**Supporting Information For**

# Approach to 2-(Arylthio)imidazoles and Imidazo[2,1-b]thiazoles from Imidazo[2,1-b][1,3,4]thiadiazoles by Ring-Opening and -Reconstruction

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## Characterization Data of Compounds

**6-Phenylimidazo[2,1-b][1,3,4]thiadiazole (1a)**[21]

White solid (67 mg, 65% yield), mp 131-132 °C. IR (KBr) 3135, 3052, 1601, 1509, 1471, 1437, 726, 691. $^1$H NMR (300 MHz, $CDCl_3$) $\delta$ = 8.52 (s, 1H), 8.10 (s, 1H), 7.84 (dd, *J* = 8.0, 1.0 Hz, 2H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.31 (t, *J* = 7.4 Hz, 1H). $^{13}$C NMR (75 MHz, DMSO-$d_6$) $\delta$ = 150.3, 146.1, 144.4, 134.0, 128.7, 127.3, 124.7, 110.4. HRMS (ESI) calcd. for $C_{10}H_7N_3S$ *m/z*: $[M+H]^+$ 202.0433; found: 202.0433.

**6-(4 -Tolyl)imidazo[2,1-b][1,3,4]thiadiazole (1b)**[21]

Yellow solid (65 mg, 60% yield), mp 142-144 °C. IR (KBr) 3133, 3094, 1605, 1542, 1490, 1458, 819. 1H NMR (300 MHz, $CDCl_3$) $\delta$ = 8.51 (s, 1H), 8.07 (s, 1H), 7.73 (d, *J* = 8.2 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 2.38 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$) $\delta$ = 147.7, 146.2, 144.1, 137.5, 130.9, 129.4, 125.1, 109.1, 21.2. HRMS (ESI) calcd. for $C_{11}H_9N_3S$ *m/z*: $[M+H]^+$ 216.0590; found: 216.0591.

**6-(4-Chlorophenyl)imidazo[2,1-b][1,3,4]thiadiazole (1c)**[22]

Yellow solid (74 mg, 63% yield), mp 152-154 °C. IR (KBr) 3103, 2922, 1589, 1510, 1484, 1460, 827. $^1$H NMR (300 MHz, $CDCl_3$) $\delta$ = 8.53 (s, 1H), 8.07 (s, 1H), 7.76 (d, *J* = 2.0 Hz, 1H), 7.74 (d, *J* = 2.0 Hz, 1H), 7.39 (d, *J* = 2.0 Hz, 1H), 7.37 (d, *J* = 2.0 Hz, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$) $\delta$ = 146.6, 144.4, 133.3, 132.2, 128.9, 127.2, 126.4, 109.6. HRMS (ESI) calcd. for C10H6 ClN3S *m/z*: $[M+H]^+$ 236.0044; found: 236.0042.

**6-(Naphthalen-2-yl)imidazo[2,1-b][1,3,4]thiadiazole (1d):** Yellow solid (58 mg, 72% yield), mp 154-156 °C. IR: $\nu$ = 3145, 3099, 1591, 1508, 1477, 1459, 777, 732 cm$^{-1}$. $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ = 8.60 – 8.48 (m, 2H), 8.09 (s, 1H), 7.87 (t, *J* = 8.9 Hz, 2H), 7.74 (d, *J* = 7.2 Hz, 1H), 7.56 – 7.45 (m, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): $\delta$ = 146.6, 143.8, 133.9, 131.4, 131.1, 128.5, 128.3, 127.2, 126.4, 125.8, 125.6, 125.3, 112.5. HRMS (ESI): *m/z* calcd. for $C_{14}H_9N_3S^+$: 252.0590 $[M+H]^+$; found: 252.0588.

**4-Phenyl-2-thiocyanato-1H-imidazole (9):** White solid (120 mg, 60% yield), mp 142-143 °C. IR: $\nu$ = 3128, 3038, 1608, 1567, 1493, 1458, 1396, 758, 687 cm$^{-1}$. $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ = 13.46 (br, 1H), 7.91 (s, 1H), 7.80 (d, *J* = 7.3 Hz, 2H), 7.41 (t, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 7.3 Hz, 1H). $^{13}$C NMR (101 MHz, DMSO-$d_6$): $\delta$ = 129.2, 127.7, 127.7, 126.8, 126.8, 124.9, 110.8, 110.8. HRMS (ESI): *m/z* calcd. for $C_{10}H_7N_3S^+$: 202.0433 $[M+H]^+$; found: 202.0435.

**4-Phenyl-2-(phenylthio)-1H-imidazole (3aa):**[19] Brown solid (108 mg, 85% yield), mp 132-134 °C. IR: $\nu$ = 3062, 1607, 1582, 1493, 1478, 1450, 737, 688 cm$^{-1}$. $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ = 7.59 (d, *J* = 7.0 Hz, 2H), 7.24 – 7.14 (m, 4H), 7.09 (s, 5H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 138.1, 134.5, 129.4, 129.2, 128.8, 127.4, 127.2, 125.0. HRMS (ESI): *m/z* calcd. for $C_{15}H_{12}N_2S^+$: 253.0794 $[M+H]^+$; found: 253.0793.

**4-Phenyl-2-(4-tolylthio)-1H-imidazole (3ab):** Yellow solid (71 mg, 56% yield), mp 154-156 °C. IR: $\nu$ = 3281, 3066, 1605, 1589, 1490, 1449, 1396, 760, 695 cm$^{-1}$. $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ = 7.81 (d, *J* = 7.3 Hz, 2H), 7.38 (d, *J* = 7.3 Hz, 2H), 7.34 (d, *J* = 2.2 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 7.12 (t, *J* = 5.7 Hz, 2H), 2.31 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 149.7, 134.3, 130.5, 130.3, 128.9, 128.8, 128.3, 127.4, 126.3, 124.9, 107.9, 31.0. HRMS (ESI): *m/z* calcd. for $C_{16}H_{14}N_2S^+$: 267.0950 $[M+H]^+$; found: 267.0950. Element analysis calcd. for $C_{16}H_{14}N_2S$·1/5EtOAc (%): C 71.05, H 5.54, N 9.86; found: C 70.87, H 5.27, N 9.98.

**2-((4-Methoxyphenyl)thio)-4-phenyl-1H-imidazole (3ac):** Colorless oil (39 mg, 30% yield), IR: $\nu$ =3416, 2925, 1655, 1545, 1492, 1460, 1384, 824, 763 cm$^{-1}$. $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ = 7.63 (d, *J* = 1.4 Hz, 1H), 7.61 (s, 1H), 7.32 – 7.26 (m, 2H), 7.25 (d, *J* = 3.5 Hz, 2H), 7.24 – 7.17 (m, 2H), 6.69 (t, *J* = 1.8 Hz, 1H), 6.66 (d, *J* = 1.5 Hz, 1H), 3.65 (s, 3H). $^{13}$C NMR (101 MHz, DMSO-$d_6$) $\delta$ = 143.9, 133.9, 129.2, 127.5, 126.7, 124.9, 118.9, 118.9, 110.8, 56.6. HRMS (ESI): *m/z* calcd. for $C_{16}H_{14}N_2OS^+$: 283.0900 $[M+H]^+$; found: 283.0895.

**1-(4-((4-Phenyl-1H-imidazol-2-yl)thio)phenyl)ethanone (3ad):** Orange oil (70 mg, 47% yield), IR: $\nu$ =3428, 2926, 1656, 1545, 1459, 824, 762, 625 cm$^{-1}$. $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ = 8.06 (d, *J* = 1.9 Hz, 1H), 8.04 (d, *J* = 1.9 Hz, 2H), 7.92 (s, 1H), 7.89 (s, 1H), 7.79 (d, *J* = 1.8 Hz, 2H), 7.77 (d, *J* = 1.9 Hz, 1H), 7.43 (s, 1H), 7.40 (s, 1H), 2.65 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 141.0, 139.8, 135.8, 132.5, 130.5, 129.1, 128.6, 123.0, 122.8, 117.9, 116.3, 30.9. HRMS (ESI): *m/z* calcd. for $C_{17}H_{14}N_2OS^+$: 295.0900 $[M+H]^+$; Found: 295.0900.

**4-((4-Phenyl-1H-imidazol-2-yl)thio)benzonitrile (3ae):** Yellow solid (63 mg, 45% yield), mp 96-97 °C. IR: $\nu$ =3437, 3074, 1656, 1562, 823, 760, 624 cm$^{-1}$. $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ = 7.85 – 7.74 (m, 3H), 7.62 (s, 1H), 7.44 (ddd, *J* = 12.9, 5.9, 3.9 Hz, 4H), 7.19 (d, *J* = 8.6 Hz, 1H), 7.14 (s, 1H). $^{13}$C NMR (101 MHz, acetone-$d_6$): $\delta$ = 144.3, 143.7, 134.3, 133.7, 132.8, 128.6, 127.0, 124.7, 118.3, 116.6, 109.4. HRMS (ESI): *m/z* calcd. for $C_{16}H_{11}N_3S^+$: 278.0746 $[M+H]^+$; found: 278.0749.

**4-Phenyl-2-((4-(trifluoromethyl)phenyl)thio)-1*H*-imidazole (3af):** Yellow oil (84 mg, 52% yield), IR: $\nu$ = 3433, 2926, 1657, 1561, 823, 761, 629 cm$^{-1}$. $^1$H NMR (400 MHz, [$D_6$]acetone): $\delta$ = 7.72 (s, 3H), 7.55 (d, *J* = 8.4, 2H), 7.25 (t, *J* = 7.7 Hz, 2H), 7.21 (d, *J* = 8.5 Hz, 2H), 7.12 (t, *J* = 7.3 Hz, 1H). $^{13}$C NMR (101 MHz, DMSO-$d_6$): $\delta$ = 134.2, 129.6, 129.2, 128.7, 127.5, 127.3, 126.9, 126.8, 126.4, 125.9, 125.0. HRMS (ESI): *m/z* calcd. for $C_{16}H_{11}F_3N_2S^+$: 321.0668 $[M+H]^+$; found: 321.0671.

**4-Phenyl-2-(2-tolylthio)-1*H*-imidazole (3ag):** White solid (68 mg, 54% yield), mp 167-168 °C. IR: $\nu$ = 3300, 3063, 1606, 1588, 1508, 1458, 1379, 752, 694 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.68 – 7.63 (m, 2H), 7.32 (dd, *J* = 14.7, 7.0 Hz, 3H), 7.25 – 7.20 (m, 1H), 7.16 – 7.10 (m, 3H), 7.08 – 7.03 (m, 1H), 2.35 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 138.2, 137.8, 133.2, 130.7, 130.1, 128.7, 127.5, 127.2, 127.0, 124.8, 20.3. HRMS (ESI): *m/z* calcd. for $C_{16}H_{14}N_2S^+$: 267.0950 $[M+H]^+$; found: 267.0955. Element analysis calcd. for $C_{16}H_{14}N_2S$·1/2EtOAc·1/4HCN (%): C 69.11, H 5.80, N 9.94; found: C 68.95, H 5.75, N 9.98.

**4-Phenyl-2-(3-tolylthio)-1*H*-imidazole (3ah):** White solid (81 mg, 64% yield), mp 150-151 °C. IR: $\nu$ = 3138, 3063, 1606, 1592, 1496, 909, 852, 760 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.66 (d, *J* = 7.3 Hz, 2H), 7.32 (dd, *J* = 8.0, 7.0 Hz, 3H), 7.23 (t, *J* = 7.4 Hz, 1H), 7.13 – 7.01 (m, 3H), 6.98 (d, *J* = 7.3 Hz, 1H), 2.22 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 140.6, 139.2, 138.3, 133.9, 132.1, 129.9, 129.1, 128.7, 128.0, 127.2, 126.4, 124.8, 118.6, 21.3. HRMS (ESI): *m/z* calcd. for $C_{16}H_{14}N_2S^+$: 267.0950 $[M+H]^+$; found: 267.0953. Element analysis calcd. for $C_{16}H_{14}N_2S$·1/3EtOAc·1/3HCN (%): C 69.63, H 5.62, N 10.72; found: C 69.53, H 5.37, N 10.42.

**2-((4-Phenyl-1H-imidazol-2-yl)thio)benzonitrile (3ai):** Yellow solid (62 mg, 45% yield), mp 86-88 °C. IR: $\nu$ = 3439, 3072, 1657, 1545, 822, 760. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 13.24 (d, *J* = 32.6 Hz, 1H), 7.98 (s, 1H), 7.92 – 7.89 (m, 1H), 7.83 (s, 2H), 7.71 – 7.58 (m, 2H), 7.44 – 7.38 (m, 3H), 7.08 (d, *J* = 8.1 Hz, 1H). $^{13}$C NMR (101 MHz, DMSO-$d_6$): $\delta$ = 140.9, 134.6, 134.5, 129.3, 129.2, 128.5, 127.7, 127.5, 124.9, 117.1, 110.3. HRMS (ESI): *m/z* calcd. for $C_{16}H_{11}N_3S^+$: 278.0746 $[M+H]^+$; found: 278.0750.

**2-((4-Fluorophenyl)thio)-4-phenyl-1*H*-imidazole (3aj):** Yellow oil (42 mg, 31% yield), IR: $\nu$ = 3066, 2972, 1607, 1589, 1489, 1450, 1395, 908, 827, 760, 733, 694 $cm^{-1}$. $^1H$ NMR (400 MHz, $CDCl_3$): $\delta$ = 7.62 – 7.58 (m, 2H), 7.27 (dd, *J* = 14.5, 6.7 Hz, 3H), 7.24 – 7.19 (m, 1H), 7.15 – 7.09 (m, 2H), 6.83 – 6.76 (m, 2H). $^{13}C$ NMR (101 MHz, $CDCl_3$): $\delta$ = 138.2, 131.8, 131.7, 131.6, 129.0, 128.7, 127.3, 125.0, 124.8, 116.3 (d, *J* = 22.1). HRMS (ESI): *m/z* calcd. for $C_{15}H_{11}FN_2S^+$: 271.0700 $[M+H]^+$; found: 271.0702.

**2-((4-Chlorophenyl)thio)-4-phenyl-1*H*-imidazole (3ak):** Brown solid (64 mg, 44% yield), mp 181-182 $^oC$. IR: $\nu$ = 3426, 2926, 1655, 824, 763, 624 $cm^{-1}$. $^1H$ NMR (300 MHz, $CDCl_3$): $\delta$ = 7.82 – 7.70 (m, 2H), 7.50 – 7.37 (m, 3H), 7.36 (s, 1H), 7.26 (s, 1H), 7.23 (s, 2H), 7.14 (s, 1H). $^{13}C$ NMR (101 MHz, DMSO-$d_6$): $\delta$ = 143.3, 135.2, 135.2, 134.5, 131.7, 129.8, 129.6, 129.1, 127.1, 124.9, 117.5. HRMS (ESI): *m/z* calcd. for $C_{15}H_{11}ClN_2S^+$: 287.0404 $[M+H]^+$; found: 287.0408.

**2-((3,5-Bis(trifluoromethyl)phenyl)thio)-4-phenyl-1*H*-imidazole (3al):** Colorless oil (35 mg, 18% yield), IR: $\nu$ = 3402, 3075, 1598, 1509, 1452, 1393, 738, 697 $cm^{-1}$. $^1H$ NMR (400 MHz, $CDCl_3$): $\delta$ = 7.50 (d, *J* = 7.1 Hz, 2H), 7.44 (s, 1H), 7.32 (d, *J* = 8.6 Hz, 3H), 7.22 – 7.12 (m, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$): $\delta$ = 138.9, 134.4, 132.6, 132.2, 131.3, 128.9, 127.9, 127.2, 125.0, 124.1, 121.4, 120.4. HRMS (ESI): *m/z* calcd. for $C_{17}H_{10}F_6N_2S^+$: 389.0542 $[M+H]^+$; found: 389.0539.

**2-((5-Fluoro-2-methylphenyl)thio)-4-phenyl-1*H*-imidazole (3am):** White solid (76 mg, 53% yield), mp 145-146 $^oC$. IR: $\nu$ = 3138, 3029, 1602, 1482, 1448, 1384, 762, 692 $cm^{-1}$. $^1H$ NMR (300 MHz, acetone-$d_6$): $\delta$ = 10.52 (br, 1H) 7.51 – 7.48 (m, 2H), 7.18 – 7.09 (m, 4H), 6.81 (dd, *J* = 8.4, 5.8 Hz, 1H), 6.55 (td, *J* = 8.3 Hz, 2.6, 1H), 6.46 (dd, *J* = 9.2, 2.6 Hz, 1H), 1.99 (s, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$): $\delta$ = 162.4, 156.0, 141.0, 136.3 (d, *J* = 7.7 Hz), 131.8, 131.4 (dd, *J* = 31.7, 5.4 Hz), 128.7, 127.3, 124.8, 119.2, 114.0 (dd, *J* = 137.9, 22.6 Hz), 19.06. HRMS (ESI): *m/z* calcd. for $C_{16}H_{13}N_2FS^+$: 285.0856 $[M+H]^+$; found: 285.0857.

**2-(Phenylthio)-4-(*p*-tolyl)-1*H*-imidazole (3ba):** Yellow oil (66 mg, 49% yield), IR: $\nu$ = 3056, 2962, 1608, 1581, 1508, 740, 702 $cm^{-1}$. $^1H$ NMR (300 MHz, $CDCl_3$): $\delta$ = 7.41 (d, *J* = 8.1 Hz, 2H), 7.11 (s, 1H), 7.04 – 7.00 (m, 4H), 6.97 (dd, *J* = 8.8, 8.3 Hz, 3H), 2.20 (s, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$): $\delta$ = 140.4, 137.5, 137.0, 134.7, 129.4, 129.2, 128.9, 126.8, 126.1, 124.8, 21.2. HRMS (ESI): *m/z* calcd. for $C_{16}H_{14}N_2S^+$: 267.0950 $[M+H]^+$; found: 267.0956.

**4-(4-Tolyl)-2-(4-tolylthio)-1*H*-imidazole (3bb):** Orange solid (77 mg, 55% yield), mp 175-176 $^oC$. IR: $\nu$ = 3346, 2922, 1596, 1509, 804, 734, 652 $cm^{-1}$. $^1H$ NMR (400 MHz, $CDCl_3$): $\delta$ = 7.57 (s, 1H), 7.30 – 7.28 (m, 3H), 7.26 (d, *J* = 1.2 Hz, 2H), 7.18 (d, *J* = 7.9 Hz, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 2.36 (s, 3H), 2.32 (s, 3H). $^{13}C$ NMR (101 MHz, acetone-$d_6$): $\delta$ = 137.1, 136.8, 136.2, 131.7, 129.9, 129.2, 129.0, 124.6, 20.3, 20.1. HRMS (ESI): *m/z* calcd. for $C_{17}H_{16}N_2S^+$: 281.1107 $[M+H]^+$; found: 281.1105. Element analysis calcd. for $C_{17}H_{16}N_2S{\cdot}1/2EtOAc$ (%):C 70.34, H 6.21, N 8.63; found: C 70.51, H 5.89, N 9.00.

**4-(4-Tolyl)-2-((4-(trifluoromethyl)phenyl)thio)-1*H*-imidazole (3bf):** Yellow solid (38 mg, 23% yield), mp 173-174 $^oC$. IR: $\nu$ = 3192, 2955, 1605, 1508, 823 $cm^{-1}$. $^1H$ NMR (300 MHz, $CDCl_3$): $\delta$ = 7.49 (s, 1H), 7.47 (s, 1H), 7.34 (s, 1H), 7.31 (s, 1H), 7.28 (s, 1H), 7.10 – 7.01 (m, 4H), 2.31 (s, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$): $\delta$ = 140.6, 137.5, 135.1, 130.1, 129.5, 129.1, 127.3, 126.2, 125.9, 125.9, 124.8, 21.2. HRMS (ESI): *m/z* calcd. for $C_{17}H_{13}N_2F_3S^+$: 335.0824 $[M+H]+$; found: 335.0828.

**4-(4-Chlorophenyl)-2-(phenylthio)-1*H*-imidazole (3ca):** Yellow solid (75 mg, 52% yield), mp 154-156 $^oC$. IR: $\nu$ = 3146, 3073, 1579, 1509, 788, 740, 701 $cm^{-1}$, $^1H$ NMR (400 MHz, $CDCl_3$): $\delta$ = 12.29 (s, 1H), 7.92 (d, *J* = 8.6 Hz, 1H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.46 (dd, *J* = 24.1, 8.5 Hz, 2H), 7.34 (t, *J* = 7.6 Hz, 2H), 7.23 (t, *J* = 8.0 Hz, 3H). $^{13}C$ NMR (101 MHz, DMSO-d6): $\delta$ = 136.3, 135.9, 132.7, 131.5, 129.9, 129.3, 129.1, 128.1, 127.9, 127.1, 126.5. HRMS (ESI): *m/z* calcd. for $C_{15}H_{11}N_2ClS^+$: 287.0404 $[M+H]^+$; found: 287.0404.

**4-(4-Chlorophenyl)-2-(2-tolylthio)-1*H*-imidazole (3cb):** Yellow solid (59 mg, 40% yield), mp 193-194 $^oC$. IR: $\nu$ = 3338, 2956, 1638, 1588, 1509, 805, 733, 616 $cm^{-1}$. $^1H$ NMR (300 MHz, DMSO-$d_6$): $\delta$ = 12.52 (s, 1H), 8.09 (s, 1H), 8.07 – 8.01 (m, 2H), 7.69 – 7.64 (m, 2H), 7.41 (s, 4H), 2.33 (s, 3H). $^{13}C$ NMR (101 MHz, DMSO-$d_6$): $\delta$ = 137.1, 136.9, 132.7, 131.8, 131.4, 130.5, 129.3, 129.1, 128.9, 127.9, 126.5. HRMS (ESI): *m/z* calcd. for $C_{16}H_{13}N_2ClS^+$: 301.0561 $[M+H]^+$; found: 301.0558.

**4-(4-Chlorophenyl)-2-((4-methoxyphenyl)thio)-1*H*-imidazole (3cc):** Brown oil (67 mg, 42% yield), IR: $\nu$ = 3306, 1591, 1491, 824, 796, 733 $cm^{-1}$. $^1H$ NMR (400 MHz, $CDCl_3$): $\delta$ = 7.59 (d, *J* = 8.4 Hz, 2H), 7.47 – 7.37 (m, 3H), 7.30 (d, *J* = 8.6 Hz, 2H), 6.89 – 6.81 (m, 2H), 3.77 (s, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$): $\delta$ = 159.9, 141.0, 133.9, 133.5, 132.8, 130.8, 128.8, 126.1, 122.5, 116.7, 115.1, 55.3. HRMS (ESI): *m/z* calcd. for $C_{16}H_{13}N_2ClOS^+$: 317.0510 $[M+H]^+$; found: 317.0508.

**4-((4-(4-Chlorophenyl)-1*H*-imidazol-2-yl)thio)benzonitrile (3ce):** Brown oil (62 mg, 40% yield), IR: $\nu$ = 3256, 3077, 1592, 1553, 823, 785, 735 $cm^{-1}$.$^1H$ NMR (400 MHz, $CDCl_3$): $\delta$ = 7.64 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 8.2 Hz, 3H), 7.32 (d, *J* = 8.5 Hz, 2H), 7.13 (d, *J* = 8.4 Hz, 2H). $^{13}C$ NMR (101 MHz, $CDCl_3$): $\delta$ = 142.8, 134.5, 133.3, 132.4, 130.3, 128.9, 128.8, 126.8, 126.1, 118.3, 109.4. HRMS (ESI): *m/z* calcd. for $C_{16}H_{10}N_3ClS^+$: 312.0357 $[M+H]^+$; found: 312.0359.

**4-(4-Chlorophenyl)-2-((4-(trifluoromethyl)phenyl)thio)-1*H*-imidazole (3cf):** Yellow solid (61 mg, 34% yield), mp 154-156 $^oC$. IR: $\nu$ = 3327, 2956, 1605, 1561, 1509, 829, 734 $cm^{-1}$. $^1H$ NMR (300 MHz, $CDCl_3$): $\delta$ = 7.51 (d, *J* = 7.8 Hz, 2H), 7.32 (d, *J* = 8.2 Hz, 2H), 7.26 (s, 1H), 7.21 (s, 1H), 7.19 (s, 1H), 7.05 (d, *J* = 8.2 Hz, 2H).$^{13}C$ NMR (101 MHz, DMSO-$d_6$): $\delta$ = 142.3, 131.7, 129.2, 129.1, 127.8, 127.4, 127.0, 126.6, 126.6, 125.9, 123.2. HRMS (ESI): *m/z* calcd. for $C_{16}H_{10}N_2ClF_3S^+$: 355.0284 $[M+H]^+$; found: 355.0290.

**4-(Naphthalen-2-yl)-2-(phenylthio)-1*H*-imidazole (3da):** Brown solid (83 mg, 55% yield), mp 158-159 $^oC$. IR: $\nu$ = 3054, 1581, 1560, 1509, 735, 688 $cm^{-1}$. $^1H$ NMR (400 MHz, $CDCl_3$) $\delta$ = 8.13 (d, *J* = 16.1 Hz, 1H), 7.77 – 7.75 (m, 1H), 7.69 (dd, *J* = 7.9, 4.1 Hz, 1H), 7.45 – 7.27 (m, 4H), 7.17 – 6.96 (m, 6H). $^{13}C$ NMR (101 MHz, $CDCl_3$): $\delta$ = 138.3, 137.6, 135.0, 133.9, 131.1, 129.7, 129.2, 129.0, 128.4, 128.2, 127.0, 126.9, 126.4, 125.9, 125.6, 125.4, 123.0. HRMS (ESI): *m/z* calcd. for $C_{19}H_{14}N_2S^+$: 303.0950 $[M+H]^+$; found: 303.0947. Element analysis calcd. for $C_{19}H_{14}N_2S{\cdot}2/5EtOAc{\cdot}1/5HCN$ (%): C 73.03, H 5.26, N 8.84; found: C 72.82, H 5.07, N 8.66.

**4-(Naphthalen-2-yl)-2-(*p*-tolylthio)-1*H*-imidazole (3db):** Brown solid (82 mg, 52% yield), mp 138-139 $^oC$. IR: $\nu$ = 3287, 3052, 1595, 1561, 1509, 801, 776, 734 $cm^{-1}$. $^1H$ NMR (400 MHz, $CDCl_3$): $\delta$ = 8.24 (d, *J* = 7.7 Hz, 1H), 7.84 (d, *J* = 7.6 Hz, 1H), 7.78 (d, *J* = 8.2 Hz, 1H), 7.53 (d, *J* = 6.9 Hz, 1H), 7.48 – 7.37 (m, 3H), 7.24 (ddd, *J* = 11.6, 6.9, 2.4 Hz, 3H), 7.04 (d, *J* = 8.1 Hz, 2H), 2.26 (s, 3H). $^{13}C$ NMR (101 MHz, $CDCl_3$): $\delta$ = 138.3, 137.8, 136.9, 133.7, 131.0, 130.7, 129.8, 129.7, 128.2, 127.8, 126.7, 126.1, 125.6, 125.5, 125.2, 122.6, 20.9. HRMS (ESI): *m/z* calcd. for $C_{20}H_{16}N_2S^+$: 317.1107 $[M+H]^+$; found: 317.1105.

**3,6-Diphenylimidazo[2,1-b]thiazole (5aa):**[14] Yellow solid (117 mg, 85% yield), mp 120-121 $^oC$. IR: $\nu$ = 3105, 3063, 1558, 1494, 733, 698 $cm^{-1}$. $^1H$ NMR (400 MHz, $CDCl_3$): $\delta$ = 7.91 (s, 1H), 7.88 – 7.81 (m, 2H), 7.68 (dd, *J* = 8.0, 1.1 Hz, 2H), 7.60 – 7.47 (m, 3H), 7.41 (dd,

*J* = 11.5, 4.1 Hz, 2H), 7.34 – 7.27 (m, 1H), 6.78 (s, 1H). $^{13}$C NMR (75 MHz, $CDCl_3$): $\delta$ = 150.3, 147.9, 134.3, 132.7, 130.1, 129.8, 129.5, 128.8, 127.6, 127.0, 125.4, 108.4, 107.5. HRMS (ESI): *m/z* calcd. for $C_{17}H_{12}N_2S^+$: 277.0794 $[M+H]^+$; found: 277.0790.

**6-Phenyl-3-(*p*-tolyl)imidazo[2,1-b]thiazole (5ab):** Yellow solid (119 mg, 82% yield), mp 177-178 °C. IR: $\nu$ = 3112, 3031, 1605, 1508, 1470, 1441, 772, 709 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.88 – 7.78 (m, 3H), 7.36 (dd, *J* = 10.1, 7.0 Hz, 5H), 7.29 – 7.20 (m, 2H), 6.65 (d, *J* = 3.8 Hz, 1H), 2.40 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 150.0, 147.5, 139.1, 134.0, 132.6, 130.3, 129.8, 129.1, 128.5, 127.4, 127.3, 125.1, 123.8, 107.9, 107.3, 21.4. HRMS (ESI): *m/z* calcd. for $C_{18}H_{14}N_2S^+$: 291.0950 $[M+H]^+$; found: 291.0960. Element analysis calcd. for $C_{18}H_{14}N_2S$·1/4EtOAc (%): C 73.05, H 5.16, N 8.97; found: C 72.98, H 4.85, N 9.11.

**3-(4-Methoxyphenyl)-6-phenylimidazo[2,1-b]thiazole (5ac):** White solid (146 mg, 95% yield), mp 112-113 °C. IR: $\nu$ = 3112, 3067, 1610, 1508, 1469, 1441, 813, 772, 709 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.76 – 7.67 (m, 3H), 7.40 (dd, *J* = 8.8, 2.0 Hz, 2H), 7.27 (t, *J* = 7.5 Hz, 2H), 7.15 (dd, *J* = 10.1, 4.4 Hz, 1H), 6.88 (dd, *J* = 8.6, 1.8 Hz, 2H), 6.46 (d, *J* = 2.2 Hz, 1H), 3.71 (d, *J* = 2.1 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): $\delta$ = 160.3, 149.9, 147.4, 134.0, 132.1, 128.5, 128.1, 127.2, 125.0, 122.1, 114.5, 107.1, 106.7, 55.2. HRMS (ESI): *m/z* calcd. for $C_{18}H_{14}N_2OS^+$: 307.0900 $[M+H]^+$; found: 307.0907.

**3-(4-Fluorophenyl)-6-phenylimidazo[2,1-b]thiazole (5ad):**[20] White solid (117 mg, 80% yield), mp 131-132 °C. IR: $\nu$ = 3376, 2923, 1605, 1561, 1507, 1471, 1440, 771, 743, 708 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.87 – 7.79 (m, 3H), 7.69 – 7.60 (m, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.26 (dt, *J* = 17.0, 8.0 Hz, 3H), 6.73 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 164.5, 162.0, 150.0, 147.9, 134.0, 131.5, 128.9 (d, *J* = 8.3 Hz), 128.7, 127.5, 127.5, 126.1 (d, *J* = 2.9 Hz), 126.1 (d, *J* = 2.9 Hz), 125.2, 116.5 (d, *J* = 22.0 Hz), 107.6 (d, *J* = 125.5 Hz). HRMS (ESI): *m/z* calcd. for $C_{17}H_{11}FN_2S^+$: 295.0700 $[M+H]^+$; found: 295.0760. Element analysis calcd. for $C_{17}H_{11}FN_2S$ (%): C 69.37, H 3.77, N 9.52; found: C 69.61, H 3.64, N 9.29.

**3-(4-Chlorophenyl)-6-phenylimidazo[2,1-b]thiazole (5ae):**[20] White solid (174 mg, 98% yield), mp 89-90 °C. IR: $\nu$ = 3344, 3070, 1600, 1577, 1509, 1471, 1441, 773, 733, 709 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.85 (t, *J* = 5.6 Hz, 3H), 7.62 (dd, *J* = 8.5, 2.3 Hz, 2H), 7.52 (dd, *J* = 8.6, 2.2 Hz, 2H), 7.41 (dd, *J* = 10.5, 4.6 Hz, 2H), 7.30 (d, *J* = 7.0 Hz, 1H), 6.78 (d, *J* = 2.5 Hz, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$): $\delta$ = 150.0, 147.9, 135.6, 133.9, 131.4, 129.6, 128.6, 128.3, 128.1, 127.5, 125.2, 108.7, 107.0. HRMS (ESI): *m/z* calcd. for $C_{17}H_{11}ClN_2S^+$: 311.0404 $[M+H]^+$; found: 311.0411.

**3-(4-Bromophenyl)-6-phenylimidazo[2,1-b]thiazole (5af):**[20] Yellow solid (156 mg, 88% yield), mp 126-127 °C. IR: $\nu$ = 3149, 3062, 1607, 1537, 1509, 1470, 1440, 772, 737, 707 cm$^{-1}$, $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ = 7.83 (t, *J* = 3.6 Hz, 3H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.55 – 7.47 (m, 2H), 7.39 (t, *J* = 7.7 Hz, 2H), 7.29 (d, *J* = 7.2 Hz, 1H), 6.76 (s, 1H). $^{13}$C NMR (75 MHz, $CDCl_3$): $\delta$ = 150.0, 147.9, 133.9, 132.5, 131.4, 128.8, 128.6, 128.3, 127.5, 125.2, 123.7, 108.8, 107.0. HRMS (ESI): *m/z* calcd. for $C_{17}H_{11}BrN_2S^+$: 354.9899 $[M+H]^+$; found: 354.9910.

**6-Phenyl-3-(*m*-tolyl)imidazo[2,1-b]thiazole (5ag):**[20] Colorless oil (142 mg, 98% yield), IR: $\nu$ = 3381, 3106, 1606, 1560, 1509, 1469, 1442, 1373, 772, 737, 703 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.83 (m, 3H), 7.37 (m, 5H), 7.34 – 7.22 (m, 3H), 6.67 (s, 1H), 2.40 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 150.1, 147.5, 139.1, 134.0, 132.6, 130.3, 129.8, 129.1, 128.5, 127.4, 127.3, 125.1, 123.8, 107.9, 107.3, 21.4. HRMS (ESI): *m/z* calcd. for $C_{18}H_{14}N_2S^+$: 291.0950 $[M+H]^+$; found: 291.0958.

**3-(2-Fluorophenyl)-6-phenylimidazo[2,1-b]thiazole (5ah):**[20] Yellow solid (125 mg, 85% yield), mp 130-131 °C. IR: $\nu$ = 3329, 3070, 1599, 1505, 1473, 1440, 804, 770, 706 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.85 – 7.83 (m, 3H), 7.67 – 7.63 (m, 2H), 7.40 (t, *J* = 7.6 Hz, 2H), 7.30 – 7.22 (m, 3H), 6.73 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 164.5, 162.0, 150.0, 147.9, 134.0, 131.5, 128.9 (d, *J* = 8.5 Hz), 128.7, 127.4, 126.1 (d, *J* = 3.4 Hz), 125.2, 116.5 (d, *J* = 22.0 Hz), 108.2, 107.0. HRMS (ESI): *m/z* calcd. for $C_{17}H_{11}FN_2S^+$: 295.0700 $[M+H]^+$; found: 295.0709.

**6-Phenyl-3-(4-(trifluoromethyl)phenyl)imidazo[2,1-b]thiazole (5ai):**[20] White solid (135 mg, 78% yield), mp 122-123 °C. IR: $\nu$ = 3304, 3068, 1602, 1511, 1475, 1441, 1418, 773, 734, 710 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.86 (s, 1H), 7.84 – 7.80 (m, 2H), 7.80 – 7.75 (m, 4H), 7.38 (t, *J* = 7.6 Hz, 2H), 7.27 (t, *J* = 8.3 Hz, 1H), 6.85 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 150.2, 148.2, 133.9, 133.4, 131.2, 128.8, 127.7, 127.2, 126.46, 126.43, 125.3, 122.5, 110.2, 107.2. HRMS (ESI): *m/z* calcd. for $C_{18}H_{11}F_3N_2S^+$: 345.0668 $[M+H]^+$; found: 345.0663.

**3-(3,5-bis(Trifluoromethyl)phenyl)-6-phenylimidazo[2,1-b]thiazole (5aj):** Yellow solid (111 mg, 54% yield), mp 185-186 °C. IR: $\nu$ = 3328, 3080, 1606, 1509, 1479, 1444, 775, 740, 700 cm$^{-1}$. $^1$H NMR (300 MHz, $CDCl_3$): $\delta$ = 8.13 (s, 2H), 8.02 (s, 1H), 7.83 (dd, *J* = 8.8, 1.6 Hz, 3H), 7.44 – 7.39 (m, 2H), 7.32 (dt, *J* = 9.4, 4.3 Hz, 1H), 7.01 (s, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 150.1, 148.7, 133.5, 133.3, 132.9, 132.0, 129.5, 128.8, 127.8, 126.8, 125.4, 124.2, 123.2, 121.5, 111.5, 106.5. HRMS (ESI): *m/z* calcd. for $C_{19}H_{10}F_6N_2S^+$: 413.0542 $[M+H]^+$; found: 413.0539.

**3-Phenyl-6-(*p*-tolyl)imidazo[2,1-b]thiazole (5ba):**[21] Yellow oil (91 mg, 62% yield), mp 154-156 °C. IR: $\nu$ = 3113, 3059, 1604, 1548, 1509, 1467, 1446, 799, 728, 696 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.84 (s, 1H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.63 – 7.62 (m, 2H), 7.53 – 7.48 (m, 3H), 7.19 (d, *J* = 7.9 Hz, 2H), 6.71 (s, 1H), 2.35 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 150.1, 147.9, 137.2, 132.6, 131.4 130.1, 129.7, 129.5, 129.4, 126.9, 125.2, 108.2, 107.0, 21.3. HRMS (ESI): *m/z* calcd. for $C_{18}H_{14}N_2S^+$: 291.0950 $[M+H]^+$; found: 291.0959.

**3,6-di-*p*-Tolylimidazo[2,1-b]thiazole (5bb)**[21]

Yellow solid (102 mg, 67% yield), mp 122-123 °C. IR: $\nu$ = 3112, 3025, 1581, 1546, 1508, 1465, 1414, 815 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.79 (d, *J* = 1.5, 1H), 7.71 (d, *J*=8.1, 2H), 7.46 (dd, *J* = 8.2, 2.1, 2H), 7.27 – 7.25 (m, 2H), 7.17 (d, *J* = 7.8 Hz, 2H), 6.59 (d, *J* = 2.8 Hz, 1H), 2.39 (s, 3H), 2.33 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 149.8, 147.6, 139.5, 136.9, 132.4, 131.2, 129.8, 129.2, 126.9, 126.5, 124.9, 107.2, 106.8, 21.2, 21.1. HRMS (ESI): *m/z* calcd. for $C_{19}H_{16}N_2S^+$: 305.1107 $[M+H]^+$; found: 305.1102.

**3-(4-Methoxyphenyl)-6-(*p*-tolyl)imidazo[2,1-b]thiazole (5bc):**[21] Brown oil (93 mg, 58% yield), IR: $\nu$ = 3366, 3112, 1611, 1585, 1508, 1466, 1422, 823 cm$^{-1}$. $^1$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.81 (d, *J* = 1.5 Hz, 1H), 7.73 (d, *J* = 8.0 Hz, 2H), 7.57 (dd, *J* = 8.9, 2.3 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 7.05 – 7.02 (m, 2H), 6.63 (s, 1H), 3.87 (s, 3H), 2.36 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 139.4, 138.5, 133.7, 130.2, 129.3, 128.8, 128.3, 127.4, 126.7, 124.9, 21.4. HRMS (ESI): *m/z* calcd. for $C_{19}H_{16}N_2OS^+$: 321.1056 $[M+H]^+$; found: 321.1053.

**3-(4-Chlorophenyl)-6-(*p*-tolyl)imidazo[2,1-b]thiazole (5be):**[22] White solid (101 mg, 62% yield), mp 129-130 $^{o}$C. IR: $\nu$ = 3227, 3071, 1597, 1510, 1469, 1412, 1373, 815 cm$^{-1}$. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.80 (s, 1H), 7.72 (d, *J* = 8.1 Hz, 2H), 7.59 (d, *J* = 8.5 Hz, 2H), 7.50 (d, *J* = 8.4 Hz, 2H), 7.20 (d, *J* = 7.9 Hz, 2H), 6.75 (s, 1H), 2.37 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 149.9, 148.0, 137.2, 135.5, 131.3, 131.1, 129.5, 129.32, 128.4, 128.0, 125.1, 108.5, 106.6, 21.2. HRMS (ESI): *m/z* calcd. for $C_{18}H_{13}ClN_2S^+$: 325.0561 $[M+H]^+$; found: 325.0558.

**6-(4-Chlorophenyl)-3-phenylimidazo[2,1-b]thiazole (5ca):**[21] Yellow solid (52 mg, 34% yield), mp 146-147 $^{o}$C. IR: $\nu$ = 3342, 3119, 1594, 1510, 1465, 1404, 793, 728, 694 cm$^{-1}$. $^{1}$H NMR (400 MHz, DMSO-d6): $\delta$ = 12.28 (s, 1H), 7.92 (d, *J* = 8.0 Hz, 1H), 7.84 – 7.81 (m, 2H), 7.44 (dd, *J* = 8.0, 1.5 Hz, 2H), 7.37 – 7.32 (m, 2H), 7.24-7.21 (m, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 150.3, 146.6, 133.0, 132.6, 132.6, 129.9, 129.7, 129.4, 128.8, 126.9, 126.4, 108.4, 107.4. HRMS (ESI): *m/z* calcd. for $C_{17}H_{11}ClN_2S^+$: 311.0404 $[M+H]^+$; found: 311.0415.

**6-(4-Chlorophenyl)-3-(*p*-tolyl)imidazo[2,1-b]thiazole (5cb):** Orange solid (47 mg, 30% yield), mp 127-128 $^{o}$C. IR: $\nu$ = 3286, 3032, 1583, 1536, 1508, 1466, 1402, 812 cm$^{-1}$. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.85 (s, 1H), 7.77 – 7.74 (m, 2H), 7.53 (d, *J* = 8.1 Hz, 2H), 7.33 (dd, *J* = 8.3, 2.8 Hz, 4H), 6.71 (s, 1H), 2.44 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 150.2, 146.5, 139.9, 132.9, 132.7, 132.6, 130.0, 128.7, 126.9, 126.7, 126.4, 107.7, 107.4, 30.9. HRMS(ESI): *m/z* calcd. for $C_{18}H_{13}ClN_2S^+$: 325.0561 $[M+H]^+$; found: 325.0557. Element analysis calcd. for $C_{18}H_{13}ClN_2S$ (%): C 66.56, H 4.03, N 8.62; found: C 66.63, H 3.91, N 8.46.

**6-(4-Chlorophenyl)-3-(4-methoxyphenyl)imidazo[2,1-b]thiazole (5cc):**[21] Yellow solid (73 mg, 42% yield), mp 179-180 $^{o}$C. IR: $\nu$ = 3284, 3116, 1611, 1584, 1508, 1465, 1402, 816 cm$^{-1}$. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.83 (s, 1H), 7.75 (d, *J* = 8.5 Hz, 2H), 7.56 (d, *J* = 8.6 Hz, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 8.6 Hz, 2H), 6.65 (s, 1H), 3.88 (s, 3H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 160.6, 150.2, 146.5, 132.8, 132.6, 132.3, 128.7, 128.3, 126.3, 122.2, 114.7, 107.3, 107.0, 55.4. HRMS (ESI): *m/z* calcd. for $C_{18}H_{13}ClN_2OS^+$: 341.0510 $[M+H]^+$; found: 341.0506.

**3,6-bis(4-Chlorophenyl)imidazo[2,1-b]thiazole (5ce):**[22] Yellow solid (75 mg, 43% yield), mp 138-140 $^{o}$C. IR: $\nu$ = 3375, 3063, 1600, 1536, 1509, 1466, 1404, 834 cm$^{-1}$. $^{1}$H NMR (400 MHz, $CDCl_3$): $\delta$ = 7.88 (d, *J* = 3.5 Hz, 1H), 7.77 – 7.75 (m, 2H), 7.67 – 7.64 (m, 2H), 7.56 – 7.52 (m, 2H), 7.37 – 7.34 (m, 2H), 6.79 (d, *J* = 3.6 Hz, 1H). $^{13}$C NMR (101 MHz, $CDCl_3$): $\delta$ = 150.3, 146.6, 133.0, 132.58, 132.56, 129.9, 129.7, 129.4, 128.8, 126.9, 126.4, 108.5, 107.4. HRMS (ESI): *m/z* calcd. for $C_{17}H_{10}N_2Cl_2S^+$: 345.0015 $[M+H]^+$; found: 345.0024.

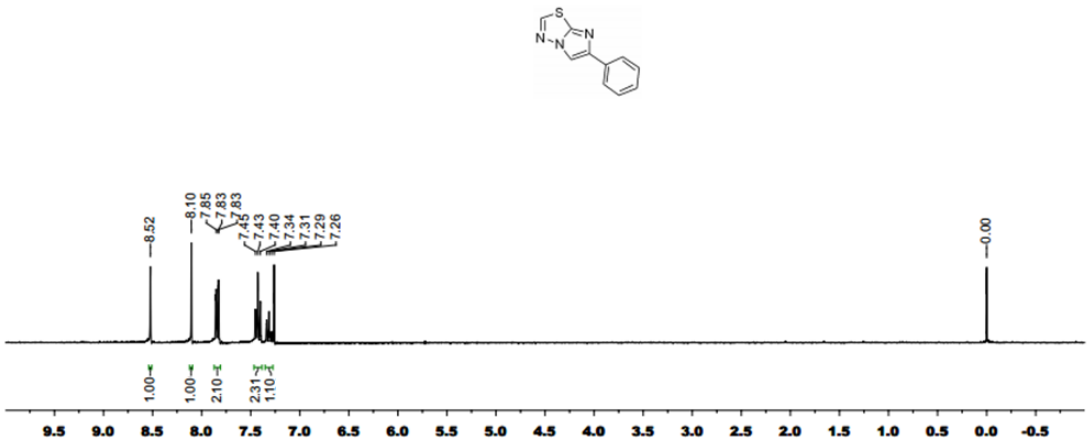
**6-(Naphthalen-2-yl)-3-phenylimidazo[2,1-b]thiazole (5da):** Yellow solid (103 mg, 63% yield), mp 198-199 $^{o}$C. IR: $\nu$ = 3362, 3058, 1592, 1546, 1509, 1461, 1428, 806, 778, 690 cm$^{-1}$. $^{1}$H NMR (300 MHz, $CDCl_3$): $\delta$ = 862 – 8.59 (m, 1H), 7.90 – 7.83 (m, 3H), 7.76 – 7.71(m, 1H), 7.70 – 7.68 (m, 2H), 7.55 – 7.48 (m, 6H), 6.82 (s, 1H). $^{13}$C NMR (75 MHz, $CDCl_3$): $\delta$ = 140.5, 137.6, 133.9, 132.6, 131.9, 131.3, 130.0, 129.6, 129.3, 128.3, 128.2, 127.1, 126.8, 126.3, 125.9, 125.7, 125.3, 110.4, 108.3. HRMS (ESI): *m/z* calcd. for $C_{21}H_{14}N_2S^+$: 327.0950 $[M+H]^+$; found: 327.0956. Element analysis calcd. for $C_{21}H_{14}N_2S{\cdot}1/4EtOAc{\cdot}1/8HCN$ (%): C 75.53, H 4.62, N 8.46; found: C 75.64, H 4.43, N 8.30.

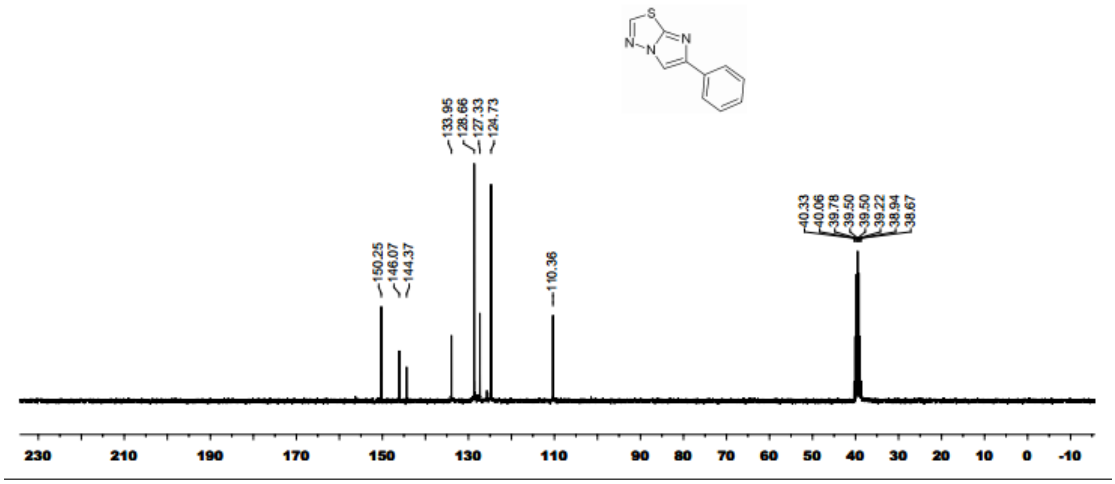
**3-(4-Methoxyphenyl)-6-(naphthalen-2-yl)imidazo[2,1-b]thiazole (5dc):** Yellow oil (82 mg, 46% yield), IR: $\nu$ = 3110, 3050, 1611, 1585, 1507, 1462, 1381, 803, 739, 673 cm$^{-1}$. $^{1}$H NMR (300 MHz, $CDCl_3$): $\delta$ = 8.51 (dd, *J* = 6.8, 2.2 Hz, 1H), 7.86 – 7.55 (m, 4H), 7.51 – 7.29 (m, 5H), 6.92 – 6.78 (m, 2H), 6.59 – 6.48 (m, 1H), 3.69 (d, *J* = 2.3 Hz, 3H). $^{13}$C NMR (75 MHz, $CDCl_3$): $\delta$ = 160.4, 149.5, 146.9, 133.8, 132.2, 131.8, 131.2, 128.2, 128.1, 128.1, 127.0, 126.2, 125.9, 125.6, 125.2, 122.2, 114.5, 110.2, 106.8, 55.3. HRMS (ESI): *m/z* calcd. for $C_{22}H_{16}N_2OS^+$: 357.1056 $[M+H]^+$; found: 357.1066.

**3-(4-Bromophenyl)-6-(naphthalen-2-yl)imidazo[2,1-b]thiazole (5df):** Yellow solid (126 mg, 62% yield), mp 163-165 oC. IR: ν = 3393, 3054, 1592, 1545, 1510, 804, 778, 669 cm-1. 1H NMR (400 MHz, CDCl3): $\delta$ = 8.48 (d, J = 7.9 Hz, 1H), 7.72 (dd, J = 19.5, 9.6 Hz, 3H), 7.59 (d, J = 7.0 Hz, 1H), 7.45 (d, J = 8.1 Hz, 2H), 7.42 – 7.28 (m, 5H), 6.61 (s, 1H). 13C NMR (101 MHz, CDCl3): $\delta$ = 149.5, 147.2, 133.8, 132.4, 131.6, 131.3, 131.1, 128.7, 128.2, 128.2, 128.1, 127.0, 126.3, 125.8, 125.7, 125.2, 123.6, 110.1, 108.8. HRMS (ESI): m/z calcd. for C21H13N2BrS+: 405.0056 [M+H]+; found: 405.0052. Element analysis calcd. for C21H13BrN2S (%): C 62.23, H 3.23, N 6.91; found: C 62.08, H 3.08, N 6.55.

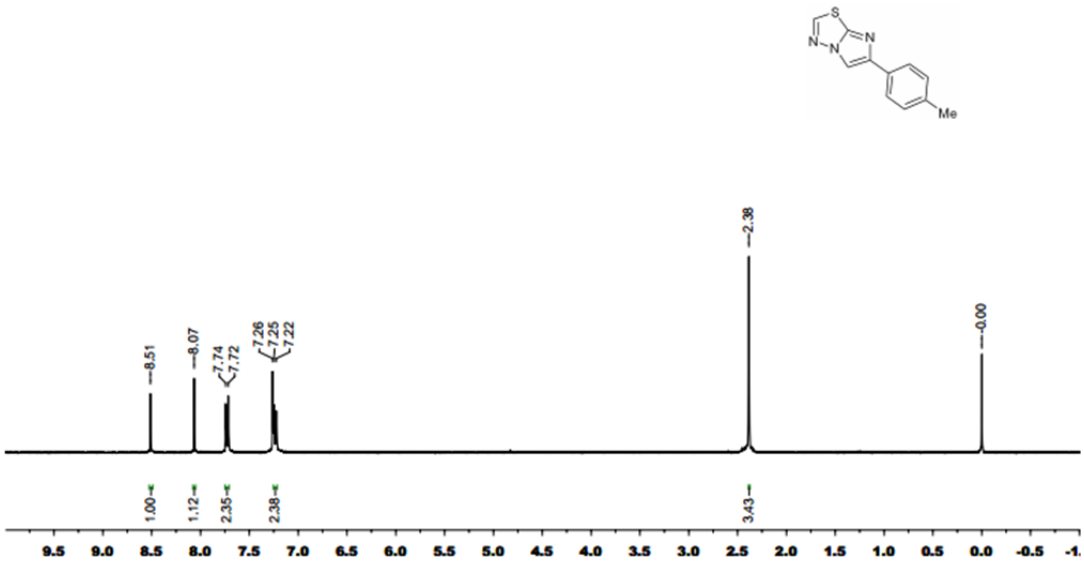
## Copies of $^{1}$H NMR and $^{13}$C NMR spectra

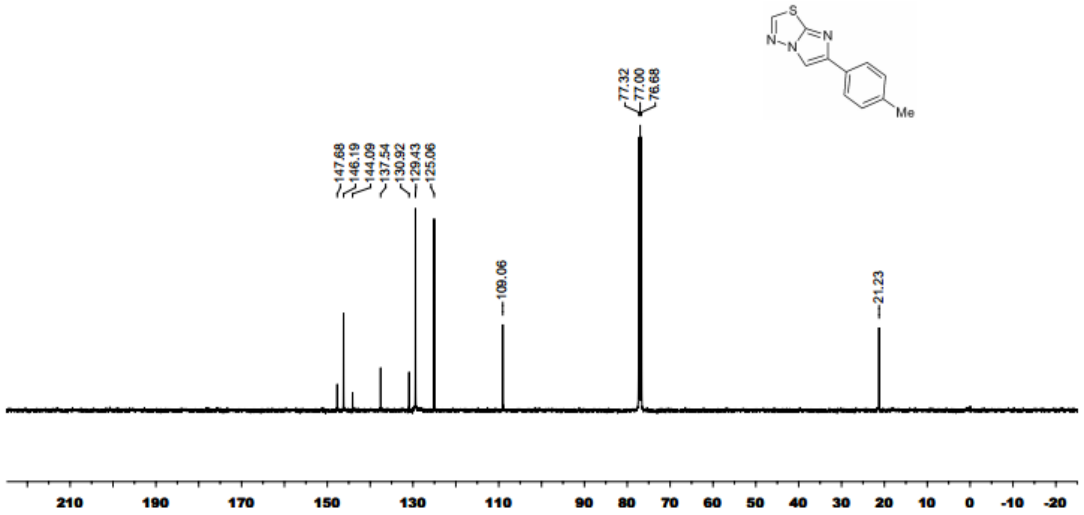
### 6-phenylimidazo[2,1-b][1,3,4]thiadiazole (1a)



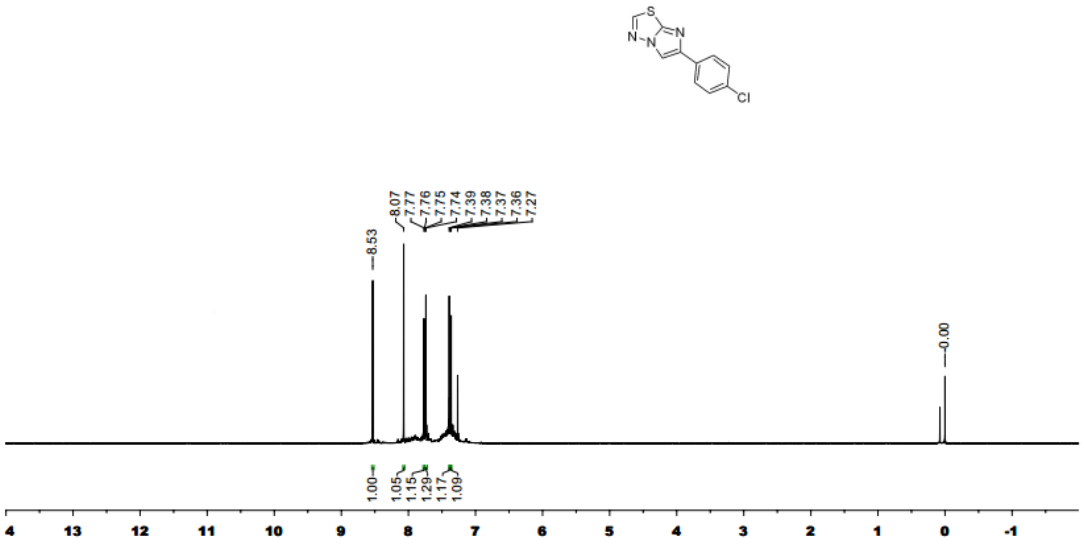



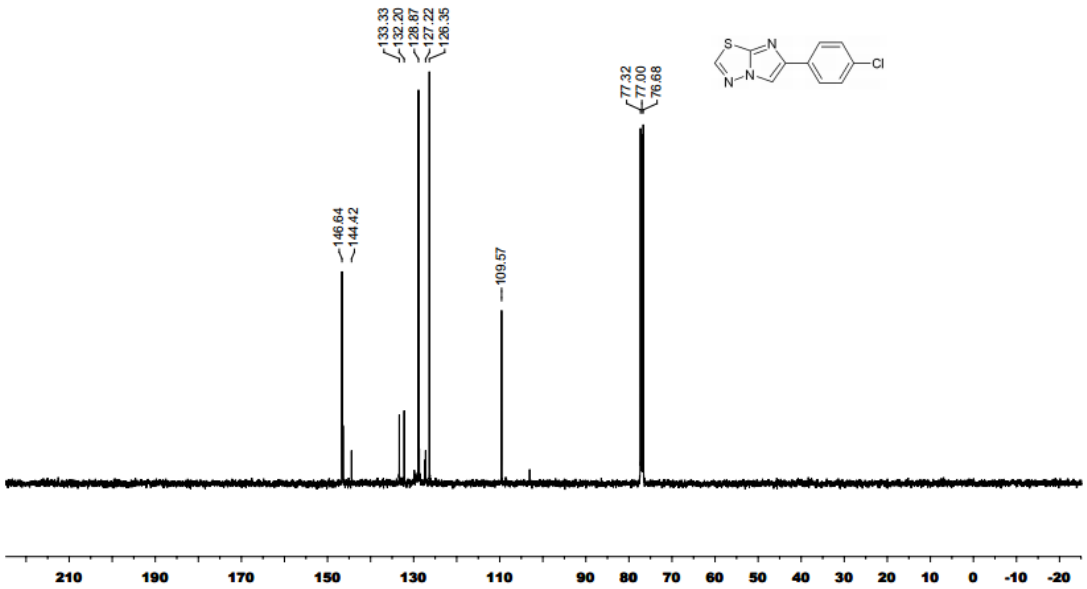
**6-(4 -tolyl)imidazo[2,1-b][1,3,4]thiadiazole (1b)**



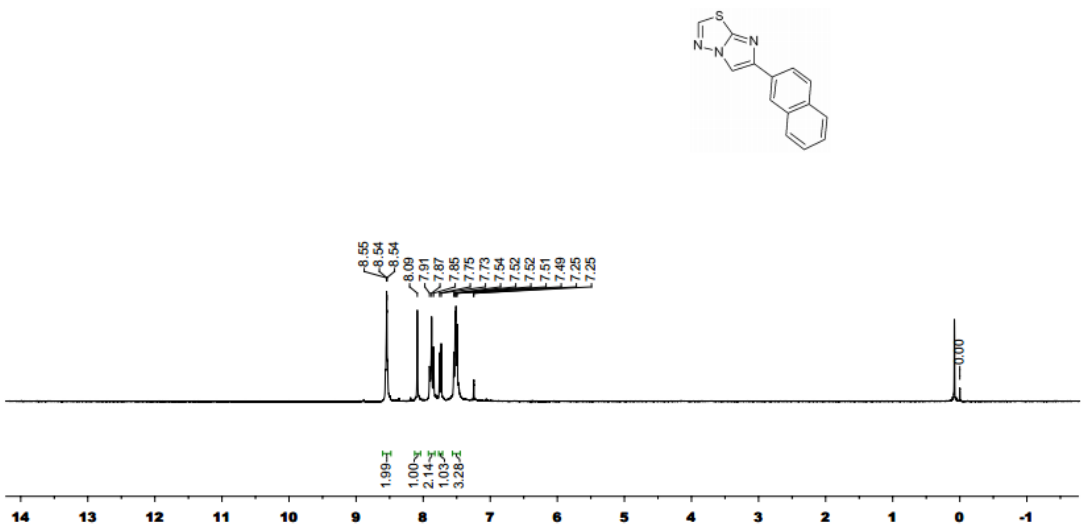



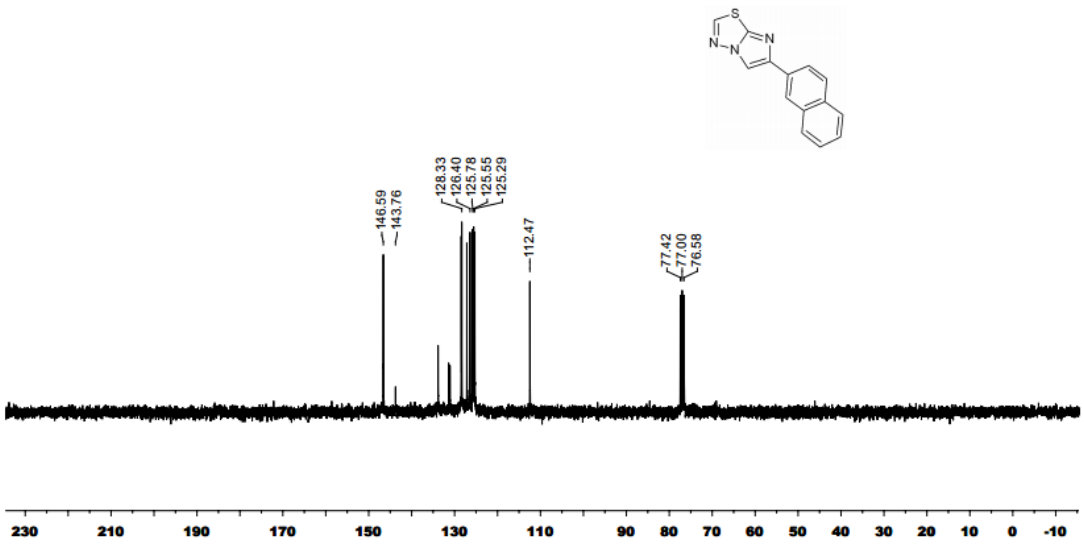
**6-(4-chlorophenyl)imidazo[2,1-b][1,3,4]thiadiazole (1c)**



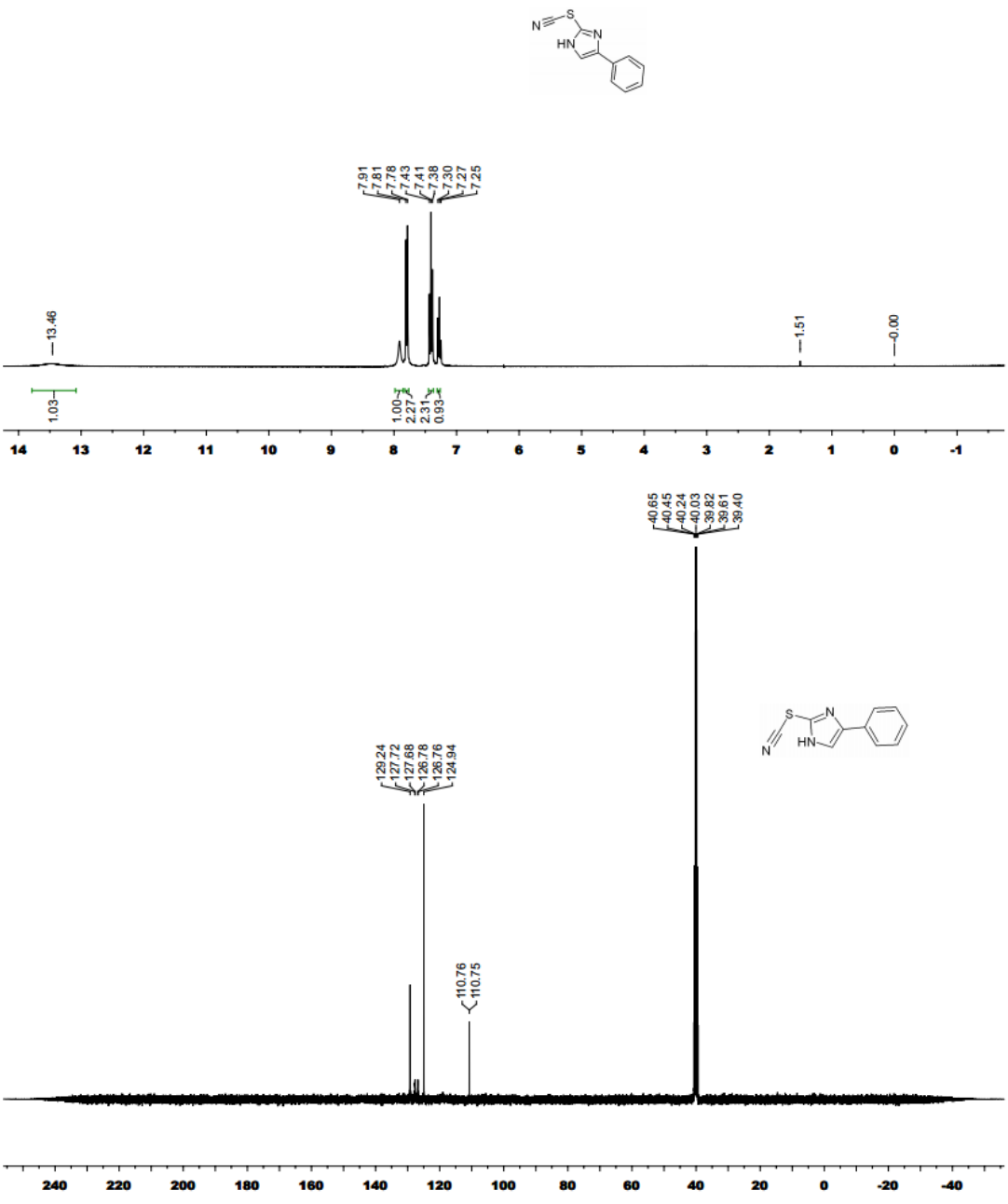



**6-(naphthalen-2-yl)imidazo[2,1-b][1,3,4]thiadiazole (1d)**

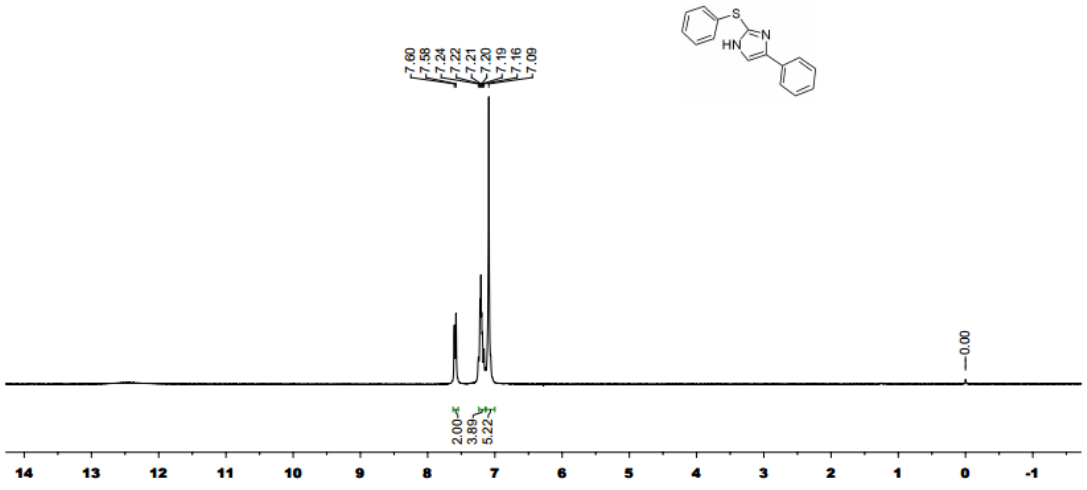


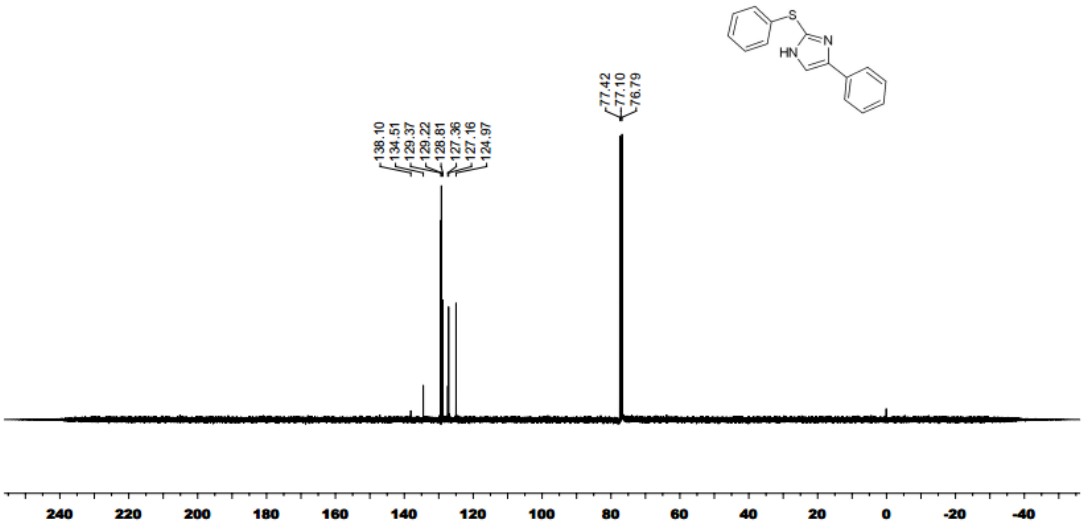



**4-phenyl-2-thiocyanato-1H-imidazole (9)**

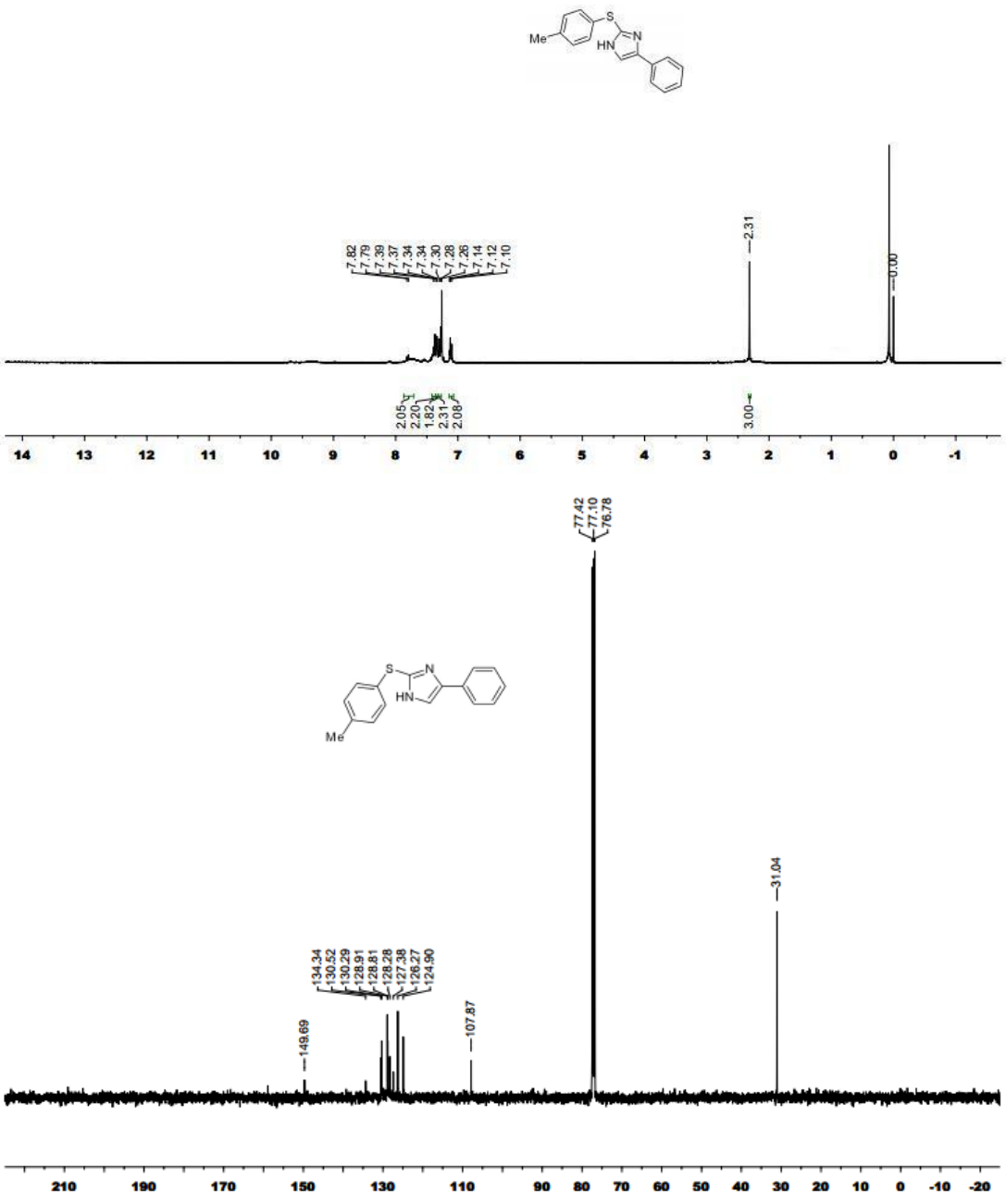


**4-phenyl-2-(phenylthio)-1H-imidazole (3aa)**

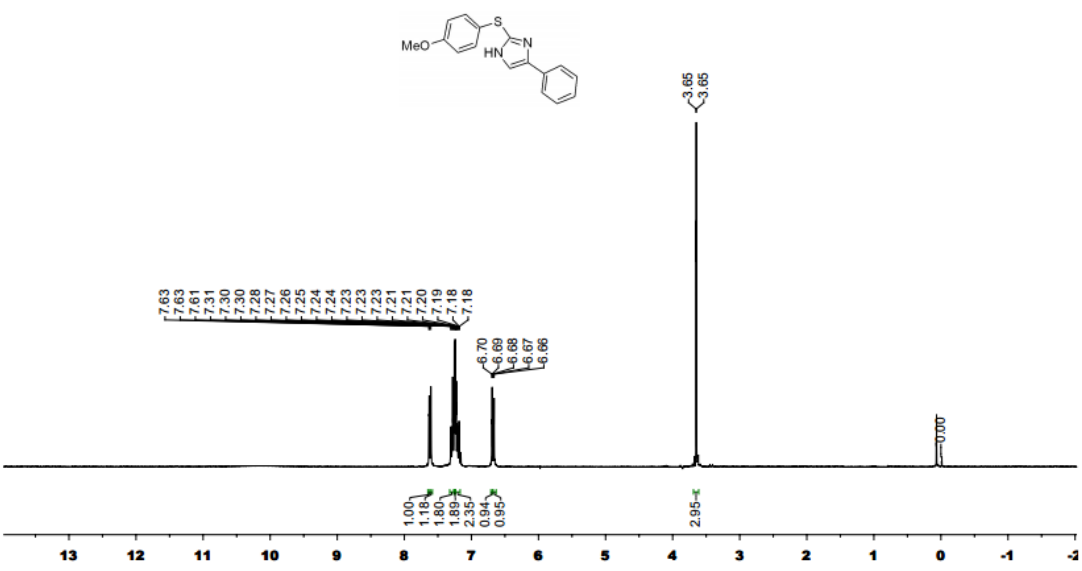


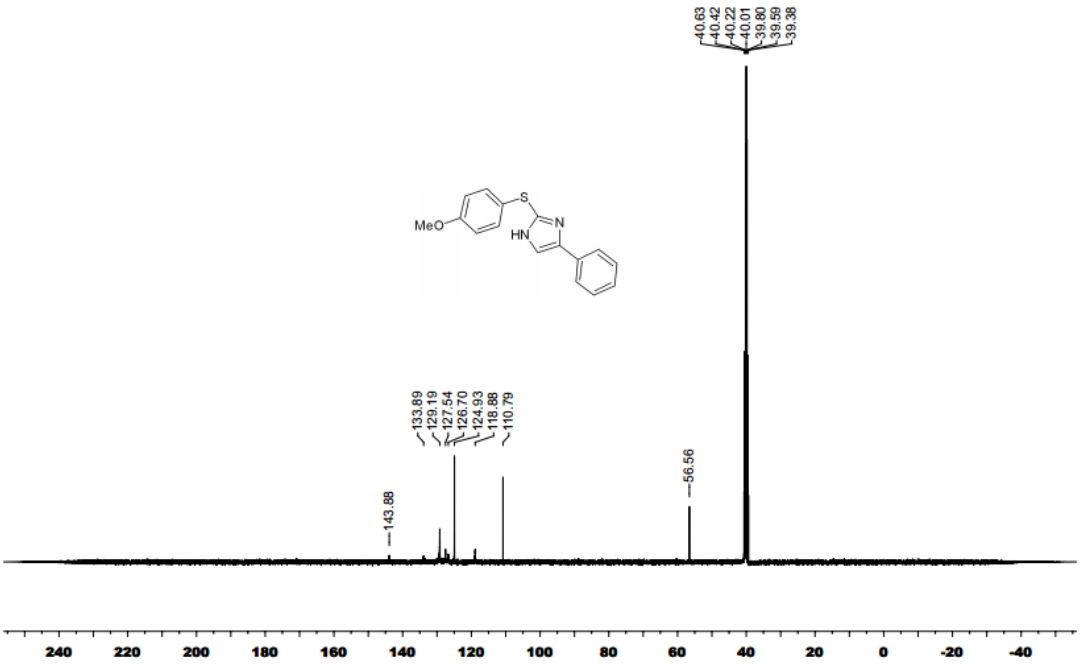



**4-phenyl-2-(4-tolylthio)-1H-imidazole (3ab)**

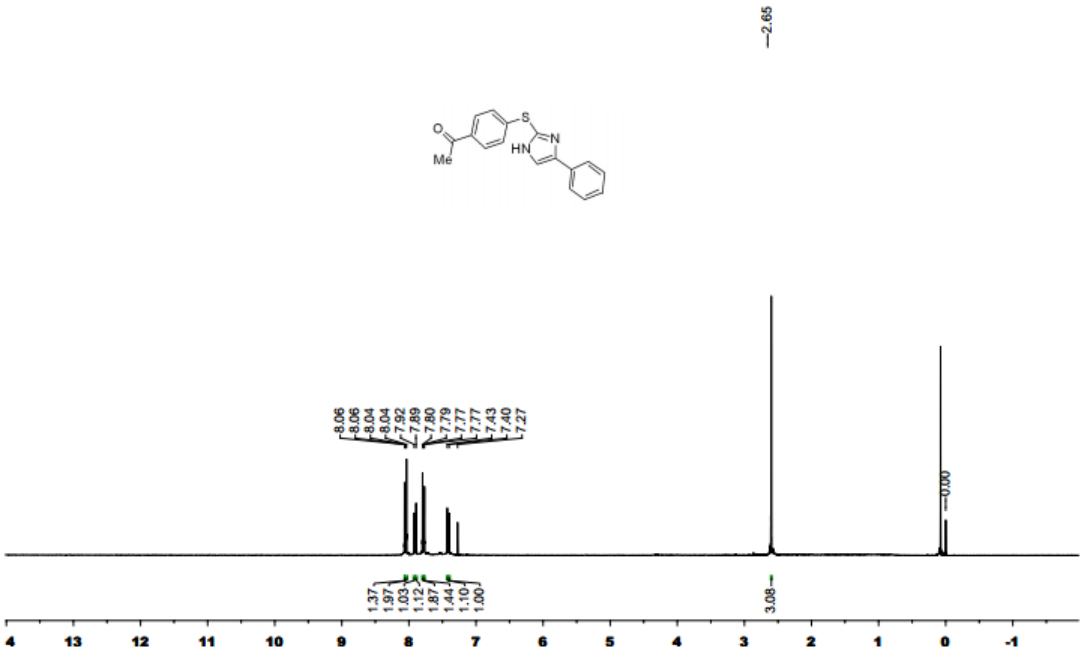


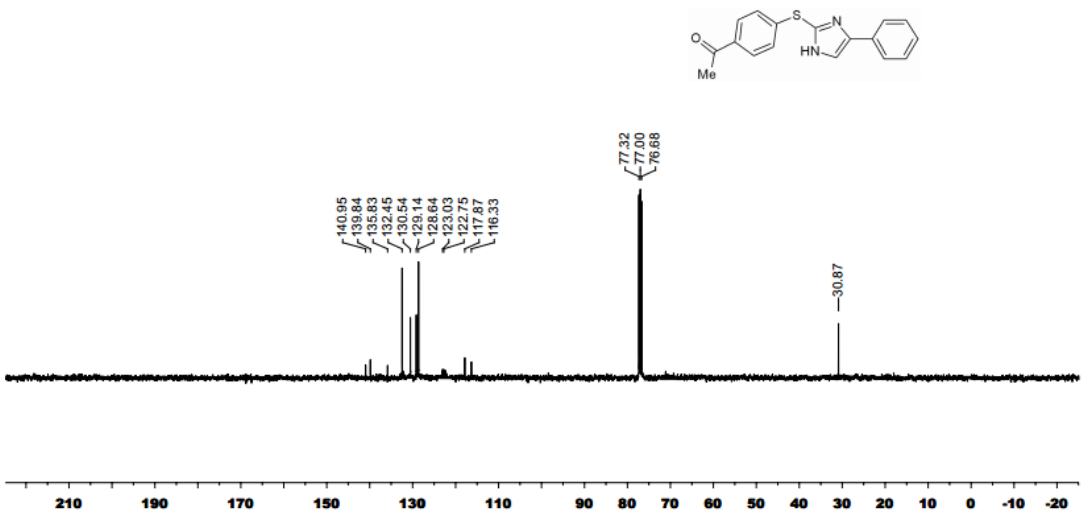
**2-((4-methoxyphenyl)thio)-4-phenyl-1H-imidazole (3ac)**



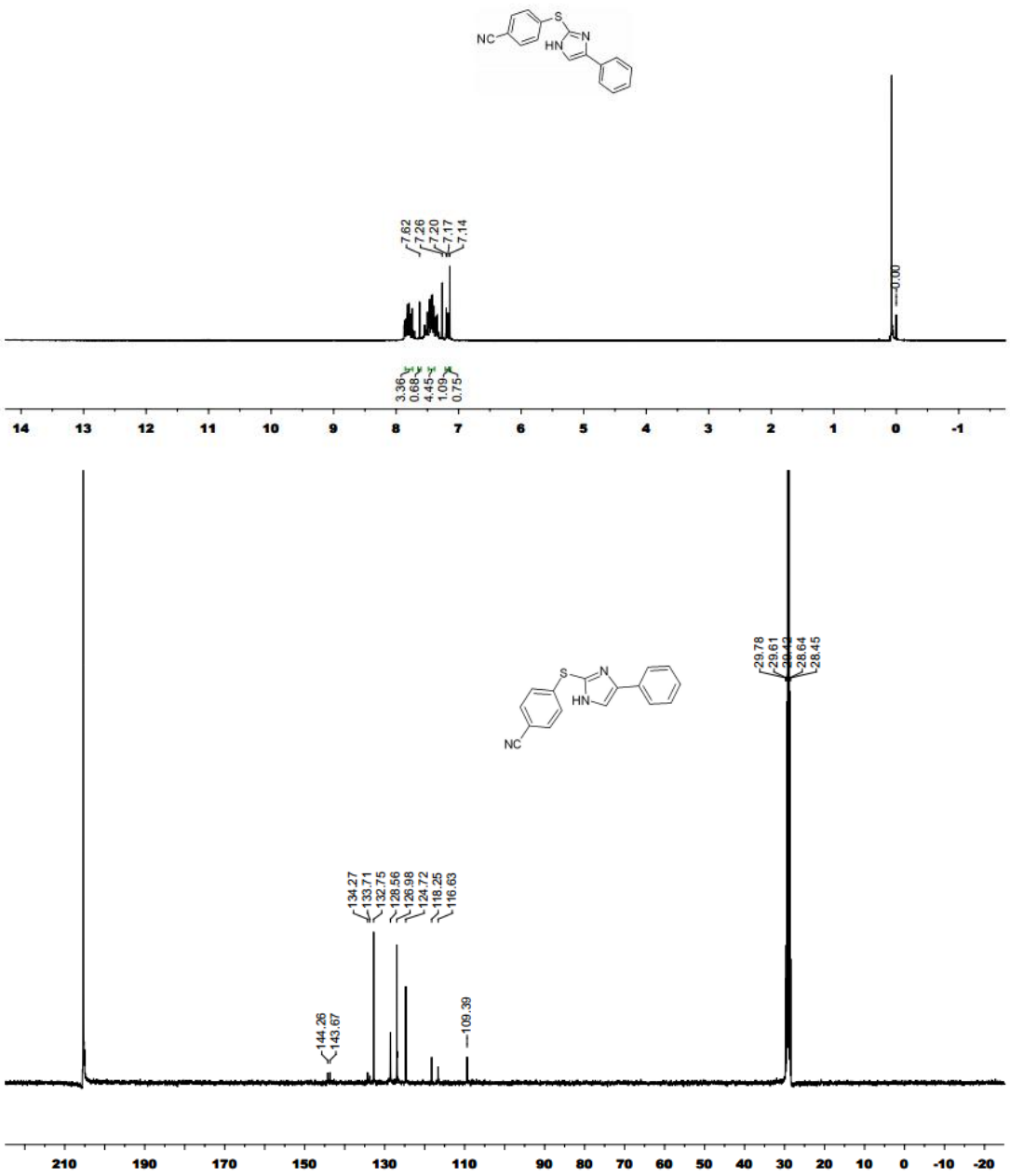



**1-(4-((4-phenyl-1H-imidazol-2-yl)thio)phenyl)ethanone (3ad)**

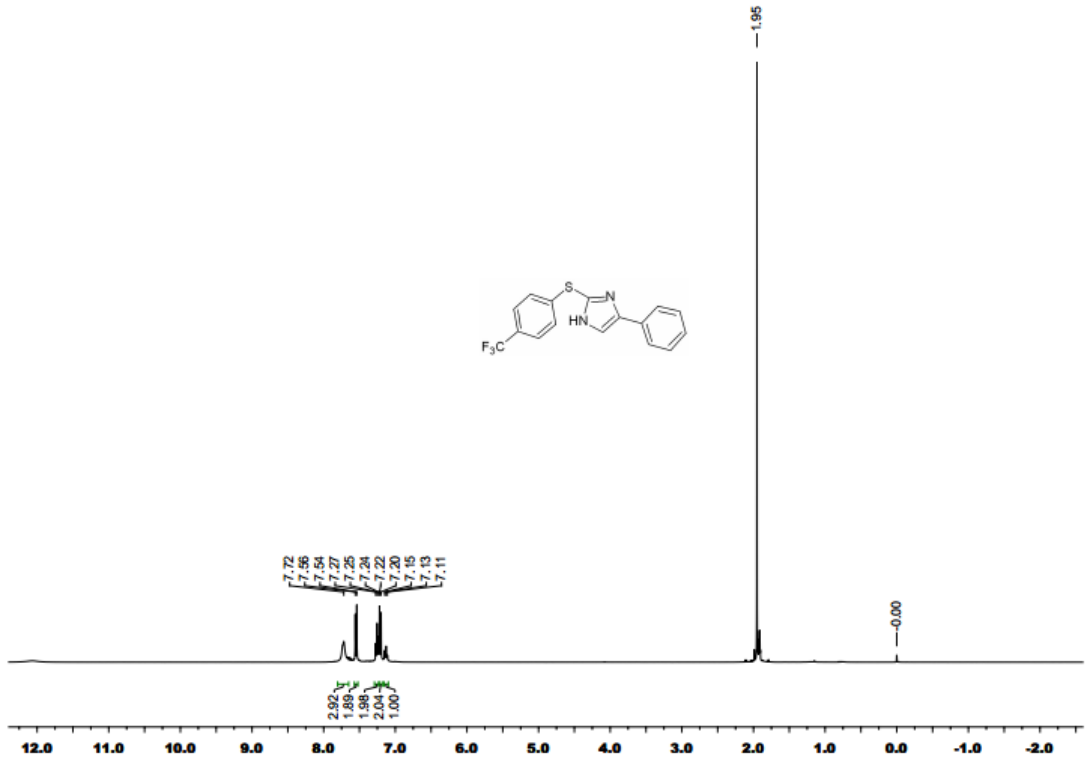


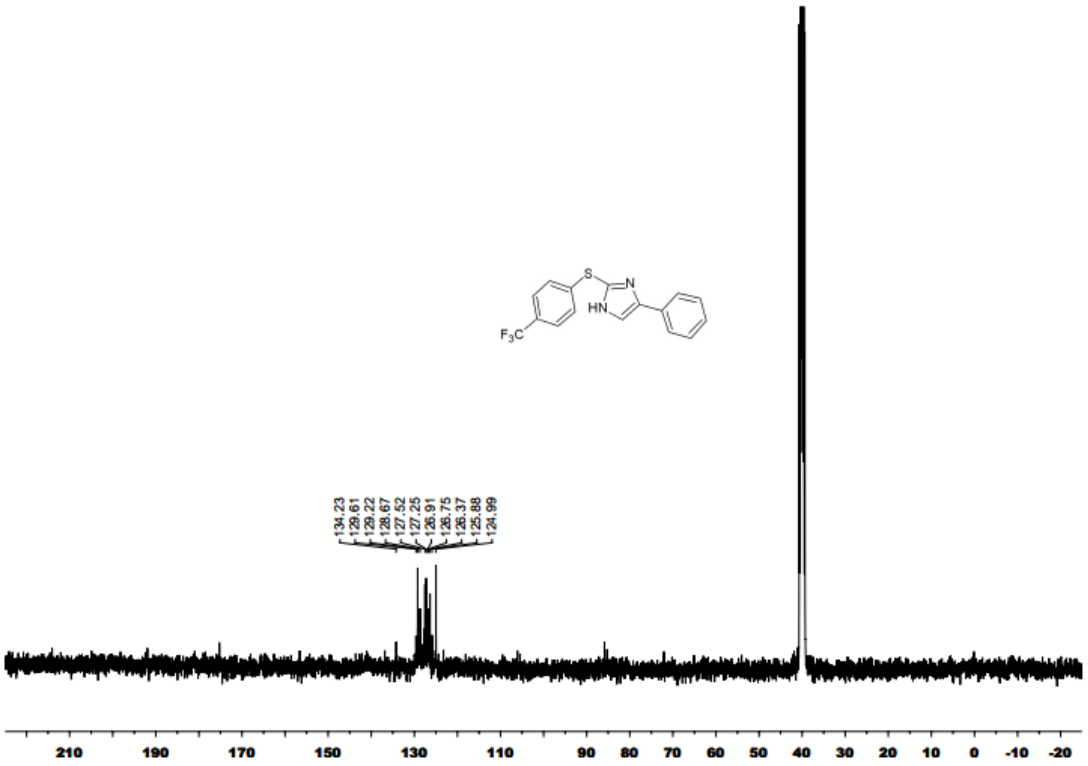



**4-((4-phenyl-1H-imidazol-2-yl)thio)benzonitrile (3ae)**

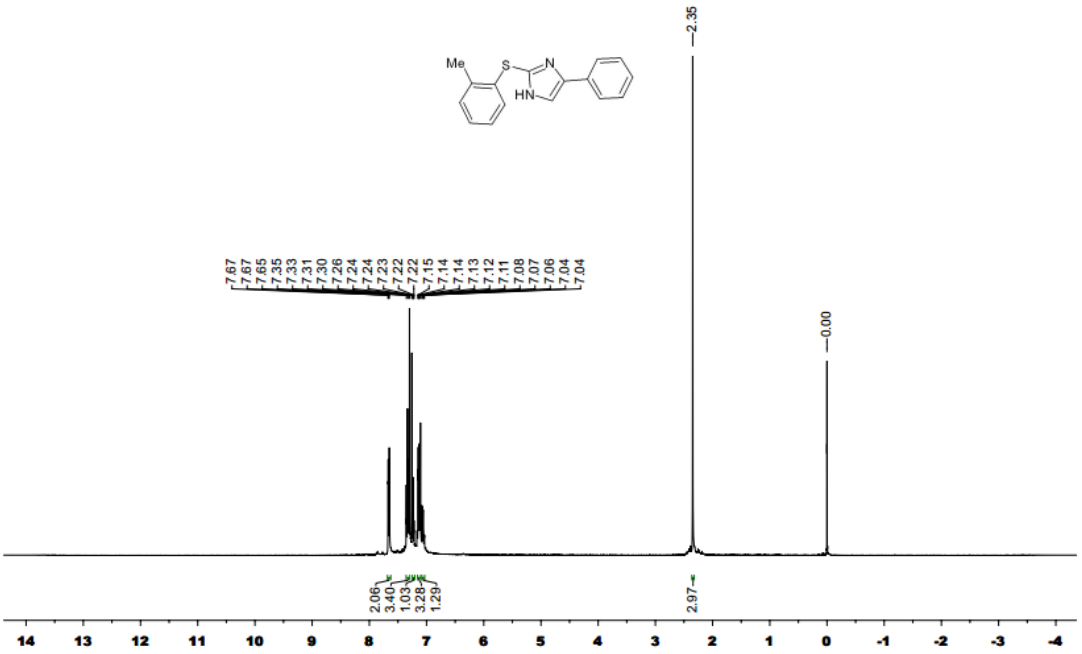


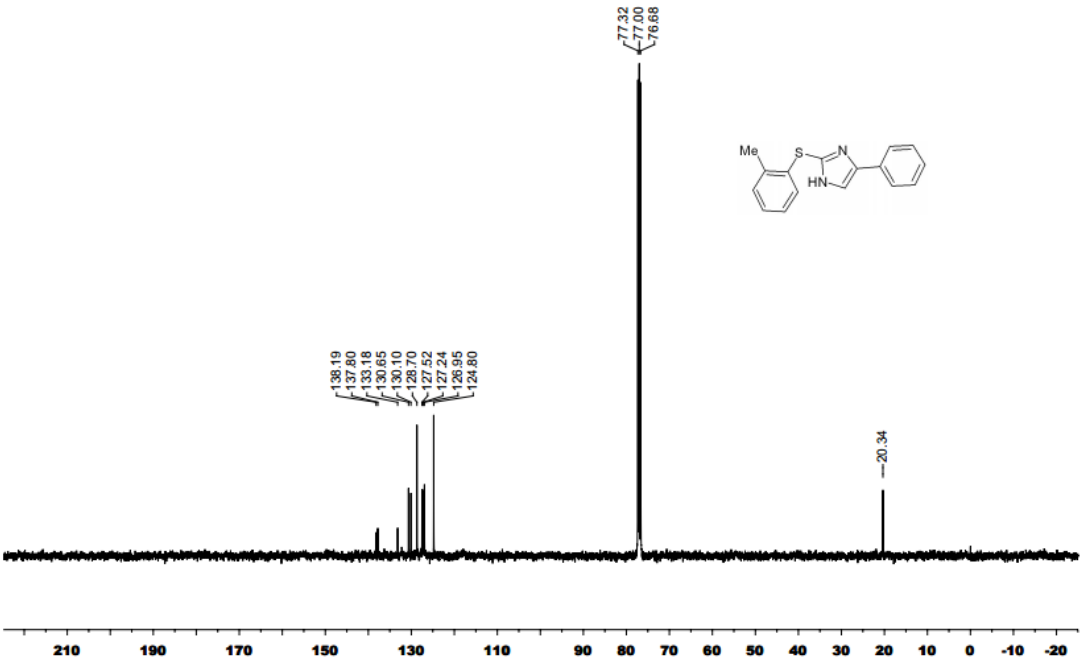
**4-phenyl-2-((4-(trifluoromethyl)phenyl)thio)-1H-imidazole (3af)**



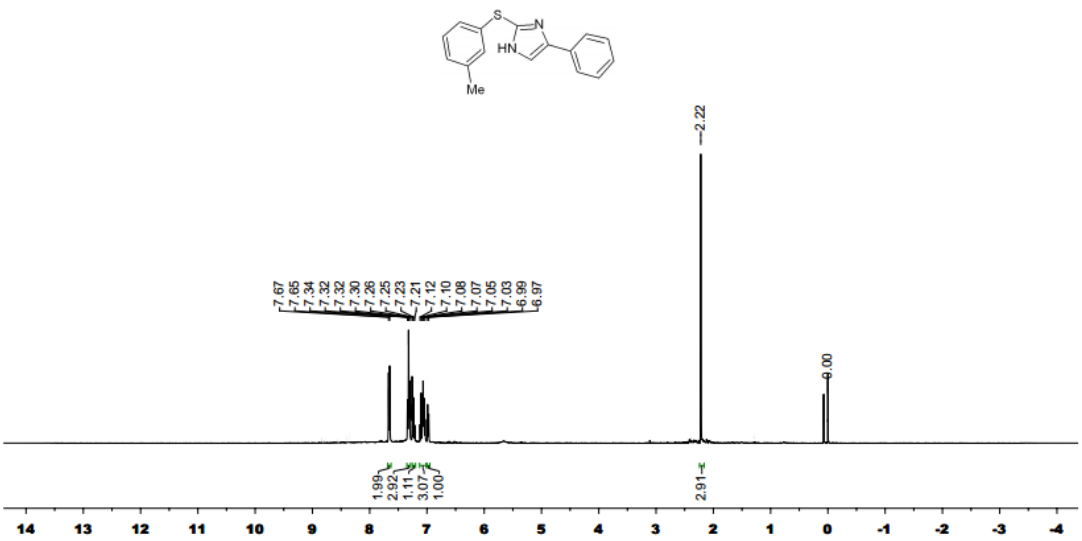



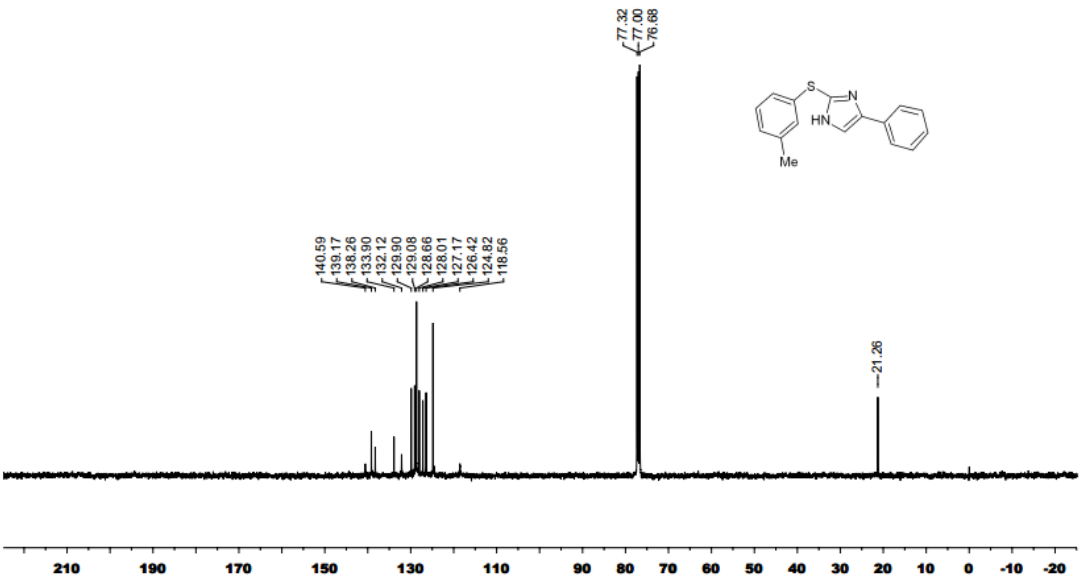
**4-phenyl-2-(2-tolylthio)-1H-imidazole (3ag)**



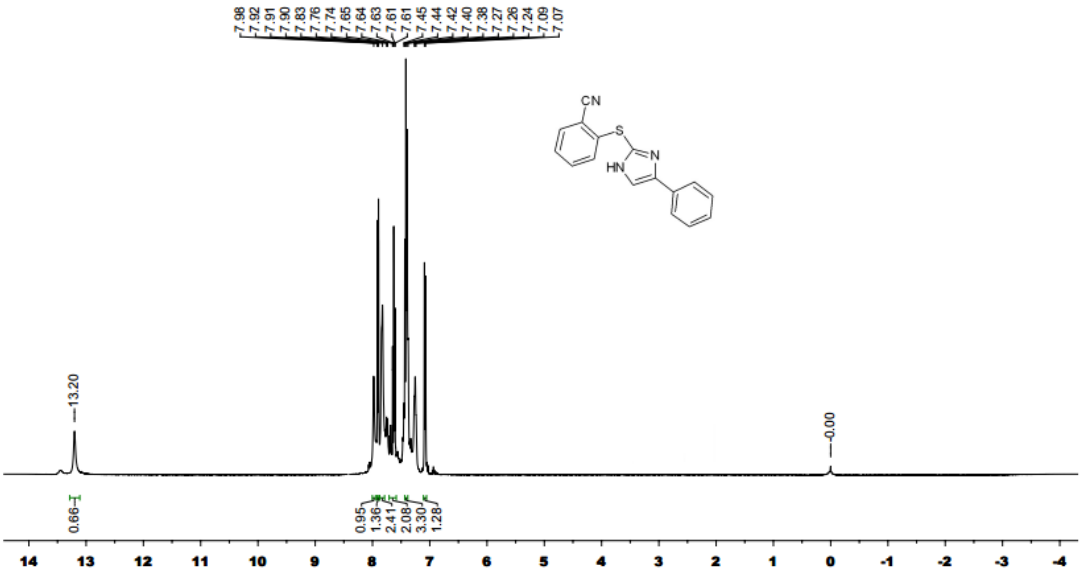



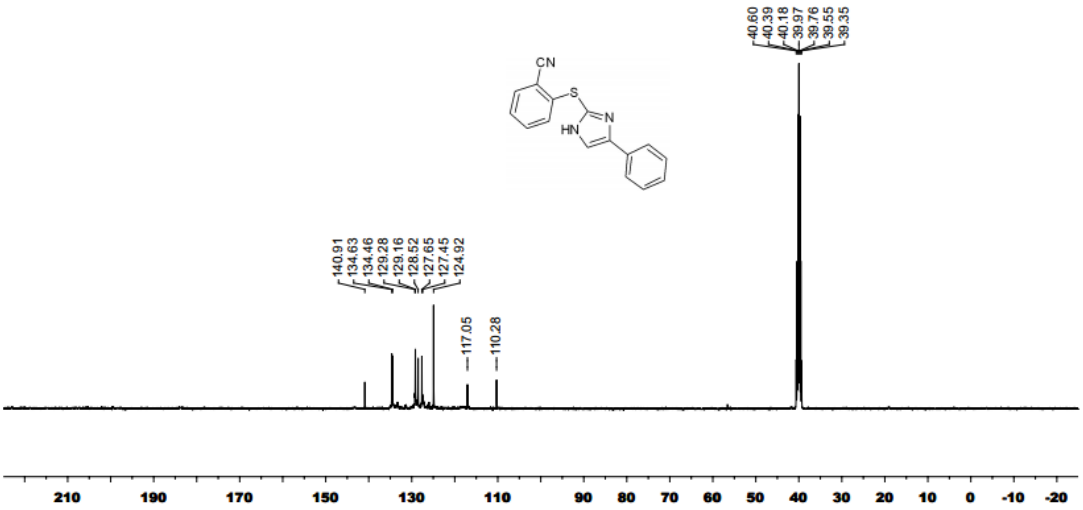
**4-phenyl-2-(3-tolylthio)-1H-imidazole (3ah)**



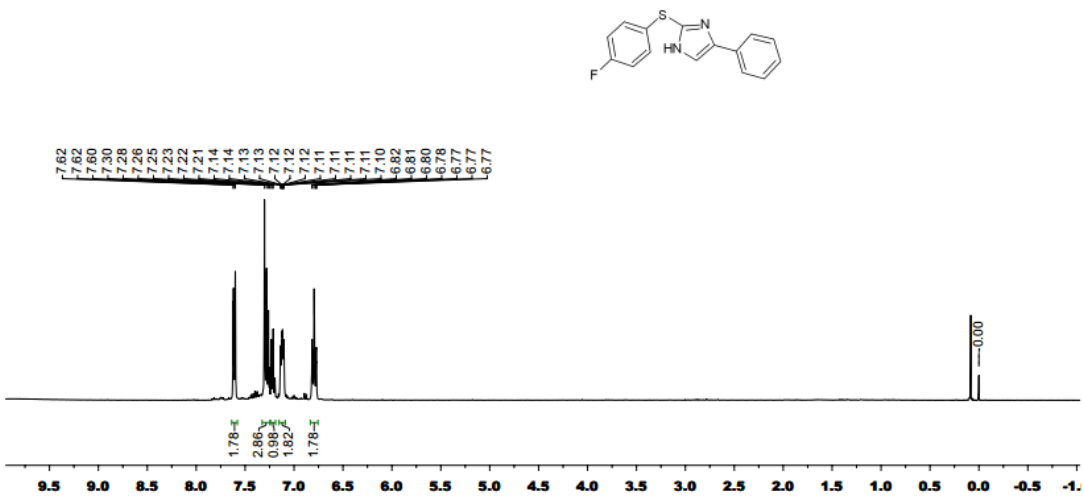



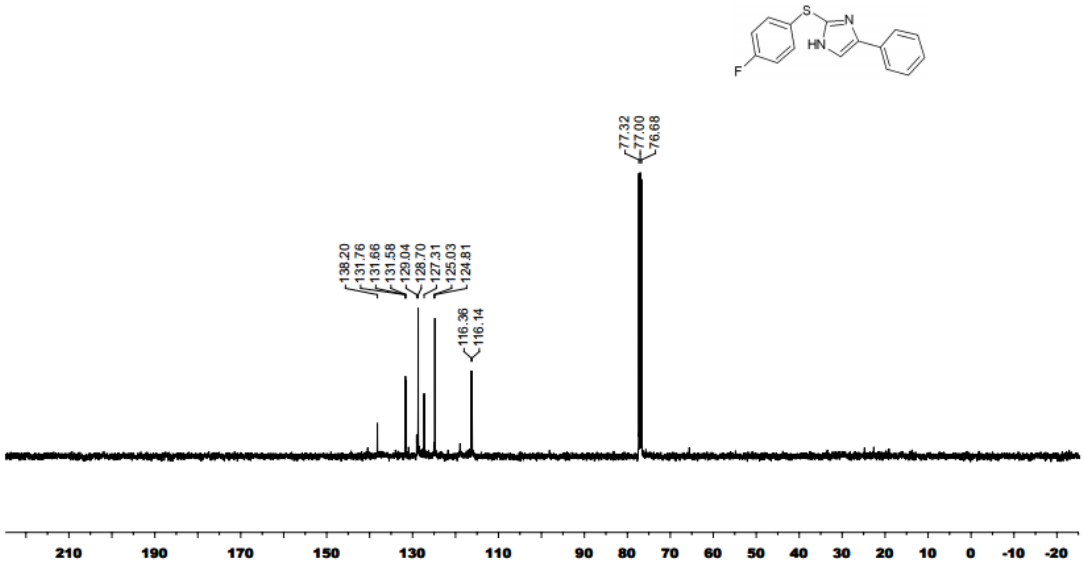
**2-((4-phenyl-1H-imidazol-2-yl)thio)benzonitrile (3ai)**



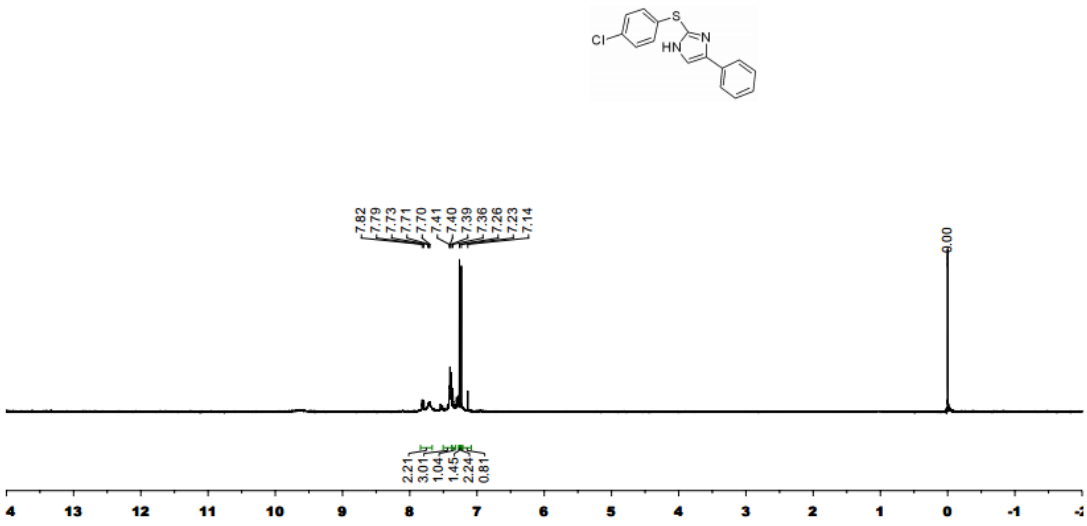



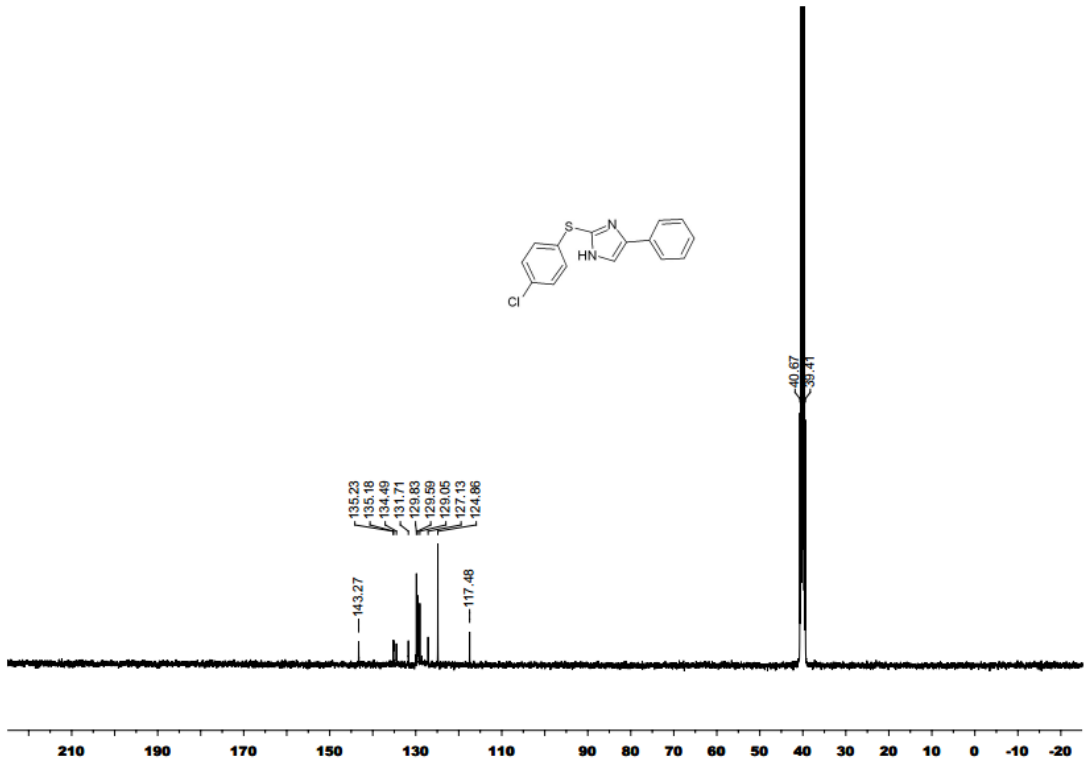
**2-((4-fluorophenyl)thio)-4-phenyl-1H-imidazole (3aj)**



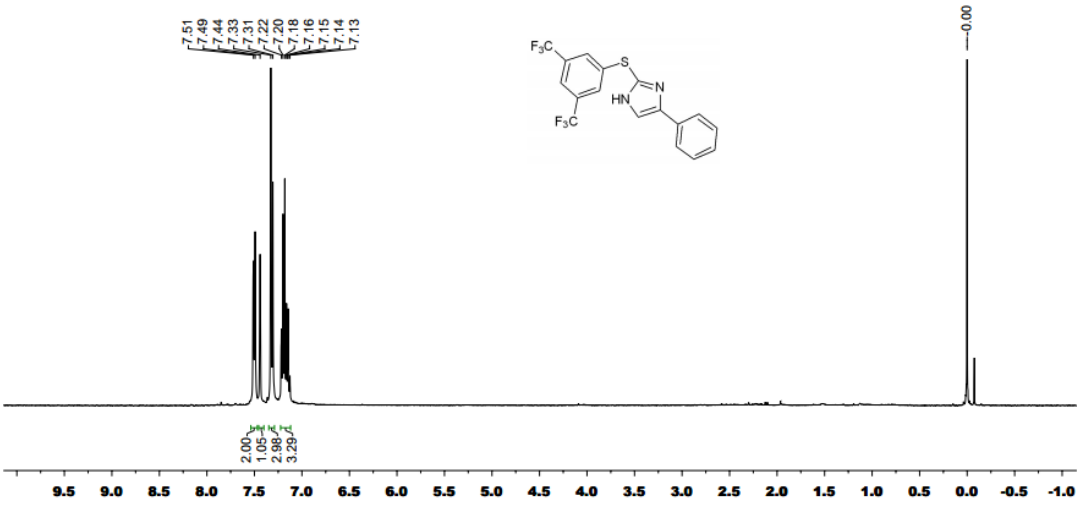



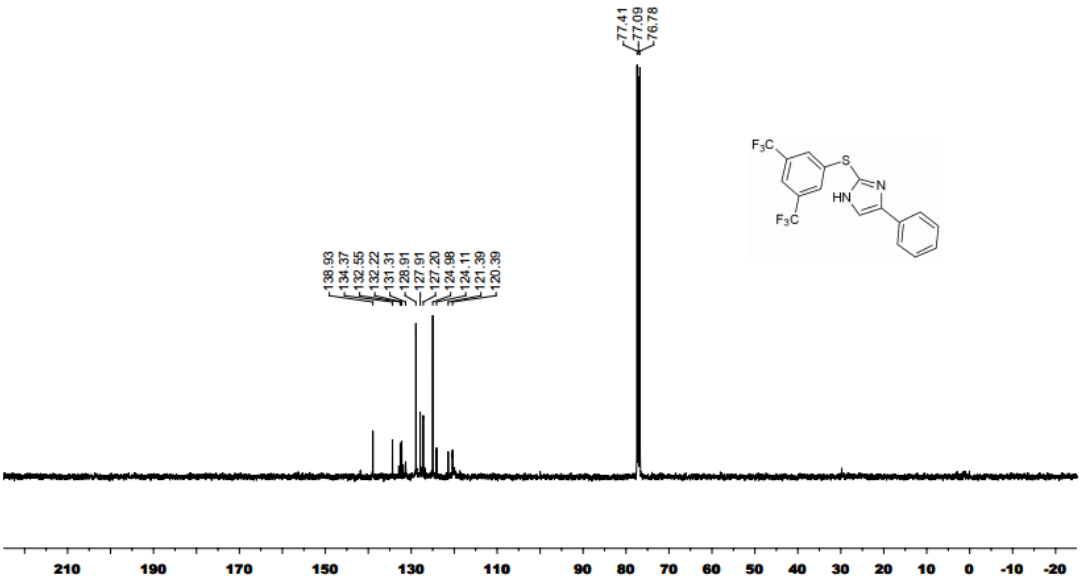
**2-((4-chlorophenyl)thio)-4-phenyl-1H-imidazole (3ak)**



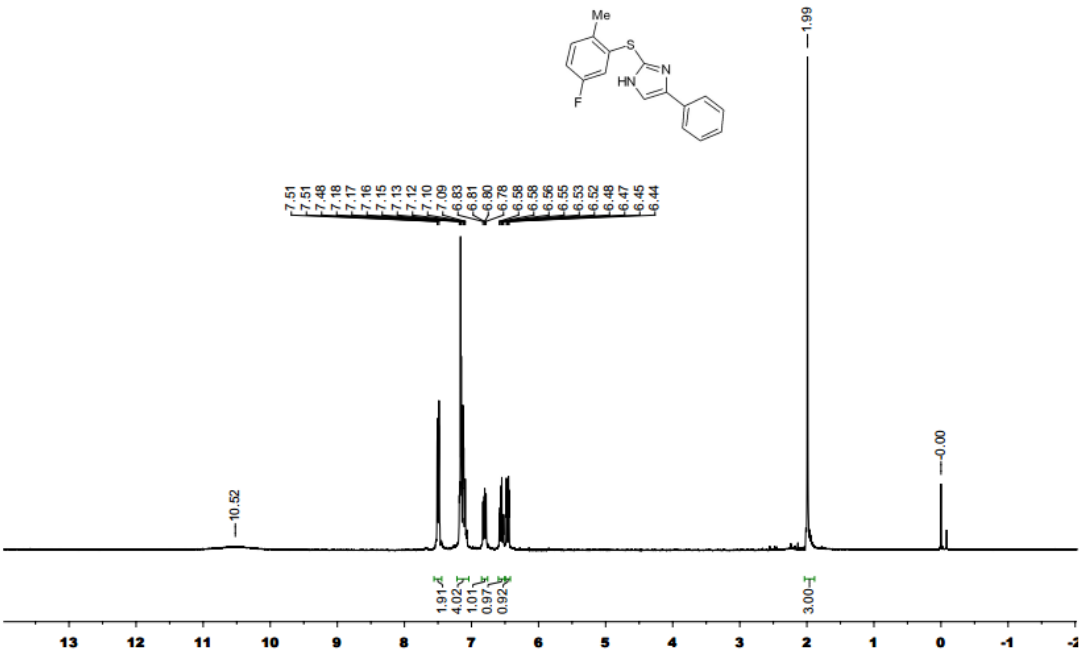



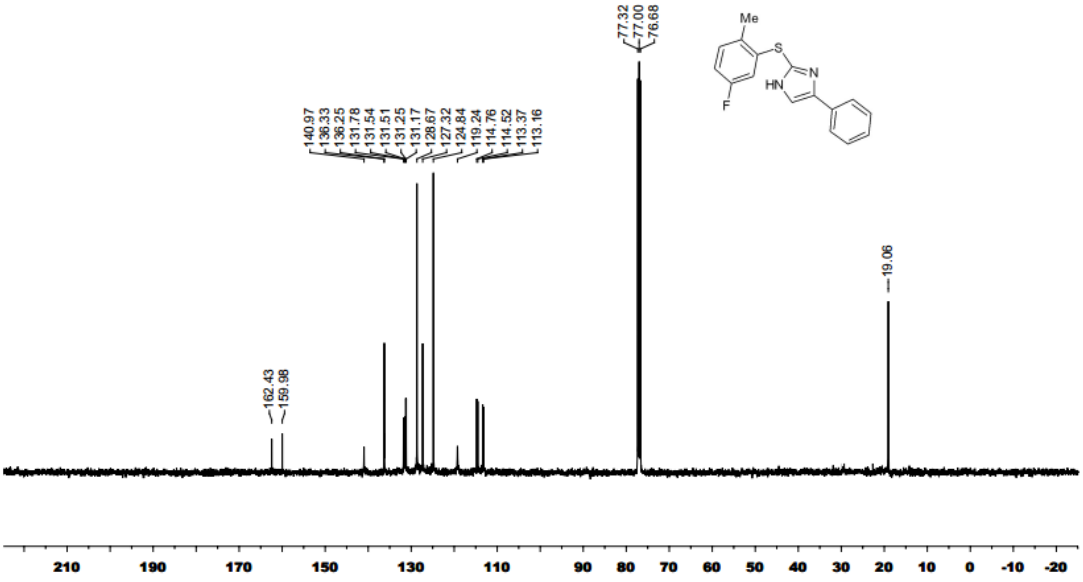
**2-((3,5-bis(trifluoromethyl)phenyl)thio)-4-phenyl-1H-imidazole (3al)**



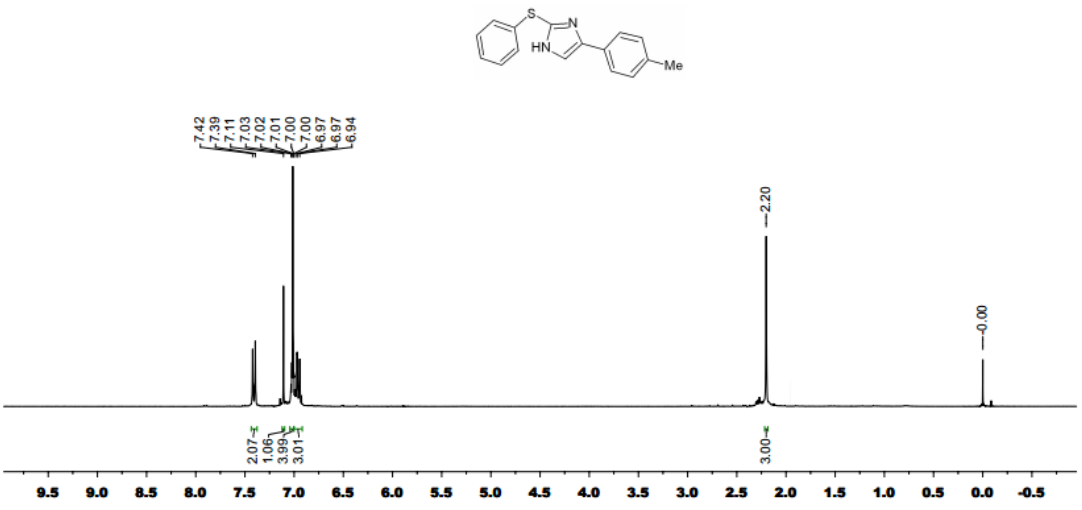



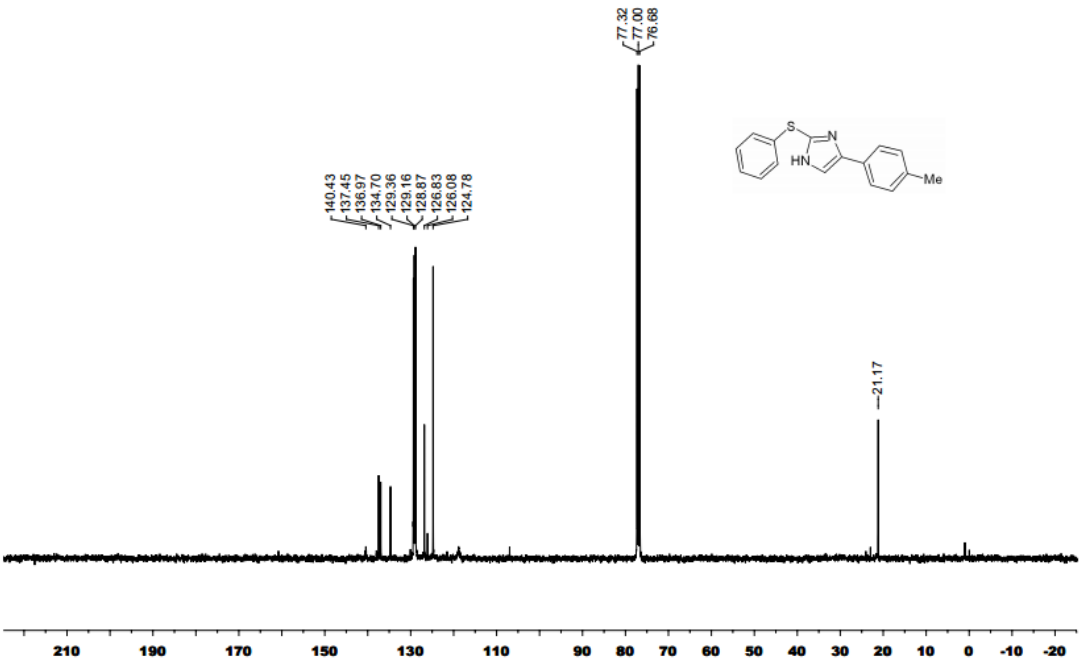
**2-((5-fluoro-2-methylphenyl)thio)-4-phenyl-1H-imidazole (3am)**



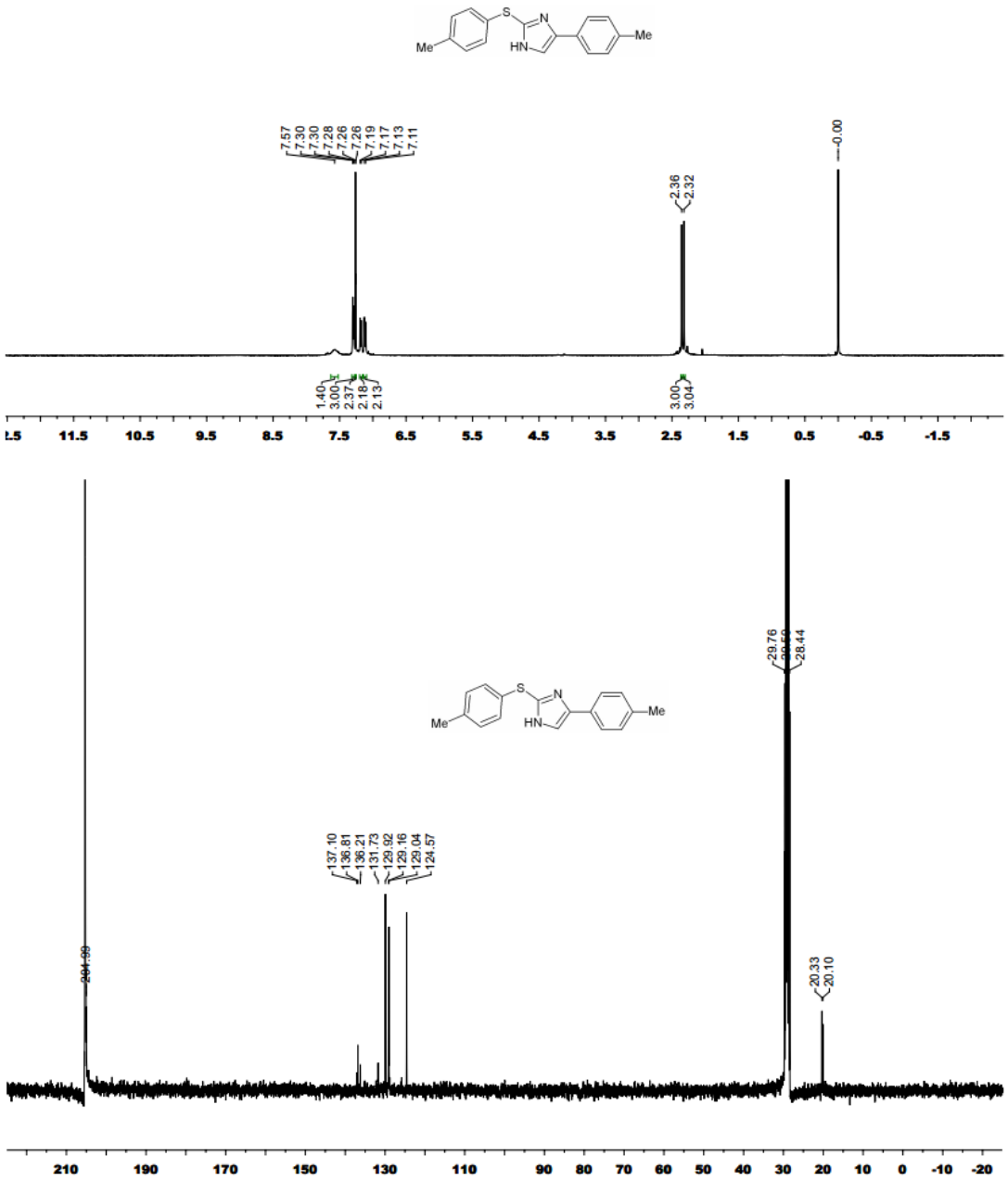



**2-(phenylthio)-4-(4-tolyl)-1H-imidazole (3ba)**



**4-(4-tolyl)-2-(4-tolylthio)-1H-imidazole (3bb)**



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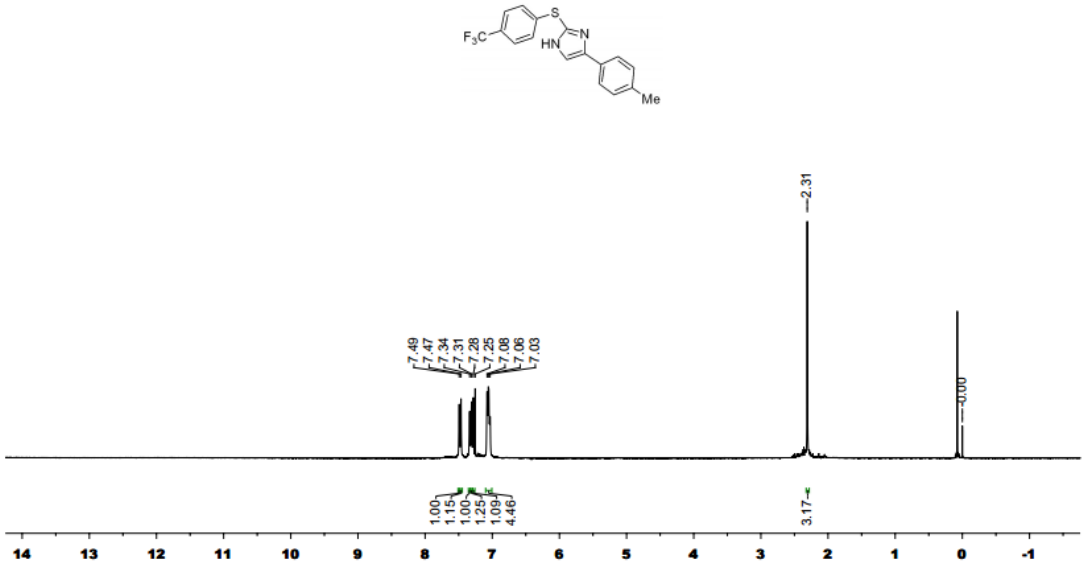
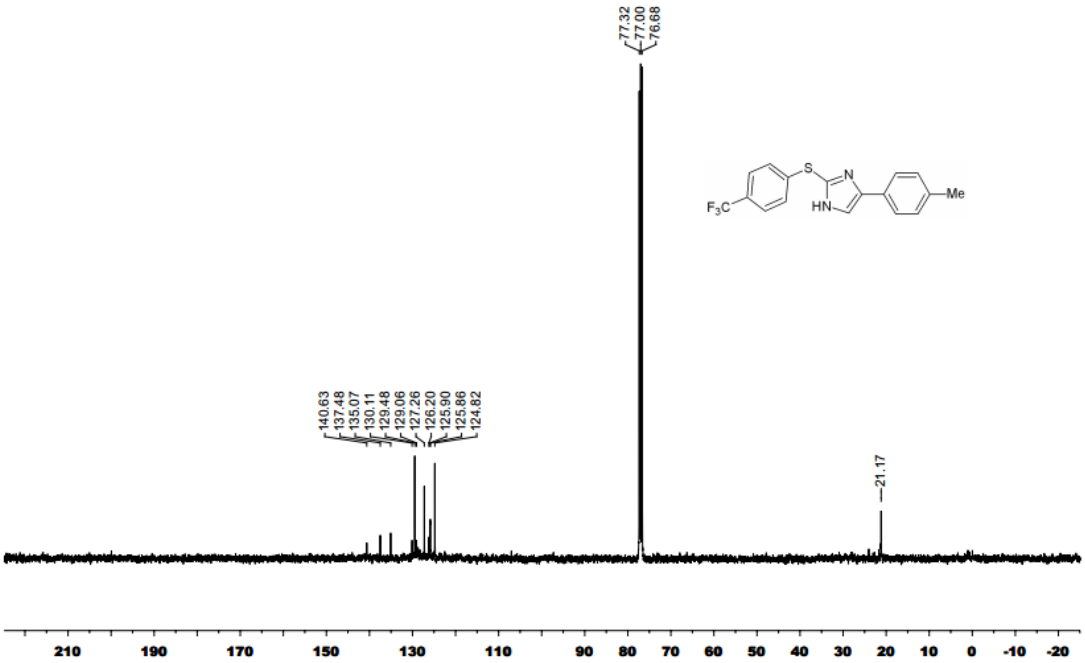
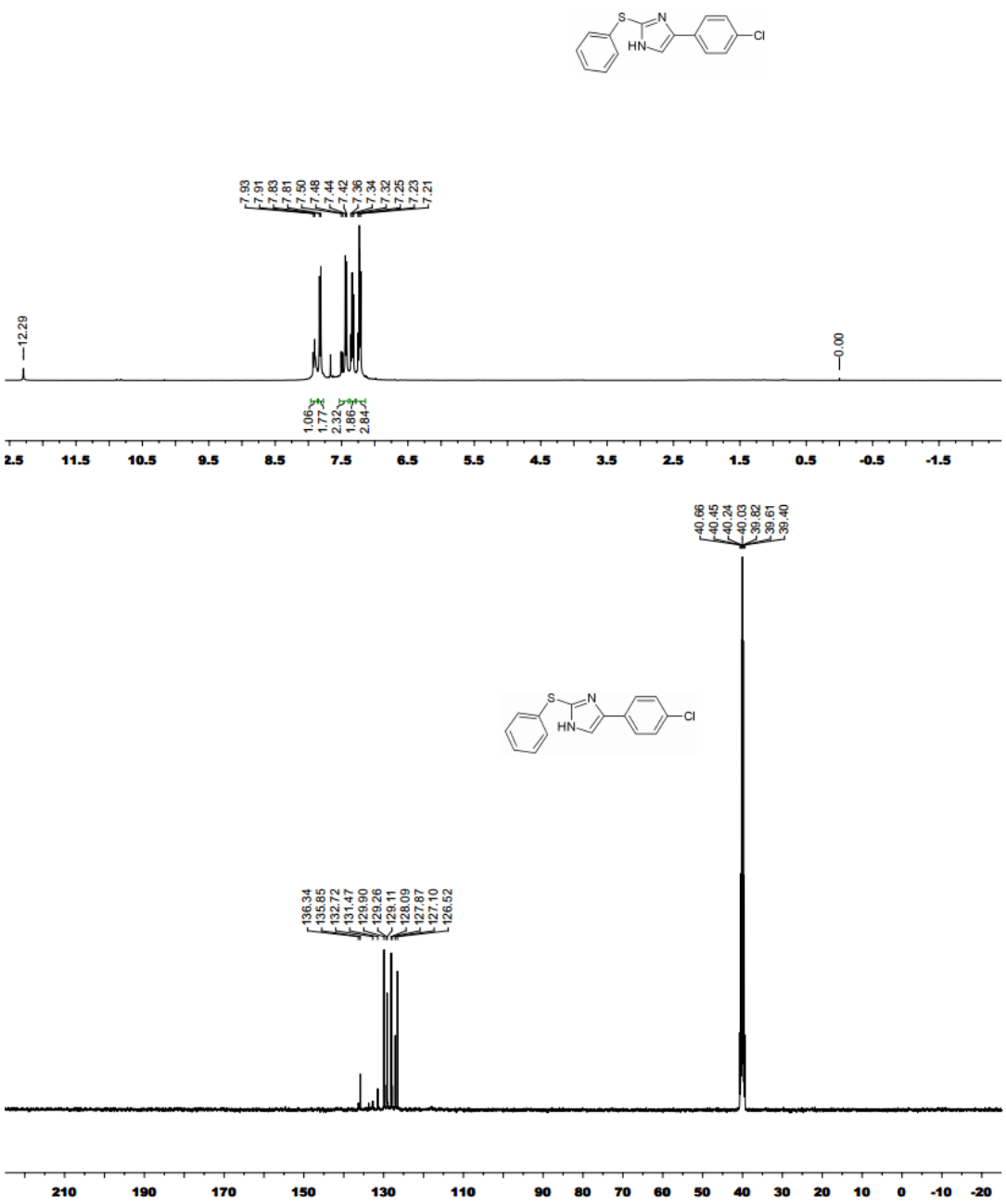
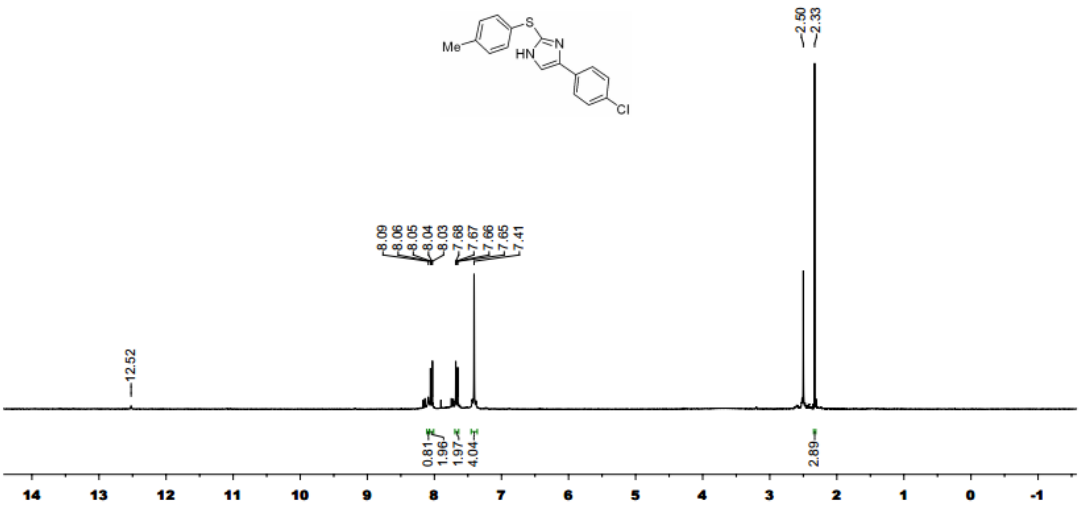


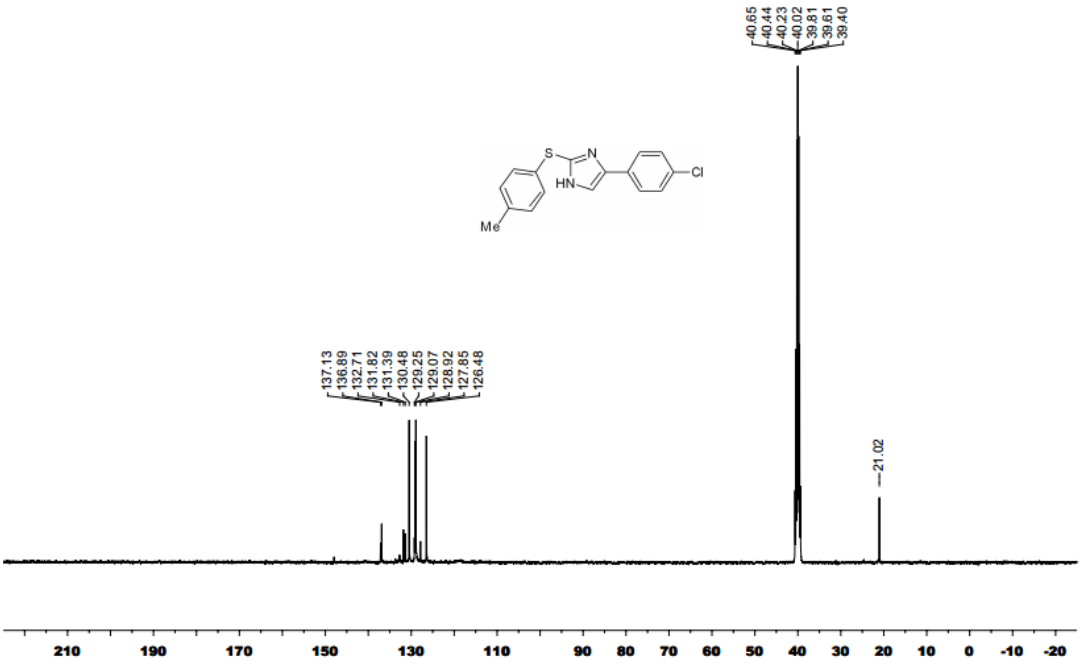



**4-(4-chlorophenyl)-2-(phenylthio)-1H-imidazole (3ca)**

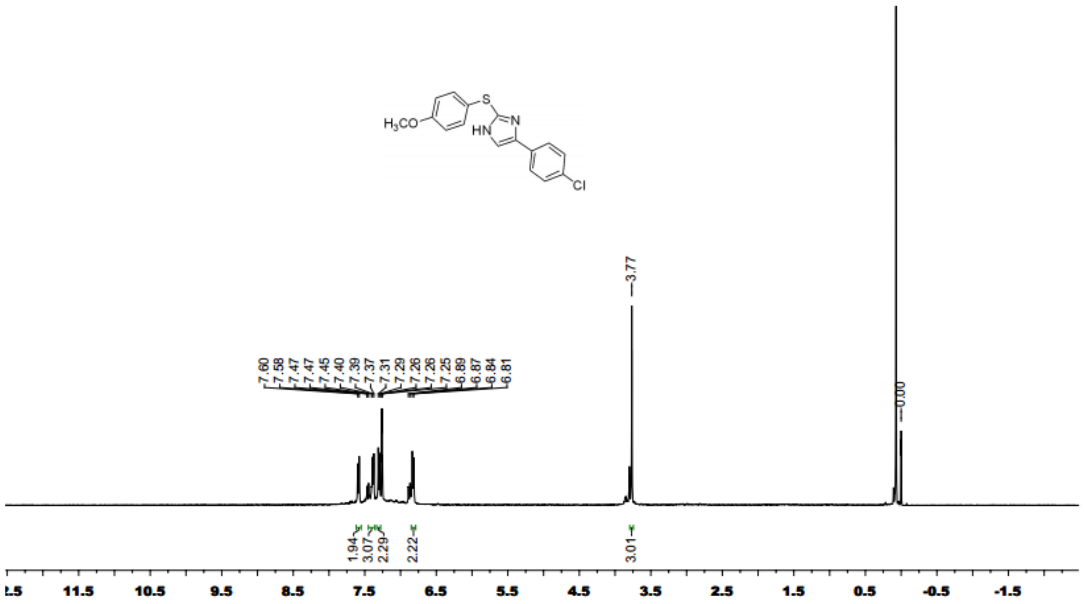


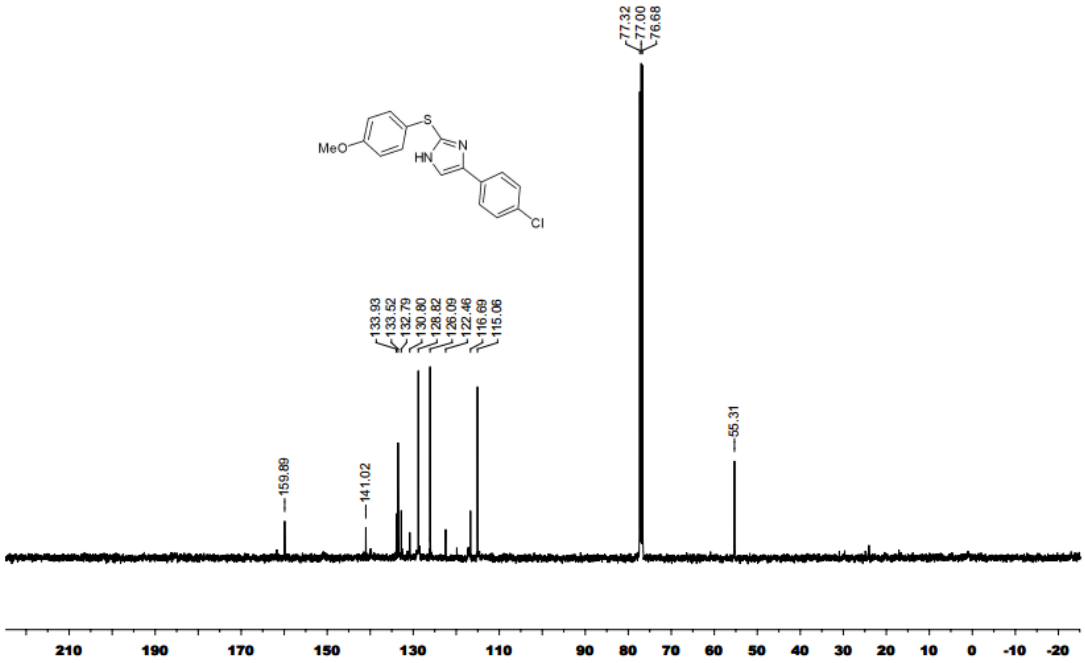
**4-(4-chlorophenyl)-2-(4-tolylthio)-1H-imidazole (3cb)**



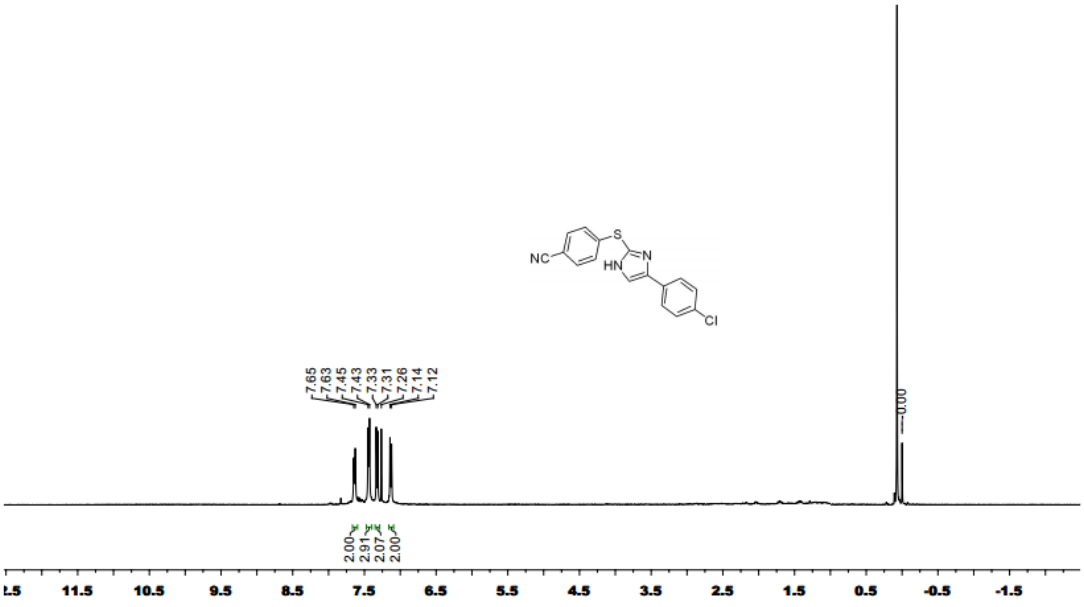



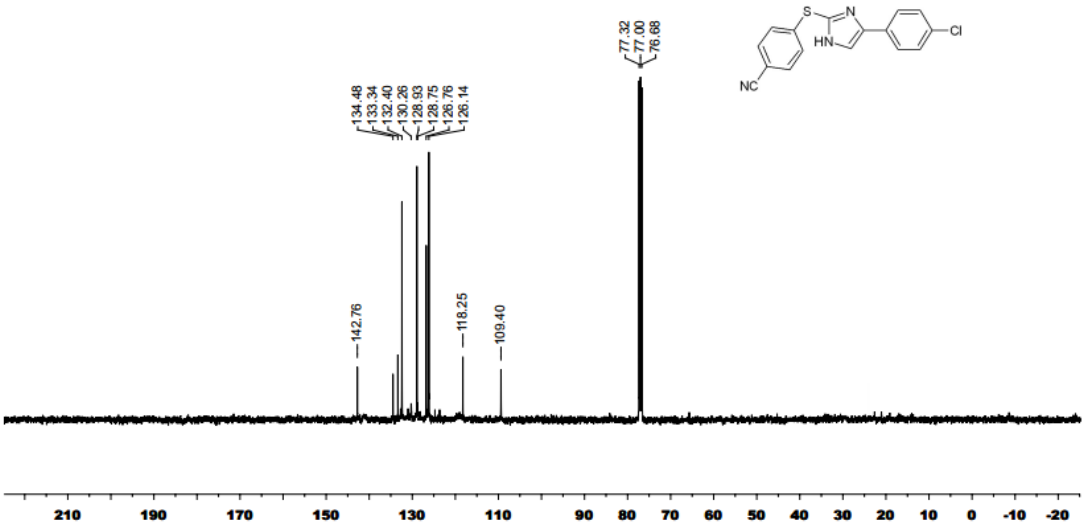
**4-(4-chlorophenyl)-2-((4-methoxyphenyl)thio)-1H-imidazole (3cc)**



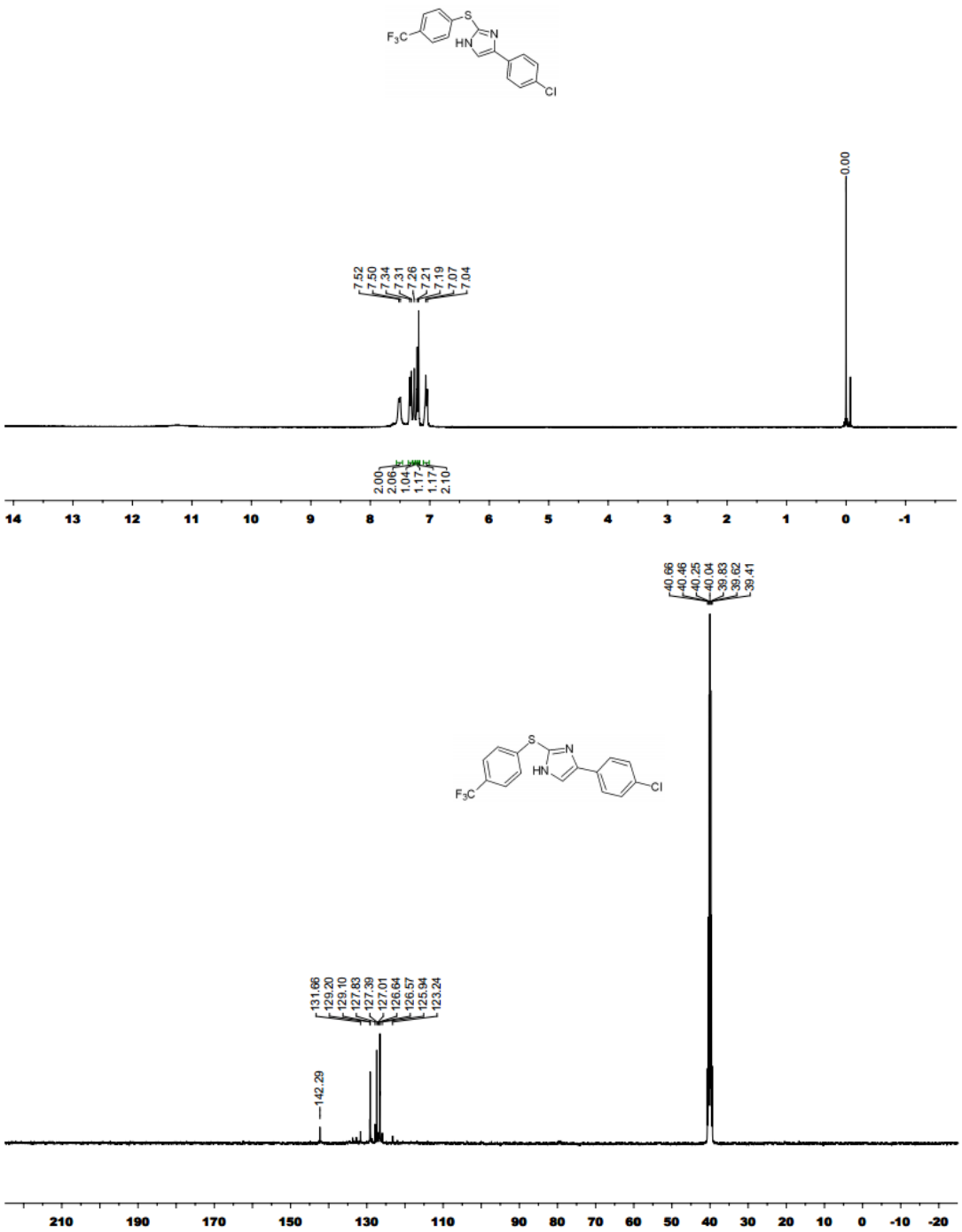



**4-((4-(4-chlorophenyl)-1H-imidazol-2-yl)thio)benzonitrile (3ce)**

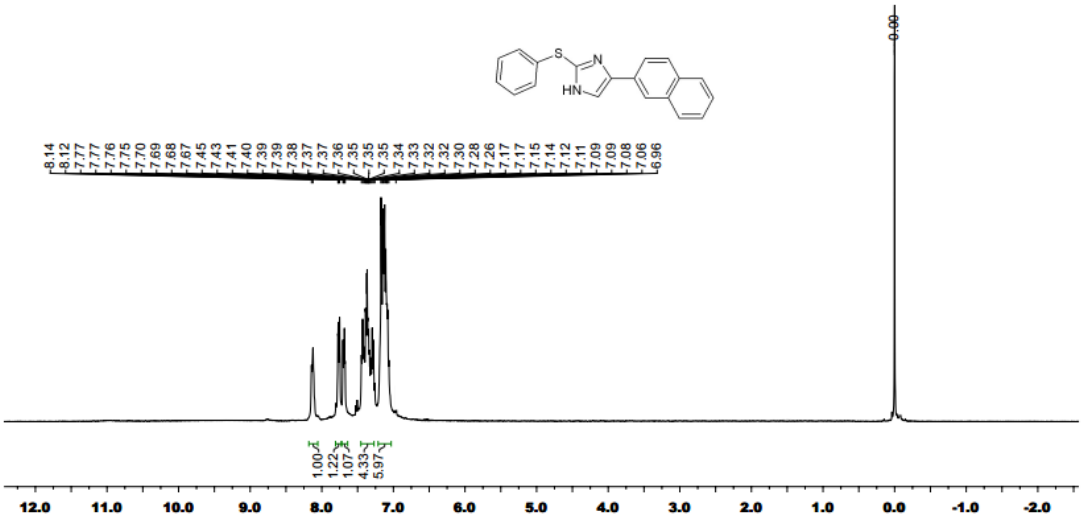


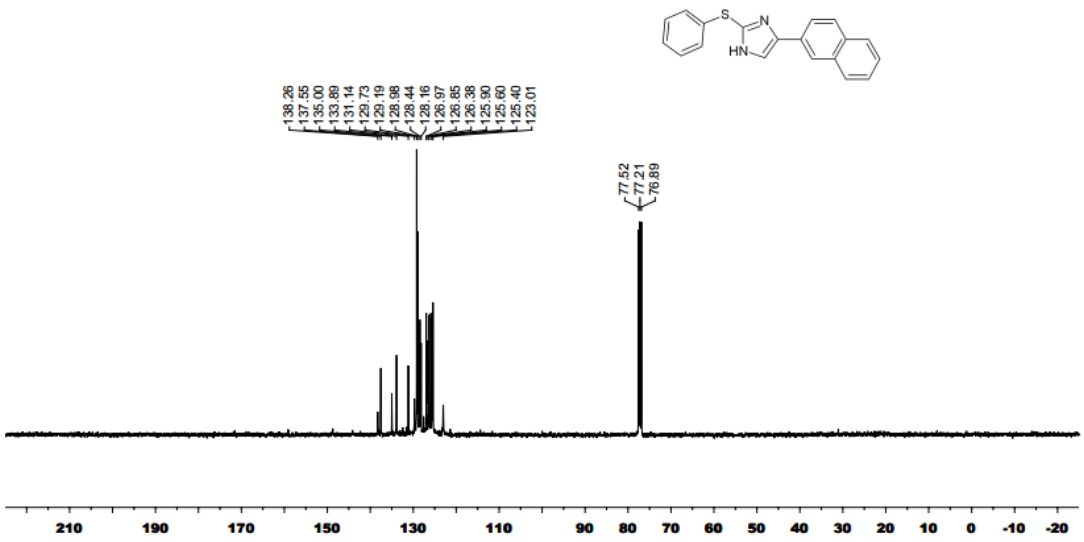



**4-(4-chlorophenyl)-2-((4-(trifluoromethyl)phenyl)thio)-1H-imidazole (3cf)**

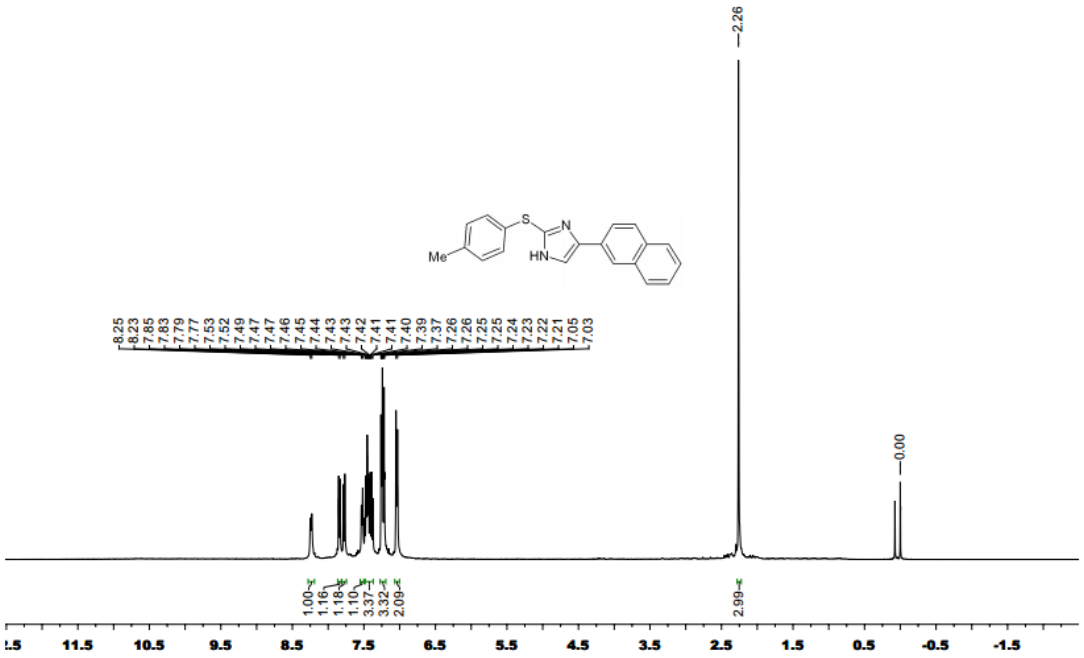


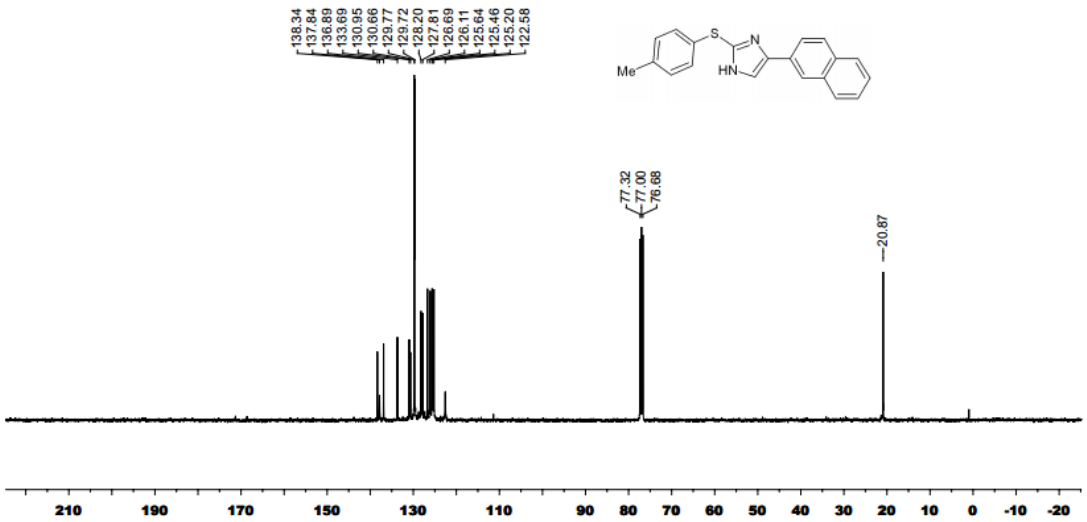
**4-(naphthalen-2-yl)-2-(phenylthio)-1H-imidazole (3da)**



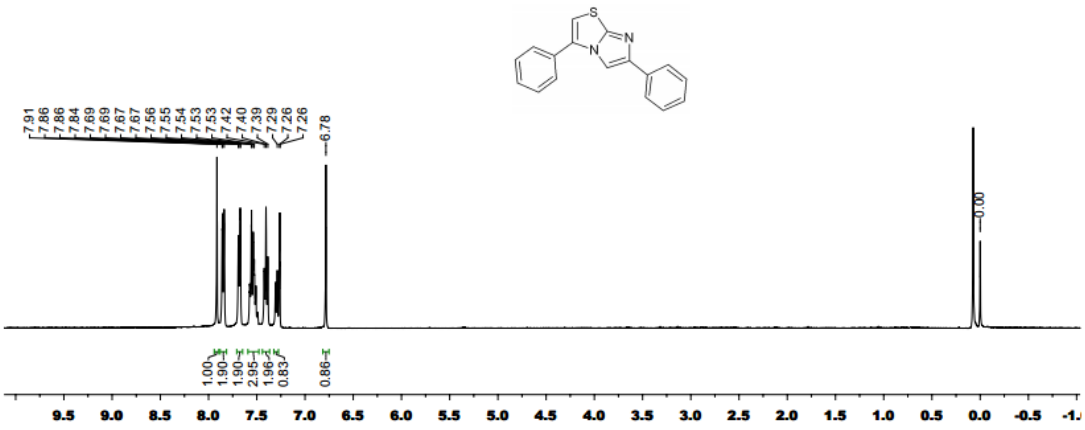



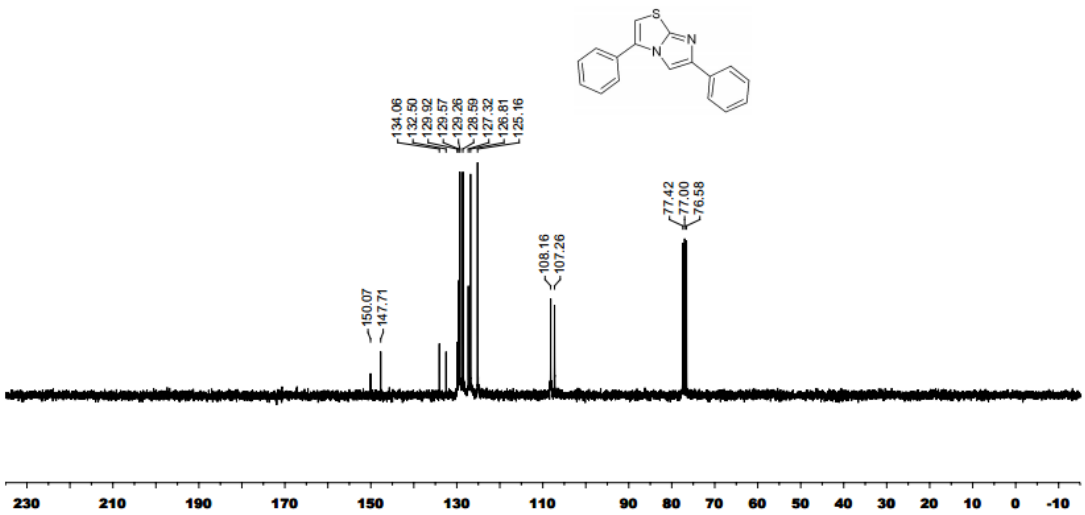
**4-(naphthalen-2-yl)-2-(4-tolylthio)-1H-imidazole (3db)**



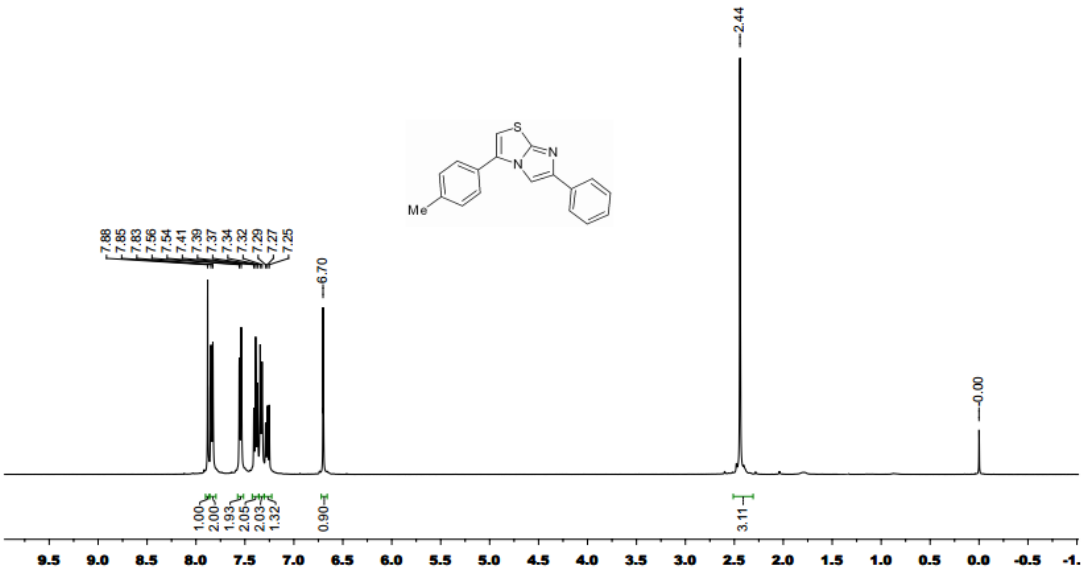



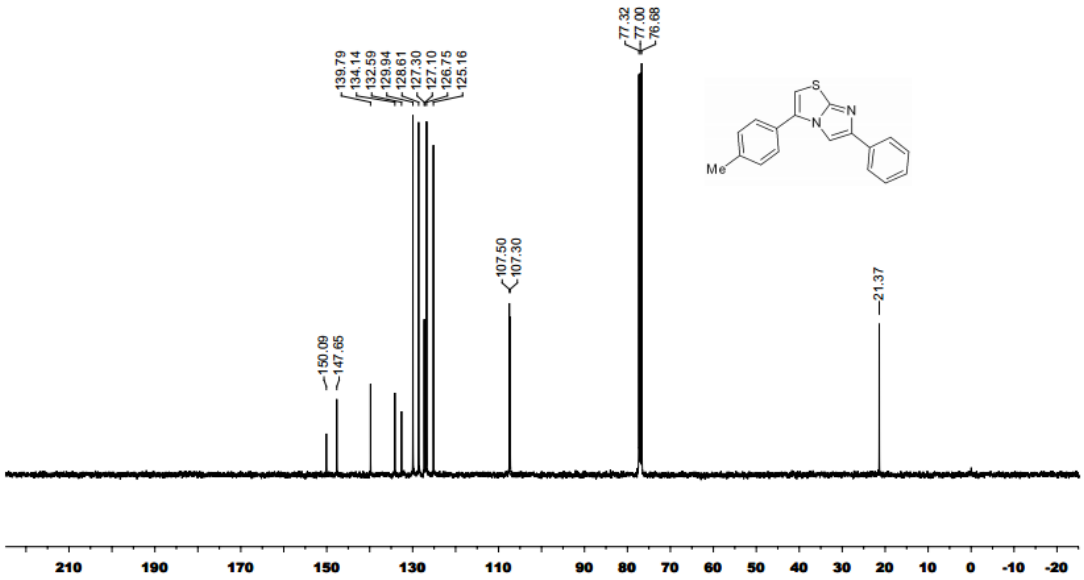
**3,6-diphenylimidazo[2,1-b]thiazole (5aa)**



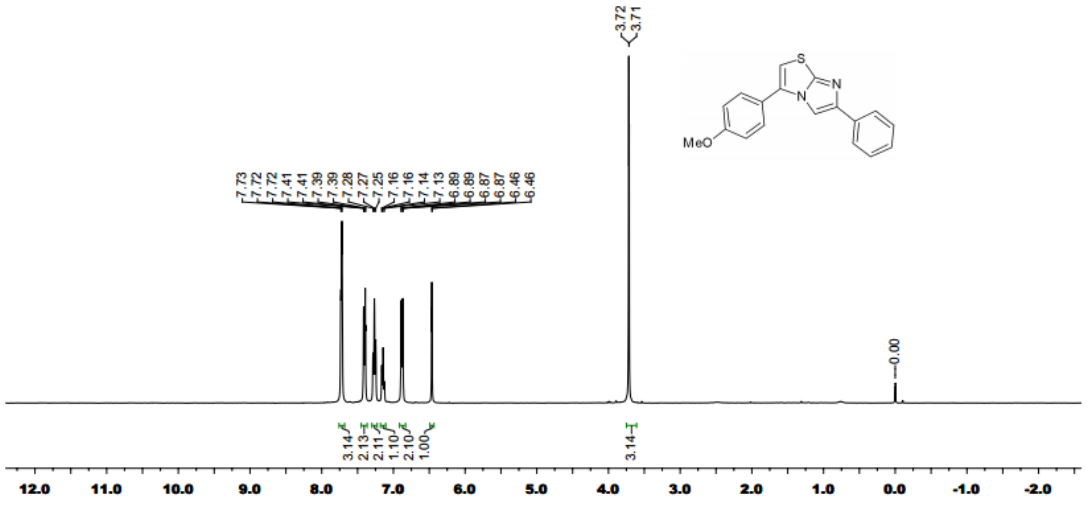



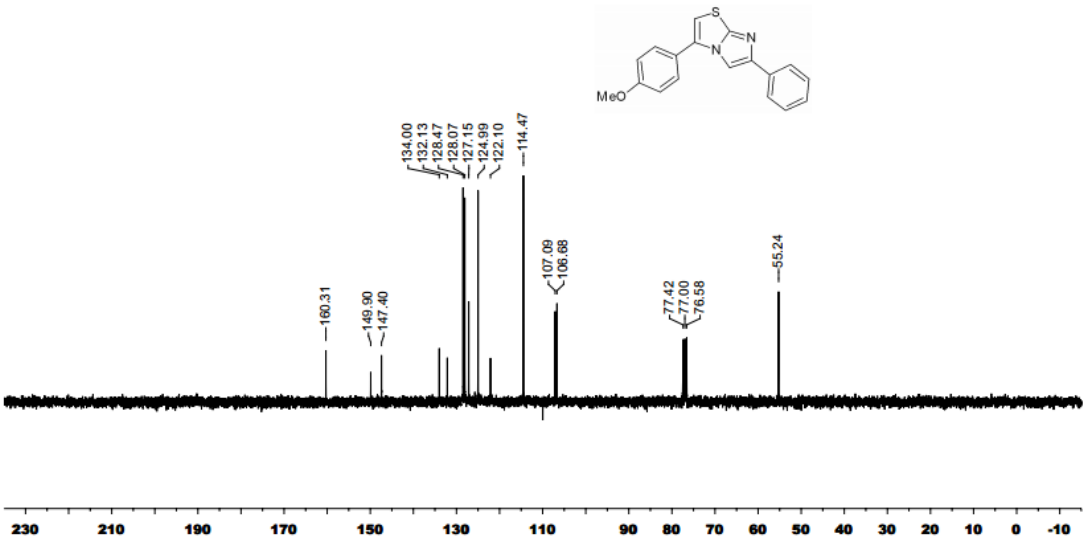
**6-phenyl-3-(3-tolyl)imidazo[2,1-b]thiazole (5ab)**



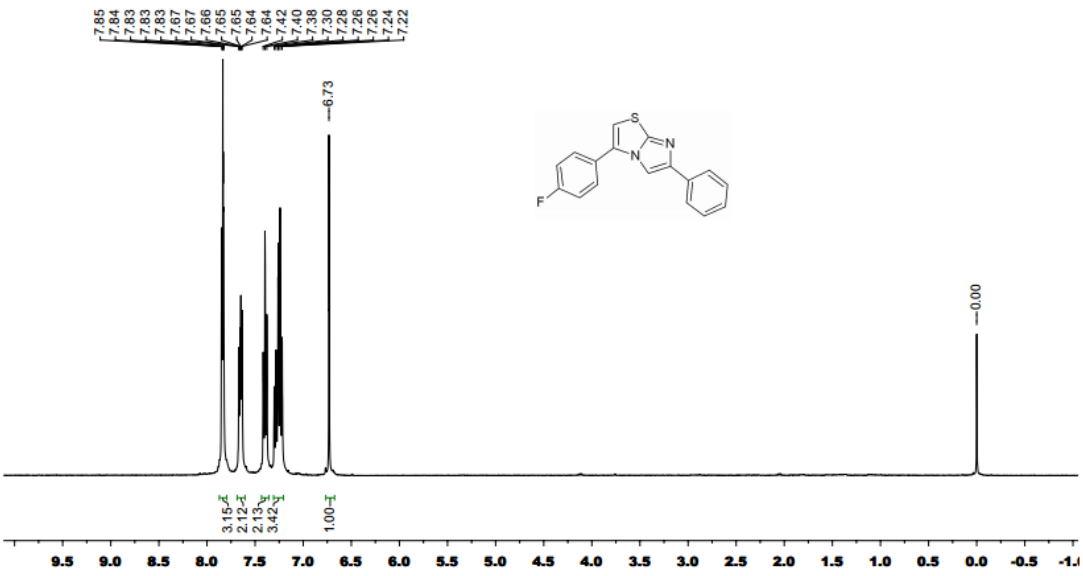



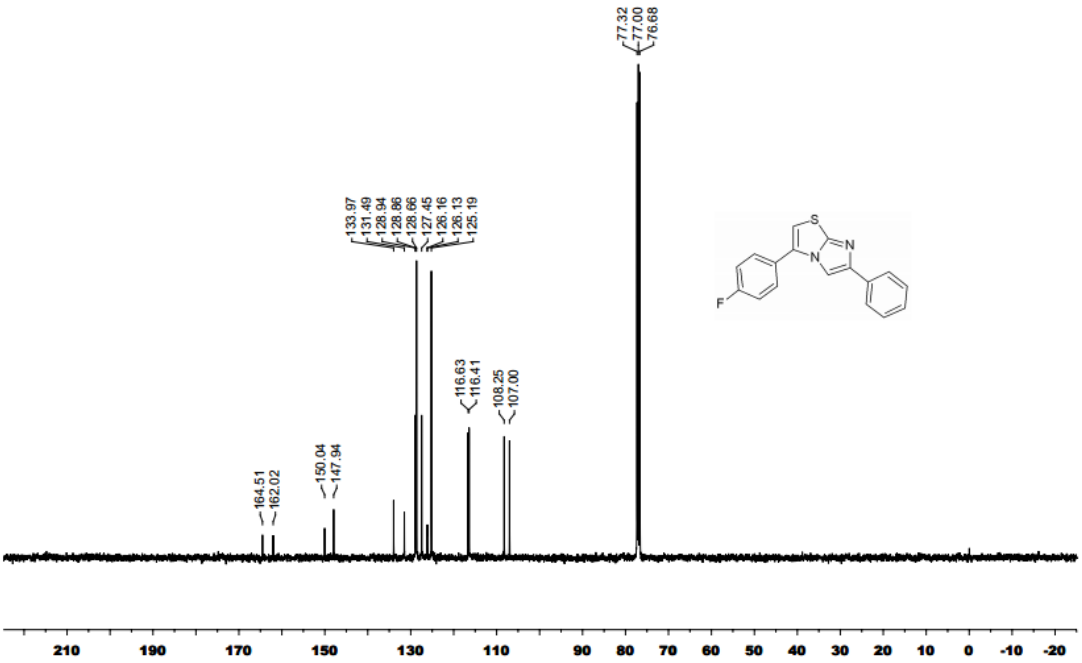
**3-(4-methoxyphenyl)-6-phenylimidazo[2,1-b]thiazole (5ac)**



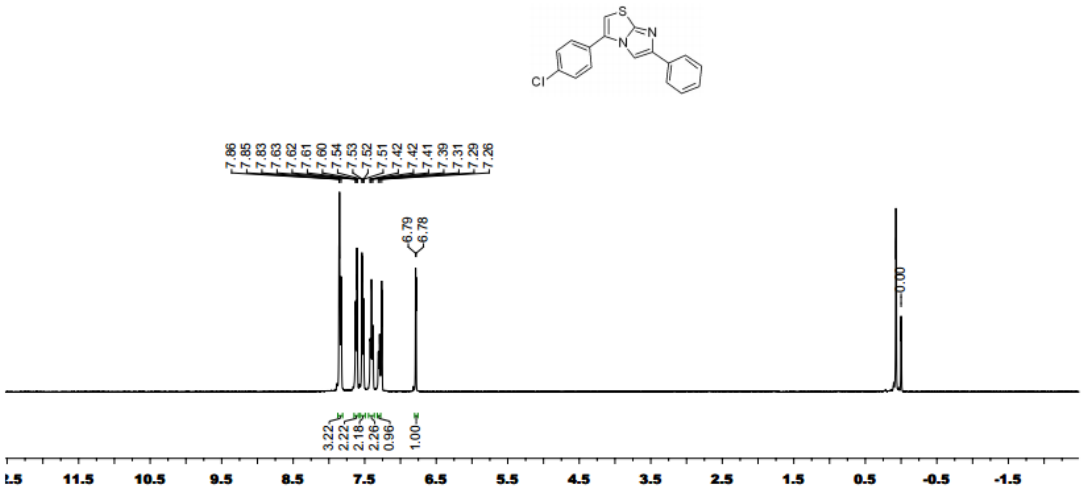



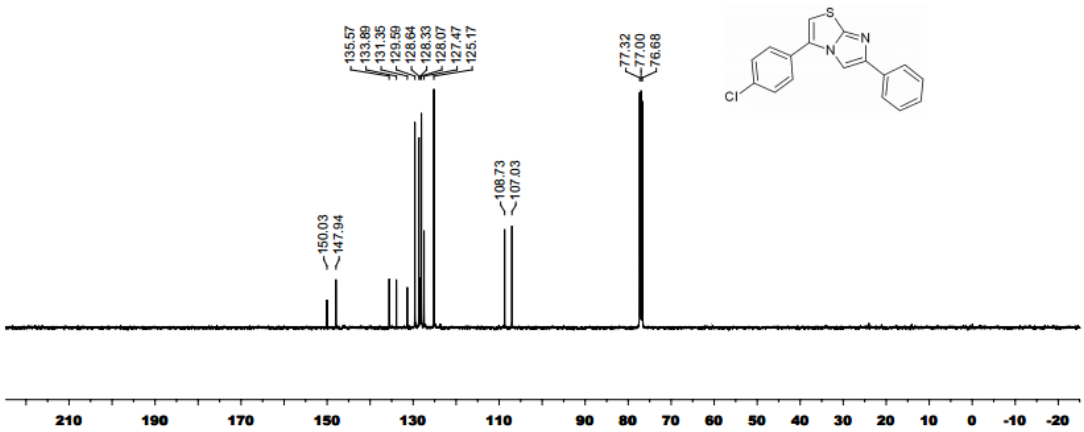
**3-(4-fluorophenyl)-6-phenylimidazo[2,1-b]thiazole (5ad)**



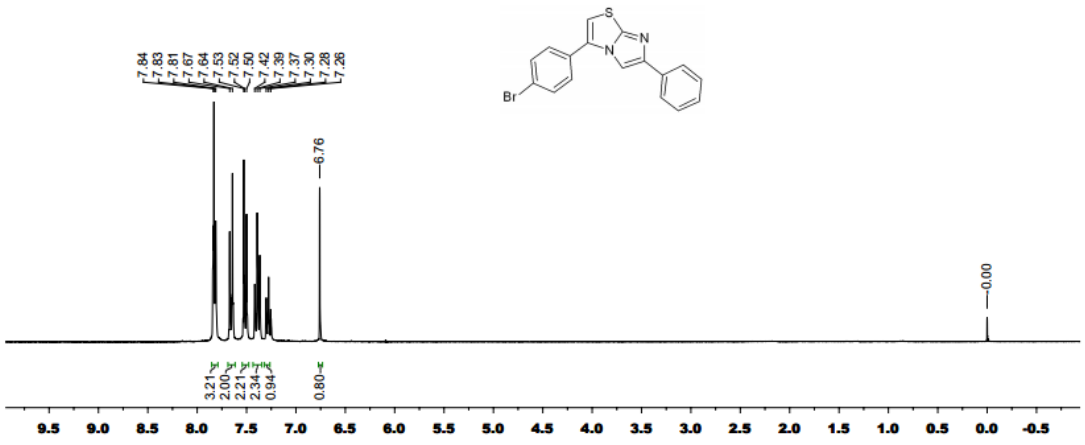



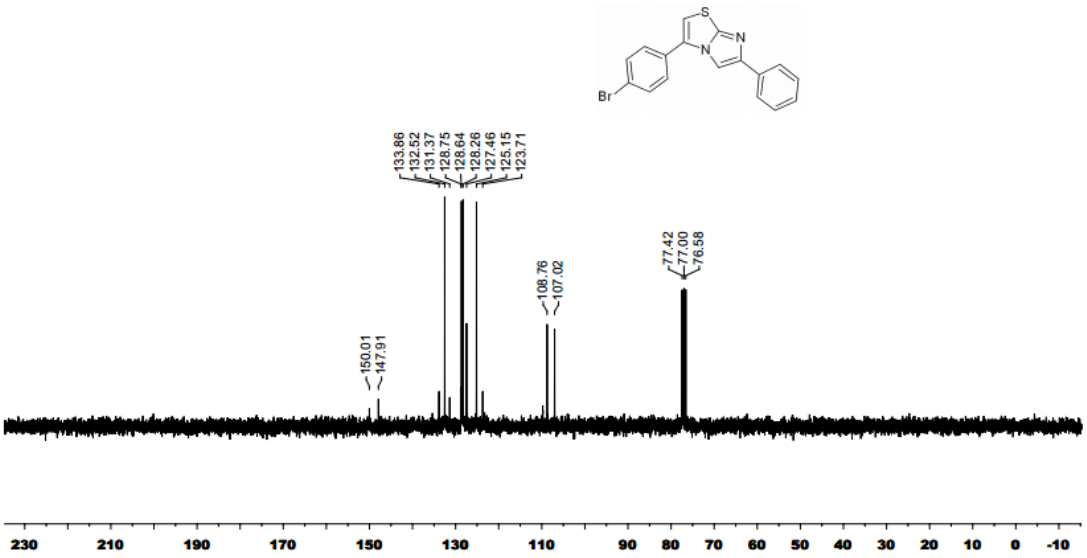
**3-(4-chlorophenyl)-6-phenylimidazo[2,1-b]thiazole (5ae)**



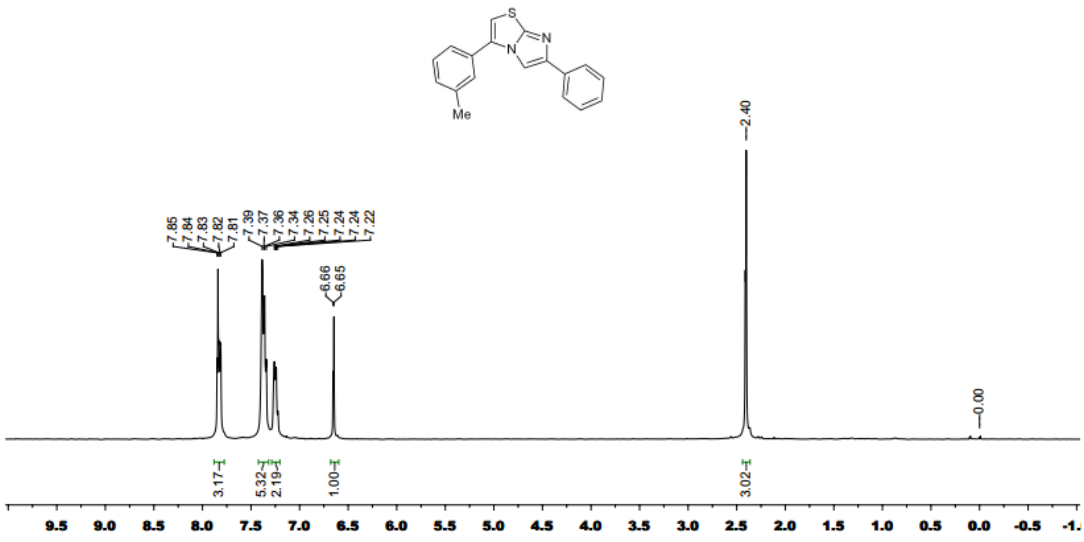



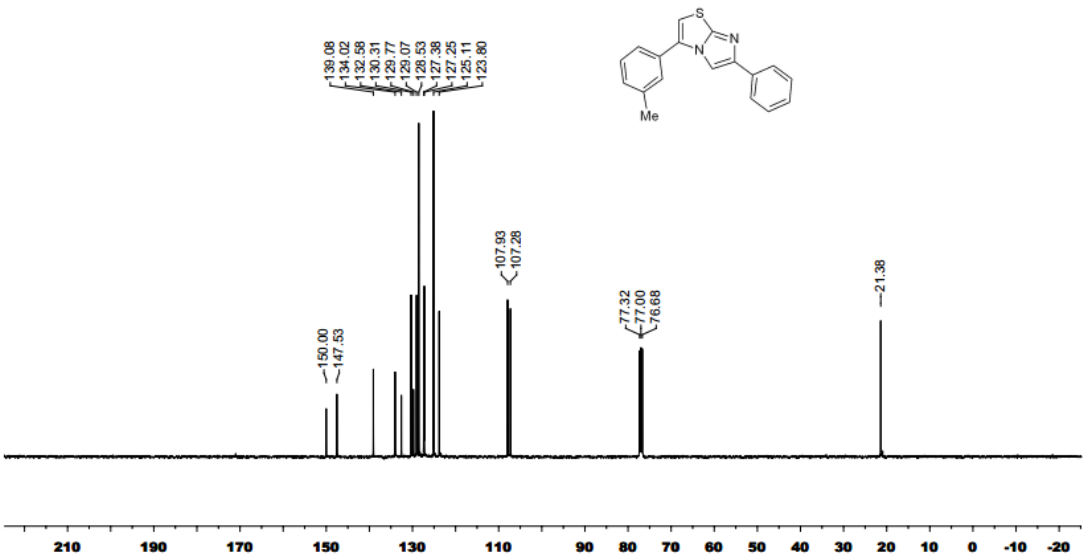
**3-(4-bromophenyl)-6-phenylimidazo[2,1-b]thiazole (5af)**



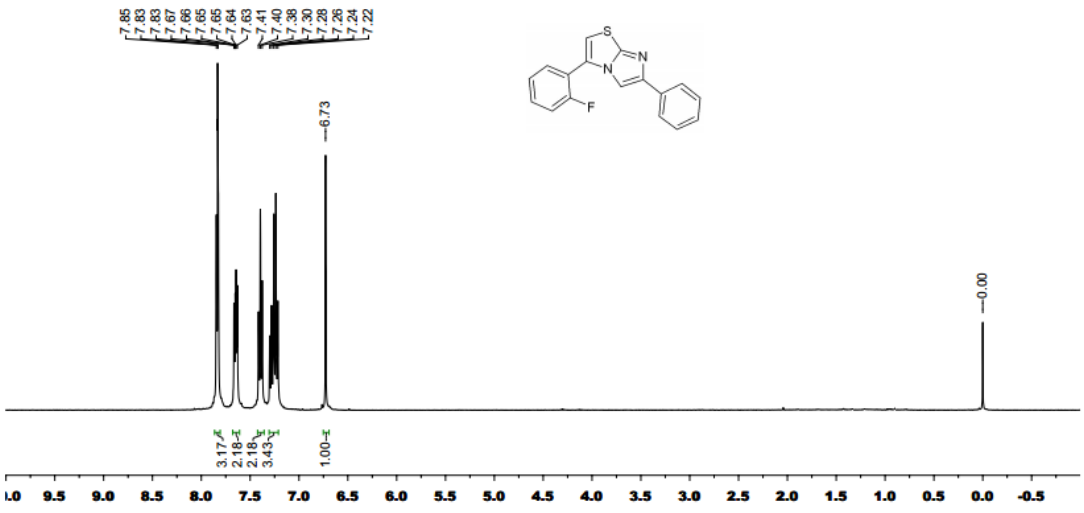



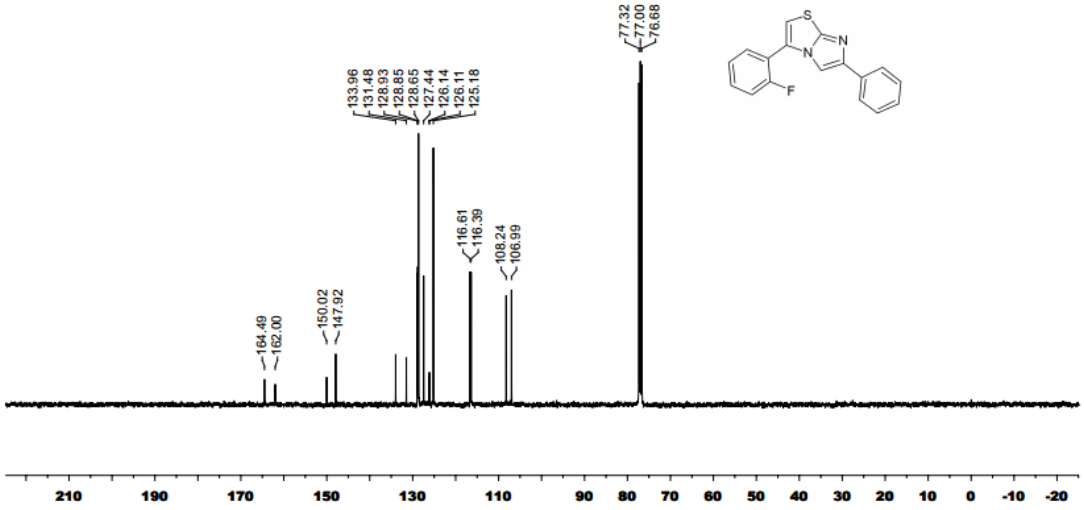
**6-phenyl-3-(3-tolyl)imidazo[2,1-b]thiazole (5ag)**



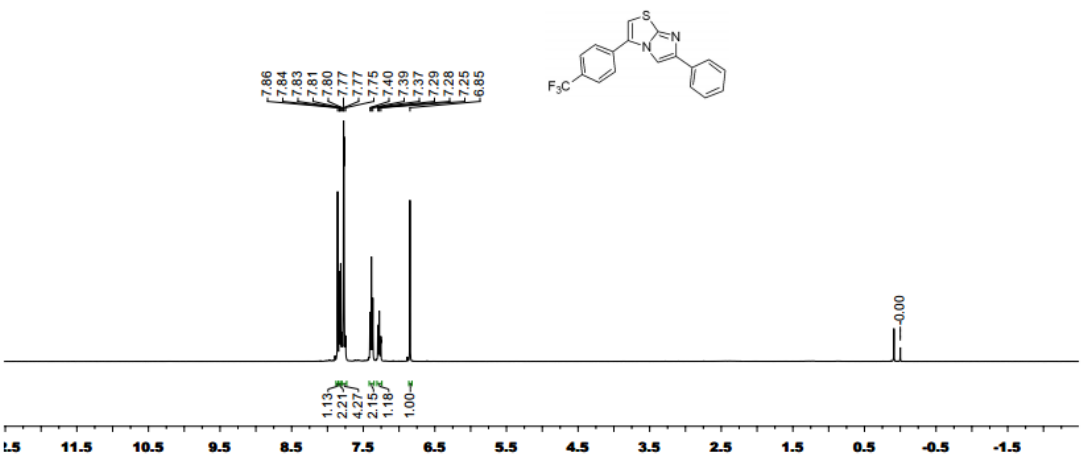



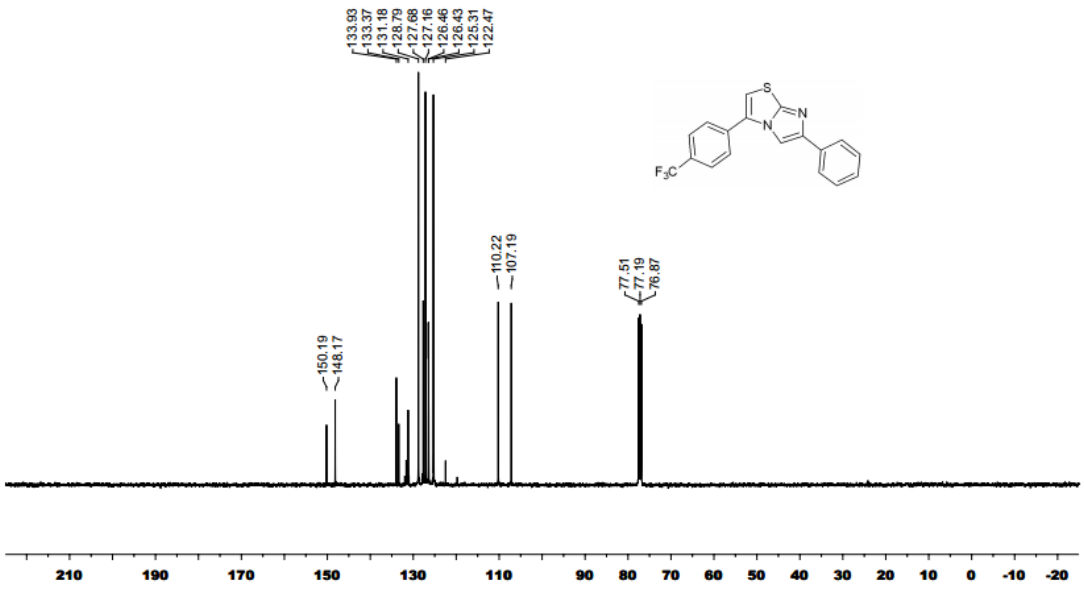
**3-(2-fluorophenyl)-6-phenylimidazo[2,1-b]thiazole (5ah)**



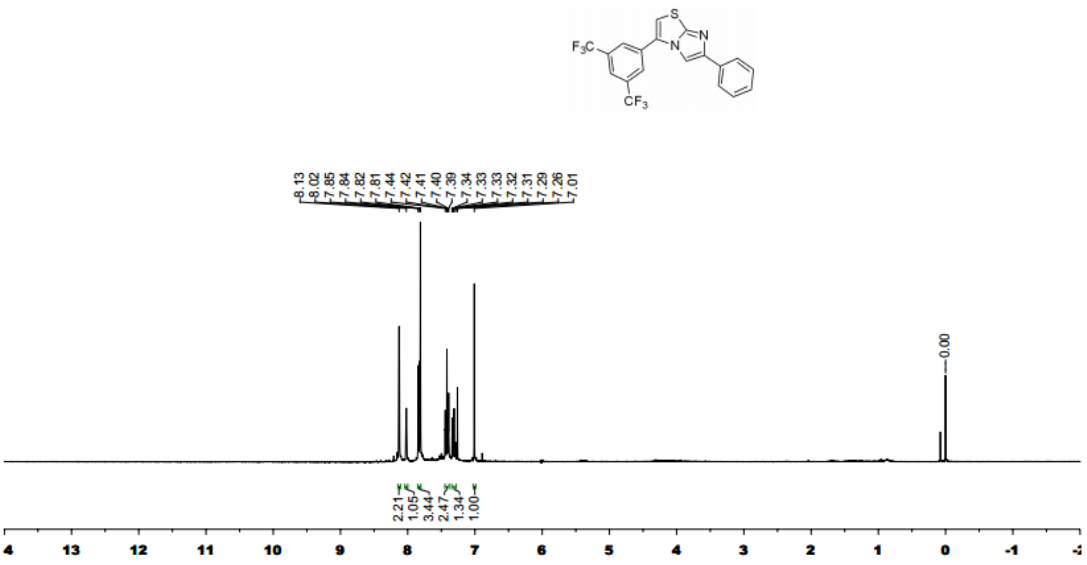



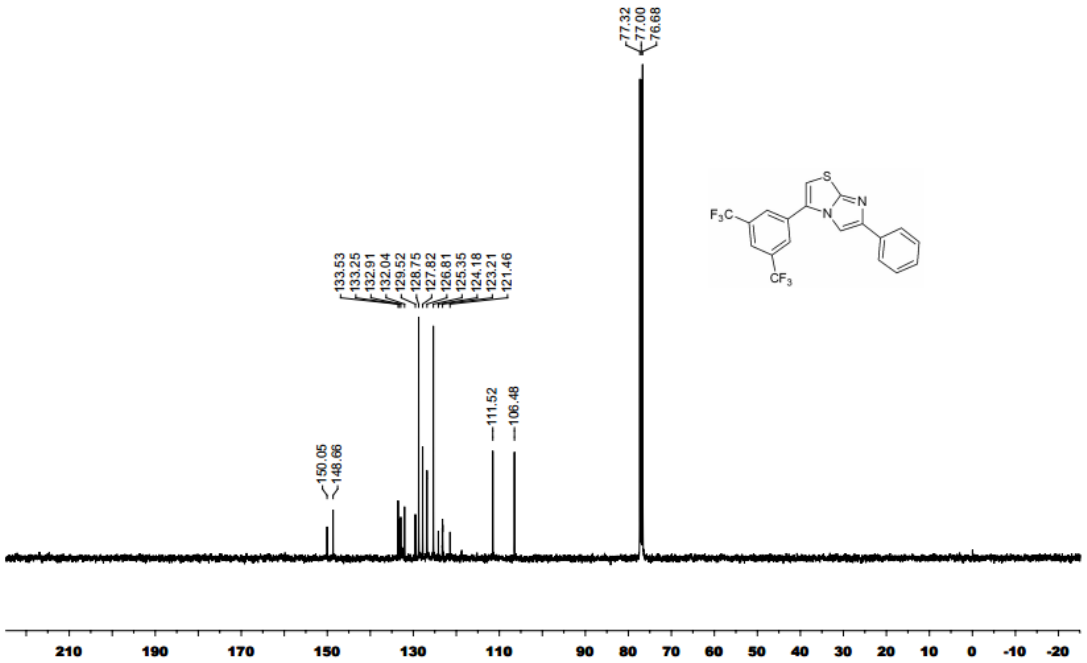
**6-phenyl-3-(4-(trifluoromethyl)phenyl)imidazo[2,1-b]thiazole (5ai)**



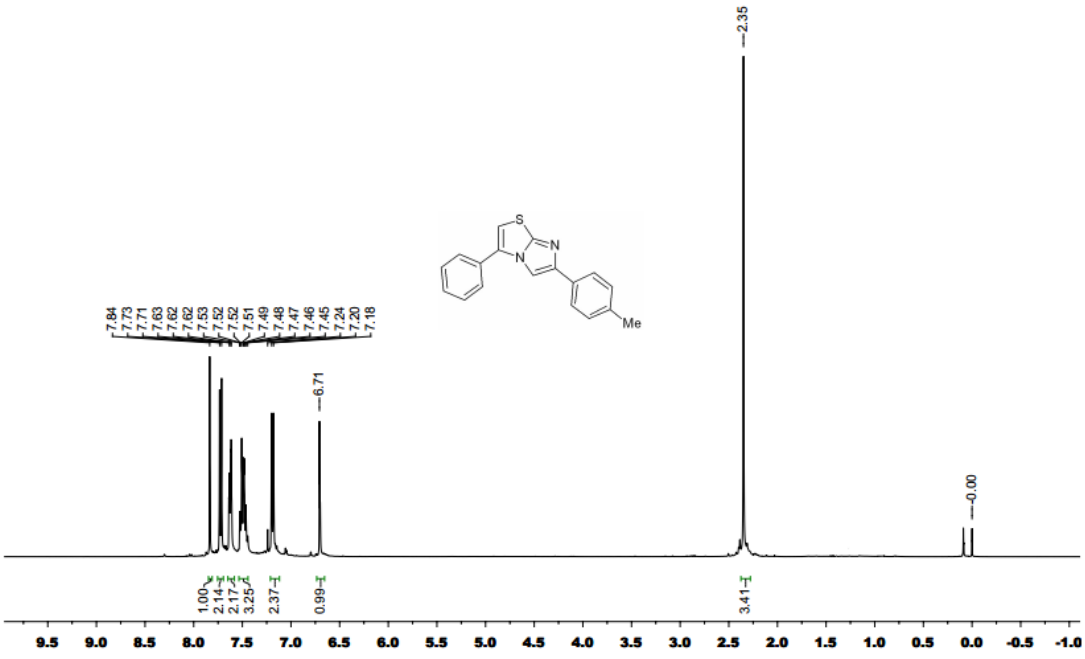



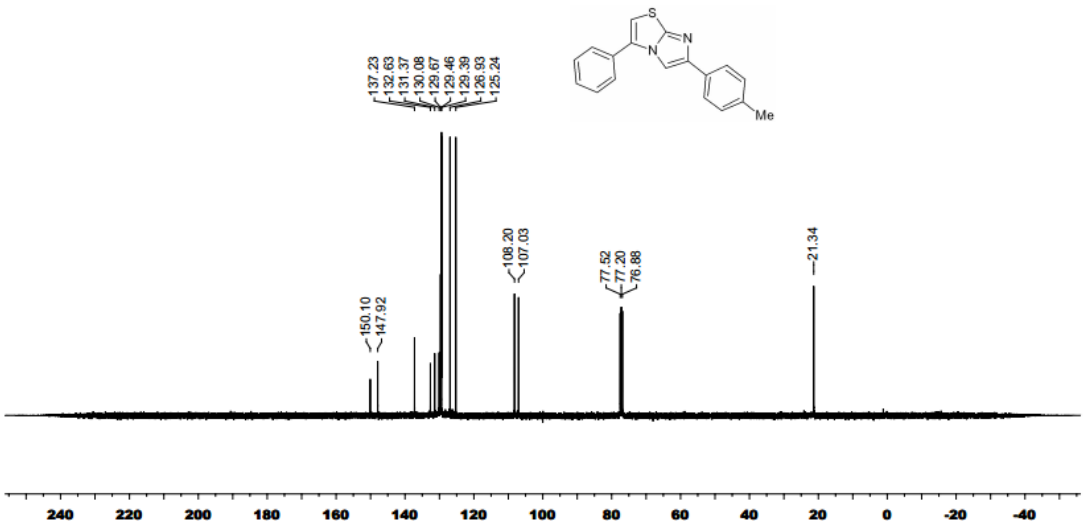
**3-(3,5-bis(trifluoromethyl)phenyl)-6-phenylimidazo[2,1-b]thiazole (5aj)**



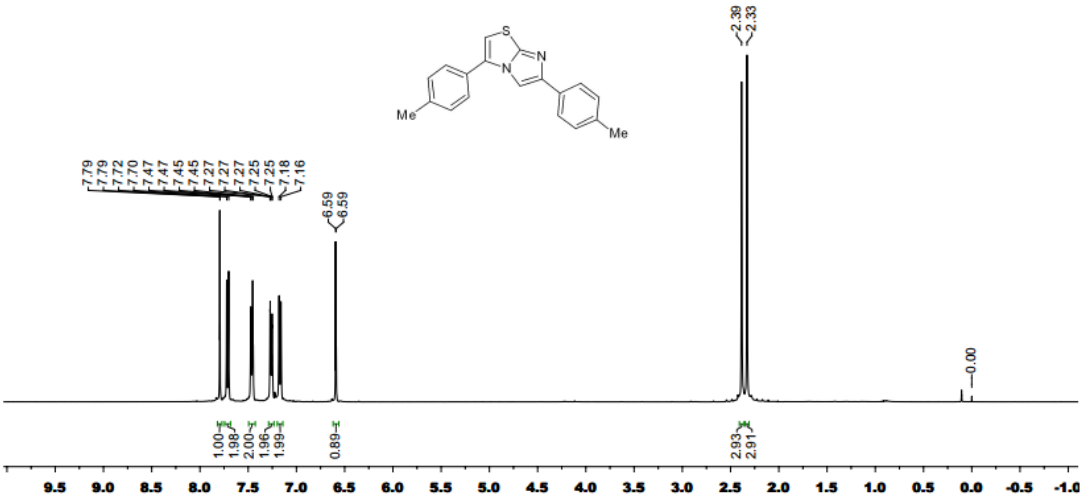



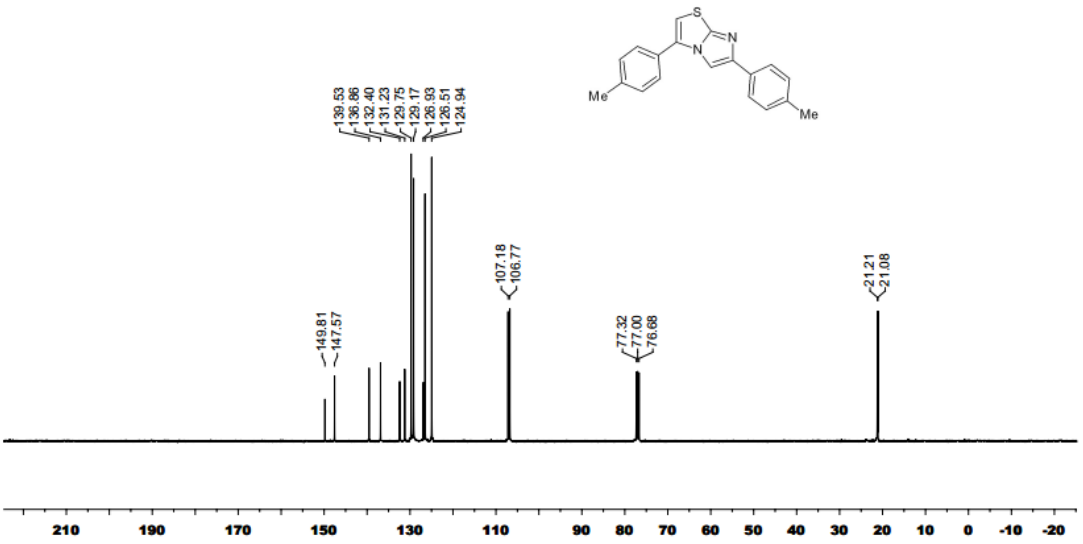
**3-phenyl-6-(4-tolyl)imidazo[2,1-b]thiazole (5ba)**



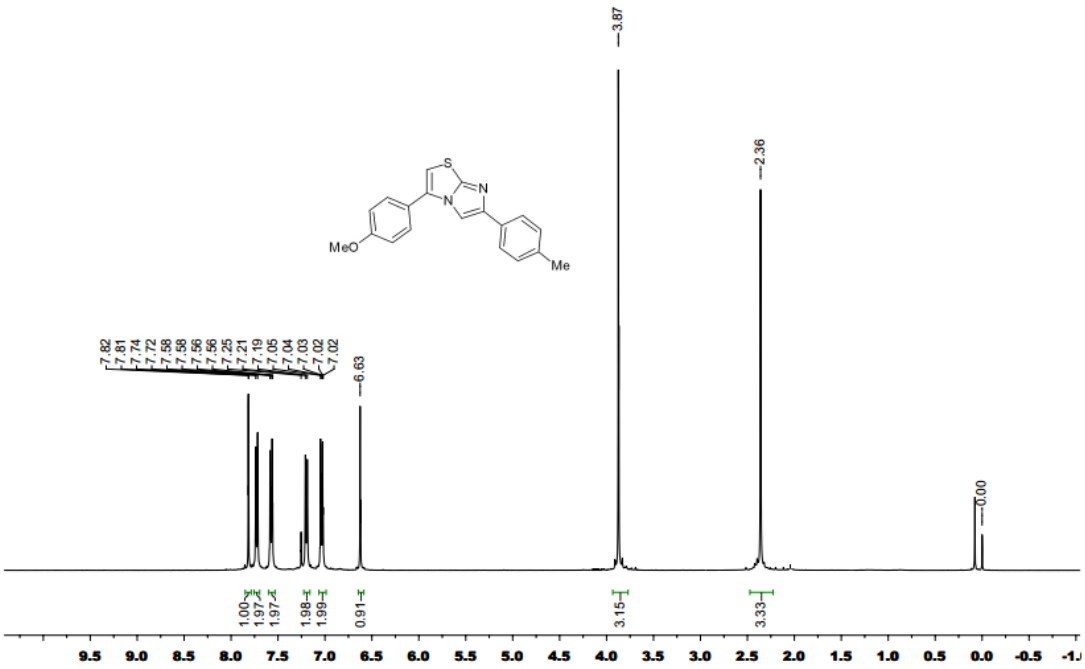



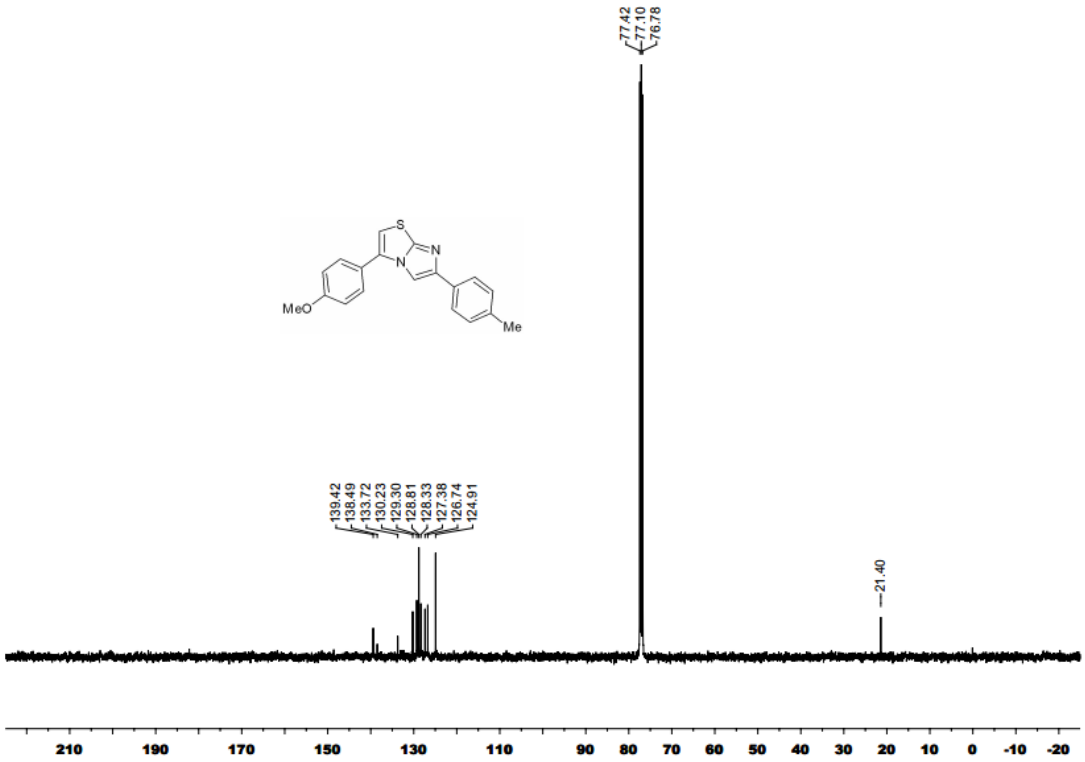
**3,6-di-4-tolylimidazo[2,1-b]thiazole (5bb)**



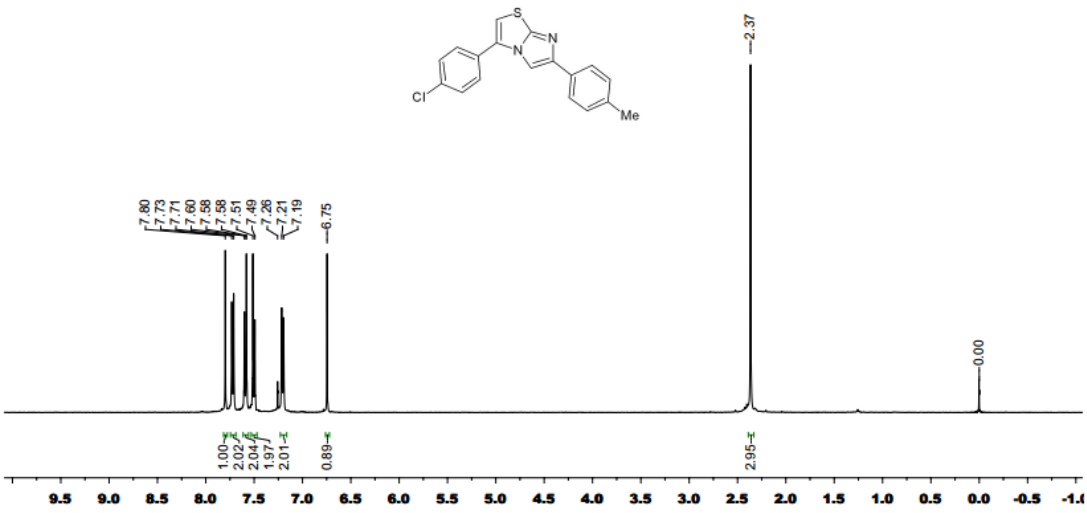



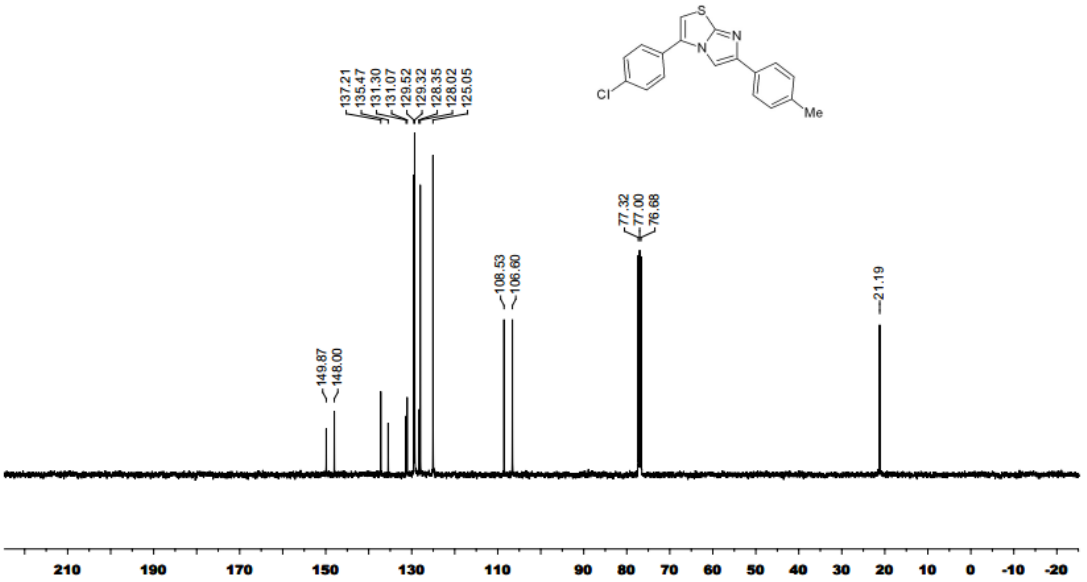
**3-(4-methoxyphenyl)-6-(4-tolyl)imidazo[2,1-b]thiazole (5bc)**



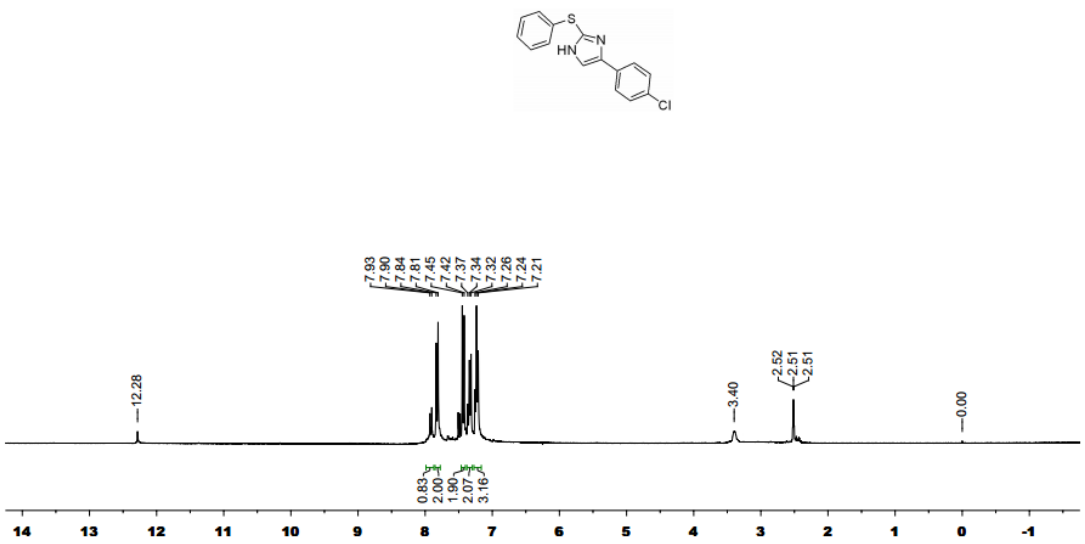



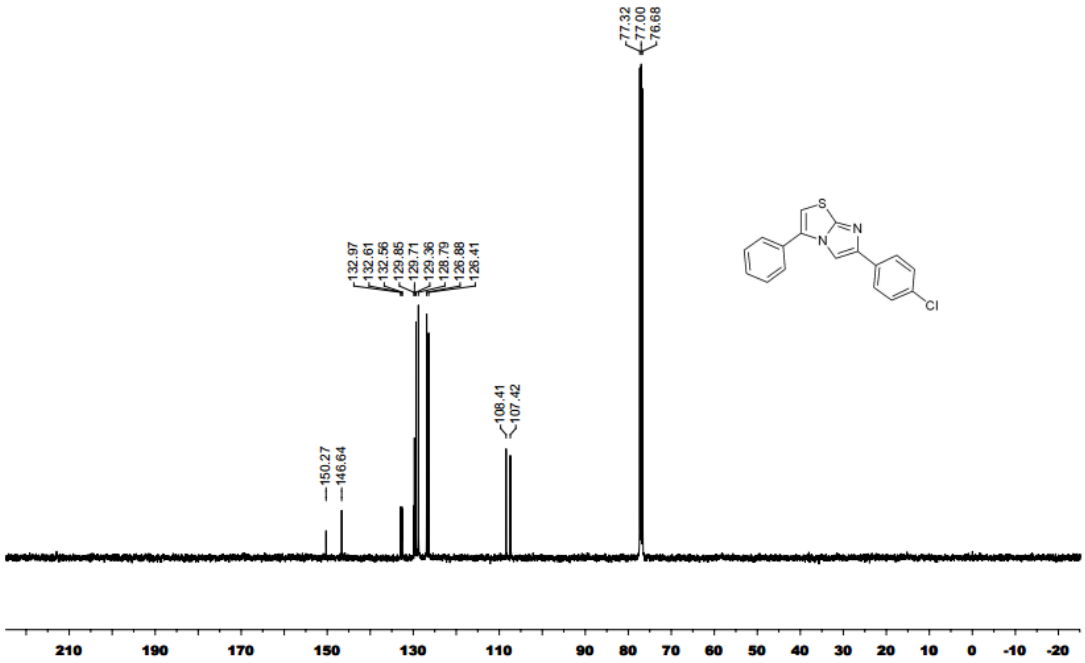
**3-(4-chlorophenyl)-6-(4-tolyl)imidazo[2,1-b]thiazole (5be)**



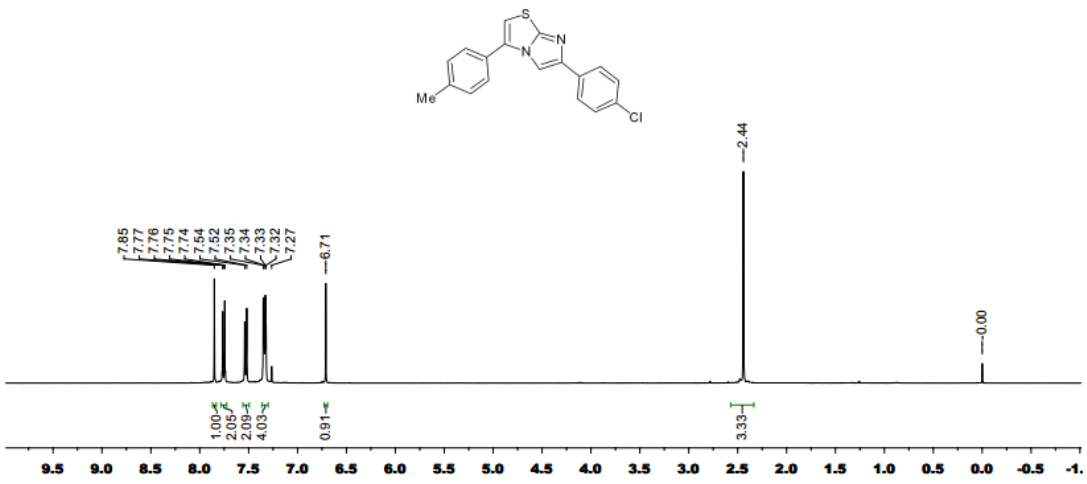



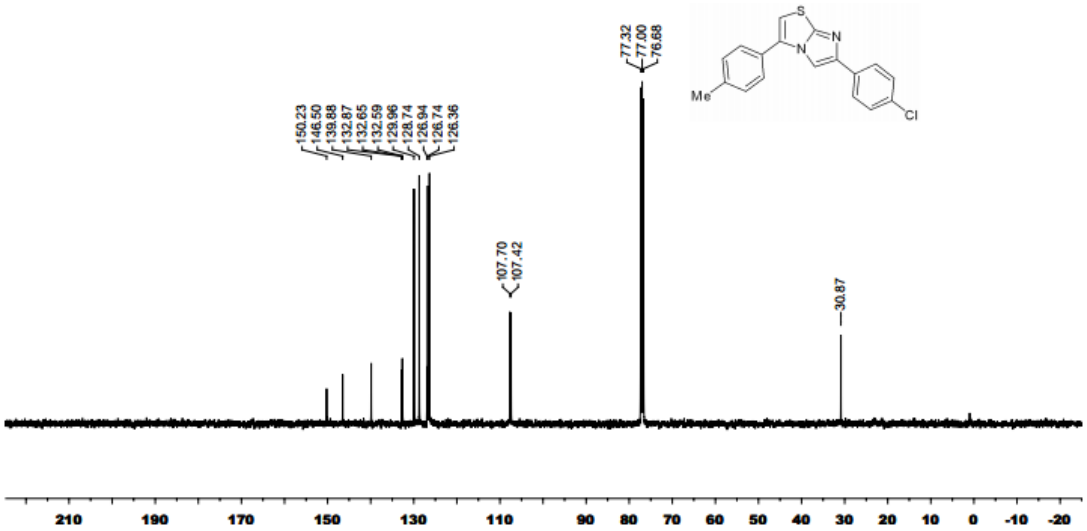
**6-(4-chlorophenyl)-3-phenylimidazo[2,1-b]thiazole (5ca)**



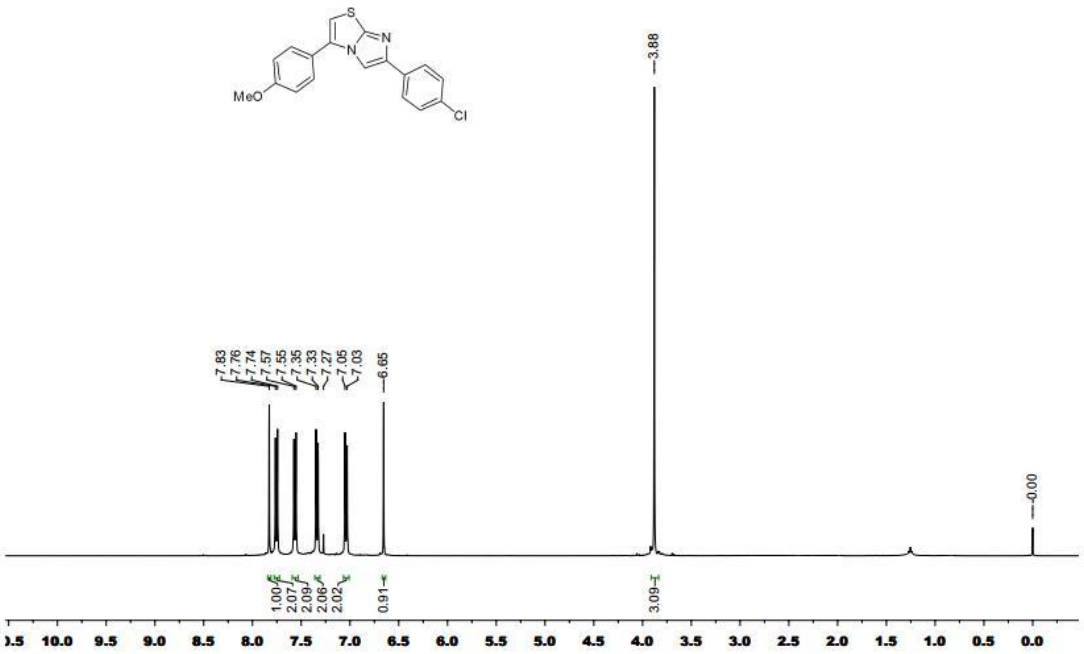



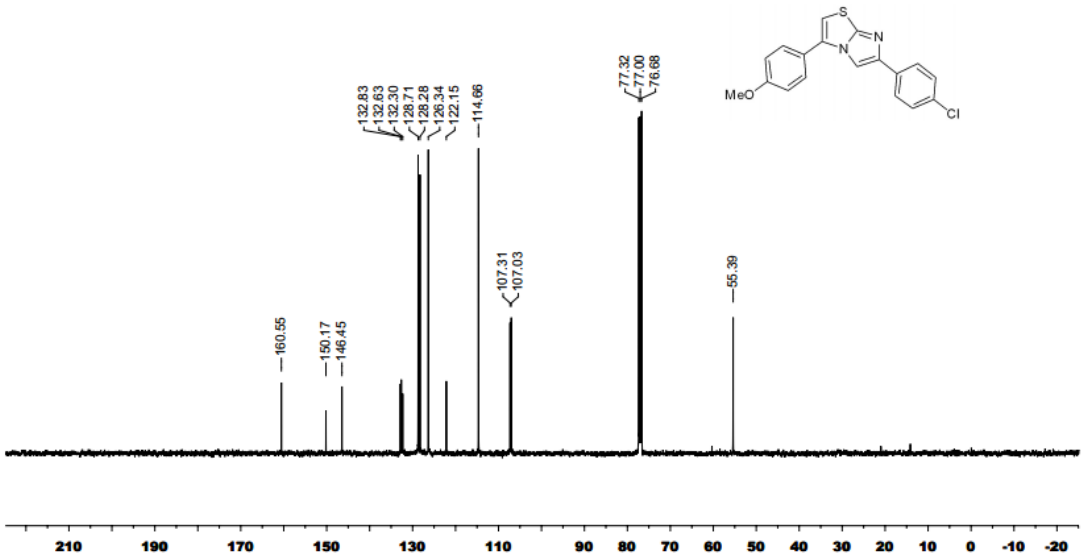
**4-(4-chlorophenyl)-2-(4-tolylthio)-1H-imidazole (5cb)**



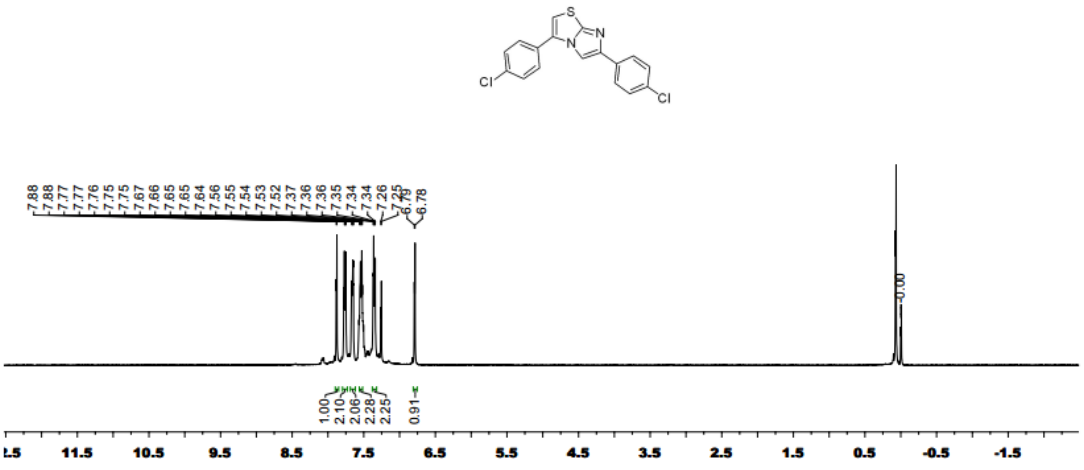



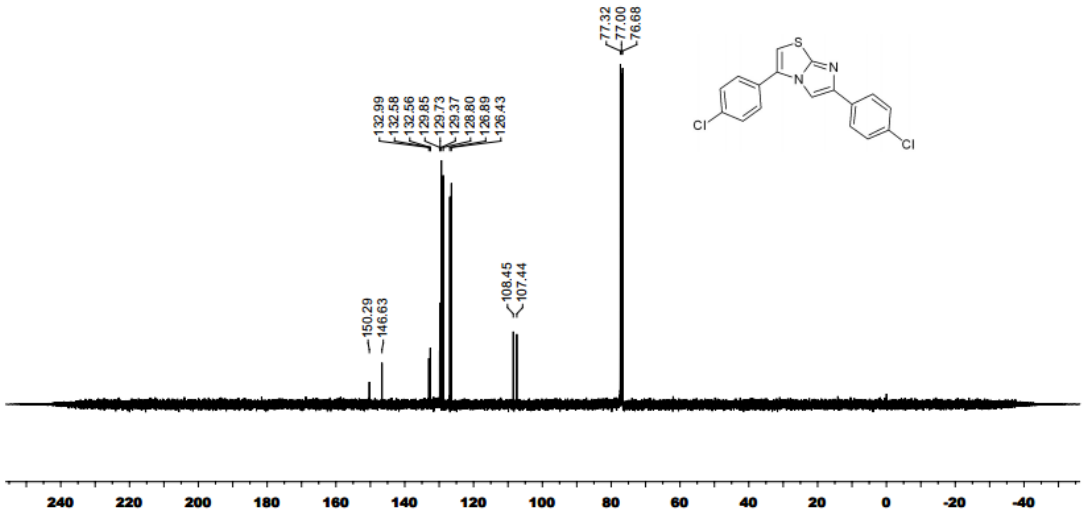
**6-(4-chlorophenyl)-3-(4-methoxyphenyl)imidazo[2,1-b]thiazole (5cc)**



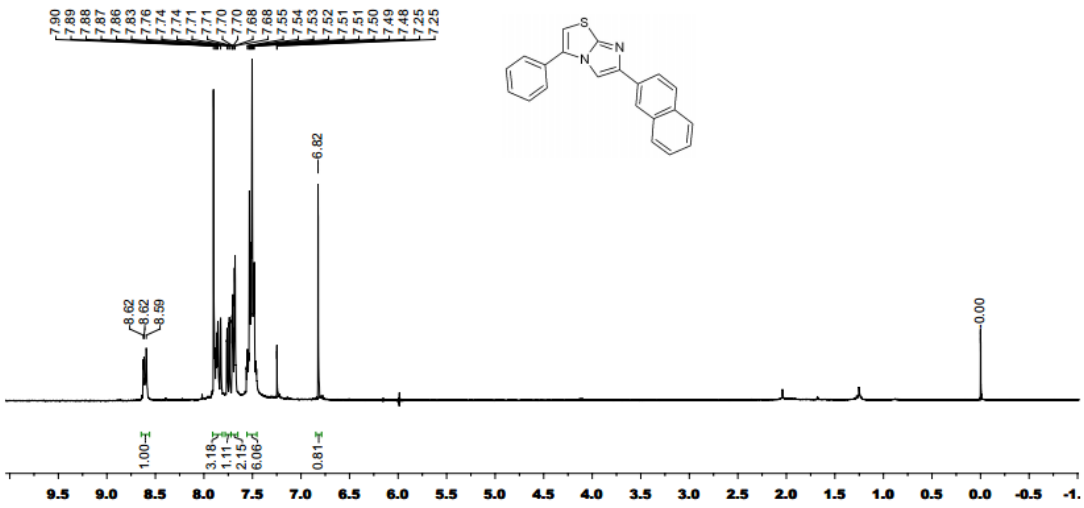



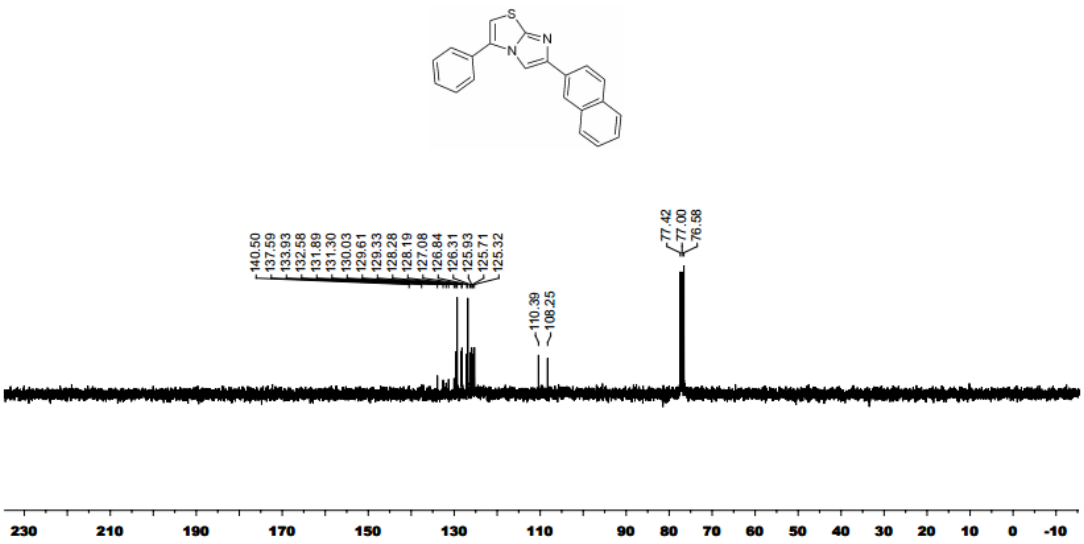
**3,6-bis(4-chlorophenyl)imidazo[2,1-b]thiazole (5ce)**



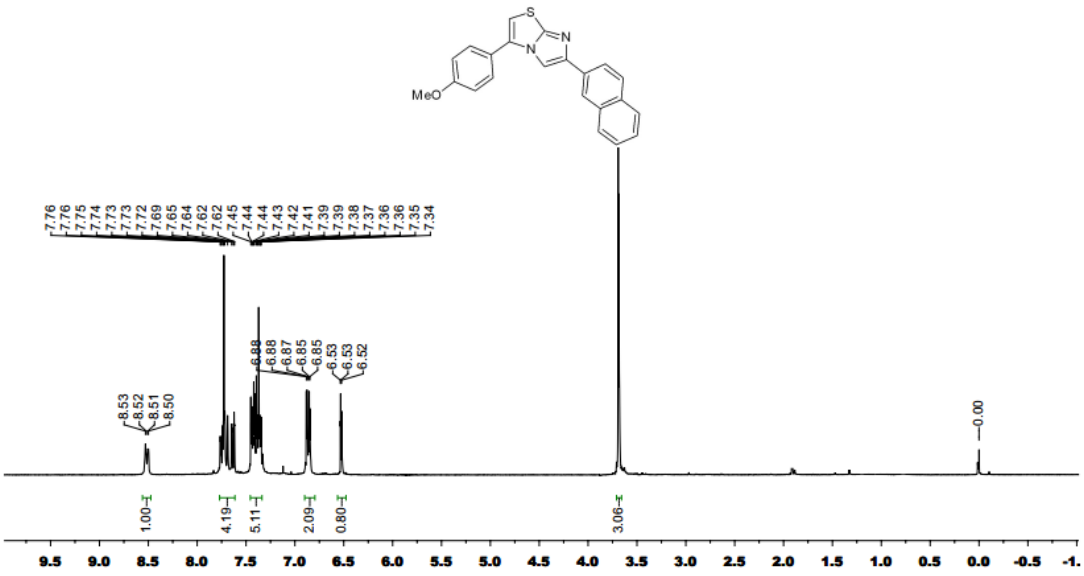



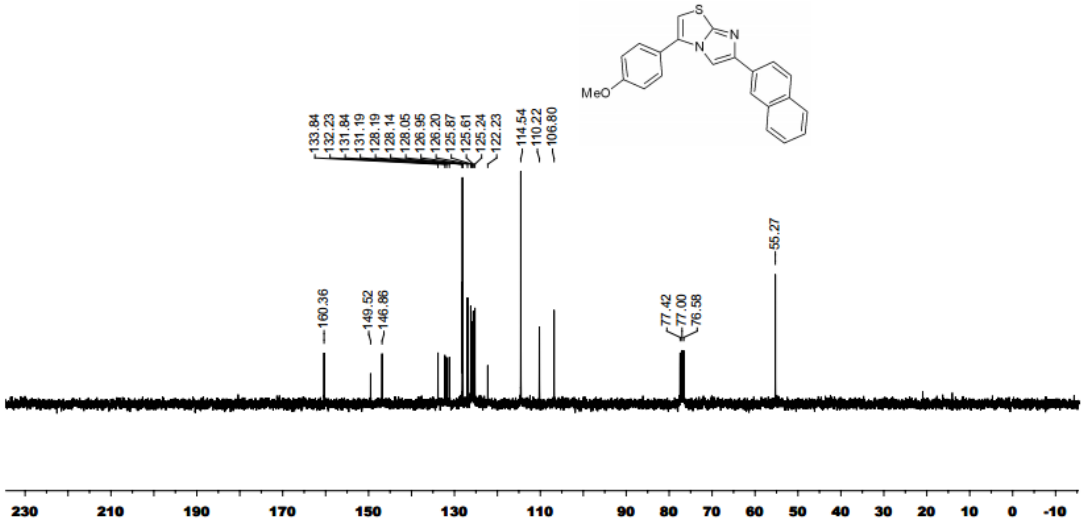
**6-(naphthalen-2-yl)-3-phenylimidazo[2,1-b]thiazole (5da)**



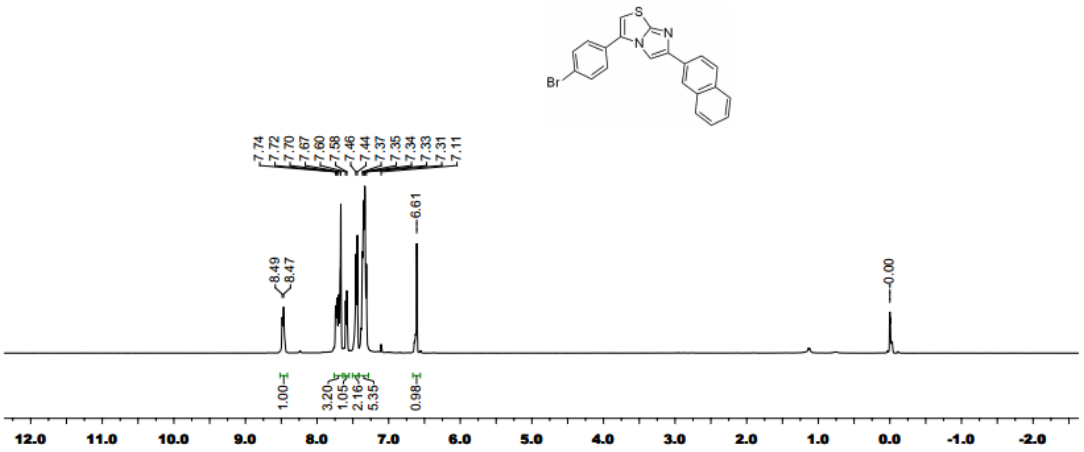



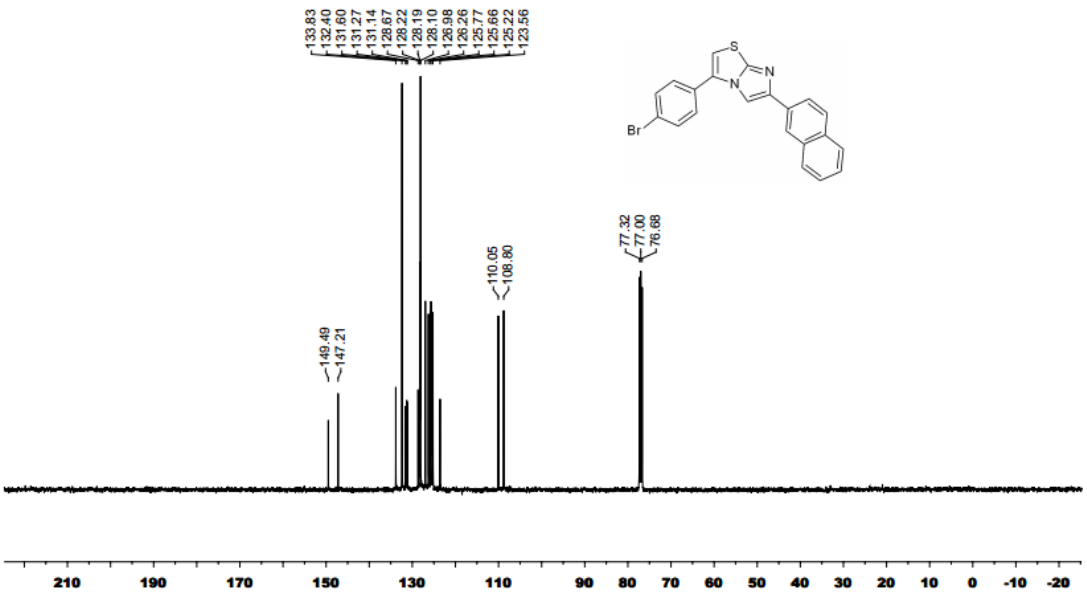
**3-(4-methoxyphenyl)-6-(naphthalen-2-yl)imidazo[2,1-b]thiazole (5dc)**



**3-(4-bromophenyl)-6-(naphthalen-2-yl)imidazo[2,1-b]thiazole (5df)**



# Part one

The Cartesian Coordinates of all stationary points.

## R1 (1a + $^{t}$BuO$^{-}$)

| | | | |
|---|---|---|---|
| C | -5.63315200 | 0.16566300 | 0.00797500 |
| C | -5.68295600 | -0.74415800 | 1.26698400 |
| H | -5.66339200 | -0.12700900 | 2.17382300 |
| H | -6.58203400 | -1.37553800 | 1.30172400 |
| H | -4.80465900 | -1.40117800 | 1.28761700 |
| C | -5.67989100 | -0.74886500 | -1.24780400 |
| H | -5.65860700 | -0.13499900 | -2.15682900 |
| H | -4.80129700 | -1.40565000 | -1.26410300 |
| H | -6.57866000 | -1.38071200 | -1.28220300 |
| C | -6.90697400 | 1.05385000 | 0.00482300 |
| H | -6.91261000 | 1.70176000 | 0.89030600 |
| H | -6.91089300 | 1.69786900 | -0.88347300 |
| H | -7.83574200 | 0.46591000 | 0.00522300 |
| O | -4.48654500 | 0.94884300 | 0.00786600 |
| C | 1.70675100 | 1.23488200 | 0.03453700 |
| C | 2.53681800 | 0.12177400 | -0.00016200 |
| C | 0.53763400 | -0.64873300 | -0.02470200 |
| C | -1.71213000 | 0.32570500 | 0.00246100 |
| H | 1.89334700 | 2.29540600 | 0.07397000 |
| H | -2.82496900 | 0.50080500 | 0.00619300 |
| N | -0.82371300 | 1.27410600 | 0.03419600 |
| N | 0.43049800 | 0.71807900 | 0.01815700 |
| N | 1.78887100 | -1.05506600 | -0.03674300 |
| S | -1.06932700 | -1.33391600 | -0.05001500 |
| C | 4.00818500 | 0.08802500 | 0.00114700 |
| C | 4.76694800 | 1.27326300 | -0.04956500 |
| C | 4.69204700 | -1.14030100 | 0.05431500 |
| C | 6.16155100 | 1.23010700 | -0.04375900 |
| H | 4.26844900 | 2.23678800 | -0.09830000 |
| C | 6.08800800 | -1.18132200 | 0.05847300 |
| H | 4.11902000 | -2.06024500 | 0.09350800 |
| C | 6.83146100 | 0.00225300 | 0.01033300 |
| H | 6.72597500 | 2.15739800 | -0.08426700 |
| H | 6.59528300 | -2.14118000 | 0.10078500 |
| H | 7.91698000 | -0.03020800 | 0.01374600 |

## TS1

| | | | |
|---|---|---|---|
| C | 0.08983400 | -5.72927900 | -2.20205500 |
| C | -0.57253900 | -5.74751600 | -0.80140800 |
| H | -1.44215900 | -5.07982000 | -0.78936600 |
| H | -0.90813300 | -6.75328800 | -0.51597300 |
| H | 0.13317700 | -5.39968500 | -0.03755400 |
| C | 1.32999800 | -6.65669600 | -2.17858600 |
| H | 1.80973200 | -6.66922300 | -3.16454600 |
| H | 2.06371500 | -6.29178100 | -1.45013200 |
| H | 1.07123100 | -7.68932000 | -1.90941700 |
| C | -0.92000300 | -6.27338300 | -3.23578200 |
| H | -1.80897100 | -5.63219000 | -3.26717800 |
| H | -0.47069400 | -6.27729200 | -4.23595200 |
| H | -1.24204000 | -7.29637500 | -3.00025500 |
| O | 0.45620400 | -4.42110100 | -2.56252300 |
| C | 4.00677900 | -0.02213800 | -0.57419400 |
| C | 4.88350500 | -0.14404300 | 0.49740800 |
| C | 3.90424200 | -2.04560400 | 0.32532900 |
| C | 2.18019500 | -3.02209900 | -1.18842200 |
| H | 3.77364600 | 0.78546600 | -1.24873300 |
| H | 1.33567300 | -3.77910100 | -1.80999300 |
| N | 2.43614200 | -1.78421100 | -1.50689100 |
| N | 3.39192800 | -1.25002800 | -0.66461400 |
| N | 4.80874800 | -1.41969900 | 1.05427300 |
| S | 3.14429700 | -3.61305000 | 0.22274100 |
| C | 5.80135700 | 0.87145700 | 1.03768300 |
| C | 5.90371600 | 2.15015600 | 0.45569300 |
| C | 6.60547500 | 0.58341700 | 2.15603800 |
| C | 6.77863900 | 3.10525900 | 0.97464400 |
| H | 5.29860800 | 2.40336000 | -0.40984500 |
| C | 7.48093200 | 1.54060500 | 2.67385300 |
| H | 6.53700400 | -0.39738600 | 2.61383000 |
| C | 7.57360400 | 2.80707100 | 2.08765200 |
| H | 6.84031200 | 4.08422400 | 0.50758800 |
| H | 8.09211100 | 1.29522700 | 3.53811100 |
| H | 8.25463400 | 3.55107000 | 2.49040400 |

## IM1

| | | | |
|---|---|---|---|
| C | -0.53670300 | 1.29003700 | 0.00061600 |
| C | 0.24399400 | 0.13943800 | 0.00012100 |
| C | -1.80237000 | -0.53285300 | 0.00003600 |

| | | | |
|---|---|---|---|
| C | -4.09260500 | 0.65266300 | -0.00045300 |
| H | -0.29897600 | 2.34146600 | 0.00095100 |
| N | -3.07523000 | 1.47367700 | -0.00029100 |
| N | -1.83467400 | 0.83534600 | 0.00001100 |
| N | -0.56068100 | -0.99755100 | -0.00001600 |
| S | -3.43869400 | -1.12614400 | -0.00024300 |
| C | 1.71193900 | 0.04061200 | 0.00001600 |
| C | 2.52540700 | 1.19146300 | -0.00001600 |
| C | 2.34479500 | -1.21710800 | 0.00000700 |
| C | 3.91681300 | 1.08746200 | -0.00006700 |
| H | 2.06991300 | 2.17737100 | -0.00001200 |
| C | 3.73775500 | -1.31945700 | -0.00003700 |
| H | 1.73249900 | -2.11231300 | 0.00004400 |
| C | 4.53381600 | -0.16935900 | -0.00007900 |
| H | 4.52092700 | 1.99057100 | -0.00009800 |
| H | 4.20190900 | -2.30205600 | -0.00004100 |
| H | 5.61694000 | -0.24940900 | -0.00011500 |

## TS2

| | | | |
|---|---|---|---|
| C | 0.49472000 | 1.32809000 | 0.00725600 |
| C | -0.28552000 | 0.16946800 | -0.00166500 |
| C | 1.76929700 | -0.43195500 | -0.00720800 |
| C | 4.17136300 | 0.43644400 | -0.00075700 |
| H | 0.22604400 | 2.37390900 | 0.01656000 |
| N | 3.45867500 | 1.47409800 | 0.00778700 |
| N | 1.79930000 | 0.90978700 | 0.00348000 |
| N | 0.54241000 | -0.94873300 | -0.01077500 |
| S | 3.39433700 | -1.14818300 | -0.01337200 |
| C | -1.75153800 | 0.05079700 | -0.00127000 |
| C | -2.58094100 | 1.19122400 | -0.00594500 |
| C | -2.37183600 | -1.21414000 | 0.00425600 |
| C | -3.97106200 | 1.07075100 | -0.00447300 |
| H | -2.13706500 | 2.18247000 | -0.01139500 |
| C | -3.76357300 | -1.33310600 | 0.00549600 |
| H | -1.74980600 | -2.10273500 | 0.00784800 |
| C | -4.57412100 | -0.19297000 | 0.00132700 |
| H | -4.58559900 | 1.96698100 | -0.00823400 |
| H | -4.21573500 | -2.32141900 | 0.01002400 |
| H | -5.65625400 | -0.28582800 | 0.00241700 |

## IM2

| | | | |
|---|---|---|---|
| C | 1.32768000 | -0.20406600 | 0.48947600 |
| C | 2.63479300 | -0.33726800 | -0.01035200 |
| C | 1.94387500 | 1.64857000 | -0.31503300 |
| C | 2.49701700 | 4.17290800 | 0.50424000 |
| H | 0.69784000 | -0.94461200 | 0.96763800 |
| N | 2.90912200 | 4.78186200 | 1.41305900 |
| N | 0.88541200 | 1.06990500 | 0.29182400 |
| N | 3.01940100 | 0.87485800 | -0.53067700 |
| S | 1.88839600 | 3.34785000 | -0.86546700 |
| C | 3.51316100 | -1.51569000 | -0.02659800 |
| C | 3.07823200 | -2.76056500 | 0.47480100 |
| C | 4.82191300 | -1.43960800 | -0.54513700 |
| C | 3.91507600 | -3.87768900 | 0.45909700 |
| H | 2.07497900 | -2.85760000 | 0.87936900 |
| C | 5.65783200 | -2.55811400 | -0.56131500 |
| H | 5.17599100 | -0.49107000 | -0.93504400 |
| C | 5.21225700 | -3.78619200 | -0.05943900 |
| H | 3.55186400 | -4.82360800 | 0.85217700 |
| H | 6.66240200 | -2.46947100 | -0.96692600 |
| H | 5.86276600 | -4.65591500 | -0.07198700 |
| C | -5.55518500 | 0.15935600 | -0.12930200 |
| C | -5.15519400 | -0.43580000 | 1.08431700 |
| C | -5.41995700 | -1.78407700 | 1.32570100 |
| C | -6.08443800 | -2.55550700 | 0.36594100 |
| C | -6.48490400 | -1.97172800 | -0.84095500 |
| C | -6.22433400 | -0.62423100 | -1.09120100 |
| H | -4.63906200 | 0.16304900 | 1.82781300 |
| H | -5.10682000 | -2.23255700 | 2.26369400 |
| H | -6.28857600 | -3.60471500 | 0.55709000 |
| H | -7.00066100 | -2.56629600 | -1.58899900 |
| H | -6.53390400 | -0.17081600 | -2.02737800 |
| C | -5.28477200 | 1.54324800 | -0.38186900 |
| C | -5.05555200 | 2.71578100 | -0.59592300 |
| H | -4.85174500 | 3.74701800 | -0.78369400 |

## IM3

| | | | |
|---|---|---|---|
| C | 0.14534400 | 1.78403700 | 0.14421300 |
| C | -0.40291100 | 0.52994400 | -0.09043700 |
| C | 1.71838300 | 0.35241900 | -0.41180500 |

| | | | |
|---|---|---|---|
| C | 3.87893000 | -0.78128600 | 0.68474700 |
| H | -0.29021300 | 2.72841200 | 0.43079200 |
| N | 4.31431100 | -1.15828500 | 1.69948300 |
| N | 1.49029100 | 1.65363400 | -0.06741400 |
| N | 0.60329200 | -0.34848300 | -0.44205400 |
| S | 3.32687100 | -0.25888100 | -0.84948800 |
| C | -1.81098900 | 0.10719400 | -0.00970700 |
| C | -2.82312200 | 1.01548000 | 0.35185800 |
| C | -2.17168400 | -1.22172500 | -0.29416900 |
| C | -4.15503700 | 0.60571700 | 0.42638900 |
| H | -2.57446200 | 2.04804200 | 0.57796600 |
| C | -3.50510300 | -1.62948500 | -0.21884600 |
| H | -1.39982300 | -1.93048400 | -0.57394200 |
| C | -4.50387700 | -0.71924800 | 0.14162800 |
| H | -4.92101000 | 1.32272000 | 0.70733900 |
| H | -3.76327700 | -2.66077300 | -0.44212200 |
| H | -5.54061000 | -1.03709800 | 0.20011200 |
| H | 2.18458400 | 2.38492600 | 0.01833700 |

## TS4

| | | | |
|---|---|---|---|
| C | 1.57264600 | -1.42542100 | 0.54643600 |
| C | 2.59179000 | -0.58360600 | 0.14572000 |
| C | 0.74492600 | 0.51374300 | -0.11865500 |
| C | 0.90179600 | 3.05474800 | -0.86596100 |
| H | 1.55865700 | -2.43770100 | 0.91966100 |
| N | 1.44834500 | 4.05037400 | -1.15286200 |
| N | 0.41018400 | -0.70869400 | 0.37378300 |
| N | 2.05121100 | 0.62939300 | -0.26891500 |
| S | -0.49365700 | 1.76597900 | -0.48567800 |
| C | 4.04067200 | -0.83452000 | 0.11208700 |
| C | 4.58793000 | -2.03074400 | 0.61618400 |
| C | 4.91909200 | 0.12046700 | -0.43251100 |
| C | 5.96294900 | -2.26333800 | 0.57321500 |
| H | 3.93717500 | -2.78522800 | 1.04859300 |
| C | 6.29556000 | -0.11343400 | -0.47348100 |
| H | 4.51053000 | 1.04499200 | -0.82544700 |
| C | 6.82686800 | -1.30589100 | 0.02794600 |
| H | 6.36108800 | -3.19347000 | 0.96898700 |
| H | 6.95401600 | 0.63856400 | -0.89972800 |
| H | 7.89709700 | -1.48756000 | -0.00399100 |
| H | -0.55279000 | -0.99246100 | 0.52798000 |
| C | -4.65962400 | -0.41291900 | -0.02853700 |

| | | | |
|---|---|---|---|
| C | -5.06088600 | -1.63358300 | -0.61615600 |
| C | -6.39709200 | -2.03463400 | -0.58712900 |
| C | -7.36530000 | -1.22938200 | 0.02404700 |
| C | -6.98288900 | -0.01687800 | 0.60938700 |
| C | -5.64754600 | 0.38818500 | 0.58664500 |
| H | -4.31409300 | -2.26105800 | -1.09342300 |
| H | -6.68349900 | -2.97775100 | -1.04430800 |
| H | -8.40492500 | -1.54275000 | 0.04372500 |
| H | -7.72680000 | 0.61564000 | 1.08599900 |
| H | -5.35616200 | 1.32913300 | 1.04356900 |
| C | -3.28797300 | 0.00286600 | -0.05822400 |
| C | -2.10005100 | 0.34365500 | -0.08133900 |

## IM4

| | | | |
|---|---|---|---|
| C | -2.23492100 | 1.46466400 | -0.55309300 |
| C | -2.56726500 | 0.27277900 | 0.07968100 |
| C | -0.76166900 | 1.00249800 | 0.99732100 |
| C | 0.23118000 | 4.41153900 | -0.77739200 |
| H | -2.70322700 | 2.01197800 | -1.35716800 |
| N | 0.69523800 | 5.41888900 | -1.17454500 |
| N | -1.09109600 | 1.91617300 | 0.04252500 |
| N | -1.62673000 | 0.00233300 | 1.05455900 |
| S | 0.64078200 | 1.20344500 | 2.07651800 |
| C | -3.70880000 | -0.62117400 | -0.17443100 |
| C | -4.72446100 | -0.26738600 | -1.08339800 |
| C | -3.80958700 | -1.85787300 | 0.48889200 |
| C | -5.80101900 | -1.12286300 | -1.32214600 |
| H | -4.67919700 | 0.68382600 | -1.60555200 |
| C | -4.88835700 | -2.71201900 | 0.24992200 |
| H | -3.03346300 | -2.14287800 | 1.19108700 |
| C | -5.89019000 | -2.35110500 | -0.65705000 |
| H | -6.57312200 | -0.82780700 | -2.02718100 |
| H | -4.94487400 | -3.66265600 | 0.77305300 |
| H | -6.72890500 | -3.01558900 | -0.84278700 |
| H | -0.57705100 | 2.79929100 | -0.20956000 |
| C | 3.96181700 | -0.75550100 | 0.06877500 |
| C | 4.54560500 | -0.19324500 | -1.08604800 |
| C | 5.63659700 | -0.81252600 | -1.69562800 |
| C | 6.16657200 | -1.99253200 | -1.16163700 |
| C | 5.59706300 | -2.55580800 | -0.01409700 |
| C | 4.50099600 | -1.94738700 | 0.59732000 |
| H | 4.13669600 | 0.72471700 | -1.49584500 |
| H | 6.07588100 | -0.37204500 | -2.58564100 |

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|---|---|---|---|
| H | 7.01812900 | -2.47020300 | -1.63686800 |
| H | 6.00517000 | -3.47146600 | 0.40322300 |
| H | 4.05515000 | -2.38565200 | 1.48449900 |
| C | 2.84288100 | -0.12402700 | 0.69728000 |
| C | 1.87929500 | 0.41390000 | 1.21684400 |

## IM5

| | | | |
|---|---|---|---|
| C | 2.05833900 | 0.32471700 | -2.27126600 |
| C | 2.49168300 | 0.29822800 | -0.93594100 |
| C | 0.68811800 | 1.42231500 | -1.08644700 |
| H | 2.51061000 | -0.12416500 | -3.14786000 |
| N | 0.90489200 | 1.04709700 | -2.36716400 |
| N | 1.59366000 | 1.01703800 | -0.18121700 |
| S | -0.70127400 | 2.45582200 | -0.63338300 |
| C | 3.67618400 | -0.34426400 | -0.35089000 |
| C | 4.58092500 | -1.07953000 | -1.14625000 |
| C | 3.95007200 | -0.24692300 | 1.02915900 |
| C | 5.70560100 | -1.68850100 | -0.58727600 |
| H | 4.40318800 | -1.17658600 | -2.21338500 |
| C | 5.07557500 | -0.85678100 | 1.58742100 |
| H | 3.26746600 | 0.31427700 | 1.65861800 |
| C | 5.96322800 | -1.58259300 | 0.78500900 |
| H | 6.38373700 | -2.24818900 | -1.22623800 |
| H | 5.26000300 | -0.76426100 | 2.65473700 |
| H | 6.83860100 | -2.05675500 | 1.21942200 |
| C | -3.90411300 | -0.28690600 | 0.42876200 |
| C | -5.15492400 | 0.23043300 | 0.83025600 |
| C | -6.19605600 | -0.63076000 | 1.17710000 |
| C | -6.01427600 | -2.01759600 | 1.13156700 |
| C | -4.77764000 | -2.53924700 | 0.73490600 |
| C | -3.72971600 | -1.68732900 | 0.38601900 |
| H | -5.30003700 | 1.30553500 | 0.86670400 |
| H | -7.15221800 | -0.21680400 | 1.48393300 |
| H | -6.82719300 | -2.68456400 | 1.40231400 |
| H | -4.62732800 | -3.61427600 | 0.69694700 |
| H | -2.77210700 | -2.09572500 | 0.07894800 |
| C | -2.83546400 | 0.59069200 | 0.07266800 |
| C | -1.91297800 | 1.33005400 | -0.23357100 |

## TS5

| | | | |
|---|---|---|---|
| C | 0.62224400 | -0.51994300 | 0.02496300 |
| C | 1.83357600 | 0.17649700 | 0.00018700 |
| C | 0.22829900 | 1.58270100 | 0.03017700 |
| H | 0.43112000 | -1.58442100 | 0.02481600 |
| N | -0.40167100 | 0.39739500 | 0.04487900 |
| N | 1.56234100 | 1.53723700 | 0.00489700 |
| S | -0.78116700 | 3.06446800 | 0.02348000 |
| C | 3.20558400 | -0.34763400 | -0.02991400 |
| C | 3.46658700 | -1.73436300 | -0.00260400 |
| C | 4.31165200 | 0.52494000 | -0.08895500 |
| C | 4.77273700 | -2.22437200 | -0.03305900 |
| H | 2.63979900 | -2.43728000 | 0.04452500 |
| C | 5.61859300 | 0.03295200 | -0.11843900 |
| H | 4.13255300 | 1.59468500 | -0.11289400 |
| C | 5.86104700 | -1.34479100 | -0.09107400 |
| H | 4.94162100 | -3.29780100 | -0.01067400 |
| H | 6.45140000 | 0.73011300 | -0.16395300 |
| H | 6.87746700 | -1.72701900 | -0.11421100 |
| C | -3.26368900 | -0.18172300 | 0.00879100 |
| C | -2.84096400 | -1.45025700 | 0.45179000 |
| C | -3.71443200 | -2.53899100 | 0.43079800 |
| C | -5.02877500 | -2.38960400 | -0.02339300 |
| C | -5.46163800 | -1.13241400 | -0.46255100 |
| C | -4.59316600 | -0.04186400 | -0.45448700 |
| H | -1.82778000 | -1.56979500 | 0.81434300 |
| H | -3.36536500 | -3.50811200 | 0.77663100 |
| H | -5.70532600 | -3.23884400 | -0.03754400 |
| H | -6.47852200 | -1.00084100 | -0.82175500 |
| H | -4.93157400 | 0.92795600 | -0.80446500 |
| C | -2.41592600 | 0.98231400 | 0.03594200 |
| C | -2.29311500 | 2.25480300 | 0.02562300 |

## IM6

| | | | |
|---|---|---|---|
| C | -0.38820200 | -0.29706800 | 0.00789700 |
| C | -1.63034800 | 0.32844700 | -0.01130800 |
| C | -0.16538200 | 1.89120800 | -0.11617300 |
| H | -0.10927400 | -1.33462700 | 0.07933800 |
| N | 0.54755000 | 0.71951000 | -0.06852400 |
| N | -1.47729700 | 1.70633300 | -0.08957700 |
| S | 0.96059500 | 3.23732500 | -0.12737900 |
| C | -2.96038300 | -0.29803800 | 0.04313900 |

| | | | |
|---|---|---|---|
| C | -3.11287600 | -1.69847400 | 0.09383100 |
| C | -4.12499500 | 0.49354400 | 0.04725400 |
| C | -4.37921600 | -2.28215800 | 0.14872600 |
| H | -2.23638600 | -2.33980000 | 0.08920500 |
| C | -5.39182400 | -0.09207700 | 0.10131500 |
| H | -4.02470700 | 1.57277400 | 0.00861700 |
| C | -5.52892100 | -1.48322600 | 0.15281600 |
| H | -4.46805600 | -3.36443700 | 0.18707800 |
| H | -6.27459700 | 0.54174900 | 0.10355900 |
| H | -6.51406300 | -1.93856300 | 0.19498500 |
| C | 2.84736400 | -0.29572100 | -0.00514400 |
| C | 2.56325700 | -1.45837100 | -0.75040800 |
| C | 3.43113200 | -2.55421400 | -0.73914700 |
| C | 4.60879400 | -2.51711300 | 0.01353600 |
| C | 4.90739000 | -1.36800000 | 0.75583600 |
| C | 4.03677700 | -0.27722100 | 0.75112800 |
| H | 1.67300300 | -1.49862000 | -1.36990400 |
| H | 3.18957100 | -3.43409000 | -1.32949600 |
| H | 5.28242900 | -3.36914600 | 0.02345000 |
| H | 5.81612200 | -1.32603900 | 1.35048700 |
| H | 4.26574700 | 0.60680000 | 1.33739100 |
| C | 1.97100500 | 0.89451900 | -0.03026400 |
| C | 2.40624600 | 2.19828000 | -0.05135600 |

## TS6

| | | | |
|---|---|---|---|
| C | 1.86336900 | 0.64052000 | -0.10414100 |
| C | 2.81618300 | -0.36957500 | -0.05616300 |
| C | 0.91721100 | -1.34836500 | -0.21793700 |
| H | 1.94897100 | 1.71387100 | -0.08709700 |
| N | 0.64194300 | -0.00307700 | -0.19974200 |
| N | 2.20842200 | -1.61699400 | -0.13121300 |
| S | -0.56542800 | -2.25495300 | -0.41535900 |
| C | 4.27724600 | -0.23209100 | 0.05542300 |
| C | 4.89071400 | 1.03291100 | 0.15031700 |
| C | 5.10297500 | -1.37202800 | 0.06911000 |
| C | 6.27715700 | 1.15178700 | 0.25406800 |
| H | 4.28314600 | 1.93297500 | 0.14451100 |
| C | 6.49054500 | -1.25131900 | 0.17352500 |
| H | 4.64516500 | -2.35256300 | -0.00334400 |
| C | 7.08741700 | 0.01020600 | 0.26661100 |
| H | 6.72564100 | 2.13875800 | 0.32621800 |
| H | 7.10654900 | -2.14644000 | 0.18191700 |

| | | | |
|---|---|---|---|
| H | 8.16640400 | 0.10381700 | 0.34765800 |
| C | -1.16773000 | 1.73463600 | -0.33656000 |
| C | -0.63704800 | 2.66378900 | 0.57914700 |
| C | -1.07861600 | 3.98922100 | 0.59126100 |
| C | -2.06218300 | 4.41462300 | -0.30748100 |
| C | -2.60060100 | 3.49988900 | -1.21910000 |
| C | -2.15438500 | 2.17707000 | -1.23749300 |
| H | 0.10626400 | 2.34564600 | 1.30378300 |
| H | -0.65862200 | 4.68705700 | 1.31025700 |
| H | -2.40381400 | 5.44553400 | -0.29828500 |
| H | -3.36282100 | 3.81869100 | -1.92463600 |
| H | -2.56548400 | 1.47244000 | -1.95291600 |
| C | -0.73544300 | 0.32154800 | -0.34943000 |
| C | -1.54474900 | -0.77267800 | -0.48037900 |
| C | -4.87206600 | -1.41907000 | 0.46745500 |
| C | -6.36151600 | -1.53656700 | 0.08362600 |
| H | -6.49357400 | -2.30883100 | -0.68356900 |
| H | -6.98853200 | -1.79852800 | 0.94602300 |
| H | -6.72201600 | -0.58556800 | -0.32627400 |
| C | -4.71729400 | -0.32823000 | 1.55498600 |
| H | -5.29502100 | -0.56267900 | 2.45865200 |
| H | -3.66455300 | -0.22209900 | 1.84046800 |
| H | -5.06240800 | 0.63791200 | 1.16826700 |
| C | -4.39470400 | -2.77565100 | 1.04156600 |
| H | -4.50430300 | -3.56265300 | 0.28579900 |
| H | -3.33690000 | -2.72160600 | 1.32261800 |
| H | -4.96828200 | -3.07158300 | 1.92981800 |
| O | -4.13365500 | -1.07899600 | -0.68285700 |
| H | -2.89135700 | -0.91433100 | -0.53511300 |

## P (5aa) + $^{t}$BuO$^{-}$

| | | | |
|---|---|---|---|
| C | 2.10199000 | 0.52633900 | -0.03136900 |
| C | 2.99167500 | -0.53844300 | -0.03093100 |
| C | 1.03768600 | -1.40639700 | -0.11457500 |
| H | 2.25075200 | 1.59253800 | -0.01237900 |
| N | 0.84124400 | -0.04460400 | -0.07600900 |
| N | 2.30866600 | -1.74869900 | -0.08774800 |
| S | -0.48665700 | -2.25092900 | -0.25072900 |
| C | 4.46195500 | -0.49156400 | 0.01943300 |
| C | 5.15343500 | 0.73237600 | 0.10695800 |
| C | 5.21405100 | -1.68010000 | -0.01964700 |
| C | 6.54763700 | 0.76495900 | 0.15149900 |

| | | | |
|---|---|---|---|
| H | 4.60233100 | 1.66736000 | 0.14280900 |
| C | 6.60954300 | -1.64549300 | 0.02597300 |
| H | 4.69393200 | -2.62945700 | -0.08673600 |
| C | 7.28530900 | -0.42404200 | 0.11129500 |
| H | 7.05873800 | 1.72119100 | 0.21924500 |
| H | 7.16952700 | -2.57603400 | -0.00574700 |
| H | 8.37043400 | -0.39745100 | 0.14657900 |
| C | -0.89008500 | 1.78734400 | -0.12158300 |
| C | -0.27583100 | 2.69028400 | 0.76578300 |
| C | -0.67349000 | 4.02842600 | 0.80385200 |
| C | -1.69208600 | 4.48621200 | -0.03803900 |
| C | -2.31208300 | 3.59455100 | -0.91947300 |
| C | -1.91215000 | 2.25801800 | -0.96551900 |
| H | 0.49569600 | 2.34397000 | 1.44613100 |
| H | -0.19176600 | 4.71068700 | 1.49809300 |
| H | -1.99900400 | 5.52741600 | -0.00791400 |
| H | -3.10198200 | 3.94082100 | -1.57949700 |
| H | -2.38485100 | 1.57260500 | -1.66145300 |
| C | -0.50676200 | 0.36351400 | -0.15826900 |
| C | -1.34139800 | -0.70720800 | -0.25835300 |
| C | -5.49241400 | -1.29886500 | 0.16880800 |
| C | -6.69332700 | -1.29963800 | -0.81878200 |
| H | -6.54038700 | -2.06526800 | -1.59008400 |
| H | -7.65520100 | -1.49897400 | -0.32486500 |
| H | -6.76230200 | -0.32637900 | -1.32130800 |
| C | -5.76876900 | -0.22160900 | 1.25580000 |
| H | -6.70433700 | -0.39825500 | 1.80571000 |
| H | -4.94492700 | -0.20578100 | 1.98059400 |
| H | -5.82853800 | 0.77066000 | 0.79122700 |
| C | -5.45121600 | -2.68564000 | 0.87139400 |
| H | -5.27420700 | -3.47400800 | 0.12894700 |
| H | -4.62555500 | -2.71250600 | 1.59387100 |
| H | -6.38171400 | -2.92293400 | 1.40700000 |
| O | -4.30357400 | -1.04290000 | -0.49441500 |
| H | -2.44291800 | -0.72716200 | -0.28244900 |

# Part two

The absolute energies of all stationary points. (Hartree/Particle)

| **R1(1a + *t*-BuO$^-$)** | **TS1** | **IM1+ *t*-BuOH** |
|---|---|---|
| -1180.928176 | -1180.926078 | -1180.936073 |
| **IM1** | **TS2** | **IM2** |
| -947.218873 | -947.206675 | -947.274146 |
| **IM3** | **TS4** | **IM4** |
| -1255.655717 | -1255.657783 | -1255.708519 |
| **IM5+HCN** | **IM5** | **TS5** |
| -1255.702836 | -1162.254408 | -1162.221537 |
| **IM6** | **IM6+*t*-BuOH** | **TS6** |
| -1162.256201 | -1395.974557 | -1395.968655 |
| **P+*t*-BuO$^-$** | | |
| -1395.975959 | | |

# Alternative mechanism

**Scheme S1**. The detailed reaction process from **1a** to **P (5aa)**.

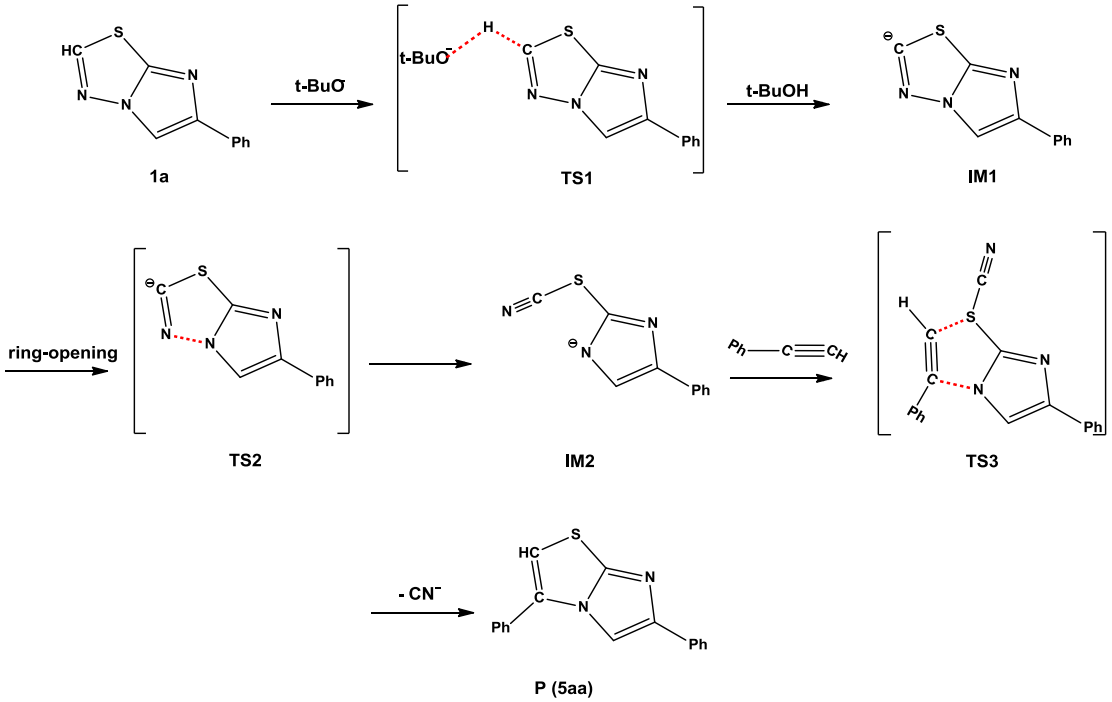
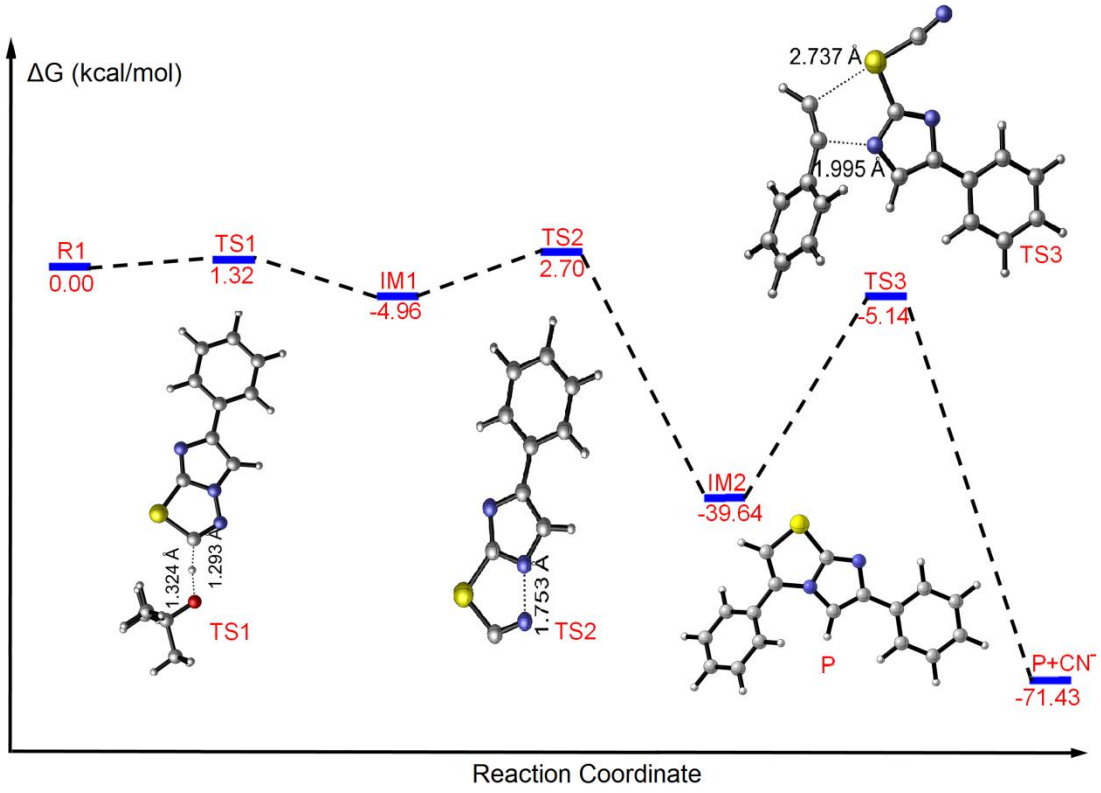


**Figure S1**. The potential energy and transition states for the **R1→P** reactions with DMF as solvent.




# Alternative Mechanism

## Part one

The Cartesian Coordinates of all stationary points.

## IM2 + phenylacetylene

| | | | |
|---|---|---|---|
| C | 1.32768000 | -0.20406600 | 0.48947600 |
| C | 2.63479300 | -0.33726800 | -0.01035200 |
| C | 1.94387500 | 1.64857000 | -0.31503300 |
| C | 2.49701700 | 4.17290800 | 0.50424000 |
| H | 0.69784000 | -0.94461200 | 0.96763800 |
| N | 2.90912200 | 4.78186200 | 1.41305900 |
| N | 0.88541200 | 1.06990500 | 0.29182400 |
| N | 3.01940100 | 0.87485800 | -0.53067700 |
| S | 1.88839600 | 3.34785000 | -0.86546700 |
| C | 3.51316100 | -1.51569000 | -0.02659800 |
| C | 3.07823200 | -2.76056500 | 0.47480100 |
| C | 4.82191300 | -1.43960800 | -0.54513700 |
| C | 3.91507600 | -3.87768900 | 0.45909700 |
| H | 2.07497900 | -2.85760000 | 0.87936900 |
| C | 5.65783200 | -2.55811400 | -0.56131500 |

| | | | |
|---|---|---|---|
| H | 5.17599100 | -0.49107000 | -0.93504400 |
| C | 5.21225700 | -3.78619200 | -0.05943900 |
| H | 3.55186400 | -4.82360800 | 0.85217700 |
| H | 6.66240200 | -2.46947100 | -0.96692600 |
| H | 5.86276600 | -4.65591500 | -0.07198700 |
| C | -5.55518500 | 0.15935600 | -0.12930200 |
| C | -5.15519400 | -0.43580000 | 1.08431700 |
| C | -5.41995700 | -1.78407700 | 1.32570100 |
| C | -6.08443800 | -2.55550700 | 0.36594100 |
| C | -6.48490400 | -1.97172800 | -0.84095500 |
| C | -6.22433400 | -0.62423100 | -1.09120100 |
| H | -4.63906200 | 0.16304900 | 1.82781300 |
| H | -5.10682000 | -2.23255700 | 2.26369400 |
| H | -6.28857600 | -3.60471500 | 0.55709000 |
| H | -7.00066100 | -2.56629600 | -1.58899900 |
| H | -6.53390400 | -0.17081600 | -2.02737800 |
| C | -5.28477200 | 1.54324800 | -0.38186900 |
| C | -5.05555200 | 2.71578100 | -0.59592300 |
| H | -4.85174500 | 3.74701800 | -0.78369400 |

## TS3

| | | | |
|---|---|---|---|
| C | 0.14245600 | -0.59421500 | -0.02792800 |
| C | 1.48207900 | -0.21544400 | 0.00408300 |
| C | 0.27053100 | 1.54579800 | 0.00787400 |
| C | 1.24677900 | 3.93507600 | 0.55491300 |
| H | -0.31520600 | -1.57310700 | -0.04989900 |
| N | 2.15849900 | 4.57260600 | 0.91548400 |
| N | -0.62437200 | 0.54332700 | -0.01475800 |
| N | 1.54663000 | 1.16966600 | 0.02454700 |
| S | -0.26055100 | 3.27425800 | -0.00455400 |
| C | 2.68958400 | -1.05161300 | 0.01753200 |
| C | 2.60990800 | -2.45716100 | -0.07474600 |
| C | 3.97011800 | -0.47256700 | 0.12548100 |
| C | 3.75993400 | -3.24734100 | -0.05796800 |
| H | 1.63985300 | -2.93775200 | -0.16421100 |
| C | 5.12033400 | -1.26487400 | 0.14111700 |
| H | 4.05238300 | 0.60672300 | 0.19839200 |
| C | 5.02560600 | -2.65783300 | 0.05013800 |
| H | 3.66740800 | -4.32774700 | -0.13100500 |
| H | 6.09489400 | -0.79100500 | 0.22600600 |
| H | 5.92026800 | -3.27356300 | 0.06260100 |

| | | | |
|---|---|---|---|
| C | -3.13613600 | -0.37066800 | -0.20695600 |
| C | -3.00630700 | -1.05448400 | 1.01645200 |
| C | -3.67174200 | -2.26265200 | 1.22892500 |
| C | -4.47265600 | -2.81556200 | 0.22253100 |
| C | -4.60466700 | -2.14776500 | -0.99905300 |
| C | -3.94251500 | -0.93625800 | -1.21370200 |
| H | -2.38084800 | -0.63116500 | 1.79536800 |
| H | -3.56535200 | -2.77397700 | 2.18153200 |
| H | -4.98666600 | -3.75773200 | 0.38901400 |
| H | -5.22011000 | -2.57051900 | -1.78813200 |
| H | -4.04548900 | -0.41878000 | -2.16273500 |
| C | -2.53482900 | 0.93610000 | -0.43620800 |
| C | -2.63301900 | 2.14750000 | -0.77526300 |
| H | -3.45180900 | 2.79312600 | -1.05318700 |

## P(5aa) + $CN^-$

| | | | |
|---|---|---|---|
| C | 1.15694200 | 0.52001300 | 0.00711000 |
| C | 1.95446200 | -0.61420200 | -0.02121100 |
| C | -0.06019300 | -1.31446100 | -0.18372900 |
| C | -6.53574900 | -4.05374000 | 0.05102900 |
| H | 1.38861000 | 1.56706600 | 0.10462000 |
| N | -7.38368000 | -4.86249200 | 0.20363100 |
| N | -0.14446800 | 0.05910600 | -0.10782100 |
| N | 1.17474800 | -1.76134700 | -0.13754600 |
| S | -1.64971800 | -2.04067100 | -0.25951300 |
| C | 3.42219700 | -0.69547300 | 0.05901400 |
| C | 4.21796400 | 0.46425200 | 0.12925200 |
| C | 4.06424600 | -1.94724300 | 0.06847000 |
| C | 5.60805600 | 0.37335000 | 0.20884900 |
| H | 3.75263700 | 1.44528100 | 0.11942900 |
| C | 5.45577700 | -2.03603600 | 0.14750400 |
| H | 3.46226000 | -2.84774000 | 0.01420100 |
| C | 6.23608900 | -0.87766600 | 0.21847600 |
| H | 6.20192600 | 1.28146200 | 0.26176500 |
| H | 5.93048900 | -3.01329000 | 0.15383700 |
| H | 7.31819100 | -0.94709200 | 0.27969500 |
| C | -1.73158500 | 2.01998500 | -0.02557000 |
| C | -0.98954000 | 2.94503700 | -0.78244800 |
| C | -1.29046400 | 4.30717000 | -0.72498000 |
| C | -2.33646100 | 4.76520200 | 0.08266700 |
| C | -3.08166800 | 3.85140200 | 0.83489500 |
| C | -2.77968400 | 2.48934800 | 0.78631900 |

| | | | |
|---|---|---|---|
| H | -0.19401800 | 2.60037300 | -1.43555000 |
| H | -0.71184200 | 5.00891700 | -1.31830200 |
| H | -2.56756400 | 5.82527800 | 0.12651100 |
| H | -3.89182700 | 4.19898000 | 1.46900100 |
| H | -3.34585700 | 1.78644800 | 1.38961900 |
| C | -1.45287200 | 0.57394200 | -0.09845700 |
| C | -2.36362200 | -0.43359200 | -0.17364900 |
| H | -3.43709000 | -0.32552800 | -0.22171400 |

# Part two

The absolute energies of all stationary points. (Hartree/Particle)

| IM2 + phenylacetylene | TS3 | P (5aa) + $CN^-$ |
|---|---|---|
| -1255.696095 | -1255.641119 | -1255.746762 |

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