

Supplementary data

Ligand-free Copper(I)-Catalysed Intramolecular Direct C-H Functionalization Of Azaheterocycles

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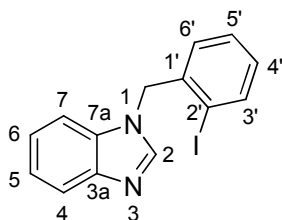
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General Remarks

General procedures.

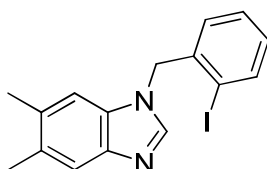
All reagents were purchased and used as received. Chemical shifts (δ) are given in ppm downfield from Me₄Si and refer as internal standard to the residual solvent CDCl₃: (δ = 7.26 for ¹H and 77.0 for ¹³C). Coupling constants, *J*, are reported in hertz (Hz). Melting points were determined in a capillary tube and are uncorrected. TLC was carried out on SiO₂, and the spots were located with UV light. Flash chromatography was carried out on SiO₂. Drying of organic extracts during work-up of reactions was performed over anhydrous Na₂SO₄. Evaporation of solvents was accomplished with a rotatory evaporator.

General Procedure for the *N*-benzylation¹

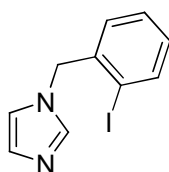


Preparation of 1-(2-Iodobenzyl)-1*H*-benzo[*d*]imidazole (1a). Commercial DMSO (13.5 mL) was added to previously crushed KOH (760 mg, 13.5 mmol) and the solution was stirred vigorously for 5 minutes. After adding the benzimidazole (807.7 mg, 6.89 mmol) the mixture was stirred for additional 45 minutes. Then, 2-iodobenzyl bromide (2.5 g, 8.46 mmol) was added and the resulting mixture was stirred for 2 h. The reaction was quenched with distilled water (15 mL) and the aqueous layer was extracted with Et₂O (3x20 mL). The combined organic layers were washed with distilled H₂O, and dried over anhydrous Na₂SO₄. The solvent was concentrated *in vacuo* and the resulting brown oily residue was redissolved and purified by flash chromatography (AcOEt) affording the title **1a** compound as a white solid. (1.79 g, 78%). Mp 102-104°C; IR_{max}(film)/cm⁻¹ 1202, 1360, 1496, 3048; ¹H NMR (300 MHz, CDCl₃, SiMe₄) (δ _H, ppm): 5.29 (s, 2H, CH₂), 6.68 (d, *J*=7.5 Hz, 1H, H_{arom}), 6.97 (apparent t, *J*=7.4 Hz, 1H, H_{arom}),

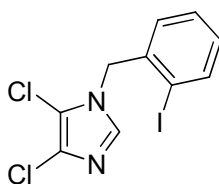
7.15-7.30 (m, 4H, H_{arom}), 7.83-7.90 (m, 3H, H_{arom}); ¹³C-NMR (75 MHz, CDCl₃, SiMe₄) (δ_C, ppm) 53.4 (CH₂), 97.6 (C_{arom}-I), 109.8 (C₇), 120.3, 122.2, 123.0, 127.8, 128.6, 129.7 (C_{arom}-H), 133.6 (C_{7a}), 137.5 (C_{arom}-C), 139.6 (C_{3'}), 143.2 (C₂), 143.7 (C_{1'}); MS-EI (CI) m/z 335 (M+1, 100), 334 (M⁺, 20), 237 (17), 235 (11), 217 (14), 209 (75), 208 (35), 207 (41); HRMS (CI) calculated for C₁₄H₁₂IN₂ 335.0045, found 335.0036.



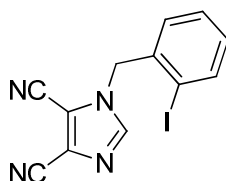
1-(2-Iodobenzyl)-5,6-dimethyl-1H-benzo[d]imidazole (1b) (63%): Mp: 120-122°C; IR_{max}(film)/cm⁻¹ 1490, 1432; ¹H NMR (300 MHz, CDCl₃, SiMe₄) (δ_H, ppm): 2.34 (s, 3H, CH₃), 2.38 (s, 3H, CH₃), 5.30 (s, 2H, CH₂), 6.66 (d, *J*=7.7 Hz, 1H, H_{arom}), 6.98-7.03 (m, 2H, H_{arom}), 7.21 (d, *J*=7.5 Hz, 1H, H_{arom}), 7.61 (s, 1H, H₄, H₇), 7.82 (s, 1H, H₂), 7.90 (d, *J*=7.8 Hz, 1H, H₂); ¹³C-NMR (75 MHz, CDCl₃, SiMe₄) (δ_C, ppm) 20.2, 20.5 (CH₃), 53.5 (CH₂), 97.4 (C_{arom}-I), 110.0 (C₇), 120.4, 127.8, 128.8, 129.7 (C_{arom}-H), 131.3, 132.3, 132.4, 137.8 (C_{arom}-C), 139.7 (C_{3'}), 142.4 (C_{1'}), 142.6 (C₂); MS-EI (CI) m/z 363 (M+1, 100), 362 (M⁺, 38); HRMS (CI) calculated for C₁₆H₁₆IN₂ 363.0358, found 363.0341.



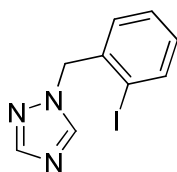
1-(2-Iodobenzyl)-1H-imidazole (1c) (66%): Mp: 55-57°C. The experimental data were compared to those reported on the bibliography.²



4,5-Dichloro-1-(2-iodobenzyl)-1H-imidazole (1d) (33%): Mp: 71-73°C; IR_{max}(film)/cm⁻¹ 1249, 1420, 1473, 1508; ¹H NMR (300 MHz, CDCl₃, SiMe₄) (δ_H, ppm): 5.10 (s, 2H, CH₂), 6.83 (d, *J*=7.6 Hz, 1H, H_{arom}), 7.05 (apparent t, *J*=7.6 Hz, 1H, H_{arom}), 7.32-7.37 (m, 2H, H_{arom}), 7.90 (d, *J*=7.9 Hz, 1H, H_{3'}); ¹³C-NMR (75 MHz, CDCl₃, SiMe₄) (δ_C, ppm) 54.4 (CH₂), 97.8 (C_{arom}-I), 113.7, 16.5 (C_{arom}-Cl), 128.2, 129.0, 130.2, 134.6 (C_{arom}-H), 136.6 (C_{1'}), 139.9 (C₂); HRMS (CI) calculated for C₁₀H₈ICl₂N₂ 352.9109, found 352.9097.

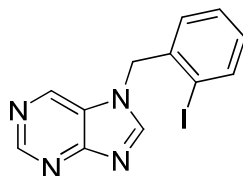


1-(2-Iodobenzyl)-1H-imidazole-4,5-dicarbonitrile (1e) (48%): Mp: 172-174°C; IR_{max}(film)/cm⁻¹ 1414, 1525, 1672, 2226; ¹H NMR (300 MHz, DMSO-d₆, SiMe₄) (δ_H, ppm): 5.45 (s, 2H, CH₂), 6.57 (d, *J*=7.0 Hz, 1H, H_{arom}), 7.06-7.11 (m, 1H, H_{arom}), 7.33-7.39 (m, 1H, H_{arom}), 7.90-7.95 (m, 1H, H_{arom}), 8.06 (s, 1H, H₂); ¹³C-NMR (75 MHz, DMSO-d₆, SiMe₄) (δ_C, ppm) 54.1 (CH₂), 97.7 (C_{arom}-I), 113.8, 114.4 (C≡N) 127.1, 128.8, 129.8 (C_{arom}-H), 134.5, 138.3 (C_{arom}-C), 139.3 (C_{arom}-H), 142.0 (C₂), 159.2 (C_{arom}-C); MS-EI (CI) m/z 335 (M+1, 5), 286 (100), 266 (32), 217 (12); HRMS (CI) calculated for C₁₂H₈IN₄ 334.9794, found 334.9794.

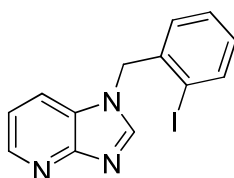


1-(2-Iodobenzyl)-1H-1,2,4-triazole (1f) (56%): Mp: 59-61°C; IR_{max}(film)/cm⁻¹ 1014, 1132, 1273, 1502, 3131; ¹H NMR (300 MHz, CDCl₃, SiMe₄) (δ_H, ppm): 5.31 (s, 2H, CH₂), 6.91 (apparent dt, *J*=7.8, 7.7, 1.6 Hz, 1H, H_{arom}), 7.0 (dd, *J*=7.7, 1.4 Hz, 1H, H_{arom}), 7.24 (apparent dt, *J*=7.6, 7.5, 1.1 Hz, 1H, H_{arom}), 7.77 (dd, *J*=7.9, 1.1 Hz, 1H, H_{arom}), 7.89 (s, 1H, H₃), 8.09 (s, 1H, H₅); ¹³C-NMR (75 MHz, CDCl₃, SiMe₄) (δ_C, ppm) 57.5 (CH₂), 98.4

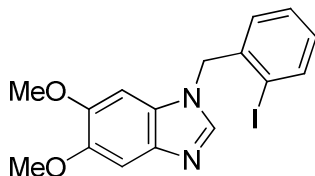
(C_{arom-I}), 128.6, 129.4, 130.0 (C_{arom-H}), 136.7 (C_{1'}), 139.5 (C_{3'}), 143.4 (C₅), 151.9 (C₃); HRMS (CI) calculated for C₉H₉IN₃ 285.9841, found 285.9841.



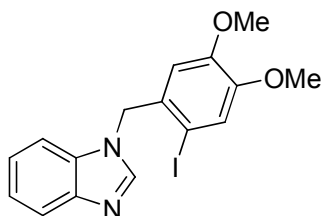
1-(2-Iodobenzyl)-1H-1,2,4-triazole (1h) (32%): Mp: 101-103°C; IR_{max}(film)/cm⁻¹ 1702, 1508, 1443, 1361, 1190; ¹H NMR (300 MHz, CDCl₃, SiMe₄) (δ_H, ppm): 5.49 (s, 2H, CH₂), 6.99-7.04 (m, 1H, H_{arom}), 7.15-7.18 (m, 1H, H_{arom}), 7.28 (apparent t, *J*=7.8 Hz, 1H, H_{arom}), 7.87 (d, *J*=7.9 Hz, 1H, H_{arom}), 8.14 (s, 1H, H₂), 8.98 (s, 1H, H₅), 9.13 (s, 1H, H₇); ¹³C-NMR (75 MHz, CDCl₃, SiMe₄) (δ_C, ppm) 51.7 (CH₂), 98.7 (C_{arom-I}), 128.9, 129.6, 130.3 (C_{arom-H}), 133.7, 137.1 (C_{arom-C}), 139.9 (C_{3'}), 145.0 (C₇), 148.7 (C₂), 151.4 (C_{3a}), 152.7 (C₅); MS-EI (CI) *m/z* 338 (M+2, 13), 337 (M+1, 100), 217 (10), 209 (21); HRMS (CI) calculated for C₁₂H₁₀IN₄ 336.9950, found 336.9939.



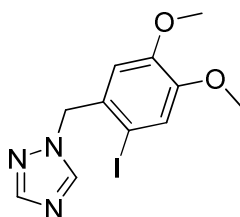
1-(2-Iodobenzyl)-1H-imidazo[4,5-*b*]pyridine (1i) (35%): Mp: 120-122°C (from hexane); IR_{max}(KBr)/cm⁻¹ 1191, 1279, 1396, 1484; ¹H NMR (300 MHz, CDCl₃, SiMe₄) (δ_H, ppm): 5.48 (s, 2H, CH₂), 6.92-7.01 (m, 2H, H_{arom}), 7.18-7.24 (m, 2H, H_{arom}), 7.83 (d, *J*=7.8 Hz, 1H, H_{arom}), 8.04-8.07 (m, 2H, H_{arom}), 8.37-8.39 (m, 1H, H_{arom}); ¹³C NMR (75 MHz, CDCl₃, SiMe₄) (δ_C, ppm): 51.6 (CH₂), 98.3 (C_{arom-I}), 118.3, 127.9, 128.6, 128.9, 129.8 (C_{arom-H}), 135.0, 137.9 (C_{arom-C}), 139.6, 143.8, 144.4 (C_{arom-H}), 146.9 (C_{arom-C}); MS (CI) *m/z*: 337 (M+2, 14), 336 (M+1, 100), 282 (18, 11), 208 (43). HRMS (CI) [M+1]: calculated for C₁₃H₁₁N₃I, 335.9998; found, 335.9982.



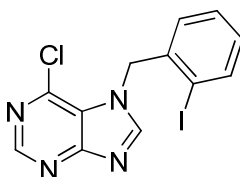
1-(2-Iodobenzyl)-5,6-dimethoxy-1H-benzo[d]imidazole (1k) (75%): Mp: 158-161°C (from hexane); IR_{max}(KBr)/cm⁻¹ 3072, 1490, 1237; ¹H NMR (300 MHz, CDCl₃, SiMe₄) (δ_H, ppm): 3.74 (s, 3H, OCH₃), 3.83 (s, 3H, OCH₃), 5.17 (s, 2H, CH₂), 6.61 (s, 2H, H_{arom}), 6.89 (apparent t, *J*=7.2 Hz, 1H, H_{arom}), 7.10 (apparent t, *J*=7.3 Hz, 1H, H_{arom}), 7.21 (s, 1H, H_{arom}), 7.69 (s, 1H, H_{arom}), 7.78 (d, *J*=7.7 Hz, 1H, H_{arom}); ¹³C NMR (75 MHz, CDCl₃, SiMe₄) (δ_C, ppm): 53.2 (CH₂), 55.9, 56.0 (OCH₃), 92.5 (C_{arom}-H), 97.4 (C_{arom}-C), 101.9 (C_{arom}-H), 127.2 (C_{arom}-C), 127.6, 128.5, 129.5, (C_{arom}-H), 136.9, 137.3 (C_{arom}-C), 139.3, 141.4 (C_{arom}-H), 146.5, 147.3 (C_{arom}-OCH₃); MS (CI) *m/z*: 395 (M+1, 100), 394 (M⁺, 51), 269 (24). HRMS (CI) [M+1]: calculated for C₁₆H₁₆IN₂O₂, 395.0257; found, 395.0245.



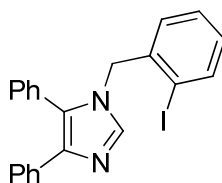
1-(2-Iodo-4,5-dimethoxybenzyl)-1H-benzo[d]imidazole (1l) (82%): Mp: 136-138°C (from hexane); IR_{max}(KBr)/cm⁻¹ 1496, 1255, 1202; ¹H NMR (300 MHz, CDCl₃, SiMe₄) (δ_H, ppm): 3.60 (s, 3H, OCH₃), 3.87 (s, 3H, OCH₃), 5.32 (s, 2H, CH₂), 6.38 (s, 1H, H_{arom}), 7.26-7.32 (m, 4H, H_{arom}), 7.82-7.85 (m, 1H, H_{arom}), 7.92 (s, 1H, H_{arom}); ¹³C NMR (75 MHz, CDCl₃, SiMe₄) (δ_C, ppm): 53.3 (CH₂), 55.7, 56.1 (OCH₃), 86.3 (C_{arom}-I), 110.0, 111.3, 120.3, 121.8, 122.3, 123.1 (C_{arom}-H), 129.6, 133.7 (C_{arom}-C), 143.0 (C_{arom}-H), 143.7, 149.4, 149.7 (C_{arom}-C); MS (CI) *m/z*: 395 (M+1, 46), 394 (M⁺, 27), 277 (100), 268 (25). HRMS (CI) [M+1]: calculated for C₁₆H₁₆N₂O₂I, 395.0257; found, 395.0242.



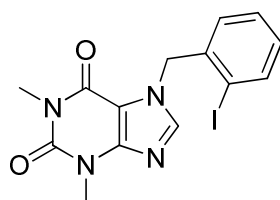
1-(2-Iodo-4,5-dimethoxybenzyl)-1H-1,2,4-triazole (1m) (17%): Mp: 101-103°C (from hexane); IR max(KBr)/cm^{-1} 3566, 1504, 1262, 1210, 1158; $^1\text{H NMR}$ (300 MHz, CDCl_3 , SiMe_4) (δ_{H} , ppm): 3.73, 3.79 (OCH_3), 5.28 (s, 2H, CH_2), 6.71 (s, 1H, H_{arom}), 7.18 (s, 1H, H_{arom}), 7.90 (s, 1H, H_{arom}), 8.08 (s, 1H, H_{arom}); $^{13}\text{C NMR}$ (75 MHz, CDCl_3 , SiMe_4) (δ_{C} , ppm): 55.7, 56.0 (OCH_3), 57.5 (CH_2), 87.2 ($\text{C}_{\text{arom-C}}$), 112.6, 121.5 ($\text{C}_{\text{arom-H}}$), 129.0 ($\text{C}_{\text{arom-C}}$), 143.2 ($\text{C}_{\text{arom-H}}$), 149.53, 149.58 ($\text{C}_{\text{arom-OCH}_3}$), 151.9 ($\text{C}_{\text{arom-H}}$); MS (CI) m/z : 346 ($\text{M}+1$, 10), 345 (M^+ , 5), 277 (100). HRMS (CI) [$\text{M}+1$]: calculated for $\text{C}_{11}\text{H}_{13}\text{IN}_3\text{O}_2$, 346.0053; found, 346.0039.



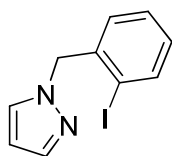
6-Chloro-7-(2-iodobenzyl)-7H-purine (31%): Mp: 89-91°C (from hexane); IR max(KBr)/cm^{-1} 1570, 1561, 1437, 1337, 1173; $^1\text{H NMR}$ (300 MHz, CDCl_3 , SiMe_4) (δ_{H} , ppm): 5.49 (s, 2H, CH_2), 7.06 (apparent t, $J=7.3$ Hz, 1H, H_{arom}), 7.19 (d, $J=7.1$ Hz, 1H, H_{arom}), 7.30 (apparent t, $J=7.4$ Hz, 1H, H_{arom}), 7.87 (d, $J=7.8$ Hz, 1H, H_{arom}), 8.11 (s, 1H, H_{arom}), 8.74 (s, 1H, H_{arom}); $^{13}\text{C NMR}$ (75 MHz, CDCl_3 , SiMe_4) (δ_{C} , ppm): 52.5 (CH_2), 98.8 ($\text{C}_{\text{arom-I}}$), 129.0, 129.9, 130.6 ($\text{C}_{\text{arom-H}}$), 131.4, 136.8 ($\text{C}_{\text{arom-C}}$), 140.1, 145.1 ($\text{C}_{\text{arom-H}}$), 151.1, 151.9 ($\text{C}_{\text{arom-C}}$), 152.1 ($\text{C}_{\text{arom-H}}$); MS (CI) m/z : 371 ($\text{M}+1$, 100), 335 (13), 243 (38), 217 (30). HRMS (CI) [$\text{M}+1$]: calculated for $\text{C}_{12}\text{H}_9\text{N}_4\text{ICl}$, 370.9561; found, 370.9544.



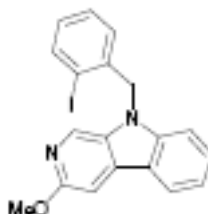
1-(2-Iodobenzyl)-4,5-diphenyl-1H-imidazole (1j) (65%): Mp: 92-94°C (from hexane); IR max(KBr)/cm^{-1} 1484, 1437, 1331, 1231; $^1\text{H NMR}$ (300 MHz, CDCl_3 , SiMe_4) (δ_{H} , ppm): 4.96 (s, 2H, CH_2), 6.76 (d, $J=7.6$ Hz, 1H, H_{arom}), 6.96 (apparent t, $J=7.6$ Hz, 1H, H_{arom}), 7.12-7.29 (m, 6H, H_{arom}), 7.34-7.38 (m, 3H, H_{arom}), 7.54 (d, $J=7.1$ Hz, 2H, H_{arom}), 7.59 (s, 1H, H_{arom}), 7.79 (d, $J=7.9$ Hz, 1H, H_{arom}); $^{13}\text{C NMR}$ (75 MHz, CDCl_3 , SiMe_4) (δ_{C} , ppm): 53.6 (CH_2), 97.3 ($\text{C}_{\text{arom-I}}$), 126.3, 126.4, 127.9, 128.0, 128.64, 128.69, 128.9, 129.5 ($\text{C}_{\text{arom-H}}$), 130.0 ($\text{C}_{\text{arom-C}}$), 130.6 ($\text{C}_{\text{arom-H}}$), 134.3 ($\text{C}_{\text{arom-C}}$), 137.1 ($\text{C}_{\text{arom-H}}$), 138.3, 138.7 ($\text{C}_{\text{arom-C}}$), 139.4 ($\text{C}_{\text{arom-H}}$); MS (CI) m/z : 438 (M+2, 22), 437 (M+1, 100), 436 (M^+ , 42), 311 (20), 310 (19), 309 (38), 308 (18). HRMS (CI) [M+1]: calculated for $\text{C}_{22}\text{H}_{18}\text{N}_2\text{I}$, 437.0515; found, 437.0500. Found C 57.5, H 3.9, N 6.0%. Calculated for $\text{C}_{22}\text{H}_{17}\text{N}_2\text{I}$: C 60.5, H 3.9, N 6.4.



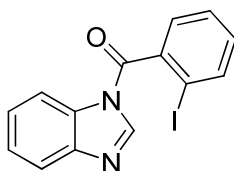
7-(2-Iodobenzyl)-1,3-dimethyl-1H-purine-2,6(3H,7H)-dione (1p) (19%): Mp: 171-173°C (from hexane); IR max(KBr)/cm^{-1} 1649, 1543, 1461, 1226; $^1\text{H NMR}$ (300 MHz, CDCl_3 , SiMe_4) (δ_{H} , ppm): 3.38 (s, 3H, CH_3), 3.57 (s, 3H, CH_3), 5.56 (s, 2H, CH_2), 7.02 (apparent t, $J=7.5$ Hz, 1H, H_{arom}), 7.15 (d, $J=7.4$ Hz, 1H, H_{arom}), 7.31 (apparent t, $J=7.45$ Hz, 1H, H_{arom}), 7.60 (s, 1H, H_{arom}), 7.87 (d, $J=7.8$ Hz, 1H, H_{arom}); $^{13}\text{C NMR}$ (75 MHz, CDCl_3 , SiMe_4) (δ_{C} , ppm): 27.9, 29.7 (CH_3), 54.5 (CH_2), 98.6, 106.9 ($\text{C}_{\text{arom-C}}$), 128.9, 129.3, 130.2 ($\text{C}_{\text{arom-H}}$), 137.6 ($\text{C}_{\text{arom-C}}$), 139.9, 141.1 ($\text{C}_{\text{arom-H}}$), 148.7, 151.5, 155.1 ($\text{C}_{\text{arom-C}}$); MS (CI) m/z : 398 (M+2, 16), 397 (M+1, 100), 396 (M^+ , 13), 269 (21). HRMS (CI) [M+1]: calculated for $\text{C}_{14}\text{H}_{14}\text{N}_4\text{I}$, 397.0162; found, 397.0153.



1-(2-iodobenzyl)-1H-pyrazole (1g) (96%): Mp: 83-85°C (from hexane); ^1H NMR (300 MHz, CDCl_3 , SiMe_4) (δ_{H} , ppm): 6.29 (s, 2H, CH_2), 6.24 (apparent t, $J=2.1$ Hz, 1H, H_{arom}), 6.78 (d, $J=7.7$ Hz, 1H, H_{arom}), 6.89 (apparent dt, $J=7.8$, 1.6 Hz, 1H, H_{arom}), 7.19 (apparent dt, $J=7.6$, 1.1 Hz, 1H, H_{arom}), 7.39 (d, $J=2.1$ Hz, 1H, H_{arom}), 7.54 (d, $J=1.3$ Hz, 1H, H_{arom}), 7.72 (dd, $J=7.9$, 1.0 Hz, 1H, H_{arom}); ^{13}C NMR (75 MHz, CDCl_3 , SiMe_4) (δ_{C} , ppm): 59.8 (CH_2), 97.7 ($\text{C}_{\text{arom-I}}$), 105.6, 128.3, 128.4, 129.1, 129.5 ($\text{C}_{\text{arom-H}}$), 138.8 ($\text{C}_{\text{arom-C}}$), 138.9, 139.4 ($\text{C}_{\text{arom-H}}$).

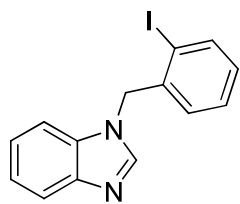


***N*-(2-Iodobenzyl)-5-methoxy-1H-indolo[2,3-*c*]pyridine (1o)** (78%): Mp: 68-70°C (from hexane); IR $_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 1492, 1241; ^1H NMR (300 MHz, CDCl_3 , SiMe_4) (δ_{H} , ppm): .93 (s, 3H, OCH_3), 5.27 (s, 2H, CH_2), 6.41 (d, $J=3.0$ Hz, 1H, H_3), 6.63 (d, $J=7.7$ Hz, 1H, H_{arom}), 6.91-6.98 (m, 2H, H_{arom}), 7.15-7.19 (m, 2H, H_{arom}), 7.85 (d, $J=7.1$ Hz, 1H, $\text{H}_{3'}$), 8.20 (s, 1H, H_7); ^{13}C NMR (75 MHz, CDCl_3 , SiMe_4) (δ_{C} , ppm): 53.9 (OCH_3), 55.3 (CH_2), 97.4 ($\text{C}_{\text{arom-I}}$), 97.8 (C_3 , C_4), 100.4 (C_4 , C_3), 127.8, 128.6, 128.8, 129.5 ($\text{C}_{\text{arom-H}}$), 130.6 ($\text{C}_{\text{arom-C}}$), 133.7 (C_7), 137.7, 138.6 ($\text{C}_{\text{arom-C}}$), 139.5 ($\text{C}_{3'}$), 158.2 ($\text{C}_{\text{arom-OCH}_3}$); MS (CI) m/z : 366 ($\text{M}+2$, 16), 365 ($\text{M}+1$, 100), 364 (46). HRMS (CI) [$\text{M}+1$]: calculated for $\text{C}_{15}\text{H}_{14}\text{IN}_2\text{O}$, 365.0151; found, 365.0140.

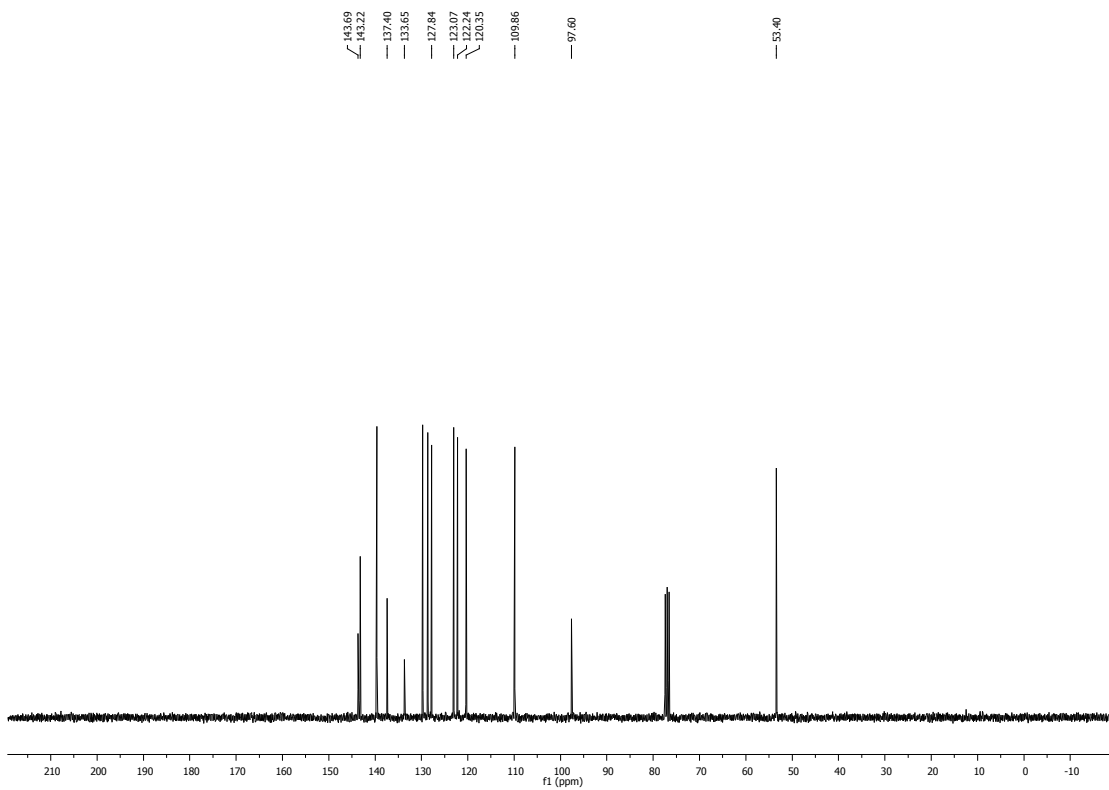
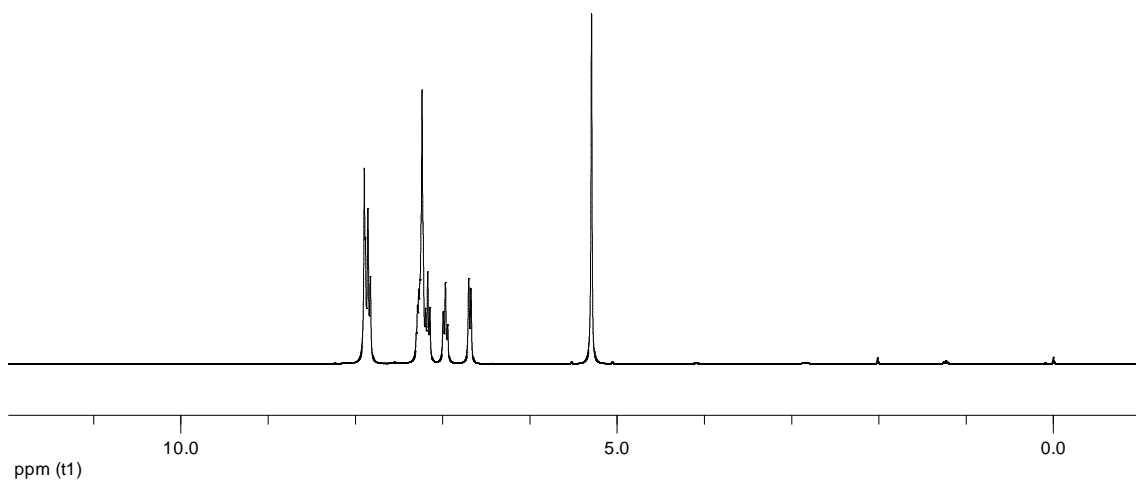


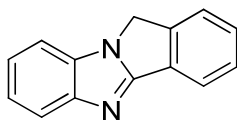
***H*-Benzo[*d*]imidazol-1-yl(2-iodophenyl)methanone (1n)** (35%): Mp: 120-122°C (from hexane); IR $_{\text{max}}(\text{KBr})/\text{cm}^{-1}$ 1191, 1279, 1396, 1484; ^1H NMR (300 MHz, CDCl_3 , SiMe_4) (δ_{H} , ppm): 7.24 (apparent t, $J=7.4$ Hz, 1H, H_{arom}), 7.37-7.52 (m, 4H, H_{arom}), 7.76-7.79 (m, 1H, H_{arom}), 7.85 (bs, 1H, H_{arom}), 7.92 (d, $J=7.9$ Hz, 1H, H_{arom}), 8.11 (d, $J=4.7$ Hz,

^1H , H_{arom}); ^{13}C NMR (75 MHz, CDCl_3 , SiMe_4) (δ_{C} , ppm): 92.3 ($\text{C}_{\text{arom-I}}$), 115.3, 120.4, 125.4, 125.8, 128.3, 128.6 ($\text{C}_{\text{arom-H}}$), 131.1 ($\text{C}_{\text{arom-C}}$), 132.3 ($\text{C}_{\text{arom-H}}$), 139.1 ($\text{C}_{\text{arom-C}}$), 139.7, 142.5 ($\text{C}_{\text{arom-H}}$), 144.1, 166.4 ($\text{C}_{\text{arom-C}}$); MS (CI) m/z : 349 ($\text{M}+1$, 100), 348 (M^+ , 21), 231 (86). HRMS (CI) [$\text{M}+1$]: calculated for $\text{C}_{14}\text{H}_{10}\text{N}_2\text{OI}$, 348.9838; found, 348.9823.

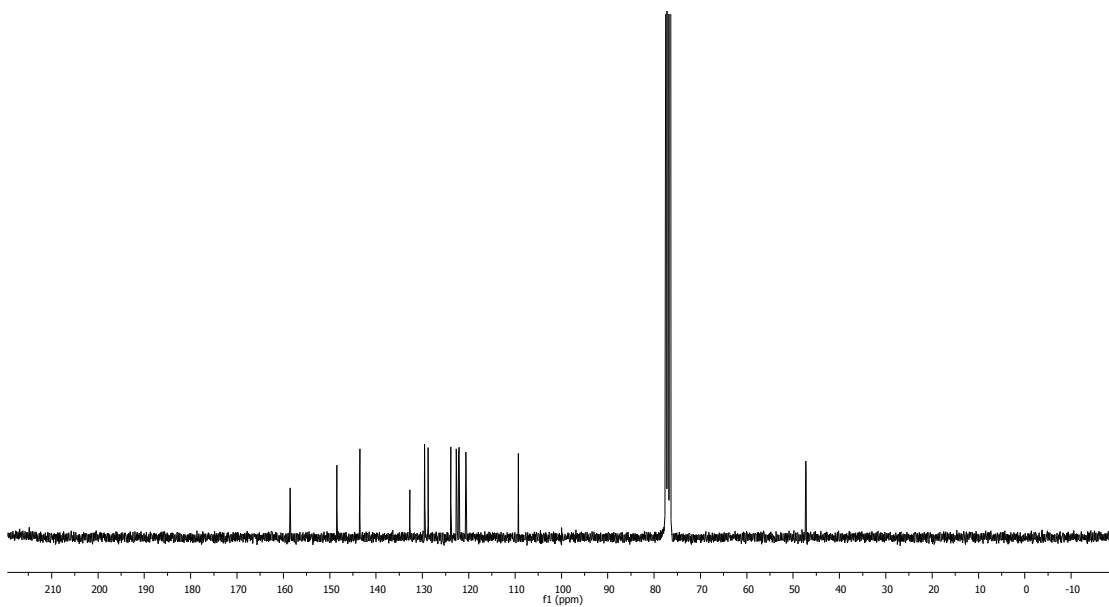
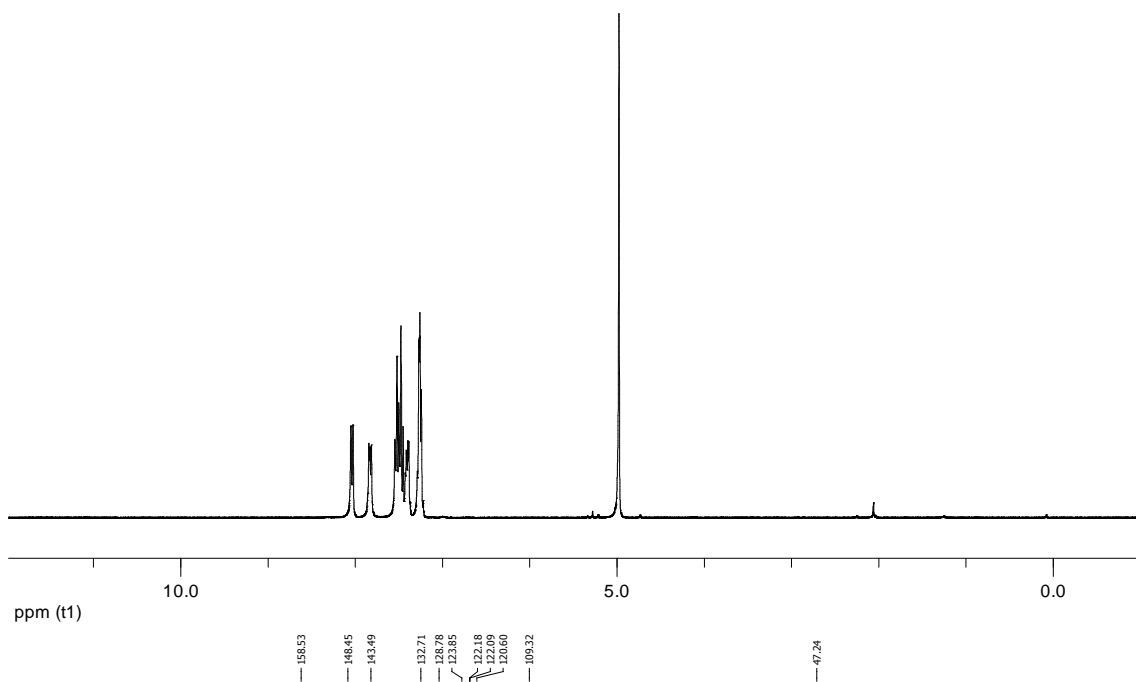


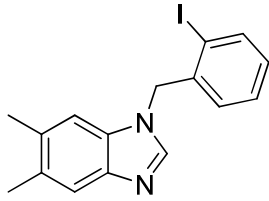
1-(2-Iodobenzyl)-1*H*-benzo[*d*]imidazole



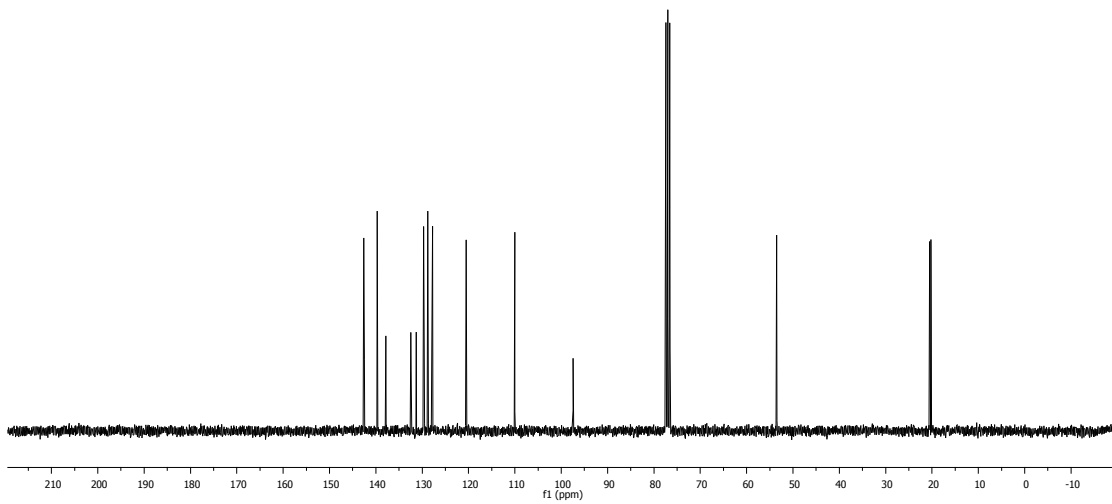
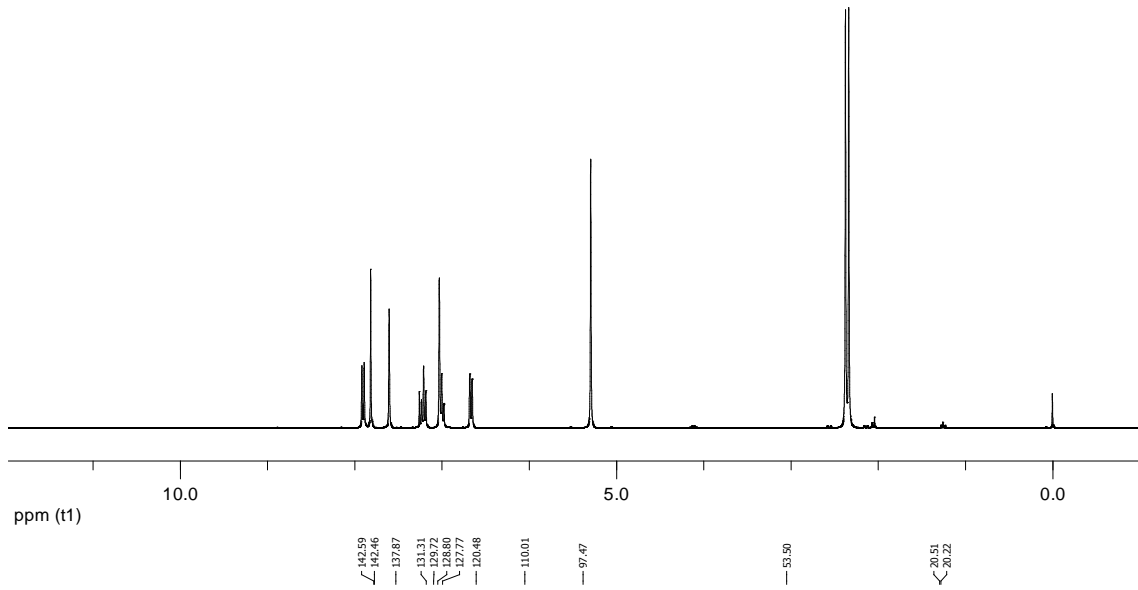


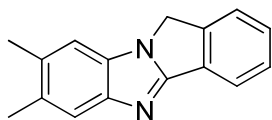
11*H*-Isoindolo[2,1-*a*]benzimidazole



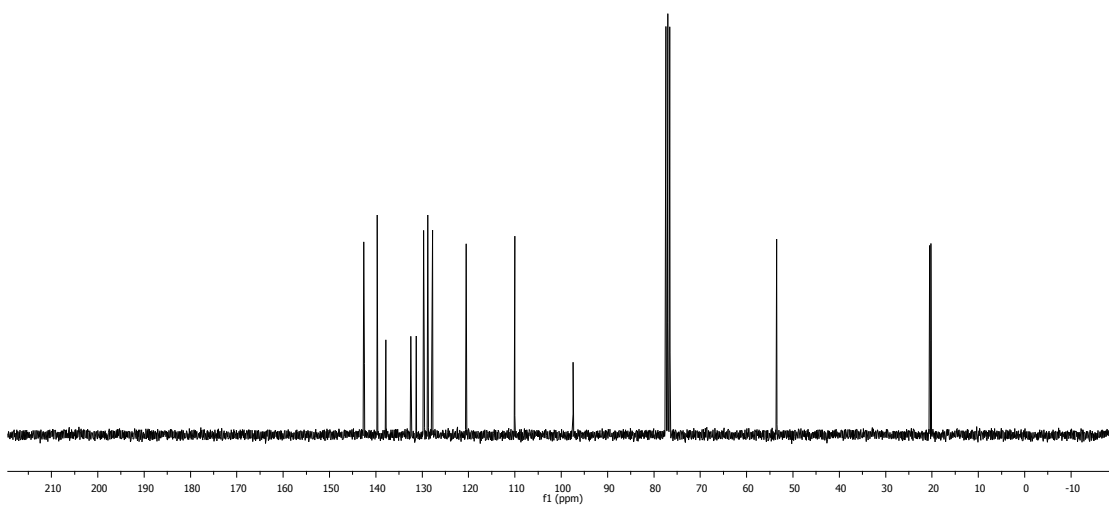
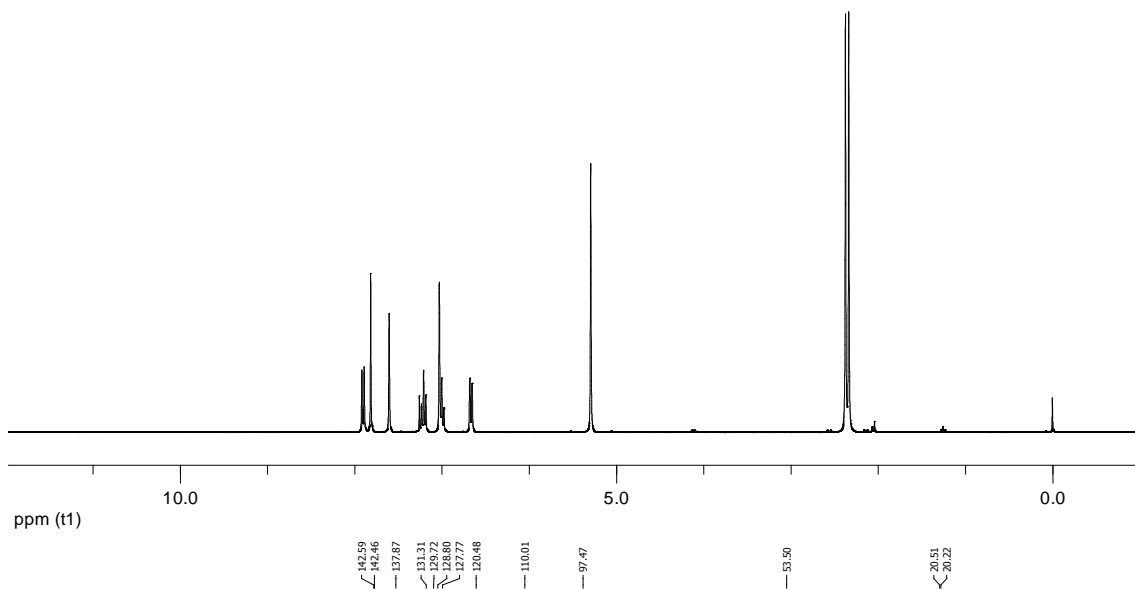


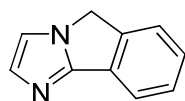
1-(2-Iodobenzyl)-5,6-dimethyl-1H-benzo[d]imidazole



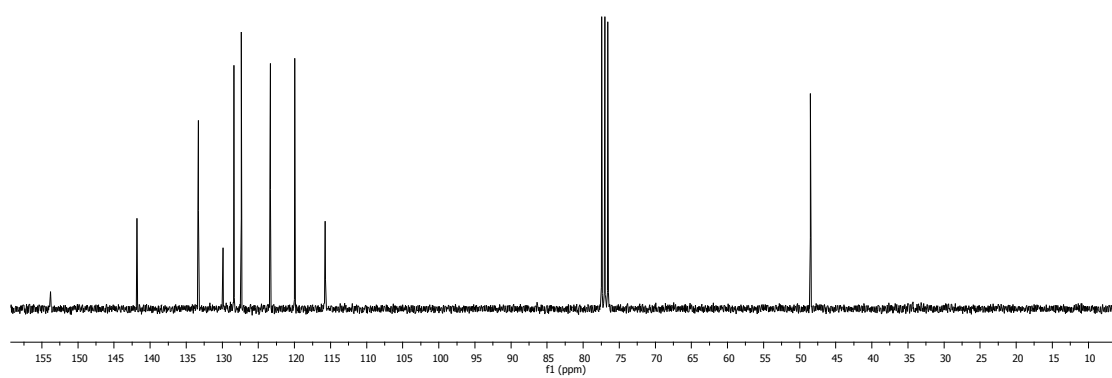
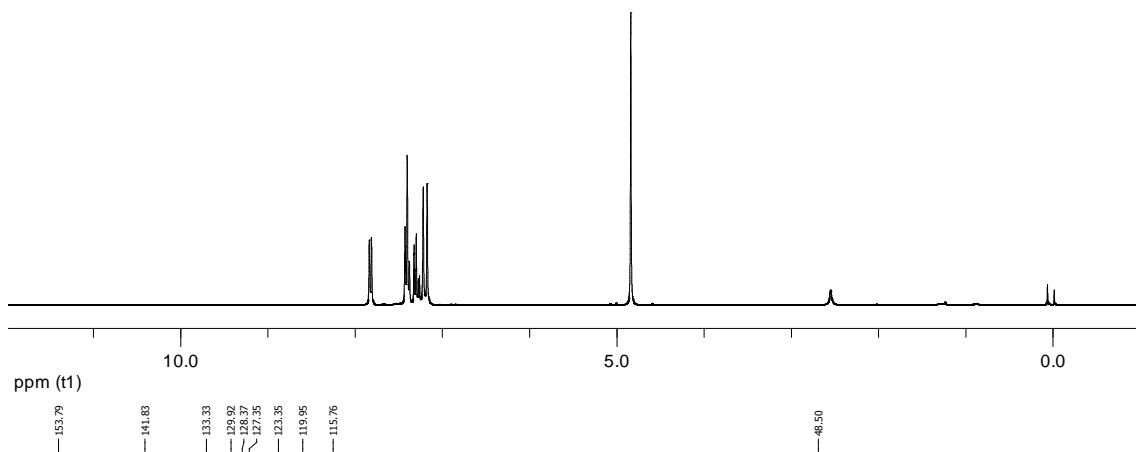


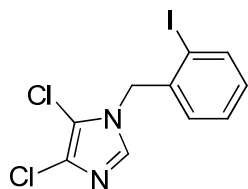
7,8-Dimethyl-11*H*-isoindolo[2,1-*a*]benzimidazole



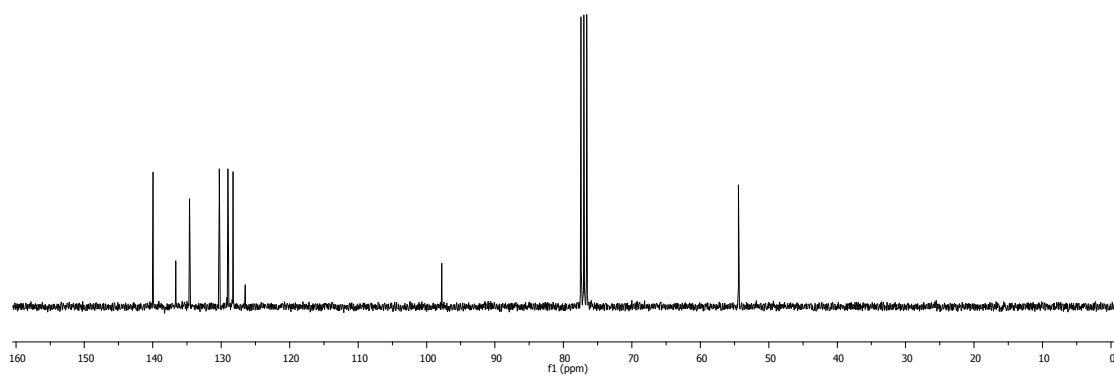
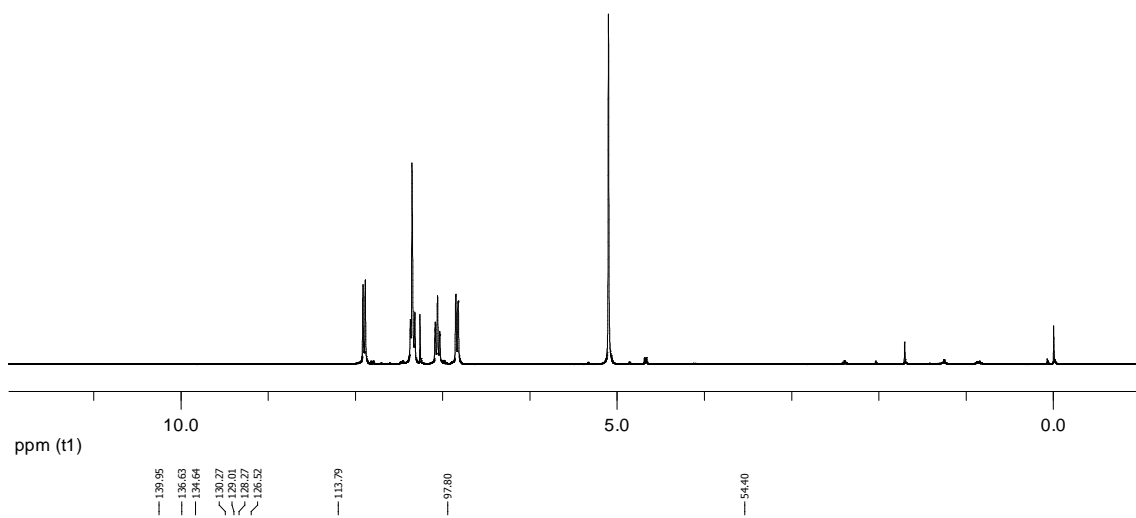


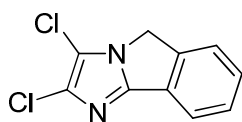
5H-Imidazo[2,1-a]-isoindole



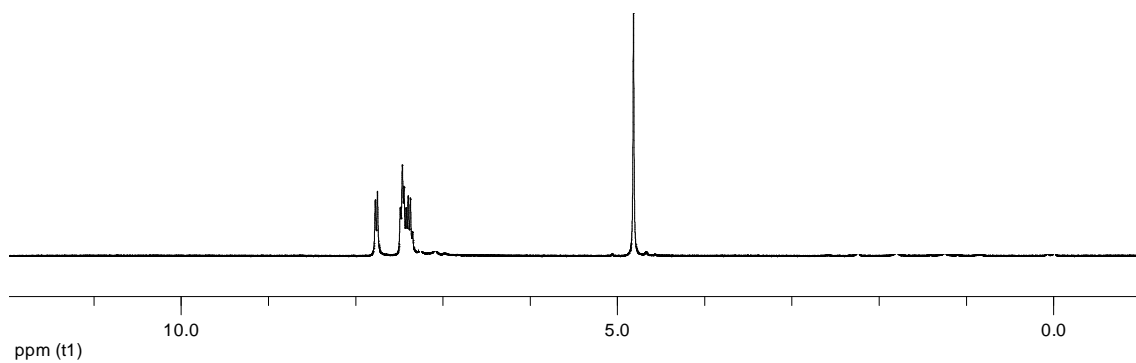


4,5-Dichloro-1-(2-iodobenzyl)-1*H*-imidazole

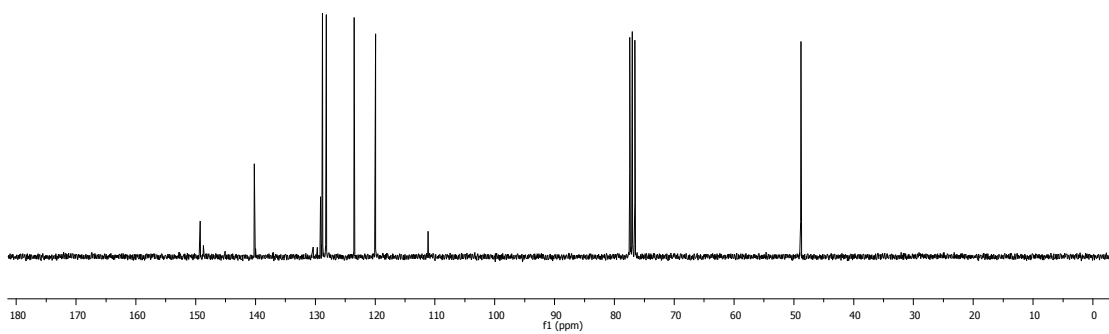


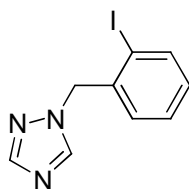


2,3-Dichloro-5*H*-imidazo[2,1-*a*]-isoindole

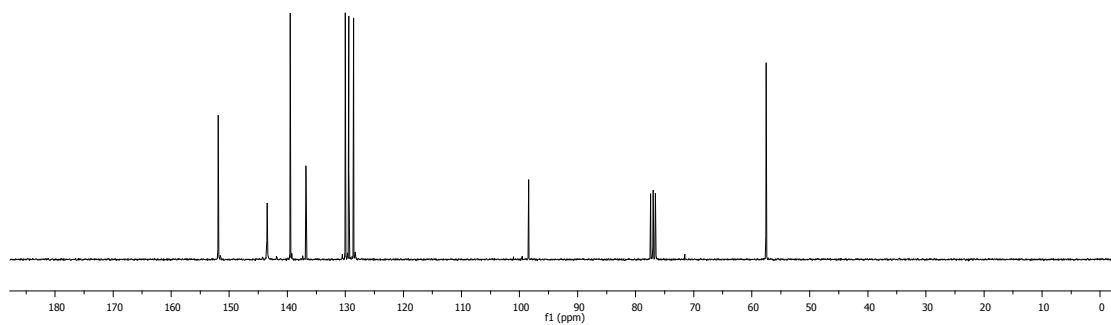
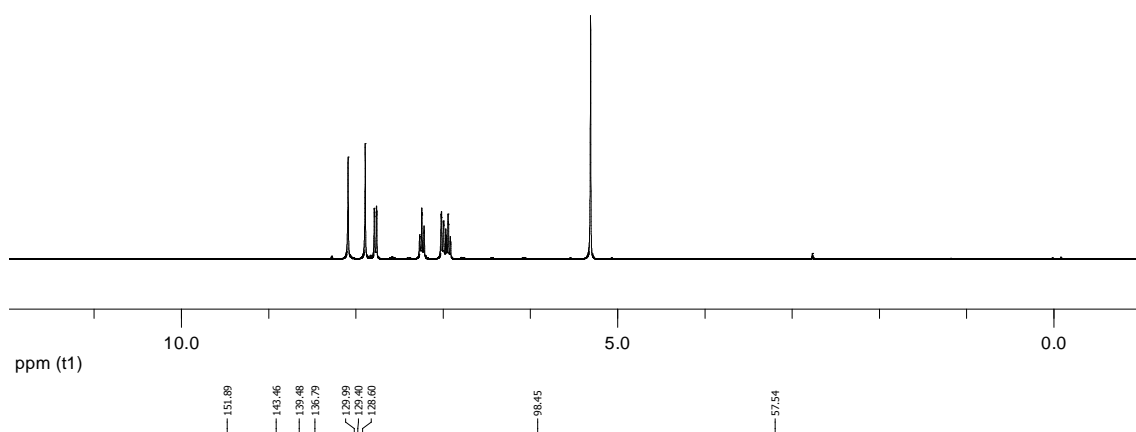


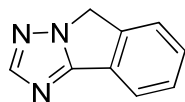
140.27
140.21
128.15
128.81
128.76
128.16
123.52
119.95
111.16
48.82



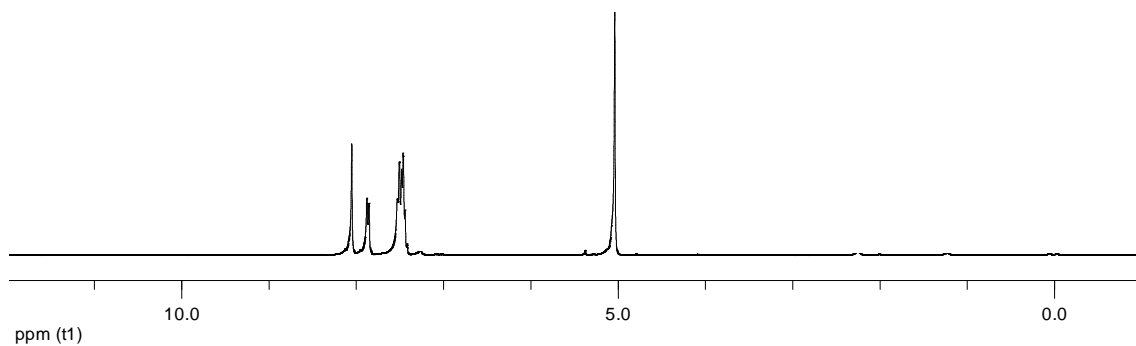


1-(2-Iodobenzyl)-1H-1,2,4-triazole

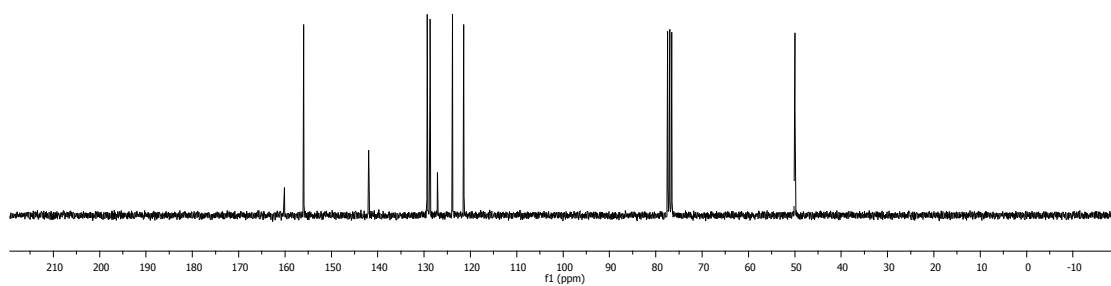


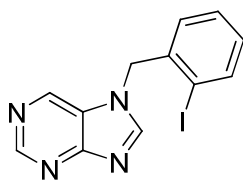


5H-[1,2,4]triazolo[5,1-a]isoindole

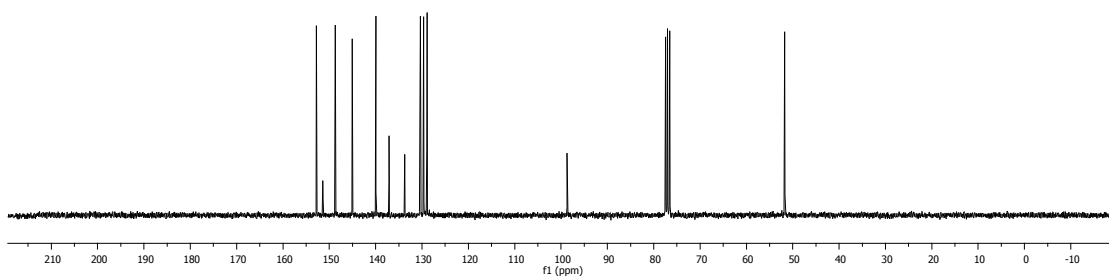
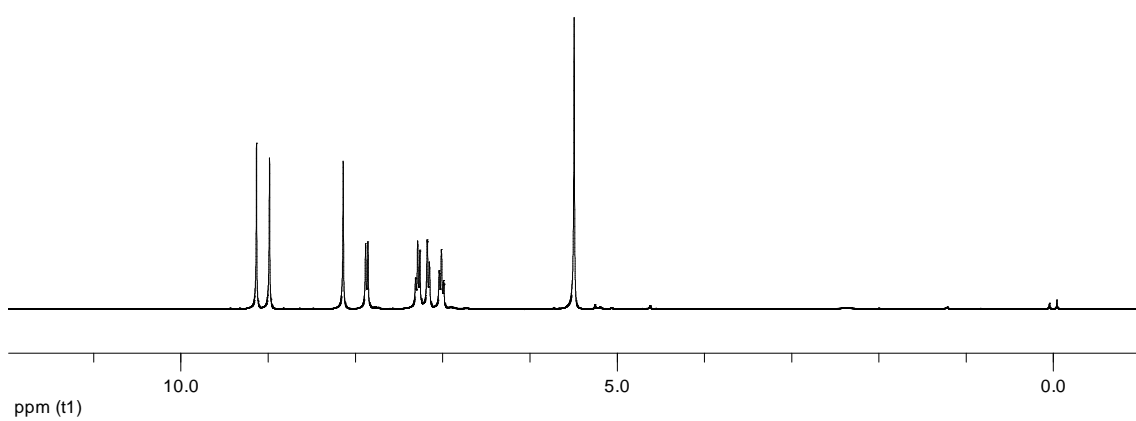


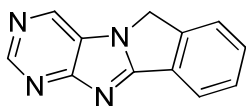
160.11
155.97
141.95
128.30
127.62
127.09
123.86
121.42
49.99



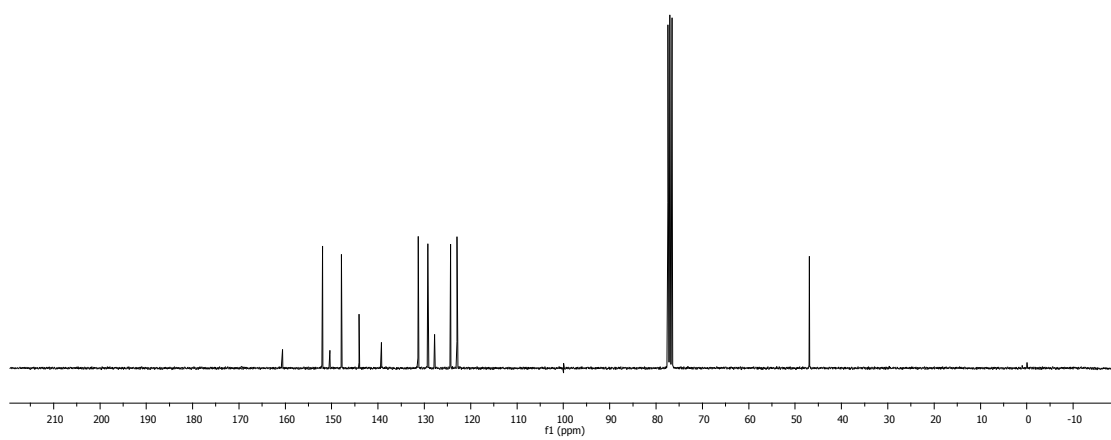
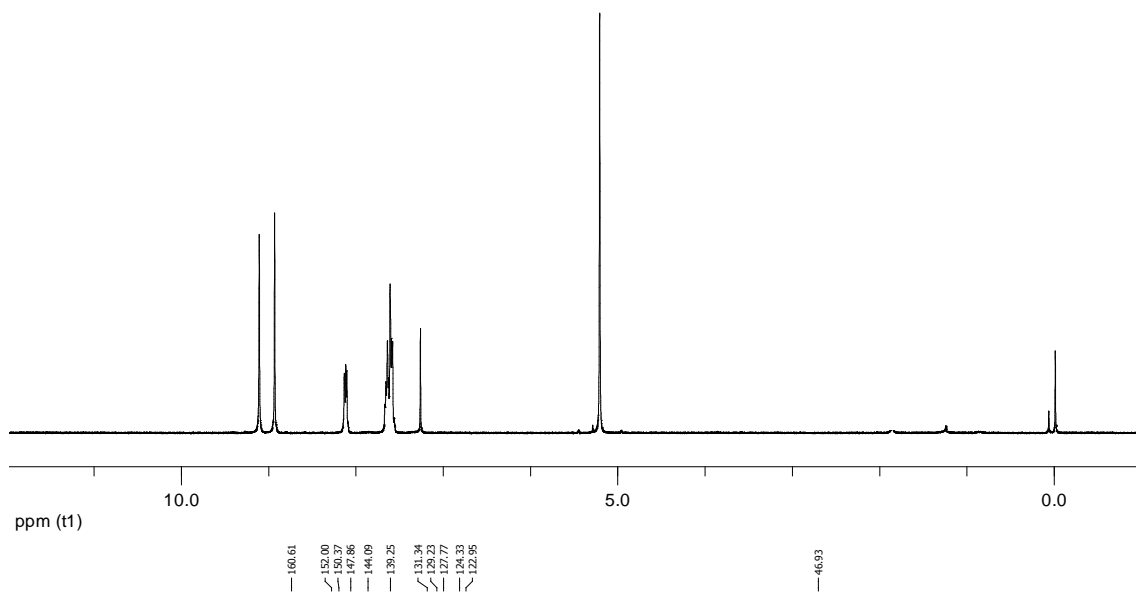


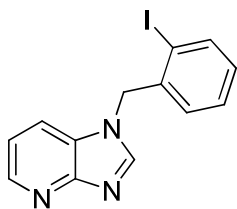
7-(2-Iodobenzyl)-7H-purine



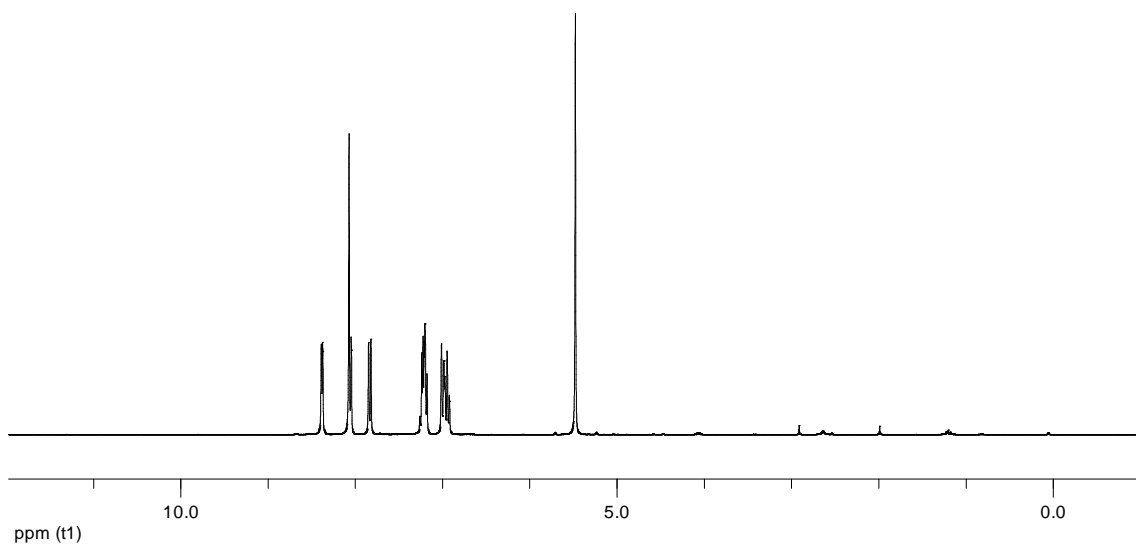


6H-Isoindolo[2,1-f]purine

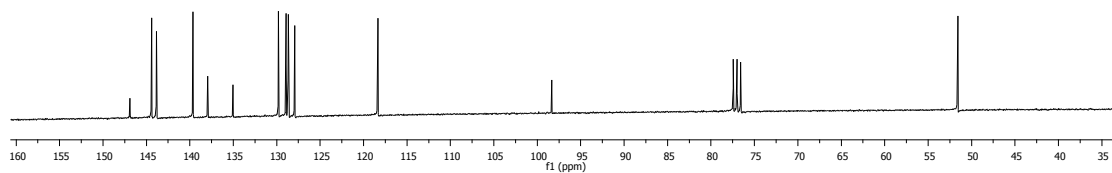


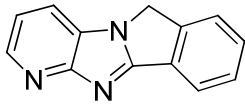


1-(2-Iodobenzyl)-1*H*-imidazo[4,5-*b*]pyridine

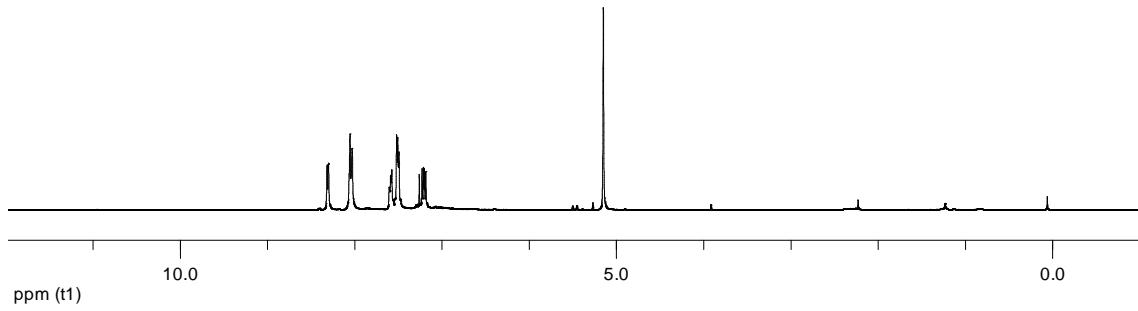


146.89
144.40
143.84
139.65
137.94
135.03
129.79
128.62
128.67
127.93
118.36

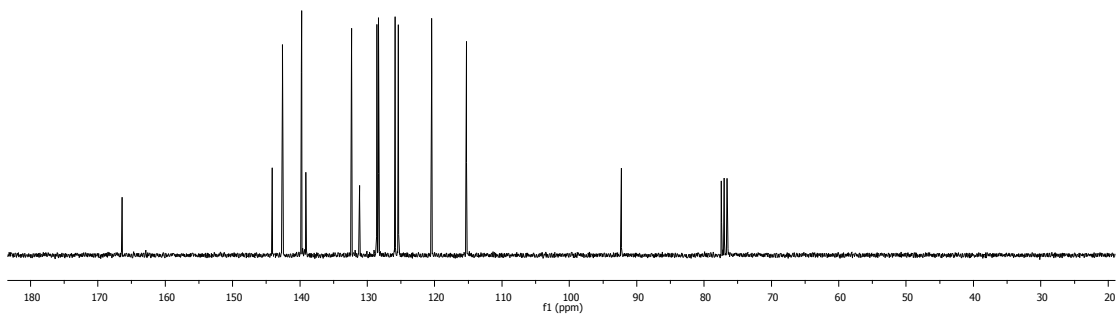


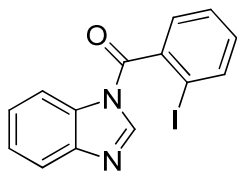


6*H*-Pyrido[2',3',4,5]imidazo[2,1-*a*]isoindole

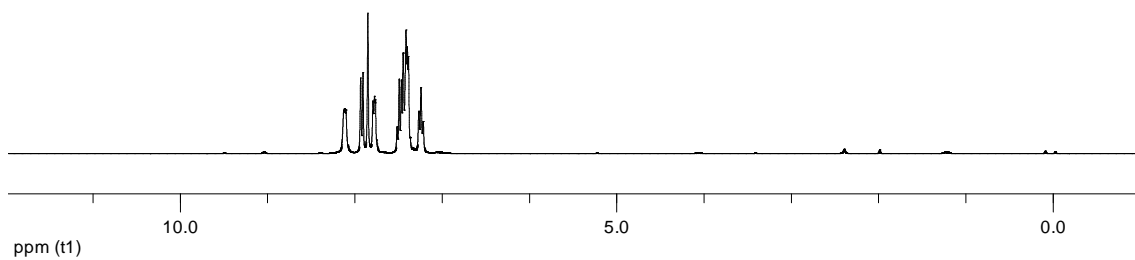


166.42
144.13
142.58
139.76
139.11
132.34
131.16
128.32
125.87
125.40
120.46
115.28
92.29

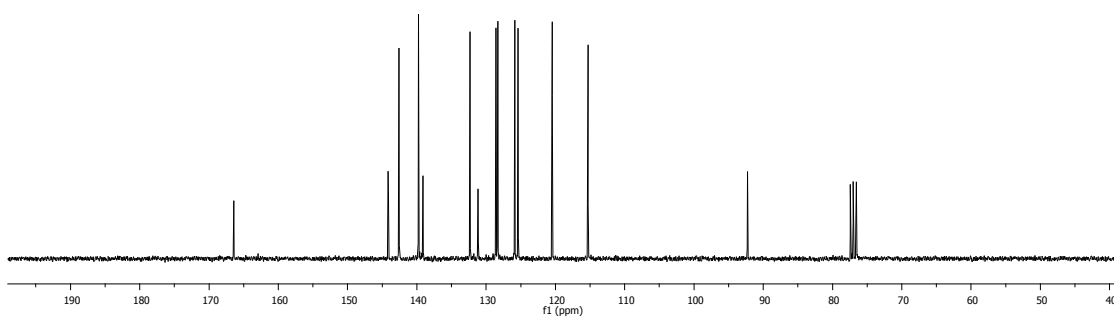


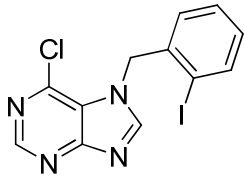


(1*H*-Benzo[d]imidazol-1-yl)(2-iodophenyl)methanone

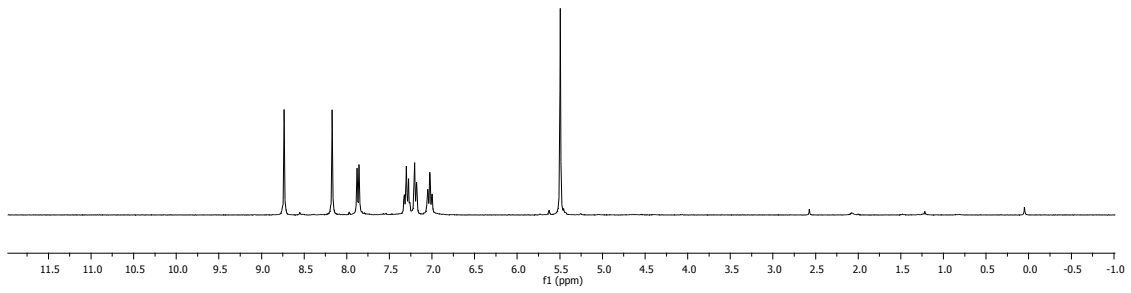


166.42
144.13
142.58
139.76
139.11
132.94
131.16
128.32
125.87
125.40
120.46
115.28
92.29





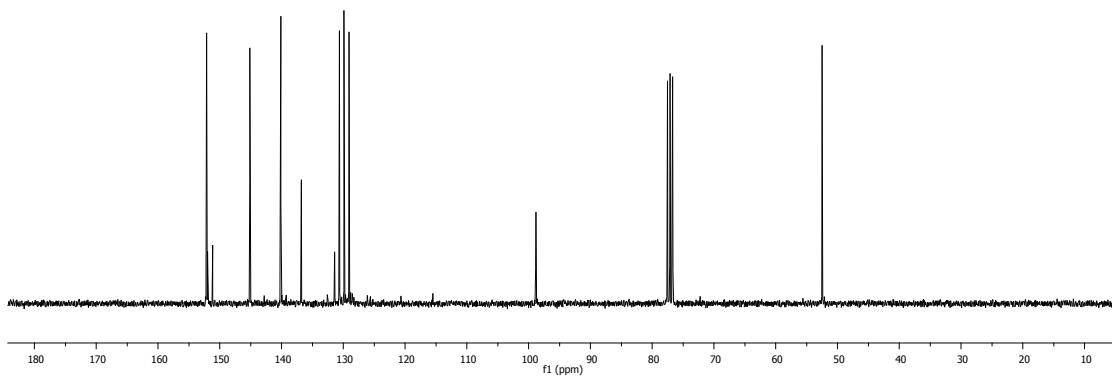
6-Chloro-7-(2-iodobenzyl)-7H-purine

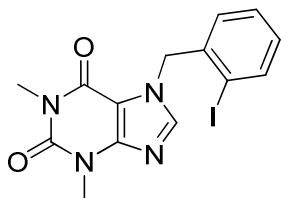


152.15
151.95
151.16
145.13
140.13
136.79
131.43
130.62
129.88
129.07

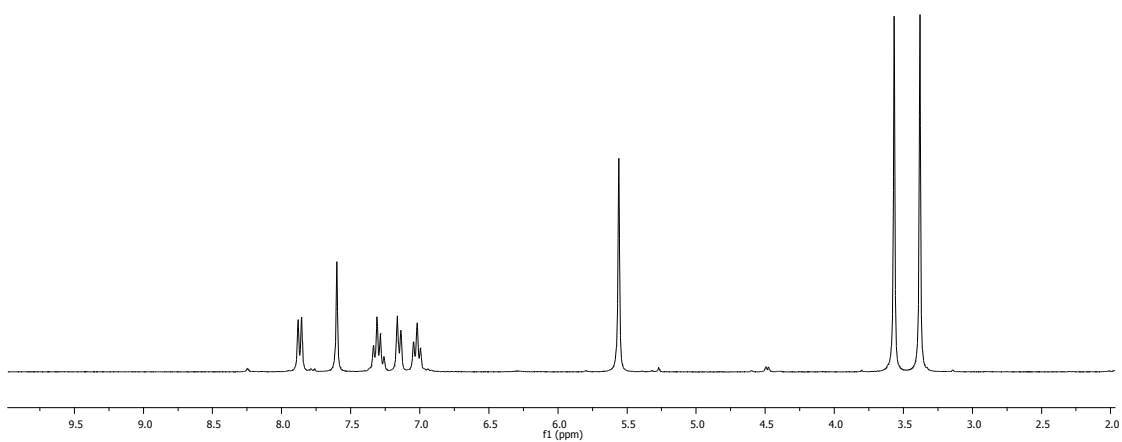
98.83

52.48

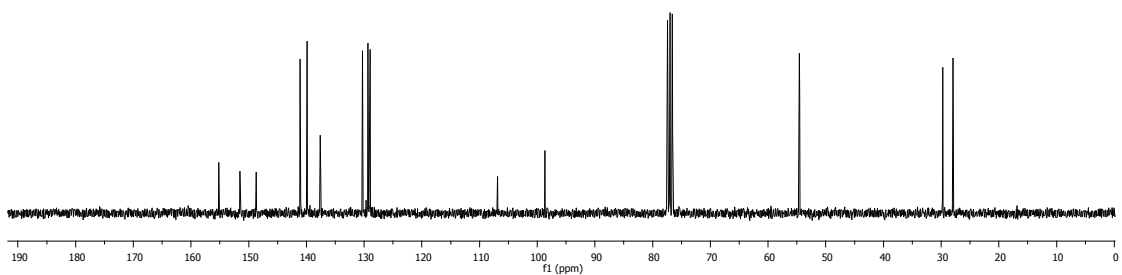


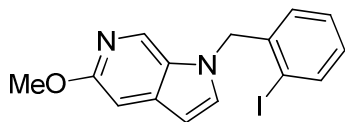


7-(2-Iodobenzyl)-1,3-dimethyl-1*H*-purine-2,6(3*H*,7*H*)-dione

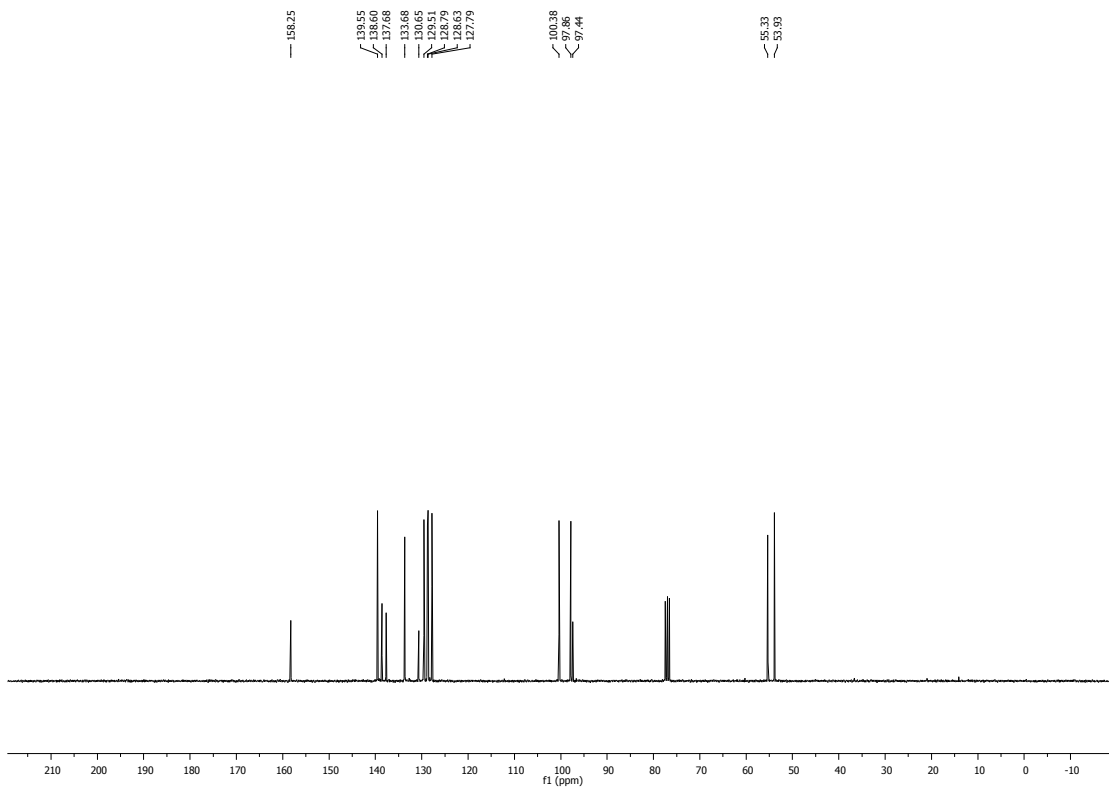
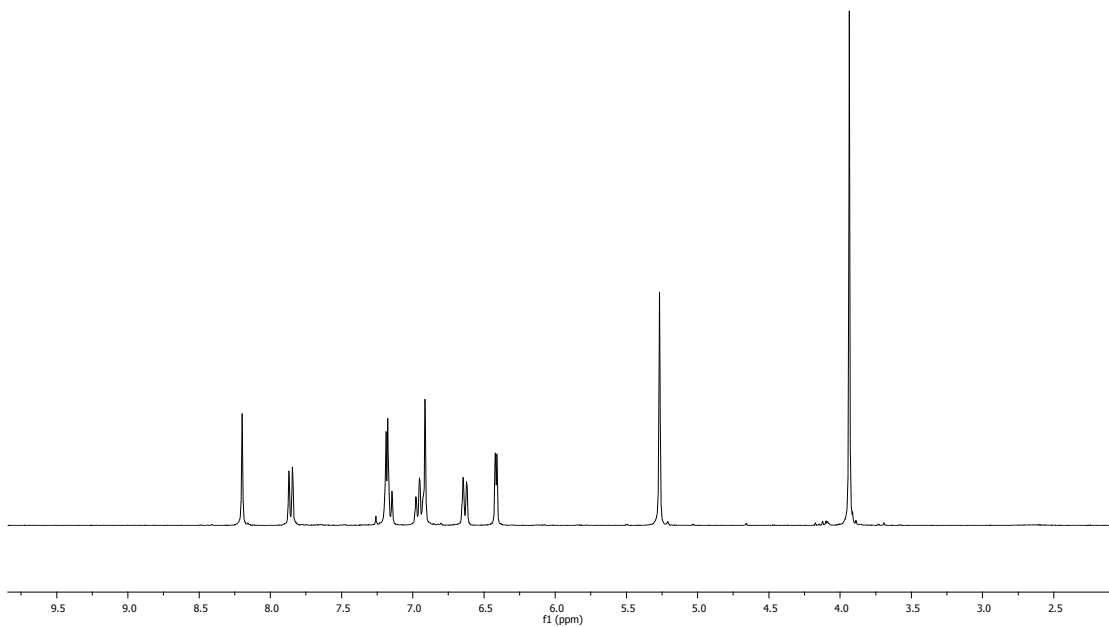


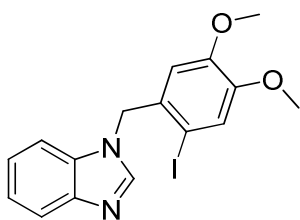
155.17
151.53
148.72
141.09
138.89
137.63
130.28
129.33
128.99
106.91
98.68
54.55
29.73
27.95



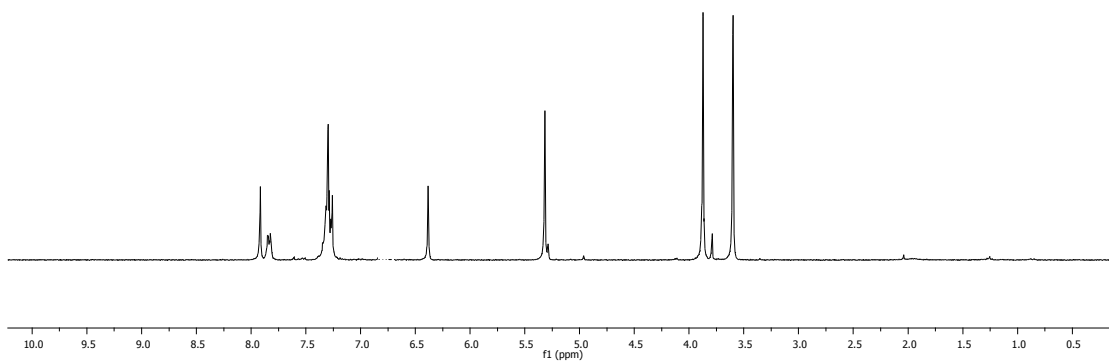


N-(2-Iodobenzyl)-5-methoxy-1*H*-pyrrolo[2,3-*c*]pyridine

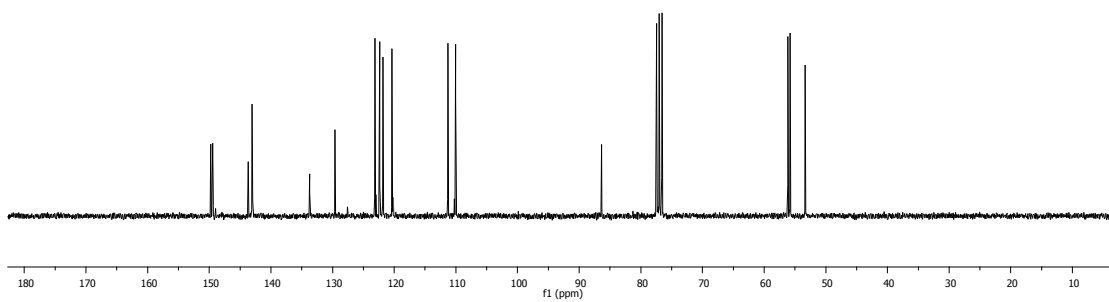


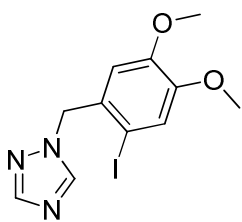


1-(2-Iodo-4,5-dimethoxybenzyl)-1*H*-benzo[*d*]imidazole

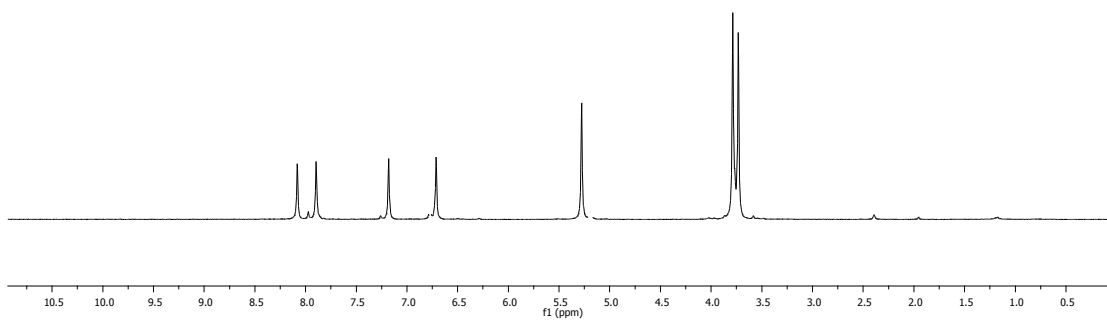


149.76
149.46
143.67
143.04
133.71
128.60
123.14
122.36
120.35
111.29
110.03
86.37
56.16
55.78
53.33

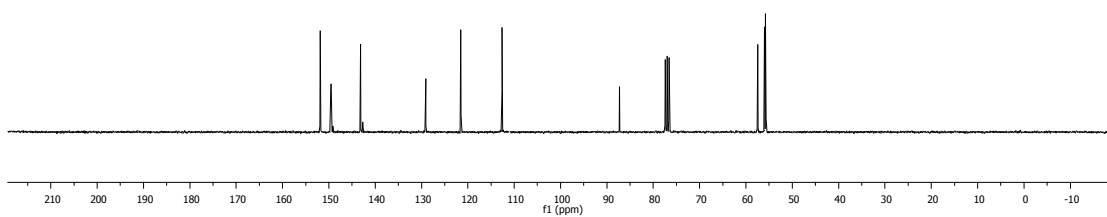


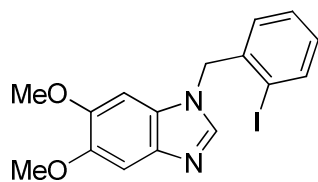


1-(2-Iodo-4,5-dimethoxybenzyl)-1H-1,2,4-triazole

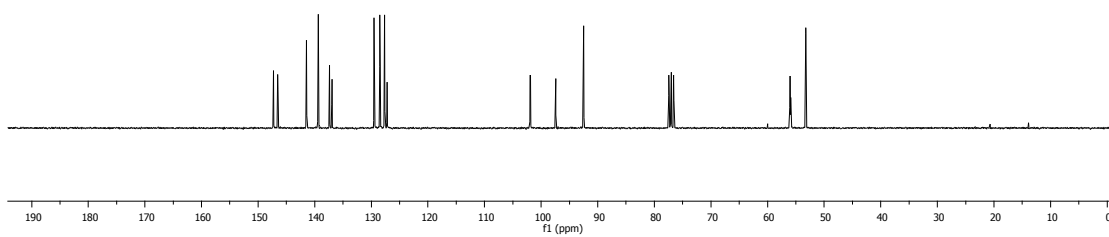
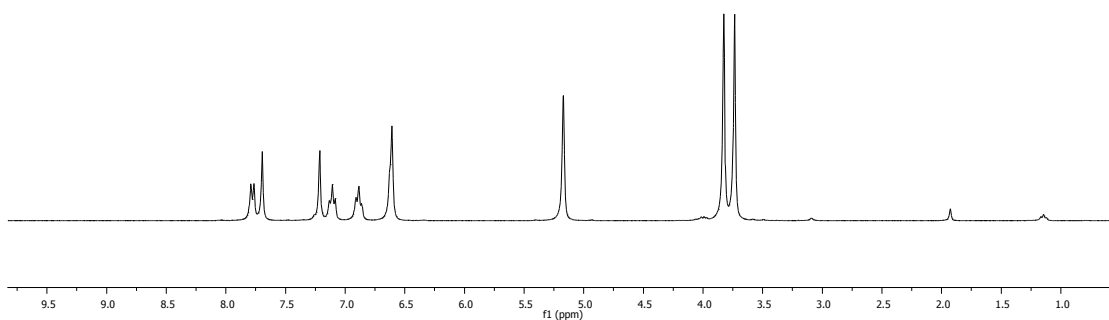


151.08
149.88
149.53
143.19
129.08
121.53
112.63
87.26
57.48
56.01
55.77





1-(2-Iodobenzyl)-5,6-dimethoxy-1*H*-benzo[d]imidazole



¹ R. Sanz, J. M. Ignacio, M. P. Castroviejo,; Fañanas, F. J. *Arkivok* 2007, 84-91.

² N. Arai,; M. Takahashi, M. Mitani, A.Mori, *Synlett* 2006, 3170-3172.