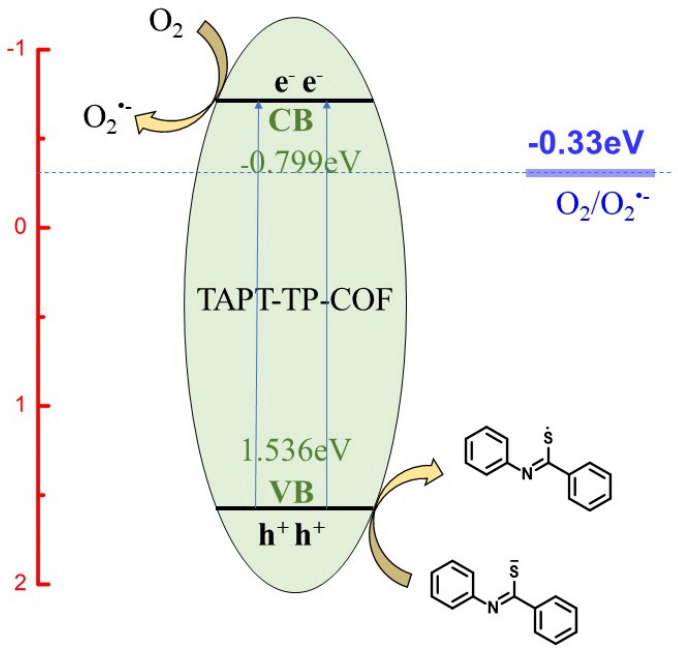


Figure S10 Possible catalytic cycles for the cyclization by TAPT-TP-COF via energy transfer.

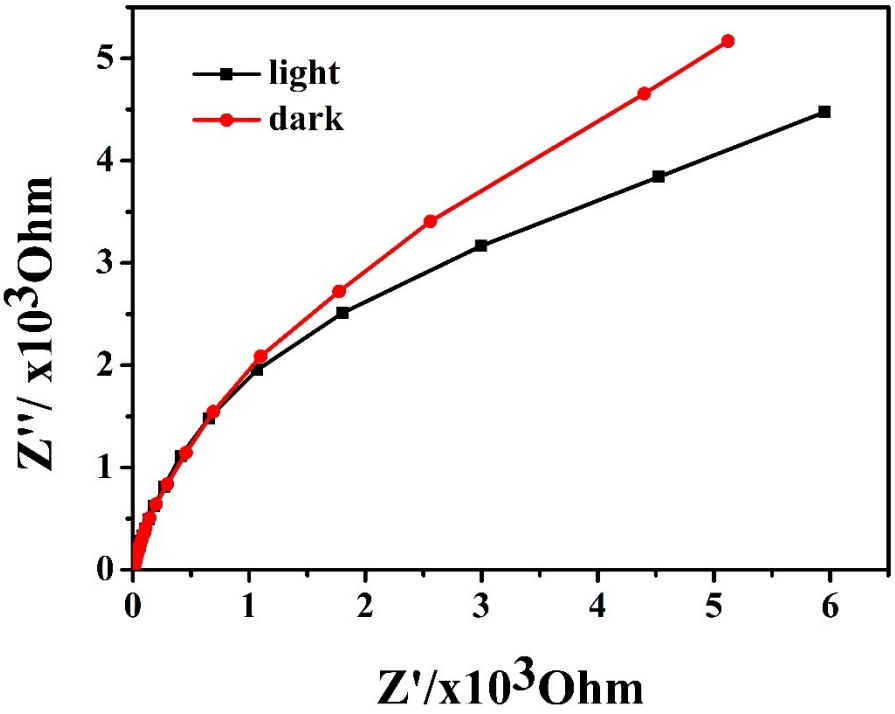


Figure S11 EIS Nyquist plots of TAPT-TP-COF under light and dark.

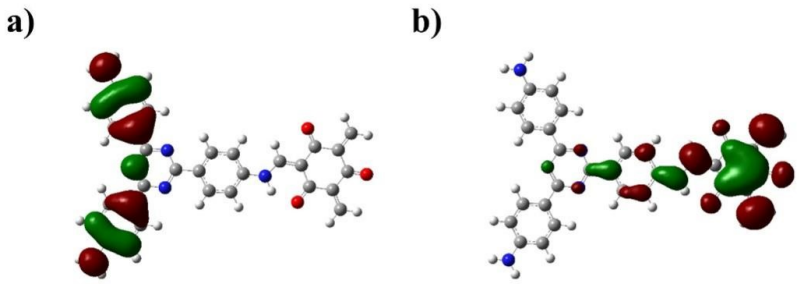


Figure S12. HOMO spectra (a) and LUMO spectra (b) of TAPT-TP-COF

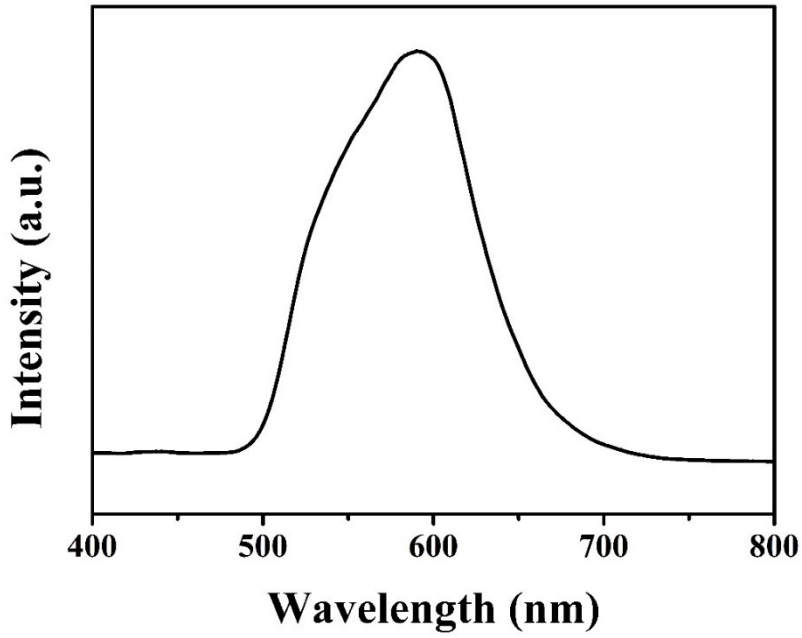


Figure S13. Photoluminescence spectra of TAPT-TP-COF

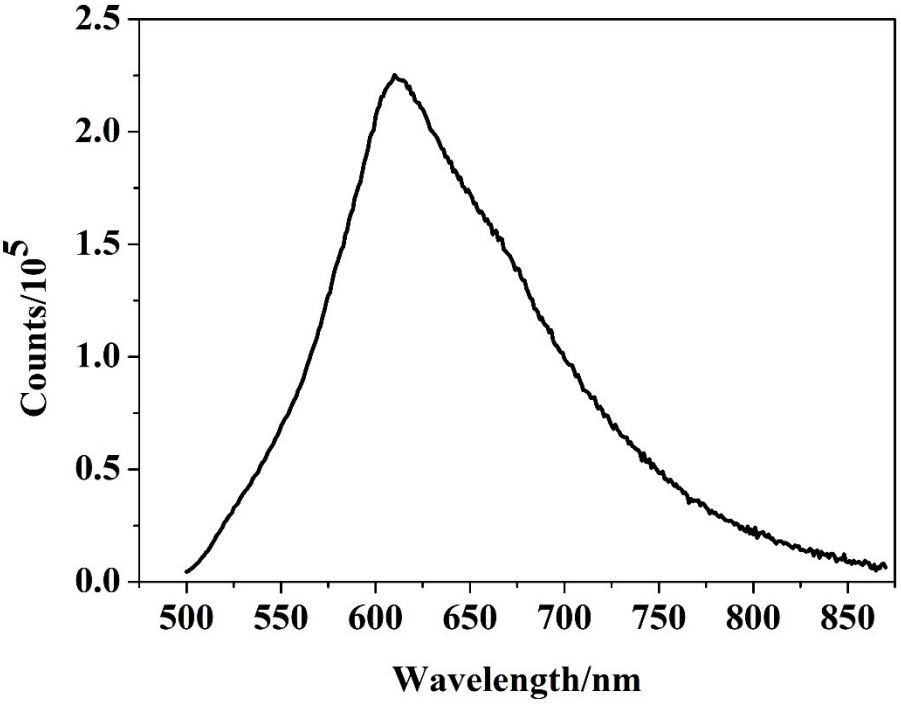


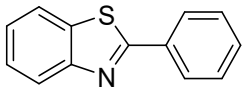
Figure S14. Emission spectrum of TAPT-TP-COF under the 10 W Blue LED

6. References

1. S. Zhang, Y. Zheng, H. An, B. Aguila, C.-X. Yang, Y. Dong, W. Xie, P. Cheng, Z. Zhang, Y. Chen and S. Ma, *Angewandte Chemie International Edition*, 2018, **57**, 16754–16759.
2. J. H. Chong, M. Sauer, B. O. Patrick and M. J. MacLachlan, *Org. Lett.*, 2003, **5**, 3823–3826.

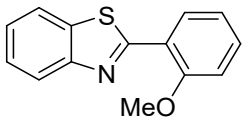
7. Data and NMR spectra of the products

2-phenylbenzo [d]thiazole (2a):



The pure product was obtained as a white solid (49 mg, 98%); m.p. 113-114^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 – 8.07 (m, 3H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.50 (dd, *J* = 9.2, 5.5 Hz, 4H), 7.38 (t, *J* = 7.6 Hz, 1H) **(Figure S15)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 154.2, 135.1, 133.7, 131.0, 129.1, 127.6, 126.4, 125.2, 123.3, 121.7 **(Figure S16)**. HRMS: $C_{13}H_9NS$ for $[M+H]^+$: 212.0534. Found: 212.0531. Anal.calcd for: $C_{13}H_9NS$: C 73.90, H 4.29, N 6.63, S 15.17; Found: C 73.89, H 4.30, N 6.62, S 15.18. FT-IR (KBr disc): v= 1638.2, 1550, 1473.6, 1435, 1311, 1226, 1157, 1072, 964, 763 cm^{-1}

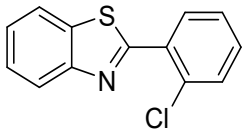
2-(2-methoxyphenyl) benzo[d]thiazole (2b):



The pure product was obtained as a white solid (41.5 mg, 83%); m.p. 104-105^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (dd, *J* = 7.8, 1.5 Hz, 1H), 8.15 (d, *J* = 8.2 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.60 – 7.47 (m, 1H), 7.40 (dddd, *J* = 8.8, 8.0, 7.5, 1.3 Hz,

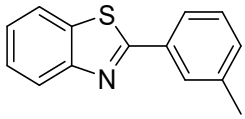
2H), 7.14 (t, *J* = 7.6 Hz, 1H), 7.01 (d, *J* = 8.3 Hz, 1H), 3.99 (s, 3H) **(Figure S17)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.2, 157.3, 152.2, 136.2, 131.8, 129.6, 126.0, 124.6, 122.8, 122.3, 121.3, 121.2, 111.7, 55.7 **(Figure S18)**. HRMS: $C_{14}H_{11}NOS$ for $[M+H]^+$: 242.0640. Found: 242.0637. Anal.calcd for: $C_{14}H_{11}NOS$ C 69.68, H 4.59, N 5.80, S 13.29; Found: C 69.66, H 4.60, N 5.81, S 13.30. FT-IR (KBr disc): v= 2850, 1589, 1496, 1458, 1427, 1288.5, 1249, 1111, 1010, 964.4, 756.1 cm^{-1}

2-(2-chlorophenyl) benzo[d]thiazole (2c):



The pure product was obtained as a white solid (35.5 mg, 71%); m.p. 83-85^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.26 – 8.19 (m, 1H), 8.15 (d, *J* = 8.1 Hz, 1H), 7.94 (d, *J* = 7.8 Hz, 1H), 7.57 – 7.49 (m, 2H), 7.46 – 7.37 (m, 3H) **(Figure S19)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 152.5, 136.1, 132.7, 132.3, 131.8, 131.2, 130.8, 127.1, 126.3, 125.5, 123.5, 121.4 **(Figure S20)**. HRMS: $C_{13}H_8ClNS$ for $[M+H]^+$: 246.0144. Found: 246.0138. Anal.calcd for: $C_{13}H_8ClNS$: C 63.54, H 3.28, Cl 14.43, N 5.70, S 13.05; Found: C 63.55, H 3.27, Cl 14.44, N 5.70, S 13.04; FT-IR (KBr disc): v=1558, 1481, 1427, 1311, 1265, 1219, 1157, 1056, 964, 756 cm^{-1}

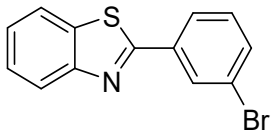
2-(*m*-tolyl) benzo[d]thiazole (2d):



The pure product was obtained as a white solid (43.5 mg, 87%); m.p. 65-67^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (d, *J* = 8.2 Hz, 1H), 7.96 (s, 1H), 7.88 (d, *J* = 7.8 Hz, 2H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 2H), 7.30 (d, *J* = 7.5 Hz, 1H), 2.45 (s, 3H) **(Figure S21)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.4, 154.2, 138.9, 135.1, 133.6, 131.8, 128.9, 128.0, 126.3, 125.2, 124.9, 123.2, 121.6, 21.4 **(Figure S22)**. HRMS: $C_{14}H_{11}NS$ for $[M+H]^+$: 226.0690. Found: 226.0687. Anal.calcd for: $C_{14}H_{11}NS$: C 74.63, H 4.92, N 6.22, S 14.23; Found: C 74.62, H 4.93, N 6.23, S 14.22. FT-IR

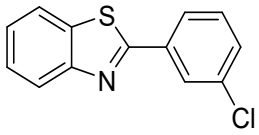
(KBr disc): v=2916, 1612, 1589, 1481, 1427, 1311, 1234, 1180, 1087, 979, 756.1 cm^{-1}

2-(3-bromophenyl) benzo[d]thiazole (2e):



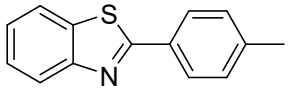
The pure product was obtained as a white solid (41 mg, 82%); m.p. 84-86^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.28 (s, 1H), 8.08 (d, *J* = 8.2 Hz, 1H), 7.98 (d, *J* = 7.8 Hz, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 7.38 (dt, *J* = 21.4, 7.8 Hz, 2H) **(Figure S23)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 154.0, 135.5, 135.1, 133.8, 130.5, 130.3, 126.6, 126.2, 125.6, 123.5, 123.2, 121.7 **(Figure S24)**. HRMS: $C_{13}H_8BrNS$ for $[M+H]^+$: 289.9639. Found: 289.9641. Anal.calcd for: $C_{13}H_8BrNS$: C 53.81, H 2.78, Br 27.54, N 4.83, S 11.05; Found: C 53.82, H 2.77, Br 27.53, N 4.82, S 11.07; FT-IR (KBr disc): v= 1596, 1491, 1455, 1315, 1226, 1097, 956, 724, 716 cm^{-1}

2-(3-chlorophenyl) benzo[d]thiazole (2f):



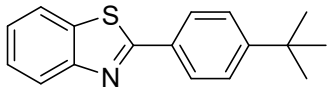
The pure product was obtained as a white solid (40 mg, 80%); m.p.96-97^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (s, 1H), 8.08 (d, *J* = 8.2 Hz, 1H), 7.93 (d, *J* = 7.4 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 7.51 (t, *J* = 7.3 Hz, 1H), 7.48 – 7.31 (m, 3H) **(Figure S25)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.3, 154.0, 135.3, 135.2, 135.1, 130.9, 130.3, 127.4, 126.6, 125.7, 125.6, 123.5, 121.7 **(Figure S26).** HRMS: $C_{13}H_8ClNS$ for $[M+H]^+$: 246.0144. Found: 246.0141. Anal.calcd for: $C_{13}H_8ClNS$: C 63.54, H 3.28, Cl 14.43, N 5.70, S 13.05; Found: C 63.53, H 3.27, Cl 14.44, N 5.70, S 13.06. FT-IR (KBr disc): v= 1562, 1457, 1410, 1313, 1228, 1173, 1077, 975, 783 cm^{-1}

2-(*p*-tolyl) benzo[d]thiazole (2g):



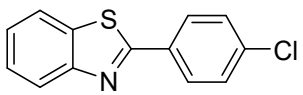
The pure product was obtained as a white solid (45 mg, 90%); m.p.84-85^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.2 Hz, 1H), 7.99 (d, *J* = 8.1 Hz, 2H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.49 (t, *J* = 7.4 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 2H), 2.43 (s, 3H) **(Figure S27)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.3, 154.2, 141.4, 135.0, 131.0, 129.7, 127.5, 126.3, 125.0, 123.1, 121.6, 21.6 **(Figure S28)**. HRMS: $C_{14}H_{11}NS$ for $[M+H]^+$: 226.0690. Found: 226.0685. Anal.calcd for: $C_{14}H_{11}NS$: C 74.63, H 4.92, N 6.22, S 14.23; Found: C 74.63, H 4.91, N 6.21, S 14.25. FT-IR (KBr disc): v= 2954, 1566, 1519, 1481, 1427, 1311, 1288, 1249, 1172, 956, 756 cm^{-1}

2-(4-(tert-butyl) phenyl) benzo[d]thiazole (2h):



The pure product was obtained as a white solid (46 mg, 92%); m.p.107-108^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.1 Hz, 1H), 8.03 (d, *J* = 8.4 Hz, 2H), 7.90 (d, *J* = 7.9 Hz, 1H), 7.58 – 7.44 (m, 3H), 7.37 (t, *J* = 7.6 Hz, 1H), 1.38 (s, 9H) **(Figure S29)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.2, 154.6, 154.2, 135.0, 130.9, 127.4, 126.2, 126.0, 125.0, 123.1, 121.6, 35.0, 31.2 **(Figure S30)**. HRMS: $C_{17}H_{17}NS$ for $[M+H]^+$: 268.1160. Found: 268.1156. Anal.calcd for: $C_{17}H_{17}NS$: C 76.36, H 6.41, N 5.24, S 11.99; Found: C 76.37, H 6.40, N 5.25, S 11.98. FT-IR (KBr disc): v= 2956, 1504, 1473, 1427, 1311, 1219, 1157, 1111, 1072, 964, 763 cm^{-1}

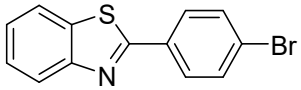
2-(4-chlorophenyl)benzo[d]thiazole (2i):



The pure product was obtained as a pale solid (41.5 mg, 83%); m.p.113-114^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.3 Hz, 1H), 8.01 (d, *J* = 8.5 Hz, 2H), 7.89 (d, *J* = 8.2 Hz, 1H), 7.52 – 7.44 (m, 3H), 7.39 (t, *J* = 7.4 Hz, 1H) **(Figure S31)**. ^{13}C

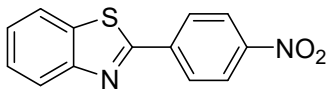
NMR (100 MHz, $CDCl_3$) δ 166.6, 154.1, 137.0, 135.1, 132.1, 129.3, 128.7, 126.5, 125.4, 123.3, 121.7 **(Figure S32)**. HRMS: $C_{13}H_8ClNS$ for $[M+H]^+$: 246.0144. Found: 246.0142. Anal.calcd for: $C_{13}H_8ClNS$: C 63.54, H 3.28, Cl 14.43, N 5.70, S 13.05; Found: C 63.52, H 3.29, Cl 14.43, N 5.70, S 13.06. FT-IR (KBr disc): v= 1589, 1507, 1473, 1431, 1315, 1249, 1111, 1086, 964, 754 cm^{-1}

2-(4-bromophenyl) benzo[d]thiazole (2j):



The pure product was obtained as a white solid (42.5 mg, 85%); m.p. 131-132°C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 8.1 Hz, 1H), 7.95 (d, *J* = 8.5 Hz, 2H), 7.89 (d, *J* = 7.9 Hz, 1H), 7.61 (d, *J* = 8.5 Hz, 2H), 7.50 (t, *J* = 7.6 Hz, 1H), 7.39 (t, *J* = 7.2 Hz, 1H) **(Figure S33)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.7, 154.1, 135.1, 132.6, 132.2, 128.9, 126.5, 125.5, 125.4, 123.3, 121.7 **(Figure S34)**. HRMS: $C_{13}H_8BrNS$ for $[M+H]^+$: 289.9639. Found: 289.9631. Anal.calcd for: $C_{13}H_8BrNS$: C 53.81, H 2.78, Br 27.54, N 4.83, S 11.05; Found: C 53.80, H 2.77, Br 27.55, N 4.83, S 11.06. FT-IR (KBr disc): v= 1581, 1504, 1473, 1427, 1396, 1311, 1226, 1064, 1010, 964, 825, 756, 717 cm^{-1}

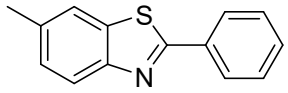
2-(4-nitrophenyl) benzo[d]thiazole (2k):



The pure product was obtained as a yellow solid (37 mg, 74%); m.p.227-229°C.^1H NMR (400 MHz, $CDCl_3$) δ 8.35 (d, *J* = 7.7 Hz, 2H), 8.27 (d, *J* = 7.3 Hz, 2H), 8.13 (d, *J* = 7.5 Hz, 1H), 7.96 (d, *J* = 7.2 Hz, 1H), 7.56 (t, *J* = 6.8 Hz, 1H), 7.47 (t, *J* = 6.7 Hz, 1H) **(Figure S35)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.9, 154.1, 149.1, 139.1, 135.5, 128.3, 127.0, 126.3, 124.3, 123.9, 121.9 **(Figure S36)**. HRMS: $C_{13}H_8N_2O_2S$ for $[M+H]^+$: 257.0385. Found: 257.0381. Anal.calcd for: $C_{13}H_8N_2O_2S$: C 60.93, H 3.15, N 10.93, S 12.51; Found: C 60.92, H 3.16, N 10.91, S 12.52. FT-IR

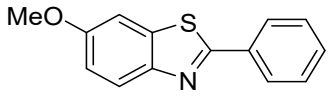
(KBr disc): 1597, 1519, 1473, 1342, 1311, 1219, 1103, 1103, 972, 763 cm^{-1}

6-methyl-2-phenylbenzo[d]thiazole (2l):



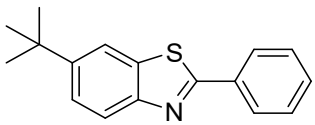
The pure product was obtained as a white solid (44 mg, 88%); m.p. 126-127^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 6.6, 2.8 Hz, 2H), 7.96 (d, *J* = 8.3 Hz, 1H), 7.69 (s, 1H), 7.49 (dd, *J* = 4.9, 1.6 Hz, 3H), 7.31 (d, *J* = 8.3 Hz, 1H), 2.50 (s, 3H) **(Figure S37)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 152.3, 135.4, 135.2, 133.8, 130.8, 129.0, 127.9, 127.4, 122.7, 121.4, 21.6 **(Figure S38)**. HRMS: $C_{14}H_{11}NS$ for $[M+H]^+$: 226.0690. Found: 226.0684. Anal.calcd for: $C_{14}H_{11}NS$: C 74.63, H 4.92, N 6.22, S 14.23; Found: C 74.64, H 4.91, N 6.21, S 14.24. FT-IR (KBr disc): v= 2916, 1604, 1508, 1481, 1427, 1311, 1249, 1226, 1172, 956, 756 cm^{-1}

6-methoxy-2-phenylbenzo[d]thiazole (2m):



The pure product was obtained as a white solid (47 mg, 94%); m.p. 116-117^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.0 Hz, 2H), 7.96 (d, *J* = 8.9 Hz, 1H), 7.47 (d, *J* = 5.2 Hz, 3H), 7.35 (d, *J* = 1.8 Hz, 1H), 7.09 (dd, *J* = 8.8, 1.8 Hz, 1H), 3.89 (s, 3H) **(Figure S39)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 157.8, 148.7, 136.4, 133.8, 130.6, 129.0, 127.3, 123.7, 115.7, 104.2, 55.8 **(Figure S40)**. HRMS: $C_{14}H_{11}NOS$ for $[M+H]^+$: 242.0640. Found: 242.0631. Anal.calcd for: $C_{14}H_{11}NOS$: C 69.68, H 4.59, N 5.80, S 13.29; Found: C 69.67, H 4.60, N 5.81, S 13.28. FT-IR (KBr disc): v= 2967, 1597, 1550, 1458, 1427, 1265, 1219, 1118, 1026, 964, 756.1 cm^{-1}

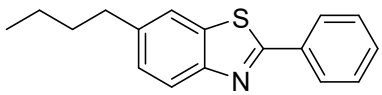
6-(tert-butyl)-2-phenylbenzo[d]thiazole (2n):



The pure product was obtained as a white solid (45.5 mg, 91%); m.p.114-116^{o}C.

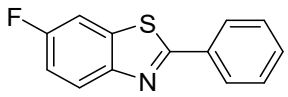
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.10 (dd, *J* = 6.5, 3.1 Hz, 2H), 8.02 (d, *J* = 8.6 Hz, 1H), 7.91 (d, *J* = 1.6 Hz, 1H), 7.57 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.50 (dd, *J* = 5.0, 1.7 Hz, 3H), 1.43 (s, 9H) **(Figure S41)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 152.1, 148.8, 135.1, 133.8, 130.8, 129.0, 127.5, 124.6, 122.5, 117.7, 35.1, 31.6 **(Figure S42)**. HRMS: $C_{17}H_{17}NS$ for $[M+H]^+$: 268.1160. Found: 268.1157. Anal.calcd for: $C_{17}H_{17}NS$: C 76.36, H 6.41, N 5.24, S 11.99; Found: C 76.37, H 6.40, N 5.24, S 11.99. FT-IR (KBr disc): v= 2936, 1597, 1512, 1473, 1396, 1311, 1226, 1111, 1026, 964, 756 cm^{-1}

6-butyl-2-phenylbenzo[d]thiazole (2o):



The pure product was obtained as a white solid (44.5 mg, 89%); m.p. 62-64^{o}C.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (dd, *J* = 6.5, 3.1 Hz, 2H), 7.98 (d, *J* = 8.3 Hz, 1H), 7.70 (s, 1H), 7.49 (dd, *J* = 5.0, 1.7 Hz, 3H), 7.32 (dd, *J* = 8.4, 1.4 Hz, 1H), 2.84 – 2.67 (m, 2H), 1.68 (dt, *J* = 15.3, 7.6 Hz, 2H), 1.40 (dq, *J* = 14.6, 7.3 Hz, 2H), 0.96 (t, *J* = 7.3 Hz, 3H) **(Figure S43)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.1, 152.4, 140.5, 135.2, 133.8, 130.8, 129.0, 127.5, 127.4, 122.8, 120.8, 35.7, 33.8, 22.4, 14.0 **(Figure S44)**. HRMS: $C_{17}H_{17}NS$ for $[M+H]^+$: 268.1160. Found: 268.1154. Anal.calcd for: $C_{17}H_{17}NS$: C 76.36, H 6.41, N 5.24, S 11.99; Found: C 76.35, H 6.42, N 5.23, S 12.00. FT-IR (KBr disc): v= 2953, 2916, 1597, 1512, 1450, 1319, 1257, 1226, 1095, 1026, 972, 763 cm^{-1}

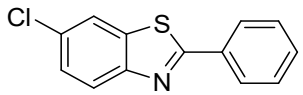
6-fluoro-2-phenylbenzo[d]thiazole (2p):



The pure product was obtained as a white solid (39 mg, 78%); m.p.134-135^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 3.9 Hz, 2H), 8.01 (dd, *J* = 7.9, 4.3Hz, 1H), 7.62 – 7.52 (dd, 1H),7.49 (d, *J* = 2.2 Hz, 1H), 7.19 (m, 1H) **(Figure S45)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.8, 160.5 (d, *J* = 245.6 Hz), 150.8, 136.0 (d, *J* = 11.3 Hz), 133.5, 131.2, 129.3, 127.6, 124.1 (d, *J* = 9.2 Hz), 114.9 (d, *J* = 24.6 Hz), 107.8 (d, *J* =

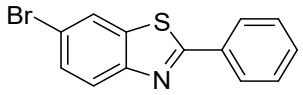
26.7 Hz) **(Figure S46)**. ^{19}F NMR (376 MHz, $CDCl_3$) δ -39.2 **(Figure S47)**. HRMS: $C_{13}H_8FNS$ for $[M+H]^+$: 230.0440. Found: 230.0435. Anal.calcd for: $C_{13}H_8FNS$: C 68.10, H 3.52, F 8.29, N 6.11, S 13.98; Found: C 68.09, H 3.52, F 8.30, N 6.12, S 13.97. FT-IR (KBr disc): v= 1561, 1512, 1492, 1454, 1447, 1249, 1196, 959, 756 cm^{-1}

6-chloro-2-phenylbenzo[d]thiazole (2q):



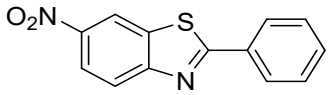
The pure product was obtained as a white solid (40.5 mg, 81%); m.p. 156-157°C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 6.7, 2.9 Hz, 2H), 7.97 (d, *J* = 8.7 Hz, 1H), 7.87 (d, *J* = 1.9 Hz, 1H), 7.55 – 7.48 (m, 3H), 7.45 (dd, *J* = 8.7, 2.0 Hz, 1H) **(Figure S48)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 152.7, 136.2, 133.2, 131.3, 131.1, 129.1, 127.6, 127.2, 124.0, 121.3 **(Figure S49)**. HRMS: $C_{13}H_8ClNS$ for $[M+H]^+$: 246.0144. Found: 246.0148. Anal.calcd for: $C_{13}H_8ClNS$: C 63.54, H 3.28, Cl 14.43, N 5.70, S 13.05; Found: C 63.55, H 3.29, Cl 14.42, N 5.69, S 13.05. FT-IR (KBr disc): v= 1581, 1543, 1512, 1473, 1435, 1303, 1219, 1103, 964, 756 cm^{-1}

6-bromo-2-phenylbenzo[d]thiazole (2r):



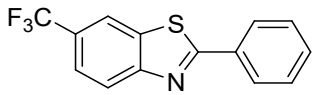
The pure product was obtained as a white solid (42.5 mg, 85%); m.p. 156-157°C. ^1H NMR (400 MHz, $CDCl_3$) δ 8.07 (dd, *J* = 6.5, 2.8 Hz, 2H), 8.03 (d, *J* = 1.7 Hz, 1H), 7.91 (d, *J* = 8.7 Hz, 1H), 7.59 (dd, *J* = 8.7, 1.7 Hz, 1H), 7.54 – 7.45 (m, 3H) **(Figure S50)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.6, 153.0, 136.7, 133.2, 131.3, 129.9, 129.1, 127.6, 124.3, 124.2, 118.8 **(Figure S51)**. HRMS: $C_{13}H_8BrNS$ for $[M+H]^+$: 289.9639. Found: 289.9633. Anal.calcd for: $C_{13}H_8BrNS$: C 53.81, H 2.78, Br 27.54, N 4.83, S 11.05; Found: C 53.80, H 2.79, Br 27.55, N 4.83, S 11.05. FT-IR (KBr disc): v= 1581, 1535, 1512, 1473, 1435, 1303, 1226, 1087, 964, 756.1 cm^{-1}

6-nitro-2-phenylbenzo[d]thiazole (2s):



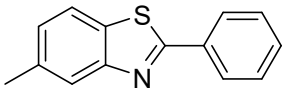
The pure product was obtained as a yellow solid (36 mg, 72%); m.p. 191-192°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.83 (d, *J* = 2.1 Hz, 1H), 8.36 (dd, *J* = 9.0, 2.2 Hz, 1H), 8.19 – 8.07 (m, 3H), 7.63 – 7.48 (m, 3H) **(Figure S52)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.8, 157.9, 144.9, 135.3, 132.7, 132.3, 129.3, 128.0, 123.3, 121.9, 118.3 **(Figure S53)**. HRMS: $C_{13}H_8N_2O_2S$ for $[M+H]^+$: 257.0385. Found: 257.0377. Anal.calcd for: $C_{13}H_8N_2O_2S$: C 60.93, H 3.15, N 10.93, S 12.51; Found: C 60.94, H 3.14, N 10.93, S 12.50. FT-IR (KBr disc): v= 1589, 1566, 1512, 1442, 1334, 1219, 1126, 1041, 964, 756 cm^{-1}

2-phenyl-6-(trifluoromethyl) benzo[d]thiazole (2t):



The pure product was obtained as a white solid (39 mg, 78%); m.p. 152-153°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 (s, 1H), 8.14 (d, *J* = 8.6 Hz, 1H), 8.10 (dd, *J* = 7.3, 1.9 Hz, 2H), 7.73 (d, *J* = 8.5 Hz, 1H), 7.52 (d, *J* = 7.0 Hz, 3H) **(Figure S54)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.2, 156.1, 135.1, 133.0, 131.7, 129.2, 127.8, 127.3 (q, *J* = 32.5 Hz), 124.2 (q, *J* = 270.1 Hz), 123.5, 123.4 (q, *J* = 3.4 Hz), 119.3 (q, *J* = 4.2 Hz) **(Figure S55)**. ^{19}F NMR (376 MHz, $CDCl_3$) δ 14.7 **(Figure S56)**. HRMS: $C_{14}H_8F_3NS$ for $[M+H]^+$: 280.0408. Found: 280.0402. Anal.calcd for: $C_{14}H_8F_3NS$: C 60.21, H 2.89, F 20.41, N 5.02, S 11.48; Found: C 60.22, H 2.90, F 20.40, N 5.01, S 11.47. FT-IR (KBr disc): v= 1512, 1481, 1410, 1319, 1249, 1111, 1087, 1049, 964, 763 cm^{-1}

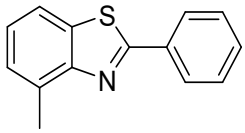
5-methyl-2-phenylbenzo[d]thiazole (2u):



The pure product was obtained as a white solid (44.5 mg, 89%); m.p. 145-146°C.

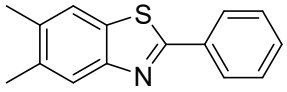
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07 (d, *J* = 3.9 Hz, 2H), 7.87 (s, 1H), 7.75 (d, *J* = 8.4 Hz, 1H), 7.51 – 7.42 (m, 3H), 7.19 (d, *J* = 8.2 Hz, 1H), 2.5 (s, 3H) **(Figure S57)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 154.5, 136.4, 133.6, 131.9, 130.8, 128.9, 127.4, 126.7, 123.1, 120.9, 21.4 **(Figure S58)**. HRMS: $C_{14}H_{11}NS$ for $[M+H]^+$: 226.0690. Found: 226.0687. Anal.calcd for: $C_{14}H_{11}NS$: C 74.63, H 4.92, N 6.22, S 14.23; Found: C 74.64, H 4.92, N 6.21, S 14.23. FT-IR (KBr disc): v = 2923, 1657, 1513, 1457, 1312, 1250, 1113, 1049, 964, 765, 682cm^{-1}

4-methyl-2-phenylbenzo[d]thiazole (2v):



The pure product was obtained as a white solid (41.5 mg, 83%); m.p.139-140^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 6.5, 2.9 Hz, 2H), 7.78 – 7.70 (m, 1H), 7.49 (dd, *J* = 5.0, 1.6 Hz, 3H), 7.32 – 7.27 (m, 2H), 2.82 (s, 3H) **(Figure S59)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.6, 153.5, 135.0, 134.0, 133.4, 130.7, 129.0, 127.5, 126.8, 125.1, 119.0, 18.4 **(Figure S60)**. HRMS: $C_{14}H_{11}NS$ for $[M+H]^+$: 226.0690. Found: 226.0685. Anal.calcd for: $C_{14}H_{11}NS$: C 74.63, H 4.92, N 6.22, S 14.23; Found: C 74.64, H 4.91, N 6.23, S 14.22. FT-IR (KBr disc): v = 3076, 1480, 1430, 1260, 1222, 1073, 969, 903, 875, 804 760 cm^{-1}

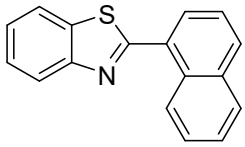
5,6-dimethyl-2-phenylbenzo[d]thiazole (2w):



The pure product was obtained as a white solid (46.5 mg, 93%); m.p. 150-151^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.19 – 8.01 (m, 2H), 7.87 (s, 1H), 7.65 (s, 1H), 7.58 – 7.41 (m, 3H), 2.41 (d, *J* = 4.8 Hz, 6H) **(Figure S61)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.0, 153.0, 135.6, 134.8, 133.9, 132.5, 130.6, 129.0, 127.4, 123.4, 121.5, 20.2, 20.2 **(Figure S62)**. HRMS: $C_{15}H_{13}NS$ for $[M+H]^+$: 240.0847. Found: 240.0849. Anal.calcd for: $C_{15}H_{13}NS$: C 75.28, H 5.48, N 5.85, S 13.40; Found: C 75.27, H 5.49, N 5.86, S

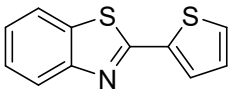
13.38. FT-IR (KBr disc): v= 2926, 1535, 1512, 1442, 1311, 1273, 1226, 1123, 1026, 949, 756 cm^{-1}

2-(naphthalen-1-yl) benzo[d]thiazole (2x):



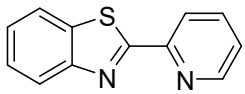
The pure product was obtained as a white solid (45.5 mg, 91%); m.p. 128-129^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.98 (d, *J* = 8.5 Hz, 1H), 8.23 (d, *J* = 8.1 Hz, 1H), 7.96 (DDD, *J* = 9.7, 8.7, 5.0 Hz, 4H), 7.65 (DDD, *J* = 8.5, 6.9, 1.4 Hz, 1H), 7.61 – 7.52 (m, 3H), 7.51 – 7.40 (m, 1H) **(Figure S63)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.5, 154.1, 135.4, 134.0, 131.0, 130.8, 130.6, 129.3, 128.4, 127.6, 126.5, 126.2, 125.8, 125.2, 124.9, 123.5, 121.3 **(Figure S64)**. HRMS: $C_{17}H_{11}NS$ for $[M+H]^+$: 262.0690. Found: 262.0684. Anal.calcd for: $C_{17}H_{11}NS$: C 78.13, H 4.24, N 5.36, S 12.27; Found: C 78.12, H 4.24, N 5.36, S 12.28. FT-IR (KBr disc): v= 1589, 1504, 1427, 1334, 1311, 1226, 1172, 1095, 933, 756.1 cm^{-1}

2-(thiophen-2-yl) benzo[d]thiazole (2y):



The pure product was obtained as a white solid (32 mg, 64%); m.p. 99-100^{o}C.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.1 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.65 (dd, *J* = 3.7, 0.9 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.48 – 7.42 (m, 1H), 7.40 – 7.33 (m, 1H), 7.18 – 7.08 (m, 1H) **(Figure S65)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.4, 153.7, 137.3, 134.7, 129.3, 128.6, 128.1, 126.5, 125.3, 123.0, 121.5 **(Figure S66)**. HRMS: $C_{11}H_7NS_2$ for $[M+H]^+$: 218.0098, Found: 218.0093. Anal.calcd for: $C_{11}H_7NS_2$: C 60.80, H 3.25, N 6.45, S 29.51; Found: C 60.81, H 3.25, N 6.44, S 29.50. FT-IR (KBr disc): v= 1535, 1473, 1411, 1311, 1219, 1080, 1049, 902, 848, 756 cm^{-1}

2-(pyridine-2-yl) benzo[d]thiazole (2z):



The pure product was obtained as a white solid (38 mg, 76%); m.p. 133-134°C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.4 Hz, 1H), 8.34 (d, *J* = 7.9 Hz, 1H), 8.08 (d, *J* = 8.1 Hz, 1H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.79 (dd, *J* = 15.4, 1.6 Hz, 1H), 7.57 – 7.43 (m, 1H), 7.38 (t, *J* = 7.6 Hz, 1H), 7.33 (dd, *J* = 6.6, 5.0 Hz, 1H) **(Figure S67)**. ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.4, 154.3, 151.4, 149.6, 137.0, 136.1, 126.3, 125.7, 125.3, 123.6, 122.0, 120.8 **(Figure S68)**. HRMS: $C_{12}H_8N_2S$ for $[M+H]^+$: 213.0486, Found: 213.0481. Anal.calcd for: $C_{12}H_8N_2S$: C 67.90, H 3.80, N 13.20, S 15.10; Found: C 67.91, H 3.79, N 13.19, S 15.11. FT-IR (KBr disc): v= 1581, 1512, 1458, 1427, 1311, 1234, 1157, 1087, 979, 756.1 cm^{-1}

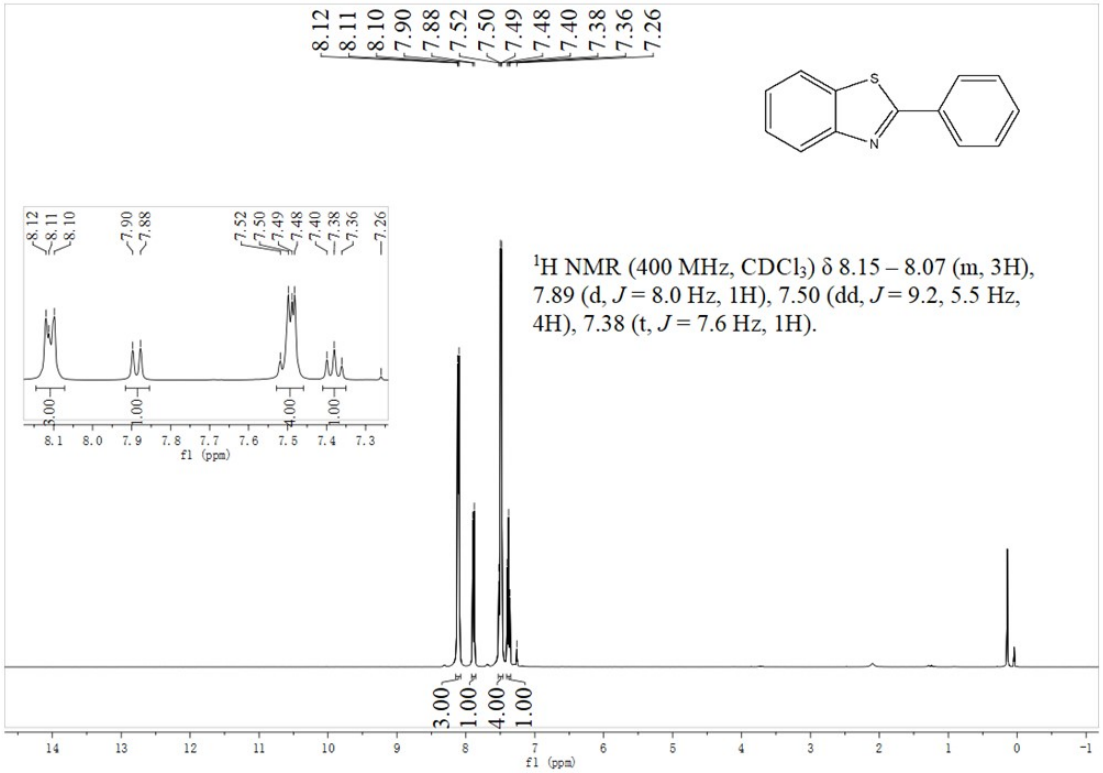


Figure S15. ^{1}H NMR of 2-phenylbenzo[d]thiazole **(2a)**

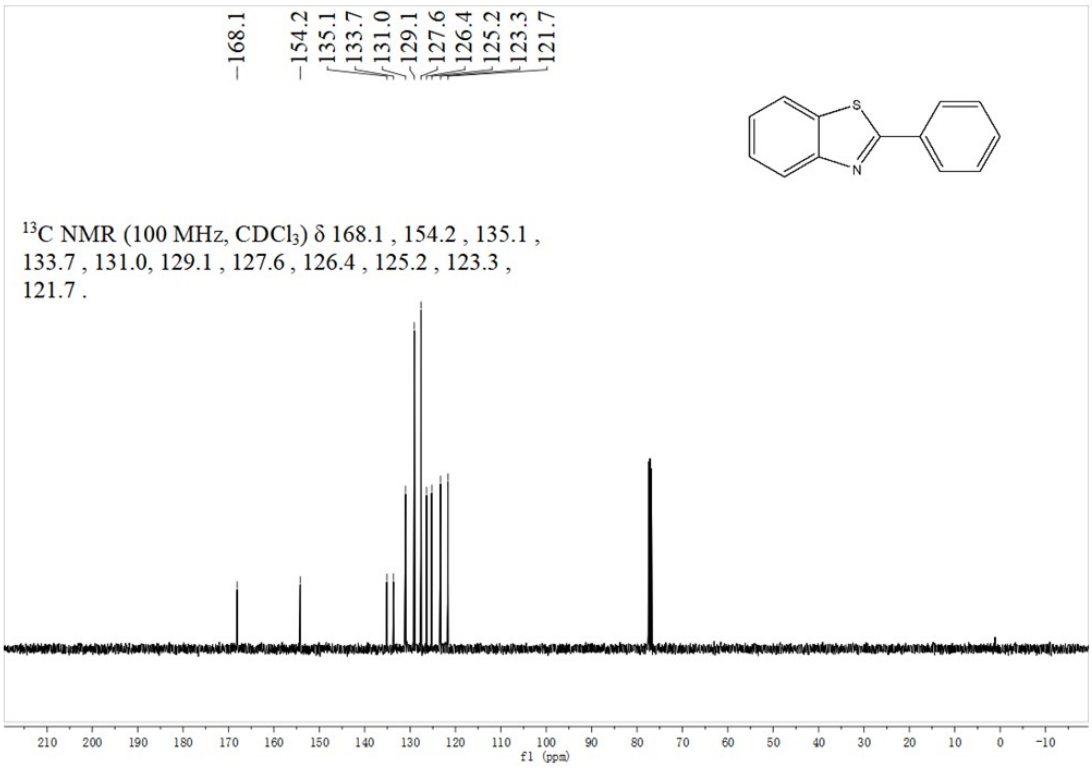


Figure S16. ^{13}C NMR of 2-phenylbenzo[d]thiazole **(2a)**

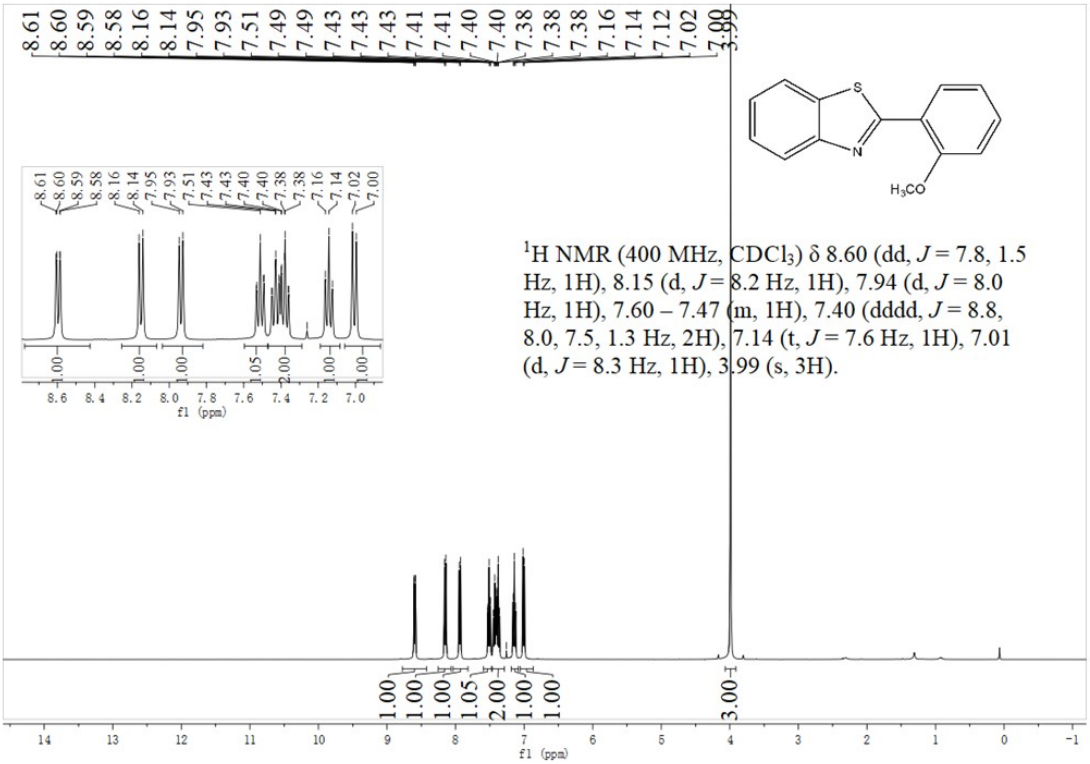


Figure S17. [1]H NMR of 2-(2-methoxyphenyl) benzo[d]thiazole **(2b)**

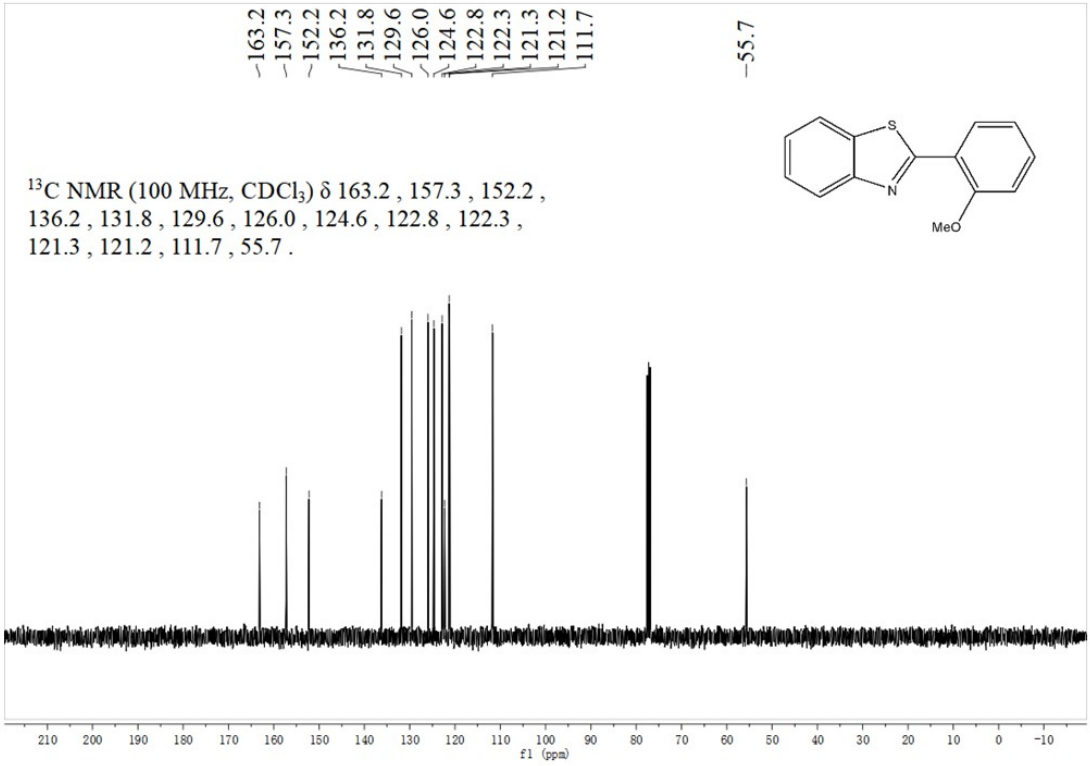


Figure S18. [13]C NMR of 2-(2-methoxyphenyl) benzo[d]thiazole **(2b)**

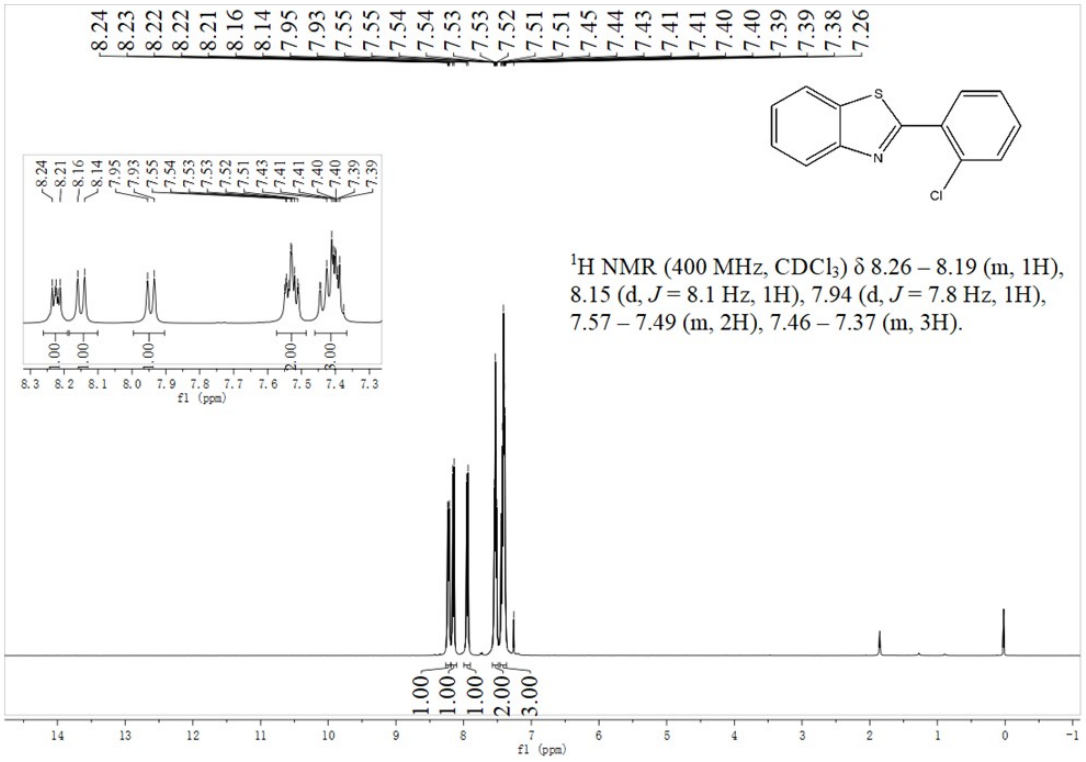


Figure S19. ^{1}H NMR of 2-(2-chlorophenyl) benzo[d]thiazole **(2c)**

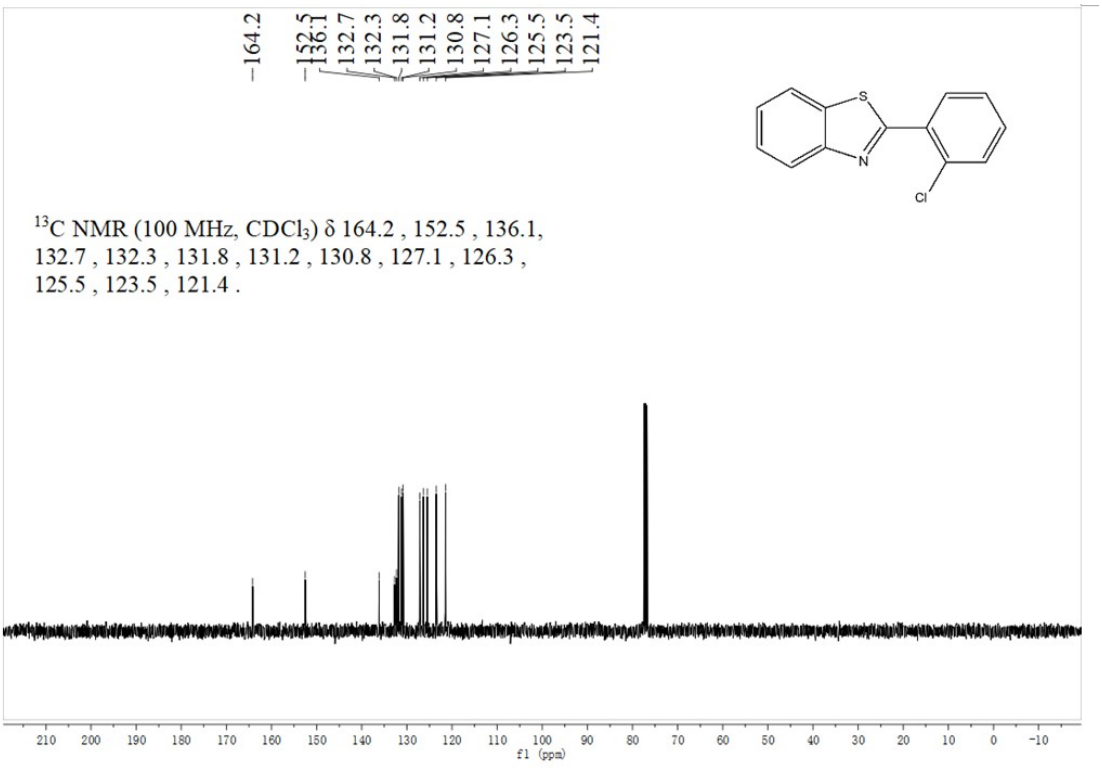


Figure S20. ^{13}C NMR of 2-(2-chlorophenyl) benzo[d]thiazole **(2c)**

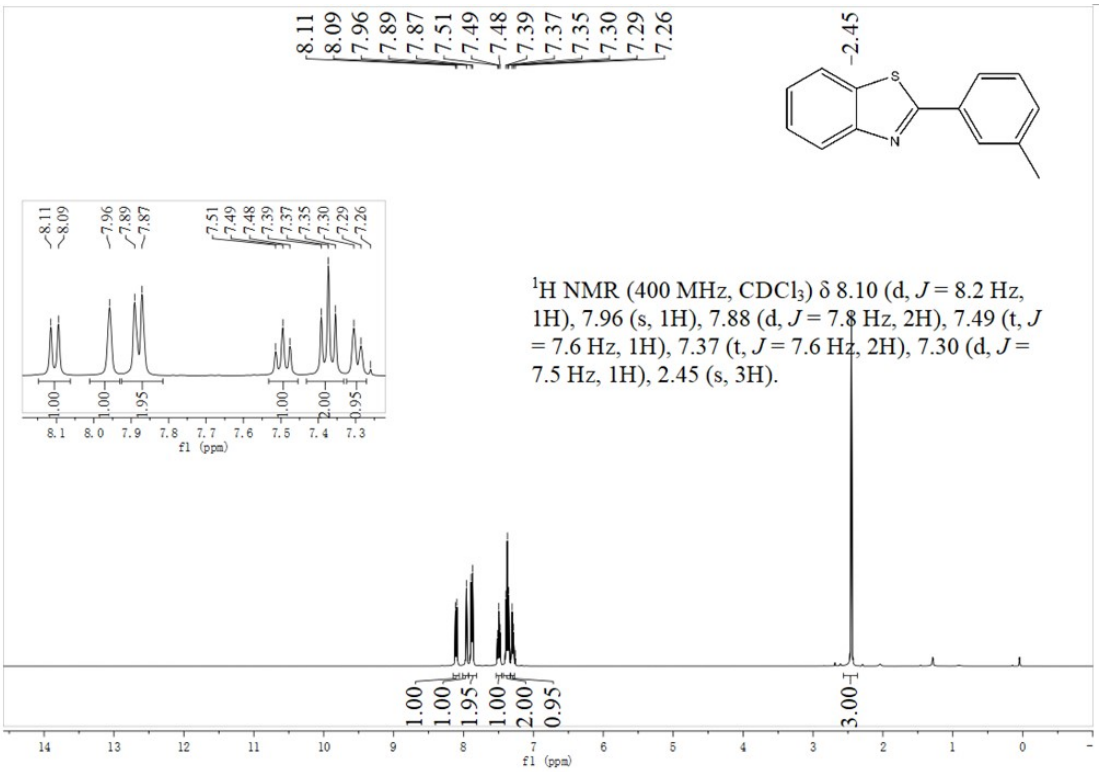


Figure S21. ^{1}H NMR of 2-(*m*-tolyl) benzo[d]thiazole **(2d)**

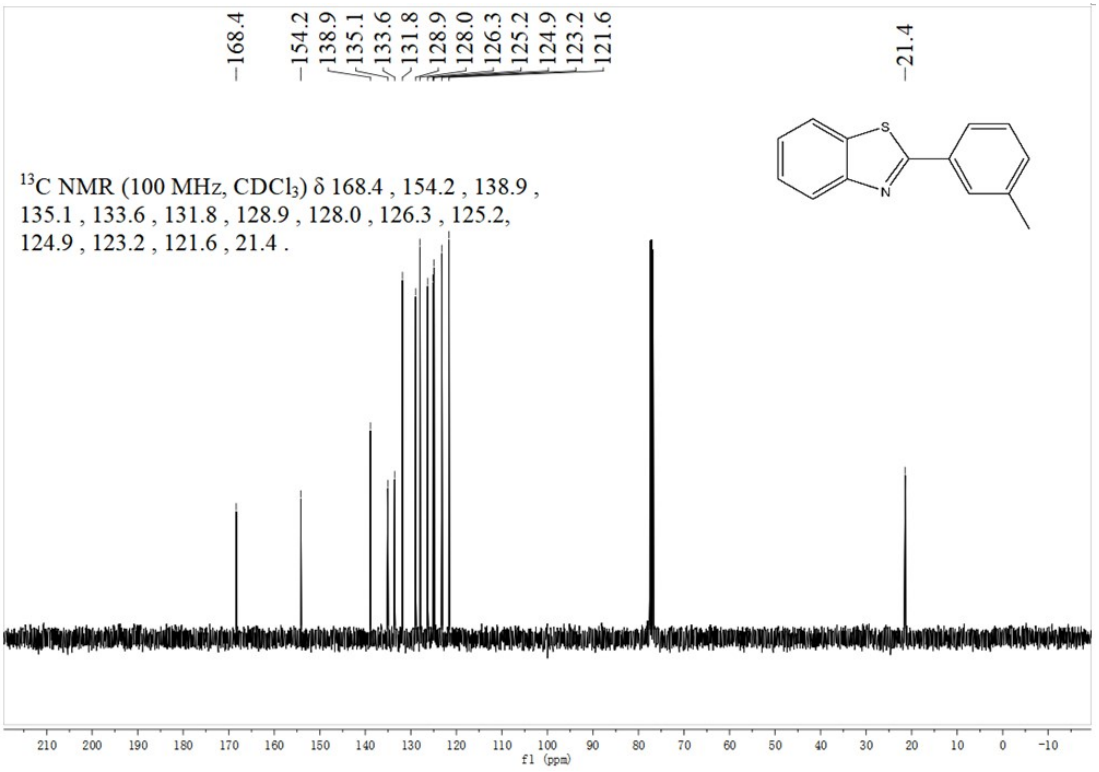


Figure S22. ^{13}C NMR of 2-(*m*-tolyl) benzo[d]thiazole **(2d)**

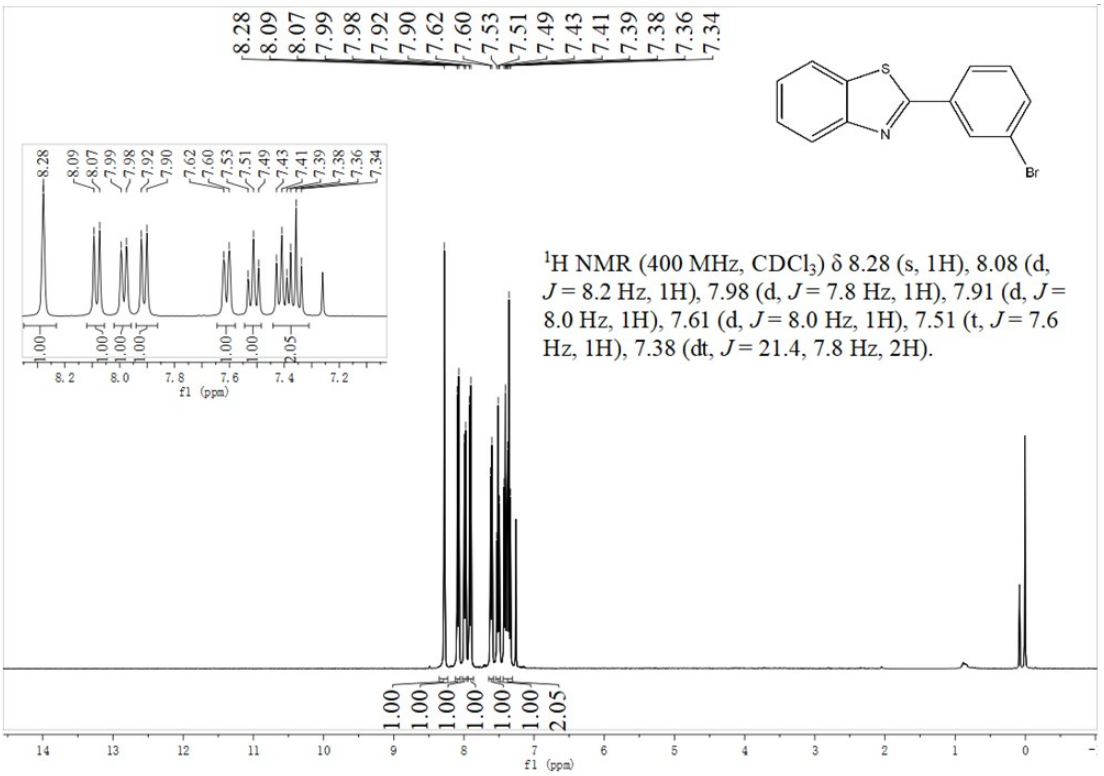


Figure S23. ^{1}H NMR of 2-(3-bromophenyl) benzo[d]thiazole **(2e)**

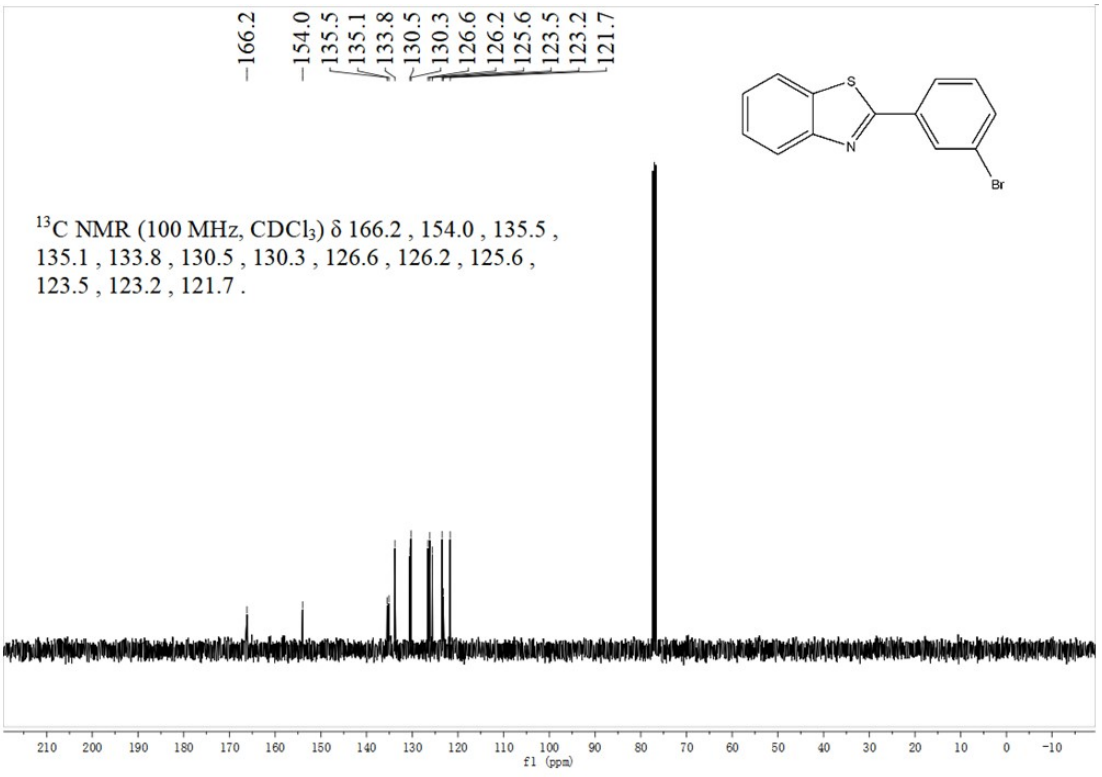


Figure S24. ^{13}C NMR of 2-(3-bromophenyl) benzo[d]thiazole **(2e)**

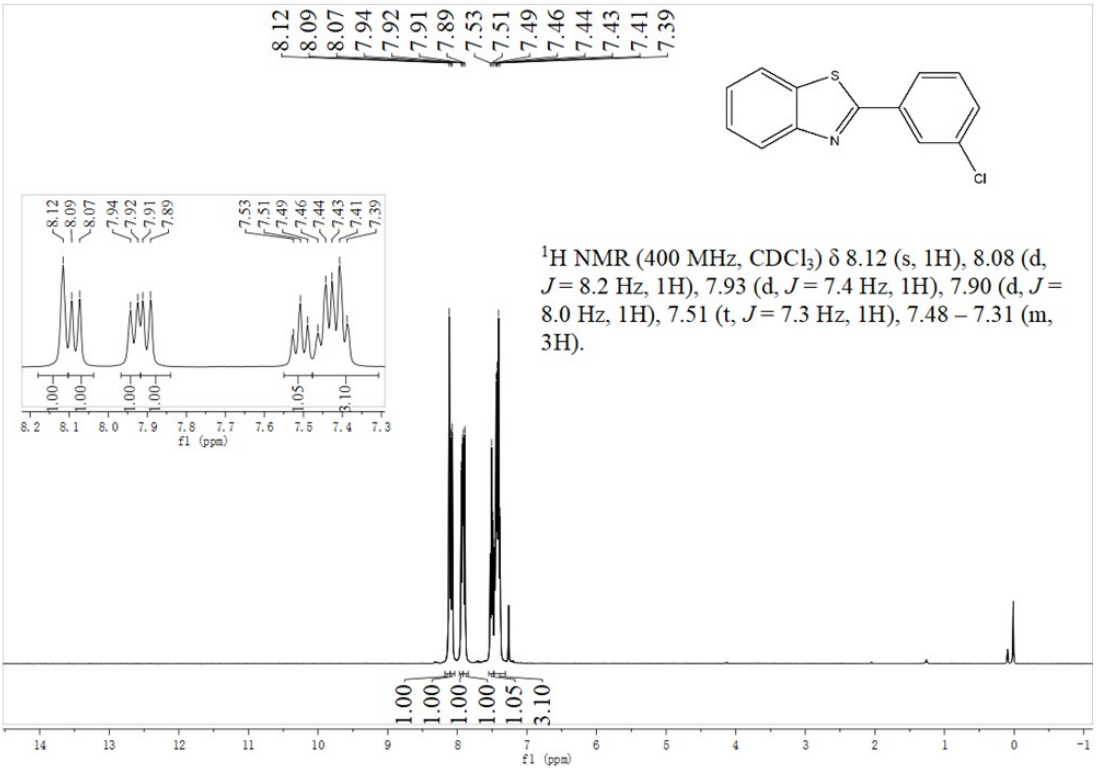


Figure S25. ^{1}H NMR of 2-(3-chlorophenyl) benzo[d]thiazole **(2f)**

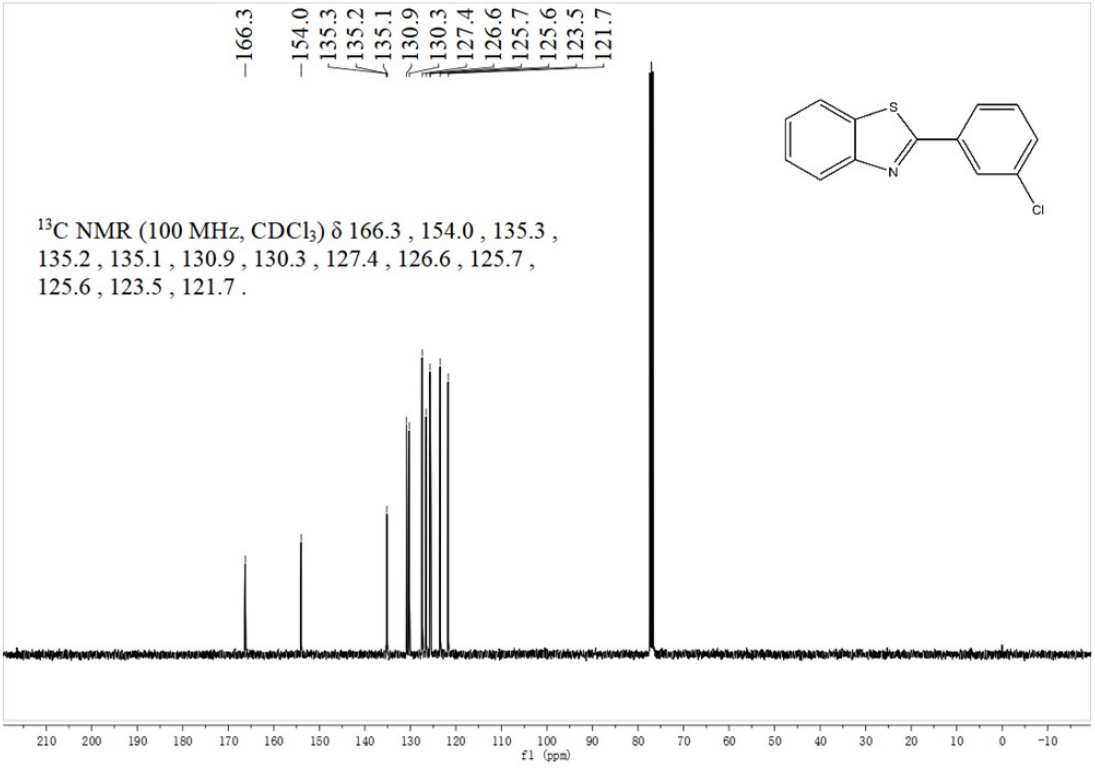


Figure S26. ^{13}C NMR of 2-(3-chlorophenyl) benzo[d]thiazole **(2f)**

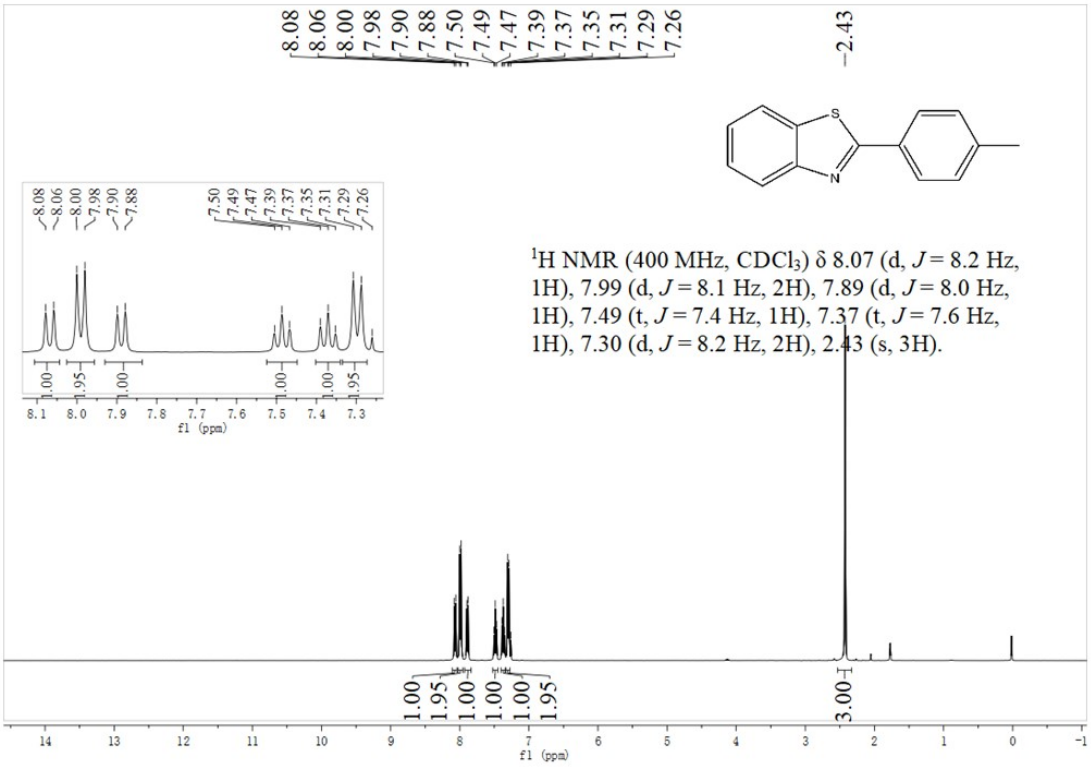


Figure S27. ^{1}H NMR of 2-(*p*-tolyl) benzo[d]thiazole **(2g)**

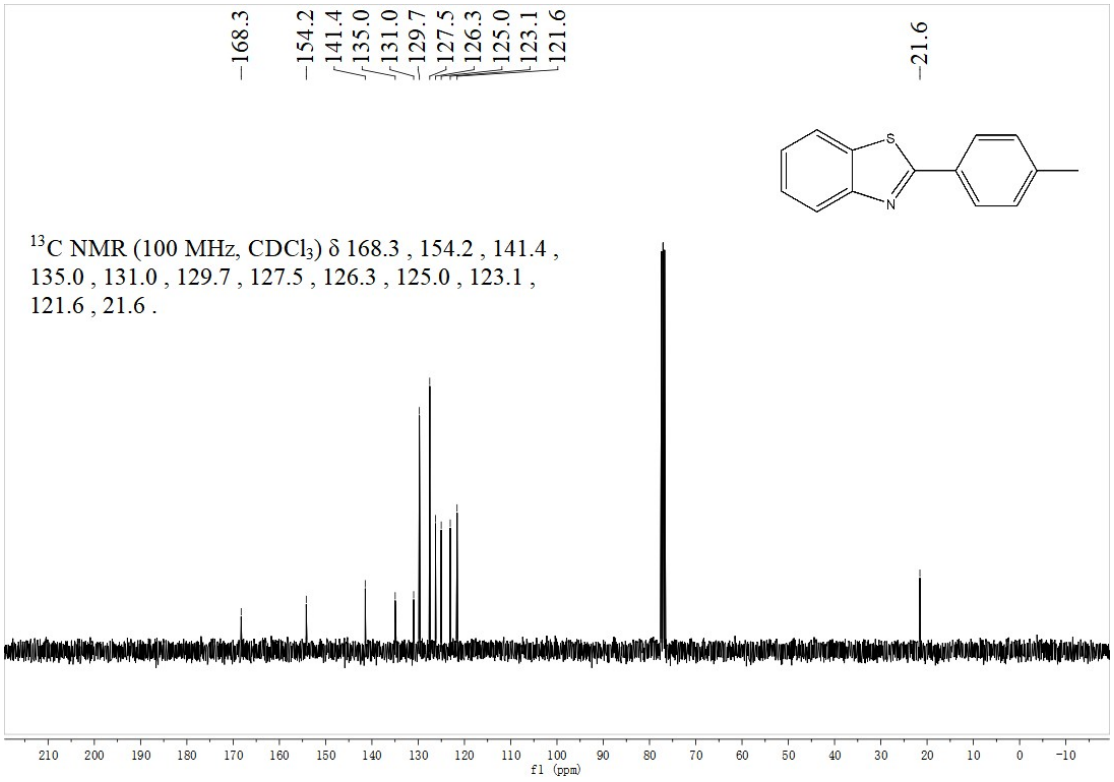


Figure S28. ^{13}C NMR of 2-(*p*-tolyl) benzo[d]thiazole **(2g)**

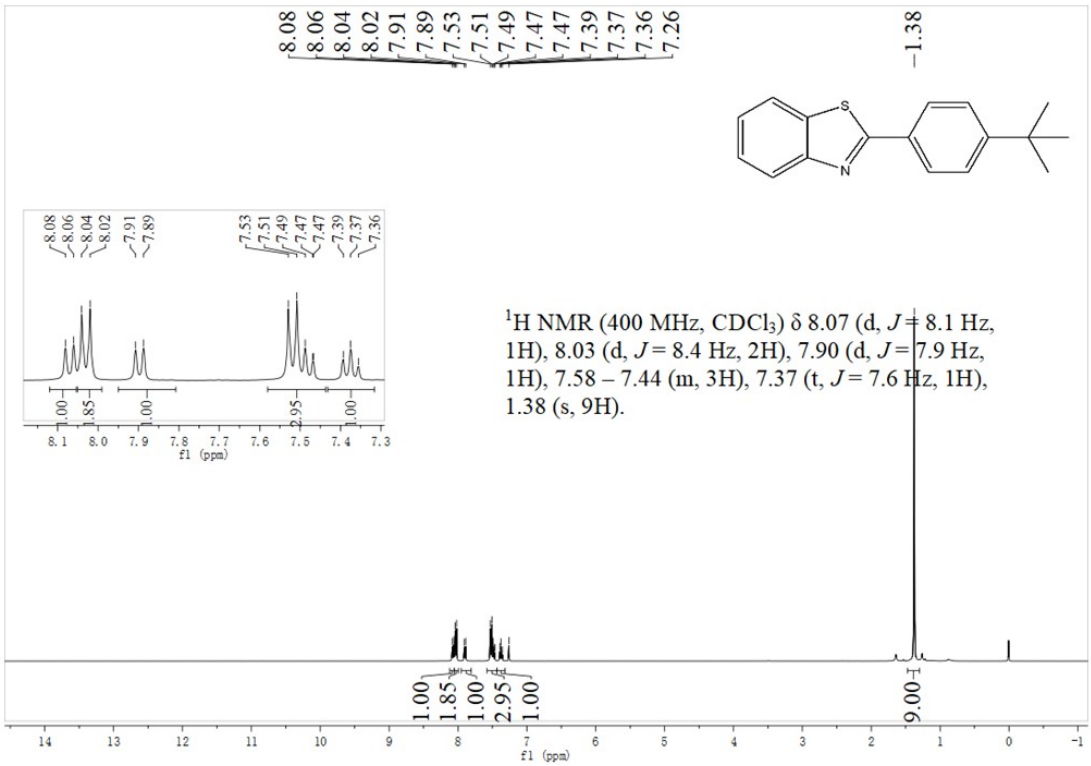


Figure S29. ^{1}H NMR of 2-(4-(tert-butyl) phenyl) benzo[d]thiazole **(2h)**

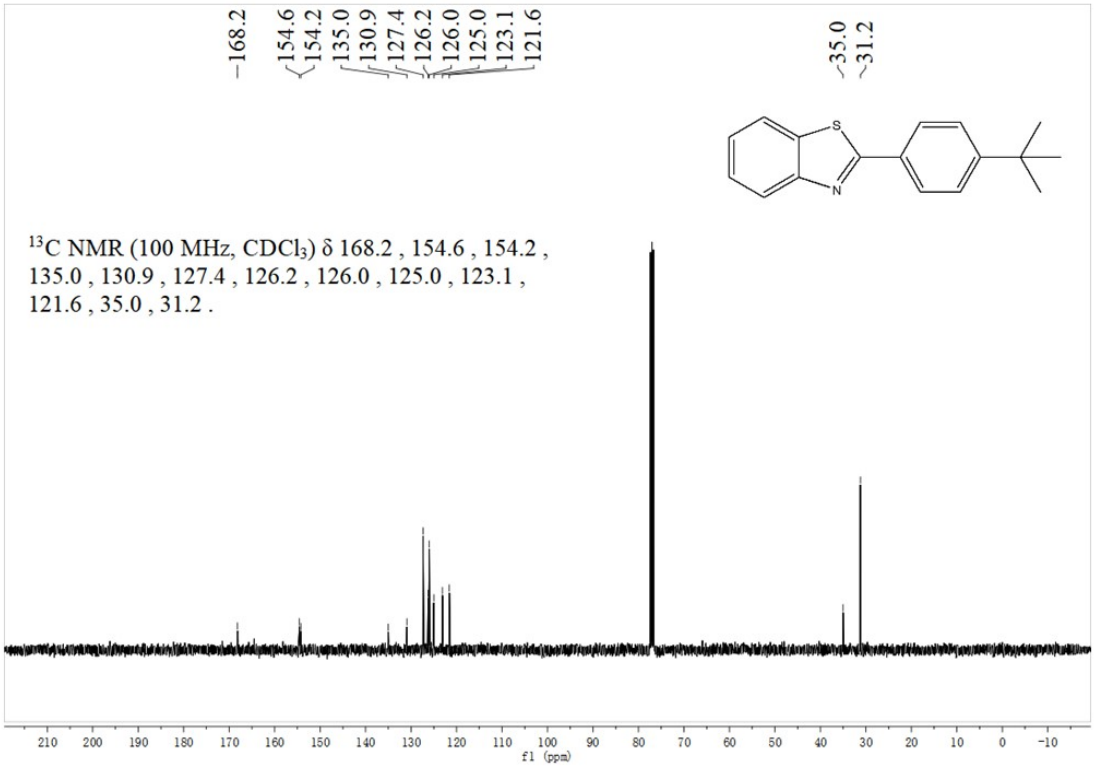


Figure S30. ^{13}C NMR of 2-(4-(tert-butyl) phenyl) benzo[d]thiazole **(2h)**

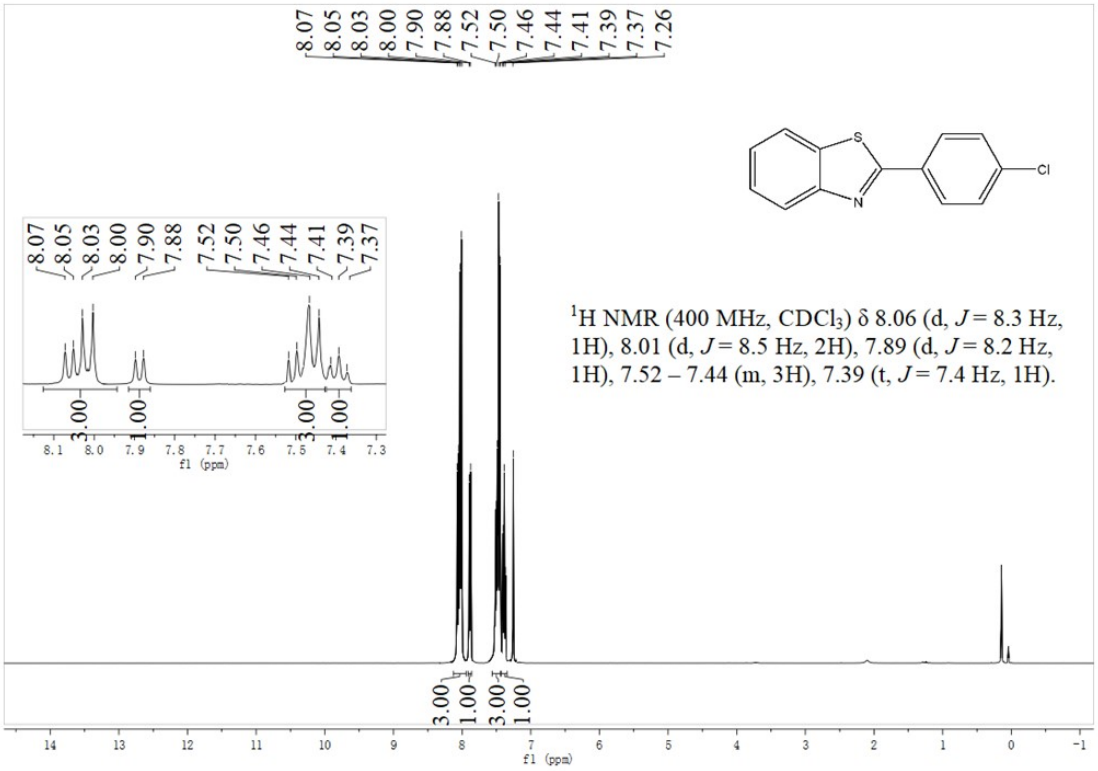


Figure S31. ^{1}H NMR of 2-(4-chlorophenyl)benzo[d]thiazole **(2i)**

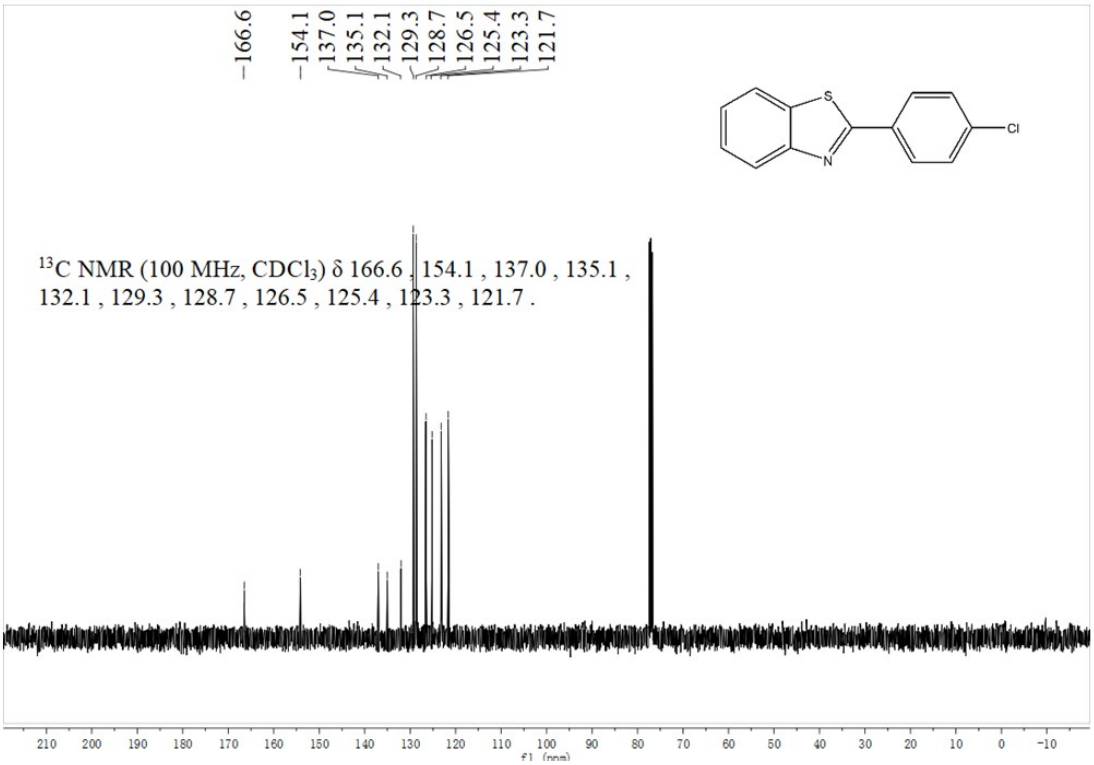


Figure S32. ^{13}C NMR of 2-(4-chlorophenyl)benzo[d]thiazole **(2i)**

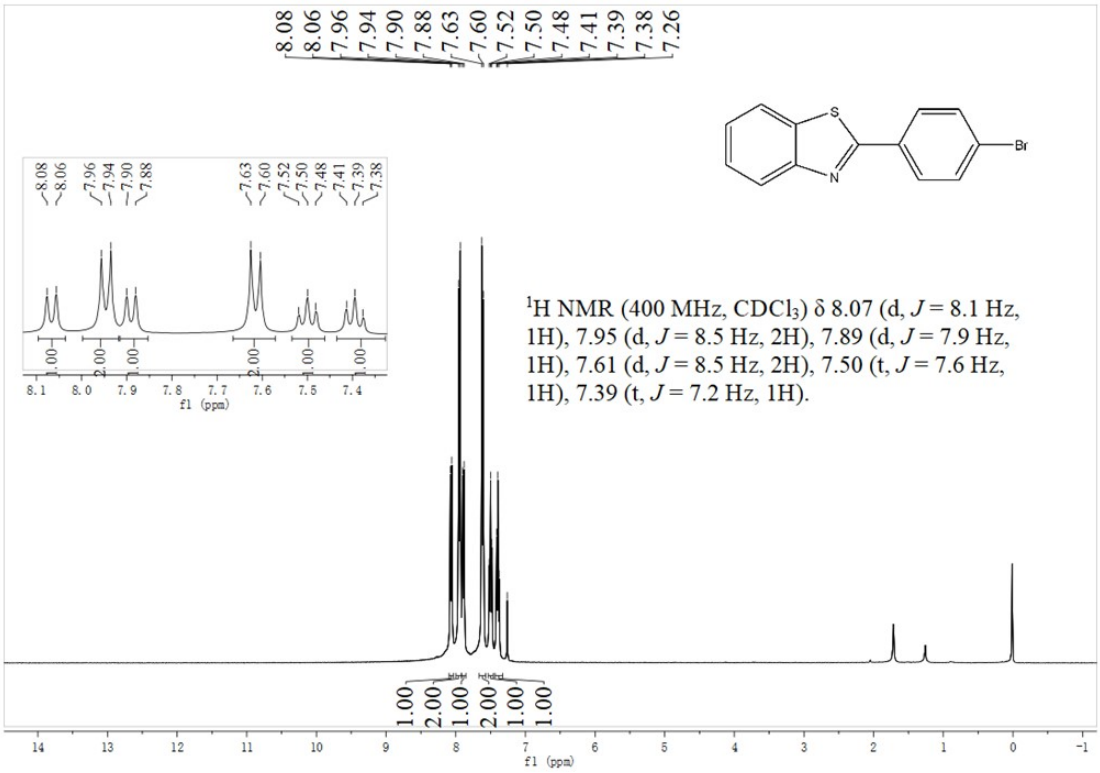


Figure S33. ^{1}H NMR of 2-(4-bromophenyl) benzo[d]thiazole **(2j)**

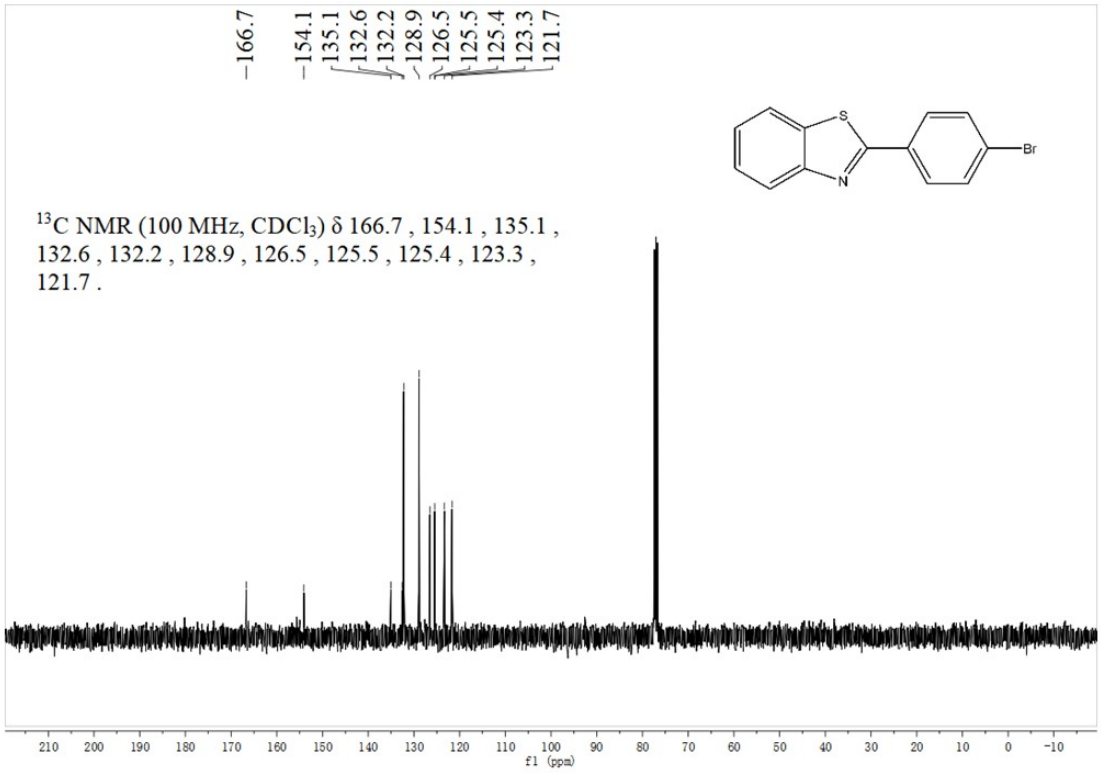


Figure S34. ^{13}C NMR of 2-(4-bromophenyl) benzo[d]thiazole **(2j)**

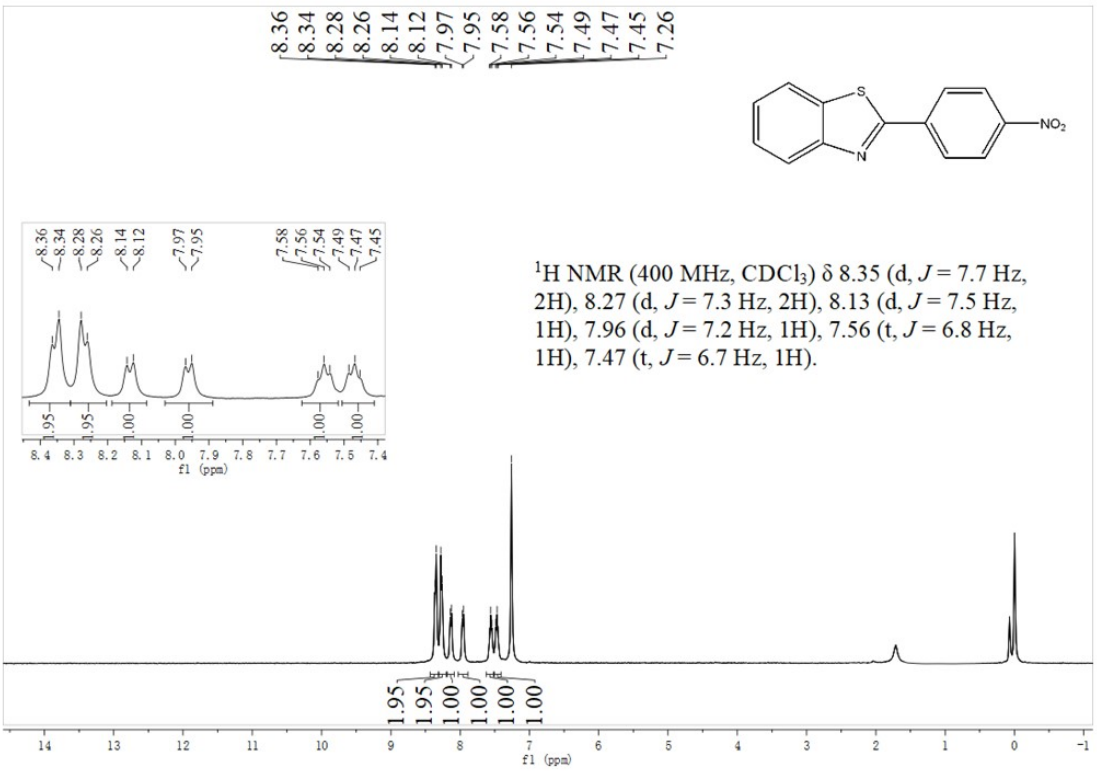


Figure S35. [1]H NMR of 2-(4-nitrophenyl) benzo[d]thiazole **(2k)**

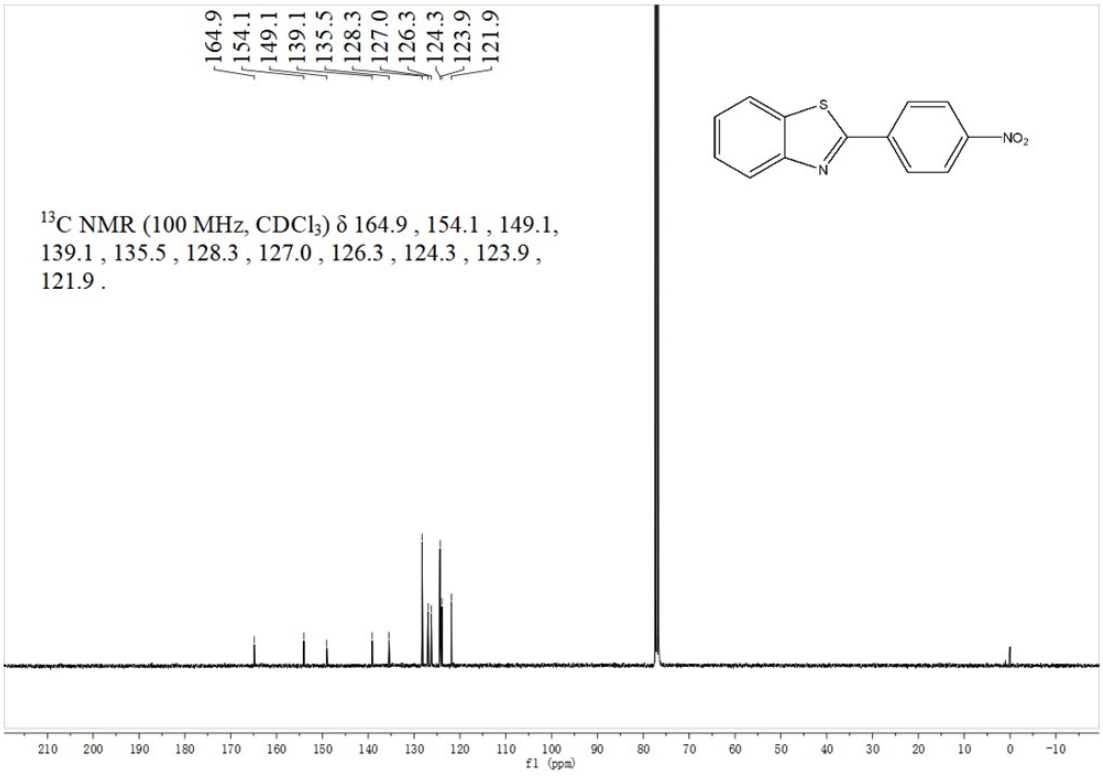


Figure S36. [13]C NMR of 2-(4-nitrophenyl) benzo[d]thiazole **(2k)**

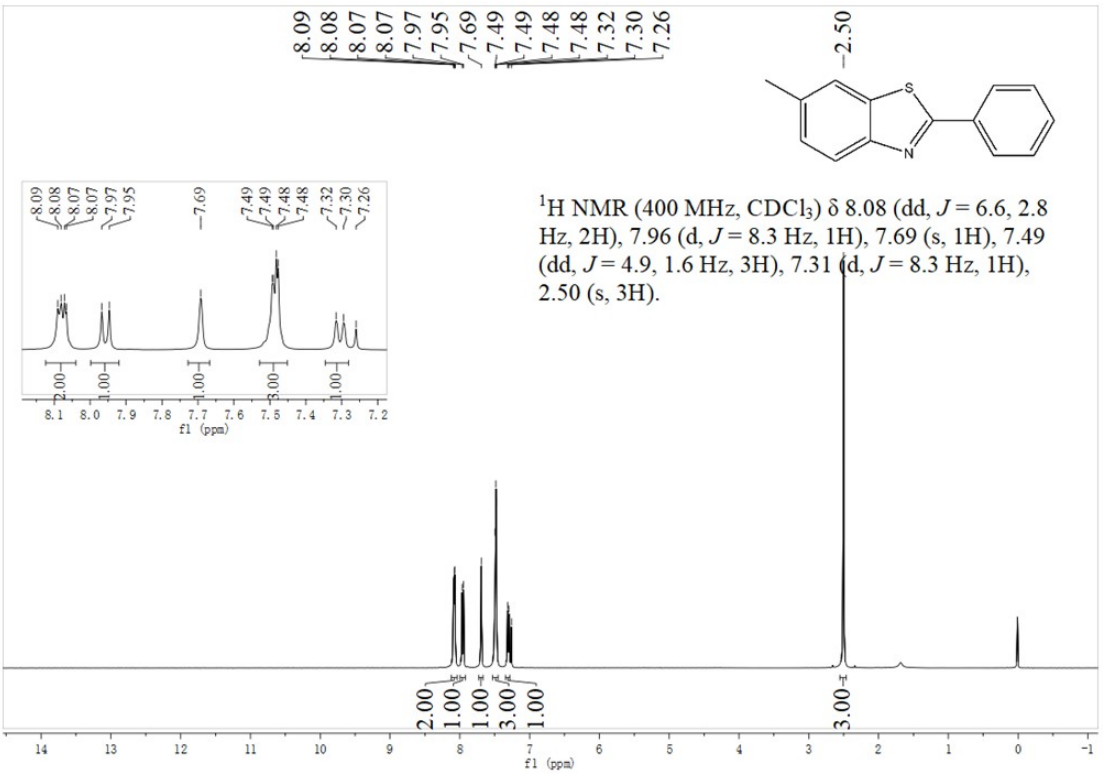


Figure S37. ^{1}H NMR of 6-methyl-2-phenylbenzo[d]thiazole **(2l)**

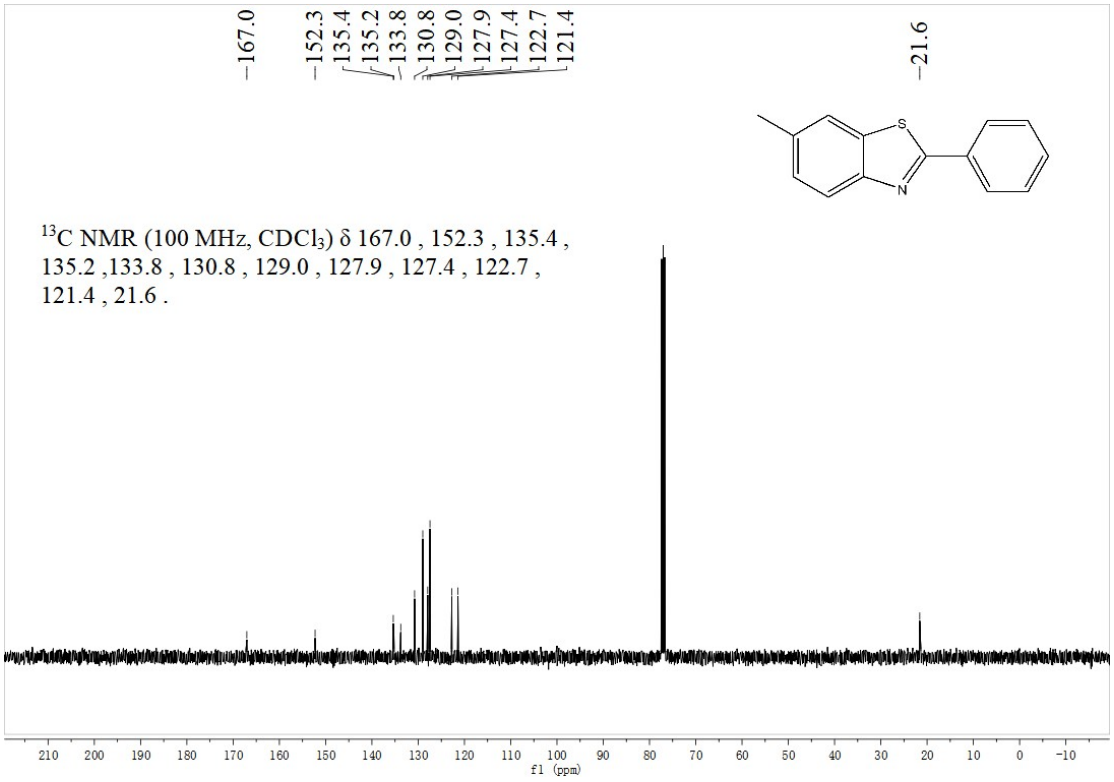


Figure S38. ^{13}C NMR of 6-methyl-2-phenylbenzo[d]thiazole **(2l)**

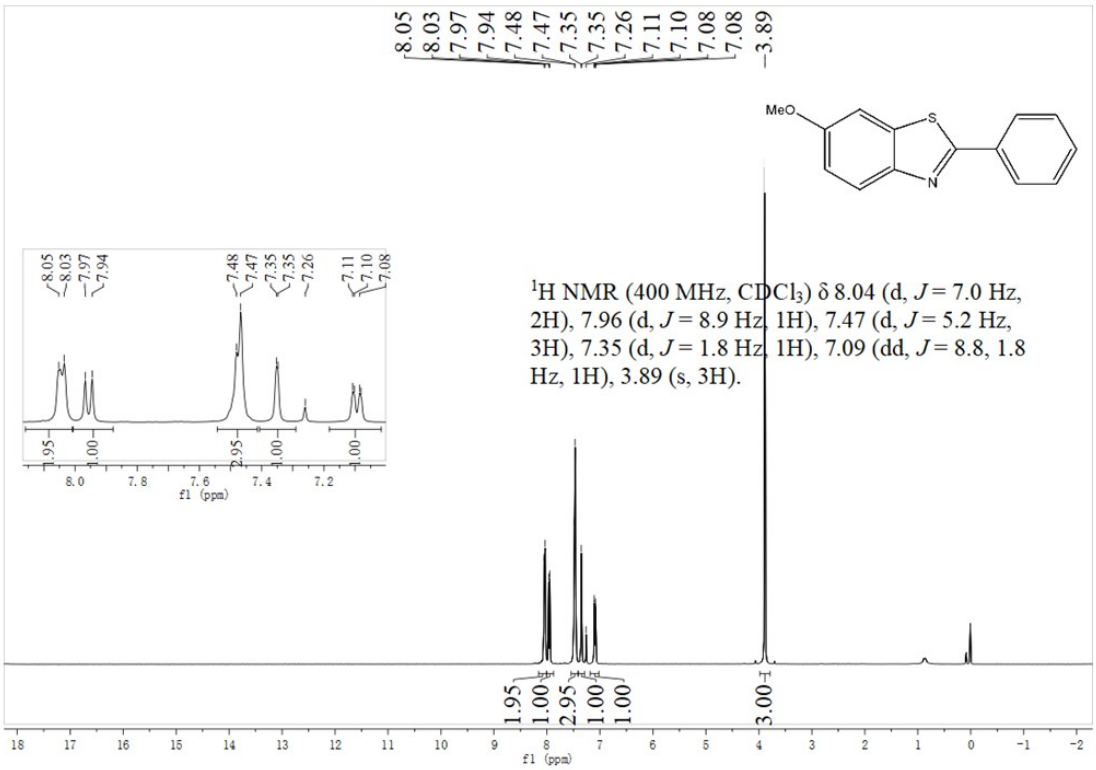


Figure S39. ^{1}H NMR of 6-methoxy-2-phenylbenzo[d]thiazole **(2m)**

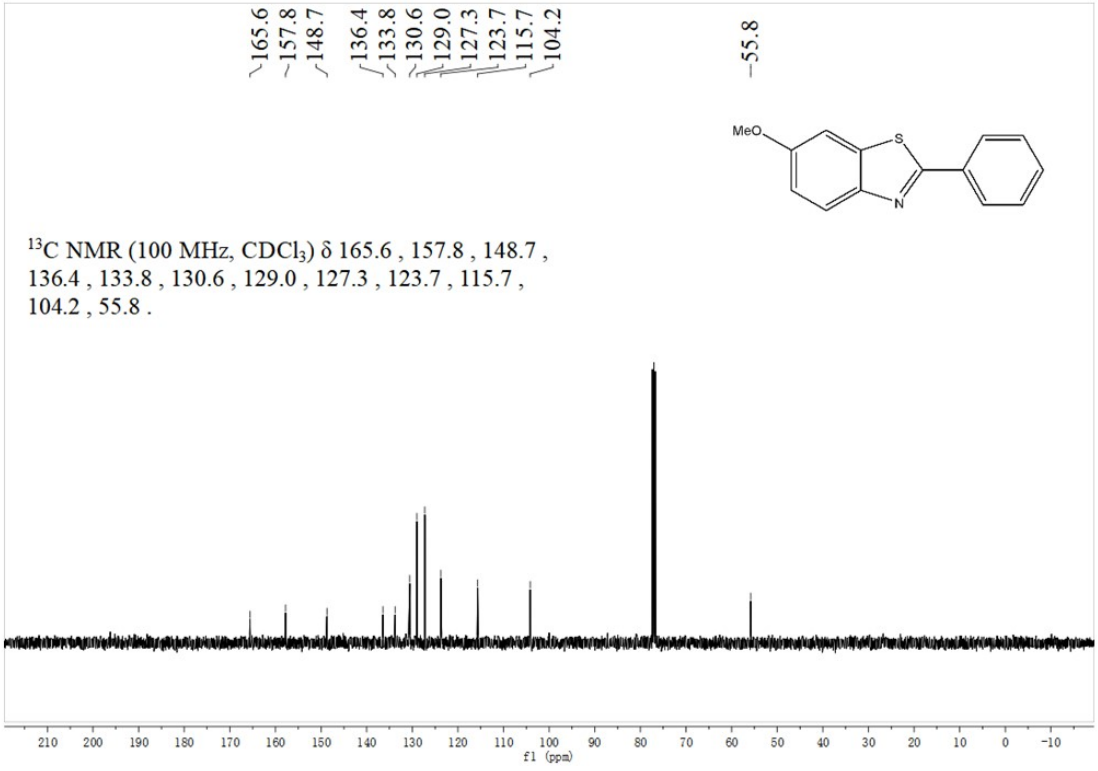


Figure S40. ^{13}C NMR of 6-methoxy-2-phenylbenzo[d]thiazole **(2m)**

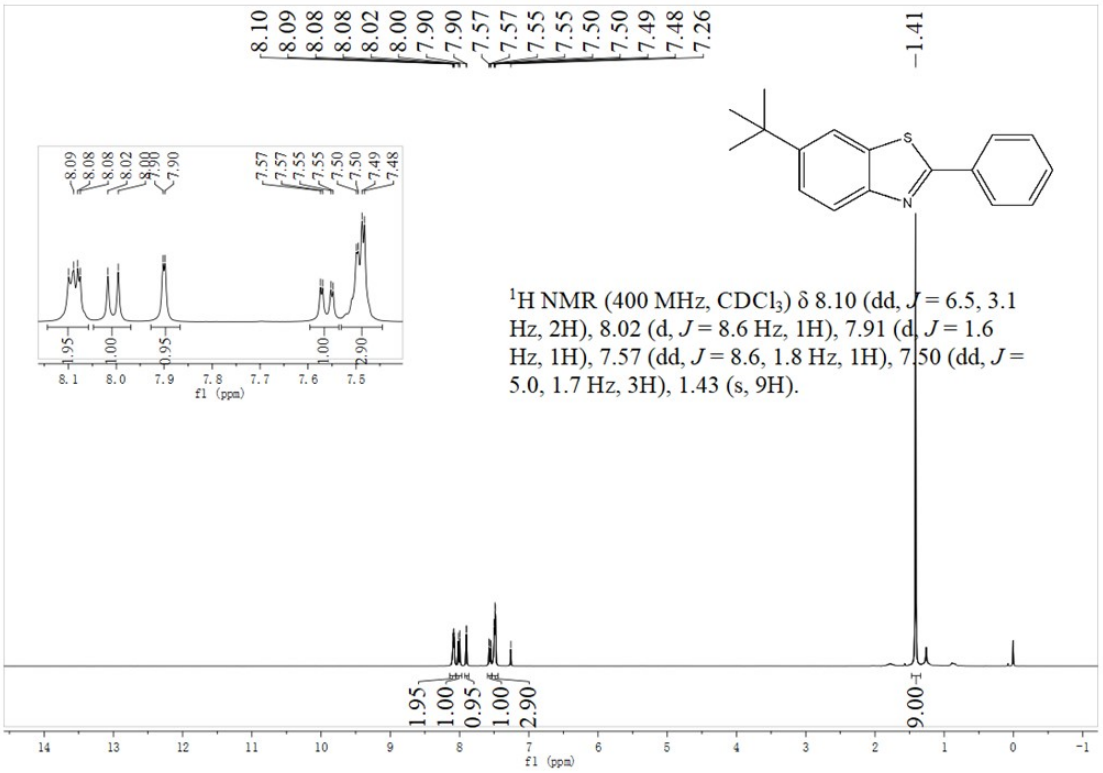


Figure S41. ^{1}H NMR of 6-(tert-butyl)-2-phenylbenzo[d]thiazole **(2n)**

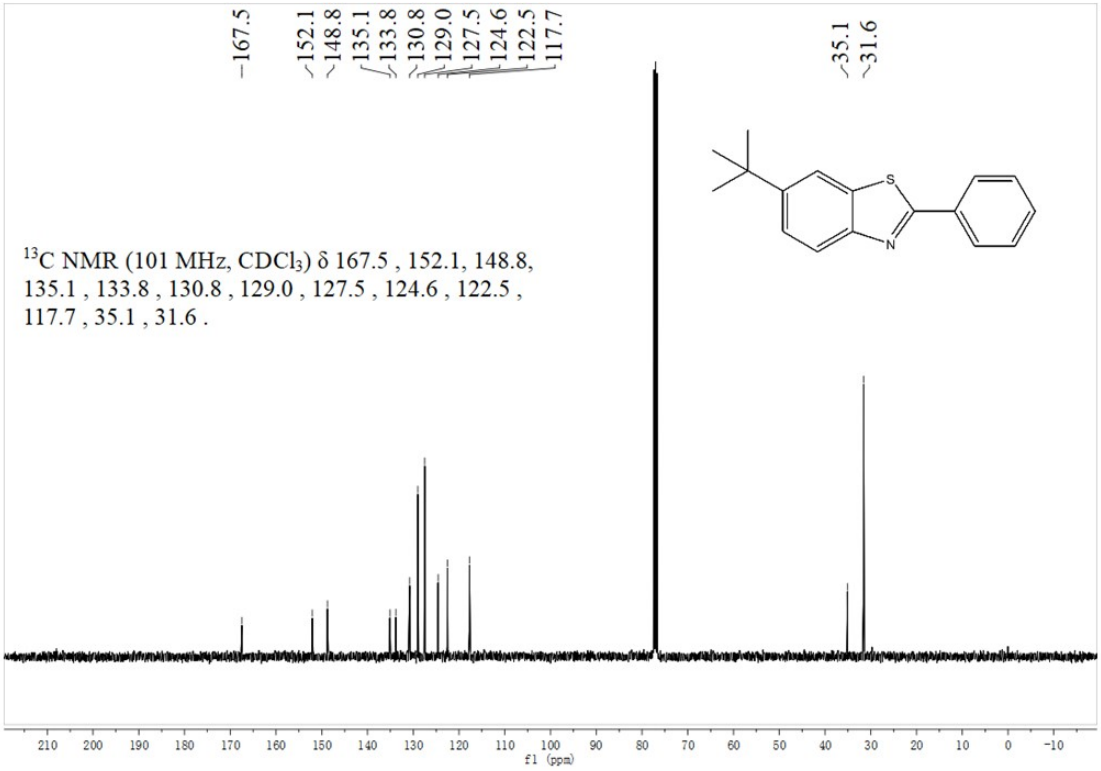


Figure S42. ^{13}C NMR of 6-(tert-butyl)-2-phenylbenzo[d]thiazole **(2n)**

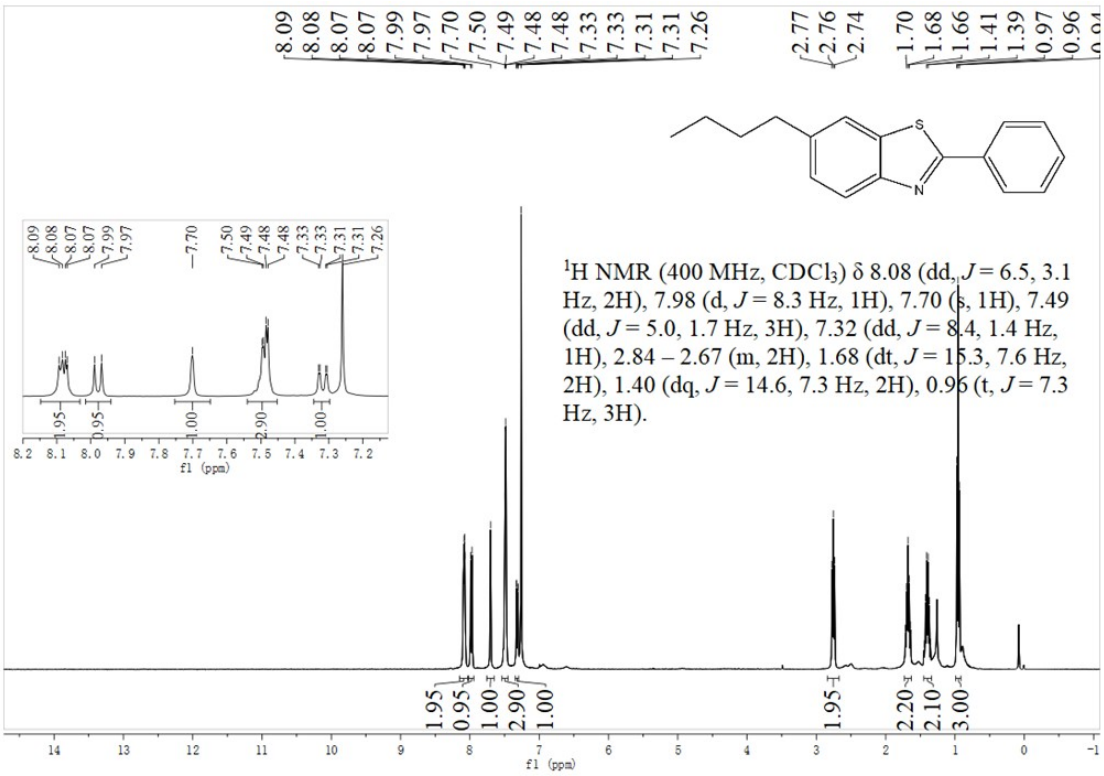


Figure S43. ^{1}H NMR of 6-butyl-2-phenylbenzo[d]thiazole **(2o)**

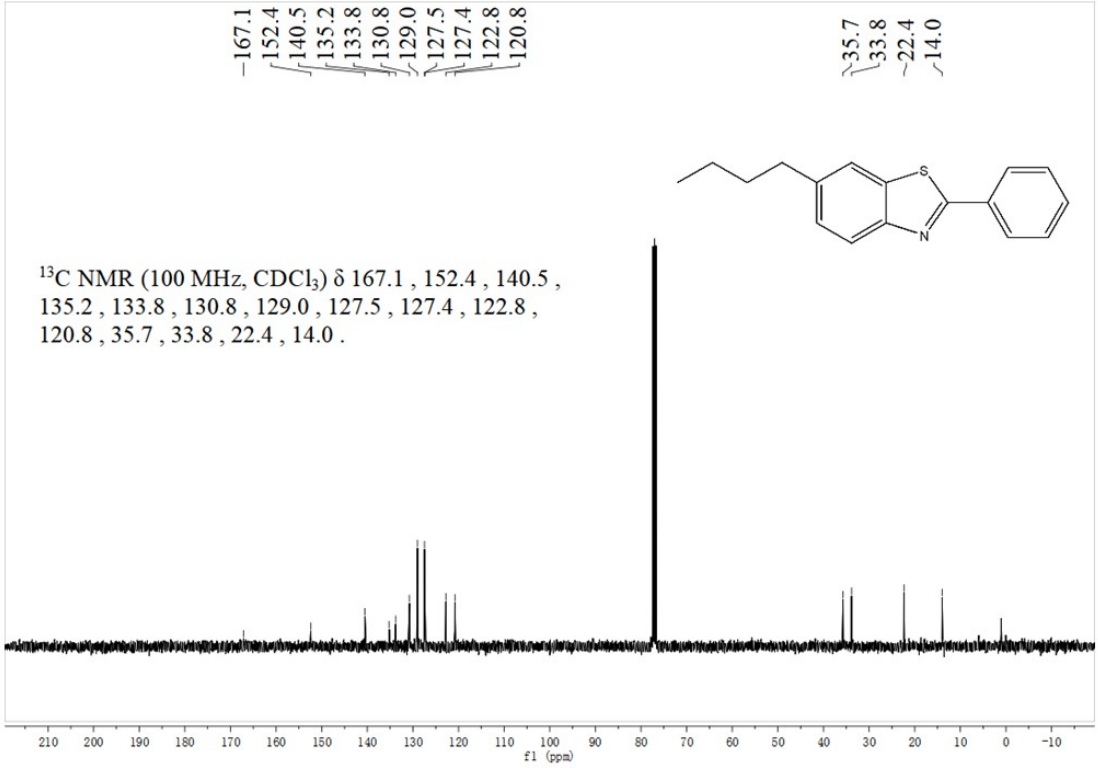


Figure S44. ^{13}C NMR of 6-butyl-2-phenylbenzo[d]thiazole **(2o)**

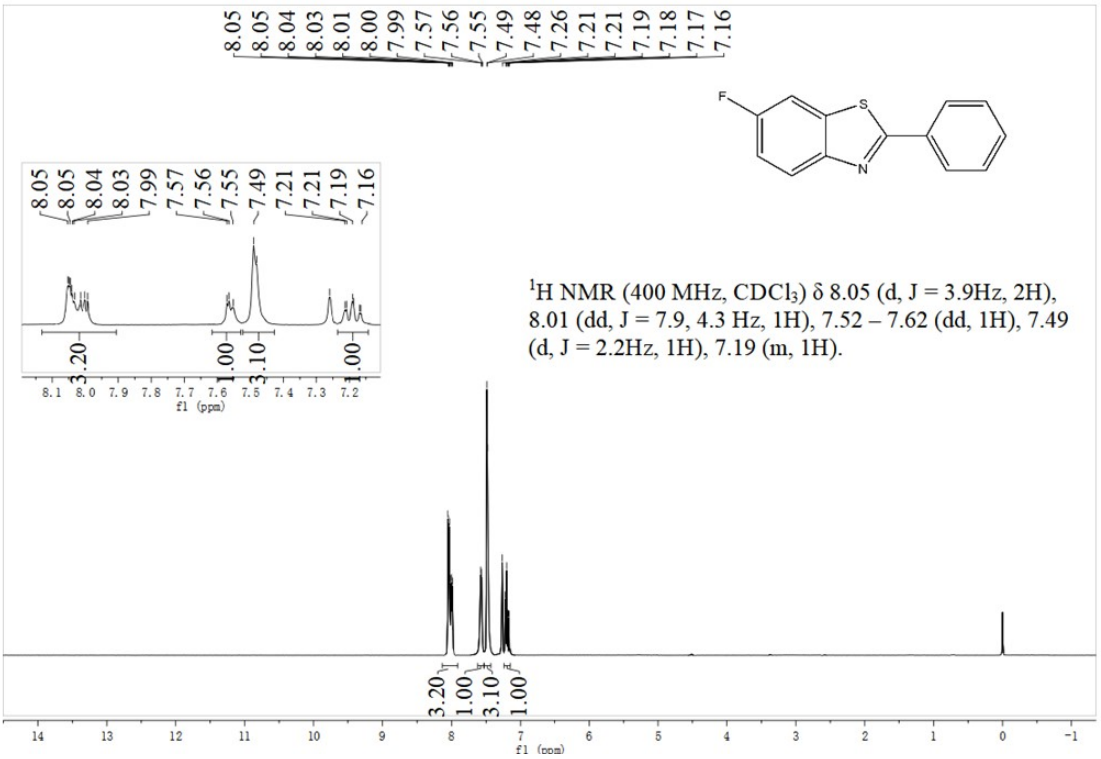


Figure S45. ^{1}H NMR of 6-fluoro-2-phenylbenzo[d]thiazole **(2p)**

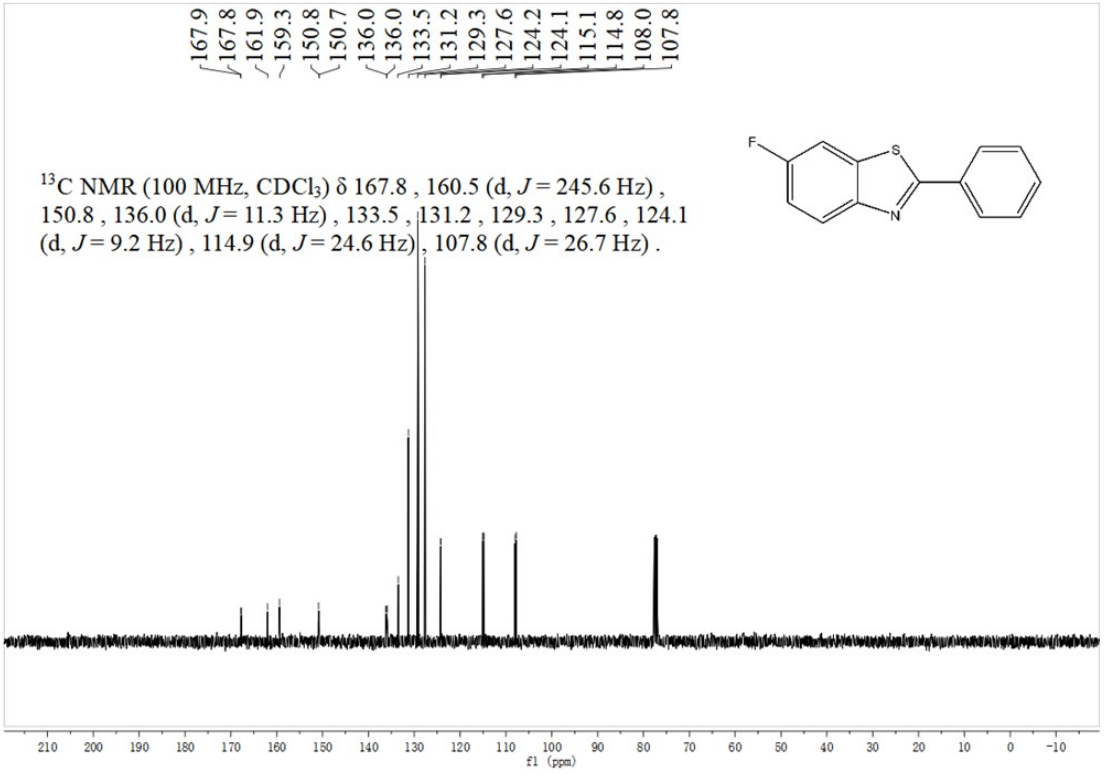


Figure S46. ^{13}C NMR of 6-fluoro-2-phenylbenzo[d]thiazole **(2p)**

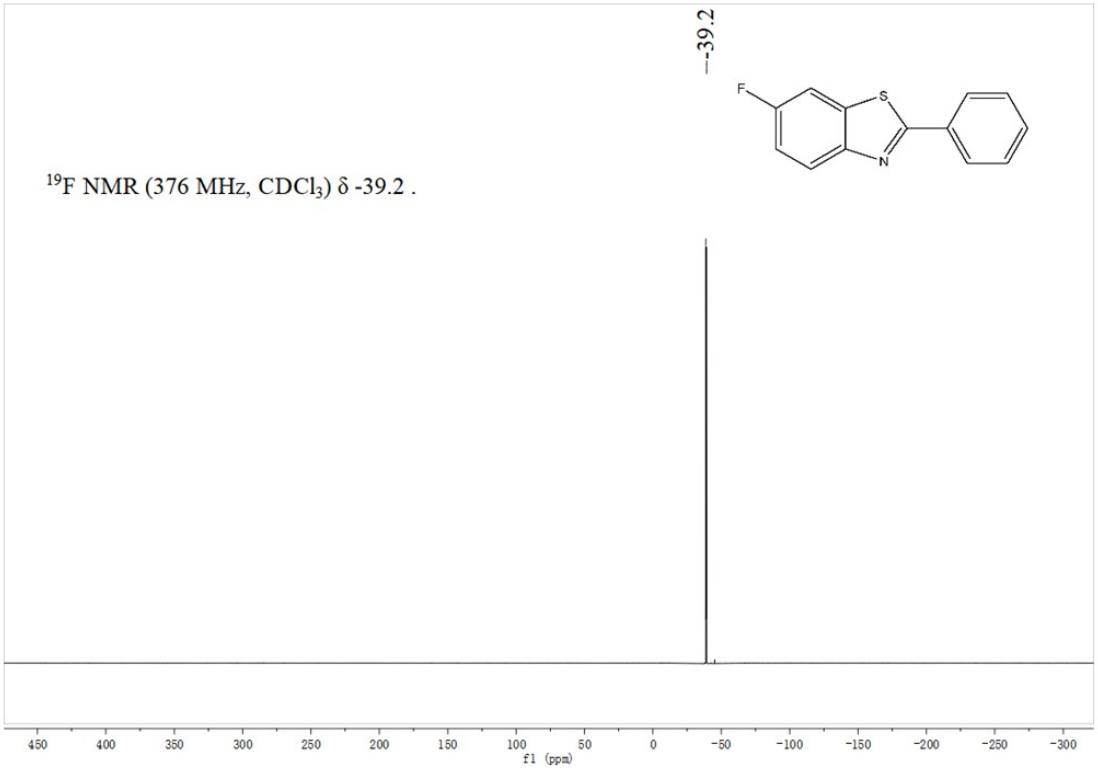


Figure S47. ^{19}F NMR of 6-fluoro-2-phenylbenzo[d]thiazole **(2p)**

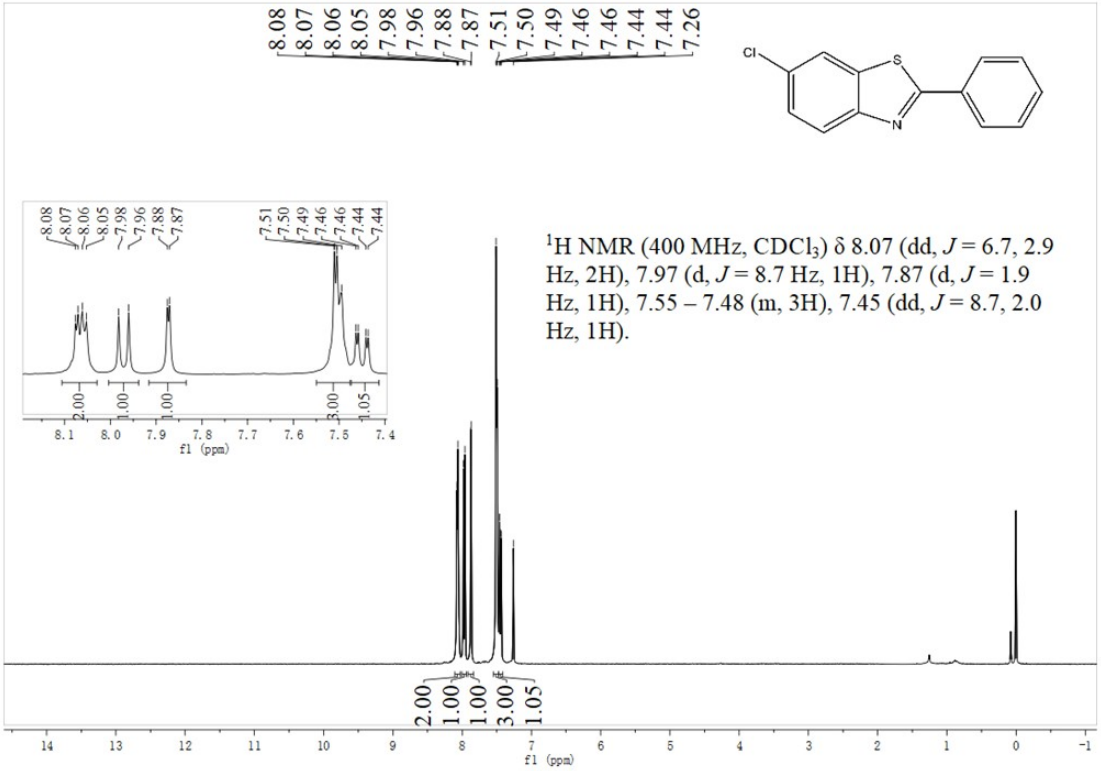


Figure S48. ^{1}H NMR of 6-chloro-2-phenylbenzo[d]thiazole **(2q)**

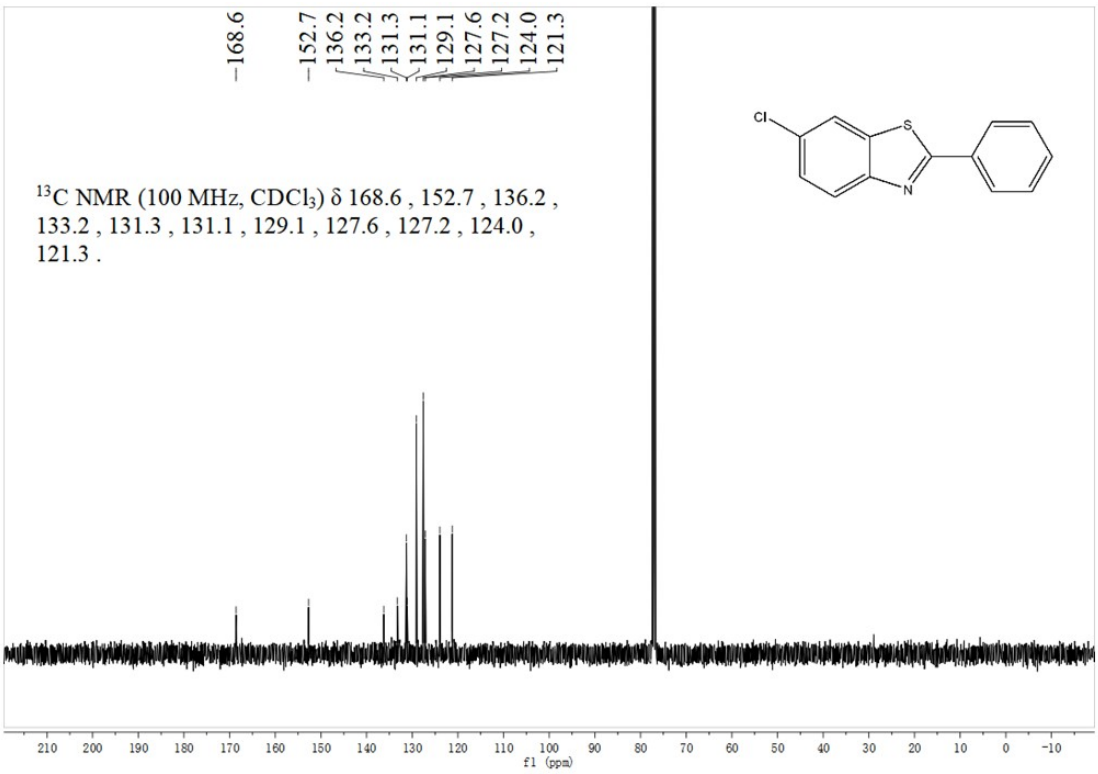


Figure S49. ^{13}C NMR of 6-chloro-2-phenylbenzo[d]thiazole **(2q)**

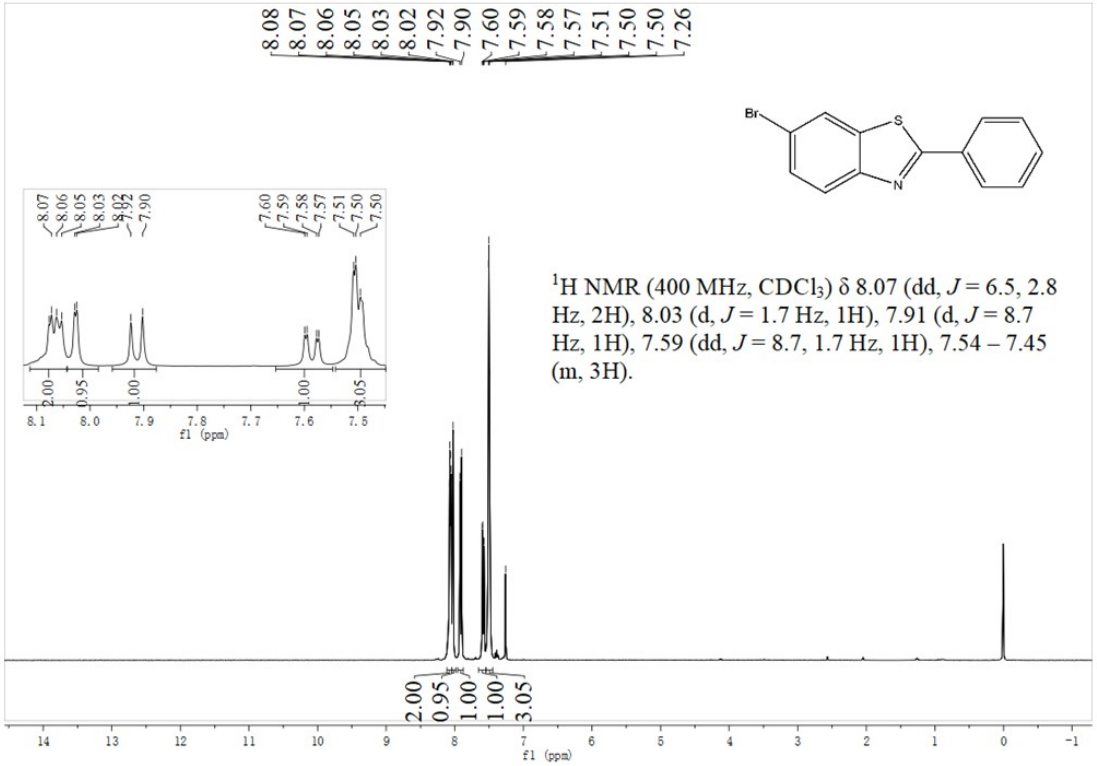


Figure S50. ^{1}H NMR of 6-bromo-2-phenylbenzo[d]thiazole **(2r)**

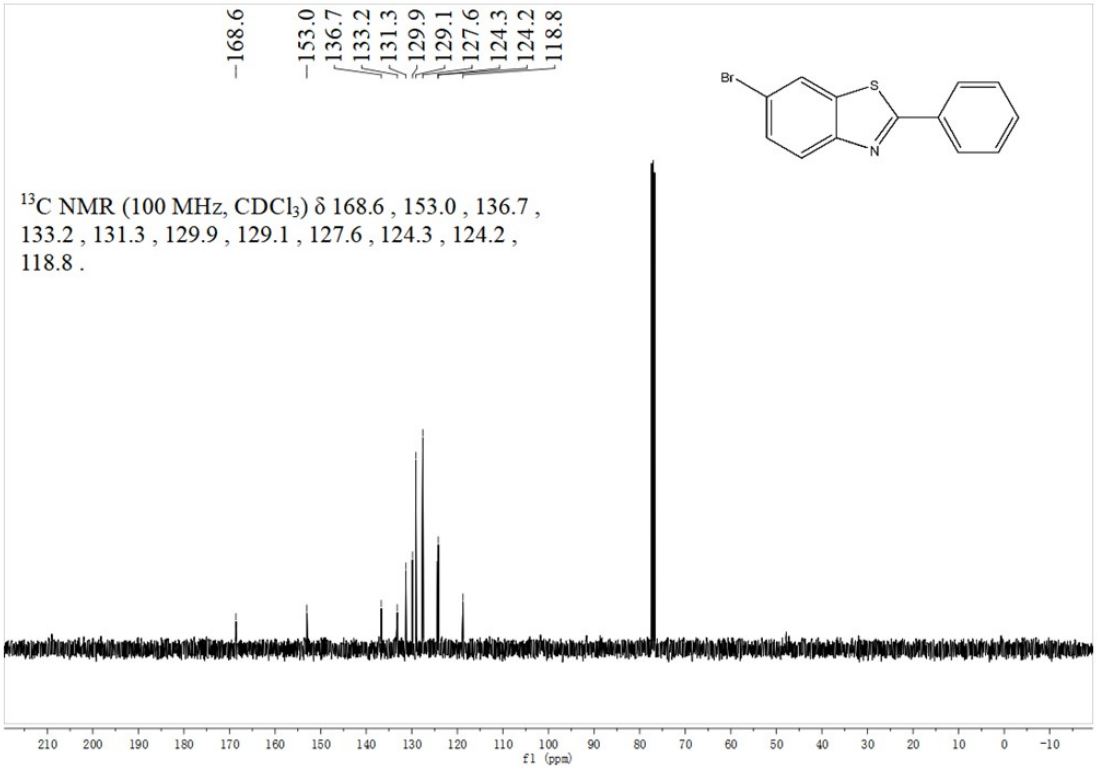


Figure S51. ^{13}C NMR of 6-bromo-2-phenylbenzo[d]thiazole **(2r)**

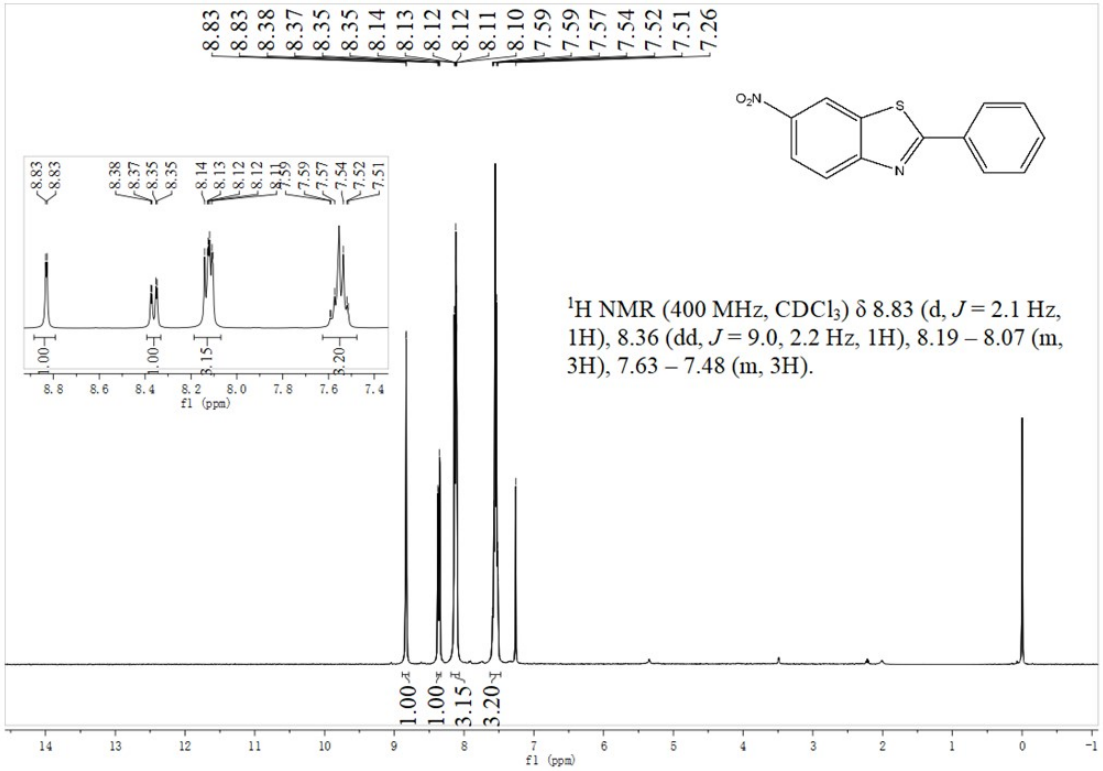


Figure S52. ^{1}H NMR of 6-nitro-2-phenylbenzo[d]thiazole **(2s)**

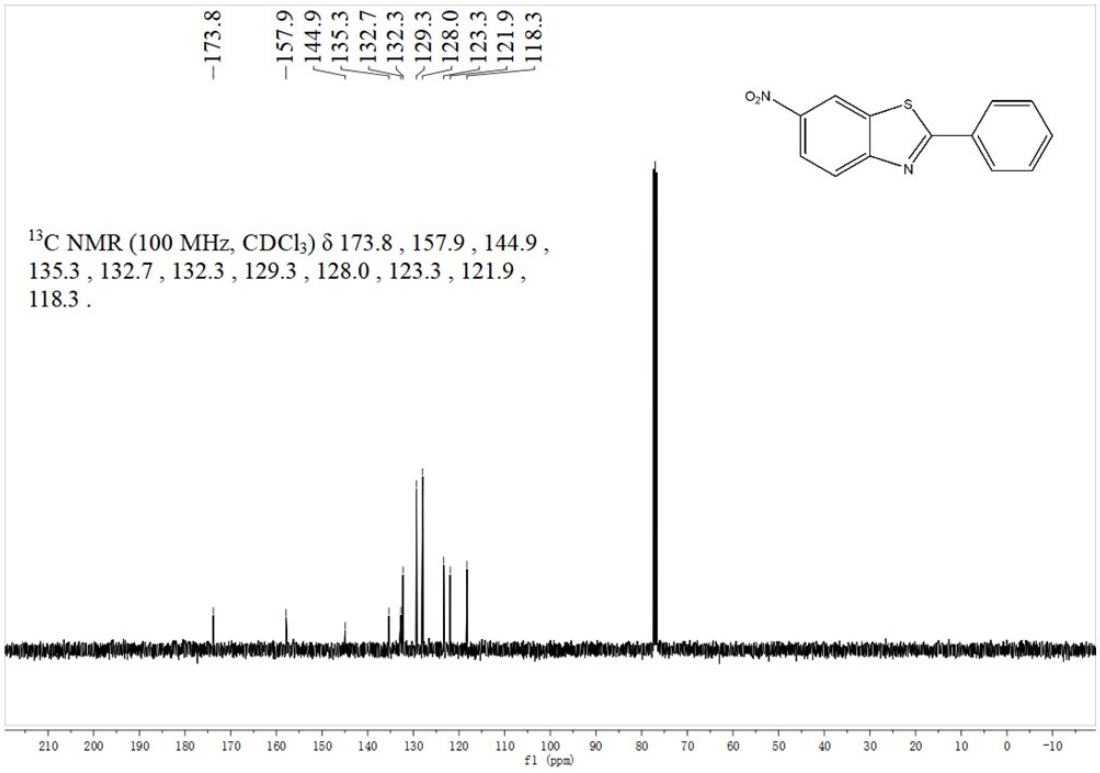


Figure S53. ^{13}C NMR of 6-nitro-2-phenylbenzo[d]thiazole **(2s)**

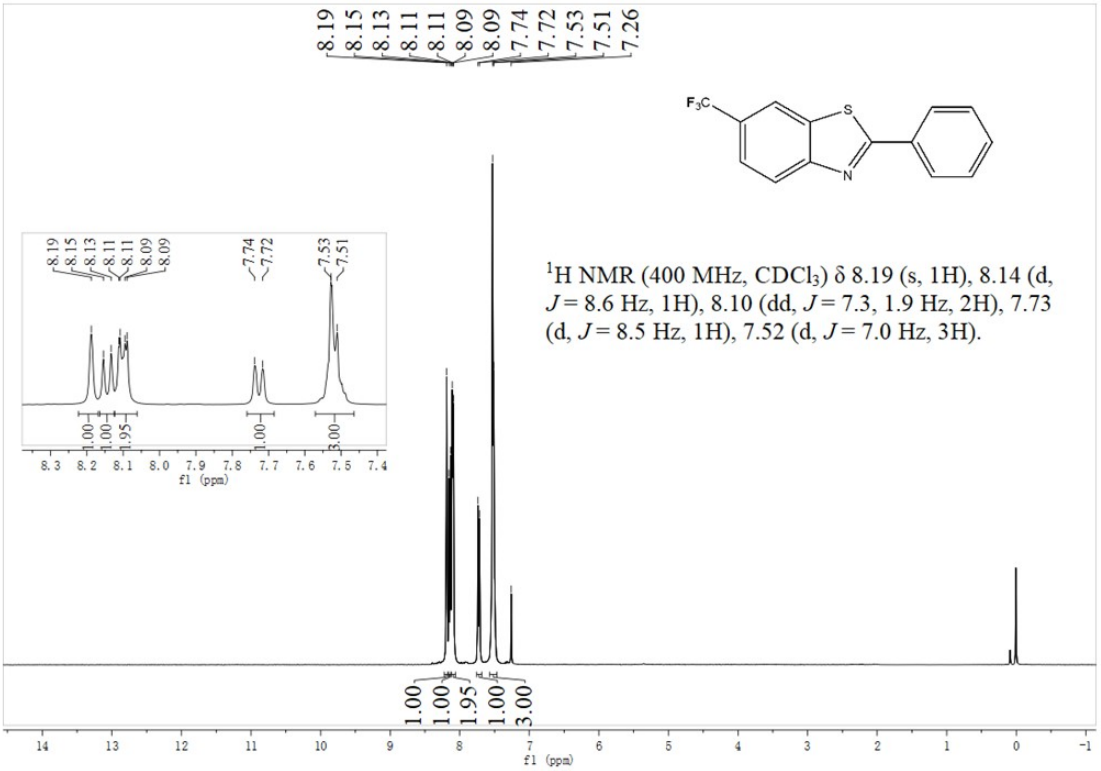


Figure S54. ^{1}H NMR of 2-phenyl-6-(trifluoromethyl) benzo[d]thiazole **(2t)**

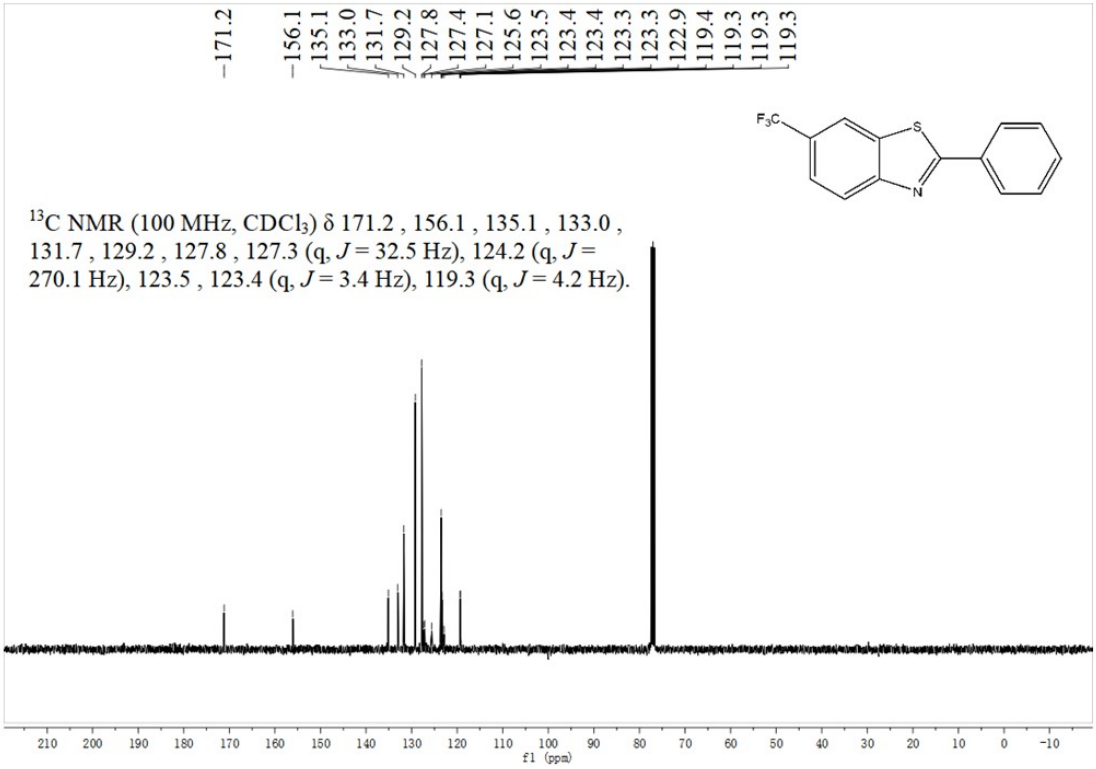


Figure S55. ^{13}C NMR of 2-phenyl-6-(trifluoromethyl) benzo[d]thiazole **(2t)**

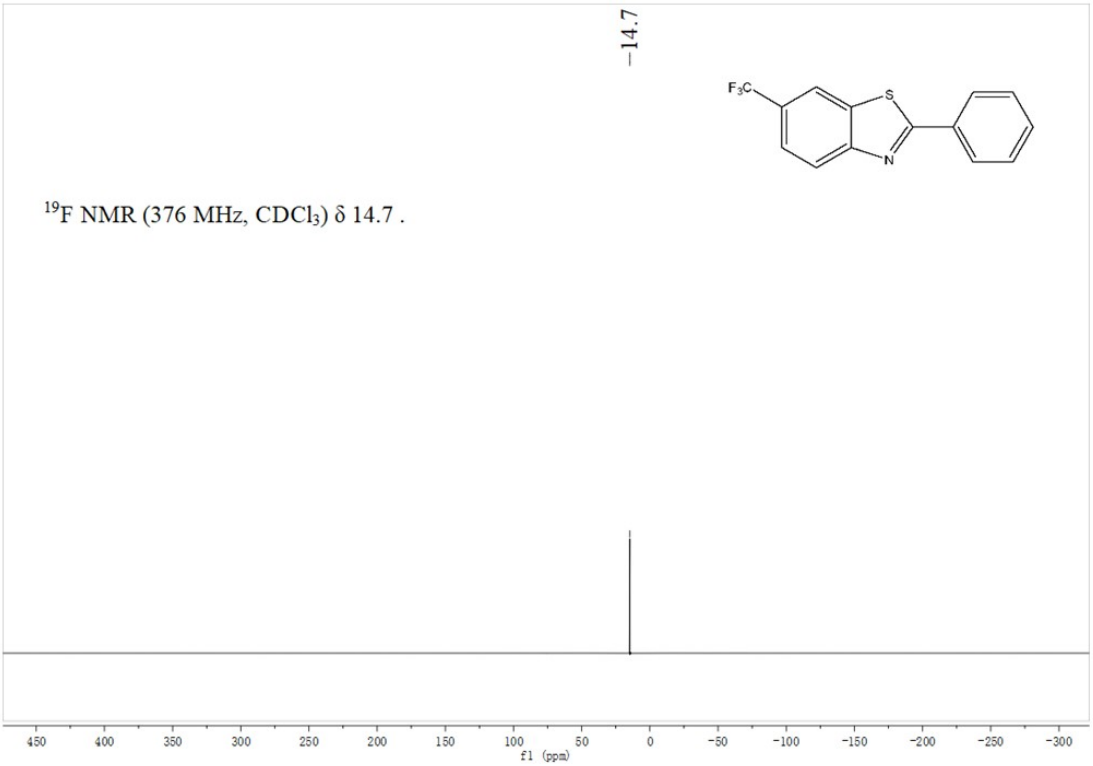


Figure S56. ^{19}F NMR of 2-phenyl-6-(trifluoromethyl) benzo[d]thiazole **(2t)**

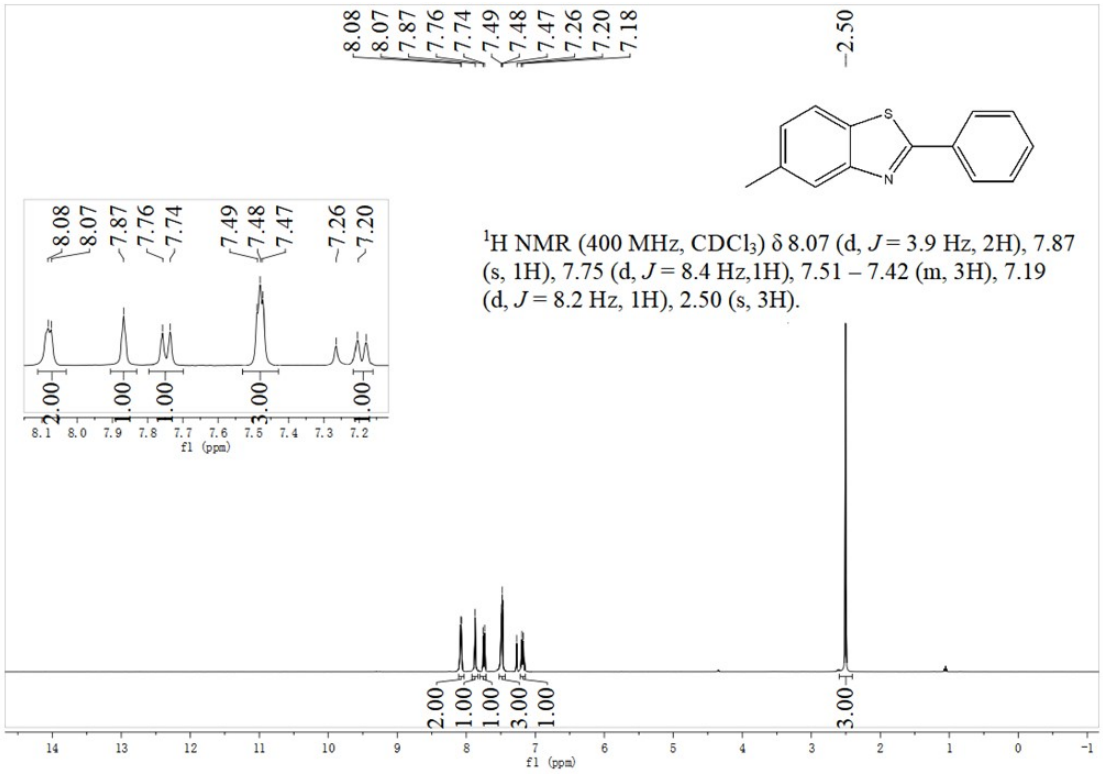


Figure S57. ^{1}H NMR of 5-methyl-2-phenylbenzo[d]thiazole **(2u)**

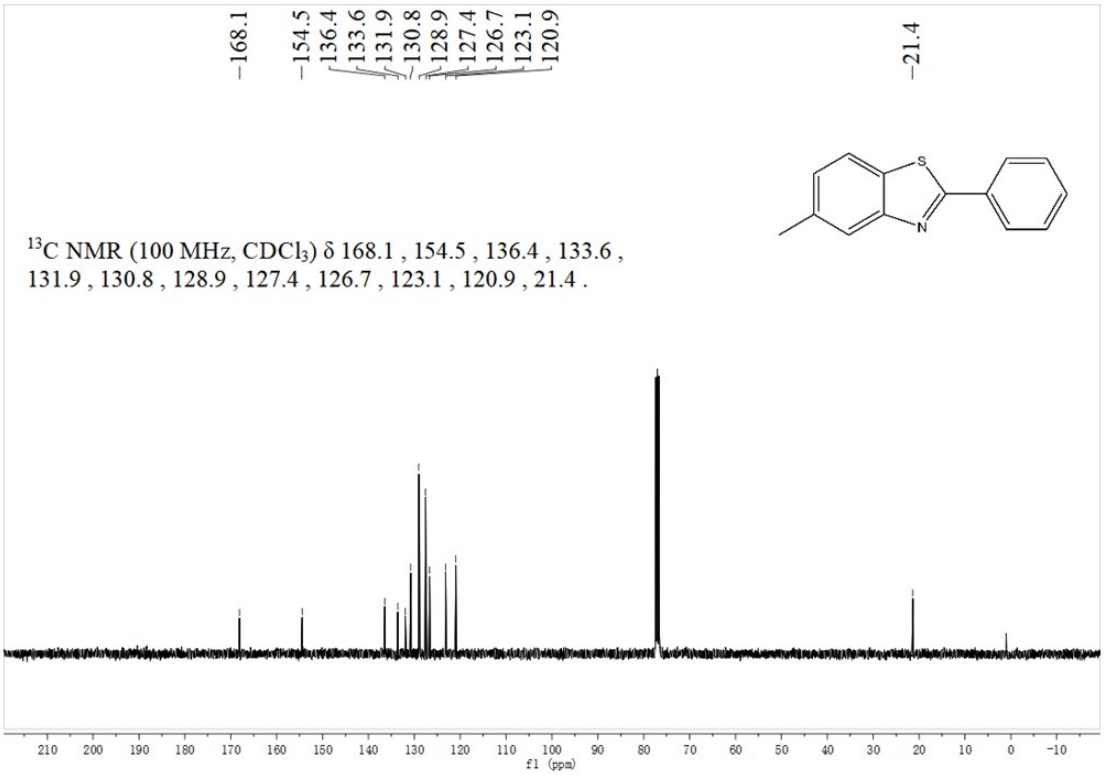


Figure S58. ^{13}C NMR of 5-methyl-2-phenylbenzo[d]thiazole **(2u)**

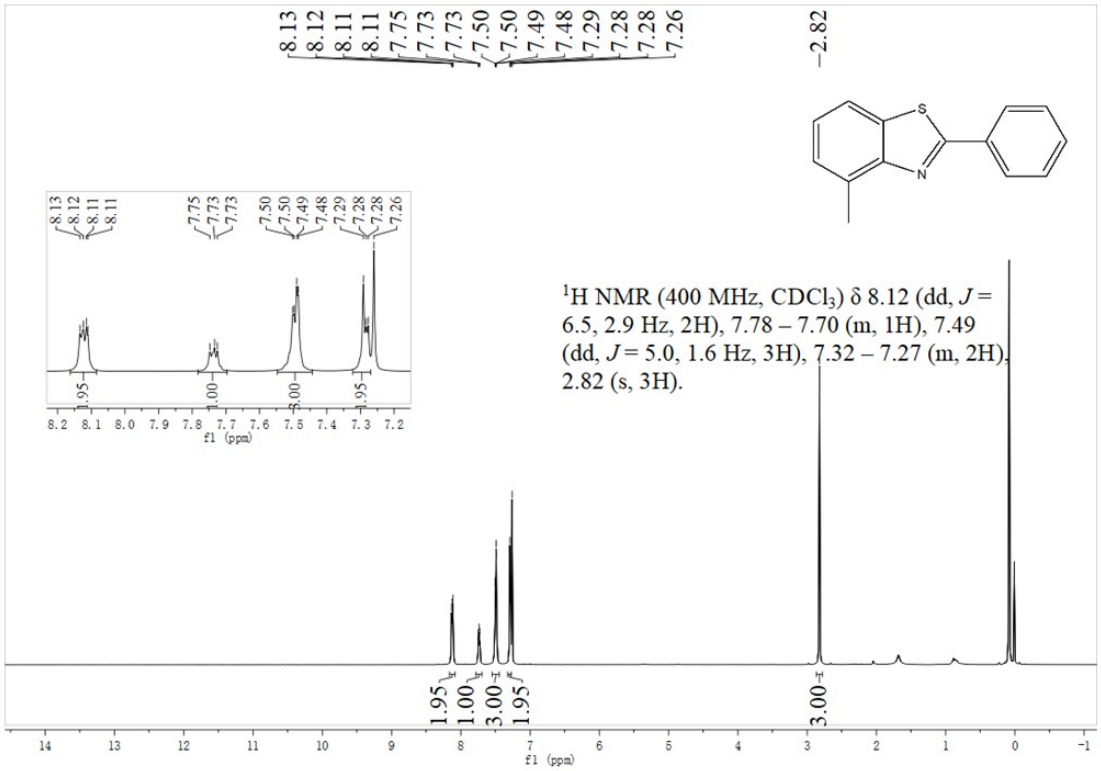


Figure S59. ^{1}H NMR of 4-methyl-2-phenylbenzo[d]thiazole **(2v)**

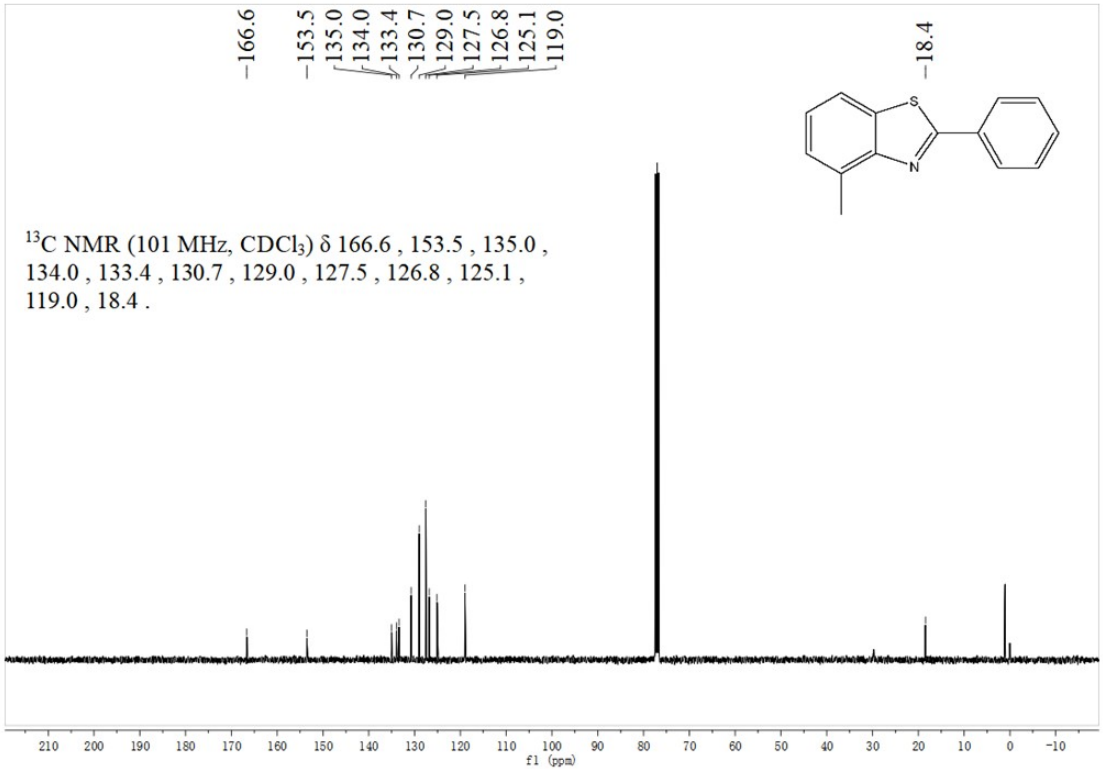


Figure S60. ^{13}C NMR of 4-methyl-2-phenylbenzo[d]thiazole **(2v)**

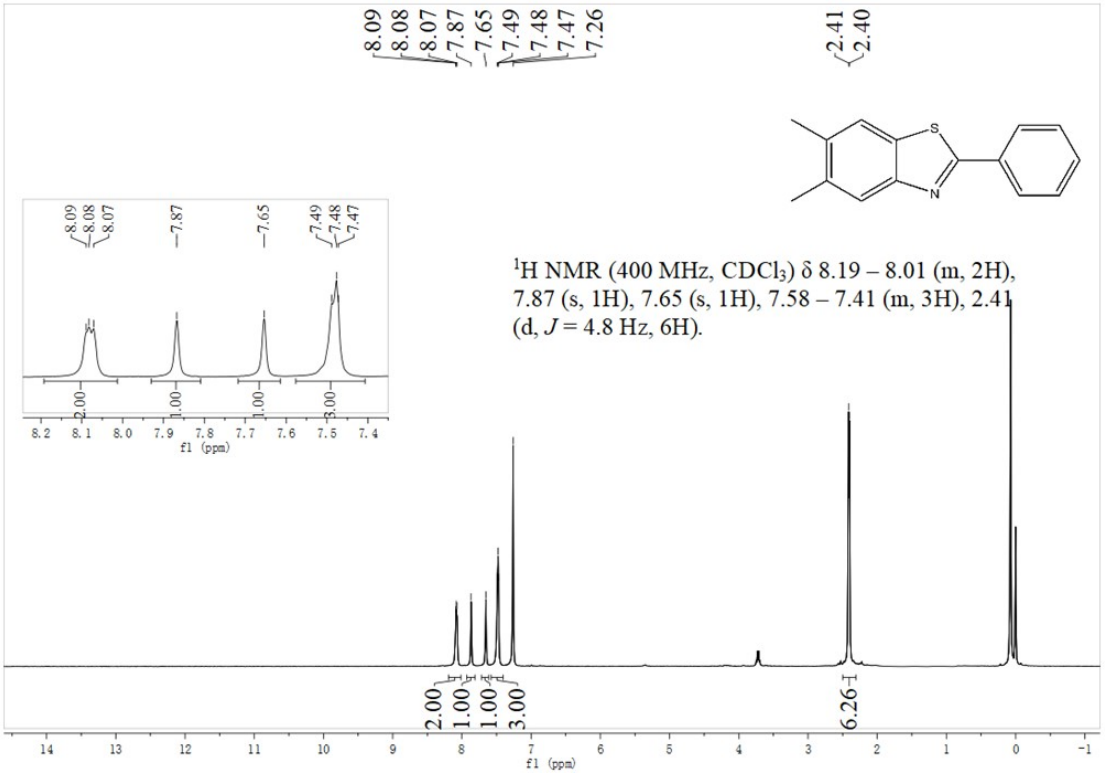


Figure S61. ^{1}H NMR of 5,6-dimethyl-2-phenylbenzo[d]thiazole **(2w)**

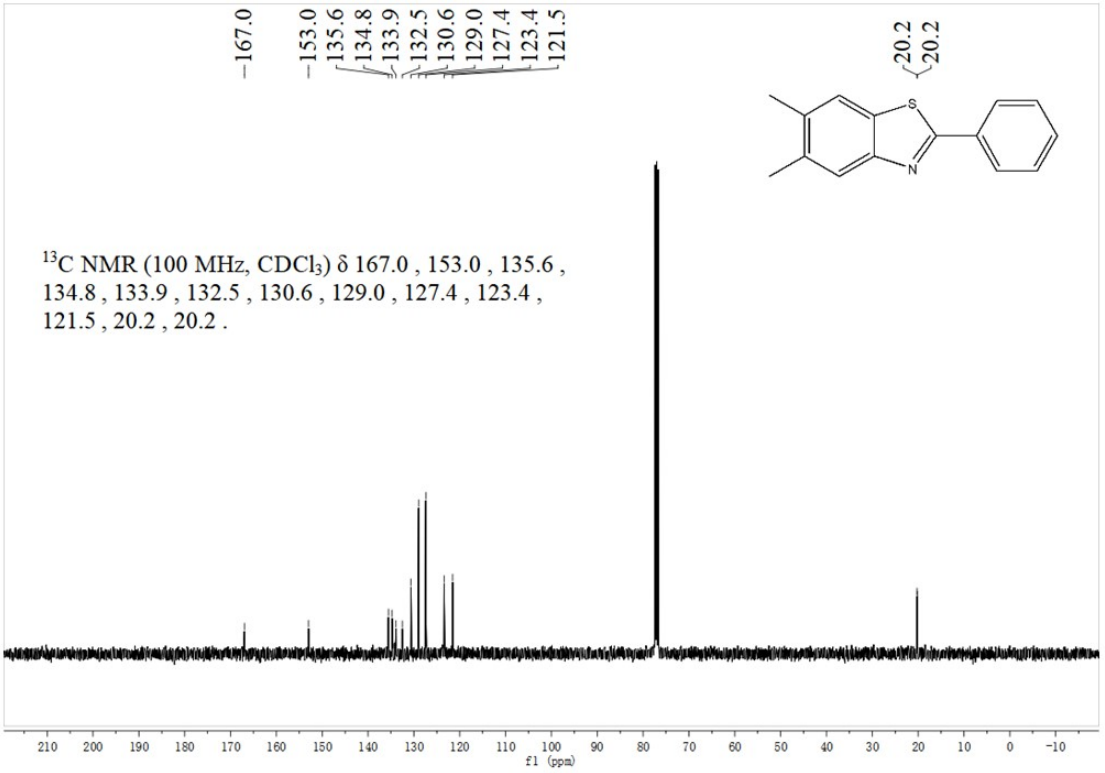


Figure S62. ^{13}C NMR of 5,6-dimethyl-2-phenylbenzo[d]thiazole **(2w)**

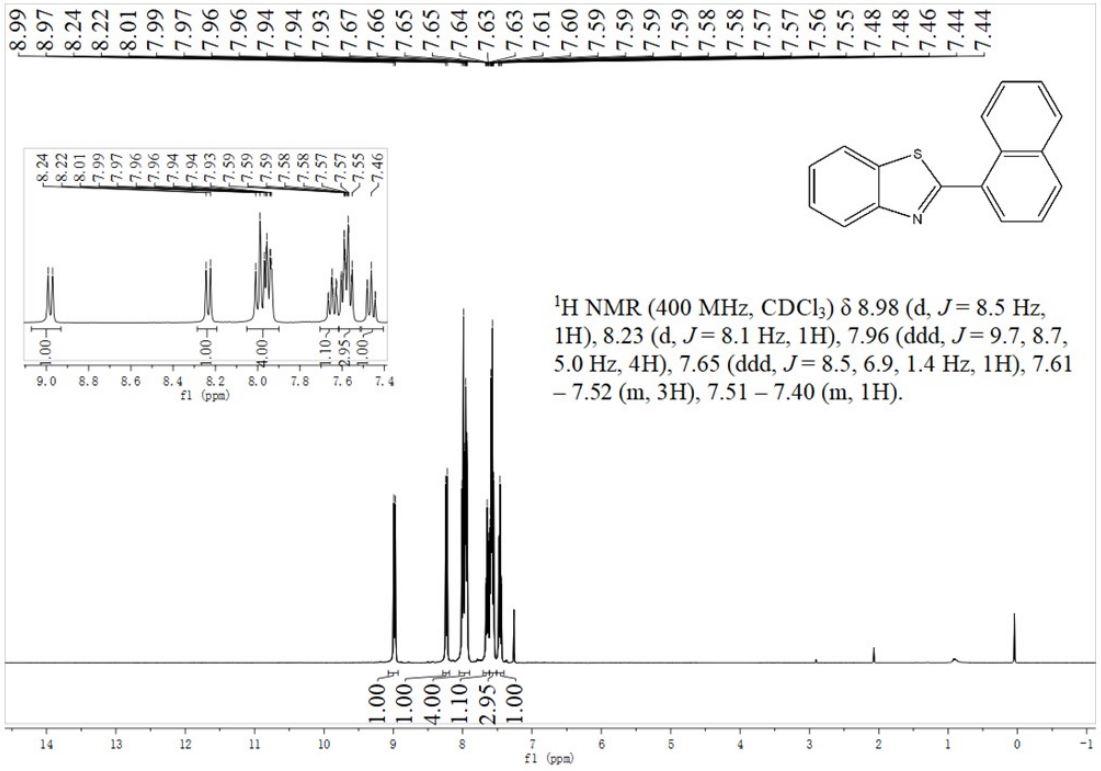


Figure S63. ^{1}H NMR of 2-(naphthalen-1-yl) benzo[d]thiazole **(2x)**

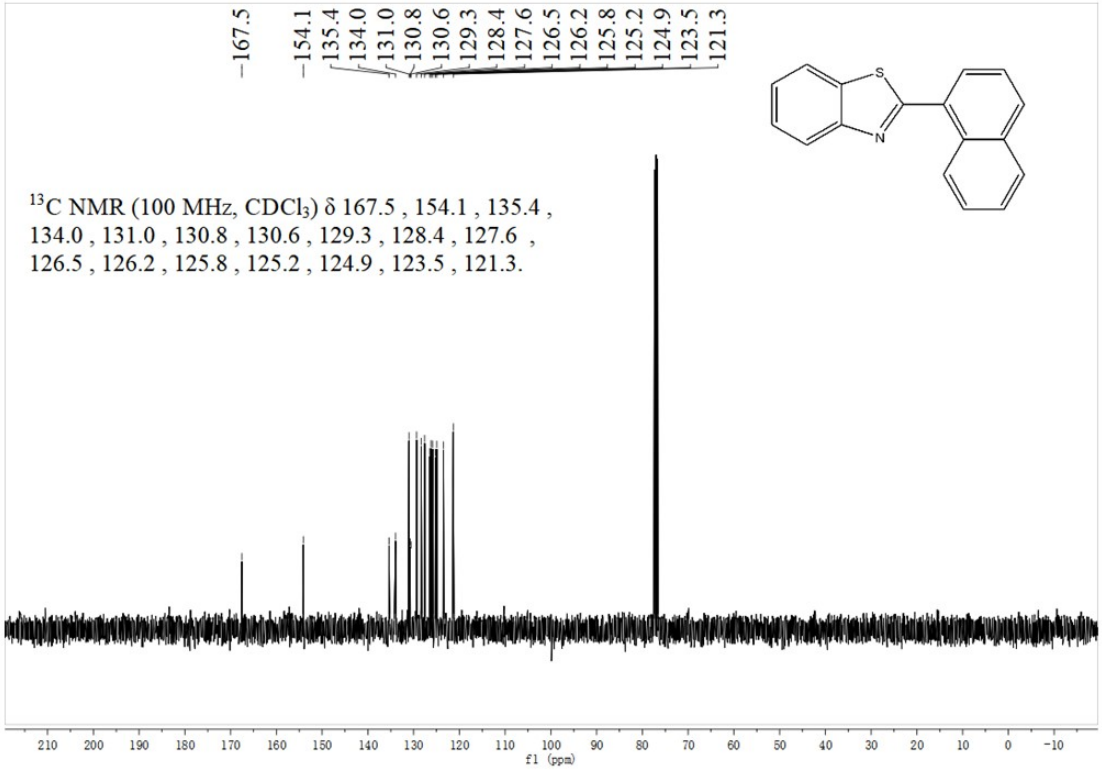


Figure S64. ^{13}C NMR of 2-(naphthalen-1-yl) benzo[d]thiazole **(2x)**

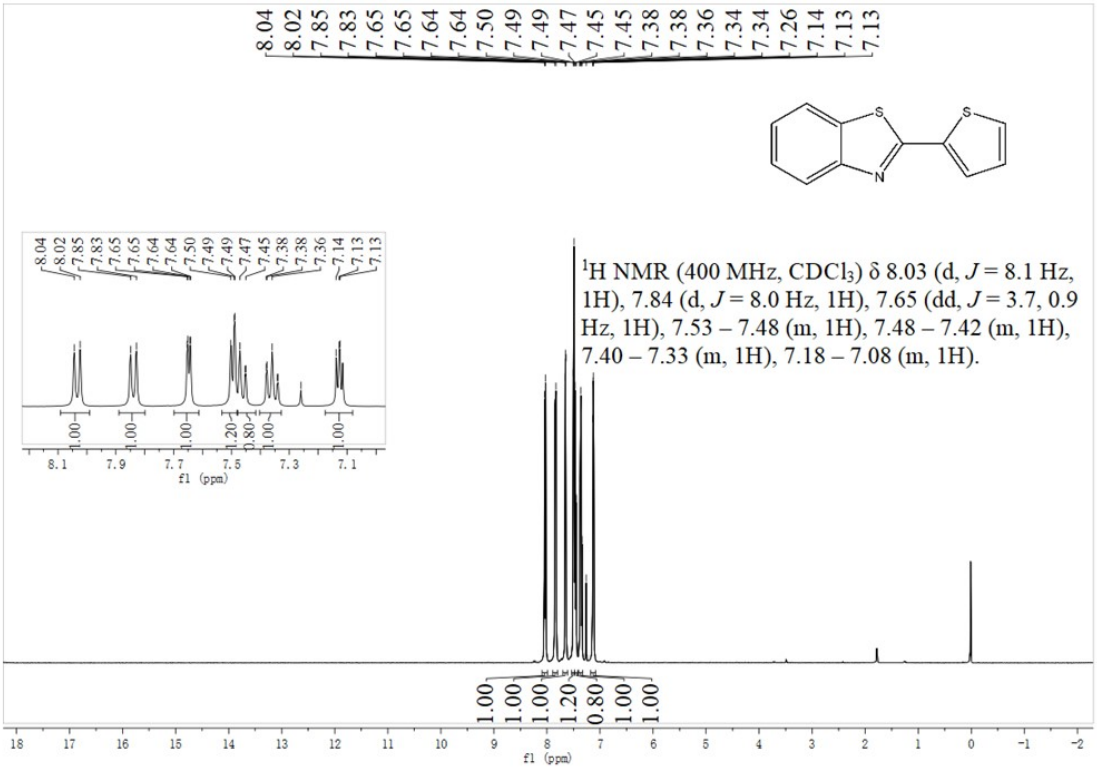


Figure S65. ^{1}H NMR of 2-(thiophen-2-yl) benzo[d]thiazole **(2y)**

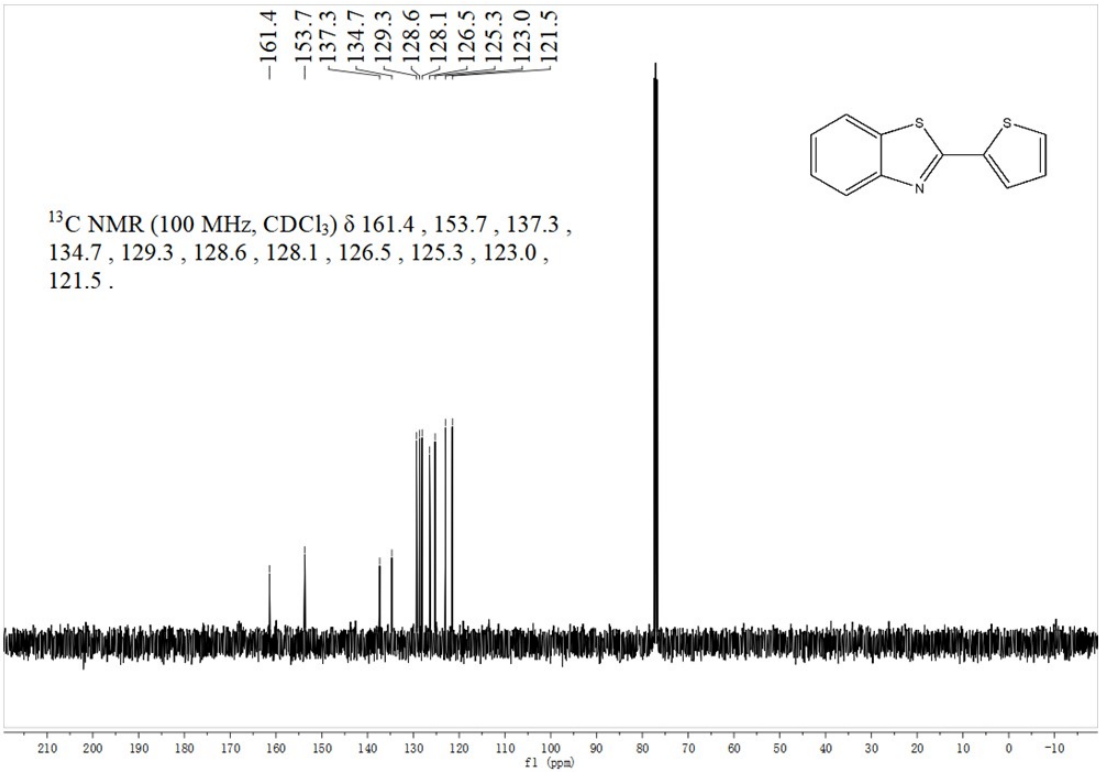


Figure S66. ^{13}C NMR of 2-(thiophen-2-yl) benzo[d]thiazole **(2y)**

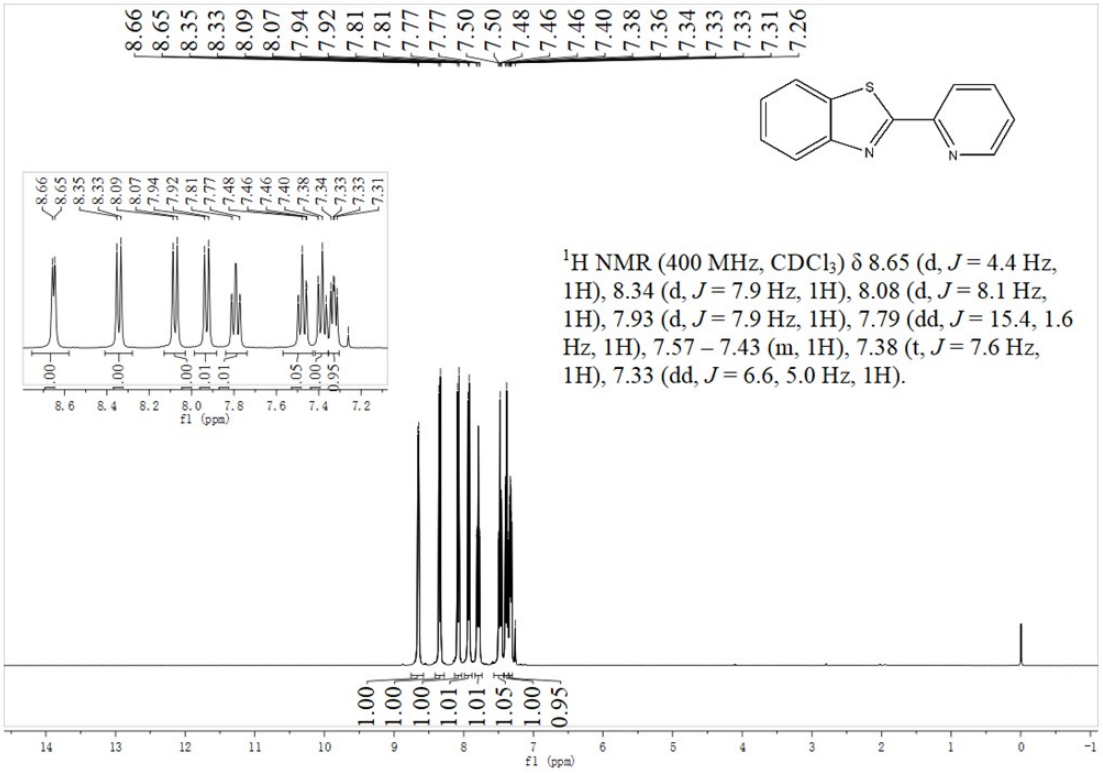


Figure S67. ^{1}H NMR of 2-(pyridine-2-yl) benzo[d]thiazole **(2z)**

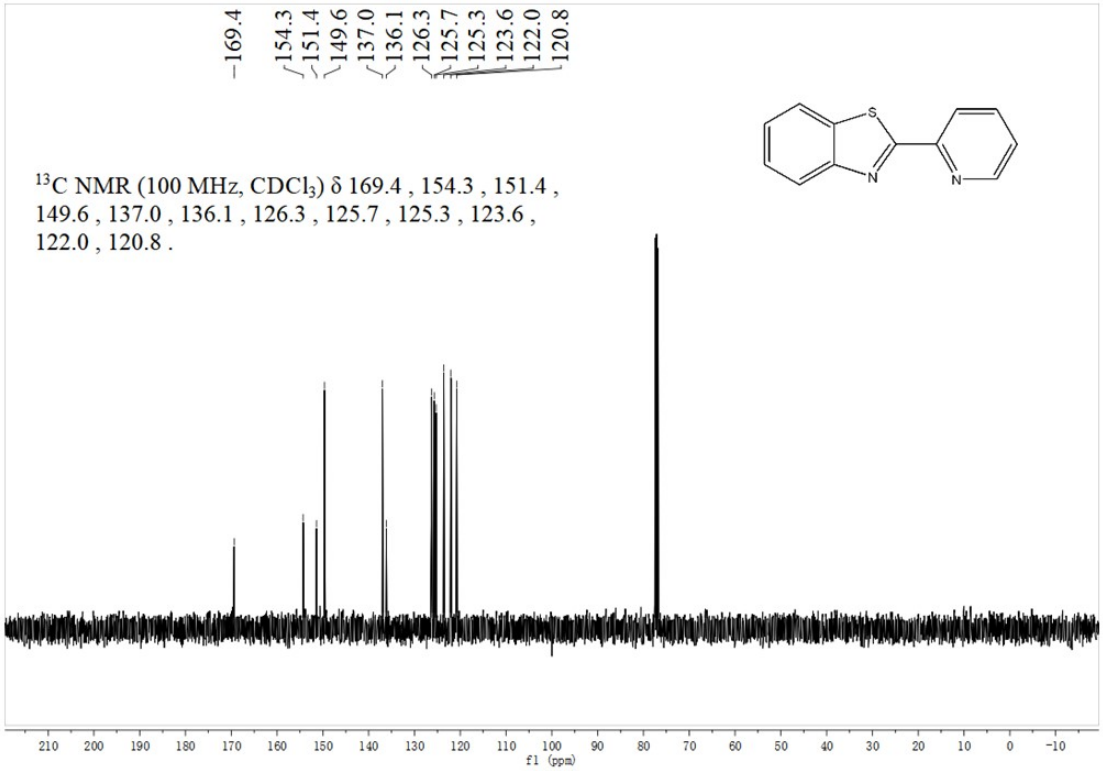


Figure S68. ^{13}C NMR of 2-(pyridine-2-yl) benzo[d]thiazole **(2z)**