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Meridianin G and its analogs as antimalarial agents

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Contents

S1. EXPERIMENTAL SECTION

General

All chemicals were obtained from Sigma-Aldrich Company and used as received. ^{1}H, ^{13}C and DEPT NMR spectra were recorded on Brucker-Avance DPX FT-NMR 500 and 400 MHz instruments. Chemical data for protons are reported in parts per million (ppm) downfield from tetramethylsilane and are referenced to the residual proton in the NMR solvent ($CDCl_3$, 7.26 ppm; CD_3OD, 3.31 ppm). Carbon nuclear magnetic resonance spectra (^{13}C NMR) were recorded at 125 MHz or 100 MHz: chemical data for carbons are reported in parts per million (ppm, δ scale) downfield from tetramethylsilane and are referenced to the carbon resonance of the solvent ($CDCl_3$, 77.16 ppm; CD_3OD, 49.0). ESI-MS and HRMS spectra were recorded on Agilent 1100 LC-Q-TOF and HRMS-6540-UHD machines. IR spectra were recorded on Perkin-Elmer IR spectrophotometer. Melting points were recorded on digital melting point apparatus.

Procedure for acetylation of indoles[1]: Synthesis of 12a-b. To a solution of indole (**11a**) or 5-bromo-indole (**11b**) in 50 mL of anhydrous toluene at 0 °C was added 2 equiv. acetyl chloride. After stirring for 15 min at 0 °C, a solution of $SnCl_4$ (2 equiv) in 24 mL anhydrous toluene was added. The resultant solution was stirred for 2 h at 0 °C and 75 ml of 8% $NaHCO_3$ was added dropwise. Resulted slurry was diluted with 150 mL of ethyl acetate, dried (Na_2SO_4), and filtered. The solvent was removed with rotary evaporator. The residue was chromatographed on a silica gel column using EtOAc/hexane as eluent to get title products **12a-b**.

1-(*1H*-Indol-3-yl) ethanone (12a). Yield: 95%, brick red solid, m. p. 252-254 °C; ^{1}H NMR (CD_3OD, 400 MHz): δ 8.21 (s, 1H), 8.13 (s, 1H), 7.42-7.44 (m, 1H), 7.17-7.24 (m, 2H), 2.51 (s, 3H); HRMS: m/z 160.0774 calcd for $C_{10}H_9NO + H^+$ (160.0757).

1-(5-Bromo-1H-indol-3-yl)ethanone (12b). Yield: 84%, brick red solid, m. p. 250-252 °C; ^{1}H NMR (CD_3OD, 400 MHz): δ 7.2 (d, 1H, J = 8.9 Hz), 6.9 (s, 1H), 5.9-6.1 (m, 2H), 2.1 (s, 3H); HRMS: m/z 237.9860 calcd for $C_{10}H_8NO + H^+$ (237.9862).

Procedure for tosylation of 12a-b[1]: Synthesis of 13a-b. To the solution of 3-acetyl indole (**12a**) or 5-bromo-3-acetyl indole (**12b**) in dichloromethane was added DMAP (0.05 equiv), p-toluenesulfonyl choride (TsCl, 1.1 equiv)) and *N*,*N*-diisopropylethylamine (DIPEA, 1.5 equiv). The mixture was stirred at room temperature for 20 h. Reaction was then quenched by

the addition of 10% HCl. Dichloromethane was added to the reaction mixture. Organic layer was separated, dried over anhydrous sodium sulphate and concentrated to get crude compound. The residue was chromatographed on a silica gel column using EtOAc/hexane as eluent to get title products **13a-b**.

1-(1-Tosyl-1H-indol-3-yl)ethanone (13a): Yield: 85%, white solid, m. p. 155-157 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.2 (s, 1H), 7.93 (t, 1H, *J* = 6.8 Hz), 7.85 (s, 1H), 7.83 (s, 2H), 7.26-7.39 (m, 4H), 2.57 (d, 3H, *J* = 3.6 Hz), 2.37 (d, 3H, *J* = 3.6 Hz); HRMS: *m/z* 314.0827 calcd for $C_{17}H_{15}NO_3S + H^+$ (314.0845).

1-(5-Bromo-1-tosyl-1H-indol-3-yl)ethanone (13b): Yield: 72%, white solid, m. p. 140-142 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.49-8.53 (m, 1H), 8.17-8.19 (t, 1H, *J* = 4.4 Hz), 7.79 (t, 3H, *J* = 8 Hz), 7.45-7.48 (m, 1H), 7.25-7.30 (m, 2H), 2.49-2.56 (m, 3H), 2.35 (d, 3H, *J* = 4.8 Hz); HRMS: *m/z* 391.9916 calcd for $C_{17}H_{14}NO_3S + H^+$ (391.9951).

Procedure for enaminone synthesis[2]: Synthesis of 14a-b

1-(1-Tosyl-*1H*-indol-3-yl)ethanone (**13a**) or 1-(5-bromo-1-tosyl-1H-indol-3-yl)ethanone (**13b**) was taken in dry DMF was added a solution of dimethyl formamide-dimethylacetal (DMF-DMA, 1.5 equiv) in the same solvent (2 mL). The resultant solution was heated at 110 °C for 4 h under N_2 atmosphere. After cooling, the solution was poured into water and then extracted with EtOAc. The combined organic layers were dried over anhydrous sodium sulphate and concentrated to dryness under reduced pressure. The residue was chromatographed on a silica gel column using EtOAc/hexane as eluent to give title products **14a-b** as yellow solids.

3-(Dimethylamino)-1-(1-tosyl-1H-indol-3-yl)prop-2-en-1-one (**14a**): Yield: 55%, pale yellow solid, m. p. 163-165 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.3 (s, 1H), 8.1 (s, 1H), 7.90 (d, 1H, *J* = 0.4 Hz), 7.76-7.80 (m, 3H), 7.22-7.34 (m, 4H), 5.6 (d, 3H, *J* = 12.4 Hz), 2.96 (d, 6H, *J* = 10.8 Hz), 2.36 (d, 3H, *J* = 10.0 Hz); HRMS: *m/z* 369.1241 calcd for $C_{20}H_{20}N_2O_3S + H^+$ (369.1267)

1-(5-Bromo-1-tosyl-1H-indol-3-yl)-3-(dimethylamino)prop-2-en-1-one (**14b**): Yield: 50%, pale yellow solid, m. p. 176-178 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.6 (s, 1H), 8.0 (s, 1H), 7.7 (m, 4H), 7.4 (t, 1H, *J* = 1.9 Hz), 7.2 (t, 2H, *J* = 4.8 Hz), 5.6 (d, 3H, *J* = 12.3 Hz), 3.1 (s, 3H), 2.9 (s, 3H), 2.4 (s, 3H); HRMS: *m/z* 447.0335 calcd for $C_{20}H_{19}BrN_2O_3S + H^+$ (447.0373)

Procedure for aminopyrimidine ring formation[3]: Synthesis of meridianin C (3) and G (7). A mixture of enaminone **14a** or **14b**, guanidine hydrochloride (1.5 equiv), anhydrous K_2CO_3 (2 equiv) and 2-methoxyethanol was heated at reflux temperature for 24 h under N_2 atmosphere. After cooling, the solution was poured into water and then extracted with EtOAc. The combined organic layers were dried (Na_2SO_4) and concentrated to dryness under reduced pressure. The residue was chromatographed on a silica gel column using DCM/methanol as eluent to give title product **3** or **7** as pale yellow solids. The side product **15** was also formed during synthesis of meridianin C (**3**).

Meridianin C (3): Yield: 55%; pale yellow solid; m. p. 104-107 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ 11.86 (brs, 1H, NH), 8.76 (d, 1H, *J* = 2.0 Hz), 8.26 (d, 1H, *J* = 2.8 Hz), 8.11 (d, 1H, *J* = 5.6 Hz), 7.42 (d, 1H, *J* = 8.8 Hz), 7.30 (dd, 1H, *J* = 2.0, 7.2 Hz), 7.01 (d, 1H, *J* = 5.6 Hz), 6.49 (s, 2H, NH_2); ^{13}C NMR (Acetone-d_6, 125 MHz): 164.85, 163.63, 158.20, 137.00, 129.69, 128.39, 125.87, 125.84, 115.11, 114.51, 114.35, 106.59; IR (Neat): ν_{max} 3400, 2921, 1580, 1450, 1022 cm^{-1}; HRMS: *m/z* 289.0081 calcd for $C_{12}H_9BrN_4 + H^+$ (289.0083).[4]

Meridianin G (7): Yield: 66%; m. p. 185-187 °C; pale yellow solid; ^{1}H NMR (CD_3OD, 400 MHz): δ 8.40-8.30 (m, 1H), 8.00 (d, 1H, *J* = 5.6 Hz), 7.93 (s, 1H), 7.35-7.31 (m, 1H), 7.12-7.05 (m, 2H), 6.96 (d, 1H, *J* = 5.6 Hz); ^{13}C NMR (CD_3OD, 125 MHz): 164.83, 163.66, 157.03, 138.24, 128.62, 126.05, 123.10, 121.88, 121.59, 114.78, 112.54, 107.59; IR (Neat): ν_{max} 3176, 2920, 1573, 1533, 1454, 1325, 1245, 1219, 1183 cm^{-1}; HRMS: *m/z* 211.0989 calcd for $C_{12}H_{10}N_4 + H^+$ (211.0978).[5]

4-(5-Bromo-1-(2-methoxyethyl)-1H-indol-3-yl)pyrimidin-2-amine (15): Yield: 35%; brown solid; m. p. 119-121 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.60 (d, 1H, *J* = 1.6 Hz), 8.20 (d, 1H, *J* = 5.6 Hz), 7.83 (s, 1H), 7.38-7.36 (m, 1H), 7.26-7.24 (m, 1H), 6.91 (d, 1H, *J* = 5.2 Hz), 5.19 (s, 2H), 4.32 (t, 2H, *J* = 5.2 Hz), 3.74 (t, 2H, *J* = 5.2 Hz), 3.31 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 165.44, 163.67, 159.20, 137.73, 134.75, 129.24, 126.51, 126.45, 115.50, 114.48, 114.37, 107.06, 72.49, 60.01, 47.92; IR ($CHCl_3$): ν_{max} 3307, 3203, 2955, 2925, 2856, 1740, 1576, 1536, 1458, 1398, 1343, 1211, 1185, 1099, 1014 cm^{-1}; HRMS: *m/z* 347.0474 calcd for $C_{15}H_{15}BrN_4O + H^+$ (347.0502).

General procedure for synthesis of *NH*-substituted meridinain analogs 17a-h and 19a-g. To a solution of meridianin G (**7**) or meridianin C (**3**) in acetonitrile, anhydrous potassium carbonate (2 equiv) and aryl acid chloride/ aryl alkyl halide (1 equiv) was added. The resultant mixture was allowed to stir for 12 h. After completion of the reaction, solvent was

evaporated, extracted with ethyl acetate, and dried over Na_2SO_4, purified by column chromatography (#100-200) using dichloromethane and methanol (99:1 to 97:3) to get the title products **17a-h** or **19a-g**.

(3-(2-Aminopyrimidin-4-yl)-1H-indol-1-yl)(morpholino) methanone (17a): Yield: 83%; pale yellow solid; m. p. 188-190 °C; ^{1}H NMR (CD_3OD, 400 MHz): δ 8.43 (d, 1H, *J* = 7.6 Hz), 8.09 (t, 2H, *J* = 3.6 Hz), 7.58 (d, 1H, *J* = 8.4 Hz), 7.29-7.19 (m, 2H), 7.03 (d, 1H, *J* = 5.2 Hz), 3.61 (d, 4H, *J* = 5.2 Hz), 3.55-3.53 (t, 4H, *J* = 4.8 Hz); ^{13}C NMR (CD_3OD, 100 MHz): 164.78, 163.95, 158.40, 154.83, 137.70, 129.53, 128.10, 125.52, 124.02, 123.73, 118.96, 114.10, 108.21, 67.65, 48.12; IR (Neat): ν_{max} 3351, 2920, 2355, 2347, 2325, 1685, 1575, 1452, 1420, 1306, 1273, 1236, 1203, 1114, 1018 cm^{-1}; HRMS: *m/z* 324.1461 calcd for $C_{12}H_{17}N_5O_2 + H^+$ (324.1455).

(3-(2-Aminopyrimidin-4-yl)-5-bromo-1H-indol-1-yl)(morpholino) methanone (17b): Yield: 87%; yellow solid; m. p. 244-246 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.86 (s, 1H), 8.44 (d, 1H, *J* = 1.6 Hz), 8.21-8.19 (m, 1H), 7.65-7.63 (m, 1H), 7.48-7.46 (t, 1H, *J* = 6.8 Hz), 7.14-7.12 (m, 1H), 6.71 (s, 1H), 5.72 (d, 1H, *J* = 2.0 Hz), 3.77 (s, 4H), 3.70 (s, 4H); ^{13}C NMR (CD_3OD + $CDCl_3$, 125 MHz): δ 162.35, 157.09, 156.14, 135.45, 131.47, 127.96, 127.05, 124.93, 123.92, 114.25, 114.03, 110.89, 106.40, 70.48, 58.43; IR ($CHCl_3$): ν_{max} 3306, 2955, 2925, 2858, 1739, 1688, 1578, 1544, 1491, 1449, 1419, 1401, 1362, 1342, 1273, 1248, 1082, 1015 cm^{-1}; HRMS: *m/z* 402.0555 calcd for $C_{17}H_{16}BrN_5O_2 + H^+$ (402.0560).

(3-(2-Aminopyrimidin-4-yl)-1H-indol-1-yl)(4-methylpiperazin-1-yl)methanone (17c): Yield: 89%; yellow solid; m. p. 195-197 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.38 (t, 1H, *J* = 7.6 Hz), 8.30 (d, 1H, *J* = 5.6 Hz), 7.97 (s, 1H), 7.66 (d, 1H, *J* = 7.6 Hz), 7.39 (m, 2H), 7.02 (t, 1H, *J* = 5.6 Hz), 5.06 (s, 2H, NH_2), 3.65 (t, 4H, *J* = 4.8 Hz), 2.52 (t, 4H, *J* = 4.8 Hz), 2.35 (s, 3H); ^{13}C NMR ($CDCl_3$, 125 MHz): 162.08, 160.81, 157.09, 153.24, 135.14, 126.74, 125.72, 123.23, 121.77, 121.33, 116.91, 112.18, 107.13, 53.75, 46.21, 45.06; IR ($CHCl_3$): ν_{max} 3341, 3210, 2955, 2924, 2854, 2802, 1684, 1623, 1574, 1545, 1454, 1421, 1330, 1294, 1263, 1248, 1153, 1082, 1050, 1018, 1001 cm^{-1}; HRMS: *m/z* 337.1773 calcd for $C_{18}H_{20}N_6O + H^+$ (337.1771).

(3-(2-Aminopyrimidin-4-yl)-5-bromo-1H-indol-1-yl)(4-methylpiperazin-1-yl)methanone (17d): Yield: 81%; pale yellow solid; m. p. 110-112 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.60 (d, 1H, *J* = 2.0 Hz), 8.31 (d, 1H, *J* = 5.6 Hz), 7.93 (s, 1H), 7.55-7.52 (t, 1H, *J* = 8.8 Hz), 7.48-7.45 (m, 1H), 6.95 (d, 1H, *J* = 5.2 Hz), 5.09 (s, 2H, NH_2), 3.64 (t, 4H, *J* = 4.4 Hz), 2.52

(t, 4H, *J* = 4.8 Hz), 2.35 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): 163.14, 161.34, 158.26, 152.84, 134.93, 128.39, 127.43, 125.05, 117.37, 116.48, 114.58, 107.89, 100.4, 54.76, 46.71, 46.01; IR ($CHCl_3$): ν_{max} 3339, 2955, 2924, 2853, 2798, 1686, 1577, 1543, 1448, 1420, 1338, 1292, 1256, 1193, 1018 cm^{-1}; HRMS: *m/z* 415.0854 calcd for $C_{18}H_{19}BrN_6O + H^+$ (415.0876).

(3-(2-Aminopyrimidin-4-yl)-1H-indol-1-yl)(phenyl)methanone (17e): Yield: 67%; pale yellow solid; m. p. 242-244 °C; ^{1}H NMR (Acetone-d_6, 400 MHz): δ 8.66 (d, 1H, *J* = 7.6 Hz), 8.39 (d, 1H, *J* = 8.4 Hz), 8.23 (d, 1H, *J* = 5.2 Hz), 8.14 (s, 1H), 7.90-7.88 (t, 2H, *J* = 6.8 Hz), 7.77-7.73 (m, 1H), 7.68-7.64 (t, 2H, *J* = 7.6 Hz), 7.48-7.39 (m, 2H), 7.09 (d, 1H, *J* = 5.2 Hz), 6.11 (s, 2H, NH_2); ^{13}C NMR ($CDCl_3$, 100 MHz): 168.62, 162.98, 161.67, 157.67, 137.08, 133.98, 132.45, 129.90, 129.37, 128.86, 128.73, 128.35, 128.01, 125.68, 124.70, 121.67, 120.08, 116.47, 108.38; IR ($CHCl_3$): ν_{max} 3307, 2955, 2924, 2857, 1695, 1571, 1450, 1400, 1360, 1330, 1275, 1235, 1201, 1082, 1015 cm^{-1}; HRMS: *m/z* 315.1236 calcd for $C_{19}H_{14}N_4O + H^+$ (315.1240).

(3-(2-Aminopyrimidin-4-yl)-5-bromo-1H-indol-1-yl)(phenyl)methanone (17f): Yield: 62%; pale yellow solid; m. p. 205-207 °C; ^{1}H NMR (Acetone-d_6, 400 MHz): δ 8.92 (d, 1H, *J* = 2.0 Hz), 8.31 (d, 1H, *J* = 8.8 Hz), 8.22-8.21 (t, 2H, J=2.0 Hz), 7.92-7.89 (m, 2H), 7.78-7.74 (m, 1H), 7.68-7.67 (m, 2H), 7.61-7.59 (m, 1H), 7.08 (d, 1H, *J* = 5.2 Hz), 6.23 (s, 2H-NH_2); ^{13}C NMR (125 MHz, DMSO) δ 168.14, 163.49, 159.93, 158.09, 135.14, 133.04, 132.62, 130.40, 129.66, 129.49, 128.79, 127.85, 125.04, 118.17, 117.40, 116.98, 105.91; IR ($CHCl_3$): ν_{max} 3391, 2955, 2924, 2857, 1693, 1579, 1445, 1362, 1345, 1263, 1193, 1020 cm^{-1}; HRMS: *m/z* 393.0325 calcd for $C_{19}H_{13}BrN_4O + H^+$ (393.0346).

N-(4-(1H-Indol-3-yl)pyrimidin-2-yl)-3-methoxybenzamide (17g): Yield: 77%; pale yellow solid; m. p. 213-215 °C; ^{1}H NMR (DMSO-d_6, 500 MHz): δ 8.67 (d, 1H, *J* = 7.6 Hz), 8.31 (d, 1H, *J* = 8.1 Hz), 8.21 (d, 1H, *J* = 5.2 Hz), 8.14 (s, 1H), 7.56 (m, 1H), 7.47 (m, 4H), 7.44 (d, 1H, *J* = 7.7 Hz), 7.38-7.36 (t, 1H, *J* = 6.9 Hz), 6.67 (s, 2H, NH_2), 3.85 (s, 3H); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 168.62, 163.98, 160.77, 159.73, 158.73, 136.83, 135.35, 130.59, 129.54, 128.39, 125.75, 124.83, 123.19, 121.79, 119.72, 118.77, 116.19, 114.70, 107.16, 55.96; IR ($CHCl_3$): ν_{max} 3391, 2955, 2924, 2855, 1736, 1692, 1577, 1450, 1384, 1361, 1329, 1277, 1200, 1152, 1020 cm^{-1}; HRMS: *m/z* 345.1327 calcd for $C_{20}H_{16}N_4O_2 + H^+$ (345.1346).

(3-(2-Aminopyrimidin-4-yl)-1H-indol-1-yl)(2-ethoxyphenyl)methanone (17h): Yield: 76%; pale yellow solid; m. p. 186-188 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.65-8.63 (m, 1H), 8.29 (d, 1H, *J* = 7.2 Hz), 8.20 (d, 1H, *J* = 5.2 Hz), 7.91 (s, 1H), 7.66-7.60 (m, 2H), 7.46-

7.39 (m, 2H), 7.26 (d, 1H, *J* = 8.4 Hz), 7.19-7.15 (t, 1H, *J* = 7.6 Hz), 7.07 (d, 1H, *J* = 5.2 Hz), 6.67 (s, 2H-NH_2), 4.10-4.05 (m, 2H), 1.03-0.99 (t, 3H, *J* = 6.8 Hz); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 167.01, 163.47, 160.17, 158.17, 155.21, 135.68, 132.92, 129.40, 128.74, 127.90, 125.21, 124.21, 123.54, 122.62, 120.81, 119.31, 115.39, 113.18, 106.38, 63.78, 14.09; IR ($CHCl_3$): ν_{max} 3325, 2955, 2925, 2857, 1696, 1599, 1571, 1548, 1450, 1359, 1333, 1292, 1250, 1227, 1201, 1150, 1115, 1041 cm^{-1}; HRMS: *m/z* 359.1480 calcd for $C_{21}H_{18}N_4O_2$ + H^+ (359.1503).

4-(1-((3,5-Dimethylisoxazol-4-yl)methyl)-1H-indol-3-yl)pyrimidin-2-amine (19a): Yield: 64%; pale yellow solid; m. p. 183-185 °C; ^{1}H NMR (CD_3OD, 400 MHz): δ 8.47-8.45 (t, 1H, *J* = 7.6 Hz), 8.11 (d, 1H, *J* = 5.6 Hz), 7.97 (s, 1H), 7.44 (d, 1H, *J* = 7.6 Hz), 7.29-7.21 (m, 2H), 7.05 (d, 1H, *J* = 5.2 Hz), 5.27 (s, 2H), 2.37-2.33 (t, 3H, *J* = 7.6 Hz), 2.01 (d, 3H, *J* = 9.2 Hz); ^{13}C NMR (CD_3OD, 100 MHz): 168.78, 164.83, 164.64, 160.79, 157.78, 138.79, 131.65, 127.58, 123.96, 123.44, 122.55, 115.38, 111.33, 111.12, 107.60, 40.03, 10.86, 10.11; IR ($CHCl_3$): ν_{max} 3307, 2956, 2925, 2855, 1739, 1575, 1537, 1455, 1393, 1343, 1248, 1193, 1082, 1015 cm^{-1}; HRMS: *m/z* 320.1508 calcd for $C_{18}H_{17}N_5O$ + H^+ (320.1506).

4-(5-Bromo-1H-indol-3-yl)-N-((3,5-dimethylisoxazol-4-yl)methyl) pyrimidin-2-amine (19b): Yield: 85%; yellow solid; m. p. 172-174 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.59 (d, 1H, *J* = 2.0 Hz), 8.24 (d, 1H, *J* = 5.2 Hz), 7.58 (s, 1H), 7.42-7.39 (m, 1H), 7.23 (d, 1H, *J* = 8.8 Hz), 6.88 (d, 1H, *J* = 5.2 Hz), 5.05 (s, 4H, CH_2 and NH_2), 2.35 (s, 3H), 2.08 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 167.24, 162.56, 161.23, 159.07, 157.59, 135.80, 129.12, 127.65, 125.92, 124.77, 115.06, 114.39, 110.81, 108.66, 107.14, 39.39, 11.17, 10.21; IR ($CHCl_3$): ν_{max} 3326, 2955, 2924, 2854, 1727, 1576, 1537, 1458, 1392, 1191, 1020 cm^{-1}; HRMS: *m/z* 398.0588 calcd for $C_{18}H_{16}BrN_5O$ + H^+ (398.0611).

4-(1-((5-Chlorothiophen-2-yl)methyl)-1H-indol-3-yl)pyrimidin-2-amine (19c): Yield: 77%, yellow solid; m. p. 174-176 °C; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.40 (d, 1H, *J* = 8.4 Hz), 8.30 (d, 1H, *J* = 5.3 Hz), 7.90 (s, 1H), 7.40 (s, 1H), 7.20-7.30 (m, 2H), 7.00 (d, 1H, *J* = 5.3 Hz), 6.75 (s, 2H), 5.40 (s, 2H), 5.0 (s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 162.97, 162.55, 157.34, 137.31, 136.89, 130.17, 129.55, 126.25, 126.01, 125.75, 122.93, 121.89, 121.61, 114.61, 109.76, 107.33, 45.30; IR ($CHCl_3$): ν_{max} 3307, 2956, 2924, 2854, 1737, 1575, 1537, 1455, 1391, 1214, 1190, 1157, 1082, 1016 cm^{-1}; HRMS: *m/z* 341.0621 calcd for $C_{17}H_{13}ClN_4S$ + H^+ (341.0622).

4-(5-Bromo-1H-indol-3-yl)-N-((5-chlorothiophen-2-yl)methyl)pyrimidin-2-amine (19d): Yield: 73%; yellow solid; m. p. 175-177 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.59 (s, 1H), 8.25 (d, 1H, *J* = 5.2 Hz), 7.78 (s, 1H), 7.40-7.37 (m, 1H), 7.24 (s, 1H), 6.91 (d, 1H, *J* = 5.2 Hz), 6.91 (d, 1H, *J* = 5.2 Hz), 6.78-6.75 (m, 2H), 5.38 (s, 2H), 5.02 (s, 2H-NH_2); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 163.11, 161.99, 157.84, 136.92, 135.65, 130.62, 130.18, 127.92, 126.11, 125.98, 125.92, 124.94, 115.23, 114.68, 111.26, 107.37, 45.84; IR ($CHCl_3$): ν_{max} 3400, 2955, 2924, 2854, 1738, 1577, 1537, 1457, 1389, 1189, 1156, 1019 cm^{-1}; HRMS: *m/z* 418.9723 calcd for $C_{17}H_{12}BrClN_4S + H^+$ (418.9727).

2-((3-(2-Aminopyrimidin-4-yl)-5-bromo-1H-indol-1-yl)methyl) isoindoline-1,3-dione (19e): Yield: 32 %; pale yellow solid; m. p. 110-113 °C; ^{1}H NMR ($CDCl_3$, 500 MHz): δ 8.57 (s, 1H), 8.25 (s, 1H), 8.10 (s, 1H), 7.87-7.86 (t, 2H, *J* = 3.0 Hz), 7.77-7.74 (m, 3H), 7.40 (d, 1H), 6.94 (d, 1H, *J* = 5.5 Hz), 5.98 (s, 2H), 5.14 (s, 2H-NH_2); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.42, 163.04, 162.10, 157.57, 135.42, 134.74, 131.79, 131.43, 127.66, 126.32, 124.69, 123.97, 115.56, 115.07, 112.08, 107.43, 47.30; IR ($CHCl_3$): ν_{max} 3368, 2955, 2925, 2855, 1775, 1721, 1577, 1540, 1459, 1401, 1334, 1219, 1151, 1082, 1019 cm^{-1}; HRMS: *m/z* 448.0401 calcd for $C_{21}H_{14}BrN_5O_2 + H^+$ (448.0404).

4-(1-(Anthracen-10-ylmethyl)-1H-indol-3-yl)pyrimidin-2-amine (19f): Yield: 86%; pale yellow solid; m. p. 246-248 °C; ^{1}H NMR (DMSO-d_6, 500 MHz): δ 8.87 (s, 1H), 8.41 (d, 1H, *J* = 3.4 Hz), 8.39 (s, 2H), 8.29-8.27 (m, 2H), 8.04-8.02 (m, 2H), 7.65-7.63 (m, 3H), 7.37 (s, 3H), 6.77 (d, 1H, *J* = 5.3 Hz), 6.48 (s, 2H-NH_2), 6.36 (s, 2H); ^{13}C NMR (DMSO-d_6, 125 MHz): δ 163.26, 161.24, 157.38, 137.37, 131.02, 130.75, 129.22, 128.96, 128.52, 127.19, 125.75, 125.59, 125.56, 125.40, 123.62, 122.34, 121.86, 121.01, 113.36, 113.33, 110.77, 105.32, 105.29, 42.03; IR ($CHCl_3$): ν_{max} 3307, 2954, 2924, 2855, 1738, 1572, 1561, 1452, 1399, 1309, 1219, 1203, 1156, 1082, 1019 cm^{-1}; HRMS: *m/z* 401.1760 calcd for $C_{27}H_{20}N_4 + H^+$ (401.1761).

4-(1-(Anthracen-10-ylmethyl)-5-bromo-1H-indol-3-yl)pyrimidin-2-amine (19g): Yield: 84%; pale yellow solid; m. p. 247-249 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ 8.80 (s, 1H), 8.67 (d, 1H, *J* = 2.0 Hz), 8.33-8.31 (m, 2H), 8.23-8.21 (m, 2H), 7.96-7.91 (m, 2H), 7.60-7.57 (m, 4H), 7.49-7.46 (dd, 1H, *J* = 2.0 Hz), 7.34 (s, 1H), 6.64 (d, 1H, *J* = 5.2 Hz), 6.42 (s, 2H), 6.40 (s, 2H-NH_2); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 163.34, 160.98, 157.51, 136.17, 131.10, 130.81, 129.90, 129.33, 129.18, 127.34, 127.28, 125.48, 125.06, 124.27, 123.59, 114.06, 112.97, 112.87, 105.29, 42.38; IR ($CHCl_3$): ν_{max} 3400, 2955, 2924, 2854, 1735, 1575,

1535, 1453, 1385, 1196, 1158, 1020 cm^{-1}; HRMS: *m/z* 479.0806 calcd for $C_{27}H_{19}BrN_4 + H^+$ (479.0866).

General procedure for preparation of C-ring modified meridianin analogs 22a-c. To the solution of indole-3-carboxaldehydes **20a-c** (1 mmol) in acetonitrile (5 mL) was added amberlyst-15 (50% w/w with respect to indole-3-carboxaldehyde) and anthranilamide (1 equiv) and the resulting mixture was stirred at room temperature for overnight. After completion, the reaction mixture was filtered, filtrate was concentrated and purified by silica-gel column chromatography (#100-200) to get products **22a-c**.

2-(1H-Indol-3-yl)-2,3-dihydroquinazolin-4(1H)-one (22a): Yield: 47%; off-white solid; m. p. 177-180 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.60 (s, 1H), 7.97 (dd, 1H , *J* = 7.8 & 1.2 Hz), 7.89 (d, 1H, *J* = 7.9 Hz), 7.41 (d, 1H , *J* = 8.2 Hz), 7.36 – 7.29 (m, 2H), 7.15 (t, 1H, *J* = 7.5 Hz), 6.90 (t, 1H, *J* = 7.5 Hz), 6.67 (d, 1H, *J* = 8.0 Hz), 6.18 (s, 1H), 5.98 (s, 1H), 4.55 (s, 1H); ^{13}C NMR (CD_3OD, 100 MHz): δ 168.14, 150.72, 138.58, 135.14, 128.94, 126.80, 125.73, 123.04, 120.95, 120.42, 119.20, 116.19, 116.04, 114.69, 112.63, 64.02; IR ($CHCl_3$): ν_{max} 3369, 2955, 2925, 2854, 1737, 1647, 1485, 1456, 1155, 1019 cm^{-1}; HRMS: *m/z* 264.1129 calcd for $C_{16}H_{13}N_3O + H^+$ (264.1131).

2-(5-Bromo-1H-indol-3-yl)-2,3-dihydroquinazolin-4(1H)-one (22b): Yield: 43%; light green solid; m. p. 145-147 °C; ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.66 (s, 1H), 8.05 (d, 1H , *J* = 1.5 Hz), 7.96 (dd, 1H, *J* = 7.8 &1.3 Hz), 7.40 – 7.22 (m, 4H), 6.91 (t, 1H, *J* = 7.2 Hz), 6.69 (d, 1H, *J* = 8.0 Hz), 6.12 (d, 2H, *J* = 5.6 Hz), 4.50 (s, 1H); ^{13}C NMR (CD_3OD, 125 MHz): δ 166.30, 148.22, 135.23, 133.71, 126.44, 125.55, 125.22, 124.55, 121.92, 118.32, 114.54, 114.37, 112.88, 112.32, 111.87, 62.22; IR ($CHCl_3$): ν_{max} 3305, 2955, 2924, 2857, 1651, 1611, 1489, 1464, 1401, 1191, 1157, 1082, 1016 cm^{-1}; HRMS: *m/z* 342.0248 calcd for $C_{16}H_{12}BrN_3O + H^+$ (342.0237).

2-(5-Iodo-1H-indol-3-yl)quinazolin-4(3H)-one (22c): Yield: 57%; pale yellow solid; m. p. 309-311 °C; ^{1}H NMR (DMSO-d_6, 400 MHz): δ 12.21 (s, 1H), 12.05 (s, 1H), 9.05 (d, 1H, *J* = 1.6 Hz), 8.53 (d, 1H, *J* = 2.8 Hz), 8.13-8.10 (dd, 1H, *J* = 1.2 Hz), 7.83-7.78 (m, 1H), 7.72 (d, 1H, *J* = 7.6 Hz), 7.53-7.51 (dd, 1H, *J* = 1.6 Hz), 7.46-7.42 (m, 1H), 7.36 (d, 1H, *J* = 8.4 Hz); ^{13}C NMR (DMSO-d_6, 100 MHz): δ 162.08, 149.81, 149.40, 135.92, 134.52, 130.67, 130.62, 129.82, 127.92, 126.92, 125.77, 125.41, 120.37, 114.49, 107.82, 85.29; IR ($CHCl_3$): ν_{max} 3306, 2955, 2924, 2857, 1739, 1650, 1491, 1464, 1400, 1343, 1191, 1168, 1082, 1015 cm^{-1}; HRMS: *m/z* 387.9950 calcd for $C_{16}H_{10}IN_3O + H^+$ (387.9941).

Assay for *in vitro* antimalarial activity. The assay is based on the determination of plasmodial LDH activity. For the assay, a suspension of red blood cells infected with D6 or W2 strains of *P. falciparum* (200 μL, with 2% parasitemia and 2% hematocrit in RPMI 1640 medium supplemented with 10% human serum and 60 μg/mL Amikacin) was added to the wells of a 96- well plate containing 10 μL of test samples diluted in medium at various concentrations. The plate was placed in a modular incubation chamber (Billups-Rothenberg, CA) flushed with a gas mixture of 90% N_2, 5% O_2, and 5% CO_2 and incubated at 37 ºC, for 72 h. Parasitic LDH activity was determined by using Malstat™ reagent (Flow Inc., Portland, OR) according to the procedure of Makler and Hinrichs.[6] Briefly, 20 μL of the incubation mixture was mixed with 100 μL of the Malstat™ reagent and incubated at room temperature for 30 min. Twenty microliters of a 1:1 mixture of NBT/PES (Sigma, St. Louis, MO) was then added and the plate is further incubated in the dark for 1 h. The reaction was then stopped by the addition of 100 μL of a 5% acetic acid solution. The plate was read at 650 nm using the EL-340 Biokinetics Reader (Bio-Tek Instruments, Vermont). IC_{50} values were computed from the dose response curves. Artemisinin and chloroquine were included in each assay as the drug controls. DMSO (0.25%) was used as vehicle control.

Assay for *in vitro* antileishmanial activity. Antileishmanial activity of the compounds was tested *in vitro* against a culture of *L. donovani* promastigotes. They were grown in RPMI 1640 medium supplemented with 10% fetal calf serum (Gibco Chem. Co.) at 26 ºC. A 3 day-old culture was diluted to 5×10^5 promastigotes/mL. Drug dilutions were prepared directly in cell suspension in 96-well plates. Plates were incubated at 26 ºC for 48 h and growth of leishmania promastigotes was determined by Alamar Blue assay as described earlier.[7] The standard fluorescence was measured on a Fluostar Galaxy plate reader (BMG Lab Technologies) at excitation wavelength of 544 nm and emission wavelength of 590 nm. Pentamidine and amphotericin B were used as the standard antileishmanial agents. IC_{50} and IC_{90} values were computed from dose response curves generated by plotting percent growth versus drug concentration.

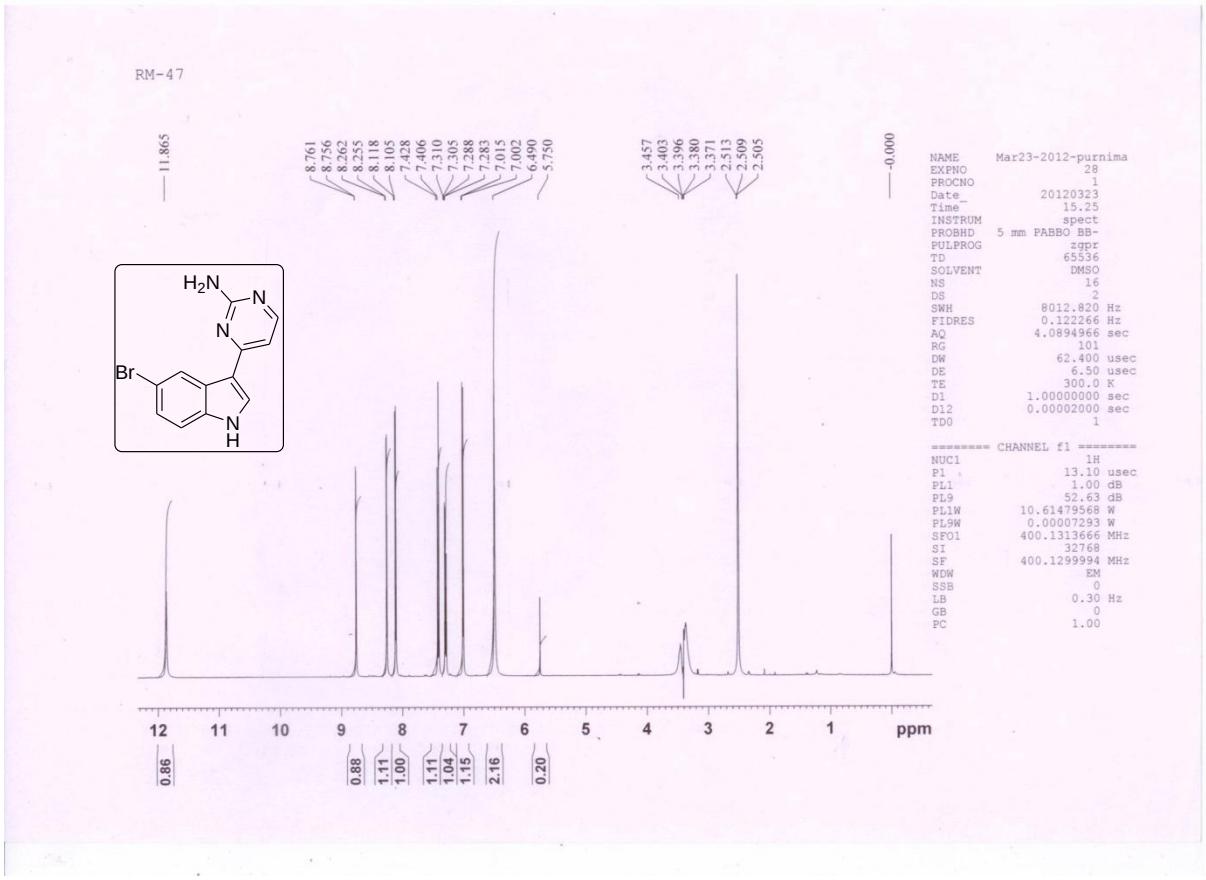
Assay for *in vitro* antimicrobial activity. Susceptibility testing against *C. albicans*, *C. neoformans*, methicillin-resistant *S. aureus* (MRS), and *A. fumigatus* was performed using a modified version of the NCCLS methods.[8] Susceptibility testing against *M. intracellulare* was done using the modified Alamar Blue procedure of Franzblau *et al.*[9] Samples (dissolved in DMSO) were serially diluted using 0.9% saline and transferred in duplicate to 96-well microplates. Microbial inocula were prepared after comparison of the absorbance at 630 nm

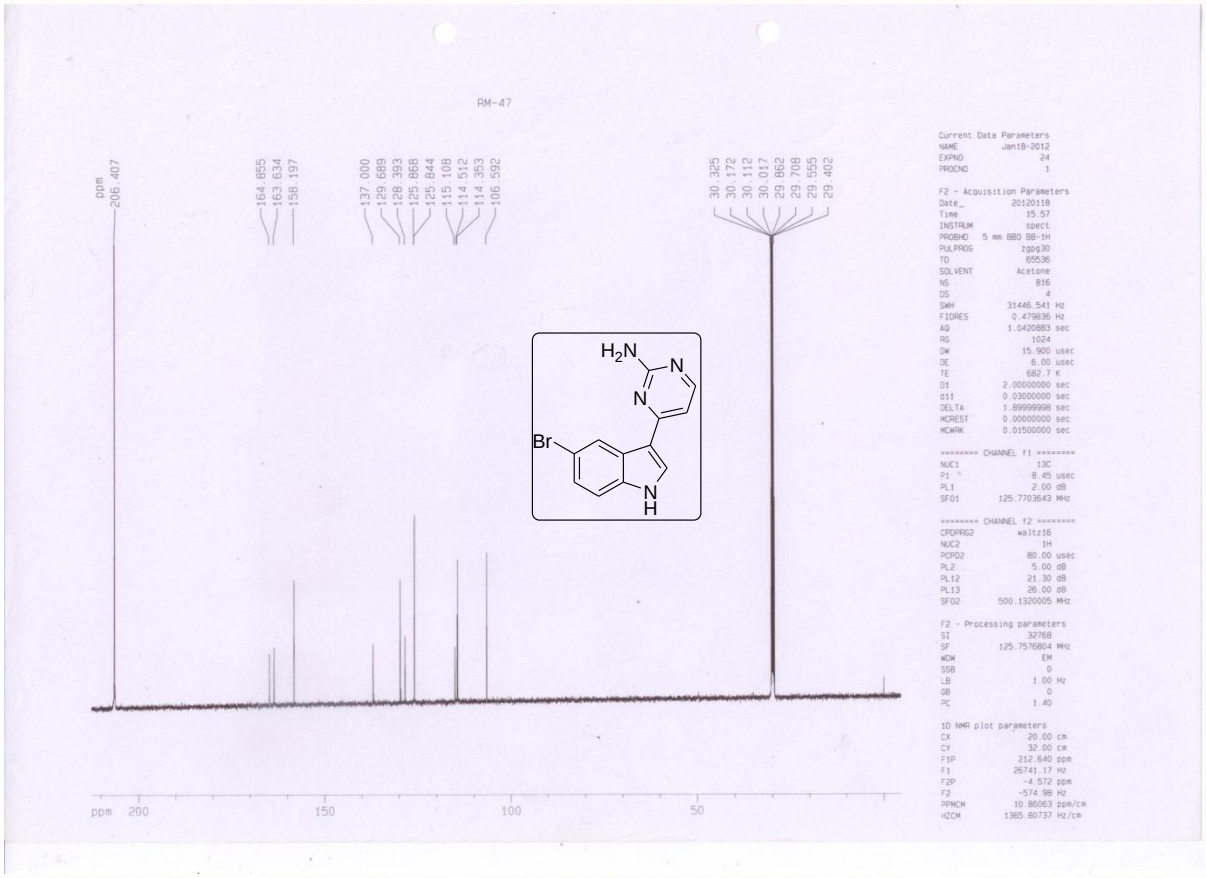
of cell suspensions to the 0.5 McFarland standard and diluting the suspensions in broth to afford recommended inocula. Microbial inocula were added to the diluted samples to achieve a final volume of 200 uL. Growth, solvent, and media controls were included in each assay. Plates were read at either 530 nm or 544ex/590em (*M. intracellulare* and *A. fumigatus*) prior to and after incubation. Percent growth was plotted versus test concentration to afford the IC_{50}.

Cytotoxicity screening. The in vitro cytotoxicity was determined against Vero (monkey kidney fibroblasts), HEPG2 (human hepatoma cells) and LLC-PK11 (pig kidney epithelial cells). The assay was performed in 96-well tissue culture-treated plates as described earlier.[10] Briefly, cells were seeded to the wells of 96-well plate (25,000 cells/well) and incubated for 24 h. Samples at different concentrations were added and plates were again incubated for 48 h. The number of via-ble cells was determined by Neutral Red assay. IC_{50} values were determined from dose curves of percent growth versus test concentrations. Doxorubicin was used as a positive control.

S2. Scanned copies of ^{1}H, ^{13}C and DEPT135 NMR spectras of all compounds

Meridianin C (3)

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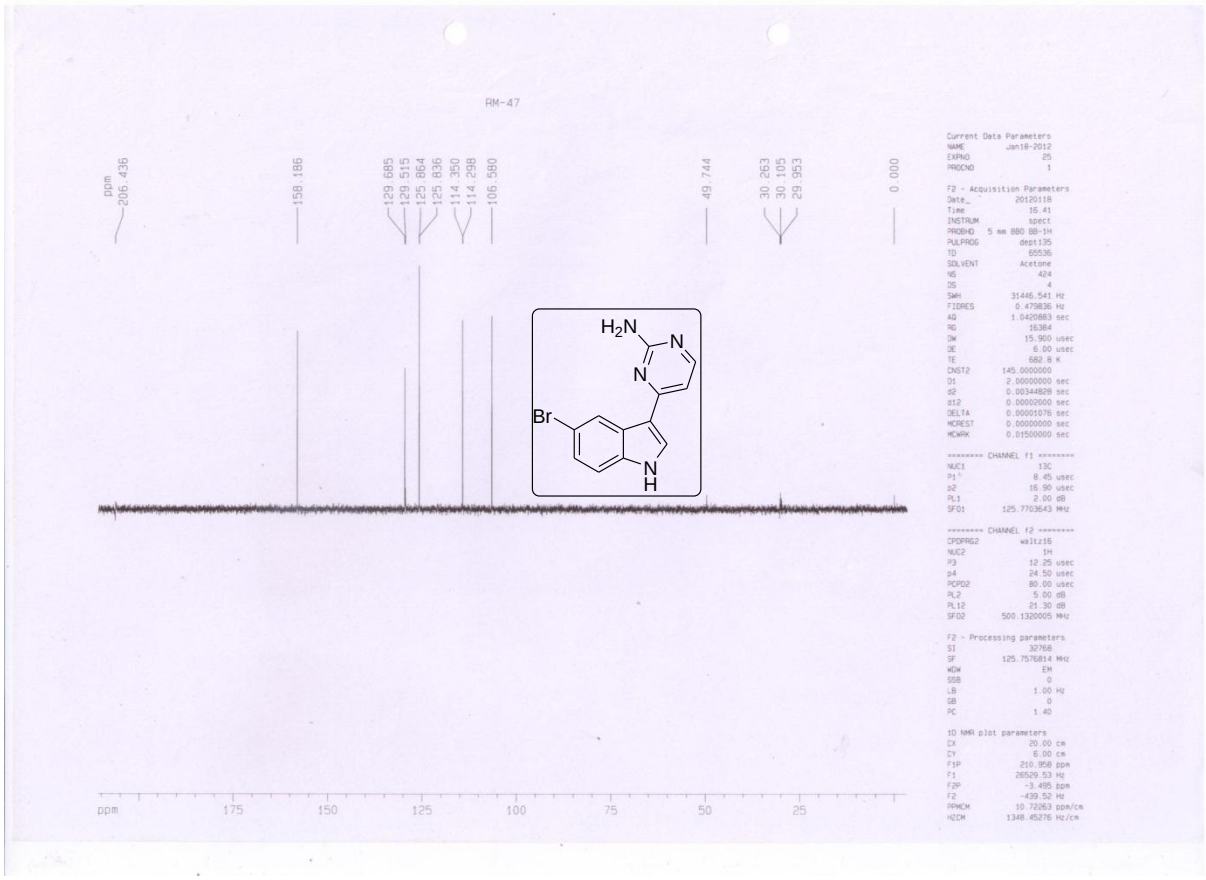
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H
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125
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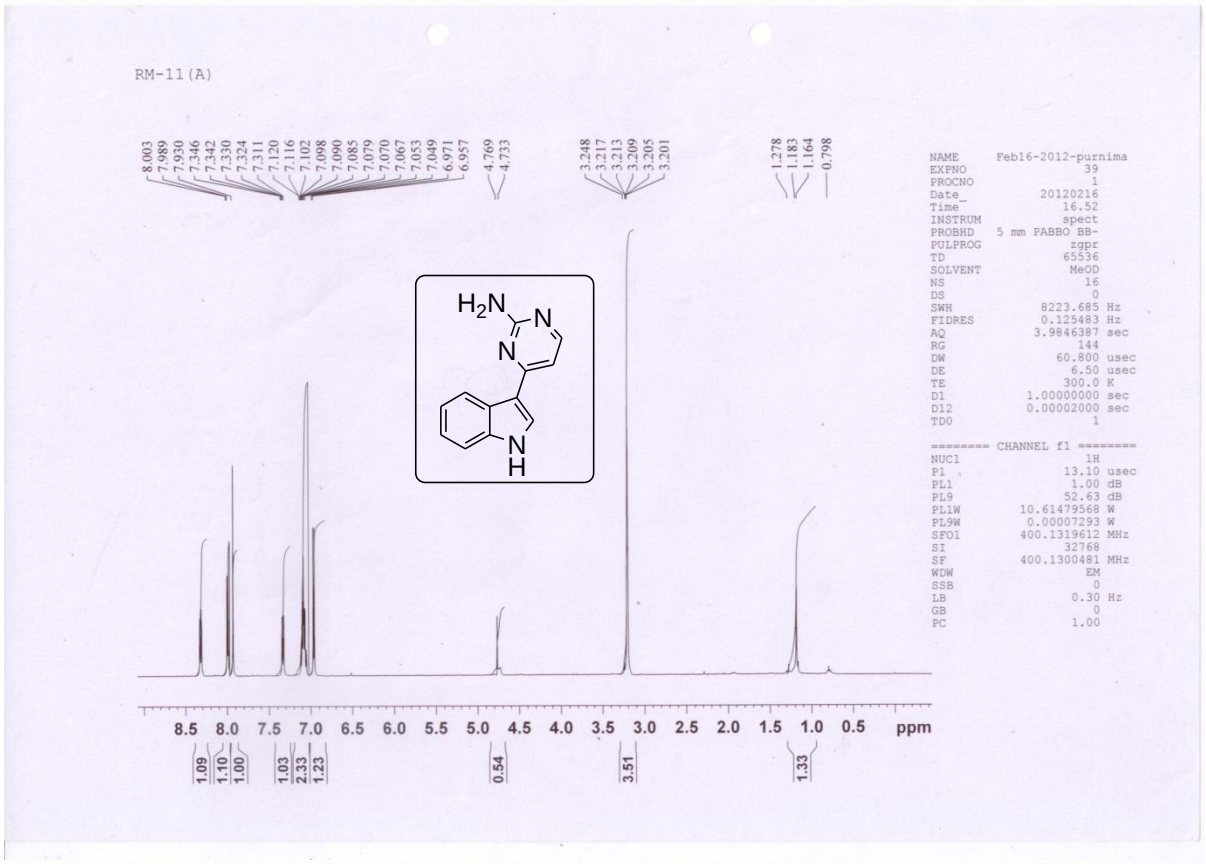
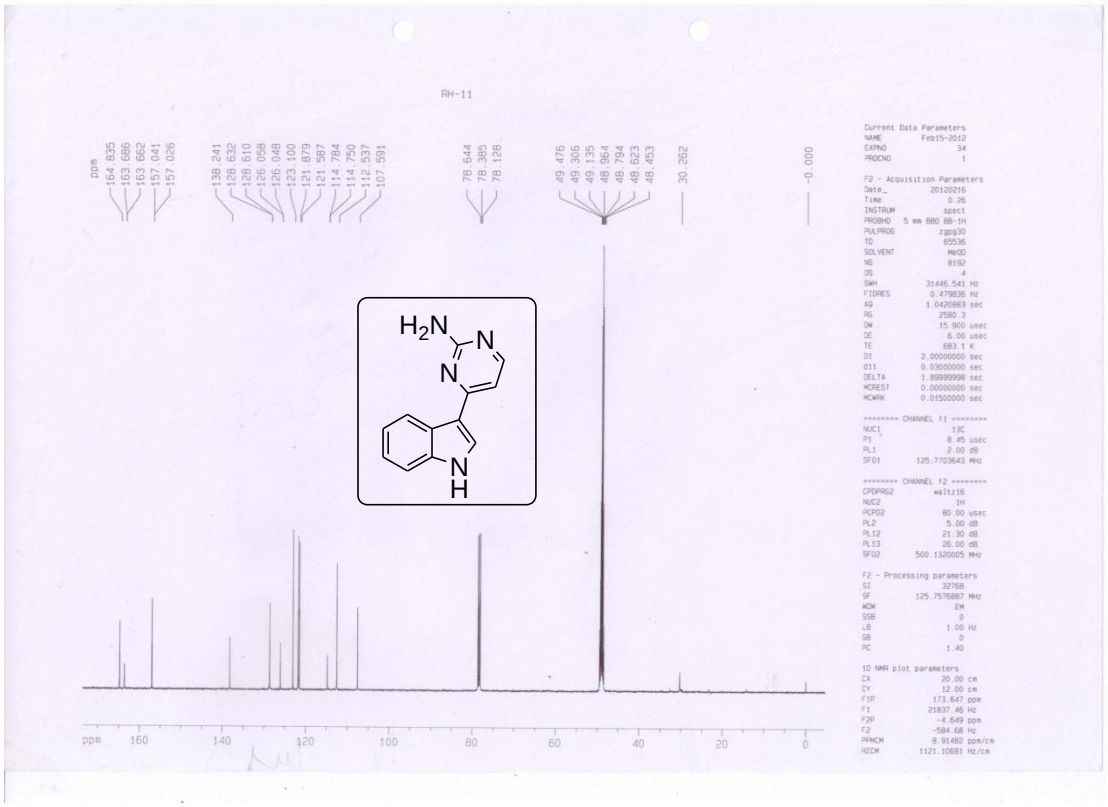
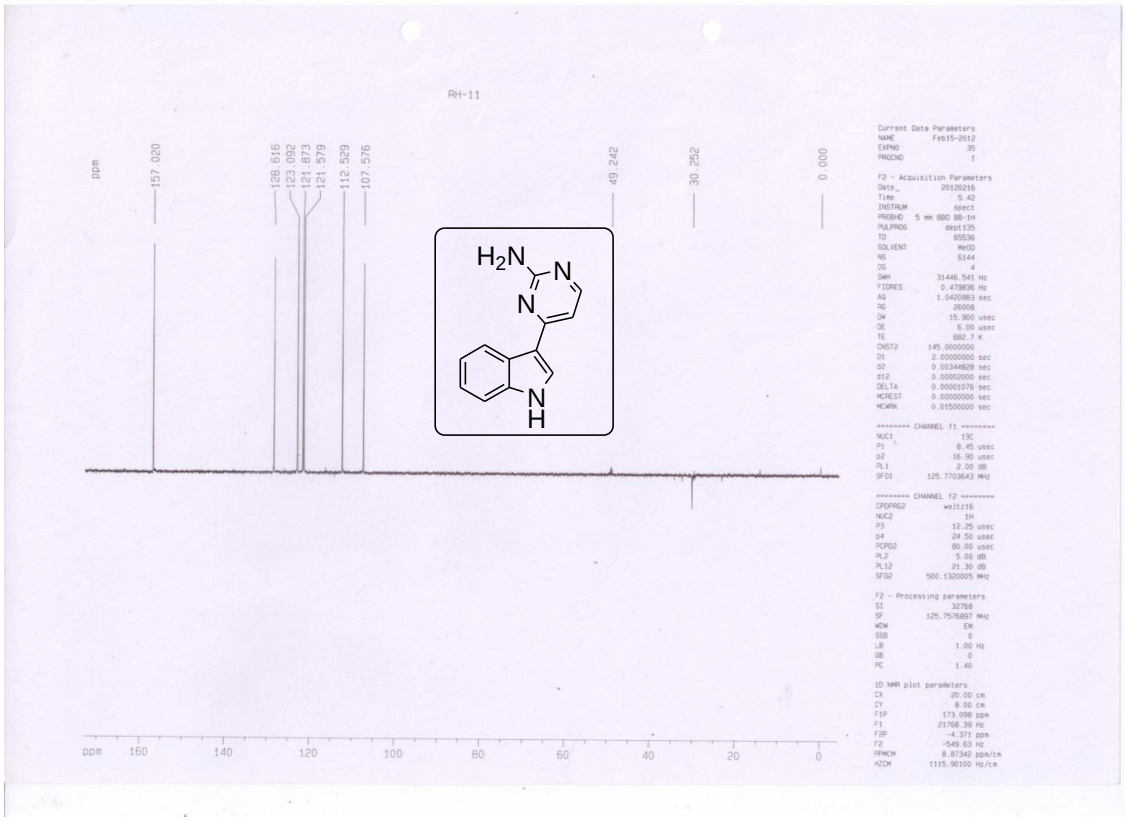
50
25

Meridianin G (7)



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F2P -4.371 ppm
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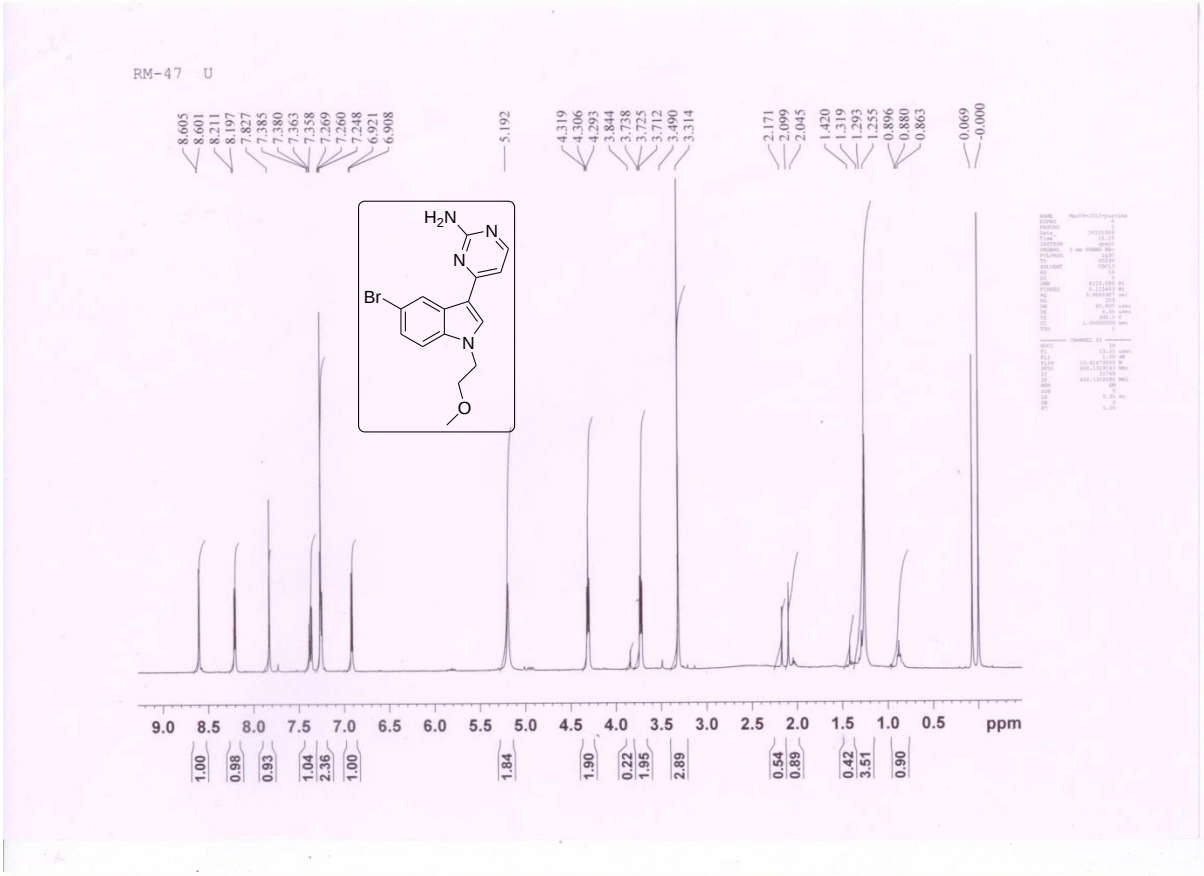
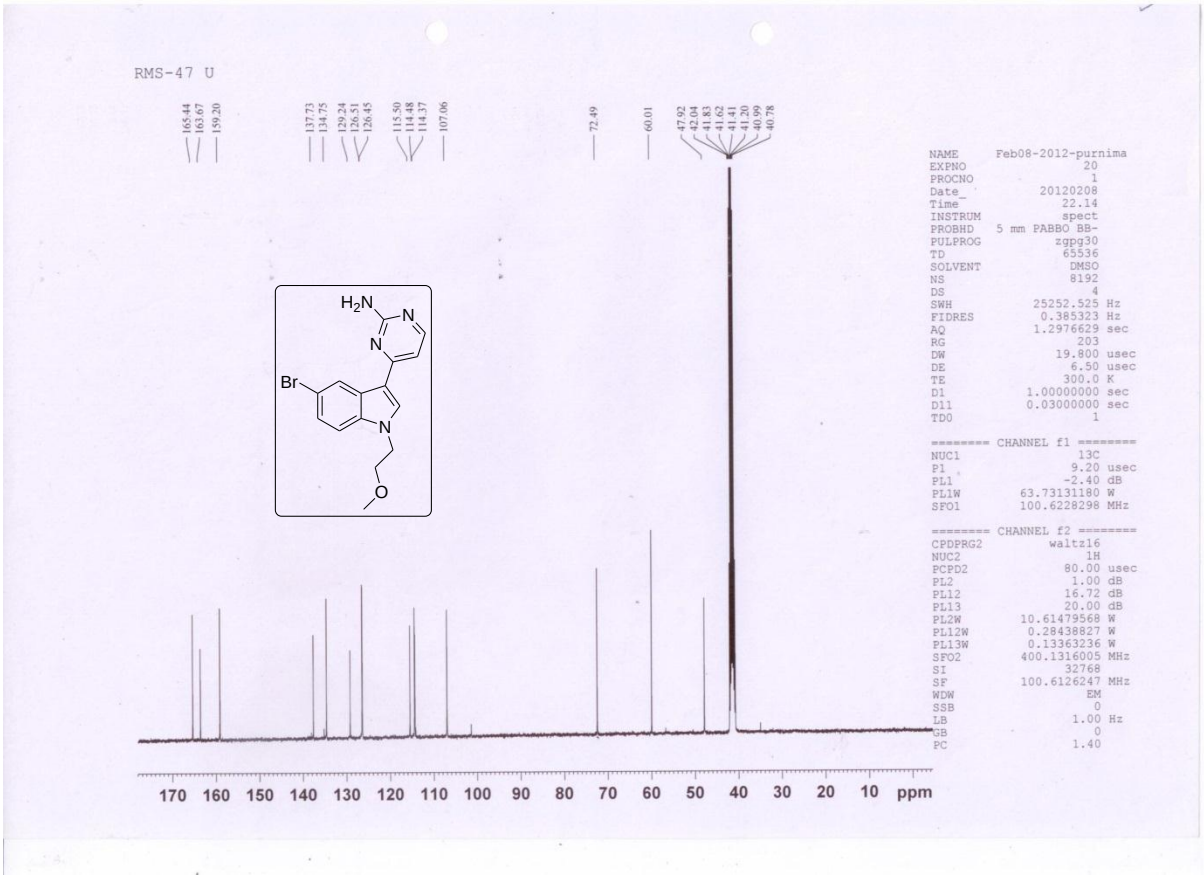
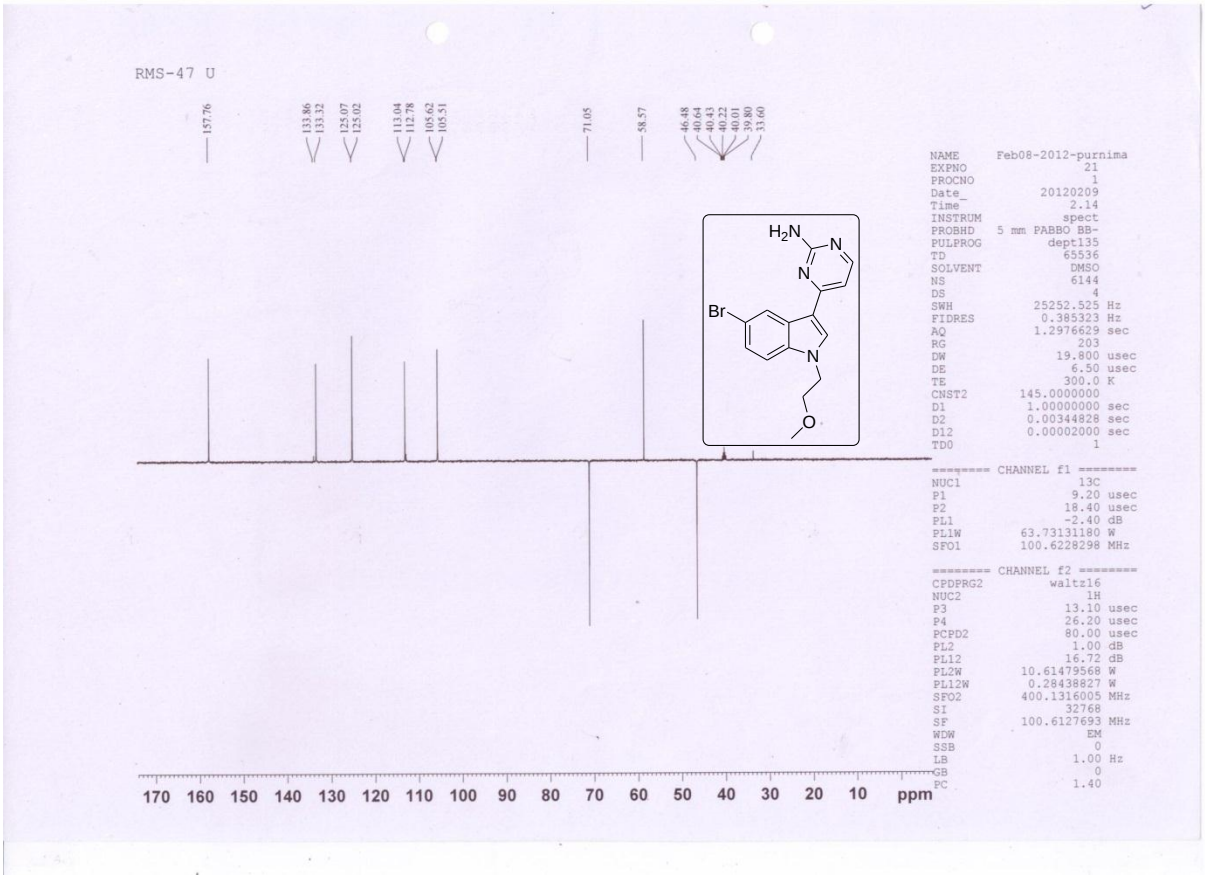
4-(5-Bromo-1-(2-methoxyethyl)-1H-indol-3-yl)pyrimidin-2-amine (15)



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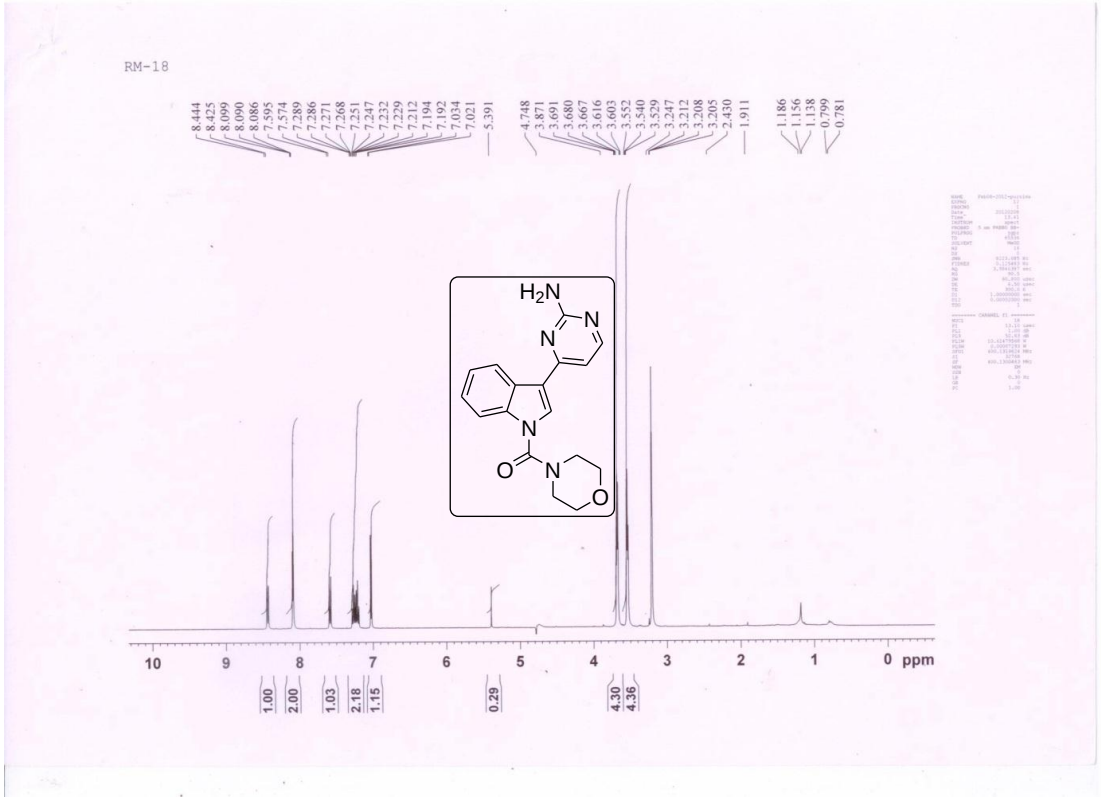
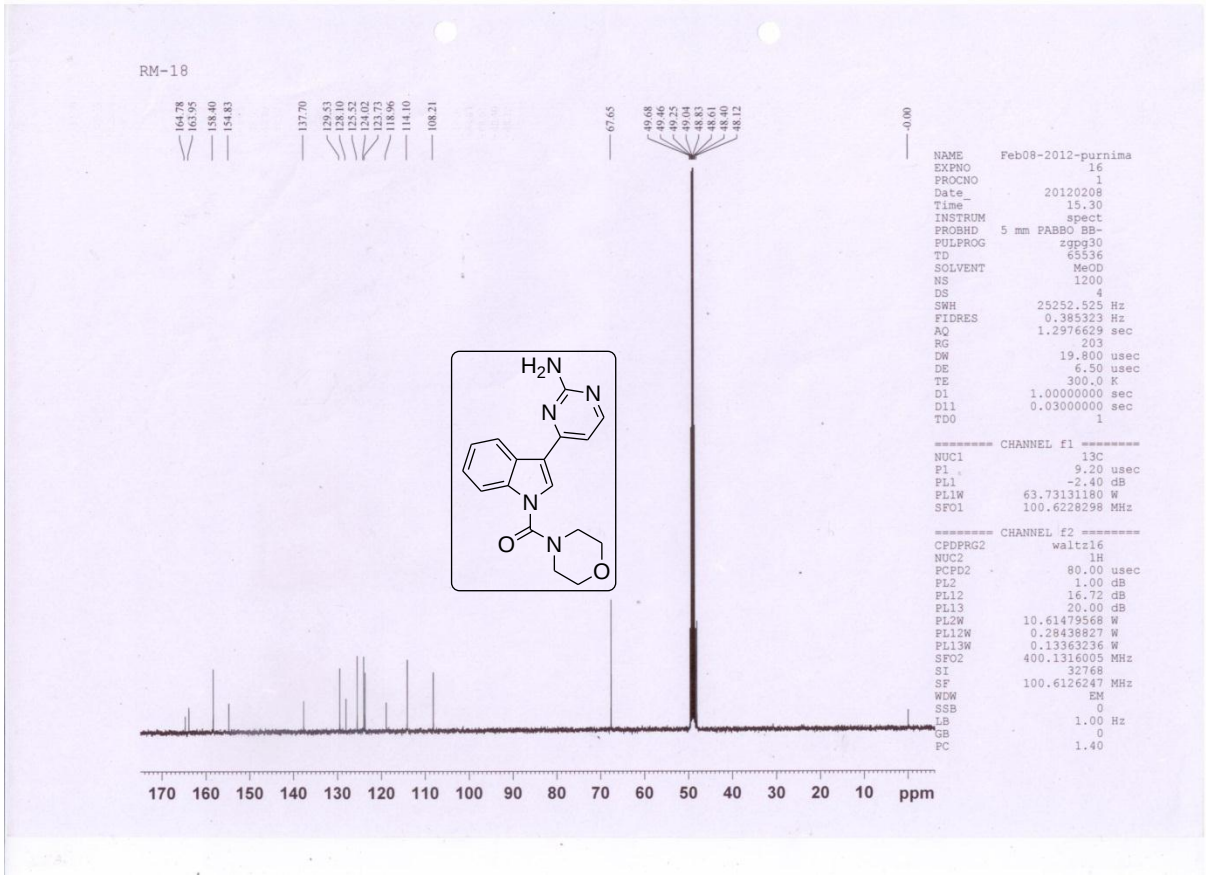
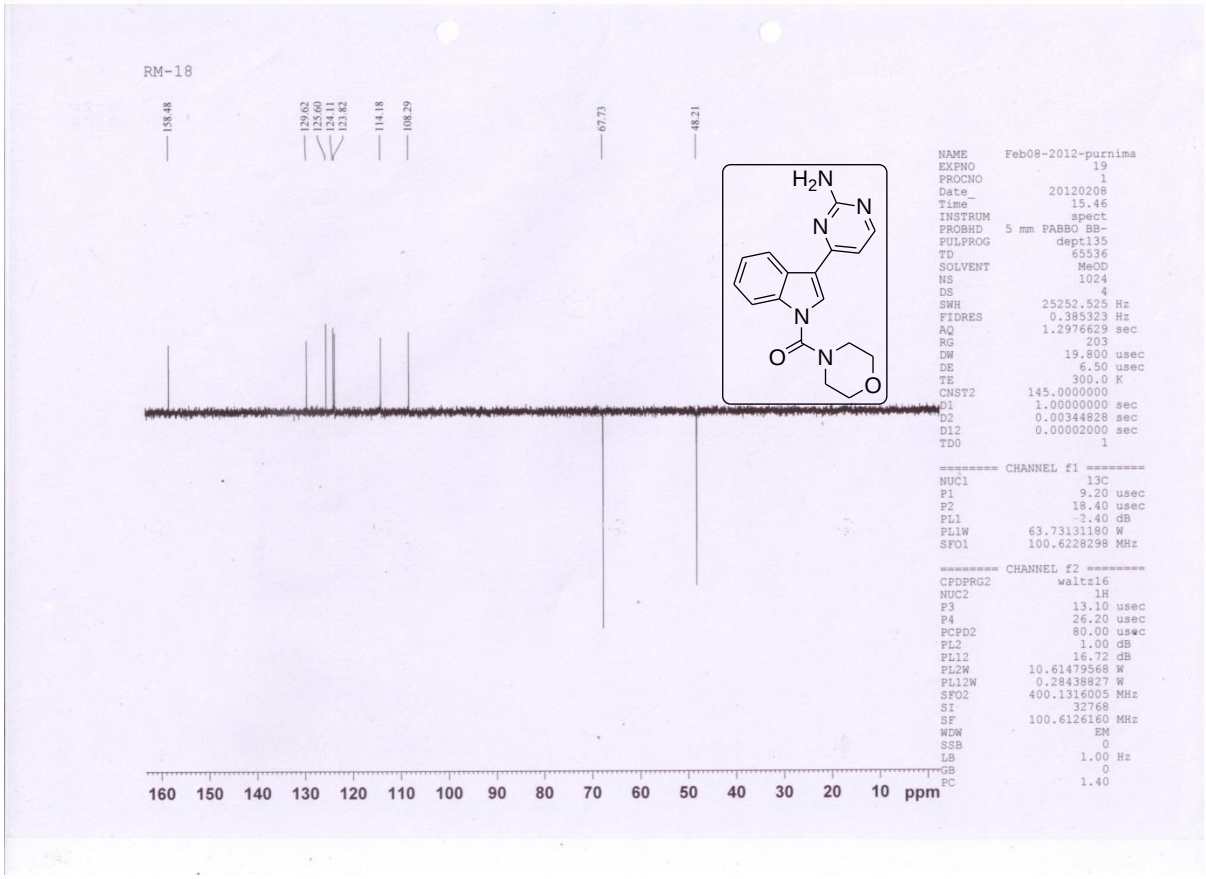
(3-(2-Aminopyrimidin-4-yl)-1H-indol-1-yl)(morpholino)methanone (17a)



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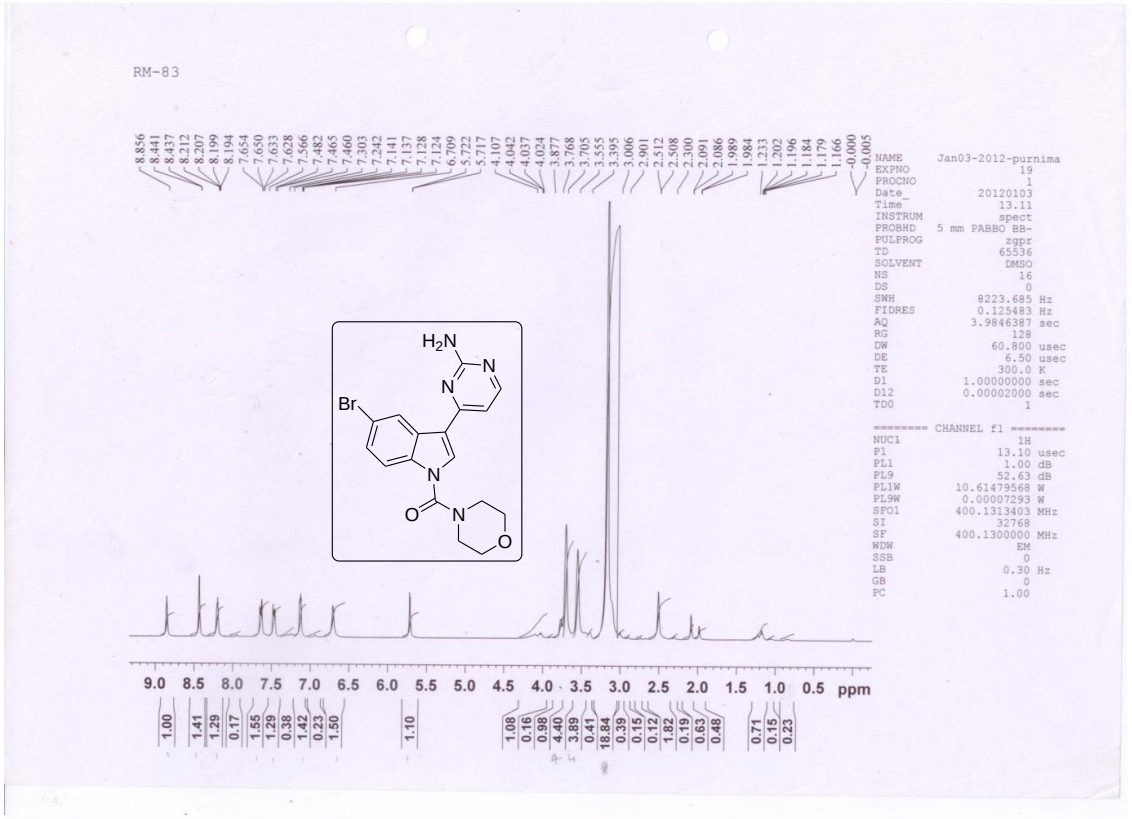
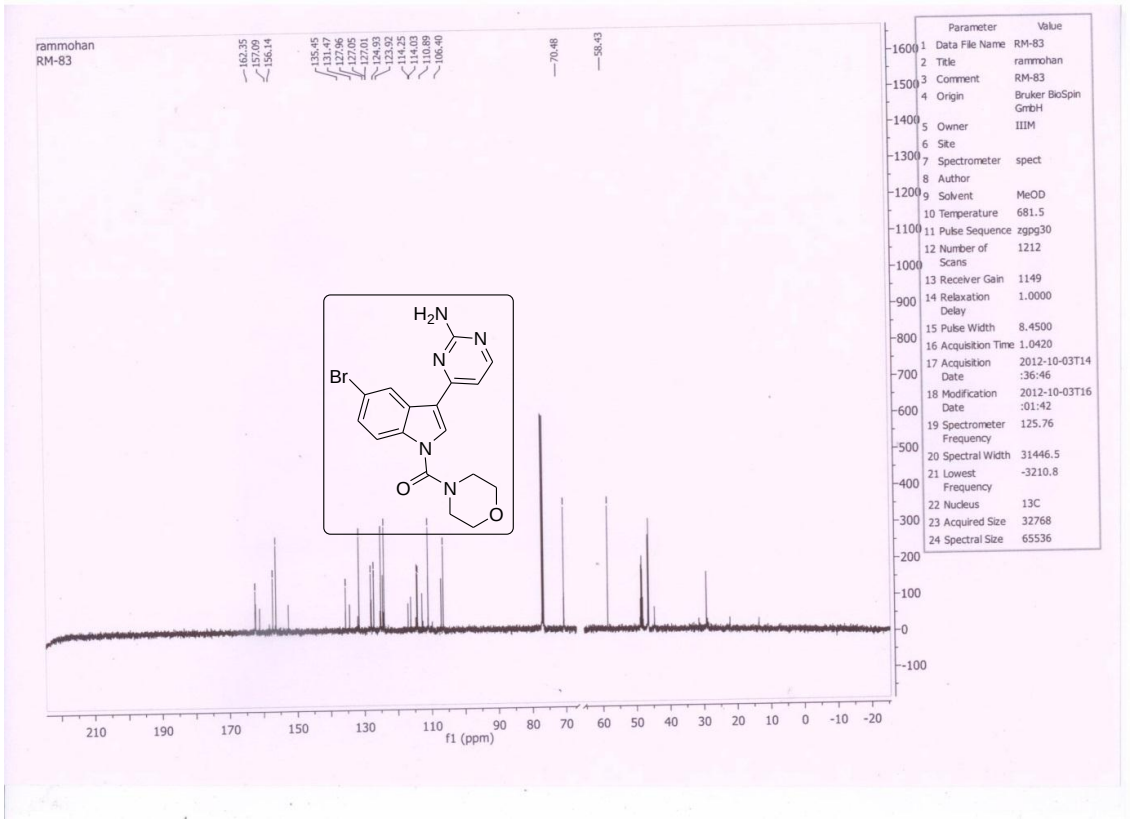
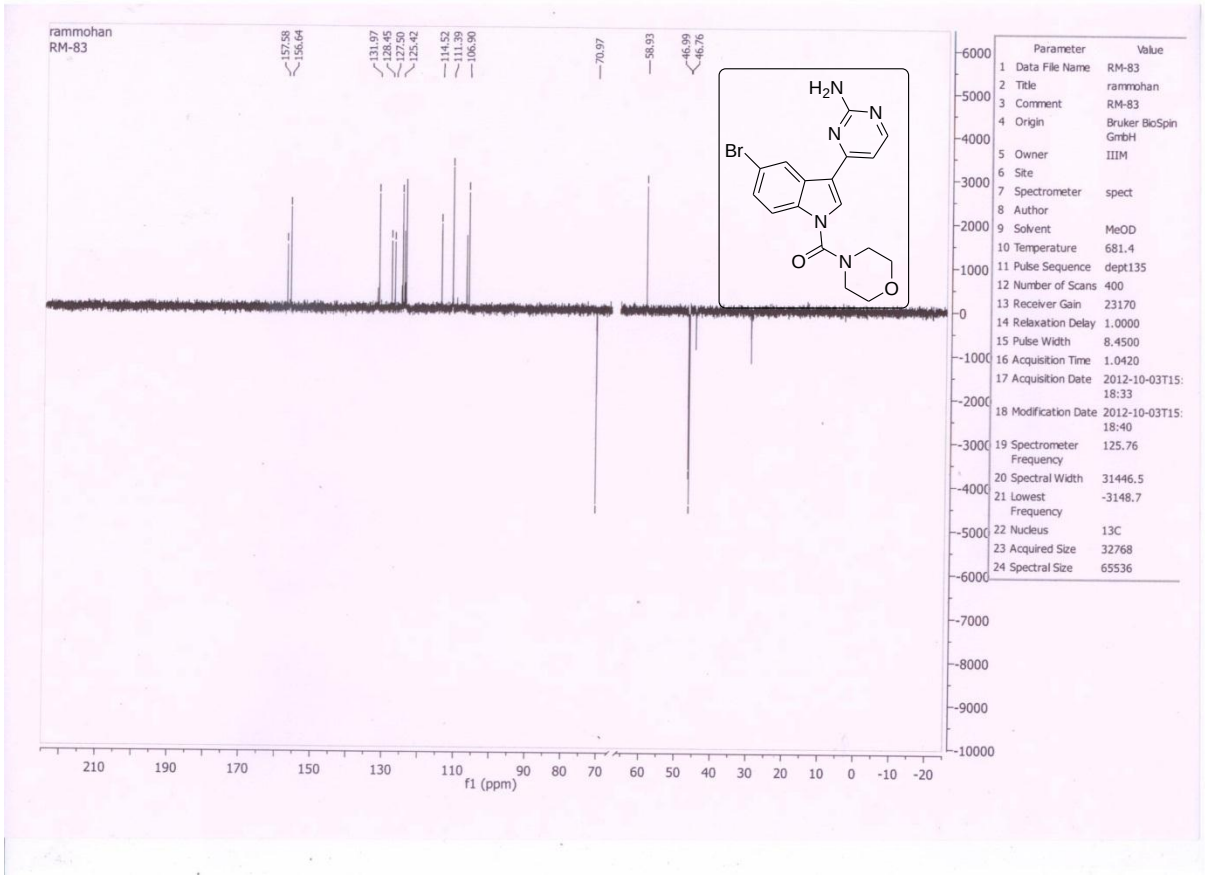
PC 1.40

(3-(2-Aminopyrimidin-4-yl)-5-bromo-1H-indol-1-yl)(morpholino)methanone(17b)

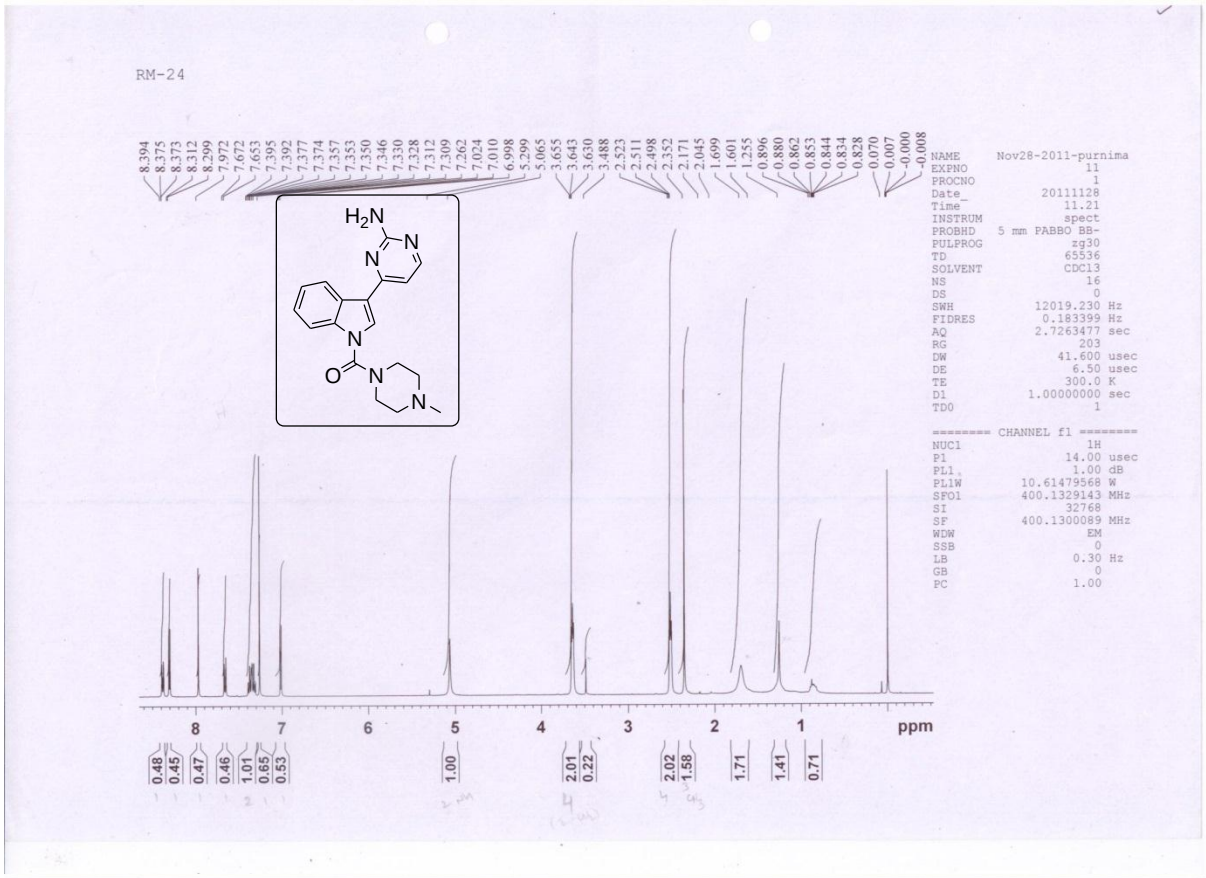


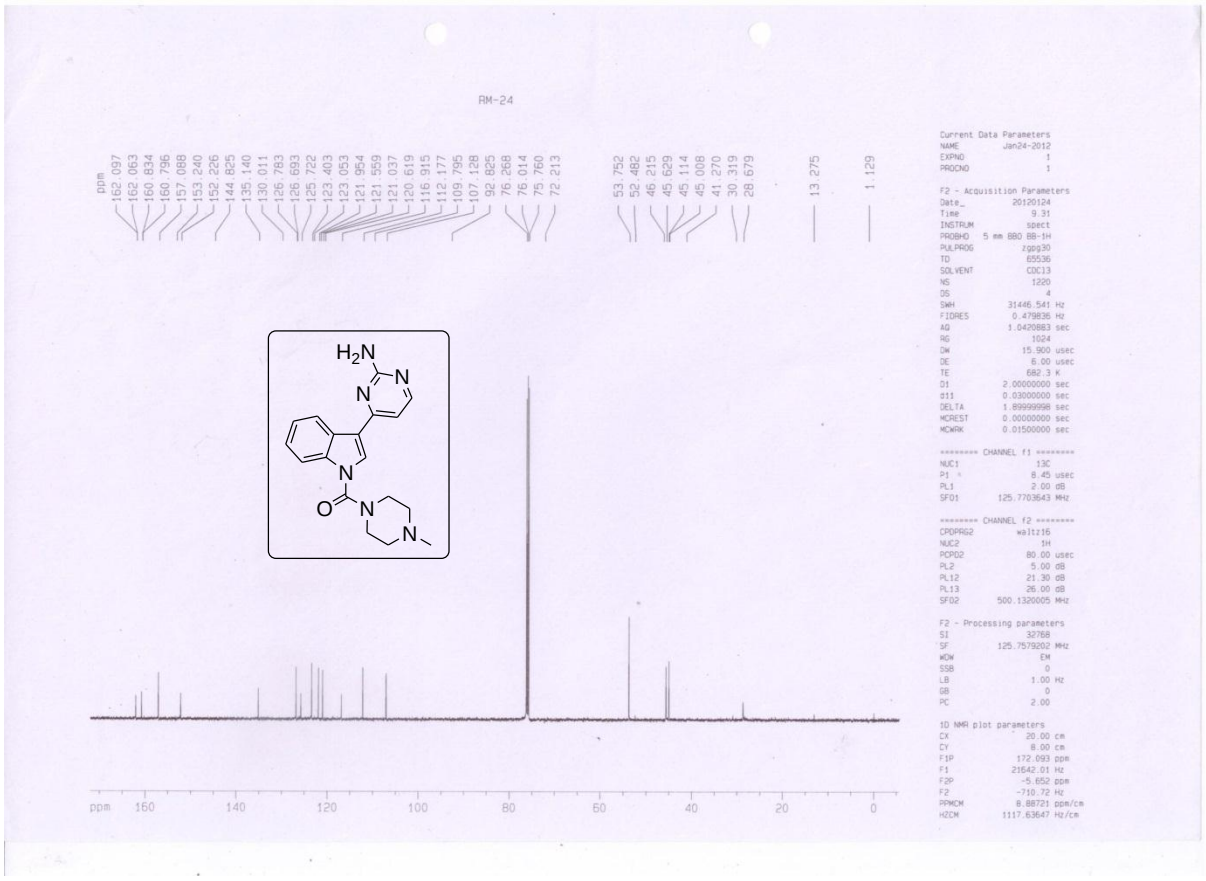


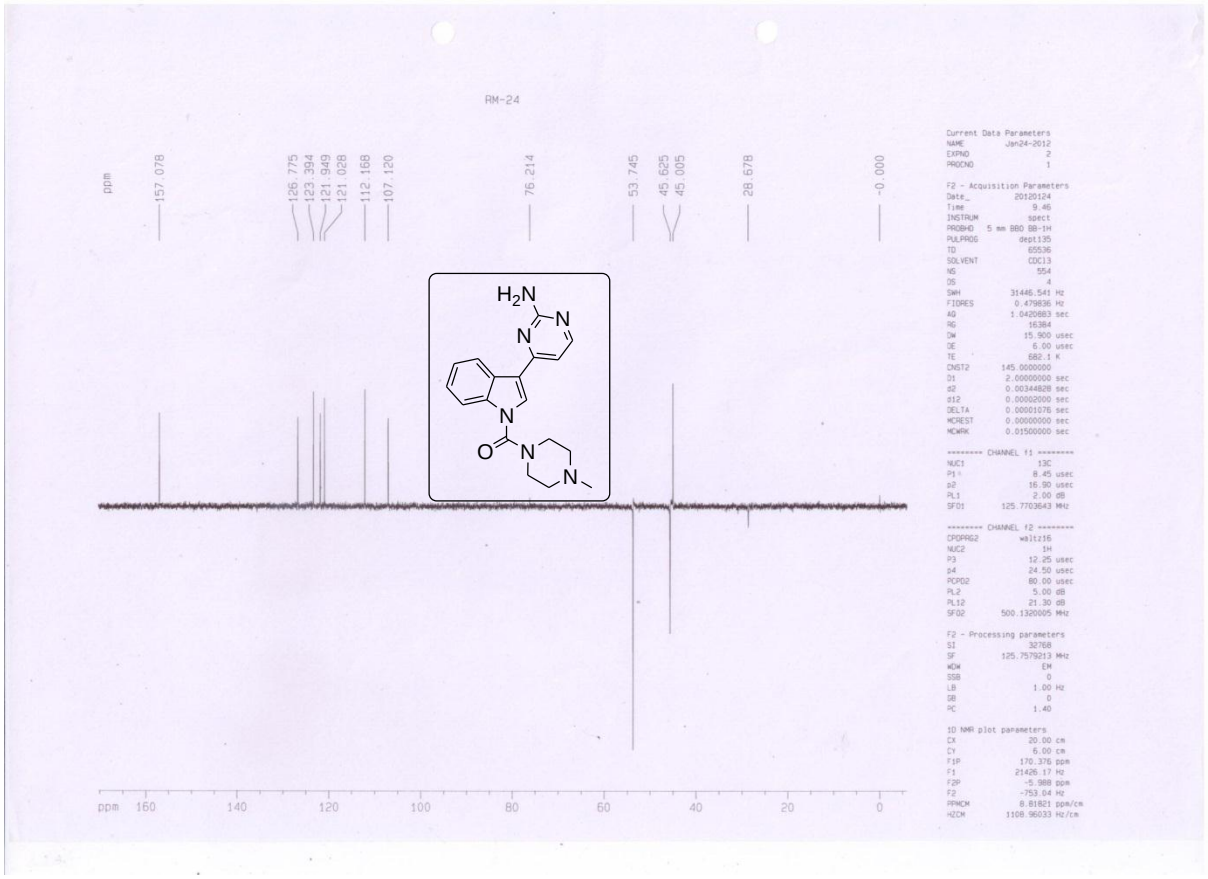

rammohan
RM-83
157.58
156.64
131.97
128.45
127.50
125.42
114.52
111.39
106.90
70.97
58.93
46.99
46.76
Br
H_2N
N
N
N
O
N
O
f1 (ppm)
Parameter Value
1 Data File Name RM-83
2 Title rammohan
3 Comment RM-83
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent MeOD
10 Temperature 681.4
11 Pulse Sequence dept135
12 Number of Scans 400
13 Receiver Gain 23170
14 Relaxation Delay 1.0000
15 Pulse Width 8.4500
16 Acquisition Time 1.0420
17 Acquisition Date 2012-10-03T15:18:33
18 Modification Date 2012-10-03T15:18:40
19 Spectrometer Frequency 125.76
20 Spectral Width 31446.5
21 Lowest Frequency -3148.7
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536

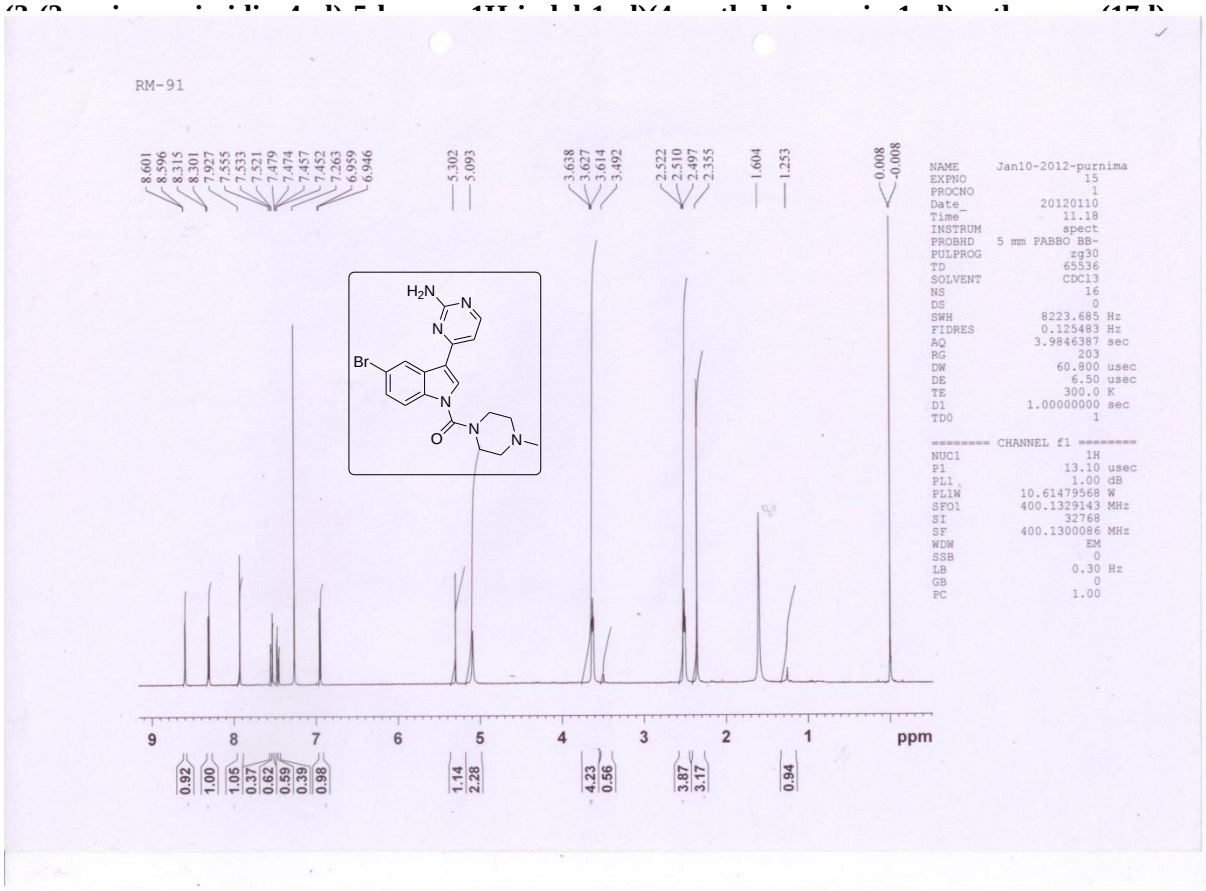
(3-(2-aminopyrimidin-4-yl)-1H-indol-1-yl)(4-methylpiperazin-1-yl)methanone

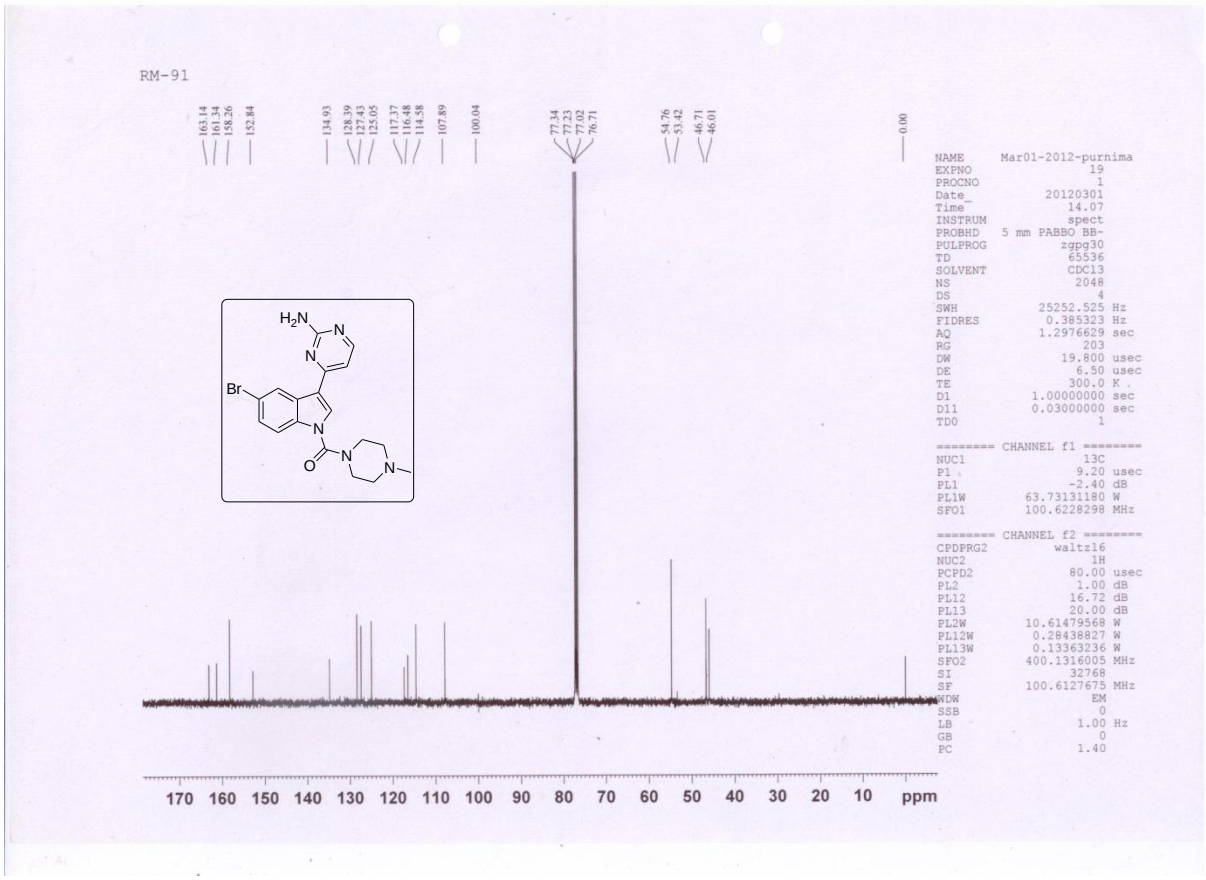
(17c)

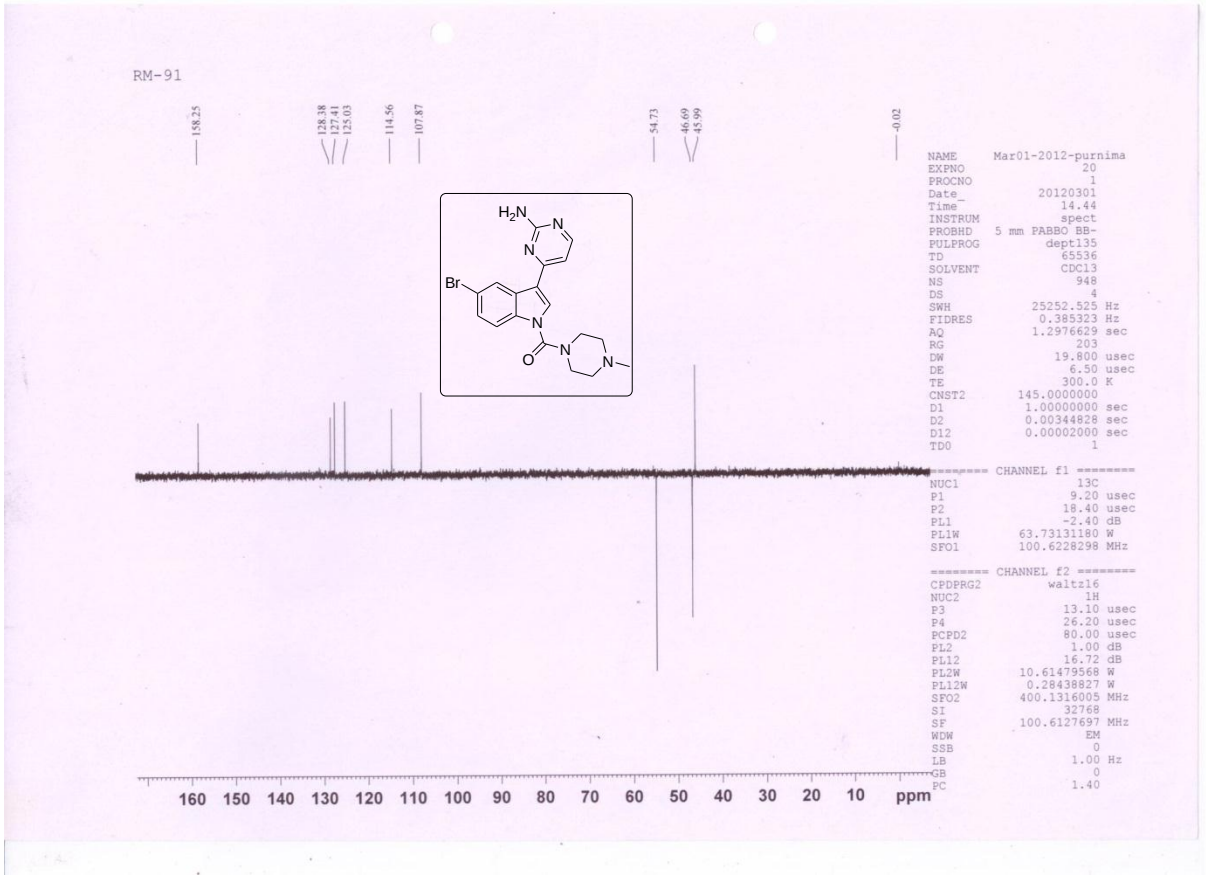




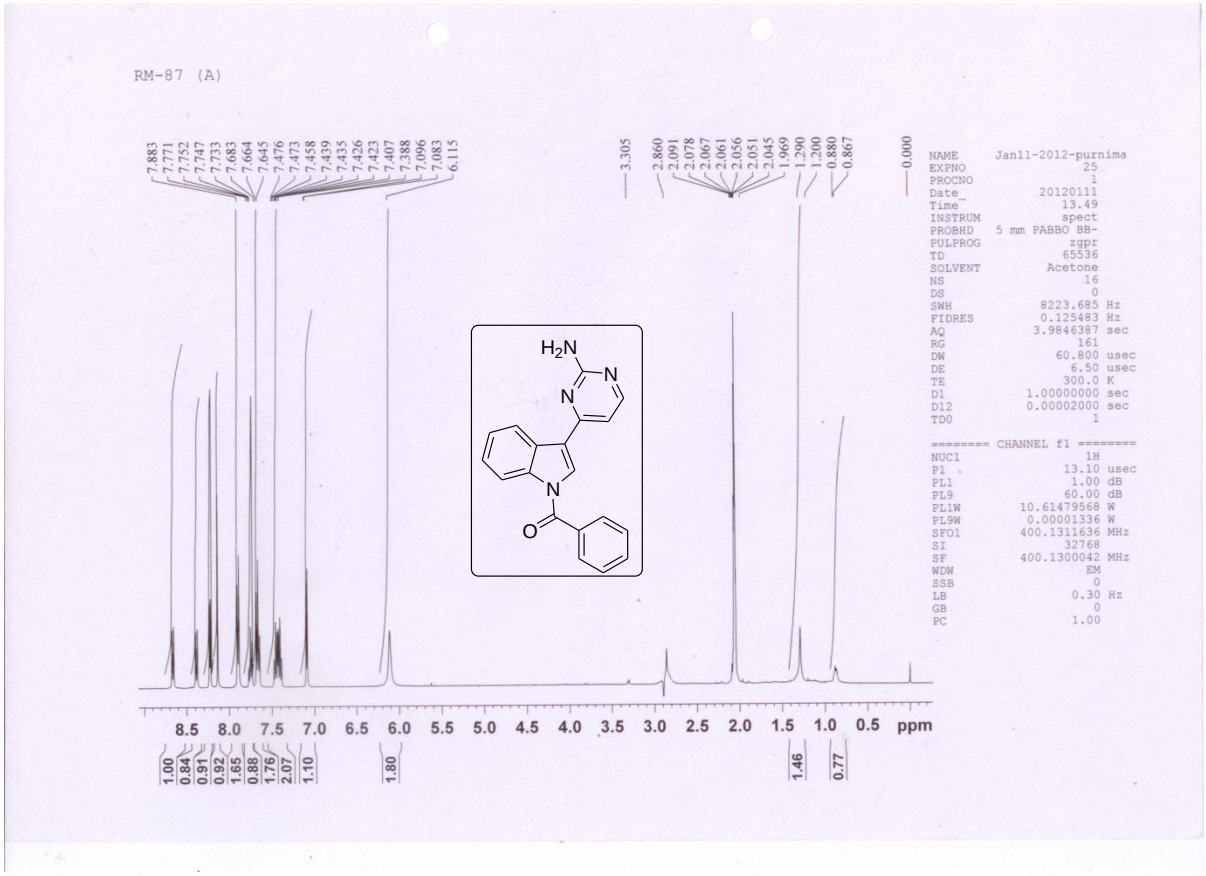

RM-24
ppm
157.078
126.775
123.394
121.949
121.028
112.168
107.120
76.214
53.745
45.625
45.005
28.678
-0.000
H_2N
N
N
N
O
N
N
ppm 160 140 120 100 80 60 40 20 0
Current Data Parameters
NAME Jan24-2012
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120124
Time 9.46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 554
DS 4
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 16384
DW 15.900 usec
DE 6.00 usec
TE 682.1 K
CNST2 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
DELTA 0.00001076 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.45 usec
P2 16.90 usec
PL1 2.00 dB
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 12.25 usec
P4 24.50 usec
PCPD2 80.00 usec
PL2 5.00 dB
PL12 21.30 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7579213 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 170.376 ppm
F1 21426.17 Hz
F2P -5.988 ppm
F2 -753.04 Hz
PPMCM 8.81821 ppm/cm
HZCM 1108.96033 Hz/cm

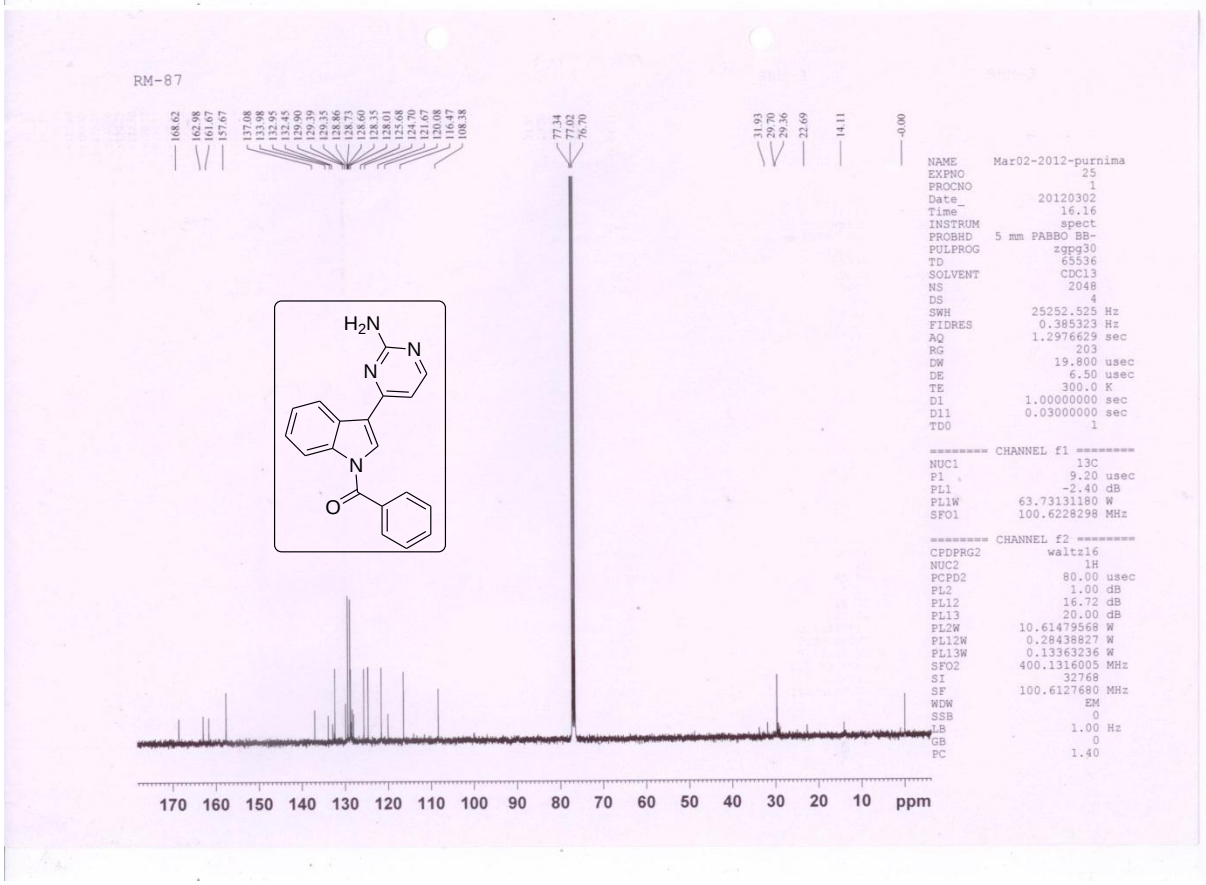

RM-91
8.601
8.596
8.315
8.301
7.927
7.555
7.533
7.521
7.479
7.474
7.457
7.452
7.263
6.959
6.946
5.302
5.093
3.638
3.627
3.614
3.492
2.522
2.510
2.497
2.355
1.604
1.253
0.008
-0.008
NAME Jan10-2012-purnima
EXPNO 15
PROCNO 1
Date_ 20120110
Time 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 0
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846387 sec
RG 203
DW 60.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 13.10 usec
PL1 1.00 dB
PL1W 10.61479568 W
SFO1 400.1329143 MHz
SI 32768
SF 400.1300086 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9 8 7 6 5 4 3 2 1 ppm
0.92 1.00 1.05 0.37 0.62 0.59 0.39 0.98 1.14 2.28 4.23 0.56 3.87 3.17 0.94

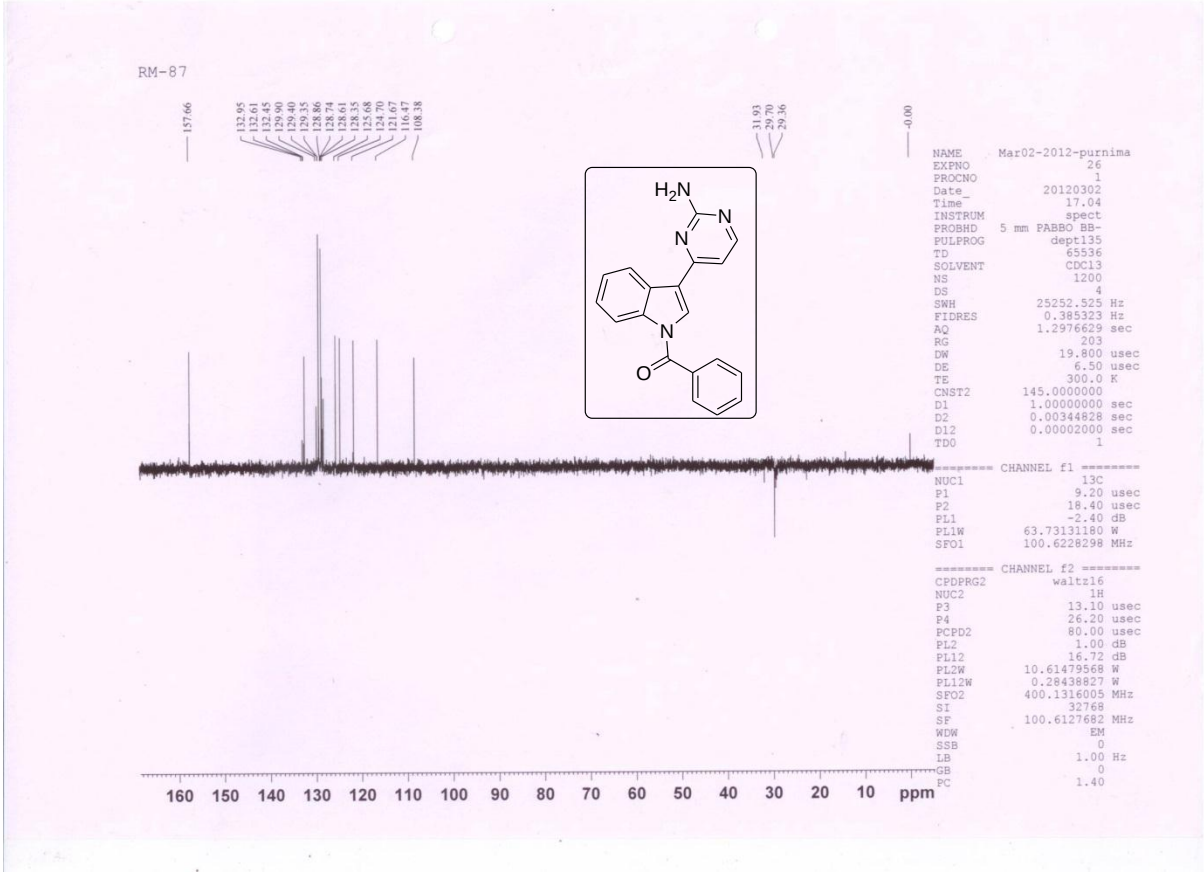

RM-91
163.14
161.34
158.26
152.84
134.93
128.39
127.43
125.05
117.37
116.48
114.58
107.89
100.04
77.34
77.23
77.02
76.71
54.76
53.42
46.71
46.01
0.00
NAME Mar01-2012-purnima
EXPNO 19
PROCNO 1
Date_ 20120301
Time 14.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.20 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL13 20.00 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
PL13W 0.13363236 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127675 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


RM-91
158.25
128.38
127.41
125.03
114.56
107.87
54.73
46.69
45.99
-0.02
H2N
N
N
Br
N
O
N
N
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
NAME Mar01-2012-purnima
EXPNO 20
PROCNO 1
Date_ 20120301
Time 14.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 948
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
P2 18.40 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 13.10 usec
P4 26.20 usec
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127697 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

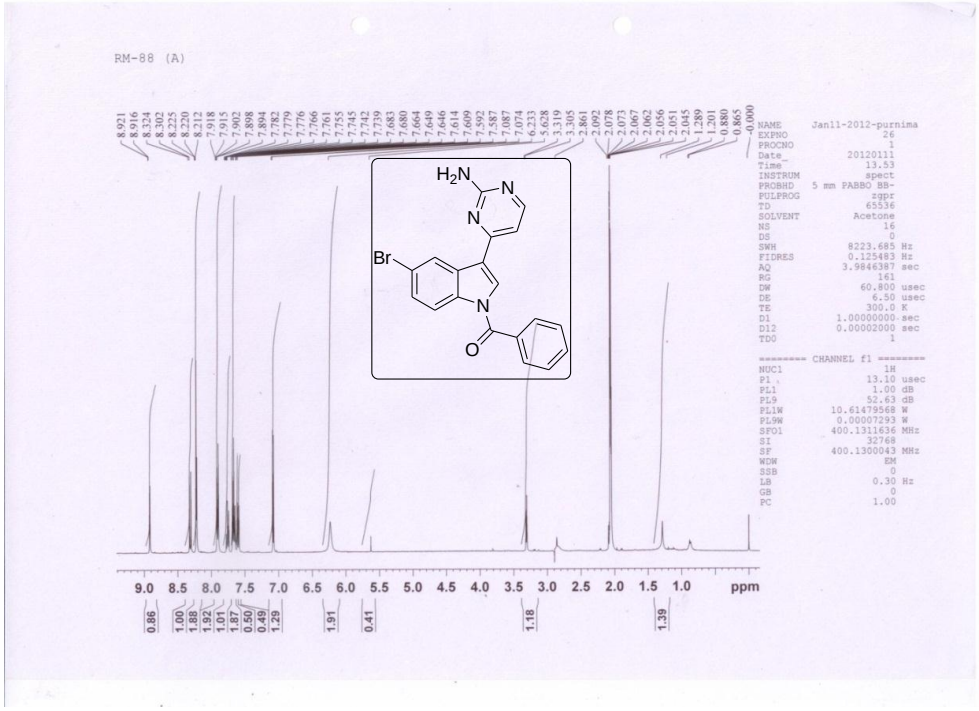
(3-(2-aminopyrimidin-4-yl)-1H-indol-1-yl)(phenyl)methanone(17e)

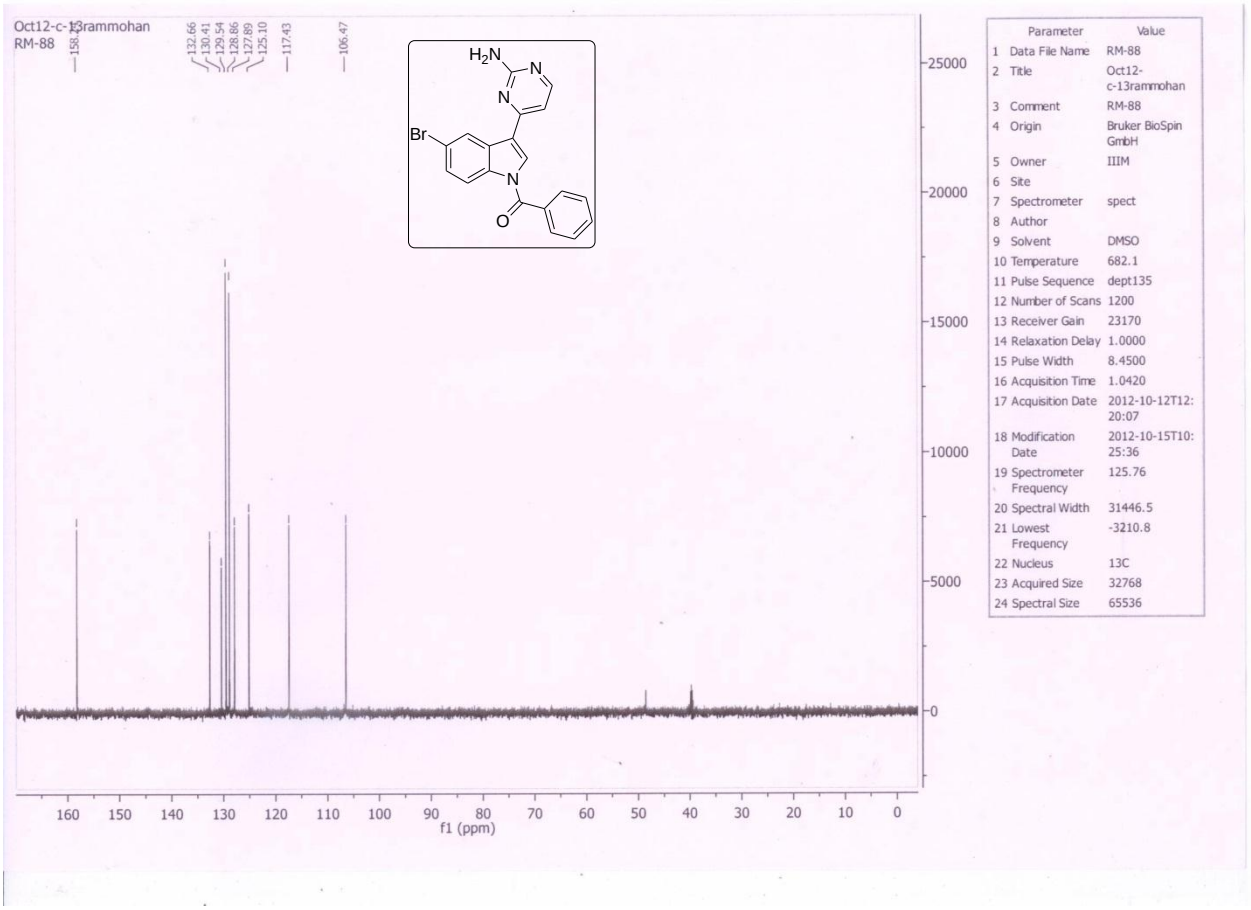


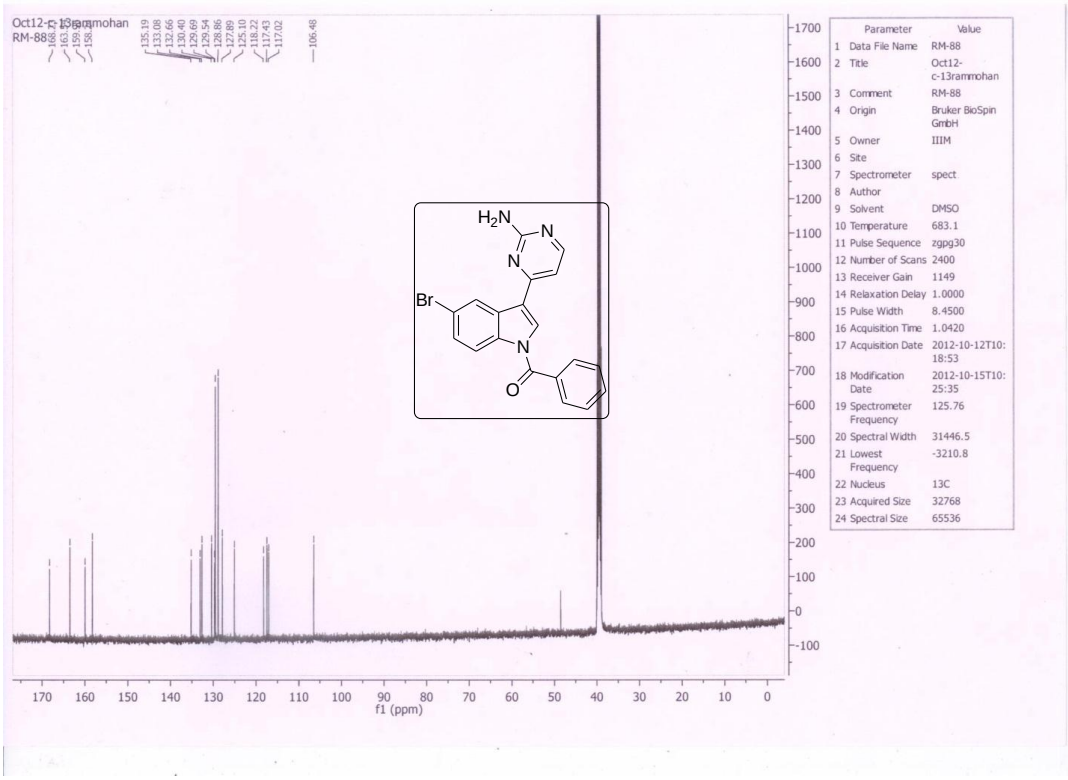



RM-87
157.66
132.95
132.61
132.45
129.90
129.40
129.35
128.86
128.74
128.61
128.35
125.68
124.70
121.67
116.47
108.38
31.93
29.70
29.36
0.00
H2N
N
N
N
O
NAME Mar02-2012-purnima
EXPNO 26
PROCNO 1
Date_ 20120302
Time 17.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 1200
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
P2 18.40 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 13.10 usec
P4 26.20 usec
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127682 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

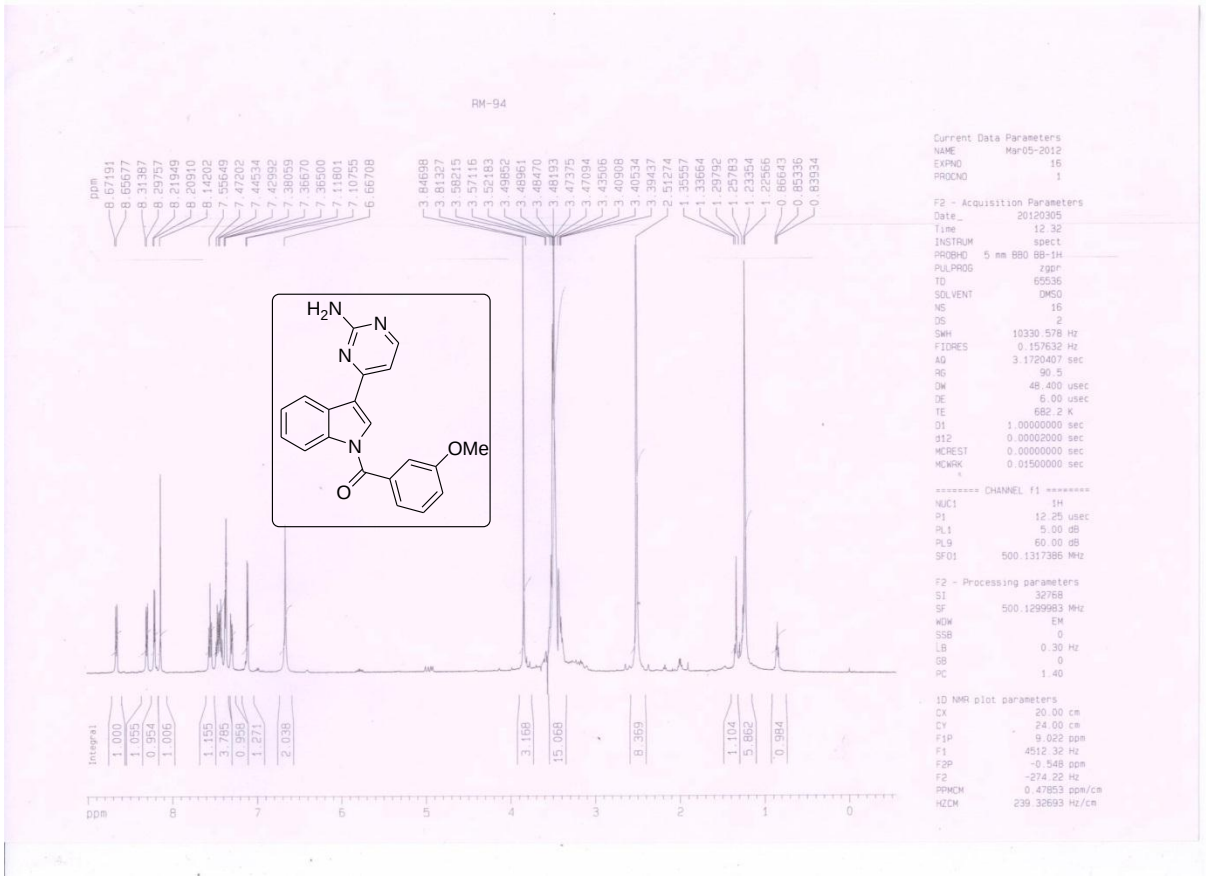
(3-(2-aminopyrimidin-4-yl)-5-bromo-1H-indol-1-yl)(phenyl)methanone (17f)

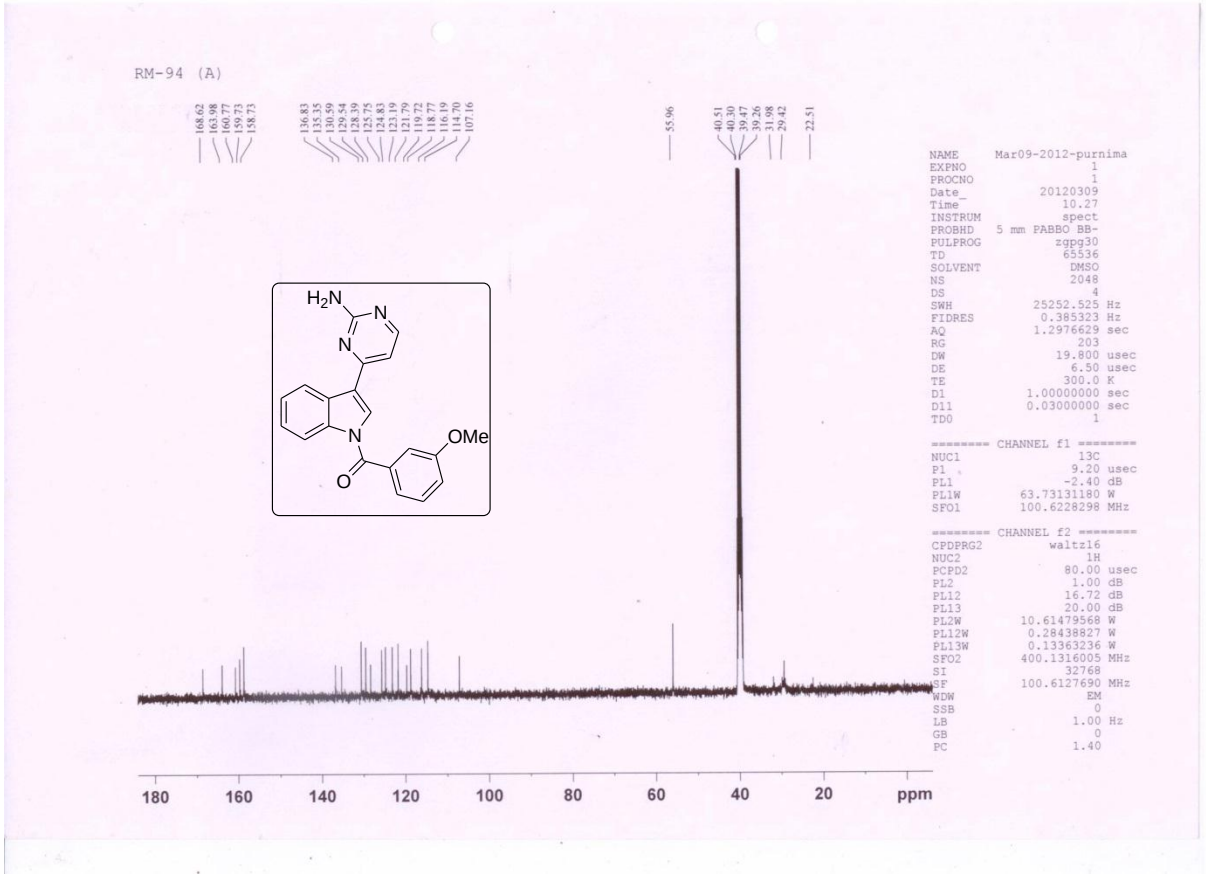


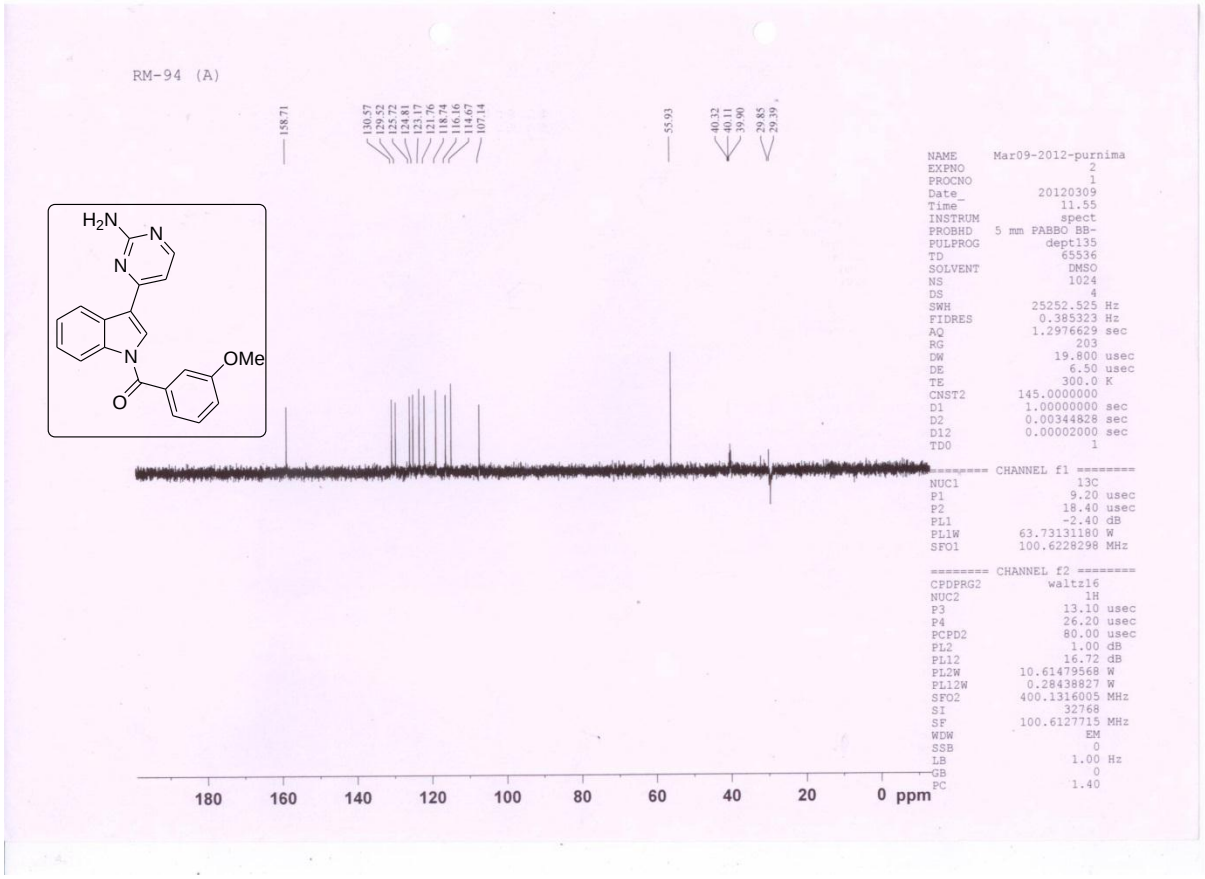

Oct12-c-13rammohan
RM-88
158.2
132.66
130.41
129.54
128.86
127.89
125.10
117.43
106.47
H2N
N
N
Br
N
O
25000
20000
15000
10000
5000
0
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Parameter Value
1 Data File Name RM-88
2 Title Oct12-c-13rammohan
3 Comment RM-88
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent DMSO
10 Temperature 682.1
11 Pulse Sequence dept135
12 Number of Scans 1200
13 Receiver Gain 23170
14 Relaxation Delay 1.0000
15 Pulse Width 8.4500
16 Acquisition Time 1.0420
17 Acquisition Date 2012-10-12T12:20:07
18 Modification Date 2012-10-15T10:25:36
19 Spectrometer Frequency 125.76
20 Spectral Width 31446.5
21 Lowest Frequency -3210.8
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536


Oct12-c-13rammohan
RM-88
168.7
163.7
159.8
158.2
135.19
133.08
132.66
130.40
129.69
129.54
128.86
127.89
125.10
118.22
117.43
117.02
106.48
H2N
N
N
Br
N
O
1700
1600
1500
1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Parameter Value
1 Data File Name RM-88
2 Title Oct12-c-13rammohan
3 Comment RM-88
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent DMSO
10 Temperature 683.1
11 Pulse Sequence zgpg30
12 Number of Scans 2400
13 Receiver Gain 1149
14 Relaxation Delay 1.0000
15 Pulse Width 8.4500
16 Acquisition Time 1.0420
17 Acquisition Date 2012-10-12T10:18:53
18 Modification Date 2012-10-15T10:25:35
19 Spectrometer Frequency 125.76
20 Spectral Width 31446.5
21 Lowest Frequency -3210.8
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536

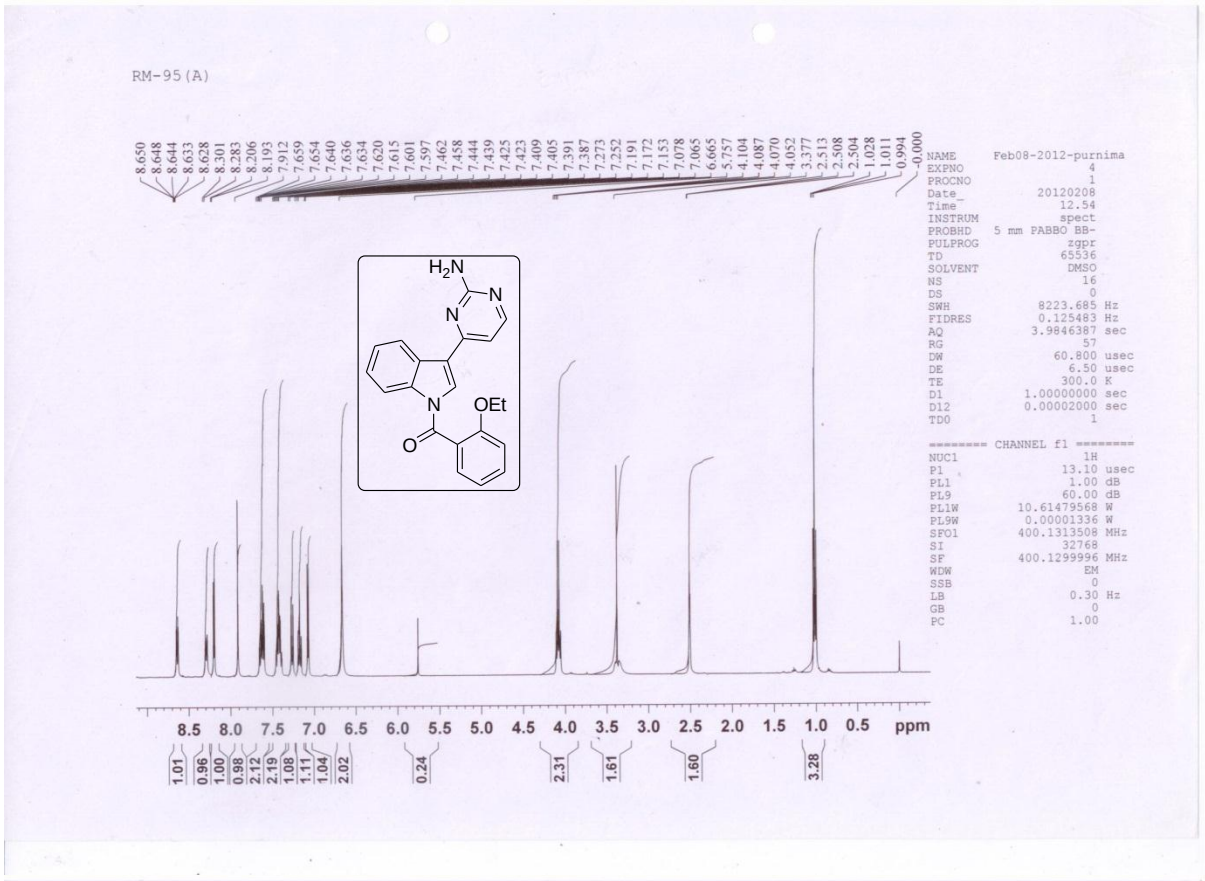
N-(4-(1H-indol-3-yl)pyrimidin-2-yl)-3-methoxybenzamide (17g)

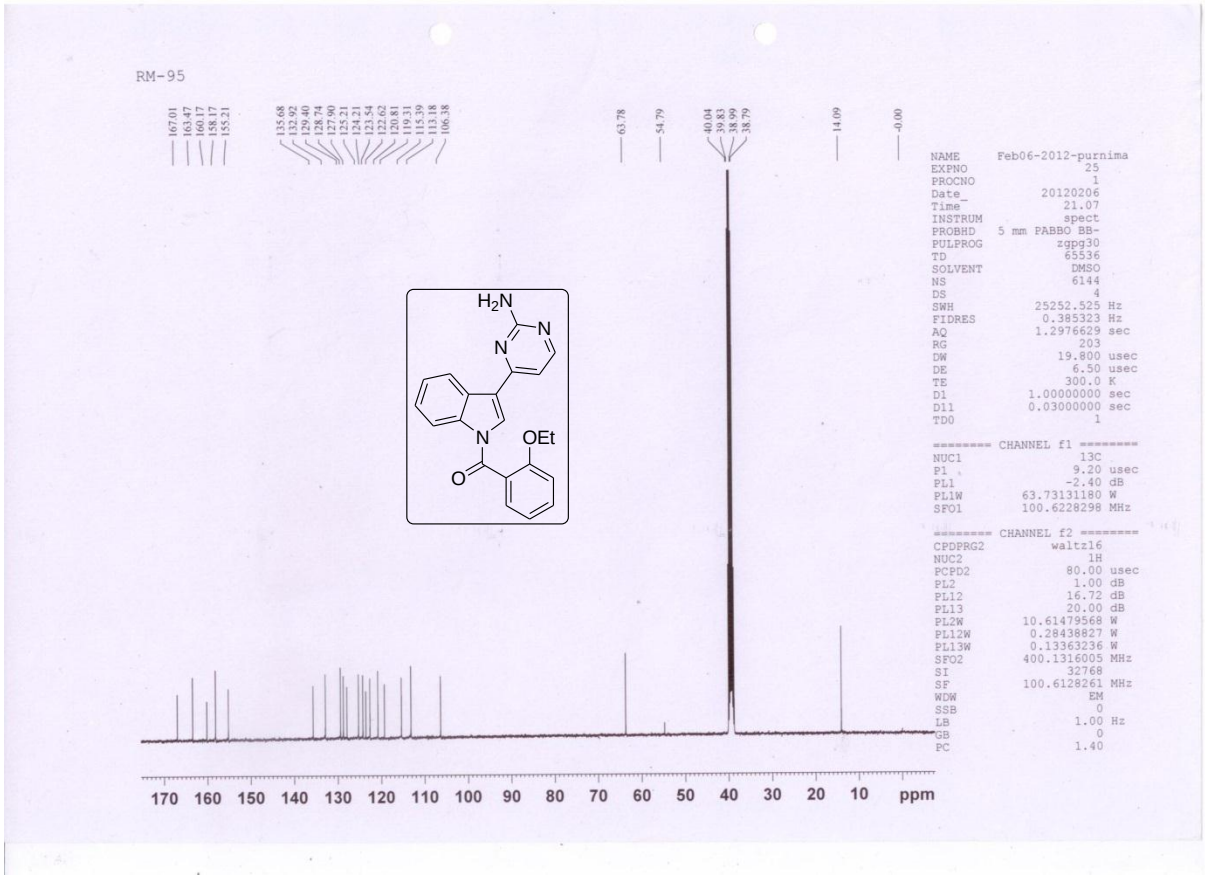


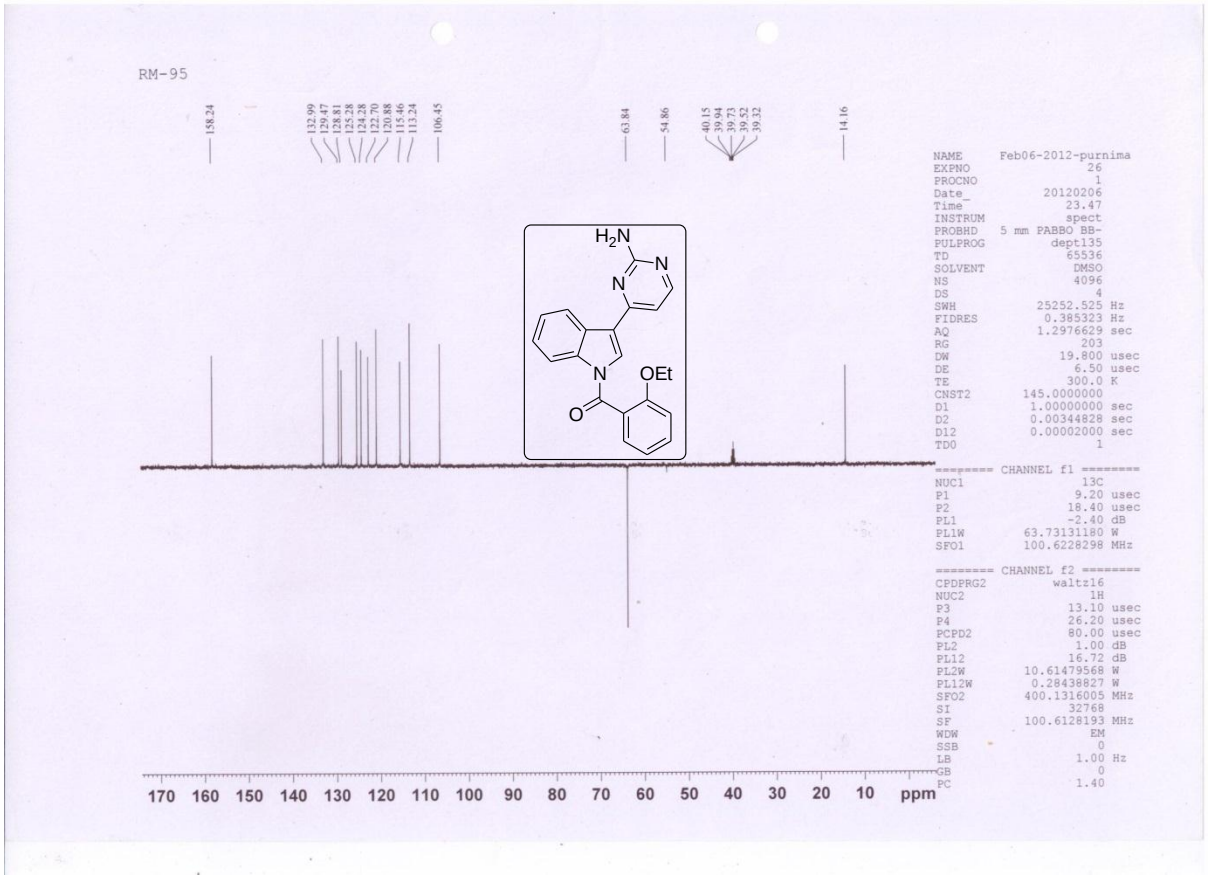



RM-94 (A)
158.71
130.57
129.52
125.72
124.81
123.17
121.76
118.74
116.46
114.67
107.14
55.93
40.32
40.11
39.90
29.85
29.39
H2N
N
N
N
O
OMe
180
160
140
120
100
80
60
40
20
0 ppm
NAME Mar09-2012-purnima
EXPNO 2
PROCNO 1
Date_ 20120309
Time 11.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
P2 18.40 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 13.10 usec
P4 26.20 usec
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127715 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

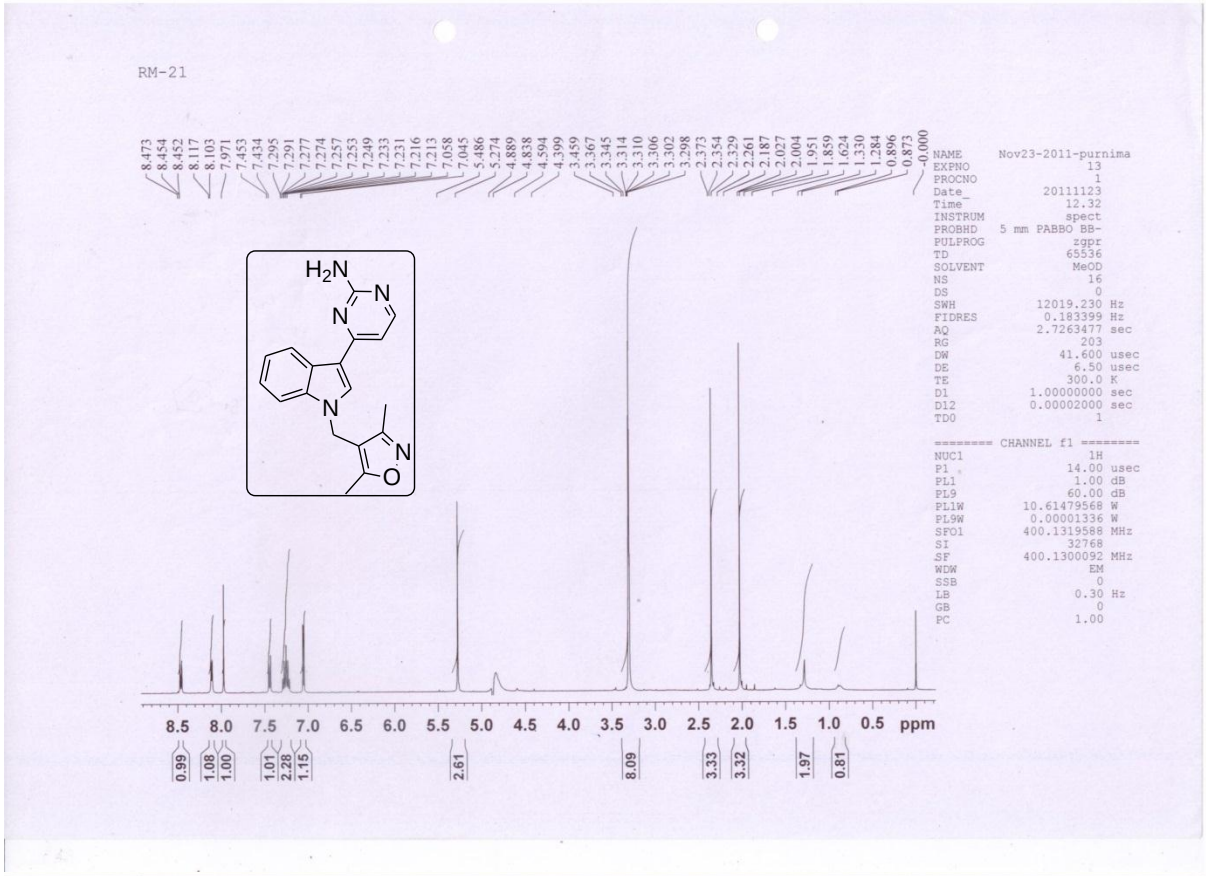
(3-(2-aminopyrimidin-4-yl)-1H-indol-1-yl)(2-ethoxyphenyl)methanone (17h)

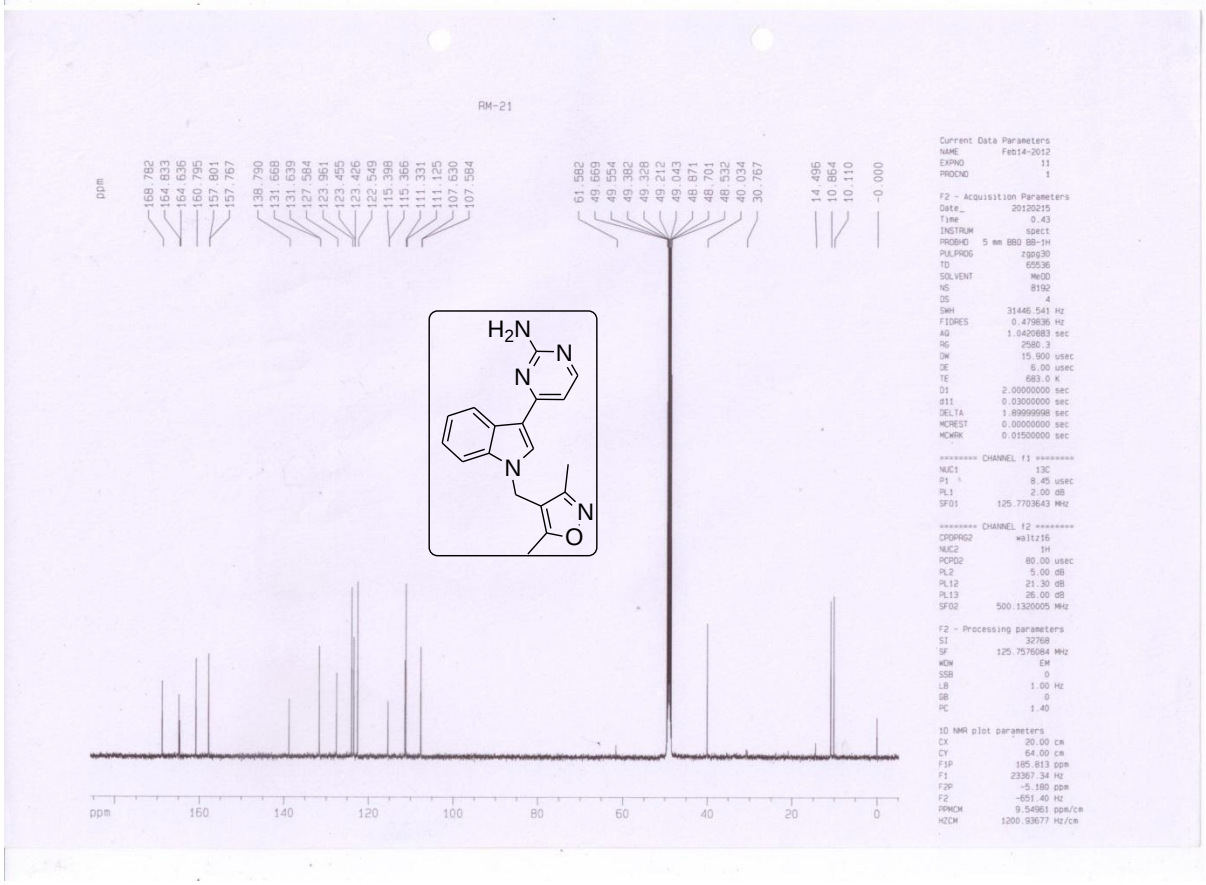


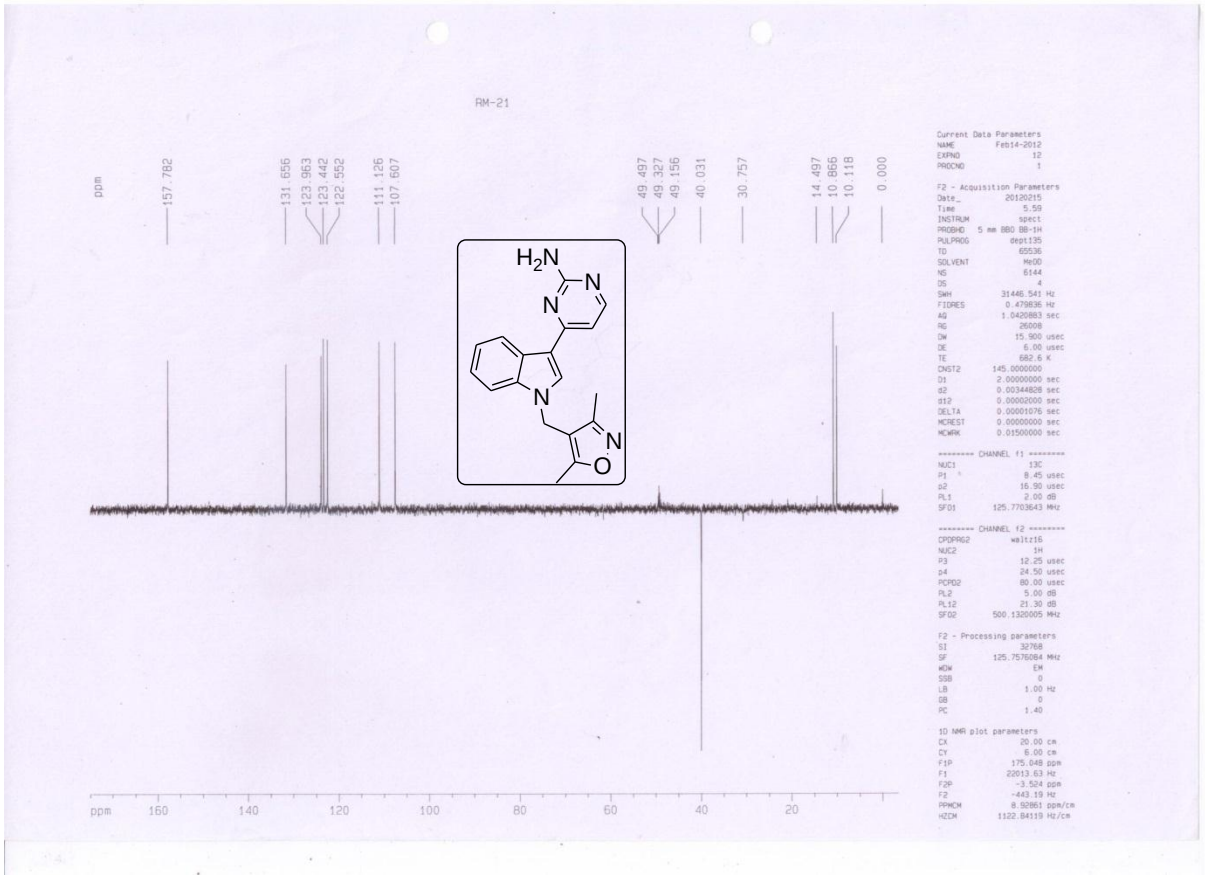



RM-95
158.24
132.99
129.47
128.81
125.28
124.28
122.70
120.88
114.46
113.24
106.45
63.84
54.86
40.15
39.94
39.73
39.52
39.32
14.16
H2N
N
N
N
OEt
O
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
NAME Feb06-2012-purnima
EXPNO 26
PROCNO 1
Date_ 20120206
Time 23.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT DMSO
NS 4096
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
P2 18.40 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 13.10 usec
P4 26.20 usec
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

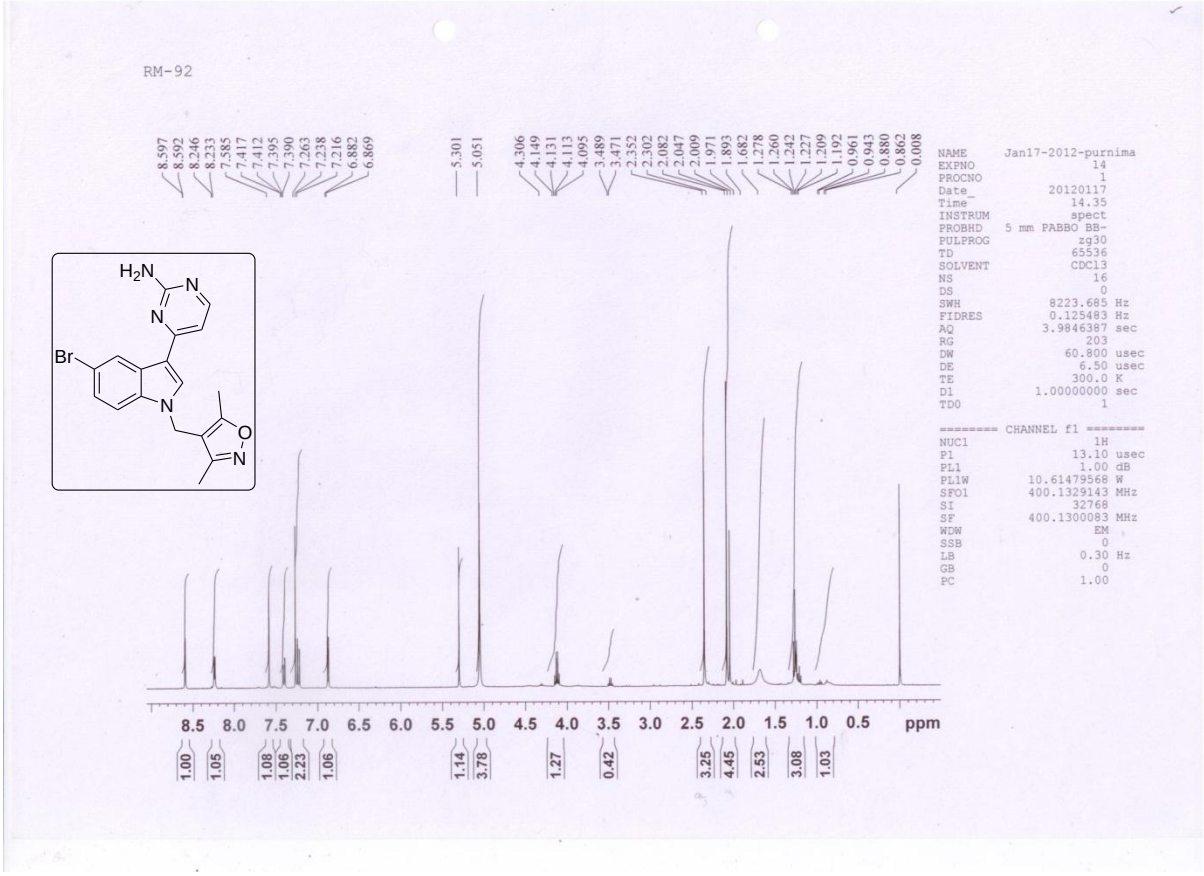
4-(1-((3,5-dimethylisoxazol-4-yl)methyl)-1H-indol-3-yl)pyrimidin-2-amine (19a)

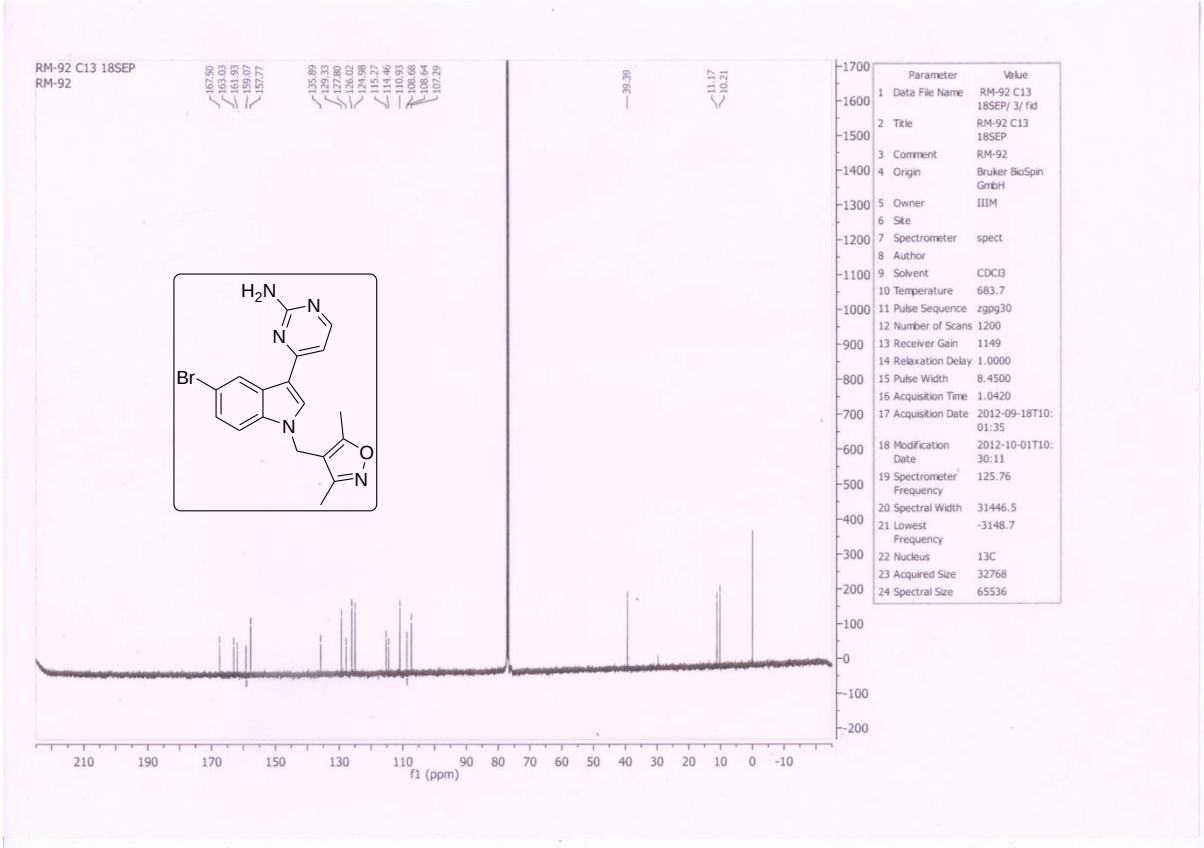


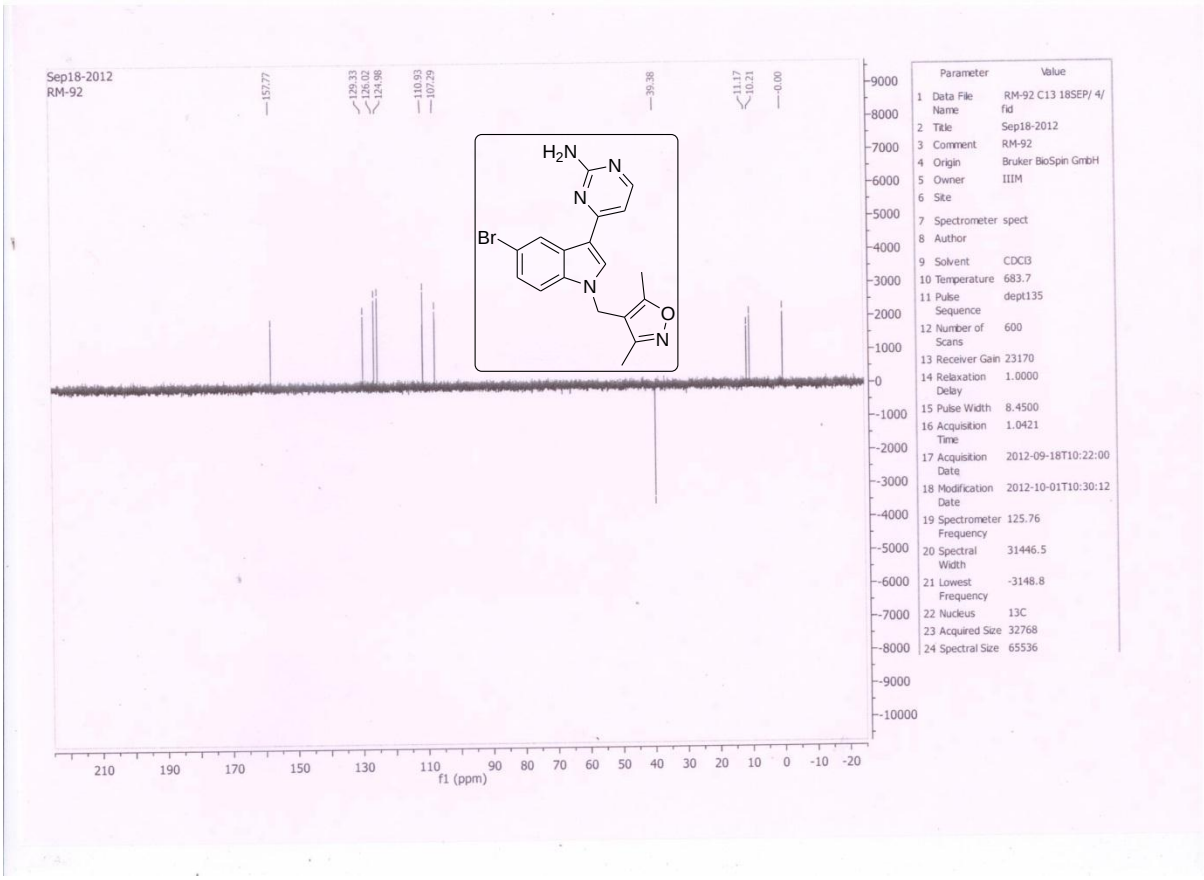



RM-21
ppm
157.782
131.656
123.963
123.442
122.552
111.126
107.607
49.497
49.327
49.156
40.031
30.757
14.497
10.866
10.118
0.000
H2N
N
N
N
N
O
ppm
160
140
120
100
80
60
40
20

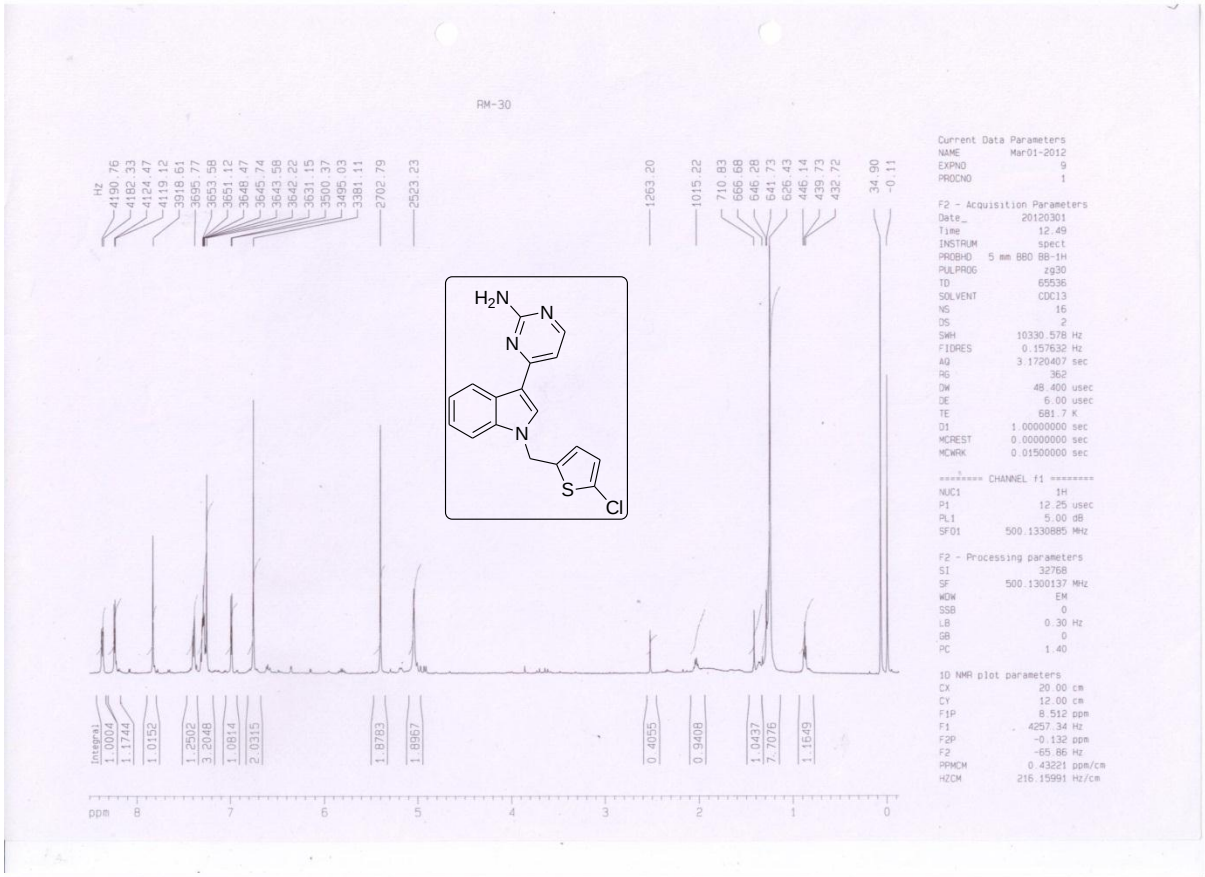
4-(5-bromo-1H-indol-3-yl)-N-((3,5-dimethylisoxazol-4-yl)methyl) pyrimidin-2-amine (19b)

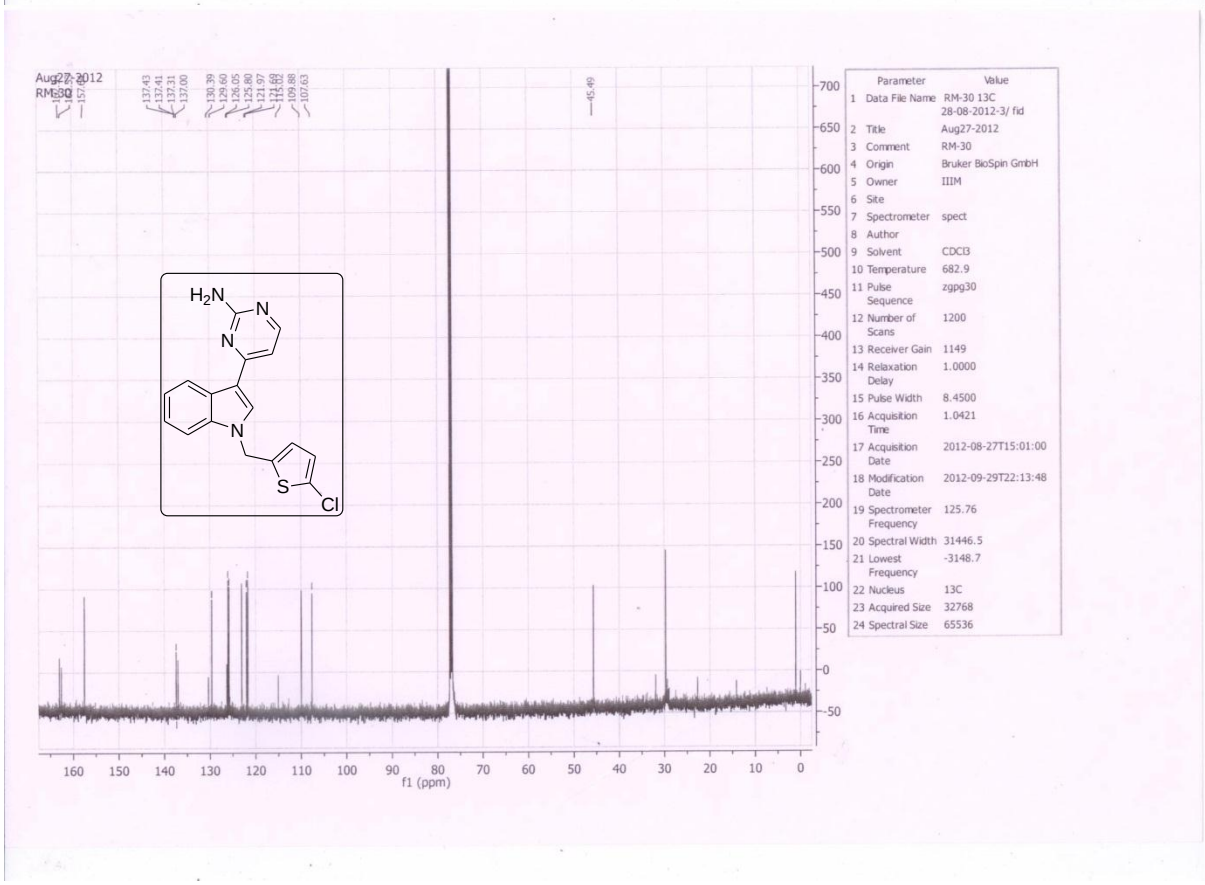


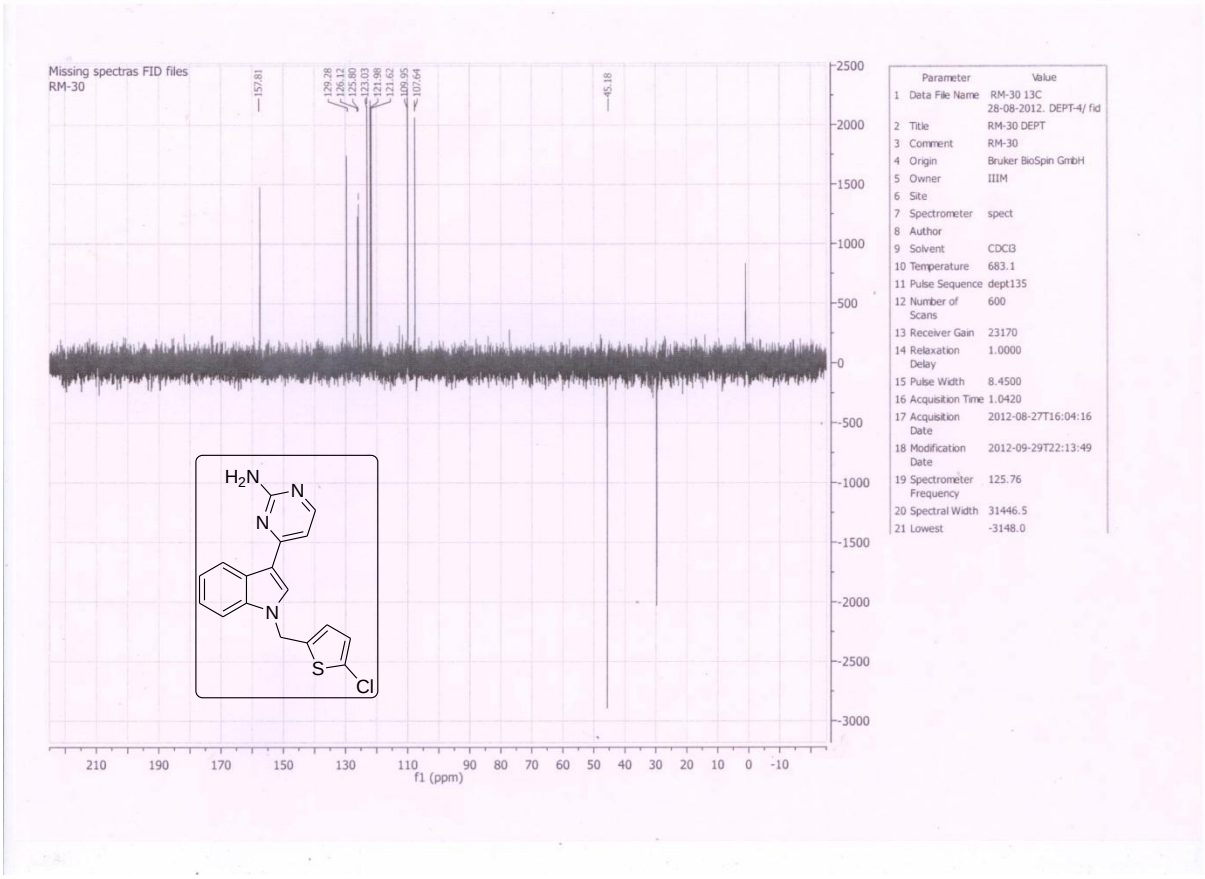

RM-92 C13 18SEP
RM-92
167.50
163.03
161.93
159.07
157.77
135.89
129.33
127.80
126.02
124.98
115.27
114.46
110.93
108.86
108.64
107.29
39.39
11.17
10.21
Br
f1 (ppm)
Parameter Value
1 Data File Name RM-92 C13 18SEP/ 3/ fid
2 Title RM-92 C13 18SEP
3 Comment RM-92
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 683.7
11 Pulse Sequence zgpg30
12 Number of Scans 1200
13 Receiver Gain 1149
14 Relaxation Delay 1.0000
15 Pulse Width 8.4500
16 Acquisition Time 1.0420
17 Acquisition Date 2012-09-18T10:01:35
18 Modification Date 2012-10-01T10:30:11
19 Spectrometer Frequency 125.76
20 Spectral Width 31446.5
21 Lowest Frequency -3148.7
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536


Sep18-2012
RM-92
157.77
129.33
126.02
124.98
110.93
107.29
39.38
11.17
10.21
0.00
Br
f1 (ppm)
Parameter Value
1 Data File Name RM-92 C13 18SEP/ 4/ fid
2 Title Sep18-2012
3 Comment RM-92
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 683.7
11 Pulse Sequence dept135
12 Number of Scans 600
13 Receiver Gain 23170
14 Relaxation Delay 1.0000
15 Pulse Width 8.4500
16 Acquisition Time 1.0421
17 Acquisition Date 2012-09-18T10:22:00
18 Modification Date 2012-10-01T10:30:12
19 Spectrometer Frequency 125.76
20 Spectral Width 31446.5
21 Lowest Frequency -3148.8
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536

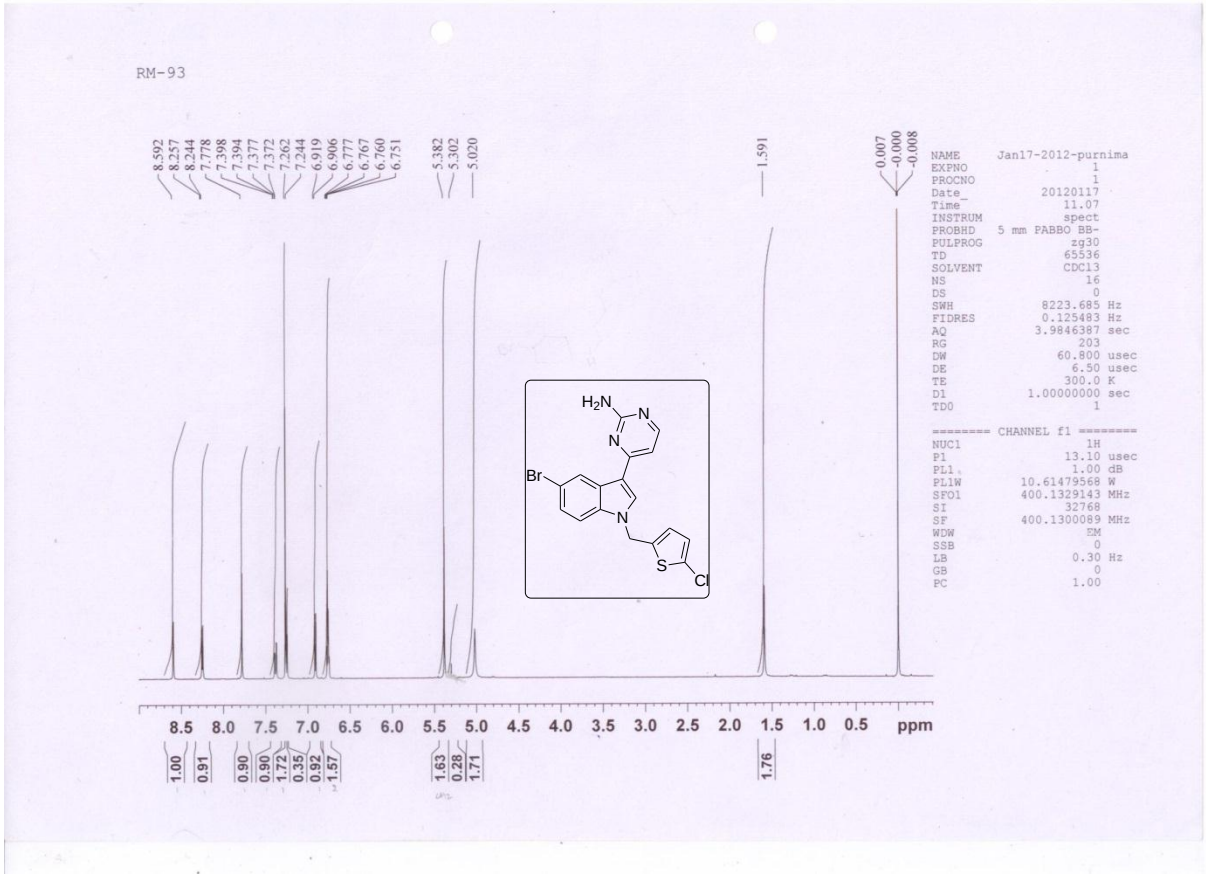
4-(1-((5-chlorothiophen-2-yl)methyl)-1H-indol-3-yl)pyrimidin-2-amine (19c)

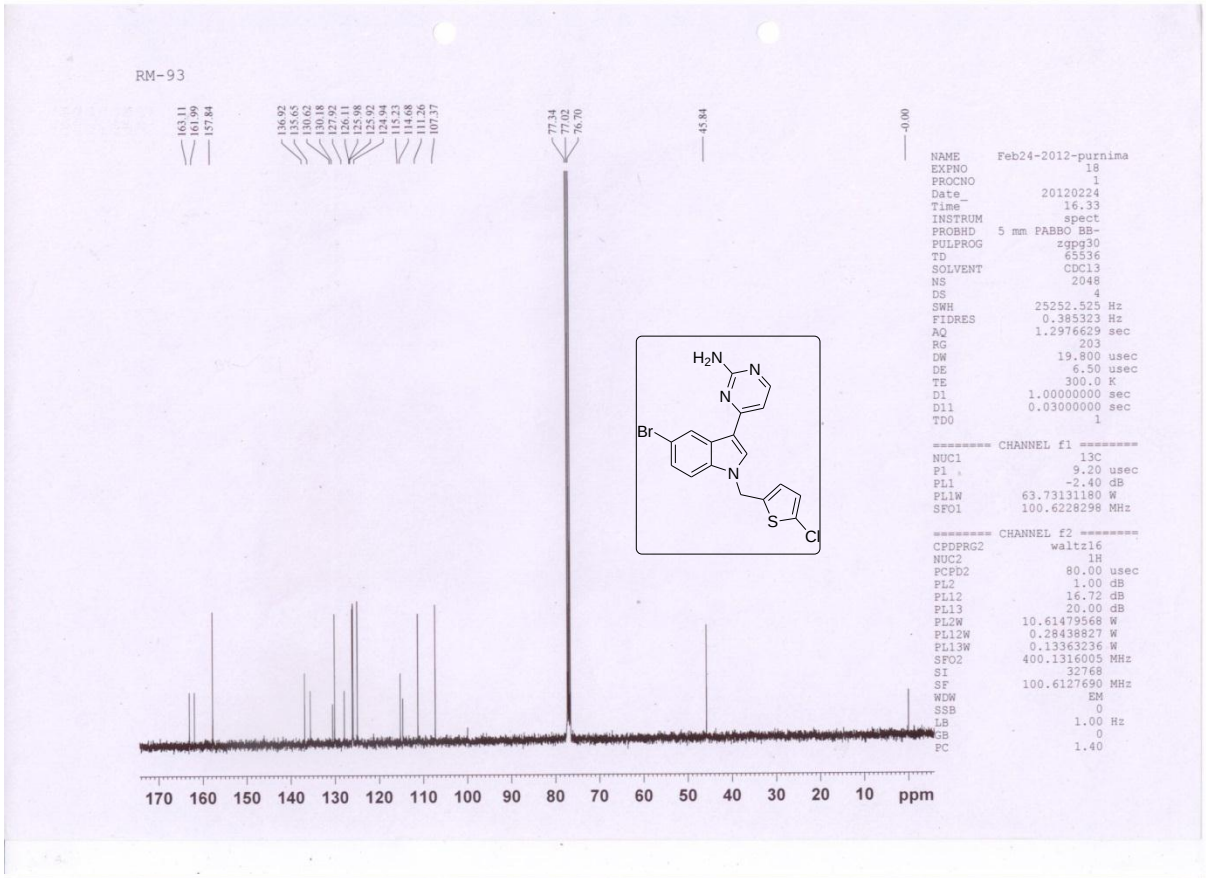


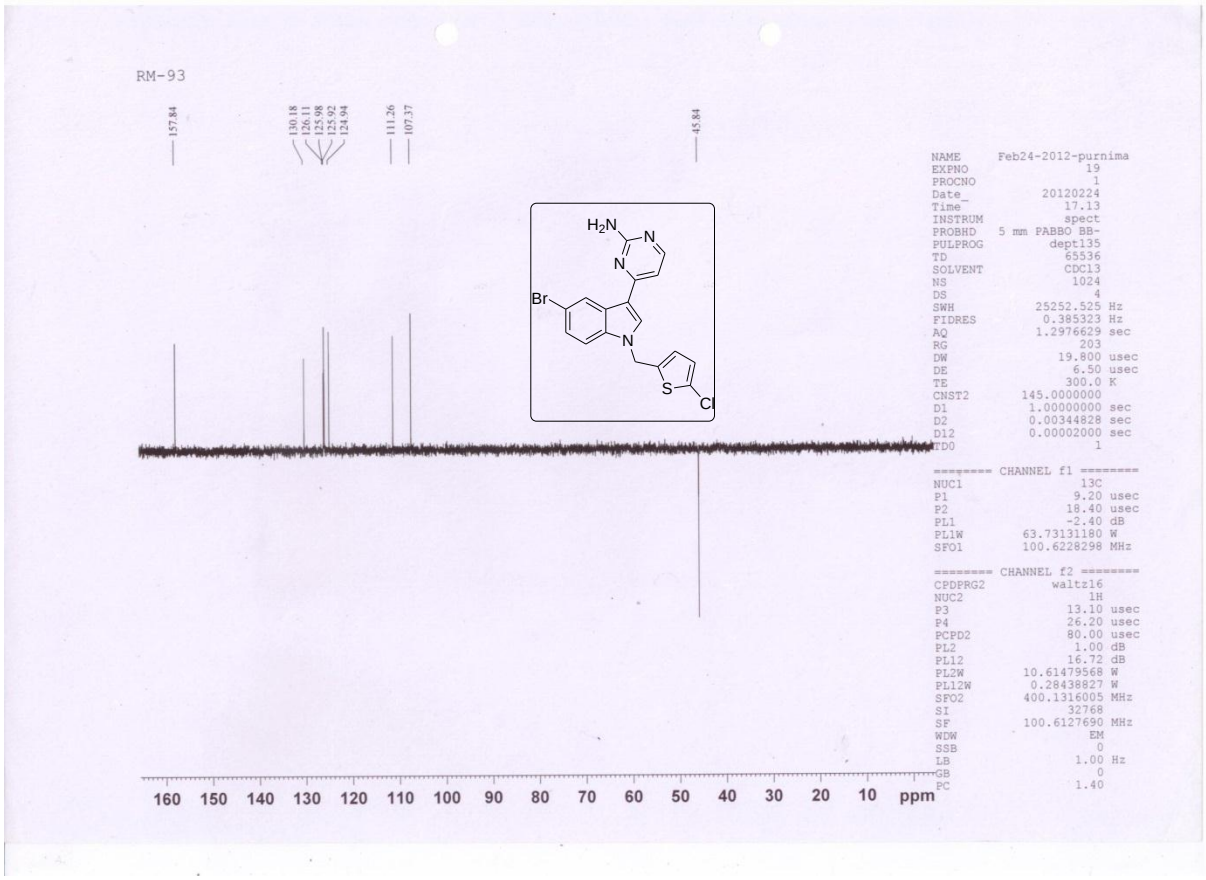



Missing spectras FID files
RM-30
157.81
129.28
126.12
125.80
123.03
121.98
121.62
109.95
107.64
65.18
2500
2000
1500
1000
500
0
-500
-1000
-1500
-2000
-2500
-3000
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)
H2N
N
N
N
S
Cl
Parameter Value
1 Data File Name RM-30 13C 28-08-2012. DEPT-4/ fid
2 Title RM-30 DEPT
3 Comment RM-30
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 683.1
11 Pulse Sequence dept135
12 Number of Scans 600
13 Receiver Gain 23170
14 Relaxation Delay 1.0000
15 Pulse Width 8.4500
16 Acquisition Time 1.0420
17 Acquisition Date 2012-08-27T16:04:16
18 Modification Date 2012-09-29T22:13:49
19 Spectrometer Frequency 125.76
20 Spectral Width 31446.5
21 Lowest -3148.0

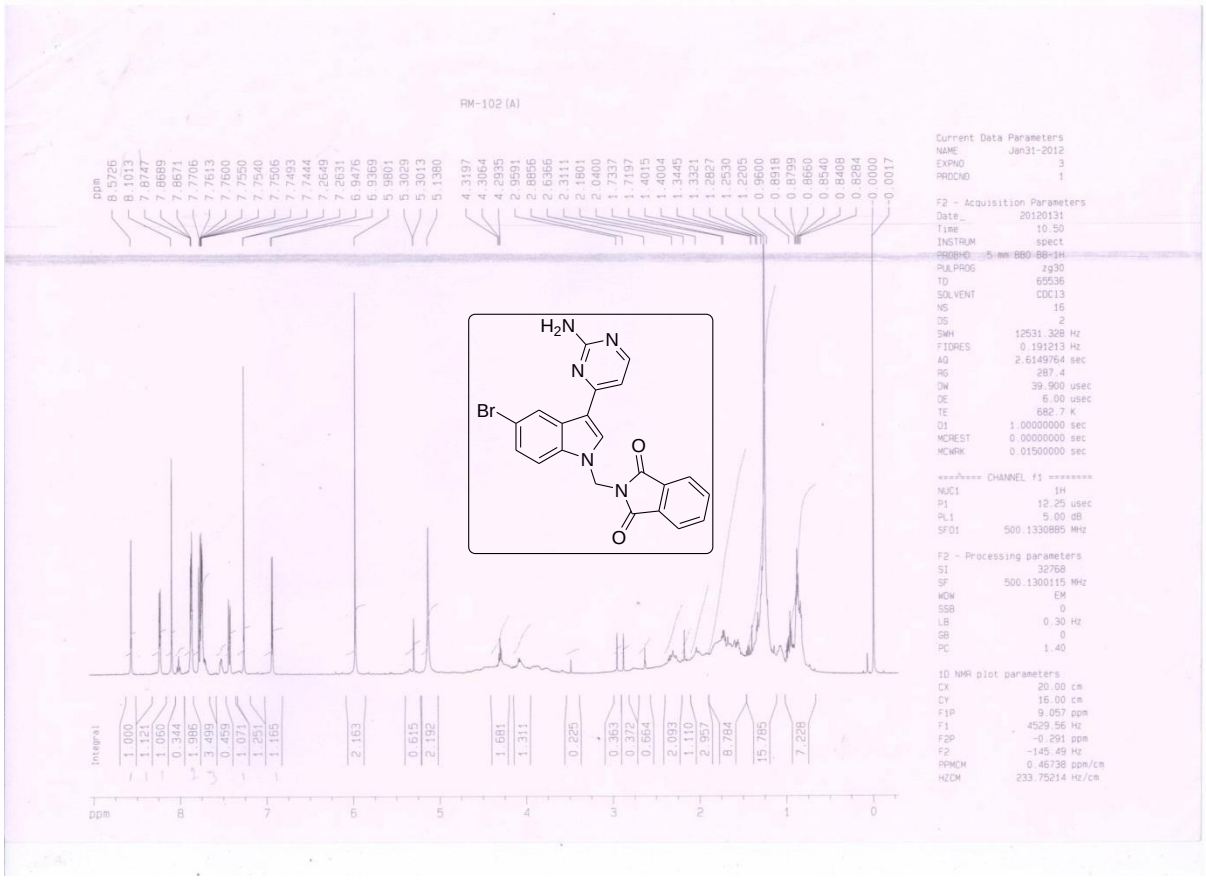
4-(5-bromo-1H-indol-3-yl)-N-((5-chlorothiophen-2-yl)methyl)pyrimidin-2-amine (19d)

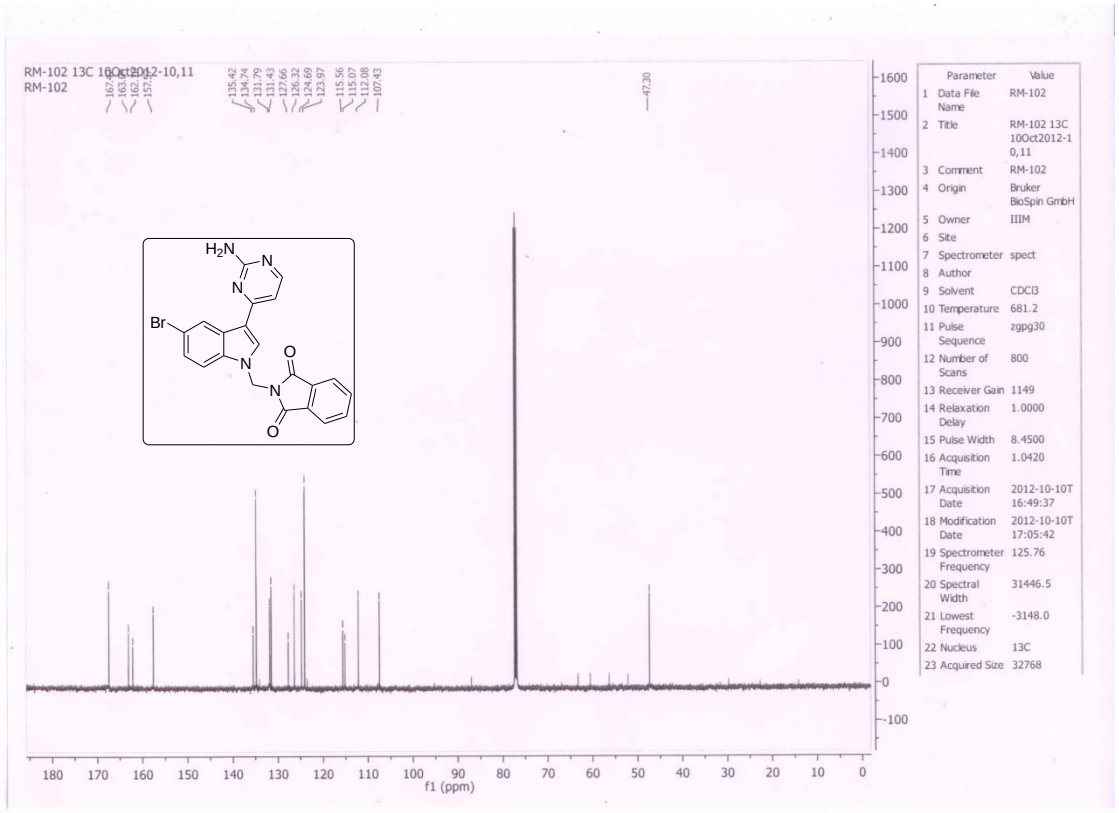


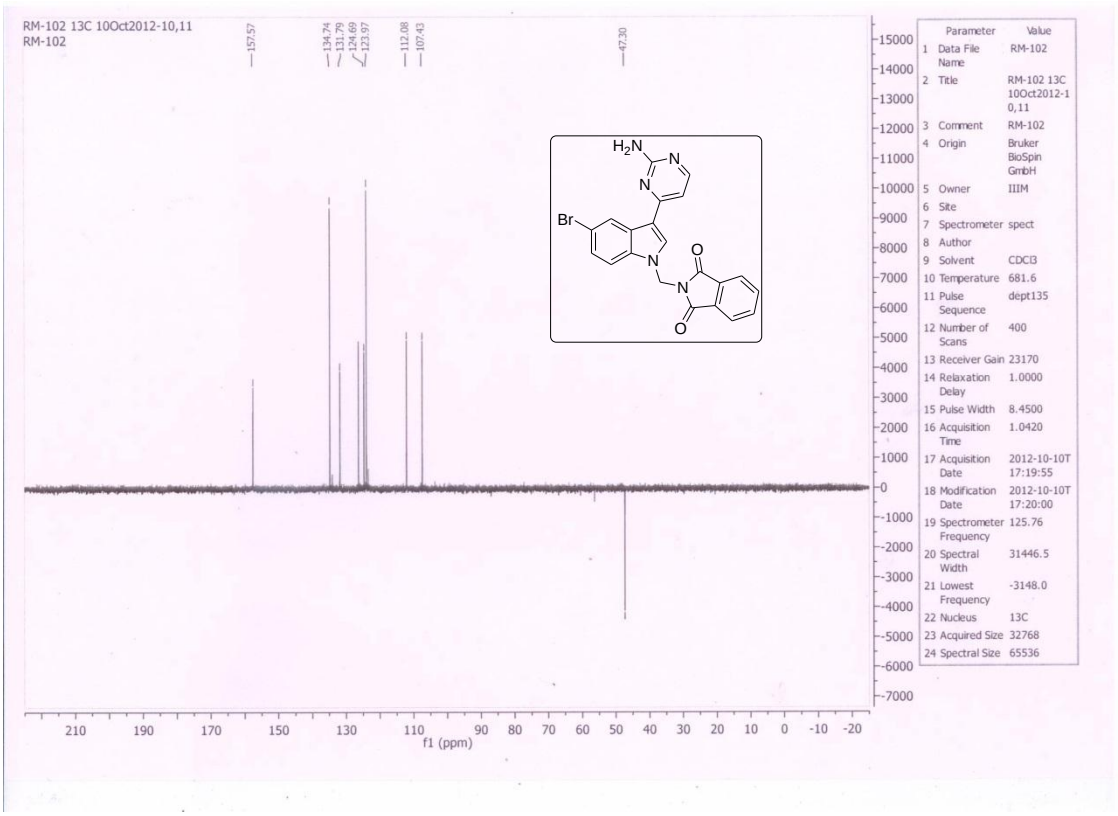

RM-93
163.11
161.99
157.84
136.92
135.65
130.62
130.18
127.92
126.11
125.98
125.92
124.94
115.23
114.68
111.26
107.37
77.34
77.02
76.70
45.84
0.00
NAME Feb24-2012-purnima
EXPNO 18
PROCNO 1
Date_ 20120224
Time 16.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL13 20.00 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
PL13W 0.13363236 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
H2N
N
N
Br
N
S
Cl
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


RM-93
157.84
130.18
126.11
125.98
125.92
124.94
111.26
107.37
45.84
NAME Feb24-2012-purnima
EXPNO 19
PROCNO 1
Date_ 20120224
Time 17.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
P2 18.40 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 13.10 usec
P4 26.20 usec
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
H2N
N
N
Br
N
S
Cl
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

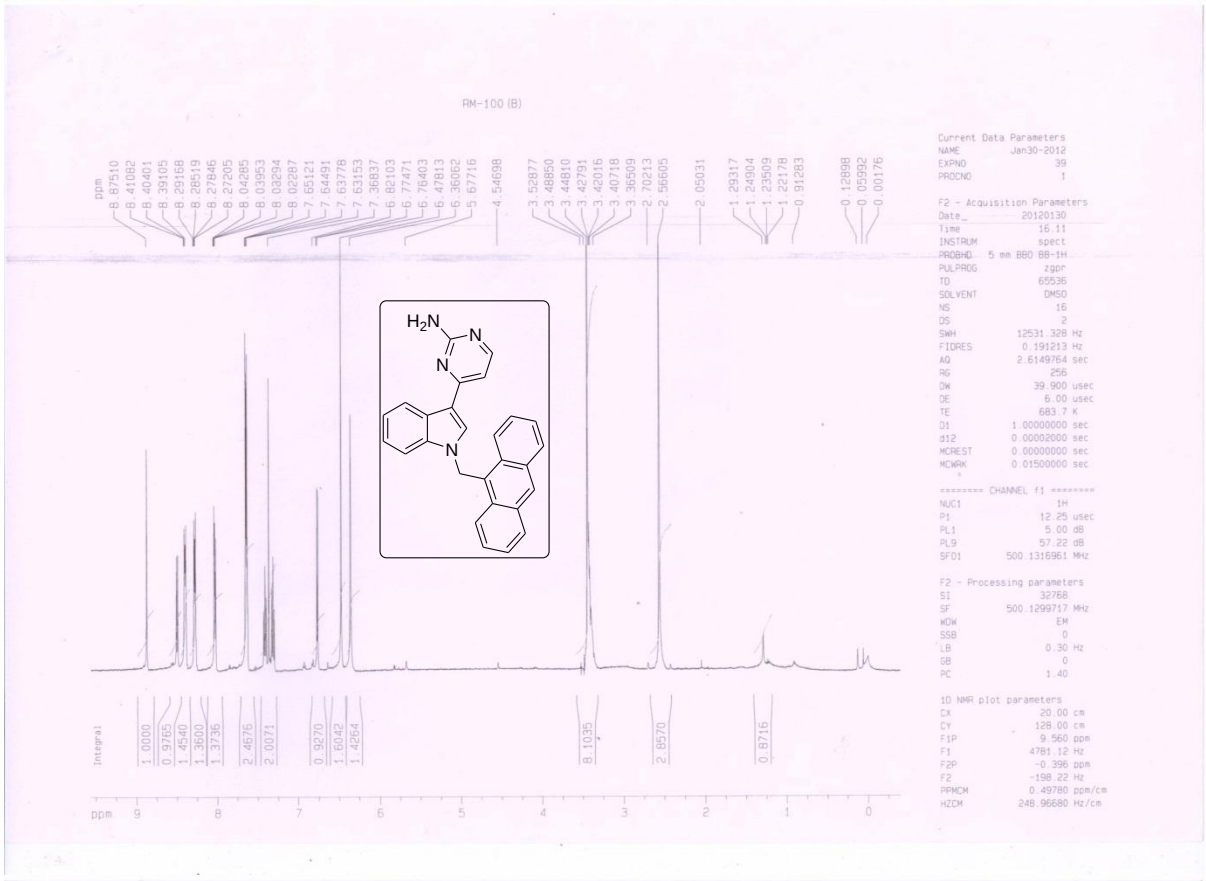
2-((3-(2-aminopyrimidin-4-yl)-5-bromo-1H-indol-1-yl)methyl) isoindoline-1,3-dione (19e)

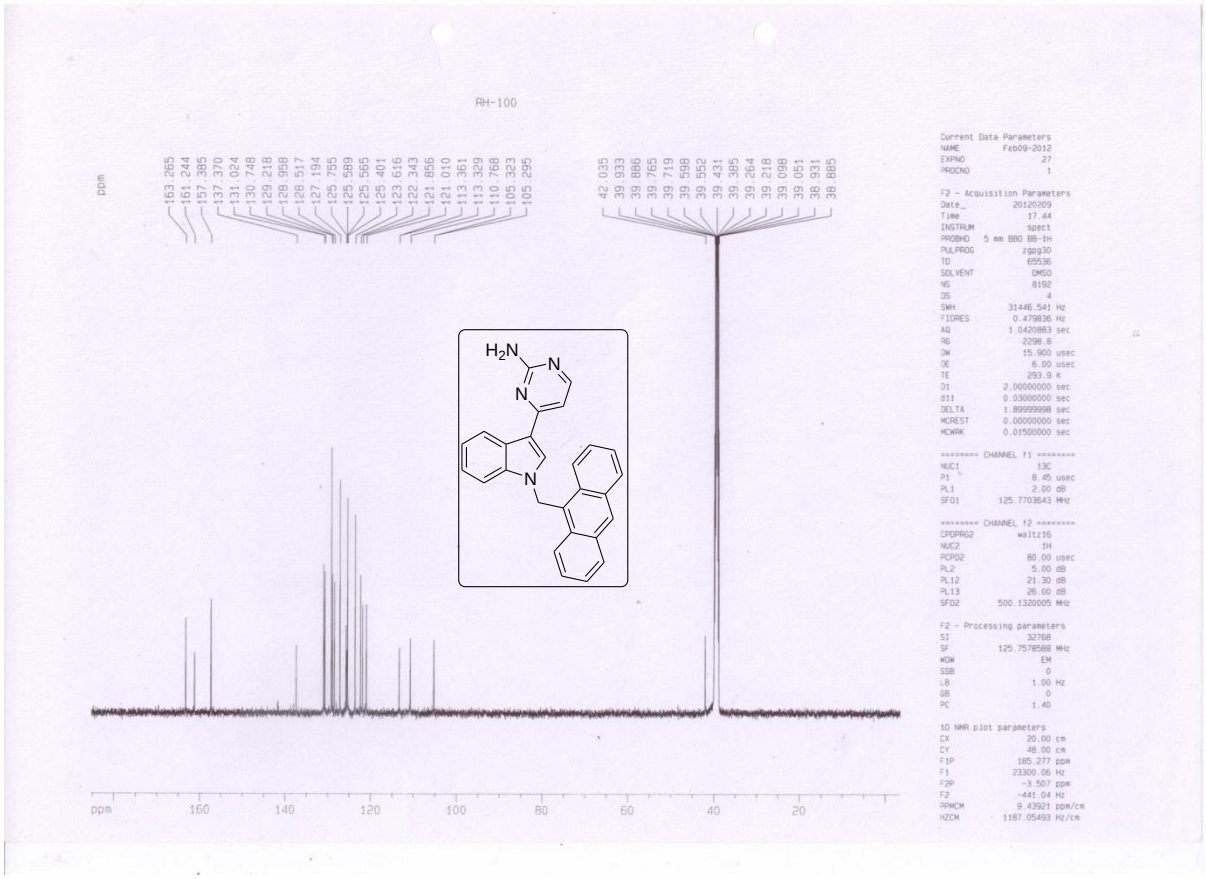


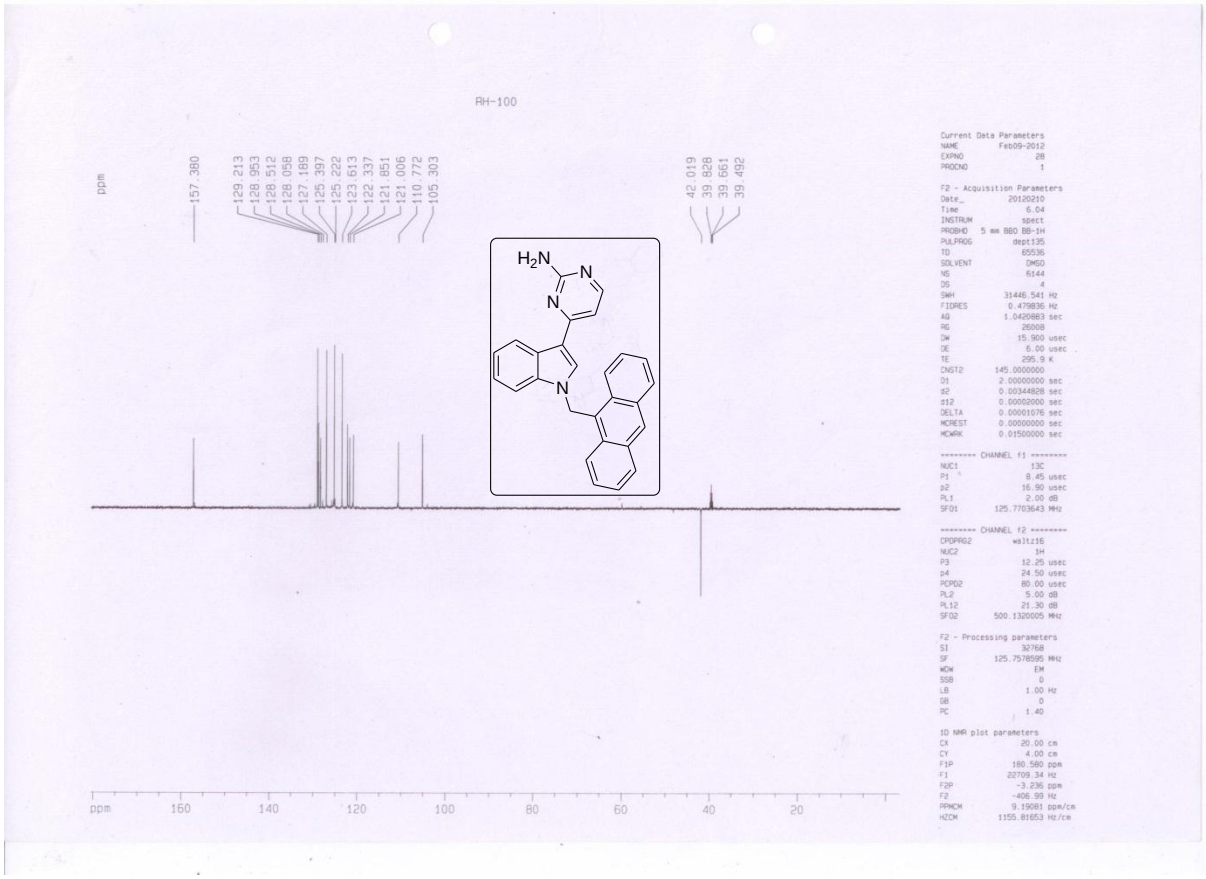



RM-102 13C 10Oct2012-10,11
RM-102
157.57
134.74
131.79
124.69
123.97
112.08
107.43
47.30
H2N
N
N
Br
N
O
N
O
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
-2000
-3000
-4000
-5000
-6000
-7000
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)
Parameter Value
1 Data File Name RM-102
2 Title RM-102 13C 10Oct2012-10,11
3 Comment RM-102
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 681.6
11 Pulse Sequence dept135
12 Number of Scans 400
13 Receiver Gain 23170
14 Relaxation Delay 1.0000
15 Pulse Width 8.4500
16 Acquisition Time 1.0420
17 Acquisition Date 2012-10-10T 17:19:55
18 Modification Date 2012-10-10T 17:20:00
19 Spectrometer Frequency 125.76
20 Spectral Width 31446.5
21 Lowest Frequency -3148.0
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536

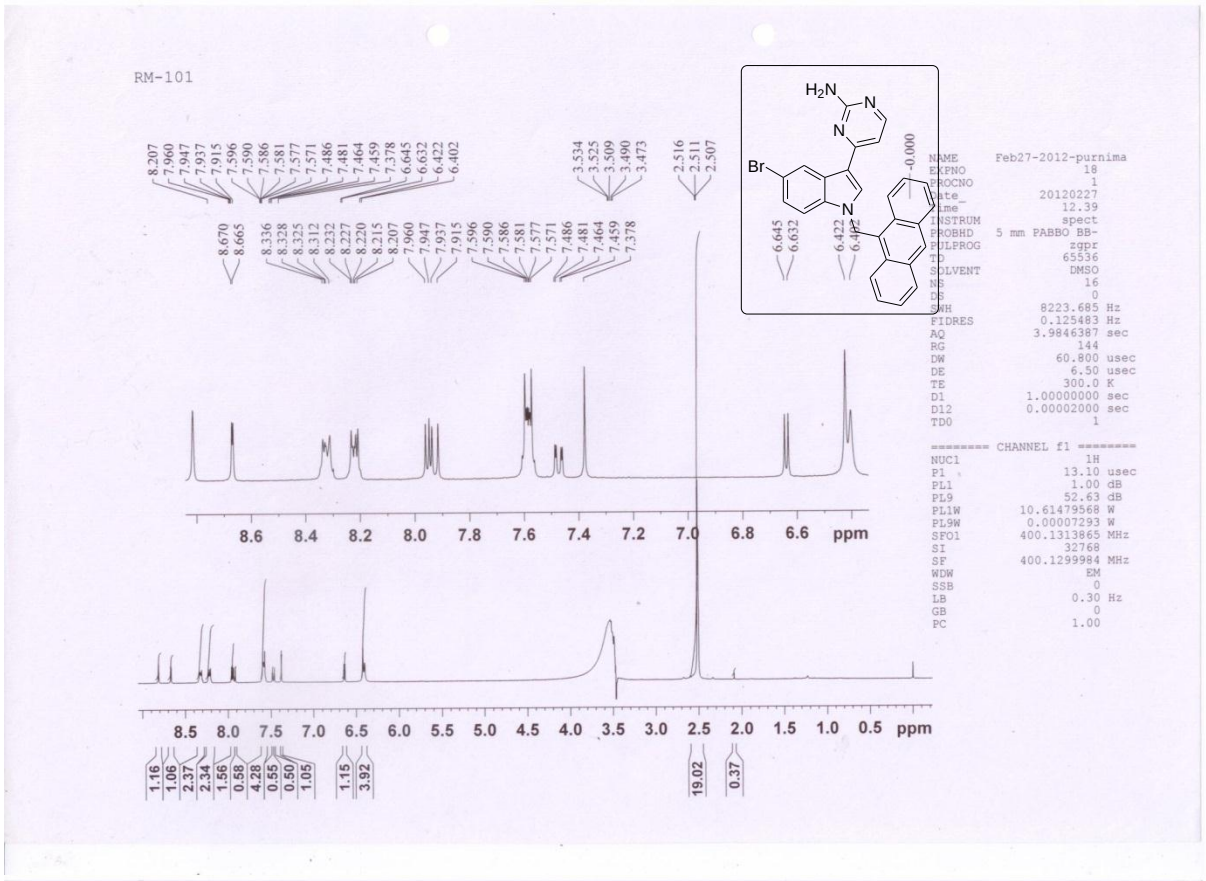
4-(1-(anthracen-10-ylmethyl)-1H-indol-3-yl)pyrimidin-2-amine (19f)

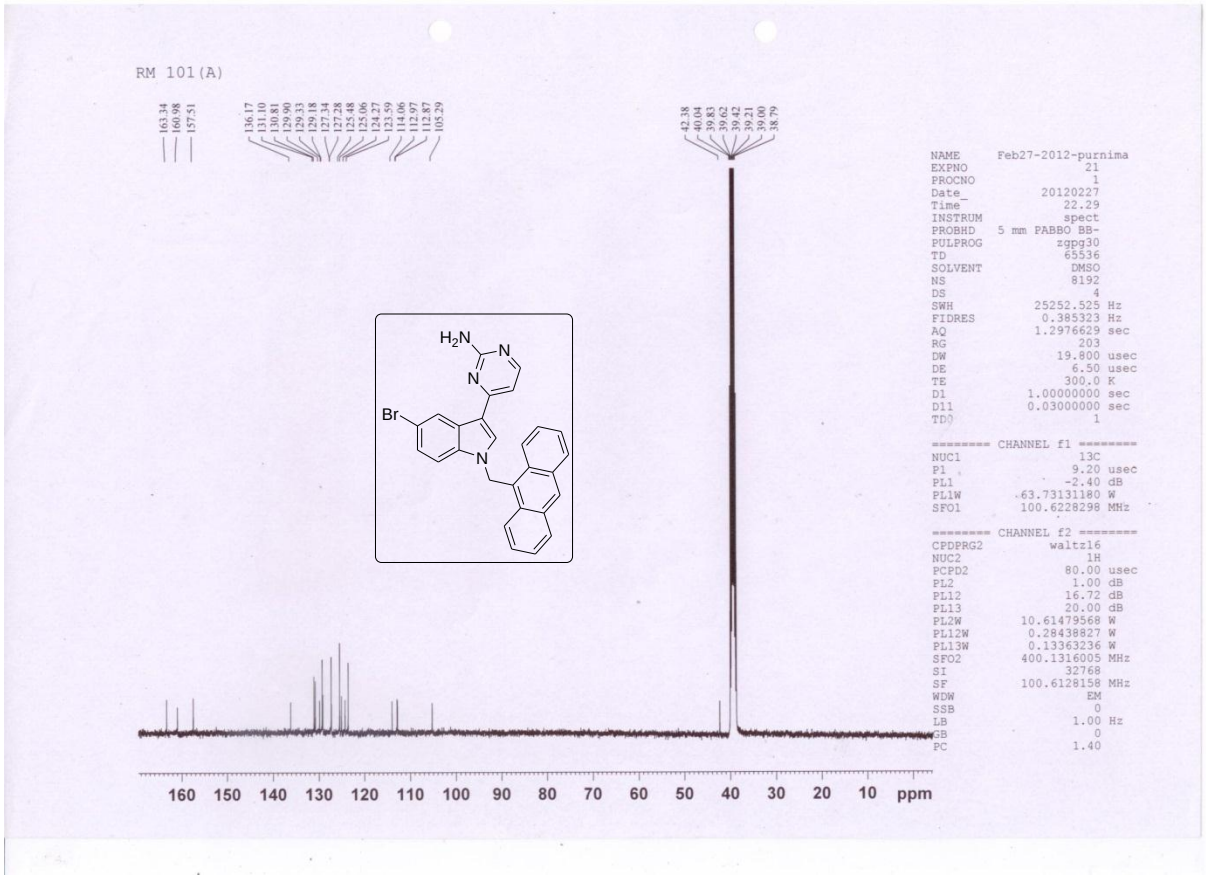


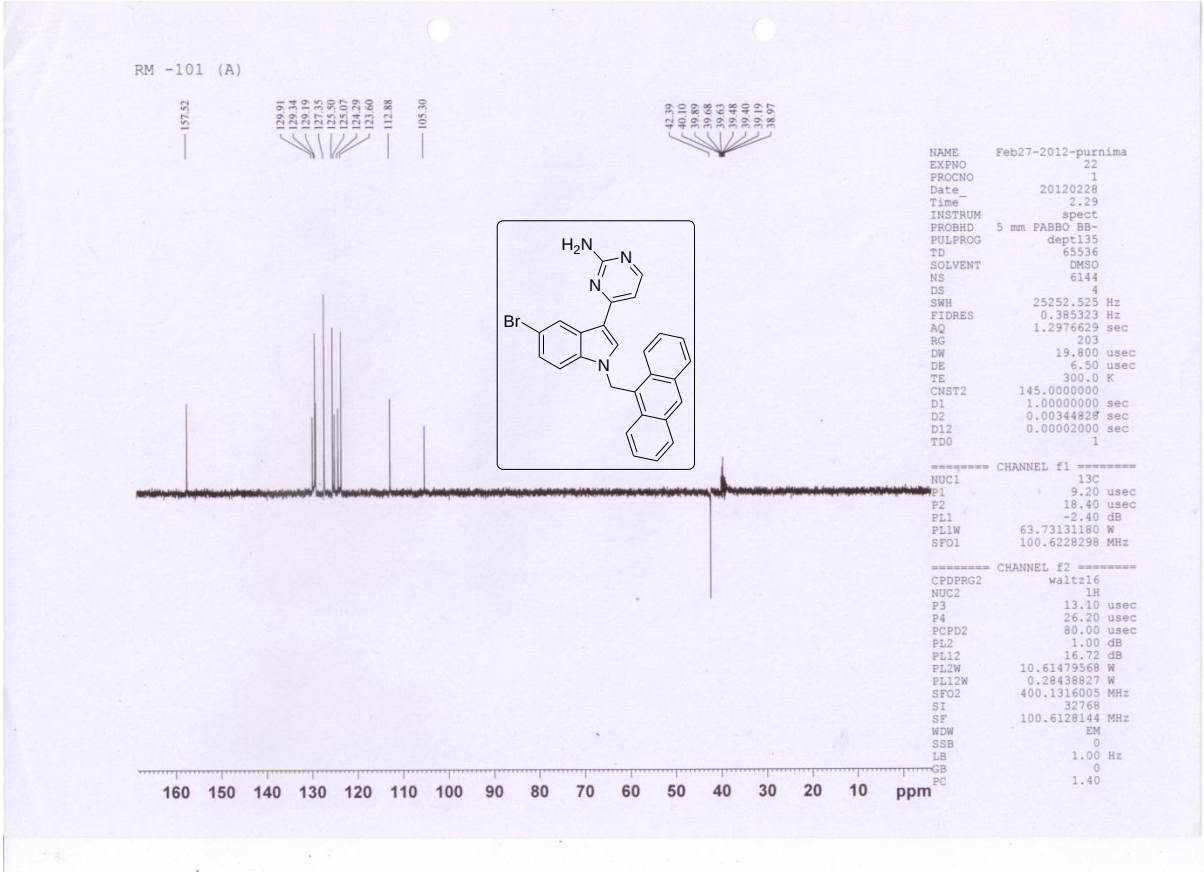



RH-100
ppm
157.380
129.213
128.953
128.512
128.058
127.189
125.397
125.222
123.613
122.337
121.851
121.006
110.772
105.303
42.019
39.828
39.661
39.492
H_2N
N
N
N
ppm
160
140
120
100
80
60
40
20
Current Data Parameters
NAME Feb09-2012
EXPNO 28
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120210
Time 6.04
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept135
TD 65536
SOLVENT DMSO
NS 6144
DS 4
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420863 sec
RG 26008
DW 15.900 usec
DE 6.00 usec
TE 295.9 K
D[2] 145.0000000
D1 2.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
DELTA 0.00001976 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
-------- CHANNEL f1 --------
NUC1 13C
P1 8.45 usec
P2 16.90 usec
PL1 2.00 dB
SFO1 125.7703643 MHz
-------- CHANNEL f2 --------
CPDPRG2 waltz16
NUC2 1H
P3 12.25 usec
P4 24.50 usec
PCPD2 80.00 usec
PL2 5.00 dB
PL12 21.30 dB
SFO2 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7578595 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 4.00 cm
F1P 180.580 ppm
F1 22709.34 Hz
F2P -3.236 ppm
F2 -406.99 Hz
PPMCM 9.19081 ppm/cm
HZCM 1155.81653 Hz/cm

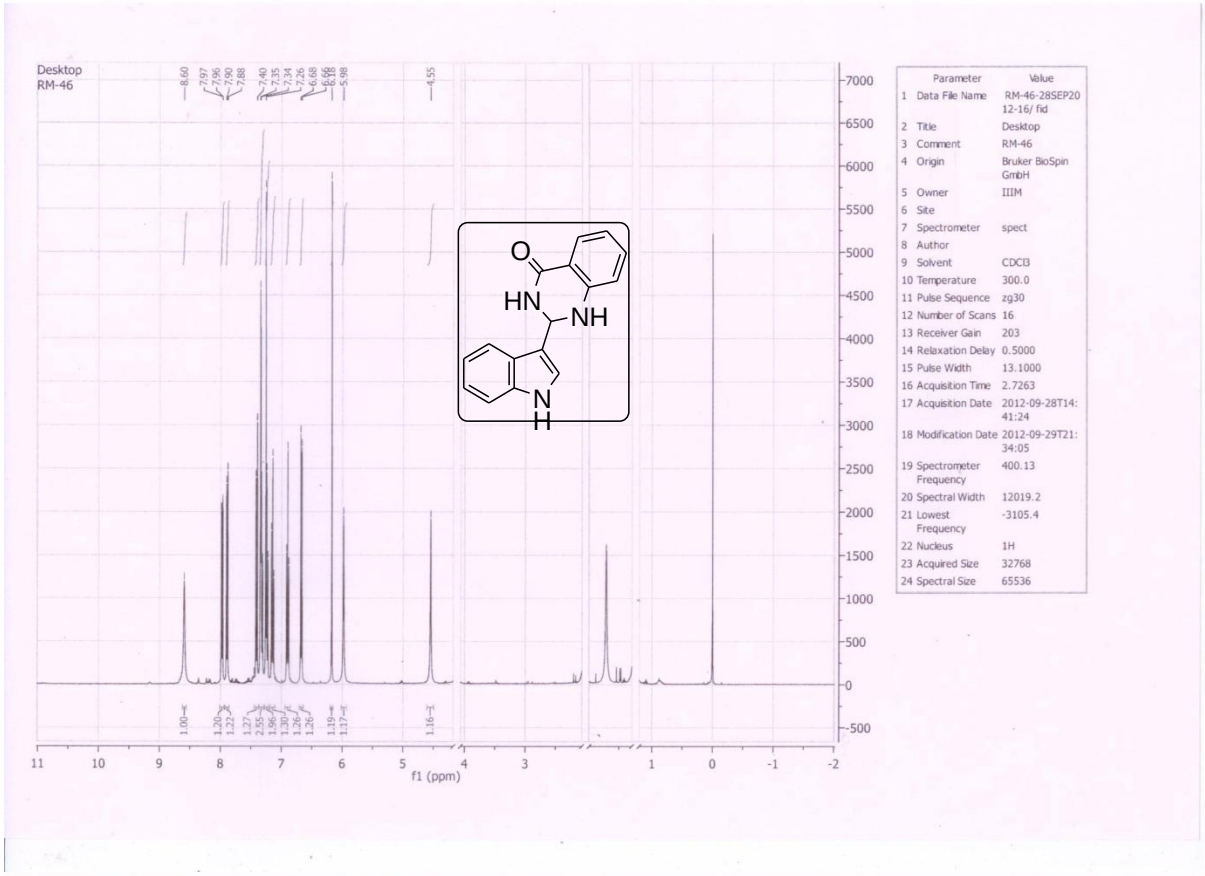
4-(1-(anthracen-10-ylmethyl)-5-bromo-1H-indol-3-yl)pyrimidin-2-amine (19g)

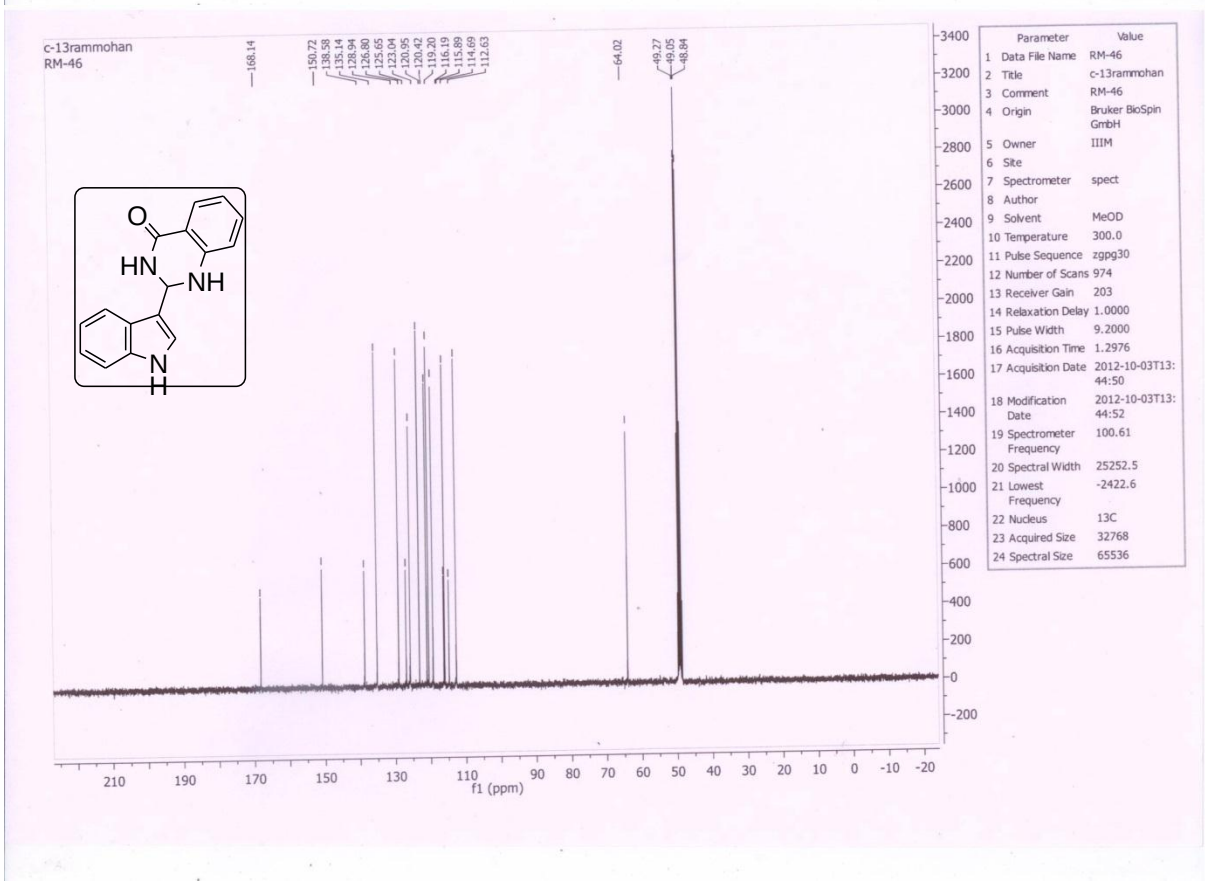


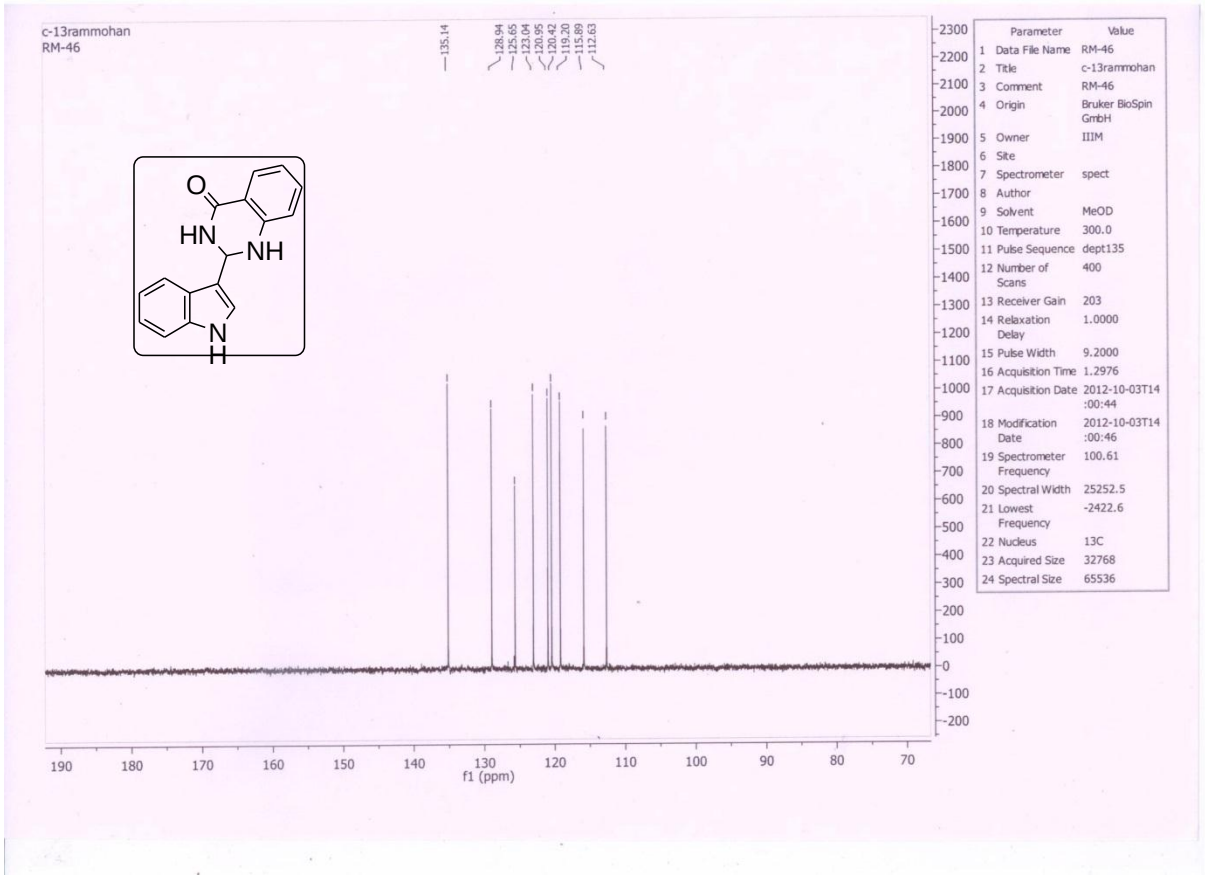



RM -101 (A)
157.52
129.91
129.34
129.19
127.35
125.50
125.07
124.29
123.60
112.88
105.30
42.39
40.10
39.89
39.68
39.47
39.48
39.40
39.19
38.97
H_2N
N
N
Br
N
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
NAME Feb27-2012-purnima
EXPNO 22
PROCNO 1
Date_ 20120228
Time 2.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT DMSO
NS 6144
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
P2 18.40 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 13.10 usec
P4 26.20 usec
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128144 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

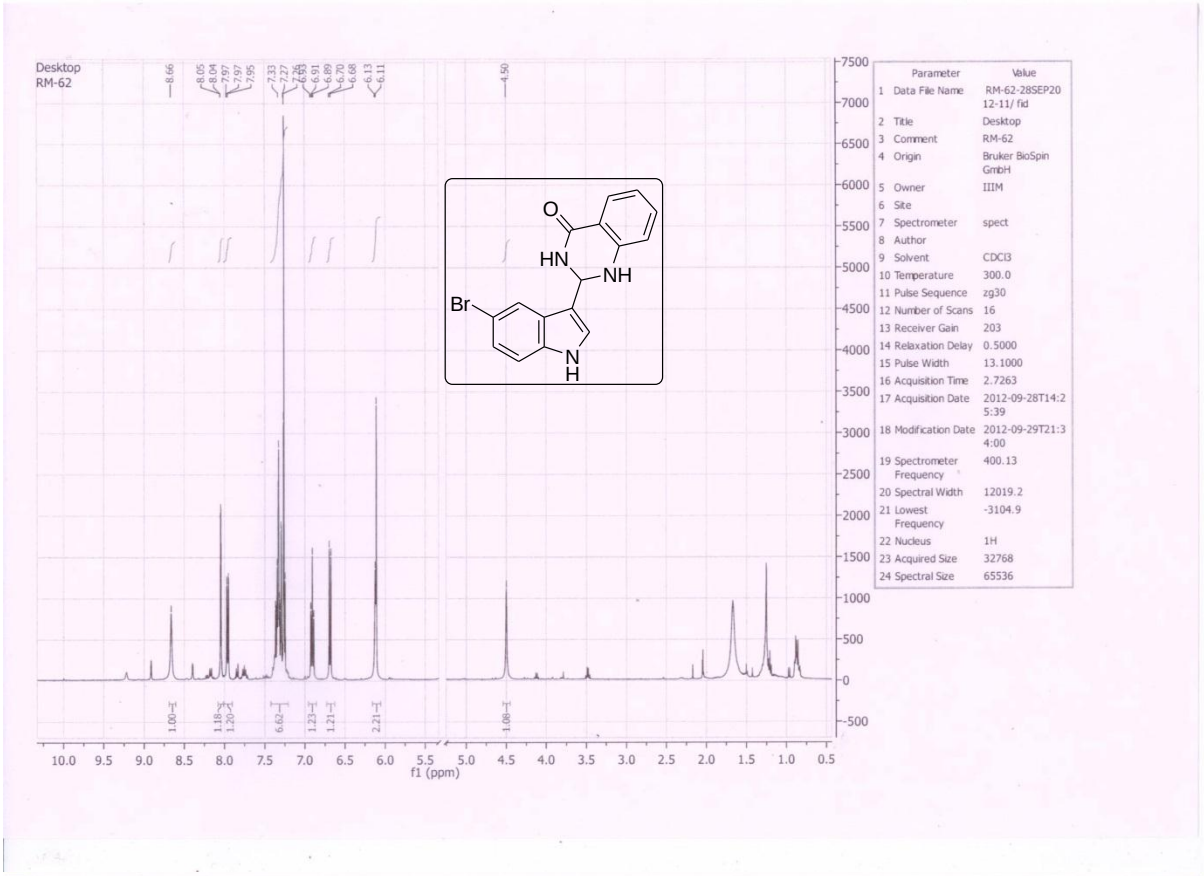
2-(1H-indol-3-yl)-2,3-dihydroquinazolin-4(1H)-one (19a)



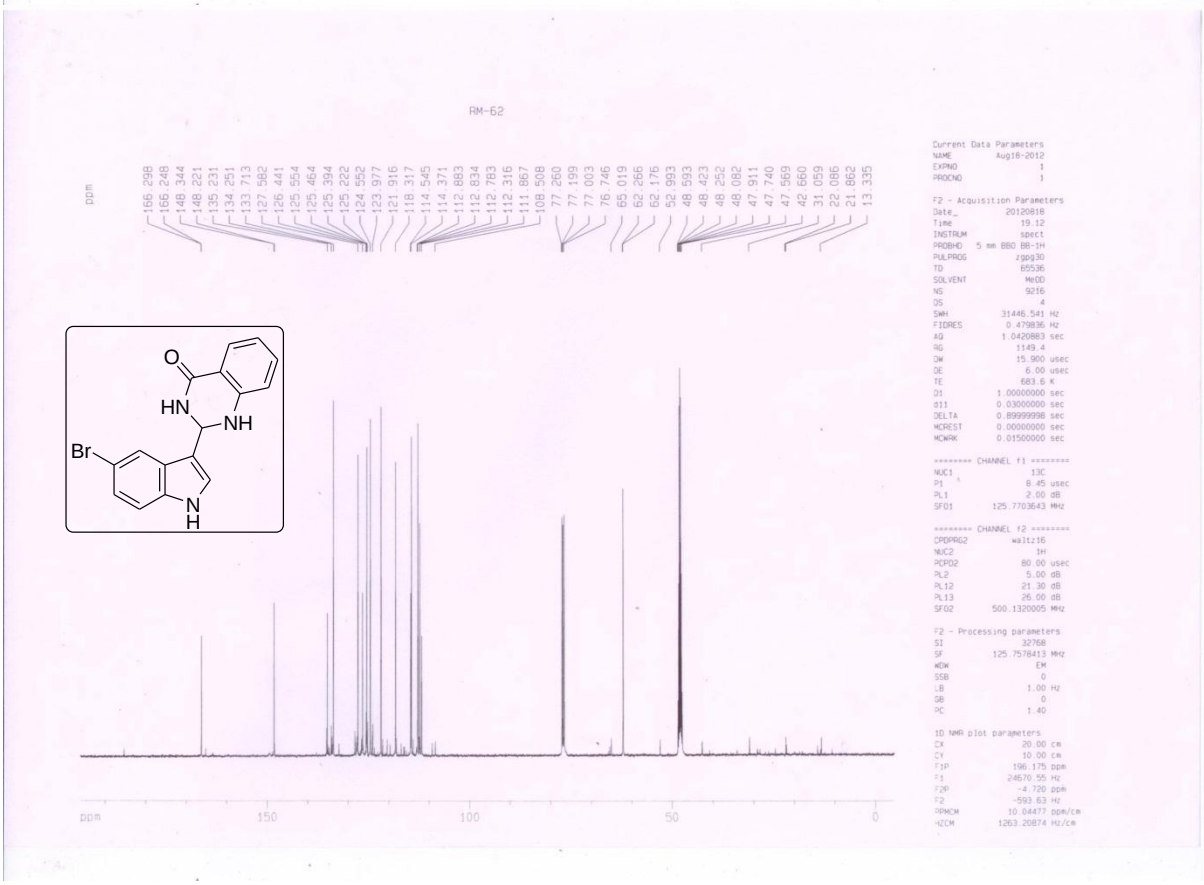


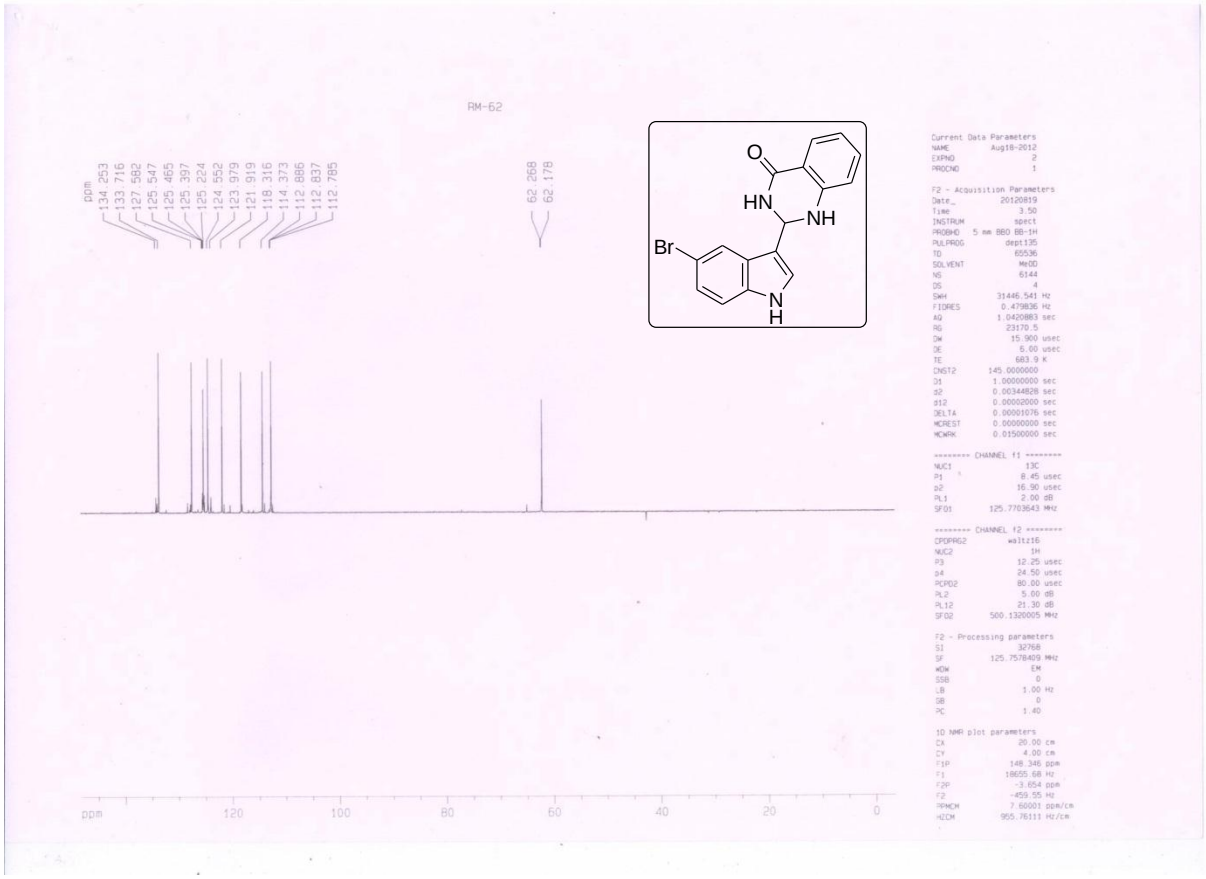

c-13rammohan
RM-46
135.14
128.94
125.65
123.04
120.95
120.42
119.20
115.89
112.63
O
HN
NH
N
H
f1 (ppm)
Parameter Value
1 Data File Name RM-46
2 Title c-13rammohan
3 Comment RM-46
4 Origin Bruker BioSpin GmbH
5 Owner IIIM
6 Site
7 Spectrometer spect
8 Author
9 Solvent MeOD
10 Temperature 300.0
11 Pulse Sequence dept135
12 Number of Scans 400
13 Receiver Gain 203
14 Relaxation Delay 1.0000
15 Pulse Width 9.2000
16 Acquisition Time 1.2976
17 Acquisition Date 2012-10-03T14:00:44
18 Modification Date 2012-10-03T14:00:46
19 Spectrometer Frequency 100.61
20 Spectral Width 25252.5
21 Lowest Frequency -2422.6
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536

2-(5-bromo-1H-indol-3-yl)-2,3-dihydroquinazolin-4(1H)-one (22b)

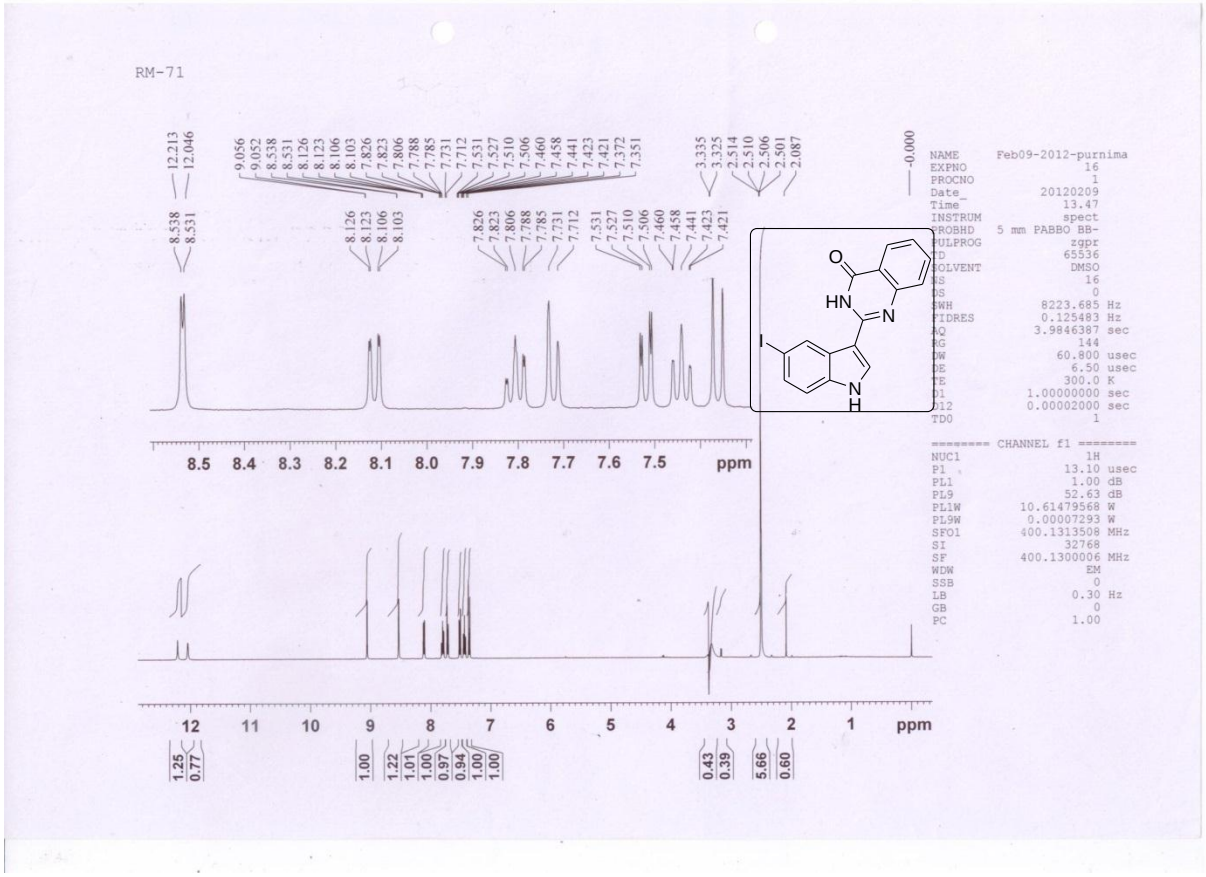


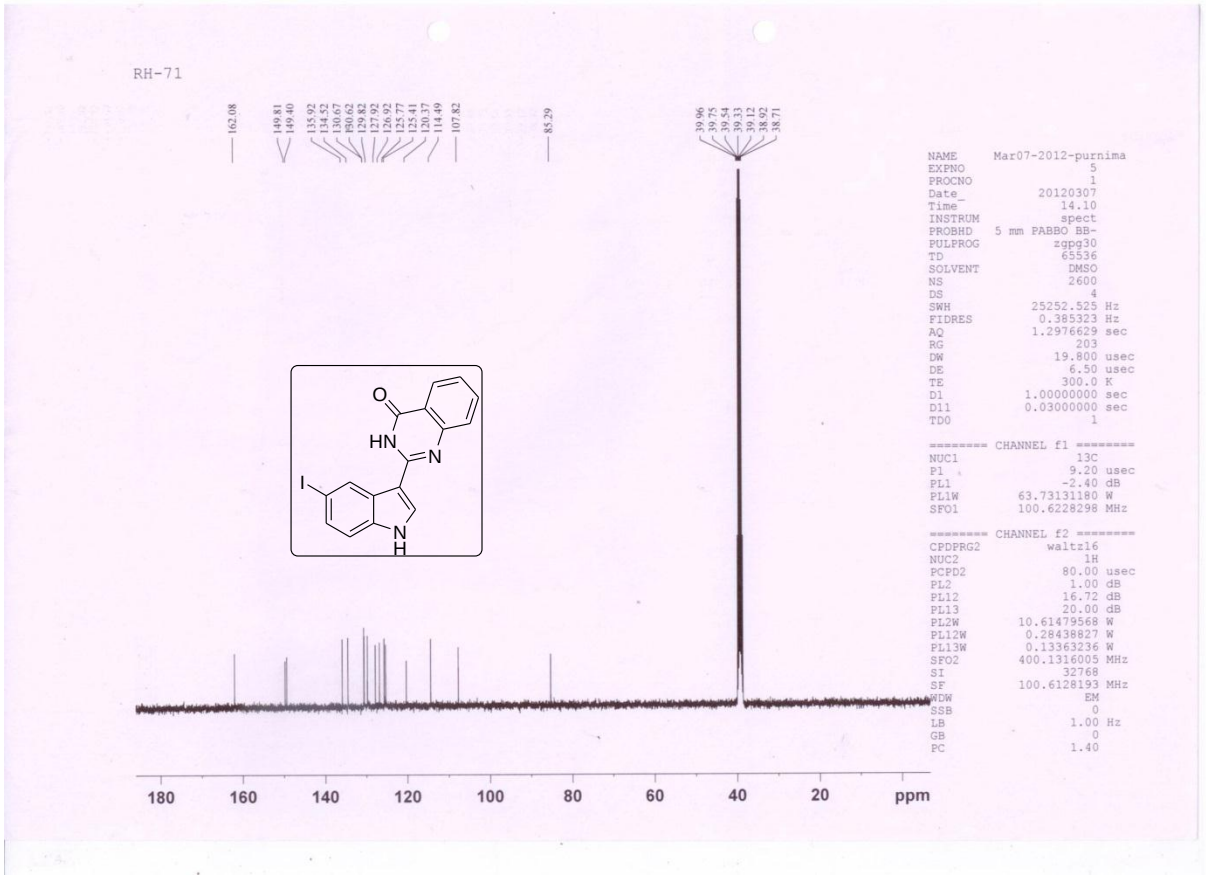
	Parameter	Value
1	Data File Name	RM-62-28SEP20 12-11/ fid
2	Title	Desktop
3	Comment	RM-62
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-09-28T14:25:39
18	Modification Date	2012-09-29T21:34:00
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3104.9
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

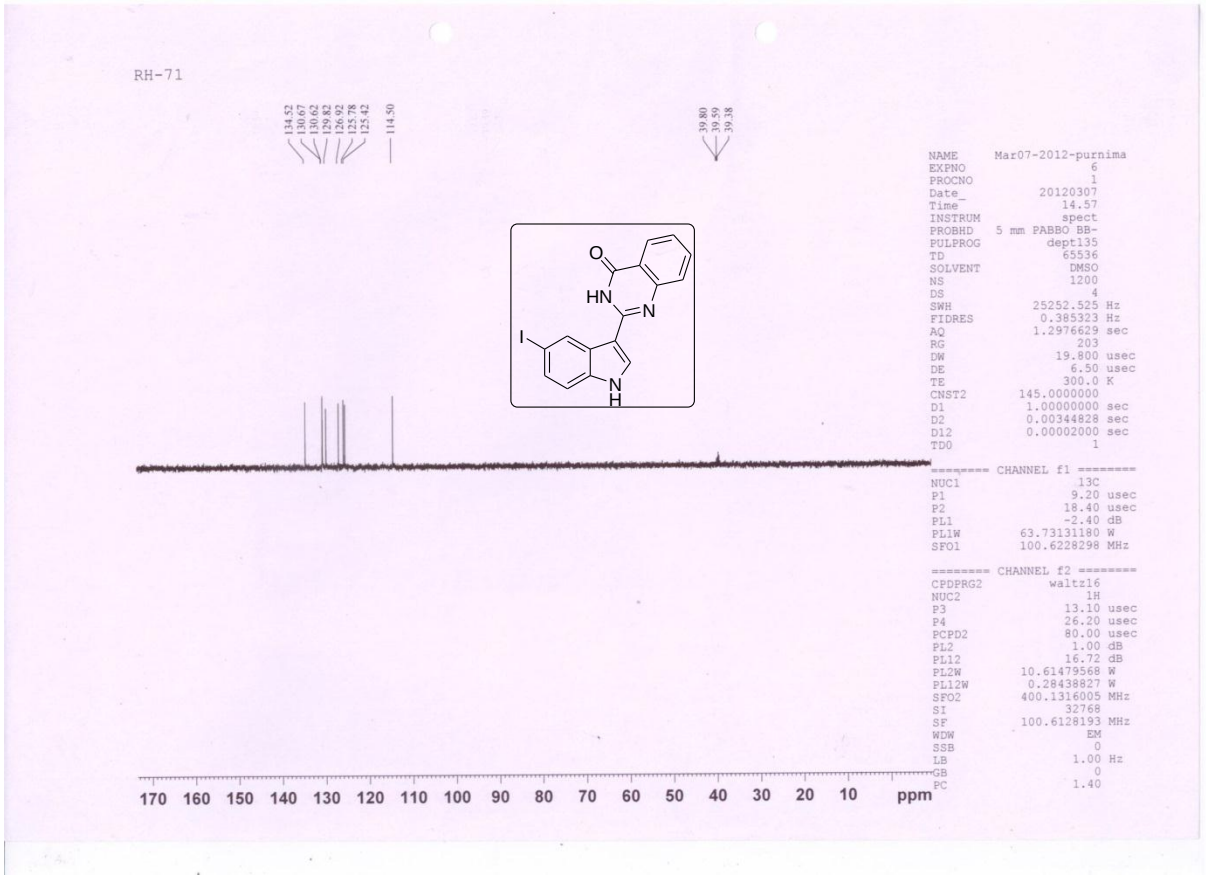



RM-62
ppm
134.253
133.716
127.582
125.547
125.465
125.397
125.224
124.552
123.979
121.919
118.316
114.373
112.886
112.837
112.785
62.268
62.178
O
HN
NH
Br
N
H
ppm
120
100
80
60
40
20
0

2-(5-iodo-1H-indol-3-yl)quinazolin-4(3H)-one (19c)




RH-71
162.08
149.81
149.40
135.92
134.52
130.67
130.62
129.82
127.92
126.92
125.77
125.41
120.37
114.49
107.82
85.29
39.96
39.75
39.54
39.33
39.12
38.92
38.71
O
HN
N
I
N
H
180 160 140 120 100 80 60 40 20 ppm
NAME Mar07-2012-purnima
EXPNO 5
PROCNO 1
Date_ 20120307
Time 14.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2600
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL13 20.00 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
PL13W 0.13363236 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40


RH-71
134.52
130.67
130.62
129.82
126.92
125.78
125.42
114.50
39.80
39.59
39.38
O
HN
N
I
N
H
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
NAME Mar07-2012-purnima
EXPNO 6
PROCNO 1
Date_ 20120307
Time 14.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT DMSO
NS 1200
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
P2 18.40 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 13.10 usec
P4 26.20 usec
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128193 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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