

## **Supporting Information**

### **CuO nanoparticles catalysed synthesis of 2*H*-indazoles under a ligand free condition**

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#### **Experimental:**

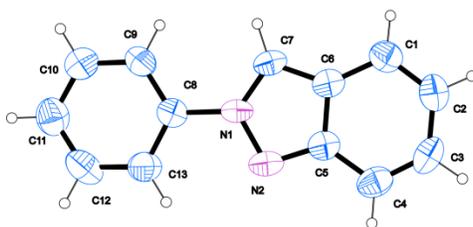
##### **General information:**

All the reagents were commercial grade and purified according to the established procedures. Organic extracts were dried over anhydrous sodium sulphate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60–120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F<sub>254</sub> (0.25 mm). NMR spectra were recorded in CDCl<sub>3</sub> with tetramethylsilane as the internal standard for <sup>1</sup>H NMR (400 MHz) CDCl<sub>3</sub> solvent as the internal standard for <sup>13</sup>C NMR (100 MHz). Elemental analysis was performed with a Perkin Elmer 2400 elemental analyzer. IR spectra were recorded in KBr or neat on a Nicolet Impact 410 spectrophotometer. Commercially available CuO nano (<50 nm) were purchased from Sigma-Aldrich.

**Crystallographic Analysis:** Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite by using graphite-monochromated Mo- $K_{\alpha}$  radiation ( $\lambda = 0.71073$  Å) at 298 K. Cell parameters were retrieved using SMART<sup>1</sup>USA, 1995 software and refined with SAINT<sup>1</sup> for all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentzian and polarization effects. Absorption corrections were applied with the SADABS program<sup>2</sup>. The structures were solved by direct methods implemented in the SHELX-97<sup>3</sup> program and refined by full-matrix least-squares methods on  $F^2$ . All non-hydrogen atom positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. The crystals were isolated in rectangular shape from ethyl acetate and hexane mixture at room temperature.

## References

1. SMART, SAINT and XPREP, Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin.
2. G. M. Sheldrick, *SADABS: Empirical Absorption and Correction Software*, University of Gottingen, Institut für Anorganische Chemie der Universität, Tammanstrasse 4, D-3400 Gottingen, Germany, 1999–2003.
3. G. M. Sheldrick, SHELXS-97, University of Gottingen, Germany, 1997.

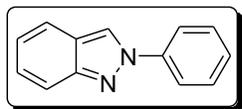


**Figure 1.** ORTEP views of 2-Phenyl-2H-indazole (**1a**)

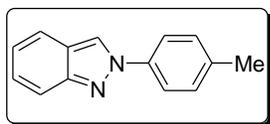
**Crystallographic description of 2-Phenyl-2H-indazole (1a):**  $C_{13}H_{10}N_2$ , crystal dimension 0.41 x 0.35 x 0.22 mm,  $M_r = 194.23$ , Monoclinic, Space group 'C c',  $a = 5.9752(9)$  Å,  $b = 25.124(4)$  Å,  $c = 13.8320(17)$  Å,  $\alpha = 90.00$ ,  $\beta = 97.080(9)$ ,  $\gamma = 90.00$ ,  $V = 2060.6(5)$  Å<sup>3</sup>,  $Z = 8$ ,  $\rho_{\text{calcd}} = 1.252$  mg/m<sup>3</sup>,  $\mu = 0.076$  mm<sup>-1</sup>,  $F(000) = 816.0$ , reflection collected / unique = 5146 / 2204, refinement method = full-matrix least-squares on  $F^2$ , final  $R$  indices [ $I > 2\sigma(I)$ ]:  $R_1 = 0.0681$ ,  $wR_2 = 0.2066$ ,  $R$  indices (all data):  $R_1(\text{all}) = 0.1370$ ,  $wR_2(\text{all}) = 0.2543$ , goodness of fit = 1.009. CCDC-961653 (for 2-phenyl-2H-indazole (**1a**)) contains the supplementary crystallographic data for this paper.

These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via [www.ccdc.cam.ac.uk/data\\_request/cif](http://www.ccdc.cam.ac.uk/data_request/cif).

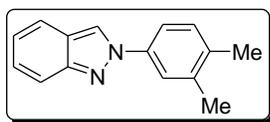
### SPECTRAL DATA



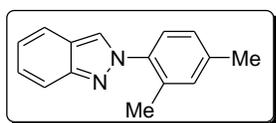
**2-Phenyl-2H-indazole (1a):** White solid; M.p. 81.5-83.5 °C (lit.<sup>4</sup> 80-82 °C); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ (ppm) 7.11 (t, 1H, *J* = 7.6 Hz), 7.32 (t, 1H, *J* = 7.6 Hz), 7.39 (t, 1H, *J* = 7.2 Hz), 7.49-7.53 (m, 2H), 7.69 (d, 1H, *J* = 8.8 Hz), 7.79 (d, 1H, *J* = 8.8 Hz), 7.89 (d, 2H, *J* = 7.6 Hz), 8.39 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ (ppm) 118.1, 120.6, 121.2, 122.6, 122.9, 127.0, 128.1, 129.7, 140.7, 149.9; IR (KBr): 3126, 2923, 1624, 1593, 1517, 1493, 1378, 1311, 1198, 1072, 1044, 944, 753 cm<sup>-1</sup>; elemental analysis calcd (%) for C<sub>13</sub>H<sub>10</sub>N<sub>2</sub> (194.2315): C 80.39, H 5.19, N 14.42; found C 80.47, H 5.12, N 14.35.



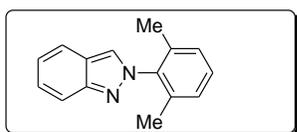
**2-p-Tolyl-2H-indazole (1b):** Yellow solid; M.p. 100-103 °C (lit.<sup>5</sup> 101-103 °C); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ (ppm) 2.41 (s, 3H), 7.09 (t, 1H, *J* = 7.6 Hz), 7.29-7.33 (m, 3H), 7.69 (d, 1H, *J* = 8.4 Hz), 7.76-7.80 (m, 3H), 8.35 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ (ppm) 21.2, 118.1, 120.5, 121.1, 122.5, 122.9, 126.8, 130.3, 138.1, 138.5, 149.9; IR (KBr): 3038, 2920, 2857, 1624, 1522, 1451, 1378, 1347, 1196, 1108, 1047, 822, 792, 757, 739 cm<sup>-1</sup>; elemental analysis calcd (%) for C<sub>14</sub>H<sub>12</sub>N<sub>2</sub> (208.2580): C 80.74, H 5.81, N 13.45; found C 80.81, H 5.89, N 13.39.



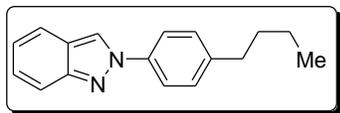
**2-(3,4-Dimethylphenyl)-2H-indazole (1c):** Brown solid; M.p. 117-119 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 2.33 (s, 3H), 2.37 (s, 3H), 7.11 (t, 1H,  $J = 8$  Hz), 7.26 (s, 1H), 7.29-7.33 (m, 1H), 7.58 (d, 1H,  $J = 8$  Hz), 7.70 (d, 2H,  $J = 8.4$  Hz), 7.79 (d, 1H,  $J = 8.8$  Hz), 8.38 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 19.5, 20.0, 117.9, 118.2, 120.4, 122.2, 122.3, 122.8, 126.7, 130.6, 136.6, 138.2, 138.5, 149.7; IR (KBr): 2925, 2851, 1611, 1517, 1500, 1465, 1448, 1379, 1129, 1056, 882, 816, 776, 757  $\text{cm}^{-1}$ ; elemental analysis calcd (%) for  $\text{C}_{15}\text{H}_{14}\text{N}_2$  (222.2845): C 81.05, H 6.35, N 12.60; found C 81.13, H 6.31, N 12.53.



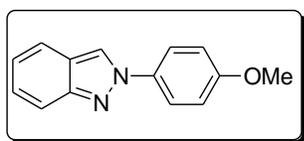
**2-(2,4-Dimethylphenyl)-2H-indazole (1d):** Liquid;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 2.18 (s, 3H), 2.39 (s, 3H), 7.10-7.16 (m, 3H), 7.28-7.34 (m, 2H), 7.72 (d, 1H,  $J = 8.4$  Hz), 7.78 (d, 1H,  $J = 8.8$  Hz), 8.05 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 17.8, 21.2, 117.9, 120.4, 122.0, 122.1, 124.5, 126.3, 126.4, 127.2, 131.9, 133.5, 138.0, 139.1, 149.3; IR (KBr): 3059, 2922, 1627, 1520, 1505, 1386, 1349, 1198, 1146, 1129, 1042, 819, 784, 756  $\text{cm}^{-1}$ ; elemental analysis calcd (%) for  $\text{C}_{15}\text{H}_{14}\text{N}_2$  (222.2845): C 81.05, H 6.35, N 12.60; found C 81.15, H 6.39, N 12.53.



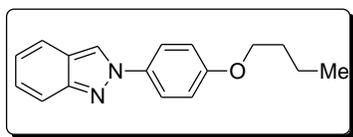
**2-(2,6-Dimethylphenyl)-2H-indazole (1e):** Semi-solid;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 1.99 (s, 6H), 7.13-7.19 (m, 3H), 7.30 (d, 1H,  $J = 8$  Hz), 7.35 (t, 1H,  $J = 7.6$  Hz), 7.76 (d, 1H,  $J = 8.8$  Hz), 7.81 (d, 1H,  $J = 9.2$  Hz), 7.98 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 17.3, 118.2, 120.5, 121.9, 122.2, 124.6, 126.3, 128.3, 129.5, 135.7, 139.9, 149.3; IR (KBr): 2922, 2853, 1624, 1515, 1482, 1376, 1267, 1184, 1095, 1045, 954, 791, 763  $\text{cm}^{-1}$ ; elemental analysis calcd (%) for  $\text{C}_{15}\text{H}_{14}\text{N}_2$  (222.2845): C 81.05, H 6.35, N 12.60; found C 81.11, H 6.38, N 12.54.



**2-(4-Butylphenyl)-2H-indazole (1f):** Yellow solid; M.p. 64-65 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 0.89-0.98 (m, 3H), 1.33-1.39 (m, 2H), 1.58-1.66 (m, 2H), 2.66 (t, 2H,  $J = 8.0$  Hz), 7.09 (t, 1H,  $J = 8.0$  Hz), 7.30 (d, 3H,  $J = 8.4$  Hz), 7.68 (dd, 1H,  $J_1 = 1.2$  Hz,  $J_2 = 8.4$  Hz), 7.77 (d, 3H,  $J = 8.8$  Hz), 8.35 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 13.9, 22.3, 33.5, 35.1, 117.9, 120.3, 120.4, 120.8, 122.3, 122.8, 126.7, 129.4, 138.4, 142.9, 149.7; IR (KBr): 2955, 2925, 2854, 1626, 1520, 1466, 1430, 1383, 1349, 1208, 1121, 1047, 815, 780, 754  $\text{cm}^{-1}$ ; elemental analysis calcd (%) for  $\text{C}_{17}\text{H}_{18}\text{N}_2$  (250.3375): C 81.56, H 7.25, N 11.19; found C 81.63, H 7.29, N 11.13.

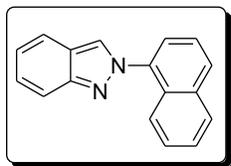


**2-(4-Methoxyphenyl)-2H-indazole (1g):** Brown solid; M.p. 130-132 °C (lit.<sup>5</sup> 130-132 °C);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 3.84 (s, 3H), 6.99 (d, 2H,  $J = 8.8$  Hz), 7.07-7.11 (m, 1H), 7.28-7.32 (m, 1H), 7.67 (d, 1H,  $J = 8.4$  Hz), 7.77 (d, 3H,  $J = 8.8$  Hz), 8.28 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 55.5, 114.6, 117.7, 120.3, 120.4, 122.19, 122.24, 122.7, 126.6, 134.0, 149.6, 159.2; IR (KBr): 3137, 2958, 2836, 1610, 1520, 1440, 1382, 1303, 1245, 1207, 1177, 1029, 837, 810, 754  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{14}\text{H}_{12}\text{N}_2\text{O}$  (224.2574): C 74.98, H 5.39, N 12.49; found C 75.05, H 5.33, N 12.43.

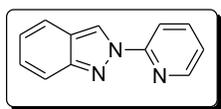


**2-(4-Butoxyphenyl)-2H-indazole (1h):** Yellow solid; M.p. 103-105 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 0.99 (t, 3H,  $J = 7.6$  Hz), 1.52 (m, 2H), 1.80 (m, 2H), 4.02 (t, 2H,  $J = 6.8$  Hz), 7.02 (d, 2H,  $J = 9.2$  Hz), 7.11 (t, 1H,  $J = 7.6$  Hz), 7.31 (t, 1H,  $J = 8.8$  Hz), 7.70 (d, 1H,  $J = 8.4$

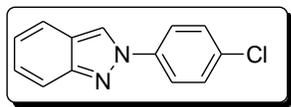
Hz), 7.78 (d, 3H,  $J = 9.2$  Hz), 8.32 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 13.9, 19.3, 31.4, 68.2, 115.3, 117.8, 120.4, 122.3, 122.4, 122.8, 126.6, 133.9, 149.7, 158.9; IR (KBr): 2954, 2937, 2870, 1609, 1521, 1382, 1306, 1303, 1246, 1180, 1110, 1047, 1009, 837, 780, 753  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{17}\text{H}_{18}\text{N}_2\text{O}$  (266.3369): C 76.66, H 6.81, N 10.52; found C 76.74, H 6.78, N 10.45.



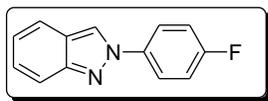
**2-(Naphthalen-1-yl)-2H-indazole (1i):** Liquid;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 7.17 (t, 1H,  $J = 8.4$  Hz), 7.37 (t, 1H,  $J = 8$  Hz), 7.48 (t, 1H,  $J = 8.4$  Hz), 7.55-7.59 (m, 2H), 7.65 (d, 1H,  $J = 7.2$  Hz), 7.72 (d, 1H,  $J = 8.4$  Hz), 7.78 (d, 1H,  $J = 8.6$  Hz), 7.84 (d, 1H,  $J = 8.8$  Hz), 7.94 (d, 1H,  $J = 8$  Hz), 7.99 (d, 1H,  $J = 8.4$  Hz), 8.29 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 118.2, 120.5, 122.2, 122.5, 123.2, 124.0, 125.1, 125.6, 126.8, 127.0, 127.8, 128.3, 129.2, 129.9, 134.3, 137.8, 149.8; IR (KBr): 3057, 2924, 2853, 1627, 1597, 1519, 1474, 1416, 1385, 1277, 1214, 1128, 1111, 1020, 939, 757, 733  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{17}\text{H}_{12}\text{N}_2$  (244.2901): C 83.58, H 4.95, N 11.47; found C 83.67, H 4.91, N 11.41.



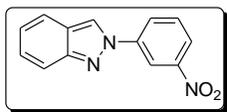
**2-(Pyridin-2-yl)-2H-indazole (1j):** Yellow solid; M.p. 106-108  $^{\circ}\text{C}$  (lit.<sup>7</sup> 103-104  $^{\circ}\text{C}$ );  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 7.09 (t, 1H,  $J = 7.6$  Hz), 7.28-7.34 (m, 2H), 7.74 (t, 2H,  $J = 8.8$  Hz), 7.89 (t, 1H,  $J = 8.4$  Hz), 8.29 (d, 1H,  $J = 8$  Hz), 8.51 (d, 1H,  $J = 4.8$  Hz), 9.11 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 114.2, 118.2, 120.7, 121.3, 122.5, 122.8, 127.7, 138.9, 148.4, 150.4, 151.9; IR (KBr): 3148, 3059, 2924, 1590, 1573, 1518, 1476, 1434, 1376, 1250, 1198, 1139, 1053, 783, 761  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{12}\text{H}_9\text{N}_3$  (195.2196): C 73.83, H 4.65, N 21.52; found C 73.90, H 4.70, N 21.43.



**2-(4-Chlorophenyl)-2H-indazole (1k):** Yellowish-white solid; M.p. 137-139 °C (lit.<sup>7</sup> 138-140 °C); <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ (ppm) 7.10 (t, 1H, *J* = 7.2 Hz), 7.31 (t, 1H, *J* = 7.6 Hz), 7.47 (d, 2H, *J* = 8.8 Hz), 7.67 (d, 1H, *J* = 8.4 Hz), 7.75 (d, 1H, *J* = 8.8 Hz), 7.83 (d, 2H, *J* = 8.8 Hz), 8.35 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ (ppm) 118.0, 120.4, 120.5, 122.0, 122.8, 123.0, 127.3, 129.8, 133.6, 139.1, 150.0; IR (KBr): 3131, 2962, 1628, 1518, 1495, 1423, 1382, 1204, 1093, 1046, 952, 825, 811, 778, 754, 727 cm<sup>-1</sup>; Elemental analysis calcd (%) for C<sub>13</sub>H<sub>9</sub>N<sub>2</sub>Cl (228.6763): C 68.28, H 3.97, N 12.25; found C 68.37, H 3.92, N 12.17.

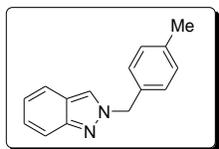


**2-(4-Fluorophenyl)-2H-indazole (1l):** Yellowish-white solid; M.p. 103-104 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ (ppm) 7.12 (t, 1H, *J* = 7.6 Hz), 7.21 (d, 1H, *J* = 8.4 Hz), 7.25 (d, 1H, *J* = 6.4 Hz), 7.33 (t, 1H, *J* = 7.6 Hz), 7.71 (d, 1H, *J* = 8.4 Hz), 7.78 (d, 1H, *J* = 8.8 Hz), 7.85-7.89 (m, 2H), 8.35 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ (ppm) 116.5 (d, *J*<sub>C-F</sub> = 22.1 Hz), 118.0, 120.6 (d, *J*<sub>C-F</sub> = 9.9 Hz), 122.7, 122.8, (d, *J*<sub>C-F</sub> = 8.4 Hz), 122.9, 127.1, 136.9, 149.9, 160.9, 163.4; IR (KBr): 3135, 2924, 1627, 1520, 1508, 1382, 1234, 1203, 1097, 1042, 951, 861, 839, 752, 779 cm<sup>-1</sup>; Elemental analysis calcd (%) for C<sub>13</sub>H<sub>9</sub>N<sub>2</sub>F (212.2220): C 73.57, H 4.27, N 13.20; found C 73.66, H 4.33, N 13.12.

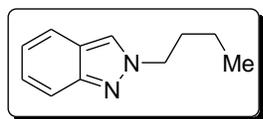


**2-(3-Nitrophenyl)-2H-indazole (1m):** Brown solid; M.p. 128-130 °C; <sup>1</sup>H NMR (CDCl<sub>3</sub>, 400 MHz): δ (ppm) 7.13 (t, 1H, *J* = 7.6 Hz), 7.34 (t, 1H, *J* = 8.8 Hz), 7.70 (d, 1H, *J* = 8 Hz), 7.75 (t, 2H, *J* = 8.8 Hz), 8.24 (d, 1H, *J* = 8 Hz), 8.32 (d, 1H, *J* = 8 Hz), 8.51 (s, 1H), 8.77 (s, 1H); <sup>13</sup>C NMR (CDCl<sub>3</sub>, 100 MHz): δ (ppm) 115.7, 118.3, 120.6, 120.7, 122.4, 123.4, 123.5, 126.4, 127.9, 130.8, 149.2, 150.5; IR (KBr): 2924, 2853, 1740, 1628, 1616, 1530, 1488, 1382, 1346, 1261,

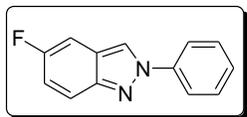
1099, 1045, 817, 802, 760, 734  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{13}\text{H}_9\text{N}_3\text{O}_2$  (239.2291): C 65.27, H 3.79, N 17.56; found C 65.33, H 3.82, N 17.49.



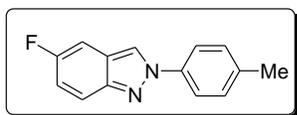
**2-(4-Methylbenzyl)-2H-indazole (1n):** Yellow solid; M.p. 80-82 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 2.33 (s, 3H), 5.54 (s, 2H), 7.06 (t, 1H,  $J = 7.2$  Hz), 7.17 (q, 4H,  $J = 8$  Hz), 7.25-7.28 (m, 1H), 7.60 (d, 1H,  $J = 8.4$  Hz), 7.72 (d, 1H,  $J = 8.8$  Hz), 7.84 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 21.3, 57.5, 117.7, 120.3, 121.8, 122.3, 122.8, 126.1, 128.3, 128.7, 129.8, 132.9, 138.4, 149.1; IR (KBr): 3119, 2921, 1623, 1512, 1465, 1440, 1421, 1385, 1350, 1136, 805, 791, 754, 729  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{15}\text{H}_{14}\text{N}_2$  (222.2845): C 81.05, H 6.35, N 12.60; found C 81.13, H 6.32, N 12.51.



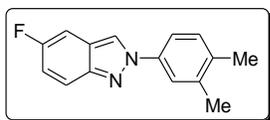
**2-Butyl-2H-indazole (1o):** Liquid;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 0.95 (t, 3H,  $J = 7.2$  Hz), 1.35 (m, 2H), 1.99 (m, 2H), 4.41 (t, 2H,  $J = 7.2$  Hz), 7.07 (t, 1H,  $J = 7.6$  Hz), 7.25-7.29 (m, 1H), 7.64 (d, 1H,  $J = 7.6$  Hz), 7.72 (d, 1H,  $J = 8.8$  Hz), 7.89 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 13.7, 19.9, 32.7, 53.5, 117.4, 120.1, 121.6, 121.8, 122.7, 125.8, 148.8; IR (KBr): 3060, 2959, 2932, 2873, 1628, 1515, 1466, 1380, 1311, 1157, 1141, 1011, 907, 757  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{11}\text{H}_{14}\text{N}_2$  (174.2417): C 75.82, H 8.10, N 16.08; found C 75.88, H 8.08, N 15.98.



**5-Fluoro-2-phenyl-2H-indazole (2a):** Yellow solid; M.p. 135.5-137.5 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 7.12 (dt, 1H,  $J_1 = 2$  Hz,  $J_2 = 8.0$  Hz), 7.27 (d, 1H,  $J = 9.6$  Hz), 7.41 (t, 1H,  $J = 7.6$  Hz), 7.53 (t, 2H,  $J = 8.0$  Hz), 7.75-7.81 (m, 1H), 7.88 (d, 2H,  $J = 8.4$  Hz), 8.37 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 102.9 (d,  $J_{\text{C-F}} = 25.2$  Hz), 118.6 (d,  $J_{\text{C-F}} = 29$  Hz), 120.2 (d,  $J_{\text{C-F}} = 9.2$  Hz), 120.6 (d,  $J_{\text{C-F}} = 9.2$  Hz), 121.0, 122.2 (d,  $J_{\text{C-F}} = 12.2$  Hz), 128.2, 129.8, 140.5, 147.4, 158.9 (d,  $J_{\text{C-F}} = 239.5$  Hz); IR (KBr): 3129, 3035, 2924, 2853, 1683, 1595, 1523, 1504, 1460, 1408, 1329, 1228, 1215, 1147, 1123, 1073, 1053, 854  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{13}\text{H}_9\text{N}_2\text{F}$  (212.2220): C 73.57, H 4.27, N 13.20; found C 73.74, H 4.22, N 13.09.

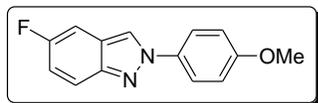


**5-Fluoro-2-p-tolyl-2H-indazole (2b):** Yellow solid; M.p. 139-141 °C (lit.<sup>7</sup> 140-142 °C);  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 2.43 (s, 3H), 7.12 (dt, 1H,  $J_1 = 2.4$  Hz,  $J_2 = 9.2$  Hz), 7.26-7.29 (m, 1H), 7.32 (d, 2H,  $J = 8.0$  Hz), 7.75 (d, 3H,  $J = 8.8$  Hz), 8.33 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 21.1, 102.8 (d,  $J_{\text{C-F}} = 24.4$  Hz), 118.4 (d,  $J_{\text{C-F}} = 29$  Hz), 120.1 (d,  $J_{\text{C-F}} = 9.9$  Hz), 120.5 (d,  $J_{\text{C-F}} = 7.7$  Hz), 120.9, 122.1 (d,  $J_{\text{C-F}} = 12.2$  Hz), 130.3, 138.2, 147.2, 158.8 (d,  $J_{\text{C-F}} = 239.5$  Hz); IR (KBr): 3137, 3036, 2922, 1638, 1526, 1379, 1337, 1323, 1217, 1146, 1121, 1051, 830, 810, 762  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{14}\text{H}_{11}\text{N}_2\text{F}$  (226.2485): C 74.32, H 4.90, N 12.38; found C 74.42, H 4.95, N 12.30.

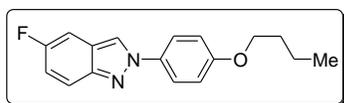


**5-Fluoro-2-(3,4-dimethylphenyl)-2H-indazole (2c):** Yellow solid; M.p. 105-106 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 2.32 (s, 3H), 2.36 (s, 3H), 7.11 (dt, 1H,  $J_1 = 2.4$  Hz,  $J_2 = 9.2$  Hz), 7.25-7.28 (m, 2H), 7.54 (dd, 1H,  $J_1 = 2$  Hz,  $J_2 = 8$  Hz), 7.67 (s, 1H), 7.73-7.77 (m, 1H), 8.32 (s,

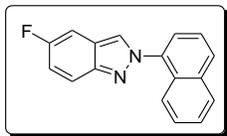
1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 19.4, 19.9, 102.8 (d,  $J_{\text{C-F}} = 24.4$  Hz), 118.1, 118.4, 120.0 (d,  $J_{\text{C-F}} = 9.9$  Hz), 120.5 (d,  $J_{\text{C-F}} = 8.4$  Hz), 121.9, 122.1, 130.6, 136.8, 138.3, 138.4, 147.1, 158.7 (d,  $J_{\text{C-F}} = 238.7$  Hz); IR (KBr): 3145, 2923, 1635, 1613, 1523, 1454, 1412, 1380, 1336, 1228, 1213, 1171, 1144, 1118, 1056, 850, 823, 805  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{15}\text{H}_{13}\text{N}_2\text{F}$  (240.2750): C 74.98, H 5.45, N 11.66; found C 75.06, H 5.49, N 11.57.



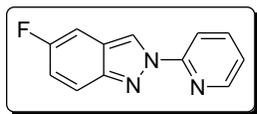
**5-Fluoro-2-(4-methoxyphenyl)-2H-indazole (2g):** Brown solid; M.p. 143-144 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 3.87 (s, 3H), 7.03 (d, 2H,  $J = 8.8$  Hz), 7.11 (dt, 1H,  $J_1 = 2.4$  Hz,  $J_2 = 9.2$  Hz), 7.25-7.28 (m, 1H), 7.70 (d, 3H,  $J = 8.8$  Hz), 8.27 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 55.7, 102.8 (d,  $J_{\text{C-F}} = 24.4$  Hz), 114.8, 118.2 (d,  $J_{\text{C-F}} = 29$  Hz), 119.9 (d,  $J_{\text{C-F}} = 9.9$  Hz), 120.5 (d,  $J_{\text{C-F}} = 8.4$  Hz), 122.4, 134.1, 147.1, 158.7 (d,  $J_{\text{C-F}} = 238.7$  Hz), 159.5; IR (KBr): 2960, 2932, 1609, 1522, 1511, 1450, 1435, 1337, 1298, 1249, 1219, 1145, 1027, 835, 814  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{14}\text{H}_{11}\text{N}_2\text{OF}$  (242.2479): C 69.41, H 4.58, N 11.56; found C 69.49, H 4.54, N 11.50.



**2-(4-Butoxyphenyl)-5-fluoro-2H-indazole (2h):** Yellow solid; M.p. 110-112 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 0.92 (t, 3H,  $J = 7.2$  Hz), 1.44 (m, 2H), 1.73 (m, 2H), 3.94 (t, 2H,  $J = 6.8$  Hz), 6.94 (d, 2H,  $J = 8.8$  Hz), 7.04 (dt, 1H,  $J_1 = 2.4$  Hz,  $J_2 = 9.2$  Hz), 7.18-7.20 (m, 1H), 7.68 (d, 3H,  $J = 8.8$  Hz), 8.19 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 13.9, 19.3, 31.3, 68.1, 102.7 (d,  $J_{\text{C-F}} = 24.4$  Hz), 115.1, 118.0 (d,  $J_{\text{C-F}} = 28.2$  Hz), 119.8 (d,  $J_{\text{C-F}} = 9.9$  Hz), 120.3 (d,  $J_{\text{C-F}} = 7.7$  Hz), 122.1, 133.7, 146.9, 158.6 (d,  $J_{\text{C-F}} = 238.7$  Hz), 158.9; IR (KBr): 3139, 2941, 2876, 1636, 1591, 1525, 1296, 1250, 1220, 1180, 1148, 1038, 1007, 836, 809, 768  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{17}\text{H}_{17}\text{N}_2\text{OF}$  (284.3274): C 71.81, H 6.03, N 9.85; found C 71.89, H 6.07, N 9.78.



**5-Fluoro-2-(naphthalen-1-yl)-2H-indazole (2i):** Yellowish-white solid; M.p. 120-122 °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 7.19 (dt, 1H,  $J_1 = 2.4$  Hz,  $J_2 = 9.2$  Hz), 7.34 (dd, 1H,  $J_1 = 2.0$  Hz,  $J_2 = 7.2$  Hz), 7.48-7.59 (m, 3H), 7.63-7.65 (m, 1H), 7.71 (d, 1H,  $J = 8.4$  Hz), 7.80-7.84 (m, 1H), 7.95 (d, 1H,  $J = 8.0$  Hz), 7.99 (d, 1H,  $J = 8.4$  Hz), 8.24 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 102.8 (d,  $J_{\text{C-F}} = 24.4$  Hz), 118.4 (d,  $J_{\text{C-F}} = 29$  Hz), 120.2 (d,  $J_{\text{C-F}} = 9.9$  Hz), 121.4 (d,  $J_{\text{C-F}} = 11.4$  Hz), 122.9, 123.9, 125.0, 125.7 (d,  $J_{\text{C-F}} = 8.4$  Hz), 126.9, 127.8, 128.2, 128.9, 129.9, 134.2, 137.5, 147.1, 158.7 (d,  $J_{\text{C-F}} = 239.5$  Hz); IR (KBr): 3058, 2924, 1634, 1595, 1522, 1420, 1387, 1227, 1175, 1147, 1120, 854, 798  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{17}\text{H}_{11}\text{N}_2\text{F}$  (262.2806): C 77.85, H 4.23, N 10.68; found C 77.93, H 4.29, N 10.60.



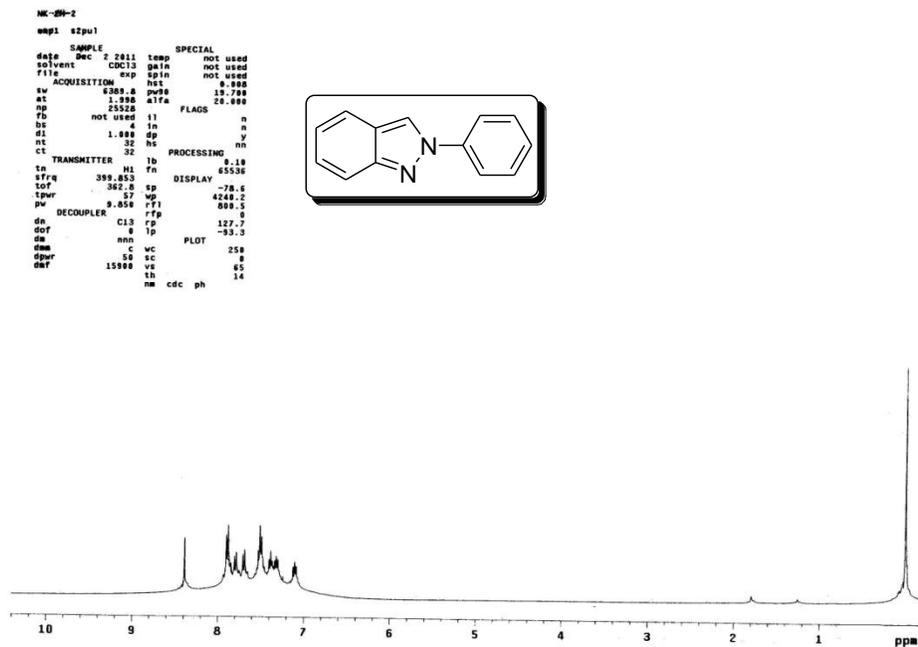
**5-Fluoro-2-(pyridin-2-yl)-2H-indazole (2j):** White solid; M.p. 133.5-135.5 (lit.<sup>7</sup> 129-130 °C) °C;  $^1\text{H}$  NMR ( $\text{CDCl}_3$ , 400 MHz):  $\delta$  (ppm) 7.11 (dt, 1H,  $J_1 = 2.4$  Hz,  $J_2 = 9.2$  Hz), 7.26-7.30 (m, 2H), 7.69-7.73 (m, 1H), 7.88 (dt, 1H,  $J_1 = 2.0$  Hz,  $J_2 = 8.4$  Hz), 8.23 (d, 1H,  $J = 8.4$  Hz), 8.49 (d, 1H,  $J = 4.8$  Hz), 9.04 (s, 1H);  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 100 MHz):  $\delta$  (ppm) 103.4 (d,  $J_{\text{C-F}} = 23.6$  Hz), 114.1, 119.6 (d,  $J_{\text{C-F}} = 29$  Hz), 120.4 (d,  $J_{\text{C-F}} = 9.1$  Hz), 120.8 (d,  $J_{\text{C-F}} = 9.1$  Hz), 121.8 (d,  $J_{\text{C-F}} = 12.2$  Hz), 123.0, 139.0, 147.9, 148.5, 151.9, 158.9 (d,  $J_{\text{C-F}} = 241$  Hz); IR (KBr): 3147, 2924, 1596, 1522, 1475, 1439, 1377, 1323, 1212, 1144, 1114, 1055, 863, 837, 808  $\text{cm}^{-1}$ ; Elemental analysis calcd (%) for  $\text{C}_{12}\text{H}_8\text{N}_3\text{F}$  (213.2101): C 67.60, H 3.78, N 19.71; found C 67.68, H 3.82, N 19.62.

## **References**

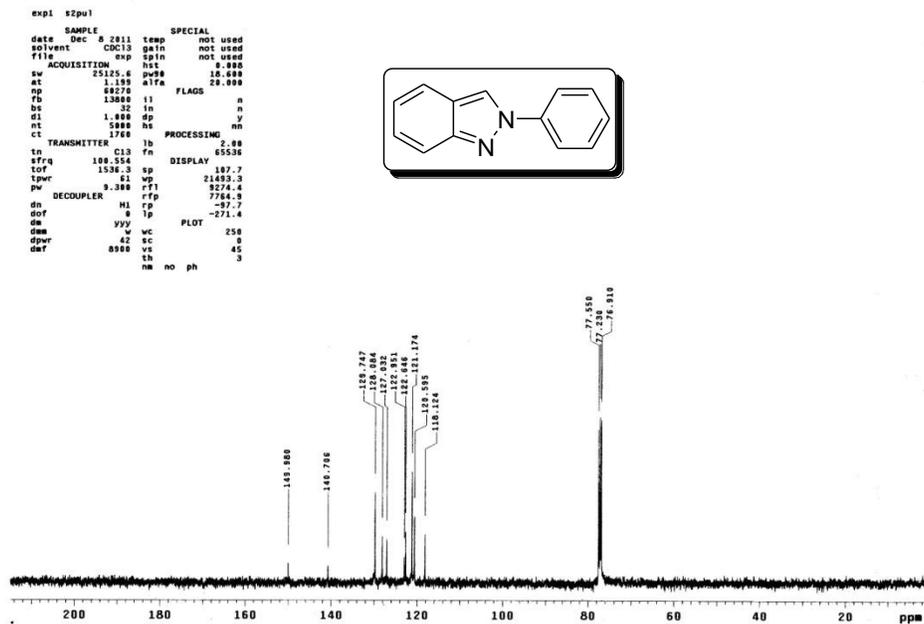
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5. Y. Fang , C. Wu, R. C. Larock and Feng Shi, *J. Org. Chem.*, 2011, **76**, 8840.
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## Spectra

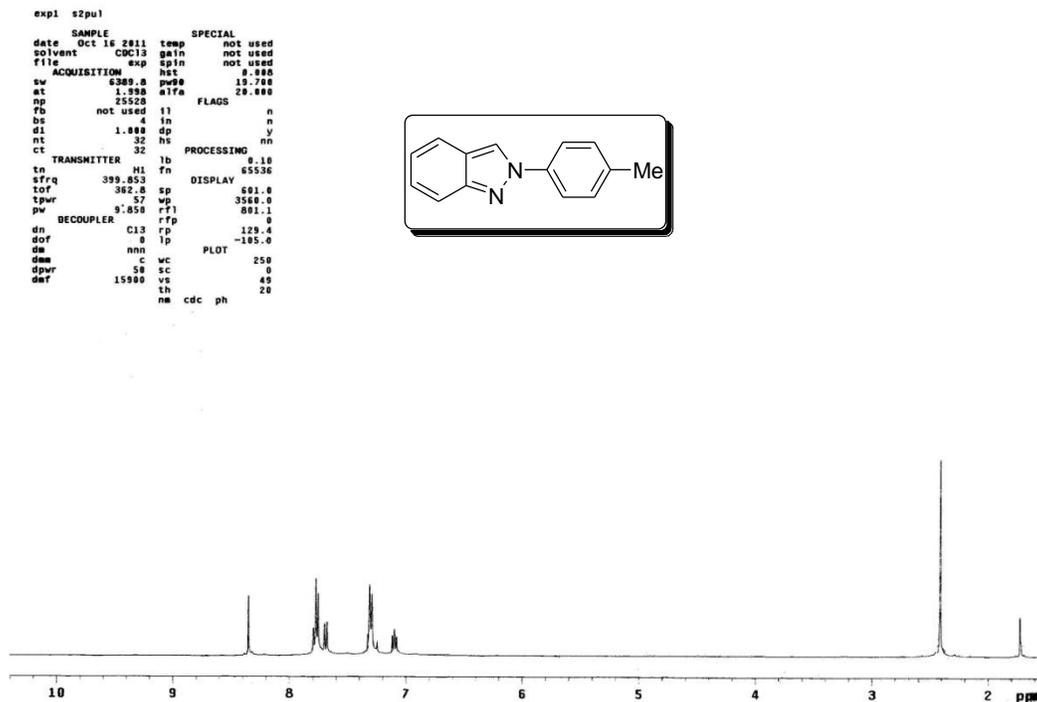
### 2-Phenyl-2H-indazole (1a): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )



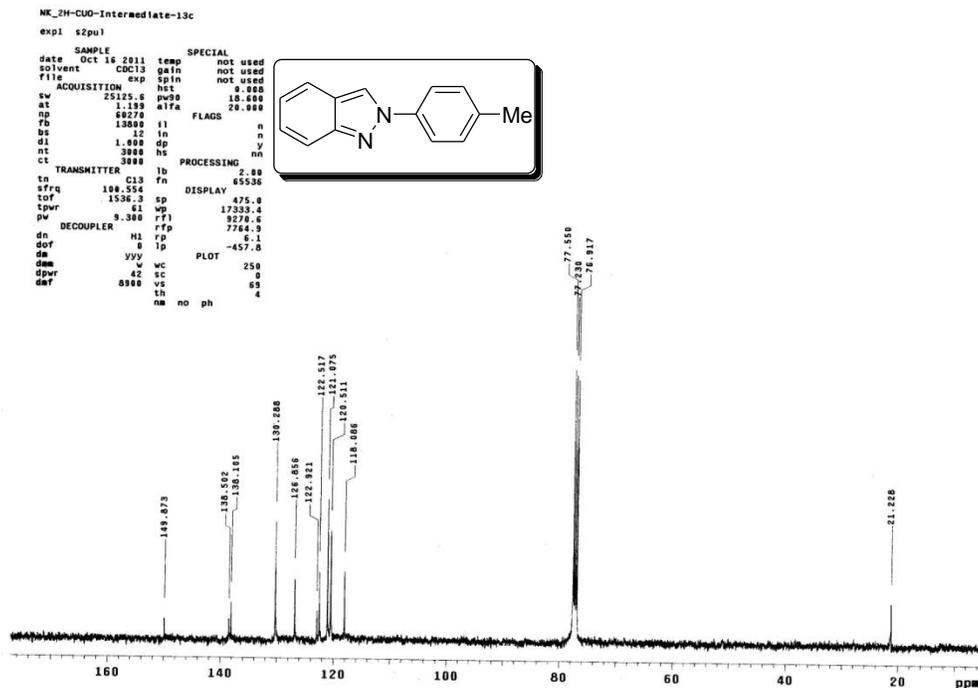
### 2-Phenyl-2H-indazole (1a): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



2-*p*-Tolyl-2H-indazole (1b):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

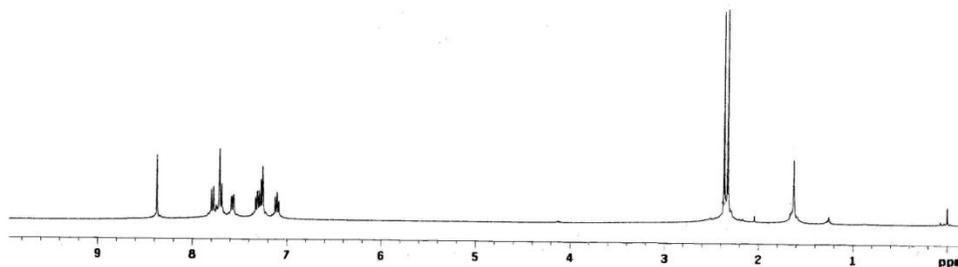
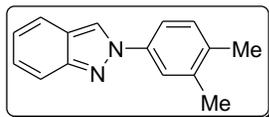


2-*p*-Tolyl-2H-indazole (1b):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )



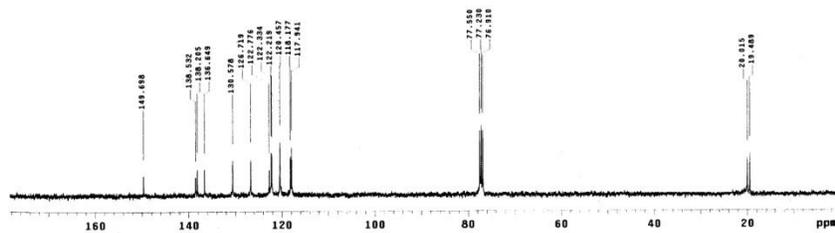
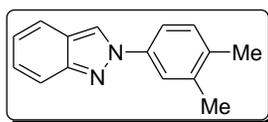
### 2-(3,4-Dimethylphenyl)-2H-indazole (1c): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

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np 25520
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ct
TRANSMITTER 32 lb PROCESSING 0.10
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pw 8.050 rfp 785.6
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dpr 50 sc 0
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### 2-(3,4-Dimethylphenyl)-2H-indazole (1c): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )

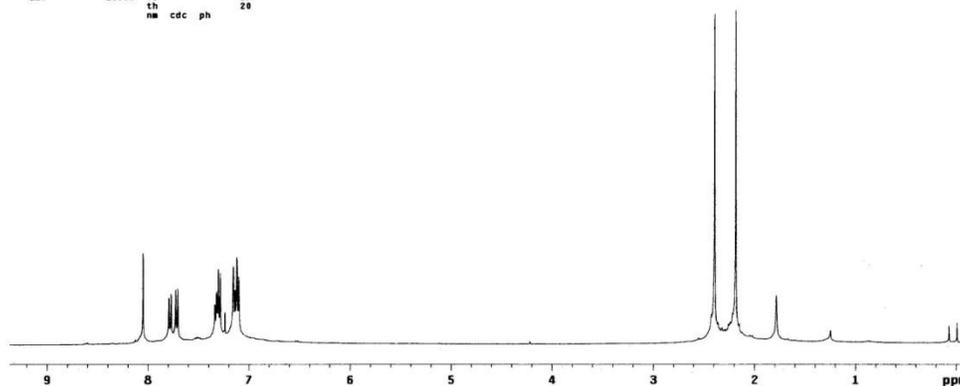
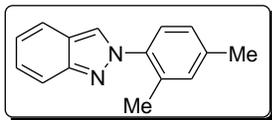
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2-(2,4-Dimethylphenyl)-2H-indazole (1d):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

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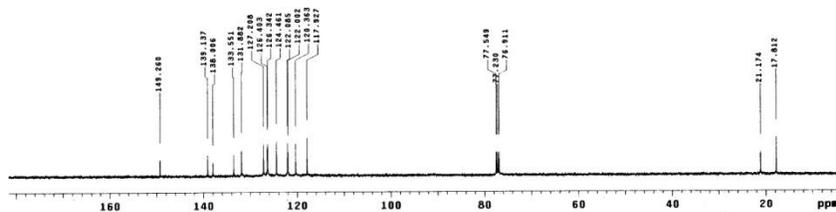
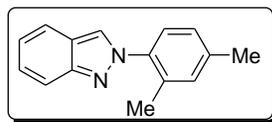
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ACQUISITION	exp	sp in	not used
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nt	25528	atfa	28.000
np	not used	fl	n
bs	4	in	n
d1	1.000	dp	y
nt	32	hs	nm
ct	32	PROCESSING	8.10
tn	TRANSMITTER	fb	fn
sfrq	399.253	sp	DISPLAY
tof	382.0	wp	-55.9
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pw	0.058	rfp	3690.1
DECOUPLER	C13	rp	2884.3
dof	0	lp	167.4
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			20



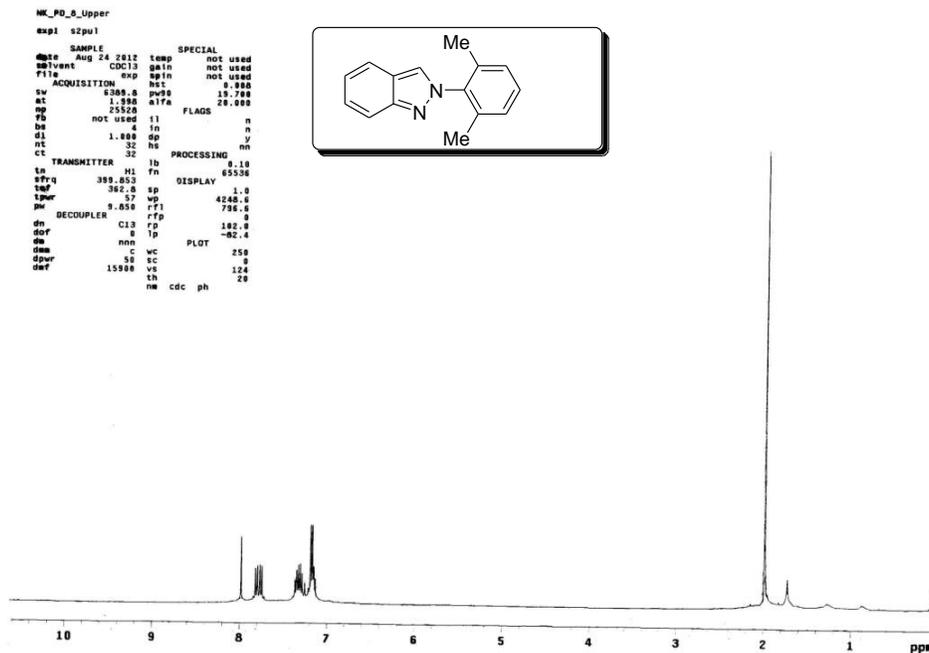
2-(2,4-Dimethylphenyl)-2H-indazole (1d):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

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 exp1 s1d13c

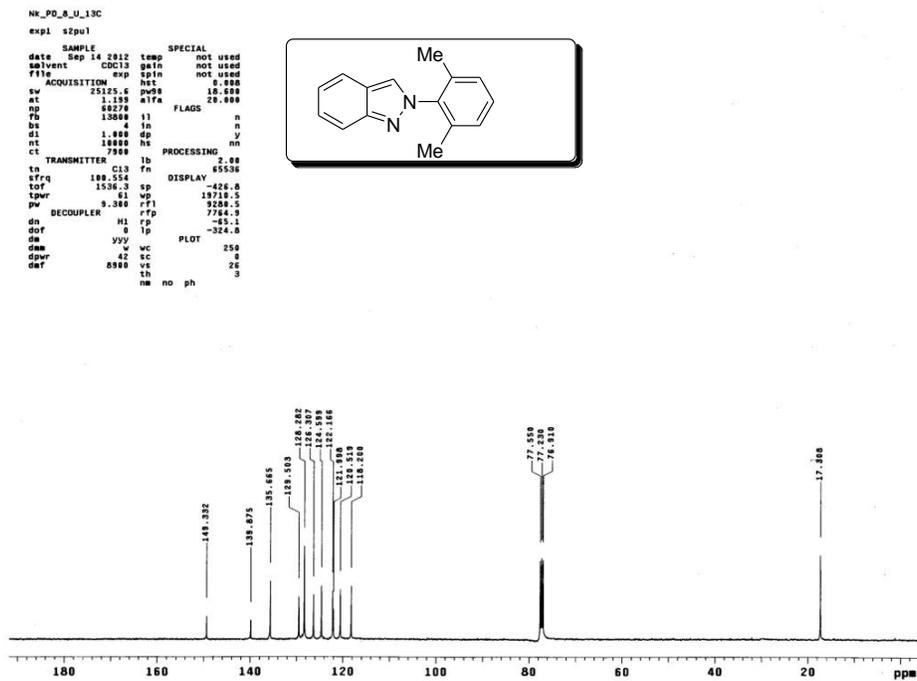
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ct	1054	PROCESSING	1.00
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daf	8500	vs	0
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		nm	no ph
			4



2-(2,6-Dimethylphenyl)-2H-indazole (1e):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



2-(2,6-Dimethylphenyl)-2H-indazole (1e):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

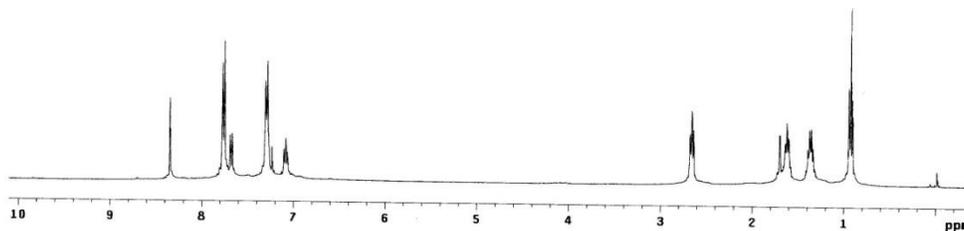
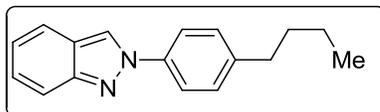


2-(4-Butylphenyl)-2H-indazole (1f):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

NK\_PD\_26\_1H  
 exp1 s2pu1

```

SAMPLE          SPECIAL
date Sep 26 2012 temp not used
solvent CDCl3 gain not used
file           exp spin not used
ACQUISITION    hst      0.000
sw 6389.8 pv90 19.700
at 1.900 a1fa 20.000
np 25528          FLAGS
fb not used i1    n
bs 4 in          n
dl 1.000 dp      y
nt 32 hs        nm
ct          32   PROCESSING
tn          11   b      8.18
sfrq 399.853 H1 fn 65536
tof 362.8 sp DISPLAY -165.3
tpwr 57 wp 4266.5
pw 9.850 rF1 3690.3
DECOUPLER C13 rfp 2894.3
dof 0 lp -116.3
dm nnn          PLOT
dwa c          250
dpwr 50 sc      0
dat 15900 vs    46
          th    20
          nm cdc ph
    
```

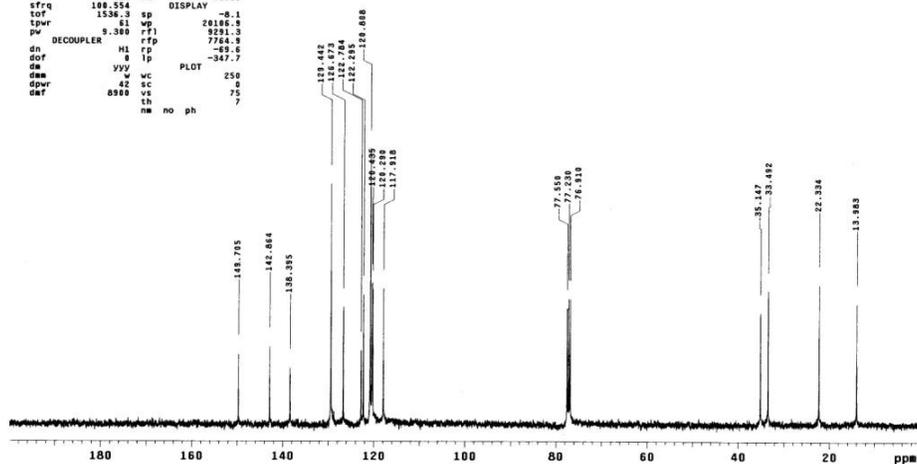
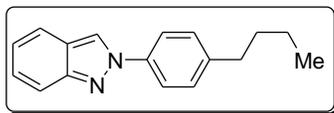


2-(4-Butylphenyl)-2H-indazole (1f):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

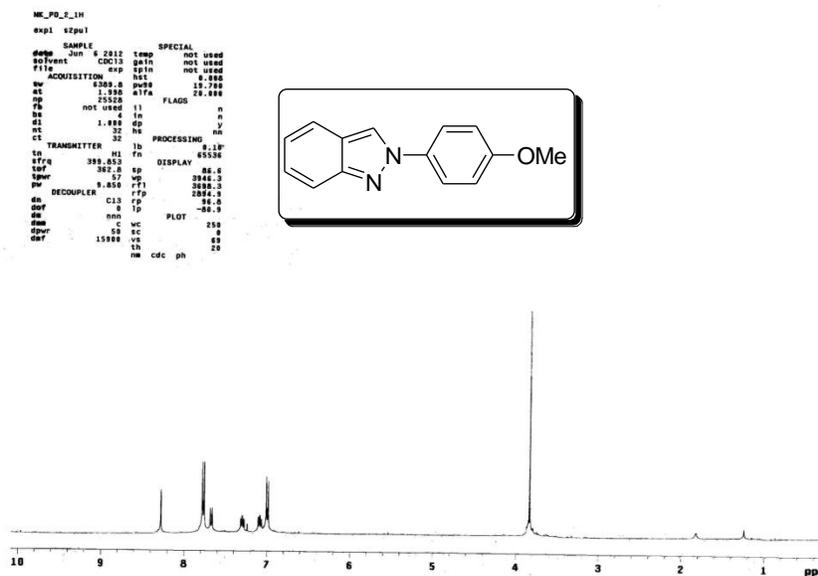
NK\_PD\_26\_13C  
 exp1 s2pu1

```

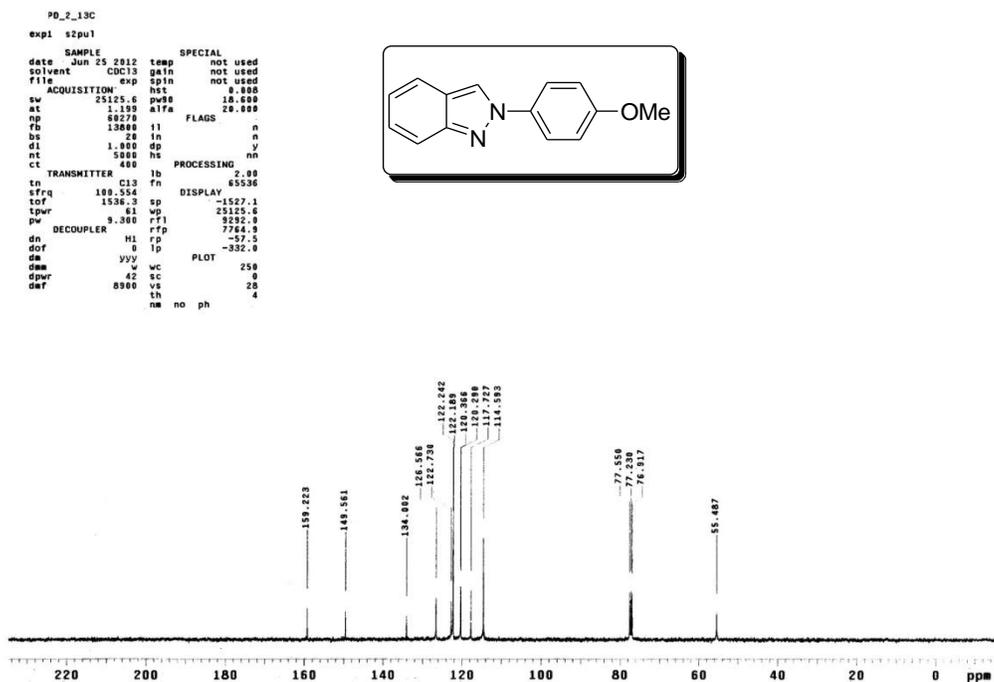
SAMPLE          SPECIAL
date Oct 2 2012 temp not used
solvent CDCl3 gain not used
file           exp spin not used
ACQUISITION    hst      0.000
sw 25125.6 pv90 18.600
at 1.100 a1fa 20.000
np 80270          FLAGS
fb 13000 i1      n
bs 32 in         n
dl 1.000 dp      y
nt 5000 hs       nm
ct          1129 PROCESSING
tn          11   b      2.00
sfrq 100.623 C13 fn 65536
tof 1536.3 sp DISPLAY -8.1
tpwr 61 wp 26100.0
pw 9.300 rF1 9291.3
DECOUPLER H1 rfp 7704.0
dof 0 lp -69.6
dm yyy          PLOT
dwa v          250
dpwr 42 sc      0
dat 8900 vs    46
          th    75
          nm no ph
    
```



2-(4-Methoxyphenyl)-2H-indazole (1g):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



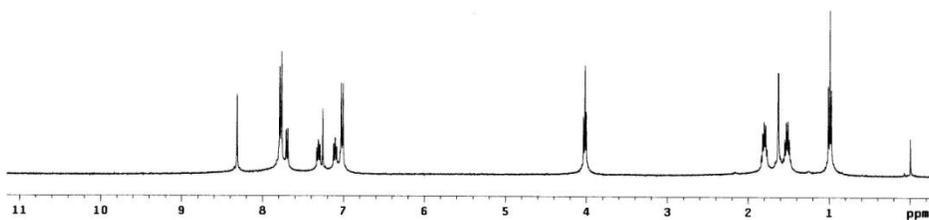
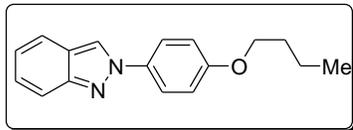
2-(4-Methoxyphenyl)-2H-indazole (1g):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )



2-(4-Butoxyphenyl)-2H-indazole (1h): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

```

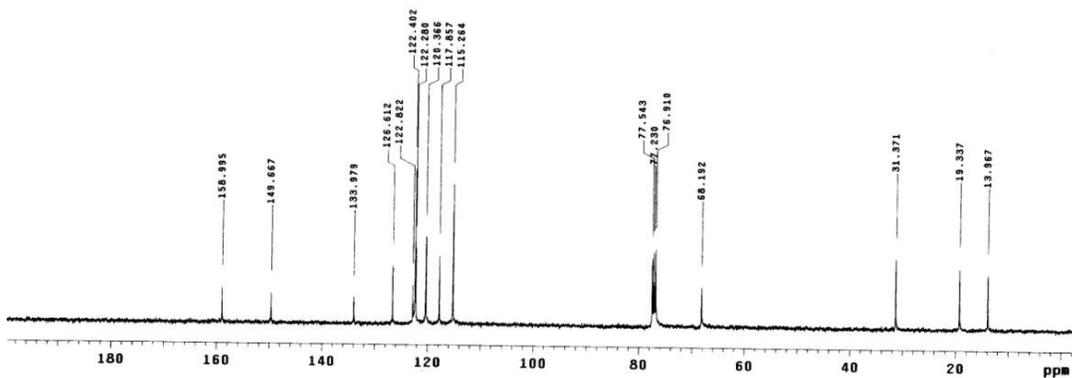
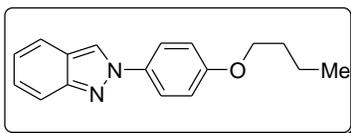
NE-PD-27
exp1 s2pu1
SAMPLE          SPECIAL
date   Sep 28 2012 temp      not used
solvent CDCl3 gain      not used
file   exp spin      not used
ACQUISITION    hst      0.000
sw      60270 pwhz     12.780
at      1.199 a1fa     20.000
np      25526
fb      not used i1      FLAGS
bs      32 in          n
d1      1.000 dp        y
nt      32 hs          nn
ct      0
TRANSMITTER    lb      0.10
tn      C13 fn        65536
sfrq     399.853 DISPLAY
tof      362.8 sp      -114.9
tpvr     57 wp        4576.0
pw      9.850 rfp      794.8
DECOUPLER      C13 rp      119.3
dn      0 lp        -79.2
dm      nnn          PLOT
dmc     w wc        250
dpcr    50 sc        0
dmf     15000 vs      56
nm      cdc ph      20
    
```



2-(4-Butoxyphenyl)-2H-indazole (1h): <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

```

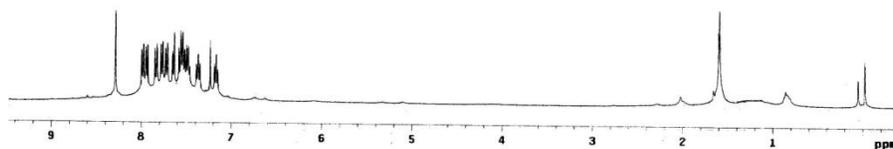
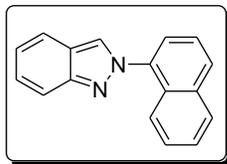
7_13C
s2pu1
SAMPLE          SPECIAL
date   Oct 8 2012 temp      not used
solvent CDCl3 gain      not used
file   exp spin      not used
ACQUISITION    hst      0.000
sw      25125.6 pwhz     10.000
at      1.199 a1fa     20.000
np      60270
fb      13600 i1      FLAGS
bs      32 in          n
d1      1.000 dp        y
nt      5000 hs          nn
ct      1632
TRANSMITTER    lb      2.00
tn      C13 fn        65536
sfrq     100.624 DISPLAY
tof      1536.3 sp      -261.2
tpvr     61 wp        20403.7
pw      9.300 rfp      9200.5
DECOUPLER      H1 rp      784.8
dn      0 lp        -67.2
dm      vvy          PLOT
dmc     w wc        250
dpcr    42 sc        0
dmf     8900 vs      36
nm      no ph      5
    
```



2-(Naphthalen-1-yl)-2H-indazole (1i):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

```

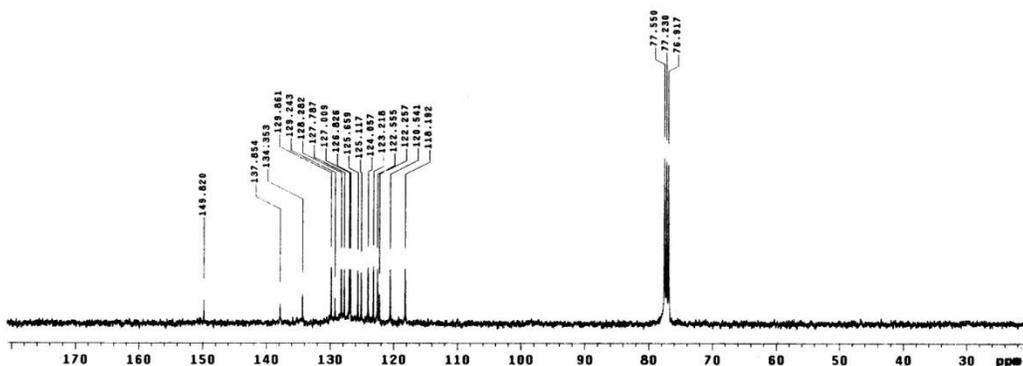
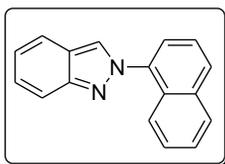
NK_PD_14
expl s2pu1
SAMPLE
date Jul 23 2012 temp not used
solvent CDCl3 gain not used
file NK_PD_14_13C spin not used
ACQUISITION exp s2pu1 hst 0.000
sw 6380.0 nu0 16.000
at 1.199 a1fa 20.000
np 0.0278
fb 13000 f1 FLAGS n
bs 32 in n
d1 1.000 sp y
nt 7800 hs nn
ct 3200
TRANSMITTER lb fb 2.00
in f1 fn 65536
sfreq 100.624 DISPLAY 2000.3
toF 1536.3 sp 16079.0
tpwr 81 wp 9275.2
pw 9.300 rf1 7764.9
DECOUPLER H1 rf 49.4
dof 0 tp -244.6
dm yvy PLOT 250
dwa v wc 0
dpwr 42 sc 0
def 8000 vs 60
th 3
nm no ph
    
```



2-(Naphthalen-1-yl)-2H-indazole (1i):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

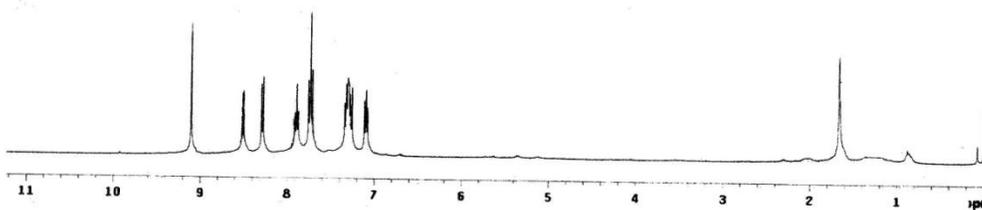
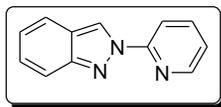
```

NK_PD_14_13C
expl s2pu1
SAMPLE
date Jul 20 2012 temp not used
solvent CDCl3 gain not used
file NK_PD_14_13C spin not used
ACQUISITION exp s2pu1 hst 0.000
sw 12525.6 nu0 16.000
at 1.199 a1fa 20.000
np 0.0278
fb 13000 f1 FLAGS n
bs 32 in n
d1 1.000 sp y
nt 7800 hs nn
ct 3200
TRANSMITTER lb fb 2.00
in f1 fn 65536
sfreq 100.624 DISPLAY 2000.3
toF 1536.3 sp 16079.0
tpwr 81 wp 9275.2
pw 9.300 rf1 7764.9
DECOUPLER H1 rf 49.4
dof 0 tp -244.6
dm yvy PLOT 250
dwa v wc 0
dpwr 42 sc 0
def 8000 vs 60
th 3
nm no ph
    
```



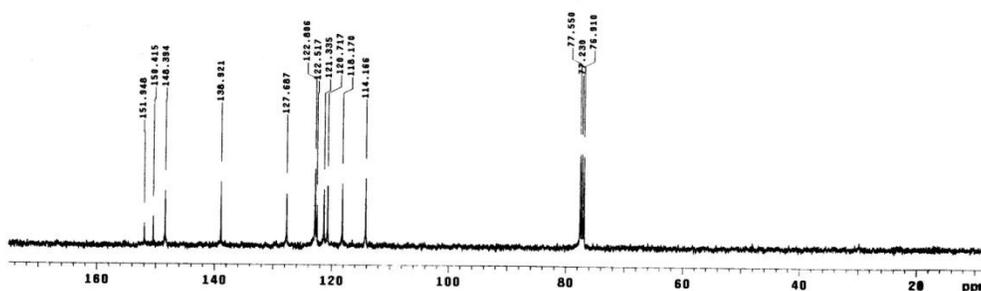
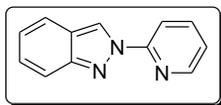
2-(Pyridin-2-yl)-2H-indazole (1j):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

```
nmr1 88pul
=====
SAMPLE          SPECIAL
date Jul 25 2012 temp not used
solvent CDCl3 gain not used
file          exp  spIn not used
ACQUISITION  hst  0.000
sv           8388.8 puse 19.700
at           1.000 alfa 20.000
ap           25520 FLAGS
fb not used  f1      n
bs           4      in  n
d1           1.000 dp  y
nt           32     hs  nn
ct
TRANSMITTER  f0      0.10
tn           M1     fn  65536
sfrq        399.853 sp  DISPLAY
tof         362.0   sp  -63.7
tpwr        57     wp  4532.7
pw          9.850  rf1  795.6
DECOUPLER   rfp    0
dn          C13   rp  113.4
dof         8     1p  -83.7
dm          nnn   PLOT
dwa         50    wc  250
dpr         15900 vs  43
dat         nm   cdc ph  20
```



2-(Pyridin-2-yl)-2H-indazole (1j):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

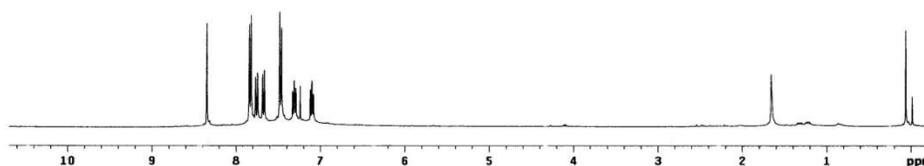
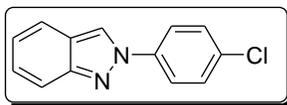
```
SAMPLE          SPECIAL
date Aug 10 2012 temp not used
solvent CDCl3 gain not used
file          exp  spIn not used
ACQUISITION  hst  0.000
sv           25125.6 puse 18.000
at           1.100 alfa 20.000
ap           60270 FLAGS
fb          130000 f1      n
bs           32     in  n
d1           1.000 dp  y
nt           5000  hs  nn
ct
TRANSMITTER  f0      2.00
tn           C13   fn  65536
sfrq        100.624 sp  DISPLAY
tof         1536.3   sp  728.8
tpwr         61     wp  10071.1
pw          9.300  rf1  3258.5
DECOUPLER   H1     rfp  7764.9
dn          8     1p  -30.7
dof         yyy   PLOT
dwa         C42   wc  250
dpr         8900 vs  24
dat         nm   no ph  4
```



### 2-(4-Chlorophenyl)-2H-indazole (1k): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

NK-PD-9  
\*xp1 s2pu1

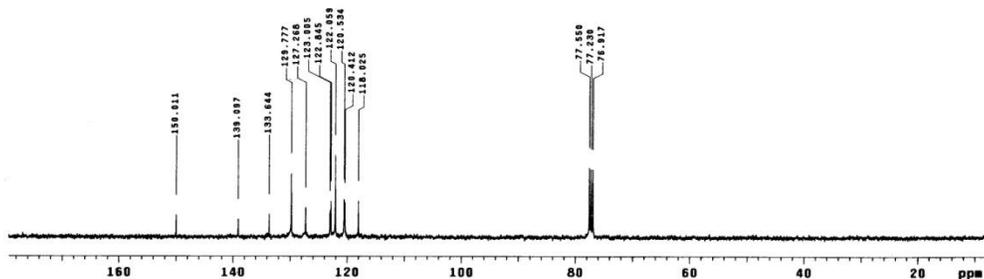
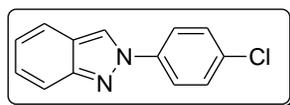
```
SAMPLE          SPECIAL
date Jul 4 2012 temp not used
solvent CDCl3 gain not used
file           exp spin not used
ACQUISITION    hsc 8.888
sv            6289.8 pu98 18.700
at           1.950 atfa 28.888
np            25528
ns not used  it  FLAGS n
ob            4 in n
ol            1.000 dp y
vc            32 hs m
ct
TRANSMITTER    32 lb PROCESSING 8.18
tn            H1 fn DISPLAY 65536
stfq          399.853
tof           362.8 sp -106.8
tpr          57 vp 4583.8
nw           9.850 rfl 3687.7
DECOUPLER     C13 rfp 2884.9
dn            8 lp 112.7
dof           0 lp PLOT -83.9
dm           C wc 250
dpr          50 sc 0
def          15900 ve th 31
nm cdc ph 26
```



### 2-(4-Chlorophenyl)-2H-indazole (1k): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )

NK\_PD\_9\_13c  
exp1 s2pu1

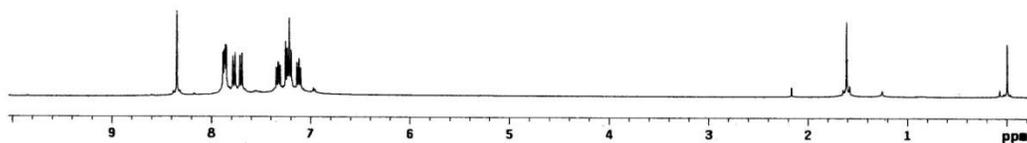
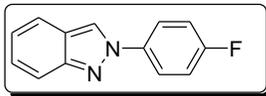
```
SAMPLE          SPECIAL
date Jul 9 2012 temp not used
solvent CDCl3 gain not used
file           exp spin not used
ACQUISITION    hsc 8.888
sv            25125.6 pu98 18.688
at           1.189 atfa 28.888
np            88278
ns not used  it  FLAGS n
ob            32 in n
ol            1.000 dp y
vc            888 hs m
ct
TRANSMITTER    888 lb PROCESSING 2.88
tn            C13 fn DISPLAY 65536
stfq          188.504
tof           1536.3 sp 784.7
tpr          61 vp 17236.5
nw           9.388 rfl 9276.8
DECOUPLER     H1 rfp 7764.9
dn            8 lp -54.7
dof           0 lp PLOT -344.3
dm           yyy wc 250
dpr          42 sc 0
def          8880 ve th 21
nm no ph 2
```



2-(4-Fluorophenyl)-2H-indazole (11):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

NK-PD-10

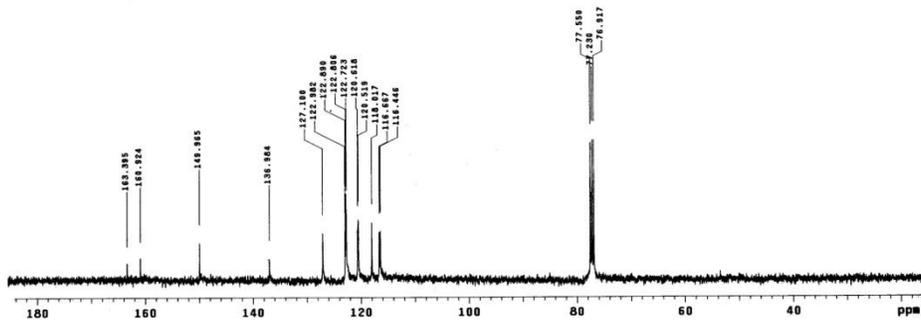
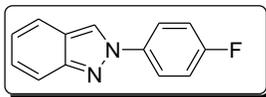
```
exp1 s2pul
SAMPLE
date Jul 9 2012 temp not used
solvent CDCl3 gain not used
file exp sp1n not used
ACQUISITION hst 0.000
sw 4388.0 pufs 15.700
at 1.998 a1fa 20.000
np 25528
fb not used i1 FLAGS n
bs 4 in n
d1 1.000 dp y
nt 32 hs nm
ct TRANSMITTER 32 PROCESSING 8.10
tn H1 fn 65536
sfrq 399.853 DISPLAY -99.6
tor 362.0 sp
tpwr 57 wp 4114.2
pw 9.050 rfl 796.4
DECOUPLER rfp 0
dn C13 rp 110.0
dof 0 lp -97.6
dm nnn PLOT 250
dwa 50 sc 0
dpwr 15900 vs 30
dnt ne cdc ph 20
```



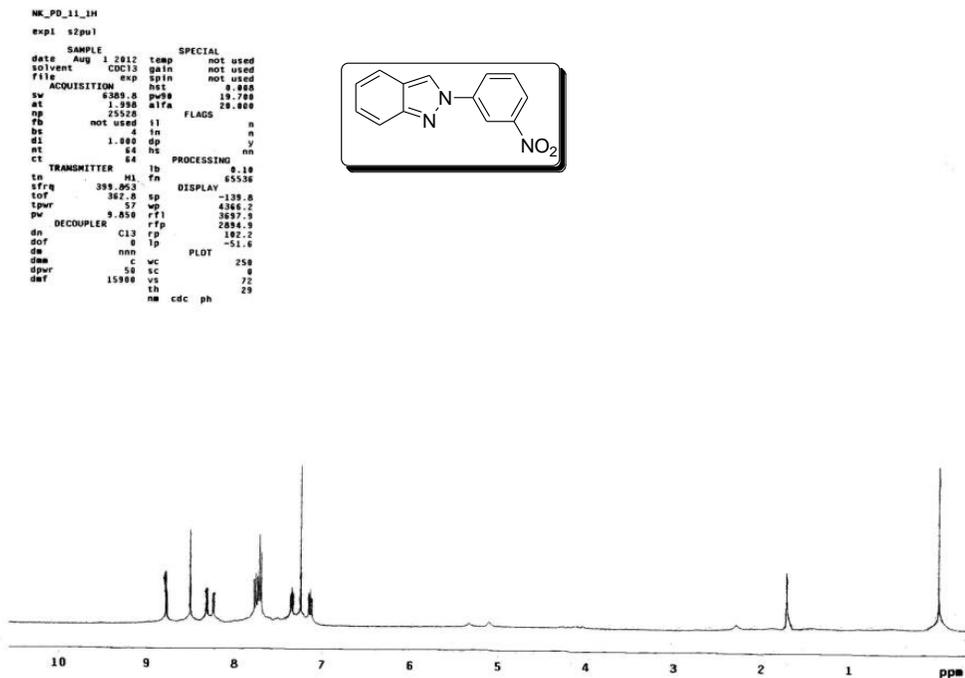
2-(4-Fluorophenyl)-2H-indazole (11):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

NK\_PD\_10\_13C

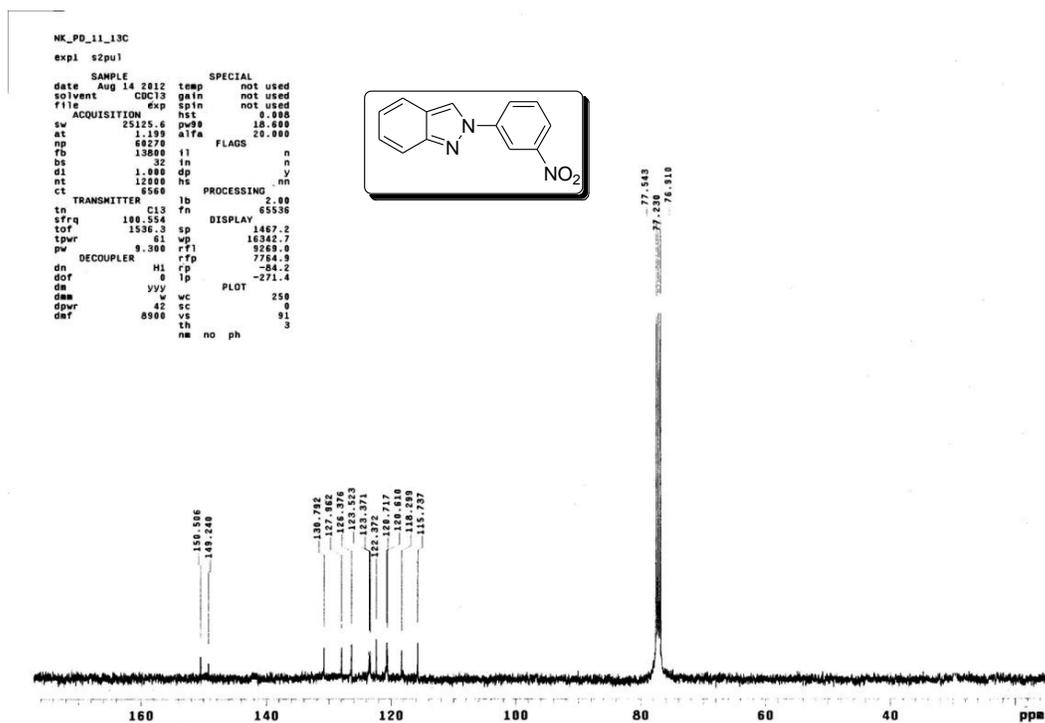
```
exp1 s2pul
SAMPLE
date Jul 9 2012 temp not used
solvent CDCl3 gain not used
file exp sp1n not used
ACQUISITION hst 0.000
sw 12125.6 pufs 10.000
at 1.199 a1fa 20.000
np 68278
fb 13000 i1 FLAGS n
bs 32 in n
d1 1.000 dp y
nt 1500 hs nm
ct TRANSMITTER 32 PROCESSING 2.00
tn C13 fn 65536
sfrq 100.626 DISPLAY 1591.4
tor 1538.3 sp
tpwr 61 wp 10937.0
pw 9.388 rfl 3276.7
DECOUPLER H1 rfp 7764.0
dn C13 rp -10.2
dof 0 lp -435.0
dm ysv PLOT 250
dwa 2 sc 0
dpwr 8900 vs 30
dnt ne no ph 4
```



### 2-(3-Nitrophenyl)-2H-indazole (1m): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

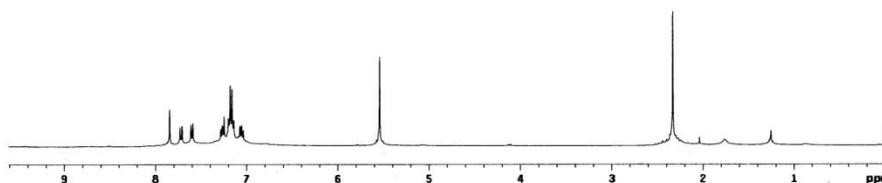
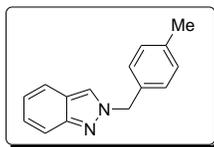


### 2-(3-Nitrophenyl)-2H-indazole (1m): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



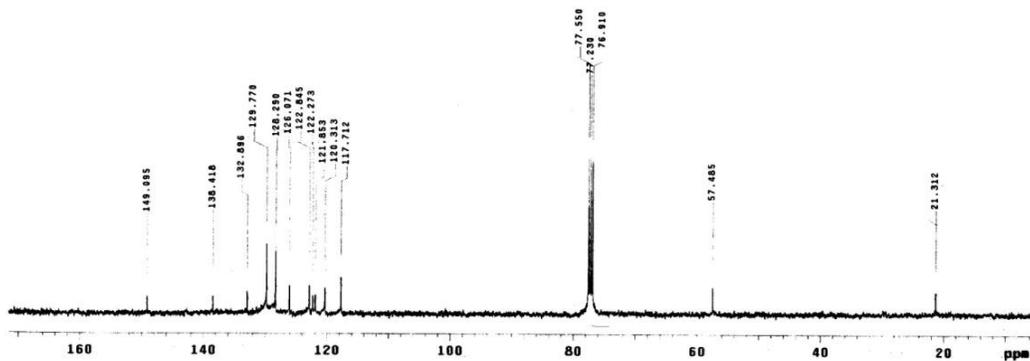
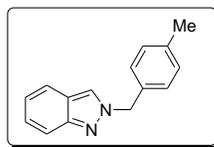
2-(4-Methylbenzyl)-2H-indazole (1n):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

```
ME_PD_5_1H
exp1 s2pm1
SPECIAL
date Jul 19 2012 temp not used
solvent CDCl3 gain not used
file ACQUISITION exp sp in not used
1.000 hst 8.000
25225.6 pwr 18.400
1.198 a1fa 20.000
25225.6
at not used f1 FLAGS n
fb 4 f2 n
ds 1.888 dp y
nt 32 hs PROCESSING nn
ct 32 ht 8.18
tn TRANSMITTER f3 f4 65536
sfrq 399.059 H1 f5 DISPLAY -28.1
tof 361.8 sp 3078.7
tpwr 57 wp 300.5
pwr 8.850 rf1 0
DECOUPLER C13 rf2 182.5
dn 0 ip -86.1
dot mm PLOT 250
dm 0 sc 0
dpr 15180 sb vs 38
dat th 20
na cdc ph
```



2-(4-Methylbenzyl)-2H-indazole (1n):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

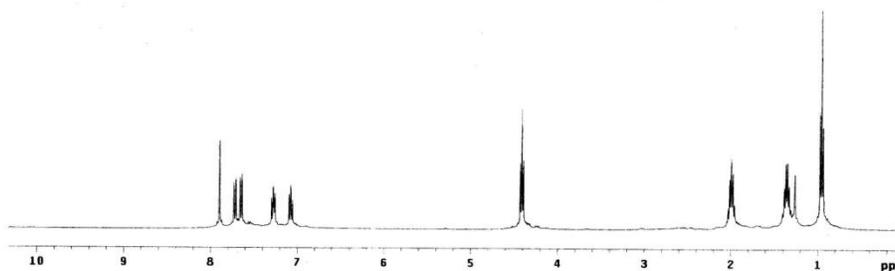
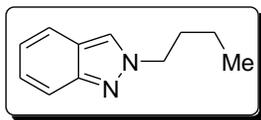
```
exp1 std13c
SPECIAL
date Jul 19 2012 temp not used
solvent CDCl3 gain not used
file ACQUISITION exp sp in not used
1.000 hst 8.000
25225.6 pwr 18.400
1.198 a1fa 20.000
25225.6
at not used f1 FLAGS n
fb 4 f2 n
ds 1.888 dp y
nt 32 hs PROCESSING nn
ct 32 ht 8.18
tn TRANSMITTER f3 f4 65536
sfrq 399.059 H1 f5 DISPLAY -28.1
tof 361.8 sp 3078.7
tpwr 57 wp 300.5
pwr 8.850 rf1 0
DECOUPLER C13 rf2 182.5
dn 0 ip -86.1
dot mm PLOT 250
dm 0 sc 0
dpr 15180 sb vs 38
dat th 20
na cdc ph
```



2-Butyl-2H-indazole (10):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

```

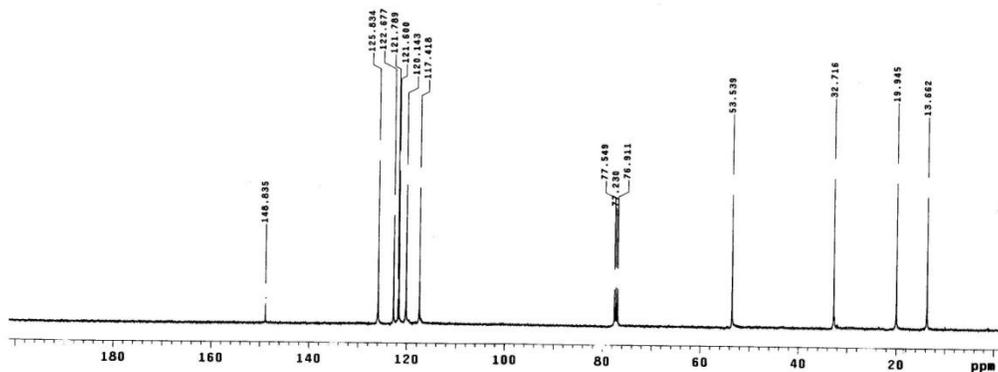
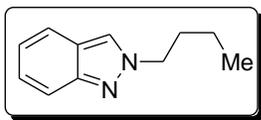
NK-PD-28
expt szpu1
SAMPLE SPECIAL
date Oct 19 2012 temp not used
solvent CDCl3 gain not used
File not used
ACQUISITION exp hst not used
sw 6389.8 pps 19.708
at 1.998 n1fa 28.000
np 25528
fb not used n1f FLAGS n
bs 4 in n
sl 1.000 dp y
nt 32 ht nm
ct 32 PROCESSING
tn 1.19
sfq M1 fn 65534
tof 399.853 DISPLAY
tof 362.8 sp -13.5
tpwr 57 wp 4142.1
pw 9.858 rfp 782.5
DECOUPLER rfp 3
dn C13 fp 110.2
dof 0 fp -92.2
dm nnn PLOT
dms 58 wc 250
dpr 58 sc 0
dwt 15988 vs 61
nm cdc ph 28
    
```



2-Butyl-2H-indazole (10):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

```

0-28
p1 std13c
SAMPLE SPECIAL
date Apr 21 2013 temp not used
solvent CDCl3 gain not used
File not used
ACQUISITION exp hst not used
sw 25000.0 pps 8.400
at 1.193 n1fa 28.000
np 59368
fb 13000 n1 FLAGS n
bs 32 in n
sl 0 dp y
nt 10000 ht nm
ct 6528 PROCESSING
tn 1.08
sfq C13 fn not used
tof 100.552 DISPLAY
tof 61 sp -132.5
tpwr 8.667 rfp 28387.3
pw 0.667 rfp 18755.5
DECOUPLER rfp 7764.9
dn H1 fp -51.1
dof 0 fp -341.0
dm yyy PLOT
dms 42 wc 250
dpr 42 sc 0
dwt 8500 vs 41
nm no ph 4
    
```

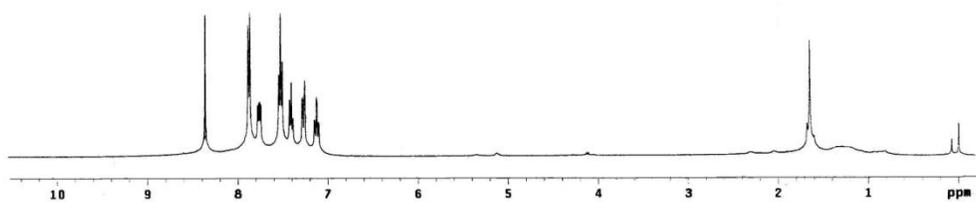
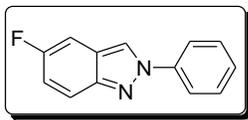


### 5-Fluoro-2-phenyl-2H-indazole (2a): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )

```
MS_PD_18_1H
exp1 s2pul

SAMPLE          SPECIAL
date Aug 2 2012 temp not used
solvent CDCl3   gain not used
file            exp  spfn not used
ACQUISITION    hsc  not used
sv 6389.8     pw90 19.700
at 1.800     a1fa 29.900
np 25528                                FLAGS
fb not used  i1      n
bs 4        in      n
d1 1.000    dp      y
nt 32      hs      nm
ct

TRANSMITTER    lb  fn  PROCESSING  0.18
tn             M1  fn  DISPLAY   65536
sfrq 399.853    sp  -73.9
tor 382.0      wp  4299.5
tpwr 57        rfl  795.8
pw 9.850      rfp  0
dn DECOUPLER  C13  rf  117.7
dor 0        ip  -89.7
dm nnn        wc  PLOT      250
dam 5        sc  0
dpwr 15900    vs  41
dof 0        th  20
nm cdc ph
```

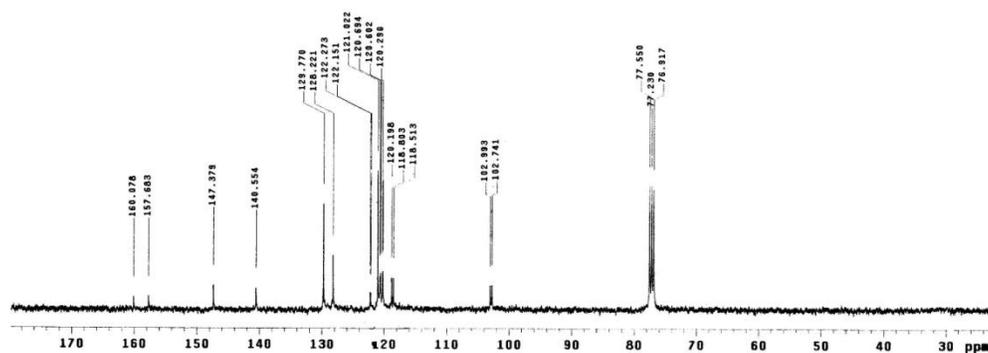
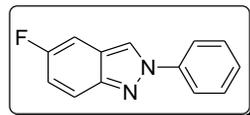


### 5-Fluoro-2-phenyl-2H-indazole (2a): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )

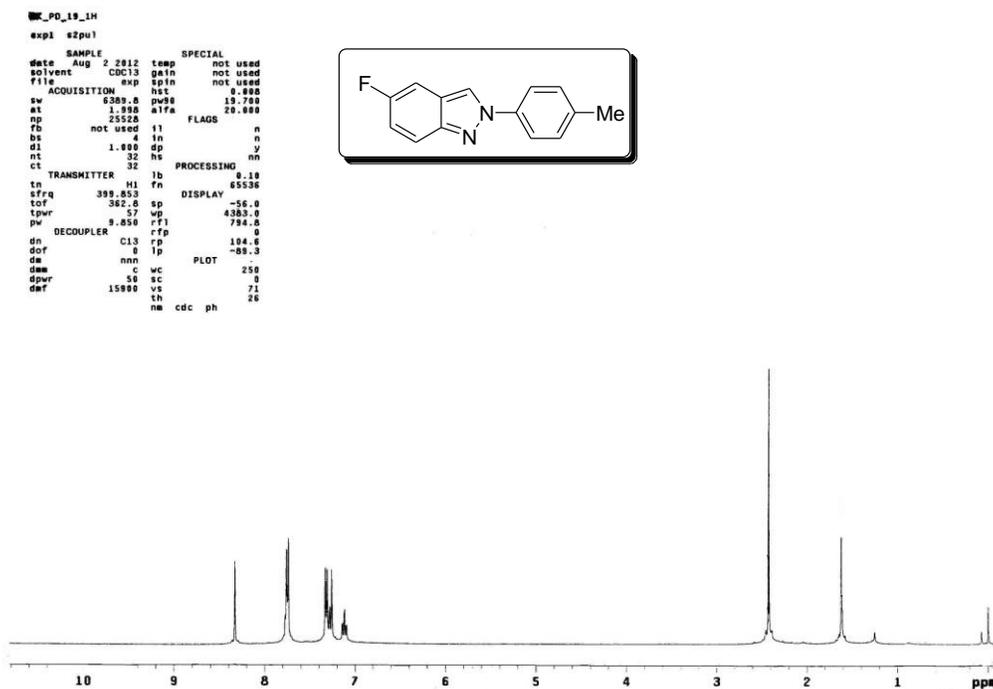
```
PD_18_13C
exp1 s2pul

SAMPLE          SPECIAL
date Aug 13 2012 temp not used
solvent CDCl3   gain not used
file            exp  spfn not used
ACQUISITION    hsc  not used
sv 25125.8     pw90 18.600
at 1.100     a1fa 29.900
np 60270                                FLAGS
fb 13000      i1      n
bs 32        in      n
d1 1.000    dp      y
nt 5800      hs      nm
ct 3264

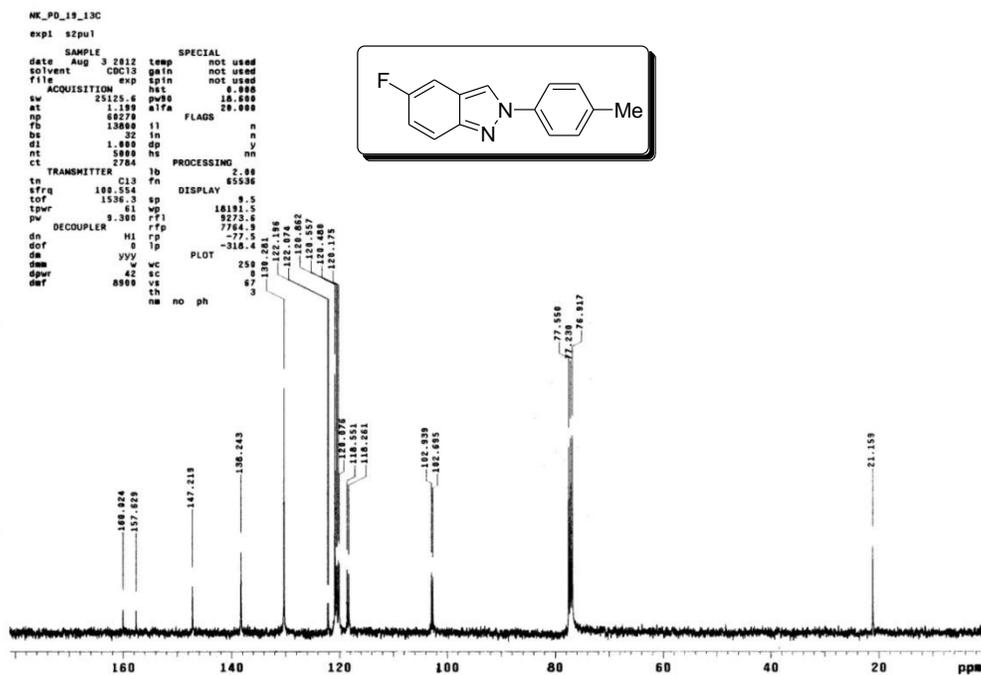
TRANSMITTER    lb  fn  PROCESSING  2.90
tn             M1  fn  DISPLAY   65536
sfrq 100.554   sp  2254.7
tor 1506.3    wp  15014.4
tpwr 81       rfl  3273.8
pw 9.800     rfp  7784.9
dn DECOUPLER  H1  rf  -30.9
dor 8        ip  -391.6
dm yyy        wc  PLOT      250
dam 42       sc  0
dpwr 8900    vs  35
dof 0        th  2
nm no ph
```



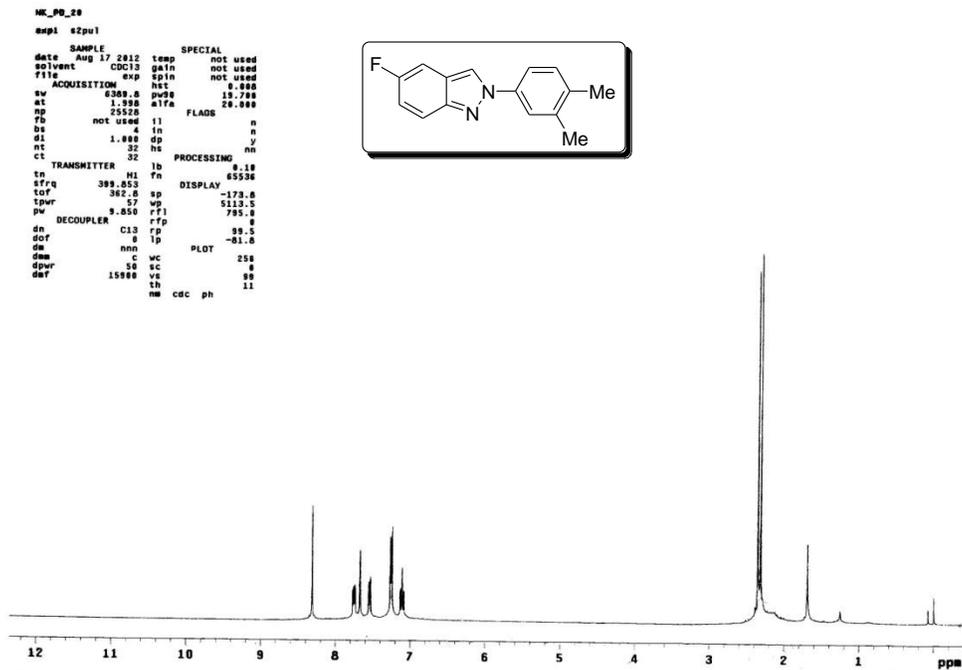
### 5-Fluoro-2-p-tolyl-2H-indazole (2b): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )



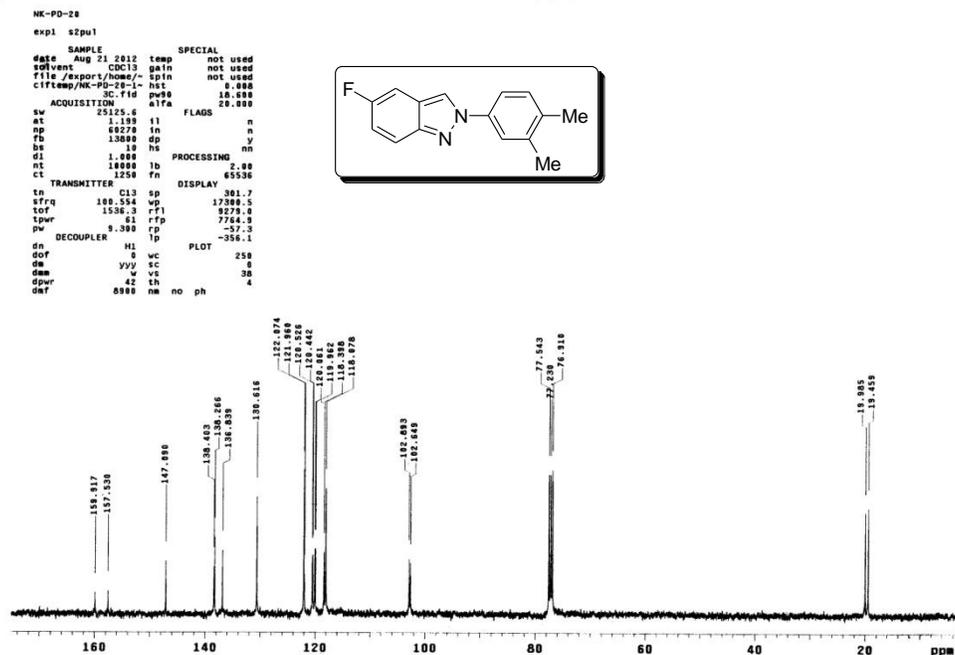
### 5-Fluoro-2-p-tolyl-2H-indazole (2b): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



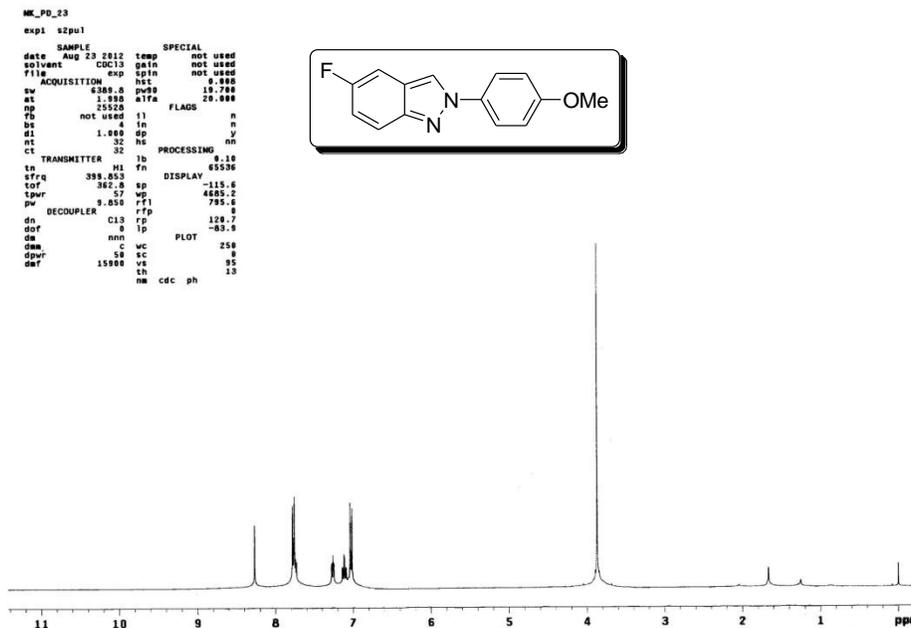
5-Fluoro-2-(3,4-dimethylphenyl)-2H-indazole (2c):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



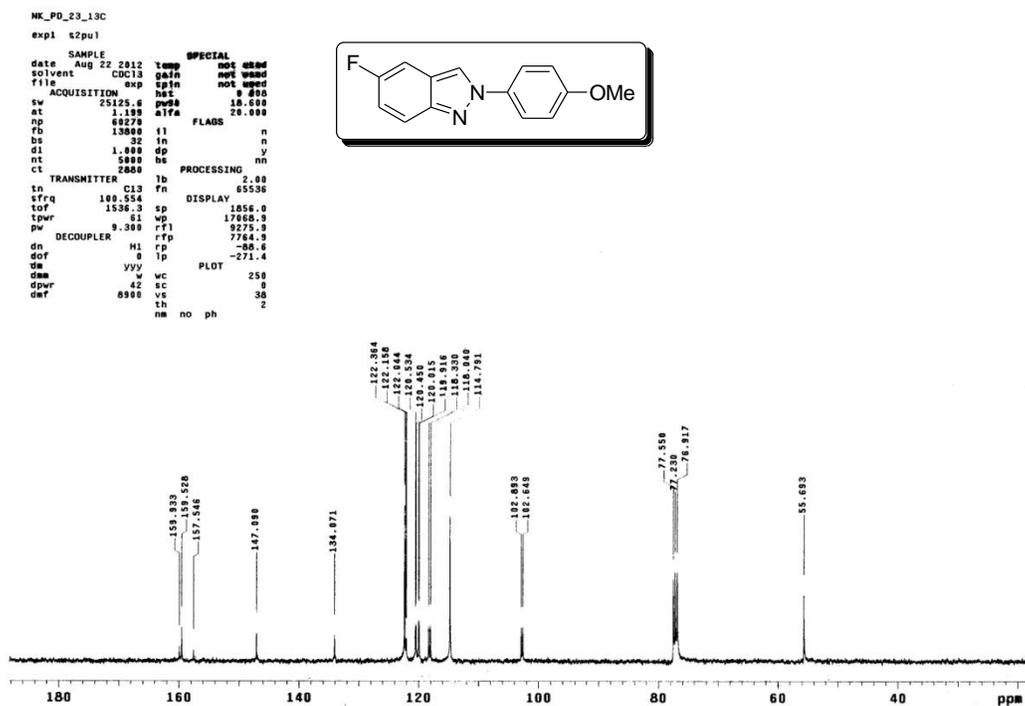
5-Fluoro-2-(3,4-dimethylphenyl)-2H-indazole (2c):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )



### 5-Fluoro-2-(4-methoxyphenyl)-2H-indazole (2g): $^1\text{H}$ NMR (400 MHz, $\text{CDCl}_3$ )



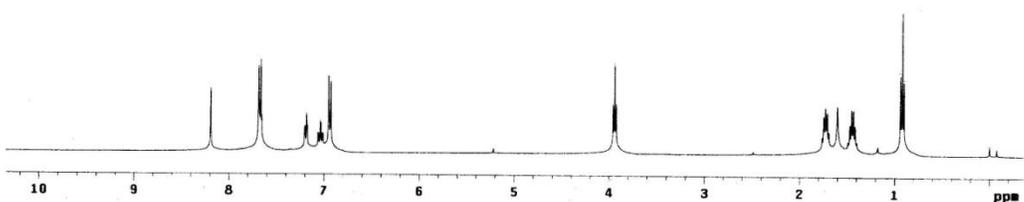
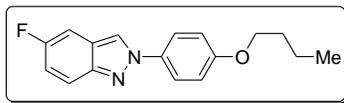
### 5-Fluoro-2-(4-methoxyphenyl)-2H-indazole (2g): $^{13}\text{C}$ NMR (100 MHz, $\text{CDCl}_3$ )



2-(4-Butoxyphenyl)-5-fluoro-2H-indazole (2h): <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)

```

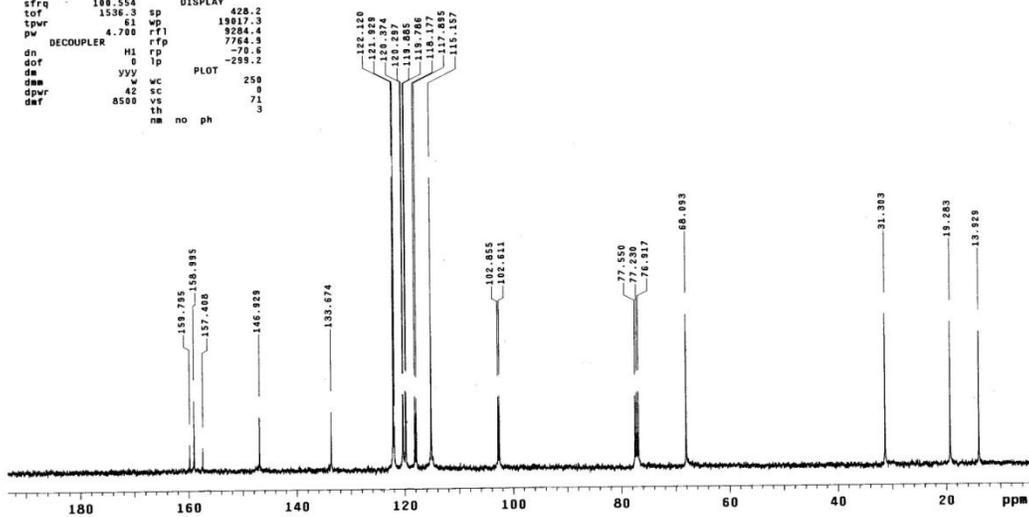
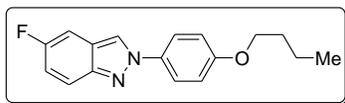
SAMPLE
date Oct 19 2012 temp not used
solvent CDCl3 gain not used
rfile exp spin not used
ACQUISITION hst 0.000
sw 6300.0 pw90 19.700
at 1.900 a1fa 28.000
np 25520
fb not used ll FLAGS n
bs 4 in n
dl 1.000 dp y
nt 32 hs nn
ct
TRANSMITTER lb 6.10
tn H1 fn 65536
sfrq 399.853 DISPLAY -144.1
tof 362.0 sp -144.1
tpwr 57 wp 8314.5
pw 9.050 rfp 824.9
DECOUPLER rfp 0
dn C13 rp 116.2
dof 0 lp -85.3
ds nnn PLOT
dms c wc 250
dpr 50 sc 0
dwt 15900 vs 35
nm cdc ph 21
    
```



2-(4-Butoxyphenyl)-5-fluoro-2H-indazole (2h): <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

```

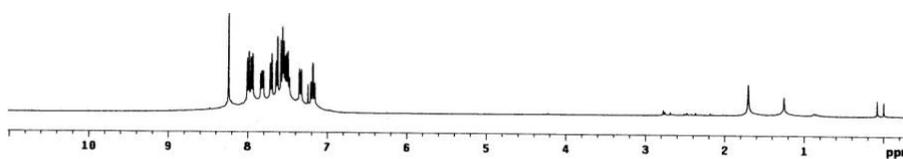
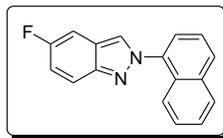
13C
pu1
SAMPLE
date Apr 28 2013 temp not used
solvent CDCl3 gain not used
rfile exp spin not used
ACQUISITION hst 0.000
sw 25125.6 pw90 9.400
at 1.190 a1fa 28.000
np 13000
fb 32 in n
dl 1.000 dp y
nt 4000 hs nn
ct
TRANSMITTER lb 2.00
tn C13 fn 65536
sfrq 100.554 DISPLAY 428.2
tof 1536.3 sp 19017.3
tpwr 61 wp 9284.4
pw 4.700 rfp 7764.3
DECOUPLER H1 rfp -70.6
dn 0 lp -299.2
ds 393 PLOT
dms w wc 250
dpr 42 sc 9
dwt 8500 vs 71
nm no ph 3
    
```



5-Fluoro-2-(naphthalen-1-yl)-2H-indazole (2i):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )

```

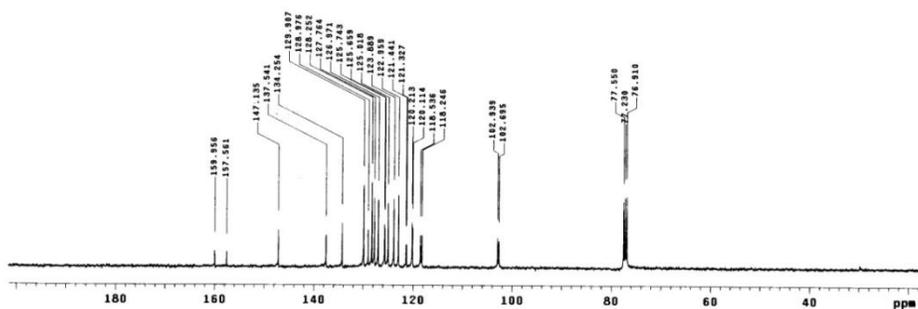
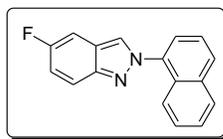
NL_P0_24
#p1 s2pu1
SAMPLE Sep 18 2012 temp SPECIAL
date Sep 18 2012 temp SPECIAL
solvent CDCl3 gain not used
f130 ACQUISITION exp gain not used
sw 400.0 hst 0.000
at 1.000 pps 10.000
ns 25528 aTfA 20.000
#b not used f1 FLAGS n
#s 4 in n
#l 1.000 sp y
#t 32 hs y
#c 32 hs nh
TRANSMITTER T0 PROCESSING
tn T0 T0 0.10
sfrq 399.950 sp DISPLAY -145.5
tot 361.0 sp 4550.0
tpr 9.850 rTf 000.0
DECOUPLER C13 rFp 0
dn 0 rFp 110.0
dot 0 lP -01.2
dm mmn PLOT
dwm C wc 250
dpr 42 sc 0
dfr 1500 th 20
nm cdc ph 20
    
```



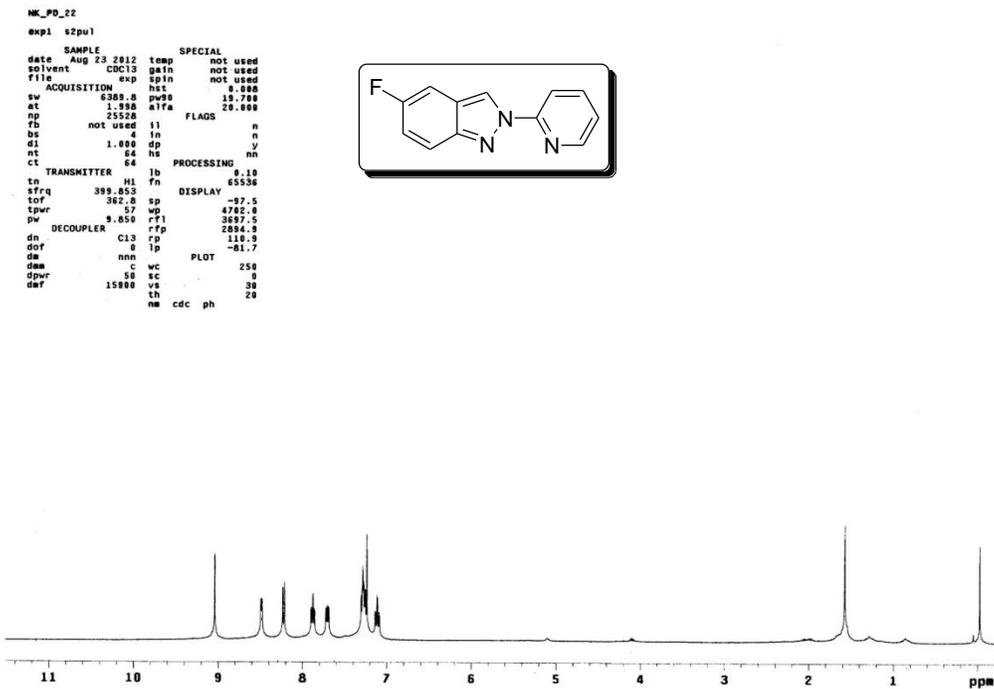
5-Fluoro-2-(naphthalen-1-yl)-2H-indazole (2i):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

```

#D-24-13c
1 s2pu1
SAMPLE Sep 18 2012 temp SPECIAL
date Sep 18 2012 temp SPECIAL
solvent CDCl3 gain not used
f130 ACQUISITION exp gain not used
sw 100.0 hst 0.000
at 1.100 pps 10.000
ns 40276 aTfA 20.000
#b not used f1 FLAGS n
#s 32 in n
#l 1.000 sp y
#t 7000 hs nh
#c 2752 hs nh
TRANSMITTER C13 T0 PROCESSING
tn T0 T0 2.00
sfrq 100.554 sp DISPLAY 65536
tot 1500.0 sp 1700.0
tpr 61 wp 10400.0
pw 9.300 rFf 9205.0
DECOUPLER 0 rFp 7754.0
dn H1 rFp -21.0
dot 0 lP -202.0
dm yyy PLOT
dwm C wc 250
dpr 42 sc 0
dfr 8000 th 20
nm no ph 2
    
```



5-Fluoro-2-(pyridin-2-yl)-2H-indazole (2j):  $^1\text{H}$  NMR (400 MHz,  $\text{CDCl}_3$ )



5-Fluoro-2-(pyridin-2-yl)-2H-indazole (2j):  $^{13}\text{C}$  NMR (100 MHz,  $\text{CDCl}_3$ )

