Supporting Information

α_2-Adrenoceptor Antagonists: Synthesis, Pharmacological Evaluation and Molecular Modelling Investigation of Pyridino Guanidine/2-Aminoimidazoline and their Derivatives

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Contents

1. Preparation of *N*-(*tert*-butoxycarbonyl)-*N'*-substituted thioureas[1]

Thiourea (1.0 eq., 6.58 mmol, 501 mg) was dissolved in dry tetrahydrofuran (70 mL) under argon at 0 °C, to which 4.5 equivalents of sodium hydride (60% suspension in mineral oil, 4.5 eq., 29.61 mmol, 788 mg) was added. The reaction was stirred at RT for 45 min to complete formation of the anion and re-cooled to 0 °C prior to the addition of di-tert-butyl dicarbonate (2.2 eq., 14.48 mmol, 3.160 g). After stirring at RT for 8 h, the reaction was re-cooled to 0 °C and sodium hydride (60% suspension in mineral oil, 1.7 eq., 11.19 mmol, 298 mg) was added. After 1 h trifluoroacetic anhydride (1.54 eq., 10.13 mmol, 1.431 mL) was added and the reaction was stirred for 1 h before the appropriate amine (1.54 eq., 10.13 mmol) was added and the reaction was allowed to come to RT overnight. The reaction was then cooled to 0 °C and dropwise H2O (20 mL) was added to quench the reaction. The product was extracted with EtOAc (3 × 20 mL) and the combined organic phases were washed with brine (sat. 30 mL) and H2O (30 mL), dried over anhydrous MgSO4, filtered and concentrated under vacuum. The resulting residue was purified by silica gel chromatography using gradient elution (hexane:EtOAc), followed by removal of solvents under vacuum to afford the product.

N-(*tert*-Butoxycarbonyl)-*N'*-(2-hydroxyethyl) thiourea

Thiourea (600 mg, 7.88 mmol) was dissolved in dry THF (60 mL) under argon at 0 °C and NaH (60% suspension in mineral oil, 4.5 eq., 851 mg, 35.47 mmol) was added. After 45 min stirring at RT and re-cooling to 0 °C di-*tert*-butyl dicarbonate (2.2 eq., 3785 mg, 17.34 mmol) was added and stirring continued at RT for 8 h. The mixture was cooled to 0 °C and further NaH (60% suspension in mineral oil, 1.7 eq., 322 mg, 13.40 mmol) was added. After 1 h trifluoroacetic anhydride (1.54 eq., 1.72 mL, 12.14 mmol) was added and the reaction was stirred for 1 h before ethanolamine (1.54 eq., 733 μL, 12.14 mmol) was added and stirring was continued for 14 h. Usual workup and purification by trituration in cold hexane yielded product (855 mg, 43%) as a white powder. M.p. 100-102 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.48 (s, 9H, Boc CH_3), 2.82 (broad s, 1H, OH), 3.82-3.88 (m, 4H, 2 CH_2), 8.36 (broad s, 1H, NH), 10.01 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 28.0 (CH_3, Boc), 47.5 (CH_2), 60.7 (CH_2), 83.7 (q ^{t}Bu, Boc), 151.9 (q CO, Boc), 180.3 (q). ν_{max} (ATR)/cm^{-1}: 3217

(NH), 2981, 2937, 2881, 1709 (C=O), 1559, 1526, 1449, 1388, 1373, 1364, 1327, 1251, 1148 (C=S), 1045, 1004. HRMS (*m/z* ESI^+): Found: 243.0781 (M^+ + Na. $C_8H_{16}N_2O_3SNa$ Requires: 243.0779).

_N_-(*tert*-Butoxycarbonyl)-_N'_-phenyl thiourea

Thiourea (600 mg, 7.88 mmol) was dissolved in dry THF (60 mL) under argon at 0 °C and NaH (60% suspension in mineral oil, 4.5 eq., 851 mg, 35.47 mmol) was added. After 45 min stirring at RT and re-cooling to 0 °C di-*tert*-butyl dicarbonate (2.2 eq., 3785 mg, 17.34 mmol) was added and stirring continued at RT for 8 h. The mixture was cooled to 0 °C and further NaH (60% suspension in mineral oil, 1.7 eq., 322 mg, 13.40 mmol) was added. After 1 h trifluoroacetic anhydride (1.54 eq., 1.72 mL, 12.14 mmol) was added and the reaction was stirred for 1 h before aniline (1.54 eq., 1.11 mL, 12.14 mmol) was added and stirring was continued for 14 h. Usual workup and purification by silica gel chromatography eluting with hexane:EtOAc yielded product (1070 mg, 54%) as a white, crystalline solid. M.p. 105-107 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.56 (s, 9H, Boc CH_3), 7.28 (t, 1H, J 7.7, Ar), 7.42 (t, 2H, J 7.7, Ar), 7.67 (d, 1H, J 7.7, Ar), 8.10 (broad s, 1H, NH), 11.54 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 28.0 (CH_3, Boc), 84.3 (q ^tBu, Boc), 124.3 (CH Ar), 126.7 (CH Ar), 128.8 (CH Ar), 137.7 (q Ar), 151.9 (q CO, Boc), 178.3 (q). ν_{max} (ATR)/cm^{-1}: 3172 (NH), 3006 (NH), 2984, 1709 (C=O), 1591, 1528, 1477, 1451, 1391, 1366, 1321, 1252, 1196, 1143, 1075, 1048, 1016, 1004. HRMS (*m/z* ESI^+): Found: 275.0828 (M^+ + Na. $C_{12}H_{16}N_2O_2SNa$ Requires: 275.0830).

_N_-(*tert*-Butoxycarbonyl)-_N'_-(2-furanylmethyl) thiourea

Thiourea (400 mg, 5.25 mmol) was dissolved in dry THF (40 mL) under argon at 0 °C and NaH (60% suspension in mineral oil, 4.5 eq., 567 mg, 23.65 mmol) was added. After 45 min stirring at RT and re-cooling to 0 °C di-*tert*-butyl dicarbonate (2.2 eq., 2523 mg, 11.56 mmol) was added and stirring continued at RT for 8 h. The mixture was cooled to 0 °C and further NaH (60% suspension in mineral oil, 1.7 eq., 215 mg, 8.93 mmol) was added. After 1 h trifluoroacetic anhydride (1.54 eq., 1.15 mL, 8.09 mmol) was added and the reaction was stirred for 1 h before furfurylamine (1.54 eq., 715 μL, 8.09 mmol) was added and stirring was continued for 14 h. Usual workup and purification by trituration in cold hexane yielded

product (764 mg, 58%) as a white powder. M.p. 99-100 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.51 (s, 9H, Boc CH_3), 4.88 (m, 2H, CH_2), 6.37 (d, 2H, J 2.9, Ar), 7.43 (s, 1H, Ar), 7.94 (broad t, 1H, J 5.4, NH), 9.66 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 27.5 (CH_3, Boc), 42.0 (CH_2), 83.4 (q ^{t}Bu, Boc), 108.1 (CH Ar), 110.0 (CH Ar), 142.2 (CH Ar), 149.0 (q CO, Boc), 151.2 (q Ar), 179.1 (q). ν_{max} (ATR)/cm^{-1}: 3279, 3251 (NH), 3174 (NH), 2983, 1711 (C=O), 1642, 1535, 1443, 1368, 1321, 1252, 1132 (C=S), 1011. HRMS (*m/z* ESI^+): Found: 279.0793 (M^+ + Na. $C_{11}H_{16}N_2O_3SNa$ Requires: 279.0779).

_N_-(_tert_-Butoxycarbonyl)-_N'_-propyl thiourea

Thiourea (600 mg, 7.88 mmol) was dissolved in dry THF (60 mL) under argon at 0 °C and NaH (60% suspension in mineral oil, 4.5 eq., 851 mg, 35.47 mmol) was added. After 45 min stirring at RT and re-cooling to 0 °C di-*tert*-butyl dicarbonate (2.2 eq., 3785 mg, 17.34 mmol) was added and stirring continued at RT for 8 h. The mixture was cooled to 0 °C and further NaH (60% suspension in mineral oil, 1.7 eq., 322 mg, 13.40 mmol) was added. After 1 h trifluoroacetic anhydride (1.54 eq., 1.72 mL, 12.14 mmol) was added and the reaction was stirred for 1 h before *n*-propylamine (1.54 eq., 1.00 mL, 12.14 mmol) was added and stirring was continued for 14 h. Usual workup and purification by silica gel chromatography eluting with hexane:EtOAc yielded product (1218 mg, 71%) as a white, crystalline solid. M.p. 58-60 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.01 (t, 3H, J 7.3, CH_3), 1.52 (s, 9H, Boc CH_3), 1.71 (app. q, 2H, J 7.3, CH_2), 3.63 (m, 2H, CH_2), 7.97 (broad s, 1H, NH), 9.74 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 11.3 (CH_3), 21.5 (CH_2), 27.8 (CH_3, Boc), 47.1 (CH_2), 83.4 (q ^{t}Bu, Boc), 151.8 (q CO, Boc), 179.4 (q2). ν_{max} (ATR)/cm^{-1}: 3245 (NH), 3175 (NH), 2961, 2934, 2875, 1720 (C=O), 1523, 1243, 1206, 1142 (C=S), 1073, 1008. HRMS (*m/z* ESI^+): Found: 219.1167 (M^+ + H. $C_9H_{19}N_2O_2S$ Requires: 219.1167).

_N_-(_tert_-Butoxycarbonyl)-_N'_-(2-acetoxyethyl) thiourea

Over a solution of *N*-(*tert*-Butoxycarbonyl)-*N'*-(2-hydroxyethyl) thiourea (600 mg, 2.73 mmol) in CH_2Cl_2 (6 mL) at 0 °C were added pyridine (3.0 eq., 658 μL, 8.18 mmol), acetic anhydride (1.5 eq., 386 μL, 4.09 mmol) and 4-(dimethylamino)pyridine (0.05 eq., 17 mg, 0.14 mmol). The mixture was stirred at RT for 3 h, after which $NaHCO_3$ (saturated, 15 mL) was added to quench the reaction. The mixture was stirred for 30 min and then extracted with

Et_2O (3 × 20 mL). The combined organic layers were washed with 0.5 M HCl (15 mL), brine (15 mL) and water (15 mL). The organic extract was dried over $MgSO_4$, filtered and concentrated under vacuum to yield product (650 mg, 91%) as a white, crystalline solid. M.p. 95-97 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.48 (s, 9H, Boc CH_3), 2.08 (s, 3H, CH_3), 3.93 (q, 2H, J 5.1, CH_2), 4.27 (t, 2H, J 5.1, CH_2), 8.39 (broad s, 1H, NH), 9.93 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 20.4 (CH_3), 27.5 (CH_3, Boc), 43.9 (CH_2), 61.6 (CH_2), 83.5 (q ^{t}Bu, Boc), 151.3 (q CO, Boc), 170.4 (q CO, Ac), 179.8 (q). ν_{max} (ATR)/cm^{-1}: 3259 (NH), 3179 (NH), 2988, 2957, 1738, 1718 (C=O), 1558, 1526, 1391, 1365, 1329, 1240, 1195, 1133, 1050, 1039. HRMS (*m/z* ESI^+): Found: 285.0876 (M^+ + Na. $C_{10}H_{18}N_2O_4SNa$ Requires: 285.0885).

2. Preparation of *S*-methyl-*N*-substituted dithiocarbamates

To a solution of carbon disulphide (1.1 eq., 3.72 mmol, 225 μL) and triethylamine (1.1 eq., 3.72 mmol, 519 μL) in CH_2Cl_2 (4 mL) at 0 °C was added starting amine (1.0 eq., 3.38 mmol). After 15 min methyl iodide (1.1 eq., 3.72 mmol, 232 μL) was added dropwise. The reaction was warmed to RT and stirred for 2 h. It was then diluted with EtOAc (30 mL) and added to a 1 M solution of H_2SO_4 (30 mL). The aqueous layer was extracted with EtOAc (2 × 30 mL) and the combined organic layers were washed with water (2 × 20 mL) and dried over $MgSO_4$. Filtration and removal of solvents yielded a residue which was purified either by recrystallisation from hexane or silica gel column chromatography, eluting with hexane:EtOAc, as appropriate.

***S*-Methyl-*N*-(2-hydroxyethyl) dithiocarbamate**

Ehanolamine (1.0 eq., 198 μL, 3.27 mmol) was added to a solution of carbon disulphide (1.1 eq., 217 μL, 3.60 mmol) and triethylamine (1.1 eq., 502 μL, 3.60 mmol) in CH_2Cl_2 (3 mL) at 0 °C. After 15 min methyl iodide (1.1 eq., 224 μL, 3.60 mmol) was added dropwise and the reaction was stirred at RT for 2 h. Usual workup, followed by silica gel chromatography, eluting with hexane:EtOAc yielded product (339 mg, 68%) as a colourless oil. The product, **54a**, was obtained as a mixture of isomers (7:2). δ_H (400 MHz, $CDCl_3$): *Major isomer;* 2.59 (s, 3H, CH_3), 3.77-3.91 (m, 4H, 2 CH_2), 8.18 (broad s, 1H, NH). δ_H (400 MHz, $CDCl_3$): *Minor isomer;* 2.64 (s, 3H, CH_3), 3.54-3.61 (m, 2H, CH_2), 3.77-3.91 (m, 2H, CH_2), 8.73

(broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): *Major isomer*; 17.8 (CH_3), 48.8 (CH_2), 59.9 (CH_2), 199.5 (q). δ_C (100 MHz, $CDCl_3$): *Minor isomer;* 18.5 (CH_3), 21.0 (CH_3), 48.0 (CH_2), 59.4 (CH_2), 201.8 (q). ν_{max} (ATR)/cm^{-1}: 3227 (NH), 3009 (NH), 2919, 2880, 1504, 1423, 1382, 1326, 1305, 1266, 1213, 1108 (C=S), 1051, 1003, 870, 789. HRMS (*m/z* ESI^-): Found: 150.0052 (M^- - H. $C_4H_8NOS_2$ Requires: 150.0047).

_S_-Methyl-_N_-phenyl dithiocarbamate

Aniline (1.0 eq., 587 μL, 6.44 mmol) was added to a solution of carbon disulphide (1.1 eq., 428 μL, 7.09 mmol) and triethylamine (1.1 eq., 988 μL, 7.09 mmol) in CH_2Cl_2 (6 mL) at 0 °C. After 15 min methyl iodide (1.1 eq., 441 μL, 7.09 mmol) was added dropwise and the reaction was stirred at RT for 2 h. Usual workup, followed by trituration in cold hexane yielded product (803 mg, 68%) as a white, crystalline solid. M.p. 90-92 °C, clean melt, lit. 92-93 °C.[2] δ_H (400 MHz, $CDCl_3$): 2.68 (s, 3H, CH_3), 7.35 (t, 1H, J 7.0), 7.42-7.49 (m, 4H, Ar), 9.03 (broad s, 1H, NH).

_S_-Methyl-_N_-(2-furanylmethyl) dithiocarbamate

Furfurylamine (1.0 eq., 546 μL, 6.18 mmol) was added to a solution of carbon disulphide (1.1 eq., 410 μL, 6.80 mmol) and triethylamine (1.1 eq., 948 μL, 6.80 mmol) in CH_2Cl_2 (6 mL) at 0 °C. After 15 min methyl iodide (1.1 eq., 423 μL, 6.80 mmol) was added dropwise and the reaction was stirred at RT for 2 h. Usual workup, followed by silica gel chromatography, eluting with hexane:EtOAc, yielded product (926 mg, 80%) as an off-white solid. M.p. 47-48 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 2.61 (s, 3H, CH_3), 4.89 (d, 2H, J 4.9, CH_2), 6.32-6.35 (m, 2H, Ar), 7.37 (s, 1H, Ar), 7.45 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 18.3 (CH_3), 43.8 (CH_2), 109.0 (CH Ar), 110.7 (CH Ar), 142.7 (CH Ar), 149.3 (q Ar), 199.2 (q). ν_{max} (ATR)/cm^{-1}: 3221 (NH), 2996, 2919, 1641, 1591, 1493, 1422, 1367, 1321, 1304, 1269, 1190, 1146 (C=S), 1086, 1063, 1010, 927, 883, 864, 843, 816, 738, 694. HRMS (*m/z* ESI^-): Found: 186.0041 (M^- - H. $C_7H_8NOS_2$ Requires: 186.0047).

_S_-Methyl-_N_-propyl dithiocarbamate

n-Propylamine (1.0 eq., 278 μL, 3.38 mmol) was added to a solution of carbon disulphide (1.1 eq., 225 μL, 3.72 mmol) and triethylamine (1.1 eq., 519 μL, 3.72 mmol) in CH_2Cl_2 (4 mL) at 0 °C. After 15 min methyl iodide (1.1 eq., 232 μL, 3.72 mmol) was added dropwise and the reaction was stirred at RT for 2 h. Usual workup, followed by silica gel chromatography, eluting with hexane:EtOAc, yielded product (450 mg, 89%) as a colourless oil. The product was obtained as a mixture of isomers. δ_H (400 MHz, $CDCl_3$): *Major isomer;* 0.91-0.97 (m, 3H, CH_3), 1.61-1.72 (m, 2H, CH_2), 2.59 (s, 3H, CH_3), 3.63-3.68 (m, 2H, CH_2), 7.31 (broad s, 1H, NH). δ_H (400 MHz, $CDCl_3$): *Minor isomer;* 0.95-1.01 (m, 3H, CH_3), 1.61-1.72 (m, 2H, CH_2), 2.63 (s, 3H, CH_3), 3.37 (t, 2H, J 7.1, CH_2), 8.21 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): *Major isomer;* 11.4 (CH_3), 18.1 (CH_3), 21.7 (CH_2), 49.0 (CH_2), 198.7 (q). δ_C (100 MHz, $CDCl_3$): *Minor isomer;* 11.3 (CH_3), 18.8 (CH_3), 22.0 (CH_2), 48.2 (CH_2), 201.5 (q). ν_{max} (ATR)/cm^{-1}: 3222 (NH), 2962, 2931, 2874, 1502, 1459, 1425, 1389, 1345, 1305, 1291, 1249, 1153 (C=S), 1062, 1002, 936, 883, 856, 771, 749, 727. HRMS (*m/z* ESI$^-$): Found: 148.0259 (M^- - H. $C_5H_{10}NS_2$ Requires: 148.0255).

_S_-Methyl-_N_-(2-acetoxyethyl) dithiocarbamate 2

Methyl (2-hydroxyethyl)carbamodithioate (1.0 eq., 1300 mg, 8.60 mmol), triethylamine (3.0 eq., 3.59 mL, 25.79 mmol) and acetic anhydride (1.1 eq., 892 μL, 9.46 mmol) were added to CH_2Cl_2 (21 mL) under stirring at 0 °C. The reaction was warmed to RT and stirred for 2 h. At this point TLC showed no starting material and the reaction was diluted with CH_2Cl_2 (30 mL). The organic layer was separated, washed with brine (30 mL) and water (2 × 30 mL), dried over $MgSO_4$ and filtered. Removal of solvents under reduced pressure yielded a residue which was purified using silica-gel chromatography (hexane:EtOAc), affording product (1609 mg, 97%) obtained as a colourless oil, in a mixture of isomers (85:15). δ_H (400 MHz, $CDCl_3$): *Major isomer;* 2.06 (s, 3H, CH_3), 2.59 (s, 3H, CH_3), 3.95-4.00 (m, 2H, CH_2), 4.27-4.33 (m, 2H, CH_2), 7.73 (broad s, 1H, NH). δ_H (400 MHz, $CDCl_3$): *Minor isomer;* 2.06 (s, 3H, CH_3), 2.60 (s, 3H, CH_3), 3.95-4.00 (m, 2H, CH_2), 4.27-4.33 (m, 2H, CH_2), 8.12 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): *Major isomer;* 18.1 (CH_3), 20.9 (CH_3), 46.2 (CH_2), 62.1 (CH_2), 171.3 (q, CO), 199.8 (q). δ_C (100 MHz, $CDCl_3$): *Minor isomer;* 18.1 (CH_3), 21.0 (CH_3), 45.0 (CH_2), 61.7 (CH_2), 171.7 (q, CO), 202.3 (q). ν_{max} (ATR)/cm^{-1}: 3292 (NH), 2919, 1720 (C=O), 1508 (C=S), 1427, 1378, 1332, 1308, 1222, 1132, 1044, 950, 881, 808, 727. HRMS (*m/z* ESI$^-$): Found: 192.0146 (M^- - H. $C_6H_{10}NO_2S_2$ Requires: 192.0153).

_S_-Methyl-_N_-(benzo[_d_][1,3]dioxol-5-ylmethyl) dithiocarbamate

Benzo[*d*][1,3]dioxol-5-ylmethanamine (1.0 eq., 934 mg, 6.18 mmol) was added to a solution of carbon disulphide (1.1 eq., 410 μL, 6.80 mmol) and triethylamine (1.1 eq., 948 μL, 6.80 mmol) in CH_2Cl_2 (6 mL) at 0 °C. After 15 min methyl iodide (1.1 eq., 423 μL, 6.80 mmol) was added dropwise and the reaction was stirred at RT for 2 h. Usual workup, followed by silica gel chromatography, eluting with hexane:EtOAc, yielded product (761 mg, 51%) as a yellow solid. M.p. 96 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 2.55 (s, 3H, CH_3), 4.73 (d, 2H, J 4.0, CH_2), 5.85 (s, 2H, CH_2, -OCH_2O-), 6.68-6.70 (m, 3H, Ar), 7.65 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 18.1 (CH_3), 50.8 (CH_2), 101.1 (CH_2, -OCH_2O-), 106.3 (CH Ar), 108.7 (CH Ar), 121.7 (CH Ar), 130.2 (q Ar), 147.4 (q Ar), 147.8 (q Ar), 198.9 (q, C=S). ν_{max} (ATR)/cm^{-1}: 3180 (NH), 2995, 2959, 2902, 1651, 1520, 1497, 1482, 1424, 1376, 1346, 1310, 1272, 1240, 1191, 1132 (C=S), 1101, 960, 935, 908, 856, 768, 729, 698. HRMS (*m/z* ESI⁻): Found: 240.0153 (M^- - H. $C_{10}H_{10}NO_2S_2$ Requires: 240.0148).

3. Preparation of non-commercial starting amines

2-amino-5,6,7,8-tetrahydroquinoline

This compound was prepared according to the procedure of Vijn *et al*.[3]

3-amino-5,6,7,8-tetrahydroquinoline

This compound was prepared according to the procedure of Tohda *et al*.[4]

2-(_N_-Ethylamino)-5-aminopyridine

N-(Pyridin-2-yl)acetamide

To a solution of 2-aminopyridine (1.0 eq., 500 mg, 5.31 mmol) in CH_2Cl_2 at RT were added triethylamine (3.0 eq., 2.22 mL, 15.94 mmol) and acetic anhydride (2.0 eq., 1.00 mL, 10.63 mmol). Stirring was continued for 6 h, after which the mixture was diluted with EtOAc (30 mL). The organic layer was washed with H_2O (2 × 15 mL), dried over $MgSO_4$, filtered, and concentrated under vacuum to yield a colourless oil which was purified by silica gel chromatography, eluting with hexane:EtOAc. Removal of solvent yielded product (650 mg, 90%) as a yellow/white solid. M.p. 75-76 °C, clean melt, lit., 70- 71 °C.231 δ_H (400 MHz, $CDCl_3$): 2.14

(s, 3H, CH_3), 6.96-6.99 (m, 1H, Ar), 7.63-7.66 (m, 1H, Ar), 8.18-8.21 (m, 2H, Ar), 9.84 (broad s, 1H, NH).

2-(N-Ethylamino)pyridine

To a solution of 33 (1.0 eq., 400 mg, 2.94 mmol) in dry tetrahydrofuran (30 mL) at 0 °C was added lithium aluminium hydride (5.0 eq., 557 mg, 14.69 mmol). The mixture was stirred at RT for 16 h, after which H_2O (30 mL) was added to quench the reaction. The mixture was filtered through celite and the organic phase was extracted with EtOAc (3 × 30 mL), washed with H2O (2 × 15 mL), dried over MgSO4, filtered, and concentrated under reduced pressure to yield product (266 mg, 74%) as a red liquid. δ_H (400 MHz, $CDCl_3$): 1.24 (t, 3H, J 7.2, CH_3), 3.28 (q, 2H, J 7.2, CH_2), 4.65 (broad s, 1H, NH), 6.37 (d, 1H, J 8.4, Ar), 6.54 (m, 1H, Ar), 7.41 (app. dt, 1H, J 8.4, 1.9, Ar), 8.06 (dd, 1H, J 5.0, 1.9, Ar). δ_C (100 MHz, $CDCl_3$): 14.8 (CH_3), 36.9 (CH_2), 106.3 (CH Ar), 112.6 (CH Ar), 137.5 (CH Ar), 148.1 (CH Ar), 158.9 (q Ar). ν_{max} (ATR)/cm^{-1}: 2959 (NH), 1610, 1571, 1482, 1443, 1320, 1273, 1253, 1150, 1046, 989, 846, 631, 550, 519. HRMS (*m/z* ESI^+): Found: 123.0921 (M^+ + H. $C_7H_{11}N_2$ Requires: 123.0922).

2-(N-Ethylamino)-5-nitropyridine

Aqueous sulfuric acid (20%, 2.5 eq., 5.10 mL, 5.10 mmol) and potassium nitrate (1.1 eq., 228 mg, 2.25 mmol) were added to 2-(*N*-Ethylamino)pyridine (1.0 eq., 250 mg, 2.05 mmol) and the mixture was stirred at RT for 5 h. The reaction was cooled to 0 °C and aqueous ammonia was added dropwise until a pH of 12 was reached. The resulting precipitate was extracted with EtOAc (3 × 30 mL), washed with brine (20 mL) and water (2 × 20 mL), dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure to yield a yellow/brown solid which was purified by silica gel column chromatography, eluting with 1:1 hexane:EtOAc. Removal of solvent yielded product (171 mg, 50%) as a yellow solid. M.p. 115-116 °C, lit., 117-119 °C.232 δ_H (400 MHz, $CDCl_3$): 1.26 (t, 3H, J 7.0, CH_3), 3.40 (broad s, 2H, CH_2), 6.13 (broad s, 1H, NH), 6.35 (d, 1H, J 9.3, Ar), 8.10 (broad s, 1H, Ar), 8.93 (s, 1H, Ar).

2-(N-Ethylamino)-5-aminopyridine

To a solution of 2-(*N*-Ethylamino)-5-nitropyridine (1.0 eq., 200 mg, 1.20 mmol) in EtOAc (12 mL) was added 10% Pd/C (25 mg, 0.02 mmol, 2 mol%). The mixture was stirred under a hydrogen atmosphere (3 atm.) for 5 h. It was then filtered through filter paper and concentrated under reduced pressure to yield product (157 mg, 95%) as a dark red solid. M.p. 96-97 °C, clean melt, lit. 95-98 °C.233 δ_H (400 MHz, DMSO-D6): 1.08 (t, 3H, J 8.0, CH_3),

3.10 (m, 2H, CH_2), 4,26 (broad s, 2H, NH_2), 5.44 (broad s, 1H, NH), 6.26 (d, 1H, J 8.0, Ar), 6.81 (dd, 1H, J 8.0, 1.9, Ar), 7.45 (s, 1H, Ar).

2-Amino-5-ethylaminopyridine

To a solution of 2,5-diaminopyridine (250 mg, 2.29 mmol) in ethanol (11 mL) was added ethyl mesylate (1.00 eq., 236 μL, 2.29 mmol). The mixture was stirred at 60 °C for 16 h. The product was extracted with a 20% solution of iPrOH/CH_2Cl_2 (3 × 20 mL), washed with saturated $NaHCO_3$ (2 × 20 mL), dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure to yield a residue that was purified by silica gel column chromatography, eluting with 4:1 CH_2Cl_2/CH_3OH. Removal of solvent afforded product (149 mg, 47%) as a red liquid. The position of alkylation was confirmed by a NOE signal from H3 to the NH_2. δ_H (400 MHz, $CDCl_3$): 1.11 (t, 3H, J 6.9, CH_3), 2.92 (q, 2H, J 6.9, CH_2), 4.66 (broad s, 1H, NH, NHEt), 5.00 (broad s, 2H, NH_2), 6.34 (d, 1H, J 8.9, Ar), 6.82 (dd, 1H, 8.9, 3.0, Ar), 7.36 (d, 1H, J 3.0, Ar). δ_C (100 MHz, $CDCl_3$): 14.6 (CH_3), 38.9 (CH_2), 108.8 (CH Ar), 124.1 (CH Ar), 131.5 (CH Ar), 137.1 (q Ar), 151.8 (q Ar). ν_{max} (ATR)/cm^{-1}: 3314 (NH), 2968, 2871, 1625, 1578, 1496, 1392, 1279, 1240, 1144, 1100, 1059, 1015, 820. HRMS (*m/z* ESI^+): Found: 138.1027 (M^+ + H. $C_7H_{12}N_3$ Requires: 138.1031).

2-Amino-3aminomethylpyridine

To a solution of 2-aminopyridine-3-carbonitrile (300mg, 2.52mmol), in 7N NH_3/CH_3OH (5ml), was added 10% Pd/C (50mg). The mixture was stirred under an atmosphere of hydrogen (3 atm.) for 12 h. The resulting solution was diluted with CH_3OH (40ml), filtered through celite, and concentrated under reduced pressure, to yield product (284 mg, 90%) as a white solid. 121 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.92 (s, 2H, $N\underline{H}_2CH_2$), 3.95 (s, 2H, CH_2), 5.21 (s, 2H, NH_2), 6.53 (m, 1H, Ar), 7.31 (d, 1H, J 4.0, Ar), 7.89 (s, 1H, Ar). δ_C (100 MHz, $CDCl_3$): 42.0 (CH_2), 112.9 (CH Ar), 114 (q Ar), 133.1 (CH Ar), 146.4 (CH Ar), 154.5 (q Ar). ν_{max} (ATR)/cm^{-1}: 3349 (NH), 3282 (NH), 3011, 2862, 2636, 1627, 1600, 1574, 1439, 1381, 1323, 1289, 1274, 1239, 1132, 1071, 1024, 975, 928, 815, 771, 760, 754, 697. HRMS (*m/z* ESI^+): Found: 124.0875 (M^+ + H, $C_6H_{10}N_3$ Requires: 124.0875). δ_C (100 MHz, $CDCl_3$): 14.2 (CH_3), 36.9 (CH_2), 132.6 (CH Ar), 146.8 (CH Ar), 161.1 (q Ar), 135.1 (CH Ar), 105.3 (q Ar). ν_{max} (ATR)/cm^{-1}: 3343 (NH), 2980, 2934, 1601, 1550 (NO_2), 1469, 1465, 1408, 1367, 1321, 1279, 1248, 1163, 1133, 1109, 1100, 1060, 994, 973, 951, 861, 824, 766, 730. HRMS (*m/z* ESI^+): Found: 168.0772 (M^+ + H. $C_7H_{10}N_3O_2$ Requires: 168.0773).

4. Synthesis and Characterisation of Boc-protected/neutral guanidine intermediates

Preparation of 1-(pyridinyl)-2,3-di(*tert*-butoxycarbonyl)guanidines, 1-(pyridinyl)-2,3-di(*tert*-butoxycarbonyl)-2-iminoimidazolidines, 1-(pyridinyl)-2-(*tert*-butoxycarbonyl)-3-substituted guanidines – Procedure A.

To a solution of starting amine (1.00 eq., 1.06 mmol), the appropriate thiourea derivative – *N,N'-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea, *N,N'*-di-(*tert*-butoxycarbonyl) imidazolidine-2-thione[5] or *N* -(*tert*-butoxycarbonyl)-*N'*-substituted thiourea – (1.05 eq., 1.11 mmol) and triethylamine (3.5 eq., 3.71 mmol, 517 μL) in CH_2Cl_2 (5.5 mL) at 0 °C was added mercury(II) chloride (1.05 eq., 1.11 mmol, 301 mg). The mixture was stirred for 30 min at 0 °C, then warmed to RT and stirred until reaction was complete, as adjudged by disappearance of starting material in TLC analysis. The reaction mixture was diluted with EtOAc (50 mL) and filtered through a pad of Celite to remove any mercury by-products. The filtrate was washed with brine (20 mL) and water (20 mL), dried over anhydrous $MgSO_4$, filtered and concentrated under reduced pressure to yield a residue that was purified by silica gel column chromatography, eluting with the appropriate hexane:EtOAc mixture. Where necessary, recrystallisation was carried out as described below for specific compounds.

Preparation of *N*-substituted- 1,4-dihydroquinazolin-2-amines and 1,4-dihydropyridopyrimidin-2-amines – Procedure C[6]

To a suspension of 2-aminobenzylamine (1.0 eq., 1.19 mmol, 145 mg) and the appropriate *S*-methyl-*N*-substituted dithiocarbamate (1.1 eq., 1.31 mmol) in dimethylformamide (4 mL) at RT were added Cu(II)O (0.2 eq., 0.24 mmol, 19 mg) and K_2CO_3 (2.0 eq., 2.37 mmol, 328 mg). The resulting mixture was heated to 60 °C and kept at this temperature for 2 h. It was then cooled to RT, diluted with EtOAc (60 mL) and filtered through Celite. The filtrate was washed with brine (30 mL) and water (4 × 30 mL) to remove traces of dimethylformamide, dried over $MgSO_4$, filtered and concentrated under vacuum. The resulting residue was purified using silica gel column chromatography, eluting with the appropriate hexane:EtOAc mixture.

1-(Pyridin-2-yl)-2,3-di(*tert*-butoxycarbonyl)guanidine (5a) – Procedure A with *N,N'-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea. Colourless crystals (79%) after recrystallisation from hexane:EtOAc. Mp. 138-140 ºC, clean melt. δ_H (600 MHz, $CDCl_3$): 1.53 (s, 18H, CH_3, Boc), 7.01 (app. t, 1H, J 5.4, Ar), 7.70 (app. t, 1H, J 7.3, Ar), 8.29 (d, 1H, J 4.0, Ar), 8.37

(broad s, 1H, Ar), 10.89 (broad s, 1H, NH), 11.53 (broad s, 1H, NH). δ_C (150 MHz, $CDCl_3$): 28.0 (CH_3,Boc), 28.1 (CH_3, Boc), 79.9 (q ^{t}Bu, Boc), 83.9 (q ^{t}Bu, Boc), 116.0 (CH Ar), 119.7 (CH Ar), 138.1 (CH Ar), 148.0 (CH Ar), 150.6 (q Ar), 152.6 (q, CO, Boc), 153.1 (q, Gua), 163.2 (q, CO, Boc). ν_{max} (ATR)/cm^{-1}: 3253 (NH), 2979, 1725 (C=O), 1621 (C=N), 1586, 1570, 1479, 1398, 1368, 1332, 1302, 1293, 1256, 1229, 1147, 1121, 1089, 1030, 994, 883, 848, 809, 763, 733, 710, 669. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{16}H_{25}N_4O_4$ 337.1876; Found: 337.1882.

1-(Pyridin-2'-yl)-2,3-di(*tert*-butoxycarbonyl)-2-iminoimidazolidine (5b) – Procedure A with *N,N'*-di-(*tert*-butoxycarbonyl) imidazolidine-2-thione. Colourless crystals (56%). Mp. 140 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.47 (s, 18H, CH_3, Boc), 3.71 (s, 4H, CH_2), 6.81 (ddd, 1H, J 7.3, 5.0, 1.0, Ar), 7.54 (app. td, 1H, J 7.3, 2.0, Ar), 7.99 (broad s, 1H, Ar), 8.17 (dd, 1H, J 2.0, 5.0, Ar). δ_C (100 MHz, $CDCl_3$): 28.2 (CH_3, Boc), 45.1 (2 CH_2), 82.6 (q ^{t}Bu, Boc), 113.1 (CH Ar), 117.6 (CH Ar), 137.7 (CH Ar), 147.7 (CH Ar), 149.8 (q Ar), 150.3 (q CO, Boc), 152.3 (q, Imi). ν_{max} (ATR)/cm^{-1}: 3266, 2981, 2934, 2884, 1805, 1696 (C=O), 1649 (C=N), 1576, 1545, 1479, 1462, 1437, 1376, 1365, 1329, 1306, 1254, 1232, 1151, 1117, 1088, 852, 841, 769, 760, 748, 677. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{18}H_{27}N_4O_4$ 363.2032; Found: 363.2026.

1-(Pyridin-2-yl)-2-(*tert*-butoxycarbonyl)-3-(phenyl)guanidine (5e) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-phenyl thiourea. Colourless oil (63%) identified as a mixture of isomers. δ_H (400 MHz, $CDCl_3$): 1.52 (s, 9H, CH_3, Boc), 6.93 (d, 1H, J 8.2, Ar), 7.03 (m, 1H, Ar), 7.11 (m, 1H, Ar), 7.36 (m, 2H, Ar), 7.67 (d, 2H, J 8.0, Ar), 7.72 (m, 1H, Ar), 8.27 (s, 1H, Ar), 12.27 (broad s, 1H, NH), 12.63 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 28.3 (CH_3, Boc), 79.3 (q ^{t}Bu, Boc), 113.7 (CH Ar), 118.4 (CH Ar), 122.4 (CH Ar), 124.3 (CH Ar), 129.1 (CH Ar), 138.3 (q Ar), 139.1 (CH Ar), 145.9 (CH Ar), 152.4 (q, CN), 155.2 (q Ar), 164.4 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 2979, 1711 (C=O), 1646 (C=N), 1587, 1561, 1498, 1448, 1417, 1357, 1292, 1245, 1157, 1097, 1010, 809, 690, 752. HRMS (ESI^+) *m/z*: $[M + Na]^+$ Calcd. for $C_{17}H_{20}N_4O_2Na$ 335.1484; Found: 335.1494.

1-(Pyridin-2-yl)-2-(*tert*-butoxycarbonyl)-3-(2-acetoxyethyl)guanidine (5f) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-(2-acetoxyethyl) thiourea. Colourless oil (43%) identified as a mixture of isomers. δ_H (400 MHz, $CDCl_3$): 1.53 (s, 9H, CH_3, Boc), 2.10 (s, 3H, CH_3), 3.80 (t, 2H, J 5.4, CH_2), 4.26 (t, 2H, J 5.4, CH_2), 6.84 (d, 1H, J 8.3, Ar), 6.95 (dd, 1H, J 6.9, 5.5, Ar), 7.64 (app. td, 1H, J 7.8, 1.6, Ar), 8.18 (d, 1H, J 5.2, Ar), 10.46 (broad s, 1H, NH), 12.09

(broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 20.8 (CH_3), 28.4 (CH_3, Boc), 39.6 (CH_2), 63.2 (CH_2), 78.8 (q ^{t}Bu, Boc), 113.3 (CH Ar), 117.8 (CH Ar), 138.5 (CH Ar), 145.8 (CH Ar), 152.9 (q Ar), 157.7 (q, CN), 164.1 (q CO, Boc), 170.8 (q CO). ν_{max} (ATR)/cm^{-1}: 2979, 1742 (C=O), 1642 (C=N), 1590, 1559, 1453, 1353, 1311, 1234, 1140, 1046. HRMS (ESI$^+$) *m/z*: [M + Na]$^+$ Calcd. for $C_{15}H_{22}N_4O_4Na$ 345.1539; Found: 345.1537.

1-(Pyridin-2-yl)-2-(*tert*-butoxycarbonyl)-3-(2-furanylmethyl)guanidine (5g) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-(2-furanylmethyl) thiourea. White solid (61%). M.p. 107-108 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.57 (s, 9H, CH_3, Boc), 4.77 (d, 1H, J 5.0, CH_2), 6.31 (d, 1H, J 3.1, Ar), 6.35-6.38 (m, 1H, Ar), 6.87 (d, 1H, J 8.3, Ar), 6.96 (dd, 1H, J 7.2, 5.2, Ar), 7.42 (dd, 1H, J 1.7, 0.7, Ar), 7.65 (app. td, 1H, J 7.7, 1.8, Ar), 8.20 (dd, 1H, J 5.2, 1.2, Ar), 10.59 (broad s, 1H, NH), 12.14 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 28.0 (CH_3, Boc), 37.7 (CH_2), 78.4 (q ^{t}Bu, Boc), 106.7 (CH Ar), 109.9 (CH Ar), 112.8 (CH Ar), 117.3 (CH Ar), 138.0 (CH Ar), 141.7 (CH Ar), 145.6 (CH Ar), 151.0 (q Ar), 152.4 (q Ar), 156.9 (q, CN), 163.6 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3062 (NH), 2976, 2926, 1646 (C=N), 1609 C=N), 1596, 1562, 1508, 1480, 1446, 1419, 1385, 1350, 1336, 1263, 1250, 1235, 1220, 1170, 1157, 1149, 1121, 1101, 1086, 1060, 1017, 998, 967, 918, 879, 850, 802, 765, 755, 740, 696. HRMS (ESI$^+$) *m/z*: [M + H]$^+$ Calcd. for $C_{16}H_{21}N_4O_3$ 317.1614; Found: 317.1622.

1-(5-Bromopyridin-2-yl)-2,3-di(*tert*-butoxycarbonyl)guanidine (6a) – Procedure A with *N,N'-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea. Colourless crystals (80%) after recrystallisation from hexane:EtOAc. Mp. 125-126 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.47 (s, 9H, CH_3, Boc), 1.49 (s, 9H, CH_3, Boc), 7.75 (dd, 1H, J 8.3, 2.1, Ar), 8.28 (d, 1H, J 2.1, Ar), 8.31 (d, 1H, J 8.3, Ar), 10.86 (broad s, 1H, NH), 11.49 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 27.8 (CH_3, Boc), 27.9 (CH_3, Boc), 79.9 (q ^{t}Bu, Boc), 83.9 (q ^{t}Bu, Boc), 114.7 (CH Ar), 117.2 (q Ar), 140.3 (CH Ar), 148.6 (CH Ar), 149.1 (q Ar), 152.5 (q CO, Boc), 152.7 (q, Gua), 162.8 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3247 (NH), 2980, 1715 (C=O), 1632 (C=N), 1593, 1553, 1453, 1404, 1367, 1324, 1287, 1252, 1232, 1148, 1129, 1101, 1057, 1028, 1004, 878, 841, 793, 745. HRMS (ESI$^+$) *m/z*: [M + H]$^+$ Calcd. for $C_{16}H_{24}{}^{79}BrN_4O_4$ 415.0981; Found: 415.0990.

1-(5-Chloropyridin-2-yl)-2,3-di(*tert*-butoxycarbonyl)guanidine (7a) – Procedure A with *N,N'-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea. Colourless crystals (35%) after recrystallisation from hexane:EtOAc. Mp. 122-124 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.53 (s, 9H, CH_3, Boc), 1.54 (s, 9H, CH_3, Boc), 7.67 (dd, 1H, J 8.9, 2.6, Ar), 8.24 (d, 1H, J

2.6, Ar), 8.40 (d, 1H, J 8.9, Ar), 10.92 (broad s, 1H, NH), 11.51 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 28.0 (CH_3, Boc), 28.1 (CH_3, Boc), 80.1 (q ^tBu, Boc), 84.1 (q ^tBu, Boc), 116.8 (CH Ar), 126.9 (q Ar), 137.7 (CH Ar), 146.6 (CH Ar), 148.9 (q Ar), 152.6 (q CO, Boc), 152.9 (q, Gua), 163.0 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3249 (NH), 2981, 1741, 1716 (C=O), 1633 (C=N), 1576, 1559, 1476, 1455, 1407, 1383, 1367, 1322, 1287, 1252, 1235, 1219, 1142, 1123, 1101, 1059, 1028, 1006, 967, 917, 880, 848, 837, 801, 782, 743, 728, 685. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{16}H_{24}{}^{35}ClN_4O_4$ 371.1486; Found: 371.1489.

1-(5-Chloropyridin-2'-yl)-2,3-di(*tert*-butoxycarbonyl)-2-iminoimidazolidine (7b) – Procedure A with *N,N'*-di-(*tert*-butoxycarbonyl) imidazolidine-2-thione. Colourless oil (56%). δ_H (400 MHz, $CDCl_3$): 1.38 (s, 18H, CH_3, Boc), 3.84 (s, 4H, CH_2), 6.95 (d, 1H, J 8.7, Ar), 7.53 (dd, 1H, J 2.6, 8.7, Ar), 8.11 (d, 1H, J 2.6, Ar). δ_C (100 MHz, $CDCl_3$): 27.8 (CH_3, Boc), 43.0 (2 CH_2), 82.9 (q ^tBu, Boc), 119.4 (CH Ar), 124.7 (q Ar), 137.3 (CH Ar), 141.8 (q Ar), 145.9 (CH Ar), 149.7 (q CO, Boc), 159.2 (q, Imi). ν_{max} (ATR)/cm^{-1}: 2980, 2933, 2251, 1765, 1712 (C=O), 1654 (C=N), 1579, 1548, 1460, 1367, 1291, 1251, 1146, 1039, 1007, 980, 910, 843, 769, 727. HRMS (ESI^+) *m/z*: $[M + Na]^+$ Calcd. for $C_{18}H_{25}N_4O_4{}^{35}ClNa$ 419.1462; Found: 419.1453.

1-(5-Chloropyridin-2-yl)-2-(*tert*-butoxycarbonyl)-3-(propyl)guanidine (7h) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-propyl thiourea. Colourless oil (39%) identified as a mixture of isomers. M.p. 79-82 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.00 (m, 3H, CH_3), 1.54 (s, 9H, CH_3, Boc), 1.65 (app. sex, 2H, J 7.3, CH_2), 3.49 (m, 2H, CH_2), 6.82 (d, 1H, J 8.8), 7.60 (dd, 1H, J 8.8, 2.3), 8.17 (d, 1H, J 2.3), 9.77 (broad s, 1H, NH), 12.28 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 11.5 (CH_3), 22.5 (CH_2), 28.2 (CH_3, Boc), 42.6 (CH_2), 78.8 (q ^tBu, Boc), 114.2 (CH Ar), 122.8 (q Ar), 138.4 (CH Ar), 144.5 (CH Ar), 151.4 (q Ar), 157.2 (q, CN), 164.4 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3359 (NH), 2968, 1730 (C=O), 1645 (C=N), 1585, 1560, 1476, 1455, 1406, 1380, 1329, 1322, 1288, 1259, 1234, 1170, 1156, 1120, 1032, 980, 832, 799, 734, 689. HRMS (ESI^+) *m/z*: $[M + Na]^+$ Calcd. for $C_{14}H_{21}N_4O_2{}^{35}ClNa$ 335.1251; Found: 335.1246.

1-(5-Methylpyridin-2-yl)-2,3-di(*tert*-butoxycarbonyl)guanidine (8a) – Procedure A with *N,N'-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea. White powder (71%). Mp. 139 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.48 (s, 9H, CH_3, Boc), 1.49 (s, 9H, CH_3, Boc), 2.23 (s, 3H, CH_3), 7.45 (dd, 1H, J 8.4, 1.9, Ar), 8.07 (d, 1H, J 1.9, Ar), 8.20 (broad s, 1H, Ar), 10.78 (broad s, 1H, NH), 11.52 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 17.8 (CH_3), 28.0 (CH_3,

Boc), 28.1 (CH_3, Boc), 79.7 (q ^{t}Bu, Boc), 83.7 (q ^{t}Bu, Boc), 115.6 (CH Ar), 129.1 (q Ar), 138.6 (CH Ar), 147.9 (CH Ar), 148.4 (q Ar), 152.7 (q CO, Boc), 153.0 (q, Gua), 163.3 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3244 (NH), 2978, 1720 (C=O), 1632 (C=N), 1585, 1560, 1475, 1454, 1404, 1374, 1324, 1305, 1289, 1268, 1252, 1230, 1151, 1136, 1107, 1058, 1025, 882, 856, 838, 803, 758, 749, 709. HRMS (ESI$^+$) *m/z*: $[M + H]^+$ Calcd. for $C_{17}H_{27}N_4O_4$ 351.2032; Found: 351.2036.

1-(5-Methylpyridin-2'-yl)-2,3-di(*tert*-butoxycarbonyl)-2-iminoimidazolidine (8b) – Procedure A with *N,N'*-di-(*tert*-butoxycarbonyl) imidazolidine-2-thione. White solid (75%). Mp. 89-91 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.44 (s, 18H, CH_3, Boc), 2.15 (s, 3H, CH_3), 3.68 (s, 4H, CH_2), 7.34 (dd, 1H, J 8.4, 2.0, Ar), 7.85 (broad s, 1H, Ar), 7.97 (d, 1H, Ar). δ_C (100 MHz, $CDCl_3$): 17.6 (CH_3), 28.1 (CH_3, Boc), 45.2 (2 CH_2), 82.4 (q ^{t}Bu, Boc), 112.6 (CH Ar), 126.6 (q Ar), 138.4 (CH Ar), 147.6 (CH Ar), 149.8 (q CO, Boc), 150.3 (q Ar), 152.3 (q, Imi). ν_{max} (ATR)/cm^{-1}: 3265, 2980, 2933, 2885, 1804, 1697 (C=O), 1647 (C=N), 1602, 1577, 1543, 1480, 1467, 1365, 1330, 1307, 1288, 1253, 1232, 1149, 1115, 1026, 879, 851, 840, 767, 748, 740, 701, 684. HRMS (ESI$^+$) *m/z*: $[M + H]^+$ Calcd. for $C_{19}H_{29}N_4O_4$ 377.2189; Found: 377.2186.

1-(5-Methylpyridin-2-yl)-2-(*tert*-butoxycarbonyl)-3-(phenyl)guanidine (8e) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-phenyl thiourea. Colourless oil (89%) identified as a mixture of isomers. δ_H (400 MHz, $CDCl_3$): 1.56 (s, 9H, CH_3, Boc), 2.33 (s, 3H, CH_3), 6.87 (d, 1H, J 7.2, Ar), 7.12 (m, 1H, Ar), 7.32-7.39 (m, 2H, Ar), 7.53 (d, 1H, J 7.7, Ar), 7.69 (d, 2H, J 8.0, Ar), 8.11 (s, 1H, Ar), 12.21 (broad s, 1H, NH), 12.41 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 17.7 (CH_3), 28.4 (CH_3, Boc), 78.9 (q ^{t}Bu, Boc), 113.1 (CH Ar), 129.0 (q Ar), 122.4 (CH Ar), 124.1 (CH Ar), 127.5 (q Ar), 128.8 (CH Ar), 139.7 (CH Ar), 145.5 (CH Ar), 150.6 (q Ar), 155.3 (q, CN), 164.2 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 2978, 1709 (C=O), 1643 (C=N), 1607, 1590, 1562, 1494, 1473, 1447, 1354, 1244, 1203, 1154, 1096, 1069, 1027, 985, 901, 808, 752, 690. HRMS (ESI$^+$) *m/z*: $[M + H]^+$ Calcd. for $C_{18}H_{23}N_4O_2$ 327.1821; Found: 327.1828.

1-(5-Methylpyridin-2-yl)-2-(*tert*-butoxycarbonyl)-3-(2-acetoxyethyl)guanidine (8f) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-(2-acetoxyethyl) thiourea. Colourless oil (54%). δ_H (400 MHz, $CDCl_3$): 1.56 (s, 9H, CH_3, Boc), 2.13 (s, 3H, CH_3), 2.31 (s, 3H, CH_3), 3.83 (app. q, 2H, J 5.4, 5.1, CH_2), 4.29 (app. t, 2H, J 5.5, 5.3, CH_2), 6.80 (d, 1H, J 8.4), 7.49 (dd, 1H, J 8.4, 2.2), 8.02 (d, 1H, J 2.2), 10.45 (broad s, 1H, NH), 12.02 (broad s, 1H, NH). δ_C

(100 MHz, $CDCl_3$): 17.6 (CH_3), 20.9 (CH_3), 28.4 (CH_3, Boc), 39.5 (CH_2), 63.3 (CH_2), 78.7 (q ^{t}Bu, Boc), 112.9 (CH Ar), 127.2 (q Ar), 139.4 (CH Ar), 145.4 (CH Ar), 150.8 (q Ar), 157.8 (q, CN), 164.1 (q CO, Boc), 170.9 (q CO). ν_{max} (ATR)/cm^{-1}: 2926, 1742 (C=O), 1641 (C=N), 1602, 1496, 1476, 1352, 1301, 1232, 1172, 1137, 1046, 808, 741. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{16}H_{25}N_4O_4$ 337.1876; Found: 337.1884.

1-(5-Methylpyridin-2-yl)-2-(*tert*-butoxycarbonyl)-3-(2-furanylmethyl)guanidine (8g) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-(2-furanylmethyl) thiourea. White solid (41%). M.p. 102-103 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.57 (s, 9H, CH_3, Boc), 2.28 (s, 3H, CH_3), 4.76 (d, 1H, J 4.8, CH_2), 6.30 (d, 1H, J 3.1, Ar), 6.36 (m, 1H, Ar), 6.79 (d, 1H, J 8.4, Ar), 7.41 (s, 1H, Ar), 7.47 (d, 1H, J 8.4, Ar), 8.01 (s, 1H, Ar), 10.57 (broad s, 1H, NH), 12.03 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 17.2 (CH_3), 28.0 (CH_3, Boc), 37.7 (CH_2), 78.3 (q ^{t}Bu, Boc), 106.6 (CH Ar), 109.9 (CH Ar), 112.3 (CH Ar), 126.7 (q Ar), 139.0 (CH Ar), 141.6 (CH Ar), 145.1 (CH Ar), 150.3 (q Ar), 151.1 (q Ar), 157.0 (q, CN), 163.7 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3005 (NH), 2963, 2981, 2929, 1640 (C=O), 1620 (C=N), 1599, 1566, 1506, 1493, 1482, 1427, 1386, 1348, 1336, 1299, 1262, 1252, 1236, 1214, 1167, 1153, 1122, 1085, 1059, 1036, 976, 964, 801, 772, 739, 698, 670. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{17}H_{23}N_4O_3$ 331.1770; Found: 331.1764.

1-(5-Methylpyridin-2-yl)-2-(*tert*-butoxycarbonyl)-3-(propyl)guanidine (8h) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-propyl thiourea. White solid (63%) as a white solid. M.p. 102-104 °C. δ_H (600 MHz, $CDCl_3$): 0.98 (t, 3H, J 7.4, CH_3), 1.51 (s, 9H, CH_3, Boc), 1.62 (app. sex, 2H, J 7.6, 7.2, CH_2), 2.24 (s, 3H, CH_3), 3.46 (m, 2H, CH_2), 6.72 (d, 1H, J 8.4, Ar), 7.42 (dd, 1H, J 8.4, 2.1, Ar), 7.98 (d, 1H, J 2.1, Ar), 10.17 (broad s, 1H, NH), 11.97 (broad s, 1H, NH). δ_C (150 MHz, $CDCl_3$): 11.5 (CH_3), 17.5 (CH_3), 22.5 (CH_2), 28.4 (CH_3, Boc), 42.4 (CH_2), 78.4 (q ^{t}Bu, Boc), 112.7 (CH Ar), 126.7 (q Ar), 139.2 (CH Ar), 145.3 (CH Ar), 150.9 (q Ar), 157.5 (q CO, Boc), 164.2 (q, CN). ν_{max} (ATR)/cm^{-1}: 3355 (NH), 2965, 2930, 2875, 1712 (C=O), 1638 (C=N), 1597, 1562, 1495, 1474, 1347, 1300, 1245, 1172, 1154, 1125, 1056, 1026, 961, 909, 821, 805, 774, 739, 665. HRMS (ESI^+) *m/z*: $[M + Na]^+$ Calcd. for $C_{15}H_{24}N_4O_2Na$ 315.1797; Found: 315.1792.

1-(5,6,7,8-Tetrahydroquinolin-2-yl)-2,3-di(*tert*-butoxycarbonyl)guanidine (9a) – Procedure A with *N,N'-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea. White powder (90%). Mp. 164-165 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.52 (s, 18H, CH_3, Boc), 1.78 (m, 2H, CH_2), 1.84 (m, 2H, CH_2), 2.70 (t, 2H, J 6.3, 6.1, CH_2), 2.78 (t, 2H, J 6.1, 6.3, CH_2), 7.35 (d,

1H, J 8.3, Ar), 8.04 (broad s, 1H, Ar), 10.64 (broad s, 1H, NH), 11.54 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 22.7 (CH_2), 22.9 (CH_2), 28.00 (CH_3, Boc), 28.02 (CH_2), 28.04 (CH_3, Boc), 32.0 (CH_2), 79.6 (q ^{t}Bu, Boc), 83.6 (q ^{t}Bu, Boc), 113.6 (CH Ar), 128.3 (q Ar), 138.7 (CH Ar), 147.6 (q Ar), 152.6 (q CO, Boc), 152.0 (q, Gua), 155.4 (q Ar), 163.3 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3251 (NH), 2979, 1714 (C=O), 1645 (C=N), 1629, 1588, 1565, 1449, 1395, 1369, 1354, 1325, 1313, 1279, 1247, 1231, 1151, 1112, 1058, 1029, 996, 941, 899, 874, 864, 840, 804, 755, 713. HRMS (ESI$^+$) *m/z*: $[M + H]^+$ Calcd. for $C_{20}H_{31}N_4O_4$ 391.2345; Found: 391.2342.

1-(5,6,7,8-Tetrahydroquinolin-2'-yl)-2,3-di(*tert*-butoxycarbonyl)-2-iminoimidazolidine (9b) – Procedure A with *N,N'*-di-(*tert*-butoxycarbonyl) imidazolidine-2-thione. Colourless oil (81%). δ_H (400 MHz, $CDCl_3$): 1.44 (s, 18H, CH_3, Boc), 1.71-1.80 (m, 4H, CH_2), 2.66 (app. t, 2H, J 5.9, 6.1, CH_2), 2.72 (app. t, 2H, J 6.1, 6.3, CH_2), 3.82 (s, 4H, CH_2), 6.75 (d, 1H, J 8.1, Ar), 7.26 (d, 1H, J 8.1, Ar). δ_C (100 MHz, $CDCl_3$): 23.0 (CH_2), 23.2 (CH_2), 27.8 (CH_3, Boc), 28.2 (CH_2), 32.5 (CH_2), 42.7 (2 CH_2), 82.3 (q ^{t}Bu, Boc), 115.7 (CH Ar), 125.5 (q Ar), 138.4 (CH Ar), 140.3 (q Ar), 150.0 (q Ar), 154.4 (q CO, Boc), 157.9 (q, Imi). ν_{max} (ATR)/cm^{-1}: 2977, 2932, 1752, 1702 (C=O), 1589, 1586, 1458, 1366, 1352, 1291, 1248, 1145, 1104, 1039, 995, 977, 936, 847, 833, 821, 767, 729, 696. HRMS (ESI$^+$) *m/z*: $[M + H]^+$ Calcd. for $C_{22}H_{33}N_4O_4$ 417.2502; Found: 417.2494.

1-(5,6,7,8-Tetrahydroquinolin-2-yl)-2-(*tert*-butoxycarbonyl)-3-(phenyl)guanidine (9e) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-phenyl thiourea. White solid (88%) identified as a mixture of isomers. M.p. 150-152 °C. δ_H (400 MHz, $CDCl_3$): 1.58 (s, 9H, CH_3, Boc), 1.80-1.98 (m, 4H, CH_2), 2.74 (app. t, 2H, J 6.3, 5.8, CH_2), 2.91 (app. t, 2H, J 6.4, 5.9, CH_2), 6.69 (d, 1H, J 8.1, Ar), 7.10 (t, 1H, J 7.3, Ar), 7.36 (app. t, 2H, J 8.0, 7.3, Ar), 7.39 (d, 1H, J 8.1, Ar), 7.71 (d, 2H, J 8.0, Ar), 12.09 (broad s, 1H, NH), 12.93 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 22.7 (CH_2), 27.9 (CH_2), 28.4 (CH_3, Boc), 32.1 (CH_2), 78.8 (q ^{t}Bu, Boc), 110.8 (CH Ar), 120.7 (q Ar), 121.8 (CH Ar), 123.8 (CH Ar), 128.7 (q Ar), 128.9 (CH Ar), 139.8 (CH Ar), 150.0 (q Ar), 153.5 (q Ar, Ar), 155.3 (q, CN), 164.5 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 2921, 2853, 1708 (C=O), 1687 (C=N), 1471, 1389, 1286, 716. HRMS (ESI$^+$) *m/z*: $[M + H]^+$ Calcd. for $C_{21}H_{27}N_4O_2$ 367.2134; Found: 367.2140.

1-(5,6,7,8-Tetrahydroquinolin-2-yl)-2-(*tert*-butoxycarbonyl)-3-(2-acetoxyethyl) guanidine (9f) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-(2-acetoxyethyl) thiourea. Colourless oil (69%). δ_H (400 MHz, $CDCl_3$): 1.52 (s, 9H, CH_3, Boc), 2.10 (s, 3H, CH_3), 1.75-

1.82 (m, 2H, CH_2), 1.82-1.90 (m, 2H, CH_2), 2.67 (app. t, 2H, J 6.3, 6.2, CH_2), 2.77 (app. t, 2H, J 6.5, 6.2, CH_2), 3.81 (app. q, 2H, J 5.4, 5.4, 5.0), 4.24 (t, 2H, J 5.4, CH_2), 6.59 (d, 1H, J 8.3), 7.30 (d, 1H, J 8.3), 10.72 (broad t, 1H, J 5.0, NH), 11.90 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 20.9 (CH_3), 22.7 (CH_2), 22.7 (CH_2), 27.8 (CH_2), 28.4 (CH_3, Boc), 32.2 (CH_2), 39.5 (CH_2), 63.7 (CH_2), 78.6 (q ^{t}Bu, Boc), 110.6 (CH Ar), 126.1 (q Ar), 139.5 (CH Ar), 150.2 (q Ar), 153.4 (q Ar), 157.9 (q, CN), 164.0 (q CO, Boc), 170.7 (q CO). ν_{max} (ATR)/cm^{-1}: 2936, 1743 (C=O), 1618 (C=N), 1592, 1459, 1335, 1236, 1172, 1138, 1046, 812, 736. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{19}H_{29}N_4O_4$ 377.2189; Found: 377.2197.

1-(5,6,7,8-Tetrahydroquinolin-2-yl]-2-(*tert*-butoxycarbonyl)-3-(2-furanylmethyl)guanidine (9g) – Procedure A with *N*-(*tert*-Butoxycarbonyl)-*N'*-(2-furanylmethyl) thiourea. White solid (65%). M.p. 79-82 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.56 (s, 9H, CH_3, Boc), 1.74-1.87 (m, 4H, 2 CH_2), 2.66 (m, 2H, CH_2), 2.70 (m, 2H, CH_2), 4.72 (d, 1H, J 4.6, CH_2), 6.29 (d, 1H, J 2.6, Ar), 6.34-6.37 (m, 1H, Ar), 6.59 (d, 1H, J 8.2, Ar), 7.29 (d, 1H, J 8.2, Ar), 7.41 (d, 1H, J 0.9, Ar), 10.98 (broad s, 1H, NH), 11.89 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 22.7 (CH_2), 22.8 (CH_2), 27.8 (CH_2), 28.5 (CH_3, Boc), 31.9 (CH_2), 38.3 (CH_2), 78.6 (q ^{t}Bu, Boc), 106.8 (CH Ar), 110.4 (CH Ar), 110.4 (CH Ar), 126.2 (q Ar), 139.4 (CH Ar), 142.0 (CH Ar), 150.2 (q Ar), 151.5 (q Ar), 153.5 (q Ar), 157.4 (q, CN), 164.0 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3119 (NH), 2979, 2938, 1713 (C=O), 1639 (C=N), 1614, 1597, 1585, 1561, 1507 1474, 1447, 1330, 1306, 1268, 1232, 117, 1092, 1007, 946, 884, 797, 778, 751, 734. HRMS (ESI^+) *m/z*: $[M + Na]^+$ Calcd. for $C_{20}H_{26}N_4O_3Na$ 393.1903; Found: 393.1893.

1-[5-(Ethylamino)pyridin-2'-yl]-2,3-di(*tert*-butoxycarbonyl)-2-iminoimidazolidine (10b) – Procedure A with *N,N'*-di-(*tert*-butoxycarbonyl) imidazolidine-2-thione. Red liquid (35%). δ_H (400 MHz, $CDCl_3$): 1.21 (t, 3H, J 7.0, CH_3), 1.52 (s, 18H, CH_3, Boc), 3.11 (q, 2H, J 7.0, CH_2), 3.75 (s, 4H, CH_2), 5.43 (broad s, 1H, NH), 6.93 (dd, 1H, J 8.9, 3.0, Ar), 7.69 (d, 1H, 8.9, Ar), 7.80 (d, 1H, J 3.0, Ar). δ_C (100 MHz, $CDCl_3$): 14.8 (CH_3), 28.2 (CH_3, Boc), 38.9 (CH_2), 45.3 (2 CH_2), 82.4 (q ^{t}Bu, Boc), 114.3 (CH Ar), 122.4 (CH Ar), 132.8 (CH Ar), 140.2 (q Ar), 149.9 (q Ar), 152.2 (q CO, Boc), 155.0 (q, Imi). ν_{max} (ATR)/cm^{-1}: 3375 (NH), 2977, 2933, 1804, 1740, 1712, 1698 (C=O), 1676 (C=N), 1604, 1571, 1502, 1477, 1457, 1367, 1303, 1268, 1245, 1144, 1081, 973, 848, 834, 813, 765, 721, 686. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{20}H_{32}N_5O_4$ 406.2454; Found: 406.2450.

1-(Pyridin-3-yl)-2,3-di(*tert*-butoxycarbonyl)guanidine (11a) – Procedure A with *N,N′-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea. Off-white powder (89%). Mp. 136-138 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.50 (s, 9H, Boc CH_3), 1.54 (s, 9H, Boc CH_3), 7.28 (dd, 1H, J 8.3, 4.1, Ar), 8.21 (dd, 1H, J 8.3, 1.5, Ar), 8.34 (d, 1H, J 4.1, Ar), 8.67 (d, 1H, J 1.5, Ar), 10.41 (broad s, 1H, NH), 11.61 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 27.6 (CH_3, Boc), 27.6 (CH_3, Boc), 79.6 (q ^{t}Bu, Boc), 83.7 (q ^{t}Bu, Boc), 123.1 (CH Ar), 129.2 (CH Ar), 133.4 (q Ar), 142.7 (CH Ar), 145.0 (q Ar), 152.8 (q CO, Boc), 153.3 (q, Gua), 162.8 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3146 (NH), 2981, 1725 (C=O), 1636 (C=N), 1587, 1561, 1477, 1396, 1367, 1329, 1280, 1252, 1226, 1151, 1132, 1101, 1057, 1029, 942, 883, 845, 801, 773, 746, 719, 702, 656. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{16}H_{25}N_4O_4$ 337.1876; Found: 337.1870.

1-(Pyridin-3'-yl)-2,3-di(*tert*-butoxycarbonyl)-2-iminoimidazolidine (11b) – Procedure A with *N,N'*-di-(*tert*-butoxycarbonyl) imidazolidine-2-thione. Colourless crystals (87%). Mp. 99-101 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.11 (s, 18H, CH_3, Boc), 3.62 (s, 4H, CH_2), 6.93 (dd, 1H, J 7.9, 4.6, Ar), 7.04 (d, 1H, J 7.9, Ar), 7.94 (d, 1H, J 3.9, Ar), 8.04 (broad s, 1H, Ar). δ_C (100 MHz, $CDCl_3$): 27.2 (CH_3, Boc), 42.7 (2 CH_2), 82.3 (q ^{t}Bu, Boc), 122.6 (CH Ar), 127.1 (CH Ar), 140.5 (q Ar), 142.5 (CH Ar), 142.5 (CH Ar), 144.5 (q CO, Boc), 149.1 (q, Imi). ν_{max} (ATR)/cm^{-1}: 2979, 2934, 1758, 1702 (C=O), 1670 (C=N), 1579, 1476, 1458, 1412, 1367, 1297, 1248, 1144, 1041, 1020, 977, 913, 846, 808, 767, 727, 709. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{18}H_{27}N_4O_4$ 363.2032; Found: 363.2033.

1-(6-Chloropyridin-3-yl)-2,3-di(*tert*-butoxycarbonyl)guanidine (12a) – Procedure A with *N,N′-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea. White powder (79%). Mp. 118-120 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.50 (s, 9H, CH_3, Boc), 1.55 (s, 9H, CH_3, Boc), 7.31 (d, 1H, J 8.7, Ar), 8.22 (dd, 1H, J 8.7, 2.8, Ar), 8.47 (d, 1H, J 2.8, Ar), 10.44 (broad s, 1H, NH), 11.60 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 28.0 (CH_3, Boc), 28.1 (CH_3, Boc), 80.1 (q ^{t}Bu, Boc), 84.4 (q ^{t}Bu, Boc), 124.1 (CH Ar), 132.5 (CH Ar), 133.0 (q Ar), 142.7 (CH Ar), 146.3 (q Ar), 153.3 (q CO, Boc), 153.6 (q, Gua), 163.1 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3249 (NH), 2981, 1741, 1716 (C=O), 1633 (C=N), 1576, 1559, 1476, 1455, 1407, 1383, 1367, 1322, 1287, 1252, 1235, 1219, 1142, 1123, 1101, 1059, 1028, 1006, 967, 917, 880, 848, 837, 801, 782, 743, 728, 685. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{16}H_{24}{}^{35}ClN_4O_4$ 371.1486; Found: 371.1488.

1-(6-Methylpyridin-3-yl)-2,3-di(*tert*-butoxycarbonyl)guanidine (13a) – Procedure A with *N,N′-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea. White powder (88%). Mp. 102 ºC, clean

melt. δ_H (400 MHz, $CDCl_3$): 1.48 (s, 9H, Boc CH_3), 1.53 (s, 9H, Boc CH_3), 2.50 (s, 3H, CH_3), 7.12 (d, 1H, J 8.0, Ar), 8.03 (d, 1H, J 8.0, Ar), 8.53 (s, 1H, Ar), 10.28 (broad s, 1H, NH), 11.61 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 23.8 (CH_3), 28.0 (CH_3, Boc), 28.1 (CH_3, Boc), 79.8 (q ^{t}Bu, Boc), 84.0 (q ^{t}Bu, Boc), 123.0 (CH Ar), 130.3 (CH Ar), 131.1 (q Ar), 142.7 (CH Ar), 153.3 (q Ar), 153.8 (q CO, Boc), 154.4 (q, Gua), 163.3 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3244 (NH), 2978, 1720 (C=O), 1632 (C=N), 1585, 1560, 1475, 1454, 1404, 1374, 1324, 1305, 1289, 1268, 1252, 1230, 1151, 1136, 1107, 1058, 1025, 882, 856, 838, 803, 758, 749, 709. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{17}H_{27}N_4O_4$ 351.2032; Found: 351.2028.

1-(5,6,7,8-tetrahydroquinolin-3-yl)-2,3-di(*tert*-butoxycarbonyl)guanidine (14a) – Procedure A with *N,N'-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea. White powder (87%). Mp. 124-125 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.50 (s, 9H, CH_3, Boc), 1.55 (s, 9H, CH_3, Boc), 1.77-1.83 (m, 2H, CH_2), 1.86-1.92 (m, 2H, CH_2), 2.80 (app. t, 2H, J 6.4, 6.1, CH_2), 2.89 (app. t, 2H, J 6.4, CH_2), 7.79 (d, 1H, J 2.0, Ar), 8.44 (d, 1H, J 2.0, Ar), 10.25 (broad s, 1H, NH), 11.63 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 22.5 (CH_2), 23.1 (CH_2), 28.1 (CH_3, Boc), 28.1 (CH_3, Boc), 28.9 (CH_2), 32.0 (CH_2), 79.8 (q ^{t}Bu, Boc), 84.0 (q ^{t}Bu, Boc), 130.7 (CH Ar), 131.1 (q Ar), 132.4 (q Ar), 140.8 (CH Ar), 153.3 (q CO, Boc), 153.7 (q Ar), 153.9 (q, Gua), 163.3 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3250 (NH), 2982 (NH), 2933, 1725 (C=O), 1634 (C=N), 1596, 1552, 1467, 1400, 1368, 1328, 1280, 1249, 1228, 1153, 1105, 1059, 1032, 943, 909, 877, 855, 808, 760, 721, 711. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{20}H_{31}N_4O_4$ 391.2345; Found: 391.2350.

1-(5,6,7,8-Tetrahydroquinolin-3'-yl)-2,3-di(*tert*-butoxycarbonyl)-2-iminoimidazolidine (14b) – Procedure A with *N,N'*-di-(*tert*-butoxycarbonyl) imidazolidine-2-thione. White solid (85%). Mp. 128-131 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.21 (s, 18H, CH_3, Boc), 1.60-1.66 (m, 2H, CH_2), 1.68-1.75 (m, 2H, CH_2), 2.57 (app. t, 2H, J 6.0, 6.3, CH_2), 2.71 (app. t, 2H, J 6.0, 6.3, CH_2), 3.71 (s, 4H, CH_2), 6.83 (d, 1H, J 2.4, Ar), 7.94 (d, 1H, J 2.4, Ar). δ_C (100 MHz, $CDCl_3$): 22.7 (CH_2), 23.3 (CH_2), 27.8 (CH_3, Boc), 28.7 (CH_2), 31.7 (CH_2), 43.1 (2 CH_2), 82.8 (q ^{t}Bu, Boc), 128.1 (CH Ar), 131.3 (q Ar), 140.2 (q Ar), 140.5 (CH Ar), 142.2 (q Ar), 149.9 (q CO, Boc), 150.6 (q, Imi). ν_{max} (ATR)/cm^{-1}: 2979, 2921, 2858, 1752, 1754, 1719(C=O), 1649 (C=N), 1594, 1560, 1465, 1368, 1333, 1293, 1257, 1233, 1202, 1187, 1107, 1037, 1005, 977, 947, 921, 844, 823, 786, 767, 746, 735, 712, 700, 682. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{22}H_{33}N_4O_4$ 417.2502; Found: 417.2496.

1-[6-(Ethylamino)pyridin-3-yl]-2,3-di(*tert*-butoxycarbonyl)guanidine (15a) – Procedure A with *N,N'-bis*-(*tert*-butoxycarbonyl)-*S*-methylisothiourea. Colourless crystals (91%). Mp. 136-138 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 1.27 (t, 3H, J 7.0, CH_3), 1.50 (s, 9H, CH_3, Boc), 1.56 (s, 9H, CH_3, Boc), 3.31 (m, 2H, CH_2), 4.44 (t, 1H, J 5.3, NH, NHEt), 6.40 (d, 1H, J 8.9, Ar), 7.77 (dd, 1H, J 8.9, 2.6, Ar), 8.15 (d, 1H, J 2.6, Ar), 10.03 (broad s, 1H, NH), 11.65 (broad s, 1H, NH). δ_C (100 MHz, $CDCl_3$): 14.9 (CH_3), 28.1 (CH_3, Boc), 28.2 (CH_3, Boc), 37.2 (CH_2), 79.5 (q ^{t}Bu, Boc), 83.6 (q ^{t}Bu, Boc), 106.5 (CH Ar), 123.7 (q Ar), 133.6 (CH Ar), 142.7 (CH Ar), 153.4 (q CO, Boc), 154.2 (q, Gua), 156.5 (q Ar), 163.6 (q CO, Boc). ν_{max} (ATR)/cm^{-1}: 3285 (NH), 3269 (NH), 3124 (NH), 2976, 2932, 1792, 1722 (C=O), 1605 (C=N), 1561, 1517, 1475, 1448, 1389, 1325, 1280, 1246, 1227, 1150, 1122, 1105, 1059, 954, 883, 843, 814, 763. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{18}H_{30}N_5O_4$ 380.2298; Found: 380.2291.

1-(6-(Ethylamino)pyridin-3'-yl)-2,3-di(*tert*-butoxycarbonyl)-2-iminoimidazolidine (15b) – Procedure A with *N,N'*-di-(*tert*-butoxycarbonyl) imidazolidine-2-thione. White solid (64%). Mp. 121-123 ºC, clean melt. δ_H (400 MHz, $CDCl_3$): 0.98 (t, 3H, J 7.1, CH_3), 1.14 (s, 18H, CH_3, Boc), 3.04 (q, 2H, J 7.1, CH_2), 3.59 (s, 4H, CH_2), 4.43 (broad s, 1H, NH), 6.12 (d, 1H, J 8.8, Ar), 6.95 (dd, 1H, 8.8, 2.6, Ar), 7.63 (dd, 1H, J 2.6, 0.3, Ar). δ_C (100 MHz, $CDCl_3$): 14.7 (CH_3), 27.7 (CH_3, Boc), 37.0 (CH_2), 43.0 (2 CH_2), 82.4 (q ^{t}Bu, Boc), 106.1 (CH Ar), 130.6 (CH Ar), 135.2 (q Ar), 139.0 (q Ar), 141.0 (CH Ar), 150.0 (q CO, Boc), 154.9 (q, Imi). ν_{max} (ATR)/cm^{-1}: 3375 (NH), 2977, 2933, 1804, 1740, 1712 (C=O), 1698, 1676 (C=N), 1604, 1571, 1502, 1477, 1457, 1367, 1303, 1268, 1245, 1144, 1081, 973, 848, 834, 813, 765, 721, 686. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{20}H_{32}N_5O_4$ 406.2454; Found: 406.2445.

***N*-Phenyl-1,4-dihydroquinazolin-2-amine (22i)** – Procedure C with *S*-Methyl-*N*-phenyl dithiocarbamate. White solid (76%). M.p. 127-128 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 4.87 (d, 2H, J 5.5, CH_2), 6.25 (broad s, 1H, NH), 6.67 (m, 2H, Ar), 7.04 (dd, J 7.7, 1.4, Ar), 7.13 (td, 1H, J 7.7, 1.4, Ar), 7.21 (dd, 2H, J 7.4, 1.1, Ar), 7.27 (t, 1H, J 7.7, Ar), 7.39 (t, 2H, J 7.4, Ar), 8.23 (broad s, 1H, NH). δ_C (100MHz, $CDCl_3$): 47.4 (CH_2), 115.8 (CH Ar), 117.8 (CH Ar), 120.5 (q Ar), 125.1 (CH Ar), 127.3 (CH Ar), 129.5 (CH Ar), 130.2 (CH Ar), 130.6 (CH Ar), 135.9 (q Ar), 145.7 (q Ar), 179.9 (q, CN). ν_{max} (ATR)/cm^{-1}: 3469, 3358 (NH), 3168 (NH), 3005, 1619 (C=N), 1592, 1524, 1492 (C=N), 1455, 1425, 1352, 1315, 1299, 1266, 1242, 1197, 1175, 1112, 1071, 1028, 965, 746, 691. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{14}H_{14}N_3$ 224.1188; Found: 224.1186.

***N*-(2-acetoxyethyl)-1,4-dihydroquinazolin-2-amine (22j)** – Procedure C with *S*-Methyl-*N*-(2-acetoxyethyl) dithiocarbamate. White solid (60%). M.p. 56-58 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 1.94 (s, 3H, CH_3), 3.65 (broad s, 2H, CH_2), 4.07 (t, 2H, J 5.3, CH_2), 4.22 (broad s, 1H, NH), 4.54 (broad s, 2H, CH_2), 6.61 (broad s, NH), 6.64 (m, 1H, Ar), 6.71 (app. t, 1H, J 5.4, Ar), 6.96 (d, 1H, J 7.3, Ar), 7.06 (td, 1H, J 7.6, 1.3, Ar). δ_C (100MHz, $CDCl_3$): 20.9 (CH_3), 43.5 (CH_2), 46.0 (CH_2), 63.1 (CH_2), 116.0 (CH Ar), 121.4 (q Ar), 118.4 (CH Ar), 129.3 (CH Ar), 130.5 (CH Ar), 145.2 (q Ar), 171.5 (q CO), 181.9 (q, CN). ν_{max} (ATR)/cm^{-1}: 3376, 3185 (NH), 3025 (NH), 2956, 2926, 1720 (C=O), 1632 (C=N), 1607, 1586, 1545, 1494, 1458, 1445, 1382, 1361, 1335, 1315, 1282, 1253, 1216, 1163, 1145, 1085, 1065, 1044, 1023, 924, 866, 813, 790, 755, 715, 676. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{12}H_{16}N_3O_2$ 234.1243; Found: 234.1239.

***N*-(2-Furanylmethyl)-1,4-dihydroquinazolin-2-amine (22k)** – Procedure C with *S*-Methyl-*N*-(2-furanylmethyl) dithiocarbamate. Yellow solid (63%). M.p. 69-71 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 4.57 (s, 2H, CH_2), 4.60 (s, 2H, CH_2), 6.23 (d, 1H, J 3.1, Ar), 6.30 (app. t, 1H, J 2.4, Ar), 6.32 (broad s, 1H, NH), 6.62 (d, 1H, J 7.6, Ar), 6.68 (t, 1H, J 7.4, Ar), 6.73 (t, 1H, J 5.1, NH), 6.94 (d, 1H, J 7.4, Ar), 7.10 (t, 1H, J 7.6, Ar), 7.32 (app. t, 1H, J 0.7, Ar). δ_C (100MHz, $CDCl_3$): 41.4 (CH_2), 46.2 (CH_2), 108.1 (CH Ar), 110.6 (CH Ar), 116.1 (CH Ar), 118.6 (CH Ar), 121.6 (q Ar), 129.4 (CH Ar), 130.7 (CH Ar), 142.3 (CH Ar), 145.1 (q Ar), 150.6 (q Ar), 181.5 (q, CN). ν_{max} (ATR)/cm^{-1}: 3256 (NH), 2937, 1673, 1633, 1609 (C=N), 1542, 1489, 1451, 1376, 1332, 1197, 1147, 1092, 1054, 1045, 1011, 884, 833, 751, 725, 669, 658. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{13}H_{14}N_3O$ 228.1137; Found: 228.1131.

***N*-(*n*-Propyl)-1,4-dihydroquinazolin-2-amine (22l)** – Procedure C with *S*-Methyl-*N*-propyl dithiocarbamate. White solid (81%). M.p. 56-58 °C, clean melt. δ_H (400 MHz, $CDCl_3$): 0.88 (t, 3H, J 7.3, CH_3), 1.53 (app. s, 2H, J 7.3, CH_2), 3.28 (broad s, 1H, NH), 4.23 (broad s, 2H, CH_2), 4.64 (broad s, 2H, CH_2), 6.34 (broad s, NH), 6.62-6.70 (m, 2H, Ar), 7.00 (d, 1H, J 7.3, Ar), 7.09 (t, 1H, J 7.6, 1.3, Ar). δ_C (100MHz, $CDCl_3$): 11.4 (CH_3), 22.2 (CH_2), 46.0 (CH_2), 46.4 (CH_2), 116.0 (CH Ar), 118.4 (CH Ar), 121.3 (q Ar), 129.4 (CH Ar), 130.6 (CH Ar), 145.3 (q Ar), 181.1 (q, CN). ν_{max} (ATR)/cm^{-1}: 3224 (NH), 3063 (NH), 2961, 2930, 2873, 1627 (C=N), 1605, 1546, 1495, 1457, 1376, 1335, 1288, 1264, 1227, 1156, 1101, 1063, 944, 870, 749. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{11}H_{16}N_3$ 190.1344; Found: 190.1932.

***N*-(2-acetoxyethyl)-1,4-dihydropyrido[2,3-*d*]pyrimidin-2-amine (23j)** – Procedure C. Yellow oil (64%). δ_H (400 MHz, $CDCl_3$): 1.92 (s, 3H, CH_3), 3.70 (broad s, 2H, CH_2), 4.09

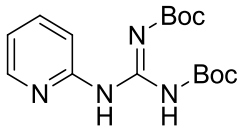
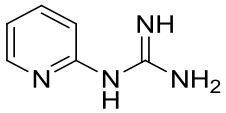
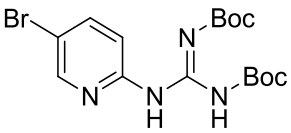
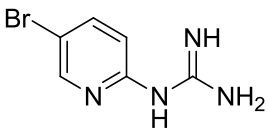
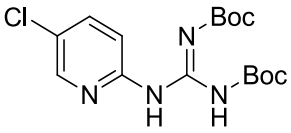
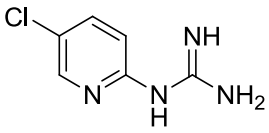
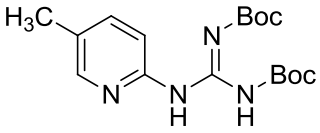
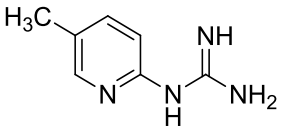
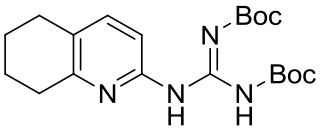
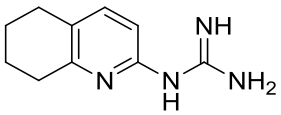
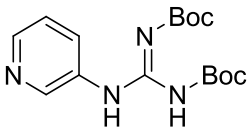
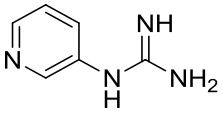
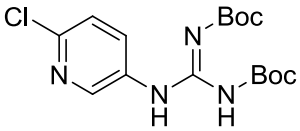
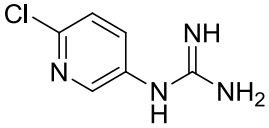
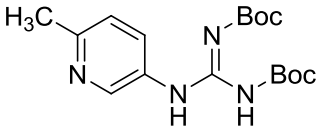
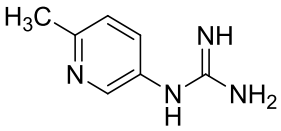
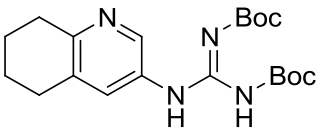
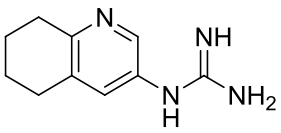
(m, 2H, CH_2) 4.62 (s, 2H, CH_2), 6.50 (t, 1H, J 4.0, 8.0, Ar), 6.81 (broad s, 1H, NH), 7.00 (broad s, 1H, NH), 7.29 (d, 1H, J 8.0, Ar), 7.80 (d, 1H, J 4.0, Ar). δ_C (100 MHz, $CDCl_3$): 20.8 (CH_3), 43.4 (CH_2), 45.6 (CH), 59.8 (CH_2), 113.6 (CH Ar), 116.2 (q Ar), 138.4 (CH Ar), 147.0 (CH Ar), 151.3 (q Ar), 171.4 (q CO), 182.7 (q CN). ν_{max} (ATR)/cm^{-1}: 3314 (NH), 2926, 1725 (C=O), 1622, 1596, 1543, 1446, 1367, 1224, 1977, 1040, 952, 773. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{11}H_{15}N_4O_2$ 235.1195; Found: 235.1199.

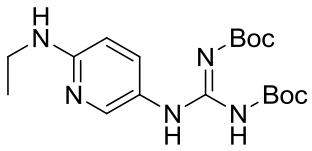
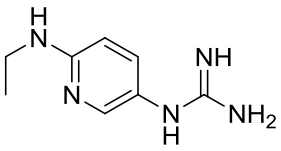
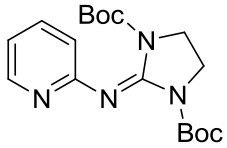
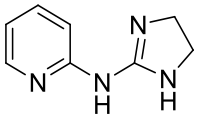
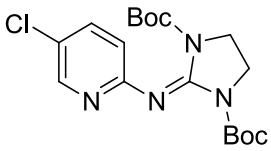
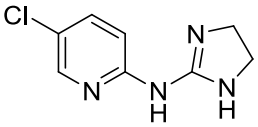
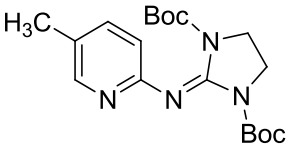
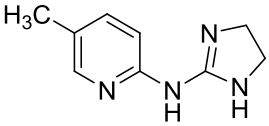
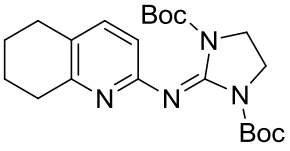
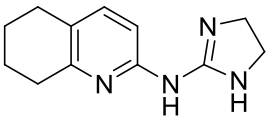
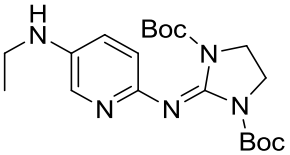
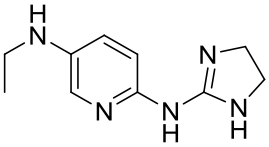
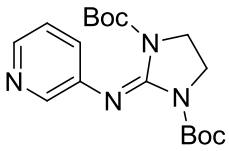
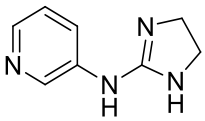
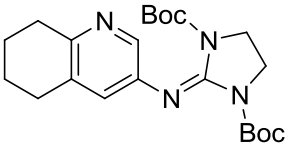
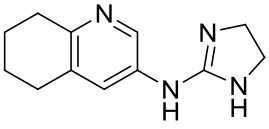
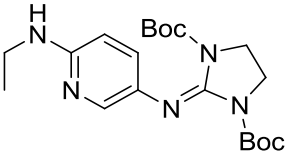
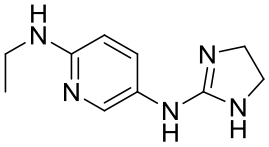
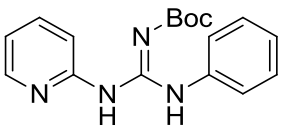
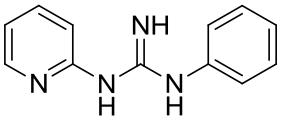
***N*-(Furan-2-ylmethyl)-1,4-dihydropyrido[2,3-*d*]pyrimidin-2-amine (23k)** – Procedure C. Yellow solid (51%). M.p. 185°C, clean melt. δ_H (400 MHz, $CDCl_3$): 4.63 (s, 2H, CH_2), 4.81 (s, 2H, CH_2), 6.23 (d, 1H, J 4.0, Ar), 6.26 (d, 1H, J 4.0, Ar), 6.50 (t, 1H, J 4.0, Ar), 6.59 (broad s, 1H, NH), 6.90 (broad s, 1H, NH), 7.25 (m, 2H, Ar), 7.83 (d, 1H, J 4.0, Ar). δ_C (100 MHz, $CDCl_3$): 41.4 (CH_2), 43.1 (CH_2), 107.1 (CH Ar), 108.1 (CH Ar), 113.1 (CH Ar), 114.2 (q Ar), 136.6 (CH Ar), 142.1 (CH Ar), 147.5 (CH Ar), 150.8 (q Ar), 171.1 (q Ar), 182.7 (q CN). ν_{max} (ATR)/cm^{-1}: 3235 (NH), 2921, 1650, 1598, 1534, 1501, 1488, 1443, 1336, 1328, 1245, 1189, 1098, 1035, 926, 883, 807, 770. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{12}H_{13}N_4O$ 229.1089; Found: 229.1090.

***N*-(1,3-Benzodioxol-5-ylmethyl)-1,4-dihydropyrido[2,3-*d*]pyrimidin-2-amine (23m)** – Procedure C. Yellow oil (39%). δ_H (400 MHz, $CDCl_3$): 4.46 (broad s, 2H, CH_2), 4.57 (s, 2H, CH_2), 5.82 (s, 2H, CH_2), 6.44 (t, 1H, J 4.0, Ar), 6.62 (s, 2H, Ar), 6.67 (s, 1H, Ar), 6.80 (broad s, 1H, NH), 7.05 (broad s, 1H, NH), 7.20 (d, 1H, J 4.0, Ar), 7.73 (d, 1H, J 4.0, Ar). δ_C (100 MHz, $CDCl_3$): 45.6 (CH_2), 48.0 (CH_2), 101.0 (CH_2), 108.2 (CH Ar), 108.9 (CH Ar), 113.4 (CH Ar), 116.4 (q Ar), 120.8 (CH Ar), 131.3 (q Ar), 138.4 (CH Ar), 146.8 (CH Ar), 146.9 (q Ar), 147.8 (q Ar), 157.1 (q Ar), 182.2 (q CN). ν_{max} (ATR)/cm^{-1}: 3229 (NH), 2921, 2852, 1783, 1653, 1543, 1500, 1488, 1443, 1377, 1327, 1245, 1097, 1037, 924, 887, 805, 769. HRMS (ESI^+) *m/z*: $[M + H]^+$ Calcd. for $C_{15}H_{15}N_4O_2$ 283.1191; Found: 283.1195.

5. Yields obtained for all compounds prepared

Table S1. Yields (% of purified material) obtained in the preparation of the Boc-protected derivatives (stage A) and final hydrochloride salts (stage B) starting from aminopyridines.

Cmpd	Structure	A	Cmpd	Structure	B
5a		79	**5c**		71
6a		80	**6c**		74
7a		35	**7c**		85
8a		71	**8c**		84
9a		90	**9c**		87
11a		89	**11c**		85
12a		79	**12c**		92
13a		88	**13c**		82
14a		87	**14c**		87

15a		91	**15c**		99
5b		56	**5d**		92
7b		56	**7d**		96
8b		75	**8d**		93
9b		81	**9d**		93
10b		35	**10d**		93
11b		87	**11d**		98
14b		85	**14d**		91
15b		64	**15d**		95
5e		63	**5i**		90

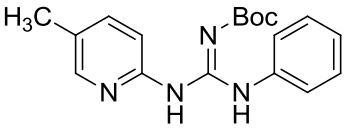
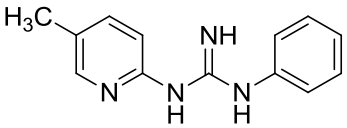
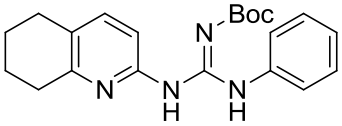
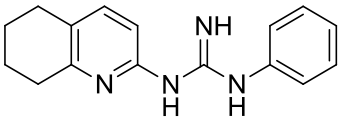
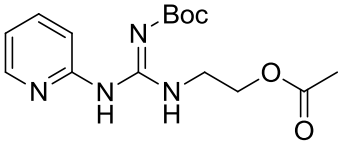
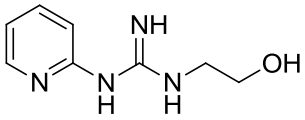
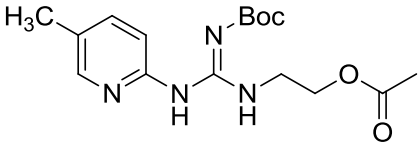
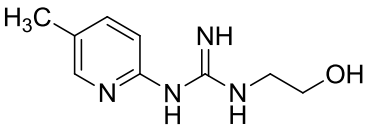
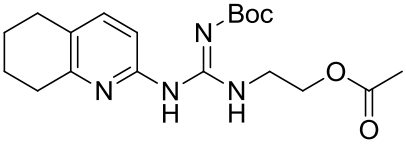
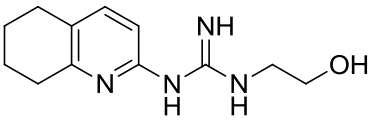
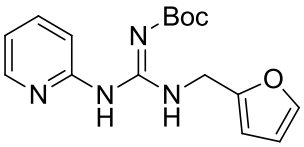
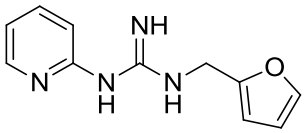
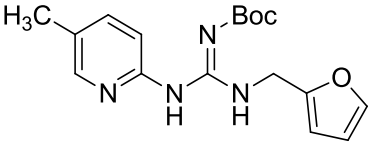
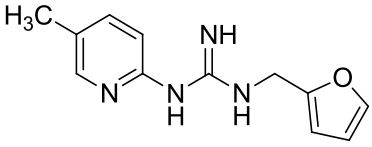
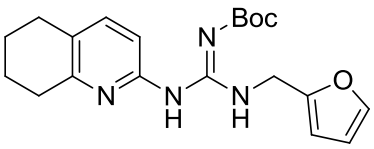
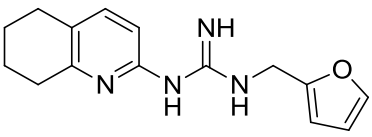
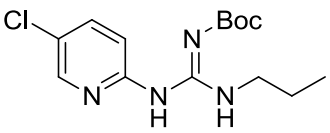
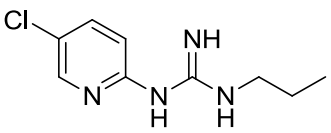
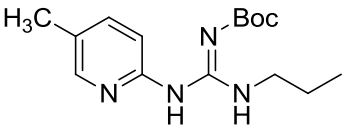
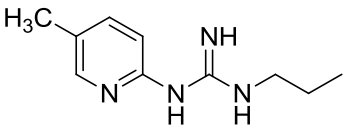
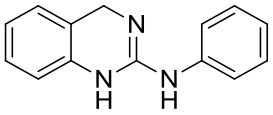
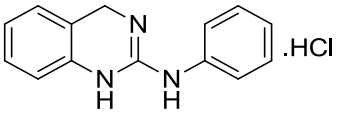
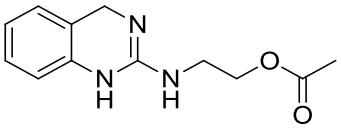
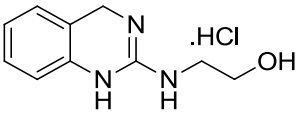
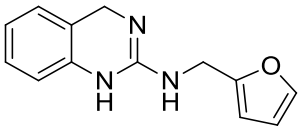
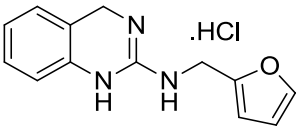
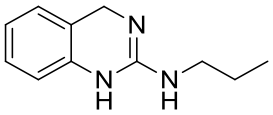
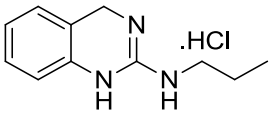
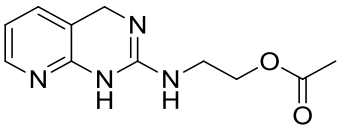
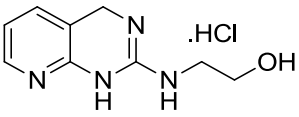
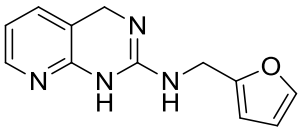
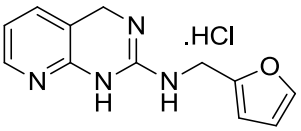
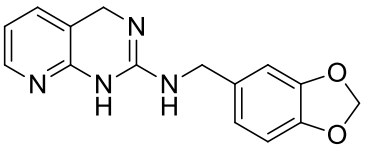
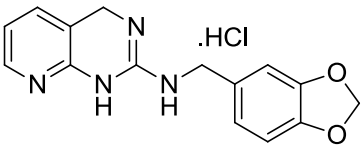
8e		89	**8i**		86
9e		88	**9i**		86
5f		43	**5j**		83
8f		54	**8j**		87
9f		69	**9j**		81
5g		61	**5k**		82
8g		41	**8k**		95
9g		65	**9k**		86
7h		39	**7l**		93
8h		63	**8l**		90

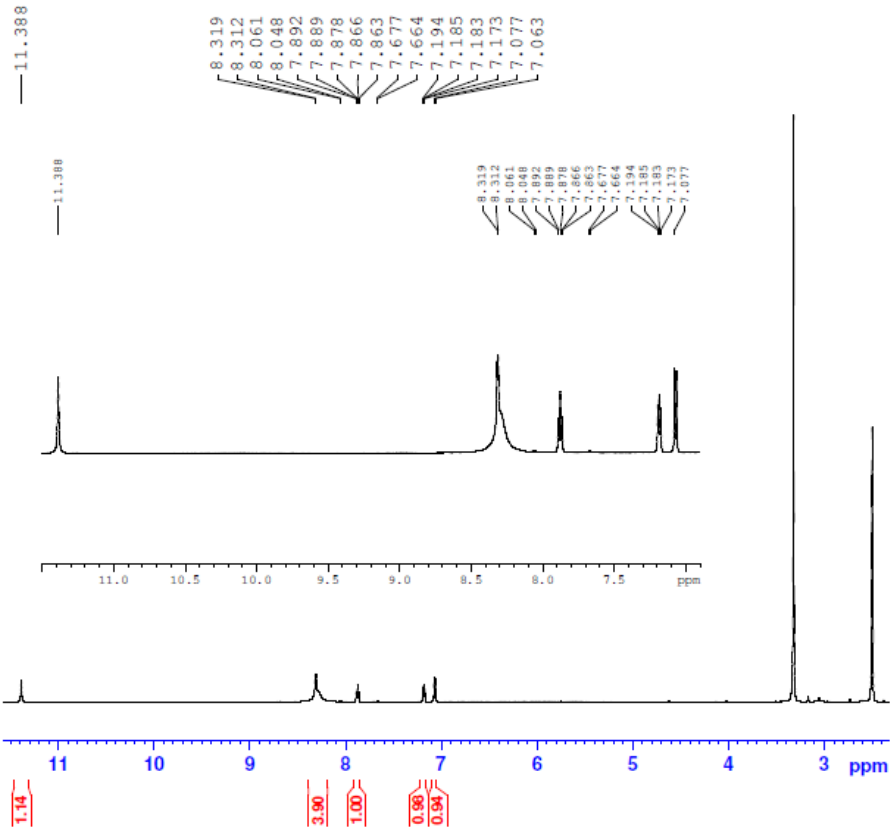
Table S2. Yields (% of purified material) obtained in the preparation of the neutral derivatives **19-25m** (stage A) and final hydrochloride salts **19-25n** (stage B).

Cmpd	Structure	A	Cmpd	Structure	B
22i		76	**19i**		93[a]
22j		60	**19j**		95[b]
22k		63	**19k**		30[a]
22l		81	**19l**		90[a]
23j		64	**20j**		98[b]
23k		51	**20k**		86[a]
23m		39	**20m**		26[a]

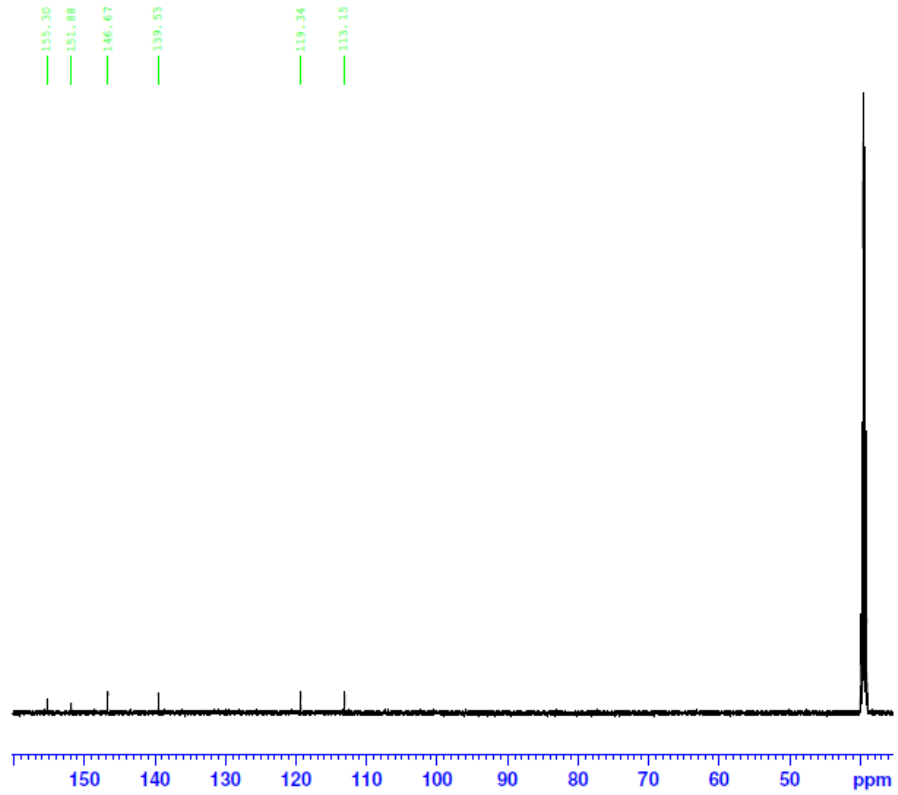
[a] 4M HCl in 1,4-dioxane, [b] 1.25M HCl in CH_3OH.

6. NMR spectra of final hydrochloride salts

1-(Pyridin-2-yl)guanidine hydrochloride (5c)

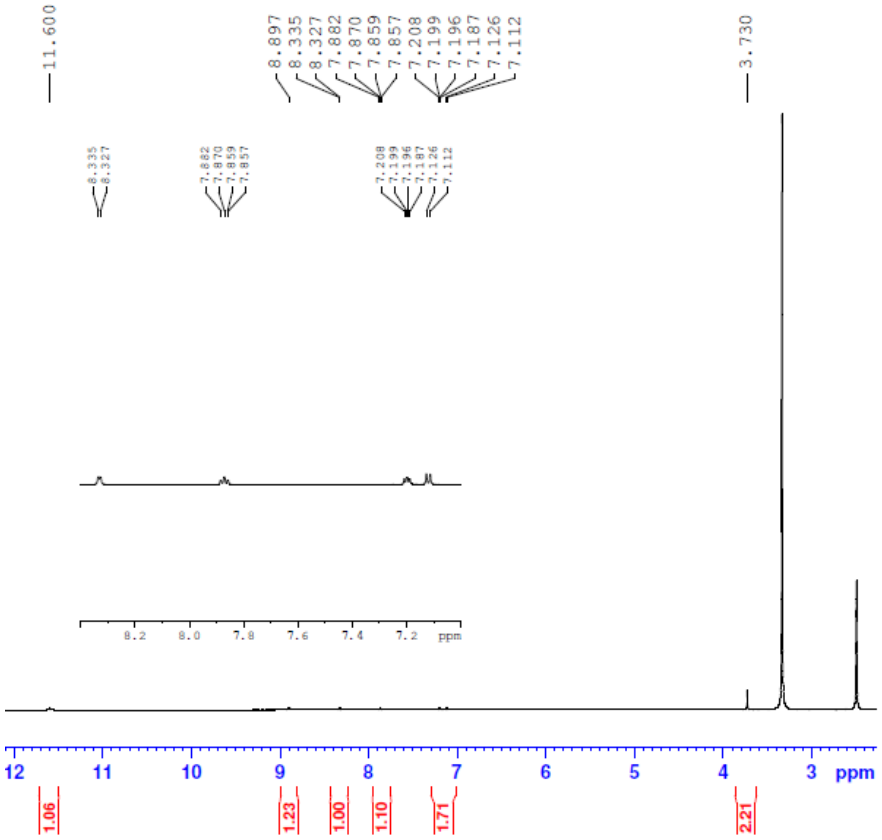



```
NAME              bki70cx
EXPNO                   1
PROCNO                  1
Date_            20100429
Time                 9.31
INSTRUM             AV600
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     2
SWH           12335.526 Hz
FIDRES        0.188225 Hz
AQ            2.6564426 sec
RG                     8
DW               40.533 usec
DE                6.00 usec
TE               300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 =======
NUC1                  1H
P1                 8.21 usec
PL1                4.05 dB
PL1W        6.03017378 W
SFO1       600.1337060 MHz
SI                 32768
SF         600.1300071 MHz
WDW                   EM
SSB                    0
LB                0.30 Hz
GB                     0
PC                1.00
```

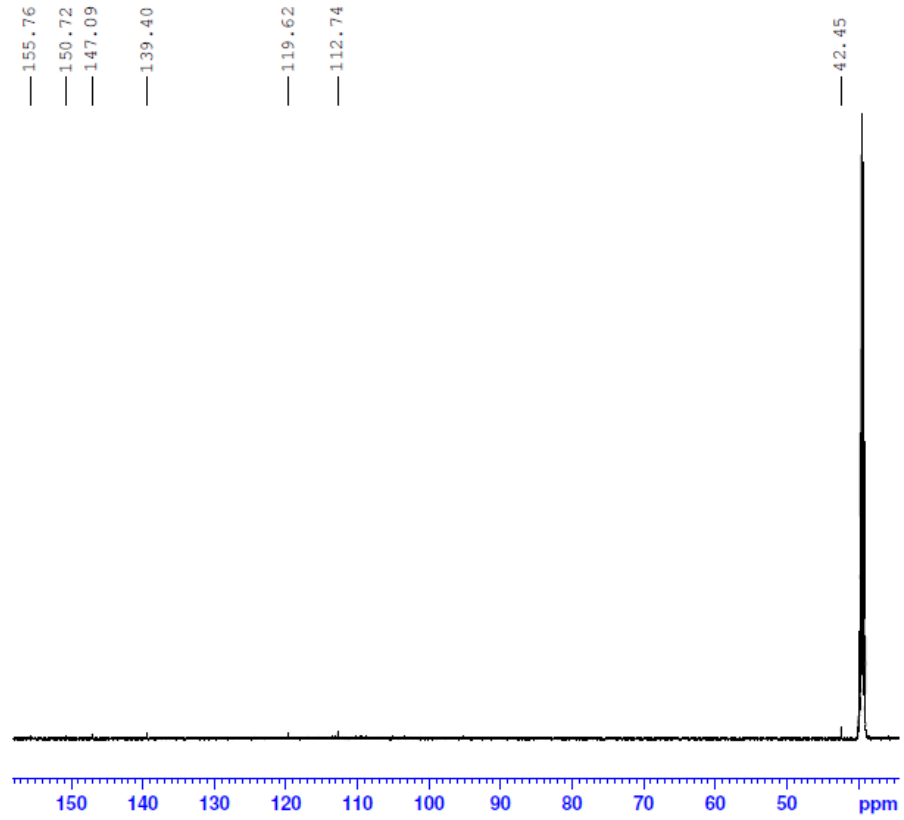



```
NAME              bki70cx
EXPNO                  13
PROCNO                  1
Date_            20100429
Time                 9.17
INSTRUM             AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   175
DS                     4
SWH           36057.691 Hz
FIDRES        0.550197 Hz
AQ            0.9088159 sec
RG                  2050
DW               13.867 usec
DE                6.00 usec
TE               300.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                  400

======== CHANNEL f1 =======
NUC1                 13C
P1                13.20 usec
PL1               -2.00 dB
PL1W       121.82079315 W
SFO1       150.9178990 MHz

======== CHANNEL f2 =======
CPDPRG2           waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                4.05 dB
PL12              24.27 dB
PL13              24.27 dB
PL2W        6.03017378 W
PL12W       0.05732312 W
PL13W       0.05732312 W
SFO2       600.1324000 MHz
SI                 32768
SF         150.9028853 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                1.40
```

1-(Pyridin-2’-yl)-2-iminoimidazolidine hydrochloride (5d)

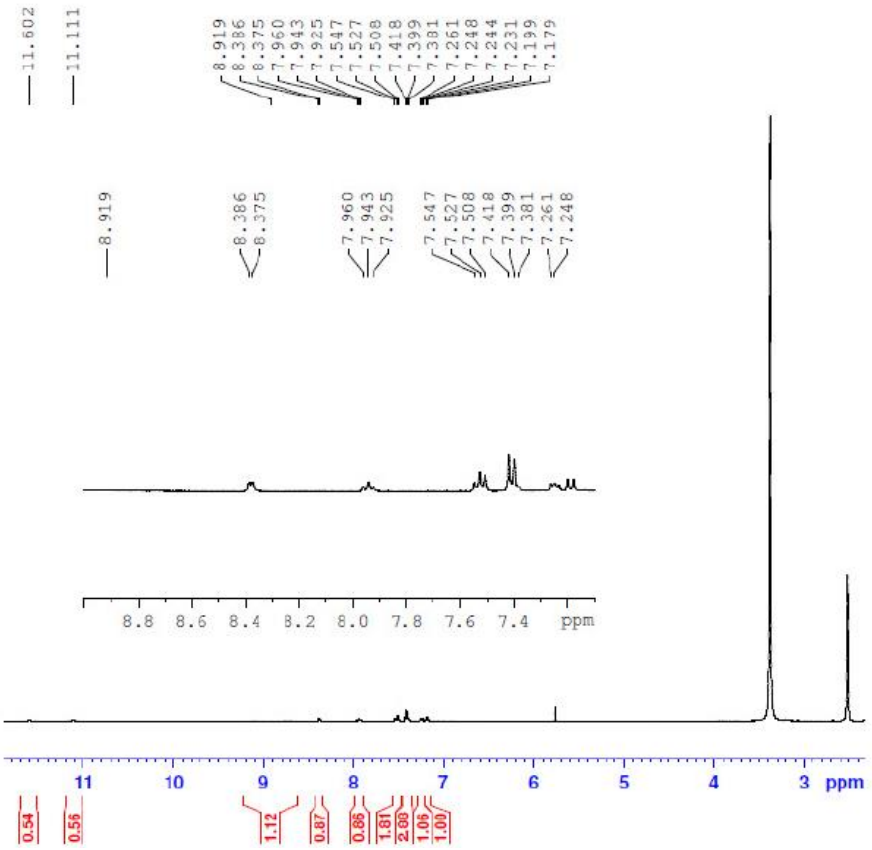



```
NAME            bki283ax
EXPNO                1
PROCNO               1
Date_         20110729
Time              8.52
INSTRUM           AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                  16
DS                   2
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                   8
DW               20.800 usec
DE                6.00 usec
TE              298.0 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               7.84 usec
PL1              4.05 dB
PL1W       6.03017378 W
SFO1      600.1337060 MHz
SI               32768
SF        600.1300067 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

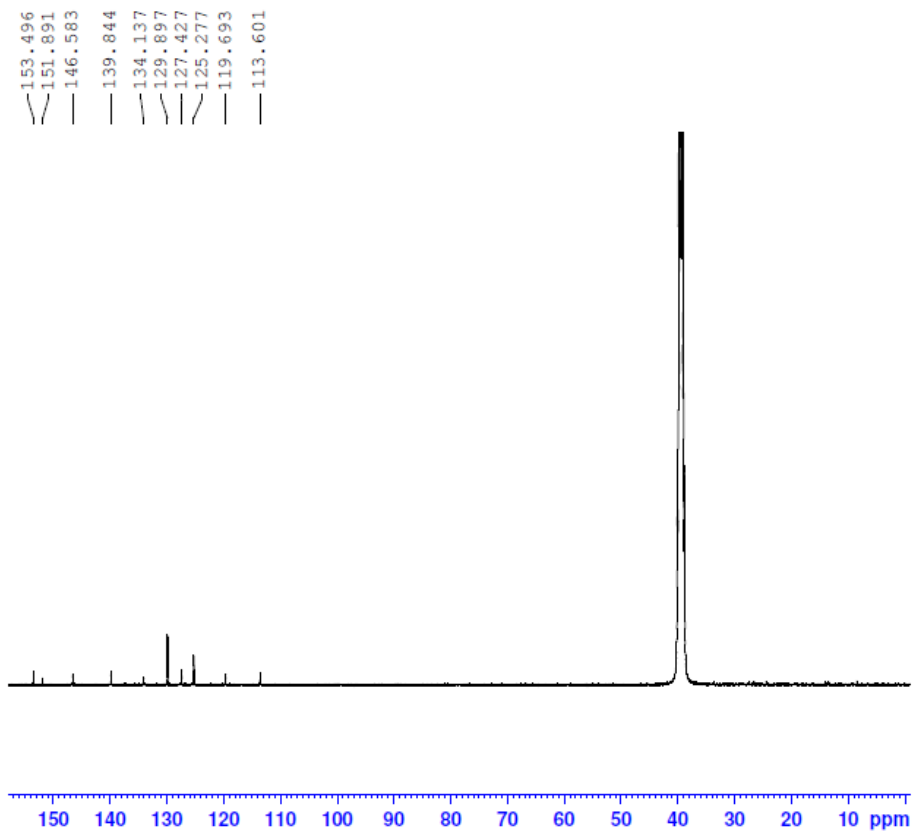



```
NAME            bki283ax
EXPNO                13
PROCNO               1
Date_         20110729
Time              9.29
INSTRUM           AV600
PROBHD   5 mm CPTCI 1H-
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                 872
DS                   4
SWH          36057.691 Hz
FIDRES        0.550197 Hz
AQ            0.9088159 sec
RG                2050
DW               13.867 usec
DE                6.00 usec
TE              298.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                400

======== CHANNEL f1 ========
NUC1               13C
P1               13.20 usec
PL1              -2.00 dB
PL1W      121.82079315 W
SFO1      150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              4.05 dB
PL12             24.27 dB
PL13             24.27 dB
PL2W       6.03017378 W
PL12W      0.05732312 W
PL13W      0.05732312 W
SFO2      600.1324000 MHz
SI               32768
SF        150.9028872 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

1-(Pyridin-2-yl)-3-(phenyl)guanidine hydrochloride (5i)

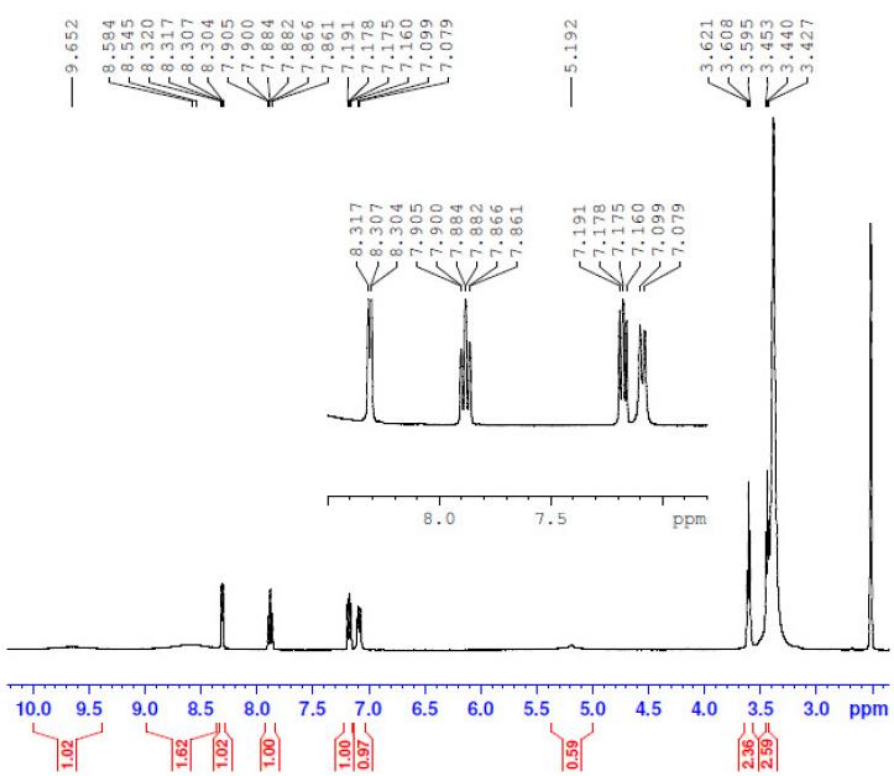


NAME	ssmmm12d
EXPNO	1
PROCNO	1
Date_	20111103
Time	15.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	32768
SOLVENT	DMSO
NS	16
DS	2
SWH	8223.685 Hz
FIDRES	0.250967 Hz
AQ	1.9923444 sec
RG	32
DW	60.800 usec
DE	6.00 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	10.00 usec
PL1	-4.00 dB
PL1W	19.30729485 W
SFO1	400.2324716 MHz
SI	32768
SF	400.2300000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

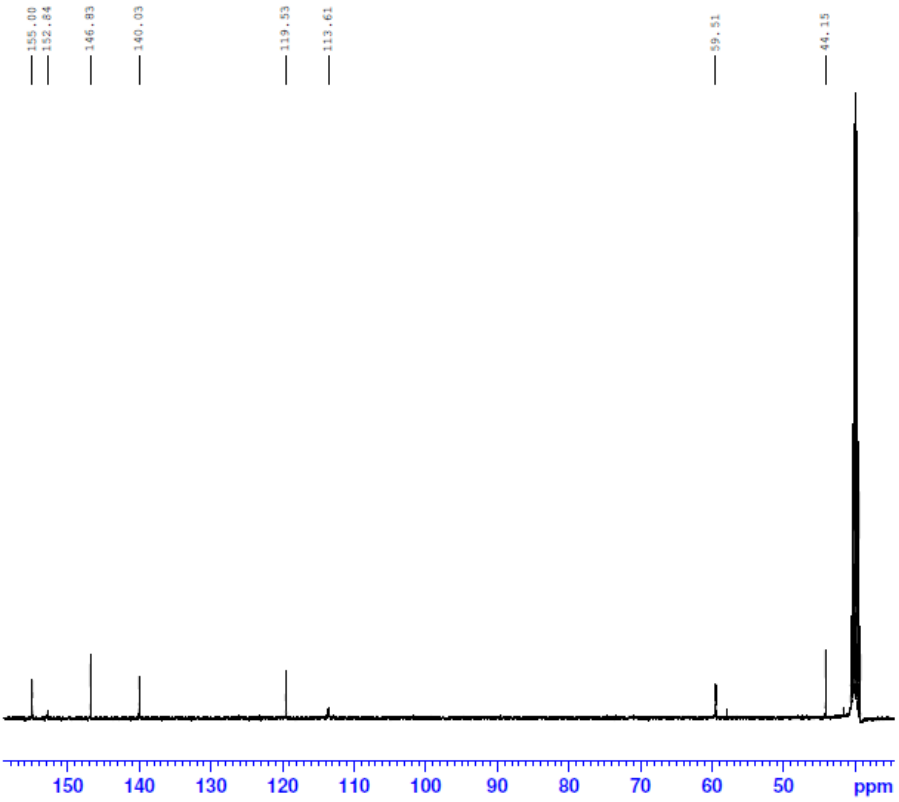


NAME	ssmmm12d
EXPNO	13
PROCNO	1
Date_	20111107
Time	18.26
INSTRUM	dpx400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	32768
SOLVENT	DMSO
NS	28688
DS	2
SWH	31847.133 Hz
FIDRES	0.971897 Hz
AQ	0.5145076 sec
RG	8192
DW	15.700 usec
DE	5.50 usec
TE	294.2 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.25 usec
PL1	-6.00 dB
SFO1	100.6254358 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	3.00 dB
PL12	19.07 dB
PL13	20.00 dB
SFO2	400.1316005 MHz
SI	32768
SF	100.6128155 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

1-(Pyridin-2-yl)-3-(2-hydroxyethyl)guanidine hydrochloride (5j)

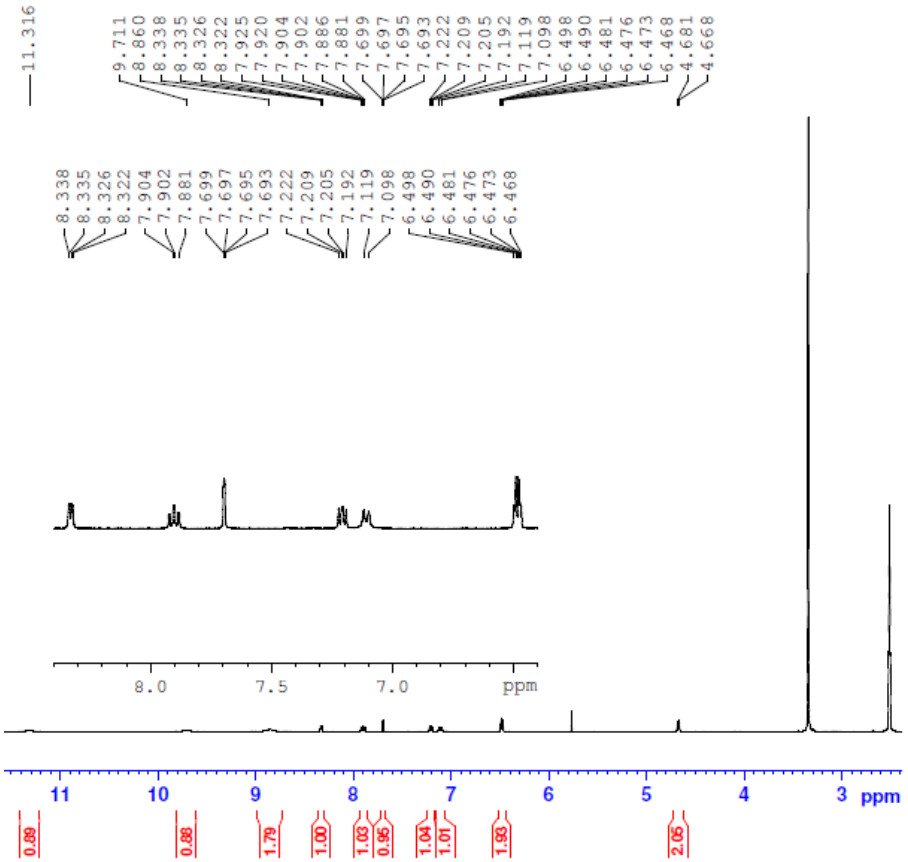



```
NAME            ssmmm20f
EXPNO                  1
PROCNO                 1
Date_           20111114
Time                11.01
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   203
DW                60.800 usec
DE                 6.00 usec
TE                298.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.00 usec
PL1                -4.00 dB
PL1W        19.30729485 W
SFO1        400.2324716 MHz
SI                 32768
SF          400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

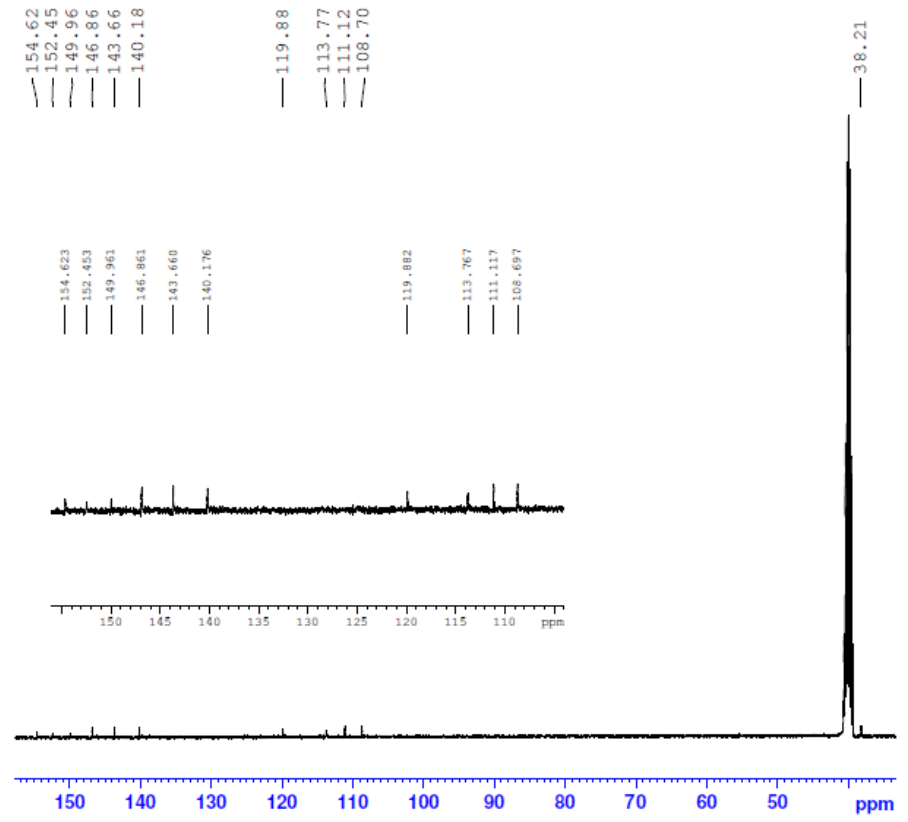



```
NAME            ssmmm20f
EXPNO                 13
PROCNO                 1
Date_           20111114
Time                11.28
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                  2980
DS                     2
SWH            32051.281 Hz
FIDRES          0.978127 Hz
AQ              0.5112308 sec
RG                   912
DW                15.600 usec
DE                 6.00 usec
TE                298.2 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  8.00 usec
PL1                -2.30 dB
PL1W        60.57429123 W
SFO1        100.6505944 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -4.00 dB
PL12               14.00 dB
PL13               14.00 dB
PL2W        19.30729485 W
PL12W        0.30599999 W
PL13W        0.30599999 W
SFO2        400.2316009 MHz
SI                 32768
SF          100.6379140 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

1-(Pyridin-2-yl)-3-(2-furanylmethyl)guanidine hydrochloride (5k)

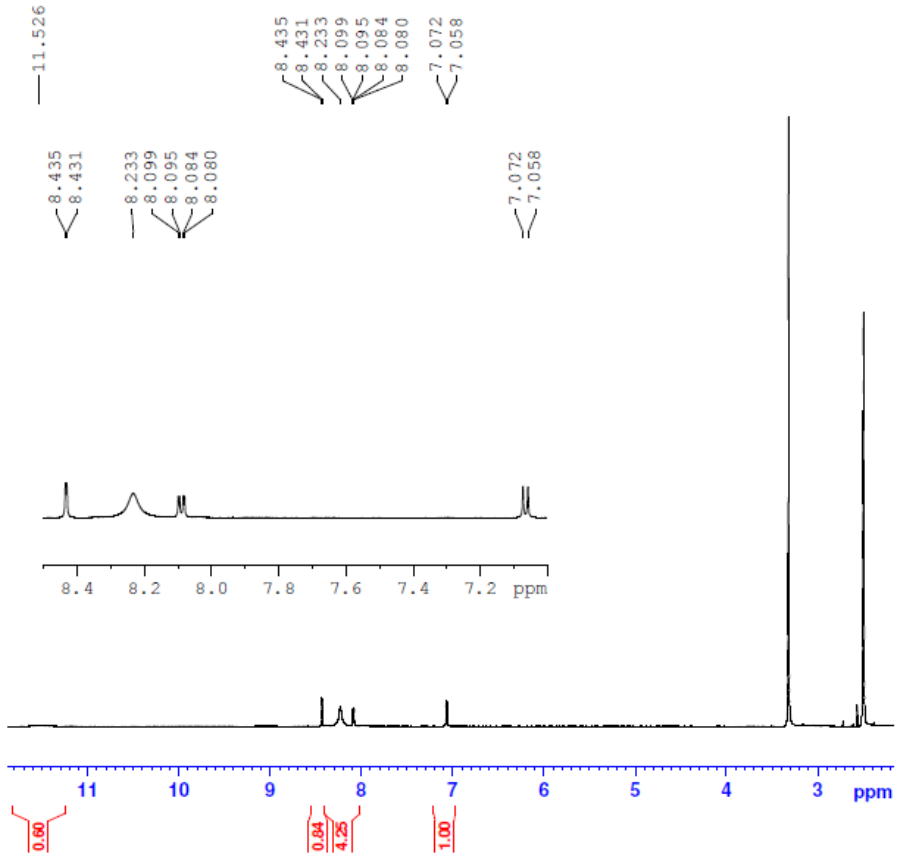



```
NAME                 ssmmm6a
EXPNO                      1
PROCNO                     1
Date_               20111005
Time                    8.56
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG                 zg30
TD                     32768
SOLVENT                DMSO
NS                         8
DS                         2
SWH                 8223.685 Hz
FIDRES              0.250967 Hz
AQ                  1.9923444 sec
RG                       256
DW                    60.800 usec
DE                     6.00 usec
TE                    298.2 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.00 usec
PL1                    -4.00 dB
PL1W               19.30729485 W
SFO1               400.2324716 MHz
SI                     32768
SF                 400.2300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

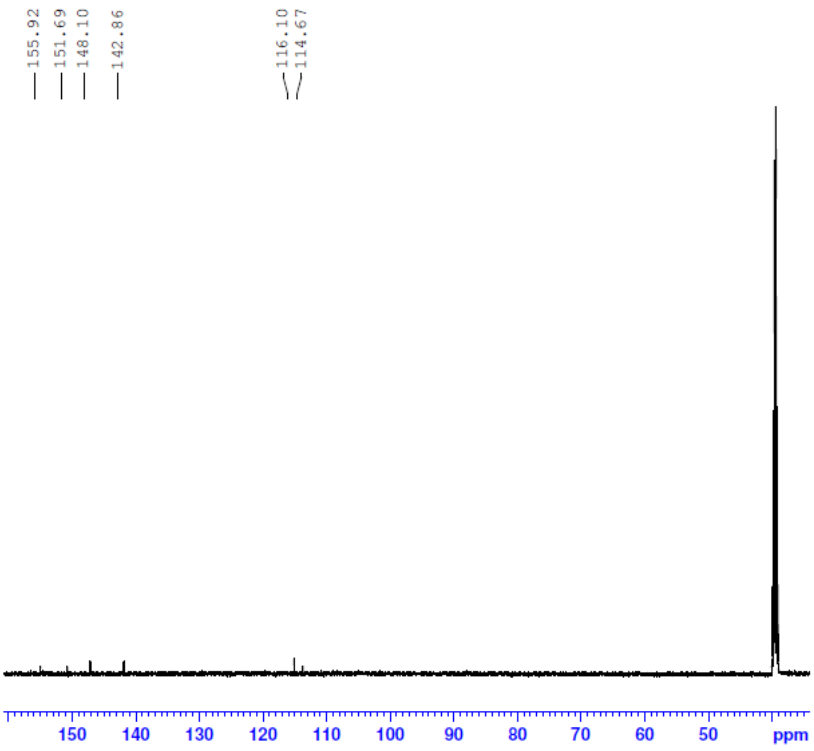



```
NAME                 ssmmm6a
EXPNO                     13
PROCNO                     1
Date_               20111005
Time                    9.28
INSTRUM                 spect
PROBHD   5 mm PABBO BB-
PULPROG              zgpg30
TD                     32768
SOLVENT                DMSO
NS                      7136
DS                         2
SWH                32051.281 Hz
FIDRES              0.978127 Hz
AQ                  0.5112308 sec
RG                       912
DW                    15.600 usec
DE                     6.00 usec
TE                    298.2 K
D1                  1.00000000 sec
D11                 0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      8.00 usec
PL1                    -2.30 dB
PL1W               60.57429123 W
SFO1               100.6505944 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -4.00 dB
PL12                   14.00 dB
PL13                   14.00 dB
PL2W               19.30729485 W
PL12W               0.30599999 W
PL13W               0.30599999 W
SFO2               400.2316009 MHz
SI                     32768
SF                 100.6379140 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

1-(5-Bromopyridin-2-yl)guanidine hydrochloride (6c)

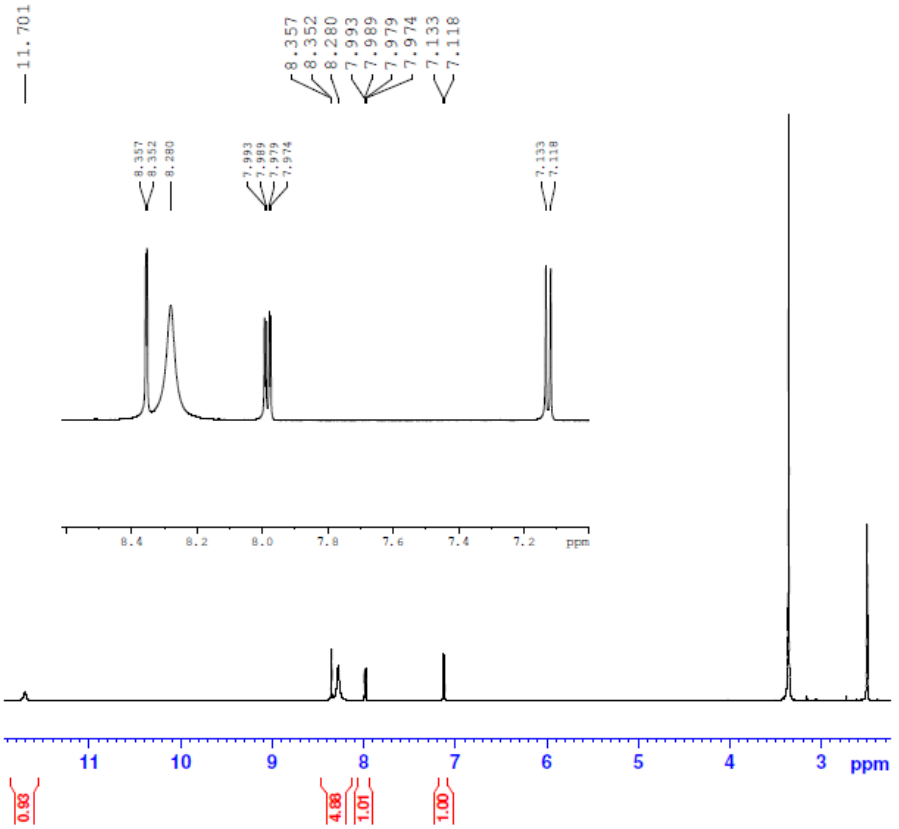



```
NAME                 bki95a
EXPNO                     1
PROCNO                    1
Date_              20100615
Time                   9.58
INSTRUM              AV600
PROBHD    5 mm CPTCI 1H-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        8
DS                        2
SWH               12335.526 Hz
FIDRES             0.188225 Hz
AQ                 2.6564426 sec
RG                        8
DW                   40.533 usec
DE                    6.00 usec
TE                   298.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                     7.80 usec
PL1                    4.05 dB
PL1W            6.03017378 W
SFO1          600.1337060 MHz
SI                    32768
SF            600.1300072 MHz
WDW                      no
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     1.00
```

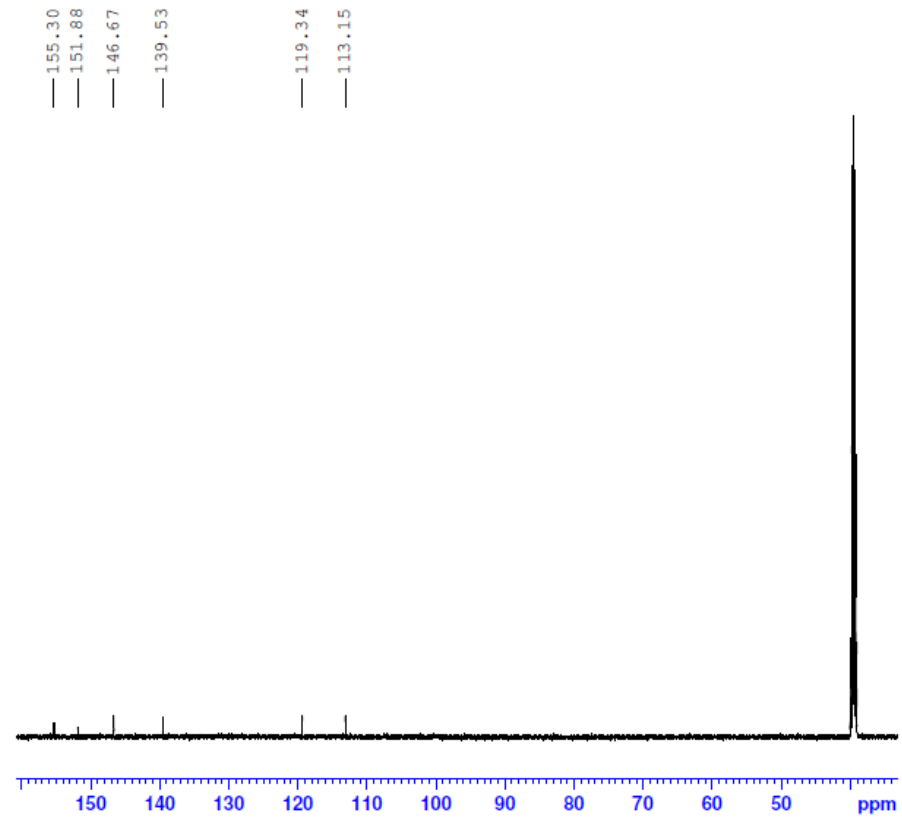



```
NAME                 bki95a
EXPNO                    13
PROCNO                    1
Date_              20100615
Time                  12.10
INSTRUM              AV600
PROBHD    5 mm CPTCI 1H-
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      262
DS                        4
SWH               36057.691 Hz
FIDRES             0.550197 Hz
AQ                 0.9088159 sec
RG                     2050
DW                   13.867 usec
DE                    6.00 usec
TE                   298.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                     400

======== CHANNEL f1 ========
NUC1                    13C
P1                    13.20 usec
PL1                   -2.00 dB
PL1W           121.82079315 W
SFO1           150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    4.05 dB
PL12                  24.27 dB
PL13                  24.27 dB
PL2W            6.03017378 W
PL12W           0.05732312 W
PL13W           0.05732312 W
SFO2          600.1324000 MHz
SI                    32768
SF            150.9028851 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

1-(5-Chloropyridin-2-yl)guanidine hydrochloride (7c)

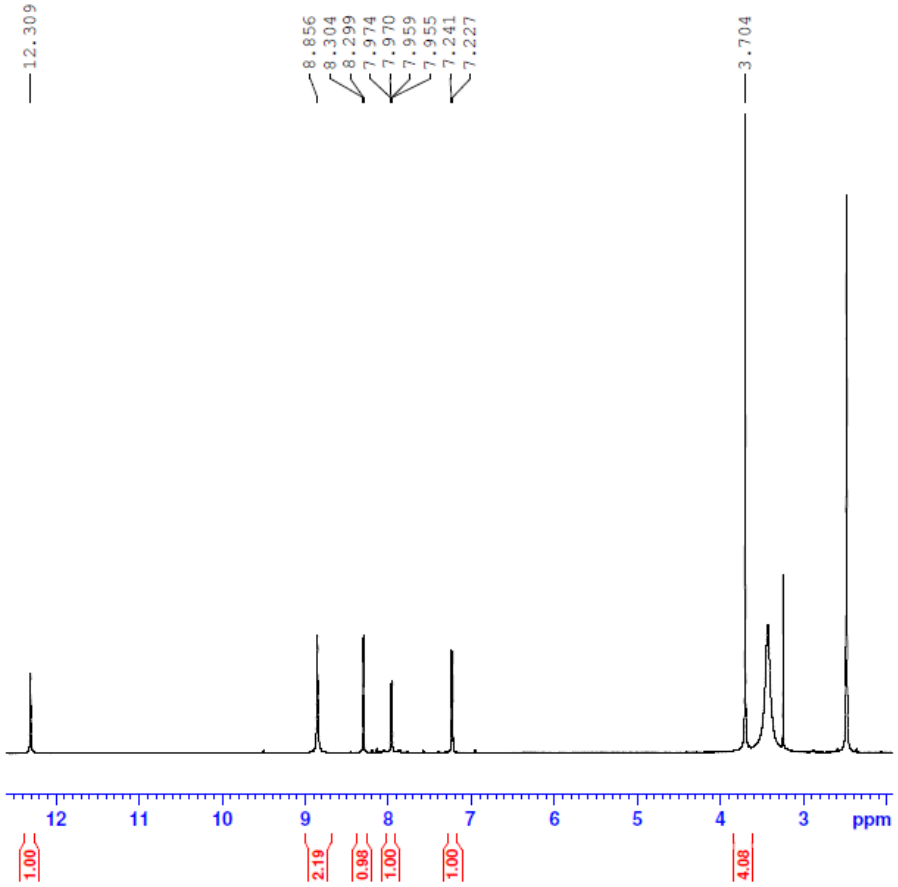



```
NAME                bki86bx
EXPNO                     1
PROCNO                    1
Date_              20100602
Time                  13.20
INSTRUM                AV600
PROBHD    5 mm CPTCI 1H-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        9
DS                        2
SWH               12335.526 Hz
FIDRES            0.188225 Hz
AQ                2.6564426 sec
RG                        8
DW                   40.533 usec
DE                    6.00 usec
TE                   298.0 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 =======
NUC1                    1H
P1                    7.80 usec
PL1                   4.05 dB
PL1W           6.03017378 W
SFO1          600.1337060 MHz
SI                    32768
SF            600.1300070 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```

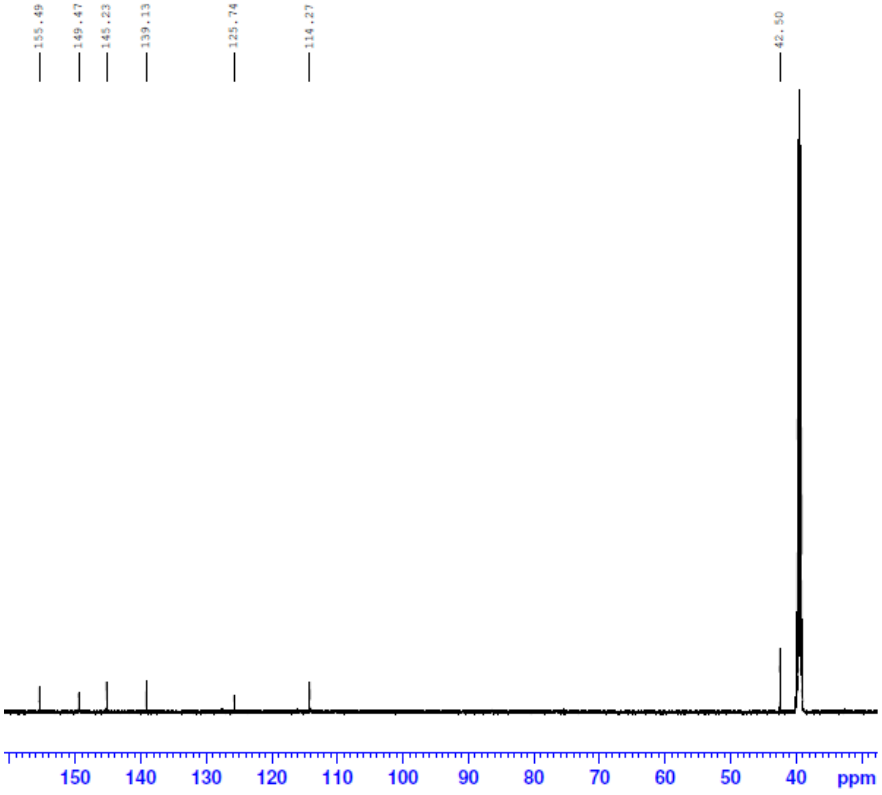



```
NAME                bki70cx
EXPNO                    13
PROCNO                    1
Date_              20100429
Time                   9.17
INSTRUM                AV600
PROBHD    5 mm CPTCI 1H-
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                      175
DS                        4
SWH               36057.691 Hz
FIDRES            0.550197 Hz
AQ                0.9088159 sec
RG                     2050
DW                   13.867 usec
DE                    6.00 usec
TE                   300.0 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                     400

======== CHANNEL f1 =======
NUC1                   13C
P1                   13.20 usec
PL1                  -2.00 dB
PL1W          121.82079315 W
SFO1          150.9178990 MHz

======== CHANNEL f2 =======
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   4.05 dB
PL12                 24.27 dB
PL13                 24.27 dB
PL2W           6.03017378 W
PL12W          0.05732312 W
PL13W          0.05732312 W
SFO2          600.1324000 MHz
SI                    32768
SF            150.9028853 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

1-(5-Chloropyridin-2’-yl)-2-iminoimidazolidine hydrochloride (7d)

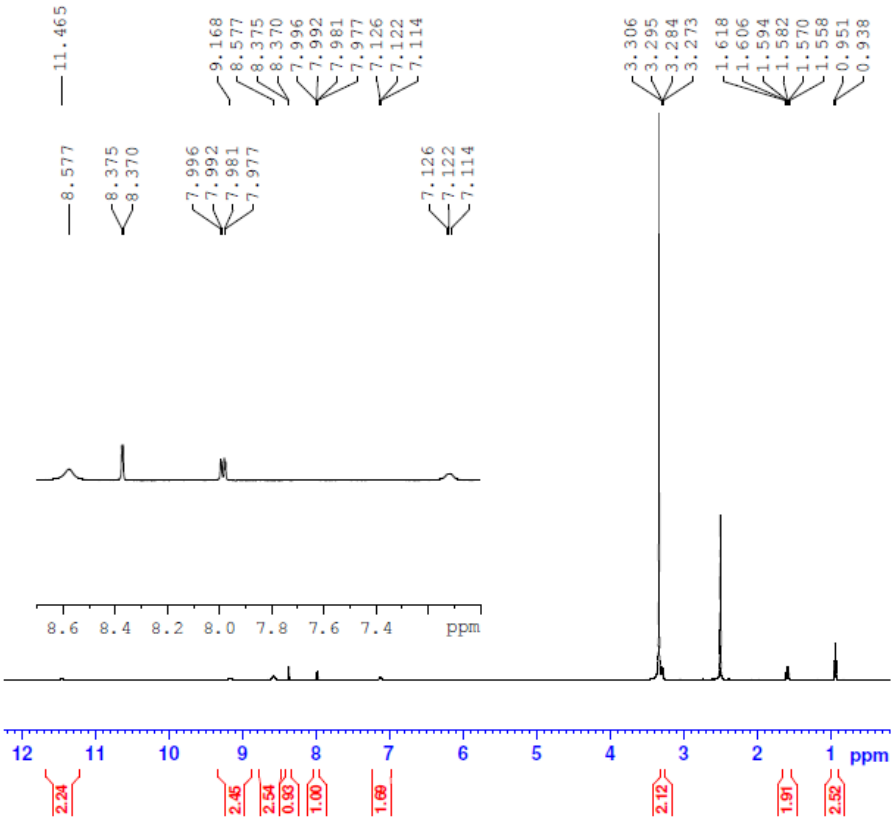



```
NAME            bki305ax
EXPNO                  1
PROCNO                 1
Date_           20110813
Time               17.41
INSTRUM           AV600
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     2
SWH           12335.526 Hz
FIDRES         0.188225 Hz
AQ            2.6564426 sec
RG                     8
DW               40.533 usec
DE                6.00 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 =======
NUC1                  1H
P1                  7.45 usec
PL1                 4.05 dB
PL1W          6.03017378 W
SFO1        600.1337060 MHz
SI                 32768
SF          600.1300173 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

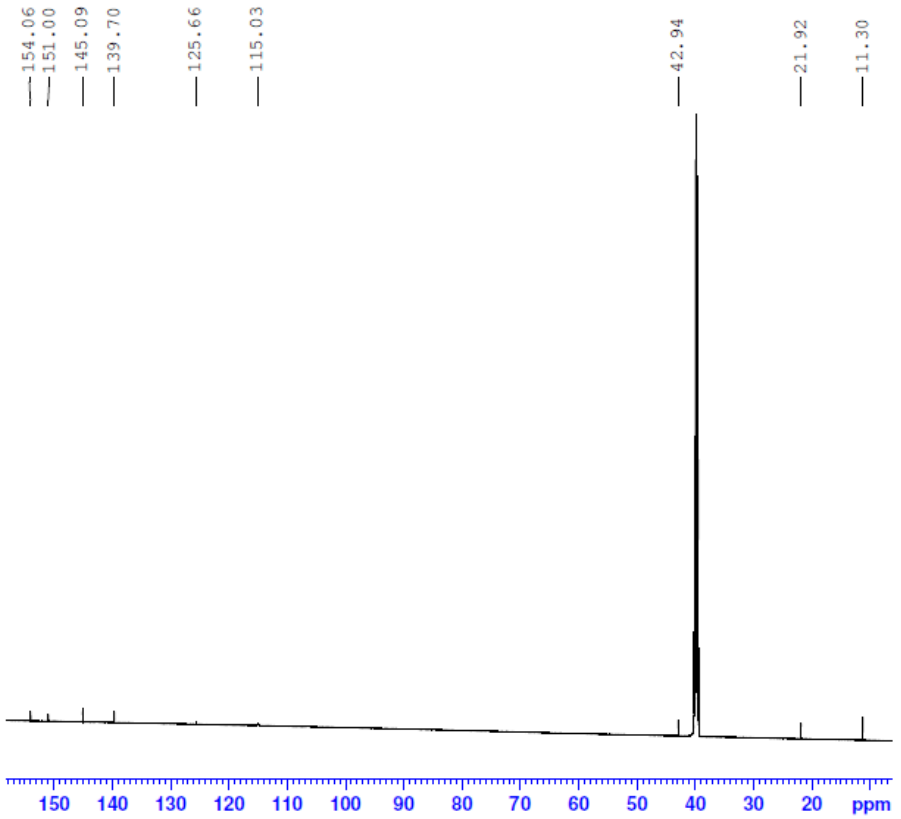



```
NAME            bki305ax
EXPNO                 13
PROCNO                 1
Date_           20110813
Time               17.47
INSTRUM           AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   129
DS                     4
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ            0.9088159 sec
RG                  2050
DW               13.867 usec
DE                6.00 usec
TE                298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  400

======== CHANNEL f1 =======
NUC1                 13C
P1                 13.20 usec
PL1                -2.00 dB
PL1W       121.82079315 W
SFO1        150.9178990 MHz

======== CHANNEL f2 =======
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 4.05 dB
PL12               24.27 dB
PL13               24.27 dB
PL2W          6.03017378 W
PL12W         0.05732312 W
PL13W         0.05732312 W
SFO2        600.1324000 MHz
SI                 32768
SF          150.9028839 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

1-(5-Chloropyridin-2-yl)-3-(propyl)guanidine hydrochloride (7l)

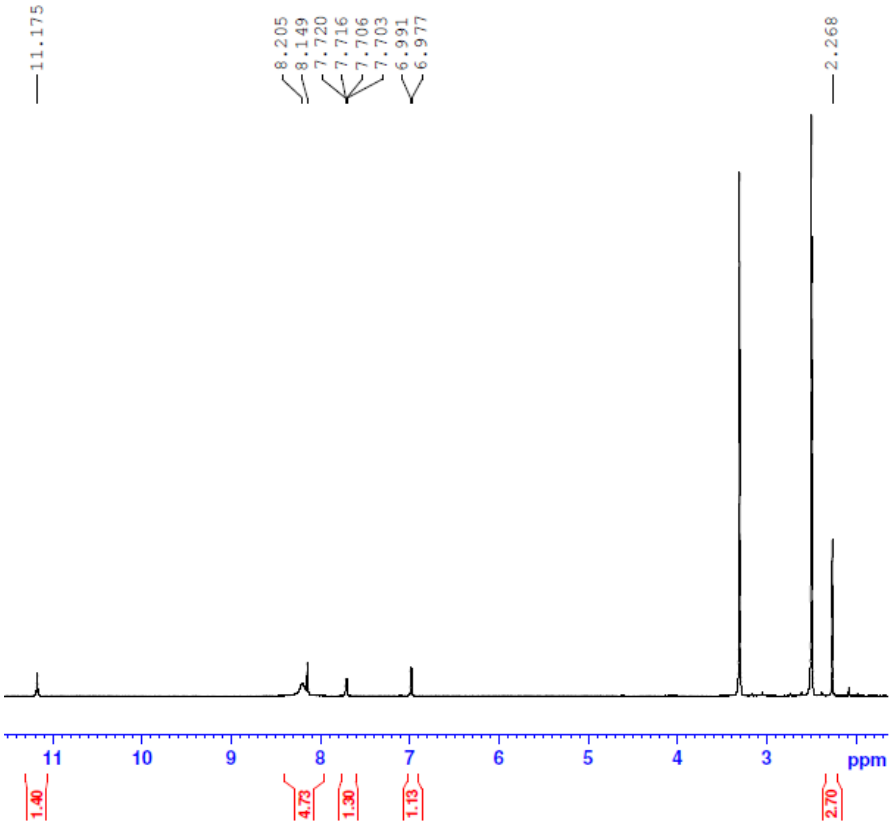



```
NAME              bki161c
EXPNO                   1
PROCNO                  1
Date_            20101111
Time                16.05
INSTRUM             AV600
PROBHD   5 mm CPTCI 1H-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                      8
DS                      2
SWH             24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631988 sec
RG                      8
DW                20.800 usec
DE                 6.00 usec
TE                298.0 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 =======
NUC1                   1H
P1                   7.92 usec
PL1                  4.05 dB
PL1W           6.03017378 W
SFO1          600.1337060 MHz
SI                   32768
SF            600.1300067 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.00
```

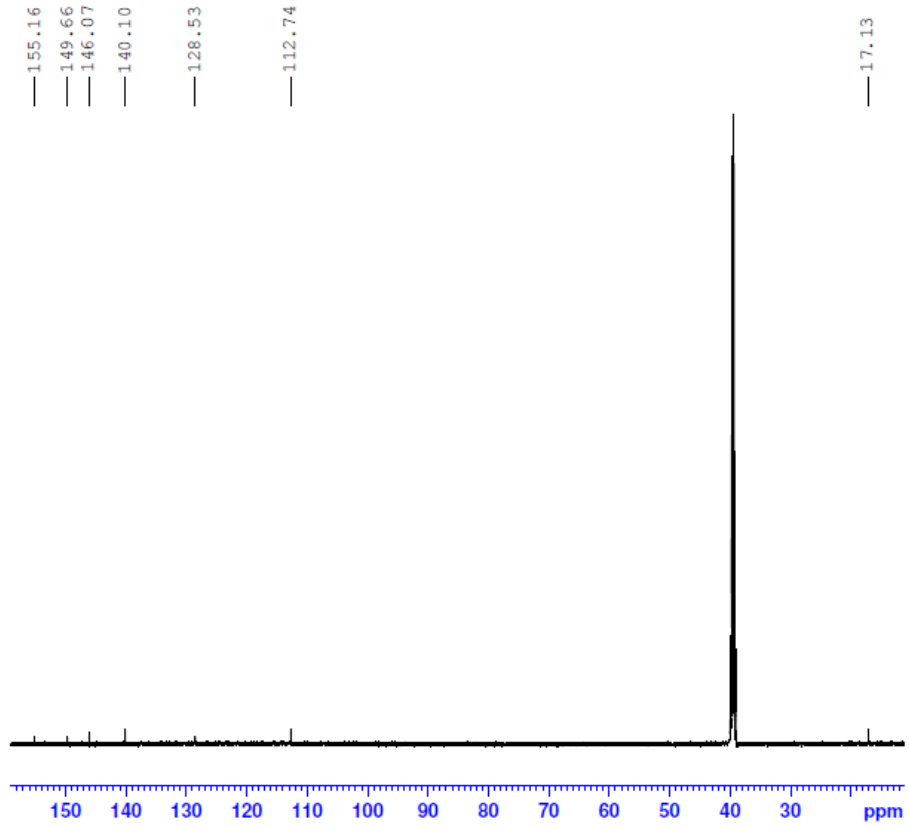



```
NAME              bki161c
EXPNO                 513
PROCNO                  1
Date_            20110118
Time                18.02
INSTRUM             AV600
PROBHD   5 mm CPTCI 1H-
PULPROG            zgpg30
TD                  65536
SOLVENT              DMSO
NS                  27143
DS                      4
SWH             36057.691 Hz
FIDRES          0.550197 Hz
AQ              0.9088159 sec
RG                   2050
DW                13.867 usec
DE                 6.00 usec
TE                298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                   400

======== CHANNEL f1 =======
NUC1                  13C
P1                  13.20 usec
PL1                 -2.00 dB
PL1W          121.82079315 W
SFO1           150.9178990 MHz

======== CHANNEL f2 =======
CPDPRG2            waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 4.05 dB
PL12                24.27 dB
PL13                24.27 dB
PL2W           6.03017378 W
PL12W          0.05732312 W
PL13W          0.05732312 W
SFO2          600.1324000 MHz
SI                   32768
SF            150.9028332 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.00
```

1-(5-Methylpyridin-2-yl)guanidine hydrochloride (8c)

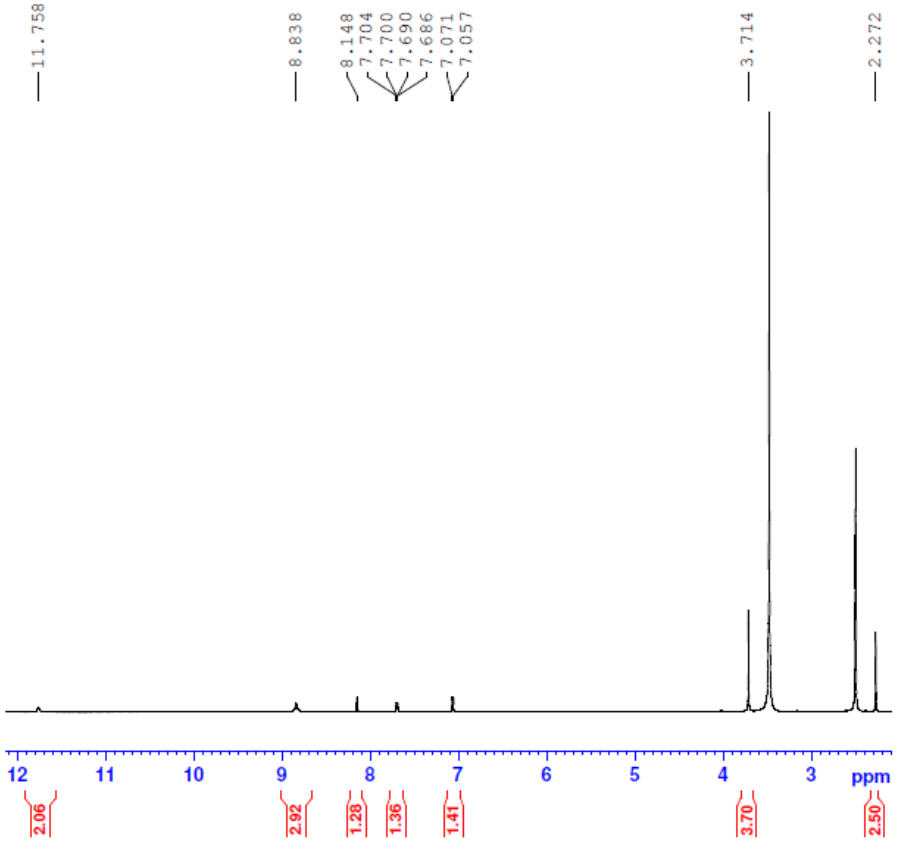



```
NAME                bki03ax
EXPNO                     1
PROCNO                    1
Date_              20100514
Time                  12.51
INSTRUM               AV600
PROBHD   5 mm CPTCI 1H-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        8
DS                        2
SWH               12335.526 Hz
FIDRES             0.188225 Hz
AQ                2.6564426 sec
RG                        8
DW                   40.533 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 =======
NUC1                     1H
P1                     8.08 usec
PL1                    4.05 dB
PL1W           6.03017378 W
SFO1          600.1337060 MHz
SI                    32768
SF            600.1300069 MHz
WDW                      no
SSB                       0
LB                     0.00 Hz
GB                        0
PC                     1.00
```

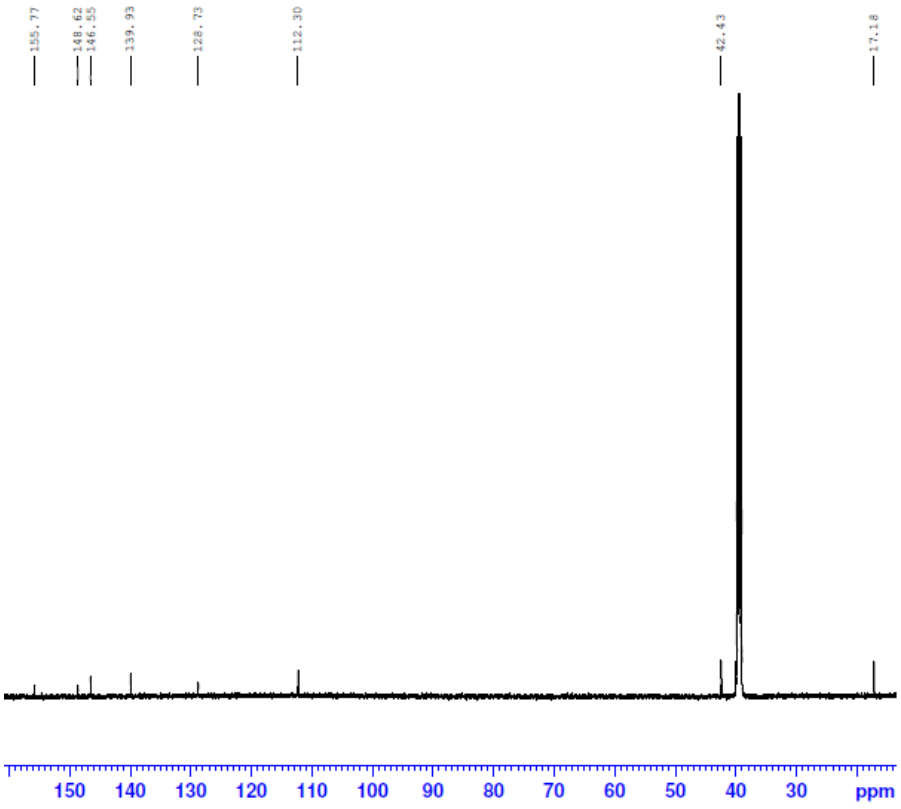



```
NAME                bki03ax
EXPNO                    13
PROCNO                    1
Date_              20100514
Time                  12.55
INSTRUM               AV600
PROBHD   5 mm CPTCI 1H-
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                      199
DS                        4
SWH               36057.691 Hz
FIDRES             0.550197 Hz
AQ                0.9088159 sec
RG                     2050
DW                   13.867 usec
DE                    6.00 usec
TE                   300.0 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                     400

======== CHANNEL f1 =======
NUC1                     13C
P1                    13.20 usec
PL1                   -2.00 dB
PL1W          121.82079315 W
SFO1          150.9178990 MHz

======== CHANNEL f2 =======
CPDPRG2              waltz16
NUC2                     1H
PCPD2                 80.00 usec
PL2                    4.05 dB
PL12                  24.27 dB
PL13                  24.27 dB
PL2W           6.03017378 W
PL12W          0.05732312 W
PL13W          0.05732312 W
SFO2          600.1324000 MHz
SI                    32768
SF            150.9028890 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

1-(5-Methylpyridin-2’-yl)-2-iminoimidazolidine hydrochloride (8d)

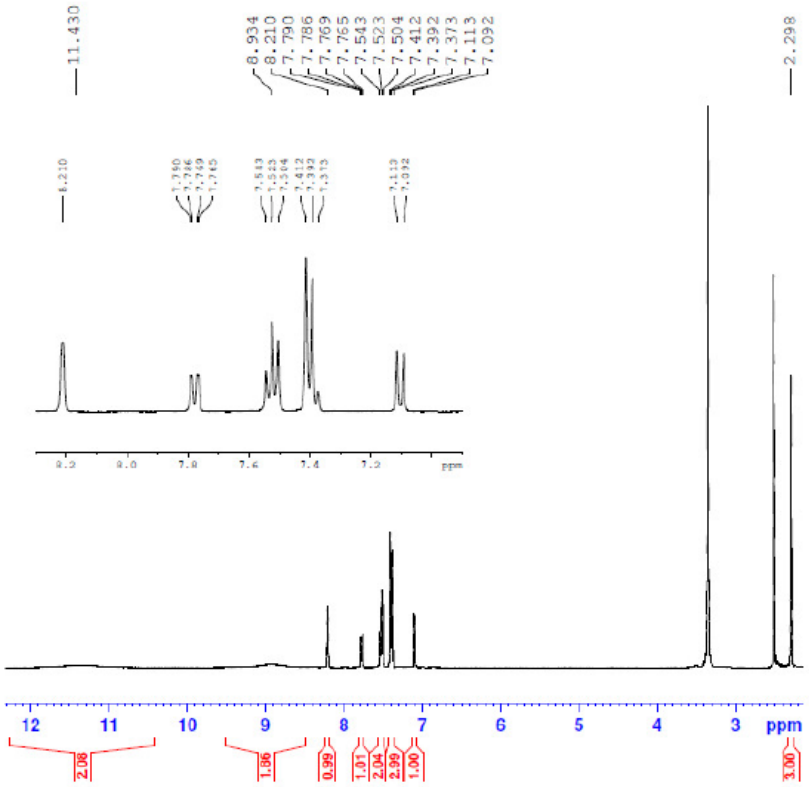



```
NAME            bki284ax
EXPNO                  1
PROCNO                 1
Date_           20110727
Time                8.54
INSTRUM           AV600
PROBHD    5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                    16
DS                     2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                     8
DW               20.800 usec
DE                6.00 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  7.79 usec
PL1                 4.05 dB
PL1W         6.03017378 W
SFO1        600.1337060 MHz
SI                 32768
SF          600.1300067 MHz
WDW                   no
SSB                    0
LB                0.00 Hz
GB                     0
PC                 1.00
```

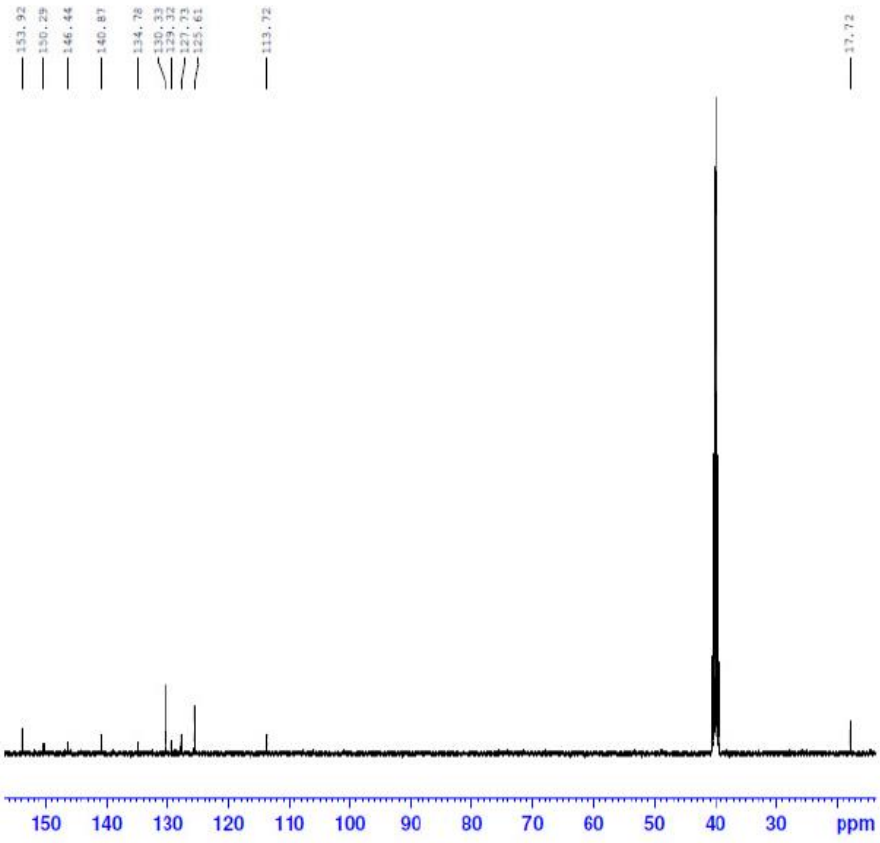



```
NAME            bki284ax
EXPNO                 13
PROCNO                 1
Date_           20110727
Time                9.28
INSTRUM           AV600
PROBHD    5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   413
DS                     4
SWH           36057.691 Hz
FIDRES        0.550197 Hz
AQ            0.9088159 sec
RG                  2050
DW               13.867 usec
DE                6.00 usec
TE                298.1 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                  400

======== CHANNEL f1 ========
NUC1                 13C
P1                13.20 usec
PL1               -2.00 dB
PL1W       121.82079315 W
SFO1        150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                 4.05 dB
PL12               24.27 dB
PL13               24.27 dB
PL2W         6.03017378 W
PL12W        0.05732312 W
PL13W        0.05732312 W
SFO2        600.1324000 MHz
SI                 32768
SF          150.9028861 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

1-(5-Methylpyridin-2-yl)-3-(phenyl)guanidine hydrochloride (8i)

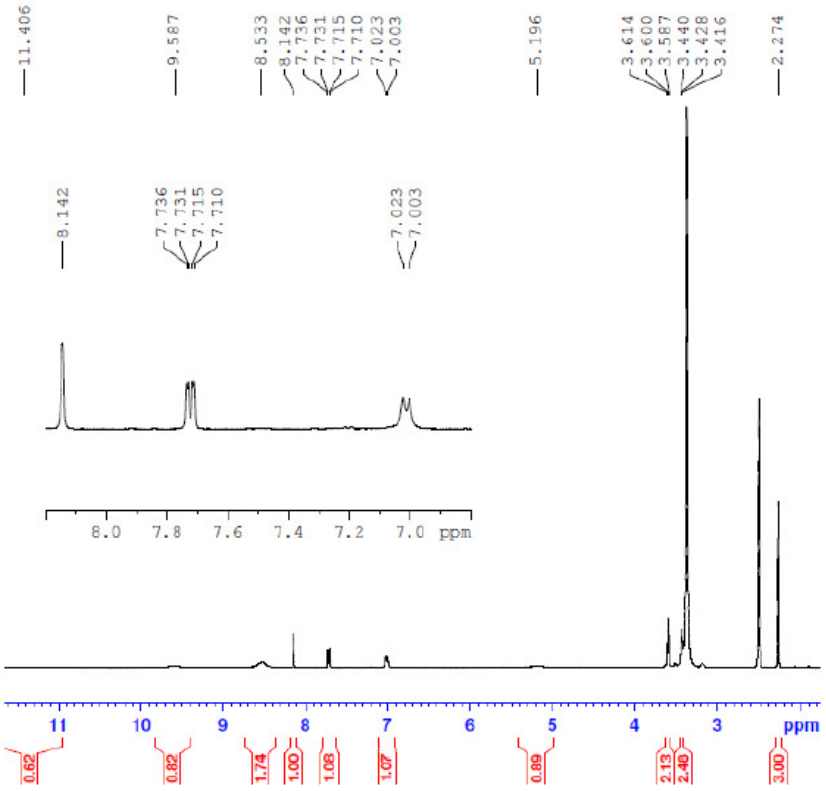



```
NAME            ssmmm11x
EXPNO                  1
PROCNO                 1
Date_           20111027
Time               10.08
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   161
DW                60.800 usec
DE                 6.00 usec
TE                298.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1                -4.00 dB
PL1W         19.30729485 W
SFO1         400.2324716 MHz
SI                 32768
SF           400.2300000 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                  1.00
```

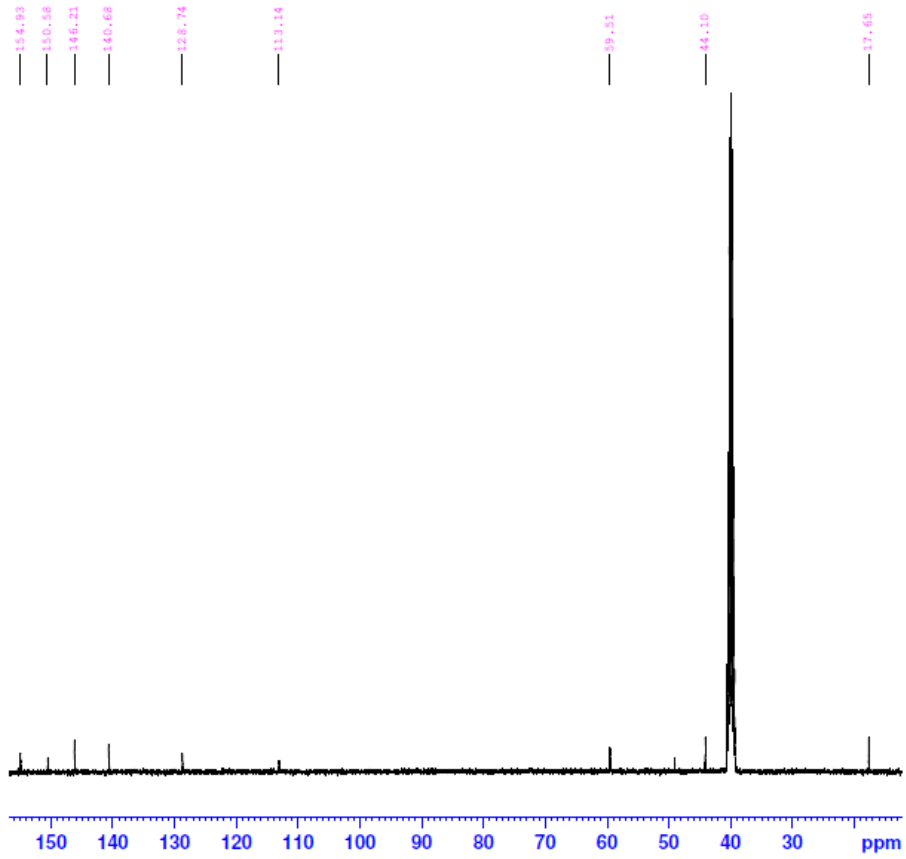



```
NAME            ssmmm11x
EXPNO                 13
PROCNO                 1
Date_           20111027
Time               10.26
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                   633
DS                     2
SWH            32051.281 Hz
FIDRES          0.978127 Hz
AQ              0.5112308 sec
RG                   912
DW                15.600 usec
DE                 6.00 usec
TE                298.2 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.00 usec
PL1                -2.30 dB
PL1W         60.57429123 W
SFO1         100.6505944 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -4.00 dB
PL12               14.00 dB
PL13               14.00 dB
PL2W         19.30729485 W
PL12W         0.30599999 W
PL13W         0.30599999 W
SFO2         400.2316009 MHz
SI                 32768
SF           100.6379140 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                  1.40
```

1-(5-Methylpyridin-2-yl)-3-(2-hydroxyethyl)guanidine hydrochloride (8j)

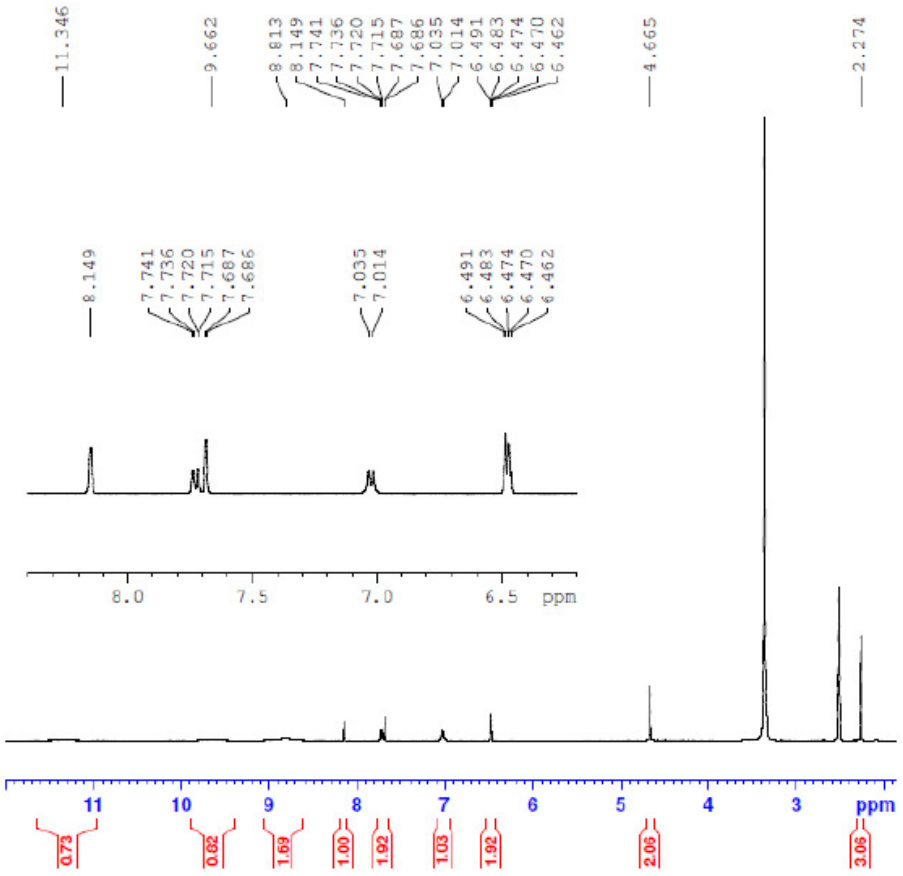



```
NAME                ssmmm8j
EXPNO                     1
PROCNO                    1
Date_              20111018
Time                  13.52
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                       16
DS                        2
SWH               8223.685 Hz
FIDRES            0.250967 Hz
AQ                1.9923444 sec
RG                      287
DW                 60.800 usec
DE                  6.00 usec
TE                  298.2 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                 10.00 usec
PL1                 -4.00 dB
PL1W           19.30729485 W
SFO1           400.2324716 MHz
SI                    32768
SF             400.2300000 MHz
WDW                      EM
SSB                       0
LB                 0.30 Hz
GB                        0
PC                     1.00
```

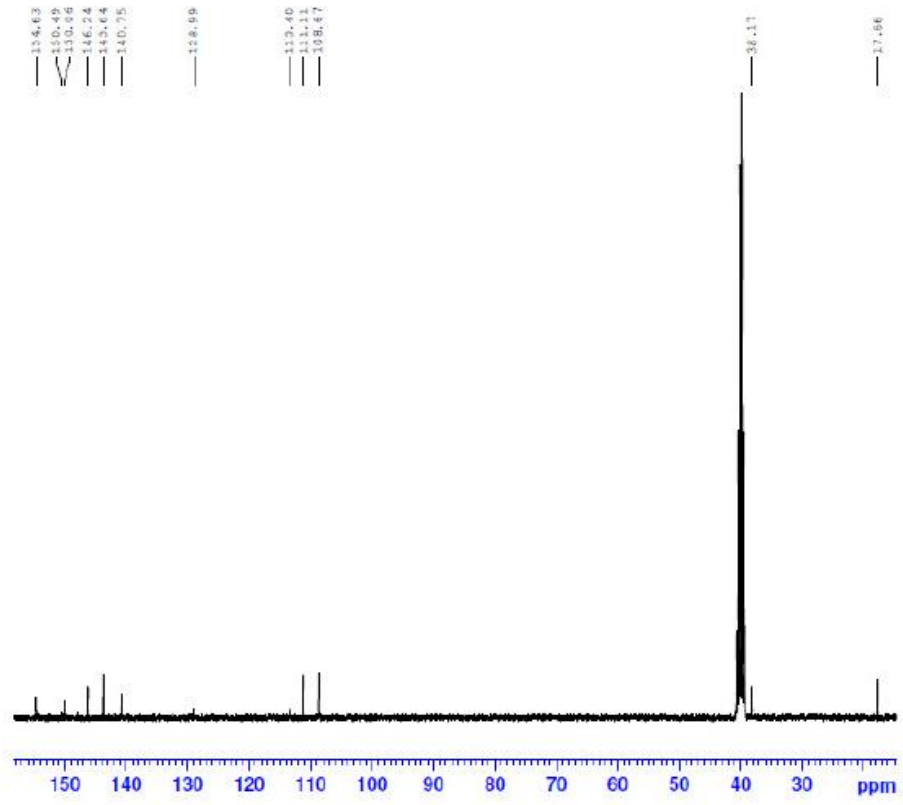



```
NAME                ssmmm8j
EXPNO                   113
PROCNO                    1
Date_              20111018
Time                  12.05
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG             zgpg30
TD                    32768
SOLVENT                DMSO
NS                      4183
DS                        2
SWH              32051.281 Hz
FIDRES            0.978127 Hz
AQ                0.5112308 sec
RG                      912
DW                 15.600 usec
DE                  6.00 usec
TE                  298.2 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     13C
P1                  8.00 usec
PL1                 -2.30 dB
PL1W          60.57429123 W
SFO1          100.6505944 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2              80.00 usec
PL2                 -4.00 dB
PL12                14.00 dB
PL13                14.00 dB
PL2W          19.30729485 W
PL12W          0.30599999 W
PL13W          0.30599999 W
SFO2          400.2316009 MHz
SI                    32768
SF            100.6379140 MHz
WDW                      EM
SSB                       0
LB                 1.00 Hz
GB                        0
PC                     1.40
```

1-(5-Methylpyridin-2-yl)-3-(2-furanylmethyl)guanidine hydrochloride (8k)

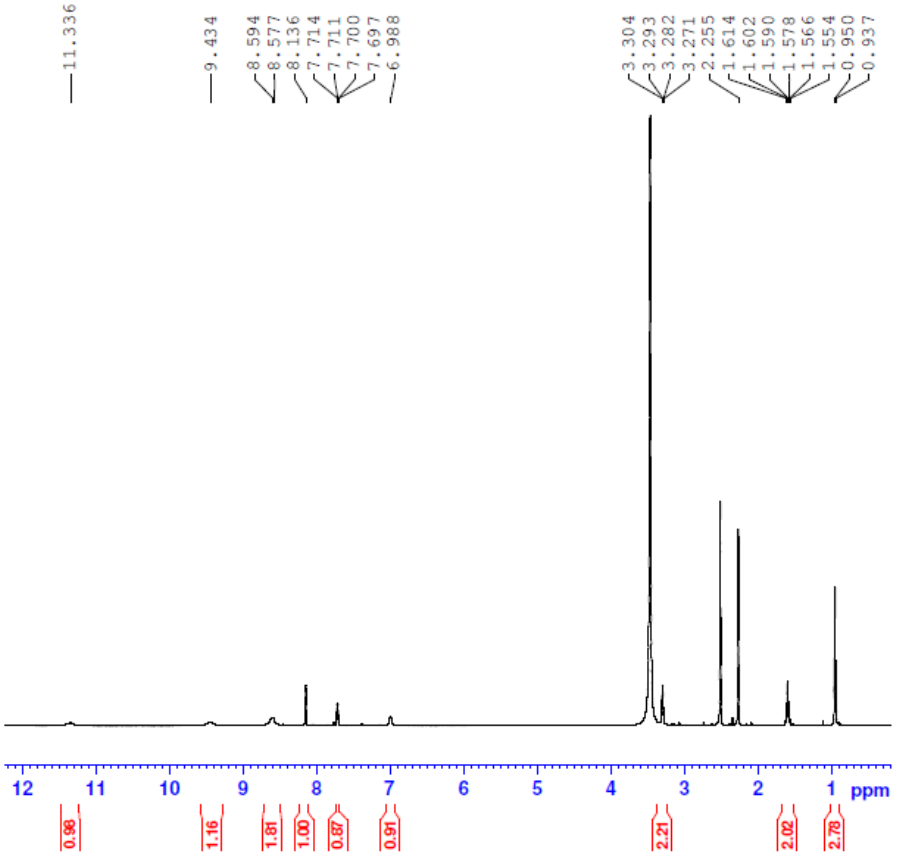



```
NAME            sammm5am
EXPNO                  1
PROCNO                 1
Date_           20111011
Time                15.51
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   203
DW                60.800 usec
DE                 6.00 usec
TE                298.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.00 usec
PL1                -4.00 dB
PL1W        19.30729485 W
SFO1        400.2324716 MHz
SI                 32768
SF          400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

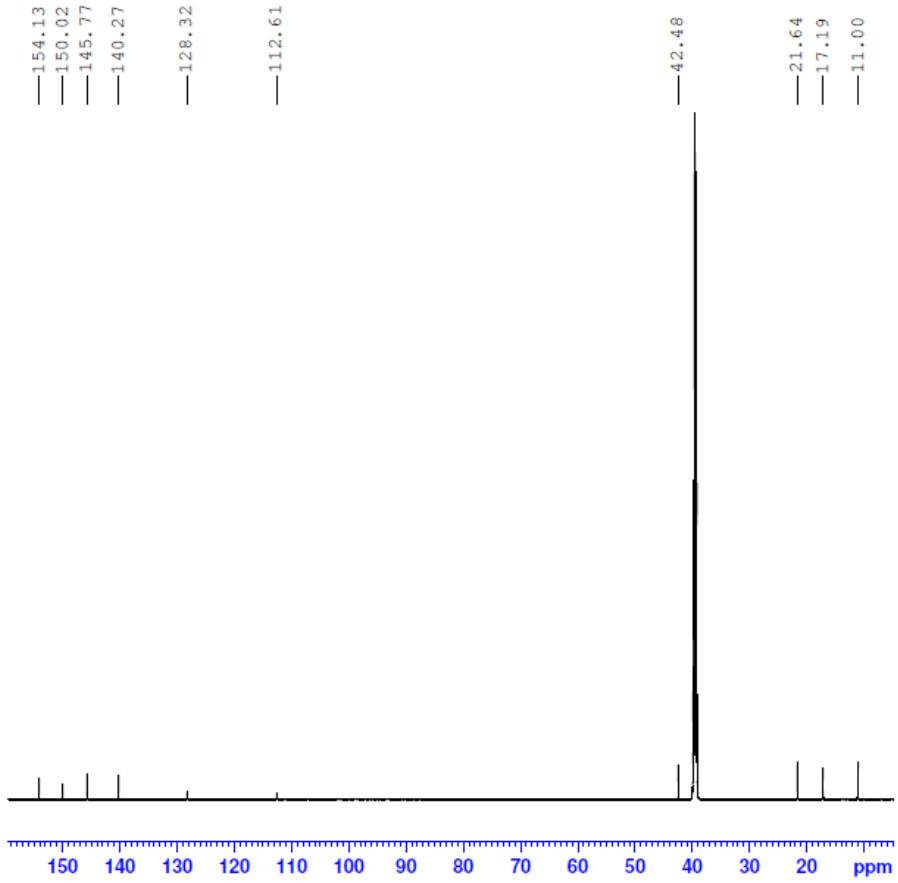



```
NAME            sammm5am
EXPNO                 13
PROCNO                 1
Date_           20111011
Time                16.37
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                   843
DS                     2
SWH            32051.281 Hz
FIDRES          0.978127 Hz
AQ              0.5112308 sec
RG                   912
DW                15.600 usec
DE                 6.00 usec
TE                298.2 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.00 usec
PL1                -2.30 dB
PL1W        60.57429123 W
SFO1        100.6565944 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -6.00 dB
PL12               14.00 dB
PL13               14.00 dB
PL2W        19.30729485 W
PL12W        0.30599999 W
PL13W        0.30599999 W
SFO2        400.2316009 MHz
SI                 32768
SF          100.6379140 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

1-(5-Methylpyridin-2-yl)-3-(propyl)guanidine hydrochloride (8l)

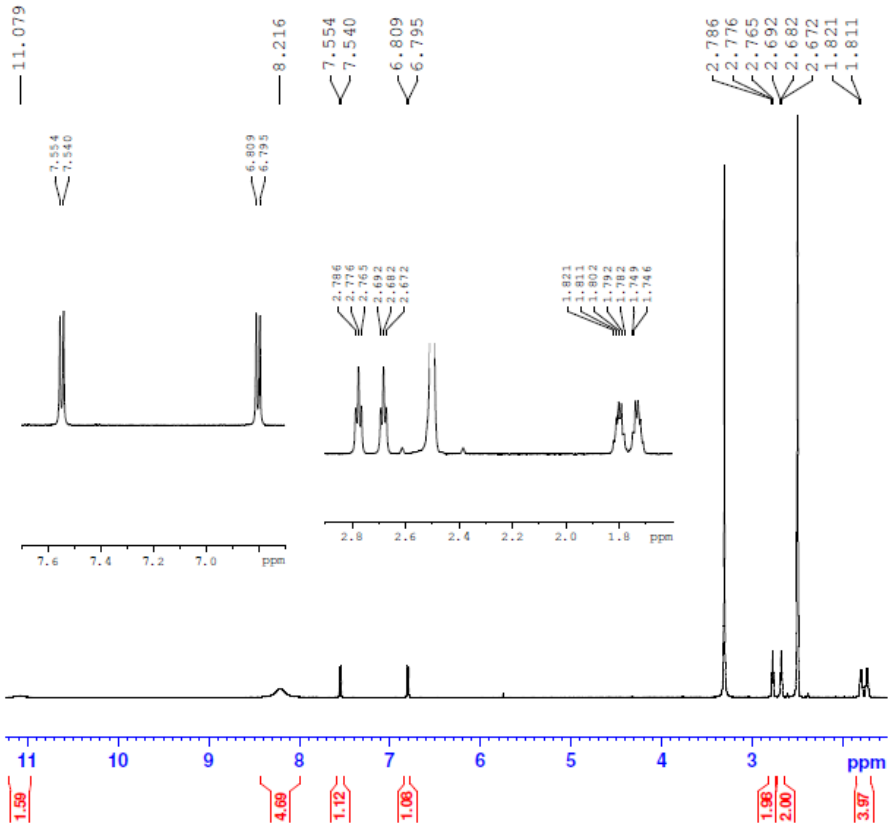



```
NAME              bki171x
EXPNO                   1
PROCNO                  1
Date_            20101203
Time                13.38
INSTRUM             AV600
PROBHD  5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                      0
DS                      2
SWH          12335.526 Hz
FIDRES        0.188225 Hz
AQ            2.6564426 sec
RG                      0
DW               40.533 usec
DE                6.00 usec
TE                298.0 K
D1           1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                   7.80 usec
PL1                  4.05 dB
PL1W          6.03017378 W
SFO1        600.1337060 MHz
SI                  32768
SF          600.1300000 MHz
WDW                    no
SSB                     0
LB                   0.00 Hz
GB                      0
PC                   1.40
```

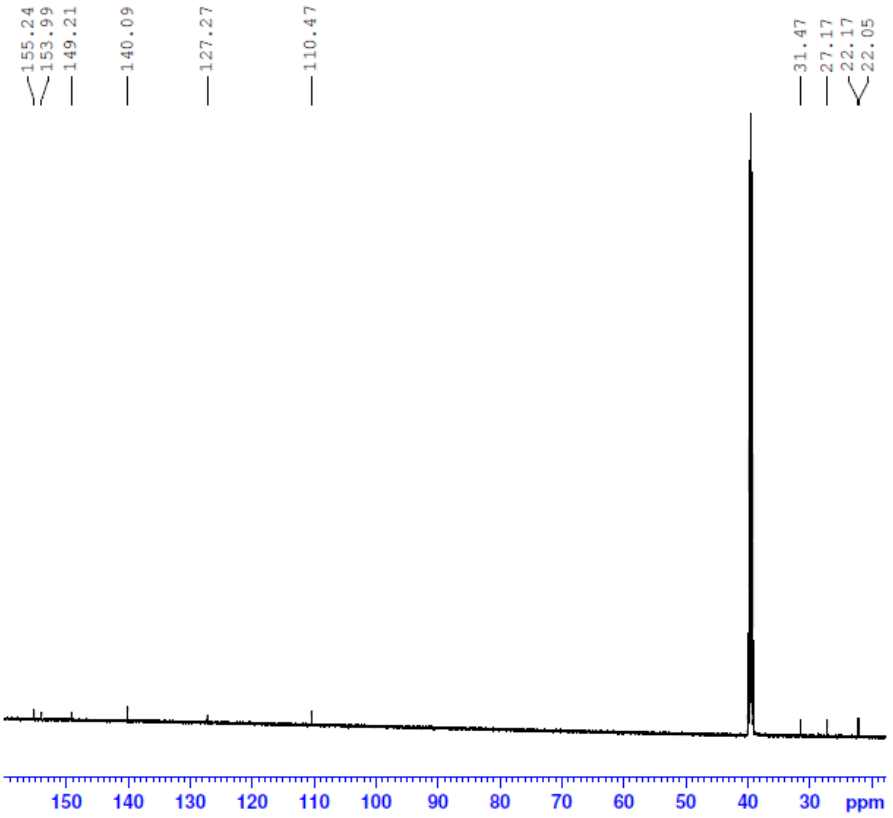



```
NAME              bki171x
EXPNO                  13
PROCNO                  1
Date_            20101203
Time                13.42
INSTRUM             AV600
PROBHD  5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                    923
DS                      4
SWH          36057.691 Hz
FIDRES        0.550197 Hz
AQ            0.9088159 sec
RG                   2050
DW               13.867 usec
DE                6.00 usec
TE                298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   400

======== CHANNEL f1 ========
NUC1                   13C
P1                  13.20 usec
PL1                 -2.00 dB
PL1W        121.82079315 W
SFO1         150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2            waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  4.05 dB
PL12                24.27 dB
PL13                24.27 dB
PL2W          6.03017378 W
PL12W         0.05732312 W
PL13W         0.05732312 W
SFO2        600.1324000 MHz
SI                  32768
SF          150.9028785 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
```

1-(5,6,7,8-Tetrahydroquinolin-2-yl)guanidine hydrochloride (9c)

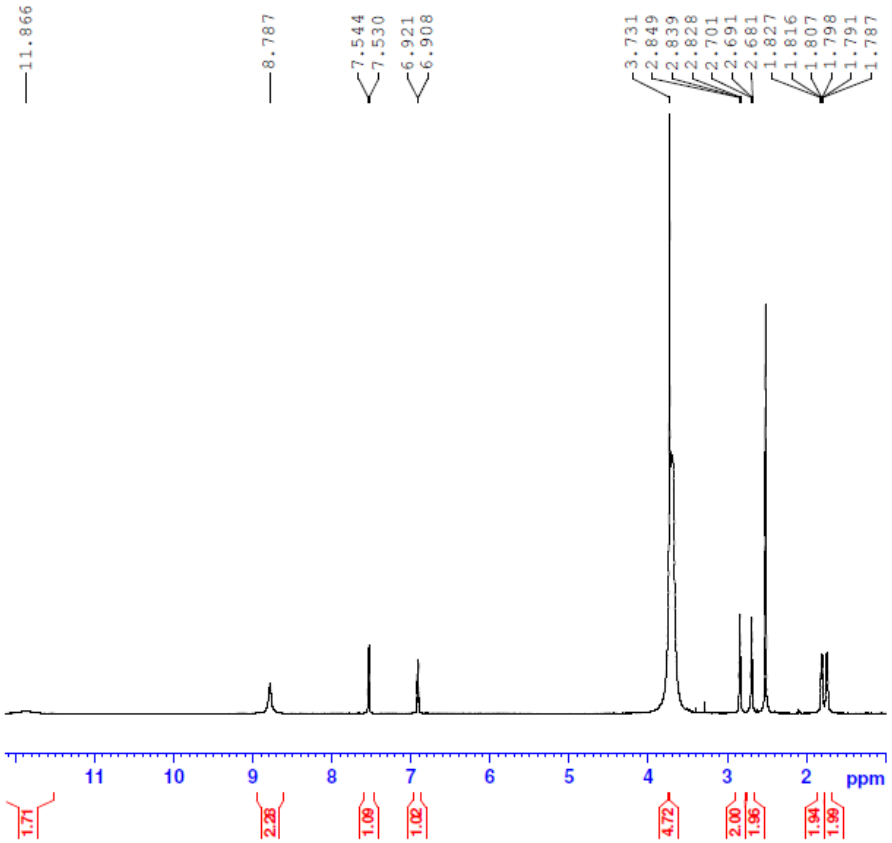



```
NAME                bki56c
EXPNO                    1
PROCNO                   1
Date_             20100413
Time                 14.51
INSTRUM              AV600
PROBHD   5 mm CPTCI 1H-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                       4
DS                       2
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631988 sec
RG                       8
DW                  20.800 usec
DE                   6.00 usec
TE                  300.0 K
D1             1.00000000 sec
TD0                      1

======== CHANNEL f1 =======
NUC1                    1H
P1                    7.94 usec
PL1                   4.05 dB
PL1W           6.03017378 W
SFO1          600.1337060 MHz
SI                   32768
SF            600.1300066 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```

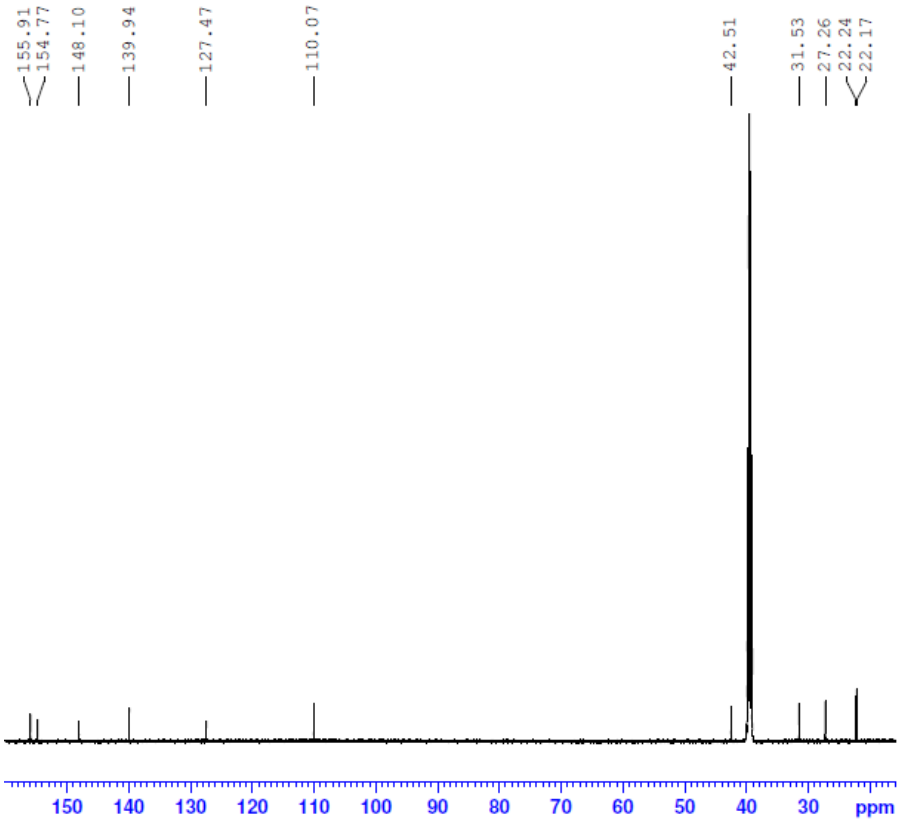



```
NAME                bki56c
EXPNO                   13
PROCNO                   1
Date_             20100412
Time                 16.18
INSTRUM              AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           zgpg30
TD                  65536
SOLVENT              DMSO
NS                     534
DS                       4
SWH              36057.691 Hz
FIDRES           0.550197 Hz
AQ               0.9088159 sec
RG                    2050
DW                  13.867 usec
DE                   6.00 usec
TE                  300.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    400

======== CHANNEL f1 =======
NUC1                   13C
P1                   13.20 usec
PL1                  -2.00 dB
PL1W         121.82079315 W
SFO1          150.9178990 MHz

======== CHANNEL f2 =======
CPDPRG2            waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   4.05 dB
PL12                 24.27 dB
PL13                 24.27 dB
PL2W           6.03017378 W
PL12W          0.05732312 W
PL13W          0.05732312 W
SFO2          600.1324000 MHz
SI                   32768
SF            150.9028880 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

1-(5,6,7,8-Tetrahydroquinolin-2’-yl)-2-iminoimidazolidine hydrochloride (9d)

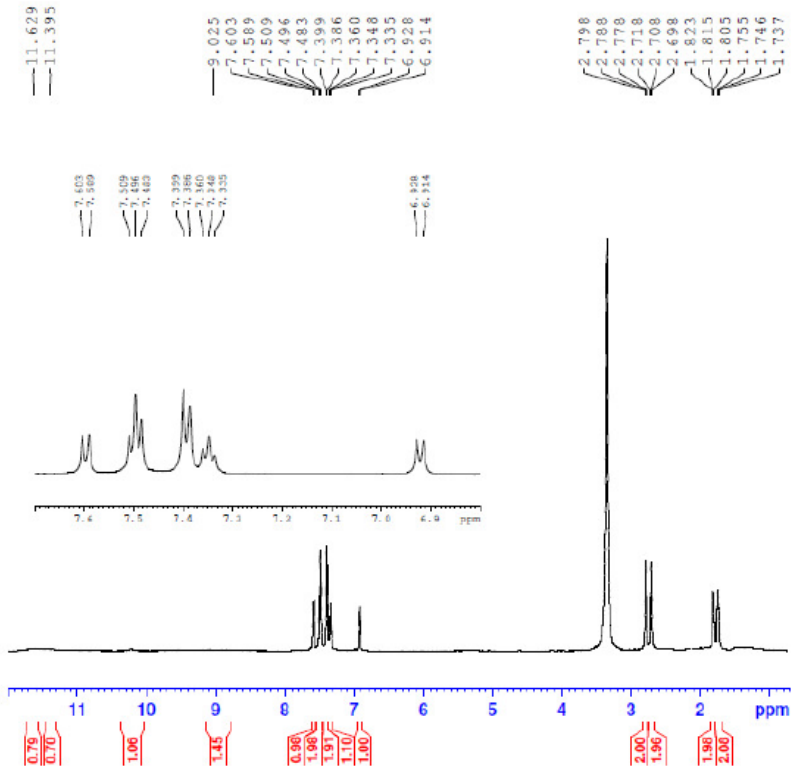


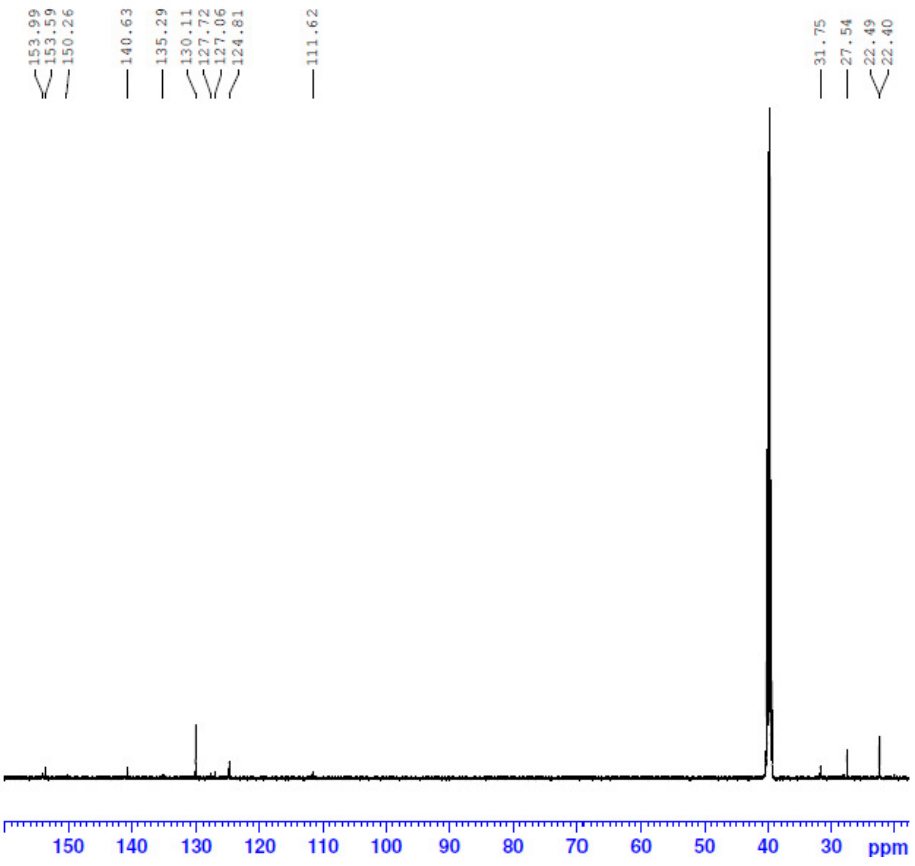

```
NAME            bki304ax
EXPNO                  1
PROCNO                 1
Date_           20110812
Time                9.45
INSTRUM            AV600
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     2
SWH           12335.526 Hz
FIDRES         0.188225 Hz
AQ             2.6564426 sec
RG                     8
DW                40.533 usec
DE                 6.00 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  8.43 usec
PL1                 4.05 dB
PL1W          6.03017378 W
SFO1        600.1337060 MHz
SI                 32768
SF          600.1300000 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```




```
NAME            bki304ax
EXPNO                 13
PROCNO                 1
Date_           20110812
Time                9.59
INSTRUM            AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   267
DS                     4
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ             0.9088159 sec
RG                  2050
DW                13.867 usec
DE                 6.00 usec
TE                298.1 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                  400

======== CHANNEL f1 ========
NUC1                 13C
P1                 13.20 usec
PL1                -2.00 dB
PL1W         121.82079315 W
SFO1         150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 4.05 dB
PL12               24.27 dB
PL13               24.27 dB
PL2W          6.03017378 W
PL12W         0.05732312 W
PL13W         0.05732312 W
SFO2        600.1324000 MHz
SI                 32768
SF          150.9028794 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

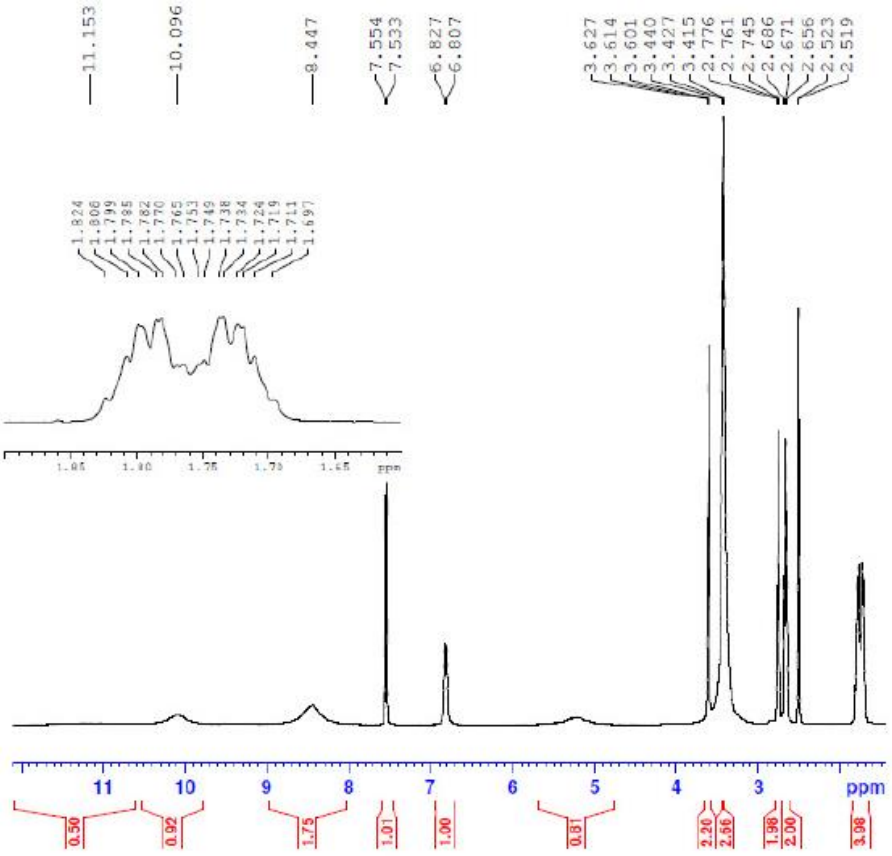
1-(5,6,7,8-Tetrahydroquinolin-2-yl)-3-(phenyl)guanidine hydrochloride (9i)



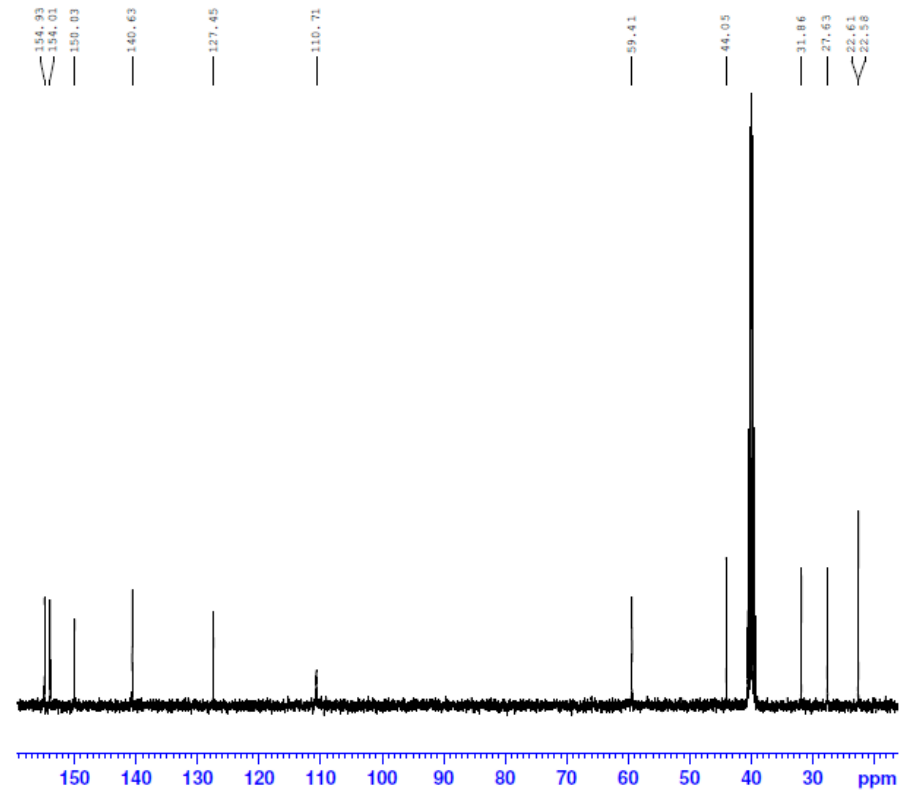


`

1-(5,6,7,8-Tetrahydroquinolin-2-yl)-3-(2-hydroxyethyl)guanidine hydrochloride (9j)

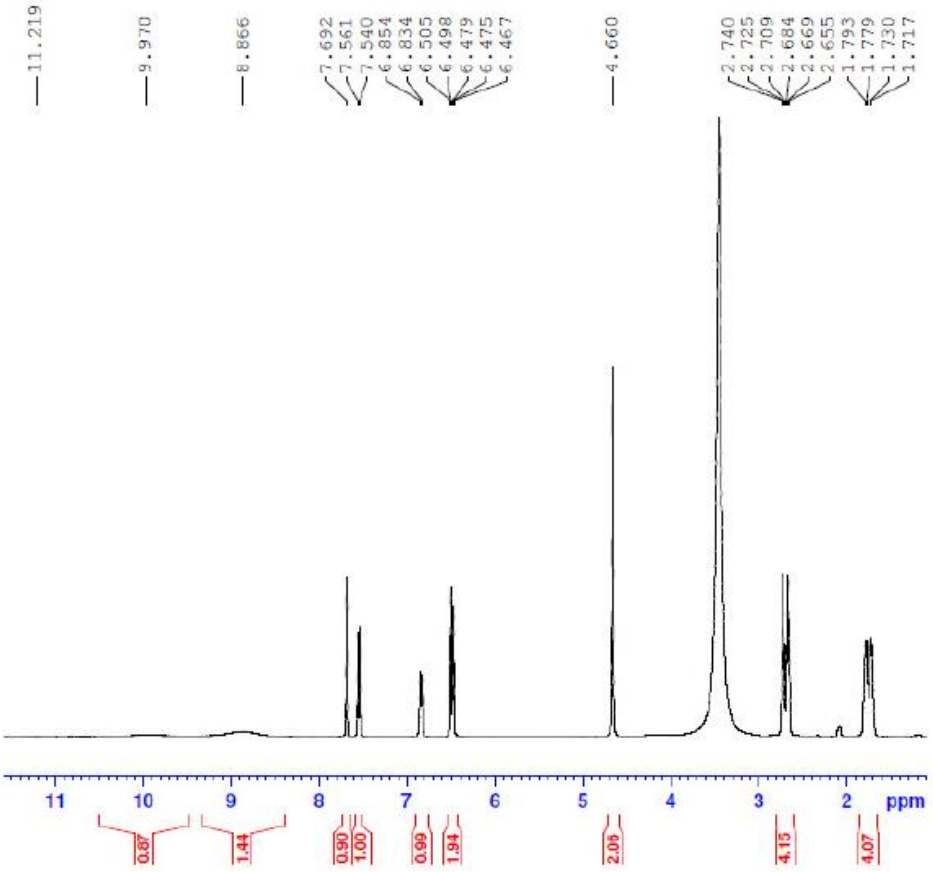



```
NAME            ssmmm21m
EXPNO                  1
PROCNO                 1
Date_           20111118
Time                8.03
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                  80.6
DW                 60.800 usec
DE                  6.00 usec
TE                298.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.00 usec
PL1                -4.00 dB
PL1W           19.30729485 W
SFO1           400.2324716 MHz
SI                 32768
SF             400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

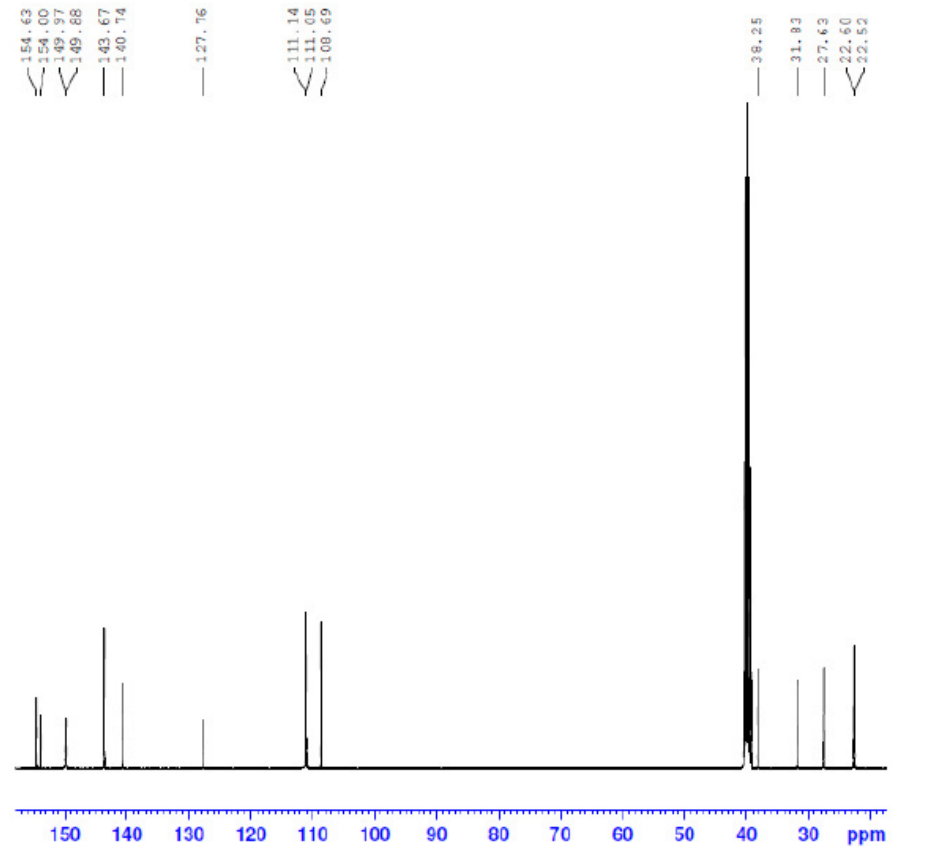



```
NAME            ssmmm21m
EXPNO                 13
PROCNO                 1
Date_           20111118
Time                8.12
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT             DMSO
NS                   175
DS                     2
SWH            32051.281 Hz
FIDRES          0.978127 Hz
AQ              0.5112308 sec
RG                   912
DW                 15.600 usec
DE                  6.00 usec
TE                298.2 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.00 usec
PL1                -2.30 dB
PL1W           60.57429123 W
SFO1           100.6505944 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                -4.00 dB
PL12               14.00 dB
PL13               14.00 dB
PL2W           19.30729485 W
PL12W           0.30599999 W
PL13W           0.30599999 W
SFO2           400.2316009 MHz
SI                 32768
SF             100.6379140 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

1-(5,6,7,8-Tetrahydroquinolin-2-yl)-3-(2-furanylmethyl)guanidine hydrochloride (9k)

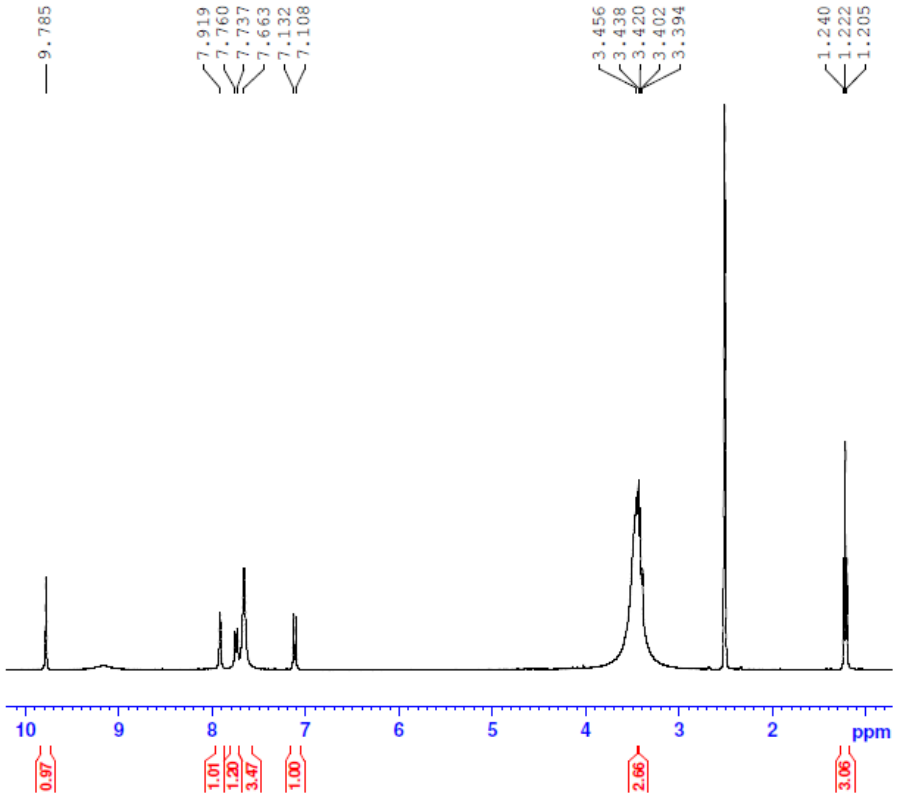



```
NAME            asmmm23d
EXPNO                  1
PROCNO                 1
Date_           20111121
Time               18.32
INSTRUM            spect
PROBHD  5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   101
DW                60.800 usec
DE                 6.00 usec
TE                298.2 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.00 usec
PL1                -4.00 dB
PL1W          19.30729485 W
SFO1          400.2324716 MHz
SI                 32768
SF            400.2300000 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

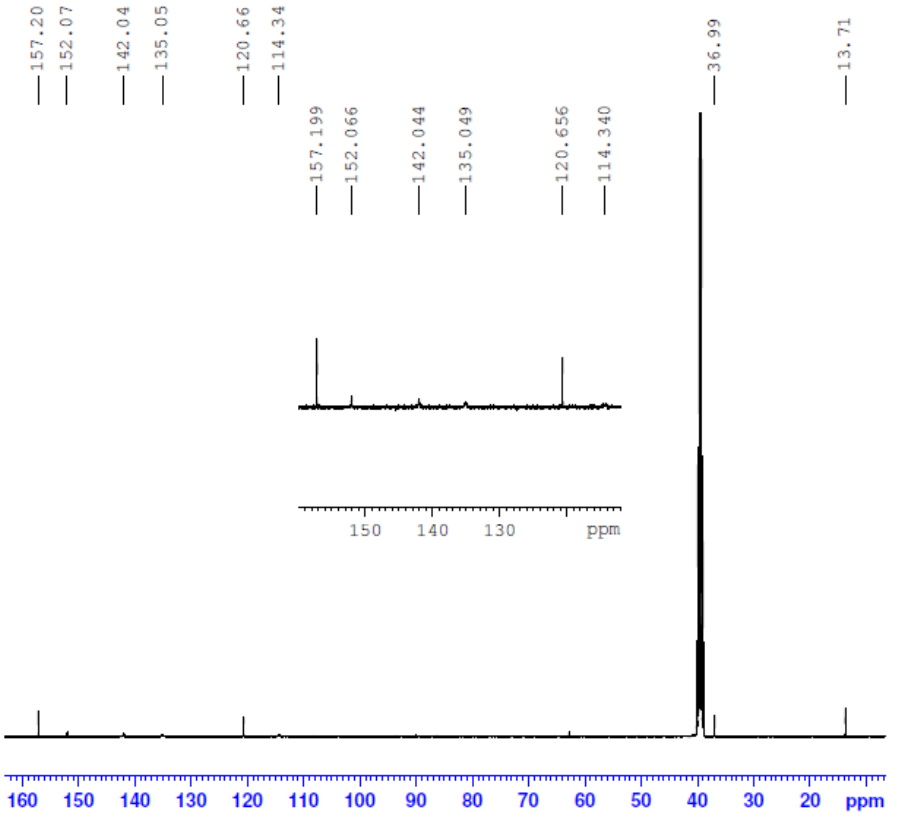



```
NAME            asmmm23d
EXPNO                 13
PROCNO                 1
Date_           20111121
Time               18.33
INSTRUM            spect
PROBHD  5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT             DMSO
NS                 31006
DS                     2
SWH            32051.281 Hz
FIDRES          0.978127 Hz
AQ              0.5112308 sec
RG                   912
DW                15.600 usec
DE                 6.00 usec
TE                298.2 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                 1009

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.00 usec
PL1                -2.30 dB
PL1W          60.57429123 W
SFO1          100.6505944 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -4.00 dB
PL12               14.00 dB
PL13               14.00 dB
PL2W          19.30729485 W
PL12W          0.30599999 W
PL13W          0.30599999 W
SFO2          400.2316009 MHz
SI                 32768
SF            100.6379140 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

1-[5-(Ethylamino)pyridin-2-yl]guanidine hydrochloride (10c)

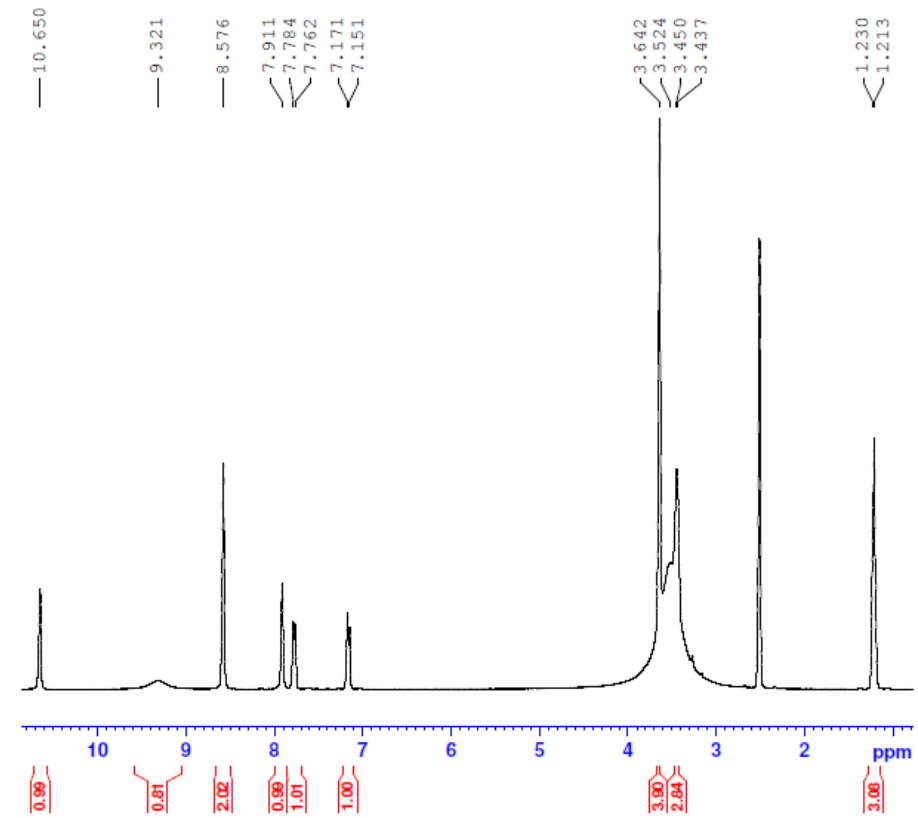



```
NAME            bki448fx
EXPNO                  1
PROCNO                 1
Date_           20120501
Time               13.13
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    16
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   161
DW                60.800 usec
DE                 6.00 usec
TE                293.5 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 10.00 usec
PL1                -4.00 dB
PL1W         19.30729485 W
SFO1         400.2324716 MHz
SI                 32768
SF           400.2300000 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

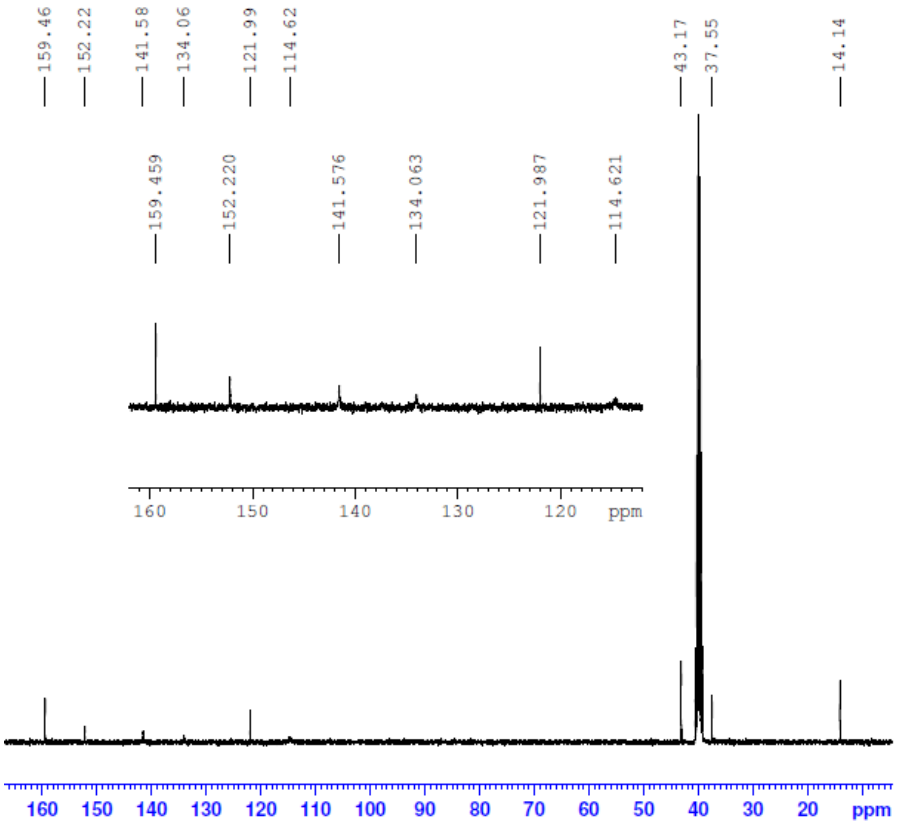



```
NAME            bki448fx
EXPNO                 13
PROCNO                 1
Date_           20120501
Time               13.18
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 32768
SOLVENT             DMSO
NS                  7034
DS                     2
SWH            32051.281 Hz
FIDRES          0.978127 Hz
AQ              0.5112308 sec
RG                   912
DW                15.600 usec
DE                 6.00 usec
TE                294.5 K
D1              1.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 8.00 usec
PL1                -2.30 dB
PL1W         60.57429123 W
SFO1         100.6505944 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -4.00 dB
PL12               14.00 dB
PL13               14.00 dB
PL2W         19.30729485 W
PL12W         0.30599999 W
PL13W         0.30599999 W
SFO2         400.2316009 MHz
SI                 32768
SF           100.6379595 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

1-[5-(Ethylamino)pyridin-2’-yl]2-iminoimidazolidine hydrochloride (10d)

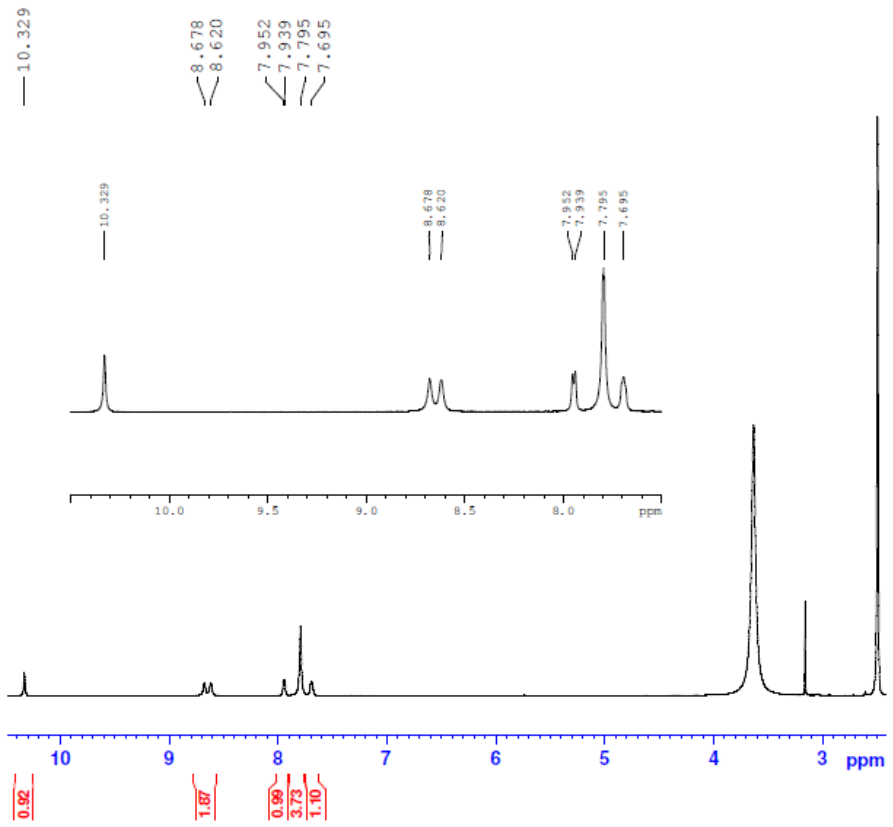



```
NAME            bki449fx
EXPNO                1
PROCNO               1
Date_         20120503
Time             10.11
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG          zg30
TD              32768
SOLVENT          DMSO
NS                  16
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9923444 sec
RG                 128
DW              60.800 usec
DE               6.00 usec
TE              295.1 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               10.00 usec
PL1              -4.00 dB
PL1W        19.30729485 W
SFO1        400.2324716 MHz
SI              32768
SF          400.2300000 MHz
WDW                 EM
SSB                  0
LB               0.30 Hz
GB                   0
PC                1.00
```

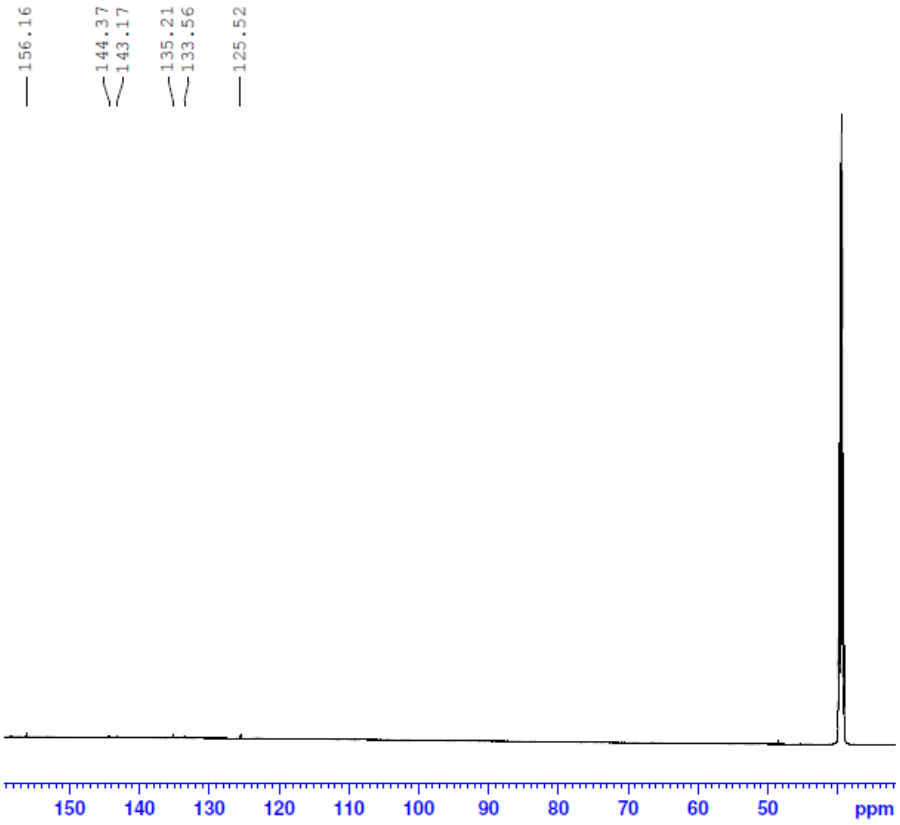



```
NAME            bki449fx
EXPNO               13
PROCNO               1
Date_         20120503
Time             10.24
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD              32768
SOLVENT          DMSO
NS                 766
DS                   2
SWH          32051.281 Hz
FIDRES        0.978127 Hz
AQ            0.5112308 sec
RG                 912
DW              15.600 usec
DE               6.00 usec
TE              296.3 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                8.00 usec
PL1              -2.30 dB
PL1W        60.57429123 W
SFO1        100.6505944 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2            80.00 usec
PL2              -4.00 dB
PL12             14.00 dB
PL13             14.00 dB
PL2W        19.30729485 W
PL12W        0.30599999 W
PL13W        0.30599999 W
SFO2        400.2316009 MHz
SI              32768
SF          100.6379140 MHz
WDW                 EM
SSB                  0
LB               1.00 Hz
GB                   0
PC                1.40
```

1-(Pyridin-3-yl)guanidine hydrochloride (11c)

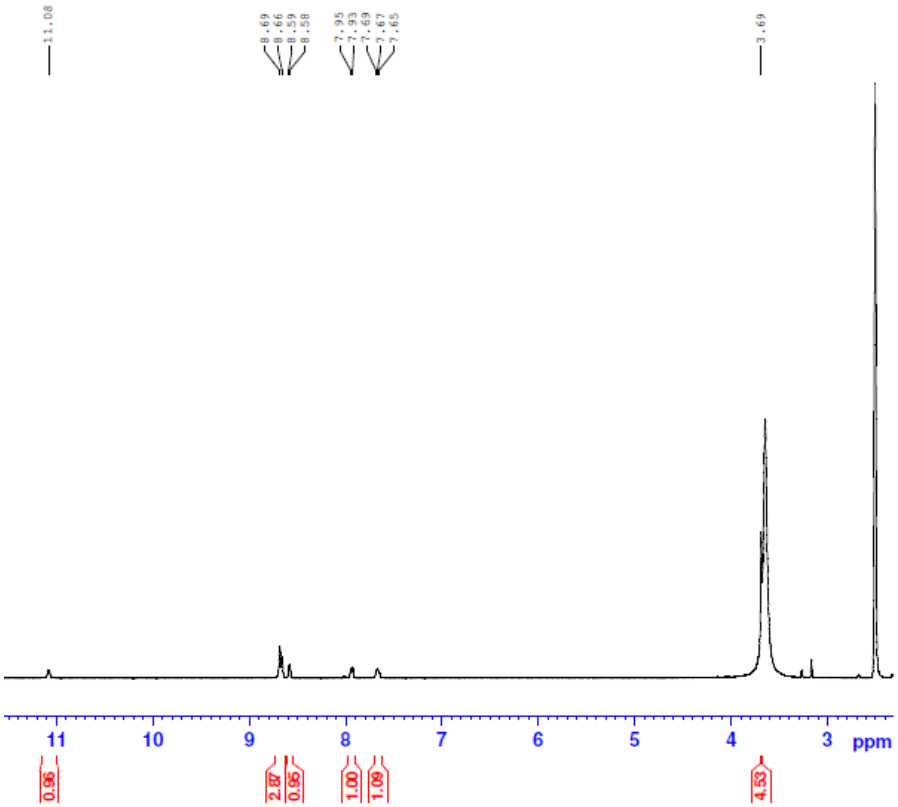



```
NAME            bki21cx
EXPNO                 1
PROCNO                1
Date_          20100504
Time              15.49
INSTRUM           AV600
PROBHD   5 mm CPTCI 1H-
PULPROG            zg30
TD                65536
SOLVENT             DMSO
NS                    8
DS                    2
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                    8
DW               20.800 usec
DE                6.00 usec
TE               300.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                7.80 usec
PL1               4.05 dB
PL1W       6.03017378 W
SFO1       600.1337060 MHz
SI                32768
SF         600.1300093 MHz
WDW                  no
SSB                   0
LB                0.00 Hz
GB                    0
PC                1.00
```

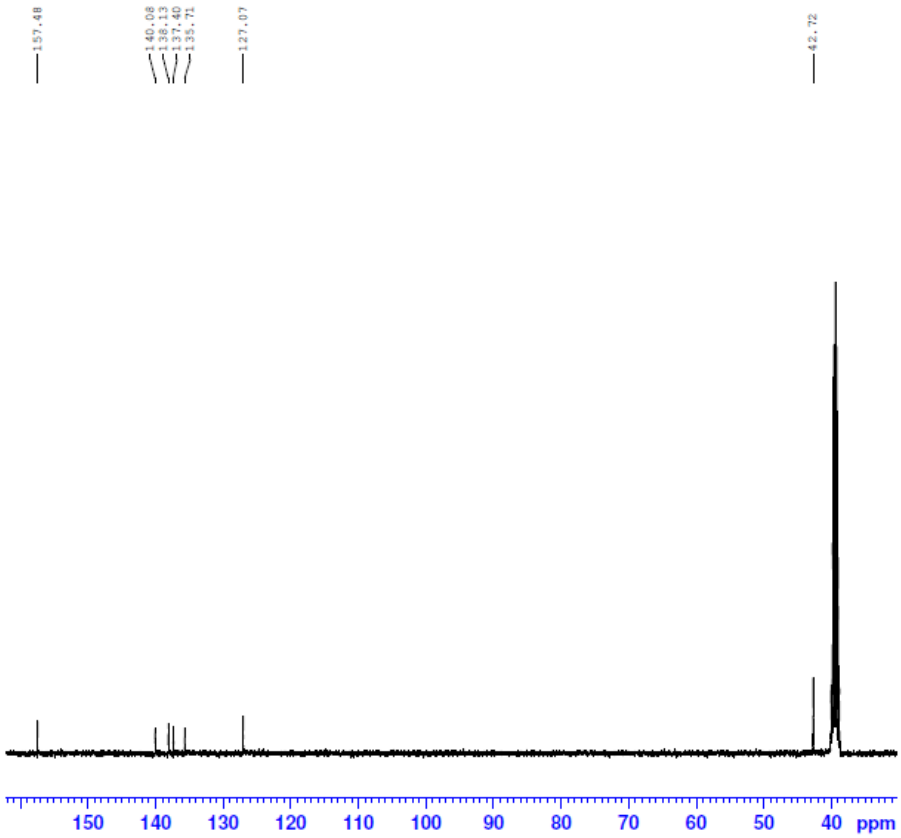



```
NAME            bki21cx
EXPNO                13
PROCNO                1
Date_          20100504
Time              16.58
INSTRUM           AV600
PROBHD   5 mm CPTCI 1H-
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                29636
DS                    4
SWH           36057.691 Hz
FIDRES        0.550197 Hz
AQ            0.9088159 sec
RG                 2050
DW               13.867 usec
DE                6.00 usec
TE               300.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                 400

======== CHANNEL f1 ========
NUC1                 13C
P1               13.20 usec
PL1               -2.00 dB
PL1W      121.82079315 W
SFO1       150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            80.00 usec
PL2               4.05 dB
PL12             24.27 dB
PL13             24.27 dB
PL2W       6.03017378 W
PL12W      0.05732312 W
PL13W      0.05732312 W
SFO2       600.1324000 MHz
SI                32768
SF         150.9028875 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

1-(Pyridin-3’-yl)-2-iminoimidazolidine hydrochloride (11d)

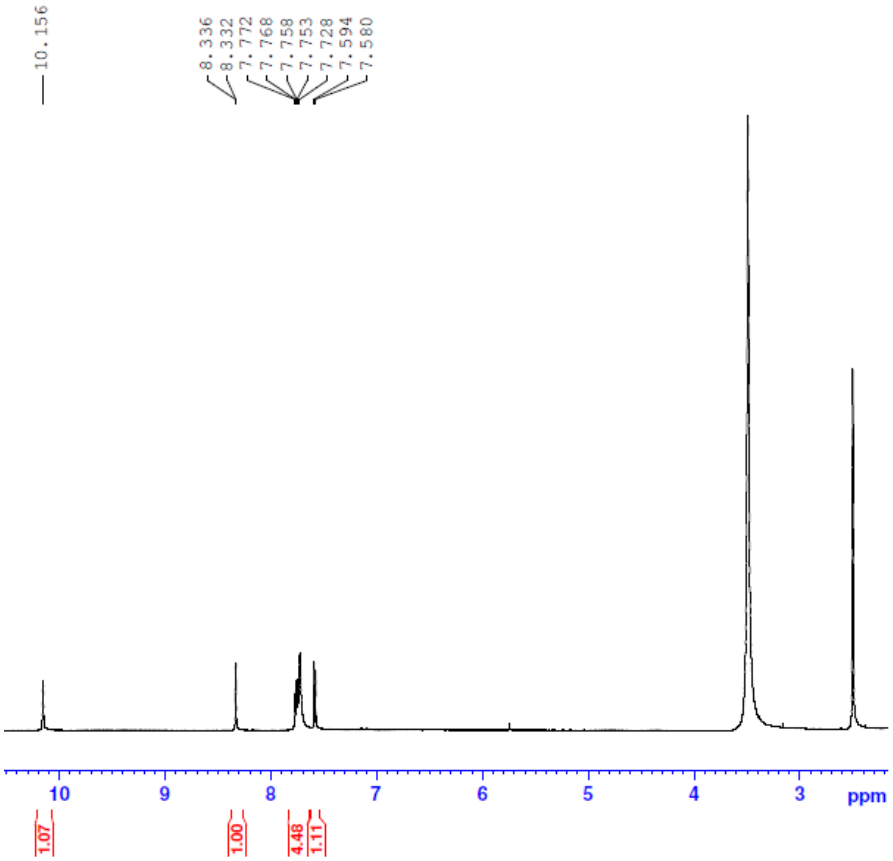



```
NAME              bki332a
EXPNO                   1
PROCNO                  1
Date_            20110908
Time                15.09
INSTRUM          dpx400
PROBHD    5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT             DMSO
NS                    51
DS                     2
SWH             8223.685 Hz
FIDRES          0.250967 Hz
AQ              1.9923444 sec
RG                   256
DW                60.800 usec
DE                 5.50 usec
TE                292.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  9.75 usec
PL1                 3.00 dB
SFO1       400.1336012 MHz
SI                 16384
SF         400.1299998 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

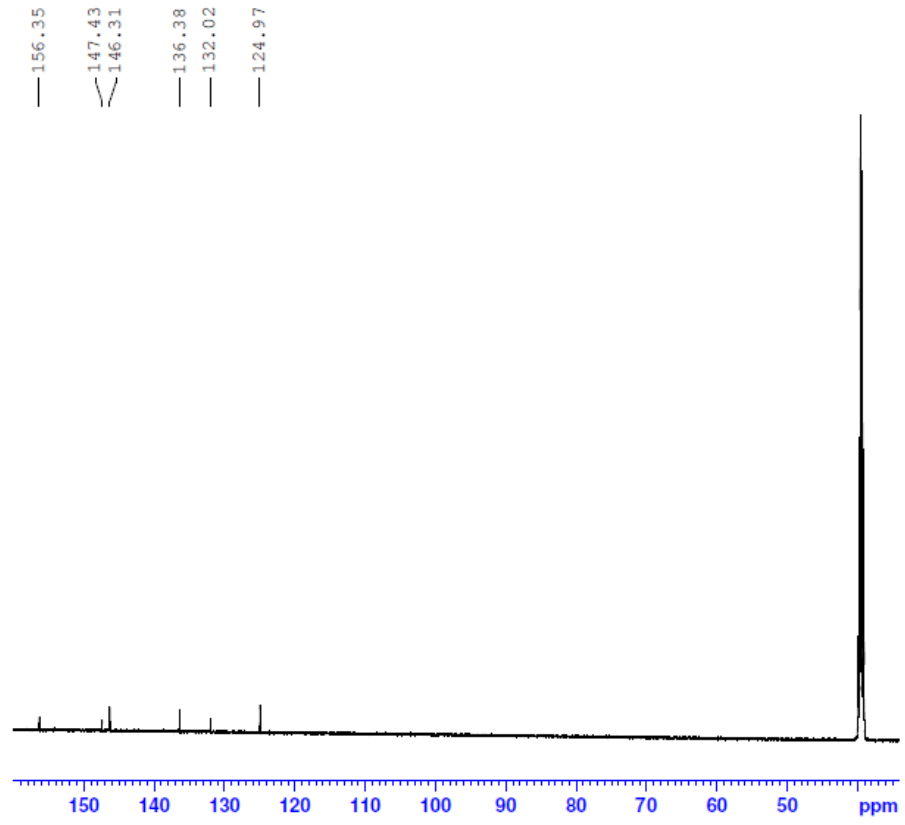



```
NAME              bki332a
EXPNO                  13
PROCNO                  1
Date_            20110909
Time                16.10
INSTRUM          dpx400
PROBHD    5 mm QNP 1H/13
PULPROG          zgpg30
TD                 32768
SOLVENT             CDCl3
NS                   184
DS                     2
SWH            31847.133 Hz
FIDRES          0.971897 Hz
AQ              0.5145076 sec
RG                  8192
DW                15.700 usec
DE                 5.50 usec
TE                293.2 K
D1           1.00000000 sec
d11          0.03000000 sec
DELTA        0.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  8.25 usec
PL1                -6.00 dB
SFO1       100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2              70.00 usec
PL2                 3.00 dB
PL12               19.07 dB
PL13               20.00 dB
SFO2       400.1316005 MHz
SI                 32768
SF         100.6128155 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

1-(6-Chloropyridin-3-yl)guanidine hydrochloride (12c)

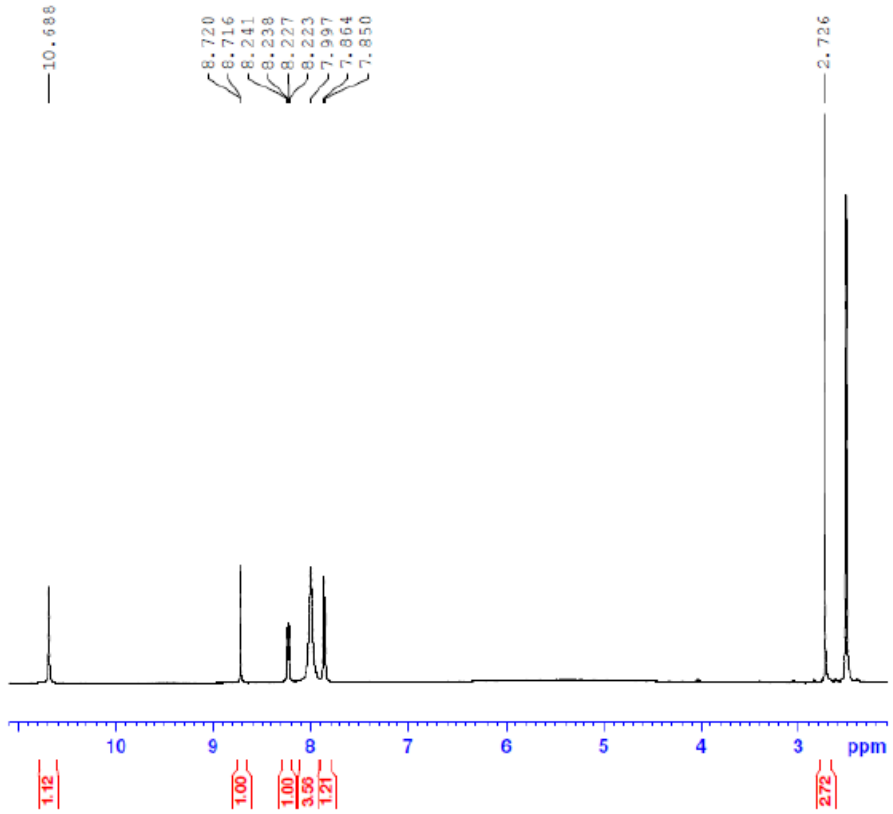



```
NAME                bki235b
EXPNO                     1
PROCNO                    1
Date_              20110426
Time                 14.09
INSTRUM              AV600
PROBHD   5 mm CPTCI 1H-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        8
DS                        2
SWH              12335.526 Hz
FIDRES            0.188225 Hz
AQ                2.6564426 sec
RG                        8
DW                  40.533 usec
DE                    6.00 usec
TE                  298.0 K
D1                1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                    1H
P1                    7.65 usec
PL1                   4.05 dB
PL1W           6.03017378 W
SFO1          600.1337060 MHz
SI                    32768
SF            600.1300070 MHz
WDW                     no
SSB                      0
LB                    0.00 Hz
GB                       0
PC                    1.00
```

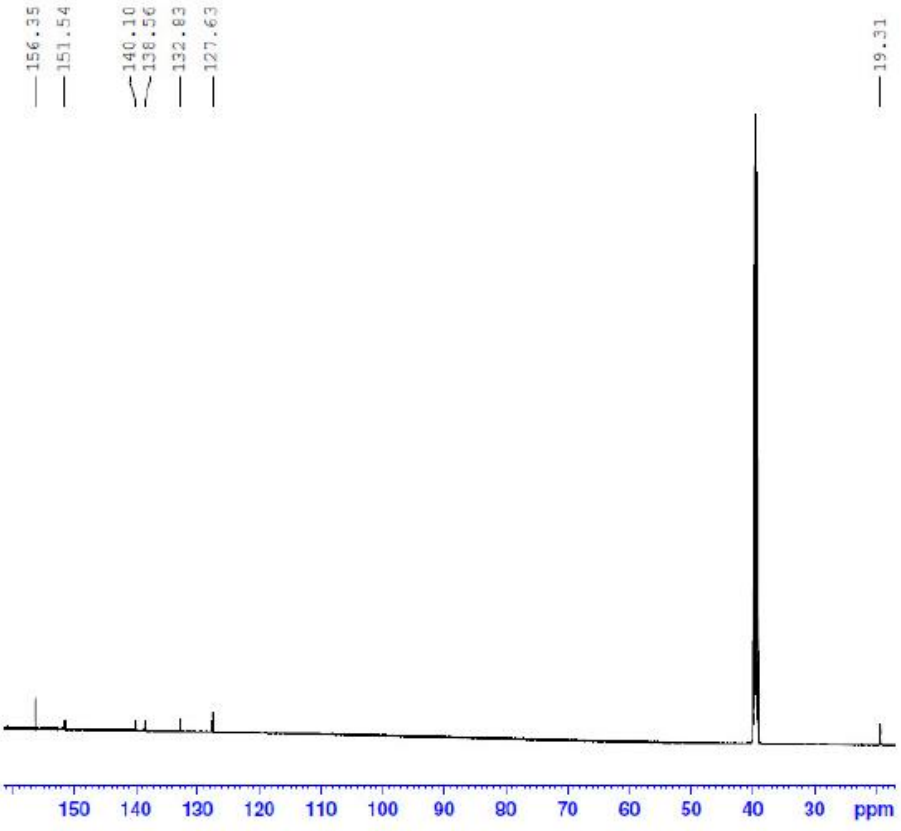



```
NAME                bki235b
EXPNO                    13
PROCNO                    1
Date_              20110426
Time                 13.19
INSTRUM              AV600
PROBHD   5 mm CPTCI 1H-
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                      205
DS                        4
SWH              36057.691 Hz
FIDRES            0.550197 Hz
AQ                0.9088159 sec
RG                     2050
DW                  13.867 usec
DE                    6.00 usec
TE                  298.1 K
D1                1.00000000 sec
D11               0.03000000 sec
TD0                     400

======== CHANNEL f1 ========
NUC1                   13C
P1                   13.20 usec
PL1                  -2.00 dB
PL1W          121.82079315 W
SFO1          150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                80.00 usec
PL2                   4.05 dB
PL12                 24.27 dB
PL13                 24.27 dB
PL2W           6.03017378 W
PL12W          0.05732312 W
PL13W          0.05732312 W
SFO2          600.1324000 MHz
SI                    32768
SF            150.9028816 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

1-(6-Methylpyridin-3-yl)guanidine hydrochloride (13c)

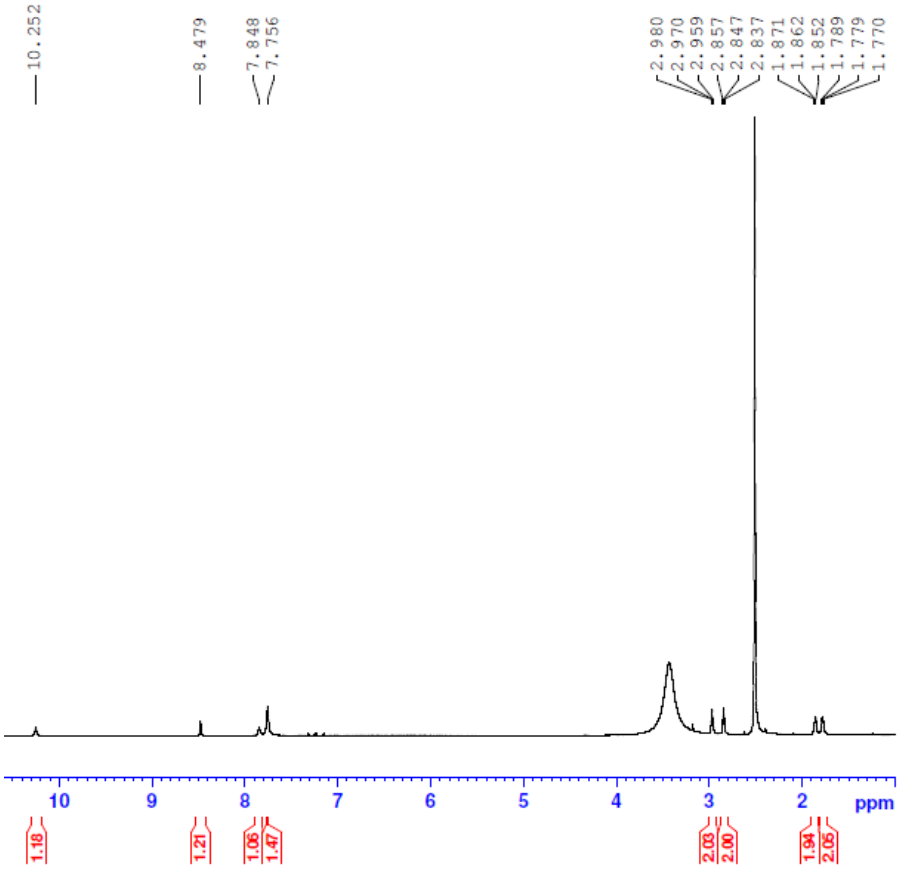



```
NAME                bk1230k
EXPNO                     1
PROCNO                    1
Date_              20110428
Time                   9.45
INSTRUM                AV600
PROBHD  5 mm CPTCI 1H-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        8
DS                        2
SWH              12335.526 Hz
FIDRES           0.188225 Hz
AQ               2.6564426 sec
RG                        8
DW                  40.533 usec
DE                   6.00 usec
TE                  298.0 K
D1               1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     7.80 usec
PL1                    4.05 dB
PL1W             6.03017378 W
SFO1           600.1337060 MHz
SI                    32768
SF             600.1300000 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```

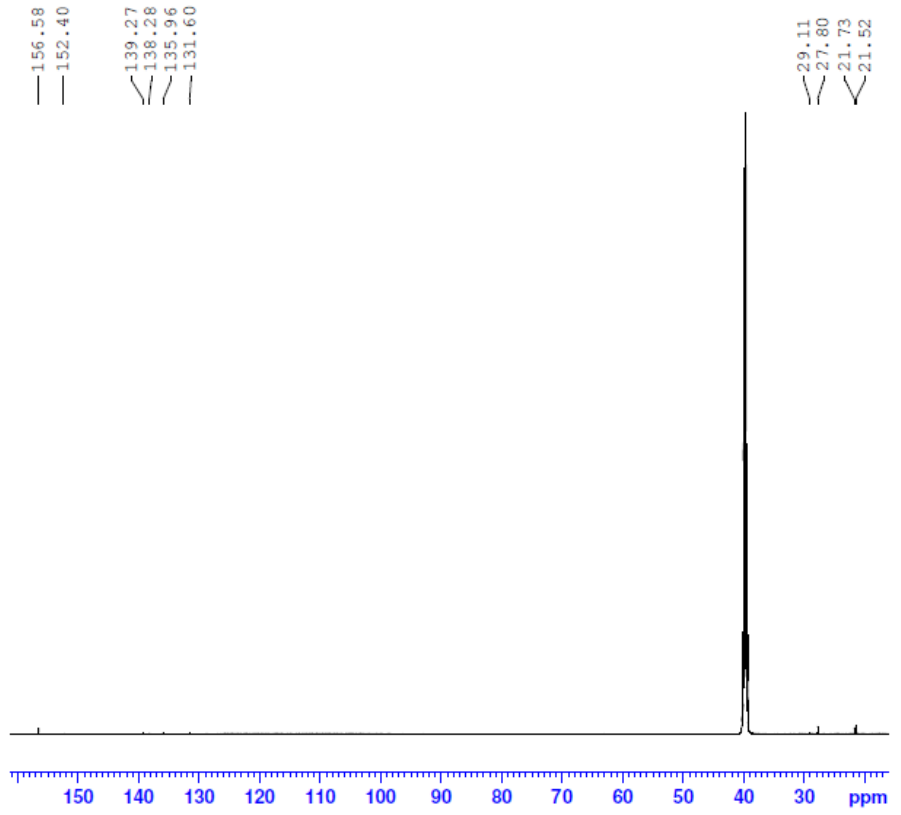



```
NAME                bk1230k
EXPNO                    13
PROCNO                    1
Date_              20110428
Time                   8.42
INSTRUM                AV600
PROBHD  5 mm CPTCI 1H-
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                      803
DS                        4
SWH              36057.691 Hz
FIDRES           0.550197 Hz
AQ               0.9088159 sec
RG                     2050
DW                  13.867 usec
DE                   6.00 usec
TE                  298.0 K
D1               1.00000000 sec
D11              0.03000000 sec
TD0                     400

======== CHANNEL f1 ========
NUC1                      13C
P1                    13.20 usec
PL1                   -2.00 dB
PL1W            121.82079315 W
SFO1           150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                    4.05 dB
PL12                  24.27 dB
PL13                  24.27 dB
PL2W             6.03017378 W
PL13W            0.05732312 W
PL13W            0.05732312 W
SFO2           600.1324000 MHz
SI                    32768
SF             150.9028848 MHz
WDW                      EM
SSB                       0
LB                     1.00 Hz
GB                        0
PC                     1.40
```

1-(5,6,7,8-Tetrahydroquinolin-3-yl)guanidine hydrochloride (14c)

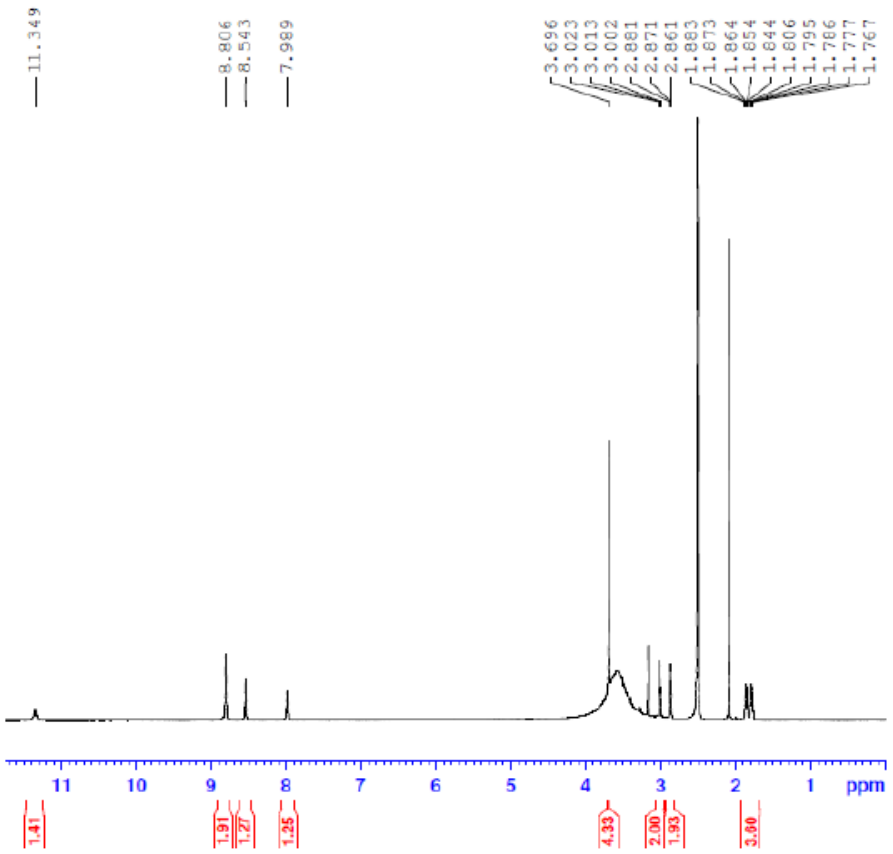



```
NAME            bki282ax
EXPNO                 1
PROCNO                1
Date_          20110726
Time               9.25
INSTRUM          AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                    8
DS                    2
SWH           12335.526 Hz
FIDRES        0.188225 Hz
AQ            2.6564426 sec
RG                    8
DW               40.533 usec
DE                6.00 usec
TE               298.0 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                7.96 usec
PL1               4.05 dB
PL1W        6.03017378 W
SFO1        600.1337060 MHz
SI                32768
SF          600.1300000 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                1.00
```

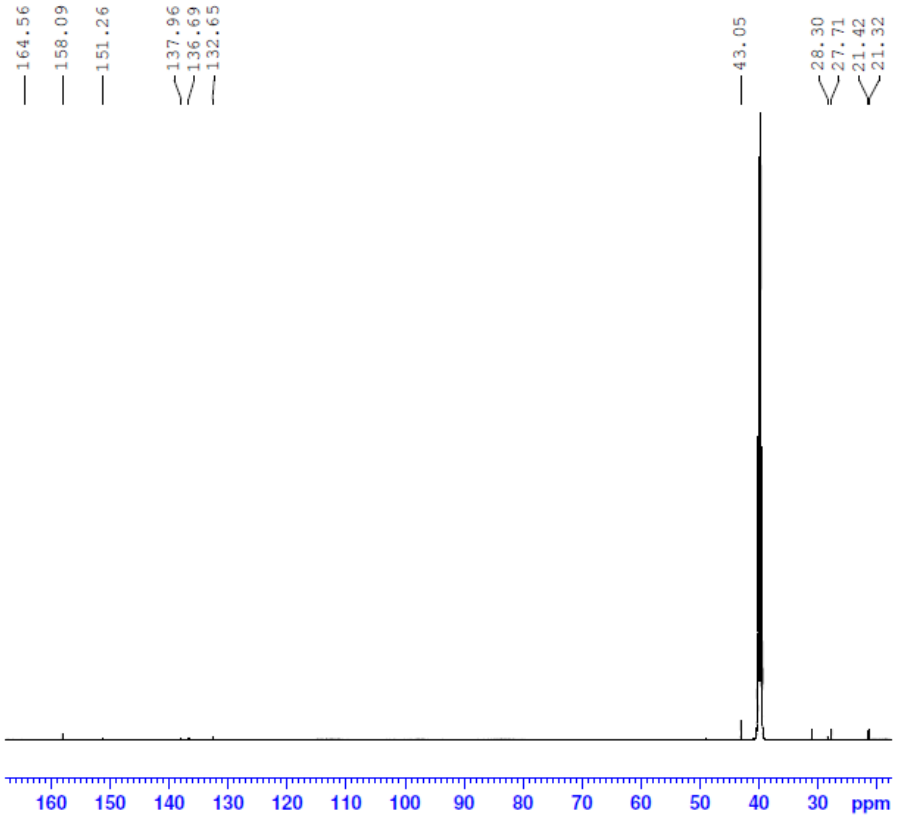



```
NAME            bki282ax
EXPNO                13
PROCNO                1
Date_          20110808
Time              15.12
INSTRUM          AV600
PROBHD   5 mm CPTCI 1H-
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                33368
DS                    4
SWH           36057.691 Hz
FIDRES        0.550197 Hz
AQ            0.9088159 sec
RG                 2050
DW               13.867 usec
DE                6.00 usec
TE               298.1 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                 400

======== CHANNEL f1 ========
NUC1                13C
P1               13.20 usec
PL1              -2.00 dB
PL1W       121.82079315 W
SFO1        150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               4.05 dB
PL12             24.27 dB
PL13             24.27 dB
PL2W        6.03017378 W
PL12W       0.05732312 W
PL13W       0.05732312 W
SFO2        600.1324000 MHz
SI                32768
SF          150.9028332 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

1-(5,6,7,8-Tetrahydroquinolin-3’-yl)-2-iminoimidazolidine hydrochloride (14d)

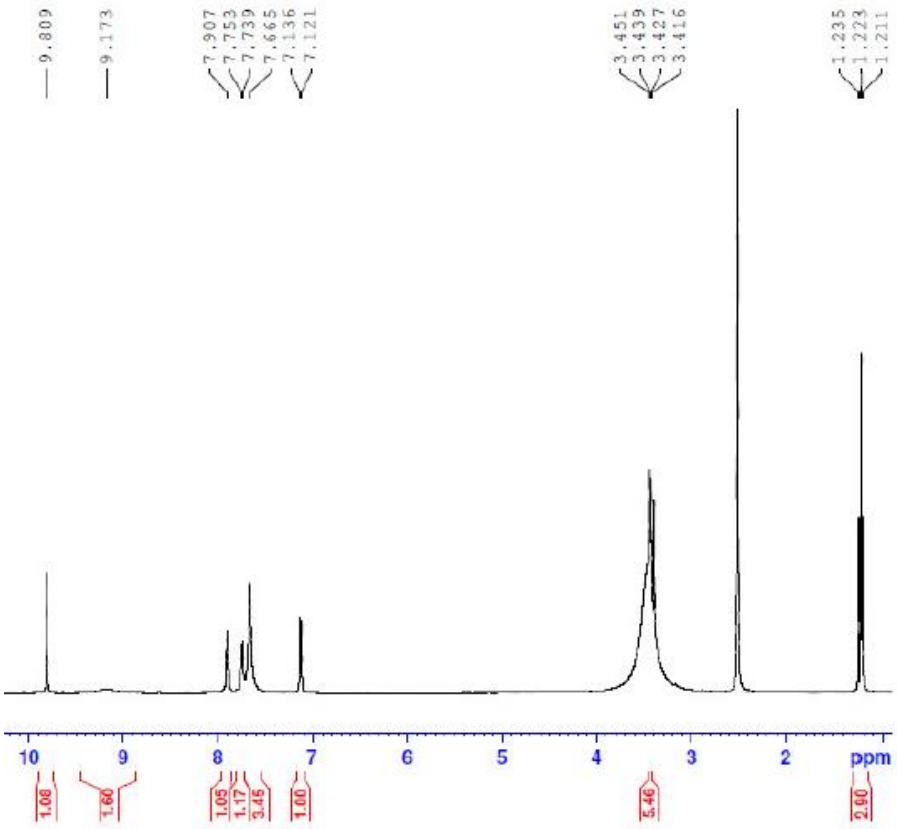



```
NAME            DK1320SX
EXPNO                1
PROCNO               1
Date_         20110826
Time              16.58
INSTRUM           AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                   8
DS                   2
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631988 sec
RG                   8
DW              20.800 usec
DE               6.00 usec
TE              298.0 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1               7.49 usec
PL1              4.05 dB
PL1W       6.03017378 W
SFO1     600.1337060 MHz
SI               32768
SF       600.1300000 MHz
WDW                 no
SSB                  0
LB                0.00 Hz
GB                   0
PC                1.00
```

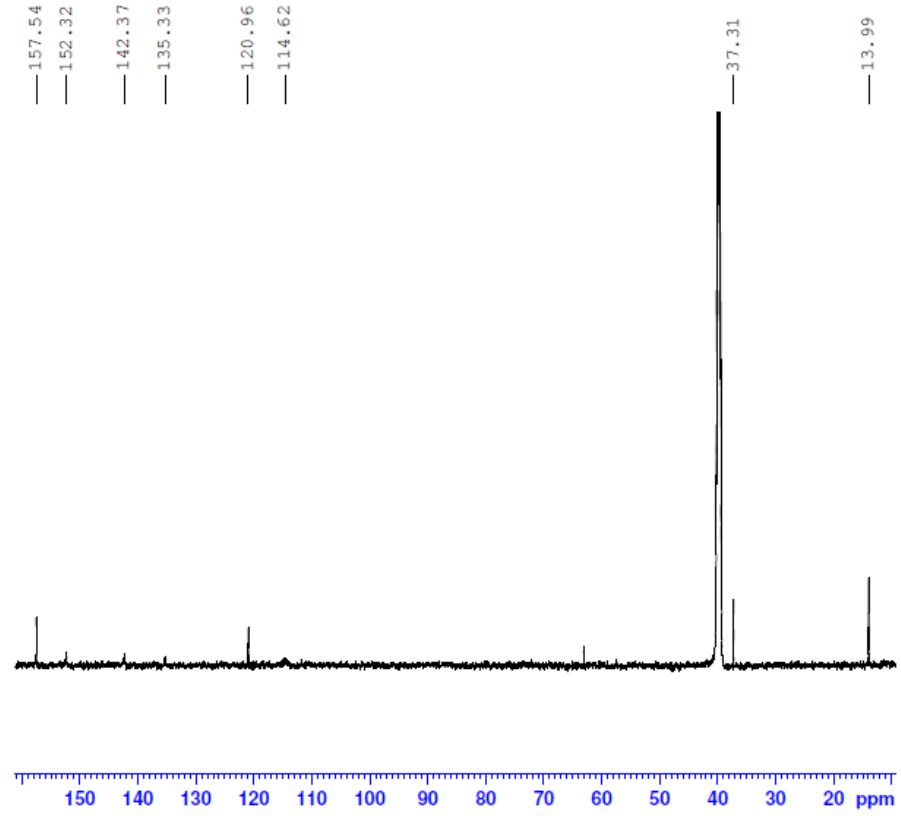



```
NAME            bki320sx
EXPNO                13
PROCNO                1
Date_         20110827
Time              19.49
INSTRUM           AV600
PROBHD   5 mm CPTCI 1H-
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                68340
DS                    4
SWH          36057.691 Hz
FIDRES        0.550197 Hz
AQ            0.9088159 sec
RG                 2050
DW              13.867 usec
DE               6.00 usec
TE              298.0 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                400

======== CHANNEL f1 ========
NUC1               13C
P1              13.20 usec
PL1             -2.00 dB
PL1W      121.82079315 W
SFO1      150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2           80.00 usec
PL2              4.05 dB
PL12            24.27 dB
PL13            24.27 dB
PL2W       6.03017378 W
PL12W      0.05732312 W
PL13W      0.05732312 W
SFO2     600.1324000 MHz
SI               32768
SF       150.9028332 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

1-[6-(*N*-ethylamino)pyridin-3-yl]guanidine hydrochloride (15c)

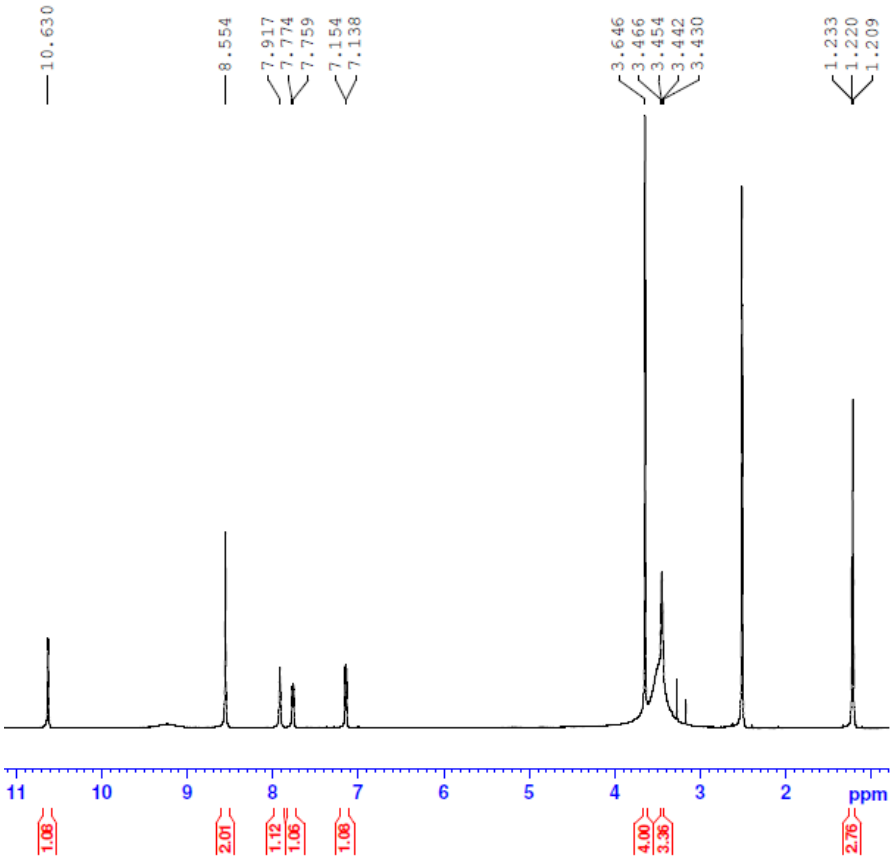



```
NAME                DX1266CX
EXPNO                      1
PROCNO                     1
Date_               20110607
Time                   15.36
INSTRUM                AV600
PROBHD     5 mm CPTCI 1H-
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                        16
DS                         2
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631988 sec
RG                         8
DW                    20.800 usec
DE                     6.00 usec
TE                    298.0 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     7.80 usec
PL1                    4.05 dB
PL1W               6.03017378 W
SFO1             600.1337060 MHz
SI                        65536
SF               600.1300000 MHz
WDW                       no
SSB                        0
LB                     0.00 Hz
GB                         0
PC                     1.00
```

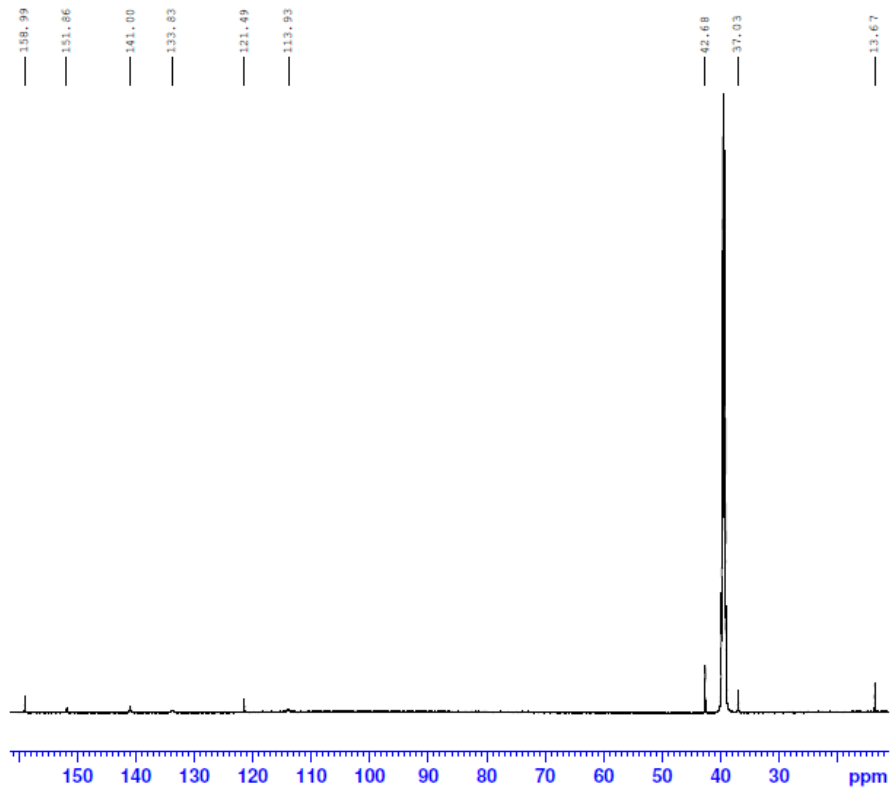



```
NAME                bki266cx
EXPNO                     13
PROCNO                     2
Date_               20110607
Time                   15.43
INSTRUM                AV600
PROBHD     5 mm CPTCI 1H-
PULPROG             zgpg30
TD                    65536
SOLVENT                DMSO
NS                       227
DS                         4
SWH                36057.691 Hz
FIDRES             0.550197 Hz
AQ                 0.9088159 sec
RG                      2050
DW                    13.867 usec
DE                     6.00 usec
TE                    298.1 K
D1                 1.00000000 sec
D11                0.03000000 sec
TD0                      400

======== CHANNEL f1 ========
NUC1                      13C
P1                    13.20 usec
PL1                   -2.00 dB
PL1W             121.82079315 W
SFO1             150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                 80.00 usec
PL2                    4.05 dB
PL12                  24.27 dB
PL13                  24.27 dB
PL2W               6.03017378 W
PL12W              0.05732312 W
PL13W              0.05732312 W
SFO2             600.1324000 MHz
SI                        32768
SF               150.9028332 MHz
WDW                       EM
SSB                        0
LB                     4.00 Hz
GB                         0
PC                     1.40
```

1-(6-(Ethylamino)pyridin-3’-yl)-2-iminoimidazolidine hydrochloride (15d)

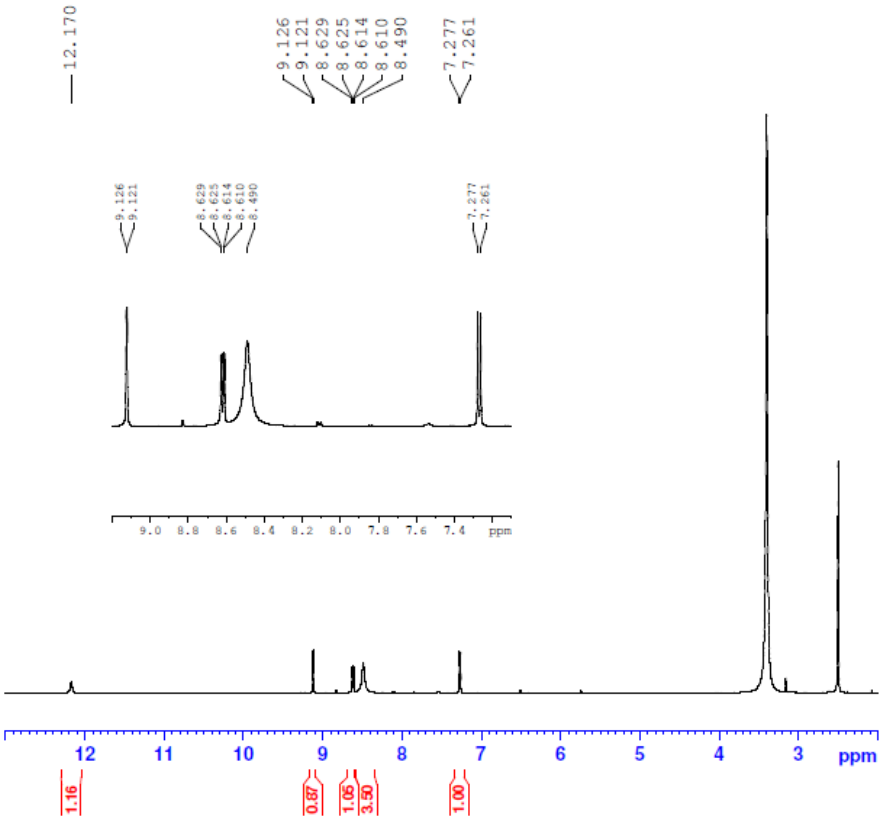



```
NAME            bki310ax
EXPNO                  1
PROCNO                 1
Date_           20110822
Time                9.20
INSTRUM           AV600
PROBHD    5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631988 sec
RG                     8
DW                20.800 usec
DE                 6.00 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  7.94 usec
PL1                 4.05 dB
PL1W          6.03017378 W
SFO1        600.1337060 MHz
SI                 32768
SF          600.1300000 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

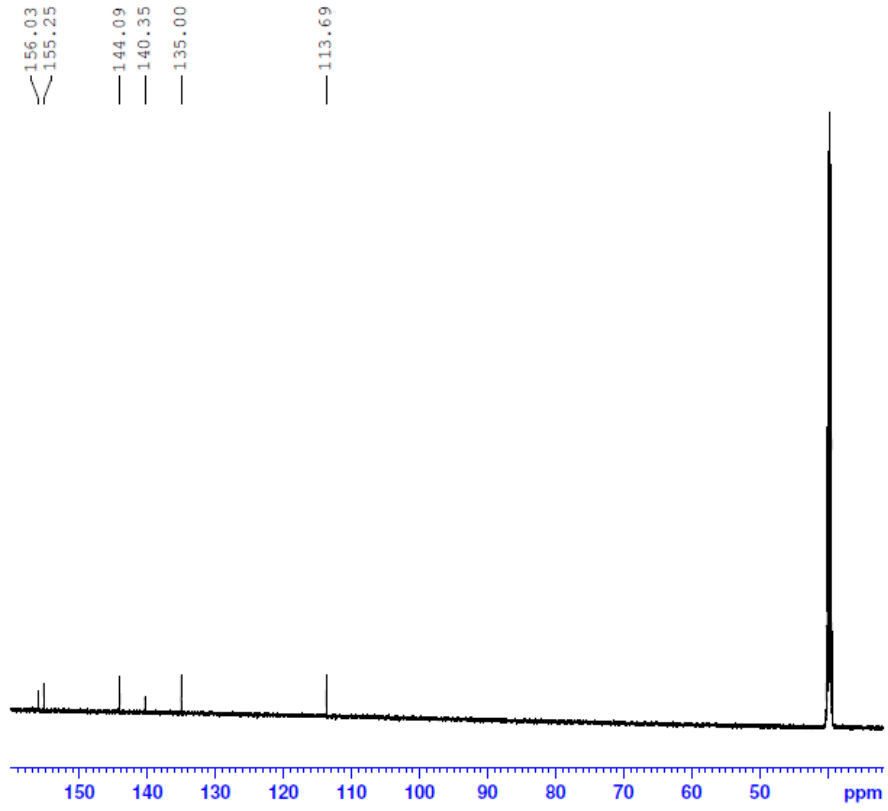



```
NAME            bki310ax
EXPNO                 13
PROCNO                 2
Date_           20110822
Time                9.24
INSTRUM           AV600
PROBHD    5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   770
DS                     4
SWH           36057.691 Hz
FIDRES         0.550197 Hz
AQ             0.9088159 sec
RG                  2050
DW                13.867 usec
DE                 6.00 usec
TE                298.0 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                  400

======== CHANNEL f1 ========
NUC1                 13C
P1                 13.20 usec
PL1                -2.00 dB
PL1W         121.82079315 W
SFO1        150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 4.05 dB
PL12               24.27 dB
PL13               24.27 dB
PL2W          6.03017378 W
PL12W         0.05732312 W
PL13W         0.05732312 W
SFO2        600.1324000 MHz
SI                 32768
SF          150.9028844 MHz
WDW                   EM
SSB                    0
LB                  6.00 Hz
GB                     0
PC                  1.40
```

1-(5-Nitropyridin-2-yl)guanidine hydrochloride (17c)

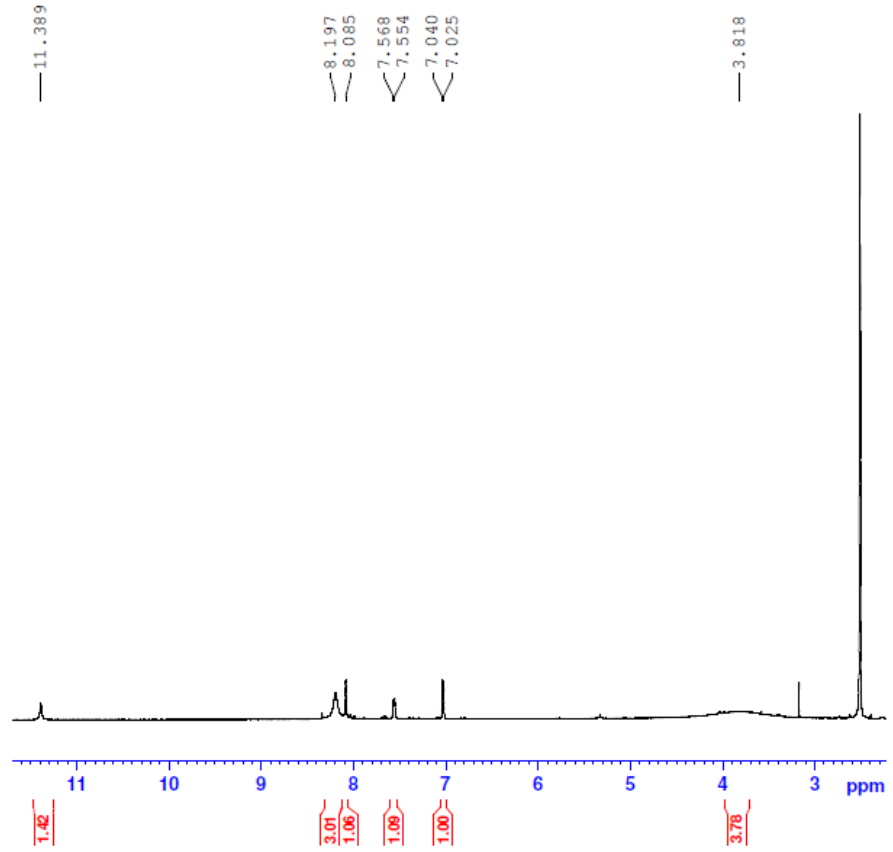



```
NAME            bki169bx
EXPNO                  1
PROCNO                 1
Date_           20101124
Time               16.05
INSTRUM            AV600
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     2
SWH            12335.526 Hz
FIDRES         0.188225 Hz
AQ             2.6564426 sec
RG                     8
DW                40.533 usec
DE                 6.00 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 7.80 usec
PL1                4.05 dB
PL1W        6.03017378 W
SFO1       600.1337060 MHz
SI                 32768
SF         600.1300071 MHz
WDW                   EM
SSB                    0
LB                 0.30 Hz
GB                     0
PC                 1.00
```

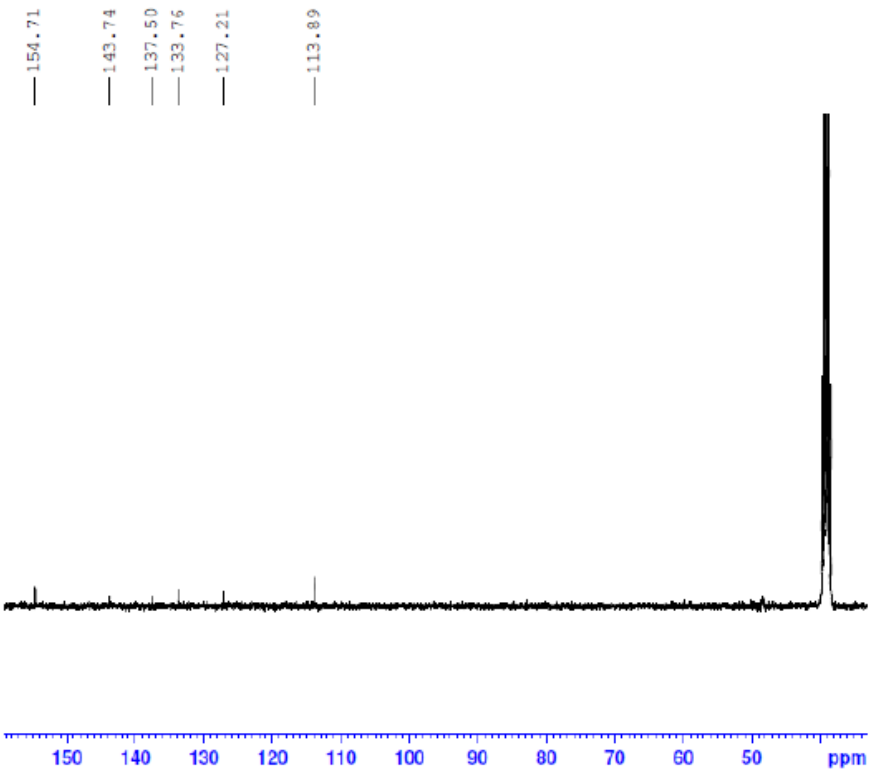



```
NAME            bki169bx
EXPNO                 13
PROCNO                 1
Date_           20101124
Time               16.11
INSTRUM            AV600
PROBHD   5 mm CPTCI 1H-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   148
DS                     4
SWH            36057.691 Hz
FIDRES         0.550197 Hz
AQ             0.9088159 sec
RG                  2050
DW                13.867 usec
DE                 6.00 usec
TE                298.0 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                  400

======== CHANNEL f1 ========
NUC1                 13C
P1                13.20 usec
PL1               -2.00 dB
PL1W       121.82079315 W
SFO1       150.9178990 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                4.05 dB
PL12               24.27 dB
PL13               24.27 dB
PL2W        6.03017378 W
PL12W       0.05732312 W
PL13W       0.05732312 W
SFO2       600.1324000 MHz
SI                 32768
SF         150.9028332 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

1-(5-Aminopyridin-2-yl)guanidine hydrochloride (18c)

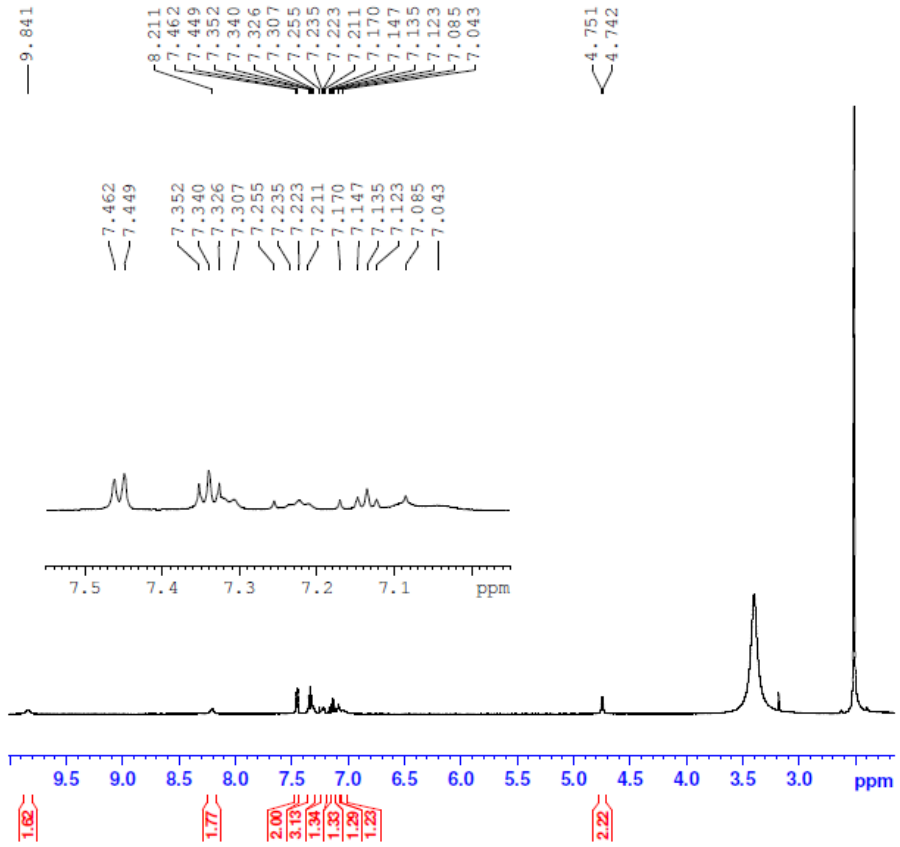



```
NAME            bki201fx
EXPNO                  1
PROCNO                 1
Date_           20110304
Time                9.21
INSTRUM           AV600
PROBHD   5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     2
SWH           12335.526 Hz
FIDRES         0.188225 Hz
AQ             2.6564426 sec
RG                     8
DW                40.533 usec
DE                 6.00 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 =======
NUC1                  1H
P1                  7.56 usec
PL1                 4.05 dB
PL1W          6.03017378 W
SFO1         600.1337060 MHz
SI                 32768
SF           600.1300000 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

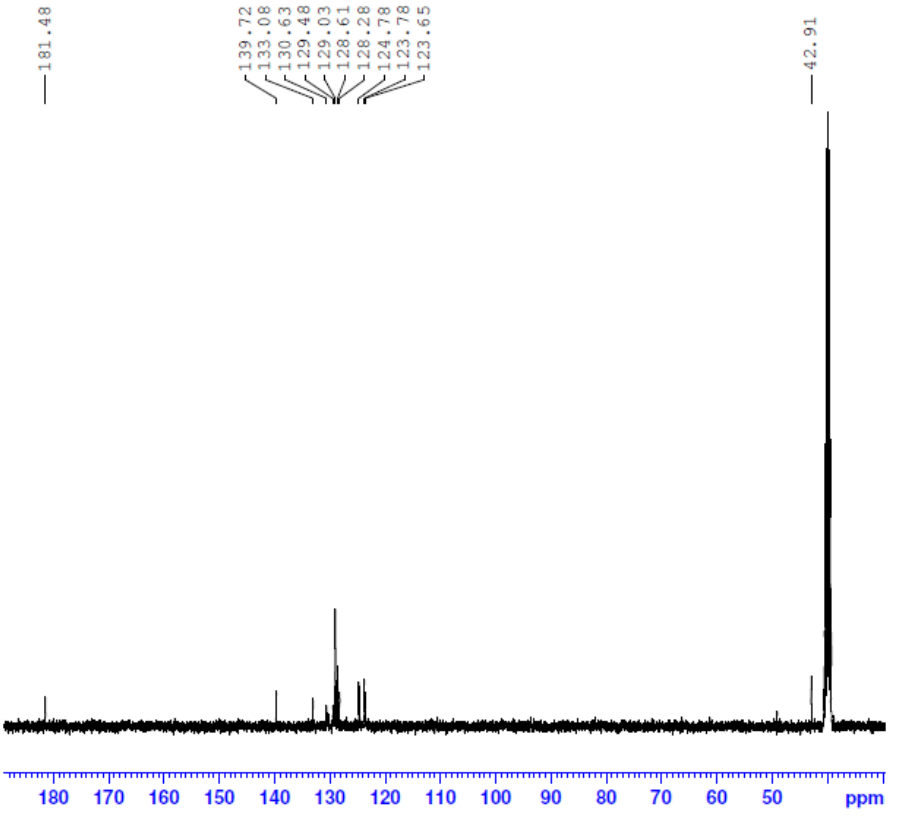



```
NAME            DK1201fx
EXPNO                 13
PROCNO                 1
Date_           20120131
TIME                15.08
INSTRUM            dpx400
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 32768
SOLVENT             CDCl3
NS                  1666
DS                     2
SWH           31847.133 Hz
FIDRES         0.971897 Hz
AQ             0.5140076 sec
RG                  8192
DW                15.700 usec
DE                 5.50 usec
TE                293.2 K
D1             1.00000000 sec
D11            0.03000000 sec
DELTA          0.89999998 sec
TD0                    1

======== CHANNEL f1 =======
NUC1                  13C
P1                  8.25 usec
PL1                -6.00 dB
SFO1         100.6256358 MHz

======== CHANNEL f2 =======
CPDPRG2             waltz16
NUC2                  1H
PCPD2              70.00 usec
PL2                 3.00 dB
PL12               19.07 dB
PL13               20.00 dB
SFO2         400.1316005 MHz
SI                 32768
SF           100.6128155 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

N-Phenyl-1,4-dihydroquinazolin-2-amine hydrochloride (19i)

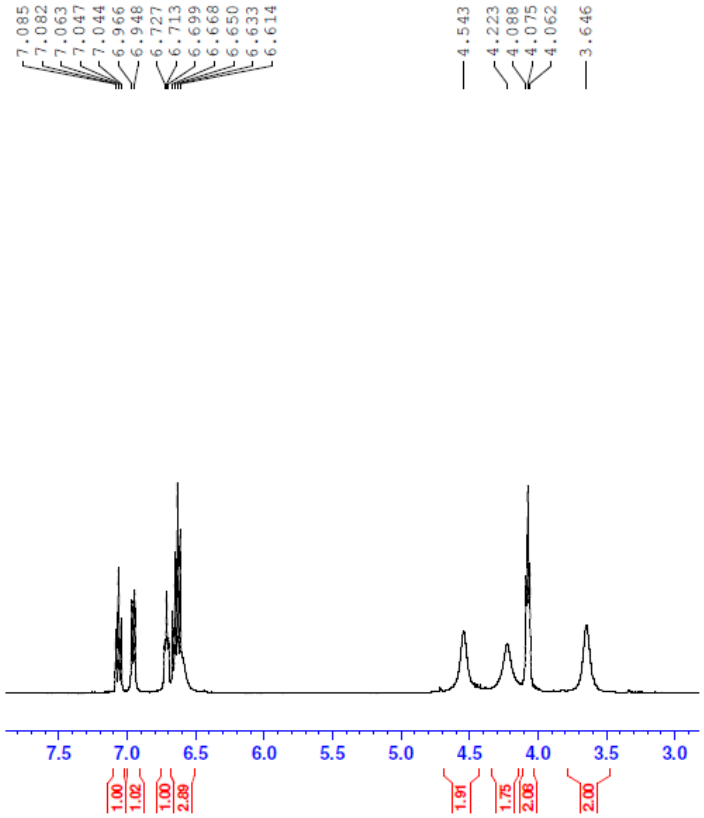



```
NAME          bki392r23xx
EXPNO                   1
PROCNO                  1
Date_            20120215
Time                16.37
INSTRUM             AV600
PROBHD    5 mm CPTCI 1H-
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     2
SWH             12335.526 Hz
FIDRES          0.188225 Hz
AQ              2.6564426 sec
RG                     8
DW                40.533 usec
DE                 6.00 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                  7.92 usec
PL1                 4.05 dB
PL1W          6.03017378 W
SFO1        600.1337060 MHz
SI                 32768
SF          600.1300000 MHz
WDW                   no
SSB                    0
LB                  0.00 Hz
GB                     0
PC                  1.00
```

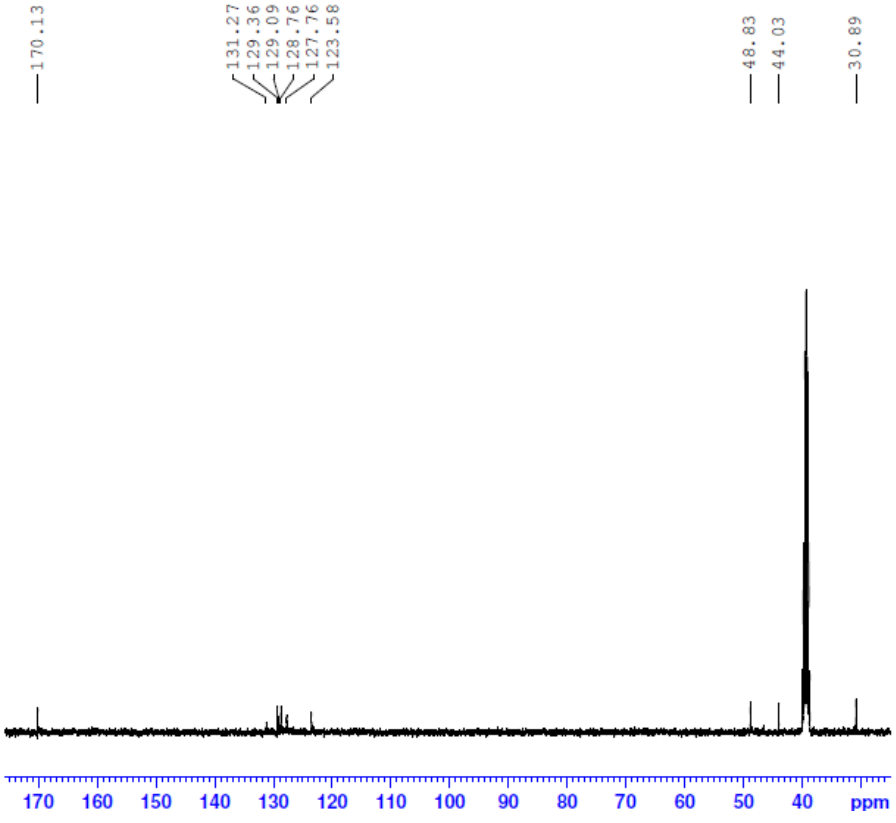



```
NAME          bki413ax
EXPNO                  13
PROCNO                  1
Date_            20120302
Time                15.22
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                 32768
SOLVENT             DMSO
NS                   181
DS                     8
SWH             32051.281 Hz
FIDRES          0.978127 Hz
AQ              0.5112308 sec
RG                   912
DW                15.600 usec
DE                 6.00 usec
TE                295.1 K
D1             1.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  8.00 usec
PL1                -2.30 dB
PL1W         60.57429123 W
SFO1        100.6505944 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                -4.00 dB
PL12               14.00 dB
PL13               14.00 dB
PL2W         19.30729485 W
PL12W         0.30599999 W
PL13W         0.30599999 W
SFO2        400.2316009 MHz
SI                 32768
SF          100.6379140 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

N-(2-hydroxyethyl)-1,4-dihydroquinazolin-2-amine hydrochloride (19j)

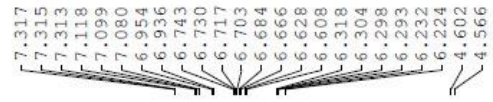



```
NAME            bki404ax
EXPNO                1
PROCNO               1
Date_         20120228
Time              9.28
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG          zg30
TD              32768
SOLVENT          CDCl3
NS                   5
DS                   2
SWH           8223.685 Hz
FIDRES        0.250967 Hz
AQ            1.9923444 sec
RG                  32
DW               60.800 usec
DE                6.00 usec
TE               296.7 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                1H
P1                10.00 usec
PL1               -4.00 dB
PL1W        19.30729485 W
SFO1       400.2324716 MHz
SI              32768
SF         400.2300000 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

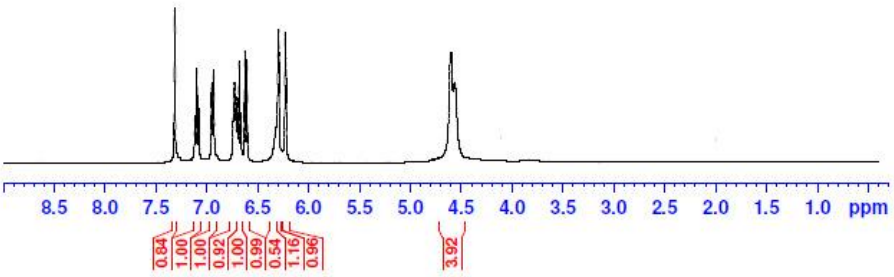


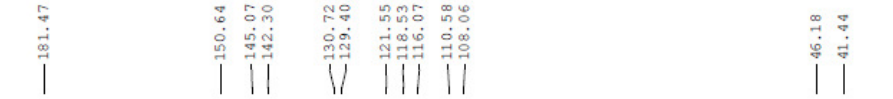

```
NAME            bki409ax
EXPNO                113
PROCNO               1
Date_         20120318
Time              13.42
INSTRUM          dpx400
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD              32768
SOLVENT          CDCl3
NS                 512
DS                   2
SWH          31847.133 Hz
FIDRES        0.971897 Hz
AQ            0.5145076 sec
RG                8192
DW               15.700 usec
DE                5.50 usec
TE               293.2 K
D1            1.00000000 sec
d11           0.03000000 sec
DELTA         0.89999998 sec
TD0                  1

======== CHANNEL f1 ========
NUC1                13C
P1                 8.25 usec
PL1               -6.00 dB
SFO1       100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                1H
PCPD2             70.00 usec
PL2                3.00 dB
PL12              19.07 dB
PL13              20.00 dB
SFO2       400.1316005 MHz
SI              32768
SF         100.6128155 MHz
WDW                EM
SSB                 0
LB                1.00 Hz
GB                  0
PC                1.40
```

N-(Furan-2-yl)-1,4-dihydroquinazolin-2-amine hydrochloride (19k)

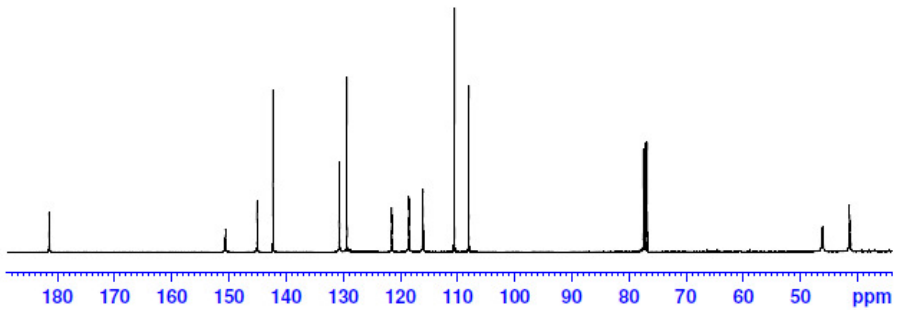



```
NAME                bk1354bx
EXPNO                      1
PROCNO                     1
Date_               20120118
Time                   17.52
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG                zg30
TD                    32768
SOLVENT               CDCl3
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.250967 Hz
AQ                  1.9923444 sec
RG                      50.8
DW                    60.800 usec
DE                     6.00 usec
TE                   293.8 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     10.00 usec
PL1                    -4.00 dB
PL1W               19.30729485 W
SFO1               400.2324716 MHz
SI                        32768
SF                 400.2300000 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

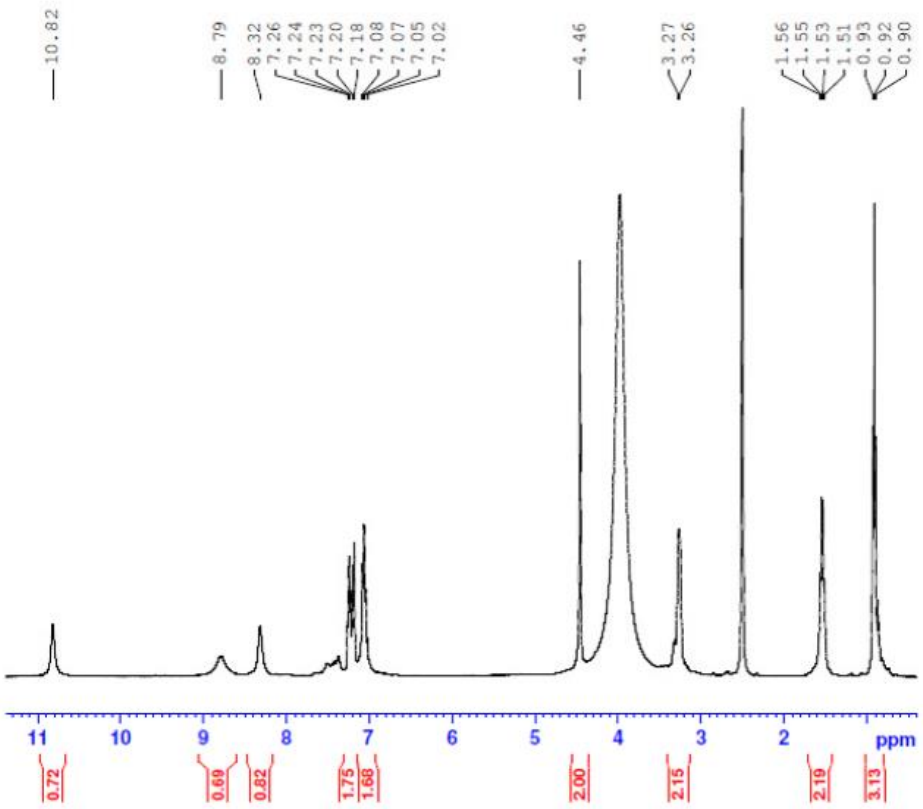




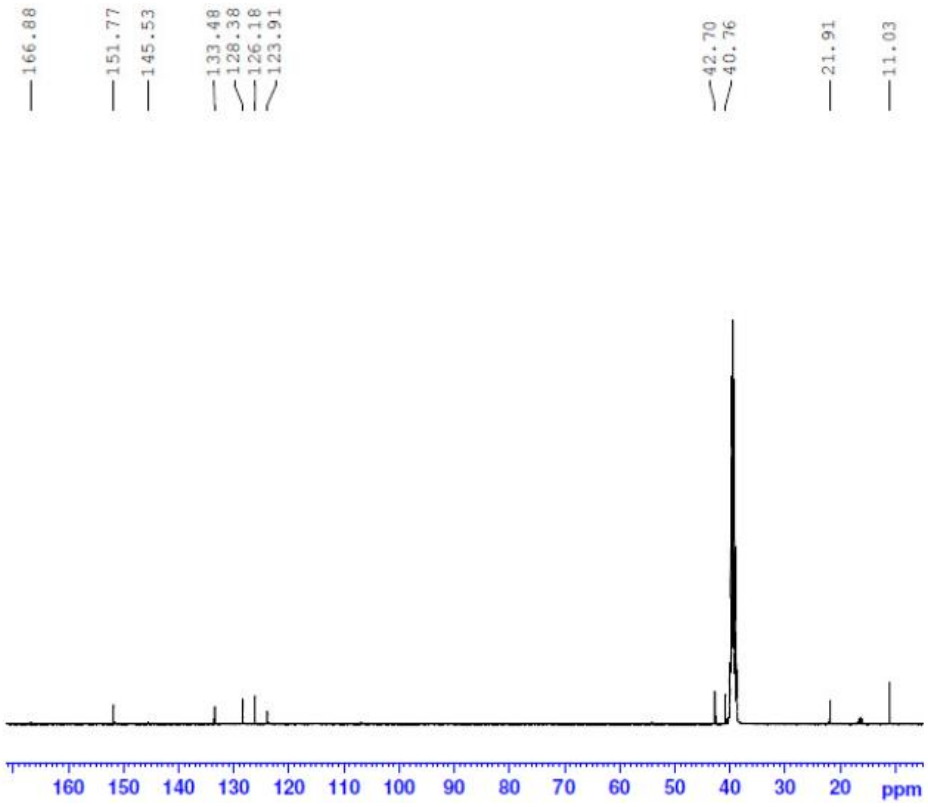

```
NAME                bk1354bx
EXPNO                     13
PROCNO                     1
Date_               20120118
Time                   18.16
INSTRUM                spect
PROBHD   5 mm PABBO BB-
PULPROG             zgpg30
TD                    32768
SOLVENT               CDCl3
NS                     31948
DS                         2
SWH                32051.281 Hz
FIDRES              0.978127 Hz
AQ                  0.5112308 sec
RG                       912
DW                    15.600 usec
DE                     6.00 usec
TE                   295.1 K
D1                  1.00000000 sec
D11                 0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                      8.00 usec
PL1                    -2.30 dB
PL1W               60.57429123 W
SFO1               100.6505944 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                      1H
PCPD2                  80.00 usec
PL2                    -4.00 dB
PL12                   14.00 dB
PL13                   14.00 dB
PL2W               19.30729485 W
PL12W               0.30599999 W
PL13W               0.30599999 W
SFO2               400.2316009 MHz
SI                        32768
SF                 100.6379140 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```



N-(*n*-Propyl)-1,4-dihydroquinazolin-2-amine hydrochloride (19l)

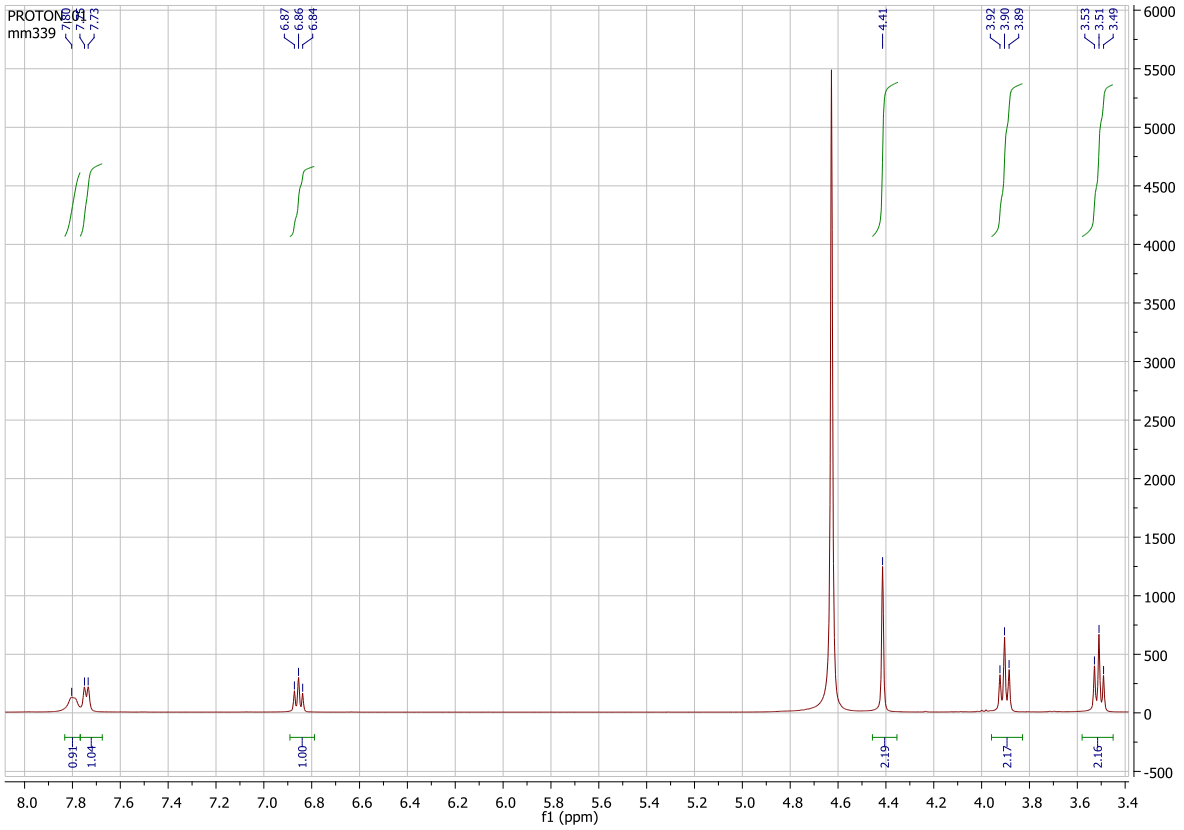


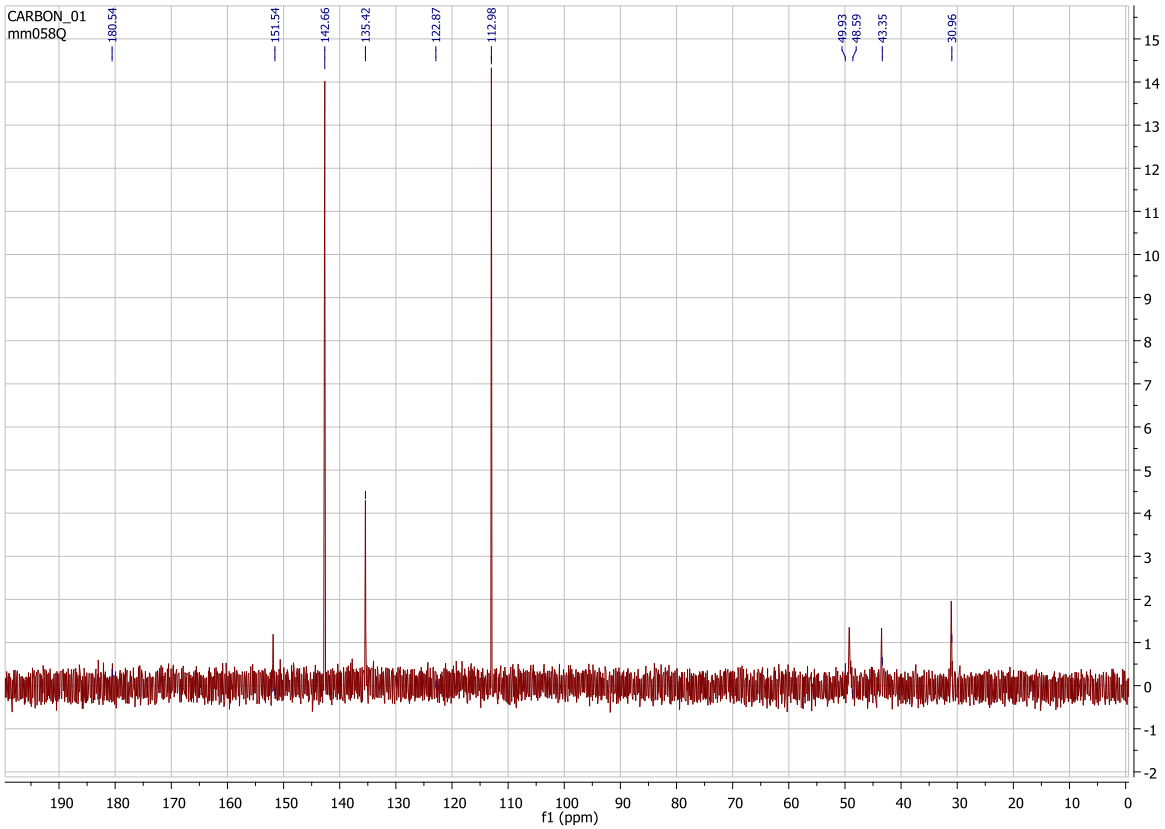

```
NAME                bki407ax
EXPNO                      1
PROCNO                     1
Date_               20120228
Time                   17.57
INSTRUM                dpx400
PROBHD   5 mm QNP 1H/13
PULPROG                zg30
TD                     32768
SOLVENT                DMSO
NS                        16
DS                         2
SWH                8223.685 Hz
FIDRES             0.250967 Hz
AQ                 1.9923444 sec
RG                      90.5
DW                    60.800 usec
DE                     5.50 usec
TE                   293.2 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                      9.75 usec
PL1                     3.00 dB
SFO1          400.1336012 MHz
SI                     16384
SF            400.1299998 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```



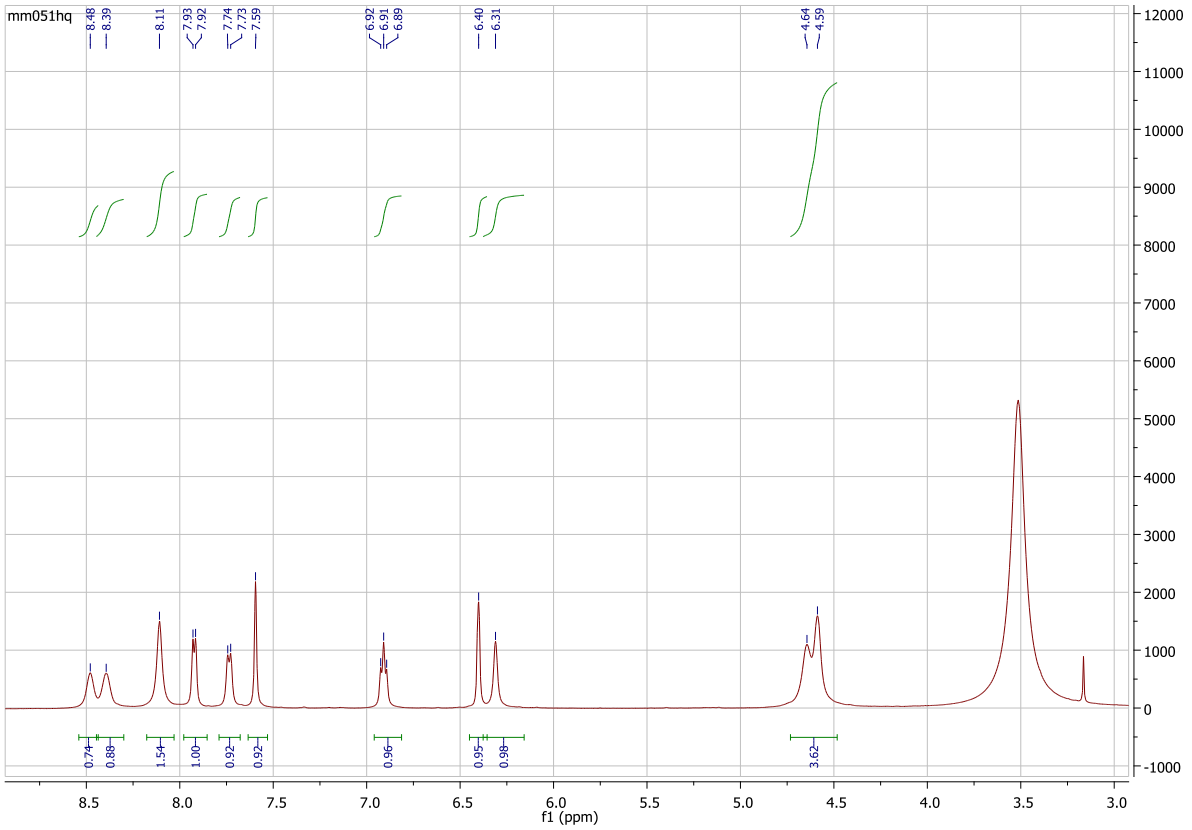

```
NAME                bki407ax
EXPNO                     13
PROCNO                     1
Date_               20120228
Time                   18.17
INSTRUM                dpx400
PROBHD   5 mm QNP 1H/13
PULPROG             xgpg30
TD                     32768
SOLVENT                CDCl3
NS                     30414
DS                         2
SWH               31847.133 Hz
FIDRES             0.971097 Hz
AQ                 0.5145076 sec
RG                      8192
DW                   15.700 usec
DE                     5.50 usec
TE                   293.2 K
D1                 1.00000000 sec
d11                0.03000000 sec
DELTA              0.89999998 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                     13C
P1                      8.25 usec
PL1                    -6.00 dB
SFO1          100.6254358 MHz

======== CHANNEL f2 ========
CPDPRG2              waltz16
NUC2                      1H
PCPD2                  70.00 usec
PL2                     3.00 dB
PL12                   19.07 dB
PL13                   20.00 dB
SFO2          400.1316005 MHz
SI                     32768
SF            100.6128155 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

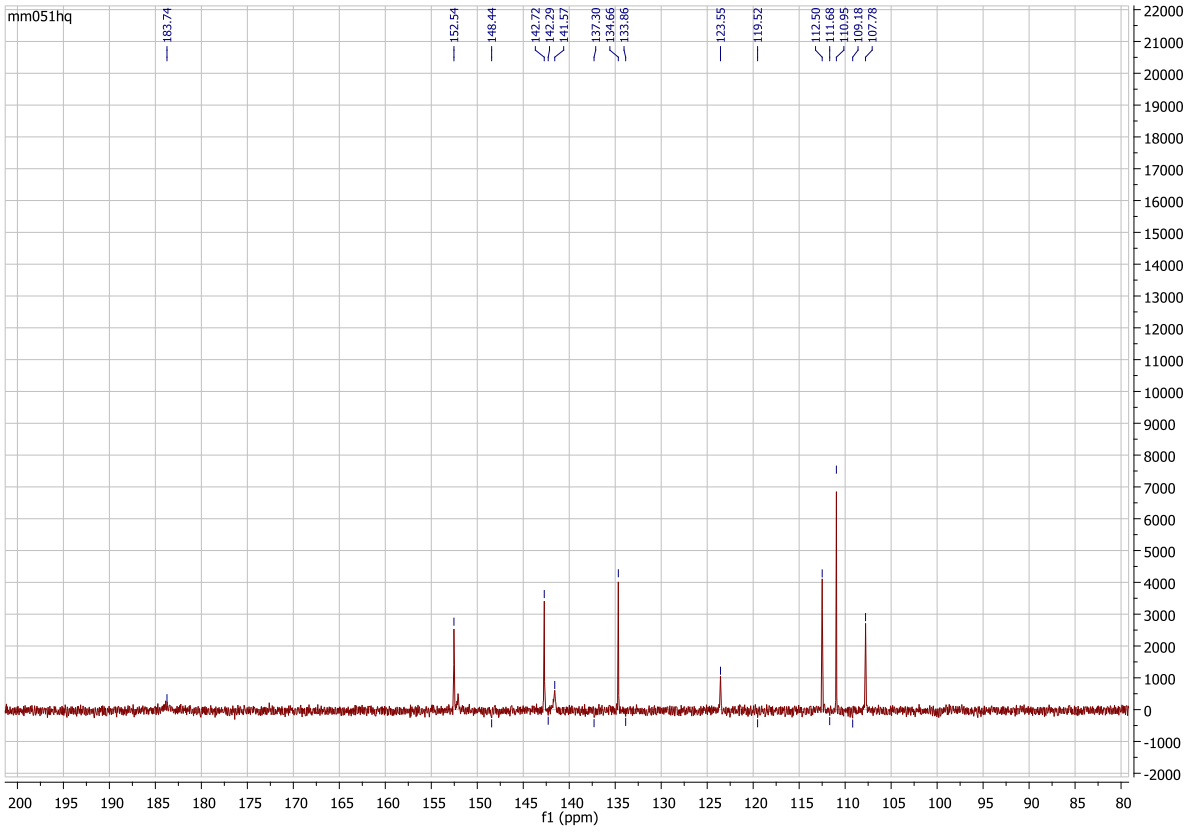
N-(2-hydroxyethyl)-1,4-dihydropyrido[2,3-d]pyrimidin-2-amine hydrochloride (20j)



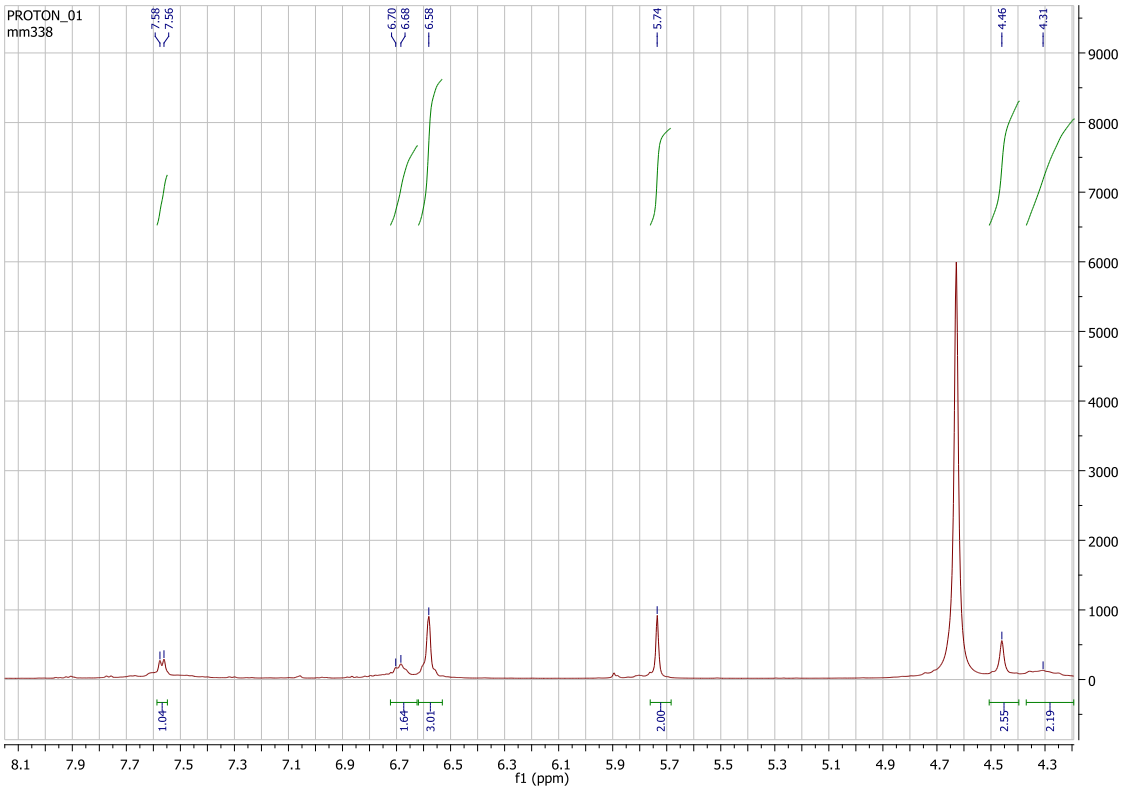


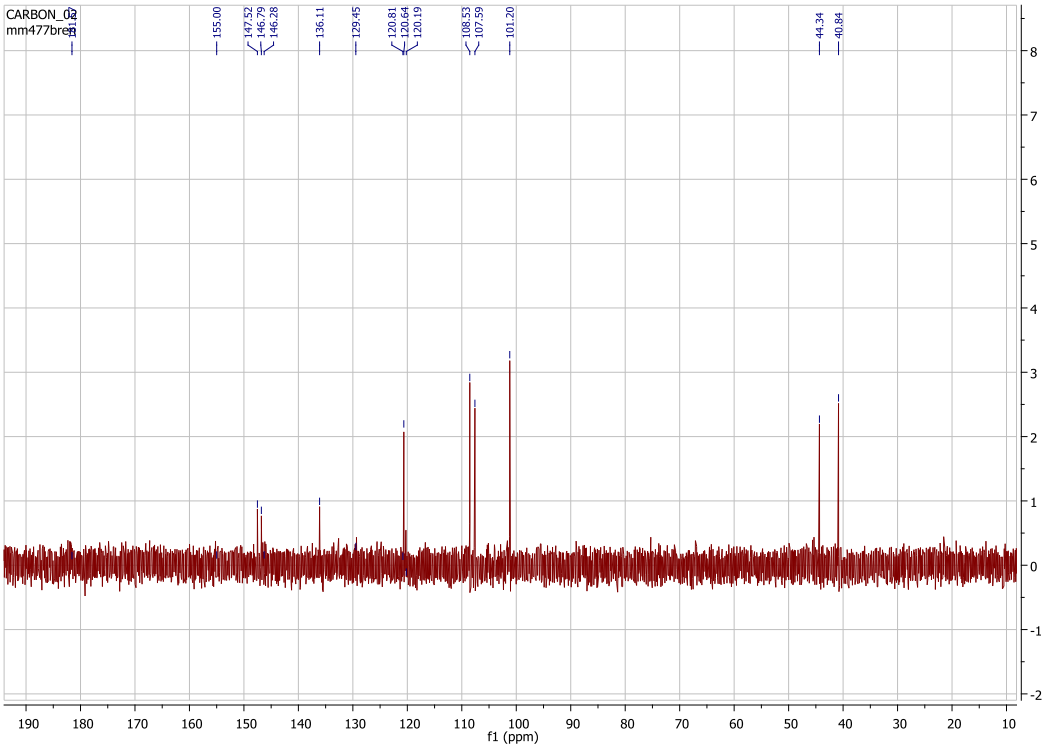
N-(furan-2-ylmethyl)-1,4-dihydropyrido[2,3-d]pyrimidin-2-amine hydrochloride (20k)





N-(1,3-benzodioxol-5-ylmethyl)-1,4-dihydropyrido[2,3-d]pyrimidin-2-amine hydrochloride (20m)





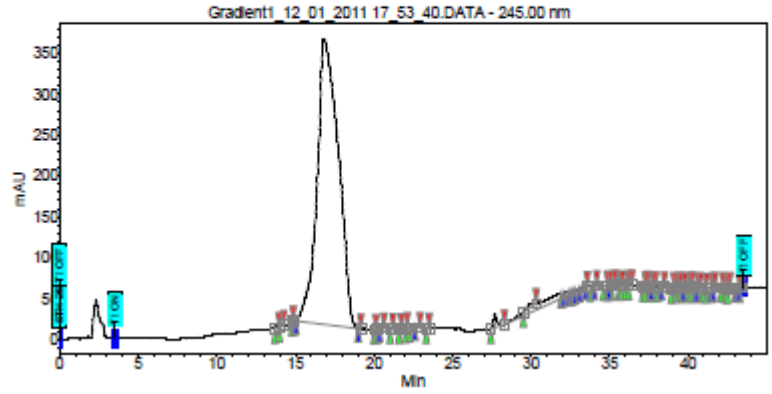
7. HPLC spectra of final hydrochloride salts

1-(Pyridin-2-yl)guanidine hydrochloride (5c)

Chromatogram : Gradient1_12_01_2011 17_53_40_channel6

System : HPLC-PDA
Method : NOT DEFINED
User : Daniel

Acquired : 12/01/2011 17:55:29
Processed : 03/02/2011 14:56:28
Printed : 03/02/2011 14:58:33



Peak results :

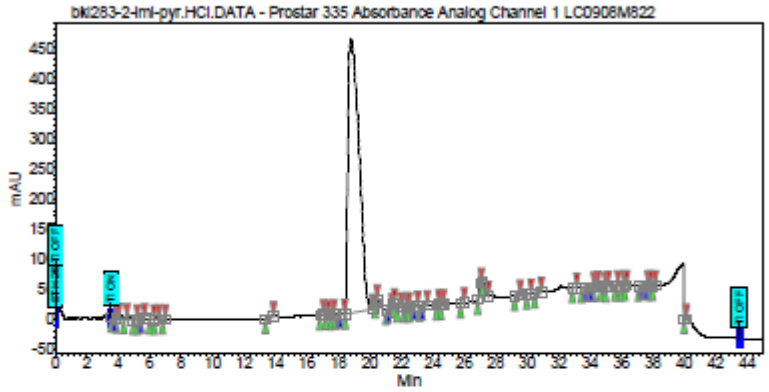
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	13.81	0.07	3.2	0.4	0.073
2	UNKNOWN	14.13	0.03	0.9	0.2	0.027
3	UNKNOWN	14.83	0.00	0.3	0.0	0.002
4	UNKNOWN	15.00	0.01	0.9	0.1	0.009
5	UNKNOWN	16.81	97.23	349.1	547.2	97.232
6	UNKNOWN	19.05	0.01	0.4	0.0	0.006
7	UNKNOWN	20.05	0.01	0.4	0.0	0.005
8	UNKNOWN	20.29	0.01	0.7	0.1	0.010
9	UNKNOWN	20.48	0.04	1.5	0.2	0.042
10	UNKNOWN	21.12	0.01	0.5	0.1	0.009
11	UNKNOWN	21.88	0.00	0.3	0.0	0.004
12	UNKNOWN	22.07	0.01	0.4	0.0	0.005
13	UNKNOWN	22.44	0.08	2.8	0.5	0.083
14	UNKNOWN	22.73	0.05	1.4	0.3	0.051
15	UNKNOWN	23.41	0.01	0.3	0.0	0.006
16	UNKNOWN	27.88	0.71	17.8	4.0	0.714
85	UNKNOWN	28.89	0.32	5.0	1.8	0.320
17	UNKNOWN	31.90	0.18	6.2	1.0	0.182
18	UNKNOWN	32.08	0.24	5.4	1.4	0.244
19	UNKNOWN	32.36	0.13	4.2	0.7	0.128
20	UNKNOWN	32.56	0.04	3.2	0.2	0.044
21	UNKNOWN	32.62	0.05	2.8	0.3	0.045
22	UNKNOWN	32.72	0.04	2.4	0.2	0.039
23	UNKNOWN	32.97	0.11	2.5	0.6	0.107
24	UNKNOWN	33.33	0.20	4.8	1.1	0.196
25	UNKNOWN	33.46	0.02	1.8	0.1	0.021
26	UNKNOWN	33.97	0.01	0.4	0.0	0.008
27	UNKNOWN	34.08	0.01	0.6	0.1	0.009
28	UNKNOWN	34.73	0.03	0.9	0.1	0.026
29	UNKNOWN	34.92	0.00	0.4	0.0	0.004
30	UNKNOWN	34.98	0.01	0.4	0.0	0.005

1-(Pyridin-2’-yl)-2-iminoimidazolidine hydrochloride (5d)

Chromatogram : bki283-2-imi-pyr.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 25/07/2011 15:03:10
Processed : 25/07/2011 17:24:37
Printed : 25/07/2011 17:24:47



Peak results :

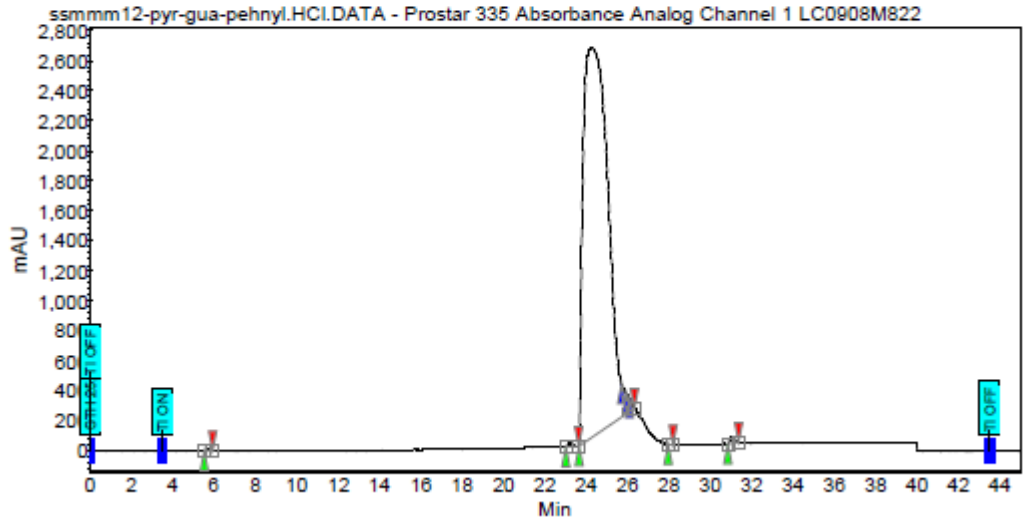
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU Min]	Area % [%]
1	UNKNOWN	3.64	0.04	1.6	0.1	0.038
2	UNKNOWN	3.79	0.02	0.9	0.1	0.017
3	UNKNOWN	3.96	0.03	0.9	0.1	0.033
4	UNKNOWN	4.47	0.07	1.6	0.3	0.067
5	UNKNOWN	5.08	0.05	1.7	0.2	0.052
6	UNKNOWN	5.35	0.04	1.3	0.1	0.038
7	UNKNOWN	5.56	0.03	0.8	0.1	0.029
8	UNKNOWN	6.12	0.05	1.4	0.2	0.053
9	UNKNOWN	6.43	0.08	2.0	0.3	0.078
10	UNKNOWN	6.89	0.01	0.6	0.1	0.015
11	UNKNOWN	13.87	0.10	1.5	0.4	0.101
12	UNKNOWN	16.96	0.02	0.6	0.1	0.023
13	UNKNOWN	17.27	0.01	0.6	0.0	0.011
14	UNKNOWN	17.61	0.02	0.9	0.1	0.024
15	UNKNOWN	17.93	0.04	1.4	0.1	0.038
16	UNKNOWN	18.05	0.01	0.5	0.0	0.008
17	UNKNOWN	18.25	0.04	1.4	0.2	0.043
18	UNKNOWN	18.80	97.24	455.8	387.9	97.236
52	UNKNOWN	20.41	0.15	8.1	0.6	0.151
19	UNKNOWN	21.11	0.01	0.6	0.1	0.015
20	UNKNOWN	21.33	0.03	1.2	0.1	0.034
53	UNKNOWN	21.58	0.01	1.0	0.0	0.009
21	UNKNOWN	21.85	0.08	2.3	0.3	0.082
22	UNKNOWN	22.24	0.01	0.6	0.0	0.012
23	UNKNOWN	22.41	0.01	0.5	0.0	0.011
24	UNKNOWN	22.77	0.05	1.1	0.2	0.048
25	UNKNOWN	22.92	0.05	1.6	0.2	0.053
26	UNKNOWN	23.25	0.02	0.6	0.1	0.015
27	UNKNOWN	23.48	0.10	2.3	0.4	0.096
28	UNKNOWN	24.32	0.01	0.3	0.0	0.007
29	UNKNOWN	24.61	0.01	0.4	0.0	0.008

1-(Pyridin-2-yl)-3-(phenyl)guanidine hydrochloride (5i)

Chromatogram :
ssmmm12-pyr-gua-pehnyl.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

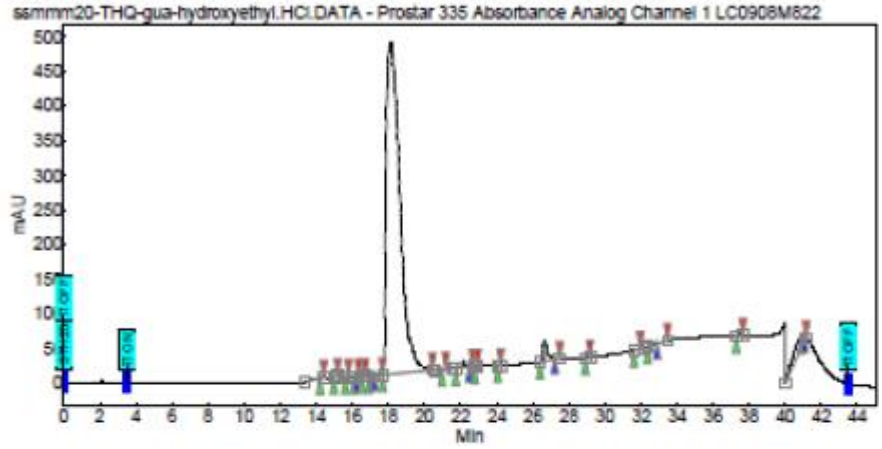
Acquired : 23/11/2011 13:48:02
Processed : 23/11/2011 14:35:31
Printed : 23/11/2011 14:36:21



Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	5.69	0.06	10.2	2.2	0.061
2	UNKNOWN	23.16	0.16	26.1	5.6	0.156
3	UNKNOWN	24.21	97.59	2594.5	3500.7	97.588
4	UNKNOWN	25.71	1.15	211.4	41.2	1.149
5	UNKNOWN	25.97	0.41	128.9	14.9	0.414
6	UNKNOWN	26.12	0.34	83.2	12.1	0.338
7	UNKNOWN	28.07	0.01	4.3	0.5	0.015
8	UNKNOWN	31.00	0.28	46.3	10.0	0.278
Total			100.00	3104.9	3587.2	100.000

1-(Pyridin-2-yl)-3-(2-hydroxyethyl)guanidine hydrochloride (5j)



Peak results :

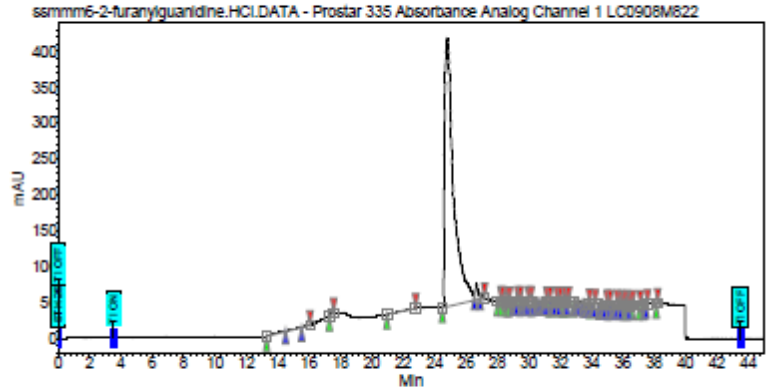
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU Min]	Area % [%]
1	UNKNOWN	14.21	0.02	0.6	0.1	0.017
2	UNKNOWN	15.11	0.02	0.6	0.1	0.016
3	UNKNOWN	15.73	0.01	0.5	0.1	0.012
4	UNKNOWN	16.19	0.01	0.6	0.1	0.013
5	UNKNOWN	16.28	0.01	0.5	0.0	0.008
6	UNKNOWN	16.65	0.01	0.4	0.0	0.010
7	UNKNOWN	17.05	0.02	0.9	0.1	0.021
8	UNKNOWN	17.15	0.03	1.2	0.1	0.033
9	UNKNOWN	17.44	0.09	1.4	0.4	0.090
25	UNKNOWN	18.11	96.44	478.9	426.7	96.442
10	UNKNOWN	21.07	0.03	0.9	0.1	0.028
11	UNKNOWN	22.12	0.40	8.1	1.8	0.404
12	UNKNOWN	22.55	0.04	1.3	0.2	0.036
13	UNKNOWN	22.87	0.01	0.6	0.0	0.010
14	UNKNOWN	24.13	0.01	0.4	0.0	0.009
15	UNKNOWN	26.65	1.81	31.7	8.0	1.811
16	UNKNOWN	27.31	0.10	2.3	0.4	0.097
17	UNKNOWN	29.04	0.04	1.2	0.2	0.036
18	UNKNOWN	31.84	0.03	0.7	0.1	0.029
19	UNKNOWN	32.59	0.09	1.2	0.4	0.086
20	UNKNOWN	33.32	0.05	0.7	0.2	0.047
21	UNKNOWN	37.48	0.04	1.0	0.2	0.043
22	UNKNOWN	40.86	0.35	17.8	1.5	0.348
23	UNKNOWN	40.97	0.27	14.1	1.2	0.275
24	UNKNOWN	41.06	0.08	6.8	0.4	0.081
Total			100.00	574.3	442.4	100.000

1-(Pyridin-2-yl)-3-(2-furanylmethyl)guanidine hydrochloride (5k)

Chromatogram :
ssmmm6-2-furanylguanidine.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 11/10/2011 15:23:39
Processed : 11/10/2011 16:11:09
Printed : 11/10/2011 16:26:46



Peak results :

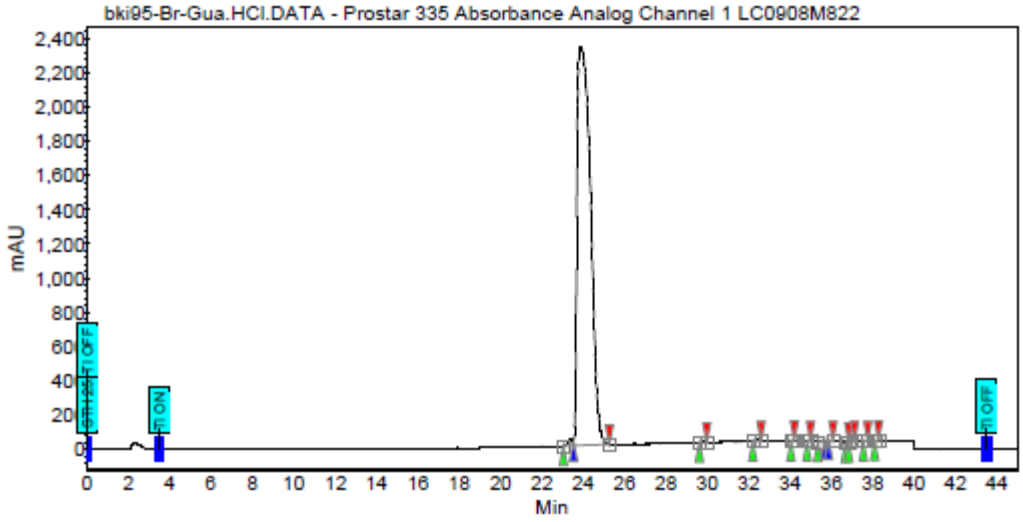
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	13.78	0.59	1.8	1.5	0.586
2	UNKNOWN	14.49	0.27	1.3	0.7	0.268
3	UNKNOWN	15.84	0.11	0.9	0.3	0.109
4	UNKNOWN	17.44	0.15	2.7	0.4	0.150
5	UNKNOWN	22.21	0.32	0.9	0.8	0.323
6	UNKNOWN	24.81	95.51	374.2	244.7	95.511
7	UNKNOWN	26.88	1.71	23.1	4.4	1.714
8	UNKNOWN	26.99	0.35	6.1	0.9	0.348
9	UNKNOWN	28.04	0.03	0.6	0.1	0.027
10	UNKNOWN	28.29	0.00	0.2	0.0	0.004
11	UNKNOWN	28.51	0.01	0.4	0.0	0.009
12	UNKNOWN	28.73	0.01	0.3	0.0	0.006
13	UNKNOWN	28.93	0.03	0.4	0.1	0.025
14	UNKNOWN	29.04	0.03	0.9	0.1	0.027
15	UNKNOWN	29.15	0.02	0.7	0.0	0.018
16	UNKNOWN	29.25	0.01	0.3	0.0	0.006
17	UNKNOWN	29.45	0.01	0.4	0.0	0.009
18	UNKNOWN	29.56	0.01	0.4	0.0	0.008
19	UNKNOWN	29.85	0.01	0.5	0.0	0.011
20	UNKNOWN	29.78	0.01	0.5	0.0	0.013
21	UNKNOWN	29.87	0.02	0.6	0.0	0.015
22	UNKNOWN	29.98	0.01	0.5	0.0	0.011
23	UNKNOWN	30.07	0.01	0.4	0.0	0.010
24	UNKNOWN	30.27	0.01	0.5	0.0	0.010
25	UNKNOWN	30.38	0.08	1.8	0.2	0.083
26	UNKNOWN	30.55	0.02	0.7	0.0	0.019
27	UNKNOWN	30.64	0.02	0.6	0.0	0.017
28	UNKNOWN	30.75	0.02	0.7	0.0	0.018
29	UNKNOWN	30.83	0.02	0.7	0.0	0.018
30	UNKNOWN	30.93	0.01	0.5	0.0	0.010
31	UNKNOWN	31.03	0.01	0.5	0.0	0.011

1-(5-Bromopyridin-2-yl)guanidine hydrochloride (6c)

Chromatogram : bki95-Br-Gua.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 08/02/2011 13:45:26
Processed : 08/02/2011 14:32:55
Printed : 08/02/2011 15:00:47



Peak results :

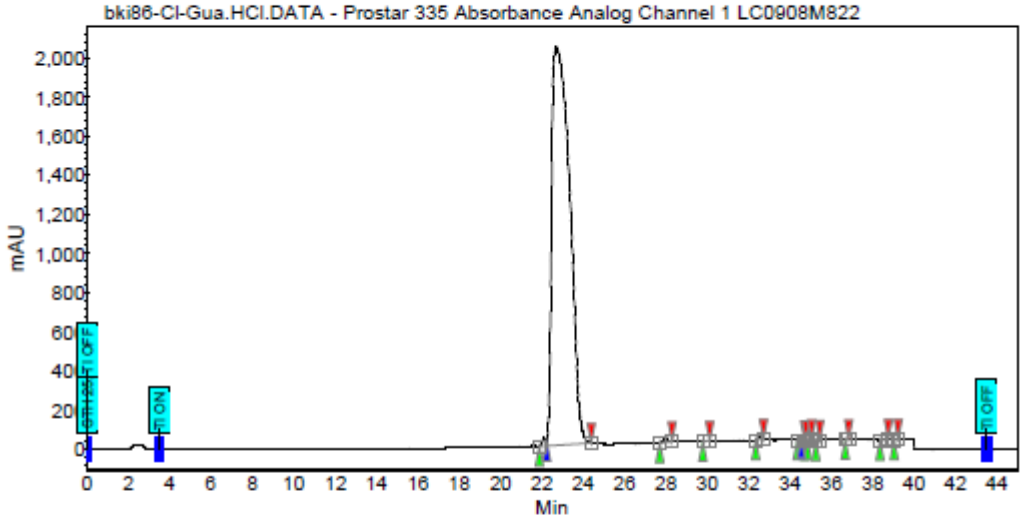
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	23.40	0.44	39.6	7.7	0.440
2	UNKNOWN	23.88	99.08	2324.8	1738.9	99.079
3	UNKNOWN	29.80	0.07	7.0	1.2	0.071
4	UNKNOWN	32.39	0.14	12.1	2.5	0.141
5	UNKNOWN	34.11	0.02	3.8	0.4	0.021
6	UNKNOWN	34.89	0.02	2.9	0.3	0.015
7	UNKNOWN	35.55	0.07	6.7	1.3	0.073
8	UNKNOWN	35.77	0.04	5.5	0.7	0.039
9	UNKNOWN	35.96	0.03	3.4	0.5	0.027
10	UNKNOWN	36.76	0.01	3.3	0.3	0.015
11	UNKNOWN	37.00	0.04	4.4	0.8	0.044
12	UNKNOWN	37.63	0.03	3.6	0.5	0.026
13	UNKNOWN	38.20	0.01	1.6	0.2	0.010
Total			100.00	2418.5	1755.1	100.000

1-(5-Chloropyridin-2-yl)guanidine hydrochloride (7c)

Chromatogram : bki86-Cl-Gua.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 08/02/2011 12:32:54
Processed : 08/02/2011 13:20:22
Printed : 08/02/2011 13:46:44



Peak results :

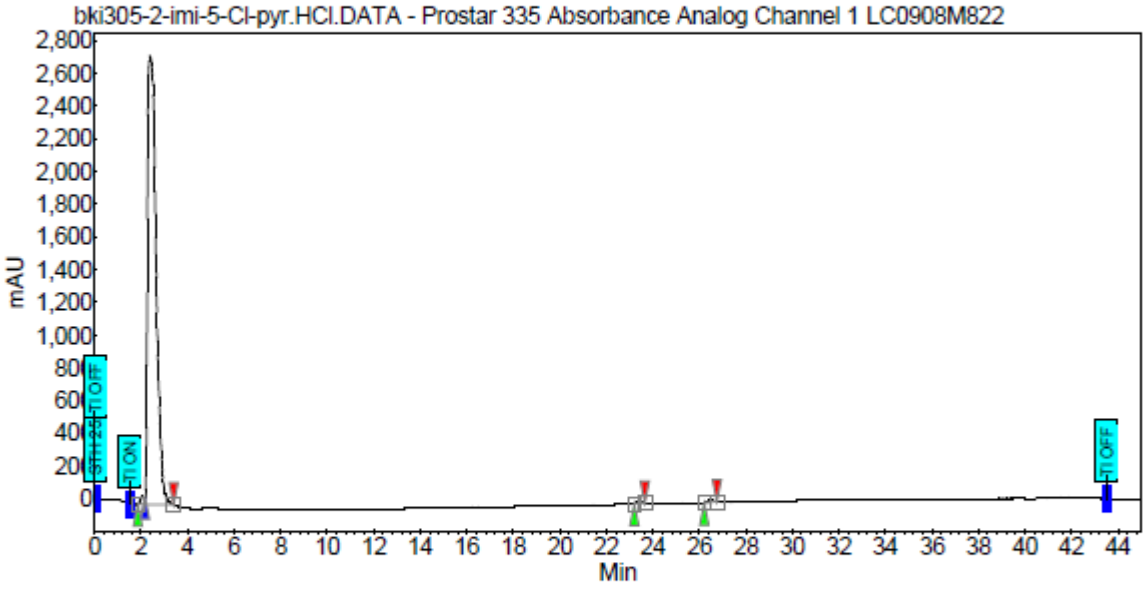
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	22.09	0.38	48.0	7.8	0.380
2	UNKNOWN	22.58	99.01	2036.4	2032.4	99.014
3	UNKNOWN	27.97	0.33	28.8	6.8	0.330
4	UNKNOWN	29.93	0.05	5.7	1.0	0.047
5	UNKNOWN	32.51	0.10	12.1	2.0	0.098
6	UNKNOWN	34.49	0.02	3.5	0.5	0.023
7	UNKNOWN	34.61	0.02	3.9	0.4	0.018
8	UNKNOWN	34.73	0.00	1.2	0.1	0.003
9	UNKNOWN	34.96	0.01	1.6	0.2	0.009
10	UNKNOWN	35.32	0.02	4.0	0.5	0.023
11	UNKNOWN	36.75	0.01	1.4	0.1	0.005
12	UNKNOWN	38.57	0.04	3.6	0.9	0.044
13	UNKNOWN	39.07	0.01	1.1	0.1	0.006
Total			100.00	2151.3	2052.7	100.000

1-(5-Chloropyridin-2’-yl)-2-iminoimidazolidine hydrochloride (7d)

Chromatogram :
bki305-2-imi-5-Cl-pyr.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 11/08/2011 12:01:26
Processed : 11/08/2011 14:26:07
Printed : 11/08/2011 14:27:17



Peak results :

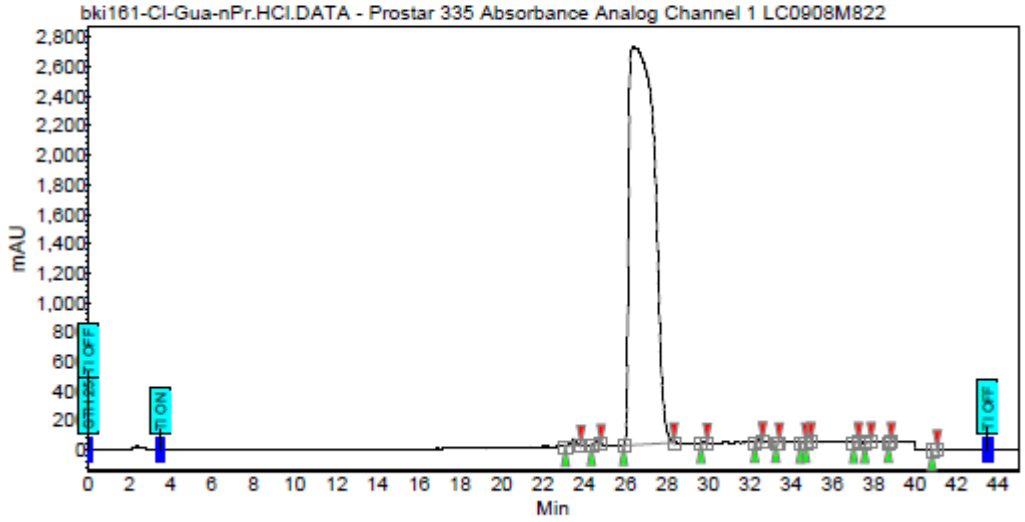
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	2.04	0.69	47.6	8.2	0.689
2	UNKNOWN	2.36	98.74	2740.3	1176.6	98.743
3	UNKNOWN	23.43	0.24	12.2	2.8	0.237
4	UNKNOWN	26.49	0.33	13.7	3.9	0.331
Total			100.00	2813.7	1191.5	100.000

1-(5-Chloropyridin-2-yl)-3-(propyl)guanidine hydrochloride (7l)

Chromatogram : bki161-Cl-Gua-nPr.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 08/02/2011 14:59:26
Processed : 08/02/2011 15:46:55
Printed : 08/02/2011 15:52:00



Peak results :

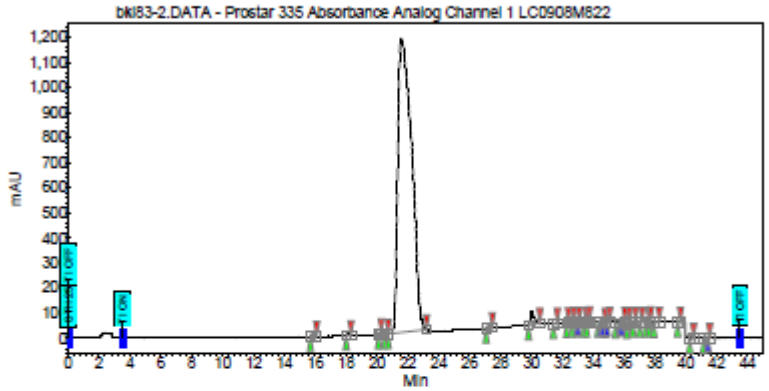
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	23.47	0.35	49.7	13.2	0.351
2	UNKNOWN	24.53	0.15	29.8	5.5	0.147
3	UNKNOWN	26.40	99.31	2700.8	3728.6	99.314
4	UNKNOWN	29.77	0.03	7.0	1.0	0.027
5	UNKNOWN	32.41	0.07	14.1	2.5	0.066
6	UNKNOWN	33.36	0.00	2.7	0.2	0.005
7	UNKNOWN	34.59	0.03	5.8	1.0	0.026
8	UNKNOWN	34.81	0.01	3.1	0.5	0.014
9	UNKNOWN	37.13	0.01	3.9	0.5	0.014
10	UNKNOWN	37.69	0.02	4.1	0.8	0.020
11	UNKNOWN	38.79	0.00	1.5	0.1	0.003
12	UNKNOWN	40.92	0.01	2.7	0.4	0.011
Total			100.00	2825.4	3754.3	100.000

1-(5-Methylpyridin-2-yl)guanidine hydrochloride (8c)

Chromatogram : bki83-2_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 31/01/2011 16:45:14
Processed : 31/01/2011 17:32:43
Printed : 03/02/2011 15:00:18



Peak results :

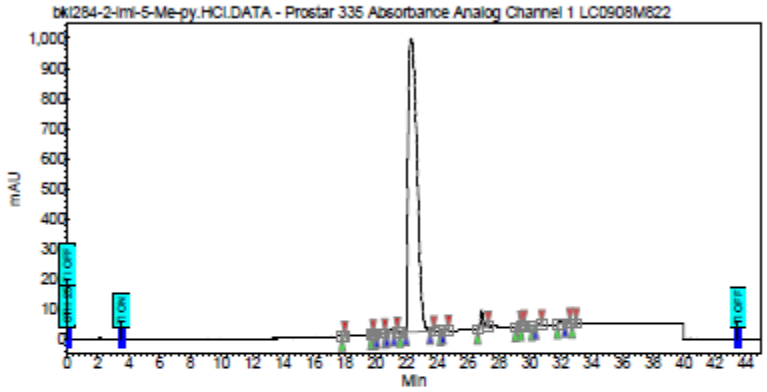
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU Min]	Area % [%]
1	UNKNOWN	15.91	0.09	5.4	1.0	0.095
2	UNKNOWN	18.15	0.04	3.4	0.5	0.041
3	UNKNOWN	20.20	0.01	1.0	0.1	0.008
4	UNKNOWN	20.80	0.03	3.3	0.3	0.028
5	UNKNOWN	21.57	98.29	1170.8	1207.7	98.294
6	UNKNOWN	27.39	0.02	1.1	0.2	0.020
7	UNKNOWN	30.04	1.05	52.9	13.0	1.054
8	UNKNOWN	31.80	0.03	2.4	0.3	0.025
9	UNKNOWN	32.35	0.00	0.7	0.0	0.003
10	UNKNOWN	32.71	0.00	0.7	0.0	0.003
11	UNKNOWN	33.00	0.00	0.8	0.0	0.003
12	UNKNOWN	33.07	0.00	0.7	0.0	0.003
13	UNKNOWN	33.48	0.01	1.6	0.1	0.012
14	UNKNOWN	33.85	0.02	1.5	0.2	0.015
15	UNKNOWN	34.40	0.02	2.9	0.3	0.025
16	UNKNOWN	34.56	0.02	3.1	0.3	0.022
17	UNKNOWN	34.68	0.04	4.2	0.5	0.039
18	UNKNOWN	34.85	0.01	1.3	0.1	0.008
19	UNKNOWN	35.01	0.01	1.4	0.1	0.011
20	UNKNOWN	35.65	0.08	5.0	1.0	0.078
21	UNKNOWN	35.80	0.03	3.1	0.3	0.028
22	UNKNOWN	35.95	0.04	3.6	0.5	0.039
23	UNKNOWN	36.27	0.02	2.8	0.3	0.023
24	UNKNOWN	36.68	0.01	1.7	0.2	0.014
25	UNKNOWN	37.12	0.01	1.2	0.1	0.008
26	UNKNOWN	37.52	0.02	1.9	0.2	0.016
27	UNKNOWN	37.71	0.00	0.7	0.0	0.003
28	UNKNOWN	38.17	0.03	1.7	0.4	0.035
29	UNKNOWN	39.57	0.01	1.2	0.1	0.009
30	UNKNOWN	40.37	0.02	1.9	0.3	0.021
31	UNKNOWN	41.29	0.02	1.8	0.3	0.023

1-(5-Methylpyridin-2’-yl)-2-iminoimidazolidine hydrochloride (8d)

Chromatogram :
bki284-2-imi-5-Me-py.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 25/07/2011 11:27:34
Processed : 25/07/2011 12:15:03
Printed : 25/07/2011 12:21:47



Peak results :

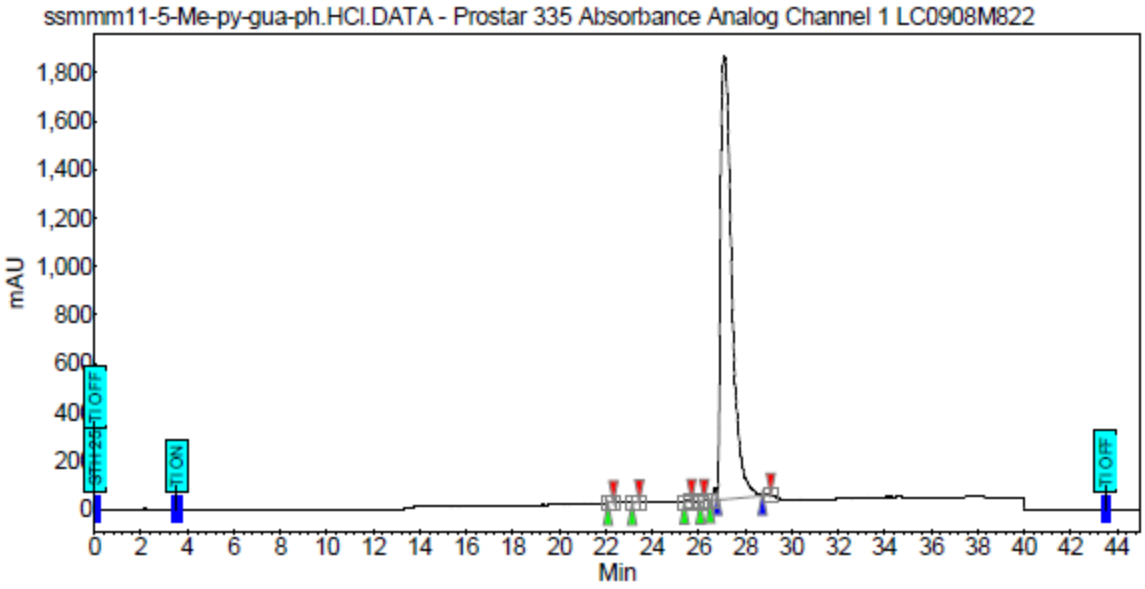
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	17.93	0.01	0.9	0.1	0.010
2	UNKNOWN	19.79	0.01	0.7	0.0	0.007
3	UNKNOWN	20.01	0.01	0.5	0.0	0.006
4	UNKNOWN	20.24	0.32	10.4	2.1	0.329
5	UNKNOWN	20.69	0.01	0.7	0.0	0.007
6	UNKNOWN	20.96	0.45	13.0	3.0	0.451
7	UNKNOWN	21.32	0.02	1.5	0.1	0.022
8	UNKNOWN	21.75	0.08	2.2	0.5	0.075
9	UNKNOWN	22.31	98.37	975.4	634.1	98.371
10	UNKNOWN	23.67	0.05	2.7	0.4	0.054
11	UNKNOWN	24.31	0.02	1.5	0.1	0.021
12	UNKNOWN	24.52	0.14	4.8	0.9	0.139
13	UNKNOWN	26.88	1.81	59.2	11.9	1.807
14	UNKNOWN	29.25	0.10	4.4	0.6	0.096
15	UNKNOWN	29.53	0.03	1.9	0.2	0.026
16	UNKNOWN	30.28	0.02	1.1	0.2	0.023
17	UNKNOWN	30.64	0.08	3.4	0.5	0.081
18	UNKNOWN	32.01	0.36	11.8	2.3	0.357
19	UNKNOWN	32.45	0.10	4.2	0.6	0.095
20	UNKNOWN	32.89	0.03	1.4	0.2	0.029
Total			100.00	1101.4	658.0	100.000

1-(5-Methylpyridin-2-yl)-3-(phenyl)guanidine hydrochloride (8i)

Chromatogram :
ssmmm11-5-Me-py-gua-ph.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 08/11/2011 11:55:22
Processed : 08/11/2011 12:42:51
Printed : 08/11/2011 12:48:40



Peak results :

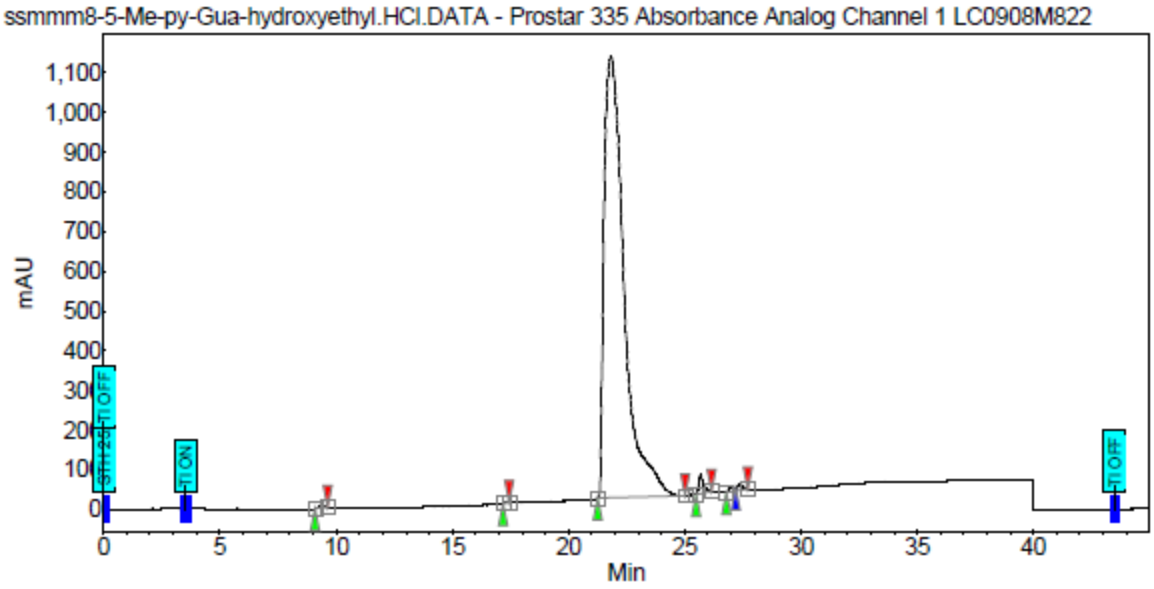
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	22.20	0.04	3.5	0.4	0.035
2	UNKNOWN	23.29	0.06	3.9	0.6	0.056
3	UNKNOWN	25.51	0.10	7.8	1.0	0.100
4	UNKNOWN	26.15	0.01	1.1	0.1	0.009
5	UNKNOWN	26.68	0.80	52.5	8.3	0.804
6	UNKNOWN	27.09	98.85	1829.3	1018.6	98.846
7	UNKNOWN	28.89	0.15	7.1	1.5	0.150
Total			100.00	1905.2	1030.5	100.000

1-(5-Methylpyridin-2-yl)-3-(2-hydroxyethyl)guanidine hydrochloride (8j)

Chromatogram :
ssmmm8-5-Me-py-Gua-hydroxyethyl.HCl_channe

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 07/11/2011 14:53:06
Processed : 07/11/2011 15:40:36
Printed : 07/11/2011 16:10:29



Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	9.37	0.11	4.2	1.3	0.113
2	UNKNOWN	17.29	0.05	4.3	0.6	0.054
3	UNKNOWN	21.83	98.20	1113.9	1106.9	98.197
4	UNKNOWN	25.68	1.00	48.0	11.3	1.003
5	UNKNOWN	27.01	0.26	13.6	2.9	0.256
6	UNKNOWN	27.36	0.38	17.2	4.2	0.376
Total			100.00	1201.3	1127.2	100.000

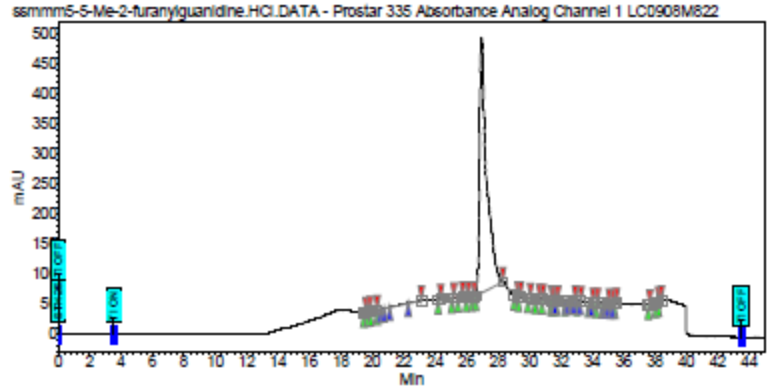
1-(5-Methylpyridin-2-yl)-3-(2-furanylmethyl)guanidine hydrochloride (8k)

Chromatogram :
ssmmm5-5-Me-2-furanylguanidine.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 11/10/2011 14:25:21
Processed : 11/10/2011 15:12:51
Printed : 11/10/2011 15:28:51

ssmmm5-5-Me-2-furanylguanidine.HCl.DATA - Prostar 335 Absorbance Analog Channel 1 LC0908M822



Peak results :

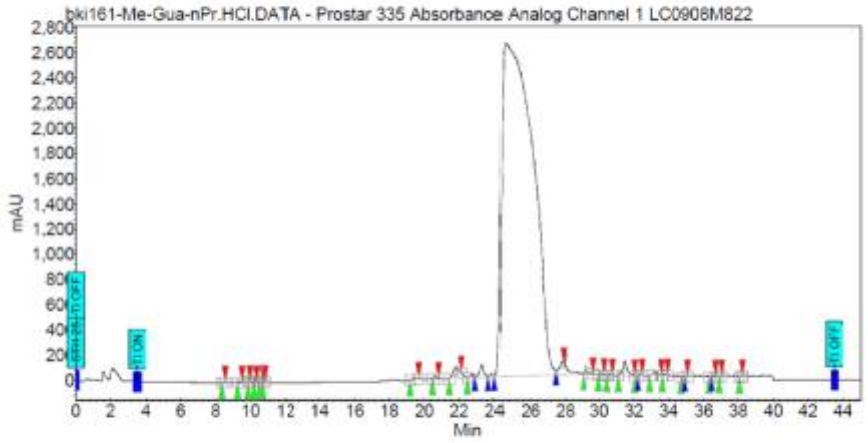
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	19.52	0.01	0.4	0.0	0.014
2	UNKNOWN	19.78	0.01	0.3	0.0	0.009
3	UNKNOWN	20.21	0.02	0.4	0.1	0.024
4	UNKNOWN	20.45	0.02	0.6	0.0	0.021
5	UNKNOWN	20.67	0.03	0.5	0.1	0.029
6	UNKNOWN	21.07	0.07	0.7	0.2	0.066
7	UNKNOWN	22.00	0.41	1.3	0.9	0.408
8	UNKNOWN	22.79	0.25	0.8	0.4	0.197
9	UNKNOWN	24.28	0.01	0.3	0.0	0.011
10	UNKNOWN	25.13	0.01	0.3	0.0	0.011
11	UNKNOWN	25.85	0.05	0.8	0.1	0.045
12	UNKNOWN	26.05	0.01	0.4	0.0	0.012
13	UNKNOWN	26.43	0.01	0.4	0.0	0.012
14	UNKNOWN	26.96	98.38	425.7	222.8	98.378
15	UNKNOWN	29.13	0.06	1.7	0.2	0.063
16	UNKNOWN	29.37	0.02	0.6	0.0	0.020
17	UNKNOWN	29.96	0.02	0.6	0.0	0.017
18	UNKNOWN	30.47	0.14	2.3	0.3	0.143
19	UNKNOWN	30.83	0.01	0.4	0.0	0.008
20	UNKNOWN	31.39	0.01	0.5	0.0	0.012
21	UNKNOWN	31.49	0.01	0.3	0.0	0.005
22	UNKNOWN	31.57	0.01	0.3	0.0	0.005
23	UNKNOWN	31.67	0.01	0.4	0.0	0.008
24	UNKNOWN	31.78	0.01	0.4	0.0	0.008
25	UNKNOWN	32.31	0.01	0.3	0.0	0.007
26	UNKNOWN	32.40	0.02	0.6	0.0	0.017
27	UNKNOWN	32.59	0.10	1.8	0.2	0.100
28	UNKNOWN	32.88	0.04	1.4	0.1	0.044
29	UNKNOWN	32.77	0.02	0.7	0.0	0.020
30	UNKNOWN	32.88	0.01	0.3	0.0	0.008
31	UNKNOWN	33.16	0.05	1.1	0.1	0.051

1-(5-Methylpyridin-2-yl)-3-(propyl)guanidine hydrochloride (8l)

Chromatogram :
bki161-Me-Gua-nPr.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 08/02/2011 15:50:31
Processed : 08/02/2011 16:38:00
Printed : 14/02/2011 13:08:45



Peak results :

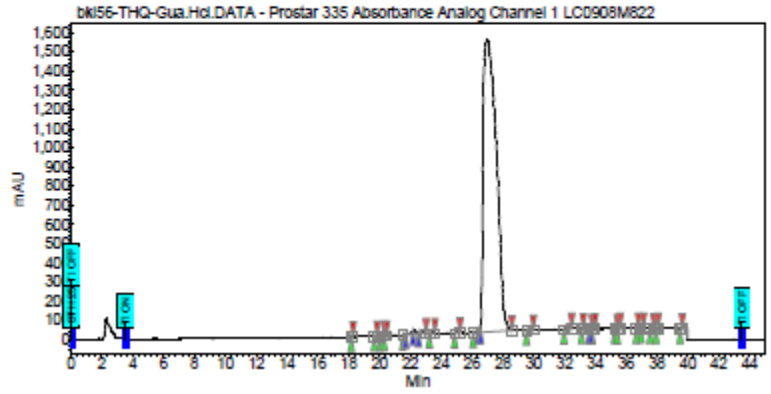
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU Min]	Area % [%]
1	UNKNOWN	8.44	0.01	3.8	0.3	0.006
2	UNKNOWN	9.33	0.02	9.3	1.0	0.019
3	UNKNOWN	9.91	0.00	3.0	0.2	0.004
4	UNKNOWN	10.23	0.00	2.0	0.2	0.004
5	UNKNOWN	10.59	0.01	5.5	0.5	0.009
6	UNKNOWN	10.77	0.00	2.5	0.1	0.003
7	UNKNOWN	19.51	0.05	9.1	2.6	0.047
8	UNKNOWN	20.64	0.05	16.8	2.5	0.046
9	UNKNOWN	21.81	0.38	68.7	20.9	0.383
10	UNKNOWN	22.76	0.11	36.1	6.0	0.110
11	UNKNOWN	23.29	0.53	96.4	28.7	0.527
12	UNKNOWN	23.89	0.11	30.3	6.0	0.110
13	UNKNOWN	24.57	96.87	2641.7	5271.8	96.873
14	UNKNOWN	27.80	0.61	105.7	33.1	0.609
15	UNKNOWN	29.24	0.28	73.4	15.3	0.282
16	UNKNOWN	30.11	0.03	11.9	1.7	0.031
17	UNKNOWN	30.60	0.02	7.4	1.2	0.023
18	UNKNOWN	31.49	0.64	119.4	35.1	0.645
19	UNKNOWN	32.17	0.00	1.1	0.1	0.002
20	UNKNOWN	32.35	0.02	7.7	1.0	0.019
21	UNKNOWN	33.20	0.16	36.1	8.8	0.162
22	UNKNOWN	33.76	0.04	15.0	1.9	0.036
23	UNKNOWN	34.83	0.02	7.3	1.0	0.018
24	UNKNOWN	34.95	0.01	3.2	0.4	0.007
25	UNKNOWN	36.43	0.01	3.6	0.3	0.006
26	UNKNOWN	36.56	0.01	4.2	0.7	0.013
27	UNKNOWN	36.97	0.00	1.7	0.1	0.002
28	UNKNOWN	38.15	0.01	2.9	0.3	0.005
Total			100.00	3319.7	5442.0	100.000

1-(5,6,7,8-Tetrahydroquinolin-2-yl)guanidine hydrochloride (9c)

Chromatogram : bki56-THQ-Gua.Hcl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 08/02/2011 11:27:01
Processed : 08/02/2011 12:14:30
Printed : 08/02/2011 12:29:16



Peak results :

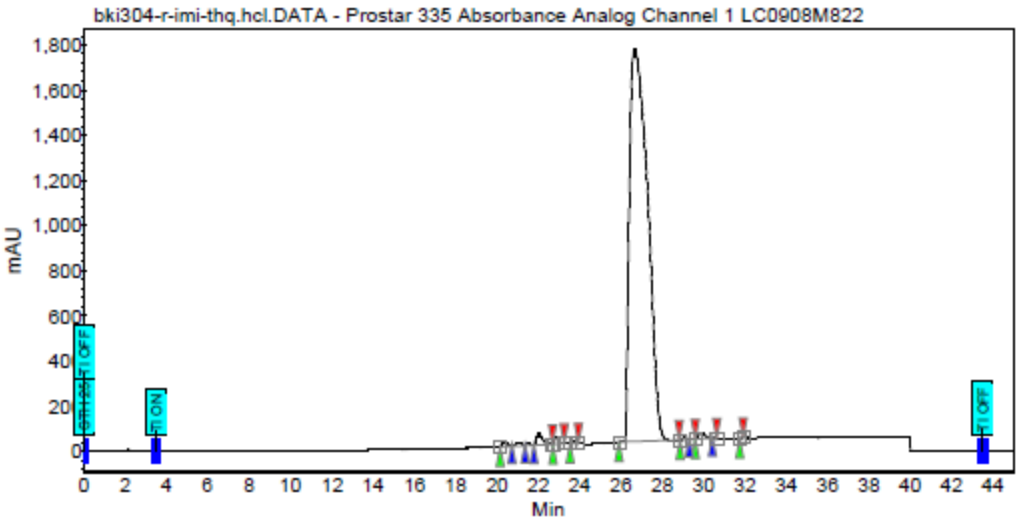
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	18.21	0.00	0.9	0.1	0.004
2	UNKNOWN	19.76	0.01	1.7	0.1	0.010
3	UNKNOWN	20.16	0.01	1.4	0.2	0.014
4	UNKNOWN	20.41	0.01	1.6	0.1	0.009
5	UNKNOWN	21.84	0.02	2.5	0.2	0.016
6	UNKNOWN	22.13	0.25	15.5	3.7	0.247
7	UNKNOWN	22.29	0.29	21.1	4.4	0.288
8	UNKNOWN	22.84	0.17	10.3	2.6	0.171
9	UNKNOWN	23.40	0.08	7.6	1.1	0.076
10	UNKNOWN	25.03	0.13	13.0	2.0	0.132
11	UNKNOWN	26.38	0.21	23.0	3.2	0.212
12	UNKNOWN	26.49	0.12	18.5	1.8	0.122
13	UNKNOWN	27.00	98.14	1530.7	1484.9	98.145
14	UNKNOWN	29.77	0.09	6.7	1.4	0.090
15	UNKNOWN	32.17	0.35	27.2	5.4	0.355
16	UNKNOWN	33.17	0.00	0.8	0.1	0.004
17	UNKNOWN	33.65	0.00	1.1	0.1	0.004
18	UNKNOWN	33.75	0.01	2.3	0.2	0.010
19	UNKNOWN	33.91	0.01	1.9	0.2	0.014
20	UNKNOWN	35.31	0.01	2.6	0.2	0.015
21	UNKNOWN	35.53	0.01	2.0	0.2	0.015
22	UNKNOWN	36.76	0.00	0.9	0.1	0.004
23	UNKNOWN	37.05	0.01	1.8	0.2	0.012
24	UNKNOWN	37.89	0.02	2.1	0.3	0.021
25	UNKNOWN	38.00	0.01	1.4	0.1	0.008
26	UNKNOWN	39.57	0.01	1.1	0.1	0.005
Total			100.00	1697.9	1513.0	100.000

1-(5,6,7,8-Tetrahydroquinolin-2’-yl)-2-iminoimidazolidine hydrochloride (9d)

Chromatogram : bki304-r-imi-thq.hcl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 11/08/2011 11:12:42
Processed : 11/08/2011 12:00:11
Printed : 11/08/2011 12:02:45



Peak results :

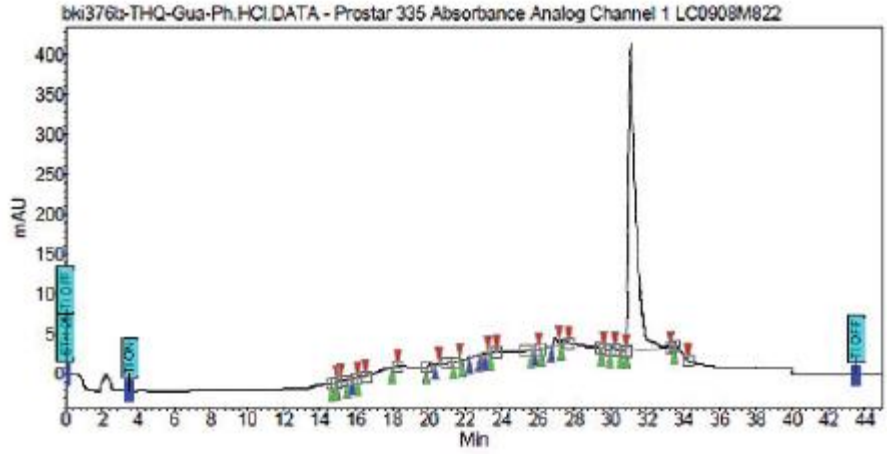
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	20.39	0.35	18.3	6.4	0.354
2	UNKNOWN	21.07	0.27	9.9	4.8	0.267
3	UNKNOWN	21.47	0.12	8.6	2.3	0.124
4	UNKNOWN	22.03	0.96	51.8	17.5	0.963
5	UNKNOWN	22.89	0.41	28.0	7.5	0.411
6	UNKNOWN	23.69	0.09	7.6	1.6	0.085
7	UNKNOWN	26.65	96.99	1737.6	1760.6	96.992
8	UNKNOWN	29.04	0.15	10.9	2.7	0.150
9	UNKNOWN	29.40	0.04	3.2	0.7	0.036
10	UNKNOWN	29.89	0.60	27.5	10.8	0.597
11	UNKNOWN	30.52	0.01	2.2	0.2	0.013
12	UNKNOWN	31.84	0.01	1.5	0.2	0.009
Total			100.00	1907.2	1815.2	100.000

1-(5,6,7,8-Tetrahydroquinolin-2-yl)-3-(phenyl)guanidine hydrochloride (9i)

bki376b-THQ-Gua-Ph.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 17/01/2012 14:49:17
Processed : 17/01/2012 15:53:15
Printed : 17/01/2012 15:53:47



Peak results :

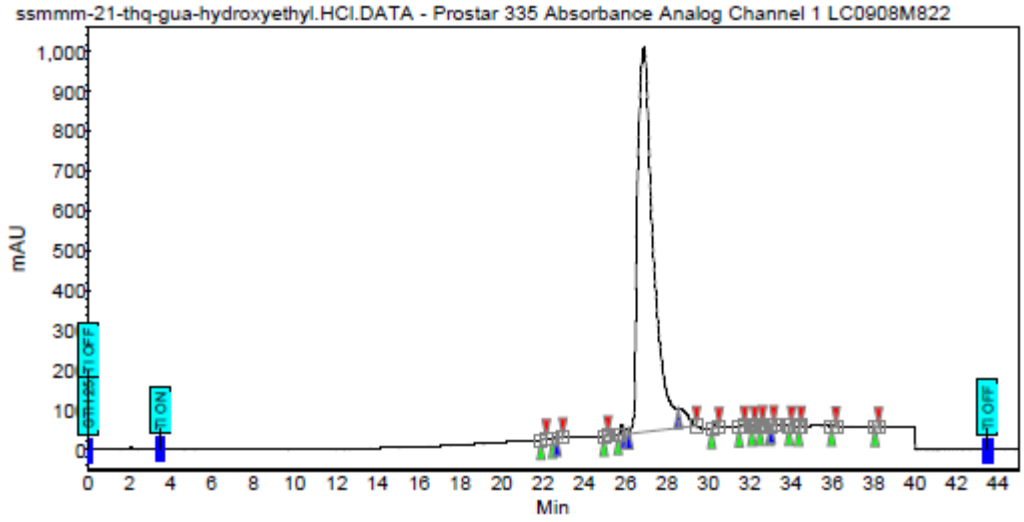
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU Min]	Area % [%]
1	UNKNOWN	14.87	0.02	0.5	0.1	0.023
2	UNKNOWN	15.04	0.03	0.6	0.1	0.030
3	UNKNOWN	15.75	0.10	1.4	0.2	0.100
4	UNKNOWN	16.53	0.09	1.3	0.2	0.087
5	UNKNOWN	16.29	0.13	1.2	0.3	0.134
6	UNKNOWN	18.00	0.09	1.2	0.2	0.090
7	UNKNOWN	20.15	0.35	3.1	0.8	0.352
8	UNKNOWN	20.43	0.10	1.5	0.2	0.103
9	UNKNOWN	21.64	0.06	0.6	0.1	0.057
10	UNKNOWN	22.04	0.11	1.0	0.3	0.110
11	UNKNOWN	22.72	0.27	1.6	0.6	0.272
12	UNKNOWN	22.85	0.07	1.3	0.2	0.071
13	UNKNOWN	23.03	0.10	1.5	0.2	0.099
14	UNKNOWN	23.19	0.08	1.4	0.2	0.080
15	UNKNOWN	23.51	0.11	1.0	0.3	0.113
16	UNKNOWN	25.76	0.03	0.6	0.1	0.027
17	UNKNOWN	25.91	0.04	0.6	0.1	0.044
18	UNKNOWN	26.61	0.17	1.2	0.4	0.170
19	UNKNOWN	26.95	1.92	19.9	2.3	1.918
20	UNKNOWN	27.41	0.78	7.8	1.8	0.780
21	UNKNOWN	28.52	0.01	0.4	0.0	0.016
22	UNKNOWN	30.12	0.12	2.3	0.3	0.124
23	UNKNOWN	30.79	0.06	0.8	0.1	0.063
24	UNKNOWN	31.11	95.60	384.4	220.6	95.605
25	UNKNOWN	33.09	0.42	3.2	1.0	0.455
Total			100.00	430.8	230.8	100.000

1-(5,6,7,8-Tetrahydroquinolin-2-yl)-3-(2-hydroxyethyl)guanidine hydrochloride (9j)

Chromatogram :
ssmmm-21-thq-gua-hydroxyethyl.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 17/11/2011 11:38:10
Processed : 17/11/2011 12:25:39
Printed : 17/11/2011 12:40:53



Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	22.04	0.02	1.6	0.2	0.023
2	UNKNOWN	22.57	0.03	2.7	0.3	0.034
3	UNKNOWN	22.80	0.05	3.3	0.5	0.051
4	UNKNOWN	25.05	0.01	0.9	0.1	0.010
5	UNKNOWN	25.79	0.38	22.2	3.4	0.382
6	UNKNOWN	26.00	0.29	14.2	2.5	0.290
7	UNKNOWN	26.89	96.37	967.1	845.7	96.372
8	UNKNOWN	28.69	2.62	46.4	23.0	2.625
9	UNKNOWN	30.31	0.13	7.1	1.2	0.132
10	UNKNOWN	31.64	0.02	2.0	0.2	0.023
11	UNKNOWN	32.17	0.01	0.7	0.0	0.005
12	UNKNOWN	32.56	0.00	0.6	0.0	0.004
13	UNKNOWN	33.03	0.00	0.4	0.0	0.002
14	UNKNOWN	33.12	0.00	0.6	0.0	0.004
15	UNKNOWN	33.96	0.00	0.8	0.0	0.005
16	UNKNOWN	34.43	0.00	0.6	0.0	0.003
17	UNKNOWN	36.07	0.02	1.9	0.2	0.023
18	UNKNOWN	38.15	0.01	1.0	0.1	0.011
Total			100.00	1074.1	877.5	100.000

1-(5,6,7,8-Tetrahydroquinolin-2-yl)-3-(2-furanylmethyl)guanidine hydrochloride (9k)

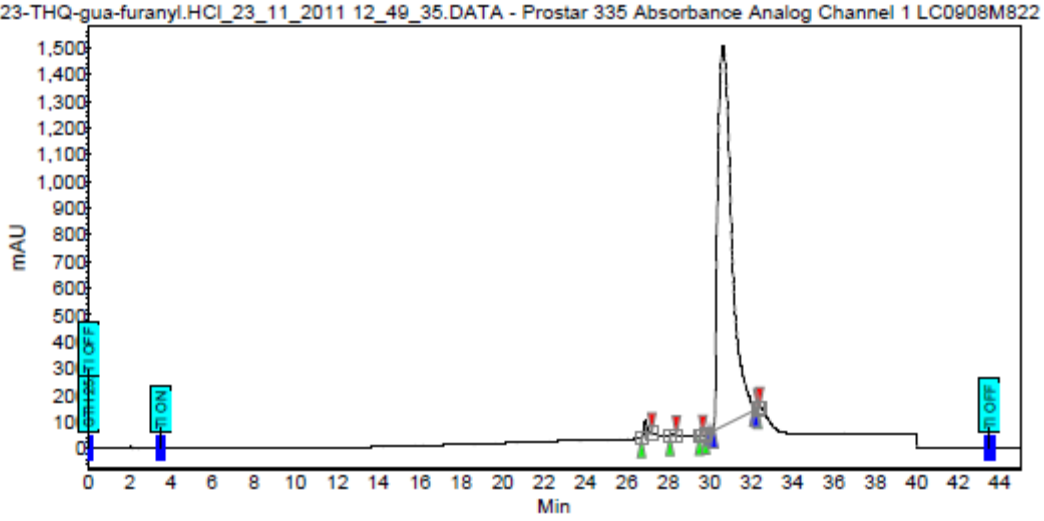
Chromatogram :

ssmmm23-THQ-gua-furanyl.HCl_23_11_2011 12_49_35.channel1

Method : GradientT
User : Daniel

Acquired : 23/11/2011 12:50:24
Processed : 23/11/2011 13:37:53
Printed : 23/11/2011 14:34:01

ssmmm23-THQ-gua-furanyl.HCl_23_11_2011 12_49_35.DATA - Prostar 335 Absorbance Analog Channel 1 LC0908M822



Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	26.88	0.94	56.0	10.4	0.938
2	UNKNOWN	28.20	0.07	5.9	0.8	0.072
3	UNKNOWN	29.59	0.01	1.0	0.1	0.007
4	UNKNOWN	29.92	0.19	24.0	2.2	0.195
5	UNKNOWN	29.96	0.19	21.3	2.2	0.194
6	UNKNOWN	30.09	0.07	8.7	0.8	0.068
7	UNKNOWN	30.64	98.42	1420.1	1093.1	98.423
8	UNKNOWN	32.13	0.06	11.2	0.7	0.063
9	UNKNOWN	32.25	0.02	4.1	0.3	0.024
10	UNKNOWN	32.36	0.01	3.3	0.2	0.014
Total			100.00	1555.5	1110.6	100.000

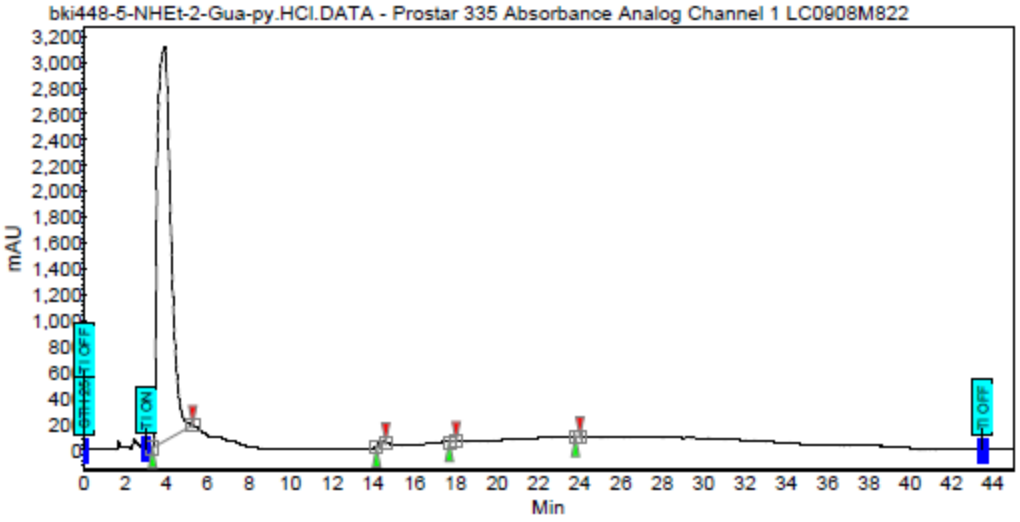
1-[5-(Ethylamino)pyridin-2-yl]guanidine hydrochloride (10c)

Chromatogram :

bki448-5-NHEt-2-Gua-py.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 25/04/2012 11:25:11
Processed : 25/04/2012 12:18:38
Printed : 25/04/2012 12:19:04



Peak results :

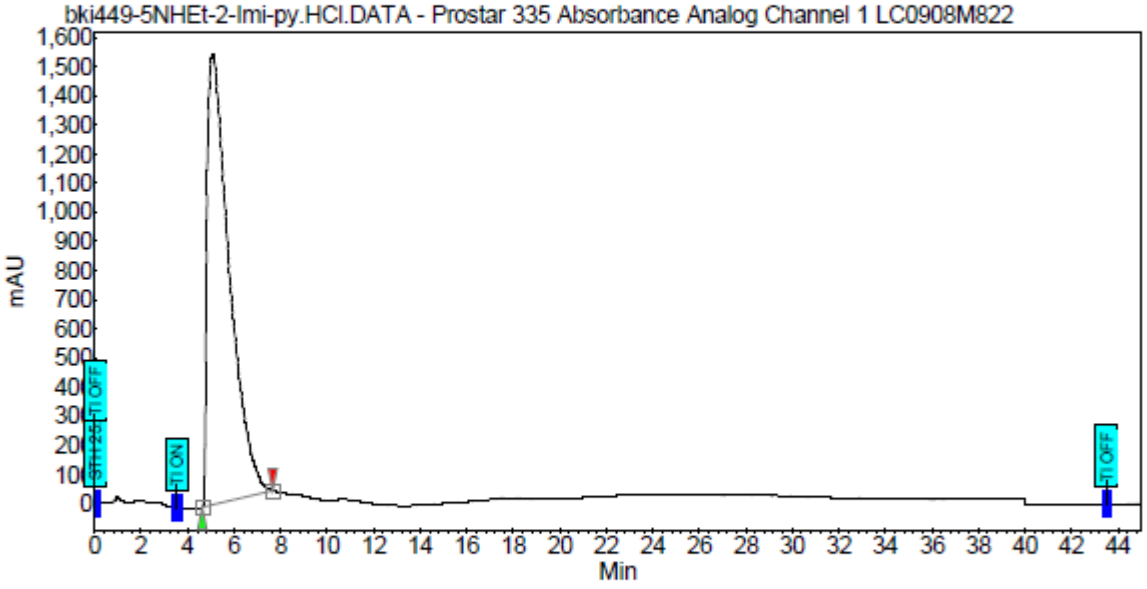
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	3.88	99.50	3053.5	2282.1	99.499
2	UNKNOWN	14.35	0.41	40.4	9.4	0.411
3	UNKNOWN	17.83	0.07	10.5	1.6	0.071
4	UNKNOWN	23.89	0.02	3.8	0.4	0.019
Total			100.00	3108.2	2293.6	100.000

1-[5-(Ethylamino)pyridin-2’-yl]2-iminoimidazolidine hydrochloride (10d)

Chromatogram :
bki449-5NHEt-2-Imi-py.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 25/04/2012 12:15:51
Processed : 25/04/2012 13:03:19
Printed : 25/04/2012 14:08:57



Peak results :

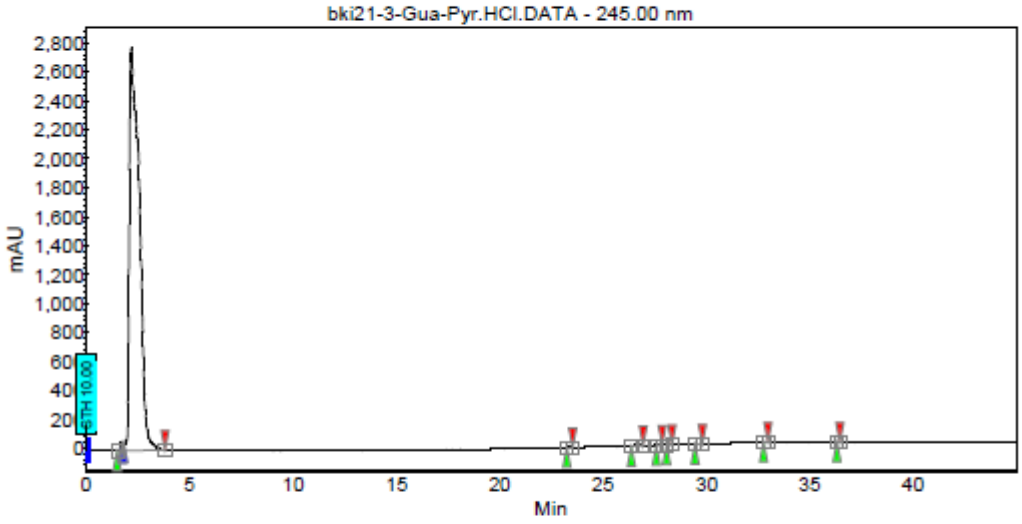
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	5.07	100.00	1543.4	1705.7	100.000
Total			100.00	1543.4	1705.7	100.000

1-(Pyridin-3-yl)guanidine hydrochloride (11c)

Chromatogram : bki21-3-Gua-Pyr.HCl_channel5

System : HPLC-PDA
Method : NOT DEFINED
User : Daniel

Acquired : 14/02/2011 13:53:21
Processed : 14/02/2011 14:59:17
Printed : 14/02/2011 14:59:48



Peak results :

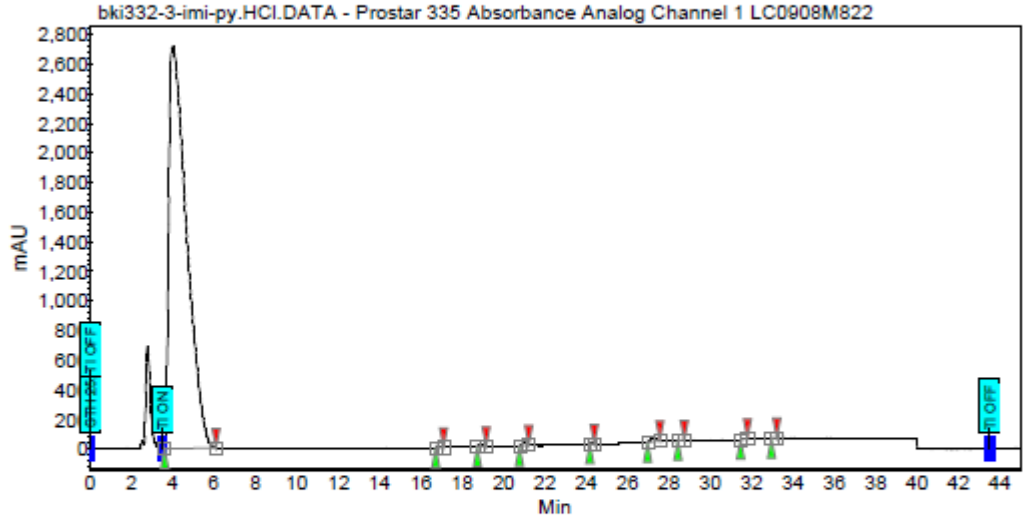
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	1.68	0.28	57.0	4.4	0.283
2	UNKNOWN	1.77	0.26	46.1	4.1	0.261
3	UNKNOWN	2.19	99.15	2785.0	1545.5	99.152
4	UNKNOWN	23.37	0.02	3.0	0.4	0.025
5	UNKNOWN	26.66	0.20	15.2	3.1	0.202
6	UNKNOWN	27.72	0.02	1.6	0.3	0.017
7	UNKNOWN	28.20	0.01	1.1	0.1	0.008
8	UNKNOWN	29.60	0.04	3.7	0.6	0.038
9	UNKNOWN	32.85	0.01	1.1	0.1	0.008
10	UNKNOWN	36.36	0.00	0.8	0.1	0.004
Total			100.00	2914.5	1558.7	100.000

1-(Pyridin-3’-yl)-2-iminoimidazolidine hydrochloride (11d)

Chromatogram : bki332-3-imi-py.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 15/09/2011 11:38:35
Processed : 15/09/2011 12:26:04
Printed : 15/09/2011 12:31:54



Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	4.00	99.23	2714.2	2684.0	99.229
2	UNKNOWN	16.91	0.04	5.7	1.1	0.042
3	UNKNOWN	18.92	0.13	17.9	3.5	0.129
4	UNKNOWN	20.97	0.17	20.8	4.5	0.166
5	UNKNOWN	24.27	0.02	3.8	0.4	0.017
6	UNKNOWN	27.25	0.33	36.6	9.1	0.335
7	UNKNOWN	28.57	0.04	5.9	1.0	0.035
8	UNKNOWN	31.69	0.03	4.3	0.9	0.032
9	UNKNOWN	33.09	0.01	3.1	0.4	0.015
Total			100.00	2812.2	2704.9	100.000

1-(6-Chloropyridin-3-yl)guanidine hydrochloride (12c)

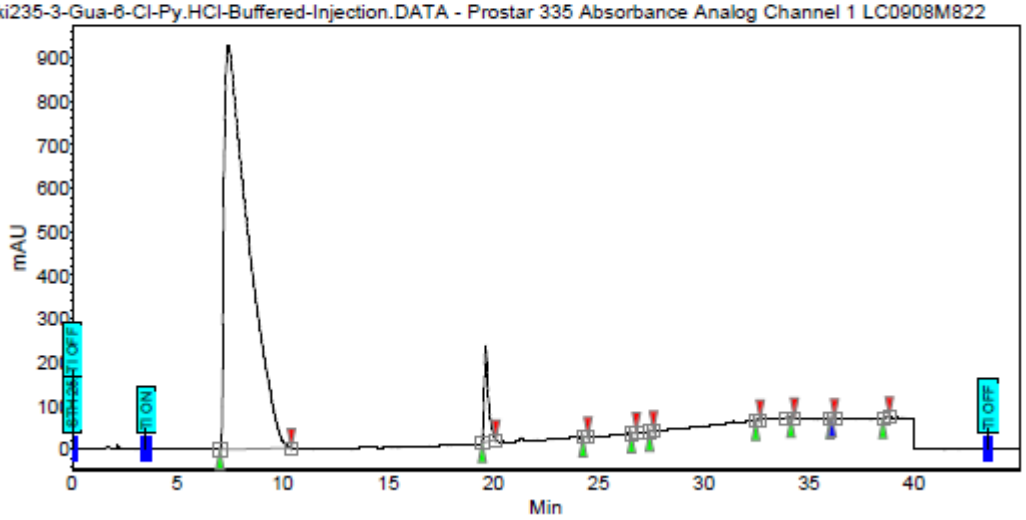
Chromatogram :

bki235-3-Gua-6-Cl-Py.HCl-Buffered-Injection_channel 1

HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 06/05/2011 11:58:11
Processed : 06/05/2011 12:53:53
Printed : 06/05/2011 12:54:36

bki235-3-Gua-6-Cl-Py.HCl-Buffered-Injection.DATA - Prostar 335 Absorbance Analog Channel 1 LC0908M822



Peak results :

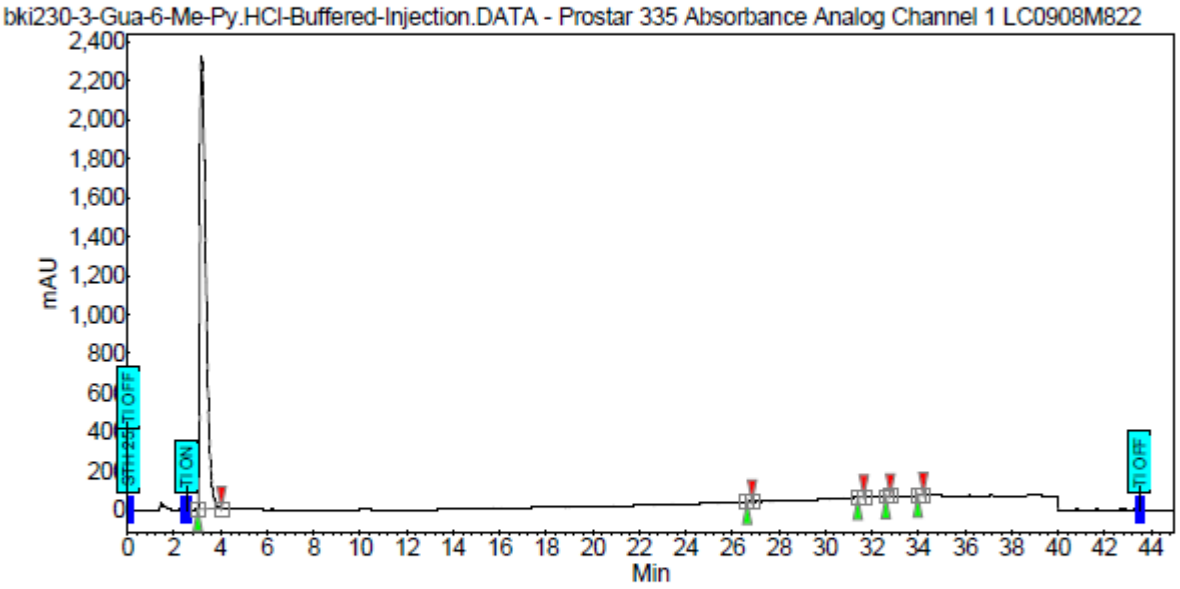
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	7.43	96.03	926.2	1226.8	96.034
10	UNKNOWN	19.64	3.88	221.2	49.6	3.881
2	UNKNOWN	24.39	0.01	1.4	0.1	0.012
3	UNKNOWN	26.67	0.01	1.5	0.2	0.014
4	UNKNOWN	27.51	0.01	1.1	0.1	0.009
5	UNKNOWN	32.60	0.01	1.1	0.1	0.010
6	UNKNOWN	34.20	0.02	2.0	0.2	0.017
7	UNKNOWN	36.05	0.00	0.7	0.0	0.003
8	UNKNOWN	36.13	0.00	0.6	0.0	0.003
9	UNKNOWN	38.72	0.02	1.5	0.2	0.017
Total			100.00	1157.2	1277.4	100.000

1-(6-Methylpyridin-3-yl)guanidine hydrochloride (13c)

Chromatogram :
bki230-3-Gua-6-Me-Py.HCl-Buffered-Injection_channel1

LC-PDA
Method : Gradient1
User : Daniel

Acquired : 06/05/2011 11:03:28
Processed : 06/05/2011 12:01:11
Printed : 06/05/2011 12:02:27



Peak results :

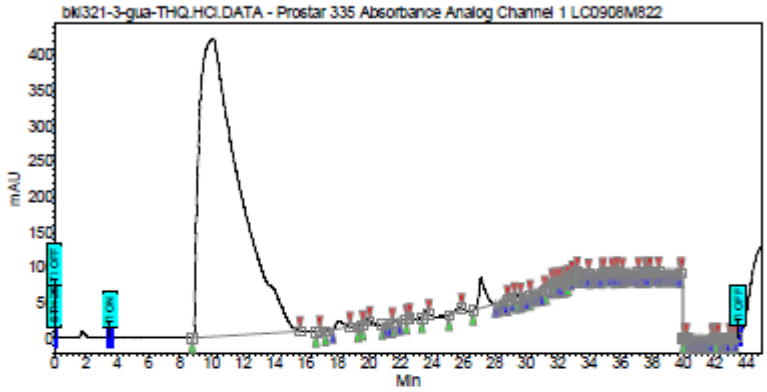
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	3.16	99.74	2322.5	683.4	99.743
2	UNKNOWN	26.75	0.04	2.5	0.3	0.039
3	UNKNOWN	31.51	0.13	7.8	0.9	0.129
4	UNKNOWN	32.68	0.03	2.0	0.2	0.032
5	UNKNOWN	34.08	0.06	3.2	0.4	0.057
Total			100.00	2337.9	685.2	100.000

1-(5,6,7,8-Tetrahydroquinolin-3-yl)guanidine hydrochloride (14c)

Chromatogram : bki321-3-gua-THQ.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 15/09/2011 15:05:50
Processed : 15/09/2011 16:27:17
Printed : 15/09/2011 16:27:43



Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
148	UNKNOWN	10.11	98.39	421.4	1231.5	98.394
1	UNKNOWN	16.76	0.01	0.7	0.1	0.008
2	UNKNOWN	17.43	0.08	3.6	1.0	0.077
3	UNKNOWN	18.07	0.50	11.0	6.4	0.488
4	UNKNOWN	19.45	0.02	1.4	0.2	0.018
5	UNKNOWN	19.77	0.13	7.2	1.6	0.129
6	UNKNOWN	21.01	0.00	0.5	0.1	0.005
7	UNKNOWN	21.19	0.01	0.6	0.1	0.007
8	UNKNOWN	21.39	0.00	0.4	0.1	0.004
9	UNKNOWN	21.77	0.02	1.4	0.3	0.024
10	UNKNOWN	21.93	0.01	0.7	0.1	0.008
11	UNKNOWN	21.99	0.01	0.8	0.2	0.012
12	UNKNOWN	22.49	0.01	0.7	0.1	0.005
13	UNKNOWN	23.55	0.11	5.7	1.4	0.107
14	UNKNOWN	25.55	0.10	2.9	1.3	0.103
15	UNKNOWN	27.13	1.81	43.0	20.6	1.614
16	UNKNOWN	28.21	0.01	0.9	0.1	0.010
17	UNKNOWN	28.45	0.02	2.1	0.2	0.015
18	UNKNOWN	28.56	0.02	2.2	0.2	0.019
19	UNKNOWN	28.65	0.01	1.9	0.2	0.014
20	UNKNOWN	28.78	0.00	0.9	0.1	0.005
21	UNKNOWN	28.99	0.04	3.6	0.6	0.045
22	UNKNOWN	29.21	0.00	0.6	0.0	0.003
23	UNKNOWN	29.51	0.02	2.2	0.3	0.022
24	UNKNOWN	29.71	0.00	0.4	0.0	0.001
25	UNKNOWN	29.81	0.01	1.4	0.1	0.008
26	UNKNOWN	29.89	0.00	0.9	0.1	0.005
27	UNKNOWN	30.00	0.00	0.6	0.0	0.003
28	UNKNOWN	30.19	0.01	0.8	0.1	0.007
29	UNKNOWN	30.40	0.03	2.9	0.3	0.026
30	UNKNOWN	30.49	0.03	3.7	0.3	0.027

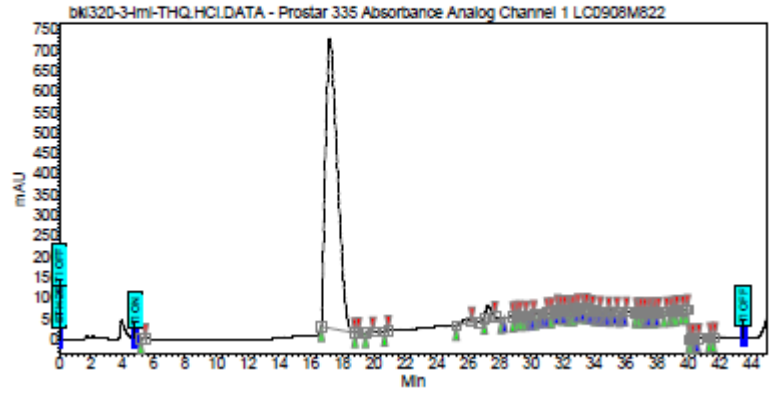
Page

1-(5,6,7,8-Tetrahydroquinolin-3’-yl)-2-iminoimidazolidine hydrochloride (14d)

Chromatogram : bki320-3-imi-THQ.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 15/09/2011 13:49:17
Processed : 15/09/2011 15:11:10
Printed : 15/09/2011 15:11:27



Peak results :

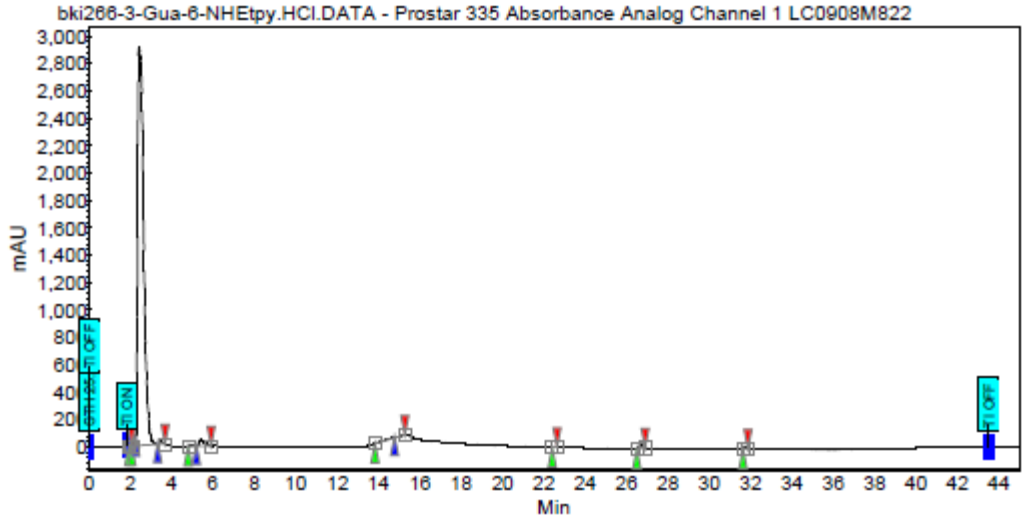
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	5.32	0.03	1.2	0.2	0.028
2	UNKNOWN	17.20	96.06	700.7	612.5	96.064
3	UNKNOWN	18.89	0.02	1.2	0.2	0.024
4	UNKNOWN	19.83	0.08	1.9	0.5	0.083
5	UNKNOWN	20.79	0.01	0.7	0.1	0.013
6	UNKNOWN	25.72	0.73	8.1	4.7	0.729
81	UNKNOWN	27.23	1.85	31.9	11.8	1.853
7	UNKNOWN	28.27	0.02	0.7	0.1	0.017
8	UNKNOWN	28.88	0.10	2.2	0.7	0.104
9	UNKNOWN	29.01	0.02	1.1	0.1	0.017
10	UNKNOWN	29.23	0.01	0.7	0.0	0.007
11	UNKNOWN	29.52	0.03	1.4	0.2	0.027
12	UNKNOWN	29.83	0.02	1.4	0.1	0.021
13	UNKNOWN	29.93	0.01	0.7	0.0	0.006
14	UNKNOWN	30.04	0.01	0.8	0.1	0.009
15	UNKNOWN	30.12	0.01	0.7	0.0	0.007
16	UNKNOWN	30.51	0.10	3.2	0.6	0.097
17	UNKNOWN	30.81	0.03	2.1	0.2	0.026
18	UNKNOWN	30.71	0.02	1.5	0.1	0.018
19	UNKNOWN	30.89	0.04	1.9	0.3	0.042
20	UNKNOWN	31.00	0.01	1.0	0.1	0.009
21	UNKNOWN	31.27	0.00	0.5	0.0	0.003
22	UNKNOWN	31.45	0.14	5.3	0.9	0.144
23	UNKNOWN	31.84	0.01	1.0	0.1	0.010
24	UNKNOWN	31.84	0.01	0.7	0.0	0.005
25	UNKNOWN	32.01	0.01	0.9	0.0	0.008
26	UNKNOWN	32.11	0.01	0.8	0.0	0.006
27	UNKNOWN	32.39	0.00	0.7	0.0	0.005
28	UNKNOWN	32.48	0.00	0.6	0.0	0.004
29	UNKNOWN	32.57	0.01	0.7	0.0	0.006
30	UNKNOWN	32.87	0.00	0.5	0.0	0.004

1-[6-(*N*-ethylamino)pyridin-3-yl]guanidine hydrochloride (15c)

Chromatogram :
bki266-3-Gua-6-NHEtpy.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 06/07/2011 16:23:43
Processed : 06/07/2011 17:29:39
Printed : 06/07/2011 17:32:11



Peak results :

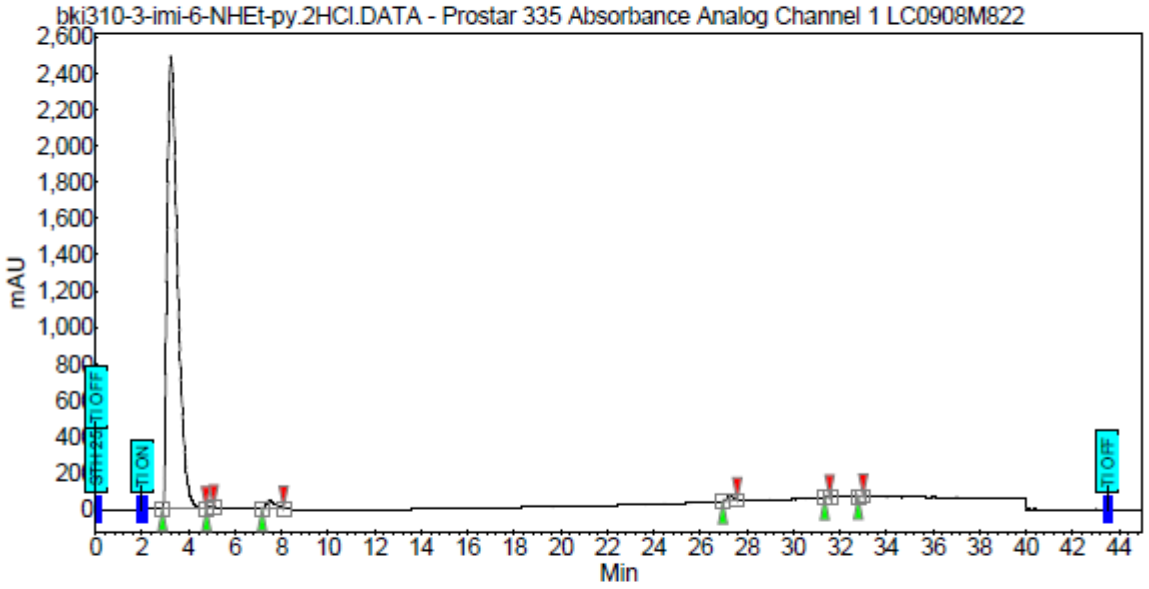
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	1.99	0.02	3.2	0.2	0.023
2	UNKNOWN	2.19	0.70	77.2	7.1	0.701
3	UNKNOWN	2.41	96.27	2906.0	976.3	96.266
4	UNKNOWN	3.45	0.35	20.2	3.5	0.348
5	UNKNOWN	4.92	0.13	6.8	1.4	0.134
6	UNKNOWN	5.39	1.41	49.2	14.3	1.405
7	UNKNOWN	14.69	0.38	8.5	3.8	0.378
8	UNKNOWN	14.76	0.15	5.5	1.5	0.147
9	UNKNOWN	22.51	0.05	4.0	0.5	0.048
10	UNKNOWN	26.64	0.48	30.5	4.9	0.480
11	UNKNOWN	31.72	0.07	6.3	0.7	0.069
Total			100.00	3117.4	1014.2	100.000

1-(6-(Ethylamino)pyridin-3’-yl)-2-iminoimidazolidine hydrochloride (15d)

Chromatogram :
bki310-3-imi-6-NHEt-py.2HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 15/09/2011 12:37:37
Processed : 15/09/2011 13:50:29
Printed : 15/09/2011 13:51:10



Peak results :

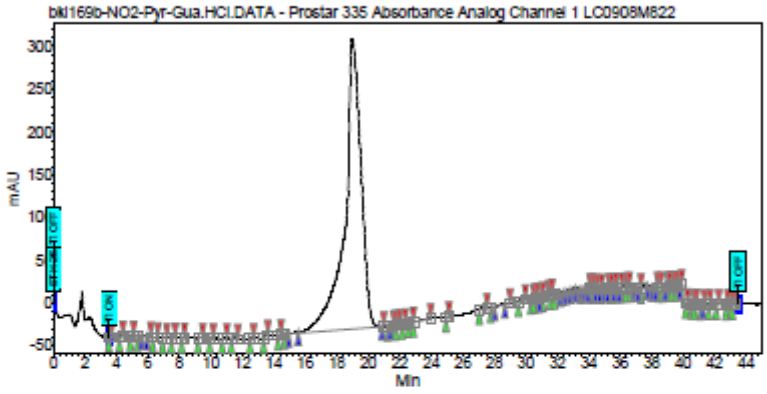
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	3.21	97.88	2494.2	1286.6	97.877
2	UNKNOWN	4.91	0.10	8.2	1.4	0.103
3	UNKNOWN	7.47	1.41	41.7	18.5	1.411
4	UNKNOWN	27.29	0.58	24.3	7.6	0.579
5	UNKNOWN	31.45	0.02	2.7	0.2	0.018
6	UNKNOWN	32.84	0.01	1.4	0.2	0.013
Total			100.00	2572.4	1314.5	100.000

1-(5-Nitropyridin-2-yl)guanidine hydrochloride (17c)

Chromatogram :
bki169b-NO2-Pyr-Gua.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 14/02/2011 13:00:41
Processed : 14/02/2011 13:48:10
Printed : 14/02/2011 13:54:08



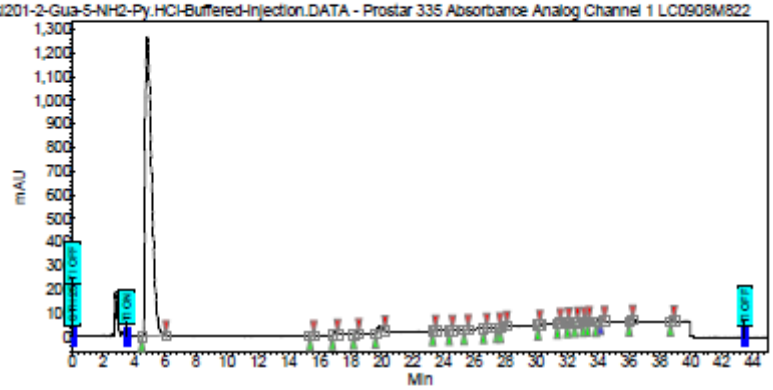
Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	3.81	0.01	0.3	0.0	0.006
2	UNKNOWN	4.32	0.01	0.4	0.0	0.011
3	UNKNOWN	4.97	0.02	0.7	0.1	0.020
4	UNKNOWN	5.51	0.03	0.8	0.1	0.035
5	UNKNOWN	5.89	0.07	1.6	0.3	0.073
6	UNKNOWN	6.00	0.03	0.8	0.1	0.031
7	UNKNOWN	6.43	0.03	0.8	0.1	0.032
8	UNKNOWN	7.04	0.06	1.9	0.2	0.059
9	UNKNOWN	7.60	0.02	0.8	0.1	0.024
10	UNKNOWN	8.23	0.01	0.6	0.0	0.011
11	UNKNOWN	9.31	0.04	1.0	0.2	0.037
12	UNKNOWN	10.03	0.01	0.6	0.1	0.015
13	UNKNOWN	10.85	0.03	0.9	0.1	0.030
14	UNKNOWN	11.47	0.06	1.3	0.2	0.058
15	UNKNOWN	12.81	0.01	0.5	0.1	0.013
16	UNKNOWN	13.51	0.04	1.5	0.2	0.042
17	UNKNOWN	14.39	0.01	0.2	0.0	0.005
18	UNKNOWN	14.92	0.02	0.6	0.1	0.022
19	UNKNOWN	15.52	0.21	1.8	0.9	0.208
20	UNKNOWN	18.97	98.79	339.8	405.8	98.792
21	UNKNOWN	20.92	0.01	0.4	0.0	0.008
22	UNKNOWN	21.31	0.01	0.5	0.0	0.009
23	UNKNOWN	21.53	0.01	0.3	0.1	0.015
24	UNKNOWN	21.88	0.01	0.4	0.0	0.006
25	UNKNOWN	21.92	0.01	0.3	0.0	0.007
26	UNKNOWN	22.23	0.00	0.2	0.0	0.004
27	UNKNOWN	22.79	0.02	0.4	0.1	0.015
28	UNKNOWN	23.75	0.09	0.8	0.4	0.090
29	UNKNOWN	25.05	0.01	0.3	0.0	0.005
30	UNKNOWN	27.37	0.07	1.1	0.3	0.072
31	UNKNOWN	27.91	0.03	0.8	0.1	0.032

1-(5-Aminopyridin-2-yl)guanidine hydrochloride (18c)

Chromatogram :
bki201-2-Gua-5-NH2-Py.HCl-Buffered-Injection_channel1-PDA
Method : Gradient1
User : Daniel
Acquired : 06/05/2011 16:13:34
Processed : 06/05/2011 17:01:04
Printed : 06/05/2011 17:06:09

bki201-2-Gua-5-NH2-Py.HCl-Buffered-Injection.DATA - Prostar 335 Absorbance Analog Channel 1 LC0908M822



Peak results :

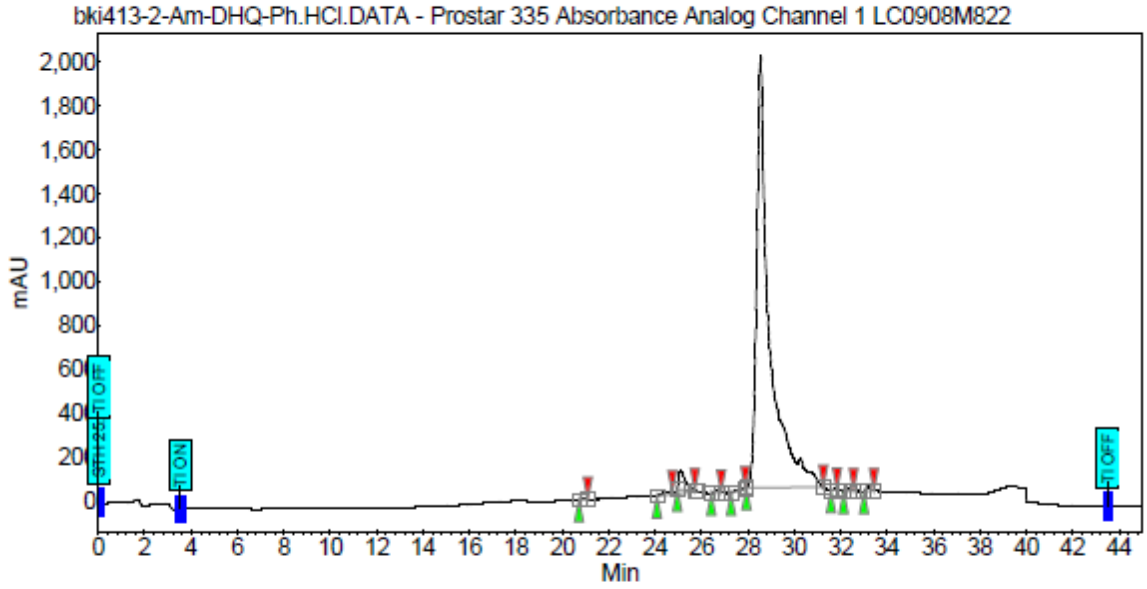
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	4.84	97.44	1264.6	803.7	97.442
2	UNKNOWN	15.51	0.03	1.7	0.2	0.032
3	UNKNOWN	16.97	0.19	8.4	1.2	0.192
4	UNKNOWN	18.33	0.29	14.5	1.8	0.287
5	UNKNOWN	19.88	1.27	22.9	7.9	1.269
6	UNKNOWN	23.41	0.03	2.2	0.2	0.034
7	UNKNOWN	24.48	0.03	1.8	0.2	0.031
8	UNKNOWN	25.49	0.04	1.8	0.2	0.039
9	UNKNOWN	26.71	0.02	1.3	0.1	0.021
10	UNKNOWN	27.56	0.02	1.1	0.1	0.021
11	UNKNOWN	27.95	0.24	7.0	1.5	0.244
12	UNKNOWN	30.20	0.01	0.5	0.0	0.008
13	UNKNOWN	31.47	0.04	1.8	0.2	0.036
14	UNKNOWN	32.09	0.01	0.7	0.0	0.005
15	UNKNOWN	32.84	0.02	1.6	0.1	0.024
16	UNKNOWN	33.11	0.01	0.8	0.0	0.006
17	UNKNOWN	33.39	0.00	0.5	0.0	0.004
18	UNKNOWN	34.05	0.10	4.0	0.6	0.099
19	UNKNOWN	34.32	0.09	4.0	0.6	0.093
20	UNKNOWN	36.17	0.08	4.0	0.5	0.075
21	UNKNOWN	38.84	0.04	1.8	0.2	0.037
Total			100.00	1347.4	819.8	100.000

N-Phenyl-1,4-dihydroquinazolin-2-amine hydrochloride (19i)

Chromatogram :
bki413-2-Am-DHQ-Ph.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 15/03/2012 15:02:29
Processed : 15/03/2012 15:59:49
Printed : 15/03/2012 16:00:07



Peak results :

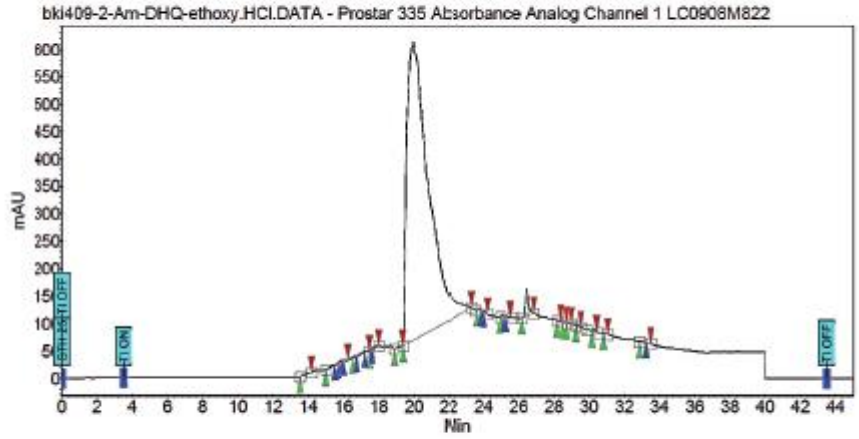
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	20.88	0.06	3.4	0.7	0.055
2	UNKNOWN	24.47	0.51	16.8	6.6	0.513
9	UNKNOWN	25.11	2.12	89.4	27.3	2.124
3	UNKNOWN	26.60	0.22	13.5	2.8	0.216
4	UNKNOWN	27.41	0.11	4.8	1.5	0.114
8	UNKNOWN	28.55	96.36	1962.0	1239.4	96.364
5	UNKNOWN	31.71	0.06	6.8	0.8	0.061
6	UNKNOWN	32.37	0.17	12.6	2.2	0.173
7	UNKNOWN	33.16	0.38	32.7	4.9	0.380
Total			100.00	2141.9	1286.1	100.000

N-(2-hydroxyethyl)-1,4-dihydroquinazolin-2-amine hydrochloride (19j)

Chromatogram :
bki409-2-Am-DHQ-ethoxy.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 15/03/2012 11:05:20
Processed : 15/03/2012 11:58:42
Printed : 15/03/2012 11:59:03



Peak results :

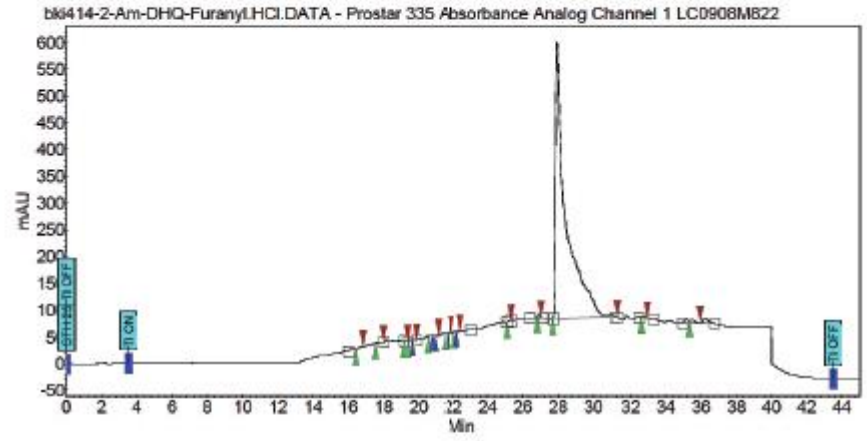
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	13.89	0.08	1.6	0.7	0.078
2	UNKNOWN	15.39	0.08	2.9	0.7	0.085
3	UNKNOWN	15.64	0.05	3.1	0.4	0.047
4	UNKNOWN	15.84	0.09	6.2	0.8	0.093
5	UNKNOWN	15.87	0.07	5.8	0.6	0.009
6	UNKNOWN	15.99	0.07	3.5	0.6	0.074
7	UNKNOWN	16.56	0.06	3.0	0.5	0.061
8	UNKNOWN	17.15	0.14	4.6	1.2	0.135
9	UNKNOWN	17.21	0.07	3.5	0.6	0.071
10	UNKNOWN	17.56	0.04	3.9	0.3	0.040
11	UNKNOWN	17.85	0.12	3.5	1.1	0.125
12	UNKNOWN	19.13	0.05	1.5	0.4	0.049
28	UNKNOWN	19.96	97.32	543.3	846.2	97.321
13	UNKNOWN	23.77	0.08	4.1	0.7	0.077
14	UNKNOWN	23.92	0.05	3.7	0.4	0.051
15	UNKNOWN	24.07	0.04	3.4	0.4	0.041
16	UNKNOWN	25.07	0.06	4.9	0.6	0.064
17	UNKNOWN	25.20	0.03	2.5	0.3	0.031
18	UNKNOWN	25.36	0.05	2.6	0.5	0.054
19	UNKNOWN	26.48	1.13	50.2	9.8	1.132
20	UNKNOWN	28.33	0.02	1.1	0.2	0.018
21	UNKNOWN	28.57	0.02	1.5	0.2	0.021
22	UNKNOWN	28.87	0.04	2.7	0.3	0.039
23	UNKNOWN	29.32	0.04	2.1	0.4	0.042
24	UNKNOWN	30.28	0.08	4.1	0.7	0.078
25	UNKNOWN	30.88	0.03	2.2	0.3	0.031
26	UNKNOWN	33.01	0.06	2.5	0.5	0.056
27	UNKNOWN	33.32	0.02	1.2	0.2	0.018
Total			100.00	675.2	869.5	100.000

N-(2-furanylmethyl)-1,4-dihydroquinazolin-2-amine hydrochloride (19k)

Chromatogram :
bki414-2-Am-DHQ-Furanyl.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 15/03/2012 14:12:24
Processed : 15/03/2012 15:05:24
Printed : 15/03/2012 15:09:11



Peak results :

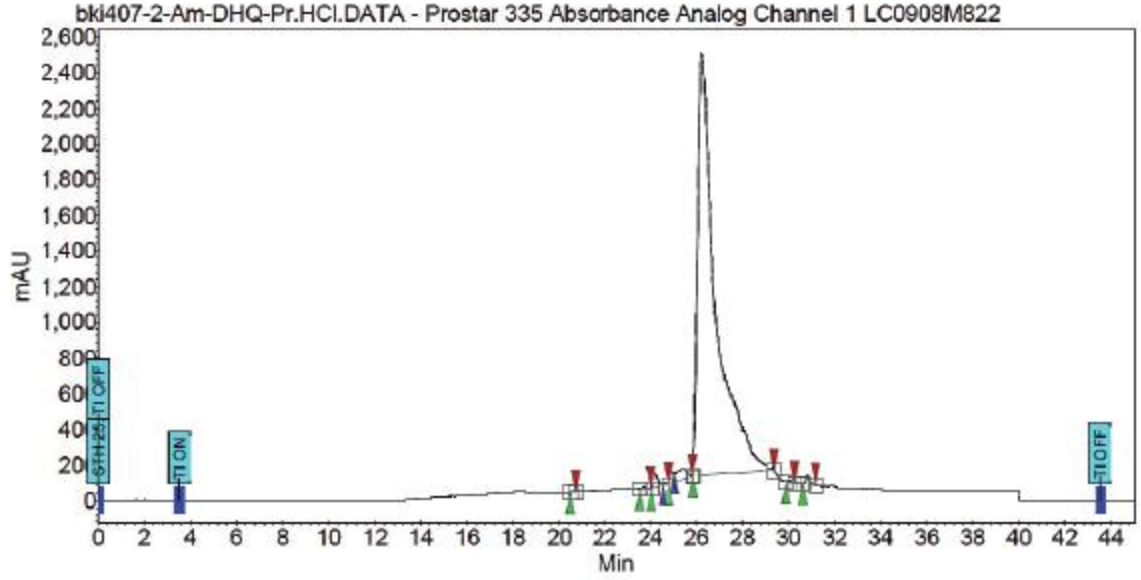
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	16.72	0.13	1.7	0.5	0.126
2	UNKNOWN	17.53	0.20	2.7	0.8	0.203
3	UNKNOWN	19.24	0.03	1.2	0.1	0.032
4	UNKNOWN	19.51	0.05	1.5	0.2	0.052
5	UNKNOWN	19.75	0.03	0.8	0.1	0.026
6	UNKNOWN	20.61	0.21	4.3	0.8	0.206
7	UNKNOWN	20.83	0.11	3.2	0.4	0.114
8	UNKNOWN	21.04	0.10	2.2	0.4	0.102
9	UNKNOWN	21.60	0.13	3.6	0.5	0.125
10	UNKNOWN	21.80	0.18	3.3	0.7	0.177
11	UNKNOWN	22.15	0.07	2.2	0.3	0.072
12	UNKNOWN	22.33	0.13	2.6	0.5	0.125
13	UNKNOWN	25.23	0.06	2.2	0.2	0.056
14	UNKNOWN	26.84	0.12	3.1	0.5	0.122
15	UNKNOWN	27.95	97.64	514.7	364.2	97.637
16	UNKNOWN	32.75	0.20	3.5	0.7	0.196
17	UNKNOWN	35.48	0.63	6.8	2.3	0.626
Total			100.00	559.6	373.0	100.000

N-(*n*-Propyl)-1,4-dihydroquinazolin-2-amine hydrochloride (19l)

Chromatogram :
bki407-2-Am-DHQ-Pr.HCl_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 15/03/2012 12:01:09
Processed : 15/03/2012 12:50:16
Printed : 15/03/2012 12:50:27



Peak results :

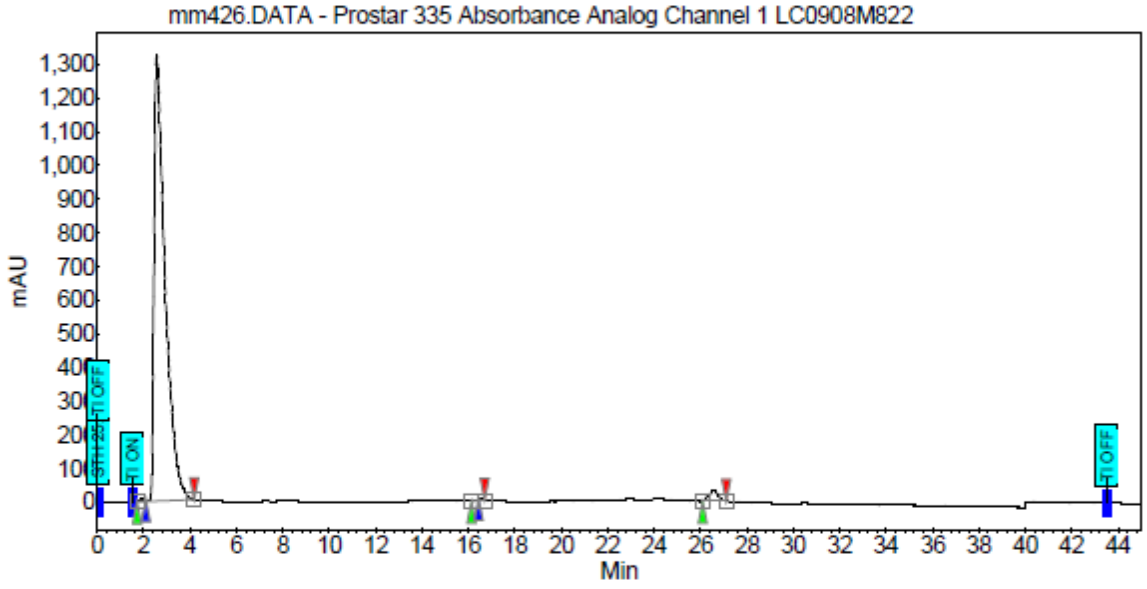
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	20.60	0.02	4.7	0.6	0.024
2	UNKNOWN	23.73	0.09	11.2	2.1	0.090
3	UNKNOWN	24.19	0.83	81.3	19.9	0.834
4	UNKNOWN	24.67	0.07	14.5	1.7	0.072
5	UNKNOWN	24.93	0.45	65.5	10.7	0.448
6	UNKNOWN	25.28	1.37	59.7	32.8	1.373
9	UNKNOWN	26.23	96.71	2370.0	2308.6	96.708
7	UNKNOWN	30.04	0.06	9.1	1.5	0.064
8	UNKNOWN	30.81	0.39	51.4	9.3	0.388
Total			100.00	2667.4	2387.2	100.000

N-(2-hydroxyethyl)-1,4-dihydropyrido[2,3-d]pyrimidin-2-amine hydrochloride (20j)

Chromatogram : mm426_channel1

System : HPLC-PDA
Method : Intergrate later Mic1
User : Daniel

Acquired : 19/02/2014 09:37:49
Processed : 19/02/2014 10:25:18
Printed : 31/03/2014 16:21:35



Peak results :

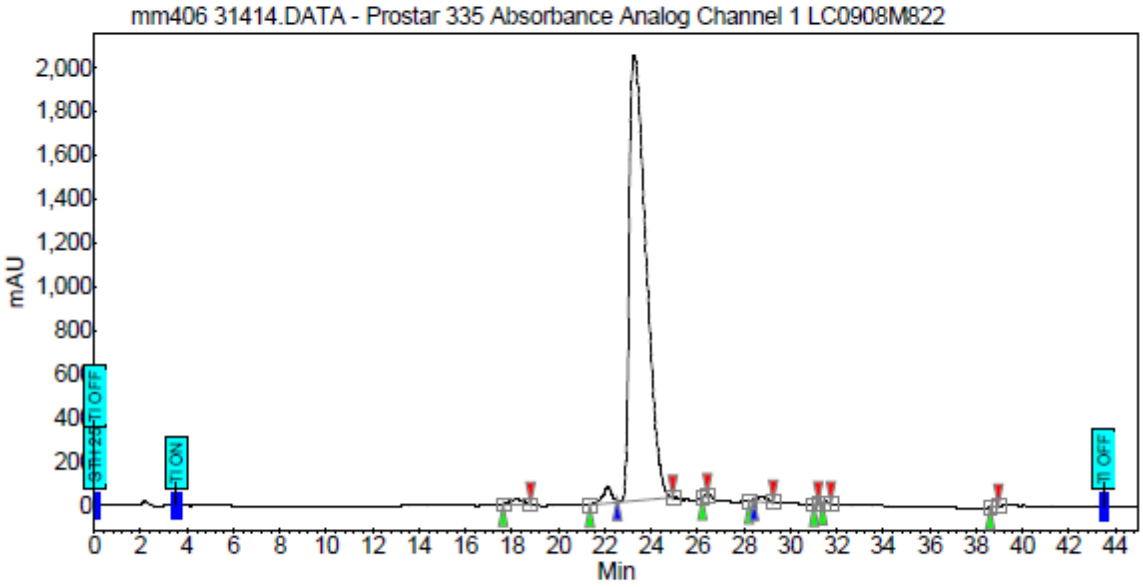
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	1.87	0.19	7.9	1.4	0.185
2	UNKNOWN	2.55	97.69	1325.1	726.8	97.694
3	UNKNOWN	16.33	0.08	2.8	0.6	0.077
4	UNKNOWN	16.55	0.08	4.3	0.6	0.085
5	UNKNOWN	26.56	1.96	34.1	14.6	1.959
Total			100.00	1374.2	744.0	100.000

N-(furan-2-ylmethyl)-1,4-dihydropyrido[2,3-d]pyrimidin-2-amine hydrochloride (20k)

Chromatogram : mm406 31414_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 31/03/2014 13:49:16
Processed : 31/03/2014 14:36:45
Printed : 31/03/2014 16:17:58



Peak results :

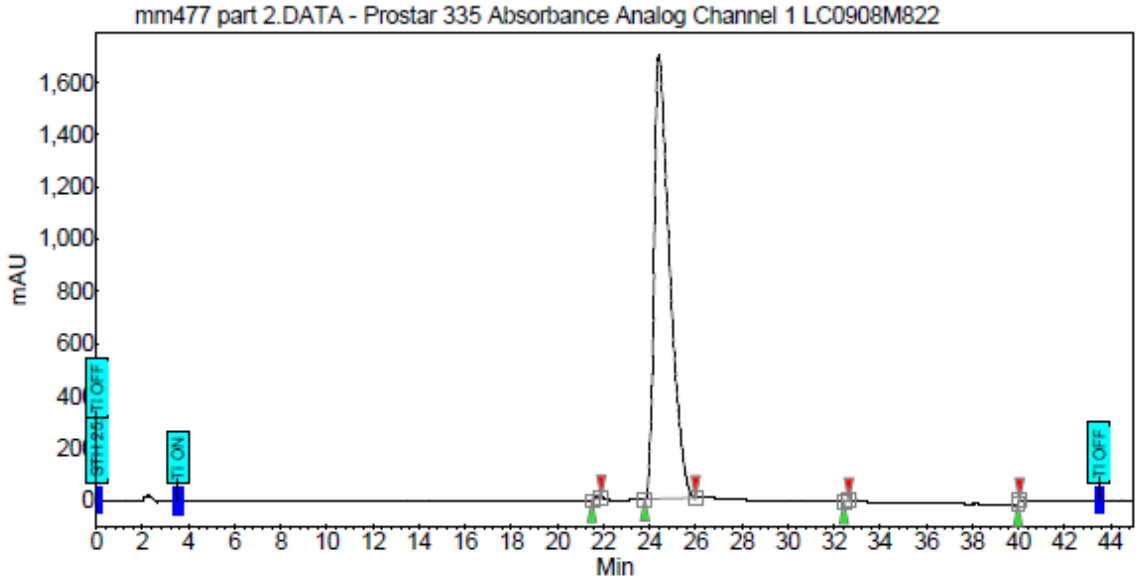
Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	18.23	0.88	23.2	15.6	0.883
2	UNKNOWN	22.15	1.95	80.1	34.5	1.954
3	UNKNOWN	23.27	96.22	2029.9	1696.7	96.215
4	UNKNOWN	26.35	0.02	3.6	0.4	0.023
5	UNKNOWN	28.44	0.07	10.2	1.3	0.072
6	UNKNOWN	28.80	0.74	26.7	13.0	0.738
7	UNKNOWN	31.12	0.01	1.7	0.2	0.009
8	UNKNOWN	31.55	0.06	6.5	1.1	0.064
9	UNKNOWN	38.79	0.04	3.6	0.7	0.042
Total			100.00	2185.4	1763.4	100.000

N-(1,3-benzodioxol-5-ylmethyl)-1,4-dihydropyrido[2,3-d]pyrimidin-2-amine hydrochloride (20m)

Chromatogram : mm477 part 2_channel1

System : HPLC-PDA
Method : Gradient1
User : Daniel

Acquired : 08/04/2014 13:29:33
Processed : 08/04/2014 14:17:03
Printed : 08/04/2014 14:18:14



Peak results :

Index	Name	Time [Min]	Quantity [% Area]	Height [mAU]	Area [mAU.Min]	Area % [%]
1	UNKNOWN	21.68	0.14	8.0	1.9	0.143
2	UNKNOWN	24.40	99.81	1699.3	1331.0	99.811
3	UNKNOWN	32.53	0.02	2.1	0.3	0.019
4	UNKNOWN	40.00	0.03	11.1	0.4	0.028
Total			100.00	1720.4	1333.6	100.000

8. Preparation of membranes

Neural membranes (P2 fractions) were prepared from the PFC of human brains obtained at autopsy in the Instituto Vasco de Medicina Legal, Bilbao, Spain, in compliance with policies of research and ethical boards for postmortem brain studies at the moment of sample obtaining. Postmortem human brain samples of each subject (~ 1 g) were homogenized using a Teflon-glass grinder (10 up-and-down strokes at 1500 rpm) in 30 volumes of homogenization buffer (1 mM $MgCl_2$, and 5 mM Tris-HCl, pH 7.4) supplemented with 0.25 M sucrose. The crude homogenate was centrifuged for 5 min at 1000 × g (4 ºC) and the supernatant was centrifuged again for 10 min at 40000 × g (4 ºC). The resultant pellet was washed twice in 20 volumes of homogenization buffer and re-centrifuged in similar conditions. Aliquots of 1 mg protein were stored at -70 ºC until assay. Protein content was measured according to the Bradford method using BSA as standard, and was similar in the different brain samples.

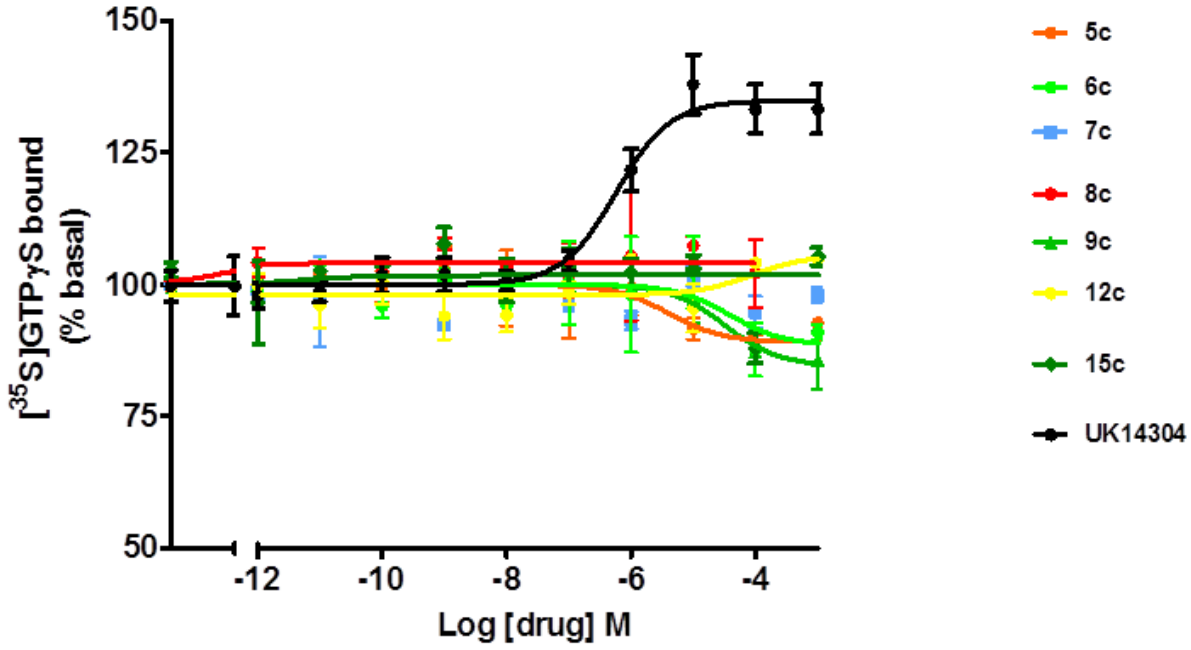
9. Analysis of binding data

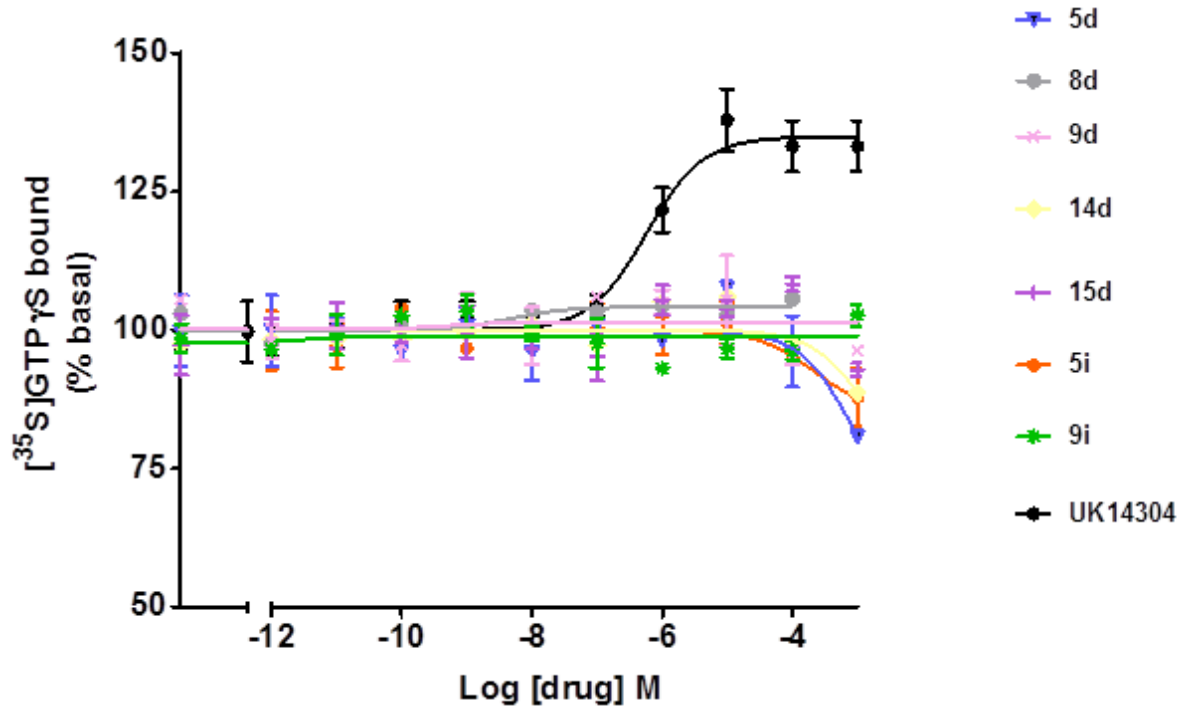
Analysis of competition experiments to obtain the inhibition constant (K_i) were performed by nonlinear regression using the GraphPad Prism program. All experiments were analysed assuming a one-site model of radioligand binding. K_i values were normalized to pK_i values.

10. Drugs used in pharmacology experiments

[^{3}H]RX821002 (specific activity 55 Ci/mmol) was obtained from Amersham International, U.K. [^{35}S]GTPγS (1250 Ci/mmol) was purchased from Perkin Elmer Life Sciences (Massachusetts, USA). GDP, GTP, GTPγS, RX821002 HCl, and UK14304 were purchased from Sigma (St. Louis, U.S.A.). All other chemicals were of the highest purity commercially available.

11. [^{35}S]GTPγS functional assays results





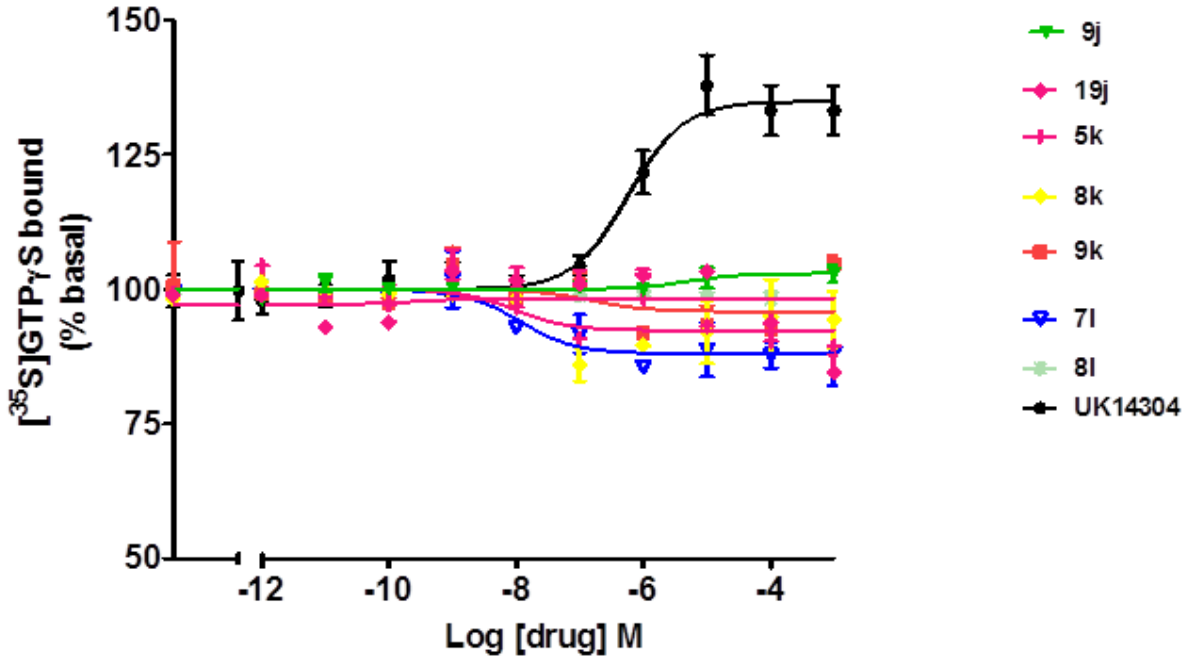
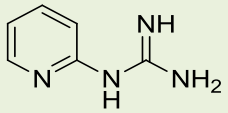
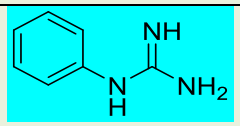
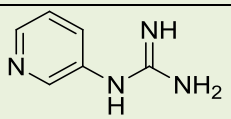
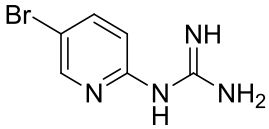
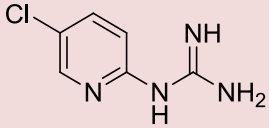
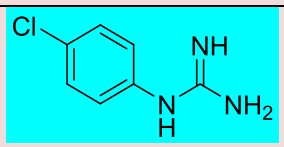


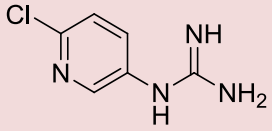
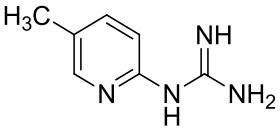
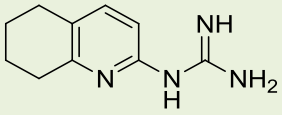
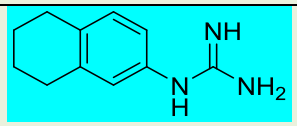
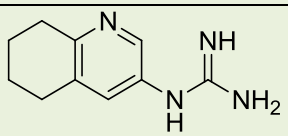
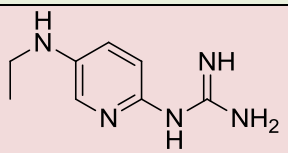
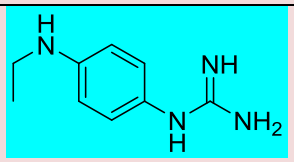
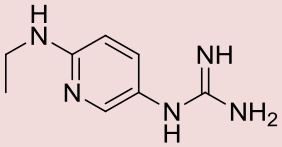
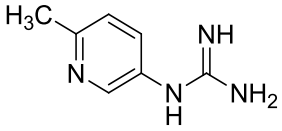
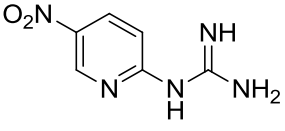
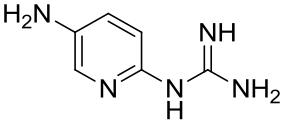
Figure S1. Dose-response curves for [^{35}S]GTPγS binding *versus* ligand concentration.

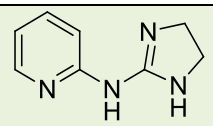
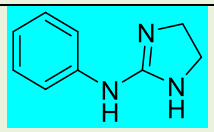
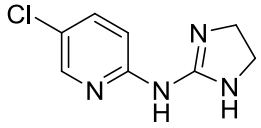
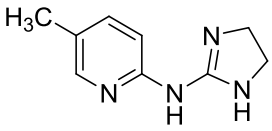
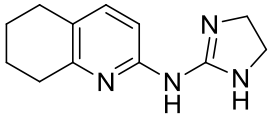
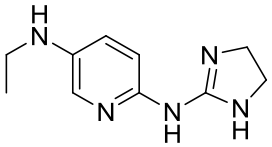
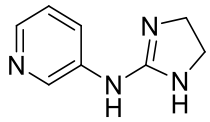
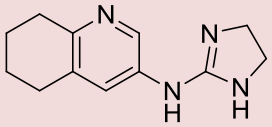
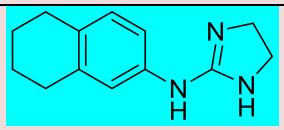
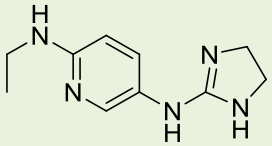
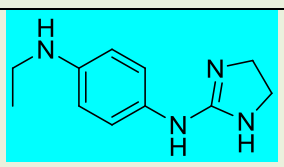
12. Computational pharmacokinetic parameters

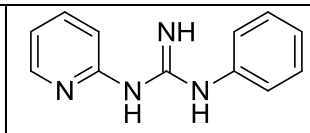
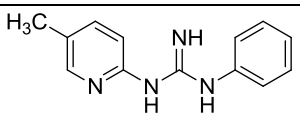
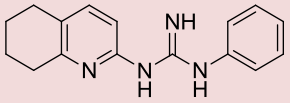
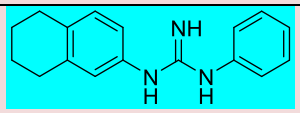
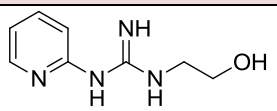
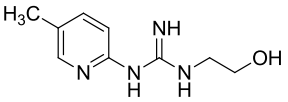
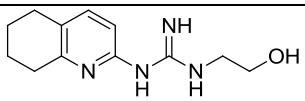
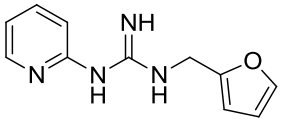
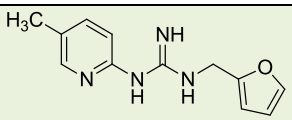
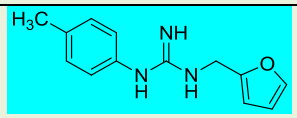
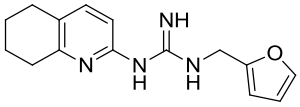
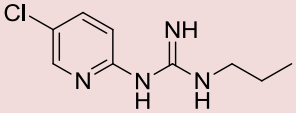
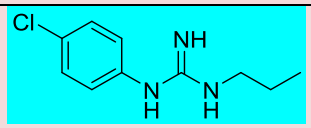
According to different authors and different databases[7] CNS drugs already in the market show the following physicochemical characteristics: MW less than 400 with a mean value of 310 g mol^{-1}, (c)logP less than 5 with a preferred value around 1.5-2.7, 2.5 or 3.43 (depending on the authors), (c)log$D_{7.4}$ greater than 0 and less than 3 (optimum value 2.1), total PSA in the range 40-90 $Å^2$ and pK_{aH} between 7.5–10.5.

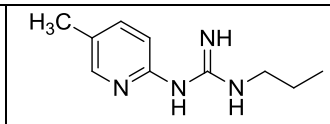
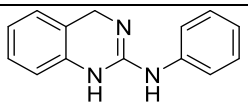
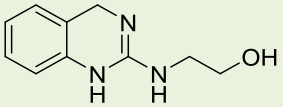
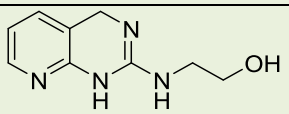
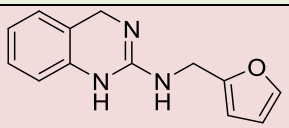
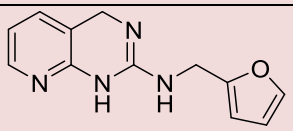
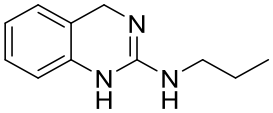
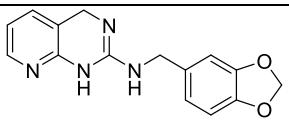
Table S3. Calculated physicochemical properties [Molecular weight (MW), total polar surface area (PSA), Partition coefficient (logP), Distribution coefficient (logD) and basicity (pK_{aH})].of all the compounds studied (and some benzene analogues highlighted in blue, for comparison) obtained from MarvinSketch. Counterions were not considered. Italicised values are within the desired range for CNS-acting drugs.

Comp.	Structure	MW	PSA ($Å^2$)	logP	logD (pH 7.40)	pK_{aH}
5c		*137.17*	*76.5*	0.3	-1.6	*9.5*
		*135.17*	*61.9*	0.9	-1.4	**11.5**
11c		*137.17*	*76.5*	-0.3	-2.5	*10.1*
6c		*216.06*	*76.5*	1.1	-0.4	*9.0*
7c		*171.61*	*76.5*	0.9	-0.6	*9.0*
		*169.61*	*61.9*	***1.5***	-0.7	**10.9**

12c		*171.61*	*76.5*	0.6	-1.5	*9.6*
8c		*151.19*	*76.5*	0.8	-1.1	*9.5*
9c		*191.26*	*76.5*	*1.7*	-0.2	*9.3*
		*189.26*	*61.9*	*2.4*	***0.1***	**10.6**
14c		*191.26*	*76.5*	1.1	-1.1	*9.9*
10c		*180.23*	*88.6*	0.2	-1.9	*9.7*
		*178.23*	*73.9*	0.8	-1.6	**10.9**
15c		*180.23*	*88.6*	0.2	-2.1	*10.3*
13c		*151.19*	*76.5*	-0.1	-2.4	*10.1*
17c		*182.16*	119.7	0.3	-0.6	*8.2*
18c		*152.18*	102.5	-0.5	-2.6	*9.8*

5d		*163.20*	50.9	0.7	-0.7	*8.7*
		*161.20*	**36.4**	1.3	-1.0	*10.1*
7d		*197.65*	50.9	1.3	*0.4*	*8.2*
8d		*177.23*	50.9	1.2	-0.1	*8.7*
9d		*217.30*	*50.9*	*2.0*	*0.9*	*8.5*
10d		*206.27*	*63.0*	0.5	-0.9	*8.8*
11d		*163.20*	*50.9*	0.1	-1.8	*9.3*
14d		*217.30*	*50.9*	1.4	-0.2	*9.1*
		*215.29*	36.4	***2.7***	***0.7***	*9.7*
15d		*206.27*	*63.0*	0.5	-1.4	*9.4*
		*204.27*	*48.5*	1.1	-1.1	*10.1*

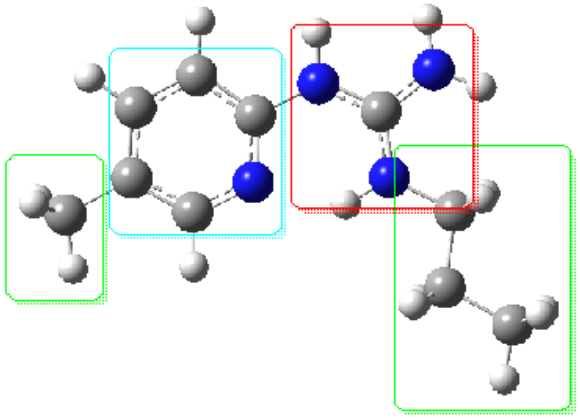
5i		*213.26*	*62.5*	*2.5*	*1.8*	*8.7*
8i		*227.29*	*62.5*	*3.0*	*2.3*	*8.6*
9i		*267.36*	*62.5*	*3.8*	*3.3*	*8.5*
		*265.35*	*47.9*	**4.6**	*3.0*	*9.1*
5j		*181.22*	*82.8*	-0.1	-2.0	*9.0*
8j		*195.25*	*82.8*	0.4	-1.5	*9.0*
9j		*235.31*	*82.8*	1.2	-0.5	*8.8*
5k		*217.25*	*75.7*	1.4	-0.2	*8.6*
8k		*231.28*	*75.7*	*1.9*	*0.3*	*8.6*
		*229.28*	*61.1*	*2.5*	*0.2*	*10.3*
9k		*271.34*	*75.7*	*2.7*	*1.3*	*8.4*
7l		*213.69*	*62.5*	*2.1*	*0.3*	*8.8*
		*211.69*	*47.9*	*2.7*	*0.4*	**10.6**

8l		*193.27*	*62.5*	*2.0*	-0.1	*9.4*
19i		*224.29*	38.0	*3.1*	*2.1*	*8.4*
19j		*192.24*	58.3	0.5	-1.4	*9.5*
20j		*193.23*	*71.2*	-0.1	-0.9	*8.2*
19k		*228.27*	51.2	*2.0*	*0.2*	*9.3*
20k		*228.26*	*62.5*	1.4	*0.7*	*9.1*
19l		*190.27*	38.0	*2.1*	-0.2	*10.2*
20m		*283.31*	*69.4*	*2.3*	*1.0*	*8.3*

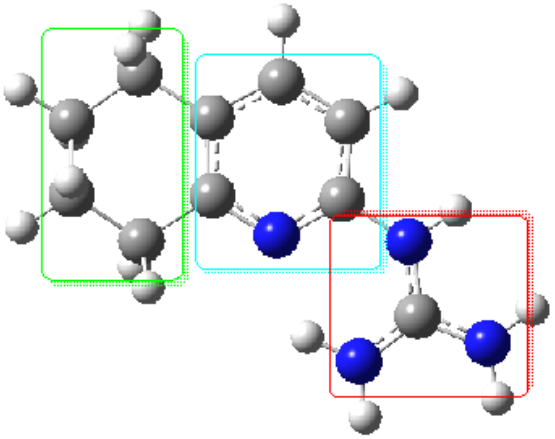
All of our compounds have molecular weights below 285 g mol^{-1} (average MW = 198.7 g mol^{-1}), average ClogP around 1.2 (only one compound with a value > 3.1 and six compounds with values < 0.2) and $logD_{(7.4)}$ values < 3.2, making them suitable for CNS penetration The majority of our compounds are within the desired range of total PSA (only two exceptions with values ~100-120), while the pK_{aH} limits of 7.5-10.5 are obeyed by all compounds (the average value being 9.1). These molecules do not contain acidic protons, an undesirable feature that leads to high plasma protein binding and low brain penetration, and are protonated at physiological pH.

We have also calculated the same properties for the benzene analogues of a selection of the compounds studied (highlighted in blue in Table S3). In all the cases MW and PSA are very similar. Regarding lipophilicity (logP and logD) in most of the cases does not make any substantial difference and only in a couple of cases the benzene derivatives have better lipophilicity (highlighted in green) for CNS absorption while in another cases the increment in lipophilicity is detrimental (highlighted in yellow). The biggest difference observed between both series is in terms of basicity. The pK_a of the benzene analogues is around one unit larger than that of the pyridine compounds, that means that the benzene analogues are more basic and this can be detrimental (highlighted in yellow) for CNS absorption since the acceptable rage is 7.5-10.5.

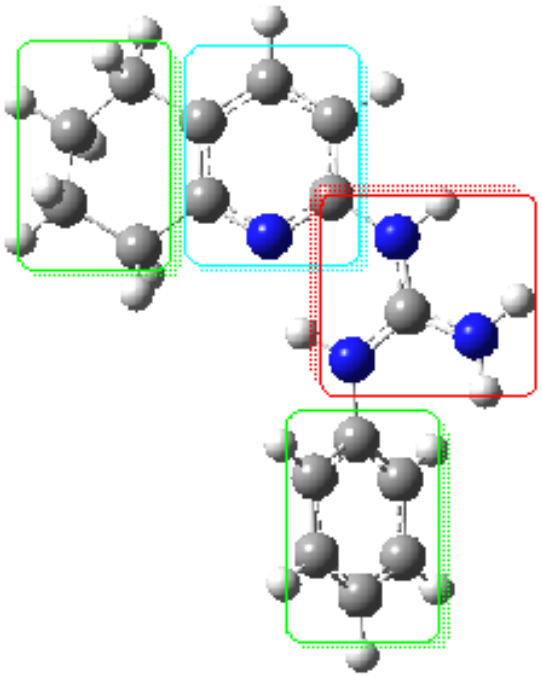
Activation of hERG is the responsible of secondary cardiac effects of many potential drugs. Recently, a ligand-based pharmacophore for the activation of hERG channels has been developed (and experimentally validated) using the Catalyst software;[8] in order to evaluate if our compounds fulfil such a pharmacophore, and hence produce cardiopathies, we have computationally optimised (DFT level: B3LYP/6-31+G*, PCM-water) four of them (**8l**, **9c**, **9i** and **14d**). The optimised structures indicating the pharmacophoric elements common to the Catalyst pharmacophore developed elsewhere, as well as the Catalyst pharmacophore are shown in Figure S2.



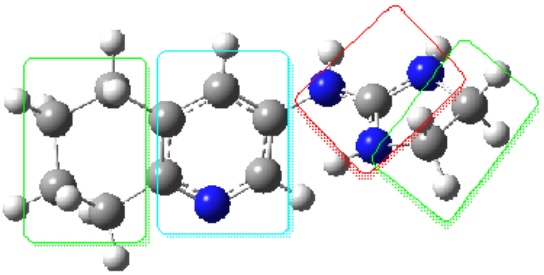
8l (pKi= 6.74)



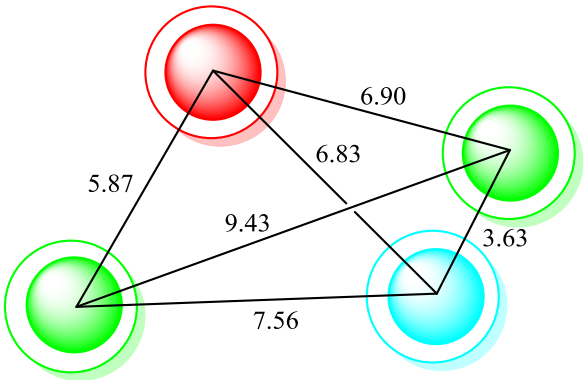
9c (pKi= 6.78)



9i (pKi= 6.75)



14d (pKi= 7.02)



Catalyst pharmacophore developed by Kratz et al.

Figure S2.- Optimised structures calculated at B3LYP/631+G* PCM(water) and Catalyst pharmacophore developed by Kratz et al.

The four Catalyst pharmacophoric elements of Kratz *et al.* are: a positively ionisable group, two hydrophobic groups and a hydrophobic aromatic group. We found that compound **9c** does not present one of the two hydrophobic groups and even though compounds **8l**, **9i** and **14d** present all four pharmacophoric elements, the distances between these elements are not those of the Catalyst pharmacophore. Hence, these compounds do not fulfil the pharmacophore, would not be able to block the hERG channel and, in principle, would not show cardiotoxicity.

Table S4. Distances (Å) between the pharmacophoric elements of the Catalyst pharmacophore developed by Kratz and those found for our compounds **8l**, **9c**, **9i** and **14d**. In italics/bold are those distances that do NOT fulfil the Catalyst pharmacophore (considering a margin of ±0.9 Å).

	Catalyst Pharm.	**8l**	**9c**	**9i**	**14d**
Positively ionisable -Hydrophobic(1)	6.90	[Me] 6.61 (C+)	6.58-7.14 (C+)	[$(CH_2)_4$] 6.57-7.13 (C+)	[$(CH_2)_4$] 6.54-7.21 (C+)
Positively ionisable -Hydrophobic(2)	5.87	[Pr] 5.00 (C+)	-	[Ph] ***3.81 (C+)***	[$Im(CH_2)_2$] ***2.31 (C+)***
Positively ionisable -Hydrophobic Ar	6.83	***3.76 (C+)***	***3.89 (C+)***	***3.89 (C+)***	***3.75 (C+)***
Hydrophobic (1) - Hydrophobic Ar	3.63	[Me] 2.97	3.75	[$(CH_2)_4$] 3.70	[$(CH_2)_4$] 3.78
Hydrophobic (2) - Hydrophobic Ar	7.56	[Pr] 7.31	-	[Ph] 6.73	[$Im(CH_2)_2$] ***5.23-5.84***
Hydrophobic (1) - Hydrophobic (2)	9.43	9.16	-	***7.85-8.90***	8.64-9.40

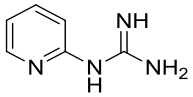
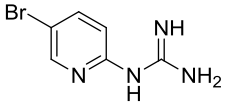
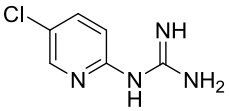
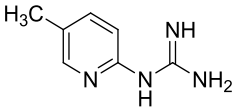
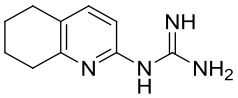
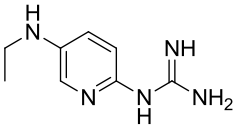
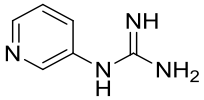
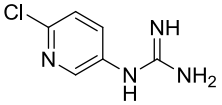
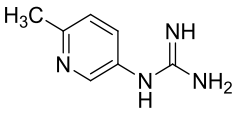
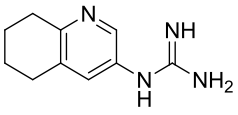
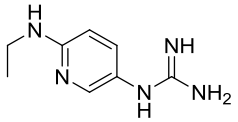
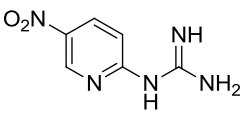
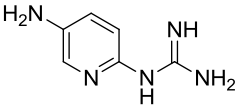
13. Molecular Modelling

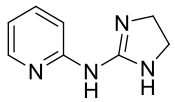
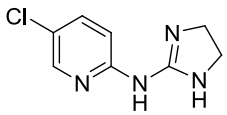
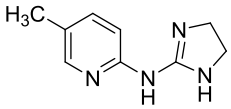
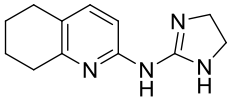
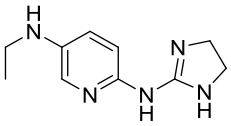
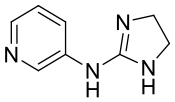
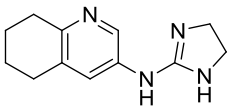
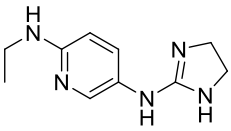
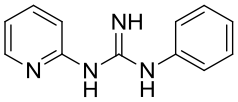
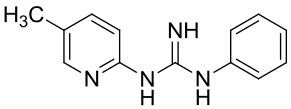
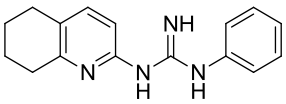
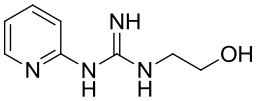
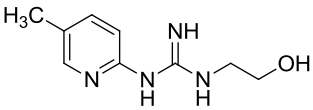
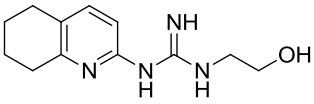
The sequences of the human α_{2A}-AR (P18825) and α_{2A}-AR (P08913) were obtained from the uniprot database. The Modeller V9.12 software was used to generate five most probable structures based on three templates of the homologous β_2-AR (2R4S[Error! Bookmark not defined.] 3D4S[Error! Bookmark not defined.] and 3SN6[Error! Bookmark not defined.]). The sequence homology for the α_{2A}-AR was 38.9%, while for the α_{2C}-AR it was 35.2%. Comparing their DOPE (Discrete optimized protein energy) score and GA431 score, the most suitable model was selected. This model was also validated by its Ramachandran plot to ensure no highly unfavoured arrangements existed. Then, the model was solvated in explicit TIP3P water in the AMBER software[Error! Bookmark not defined.] and further refined by a three-step minimisation procedure: Initially all ions and solvent molecules were relaxed with the protein constrained, then the solvent, ions and amino-acid side-chains were relaxed, and finally the entire system was minimized to give the structure which was used for docking simulations using the MOE.2010 software.[Error! Bookmark not defined.] The 3SN6 crystal structure was chosen to identify the ligand binding site applied for docking as it contains an agonist in its orthosteric site which has activated the GPCR (amino acids within 4.5 Å were included in the site).

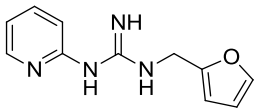
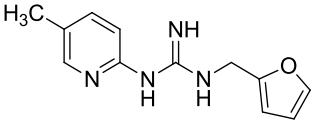
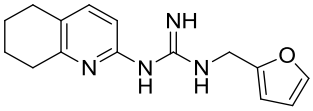
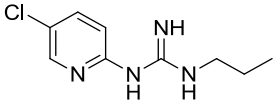
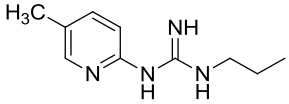
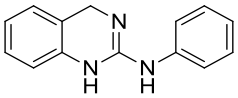
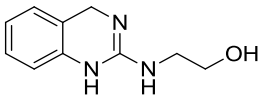
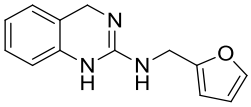
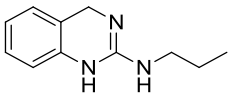
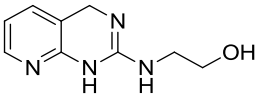
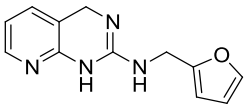
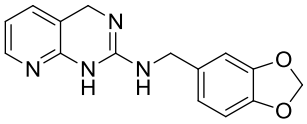
The ligands were built in MOE and minimized using the CHARMM27 force field with a 0.05 gradient. A full conformational search was conducted using the LowModeMD[9] method with a RMS gradient of 0.005, a strain cut-off of 10 kcal mol^{-1} and a minimum of 100 iterations, to generate approximately 60 conformations per ligand. The generated conformers were docked into the relevant receptors in MOE using the triangle matcher placement method and the London dG scoring function.[30] A post placement molecular mechanics forcefield refinement was carried out on the top 30 poses in which side chains of the protein were free to move and a non-interacting cut-off of 12 Å was applied. The final docking energy (E-refine) was calculated using the GB/VI solvent model.[10]

Table S5 shows the docking scores for all compounds in the α_{2A}-AR and α_{2C}-AR models, as well as their experimental binding affinity expressed as pK_i. The interactions established to form the complexes between the compounds studied and the respective binding sites illustrate the likely requirements for interacting at these receptors with high affinity.

Table S5. Compounds examined by molecular docking in homology models of the α_{2A}-AR and α_{2C}-AR, with their pK_i values and docking scores (kcal mol^{-1}).

Comp.	Structure	pK_i	S α_{2A}-AR (kcal mol^{-1})	S α_{2C}-AR (kcal mol^{-1})
5c		6.19	-6.81	-7.23
6c		5.62	-7.31	-7.75
7c		5.70	-6.94	-7.40
8c		6.03	-7.13	-7.57
9c		6.78	-7.15	-8.86
10c		4.12	-7.39	-8.58
11c		3.79	-6.84	-7.07
12c		5.18	-7.30	-7.33
13c		4.97	-7.66	-7.45
14c		5.57	-7.11	-8.27
15c		6.35	-7.62	-8.22
17c		5.00	-6.84	-8.13
18c		5.00	-6.55	-7.41

5d		6.44	-7.11	-7.85
7d		6.25	-7.10	-8.04
8d		6.41	-7.17	-8.24
9d		6.27	-8.02	-9.27
10d		5.65	-7.99	-8.66
11d		5.28	-6.69	-7.82
14d		7.02	-8.03	-9.43
15d		7.13	-8.04	-8.73
5i		6.21	-8.08	-9.32
8i		6.02	-8.34	-9.80
9i		6.75	-9.04	-10.31
5j		5.38	-7.60	-8.22
8j		5.21	-7.62	-8.91
9j		5.83	-7.98	-10.06

5k		6.32	-7.91	-9.22
8k		6.28	-8.52	-9.80
9k		6.67	-9.15	-9.91
7l		5.71	-7.88	-8.88
8l		6.74	-7.85	-9.65
19i		4.40	-8.04	-9.36
19j		6.26	-7.06	-8.63
19k		5.35	-8.41	-9.38
19l		4.33	-7.21	-8.76
20j		4.49	-7.60	-8.63
20k		4.50	-8.44	-9.51
20m		5.30	-9.25	-9.60

Homology model

>sp|**P08913**|ADA2A_HUMAN Alpha-2A adrenergic receptor OS=Homo sapiens GN=ADRA2A PE=1 SV=3

MGSLQPDAGNASWNGTEAPGGGARATPYSLQVTLTLVCLAGLLMLLTVFGNVLVII
AVFTSRALKAPQNLFLVSLASADILVATLVIPFSLANEVMGYWYFGKAWCEIYLALD
VLFCTSSIVHLCAISLDRYWSITQAIEYNLKRTPRRIKAIIITVWVISAVISFPPLISIEKK
GGGGGPQPAEPRCEINDQKWYVISSCIGSFFAPCLIMILVYVRIYQIAKRRTRVPPSRR
GPDAVAAPPGGTERRPNGLGPERSAGPGGAEAEPLPTQLNGAPGEPAPAGPRDTDAL
DLEESSSSDHAERPPGPRRPERGPRGKGKARASQVKPGDSLPRRGPGATGIGTPAAGP
GEERVGAAKASRWRGRQNREKRFTFVLAVVIGVFVVCWFPFFFTYTLTAVGCSVPR
TLFKFFFWFGYCNSSLNPVIYTIFNHDFRRAFKKILCRGDRKRIV

>sp|**P18825**|ADA2C_HUMAN Alpha-2C adrenergic receptor OS=Homo sapiens GN=ADRA2C PE=2 SV=2

MASPALAAALAVAAAAGPNASGAGERGSGGVANASGASWGPPRGQYSAGAVAGL
AAVVGFLIVFTVVGNVLVVIAVLTSRALRAPQNLFLVSLASADILVATLVMPFSLANE
LMAYWYFGQVWCGVYLALDVLFCTSSIVHLCAISLDRYWSVTQAVEYNLKRTPRR
VKATIVAVWLISAVISFPPLVSLYRQPDGAAYPQCGLNDETWYILSSCIGSFFAPCLIM
GLVYARIYRVAKLRTRTLSEKRAPVGPDGASPTTENGLGAAAGAGENGHCAPPPAD
VEPDESSAAAERRRRRGALRRGGRRRAGAEGGAGGADGQGAGPGAAESGALTASR
SPGPGGRLSRASSRSVEFFLSRRRRARSSVCRRKVAQAREKRFTFVLAVVMGVFVLC
WFPFFFSYSLYGICREACQVPGPLFKFFFWIGYCNSSLNPVIYTVFNQDFRRSFKHILF
RRRRRGFRQ

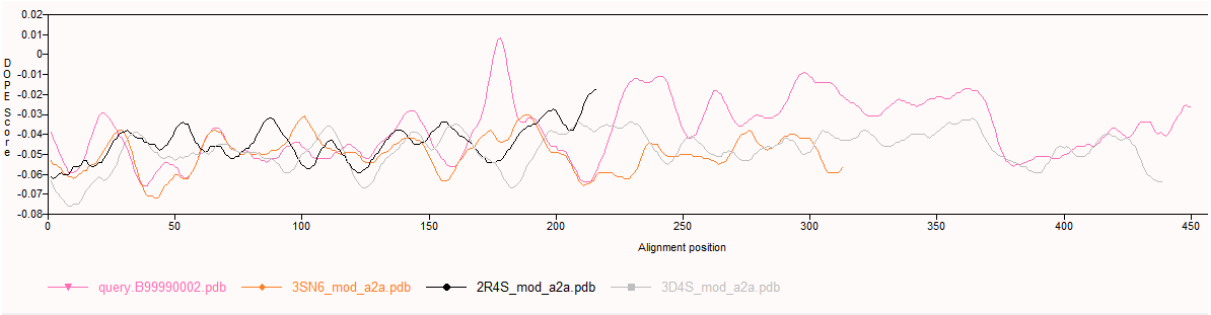
Models generated by Modeller:

Alpha 2a	**molpdf**	**DOPE Score**	**GA431 Score**
query.B99990001.pdb	11807.35	-46242.20	1.00
query.B99990002.pdb	**11759.67**	**-46738.02**	**1.00**
query.B99990003.pdb	12039.37	-46161.49	1.00
query.B99990004.pdb	11827.11	-46195.85	1.00
query.B99990005.pdb	11823.14	-46350.15	1.00
Seq ID	38.89%		

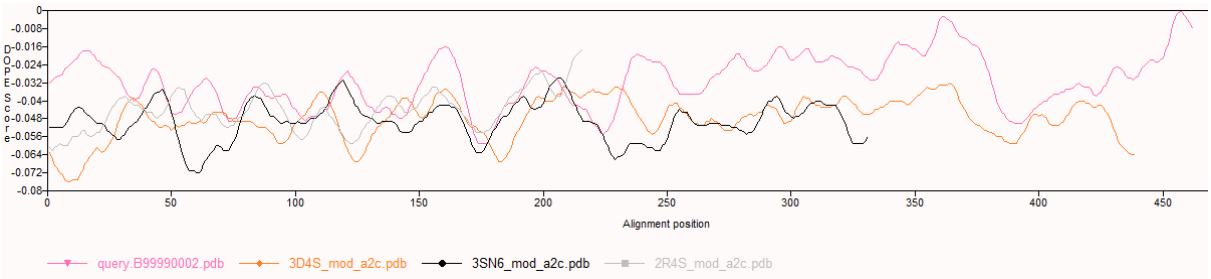
Alpha 2c	**molpdf**	**DOPE Score**	**GA431 Score**

query.B99990001.pdb	17689.31	-42877.41	0.36
query.B99990002.pdb	**17731.83**	**-43870.66**	**0.51**
query.B99990003.pdb	18312.22	-43908.57	0.25
query.B99990004.pdb	18245.95	-42806.20	0.44
query.B99990005.pdb	18349.35	-43115.01	0.44
Seq ID	35.19%		

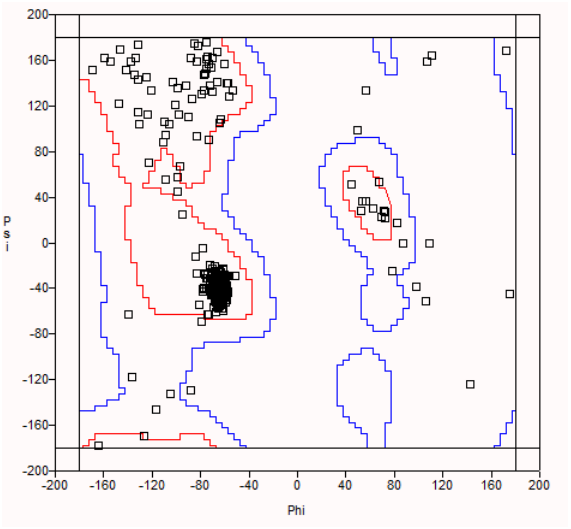
DOPE profile of **query.B99990002.pdb of the α_{2A}-AR overlaid with that of templates.**



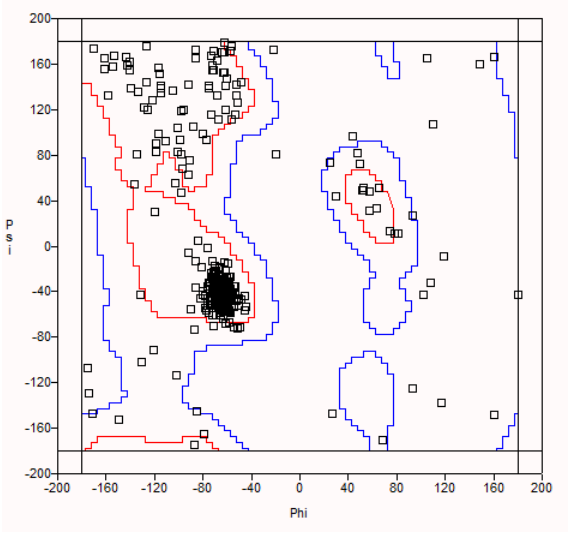
DOPE profile of **query.B99990002.pdb of the α_{2C}-AR overlaid with that of templates.**



Ramachandran plot of **query.B99990002.pdb of the α_{2A}-AR.**



Ramachandran plot of **query.B99990002.pdb of the α_{2A}-AR.**



Docking to α_{2C}-AR and α_{2A}-AR

Binding site identification:

Using the 3SN6 crystal structure and the site view tool in MOE, the ligand "site" amino acids were idenitfied. This was extrapolated to the homology model by aligning the homology models with 3SN6. Residues with identical homology are highlighted green.

3SN6	**α_{2A}-AR model**
W 239	**Y** 109
T 240	**L** 110

D 243	**D** 113
V 244	**V** 114
V 247	**C** 117
T 248	**T** 118
C 318	**C** 188
D 319	**E** 189
F 320	**I** 190
Y 326	**Y** 196
A 327	**V** 197
S 330	**S** 200
S 331	**C** 201
S 334	**S** 204
W 388	**W** 387
F 391	**F** 390
F 392	**F** 391
N 395	**Y** 394
K 407	**R** 405
Y 410	**F** 408
I 411	**K** 409
N 414	**F** 412
Y 418	**Y** 416

The corresponding amino acids were then used to define the site for docking of compounds into the homology model of the α_{2A}-AR.

The same strategy was employed for the docking of ligands into the α_{2C}-AR.

3SN6	**α_{2C}-AR model**
W 239	-
T 240	**L** 128
D 243	**D** 131
V 244	**V** 132
V 247	**C** 135

T 248	**T** 136
C 318	**C** 202
D 319	**G** 203
F 320	**L** 204
Y 326	**Y** 210
A 327	**I** 211
S 330	**S** 214
S 331	**C** 215
S 334	**S** 218
W 388	**W** 395
F 391	**F** 398
F 392	**F** 399
N 395	**Y** 402
K 407	**G** 416
Y 410	**F** 419
I 411	**K** 420
N 414	**F** 423
Y 418	**Y** 427

There is 57.3% identity between the sequences of the α_{2A}-AR and the α_{2C}-AR.

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