Supporting information for

Synthesis of C6-Azolyl Purine Nucleosides via C-N Coupling Reaction of Unprotected 6-Chloropurine Nucleosides and N-Heterocycles under Catalyst- and Solvent-Free Condition

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I. General

Melting points were recorded with a micro melting point apparatus and uncorrected. NMR spectra were recorded with a 400 NMR spectrometer for ^{1}H-NMR, 100 MHz for ^{13}C-NMR. Chemical shifts δ are given in ppm relative to tetramethylsilane in $CDCl_3$ or to the residual proton signals of the deuterated solvent DMSO-d_6 for ^{1}H and ^{13}C NMR. High resolution mass spectra were taken with a 3000 mass spectrometer, using Waters Q-TofMS/MS system. For column chromatography 200-300 mesh silica gel (GF254) was used as the stationary phase. All reactions were monitored by thin layer chromatography (TLC). All regents and solvents were purchased from commercial sources and purified commonly before used.

II. Typical Experimental Procedure

Typical Experimental Procedure for the Reaction of Unprotected 6-Chloropurine Nucleosides with Various N-Nucleophiles

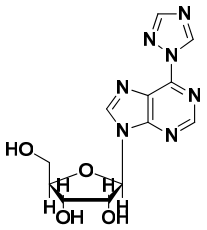
6-Chloropurine nucleosides **1** (0.2 mmol) and N-nucleophiles **2** (0.26 mmol, 1.3 eq) were added to a 5 mL round bottom flask. Then the mixture was stirred at 120 ^{o}C for 45 minutes in an oil bath. After cooling to room temperature, the resulting mixture was dissolved with methanol (2.0 mL) and evaporated in vacuo. The residue was purified by silica gel chromatography (petroleum ether ethyl acetate) to give the desired products **3**.

Typical Experimental Procedure for the Reaction of 1*H*-1,2,4-triazol with Various 6-Chloropurines

6-Chloropurine **1** (0.2 mmol) and 1*H*-1,2,4-triazol **2a** (0.26 mmol, 1.3 eq) were added to a 5 mL round bottom flask . Then the mixture was stirred at 120 ^{o}C for 45 minutes in an oil bath. After cooling to room temperature, the resulting mixture was dissolved with methanol (2.0 mL) and evaporated in vacuo. The residue was purified by silica gel chromatography (petroleum ether ethyl acetate) to give the desired products **4**.

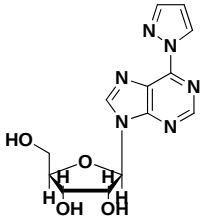
III. Characterization of Compounds

6-(1,2,4-Triazol-1-yl)-9-(*β*-D-ribofuranosyl)purine (3a)



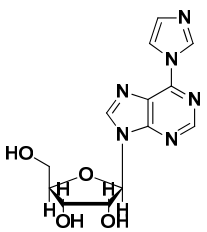
White powder. M.p. 70-72 °C. ^{1}H NMR (DMSO-d_6, 400 MHz) δ (ppm): 9.77 (s, 1H), 9.02 (s, 1H), 8.94 (s, 1H), 8.45 (s, 1H), 6.11 (d, J = 5.2 Hz, 1H), 5.67 (d, J = 3.6 Hz, 1H), 5.34 (d, J = 3.2 Hz, 1H), 5.19 (s, 1H) 4.63 (d, J = 4.8 Hz, 1H), 4.23 (d, J = 3.6 Hz, 1H), 4.02 (d, J = 4.0 Hz, 1H), 3.72 (t, J = 3.6 Hz, 1H), 3.61 (t, J = 3.6 Hz, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ (ppm) 61.4, 70.5, 74.4, 86.1, 88.4, 123.1, 144.9, 146.3, 146.5, 152.3, 153.9, 154.1. 162.0; HRMS calcd for: $C_{12}H_{13}N_7NaO_4$ $[M + Na]^+$ 342.0921, found 342.0925.

6-(1*H*-Pyrazol-1-yl)-9-(*β*-D-ribofuranosyl)purine (3b)



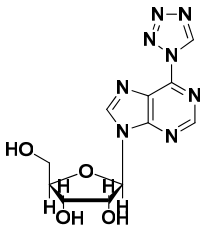
White flaky crystals. M.p. 98-100 °C. ^{1}H NMR (DMSO-d_6, 400 MHz) δ (ppm): 9.12 (q, J = 0.4 Hz, 1H）, 8.93 (s, 1H), 8.85 (s, 1H), 7.99 (s, 1H), 6.71 (s, 1H), 6.11 (d, J = 5.2 Hz, 1H), 5.62 (d, J = 5.6 Hz, 1H), 5.29 (d, J = 4.8 Hz, 1H), 5.18 (s, 1H), 4.65 (d, J = 5.2 Hz, 1H), 4.24 (d, J = 4 Hz, 1H), 4.03 (d, J = 3.6 Hz, 1H), 3.73 (m, 1H), 3.64 (m, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ (ppm) 61.6, 70.6, 74.4, 86.1, 88.3, 109.9, 122.4, 131.9, 144.3, 145.3, 146.9, 152.2, 153.9; HRMS calcd for: $C_{13}H_{14}N_6NaO_4$ $[M + Na]^+$ 341.0969, found 341.0970.

6-(1*H*-Imidazol-1-yl)-9-(*β*-D-ribofuranosyl)purine (3c)



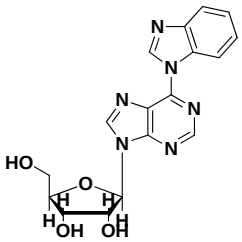
White flocculent crystals. M.p. 134-136 °C. ^{1}H NMR (DMSO-d_6, 400 MHz) δ (ppm): 9.12 (d, J = 2.8 Hz, 1H), 8.93 (s, 1H), 8.84 (s, 1H), 7.99 (s, 1H), 6.70 (d, J = 1.6 Hz, 1H), 6.12 (d, J = 5.2 Hz, 1H), 5.62 (d, J = 5.2 Hz, 1H), 5.29 (d, J = 4.0 Hz, 1H), 5.18 (s, 1H), 4.66 (d, J = 5.2 Hz, 1H), 4.26 (d, J = 4.4 Hz, 1H), 4.04 (d, J = 3.6 Hz, 1H), 3.74 (m, 1H), 3.65 (m, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ (ppm): 61.5, 70.5, 74.4, 86.1, 88.4, 117.8, 122.6, 130.9, 137.3, 145.1, 145.6, 152.4, 153.7; HRMS calcd for: $C_{13}H_{14}N_6NaO_4$ $[M + Na]^+$ 341.0969, found 341.0973.

6-(1*H*-Tetrazol-1-yl)-9-(*β*-D-ribofuranosyl)purine (3d)



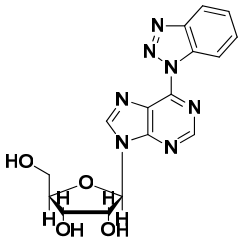
White crystals. M.p. 82-84 °C. ^{1}H NMR (DMSO-d_6, 400 MHz) δ (ppm): 10.41 (s, 1H), 9.12 (s, 1H), 9.07 (s, 1H), 6.14 (d, J = 5.2 Hz, 1H), 5.64 (s, 1H), 5.30 (s, 1H), 5.14 (s, 1H), 4.64 (s, 1H), 4.23 (s, 1H), 4.03 (d, J = 3.6 Hz, 1H), 3.74 (d, J = 11.6 Hz, 1H), 3.62 (d, J = 11.6 Hz, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ (ppm): 61.4, 70.5, 74.5, 86.2, 88.6, 123.8, 142.6. 144.4, 147.4, 152.3, 154.6; HRMS calcd for: $C_{11}H_{12}N_8NaO_4$ $[M + Na]^+$ 343.0874, found 343.0882.

6-(1*H*-Benzo[*d*]imidazol-1-yl)-9-(*β*-D-ribofuranosyl)purine (3e)



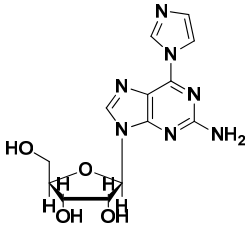
White powder. M.p. 168-170 °C. ^{1}H NMR (DMSO-d_6, 400 MHz) δ (ppm) 9.73 (s, 1H), 8.97 (s. 1H), 8.92 (s, 1H), 8.68 (d, J = 7.6 Hz, 1H), 7.78 (d, J = 7.2 Hz, 1H), 7.39 (t, J = 8.0 Hz, 2H), 6.15 (d, J = 4.8 Hz, 1H), 5.61 (s, 1H), 5.28 (s, 1H), 5.16 (s, 1H), 4.69 (d, J = 4.8 Hz, 1H), 4.28 (d, J = 4.0 Hz, 1H), 4.06 (d, J = 3.6 Hz, 1H), 3.77 (m, 1H), 3.66 (m, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ (ppm): 61.5, 70.6, 74.5, 86.2, 88.5, 170.0, 117.7, 122.1, 122.6, 130.8, 135.6, 137.3, 145.1, 145.5, 152.3, 153.8; HRMS calcd for: $C_{17}H_{16}N_6NaO_4$ $[M + Na]^+$ 391.1125, found 391.1133.

6-(1*H*-1,2,3-Benzo[*d*]triazole-1-yl)-9-(*β*-D-ribofuranosyl) purine (3f)



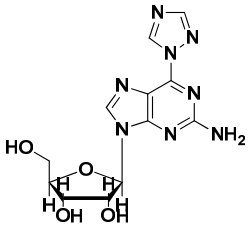
White powder. M.p. 215-217 ^{o}C. ^{1}H NMR (DMSO-d_6, 400 MHz) δ (ppm): 9.04 (s, 1H), 9.02 (s, 1H), 8.55 (d, J = 8.4 Hz, 1H), 8.23 (d, J = 8.0 Hz, 1H), 7.72 (t, J = 7.2 Hz, 1H), 7.56 (t, J = 7.6 Hz, 1H), 6.19 (d, J = 4.8 Hz, 1H), 5.59 (s, 1H), 5.25 (s, 1H), 5.12 (s, 1H), 4.70 (s, 1H), 4.29(s, 1H), 4.07 (d, J = 3.2 Hz 1H), 3.77 (m, 1H), 3.68 (m, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ (ppm): 61.5, 70.6, 74.6, 86.2, 88.5, 115.0, 120.1, 124.0, 126.2, 129.9, 131.9, 146.6, 146.2, 146.8, 152.0, 154.5; HRMS calcd for: $C_{16}H_{15}N_7NaO_4$ $[M + Na]^+$ 392.1078, found 392.1086.

6-(1*H*-Imidazol-1-yl)-2-amino-9-(*β*-D-ribofuranosyl)purine (3g)



Colorless block. M.p. 160-165 ^{o}C. ^{1}H NMR (DMSO-d_6, 400 MHz) δ (ppm): 8.91 (s, 1H), 8.44 (s, 1H), 8.22 (s, 1H), 7.18 (s, 1H), 6.83 (s, 2H), 5.86 (d, J = 6.0 Hz, 1H), 5.46 (d, J = 6.0 Hz, 1H), 5.16 (d, J = 4.8 Hz, 1H), 5.05 (t, J = 4.4 Hz, 1H), 4.50 (m, J = 5.2 Hz, 1H), 4.13 (d, J = 4.0 Hz, 1H), 3.91 (d, J = 4.0 Hz, 1H), 3.63 (m, 1H), 3.57 (m, 1H); ^{13}C NMR (DMSO-d_6, 100 MHz) δ (ppm): 61.1, 70.2, 73.5, 85.3, 86.5, 115.0, 117.0, 129.8, 136.4, 140.8, 145.0, 155.7, 159.8. HRMS calcd for: $C_{13}H_{16}N_7O_4$ $[M + H]^+$ 334.1258, found: 334.1256.

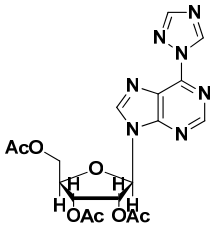
6-(1,2,4-Triazol-1-yl)-2-amino-9-(*β*-D-ribofuranosyl)purine (3h)



White powder. M.p. 188-190 ^{o}C. ^{1}H NMR (DMSO-d_6, 400 MHz) δ (ppm): 9.56 (s, 1H), 8.50 (s,

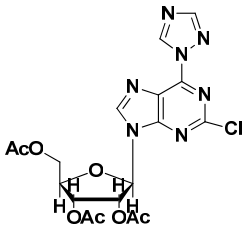
1H), 8.37 (s, 1H), 6.99 (s. 1H), 5.99 (d, *J* = 5.2 Hz, 1H), 4.53 (t, *J* = 4.8 Hz, 1H)，4.16 (t, *J* = 4.0 Hz, 1H), 3.93 (d, *J* = 3.6 Hz,1H), 3.66 (m, 1H), 3.58 (m, 1H). ^{13}C NMR (DMSO-d_6, 100 MHz) δ (ppm): 61.3, 70.4, 73.7, 85.5, 86.7, 115.6, 141.6, 145.1, 145.9, 152.9, 156.2, 160.2. HRMS calcd for: $C_{12}H_{14}N_8NaO_4$ $[M + Na]^+$ 357.1030, found: 357.1048.

6-(1,2,4-Triazol-1-yl)-9-[2,3,5-tris-*O*-(acetyl)-*β*-D-ribofuranosyl]purine (4a)



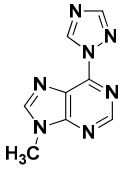
Colorless crystals. M.p. 90-92 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 9.68 (s, 1H), 8.90 (s, 1H), 8.40 (s, 1H), 8.29 (s, 1H), 8.22 (s, 1H), 6.29 (d, *J* = 5.2 Hz, 1H), 5.95 (t, *J* = 5.2 Hz, 1H), 5.65 (t, *J* = 4.8 Hz, 1H), 4.9 (t, *J* = 4.0 Hz, 1H), 4.41 (d, *J* = 4.0 Hz, 1H), 2.15 (s, 3H), 2.11 (s, 3H), 2.07 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 20.9, 21.1, 21.3, 63.5, 71.1, 73.7, 81.1, 87.4, 123.5, 144.7, 145.9, 153.1, 154.3, 154.7, 169.9, 170.1, 170.8. HRMS calcd for: $C_{18}H_{20}N_7NaO_7$ $[M + Na]^+$ 468.1238, found 468.1242.

2-Chloro-6-(1,2,4-triazol-1-yl)-9-[2,3,5-tris-*O*-(acetyl)-*β*-D-ribofuranosyl]purine (4b)



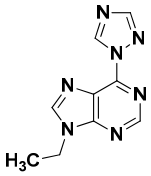
Colorless crystals. M.p. 88-90 °C. ^{1}H NMR (DMSO-d_6, 400 MHz) δ (ppm): 9.70 (s, 1H), 8.92 (s, 1H), 8.40 (s, 1H), 6.43 (d, *J* = 5.2 Hz, 1H), 6.08 (t, *J* = 5.6 Hz, 1H), 5.70 (t, *J* = 5.6 Hz, 1H), 4.50(m, 1H), 4.43 (m, 1H), 4.30 (m, 1H), 2.13 (s, 3H), 2.05 (s, 3H), 2.02 (s, 3H). ^{13}C NMR (DMSO-d_6, 100 MHz) δ (ppm): 20.5, 20.7, 20.8, 63.1, 70.4, 72.7, 80.2, 86.6, 123.1, 145.0, 146.3, 146.7, 152.4, 153.7, 153.9, 169.8, 169.9, 170.5. HRMS calcd for: $C_{18}H_{18}ClNaN_7O_7$ $[M + Na]^+$ 502.0848, found: 502.0852.

9-Methyl-6-(1*H*-1,2,4-triazol-1-yl)-9*H*-purine (4c)



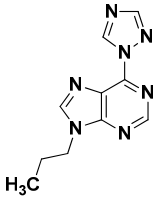
White crystals. M.p. 190-192 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 9.65 (s, 1H), 8.85 (s, 1H), 8.25 (s, 1H), 8.17 (s, 1H), 3.95 (s, 1H), ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 46.3, 120.0, 130.8, 144.9, 145.6, 152.2, 153.9; HRMS calcd for: $C_8H_8N_7$ $[M + H]^+$ 202.0836, found 202.0844.

9-Ethyl-6-(1*H*-1,2,4-triazol-1-yl)-9*H*-purine (4d)



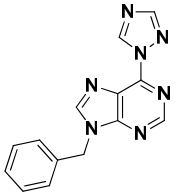
White crystals. M.p. 124-126 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 9.65 (s, 1H), 8.82 (s, 1H), 8.23 (s, 1H), 8.22 (s, 1H), 4.35 (q, J = 7.2 Hz, 2H), 1.54 (t, J = 7.6 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 15.4, 39.6, 122.4, 144.9, 145.3, 145.5, 152.1, 153.9, 154.3. HRMS calcd for: $C_9H_9N_7Na$ $[M + Na]^+$ 238.0812, found 238.0819.

9-Propyl-6-(1*H*-1,2,4-triazol-1-yl)-9*H*-purine (4e)



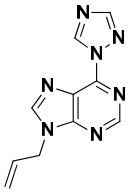
White crystals. M.p. 100-102 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 9.64 (s, 1H), 8.83 (s, 1H), 8.29 (s, 1H), 8.24 (s, 1H), 4.29 (t, J = 7.2 Hz, 2H), 1.94 (q, J = 7.2 Hz, 2H), 0.94 (t, J = 7.2 Hz, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 11.1, 23.2, 46.0, 121.8, 140.8, 144.8, 145.1, 145.9, 152.0, 153.8. HRMS calcd for: $C_{10}H_{11}N_7Na$ $[M + Na]^+$ 252.0968, found 252.0970.

9-Benzyl-6-(1*H*-1,2,4-triazol-1-yl)-9*H*-purine (4f)



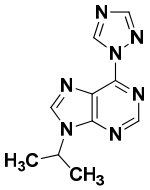
White crystals. M.p. 140-142 °C.^{1}H NMR ($CDCl_3$, 400 MHz): δ (ppm): 9.68 (s, 1H), 8.90 (s, 1H), 8.26 (s, 1H), 8.18 (s, 1H), 7.33 (m, 5H), 5.49 (s, 2H); ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 47.6, 122.0, 127.8, 128.7, 129.1, 134.4, 145.1, 152.2, 153.9, 154.2. HRMS calcd for: $C_{14}H_{12}N_7$ $[M + H]^+$ 278.1149, found 278.1158.

9-Allyl-6-(1*H*-1,2,4-triazol-1-yl)-9*H*-purine (4g)



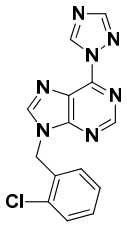
White powder. M.p. 92-94 °C. ^{1}HNMR ($CDCl_3$, 400 MHz) δ (ppm): 9.64 (s, 1H), 8.83 (s, 1H), 8.24 (s, 1H), 6.02 (m, 1H), 5.32 (d, *J* = 10 Hz, 1H), 5.22 (d, *J* = 16.8 Hz, 1H), 4.93 (d, *J* = 5.6 Hz, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 46.1, 120.0, 121.9, 130.7, 145.1, 145.6, 146.6, 152.0, 153.7, 154.1. HRMS calcd for: $C_{10}H_9N_7Na$ $[M + Na]^+$ 250.0812, found 250.0819.

9-Isopropyl-6-(1*H*-1,2,4-triazol-1-yl)-9*H*-purine (4h)



White powder. M.p. 188-190 °C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 9.66 (s, 1H), 8.83 (s, 1H), 8.28 (s, 1H), 8.24 (s, 1H), 4.97 (m, 1H), 1.65 (d, *J* = 6.8 Hz, 6H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 22.5, 48.0, 107.0, 122.4, 143.6, 144.8, 145.2, 151.7, 153.9. HRMS calcd for: $C_{10}H_{12}N_7$ $[M+H]^+$ 230.1149, found 230.1151.

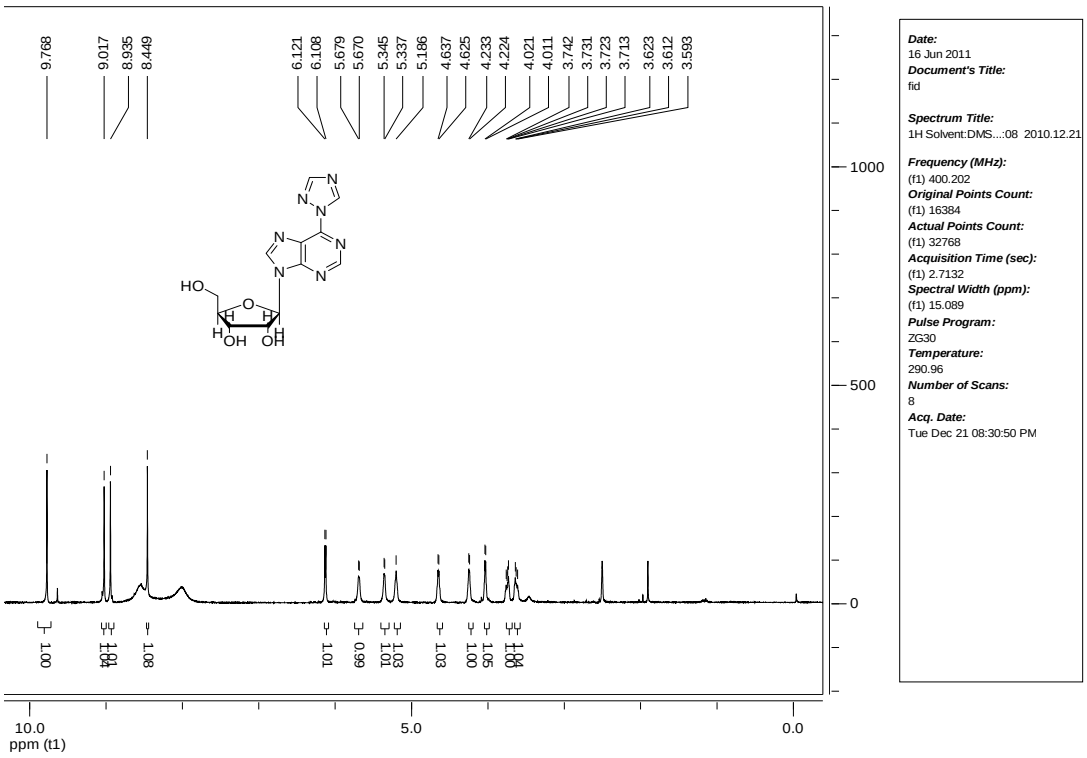
9-(2-Chlorobenzyl)-6-(1*H*-1,2,4-triazol-1-yl)-9*H*-purine (4i)



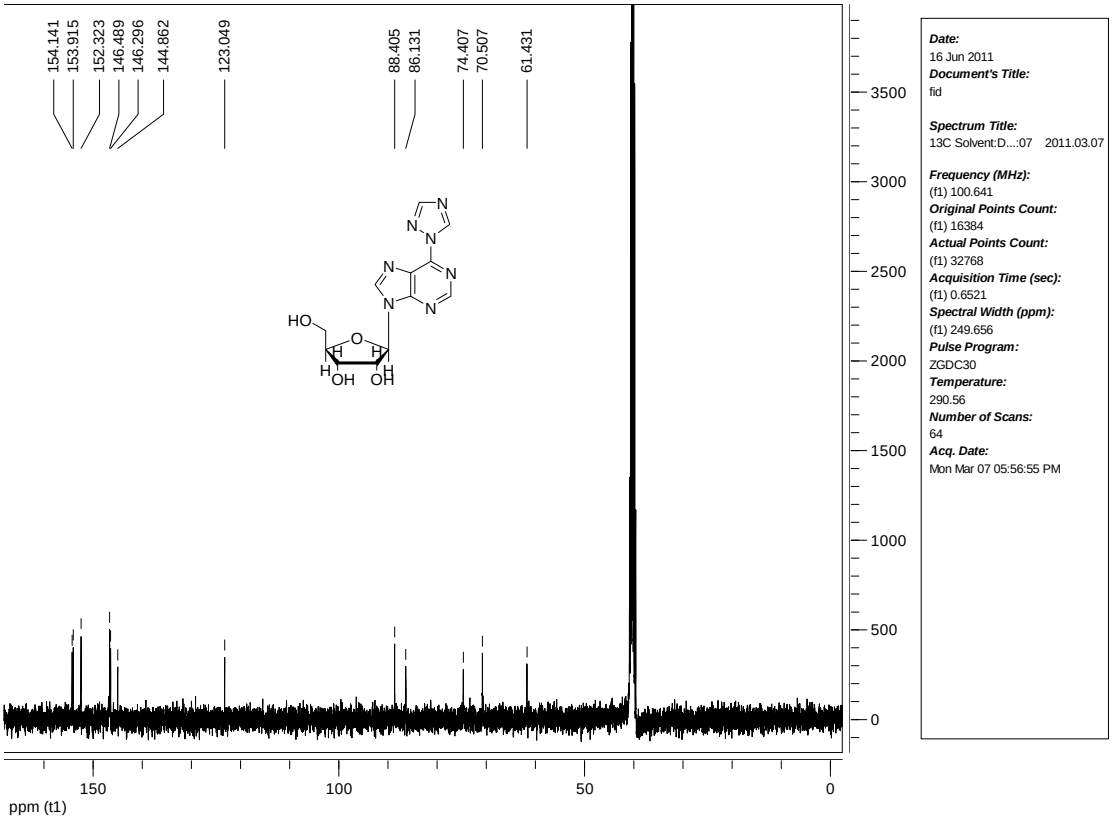
White powder. M.p. 122-124 ^{o}C. ^{1}H NMR ($CDCl_3$, 400 MHz) δ (ppm): 9.70 (s, 1H), 8.91 (s, 1H), 8.28 (s, 1H), 8.27 (s, 1H), 7.31 (m, 4H), 5.62 (s, 2H). ^{13}C NMR ($CDCl_3$, 100 MHz) δ (ppm): 45.3, 121.2, 127.4, 129.9, 130.2, 130.5, 131.9, 133.4, 144.8, 145.1, 145.6, 152.1, 153.7, 154.2. HRMS calcd for: $C_{14}H_{10}ClN_7Na$ $[M + Na]^+$ 334.0578, found: 334.0585.

IV. Copies of ^{1}H and ^{13}C NMR spectra

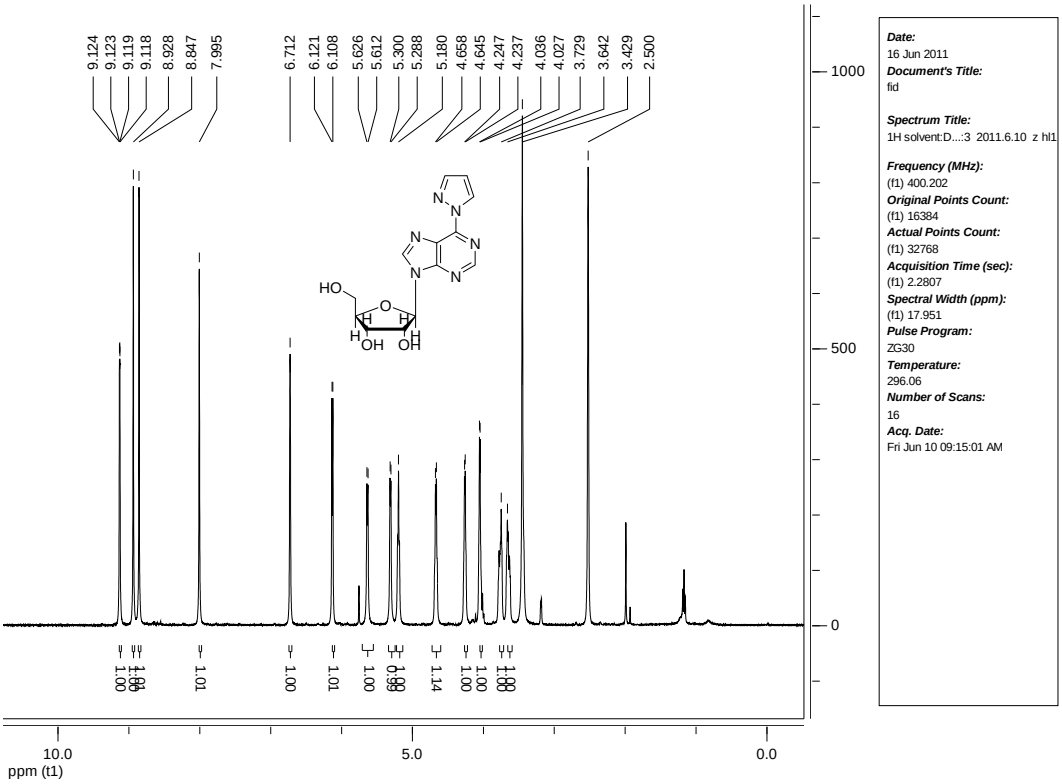
^{1}H NMR for **3a**



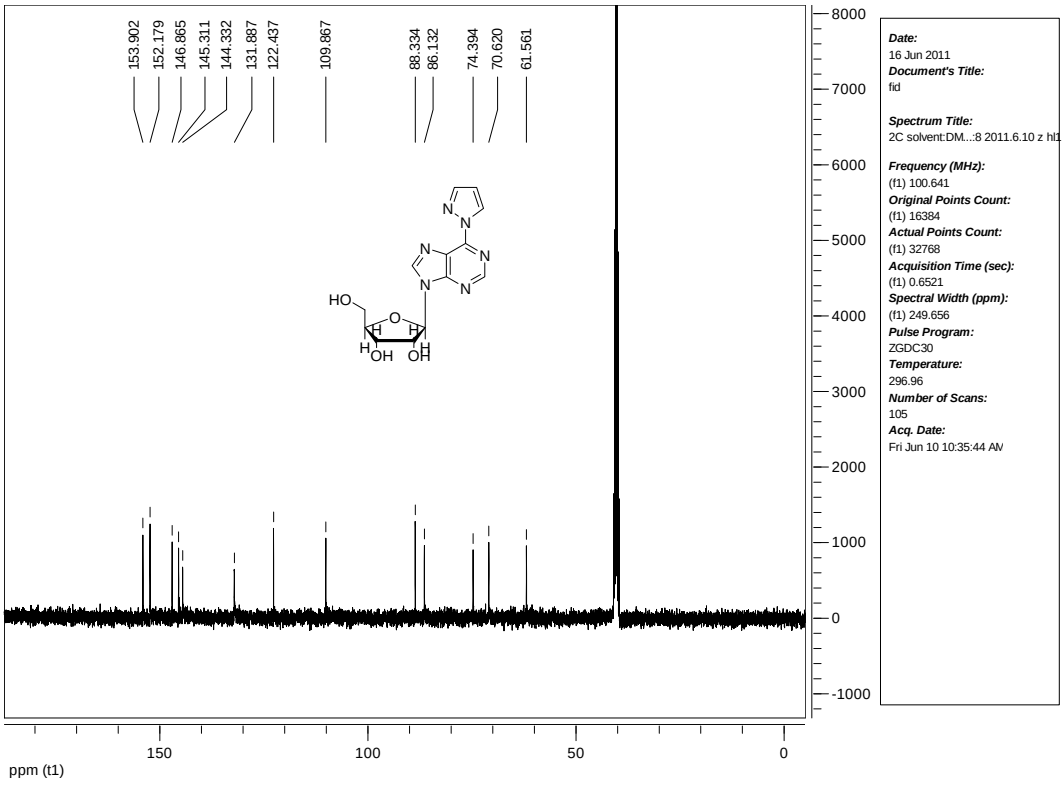
^{13}C NMR for **3a**



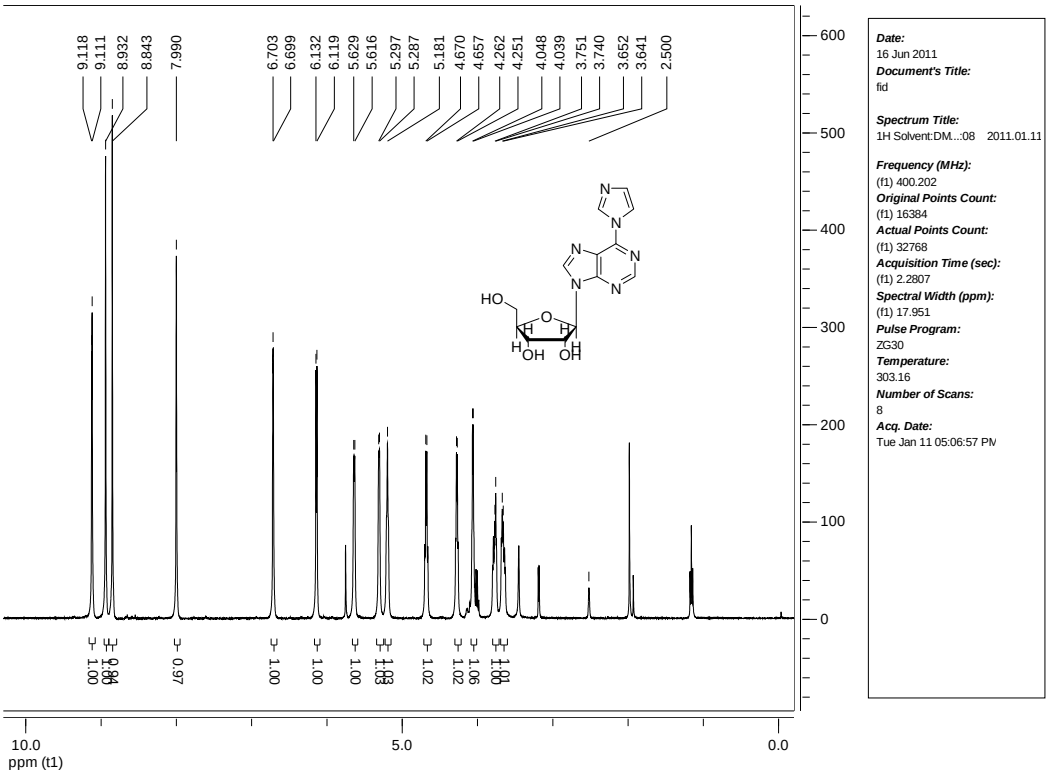
^{1}H NMR for **3b**



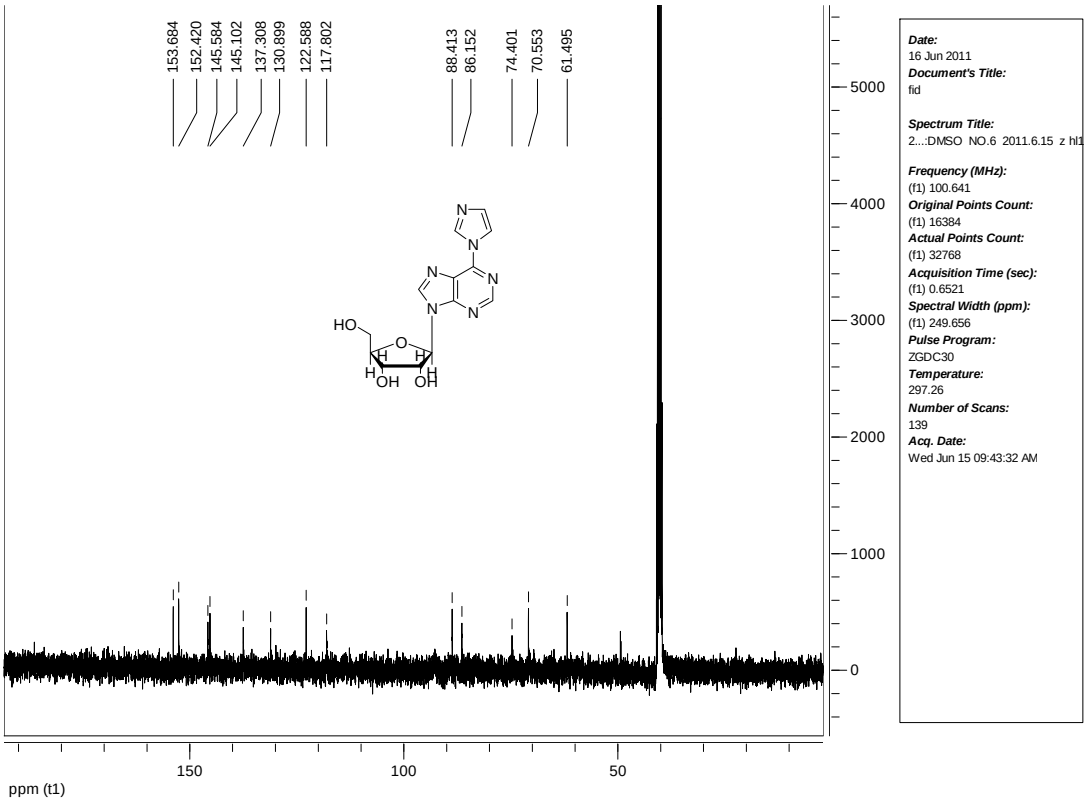
^{13}C NMR for **3b**



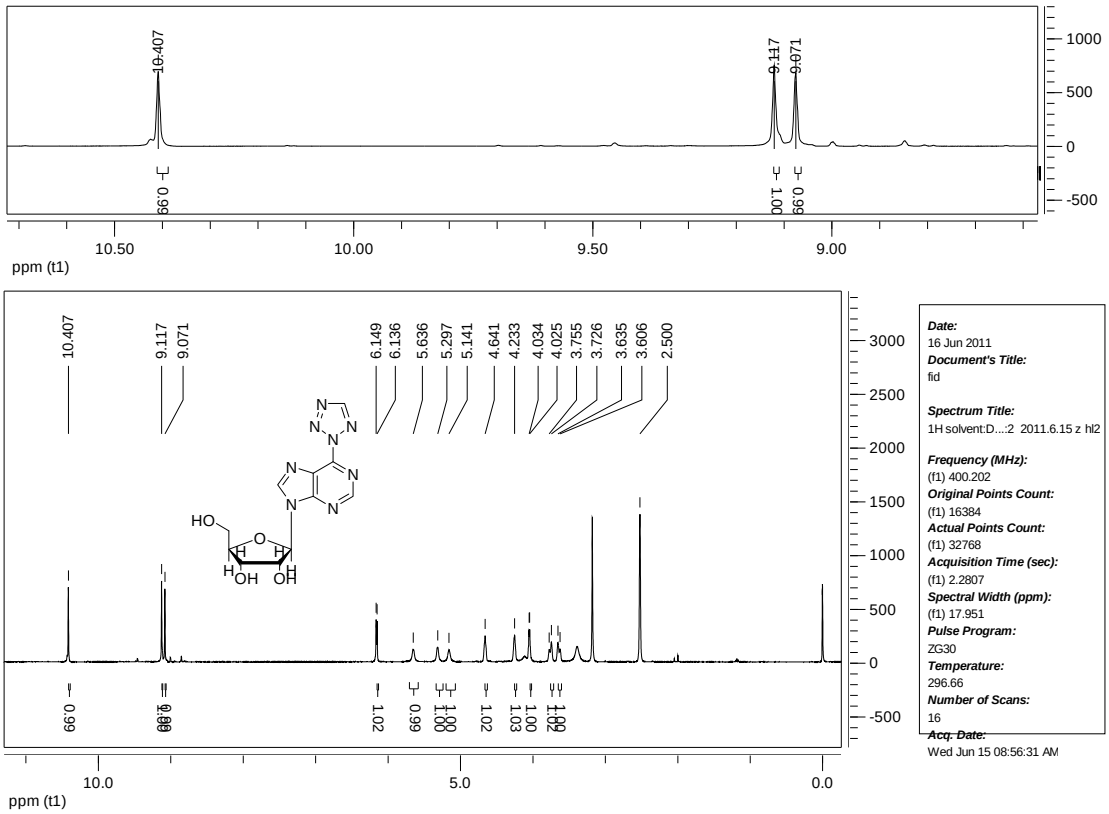
^{1}H NMR for **3c**



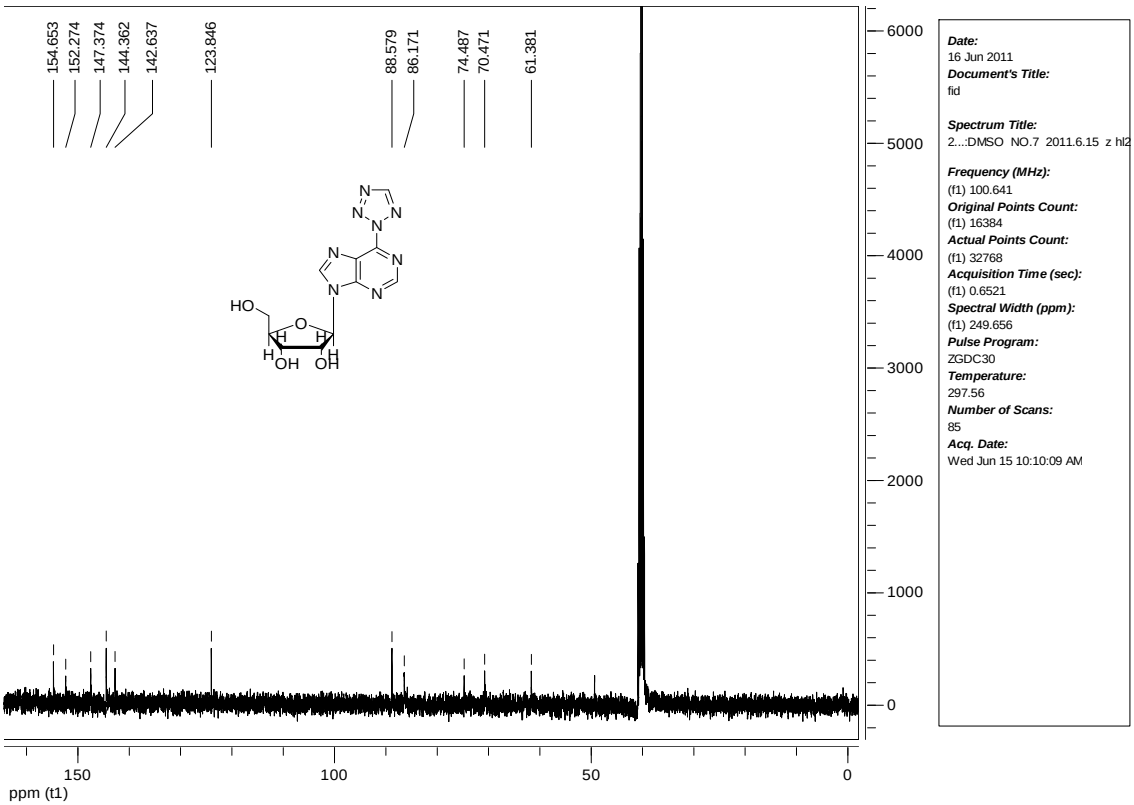
^{13}C NMR for **3c**



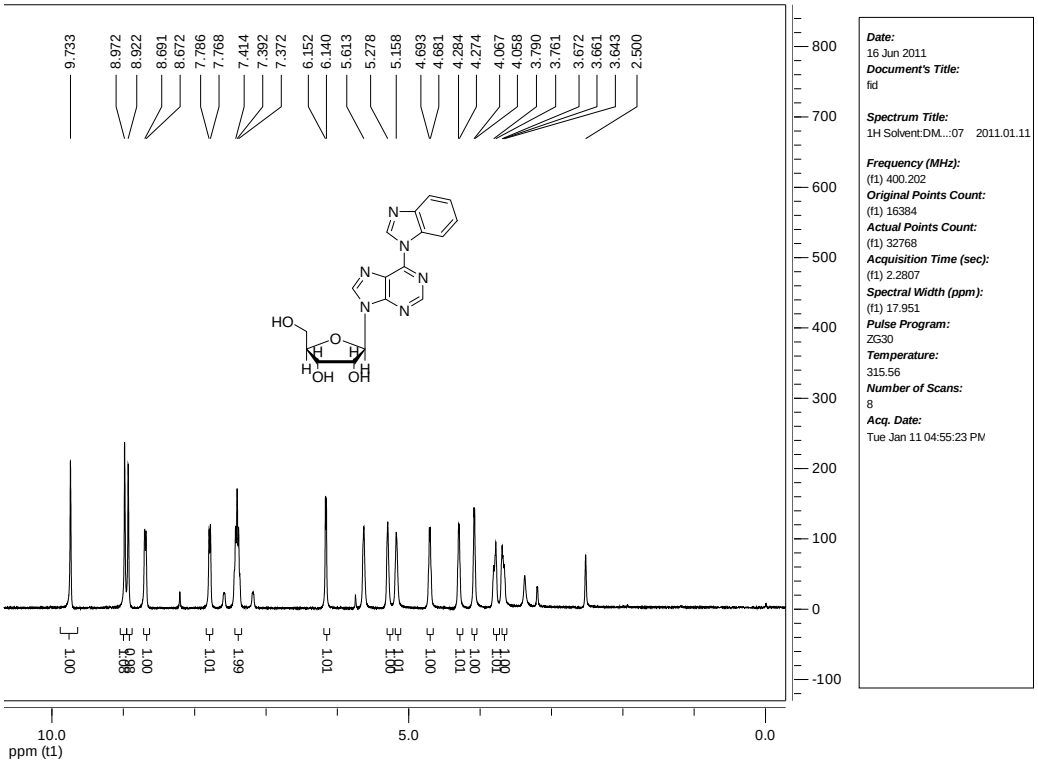
^{1}H NMR for **3d**



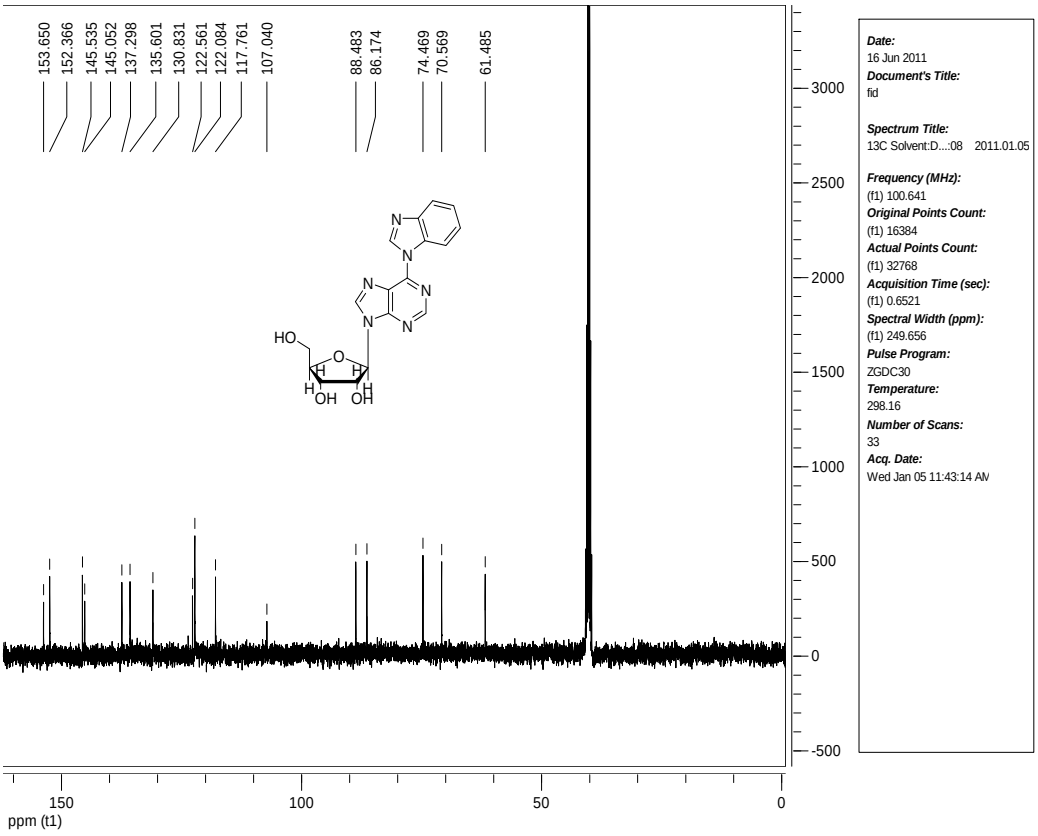
^{13}C NMR for **3d**



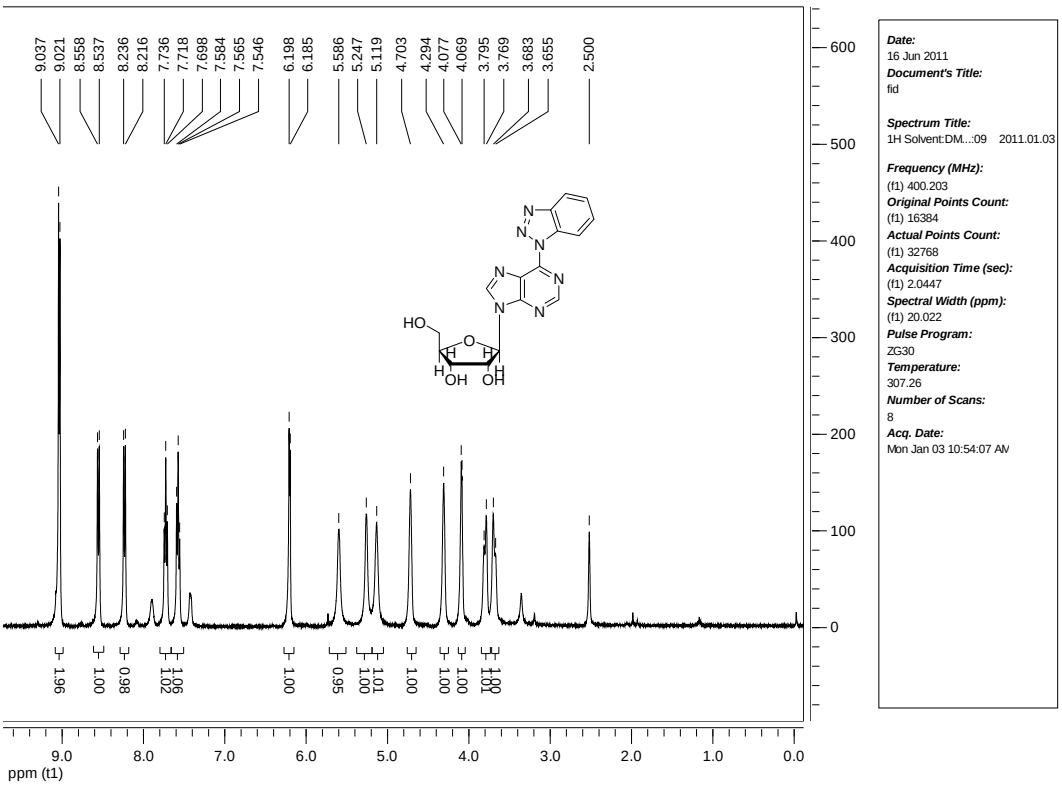
^{1}H NMR for **3e**



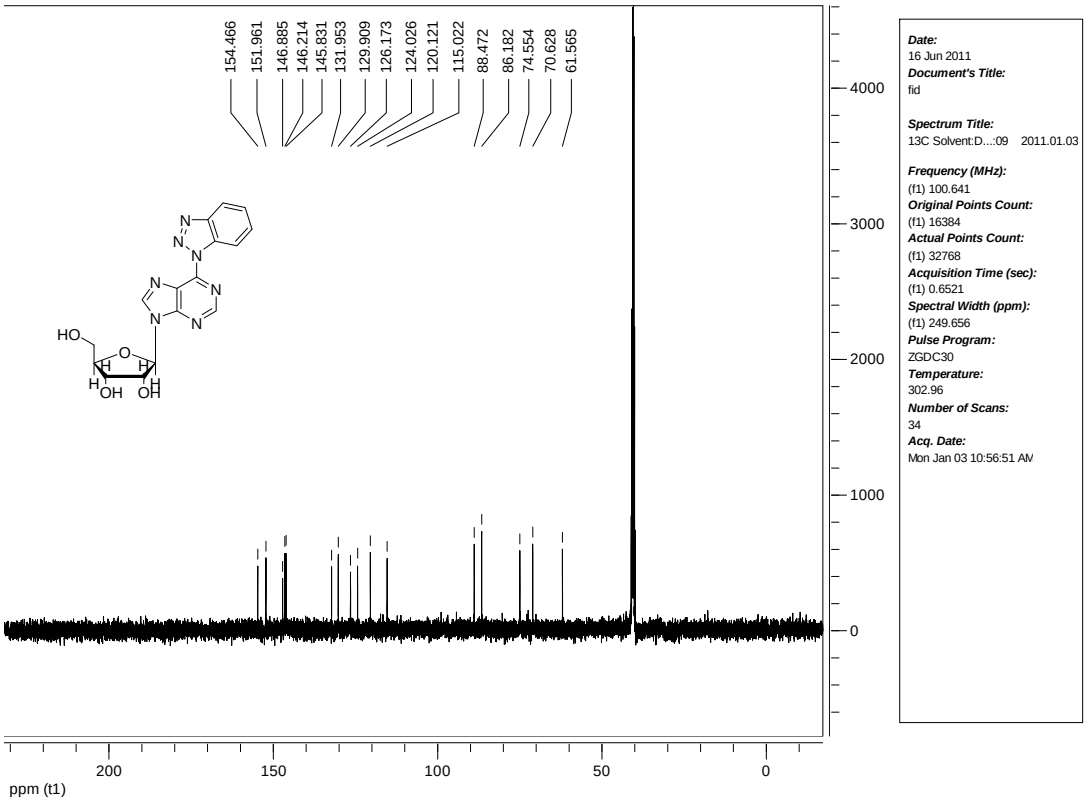
^{13}C NMR for **3e**



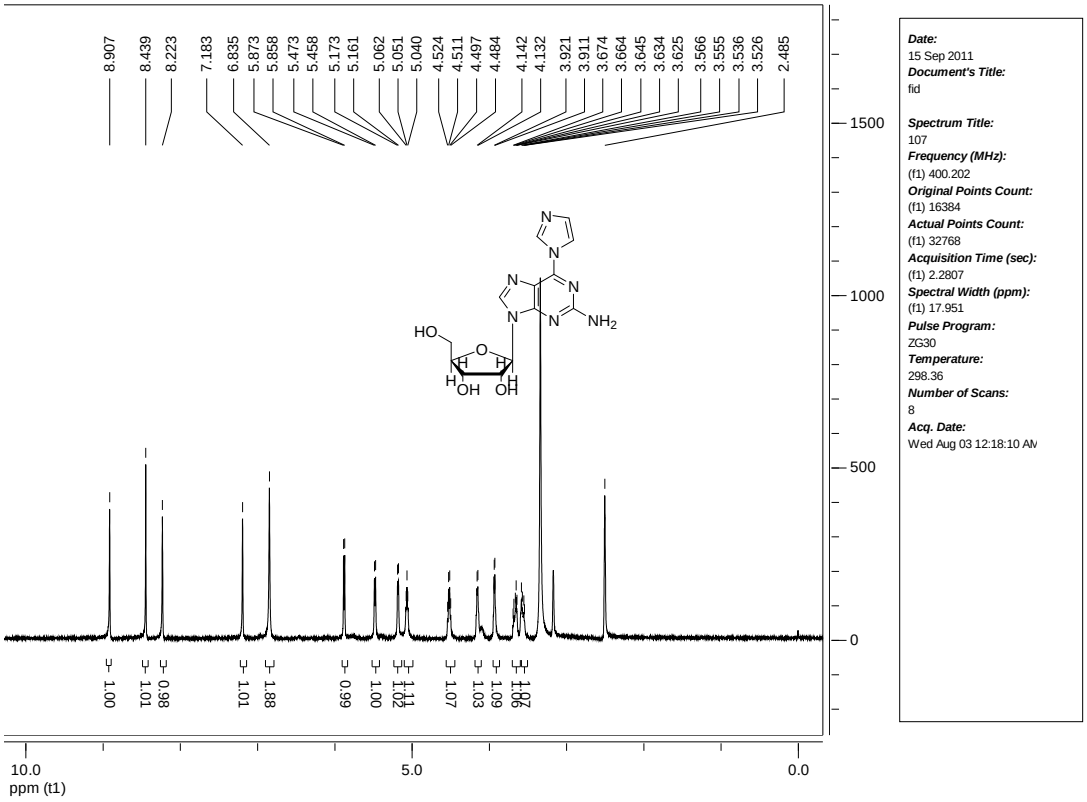
^{1}H NMR for **3f**



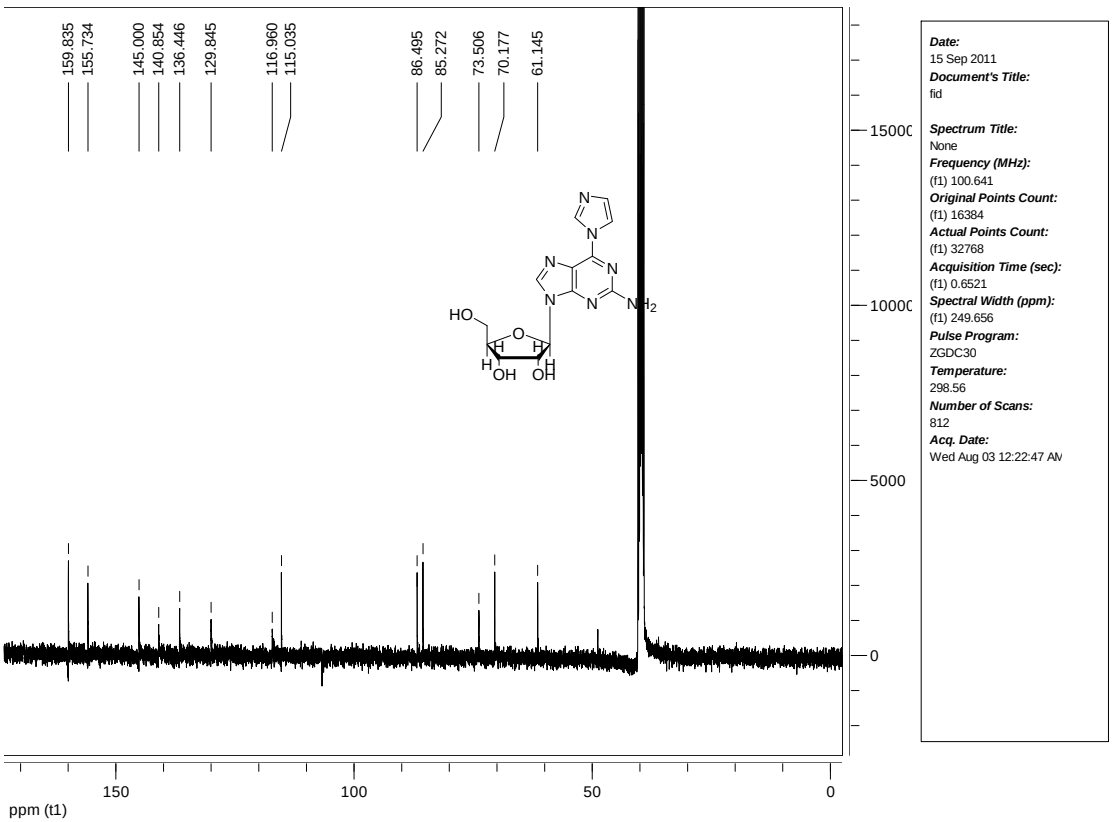
^{13}C NMR for **3f**



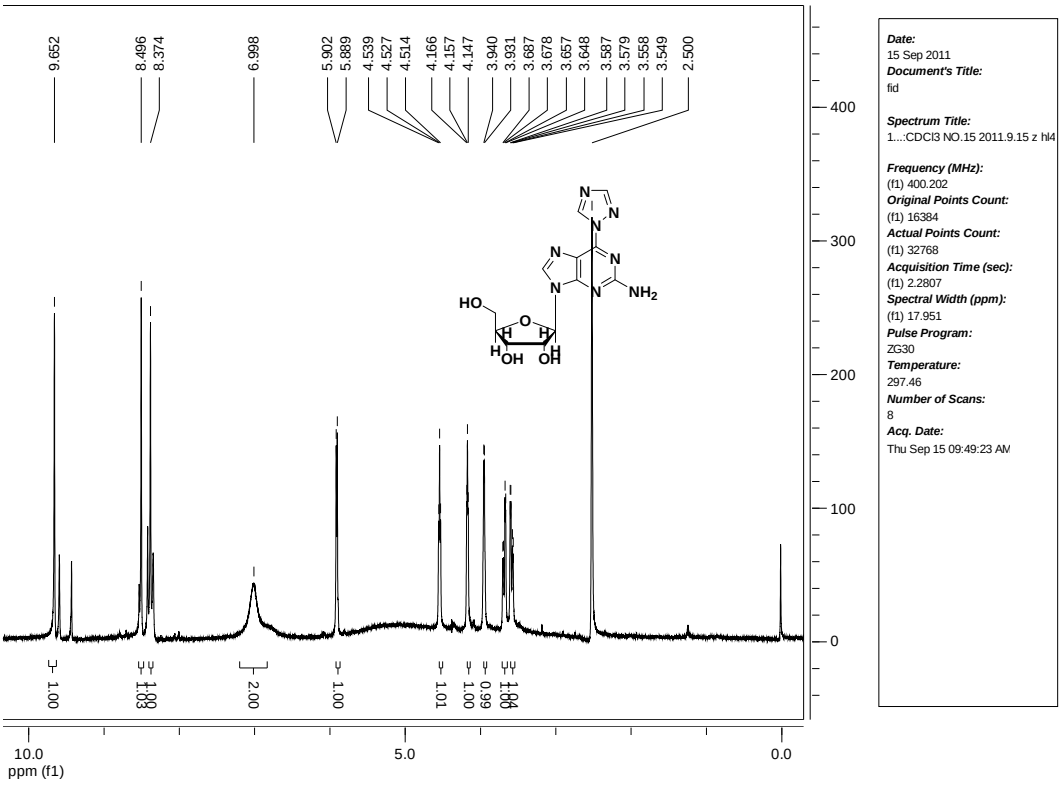
^{1}H NMR for **3g**



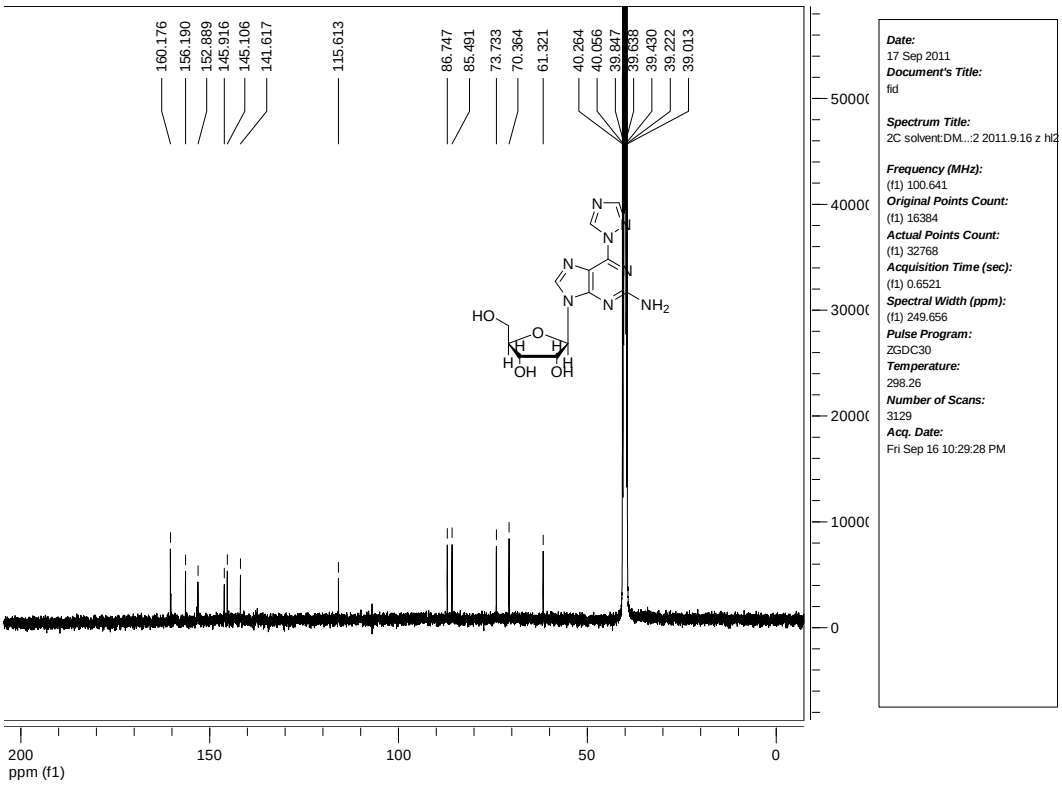
^{13}C NMR for **3g**



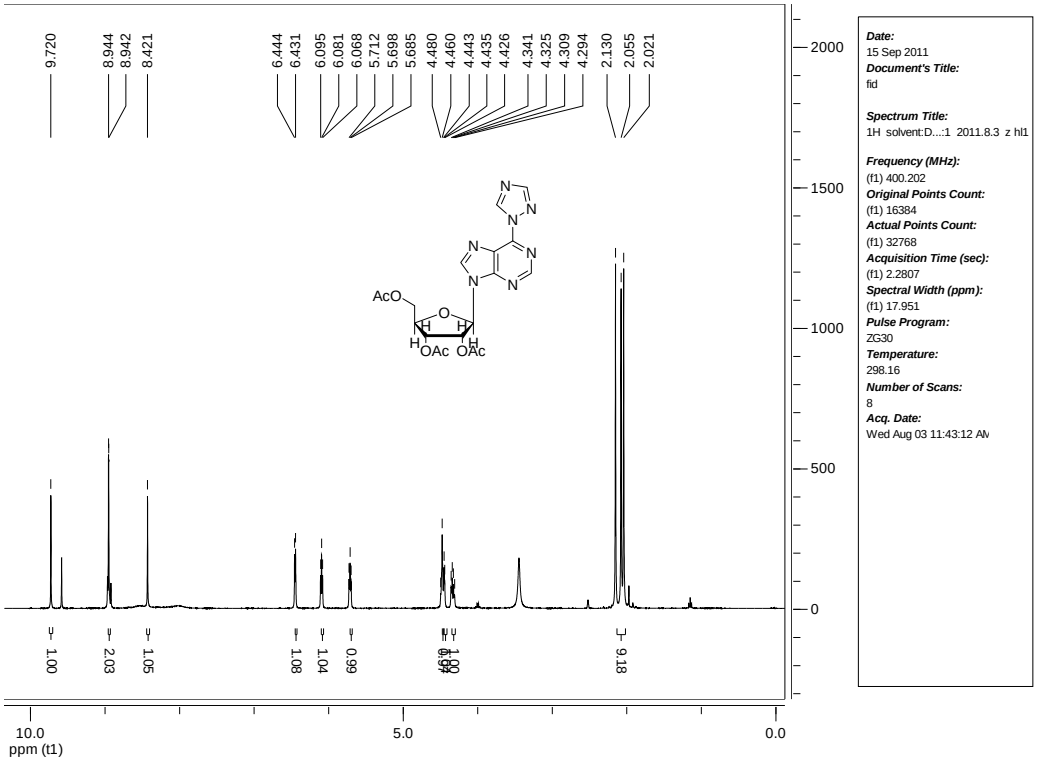
^{1}H NMR for **3h**



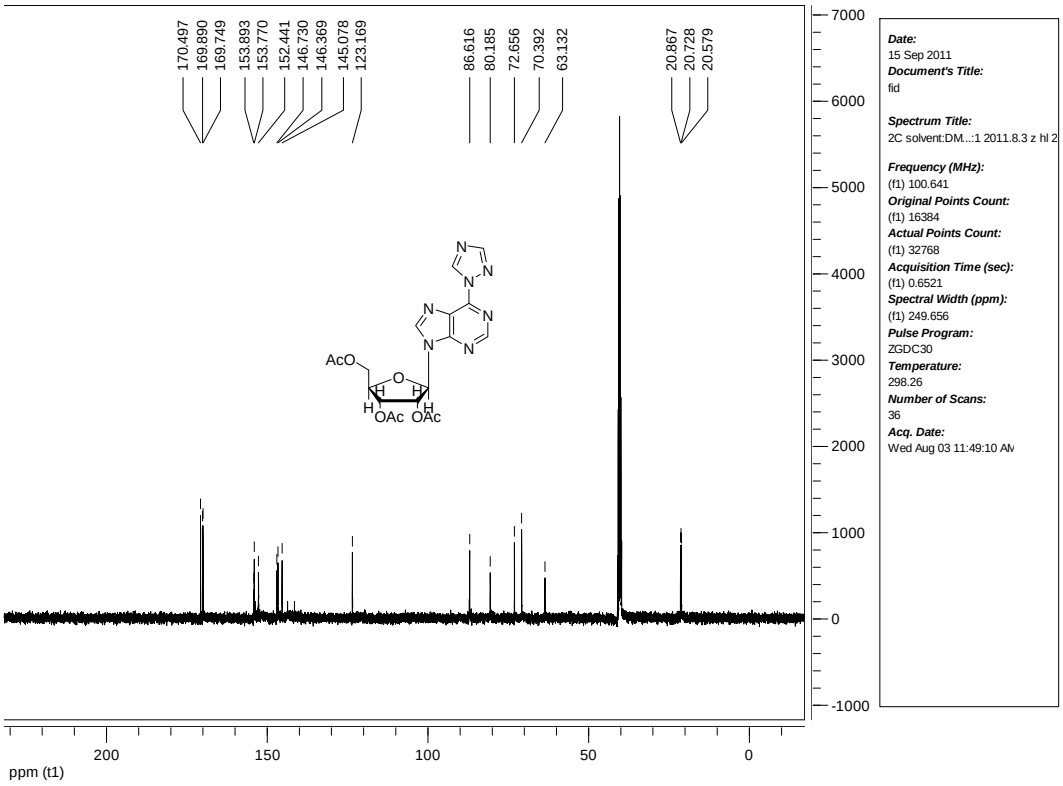
^{13}C NMR for **3h**



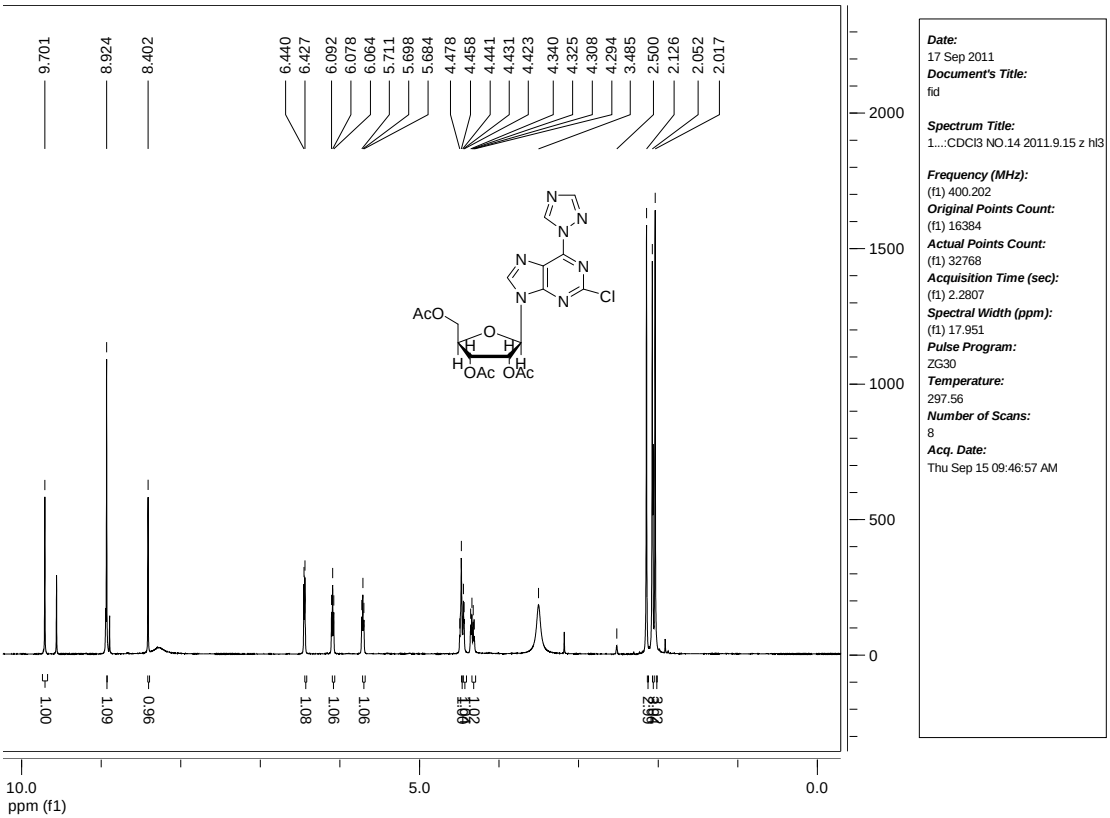
^{1}H NMR for **4a**



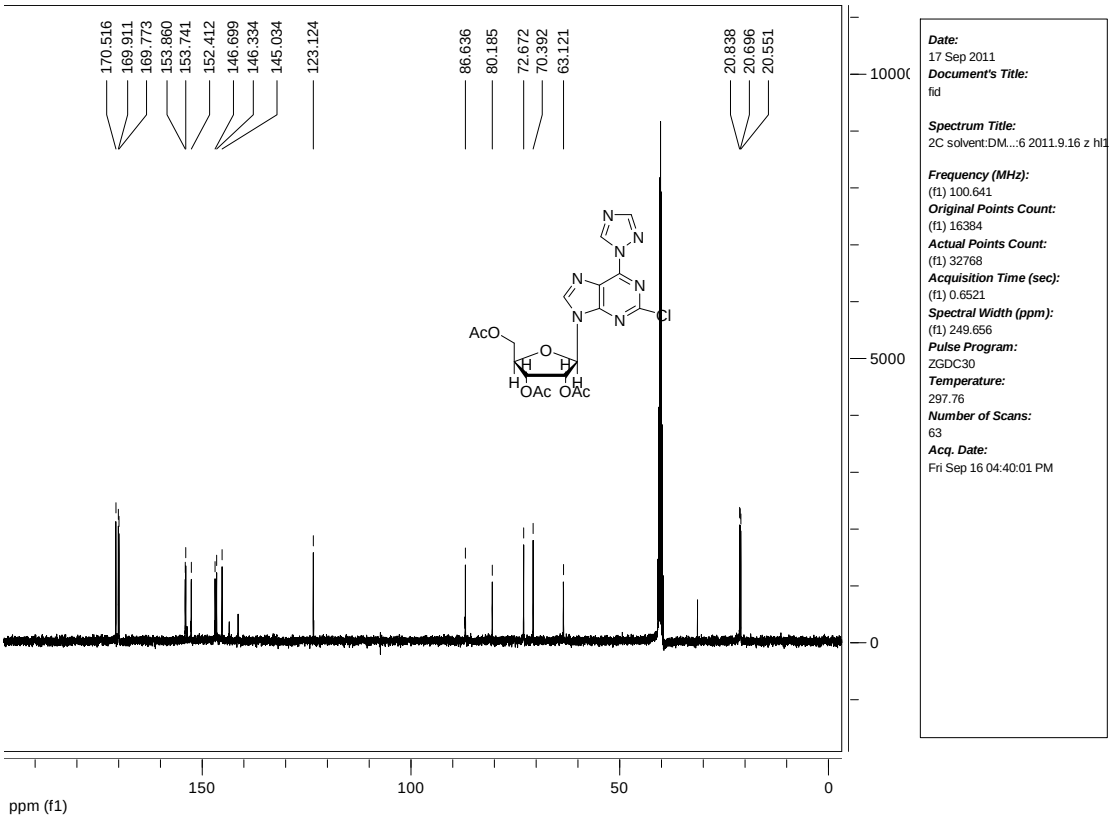
^{13}C NMR for **4a**



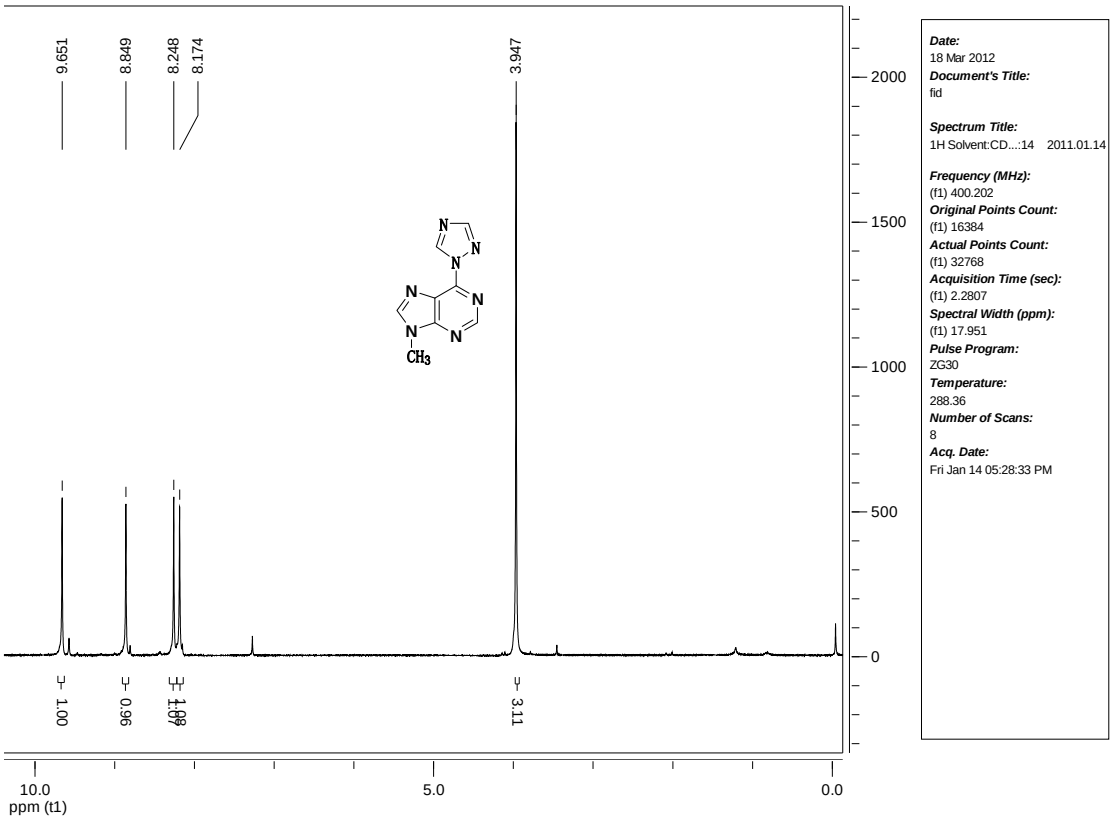
^{1}H NMR for **4b**



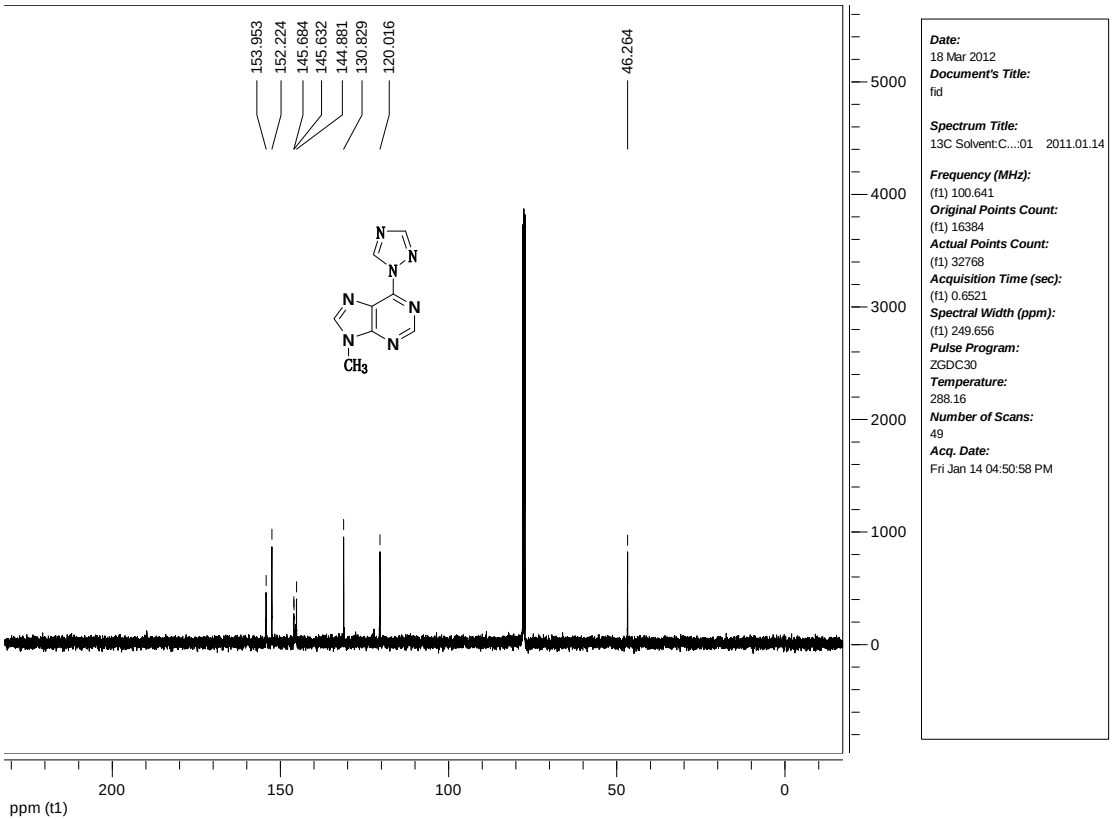
^{13}C NMR for **4b**



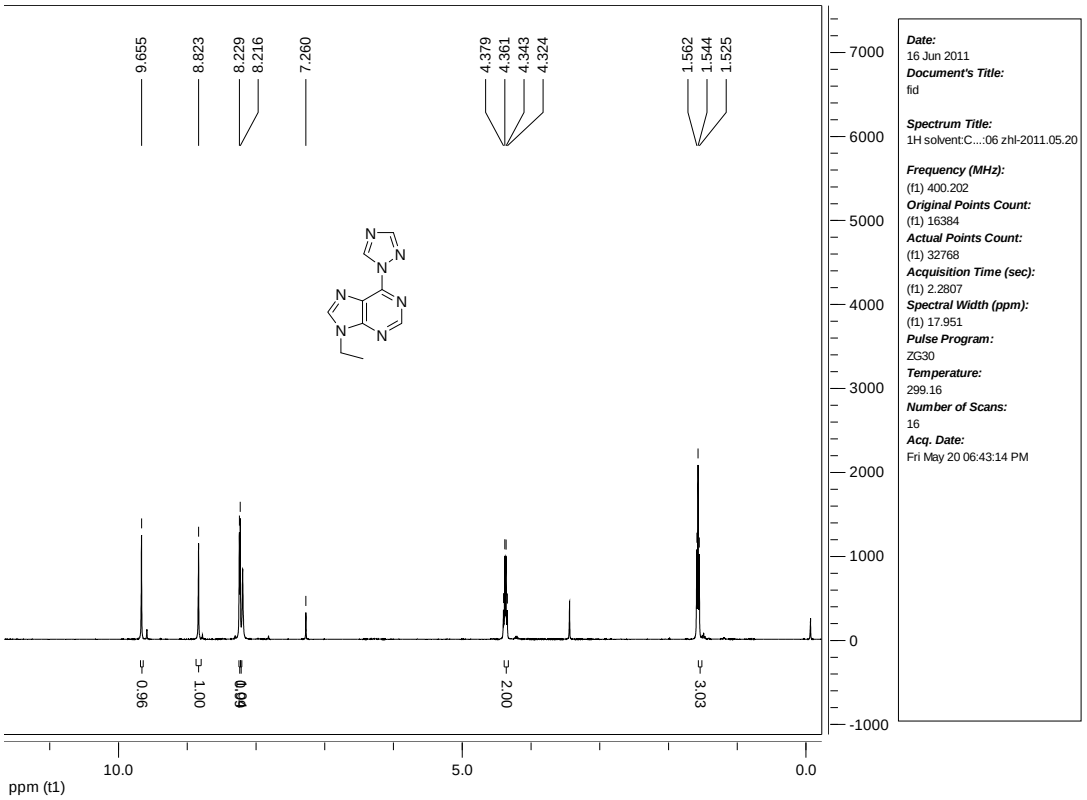
^{1}H NMR for **4c**



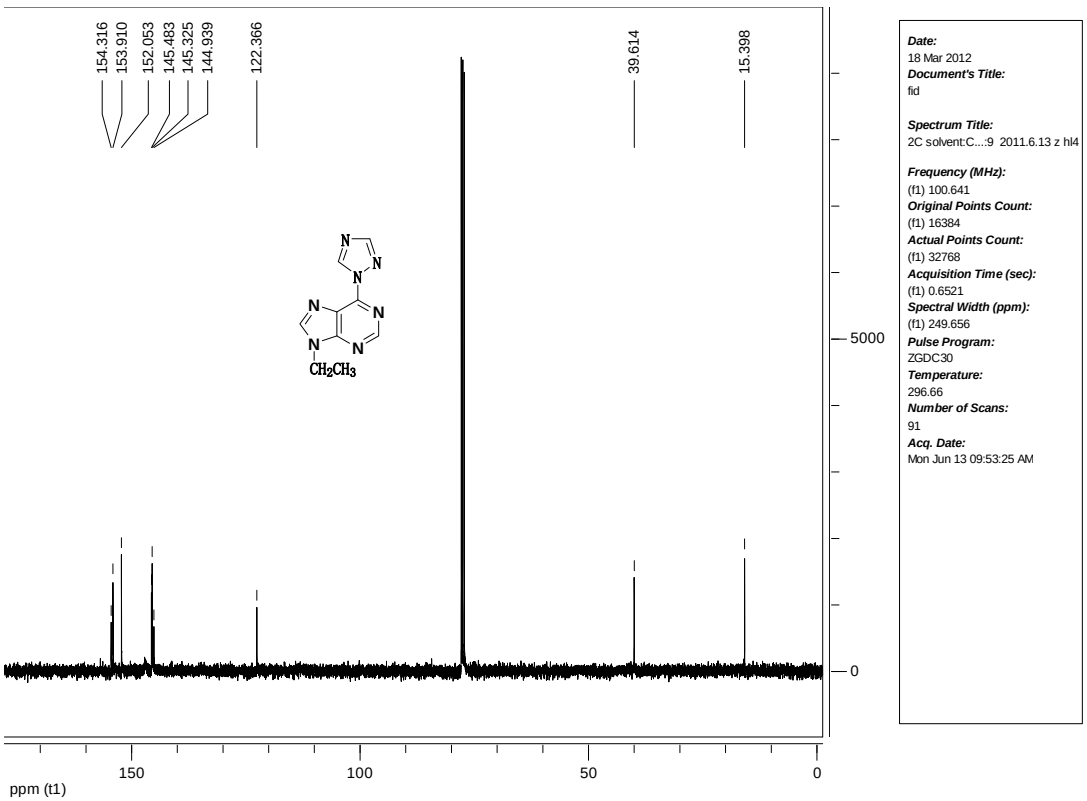
^{13}C NMR for **4c**



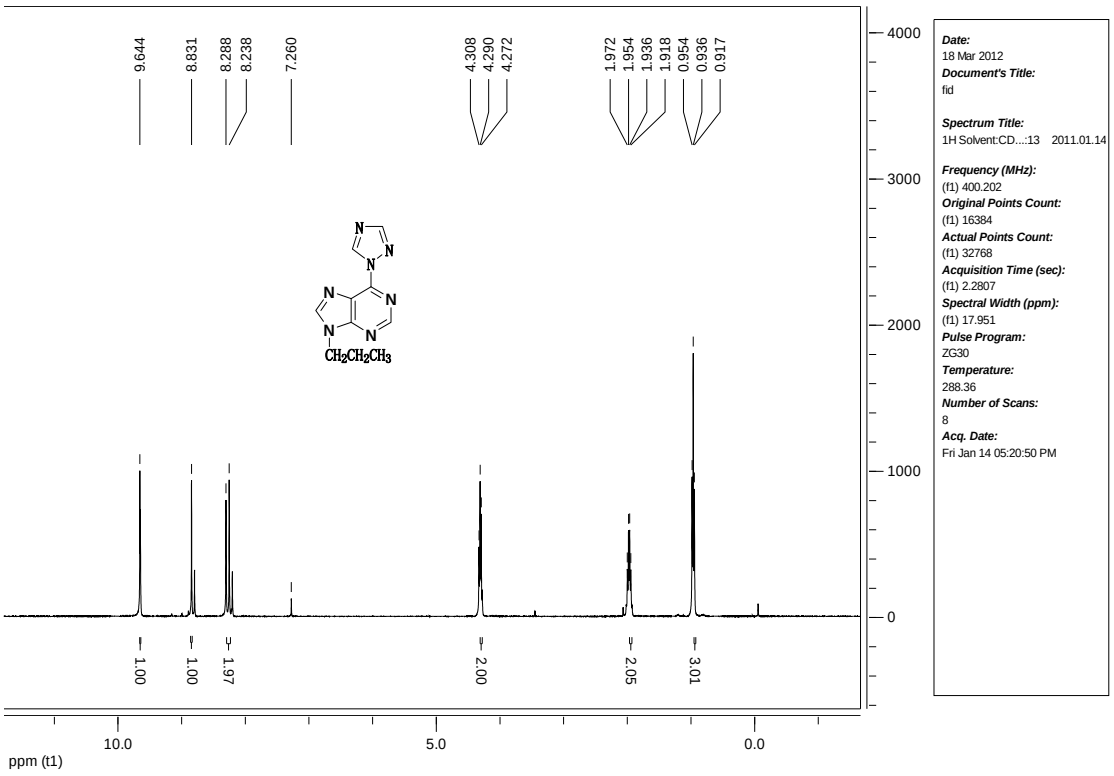
^{1}H NMR for **4d**



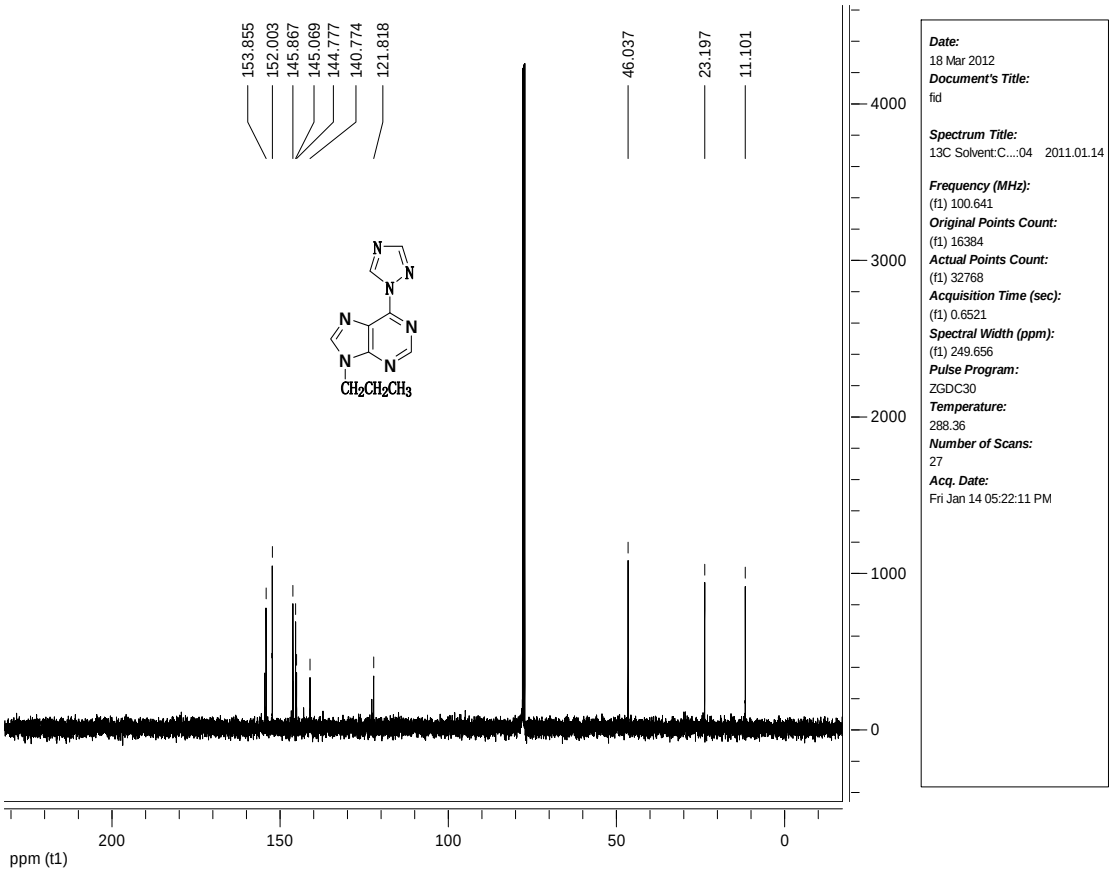
^{13}C NMR for **4d**



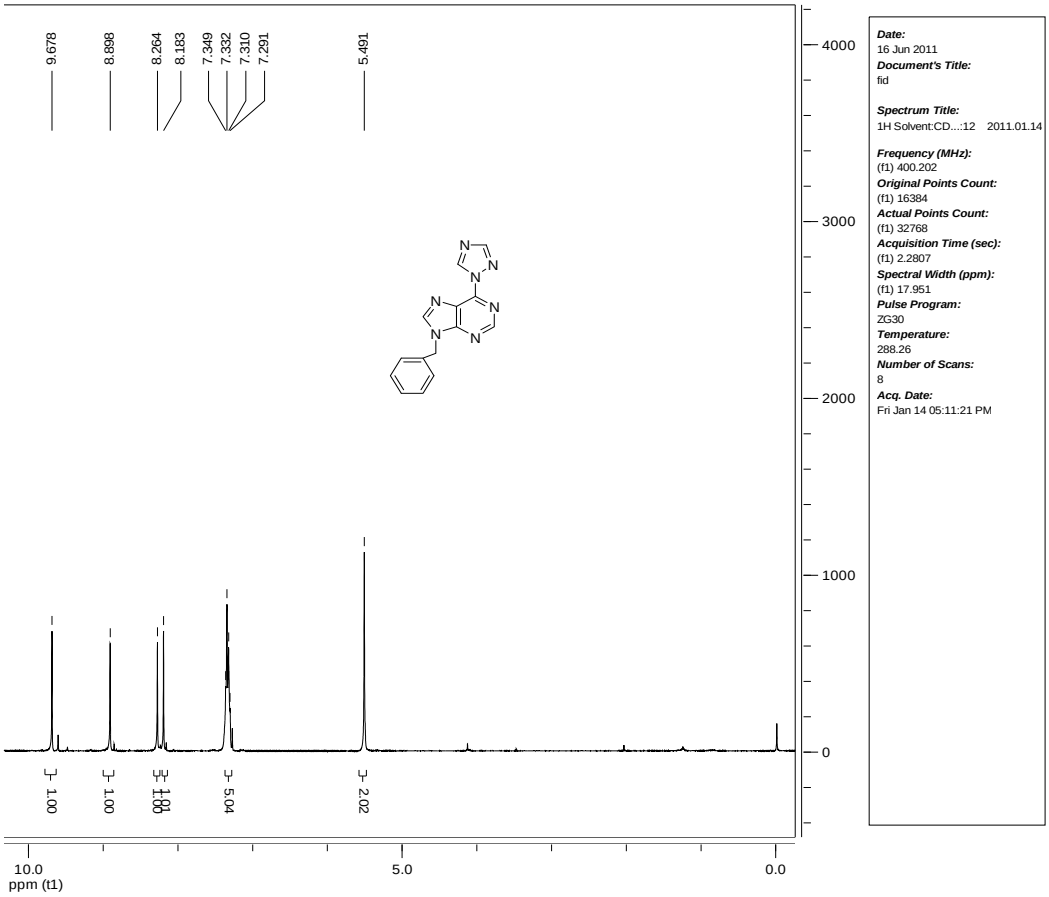
^{1}H NMR for **4e**



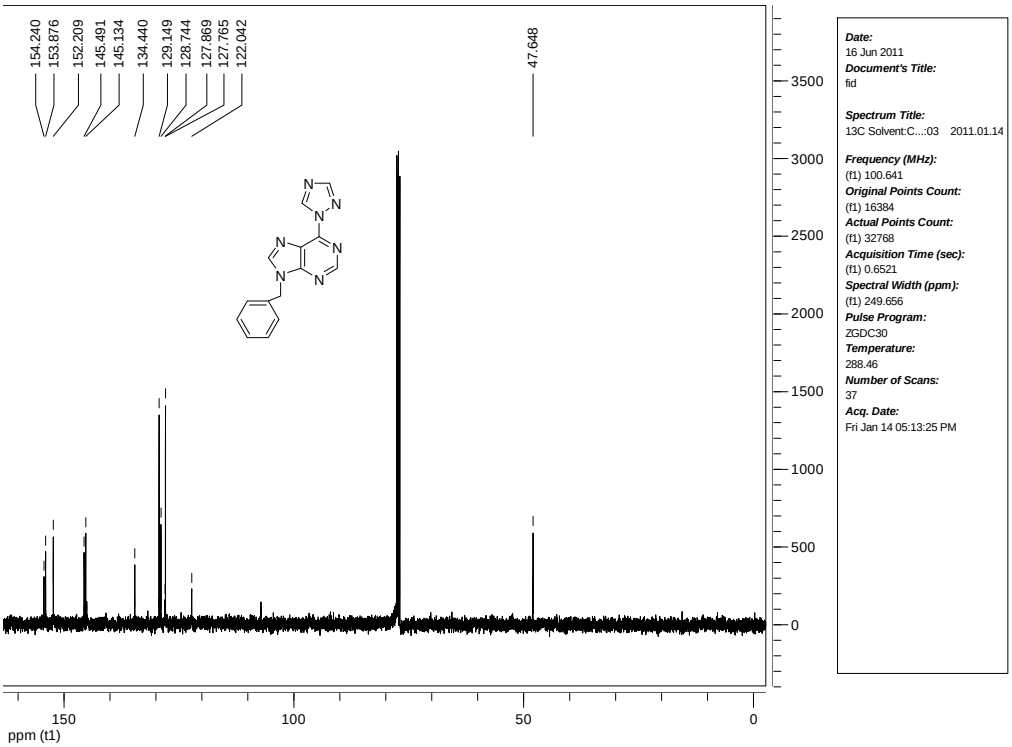
^{13}C NMR for **4e**



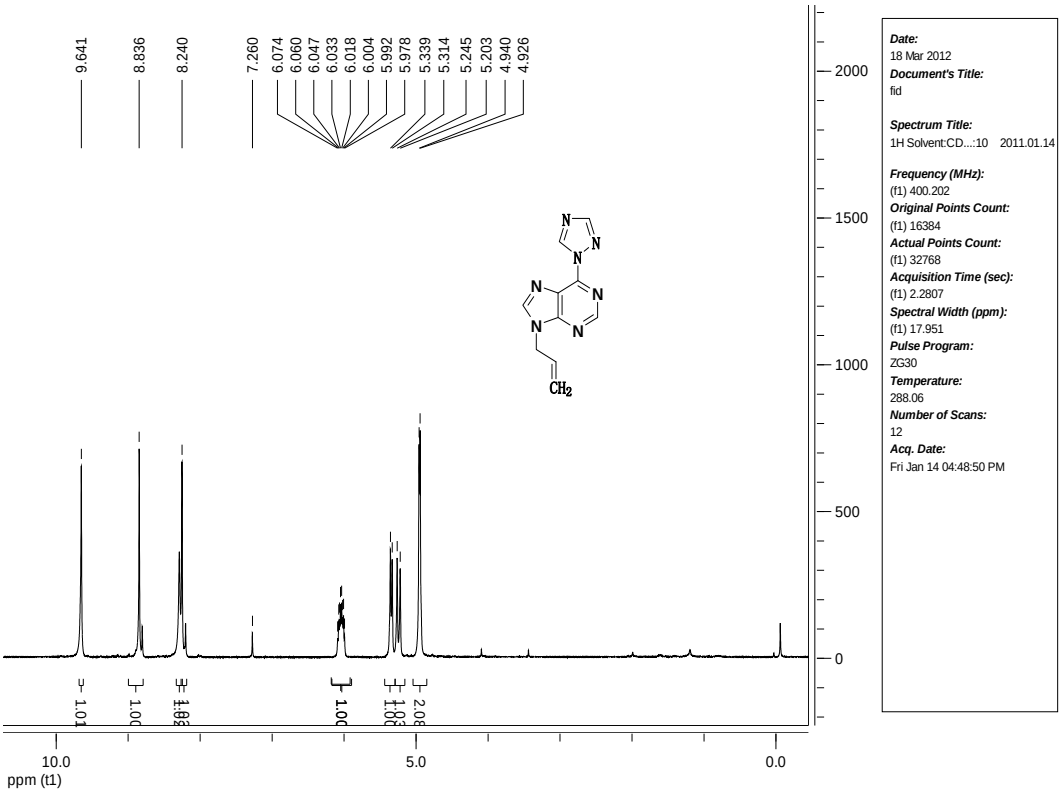
^{1}H NMR for **4f**



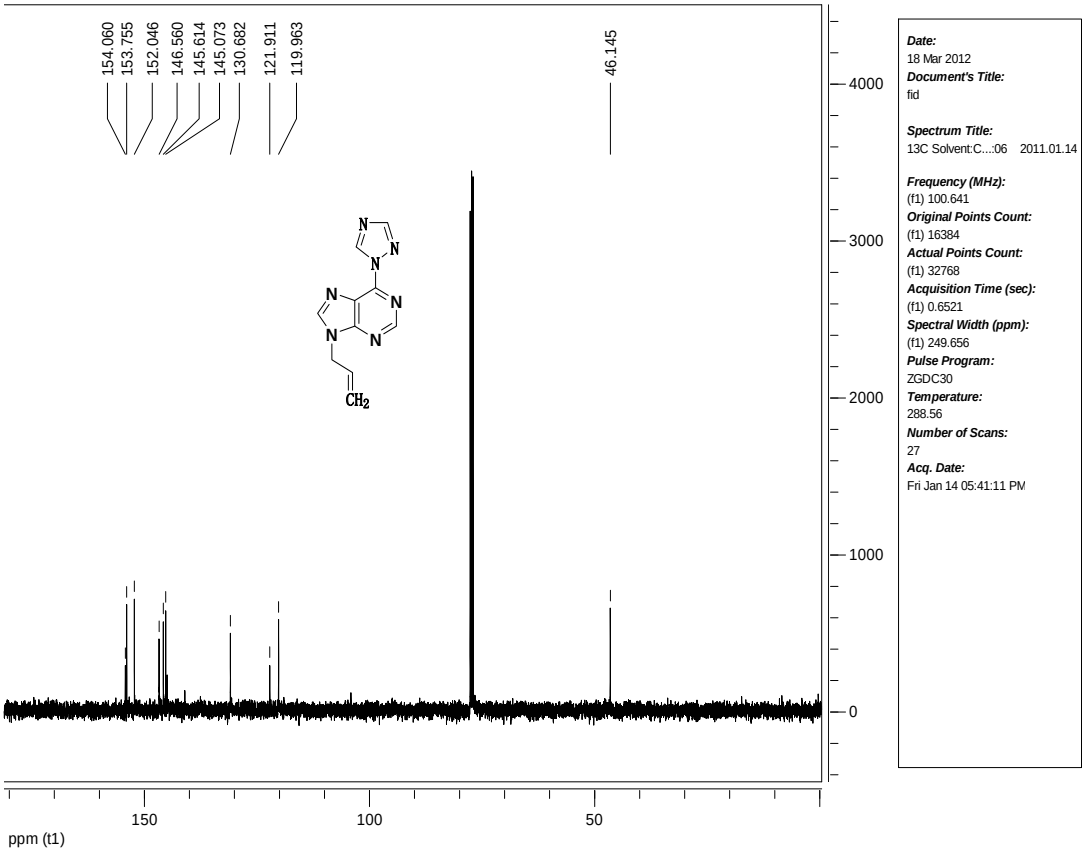
^{13}C NMR for **4f**



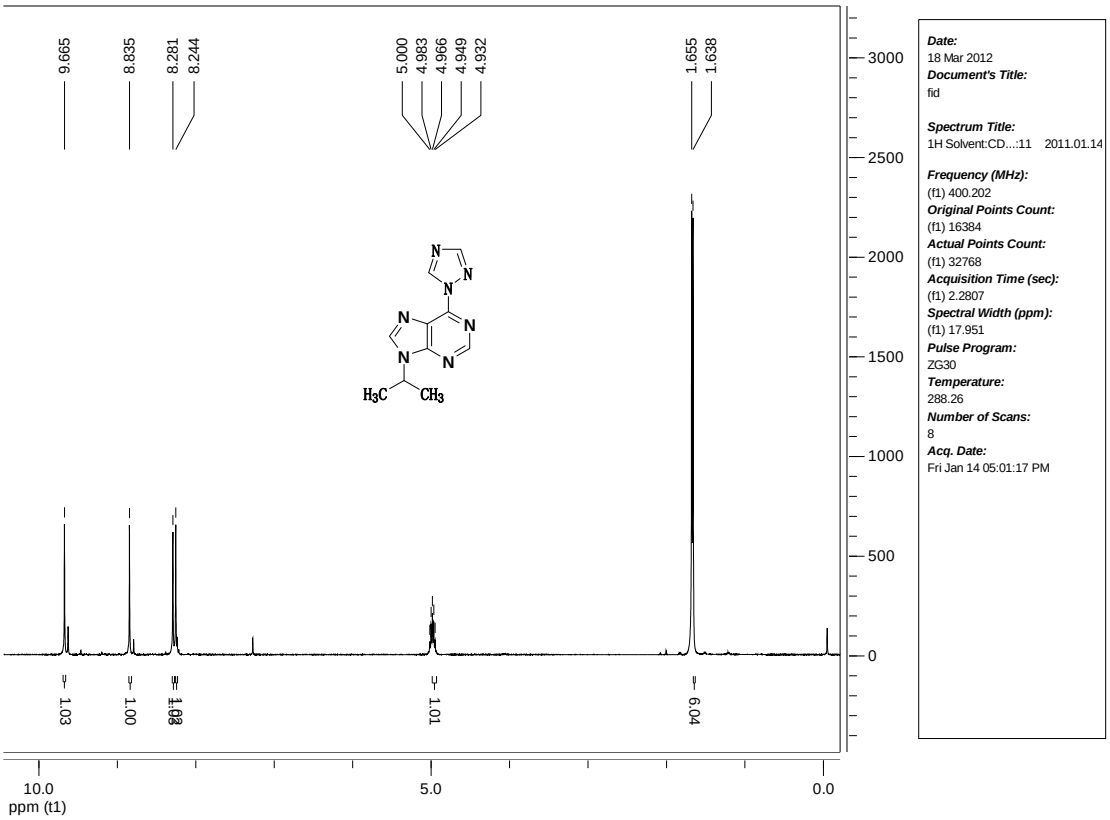
^{1}H NMR for **4g**



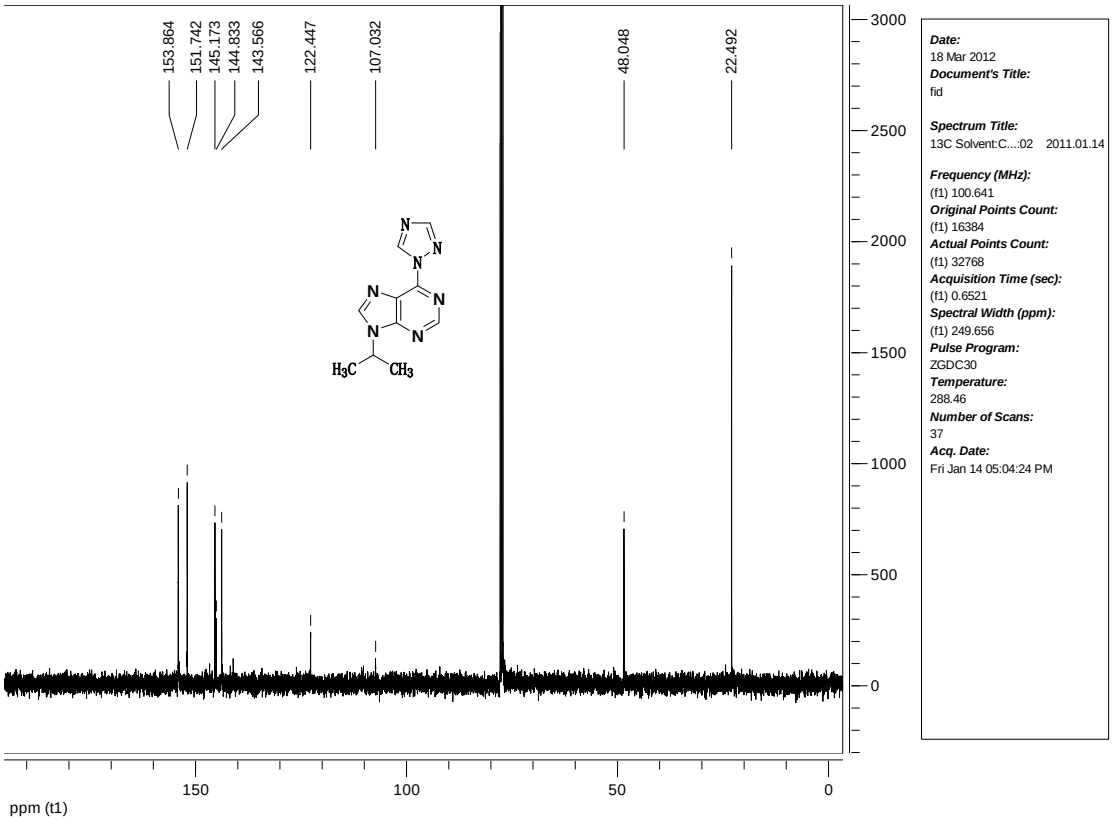
^{13}C NMR for **4g**



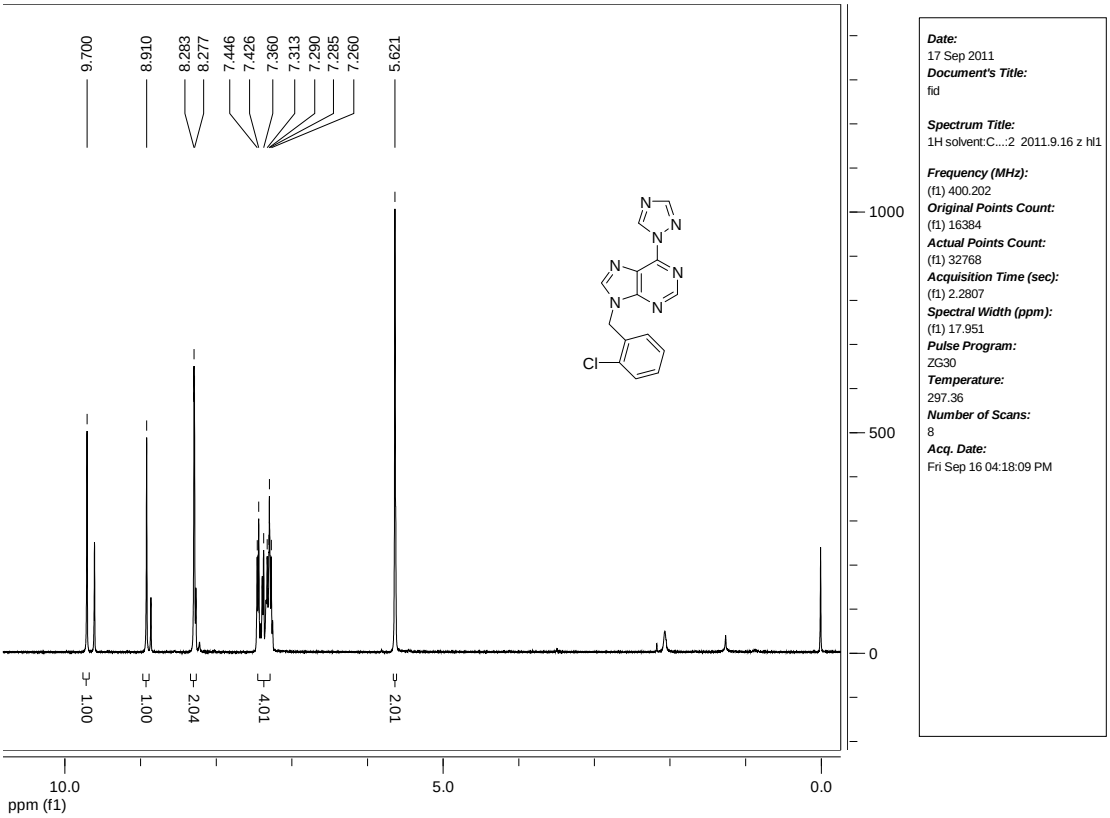
^{1}H NMR for **4h**



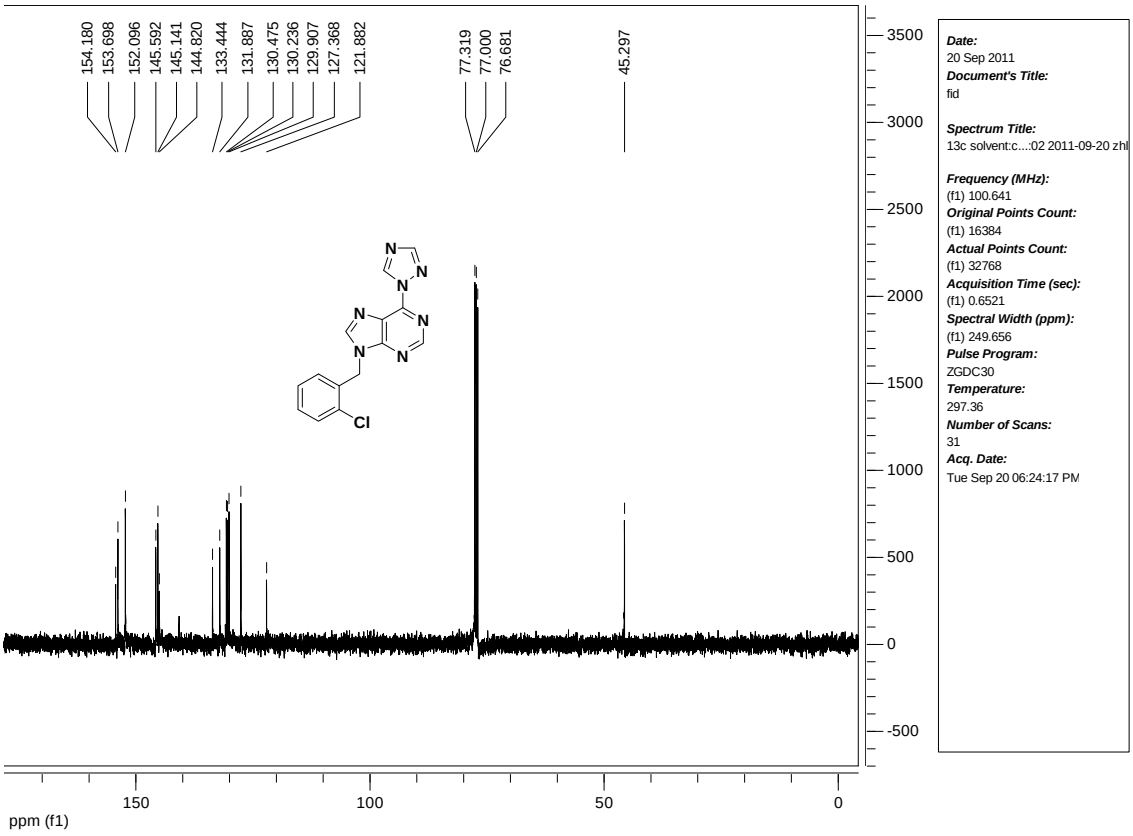
^{13}C NMR for **4h**



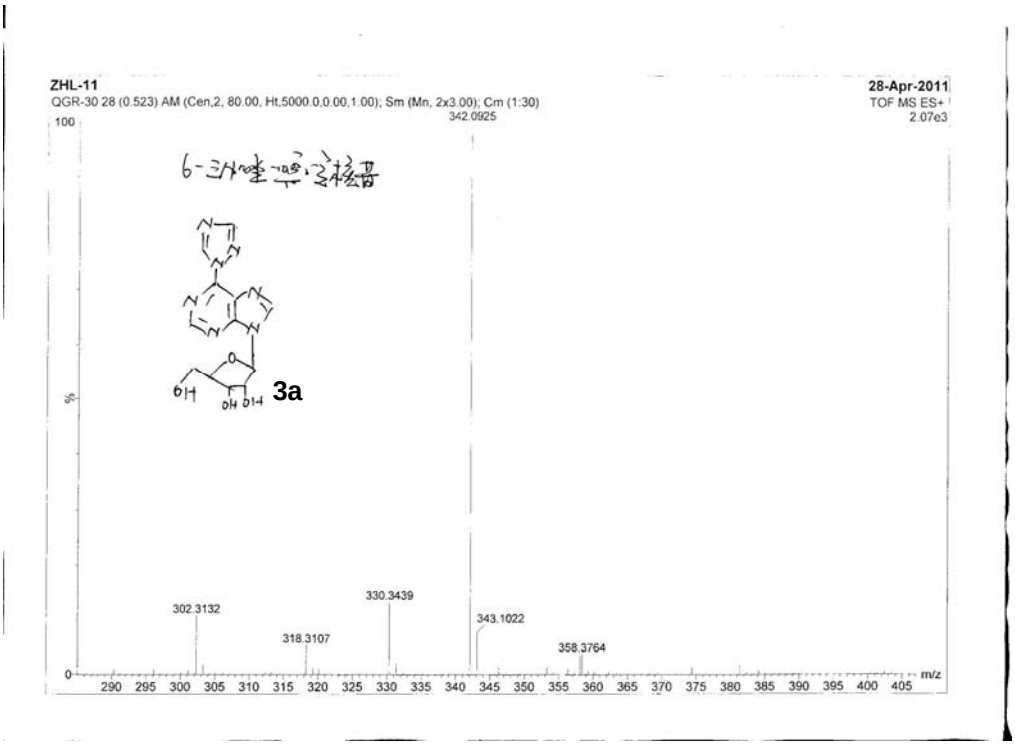
^{1}H NMR for **4i**



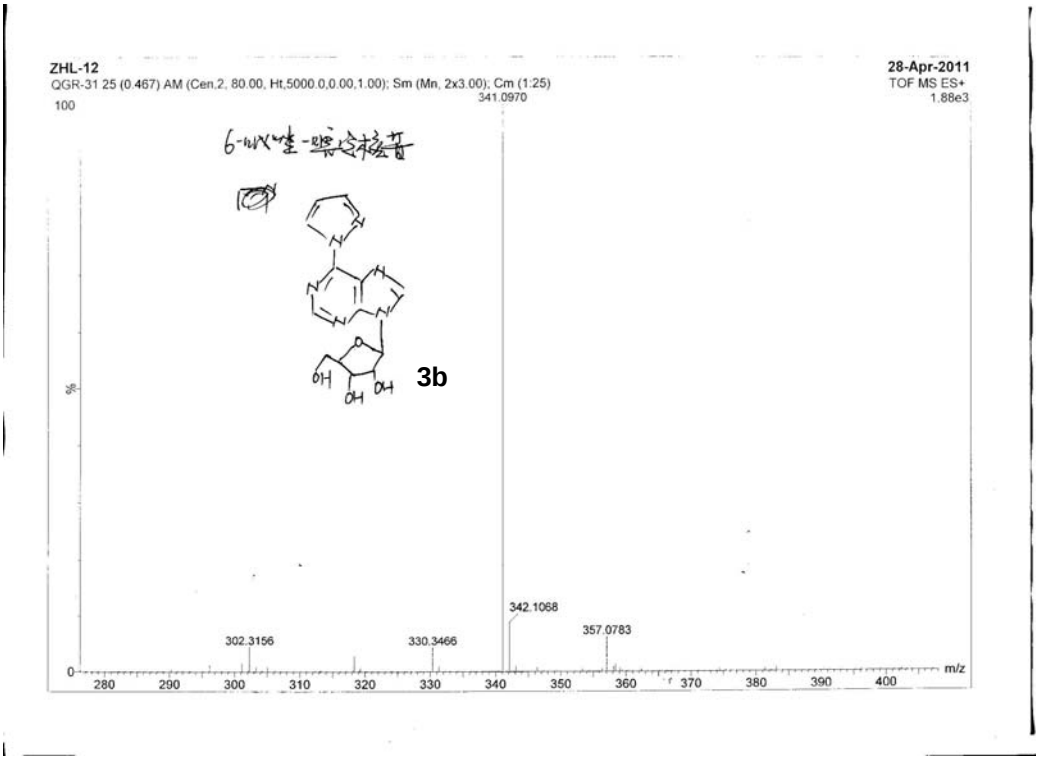
^{13}C NMR for **4i**



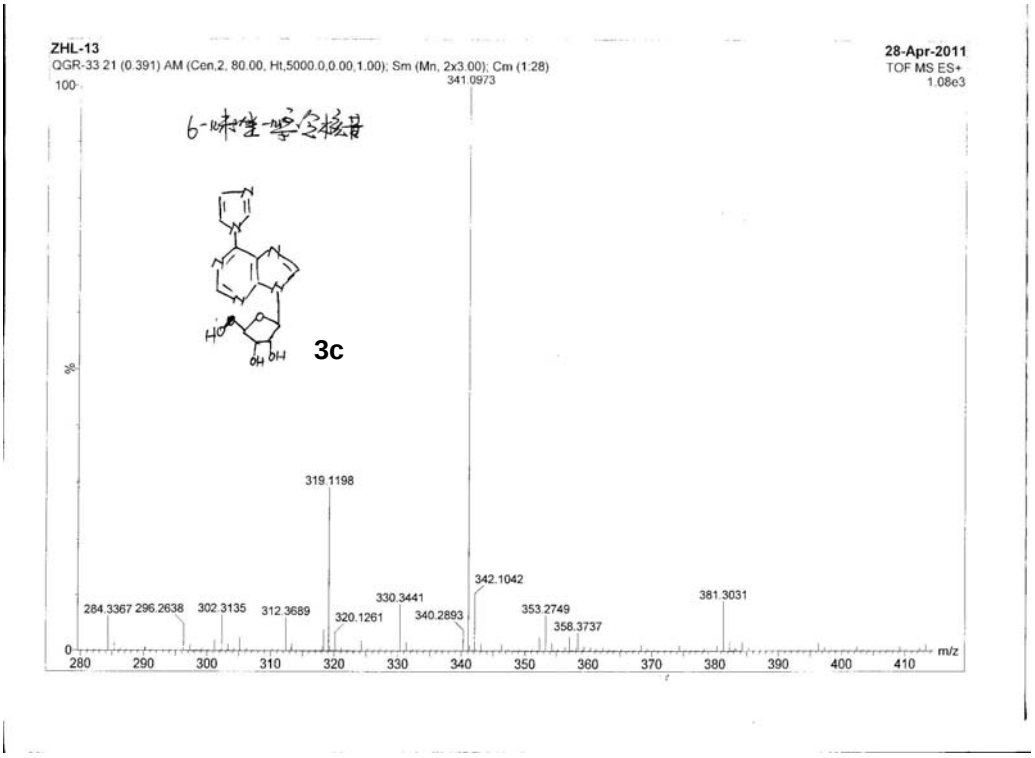
Copies of HRMS

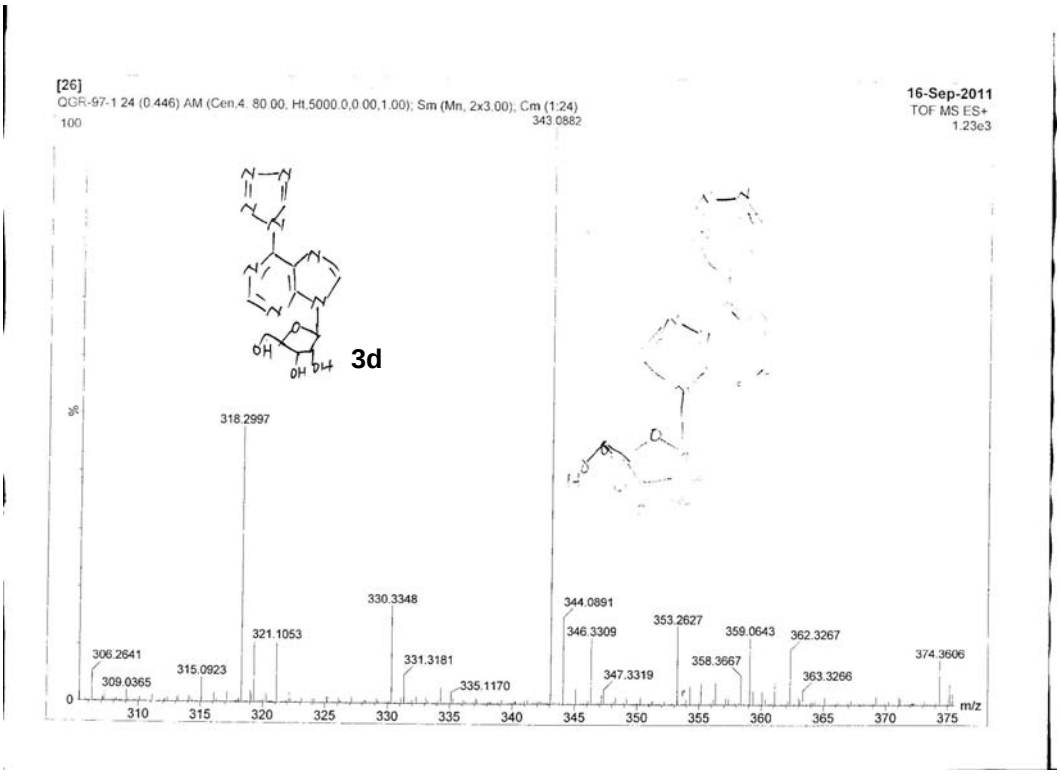


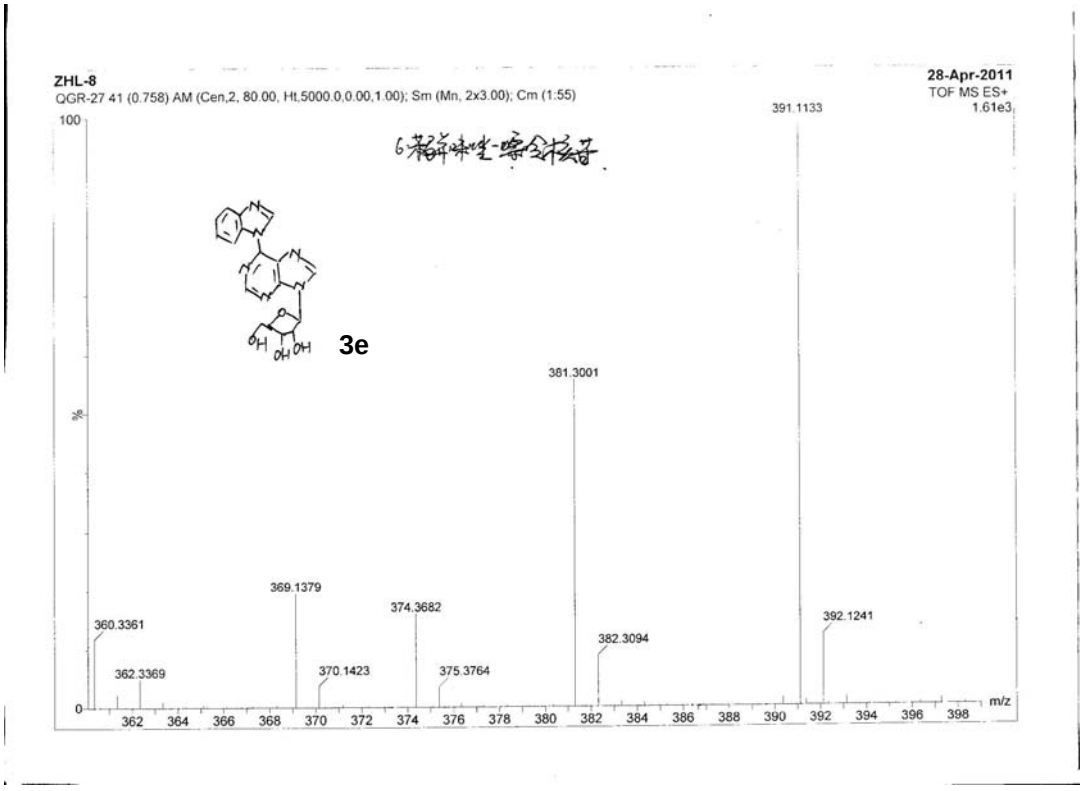
3a



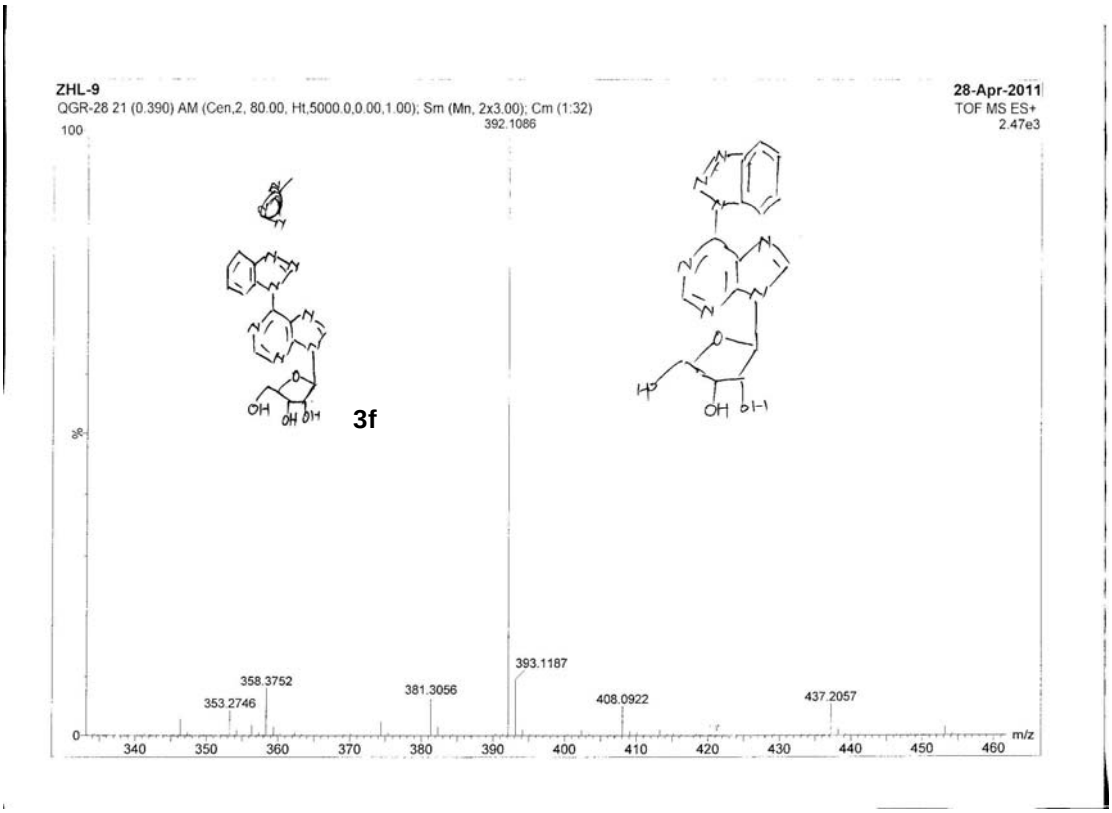
3b


ZHL-13
QGR-33 21 (0.391) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:28)
28-Apr-2011
TOF MS ES+
1.08e3
100
341.0973
6-氨基嘌呤核苷
3c
319.1198
342.1042
330.3441
381.3031
284.3367 296.2638 302.3135 312.3689 320.1261 340.2893 353.2749 358.3737
%
0
280 290 300 310 320 330 340 350 360 370 380 390 400 410
m/z

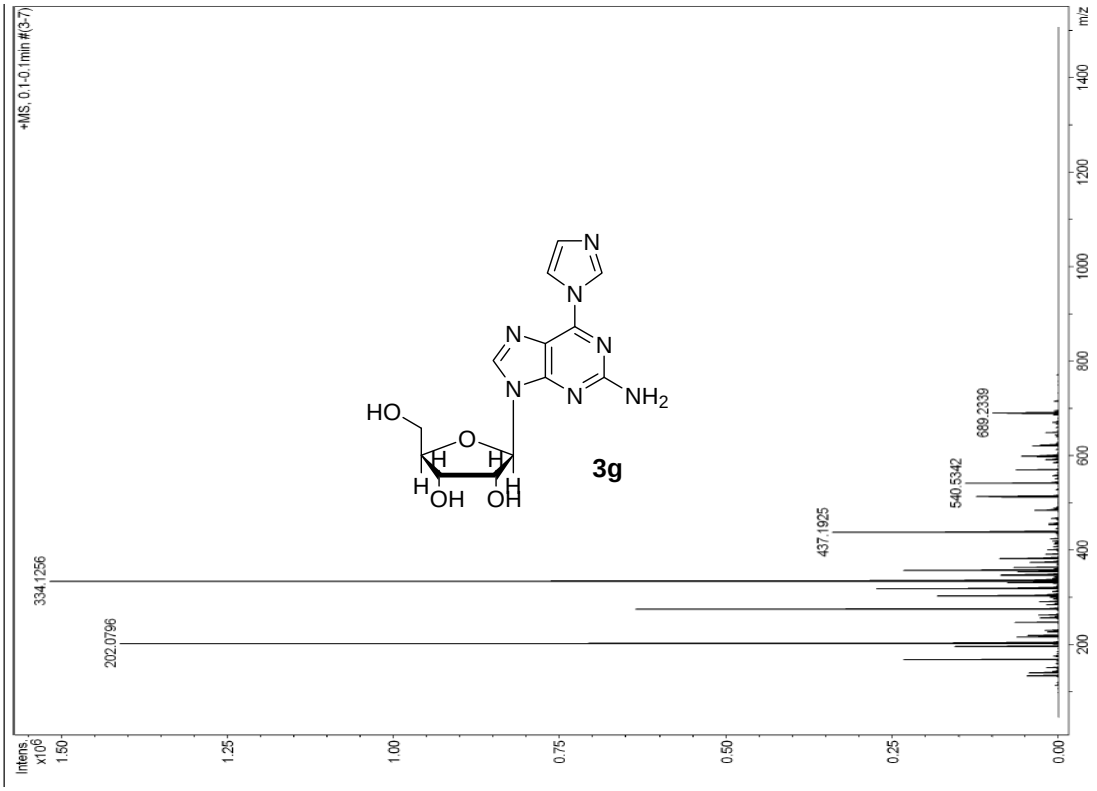

[26]
QGR-97-1 24 (0.446) AM (Cen,4, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:24)
16-Sep-2011
TOF MS ES+
1.23e3
100
343.0882
3d
318.2997
330.3348
344.0891
353.2627
321.1053
346.3309
359.0643
362.3267
306.2641
331.3181
358.3667
374.3606
315.0923
347.3319
309.0365
335.1170
363.3266
%
0
310 315 320 325 330 335 340 345 350 355 360 365 370 375
m/z

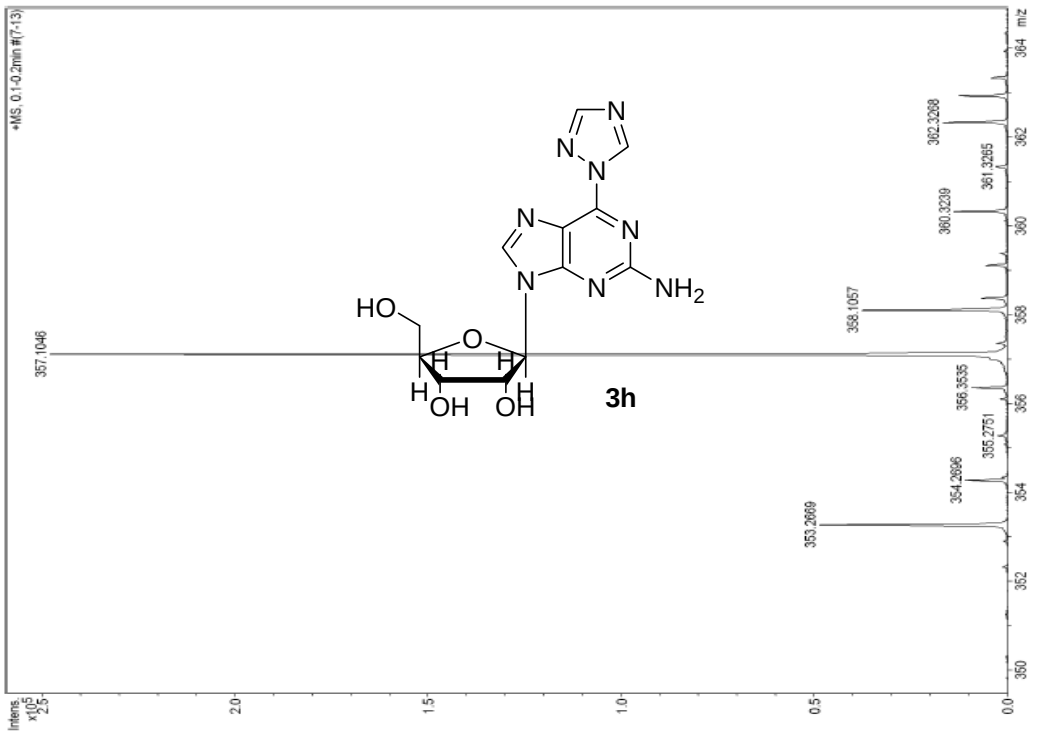

ZHL-8
QGR-27 41 (0.758) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:55)
28-Apr-2011
TOF MS ES+
1.61e3
100
%
0
391.1133
381.3001
369.1379
374.3682
392.1241
360.3361
382.3094
362.3369
370.1423
375.3764
362 364 366 368 370 372 374 376 378 380 382 384 386 388 390 392 394 396 398
m/z

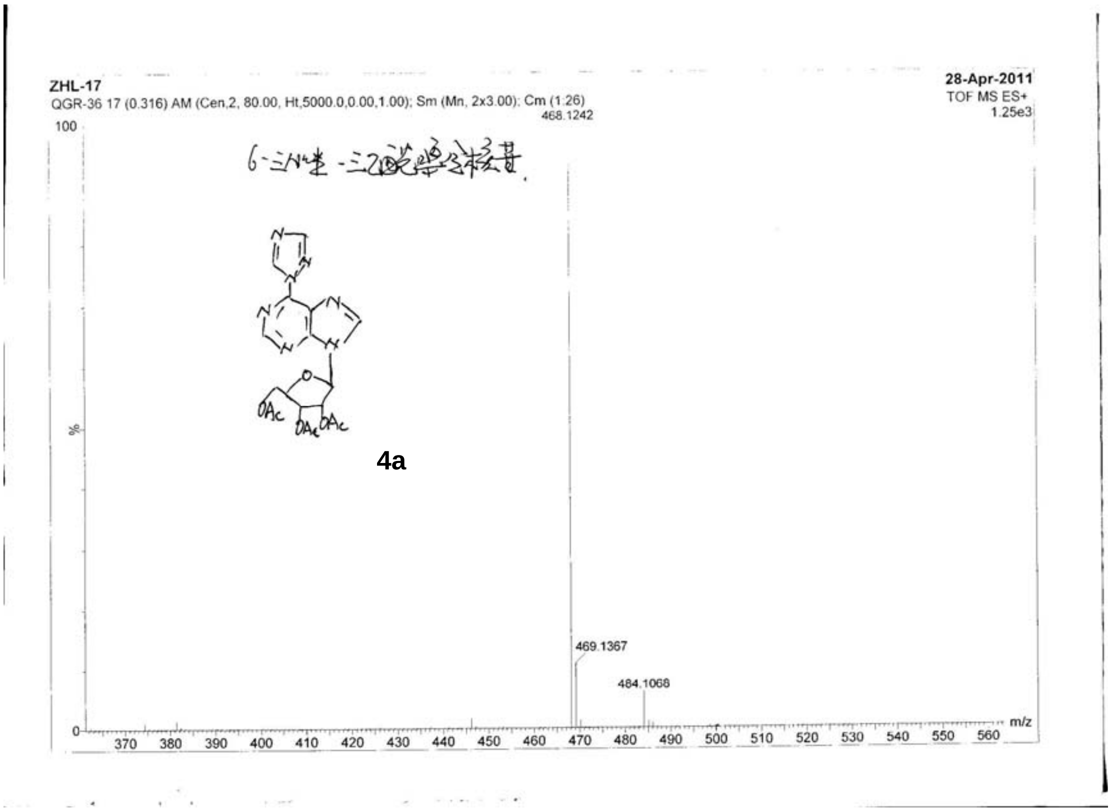
3e


ZHL-9
QGR-28 21 (0.390) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:32)
28-Apr-2011
TOF MS ES+
2.47e3
100
%
0
392.1086
393.1187
358.3752
353.2746
381.3056
408.0922
437.2057
340 350 360 370 380 390 400 410 420 430 440 450 460
m/z

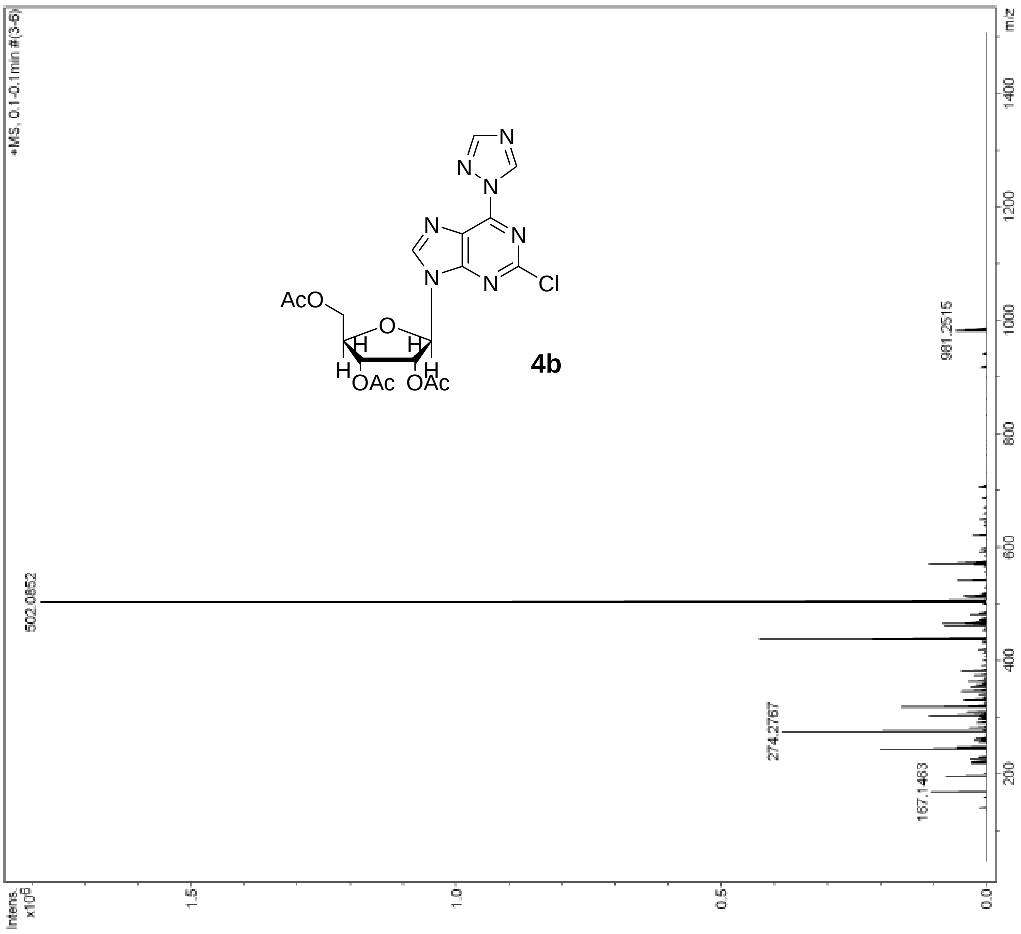
3f



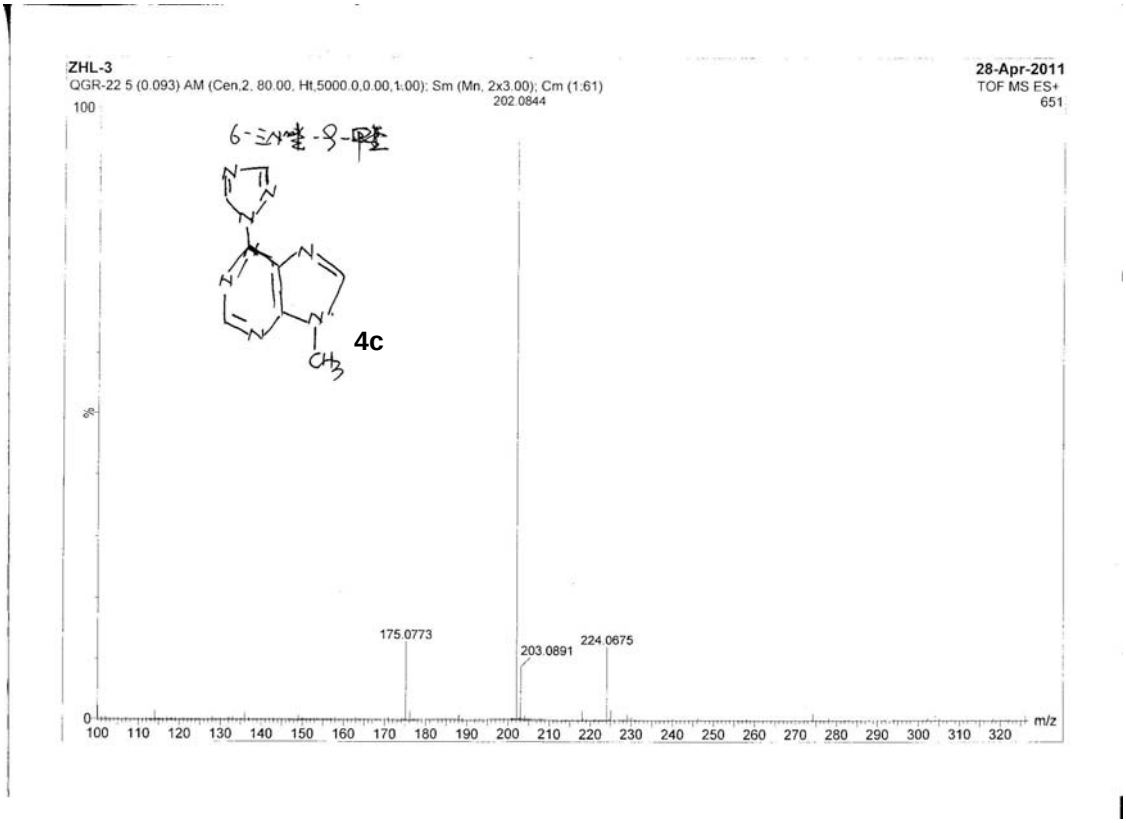


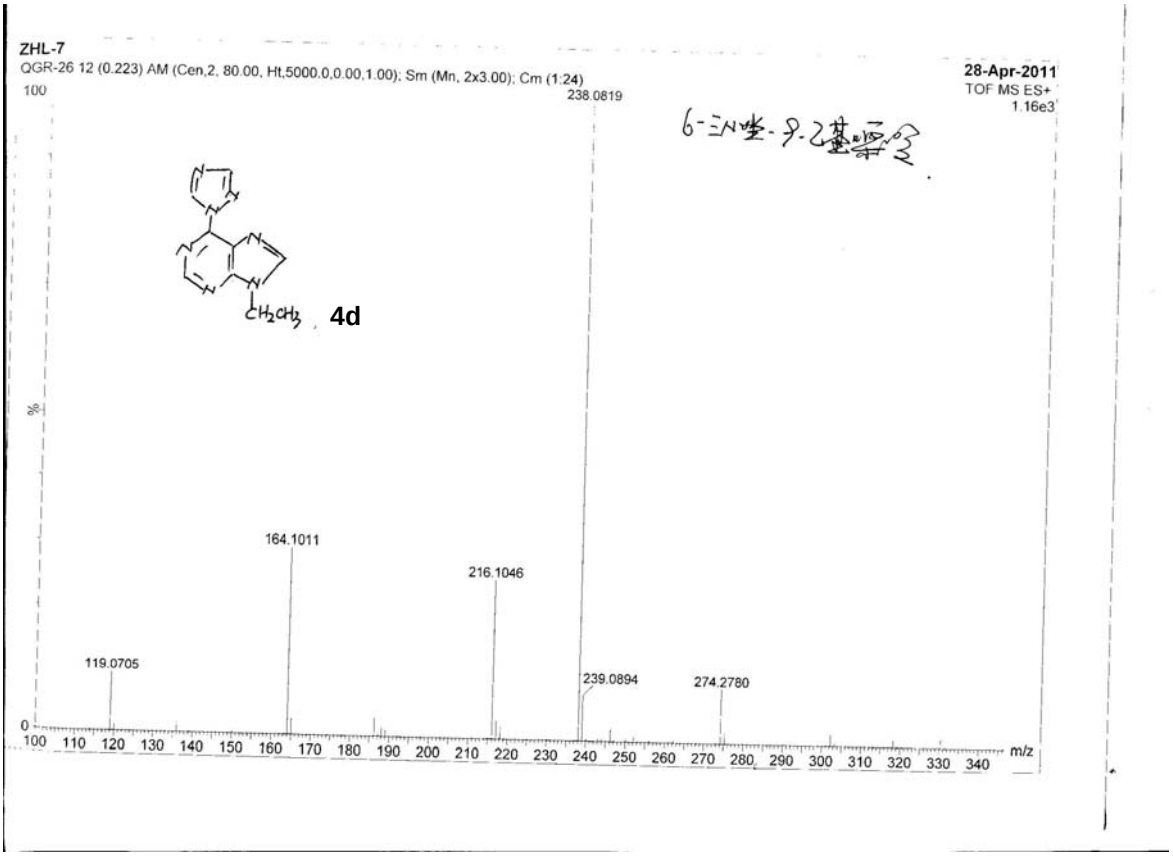

ZHL-17
QGR-36 17 (0.316) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:26)
28-Apr-2011
TOF MS ES+
1.25e3
468.1242
469.1367
484.1068
m/z
%

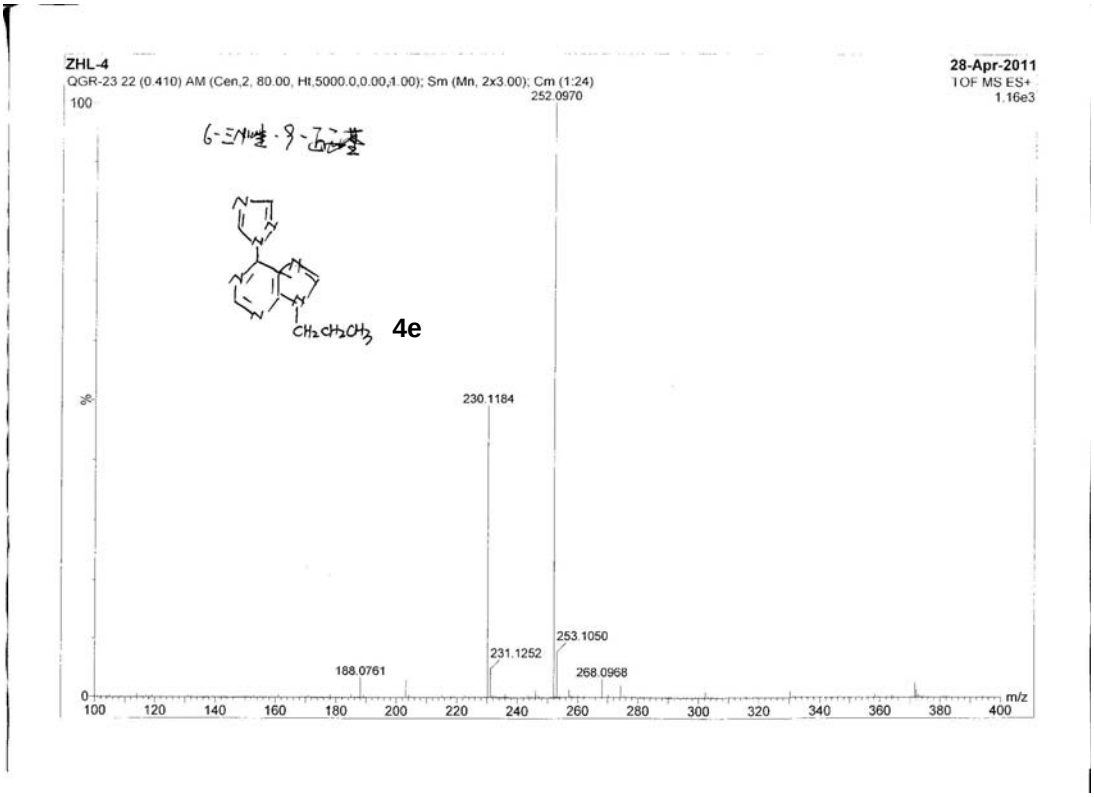
4a

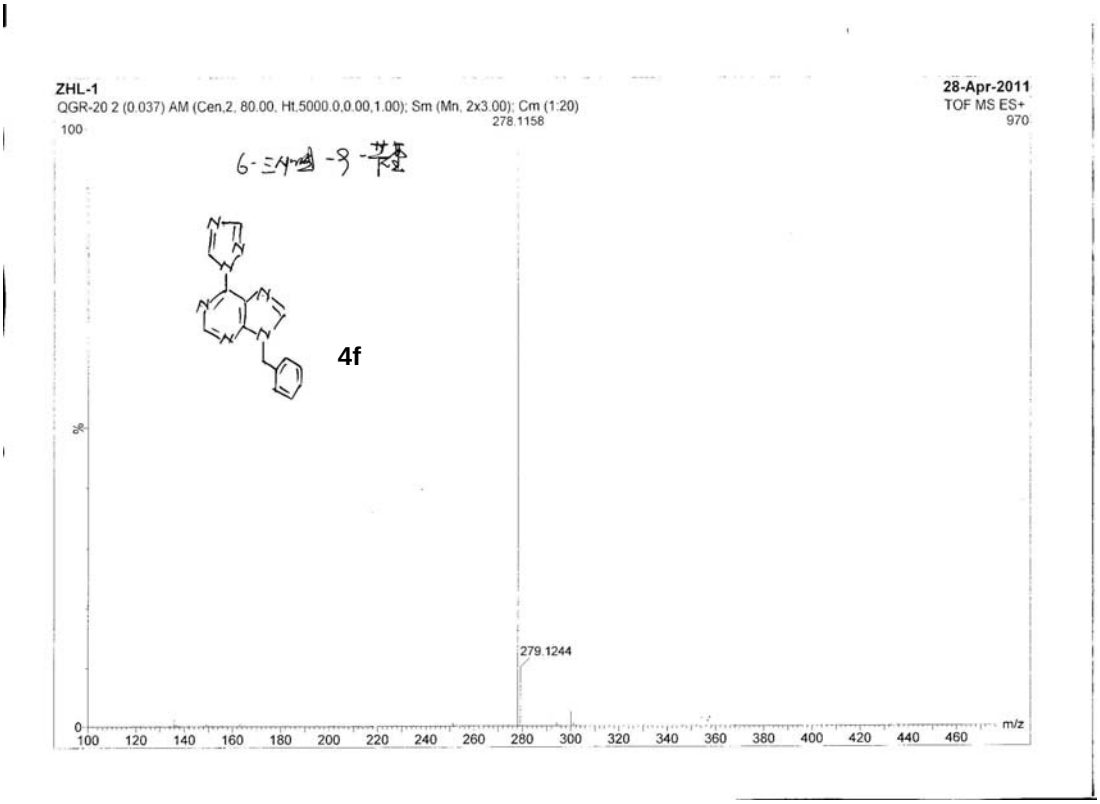

+MS, 0.1-0.1min #(3-6)
502.0852
981.2515
274.2767
167.1463
Intens.
x10^6
m/z
AcO
OAc
Cl

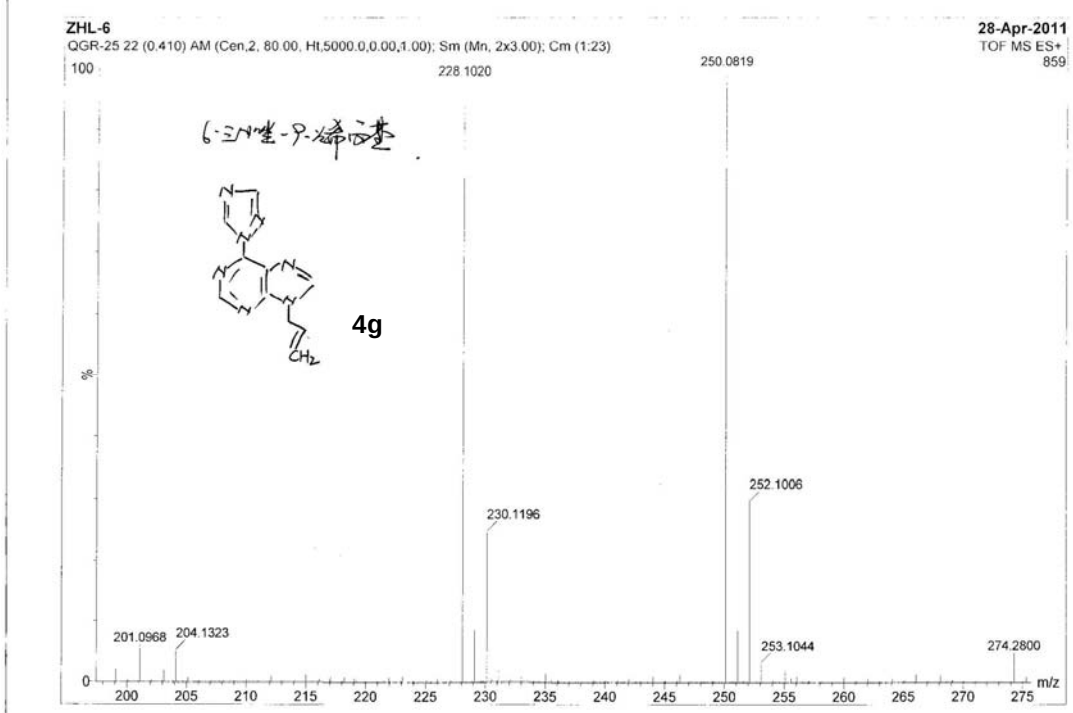
4b

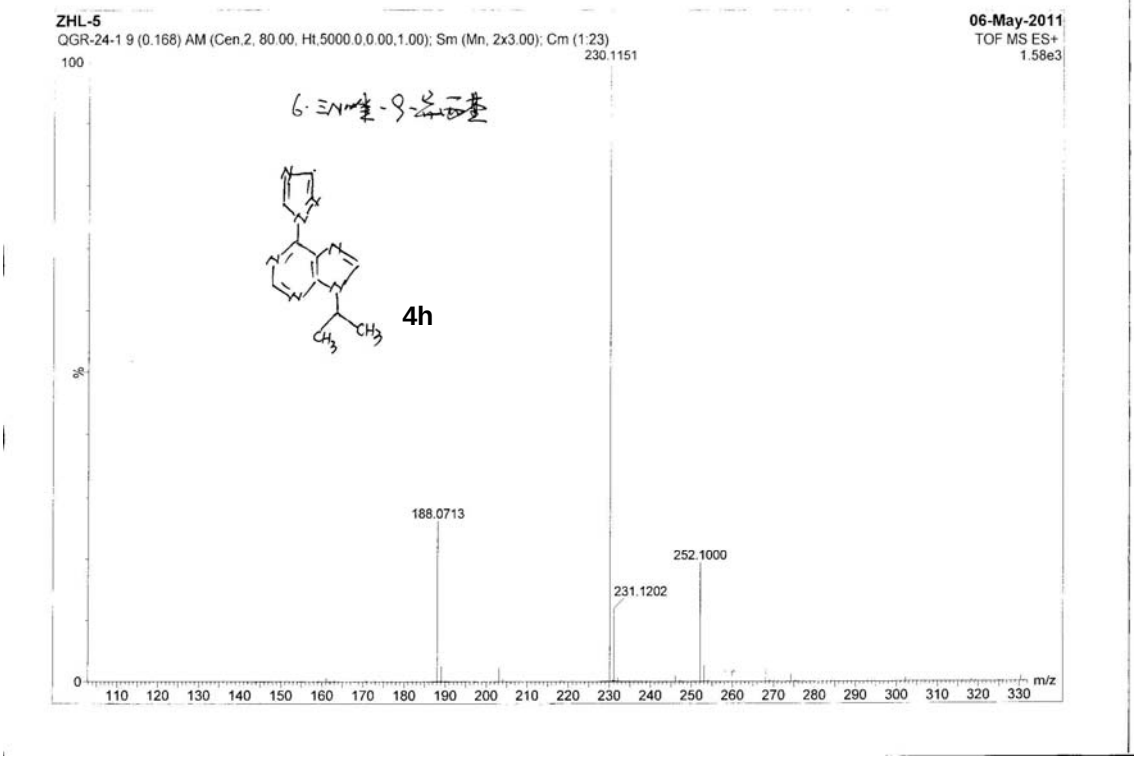

ZHL-3
QGR-22 5 (0.093) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:61)
28-Apr-2011
TOF MS ES+
651
202.0844
100
%
175.0773
203.0891
224.0675
0
100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320
m/z
4c

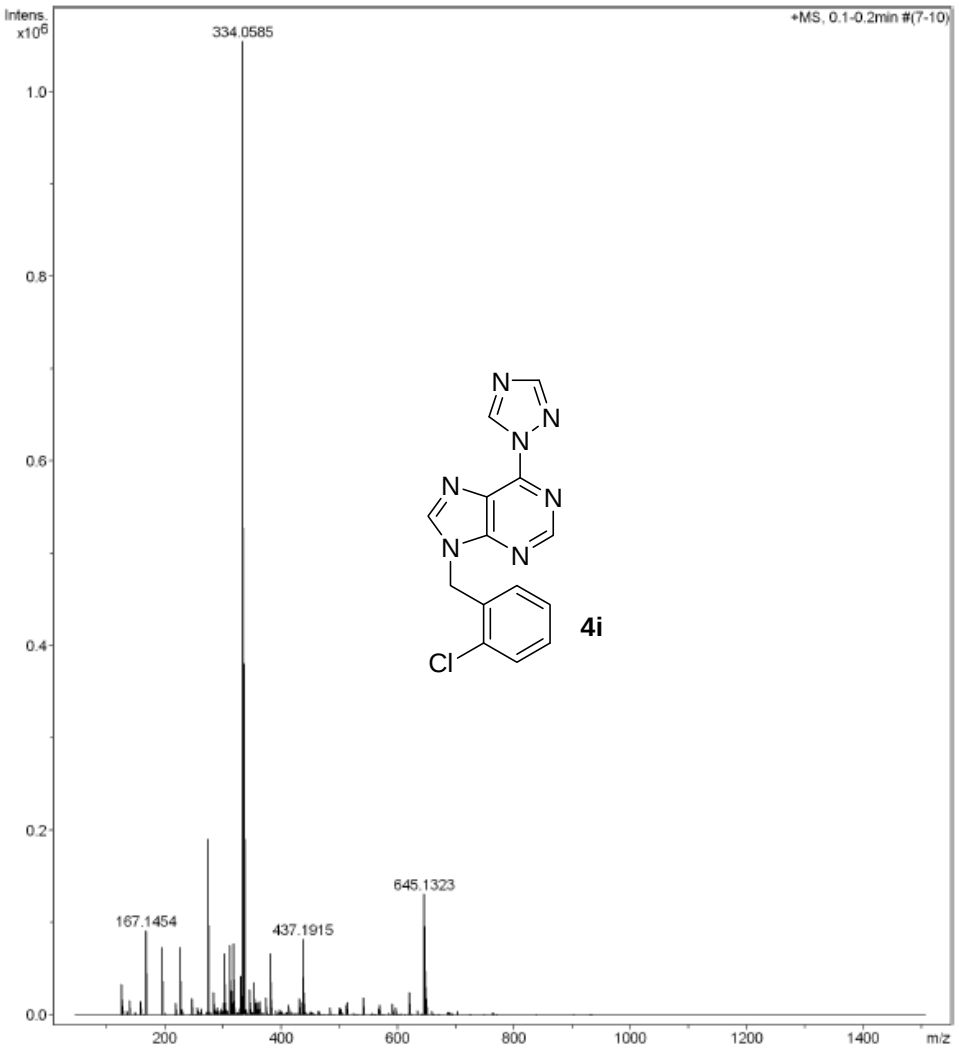

ZHL-7
QGR-26 12 (0.223) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:24)
28-Apr-2011
TOF MS ES+
1.16e3
100
238.0819
%
164.1011
216.1046
119.0705
239.0894
274.2780
0
100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340
m/z
4d


ZHL-4
QGR-23 22 (0.410) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:24)
28-Apr-2011
TOF MS ES+
1.16e3
252.0970
100
4e
230.1184
253.1050
231.1252
188.0761
268.0968
%
0
m/z
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400


ZHL-1
QGR-20 2 (0.037) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:20)
28-Apr-2011
TOF MS ES+
970
278.1158
100
4f
279.1244
%
0
m/z
100 120 140 160 180 200 220 240 260 280 300 320 340 360 380 400 420 440 460


ZHL-6
QGR-25 22 (0.410) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:23)
28-Apr-2011
TOF MS ES+
859
100
228.1020
250.0819
6-三氮唑-9-烯丙基
4g
252.1006
230.1196
201.0968
204.1323
253.1044
274.2800
%
0
200 205 210 215 220 225 230 235 240 245 250 255 260 265 270 275
m/z


ZHL-5
QGR-24-1 9 (0.168) AM (Cen,2, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 2x3.00); Cm (1:23)
06-May-2011
TOF MS ES+
1.58e3
100
230.1151
6-三氮唑-9-异丙基
4h
188.0713
252.1000
231.1202
%
0
110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330
m/z


Intens.
x10^6
+MS, 0.1-0.2min #(7-10)
334.0585
645.1323
437.1915
167.1454
1.0
0.8
0.6
0.4
0.2
0.0
200
400
600
800
1000
1200
1400
m/z
N
N
N
N
N
N
Cl
4i