

Palladium-catalyzed microwave-assisted direct arylation of imidazo[2,1-b]thiazoles with aryl bromides: synthesis and mechanistic study

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1. Characterization data

5-(4-Nitrophenyl)-6-phenylimidazo[2,1-b]thiazole (3aa)

Orange solid (58 mg, 72% yield), mp 154-156 °C. IR (KBr) 3065, 1597, 1514, 1460, 1442, 1344, 852, 732, 696 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.27 (d, *J* = 8.7 Hz, 2H), 7.60 (d, *J* = 8.7 Hz, 2H), 7.54-7.53 (m, 2H), 7.51 (d, *J* = 4.5 Hz, 1H), 7.36-7.28 (m, 3H), 6.94 (d, *J* = 4.5 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 150.6, 146.8, 145.7, 137.0, 133.6, 129.0, 128.6, 128.0, 124.5, 120.7, 117.2, 113.7. HRMS (ESI) calcd. for C₁₇H₁₁N₃O₂S [MH⁺]: 322.0645; Found: 322.0658.

5-(3-Nitrophenyl)-6-phenylimidazo[2,1-b]thiazole (3ab)

Yellow solid (44 mg, 55% yield), mp 200-202 °C. IR (KBr) 3080, 1603, 1529, 1462, 1442, 1348, 874, 811, 754, 736, 700 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.35 (t, *J* = 1.9 Hz, 1H), 8.24 (d, *J* = 8.2 Hz, 1H), 7.74 (d, *J* = 7.9 Hz, 1H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.58-7.53 (m, 2H), 7.45 (d, *J* = 4.5 Hz, 1H), 7.35-7.27 (m, 3H), 6.93 (d, *J* = 4.5 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 150.1, 148.8, 145.1, 135.1, 133.7, 132.3, 130.2, 128.5, 127.7, 125.2, 123.1, 122.8, 120.2, 117.0, 113.4. HRMS (ESI) calcd. for C₁₇H₁₁N₃O₂S [MH⁺]: 322.0645; Found: 322.0640.

5-(2-Nitrophenyl)-6-phenylimidazo[2,1-b]thiazole (3ac)

Yellow solid (18 mg, 22% yield), mp 62-64 °C. IR (KBr) 3062, 1603, 1527, 1462, 1442, 1346, 853, 735, 700 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.22-8.17 (m, 1H), 7.69-7.64 (m, 2H), 7.47 (ddd, *J* = 9.6, 7.3, 2.7 Hz, 4H), 7.26-7.23 (m, 2H), 7.06 (d, *J* = 4.5 Hz, 1H), 6.84 (d, *J* = 4.5 Hz, 1H). ¹³C NMR (100 MHz, CDCl₃) δ 149.9, 149.1, 145.1, 134.3, 133.8, 133.6, 130.2, 128.4, 127.4, 127.2, 125.3, 125.2, 117.5, 117.4, 112.8. HRMS (ESI) calcd. for C₁₇H₁₁N₃O₂S [MH⁺]: 322.0645; Found: 322.0656.

4-(6-Phenylimidazo[2,1-b]thiazol-5-yl)benzotrile (3ad)

White solid (49 mg, 65% yield), mp 180-182 °C. IR (KBr) 3065, 2228, 1605, 1536, 1461, 1443, 1371, 850, 734, 700 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.72 (d, *J* = 8.6 Hz, 2H), 7.58-7.52 (m, 4H), 7.46 (d, *J* = 4.5 Hz, 1H), 7.33-7.29 (m, 3H), 6.92 (d, *J* = 4.5 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 150.3, 145.3, 135.1, 133.7, 132.9, 129.0, 128.5, 127.9, 120.9, 118.4, 117.1, 113.4, 111.3. HRMS (ESI) calcd. for C₁₈H₁₁N₃S [MH⁺]: 302.0746; Found: 302.0749.

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

White solid (47 mg, 55% yield), mp 38-40 °C. IR (KBr) 3065, 1613, 1542, 1462, 1443, 1325, 1165, 1123, 852, 734, 702 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.70 (d, *J* = 8.2 Hz, 2H), 7.57 (d, *J* = 8.0 Hz, 4H), 7.43 (d, *J* = 4.5 Hz, 1H), 7.35–7.27 (m, 3H), 6.89 (d, *J* = 4.5 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 149.8, 144.6, 134.1, 133.9, 129.0, 128.5, 127.8, 127.6, 126.2, 125.7, 122.1, 121.3, 117.2, 113.1. HRMS (ESI) calcd. for C₁₈H₁₁F₃N₂S [MH⁺]: 345.0668; Found: 345.0680.

1-(4-(6-Phenylimidazo[2,1-b]thiazol-5-yl)phenyl)ethanone (3af)

Yellow solid (40 mg, 50% yield), mp 64-66 °C. IR (KBr) 3061, 2981, 1736, 1683, 1604, 1537, 1477, 1443, 1371, 1266, 1246, 852, 720, 700 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.05–7.99 (m, 2H), 7.57 (ddd, *J* = 10.3, 6.5, 2.0 Hz, 4H), 7.47 (d, *J* = 4.5 Hz, 1H), 7.32–7.26 (m, 3H), 6.89 (d, *J* = 4.5 Hz, 1H), 2.65 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 197.3, 149.9, 144.8, 136.2, 135.2, 134.0, 129.2, 128.7, 128.4, 127.9, 127.6, 121.7, 117.4, 113.1, 26.7. HRMS (ESI) calcd. for C₁₉H₁₄N₂SO [MH⁺]: 319.0900; Found: 319.0908.

Methyl 4-(6-phenylimidazo[2,1-b]thiazol-5-yl)benzoate(3ag)

Yellow solid (25 mg, 30% yield), mp 68-69 °C. IR (KBr) 3060, 2923, 1720, 1608, 1545, 1460, 1438, 1374, 1277, 1184, 1112, 859, 733, 701 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.10 (d, *J* = 8.3 Hz, 2H), 7.57 (dd, *J* = 7.7, 1.8 Hz, 2H), 7.52 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 4.5 Hz, 1H), 7.33–7.24 (m, 3H), 6.87 (d, *J* = 4.5 Hz, 1H), 3.95 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 166.5, 149.8, 144.6, 135.0, 134.0, 130.4, 129.5, 128.6, 128.4, 127.8, 127.5, 121.8, 117.4, 113.0, 52.3. HRMS (ESI) calcd. for C₁₉H₁₄N₂O₂S [MH⁺]: 335.0849; Found: 335.0847.

6-Phenyl-5-(p-tolyl)imidazo[2,1-b]thiazole (3ah)

Yellow solid (15 mg, 20% yield), mp 139-140 °C. IR (KBr) 3060, 1603, 1540, 1511, 1464, 1442, 1370, 856, 734, 699 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.64–7.59 (m, 2H), 7.44–7.40 (m, 1H), 7.31 (dd, *J* = 8.1, 3.4 Hz, 3H), 7.27–7.22 (m, 4H), 6.75 (d, *J* = 4.5 Hz, 1H), 2.41 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 148.6, 143.0, 138.2, 134.5, 129.9, 129.5, 128.9, 128.2, 127.4, 126.9, 122.8, 117.4, 112.3, 21.3. HRMS (ESI) calcd. for C₁₈H₁₄N₂S [MH⁺]: 291.0950; Found: 291.0959.

5-(3,5-Bis(trifluoromethyl)phenyl)-6-phenylimidazo[2,1-b]thiazole (3ai)

White solid (46 mg, 44% yield), mp 146-147 °C. IR (KBr) 3064, 1603, 1540, 1463, 1444, 1344, 1280, 1180, 1133, 847, 799, 735, 706 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.88 (s, 3H), 7.53 (d, *J* = 5.3 Hz, 2H), 7.42 (d, *J* = 4.3 Hz, 1H), 7.32-7.26 (m, 3H), 6.94 (d, *J* = 4.3 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 150.5, 145.6, 133.3, 132.8, 132.4, 128.6, 128.1, 127.7, 124.7, 121.4, 119.6, 116.8, 113.8. HRMS (ESI) calcd. for C₁₉H₁₀F₆N₂S [MH⁺]: 413.0542; Found: 413.0542.

5-(4-Nitro-3-(trifluoromethyl)phenyl)-6-phenylimidazo[2,1-b]thiazole (3aj)

Orange solid (53 mg, 54% yield), mp 176-177 °C. IR (KBr) 3064, 1607, 1537, 1460, 1444, 1355, 1182, 1151, 867, 853, 735, 704 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.94 (d, *J* = 8.4 Hz, 1H), 7.88 (s, 1H), 7.73 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.56-7.48 (m, 3H), 7.39-7.31 (m, 3H), 6.99 (d, *J* = 4.5 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 151.2, 146.7, 146.3, 135.7, 133.2, 132.2, 128.7, 128.4, 128.0, 127.2, 126.3, 125.1, 124.7, 119.8, 119.4, 116.9, 114.1. HRMS (ESI) calcd. for C₁₈H₁₀F₃N₃O₂S [MH⁺]: 390.0519; Found: 390.0519.

3-(4-Nitrophenyl)-2-phenylbenzo[d]imidazo[2,1-b]thiazole (3ba)

Yellow solid (91 mg, 98% yield), mp 223-224 °C. IR (KBr) 3062, 1596, 1515, 1482, 1440, 1348, 853, 742, 699 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.40 (d, *J* = 8.4 Hz, 2H), 7.80-7.68 (m, 3H), 7.46 (d, *J* = 5.5 Hz, 2H), 7.35-7.17 (m, 5H), 6.96 (d, *J* = 8.0 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 148.7, 148.1, 145.1, 137.1, 133.3, 132.7, 132.1, 130.5, 128.5, 127.7, 127.5, 126.0, 124.9, 124.6, 124.4, 121.9, 113.2. HRMS (ESI) calcd. for C₂₁H₁₃N₃O₂S [MH⁺]: 372.0801; Found: 372.0805.

3-(3-Nitrophenyl)-2-phenylbenzo[d]imidazo[2,1-b]thiazole (3bb)

Yellow solid (64 mg, 69% yield), mp 249-250 °C. IR (KBr) 3051, 1599, 1523, 1483, 1442, 1345, 870, 815, 768, 738, 692 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.43 (d, *J* = 10.7 Hz, 2H), 7.90 (d, *J* = 7.4 Hz, 1H), 7.78-7.70 (m, 2H), 7.48 (d, *J* = 5.8 Hz, 2H), 7.34-7.13 (m, 5H), 6.82 (d, *J* = 7.8 Hz, 1H). ¹³C NMR (75 MHz, CDCl₃) δ 148.7, 148.2, 144.8, 137.4, 133.3, 132.6, 132.2, 130.5, 130.4, 128.5, 127.6, 127.2, 126.0, 124.8, 124.6, 124.2, 121.4, 112.9. HRMS (ESI) calcd. for C₂₁H₁₃N₃O₂S [MH⁺]: 372.0801; Found: 372.0806.

4-(2-Phenylbenzo[d]imidazo[2,1-b]thiazol-3-yl)benzotrile (3bc)

White solid (69 mg, 79% yield), mp 193-195 °C. IR (KBr) 3066, 2232, 1599, 1550, 1488, 1441, 1368, 842, 733, 700 cm^{-1} . ^1H NMR (300 MHz, CDCl_3) δ 7.83 (d, $J = 7.8$ Hz, 2H), 7.69-7.66 (m, 3H), 7.45 (d, $J = 5.6$ Hz, 2H), 7.33-7.16 (m, 5H), 6.91 (d, $J = 8.0$ Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 148.3, 144.6, 135.0, 133.3, 132.8, 132.6, 131.8, 130.4, 128.4, 127.5, 127.3, 125.8, 124.8, 124.4, 122.1, 118.2, 113.0, 112.9. HRMS (ESI) calcd. for $\text{C}_{22}\text{H}_{13}\text{N}_3\text{S}$ [MH^+]: 352.0903; Found: 352.0907.

2-Phenyl-3-(4-(trifluoromethyl)phenyl)benzo[d]imidazo[2,1-b]thiazole (3bd)

White solid (76 mg, 77% yield), mp 219-222 °C. IR (KBr) 3063, 1600, 1512, 1490, 1442, 1369, 1333, 1159, 1120, 849, 743, 700 cm^{-1} . ^1H NMR (300 MHz, CDCl_3) δ 7.82 (d, $J = 8.2$ Hz, 2H), 7.71-7.68 (m, 3H), 7.49 (dd, $J = 7.9, 1.6$ Hz, 2H), 7.31-7.15 (m, 5H), 6.87 (d, $J = 8.3$ Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 148.0, 144.3, 134.1, 133.6, 132.8, 131.6, 131.1, 130.5, 128.4, 127.4, 127.2, 126.2, 125.9, 124.7, 124.4, 122.6, 122.1, 113.2. HRMS (ESI) calcd. for $\text{C}_{22}\text{H}_{13}\text{F}_3\text{N}_2\text{S}$ [MH^+]: 395.0824; Found: 395.0820.

3-(3,5-Bis(trifluoromethyl)phenyl)-2-phenylbenzo[d]imidazo[2,1-b]thiazole (3be)

White solid (99 mg, 85% yield), mp 189 °C. IR (KBr) 3051, 1601, 1553, 1478, 1444, 1344, 1276, 1173, 1119, 846, 804, 745, 697 cm^{-1} . ^1H NMR (300 MHz, CDCl_3) δ 8.05 (d, $J = 5.5$ Hz, 3H), 7.72 (d, $J = 7.8$ Hz, 1H), 7.46 (dd, $J = 7.7, 1.9$ Hz, 2H), 7.35-7.18 (m, 5H), 6.83 (d, $J = 7.7$ Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 148.7, 145.2, 133.3, 133.0, 132.7, 132.0, 131.4, 130.6, 128.5, 127.8, 127.3, 126.0, 124.9, 124.7, 122.8, 121.1, 120.8, 112.8. HRMS (ESI) calcd. for $\text{C}_{23}\text{H}_{12}\text{F}_6\text{N}_2\text{S}$ [MH^+]: 463.0698; Found: 463.0691.

3-(4-Nitro-3-(trifluoromethyl)phenyl)-2-phenylbenzo[d]imidazo[2,1-b]thiazole (3bf)

Orange solid (66 mg, 61% yield), mp 247-248 °C. IR (KBr) 3030, 1592, 1534, 1486, 1443, 1353, 1180, 1140, 860, 808, 742, 698 cm^{-1} . ^1H NMR (300 MHz, CDCl_3) δ 8.06 (d, $J = 8.3$ Hz, 1H), 8.03 (d, $J = 1.5$ Hz, 1H), 7.91 (dd, $J = 8.3, 1.8$ Hz, 1H), 7.76 (dd, $J = 7.9, 1.0$ Hz, 1H), 7.47-7.41 (m, 2H), 7.39-7.27 (m, 5H), 6.97 (d, $J = 8.0$ Hz, 1H). ^{13}C NMR (75 MHz, CDCl_3) δ 149.3, 147.6, 145.9, 135.4, 132.8, 132.4, 130.50, 130.3, 128.6, 128.0, 127.6, 126.1, 125.1, 124.9, 124.4, 123.4, 120.4, 119.8, 112.9. HRMS (ESI) calcd. for $\text{C}_{22}\text{H}_{12}\text{F}_3\text{N}_3\text{O}_2\text{S}$ [MH^+]: 440.0675; Found: 440.0666.

3-(4-Nitrophenyl)-2-phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole (3ca)

Golden yellow solid (85 mg, 91% yield), mp 210-212 °C. IR (KBr) 3065, 2935, 1599, 1520, 1477, 1443, 1346, 854, 733, 706 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.29 (d, *J* = 8.6 Hz, 2H), 7.61 (d, *J* = 8.6 Hz, 2H), 7.40 (dd, *J* = 7.7, 2.0 Hz, 2H), 7.25–7.18 (m, 3H), 2.70 (t, *J* = 5.1 Hz, 2H), 2.10 (t, *J* = 6.1 Hz, 2H), 1.90–1.69 (m, 4H). ¹³C NMR (75 MHz, CDCl₃) δ 148.8, 147.7, 143.7, 137.7, 133.9, 132.4, 128.3, 127.3, 127.2, 126.8, 123.6, 122.7, 120.6, 24.7, 22.5, 21.9. HRMS (ESI) calcd. for C₂₁H₁₇N₃O₂S [MH⁺]: 376.1114; Found: 376.1109.

3-(3-Nitrophenyl)-2-phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole (3cb)

Yellow solid (50 mg, 53% yield), mp 269-270 °C. IR (KBr) 3041, 2925, 1597, 1520, 1465, 1437, 1341, 867, 816, 753, 740, 694 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.36–8.29 (m, 2H), 7.77 (dt, *J* = 7.6, 1.2 Hz, 1H), 7.61 (t, *J* = 8.1 Hz, 1H), 7.42 (dd, *J* = 7.9, 1.8 Hz, 2H), 7.25–7.18 (m, 3H), 2.70 (t, *J* = 5.8 Hz, 2H), 2.05 (t, *J* = 5.1 Hz, 2H), 1.89–1.67 (m, 4H). ¹³C NMR (75 MHz, CDCl₃) δ 148.4, 148.0, 143.6, 137.8, 133.9, 132.7, 129.5, 128.3, 127.2, 126.7, 126.3, 123.7, 122.6, 120.2, 24.7, 24.6, 22.4, 21.9. HRMS (ESI) calcd. for C₂₁H₁₇N₃O₂S [MH⁺]: 376.1114; Found: 376.1130.

4-(2-Phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazol-3-yl)benzotrile (3cc)

White solid (59 mg, 66% yield), mp 214-215 °C. IR (KBr) 3064, 2942, 2226, 1605, 1538, 1481, 1441, 1379, 840, 736, 703 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.72 (d, *J* = 8.2 Hz, 2H), 7.55 (d, *J* = 8.2 Hz, 2H), 7.39 (dd, *J* = 7.7, 1.5 Hz, 2H), 7.26–7.14 (m, 3H), 2.68 (d, *J* = 6.0 Hz, 2H), 2.08 (d, *J* = 6.0 Hz, 2H), 1.90–1.67 (m, 4H). ¹³C NMR (75 MHz, CDCl₃) δ 148.5, 143.4, 135.7, 133.9, 132.3, 132.1, 128.2, 127.2, 127.0, 126.7, 122.5, 120.9, 118.4, 112.4, 24.6, 24.5, 22.4, 21.9. HRMS (ESI) calcd. for C₂₂H₁₇N₃S [MH⁺]: 356.1216; Found: 356.1209.

2-Phenyl-3-(4-(trifluoromethyl)phenyl)-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole (3cd)

White solid (65 mg, 65% yield), mp 187-189 °C. IR (KBr) 3070, 2943, 1603, 1547, 1485, 1442, 1380, 1323, 1169, 1129, 859, 736, 703 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.68 (d, *J* = 8.1 Hz, 2H), 7.56 (d, *J* = 8.1 Hz, 2H), 7.46–7.39 (m, 2H), 7.24–7.12 (m, 3H), 2.67 (dd, *J* = 7.0, 5.1 Hz, 2H), 2.04 (dd, *J* = 7.1, 5.0 Hz, 2H), 1.88–1.65 (m, 4H). ¹³C NMR (75 MHz, CDCl₃) δ 148.1, 143.0, 134.7, 134.2,

132.0, 130.9, 130.5, 128.2, 127.0, 126.8, 125.7, 125.3, 122.1, 121.4, 24.6, 24.3, 22.5, 21.9. HRMS (ESI) calcd. for C₂₂H₁₇F₃N₂S [MH⁺]: 399.1137; Found: 399.1152.

3-(3,5-Bis(trifluoromethyl)phenyl)-2-phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole (3ce)

White solid (84 mg, 72% yield), mp 239 °C. IR (KBr) 3060, 2921, 1601, 1548, 1466, 1443, 1350, 1280, 1178, 1133, 845, 800, 729, 697 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.96 (s, 1H), 7.90 (s, 2H), 7.42–7.36 (m, 2H), 7.28–7.19 (m, 3H), 2.71 (t, *J* = 6.0 Hz, 2H), 2.03 (t, *J* = 5.9 Hz, 2H), 1.92–1.69 (m, 4H). ¹³C NMR (75 MHz, CDCl₃) δ 148.8, 143.9, 133.6, 133.2, 132.0, 131.6, 128.4, 127.1, 126.5, 124.8, 123.0, 122.3, 121.2, 119.6, 24.7, 24.6, 22.4, 22.0. HRMS (ESI) calcd. for C₂₃H₁₆F₆N₂S [MH⁺]: 467.1011; Found: 467.1000.

3-(4-Nitro-3-(trifluoromethyl)phenyl)-2-phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole (3cf)

Orange solid (68 mg, 62% yield), mp 286–287 °C. IR (KBr) 3036, 2945, 1593, 1533, 1481, 1442, 1391, 1356, 1183, 1136, 858, 734, 697 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.94 (d, *J* = 8.3 Hz, 1H), 7.89 (d, *J* = 1.6 Hz, 1H), 7.75 (dd, *J* = 8.3, 1.8 Hz, 1H), 7.37 (dt, *J* = 5.7, 2.1 Hz, 2H), 7.31–7.27 (m, 2H), 7.25 (d, *J* = 3.6 Hz, 1H), 2.73 (t, *J* = 6.0 Hz, 2H), 2.12 (t, *J* = 6.0 Hz, 2H), 1.93–1.76 (m, 4H). ¹³C NMR (75 MHz, CDCl₃) δ 149.4, 147.3, 144.7, 136.1, 135.6, 133.4, 130.6, 128.5, 127.5, 126.6, 125.3, 124.1, 123.7, 123.3, 119.8, 119.2, 25.0, 24.7, 22.4, 22.0. HRMS (ESI) calcd. for C₂₂H₁₆F₃N₃O₂S [MH⁺]: 444.0988; Found: 444.1002.

3-Methyl-5-(4-nitrophenyl)-6-phenylimidazo[2,1-b]thiazole (3da)

Yellow solid (49 mg, 58% yield), mp 230 °C. IR (KBr) 3087, 1598, 1516, 1480, 1441, 1344, 852, 735, 702 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.30 (d, *J* = 8.7 Hz, 2H), 7.64 (d, *J* = 8.7 Hz, 2H), 7.40 (dd, *J* = 6.8, 2.6 Hz, 2H), 7.27–7.21 (m, 3H), 6.42 (s, 1H), 1.96 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 150.7, 148.0, 144.8, 137.3, 133.7, 132.8, 129.1, 128.3, 127.4, 123.6, 120.9, 108.1, 15.5. HRMS (ESI) calcd. for C₁₈H₁₃N₃O₂S [MH⁺]: 336.0801; Found: 336.0806.

5-(3,5-Bis(trifluoromethyl)phenyl)-3-methyl-6-phenylimidazo[2,1-b]thiazole (3db)

White solid (44 mg, 41% yield), mp 176-178 °C. IR (KBr) 3061, 1603, 1543, 1472, 1443, 1342, 1280, 1171, 1134, 847, 807, 738, 708 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.98 (s, 1H), 7.94 (s, 2H), 7.41 (dd, *J* = 7.7, 1.8 Hz, 2H), 7.30–7.18 (m, 3H), 6.43 (s, 1H), 1.91 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 150.8, 145.1, 133.4, 132.8, 132.0, 128.9, 128.4, 127.5, 127.2, 124.7, 122.5, 121.1, 119.9, 108.4, 15.4. HRMS (ESI) calcd. for C₂₀H₁₂F₆N₂S [MH⁺]: 427.0698; Found: 427.0713.

3-Methyl-5-(4-nitro-3-(trifluoromethyl)phenyl)-6-phenylimidazo[2,1-b]thiazole (3dc)

Orange solid (61 mg, 61% yield), mp 188-189 °C. IR (KBr) 3046, 1593, 1537, 1480, 1443, 1356, 1185, 1140, 861, 831, 723, 700 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 7.96 (d, *J* = 8.0 Hz, 1H), 7.92 (s, 1H), 7.78 (d, *J* = 9.5 Hz, 1H), 7.38 (dd, *J* = 7.3, 1.8 Hz, 2H), 7.31–7.23 (m, 3H), 6.47 (s, 1H), 2.00 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 151.3, 147.4, 145.7, 136.0, 135.7, 133.2, 130.9, 128.9, 128.5, 127.6, 125.3, 123.4, 119.8, 119.5, 109.9, 108.7, 15.7. HRMS (ESI) calcd. for C₁₉H₁₂F₃N₃O₂S [MH⁺]: 404.0675; Found: 404.0692.

3-Methyl-2,5-bis(3-nitrophenyl)-6-phenylimidazo[2,1-b]thiazole (3dd)

White solid (59 mg, 86% yield), mp 207-208 °C. IR (KBr) 3082, 1601, 1528, 1481, 1442, 1347, 869, 807, 753, 736, 706 cm⁻¹. ¹H NMR (300 MHz, CDCl₃) δ 8.39 (ddd, *J* = 9.3, 6.0, 2.1 Hz, 2H), 8.28 (ddd, *J* = 6.8, 3.2, 1.4 Hz, 2H), 7.87–7.82 (m, 1H), 7.79–7.75 (m, 1H), 7.67 (td, *J* = 7.8, 4.4 Hz, 2H), 7.47–7.42 (m, 2H), 7.28 (dd, *J* = 4.2, 1.4 Hz, 1H), 7.25–7.22 (m, 2H), 1.99 (s, 3H). ¹³C NMR (75 MHz, CDCl₃) δ 148.4, 148.1, 144.7, 138.0, 135.3, 133.4, 133.3, 132.2, 130.1, 129.7, 128.4, 127.5, 127.3, 126.6, 126.0, 124.2, 124.1, 123.4, 122.1, 120.8, 13.8. HRMS (ESI) calcd. for C₂₄H₁₆N₄O₄S [MH⁺]: 457.0965; Found: 457.0981.

2. Crystal data and structure refinement for 3aa

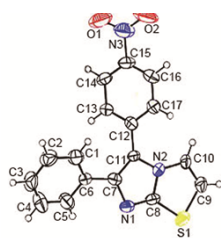


Figure S1. Representation ORTEP of **3aa**

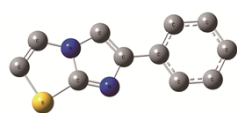
Compound	3aa
Empirical formula	C ₁₇ H ₁₁ N ₃ O ₂ S
Formula weight (g.mol ⁻¹)	321.52
Temperature (K)	296.24(11)
Crystal system	Trigonal
Space group	<i>P</i> 3 ₂
<i>a</i> (Å)	18.3921(7)
<i>b</i> (Å)	18.3921(7)
<i>c</i> (Å)	23.2883(17)
<i>α</i> (deg)	90.00
<i>β</i> (deg)	90.00
<i>γ</i> (deg)	120.00
Volume (Å ³)	6822.3(6)
<i>Z</i>	18
ρ_{calcd} (g mm ⁻³)	1409
μ (mm ⁻¹)	0.226
<i>F</i> (000)	2991.0
Crystal size (mm ³)	0.21 × 0.12 × 0.08
Theta range for data collection (deg)	5.84 to 52.04
Index ranges	-17 ≤ <i>h</i> ≤ 22, -17 ≤ <i>k</i> ≤ 22, -28 ≤ <i>l</i> ≤ 16
Reflections collected	18450

Independent reflections	11422 [R(int) = 0.0495]
Data/restraints/parameters	11422/91/1244
Goodness-of-fit on F^2	1.104
Final R indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0619$, $wR_2 = 0.1242$
Final R indexes [all data]	$R_1 = 0.1152$, $wR_2 = 0.1454$
Largest diff. peak/hole (e. \AA^{-3})	0.24/-0.26
Flack parameter	0.01(9)
CCDC deposition number:	942540

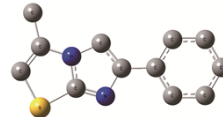
3. Computational Details

Geometries, energies, and first- and second-energy derivatives of all of the stationary points found here were fully optimized by hybrid density functional theory (DFT) using the GAUSSIAN 09 program suite.¹ For the DFT calculations, we used the hybrid gradient-corrected exchange functional of Lee, Yang, and Parr.^{2, 3} The 6-31G⁴ basis set with polarization (d and p) were selected for all the atoms except Palladium, for which the Stuttgart-Dresden effective core potential⁵ was utilized to accurately account for relativistic effects and to substantially reduce the number of electrons in the system. Vibrational frequency calculations done at the B3LYP /6-31G (d, p) level of theory were used to characterize all of the stationary points as either minima (the number of imaginary frequencies (NIMAG=0) or transition states (NIMAG=1)). The relative energies are, thus, corrected for the vibrational zero-point energies (ZPE, not scaled). To minimize the computation times, the Pd catalyst was modeled with the PMe₃ to replace PPh₃ ligand, as well as the acetate base (Figure S2, A and B).⁶

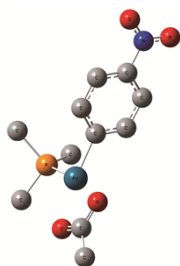
Figure S2. The optimized structures of substrates (1a, 1d) and [Pd(PMe₃)(PhNO₂)(OAc)] catalyst.



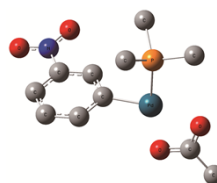
1a



1d

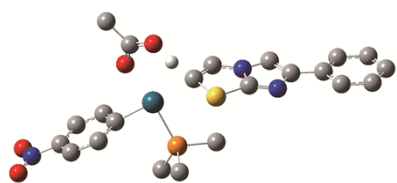


[Pd(PMe₃)(*p*-NO₂Ph)(OAc)] catalyst (A)

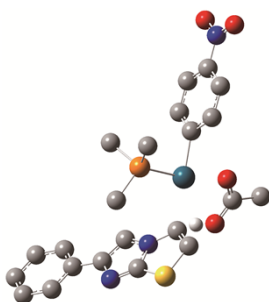


[Pd(PMe₃)(*m*-NO₂Ph)(OAc)] catalyst (B)

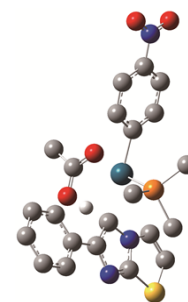
Figure S3. CMD TS structures at different sites (C2, C3, C5 of 1a and C2, C5 of 1d).



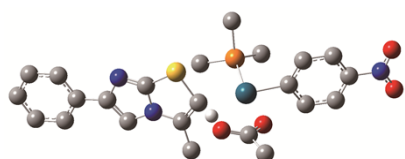
TS-2a (C)



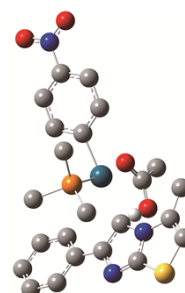
TS-3a (D)



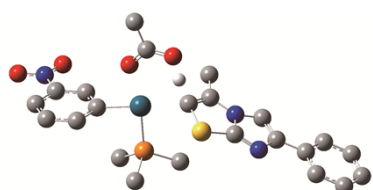
TS-1a (E)



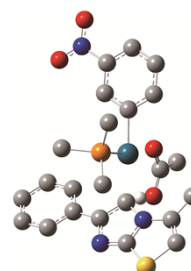
TS-2da (F)



TS-1da (G)

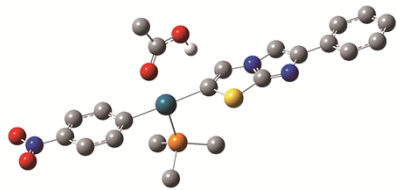


TS-2db (H)

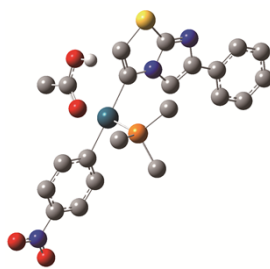


TS-1db (I)

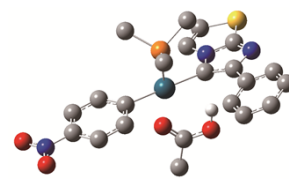
Figure S4. CMD intermediates structures at different sites (C2, C3, C5 of 1a and C2, C5 of 1d).



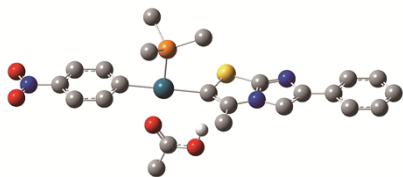
I-2a + HOAc (J)



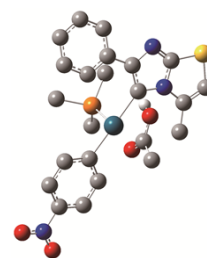
I-3a + HOAc (K)



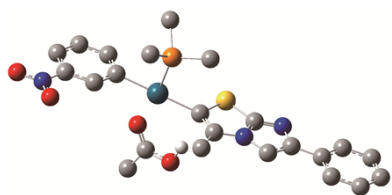
I-1a + HOAc (L)



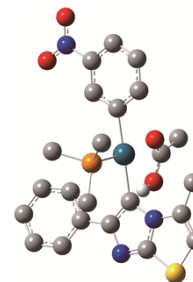
I-2da + HOAc (M)



I-1da + HOAc (N)



I-2db + HOAc (O)



I-1db + HOAc (P)

Sum of electronic and zero-point Energies (E, Hartree), Sum of electronic and thermal Free Energies (G, Hartree) and Cartesian coordinates of all geometries for CMD transition states and

intermediates with the [Pd(PMe₃)(PhNO₂)(OAc)] catalyst.

1a

E= -931.509599

G= -931.547501

C	-1.72921000	-0.49644500	-0.00015300
C	-3.07744800	1.40844500	0.00078500
C	-0.47947000	1.32563300	0.00067400
C	0.29380800	0.17560600	0.00007400
N	-1.79083800	0.88429900	0.00075900
C	-4.02277200	0.44286100	0.00015800
N	-0.50739700	-0.96081200	-0.00045400
C	1.75873200	0.06140700	-0.00004300
C	2.58633400	1.19685600	-0.00105000
C	2.36063300	-1.20741000	0.00091100
C	3.97278200	1.06721100	-0.00099700
H	2.14614500	2.18997400	-0.00201400
C	3.74791400	-1.33391100	0.00091900
H	1.72196100	-2.08351600	0.00163800
C	4.56143000	-0.19936600	-0.00000400
H	4.59547200	1.95737300	-0.00179100
H	4.19567800	-2.32371900	0.00167200
H	5.64282300	-0.29965800	0.00001700
H	-5.09300500	0.58329500	0.00012400
H	-3.23240000	2.47791100	0.00148300
H	-0.23013600	2.37382800	0.00160300
S	-3.34345600	-1.18657600	-0.00078300

1d

E= -970.807193

G= -970.846717

C	-1.41742000	-0.86142700	-0.00039600
C	-2.94718900	0.91972800	0.00071500
C	-0.35116400	1.07302300	-0.00000300
C	0.53090200	0.00371700	-0.00017000
N	-1.61344800	0.50496600	0.00026900
C	-3.78469400	-0.14491700	0.00056900
N	-0.15564100	-1.20490200	-0.00062800
C	1.99989000	0.03316000	-0.00015800
C	2.71315400	1.24383900	-0.00083100
C	2.72327200	-1.17061800	0.00051300
C	4.10566900	1.25030100	-0.00075500
H	2.17818000	2.18935700	-0.00148800
C	4.11627600	-1.16101600	0.00055500
H	2.17330800	-2.10497900	0.00099400
C	4.81537400	0.04742200	-0.00005800
H	4.63833500	2.19714000	-0.00128400
H	4.65853000	-2.10243000	0.00108500
H	5.90141300	0.05325300	-0.00001800
H	-4.86385900	-0.11040200	0.00094000

H	-0.20279300	2.14003400	0.00038500
S	-2.95532900	-1.70431200	-0.00069900
C	-3.28613400	2.37394700	0.00140400
H	-2.87634000	2.87558700	0.88602200
H	-2.87661300	2.87638100	-0.88289200
H	-4.36889300	2.51163900	0.00163800

[Pd(PMe₃)(*p*-NO₂Ph)(OAc)] catalyst (A)

E= -1253.477185

G= -1253.532074

Pd	-1.25875400	-0.26782800	-0.00092000
P	-1.31623800	1.98684400	-0.00004600
C	-3.06155400	2.57007700	-0.00109800
H	-3.57357900	2.17781700	0.88079200
H	-3.11204900	3.66355900	-0.00092300
H	-3.57233300	2.17816600	-0.88386300
C	-0.55803800	2.83383000	-1.44712700
H	-0.67899800	3.91887500	-1.36924100
H	0.50512100	2.58856000	-1.49628700
H	-1.03612400	2.48381800	-2.36564300
C	-0.55999300	2.83316700	1.44845000
H	-0.68141100	3.91820200	1.37117800
H	-1.03887000	2.48228100	2.36621800
H	0.50325000	2.58845900	1.49853700
C	0.73613200	-0.20124000	-0.00004200
C	1.45437500	-0.25125600	-1.20930400
C	1.45432200	-0.24588300	1.20945600
C	2.84501300	-0.34994800	-1.21730400
H	0.92557900	-0.22861900	-2.15800000
C	2.84496700	-0.34462600	1.21794800
H	0.92555600	-0.21882400	2.15806100
C	3.52339600	-0.39038800	0.00043600
H	3.40860600	-0.39623500	-2.14139200
H	3.40853400	-0.38687100	2.14224600
N	4.98673400	-0.47985700	0.00067100
O	5.56063000	-0.51049800	1.09082600
O	5.56067500	-0.51537200	-1.08930700
C	-2.95078100	-2.12951000	-0.00353200
O	-3.34481900	-0.91480100	-0.00303700
O	-1.70104500	-2.38742000	-0.00387500
C	-3.94626300	-3.26039600	0.00715900
H	-3.70999400	-3.96546100	-0.79437900
H	-3.86474400	-3.80336600	0.95409700
H	-4.96242200	-2.88216100	-0.11021200
Pd	0.57250009	3.99335237	3.12376829
P	0.51501609	6.24802437	3.12464229
C	-1.23029991	6.83125737	3.12359029
H	-1.74232491	6.43899737	4.00548029
H	-1.28079491	7.92473937	3.12376529
H	-1.74107891	6.43934637	2.24082529
C	1.27321609	7.09501037	1.67756129

H	1.15225609	8.18005537	1.75544729
H	2.33637509	6.84974037	1.62840129
H	0.79513009	6.74499837	0.75904529
C	1.27126109	7.09434737	4.57313829
H	1.14984309	8.17938237	4.49586629
H	0.79238409	6.74346137	5.49090629
H	2.33450409	6.84963937	4.62322529
C	2.56738609	4.05994037	3.12464629
C	3.28562909	4.00992437	1.91538429
C	3.28557609	4.01529737	4.33414429
C	4.67626709	3.91123237	1.90738429
H	2.75683309	4.03256137	0.96668829
C	4.67622109	3.91655437	4.34263629
H	2.75681009	4.04235637	5.28274929
C	5.35465009	3.87079237	3.12512429
H	5.23986009	3.86494537	0.98329629
H	5.23978809	3.87430937	5.26693429
N	6.81798809	3.78132337	3.12535929
O	7.39188409	3.75068237	4.21551429
O	7.39192909	3.74580837	2.03538129
C	-1.11952691	2.13167037	3.12115629
O	-1.51356491	3.34637937	3.12165129
O	0.13020909	1.87376037	3.12081329
C	-2.11500891	1.00078437	3.13184729
H	-1.87873991	0.29571937	2.33030929
H	-2.03348991	0.45781437	4.07878529
H	-3.13116791	1.37901937	3.01447629

[Pd(PMe₃)(*m*-NO₂Ph)(OAc)] catalyst (B)

E= -1253.476559

G= -1253.530372

Pd	1.14412800	-0.22453300	0.04551900
P	1.00505500	2.02635400	0.02564500
C	2.64520800	2.75491600	-0.38171500
H	2.96317600	2.39766300	-1.36407600
H	2.60206800	3.84871300	-0.38430000
H	3.38251600	2.41705200	0.35034700
C	0.53690000	2.82389800	1.61679000
H	0.53148700	3.91432900	1.52258900
H	-0.45567700	2.47853200	1.91454200
H	1.25018400	2.53256300	2.39208300
C	-0.13715200	2.78675300	-1.20067100
H	-0.08001700	3.87886600	-1.15661200
H	0.13184100	2.45267000	-2.20605200
H	-1.16198500	2.46974100	-0.99596000
C	-0.78472400	-0.33899800	0.56112000
C	-1.13072800	-0.67934000	1.88140400
C	-1.80834300	-0.25181200	-0.39087700
C	-2.45871900	-0.93895400	2.23968000
H	-0.35563300	-0.76272000	2.63852700
C	-3.12695900	-0.51195200	-0.01080100

H	-1.60975400	-0.00282000	-1.42617900
C	-3.47702400	-0.85784100	1.29237800
H	-2.69836800	-1.20950600	3.26412700
C	2.92929200	-1.94964400	-0.36174000
O	3.20733100	-0.70911800	-0.48297400
O	1.75191900	-2.30226400	-0.01913700
C	3.97290900	-2.99702600	-0.65143400
H	3.86517900	-3.83627300	0.03900700
H	3.82107800	-3.37800900	-1.66718600
H	4.97445700	-2.56932700	-0.58430000
H	-4.51330700	-1.05196900	1.53750800
N	-4.18924000	-0.40533200	-1.02531800
O	-5.33750800	-0.69201800	-0.68638200
O	-3.87077000	-0.02772200	-2.15403100

TS-2a (C)

E= -2184.951392

G= -2185.022488

C	3.23033900	0.44402400	0.83487400
C	1.66383300	1.11567100	-0.75424100
C	4.13573200	0.46202300	-1.19088700
C	5.04637400	0.06365900	-0.22631600
N	2.95731800	0.70490900	-0.50340100
C	0.84631100	1.18156100	0.34801800
N	4.46202600	0.05611100	1.03787200
C	6.45421700	-0.31567900	-0.40308800
C	7.04468800	-0.38355500	-1.67680700
C	7.24142500	-0.61875300	0.72015400
C	8.38318200	-0.73992700	-1.82191900
H	6.45557900	-0.15977300	-2.56184500
C	8.58007300	-0.97587600	0.57154300
H	6.78475900	-0.56619200	1.70223400
C	9.15813200	-1.03776500	-0.69810500
H	8.82240000	-0.78673500	-2.81449700
H	9.17479800	-1.20543200	1.45132800
H	10.20193500	-1.31556400	-0.81242200
H	0.13704400	2.30206700	0.52330400
H	-1.49968600	-4.06996200	-0.08942200
C	-1.87636400	-3.06768500	-0.31645600
P	-0.76539400	-1.79655200	0.42301600
H	-2.88723100	-2.95810600	0.07881800
H	-1.91833300	-2.93560900	-1.40037700
Pd	-1.29559300	0.40213600	0.05386600
C	0.88464900	-2.34000600	-0.19098300
C	-0.73824000	-2.25856600	2.20654400
C	-3.22445800	-0.16763900	-0.13390600
O	-2.05695000	2.33802200	-0.41305500
H	1.67827700	-1.77803400	0.30243200
H	0.94980100	-2.17203900	-1.26867200
H	1.02431700	-3.40617200	0.01351100
H	-0.47328900	-3.31398000	2.32580900

H	-0.00622500	-1.64004500	2.73010400
H	-1.72468900	-2.08575300	2.64420500
C	-4.03146100	-0.38697600	0.99568800
C	-3.81734500	-0.22914000	-1.40658100
C	-1.51816700	3.40114100	0.02053200
C	-5.39264500	-0.66442500	0.86625200
H	-3.60367900	-0.33150900	1.99313400
C	-5.17483500	-0.50772800	-1.55427700
H	-3.22097100	-0.04420500	-2.29525000
O	-0.39997600	3.44305800	0.62747500
C	-2.26803300	4.69939000	-0.17604700
H	-6.02663000	-0.83130000	1.72881300
C	-5.94521700	-0.72700900	-0.41203800
H	-5.64497000	-0.55583300	-2.52918700
H	1.37911900	1.37938000	-1.76556300
N	-7.37227000	-1.03078600	-0.55913000
O	-7.83469100	-1.08013400	-1.70021000
O	-8.02781300	-1.22263600	0.46665300
H	4.21432700	0.60146800	-2.25654700
S	1.79942400	0.72951200	1.80094000
H	-1.58075200	5.54609700	-0.16508000
H	-2.97960500	4.81763300	0.64833300
H	-2.83610300	4.66886800	-1.10730800

TS-3a (D)

E= -2184.950655

G= -2185.020656

C	-3.28926400	1.48897400	-0.84543200
C	-1.06458300	1.79297700	-0.06039700
C	-2.80164600	0.02640800	0.72643100
C	-4.09173500	-0.15585600	0.24572200
N	-2.28638300	1.09100800	0.01298500
C	-1.18639900	2.76985800	-1.01514900
N	-4.37985800	0.77077800	-0.74977300
C	-5.08914500	-1.15305400	0.65947600
C	-4.83158200	-2.06547300	1.69713900
C	-6.33391500	-1.20881200	0.01077800
C	-5.78723700	-3.00755700	2.07083900
H	-3.88094700	-2.03618000	2.22262000
C	-7.28821000	-2.15174900	0.38745800
H	-6.53469900	-0.50157300	-0.78640700
C	-7.02099200	-3.05646000	1.41720600
H	-5.56958600	-3.70292600	2.87680000
H	-8.24577900	-2.17959400	-0.12529400
H	-7.76626300	-3.79039500	1.70994200
H	-0.43392300	3.50337000	-1.27078500
H	1.19922700	-1.57676900	-3.90644400
C	1.50886500	-0.81689200	-3.18219200
P	0.39035100	-0.83614900	-1.71756400
H	1.46743000	0.16633300	-3.65863000
H	2.53686300	-1.00715300	-2.86939000

Pd	0.96579600	0.69787900	-0.11259500
C	0.42490900	-2.59409700	-1.16875400
C	-1.27208200	-0.69594000	-2.49254800
C	2.76966500	-0.21521800	-0.03962800
O	1.83904500	2.02769700	1.31136200
H	-0.30297900	-2.73872500	-0.36621100
H	1.41725700	-2.84759100	-0.79210200
H	0.17060500	-3.25605900	-2.00242500
H	-1.36254000	-1.43364000	-3.29602100
H	-2.05186300	-0.87979600	-1.75108700
H	-1.41110600	0.30433500	-2.90822300
C	3.85507400	0.31120300	-0.76095500
C	3.00603100	-1.27545500	0.85186100
C	1.13689000	2.57805900	2.21224000
C	5.14102500	-0.20487200	-0.60512600
H	3.70551600	1.14357200	-1.44267700
C	4.28651200	-1.80247300	1.02147300
H	2.18981700	-1.69179100	1.43549300
O	-0.13665600	2.54344700	2.24645200
C	1.85443100	3.29925300	3.32997000
H	5.98660900	0.19464000	-1.15205400
C	5.33798600	-1.26091400	0.28395600
H	4.48287000	-2.61620800	1.70923900
H	-0.52457600	2.09993800	1.12986800
N	6.68635800	-1.81522300	0.44881100
O	6.83086600	-2.74692500	1.24191900
O	7.59648200	-1.31893700	-0.21686700
H	-2.23016900	-0.46795900	1.49524100
S	-2.74857700	2.83767300	-1.82926000
H	2.00133000	2.59734500	4.15817300
H	2.83389700	3.64143300	2.99377600
H	1.25203900	4.13278200	3.69429400

TS-1a (E)

E= -2184.957357

G= -2185.026593

C	3.77342300	-1.36199300	-0.33347200
C	2.26131200	-2.99293100	0.31889000
C	1.90174700	-0.41620200	0.50983100
C	2.88776100	0.51863000	0.09770500
N	2.54543500	-1.64045700	0.20536200
C	3.26802300	-3.77229000	-0.13935200
N	4.02084500	-0.07065300	-0.42575000
C	2.81879200	1.98472900	0.20554900
C	1.78385900	2.62396400	0.91380500
C	3.80738100	2.78041200	-0.40097900
C	1.73644200	4.01378800	1.00313400
H	1.02325500	2.02828100	1.40794100
C	3.75442100	4.17009600	-0.31160800
H	4.61431900	2.28885600	-0.93317200
C	2.71888100	4.79420200	0.38823200

H	0.93385200	4.48818900	1.56105700
H	4.52675300	4.76816300	-0.78730300
H	2.68048000	5.87739600	0.45914700
H	3.30422500	-4.85113000	-0.15797100
H	-1.22475100	-0.33022500	-4.18724400
C	-1.45558200	-0.54195000	-3.13832600
P	-0.07780500	0.03831800	-2.05928200
H	-1.59709800	-1.61819500	-3.01159900
H	-2.38402700	-0.04206100	-2.85853200
Pd	-0.30166000	-0.29868300	0.18489700
C	0.07651200	1.81759500	-2.50838100
C	1.38474800	-0.73570900	-2.86776900
C	-2.31792500	-0.17037100	-0.04829300
O	-0.78144700	-0.63292300	2.25184100
H	0.93167700	2.25496400	-1.98880300
H	-0.82783200	2.34949300	-2.20237600
H	0.20804300	1.92838200	-3.58958800
H	1.36441800	-0.53460900	-3.94361400
H	2.30732800	-0.33459600	-2.44511000
H	1.36645200	-1.81683800	-2.70875900
C	-3.10542400	-1.33642100	-0.05303000
C	-2.97661700	1.07246300	-0.08225400
C	0.05433000	-0.56103400	3.19515700
C	-4.49689900	-1.27365100	-0.09198600
H	-2.63029400	-2.31295400	-0.01331300
C	-4.36854100	1.15738500	-0.12077600
H	-2.40173200	1.99487200	-0.06576800
O	1.30775200	-0.35736100	3.03832700
C	-0.44429400	-0.70053600	4.61551600
H	-5.11021200	-2.16681900	-0.09218600
C	-5.11220800	-0.02195000	-0.13008600
H	-4.88352300	2.11041400	-0.14324500
H	1.31879400	-3.31342800	0.74012700
N	-6.57462200	0.05525600	-0.18184300
O	-7.09148500	1.17381300	-0.21970400
O	-7.20738700	-1.00266800	-0.18746600
H	1.55393600	-0.33879600	1.84410400
S	4.63601200	-2.82870500	-0.73630000
H	-0.44018800	0.28764900	5.08743900
H	-1.45914000	-1.09780300	4.62776600
H	0.23056200	-1.34056400	5.18836000

TS-2da (F)

E= -2224.248639

G= -2224.321098

C	-3.17113100	0.29812300	-0.90020000
C	-1.67834700	1.06970900	0.73524700
C	-4.17538100	0.45748300	1.07147000
C	-5.04134800	0.00144400	0.09134000
N	-2.96130900	0.64486900	0.42818300
C	-0.81260600	1.05775400	-0.34002400

N	-4.39505600	-0.09499900	-1.13832600
C	-6.46019400	-0.35482100	0.22222500
C	-7.11994700	-0.31059000	1.46261500
C	-7.18823600	-0.74869700	-0.91273400
C	-8.46755300	-0.64717300	1.56386200
H	-6.57830600	-0.01285100	2.35616100
C	-8.53624100	-1.08564500	-0.80803200
H	-6.67840900	-0.78189500	-1.86915500
C	-9.18304700	-1.03641600	0.42860000
H	-8.96065200	-0.60624800	2.53109300
H	-9.08440900	-1.38663800	-1.69648200
H	-10.23412100	-1.29840600	0.50857100
H	-0.17965600	2.21623500	-0.53903900
H	1.56499000	-4.05587700	0.61584100
C	1.93431800	-3.03070200	0.71789600
P	0.82528200	-1.86765500	-0.18505100
H	2.94791900	-2.96520300	0.32011400
H	1.96660900	-2.76382300	1.77717500
Pd	1.33965000	0.36064900	-0.07420500
C	-0.83187600	-2.36750100	0.44732700
C	0.84666900	-2.52259700	-1.90645600
C	3.28386600	-0.18412700	0.07981100
O	2.12688400	2.33776900	0.08995600
H	-1.61986800	-1.86718200	-0.11643500
H	-0.92169800	-2.09490800	1.50177200
H	-0.95637000	-3.45053400	0.34840200
H	0.61279100	-3.59182500	-1.91539200
H	0.10974500	-1.98458400	-2.50685500
H	1.83757300	-2.36765400	-2.34032100
C	4.04676900	-0.48376300	-1.06223900
C	3.93181800	-0.14670100	1.32694500
C	1.50526000	3.37288200	-0.29626300
C	5.41458400	-0.74271800	-0.97042200
H	3.57879900	-0.50471000	-2.04290100
C	5.29700900	-0.40355100	1.43803300
H	3.37179900	0.09740200	2.22523200
O	0.29817600	3.37981800	-0.69952100
C	2.25994900	4.68377900	-0.30335800
H	6.01321500	-0.97083100	-1.84417000
C	6.02120800	-0.70419900	0.28408600
H	5.80790500	-0.37467700	2.39300900
N	7.45578900	-0.98665100	0.39317300
O	7.96653500	-0.94405700	1.51387200
O	8.06965100	-1.25369000	-0.64158300
H	-4.30663800	0.66436600	2.12058100
S	-1.69500700	0.51347200	-1.81026400
C	-1.37791900	1.53573200	2.12387000
H	-2.03813200	2.36419100	2.40844400
H	-1.52836900	0.73137200	2.85509900
H	-0.34222900	1.87153300	2.19189000
H	3.00270000	4.69668400	0.49576500
H	2.78895300	4.77354100	-1.25841600

H 1.57112900 5.52447100 -0.21116300

TS-1da (G)

E= -2224.25381

G= -2224.324779

C	3.86676700	-0.96689100	-0.40552900
C	2.57550600	-2.80197300	0.22385000
C	1.90963700	-0.28376900	0.49640100
C	2.77214300	0.77588600	0.11057000
N	2.69074200	-1.41261800	0.13749800
C	3.66909600	-3.41762500	-0.29094000
N	3.95671800	0.34679700	-0.45207500
C	2.53005700	2.22081000	0.26071400
C	1.46092600	2.71811300	1.02908800
C	3.38482800	3.14254900	-0.37090400
C	1.24773100	4.09013500	1.14956000
H	0.80219500	2.02707300	1.54433300
C	3.16700000	4.51387000	-0.24988800
H	4.22036700	2.76272000	-0.94852300
C	2.09671600	4.99542800	0.50769100
H	0.42057100	4.45289900	1.75352700
H	3.83778700	5.20941900	-0.74671100
H	1.92933400	6.06441100	0.60291000
H	3.84566500	-4.48190800	-0.33922500
H	-1.17935600	-0.44654500	-4.22386000
C	-1.40516600	-0.65063700	-3.17237900
P	-0.07841400	0.04289700	-2.09594600
H	-1.47534800	-1.73128400	-3.02429100
H	-2.36775400	-0.20892100	-2.91091500
Pd	-0.29890500	-0.25785700	0.15134500
C	-0.04747700	1.82276600	-2.56649200
C	1.44083200	-0.63149000	-2.88783000
C	-2.31813300	-0.18469200	-0.09690500
O	-0.79644000	-0.49422500	2.23798500
H	0.77277300	2.32454900	-2.04839500
H	-0.98795700	2.29304000	-2.26964300
H	0.08169400	1.93062100	-3.64837100
H	1.40557700	-0.45388300	-3.96737800
H	2.32704100	-0.14772000	-2.47408500
H	1.51139100	-1.70694400	-2.70713600
C	-3.07158800	-1.37281100	-0.12996100
C	-3.01350400	1.03842100	-0.10233200
C	0.03767700	-0.51897800	3.18063600
C	-4.46446500	-1.35082300	-0.16419200
H	-2.56800200	-2.33598800	-0.11796500
C	-4.40739100	1.08285300	-0.13736600
H	-2.46600300	1.97660400	-0.06409300
O	1.30954500	-0.43797700	3.02592800
C	-0.46707700	-0.62700400	4.60070400
H	-5.05116000	-2.26147900	-0.18460600
C	-5.11628900	-0.11728100	-0.17143800

H	-4.95026600	2.02055700	-0.13725900
N	-6.58052700	-0.08243900	-0.21654900
O	-7.13058100	1.02071600	-0.22584500
O	-7.18156600	-1.15839900	-0.24509000
H	1.55114100	-0.33454700	1.86603400
S	4.89656700	-2.29410400	-0.88024300
C	1.38071300	-3.43446800	0.85950400
H	1.31621100	-3.15563600	1.91687900
H	0.45354100	-3.10018700	0.38018900
H	1.44441300	-4.52238700	0.78949200
H	-1.50805600	-0.94971800	4.61191400
H	-0.39238500	0.35703900	5.07558900
H	0.15993200	-1.31556500	5.17148400

TS-2db (H)

E= -2224.248533

G= -2224.321527

C	-3.09373400	0.49826500	-0.80974800
C	-1.48706600	0.95547700	0.83592300
C	-3.97547700	0.33891400	1.21991100
C	-4.90858700	0.06528100	0.23352000
N	-2.79755600	0.61480100	0.54225100
C	-0.68633700	1.11012400	-0.27819400
N	-4.33850100	0.16635400	-1.03298200
C	-6.32470500	-0.29090600	0.39145300
C	-6.92094600	-0.39747100	1.65986400
C	-7.11451400	-0.53238700	-0.74491700
C	-8.26607500	-0.73494200	1.78751800
H	-6.33226600	-0.21419000	2.55443500
C	-8.46000000	-0.87023400	-0.61387200
H	-6.65401900	-0.44775800	-1.72296300
C	-9.04290800	-0.97338000	0.65087200
H	-8.70959100	-0.81136800	2.77635900
H	-9.05626600	-1.05267500	-1.50362200
H	-10.09209300	-1.23586500	0.75142000
H	-0.04203700	2.27043100	-0.29301800
H	1.52688200	-4.13161400	-0.01567300
C	1.93553400	-3.13190400	0.16226200
P	0.84489700	-1.85873300	-0.60523000
H	2.94058000	-3.06699100	-0.25641600
H	2.00411900	-2.95897400	1.23937600
Pd	1.45131300	0.32957500	-0.33312500
C	-0.81176200	-2.36392300	0.02357500
C	0.79375000	-2.36121700	-2.37699300
C	3.37856600	-0.29497600	-0.44660100
O	2.35117400	2.24769700	-0.10379300
H	-1.59673700	-1.80026500	-0.48165900
H	-0.87394600	-2.17439600	1.09773600
H	-0.96735400	-3.43191400	-0.15885600
H	0.51258200	-3.41478000	-2.47207200
H	0.06530200	-1.74230200	-2.90592600

H	1.77820800	-2.20898600	-2.82585100
C	4.03788600	-0.42469600	-1.67920600
C	4.12434500	-0.46634800	0.72578600
C	1.71738600	3.34464400	-0.15094700
C	5.40707800	-0.71606100	-1.74575100
H	3.48852500	-0.28353000	-2.60686300
C	5.48599100	-0.75996800	0.63865000
H	3.67891900	-0.36670600	1.70824700
O	0.45531000	3.44482100	-0.27349700
C	2.52477700	4.62273700	-0.08530700
H	5.89487500	-0.80487200	-2.71248200
C	6.14909300	-0.89028500	-0.58093600
H	-4.03759300	0.36406100	2.29513500
S	-1.66794300	0.83753600	-1.76136400
C	-1.09144200	1.17414300	2.26104100
H	-1.71328200	1.95021300	2.72371500
H	-1.21575700	0.25891200	2.85379400
H	-0.04603300	1.48031600	2.31871200
H	7.20697100	-1.11894100	-0.59582100
N	6.25230100	-0.94563500	1.88302400
O	7.45791300	-1.17638500	1.78514600
O	5.64460100	-0.86478600	2.95137400
H	3.40987100	4.47828600	0.53621700
H	1.91354100	5.44428500	0.29039500
H	2.85905000	4.87482600	-1.09759400

TS-1db (I)

E= -2224.253423

G= -2224.324379

C	3.91397300	-0.14800400	-0.43885800
C	3.14285100	-2.29755800	0.02530000
C	1.85097200	-0.06527900	0.48159000
C	2.40789000	1.20820700	0.19021000
N	2.89607500	-0.92327300	0.05020200
C	4.35453900	-2.56855800	-0.52120600
N	3.66154600	1.14375800	-0.38286400
C	1.80053200	2.52567800	0.44397900
C	0.62267600	2.66632400	1.20151100
C	2.40354100	3.68557100	-0.07571400
C	0.06069300	3.92292600	1.41917400
H	0.14939400	1.78829000	1.62851400
C	1.83800100	4.94045100	0.14303600
H	3.32026700	3.58202900	-0.64565200
C	0.66306000	5.06625700	0.88807400
H	-0.84769700	4.00900000	2.00879900
H	2.31797600	5.82415000	-0.26841000
H	0.22318300	6.04477000	1.05765300
H	4.79896600	-3.54426800	-0.65038700
H	-1.11529300	-0.70207500	-4.26097800
C	-1.26130000	-1.03461700	-3.22841500
P	-0.18010700	-0.06502800	-2.09192100

H	-1.01450000	-2.09705800	-3.15619700
H	-2.30728500	-0.90682800	-2.94686100
Pd	-0.28755700	-0.58648900	0.12400000
C	-0.65715100	1.67847500	-2.44060600
C	1.46285700	-0.22537200	-2.90707800
C	-2.27299400	-0.98888600	-0.13093400
O	-0.66598100	-1.15271500	2.17185600
H	-0.01818100	2.35232500	-1.86557500
H	-1.69503300	1.84240700	-2.14194300
H	-0.55311100	1.89674700	-3.50848900
H	1.37075700	-0.00317100	-3.97488600
H	2.17594300	0.46722200	-2.45699600
H	1.84061000	-1.24344200	-2.78571800
C	-2.73636300	-2.31649300	-0.14735700
C	-3.22826500	0.03525900	-0.15655100
C	0.14864200	-1.00569300	3.12066000
C	-4.10286900	-2.61711500	-0.18462300
H	-2.02289500	-3.13635900	-0.11727400
C	-4.58895500	-0.28197200	-0.19641100
H	-2.94707300	1.08164800	-0.13409300
O	1.34007500	-0.54708100	2.98962200
C	-0.29147500	-1.36223600	4.52169400
H	-4.42996600	-3.65333000	-0.19115800
C	-5.05060800	-1.59631300	-0.21149600
H	1.53489700	-0.29975500	1.84080800
S	5.24801000	-1.12362300	-1.00137900
C	2.15604400	-3.26365400	0.59504200
H	2.05248800	-3.11360400	1.67528500
H	1.16310300	-3.12092400	0.15354500
H	2.48221500	-4.29045300	0.41643000
H	-6.11461900	-1.79262900	-0.24332000
N	-5.57247300	0.81271800	-0.23371500
O	-6.76715700	0.51300500	-0.23105000
O	-5.14745700	1.96887400	-0.27140200
H	-0.55746900	-0.43991000	5.04917600
H	-1.16413700	-2.01488600	4.49228700
H	0.52891800	-1.83147000	5.06865100

I-2a + HOAc (J)

E= -2184.957925

G= -2185.029703

C	-3.26456400	0.06343700	-0.75762000
C	-1.75389600	0.01678000	1.02644600
C	-4.35801400	-0.00265600	1.16113900
C	-5.22721300	0.03037600	0.08040200
N	-3.08962000	0.01591700	0.61035300
C	-0.83341200	0.06794300	0.01694000
N	-4.52467700	0.07307900	-1.11733800
C	-6.69636800	0.02626200	0.09153000
C	-7.42642100	-0.01089600	1.29215600
C	-7.40455300	0.06232100	-1.12139700

C	-8.81936200	-0.01178400	1.28009800
H	-6.90374500	-0.03827500	2.24434600
C	-8.79789400	0.06129800	-1.13047200
H	-6.84123900	0.09201600	-2.04754600
C	-9.51354900	0.02429600	0.06824900
H	-9.36466100	-0.04024400	2.21957700
H	-9.32772300	0.09022500	-2.07879800
H	-10.59977700	0.02405900	0.05960700
H	-0.63552900	1.95586600	0.64402000
H	2.15749000	-4.07533700	1.54403300
C	2.15645600	-2.98157000	1.58575900
P	1.31968100	-2.28280200	0.10193000
H	3.18351400	-2.61483300	1.63341700
H	1.62952200	-2.65925100	2.48767100
Pd	1.28083500	-0.02566400	0.01388200
C	-0.30561100	-3.14469500	0.09661600
C	2.19919300	-3.06777600	-1.31254400
C	3.34267500	-0.06222800	0.01420700
O	1.54656200	2.15048000	-0.17145200
H	-0.87245600	-2.85371900	-0.79050000
H	-0.88361700	-2.85313900	0.97538300
H	-0.15489600	-4.22879700	0.09810500
H	2.20606000	-4.15669500	-1.20063600
H	1.69089900	-2.80840700	-2.24498500
H	3.22414800	-2.69564800	-1.36055400
C	4.06566000	0.00945400	-1.19274900
C	4.07581900	0.00897600	1.21496100
C	0.80930900	3.08334700	0.16902800
C	5.45301500	0.14959800	-1.21121500
H	3.53879800	-0.03227900	-2.14318400
C	5.46348000	0.15104100	1.22273600
H	3.55827800	-0.03543600	2.17062800
O	-0.39668100	2.92226800	0.67364600
C	1.22846000	4.51891400	0.02761500
H	6.01087700	0.20987200	-2.13815600
C	6.13592200	0.21545500	0.00310400
H	6.02904700	0.21177300	2.14496700
H	-1.54248800	-0.03319500	2.08795600
N	7.59519400	0.35611600	-0.00246100
O	8.17221700	0.41151500	1.08541800
O	8.16416900	0.40979800	-1.09439100
H	-4.51890200	-0.03707800	2.22641000
S	-1.69826700	0.11638500	-1.55015000
H	1.06499700	5.04792200	0.97024700
H	0.60331300	5.00087300	-0.73074100
H	2.27551000	4.57450700	-0.26596000

I-3a + HOAc (K)

E= -2184.959132

G= -2185.031156

C	3.41969900	-1.60122300	-0.07503000
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C	1.03560900	-1.62273100	-0.04001900
C	2.60136000	0.43851400	0.13107800
C	3.98719900	0.44829000	0.09997200
N	2.23513900	-0.89253200	0.01680000
C	1.34870300	-2.94809500	-0.15590800
N	4.48647400	-0.84314000	-0.03058300
C	4.89602000	1.59997000	0.18374600
C	4.41457200	2.90913700	0.35767600
C	6.28394400	1.40421700	0.08900600
C	5.29265800	3.98797100	0.43161100
H	3.34575800	3.08736900	0.44033200
C	7.16011200	2.48521200	0.16363600
H	6.65518000	0.39383600	-0.04245500
C	6.67112300	3.78218000	0.33440200
H	4.90004000	4.99204700	0.56747900
H	8.23051300	2.31372600	0.08840800
H	7.35542100	4.62376500	0.39281000
H	0.65248000	-3.76990500	-0.25707500
H	-2.02738600	-1.31478600	-4.26030500
C	-2.07892200	-1.47991100	-3.17950500
P	-0.82707200	-0.44729500	-2.31028600
H	-1.89267900	-2.53626100	-2.96942000
H	-3.07639300	-1.22216400	-2.81798600
Pd	-0.85548900	-0.67290800	-0.06113800
C	-1.16033500	1.25625500	-2.92373400
C	0.74910100	-0.87730200	-3.15622300
C	-2.72034200	0.20848600	-0.05559600
O	-1.07492800	-0.67618500	2.12441000
H	-0.38828100	1.93528900	-2.55223400
H	-2.12886300	1.59924700	-2.55694300
H	-1.15122000	1.27218900	-4.01806900
H	0.65762400	-0.71060200	-4.23417000
H	1.55649000	-0.25634000	-2.76059000
H	0.99985100	-1.92229100	-2.96475700
C	-3.89023100	-0.57000600	-0.15702400
C	-2.87821500	1.58343600	0.20799100
C	-0.57434500	-1.38454800	3.00598200
C	-5.16045300	-0.01578700	0.00259200
H	-3.81732100	-1.63768600	-0.35250700
C	-4.13674600	2.16179900	0.36866700
H	-2.00281600	2.22182700	0.30224600
O	0.30878300	-2.33612600	2.78165900
C	-0.93047100	-1.21443500	4.45566800
H	-6.06092600	-0.61423600	-0.06850000
C	-5.26603500	1.35014000	0.26063600
H	-4.26006300	3.21825800	0.57549900
H	0.56081100	-2.34740000	1.81981000
N	-6.59533900	1.94728200	0.42163300
O	-6.65926200	3.15763200	0.64514100
O	-7.57507600	1.20580200	0.32313100
H	1.86351200	1.21738400	0.23587800
S	3.09552500	-3.31527900	-0.21824300

H	-0.05568400	-0.84065800	4.99731200
H	-1.75620400	-0.51194600	4.55691800
H	-1.19378200	-2.18267000	4.88943200

I-1a + HOAc (L)

E= -2184.957536

G= -2185.027587

C	3.85740900	-1.38232300	-0.30994400
C	2.16262400	-2.96256300	-0.52666500
C	1.83509100	-0.45547400	0.09250700
C	2.90926200	0.44739100	0.20926300
N	2.50301600	-1.64404600	-0.25136600
C	3.24075800	-3.73145500	-0.79951000
N	4.15023800	-0.13747200	-0.03990200
C	2.85015100	1.88537800	0.52686600
C	1.67364300	2.50630800	0.98934900
C	3.99739800	2.68322500	0.36170400
C	1.64314800	3.87396500	1.26093400
H	0.77883600	1.90918000	1.14580700
C	3.96387500	4.04931500	0.63497500
H	4.91001400	2.20842200	0.01901500
C	2.78755000	4.65504300	1.08267200
H	0.72494800	4.32832700	1.62428500
H	4.86289100	4.64435100	0.49852500
H	2.76403700	5.71949300	1.29759200
H	3.24726300	-4.78331700	-1.04286400
H	-1.15264300	0.39527900	-4.31597900
C	-1.23479900	-0.13888200	-3.36409700
P	-0.18057000	0.66671700	-2.08545500
H	-0.90831800	-1.17246100	-3.50696300
H	-2.27499300	-0.14861200	-3.03490700
Pd	-0.27698200	-0.29198700	-0.03904900
C	-0.73006700	2.42253300	-2.10054600
C	1.46148800	0.73869900	-2.91267200
C	-2.33315000	-0.13812900	-0.12516100
O	-0.64407800	-1.24707300	1.91122800
H	-0.07950100	3.00704000	-1.44506400
H	-1.75513000	2.48552400	-1.73051400
H	-0.68071500	2.82791400	-3.11607700
H	1.35702000	1.18632600	-3.90634200
H	2.15171500	1.33317600	-2.31238200
H	1.87343200	-0.26830600	-3.00986800
C	-3.12134700	-1.23946200	-0.51628700
C	-3.01095300	1.00080900	0.35395600
C	0.11096400	-1.29033300	2.89376300
C	-4.51253100	-1.21905400	-0.43058000
H	-2.64330400	-2.14317000	-0.88763900
C	-4.40182600	1.04632900	0.45102300
H	-2.44668000	1.87384600	0.67398500
O	1.35833800	-0.88125900	2.88079000
C	-0.35425900	-1.81859800	4.22219400

H	-5.11813500	-2.06765000	-0.72593400
C	-5.13728800	-0.06909600	0.05257700
H	-4.92242200	1.91968300	0.82568700
H	1.12532300	-3.26680200	-0.50243900
N	-6.59930400	-0.03303000	0.14284300
O	-7.12520200	0.99597600	0.57234800
O	-7.22358500	-1.03348400	-0.21689400
H	1.60018800	-0.59672000	1.94347100
S	4.76006700	-2.83140300	-0.71860800
H	-1.36258300	-2.21986800	4.13243300
H	0.33635900	-2.58713700	4.57925900
H	-0.34320600	-1.00463700	4.95396500
C	5.76695757	7.35055642	1.92399643
C	4.07217257	5.77031642	1.70727543
C	3.74463957	8.27740542	2.32644743
C	4.81881057	9.18027042	2.44320343
N	4.41256457	7.08883342	1.98257443
C	5.15030657	5.00142442	1.43443043
N	6.05978657	8.59540742	2.19403843
C	4.75969957	10.61825742	2.76080643
C	3.58319157	11.23918742	3.22328943
C	5.90694657	11.41610442	2.59564443
C	3.55269657	12.60684442	3.49487443
H	2.68838457	10.64205942	3.37974743
C	5.87342357	12.78219442	2.86891543
H	6.81956257	10.94130142	2.25295543
C	4.69709857	13.38792242	3.31661243
H	2.63449657	13.06120642	3.85822543
H	6.77243957	13.37723042	2.73246543
H	4.67358557	14.45237242	3.53153243
H	5.15681157	3.94956242	1.19107643
H	0.75690557	9.12815842	-2.08203857
C	0.67474957	8.59399742	-1.13015657
P	1.72897857	9.39959642	0.14848543
H	1.00123057	7.56041842	-1.27302257
H	-0.36544443	8.58426742	-0.80096657
Pd	1.63256657	8.44089242	2.19489143
C	1.17948157	11.15541242	0.13339443
C	3.37103657	9.47157842	-0.67873157
C	-0.42360143	8.59475042	2.10877943
O	1.26547057	7.48580642	4.14516843
H	1.83004757	11.73991942	0.78887643
H	0.15441857	11.21840342	0.50342643
H	1.22883357	11.56079342	-0.88213657
H	3.26656857	9.91920542	-1.67240157
H	4.06126357	10.06605542	-0.07844157
H	3.78298057	8.46457342	-0.77592757
C	-1.21179843	7.49341742	1.71765343
C	-1.10140443	9.73368842	2.58789643
C	2.02051257	7.44254642	5.12770343
C	-2.60298243	7.51382542	1.80336043
H	-0.73375543	6.58970942	1.34630143

C	-2.49227743	9.77920842	2.68496343
H	-0.53713143	10.60672542	2.90792543
O	3.26788657	7.85162042	5.11473043
C	1.55528957	6.91428142	6.45613443
H	-3.20858643	6.66522942	1.50800643
C	-3.22773943	8.66378342	2.28651743
H	-3.01287343	10.65256242	3.05962743
H	3.03487157	5.46607742	1.73150143
N	-4.68975543	8.69984942	2.37678343
O	-5.21565343	9.72885542	2.80628843
O	-5.31403643	7.69939542	2.01704643
H	3.50973657	8.13615942	4.17741143
S	6.66961557	5.90147642	1.51533243
H	0.54696557	6.51301142	6.36637343
H	2.24590757	6.14574242	6.81319943
H	1.56634257	7.72824242	7.18790543

I-2da + HOAc (M)

E= -2224.253155

G= -2224.326593

C	-3.20683900	0.08022900	-0.83453500
C	-1.72345800	0.17046400	0.98901200
C	-4.32630900	0.07805200	1.07046300
C	-5.17987700	0.02739100	-0.02192300
N	-3.05006400	0.10895200	0.53558500
C	-0.79486400	0.20156200	-0.01895100
N	-4.46099100	0.03191100	-1.21084600
C	-6.64804300	-0.02625400	-0.03016100
C	-7.39380000	-0.04498600	1.16122700
C	-7.33937800	-0.05900100	-1.25290800
C	-8.78557900	-0.09426400	1.13081800
H	-6.88425500	-0.02095200	2.12061000
C	-8.73160400	-0.10850700	-1.28034200
H	-6.76397400	-0.04407300	-2.17195900
C	-9.46291600	-0.12629600	-0.09065800
H	-9.34317300	-0.10765200	2.06339300
H	-9.24831500	-0.13275700	-2.23600900
H	-10.54826400	-0.16447800	-0.11371300
H	-0.57053900	2.07125000	0.32833100
H	2.11981500	-4.07497500	1.41105800
C	2.17243900	-2.98323800	1.47093200
P	1.26805500	-2.22081100	0.05883800
H	3.21583900	-2.66348800	1.45430000
H	1.72417300	-2.65609000	2.41284400
Pd	1.32463800	0.03868700	-0.00854800
C	-0.38773500	-3.01746800	0.15818200
C	2.01620200	-3.01989400	-1.42192400
C	3.38197200	-0.09067300	-0.02299800
O	1.70633600	2.20209300	-0.14566800
H	-1.00278800	-2.69482300	-0.68441500
H	-0.88955000	-2.71744900	1.08016000

H	-0.28051400	-4.10666100	0.13987700
H	1.97981000	-4.10964100	-1.32556500
H	1.46204200	-2.72183300	-2.31575800
H	3.05278700	-2.69545600	-1.52896400
C	4.09759800	-0.06472700	-1.23604600
C	4.12691300	-0.03640300	1.17129000
C	0.94808800	3.16227800	0.04325200
C	5.48948400	0.01816500	-1.26667700
H	3.56207800	-0.09543200	-2.18210900
C	5.51904600	0.04795200	1.16692900
H	3.61545600	-0.04878600	2.13118400
O	-0.32592200	3.04249600	0.34655800
C	1.42567500	4.58236500	-0.07081400
H	6.04195700	0.04442400	-2.19843200
C	6.18408000	0.07067500	-0.05850600
H	6.09391300	0.09606000	2.08414200
N	7.64761400	0.15184600	-0.07657700
O	8.23502600	0.19728800	1.00624300
O	8.20984700	0.16884500	-1.17323800
H	-4.50365000	0.09416300	2.13320100
S	-1.63275600	0.14112200	-1.60495500
C	-1.47566200	0.18605200	2.46675100
H	-1.95171700	1.04945200	2.94867400
H	-1.88028600	-0.71418700	2.94828900
H	-0.40229800	0.22933600	2.66336500
H	1.10881300	5.15370900	0.80548600
H	0.96213300	5.04472500	-0.94822500
H	2.50960300	4.60462500	-0.17261600

I-1da + HOAc (N)

E= -2224.25236

G= -2224.32369

C	3.94678600	-1.06225700	-0.18435300
C	2.43275600	-2.84233900	-0.25661100
C	1.83990700	-0.32346400	0.16360100
C	2.81549100	0.69297100	0.19762800
N	2.62853700	-1.46513600	-0.09276000
C	3.60479400	-3.48512100	-0.48006500
N	4.10816900	0.22347300	-0.01617100
C	2.61323400	2.13956700	0.40164500
C	1.37952300	2.68125700	0.81105500
C	3.68168700	3.02806800	0.17819300
C	1.21760200	4.05673400	0.97625300
H	0.54162500	2.01690000	1.00727000
C	3.51746200	4.40170300	0.34539900
H	4.63821200	2.61699000	-0.12456900
C	2.28520800	4.92647700	0.74208400
H	0.25668600	4.44855100	1.29978200
H	4.35806800	5.06657300	0.16574000
H	2.15976300	5.99727400	0.87429100
H	3.73290400	-4.54611000	-0.63619600

H	-1.10519800	-0.14292000	-4.35147400
C	-1.18611300	-0.55843800	-3.34206000
P	-0.18643200	0.43952300	-2.15820500
H	-0.82040700	-1.58882000	-3.35272100
H	-2.23170700	-0.56650700	-3.03020000
Pd	-0.28121500	-0.26218400	-0.00997500
C	-0.80169600	2.15658400	-2.40237000
C	1.46744600	0.46788200	-2.96474800
C	-2.33756500	-0.15718500	-0.12831900
O	-0.64800600	-0.96845900	2.05289700
H	-0.19834600	2.84286400	-1.80241900
H	-1.84109300	2.22064300	-2.07370800
H	-0.73375500	2.44049700	-3.45730900
H	1.36945600	0.78330500	-4.00860500
H	2.12702300	1.15548100	-2.43330900
H	1.91457100	-0.52820200	-2.92866000
C	-3.11226300	-1.29850900	-0.41835100
C	-3.02986600	1.01394500	0.23999100
C	0.10568600	-0.88625100	3.03431000
C	-4.50409500	-1.28576100	-0.33906000
H	-2.62336700	-2.22744500	-0.70292000
C	-4.42130500	1.05264800	0.32879200
H	-2.47526100	1.91857200	0.47838400
O	1.35135300	-0.47857500	2.97106400
C	-0.35926600	-1.24854700	4.41769500
H	-5.09918500	-2.16489300	-0.55611600
C	-5.14317300	-0.10326700	0.03387100
H	-4.95275100	1.95115400	0.61931700
N	-6.60573200	-0.07556200	0.11731100
O	-7.14398000	0.98105600	0.45450100
O	-7.21815200	-1.11030500	-0.15530000
H	1.59049800	-0.30306000	2.00411800
S	5.01207600	-2.41913200	-0.48607100
C	1.07390100	-3.45888700	-0.16819500
H	0.62702000	-3.30622500	0.82016400
H	0.38606300	-3.01645300	-0.89746900
H	1.13866400	-4.53324500	-0.35574100
H	-1.36763300	-1.65792900	4.37849300
H	-0.34756500	-0.35153800	5.04481800
H	0.33150900	-1.96778700	4.86580000

I-2db + HOAc (O)

E= -2224.253033

G= -2224.326708

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C	-1.54875100	0.15735600	0.91828100
C	-4.14038500	0.06231400	1.17988200
C	-5.06790400	0.02099800	0.14906200
N	-2.90443300	0.10032900	0.55792600
C	-0.69364800	0.19765400	-0.15236100
N	-4.43345100	0.03849800	-1.08681500

C	-6.53307100	-0.03582700	0.24157400
C	-7.19492500	-0.08029300	1.48091300
C	-7.30696200	-0.04654200	-0.93104900
C	-8.58548100	-0.13260100	1.54514700
H	-6.62048000	-0.07523800	2.40321200
C	-8.69767000	-0.09931100	-0.86384100
H	-6.79582800	-0.01228600	-1.88682800
C	-9.34530400	-0.14237900	0.37280200
H	-9.07758600	-0.16639700	2.51339600
H	-9.27885100	-0.10623100	-1.78203700
H	-10.42961300	-0.18319100	0.42385600
H	-0.43652000	2.05961500	0.23208200
H	2.34088200	-4.04000000	1.10971700
C	2.40386400	-2.94761100	1.13879400
P	1.37995700	-2.21329200	-0.20400700
H	3.44333700	-2.63676400	1.02227600
H	2.04468800	-2.59505600	2.10915000
Pd	1.41761900	0.04262400	-0.31906600
C	-0.25862000	-3.01276900	0.04825700
C	1.99872600	-3.03782300	-1.72985500
C	3.46809100	-0.07510700	-0.52850800
O	1.76357900	2.20777600	-0.52186300
H	-0.94479400	-2.69986900	-0.74152500
H	-0.68021500	-2.70520500	1.00727300
H	-0.15090800	-4.10206200	0.03158000
H	1.97999000	-4.12560600	-1.60961400
H	1.36367900	-2.76073000	-2.57534400
H	3.01873800	-2.70914900	-1.93635100
C	4.06869600	-0.01314200	-1.80012200
C	4.31876900	-0.03509600	0.58584200
C	1.03404200	3.16095700	-0.21954400
C	5.45597600	0.09499200	-1.96033500
H	3.44520200	-0.03485600	-2.69161200
C	5.70098400	0.07188500	0.41173600
H	3.93625900	-0.07285700	1.59965200
O	-0.19077900	3.03056600	0.24200800
C	1.49135700	4.58527800	-0.36158000
H	5.88494100	0.14739300	-2.95735700
C	6.29301000	0.13848000	-0.84808700
H	-4.24403200	0.06895200	2.25249700
S	-1.64000000	0.15187900	-1.67599800
C	-1.19735100	0.15767800	2.37503400
H	-1.63446600	1.01788500	2.89774500
H	-1.57062100	-0.74581000	2.87539500
H	-0.11271800	0.19573700	2.49607000
H	7.36901000	0.21999000	-0.93418000
N	6.56678000	0.10978400	1.60204800
O	7.77951000	0.23534200	1.42777200
O	6.03176100	0.01010500	2.70787100
H	2.53979900	4.61322500	-0.65407100
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I-1db + HOAc (P)

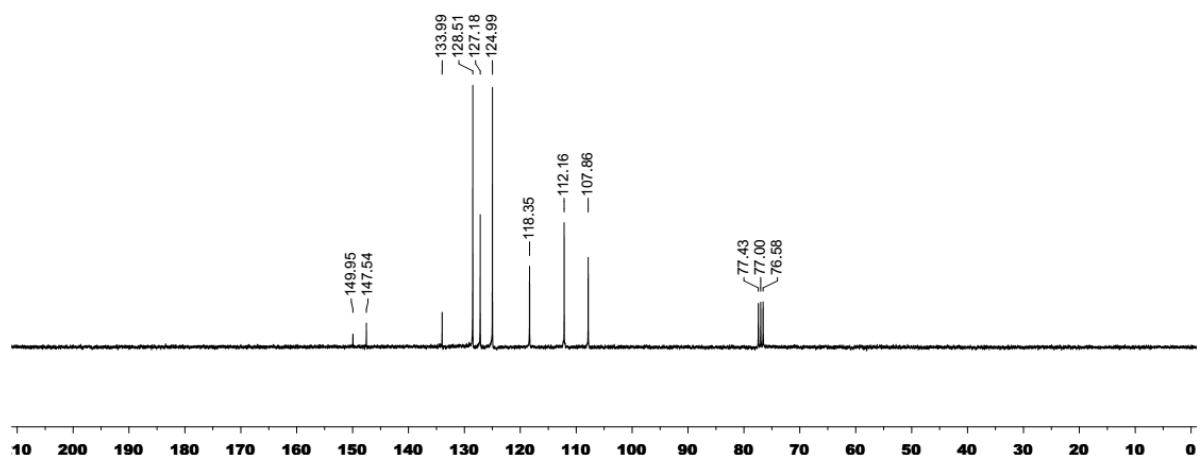
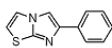
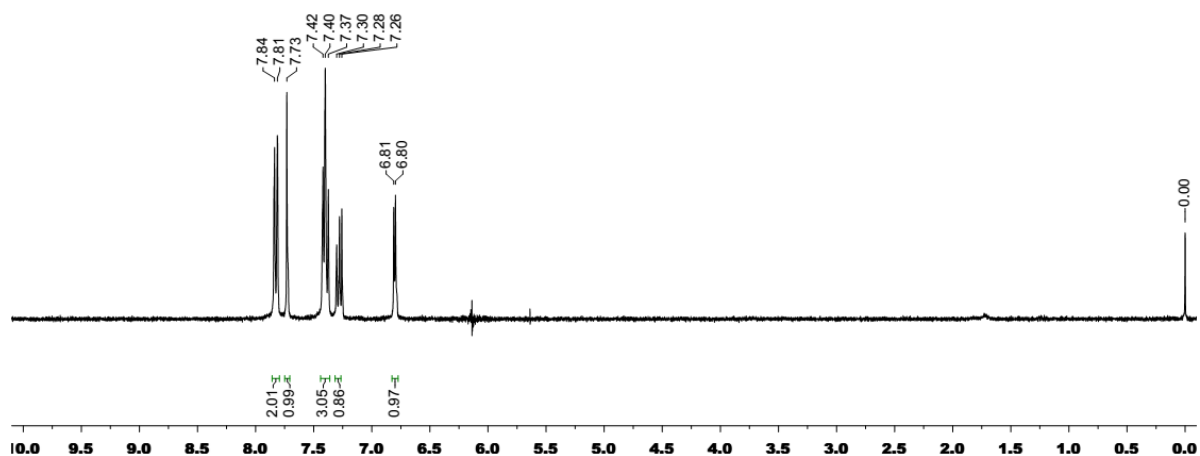
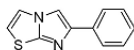
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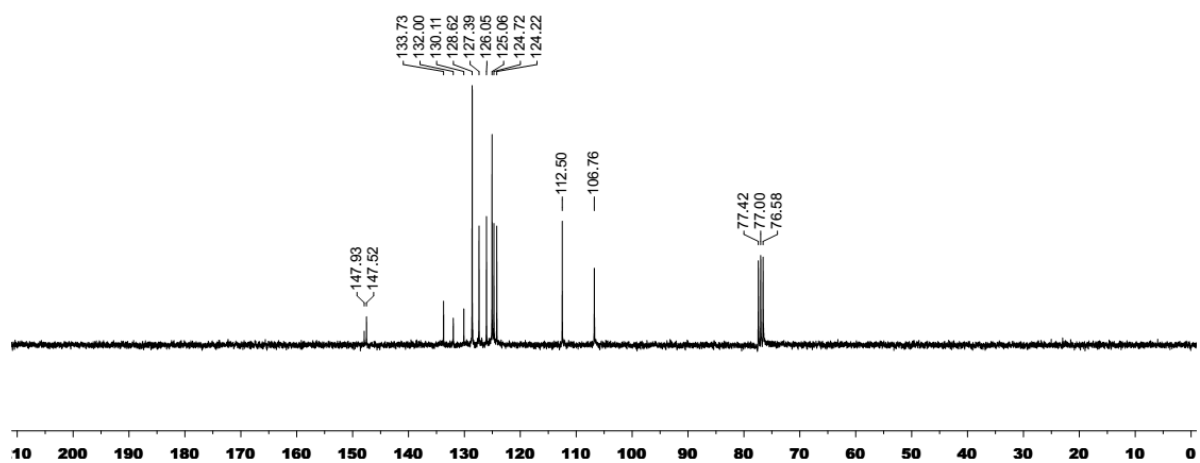
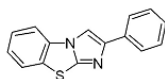
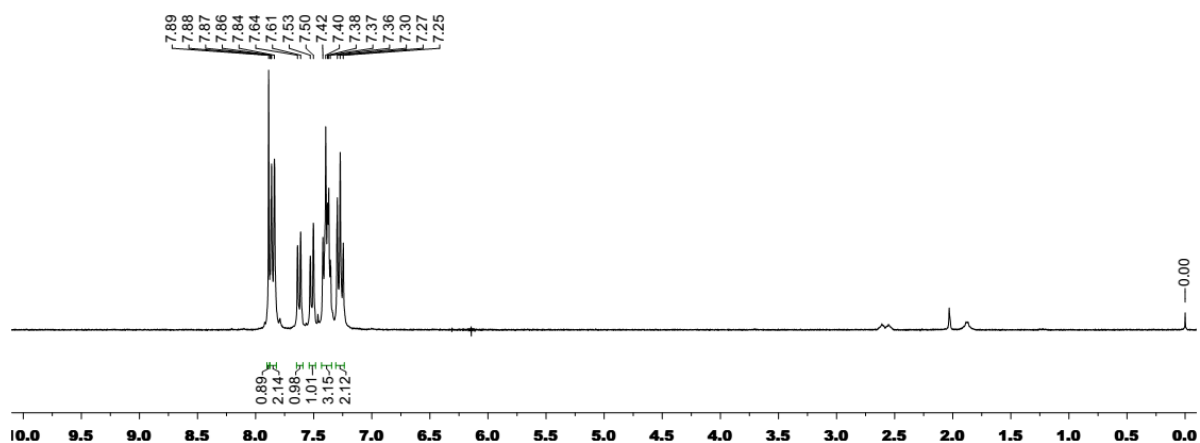
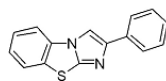
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C	2.94457700	-2.44977200	-0.12809000
C	1.78485600	-0.11860300	0.17829000
C	2.50460100	1.09246900	0.20497800
N	2.81897900	-1.05971200	-0.01198600
C	4.23828400	-2.81753200	-0.29479200
N	3.87708600	0.92100800	0.04605400
C	1.97488600	2.46102700	0.35434400
C	0.63805700	2.72072300	0.71325200
C	2.82290800	3.56152900	0.12956500
C	0.16458900	4.02779500	0.82675400
H	-0.03577600	1.89082600	0.91112800
C	2.34795200	4.86647500	0.24562700
H	3.85703600	3.36925300	-0.13360000
C	1.01648400	5.10940300	0.59113900
H	-0.87045800	4.20011200	1.10995700
H	3.02285100	5.69910800	0.06600800
H	0.64844900	6.12720300	0.68298100
H	4.60727600	-3.82647900	-0.40569100
H	-1.01994300	-0.68436000	-4.40355800
C	-1.02144200	-1.09207300	-3.38765300
P	-0.29824500	0.12519700	-2.20711700
H	-0.42976600	-2.01147300	-3.37369700
H	-2.04278900	-1.33375000	-3.08902000
Pd	-0.28426100	-0.54986700	-0.04819900
C	-1.27254900	1.65757100	-2.50261200
C	1.32496000	0.51249500	-2.98305800
C	-2.30892500	-0.93227900	-0.21872000
O	-0.53769500	-1.28434600	2.02042500
H	-0.84676200	2.47246700	-1.91190300
H	-2.30691400	1.50130600	-2.19071000
H	-1.24638600	1.92617800	-3.56352700
H	1.18138300	0.76773700	-4.03786600
H	1.79166000	1.35032700	-2.46293400
H	1.99083700	-0.34976400	-2.90510300
C	-2.79021500	-2.23990600	-0.42367600
C	-3.26385100	0.06575000	0.02868600
C	0.12491800	-0.97384600	3.02176000
C	-4.15571100	-2.54700600	-0.37589100
H	-2.08673800	-3.04764000	-0.61576100
C	-4.62371200	-0.25284500	0.07293900
H	-2.97875900	1.09728800	0.20184700
O	1.23268300	-0.27164700	2.98063200
C	-0.30717600	-1.37222700	4.40590100
H	-4.48868200	-3.56943300	-0.53352200
C	-5.09462400	-1.54900200	-0.12607700
H	1.46569900	-0.08122100	2.01549400

S	5.36880800	-1.46129300	-0.30236400
C	1.75792500	-3.35514700	-0.04796400
H	1.25874900	-3.27564100	0.92377000
H	1.01055600	-3.10274000	-0.80837400
H	2.06920600	-4.39227900	-0.19353900
H	-6.15775300	-1.74844700	-0.08455300
N	-5.59850800	0.81957700	0.33234600
O	-6.78996800	0.51241500	0.39223800
O	-5.17088300	1.96701900	0.47188800
H	-0.65612900	-0.47997300	4.93622300
H	0.54061600	-1.77538800	4.96489000
H	-1.11666400	-2.09881600	4.34994700

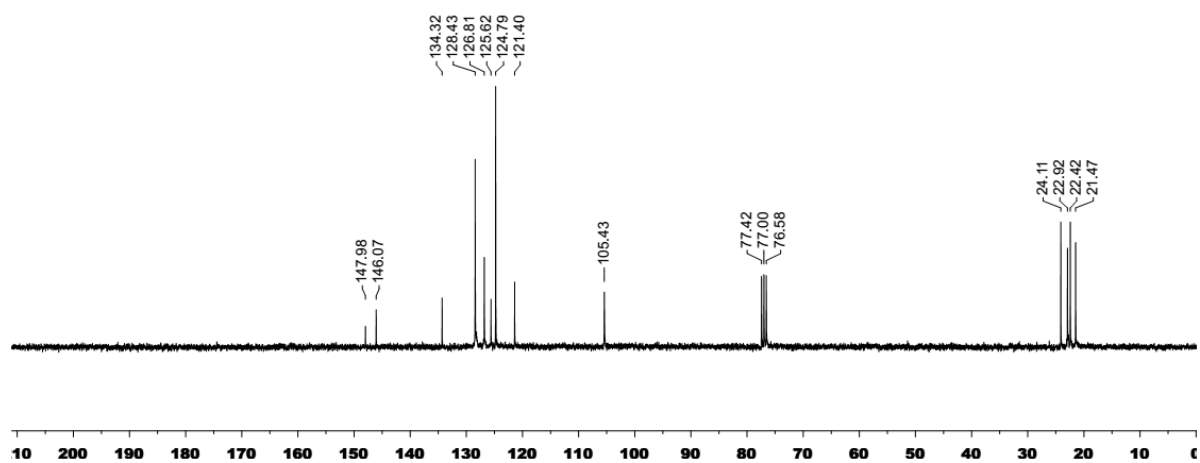
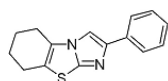
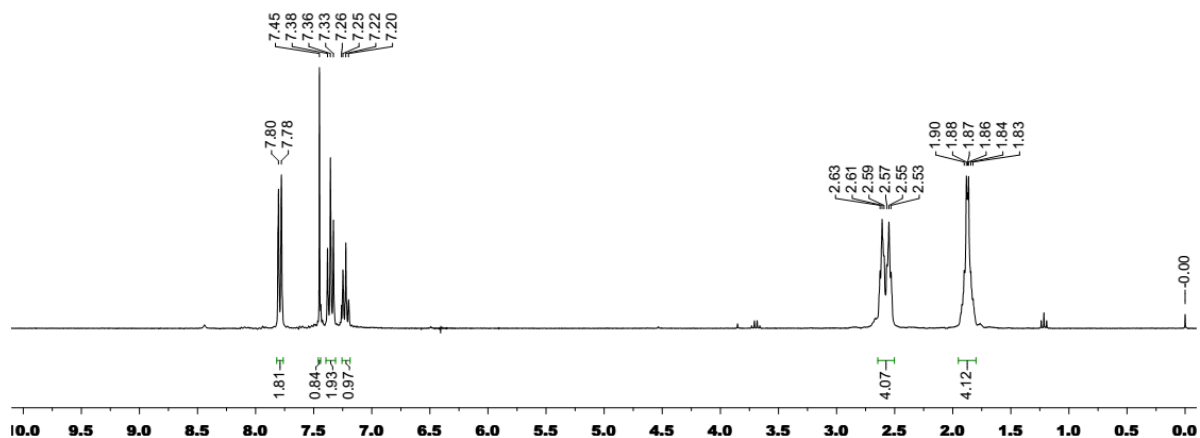
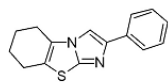
4. ^1H and ^{13}C NMR spectra
6-Phenylimidazo[2,1-b]thiazole (1a)⁷



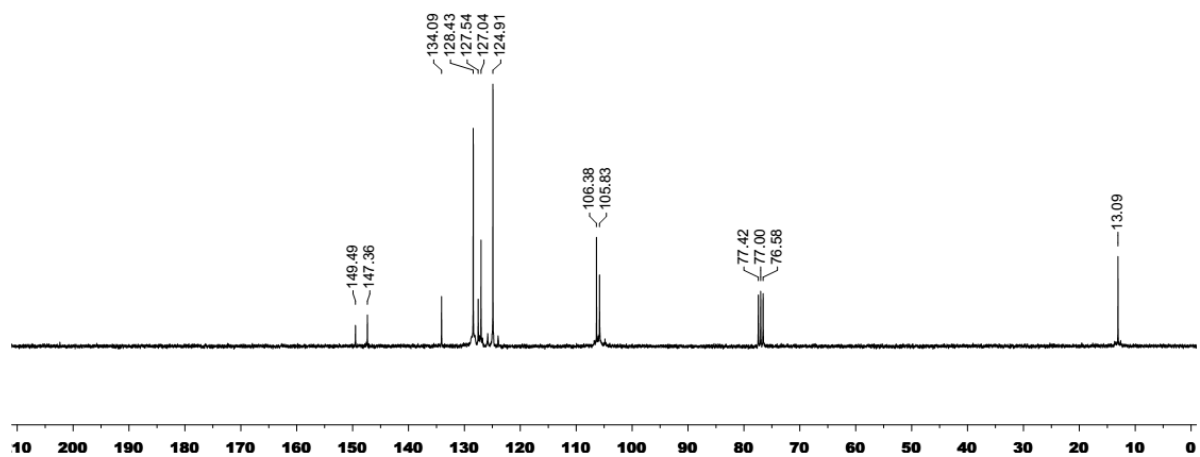
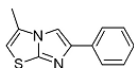
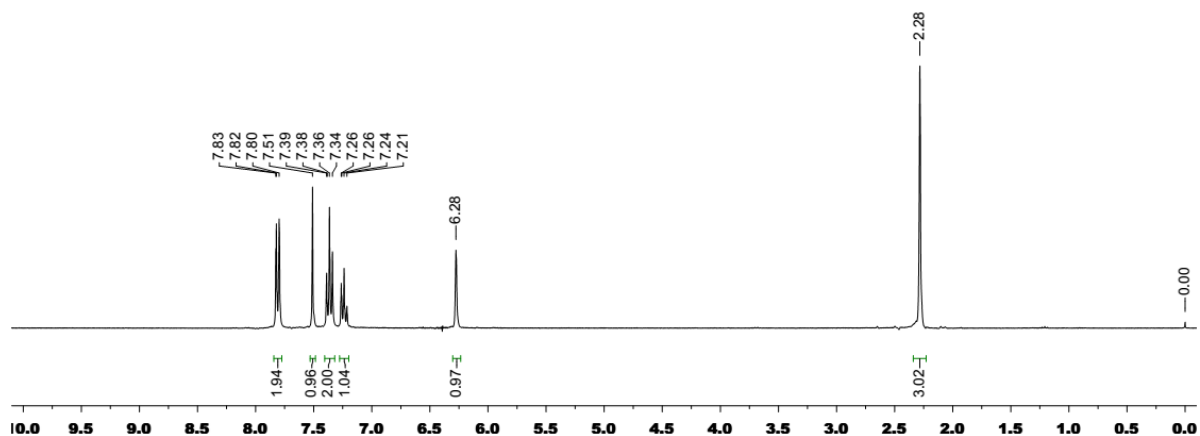
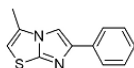
2-Phenylbenzo[d]imidazo[2,1-b]thiazole (1b)⁸



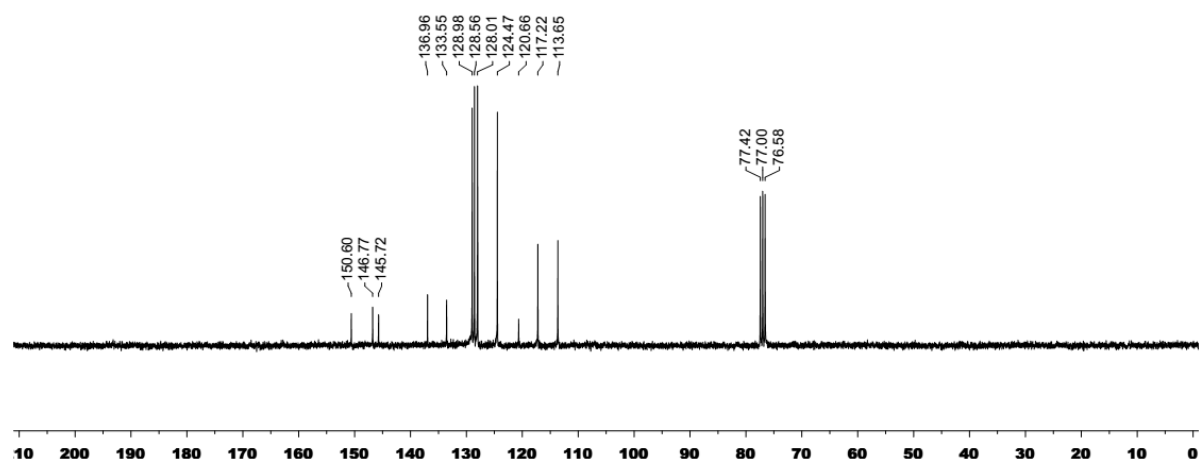
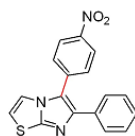
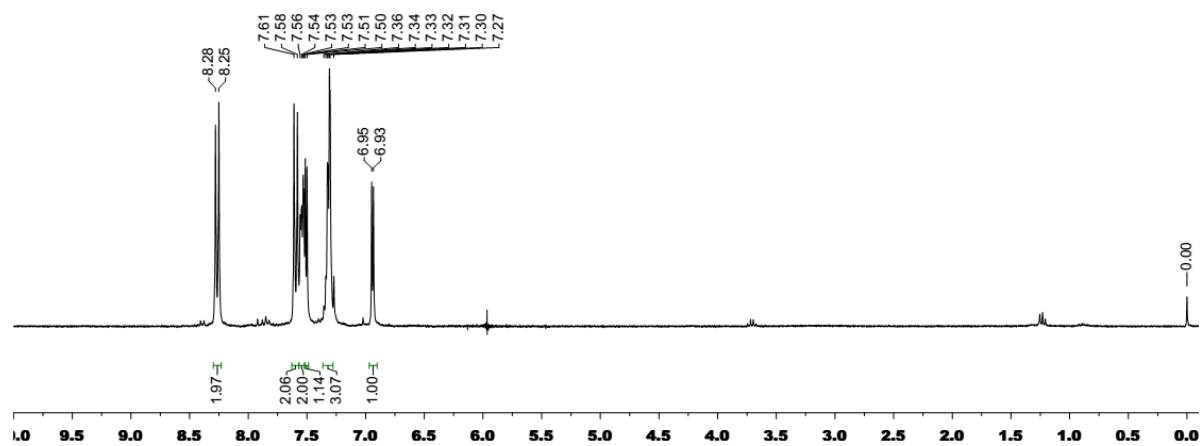
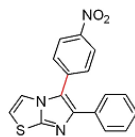
2-Phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole (1c)⁹



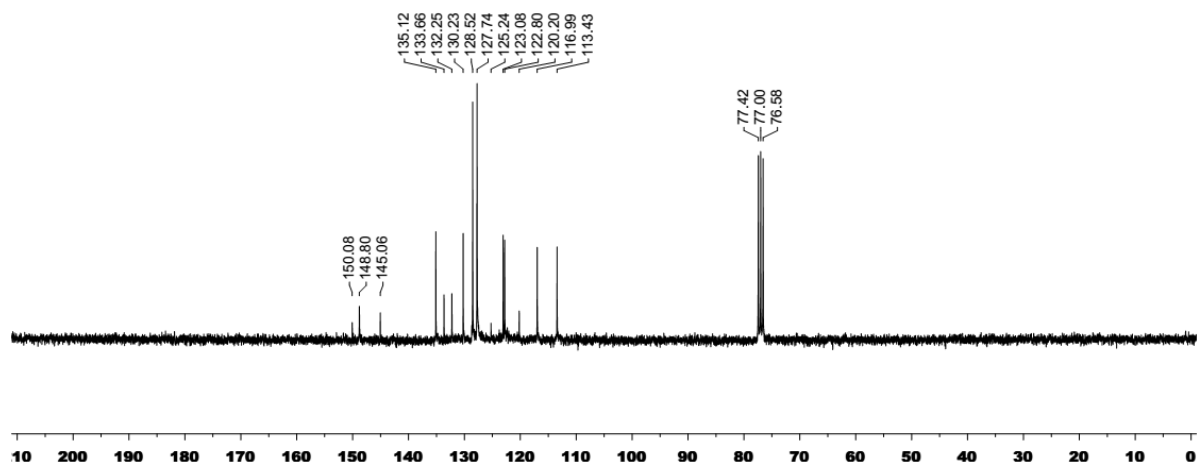
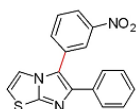
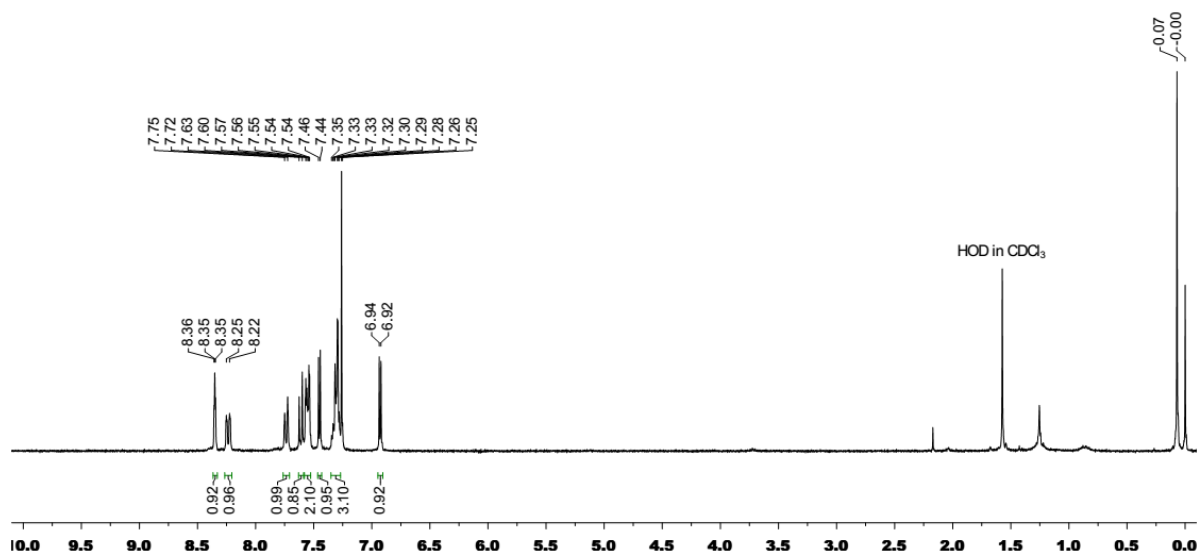
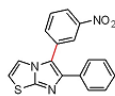
3-Methyl-6-phenylimidazo[2,1b]thiazole (1d)¹⁰



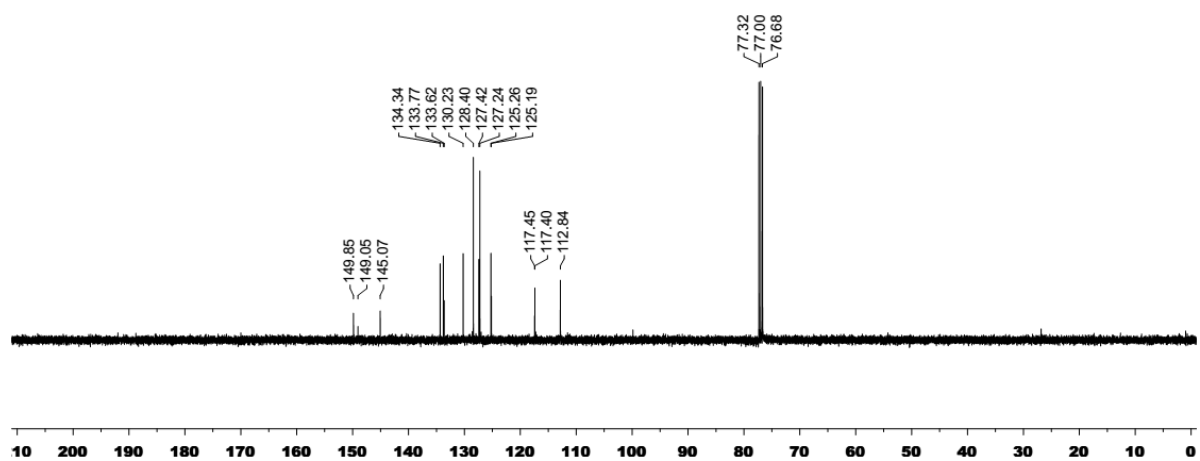
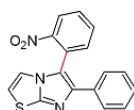
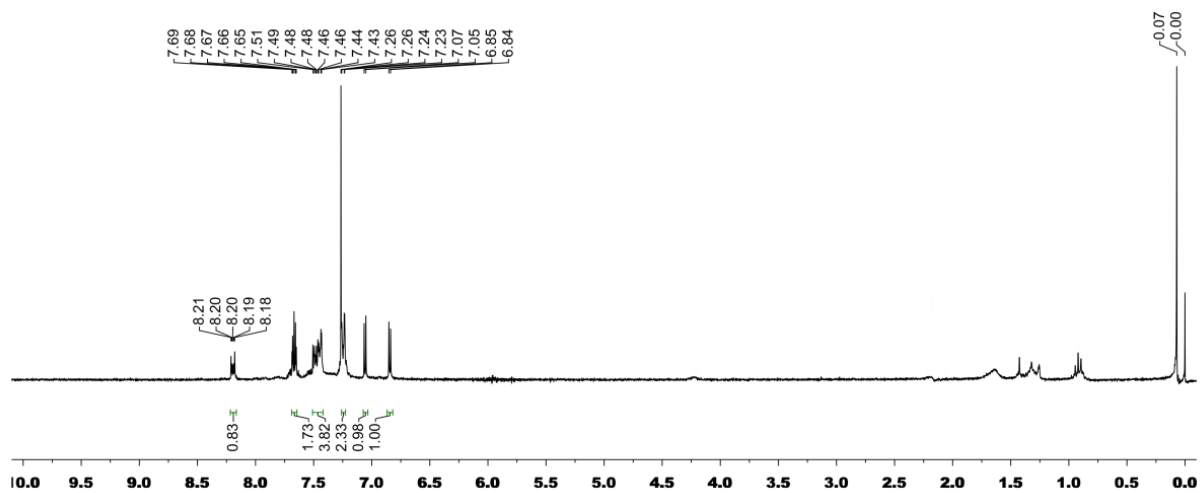
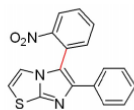
5-(4-Nitrophenyl)-6-phenylimidazo[2,1-b]thiazole (3aa)



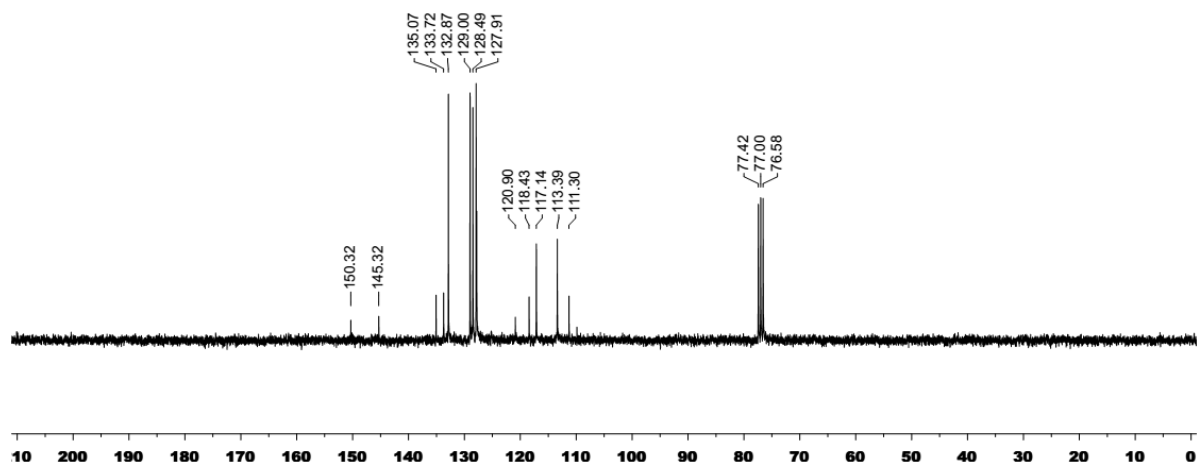
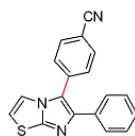
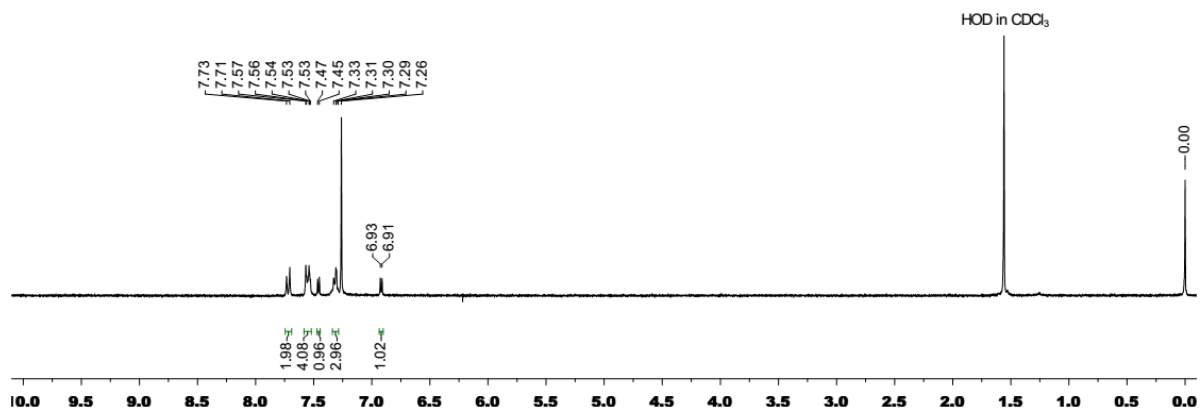
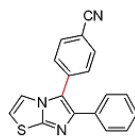
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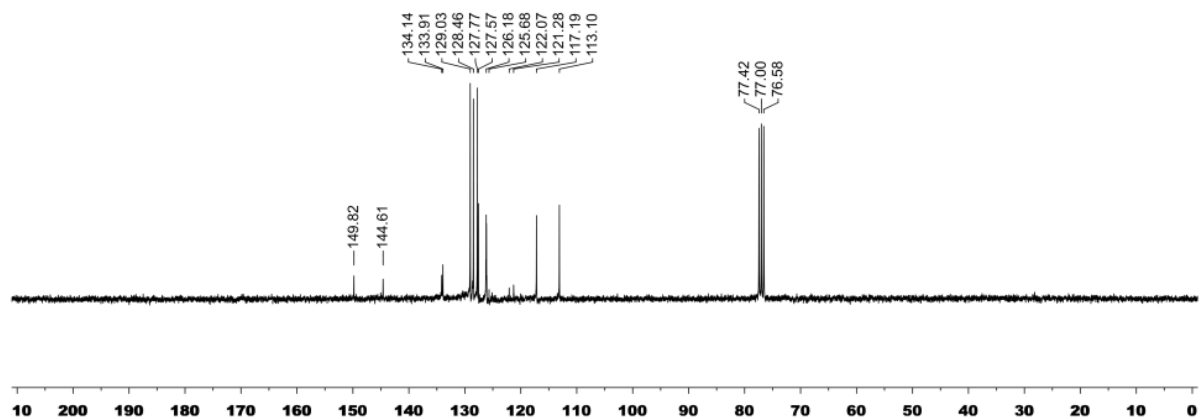
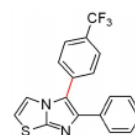
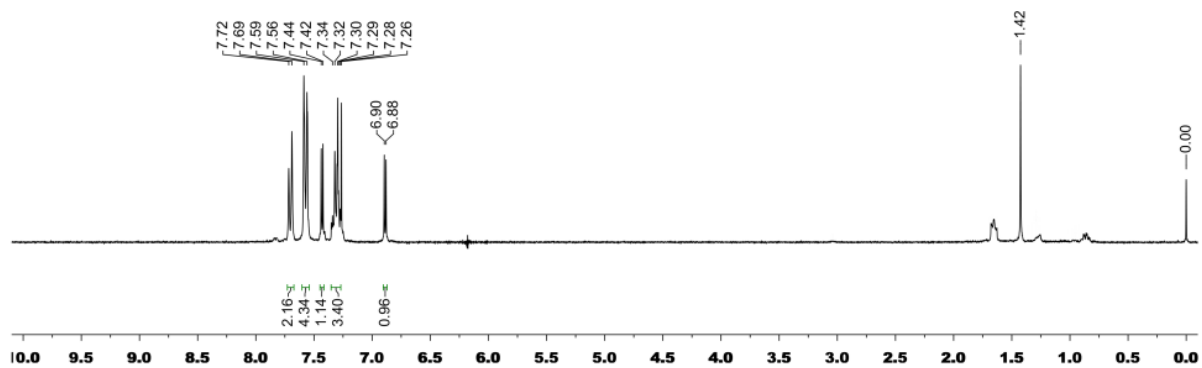
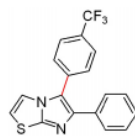
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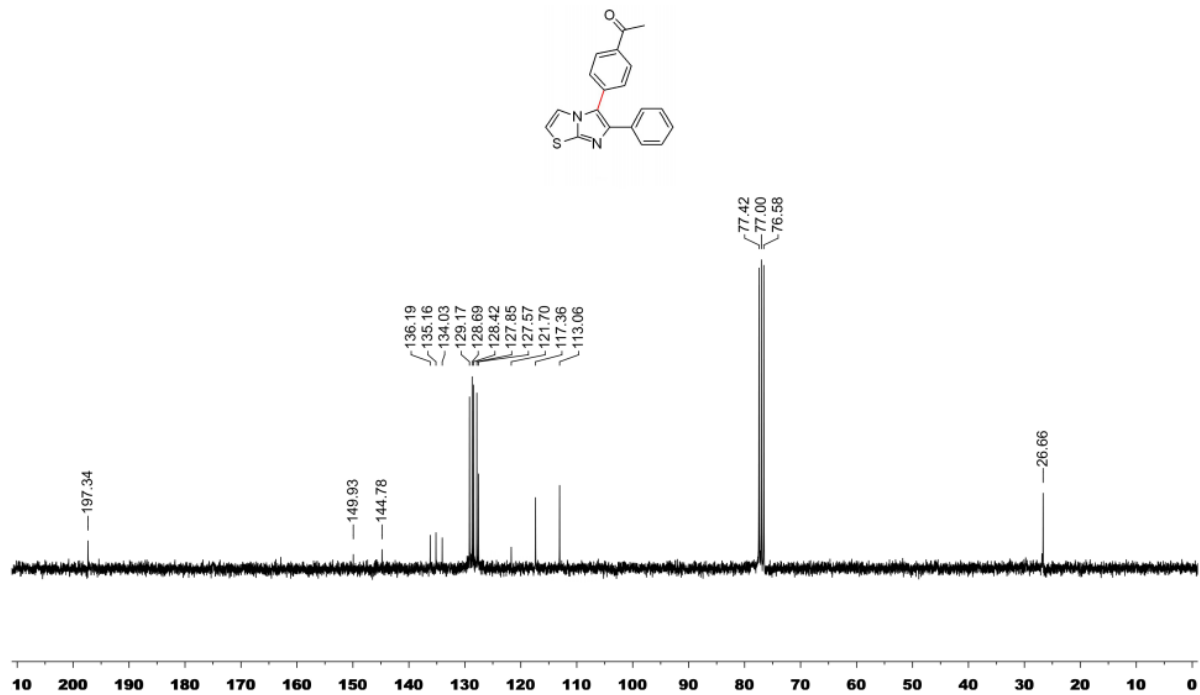
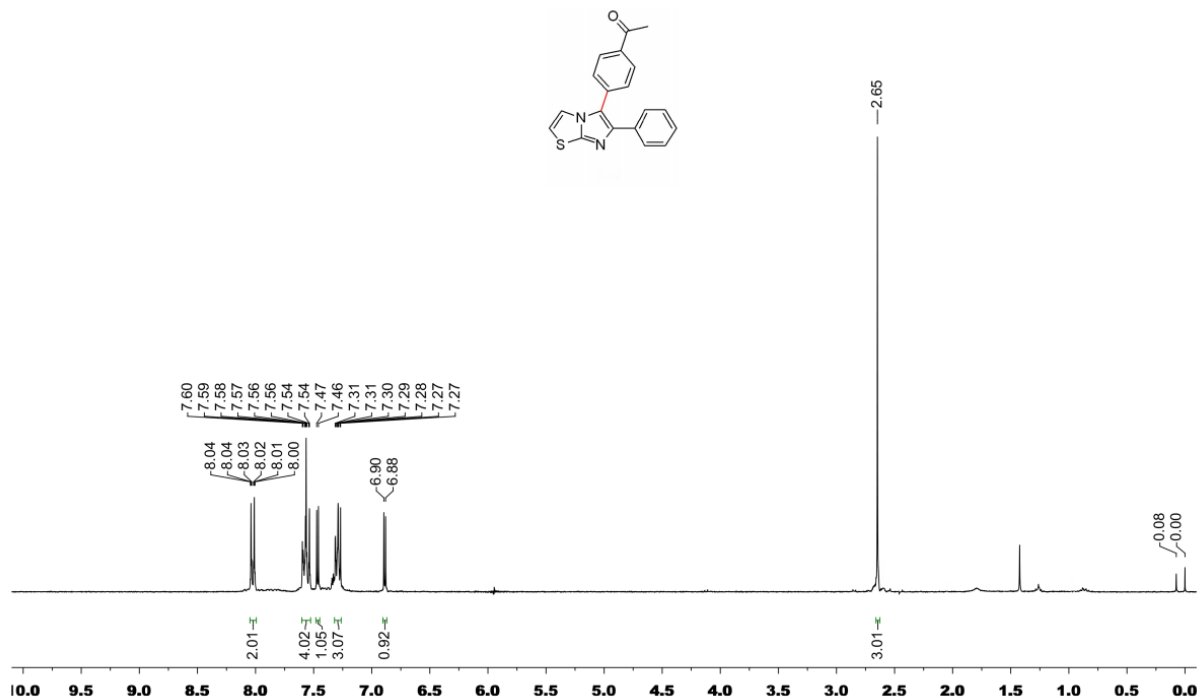
4-(6-Phenylimidazo[2,1-b]thiazol-5-yl)benzonitrile (3ad)



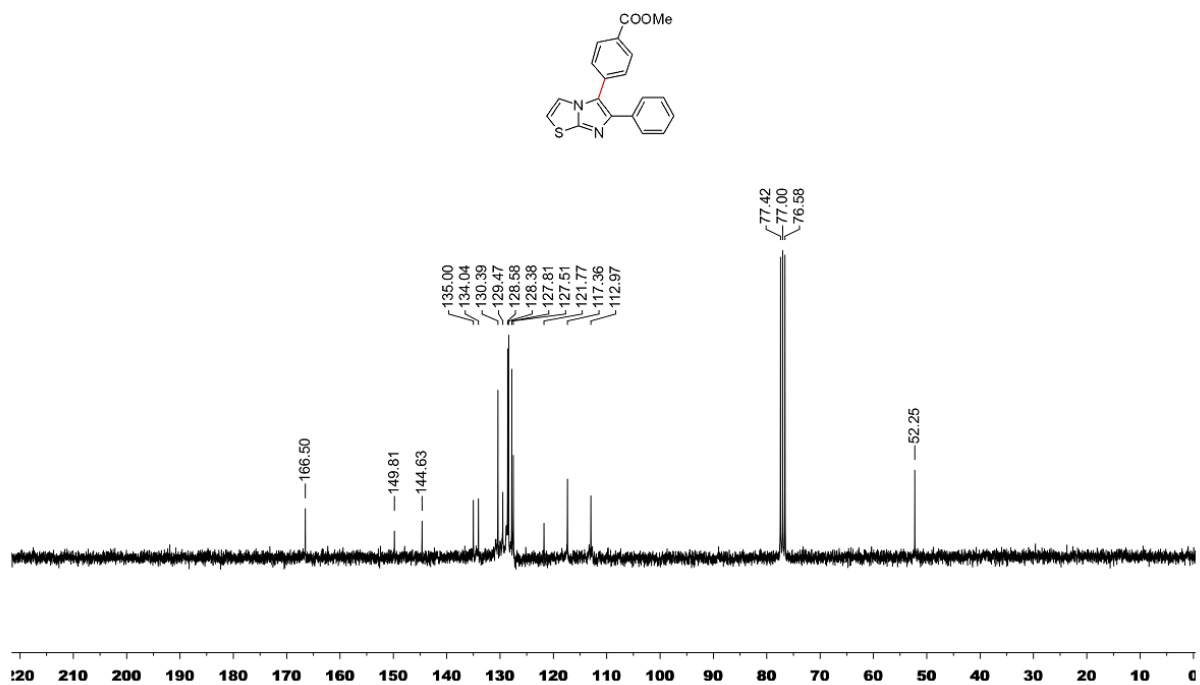
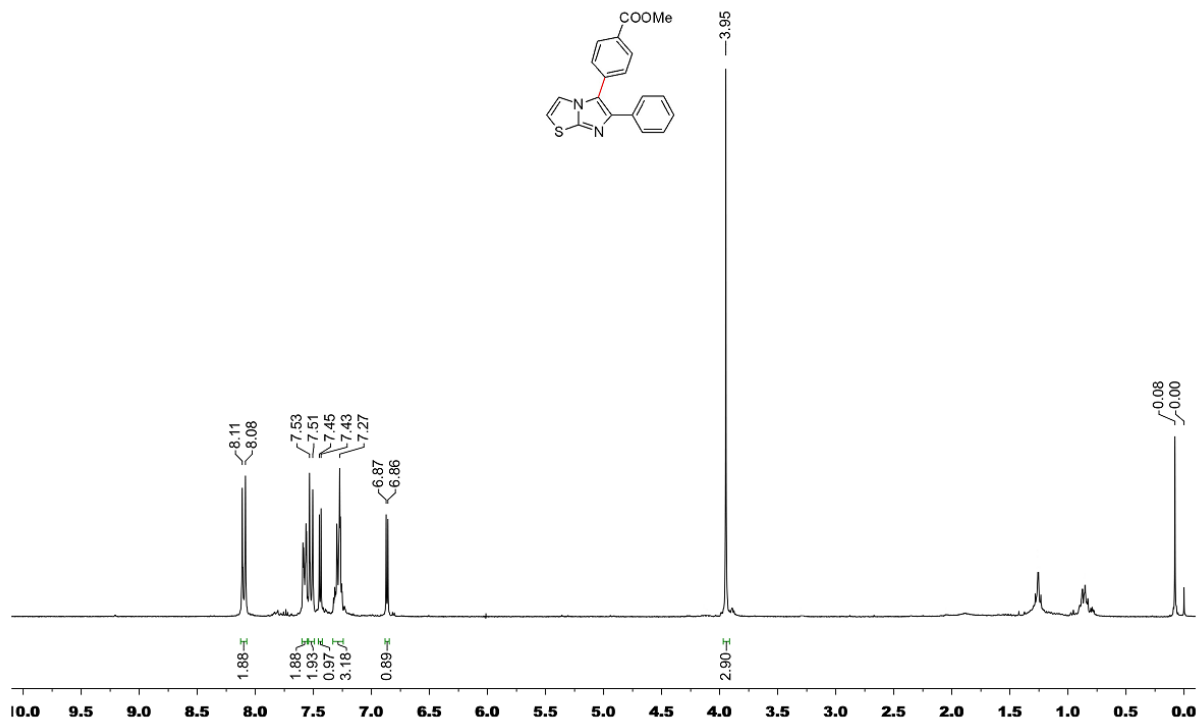
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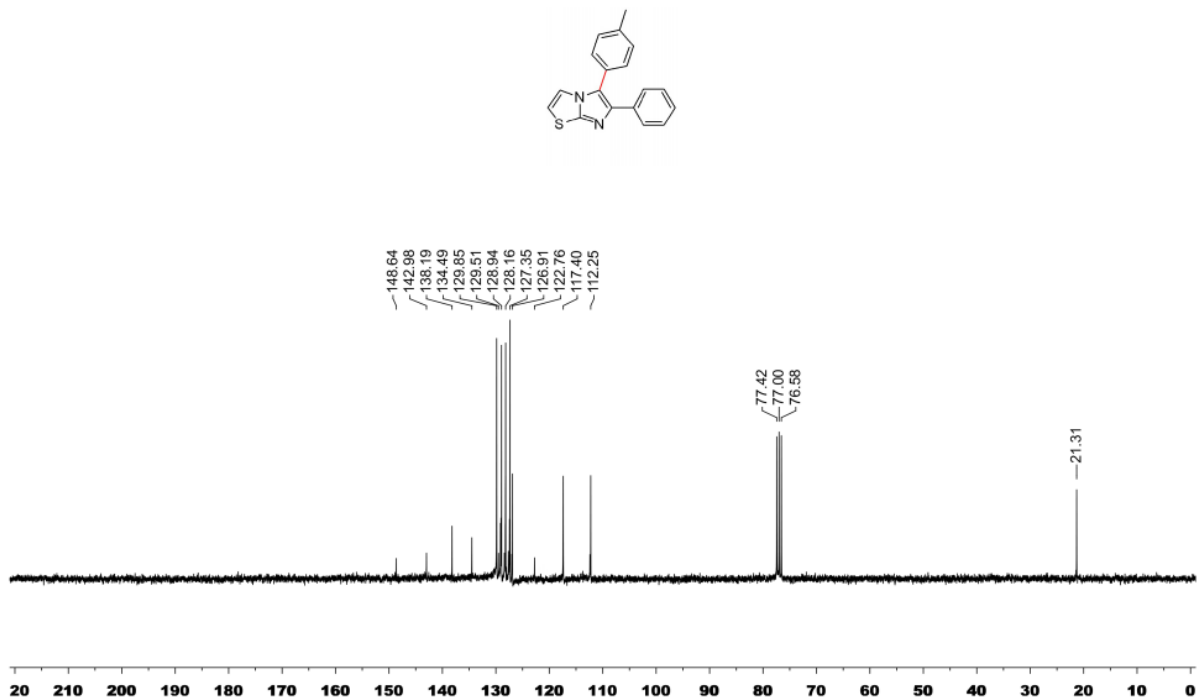
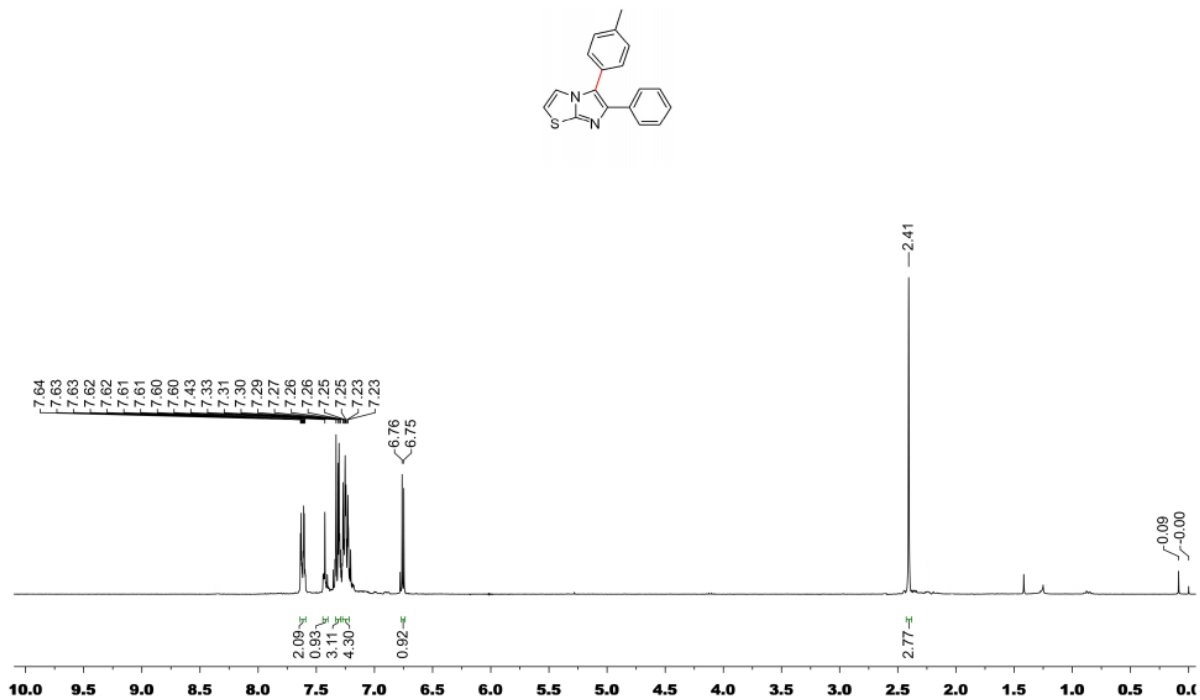
1-(4-(6-Phenylimidazo[2,1-b]thiazol-5-yl)phenyl)ethanone (3af)



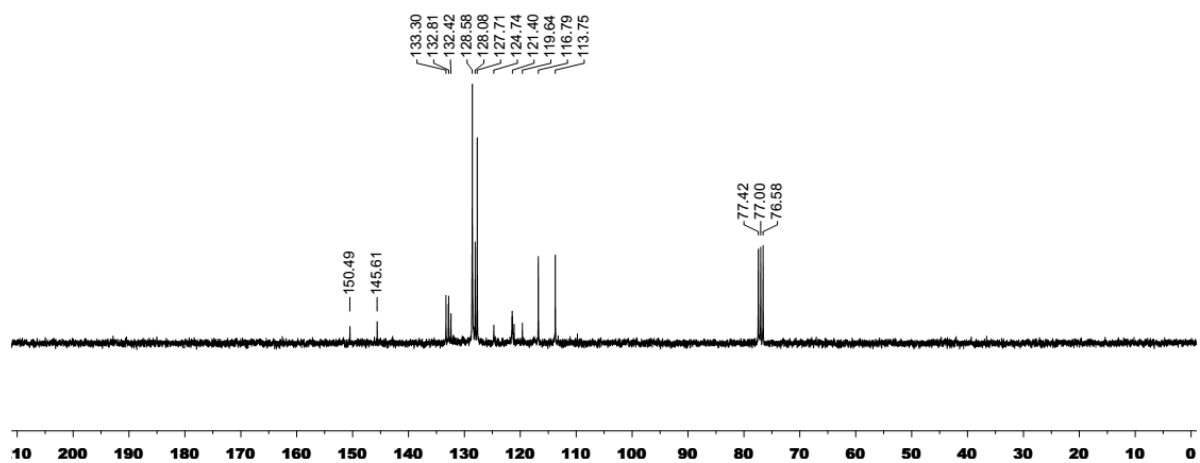
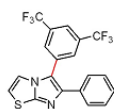
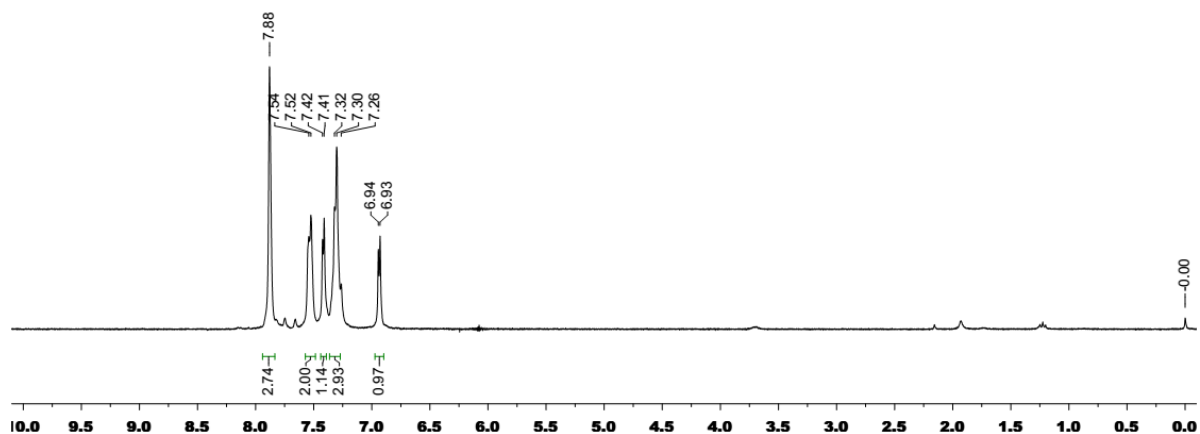
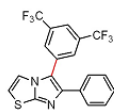
Methyl 4-(6-phenylimidazo[2,1-b]thiazol-5-yl)benzoate(3ag)



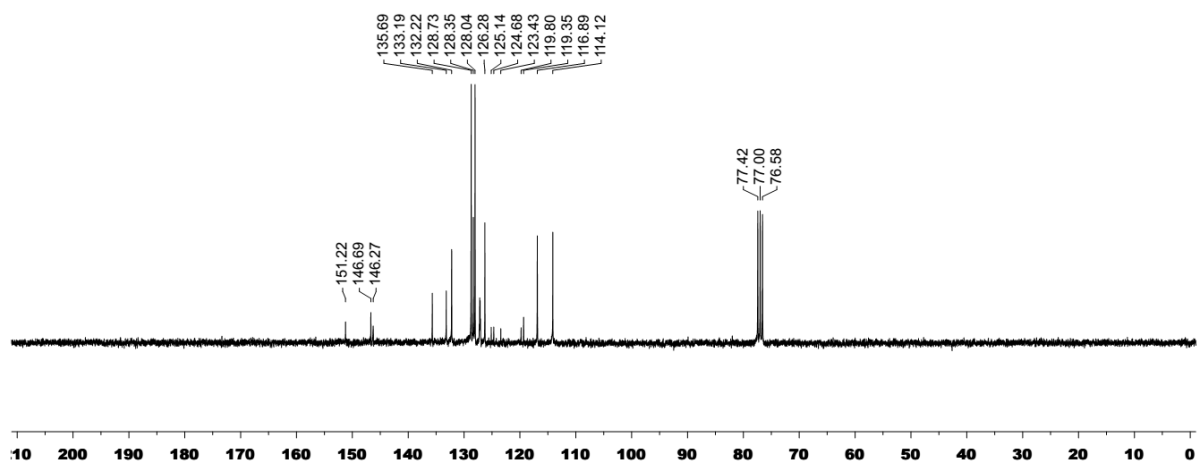
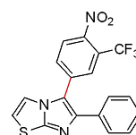
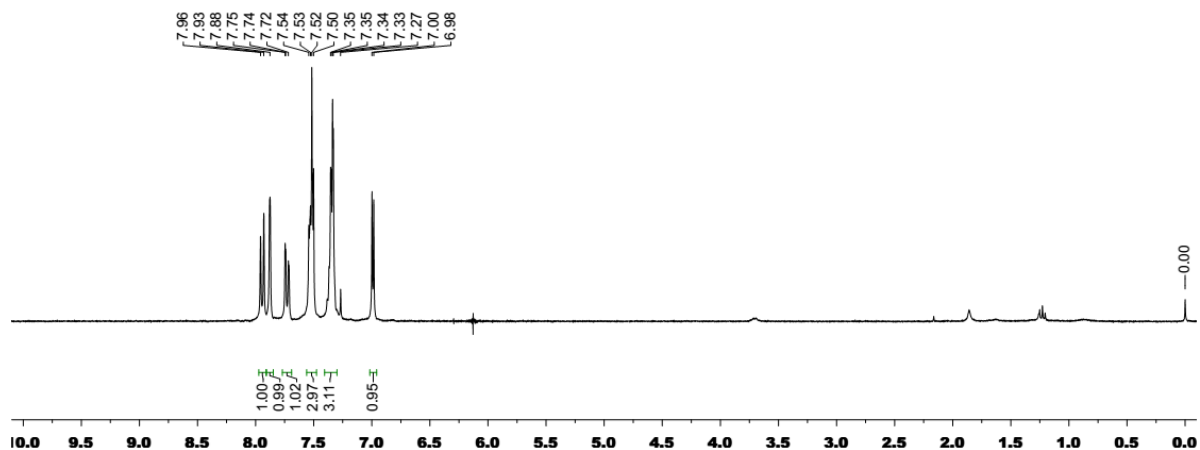
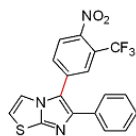
6-Phenyl-5-(p-tolyl)imidazo[2,1-b]thiazole (3ah)



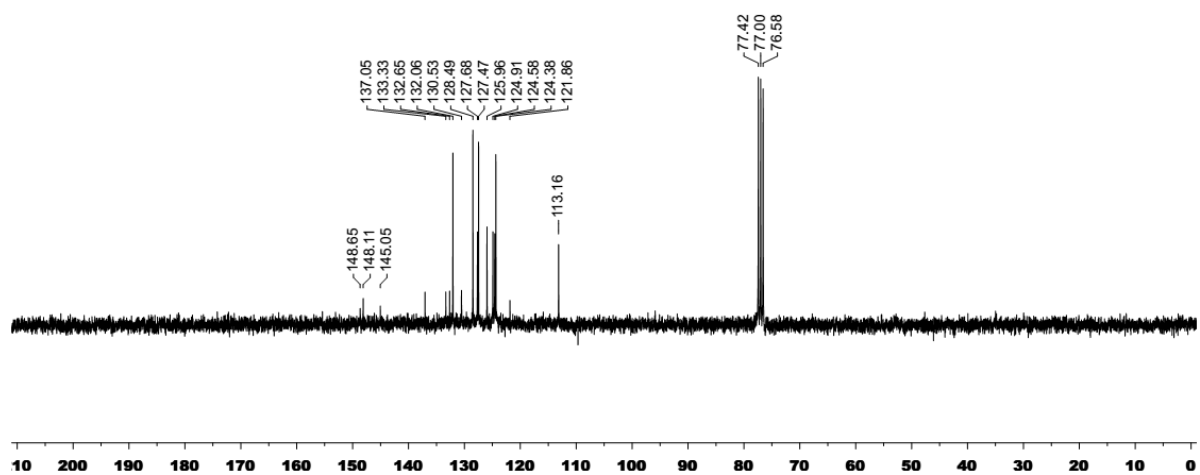
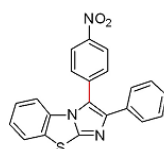
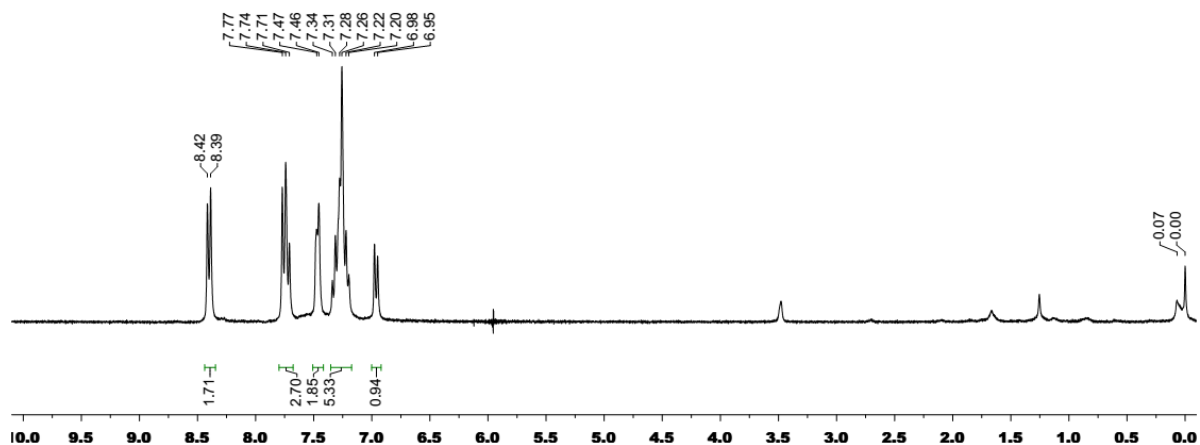
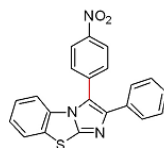
5-(3,5-Bis(trifluoromethyl)phenyl)-6-phenylimidazo[2,1-b]thiazole (3ai)



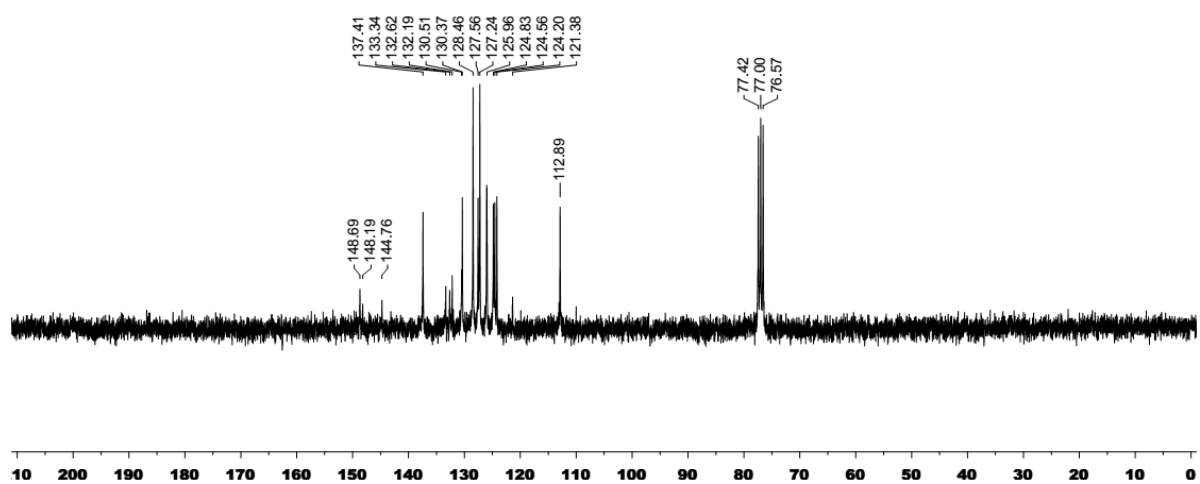
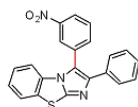
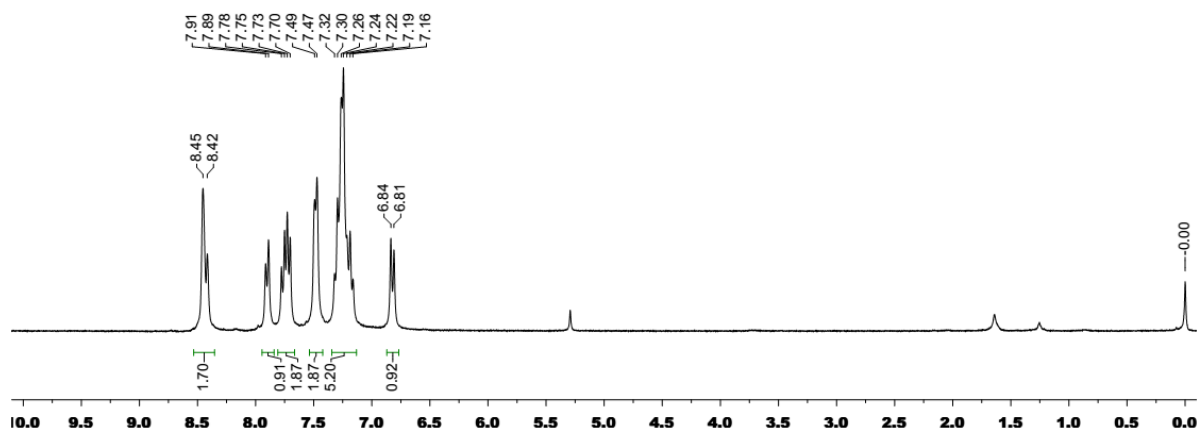
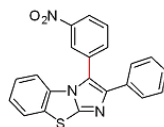
5-(4-Nitro-3-(trifluoromethyl)phenyl)-6-phenylimidazo[2,1-b]thiazole (3aj)



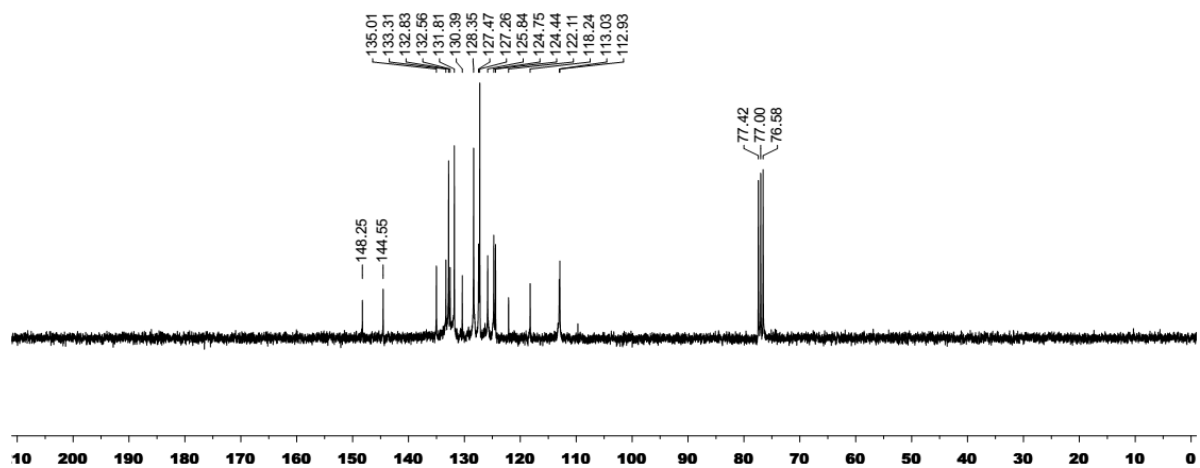
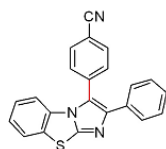
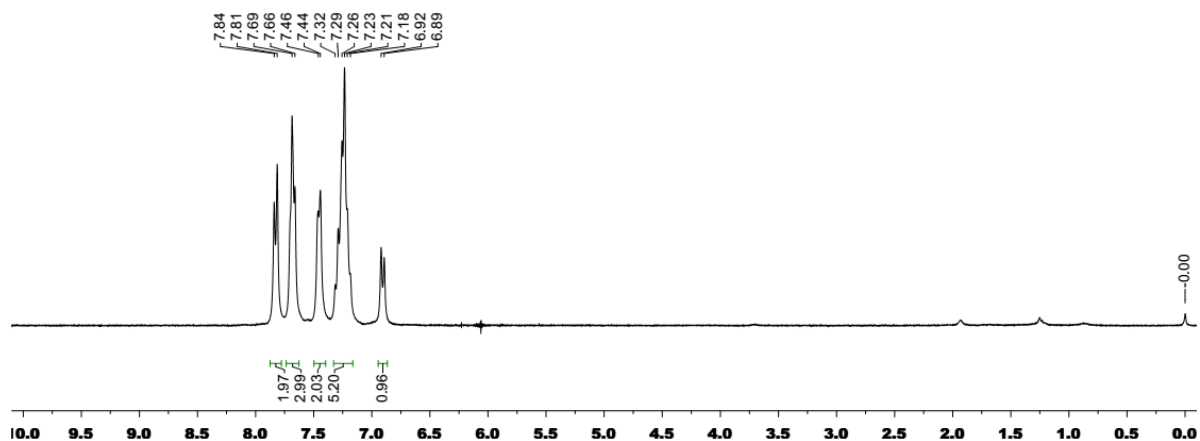
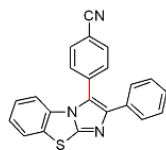
3-(4-Nitrophenyl)-2-phenylbenzo[d]imidazo[2,1-b]thiazole (3ba)



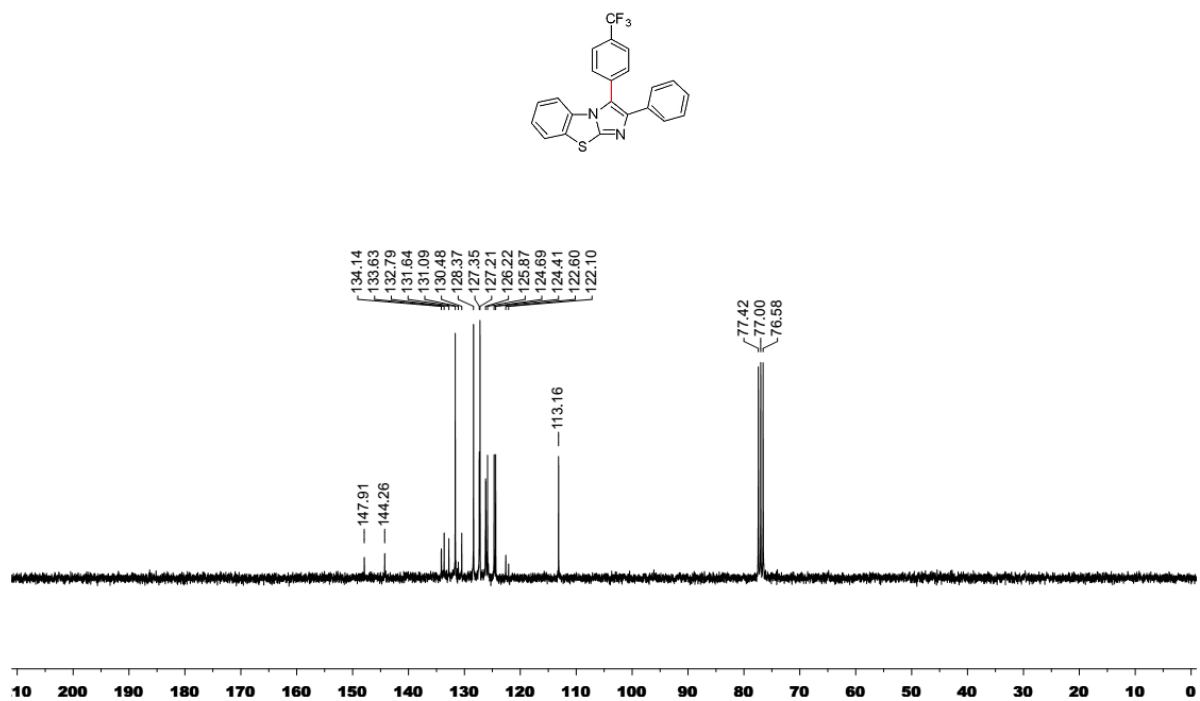
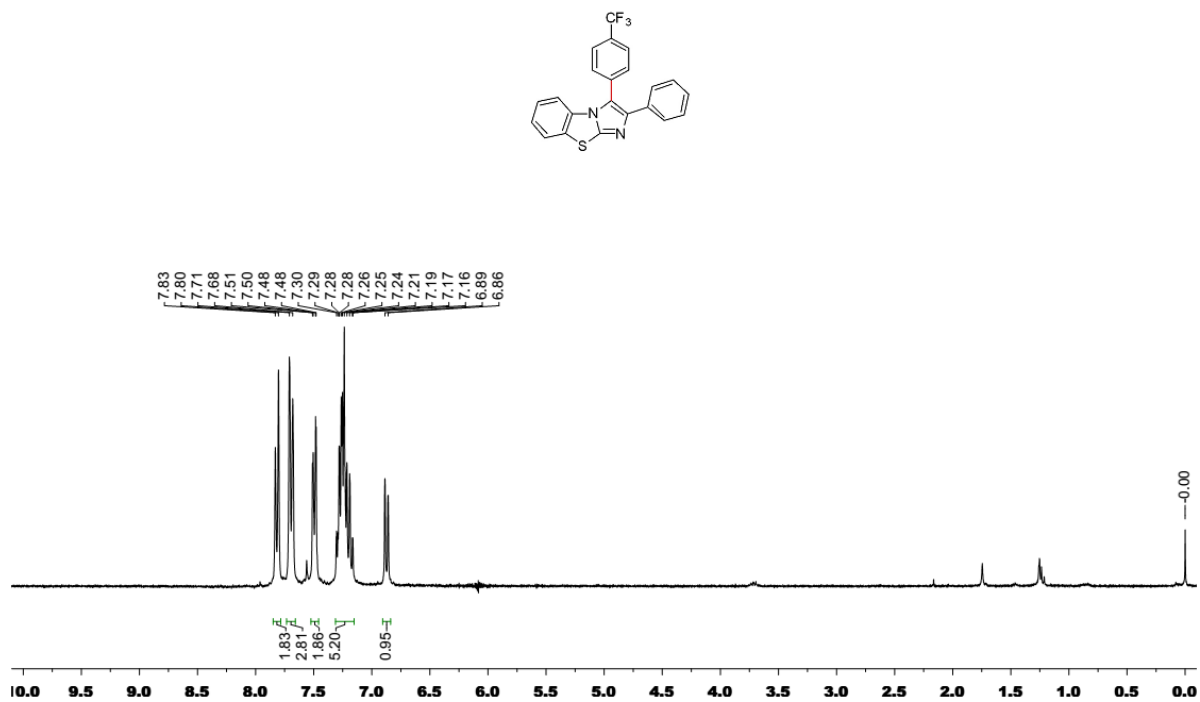
3-(3-Nitrophenyl)-2-phenylbenzo[d]imidazo[2,1-b]thiazole (3bb)



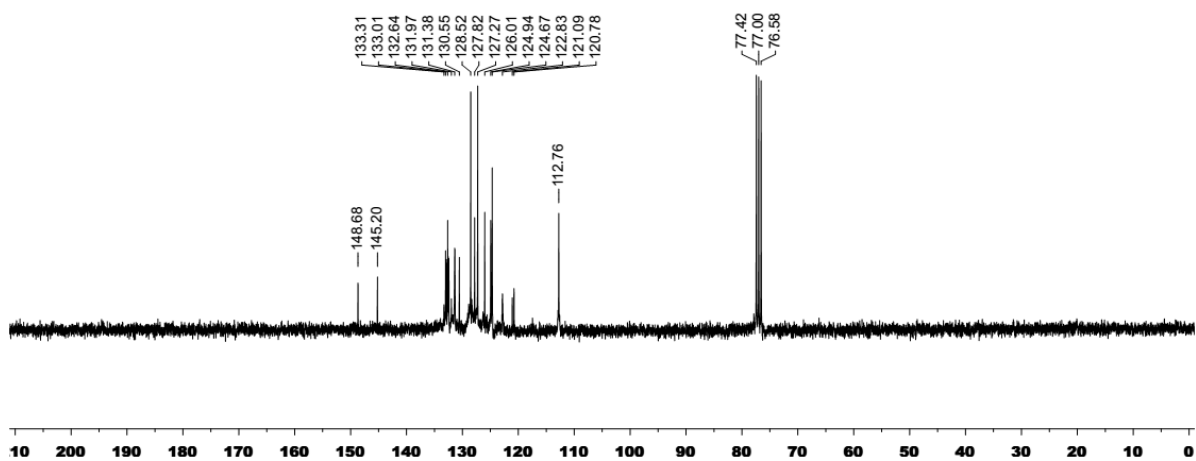
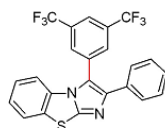
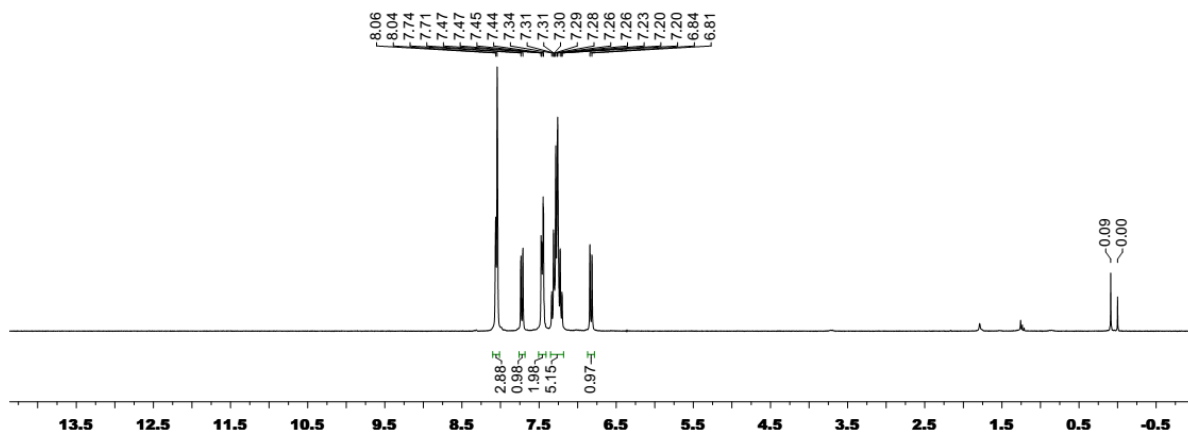
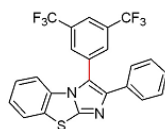
4-(2-Phenylbenzo[d]imidazo[2,1-b]thiazol-3-yl)benzonitrile (3bc)



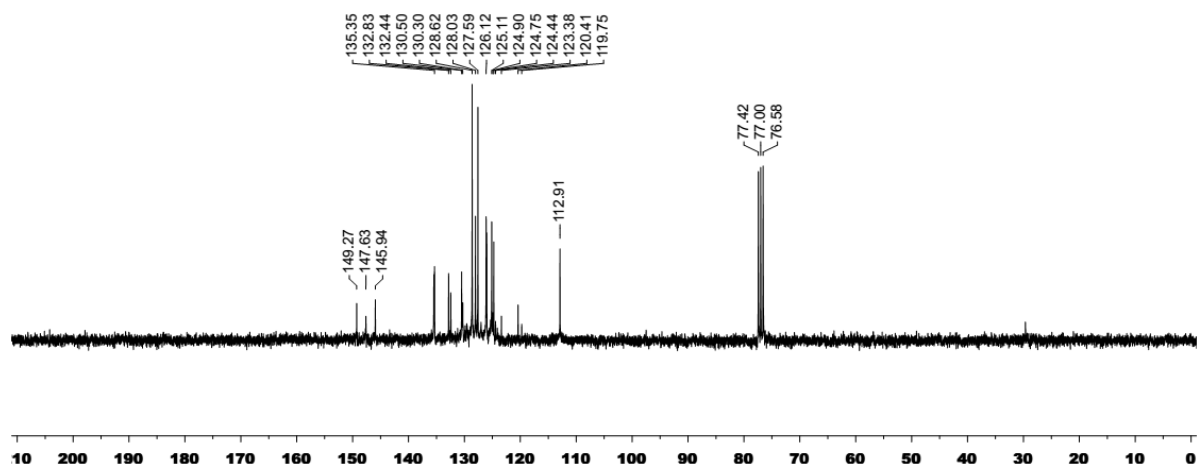
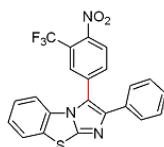
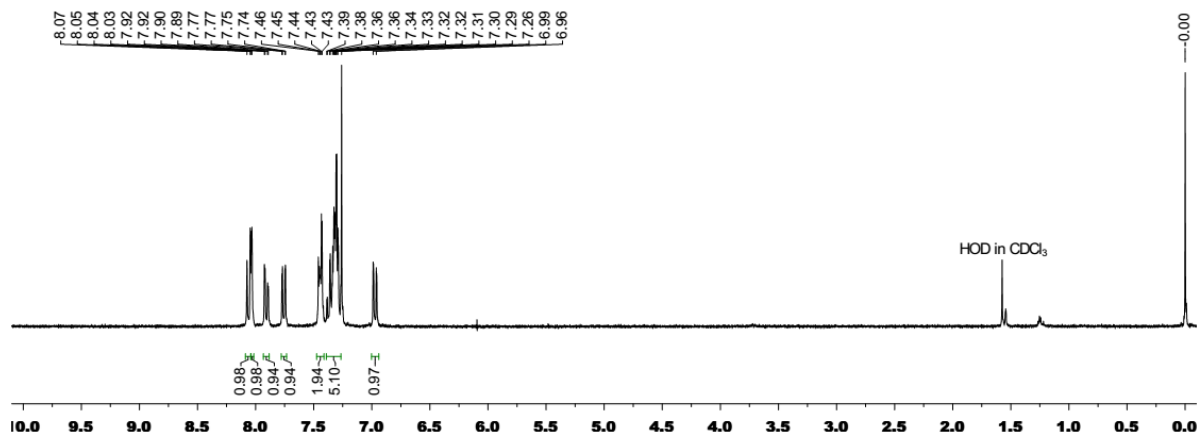
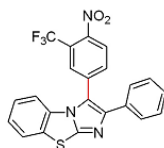
2-Phenyl-3-(4-(trifluoromethyl)phenyl)benzo[d]imidazo[2,1-b]thiazole (3bd)



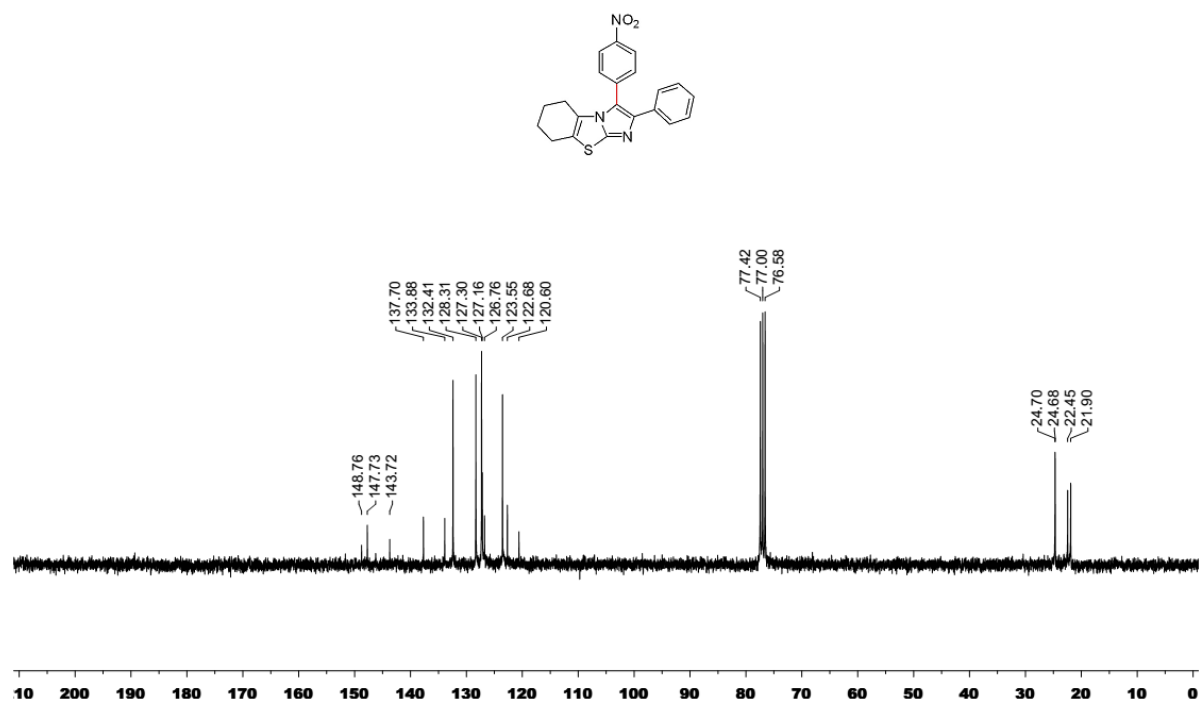
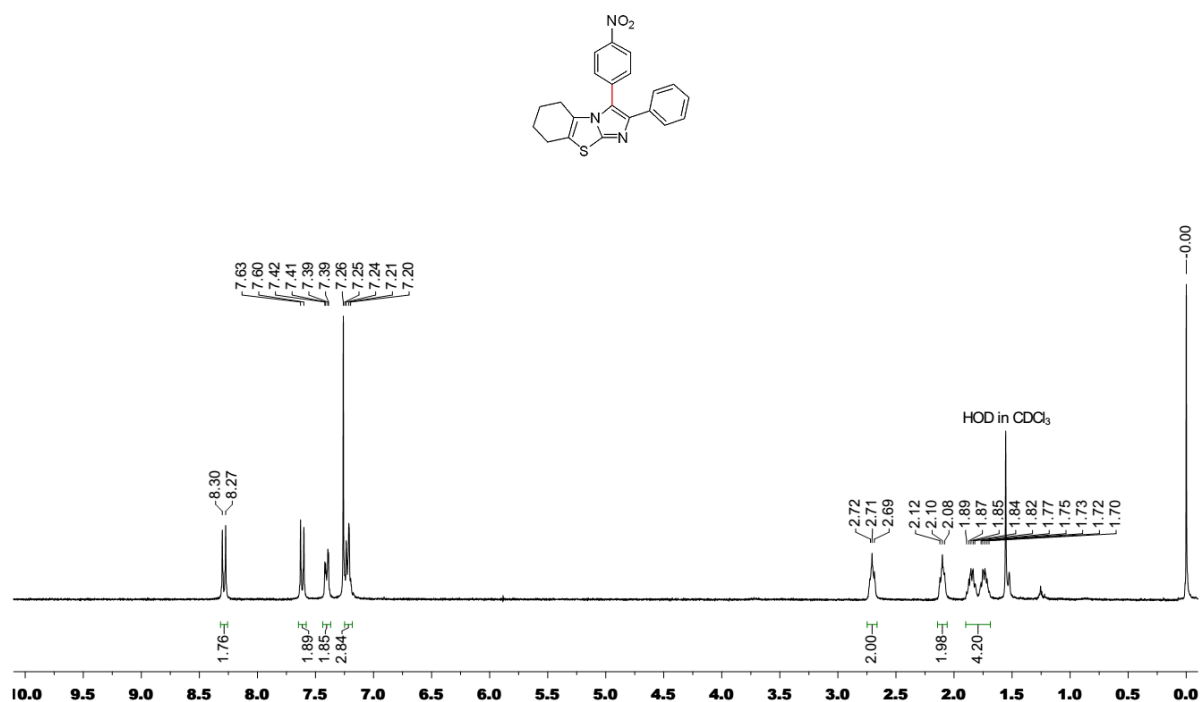
3-(3,5-Bis(trifluoromethyl)phenyl)-2-phenylbenzo[d]imidazo[2,1-b]thiazole (3be)



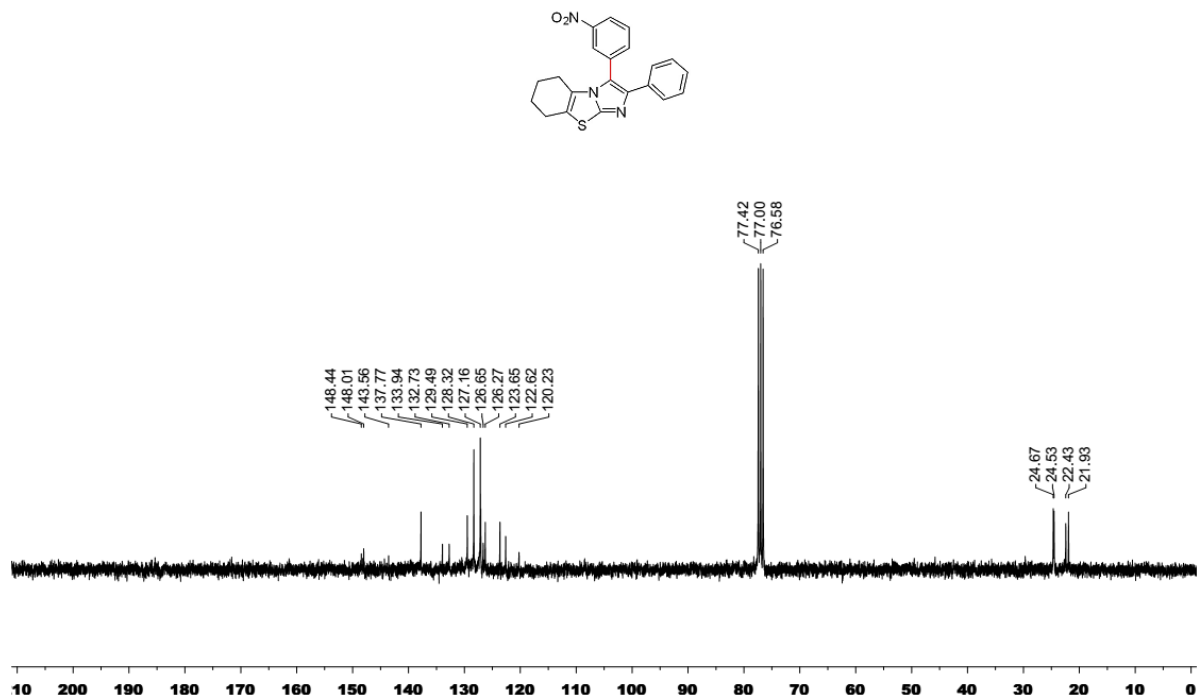
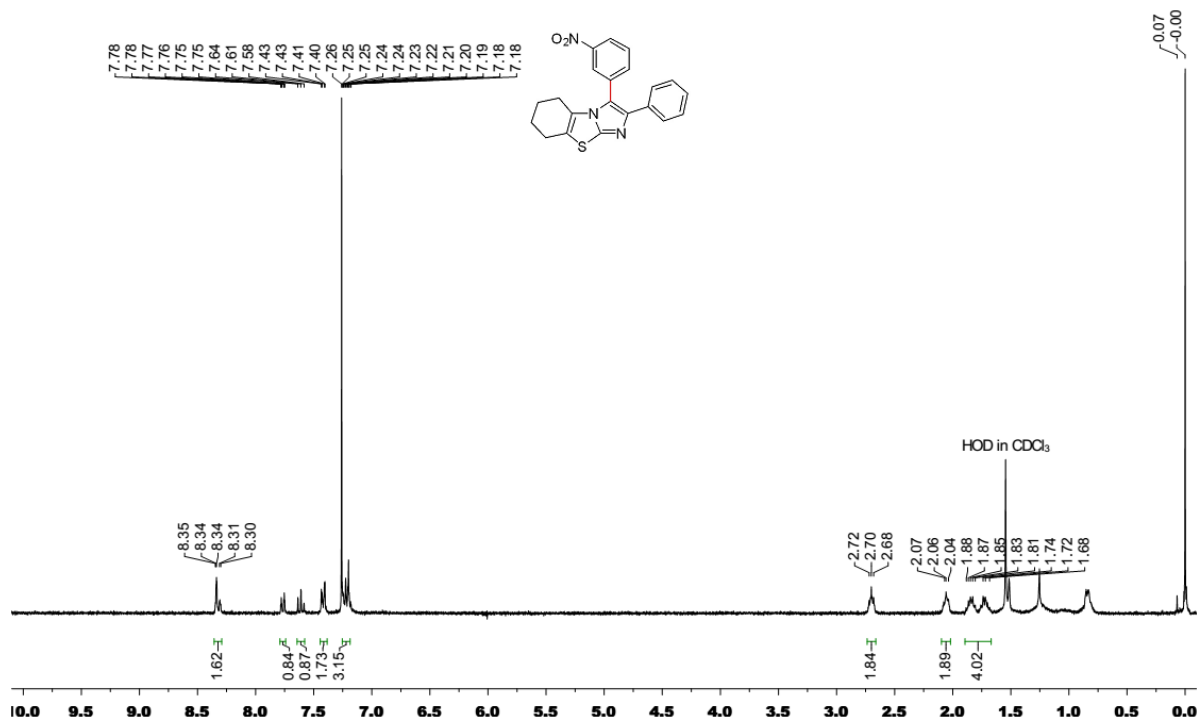
3-(4-Nitro-3-(trifluoromethyl)phenyl)-2-phenylbenzo[d]imidazo[2,1-b]thiazole (3bf)



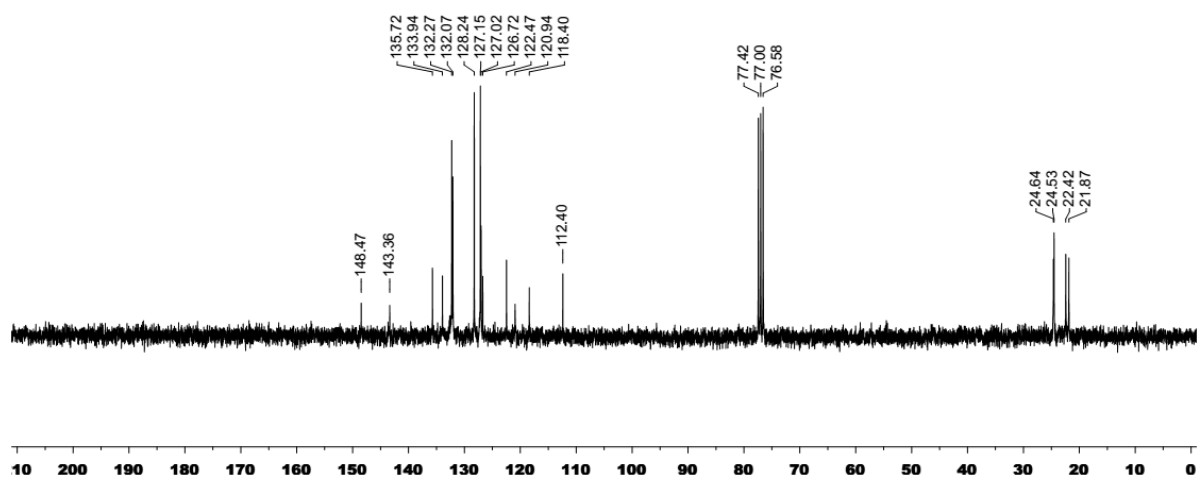
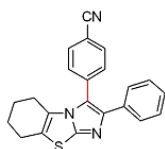
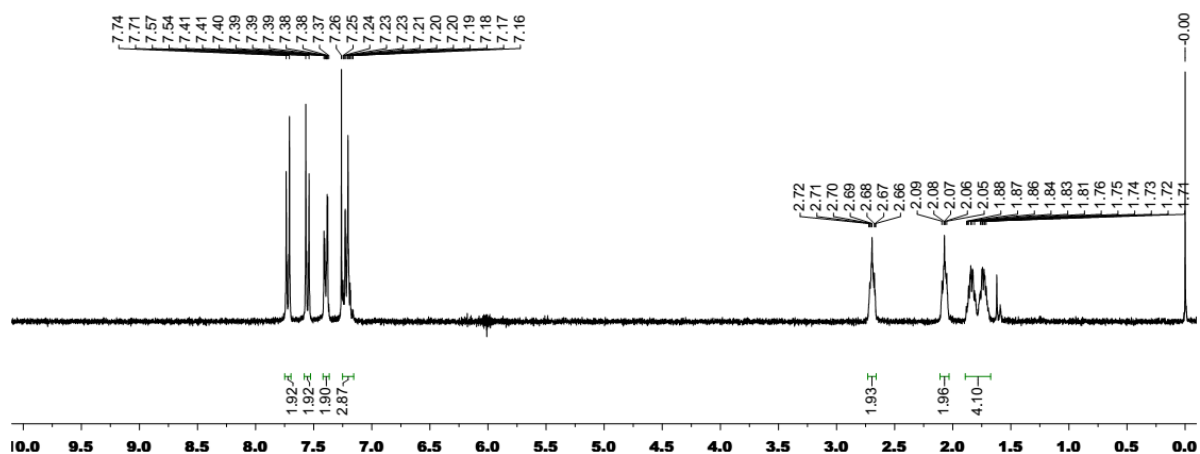
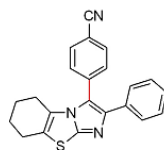
3-(4-Nitrophenyl)-2-phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole (3ca)



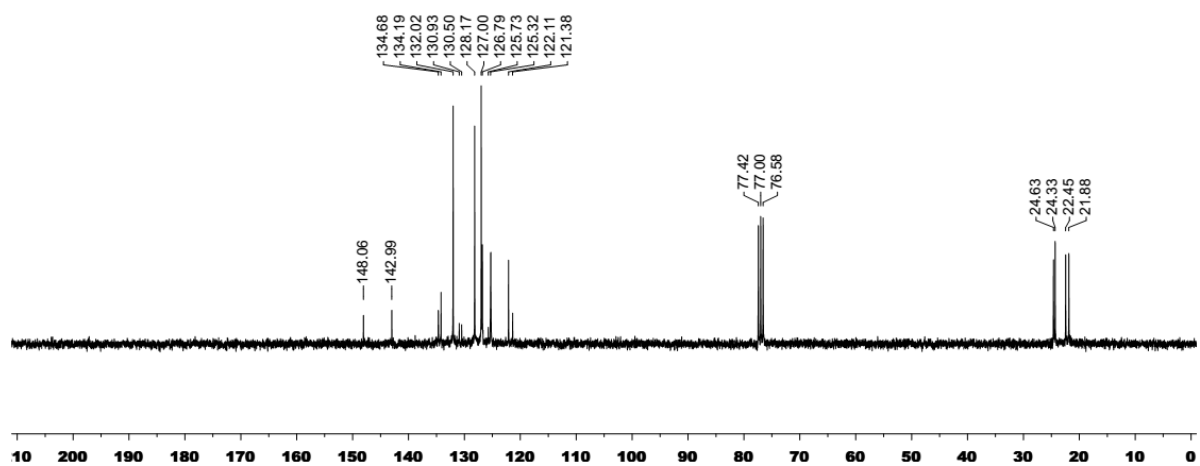
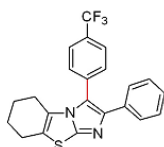
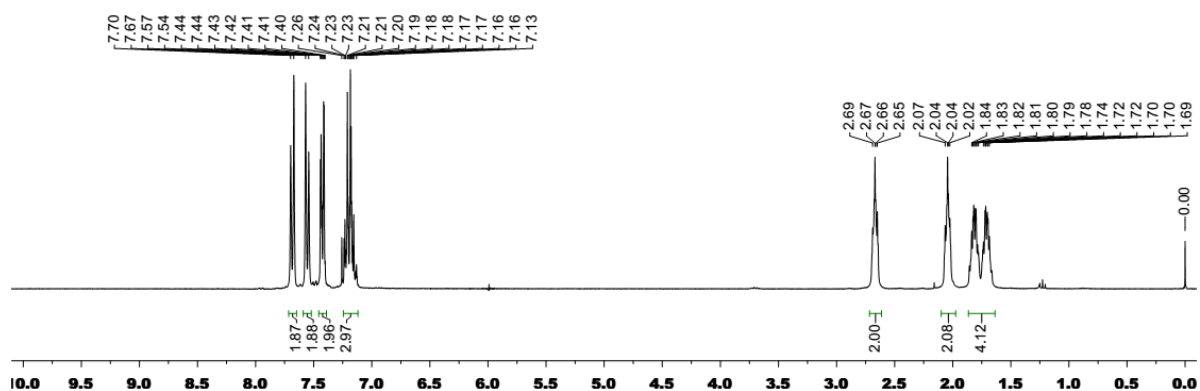
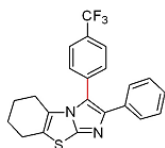
3-(3-Nitrophenyl)-2-phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole (3c)



4-(2-Phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazol-3-yl)benzotrile (3cc)

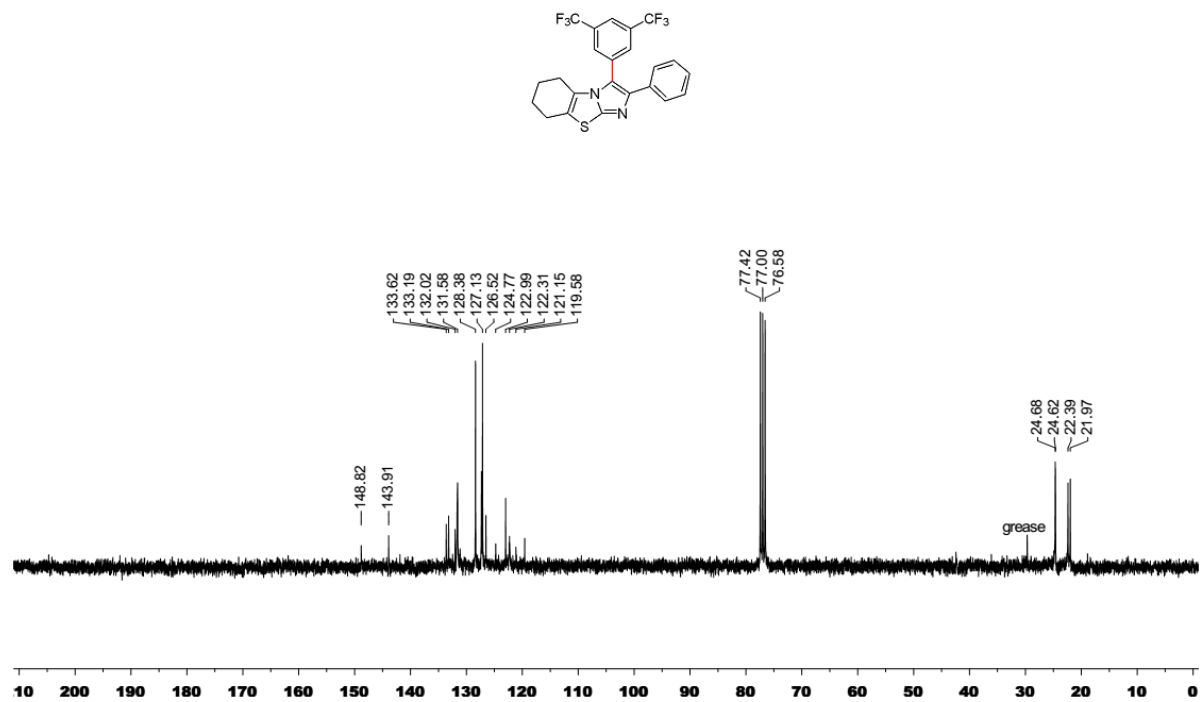
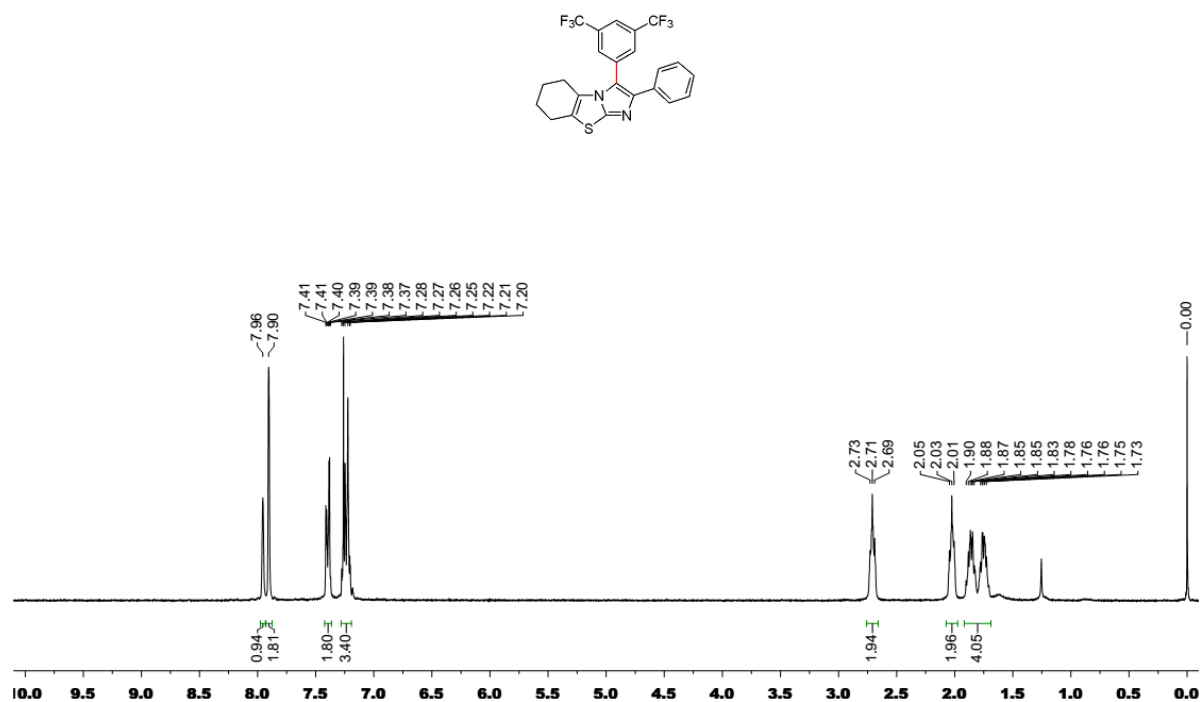


2-Phenyl-3-(4-(trifluoromethyl)phenyl)-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole (3cd)



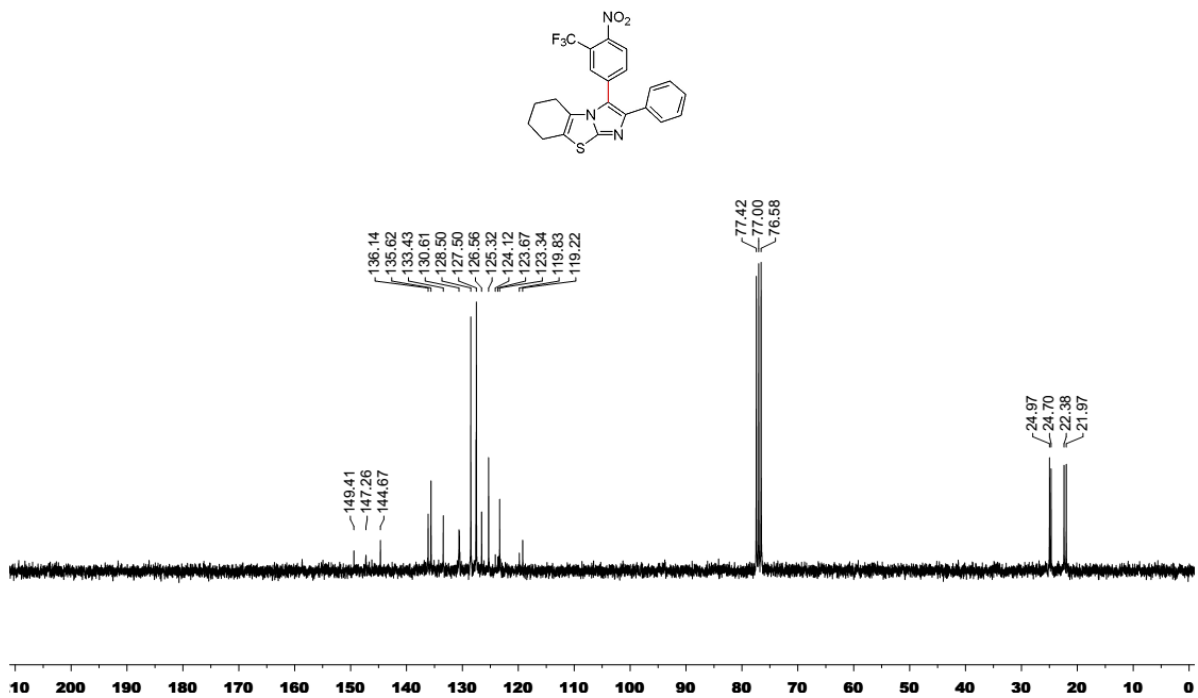
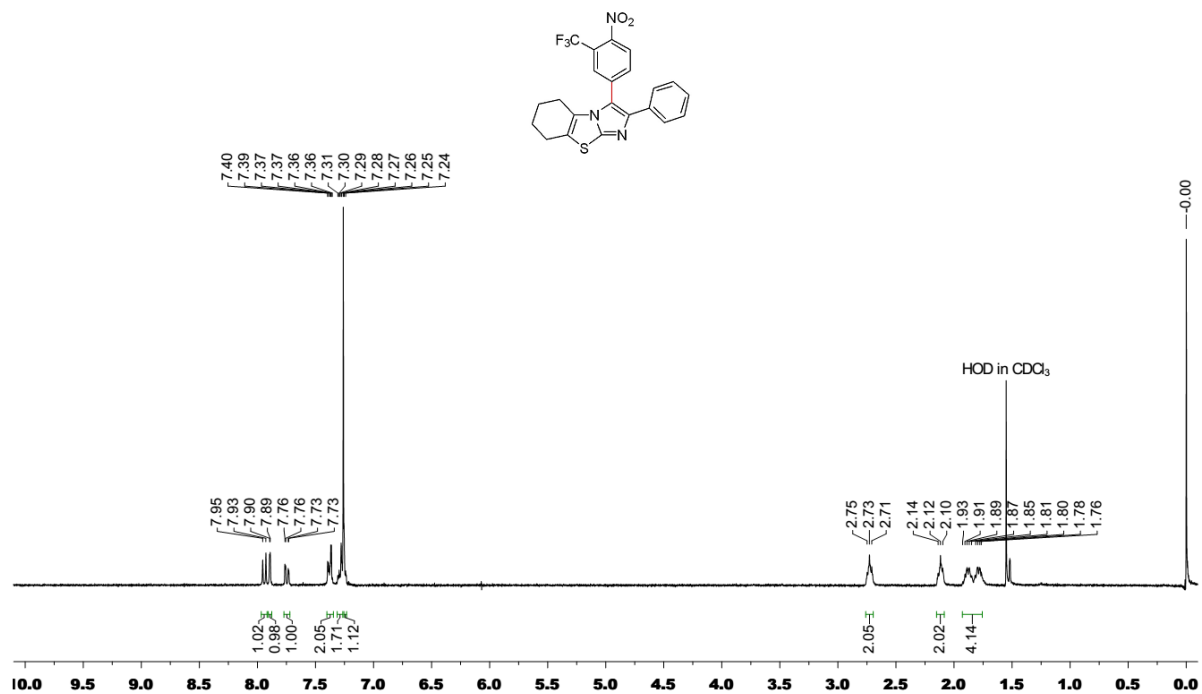
3-(3,5-Bis(trifluoromethyl)phenyl)-2-phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-b]thiazole

(3ce)

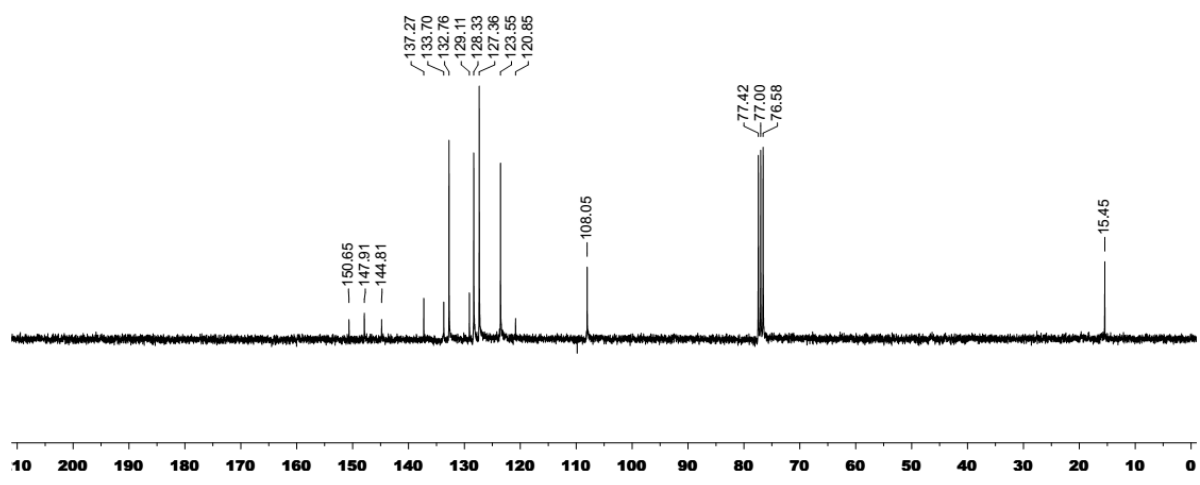
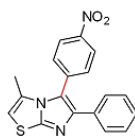
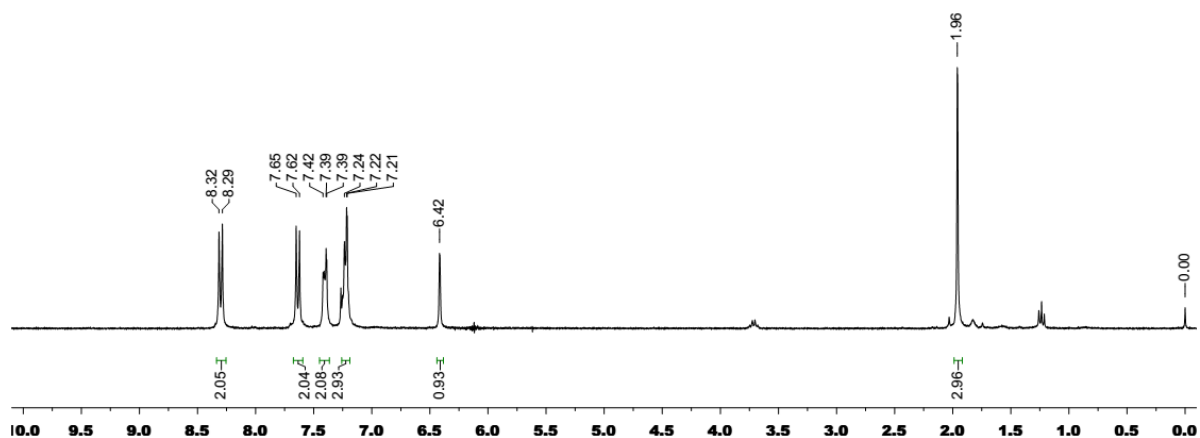
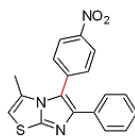


3-(4-Nitro-3-(trifluoromethyl)phenyl)-2-phenyl-5,6,7,8-tetrahydrobenzo[d]imidazo[2,1-

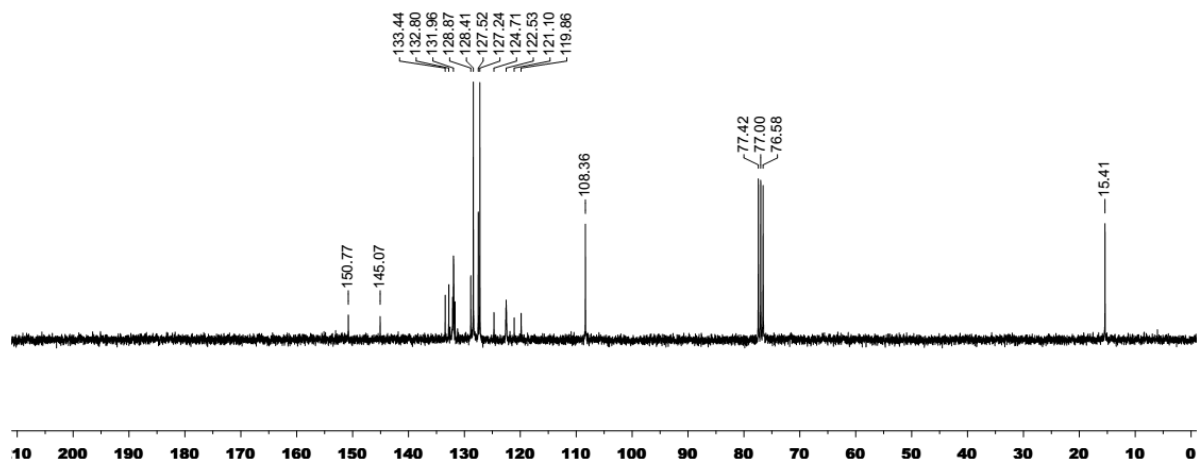
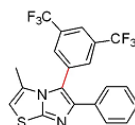
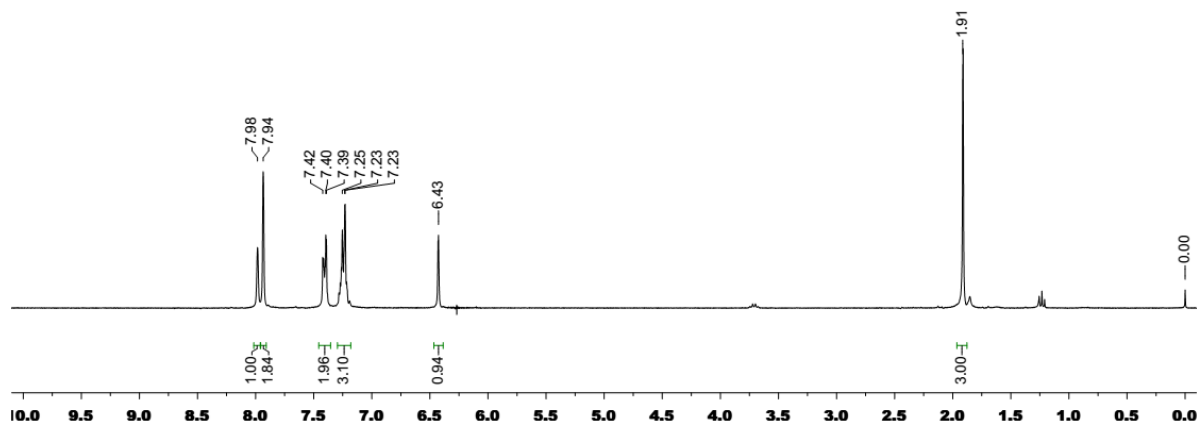
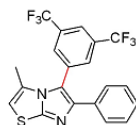
b]thiazol-e (3cf)



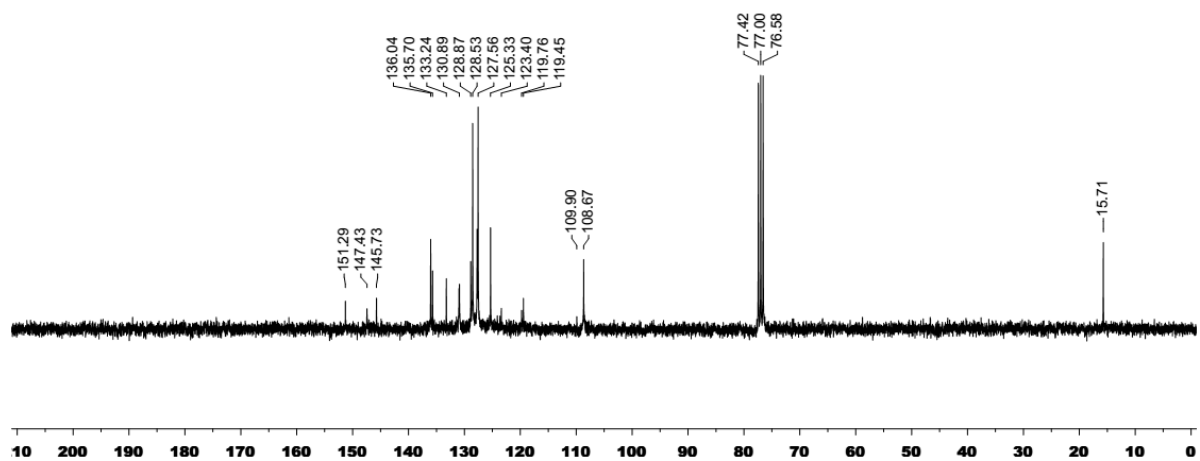
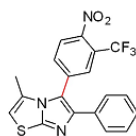
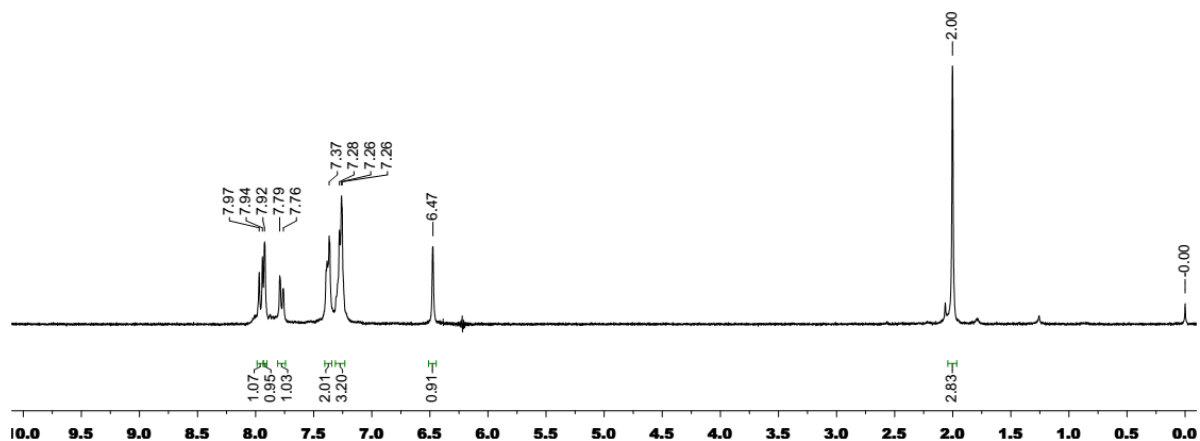
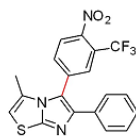
3-Methyl-5-(4-nitrophenyl)-6-phenylimidazo[2,1-b]thiazole (3da)



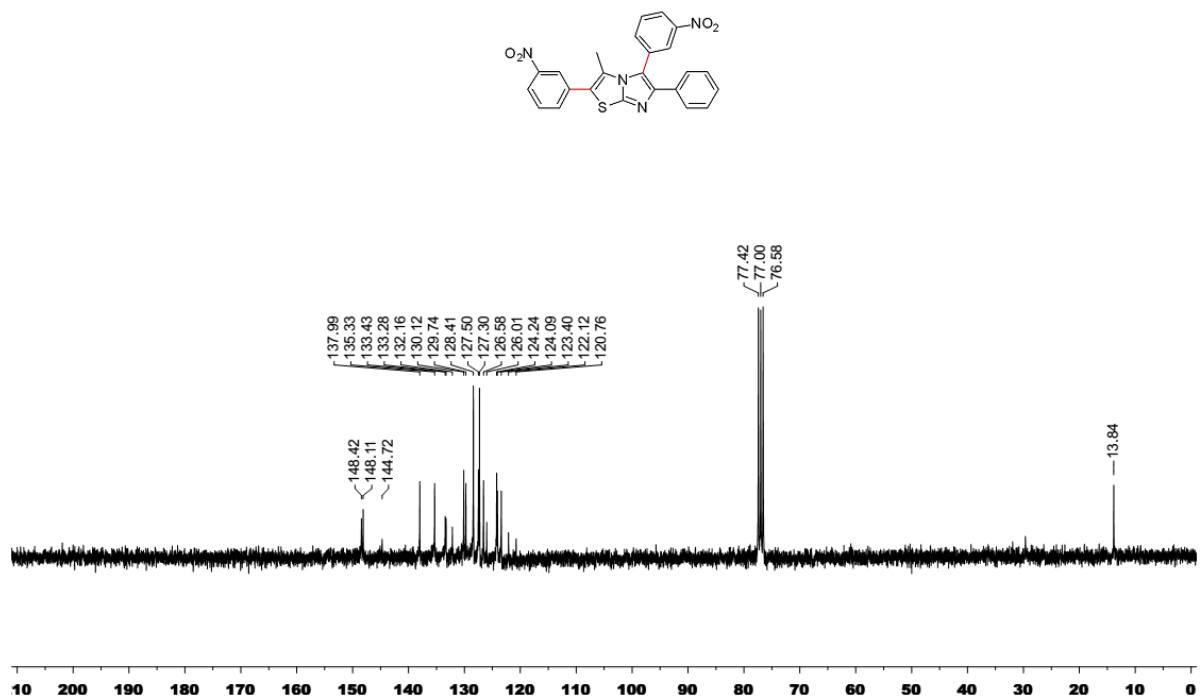
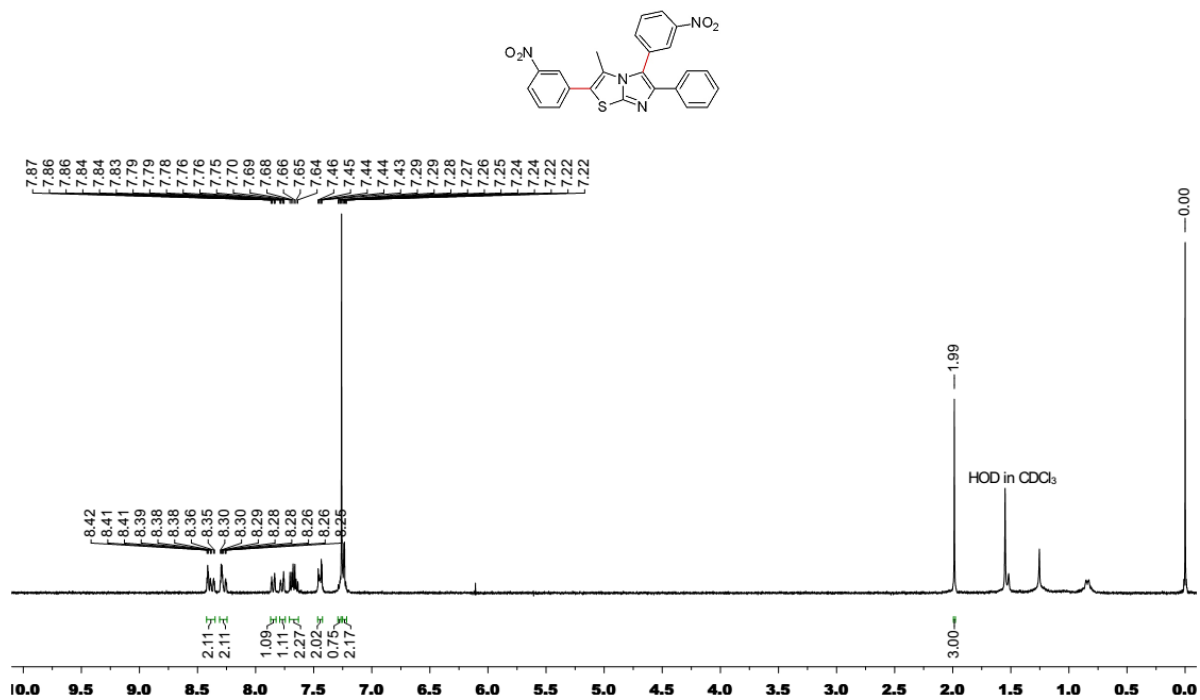
5-(3,5-Bis(trifluoromethyl)phenyl)-3-methyl-6-phenylimidazo[2,1-b]thiazole (3db)



3-Methyl-5-(4-nitro-3-(trifluoromethyl)phenyl)-6-phenylimidazo[2,1-b]thiazole (3dc)



3-Methyl-2,5-bis(3-nitrophenyl)-6-phenylimidazo[2,1-b]thiazole (3dd)



5. References

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