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Supporting Information for

Nickel-Catalyzed sp^2 C-H Bonds Arylation of N-Aromatic Heterocycles with Grignard Reagents at Room Temperature

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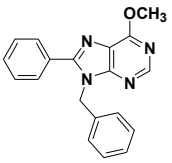
General:

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. Proton chemical shifts δ were given in ppm relative to tetramethylsilane (0.00 ppm) in $CDCl_3$ or to the residual proton signals of the deuterated solvent CD_3OD (3.31 ppm). 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 reactions were set up in air (with no use of a glove box) and carried out under nitrogen atmosphere. Ni(dppp)Cl_2 was purchased from commercial source and used as received. 1,2-Dichloroethane and THF were purified using standard methods before used. All other reagents were purchased from commercial sources and used as received.

General procedure for the Ni-catalyzed direct sp^2 C-H bond arylation of purine with Grignard reagents. An oven-dried Schlenk tube containing a stirbar was charged with purine derivatives (0.125 mmol) and Ni(dppp)Cl_2 (20 mg, 30 mol %). The Schlenk tube was fitted with a rubber cap, evacuated and back-filled with nitrogen (this sequence was repeated an additional two times). Then the 1,2-dichloroethane (0.03 mL, 3 equiv) was added to the tube along with THF (1 mL). The mixture was then stirred at room temperature. The Grignard reagent (5 equiv) was then added drop by drop via syringe and stirred for the corresponding reaction time at room temperature. After completion of the reaction, the mixture was then diluted with brine (3 mL) and extracted with ethyl acetate (3×3 mL). The organic layer was collected and dried over anhydrous Na_2SO4, filtered and concentrated under reduced pressure. The crude material was purified by column chromatography on silica gel (eluting with petroleum ether/ethyl acetate mixtures) to give the desired products.

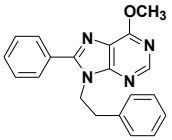
Characterization of compounds

9-Benzyl-6-methoxy-8-phenyl-9*H*-purine (3a)



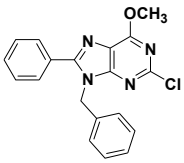
White solid. M.p. 98-100 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 7.68 (d, *J* = 7.2 Hz, 2H), 7.50-7.42 (m, 3H), 7.28 (d, *J* = 4.8 Hz, 3H), 7.07 (d, *J* = 7.6 Hz, 2H), 5.56 (s, 2H), 4.23 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 154.0, 153.3, 152.0, 136.2, 130.4, 129.3, 128.9, 128.7, 127.9, 126.5, 121.3, 54.3, 47.3. HRMS: calcd for $C_{19}H_{17}N_4O$ $[M+H]^+$ 317.1402, found 317.1404.

6-Methoxy-9-phenethyl-8-phenyl-9*H*-purine (3b)



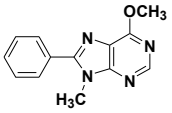
White solid. M.p. 110-112 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 7.50-7.40 (m, 5H), 7.14 (t, *J* = 2.4 Hz, 3H), 6.89 (s, 2H), 4.55 (t, *J* = 7.4 Hz, 2H), 4.19 (s, 3H), 3.08 (t, *J* = 7.4 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 153.6, 153.1, 151.6, 137.1, 130.1, 129.5, 129.1, 128.6, 126.8, 121.2, 54.1, 45.5, 35.5. HRMS: calcd for $C_{20}H_{19}N_4O$ $[M+H]^+$ 331.1559, found 331.1554.

9-Benzyl-2-chloro-6-methoxy-8-phenyl-9*H*-purine (3c)



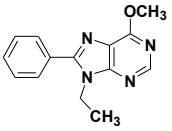
White solid. M.p. 133-135 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.2 Hz, 2H), 7.51-7.41 (m, 3H), 7.27 (s, 3H), 7.03 (t, *J* = 3.8 Hz, 2H), 5.51 (s, 2H), 4.24 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 155.4, 154.0, 152.9, 136.0, 130.8, 129.5, 129.2, 129.1, 129.0, 128.2, 126.9, 120.4, 55.3, 47.6. HRMS: calcd for $C_{19}H_{16}ClN_4O$ $[M+H]^+$ 351.1013, found 351.1010.

6-Methoxy-9-methyl-8-phenyl-9*H*-purine (3d)



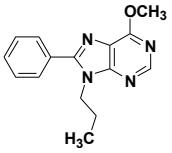
Yellow solid. M.p. 118-119 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 7.83 (q, *J* = 3 Hz, 2H), 7.53 (t, *J* = 3.2 Hz, 3H), 4.30 (s, 3H), 3.95 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 154.0, 152.9, 151.6, 130.3, 129.3, 129.2, 128.7, 121.3, 54.2, 31.0. HRMS: calcd for $C_{13}H_{13}N_4O$ $[M+H]^+$ 241.1089, found 241.1084.

9-Ethyl-6-methoxy-8-phenyl-9*H*-purine (3e)



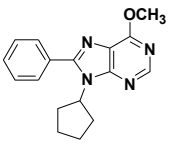
Yellow solid. M.p. 62-64 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (s, 1H), 7.71-7.69 (m, 2H), 7.44 (t, *J* = 3.2 Hz, 3H), 4.32 (q, *J* = 7.2 Hz, 2H), 4.13 (s, 3H), 1.38 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 153.5, 152.6, 151.5, 130.2, 129.6, 129.0, 128.7, 121.3, 54.0, 39.2, 15.2. HRMS: calcd for $C_{14}H_{15}N_4O$ $[M+H]^+$ 255.1246, found 255.1241.

6-Methoxy-8-phenyl-9-propyl-9*H*-purine (3f)



White solid. M.p. 76-77 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.53 (s, 1H), 7.73 (q, *J* = 3 Hz, 2H), 7.49 (t, *J* = 3.2 Hz, 3H), 4.29 (t, *J* = 7.6 Hz, 2H), 4.18 (s, 3H), 1.85-1.76 (m, 2H), 0.82 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 153.7, 152.9, 151.5, 130.2, 129.8, 129.1, 128.7, 121.2, 107.0, 54.1, 45.7, 23.1, 11.0. HRMS: calcd for $C_{15}H_{17}N_4O$ $[M+H]^+$ 269.1402, found 269.1404.

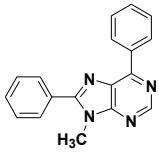
9-Cyclopentyl-6-methoxy-8-phenyl-9*H*-purine (3g)



Yellow solid. M.p. 103-105 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.52 (s, 1H), 7.68 (t, *J*

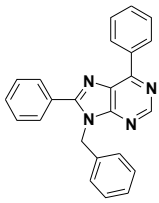
= 3.6 Hz, 2H), 7.52 (t, *J* = 2.8 Hz, 3H), 4.85-4.76 (m, 1H), 4.18 (s, 3H), 2.57 (q, *J* = 6.6 Hz, 2H), 2.12 (t, *J* = 7 Hz, 2H), 2.03 (q, *J* = 3.6 Hz, 2H), 1.65 (d, *J* = 5.6 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 153.5, 153.1, 150.8, 130.1, 129.6, 128.6, 122.0, 58.1, 53.9, 31.0, 24.8. HRMS: calcd for $C_{17}H_{19}N_4O$ $[M+H]^+$ 295.1559, found 295.1554.

9-Methyl-6,8-diphenyl-9*H*-purine (3h)



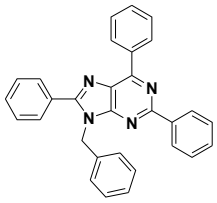
White solid. M.p. 138-140 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (s, 1H), 8.89 (d, *J* = 7.2 Hz, 2H), 7.86-7.84 (m, 2H), 7.53-7.45 (m, 6H), 3.90 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.9, 154.6, 153.6, 151.8, 135.9, 131.0, 130.7, 130.6, 129.8, 129.4, 129.3, 128.9, 128.5, 30.7. HRMS: calcd for $C_{18}H_{15}N_4$ $[M+H]^+$ 287.1297, found 287.1295.

9-Benzyl-6,8-diphenyl-9*H*-purine (3i)



White solid. M.p. 130-132 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (s, 1H), 8.92 (d, *J* = 7.6 Hz, 2H), 7.70 (d, *J* = 8 Hz, 2H), 7.56-7.42 (m, 6H), 7.25 (d, *J* = 6.4 Hz, 3H), 7.07 (d, *J* = 6.8 Hz, 2H), 5.55 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.3, 154.6, 153.9, 152.3, 136.2, 135.9, 131.0, 130.8, 130.7, 129.9, 129.5, 129.4, 128.9, 128.9, 128.6, 127.9, 126.6, 47.1. HRMS: calcd for $C_{24}H_{19}N_4$ $[M+H]^+$ 363.1610, found 363.1607.

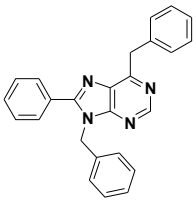
9-Benzyl-2,6,8-triphenyl-9*H*-purine (3j)



Light yellow solid. M.p. 200-202 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.11 (d, *J* = 7.6

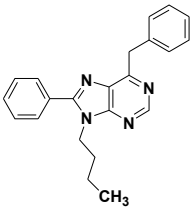
Hz, 2H), 8.73 (d, *J* = 7.2 Hz, 2H), 7.76 (d, *J* = 7.2 Hz, 2H), 7.62 (t, *J* = 7.6 Hz, 2H), 7.56-7.48 (m, 7H), 7.29 (t, *J* = 8.4 Hz, 3H), 7.20 (d, *J* = 7.2 Hz, 2H), 5.64 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.3, 155.6, 155.3, 153.4, 138.6, 136.6, 136.4, 130.7, 130.5, 129.9, 129.8, 129.7, 129.5, 128.9, 128.8, 128.6, 128.4, 128.3, 127.9, 127.1, 47.1. HRMS: calcd for $C_{30}H_{23}N_4$ $[M+H]^+$ 439.1923, found 439.1917.

6,9-Dibenzyl-8-phenyl-9*H*-purine (3k)



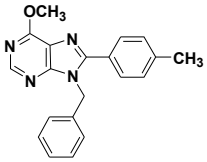
White solid. M.p. 102-104 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (s, 1H), 7.67 (d, *J* = 7.2 Hz, 2H), 7.55-7.49 (m, 5H), 7.29 (q, *J* = 7.6 Hz, 5H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.08 (d, *J* = 4.8 Hz, 2H), 5.52 (s, 2H), 4.60 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.0, 153.9, 152.5, 152.5, 144.5, 141.9, 138.4, 136.0, 133.6, 132.7, 131.7, 131.2, 130.4, 130.1, 128.8, 128.2, 127.8, 124.3, 61.8, 14.3. HRMS: calcd for $C_{25}H_{21}N_4$ $[M+H]^+$ 377.1766, found 377.1760.

6-Benzyl-9-butyl-8-phenyl-9*H*-purine (3l)



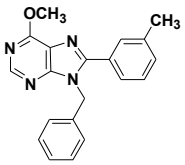
Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.92 (s, 1H), 7.77 (t, *J* = 3.6 Hz, 2H), 7.58 (t, *J* = 3 Hz, 3H), 7.51 (d, *J* = 7.2 Hz, 2H), 7.29 (t, *J* = 7.4 Hz, 2H), 7.20 (t, *J* = 7.2 Hz, 1H), 4.57 (s, 2H), 4.33 (t, *J* = 7.8 Hz, 2H), 1.79 (t, *J* = 7.6 Hz, 2H), 1.28 (q, *J* = 7.6 Hz, 2H), 0.86 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.0, 155.1, 153.1, 152.4, 138.3, 132.6, 130.8, 130.1, 129.7, 129.5, 129.2, 128.7, 126.7, 43.9, 39.4, 31.9, 20.0, 13.7. HRMS: calcd for $C_{22}H_{23}N_4$ $[M+H]^+$ 343.1927, found 343.1918.

9-Benzyl-6-methoxy-8-(*p*-tolyl)-9*H*-purine (3m)



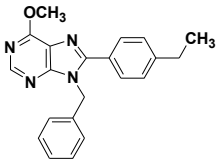
Yellow solid. M.p. 109-111 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 7.59 (d, *J* = 8 Hz, 2H), 7.27 (q, *J* = 7.6 Hz, 5H), 7.09 (d, *J* = 6.4 Hz, 2H), 5.56 (s, 2H), 4.24 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 154.0, 153.5, 151.9, 140.7, 136.3, 129.4, 129.2, 128.9, 127.8, 126.5, 126.4, 121.2, 54.2, 47.3, 21.4. HRMS: calcd for $C_{20}H_{19}N_4O$ $[M+H]^+$ 331.1559, found 331.1556.

9-Benzyl-6-methoxy-8-(*m*-tolyl)-9*H*-purine (3n)



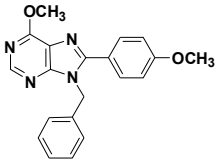
Yellow solid. M.p. 74-76 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57 (s, 1H), 7.52 (s, 1H), 7.42 (d, *J* = 6 Hz, 1H), 7.28 (q, *J* = 5.2 Hz, 5H), 7.07 (d, *J* = 6.4 Hz, 2H), 5.53 (s, 2H), 4.22 (s, 3H), 2.34 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 154.0, 153.5, 151.9, 138.6, 136.3, 131.1, 130.2, 129.1, 128.9, 128.5, 127.9, 126.6, 126.1, 121.2, 54.2, 47.4, 21.3. HRMS: calcd for $C_{20}H_{19}N_4O$ $[M+H]^+$ 331.1559, found 331.1554.

9-Benzyl-8-(4-ethylphenyl)-6-methoxy-9*H*-purine (3o)



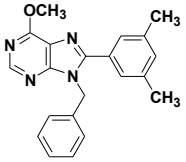
Light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (s, 1H), 7.61 (d, *J* = 8 Hz, 2H), 7.27 (t, *J* = 7.2 Hz, 5H), 7.08 (d, *J* = 6.4 Hz, 2H), 5.55 (s, 2H), 4.23 (s, 3H), 2.70 (q, *J* = 7.2 Hz, 2H), 1.26 (t, *J* = 7.6 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 154.0, 153.5, 151.8, 146.9, 136.3, 129.3, 128.9, 128.2, 127.8, 126.6, 126.4, 121.3, 54.2, 47.3, 28.7, 15.2. HRMS: calcd for $C_{21}H_{21}N_4O$ $[M+H]^+$ 345.1715, found 345.1714.

9-Benzyl-6-methoxy-8-(4-methoxyphenyl)-9*H*-purine (3p)



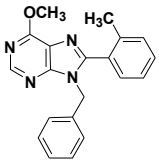
Yellow solid. M.p. 114-116 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 7.63 (d, *J* = 8.8 Hz, 2H), 7.28 (q, *J* = 7.6 Hz, 3H), 7.08 (d, *J* = 6.8 Hz, 2H), 6.94 (d, *J* = 8.4 Hz, 2H), 5.54 (s, 2H), 4.23 (s, 3H), 3.84 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.3, 160.6, 154.1, 153.3, 151.7, 136.3, 130.8, 128.9, 127.8, 126.4, 121.6, 121.2, 114.1, 55.3, 54.2, 47.3. HRMS: calcd for $C_{20}H_{19}N_4O_2$ $[M+H]^+$ 347.1508, found 347.1505.

9-Benzyl-8-(3,5-dimethylphenyl)-6-methoxy-9*H*-purine (3q)



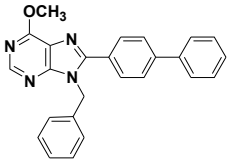
Light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 7.29 (d, *J* = 10 Hz, 5H), 7.11 (d, *J* = 6 Hz, 3H), 5.53 (s, 2H), 4.23 (s, 3H), 2.29 (s, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.7, 154.1, 153.7, 151.9, 138.3, 136.5, 132.0, 129.0, 128.8, 127.8, 127.1, 126.7, 121.2, 107.0, 54.2, 47.4, 21.1. HRMS: calcd for $C_{21}H_{21}N_4O$ $[M+H]^+$ 345.1715, found 345.1716.

9-Benzyl-6-methoxy-8-(*o*-tolyl)-9*H*-purine (3r)



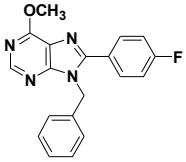
White solid. M.p. 112-114 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (s, 1H), 7.43-7.39 (m, 1H), 7.29 (s, 1H), 7.25-7.14 (m, 5H), 6.89 (d, *J* = 6.4 Hz, 2H), 5.27 (s, 2H), 4.22 (s, 3H), 2.00 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 153.2, 153.1, 152.1, 138.6, 136.0, 130.7, 130.5, 130.2, 129.4, 128.8, 128.2, 127.9, 125.9, 121.3, 54.4, 47.1, 19.7. HRMS: calcd for $C_{20}H_{19}N_4O$ $[M+H]^+$ 331.1559, found 331.1554.

8-([1,1'-Biphenyl]-4-yl)-9-benzyl-6-methoxy-9*H*-purine (3s)



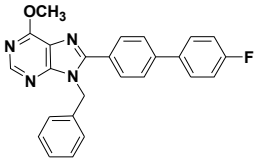
Light yellow solid. M.p. 134-136 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 7.77 (d, *J* = 8.4 Hz, 2H), 7.66 (d, *J* = 8.4 Hz, 2H), 7.61 (d, *J* = 7.6 Hz, 2H), 7.44 (t, *J* = 7.4 Hz, 2H), 7.36 (t, *J* = 7.2 Hz, 1H), 7.28 (t, *J* = 7.6 Hz, 3H), 7.11 (dt, *J* = 6.4 Hz, 2H), 5.59 (s, 2H), 4.24 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.8, 154.1, 153.0, 152.0, 143.15, 139.8, 136.2, 129.7, 129.0, 128.9, 128.1, 128.0, 127.9, 127.3, 127.1, 126.4, 121.4, 54.3, 47.4. HRMS: calcd for $C_{25}H_{21}N_4O$ $[M+H]^+$ 393.1715, found 393.1713.

9-Benzyl-8-(4-fluorophenyl)-6-methoxy-9*H*-purine (3t)



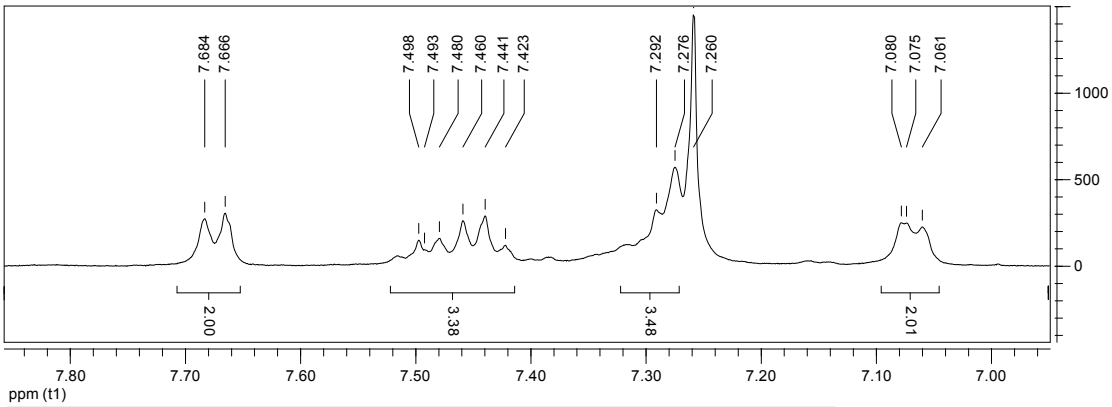
Light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 7.68-7.64 (m, 2H), 7.49-7.42 (m, 1H), 7.28 (t, *J* = 5.6 Hz, 2H), 7.13 (t, *J* = 8.6 Hz, 2H), 7.06 (t, *J* = 3.4 Hz, 2H), 5.54 (d, *J* = 8 Hz, 2H), 4.24 (d, *J* = 4.8 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 154.2, 152.5, 152.4, 136.2, 131.6, 131.6, 129.5, 129.2, 129.1, 128.9, 128.2, 126.6, 121.4, 116.3, 116.1, 54.5, 47.5. HRMS: calcd for $C_{19}H_{16}FN_4O$ $[M+H]^+$ 335.1308, found 335.1310.

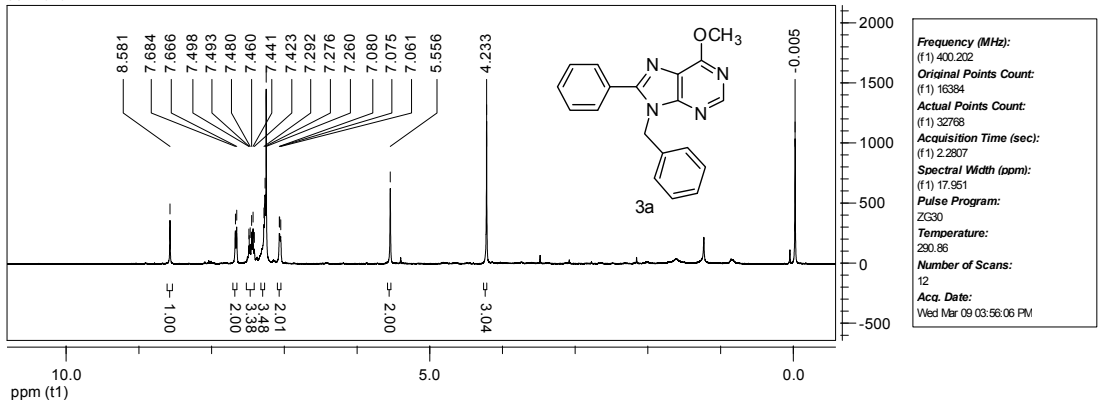
9-Benzyl-8-(4'-fluoro-[1,1'-biphenyl]-4-yl)-6-methoxy-9*H*-purine (3u)

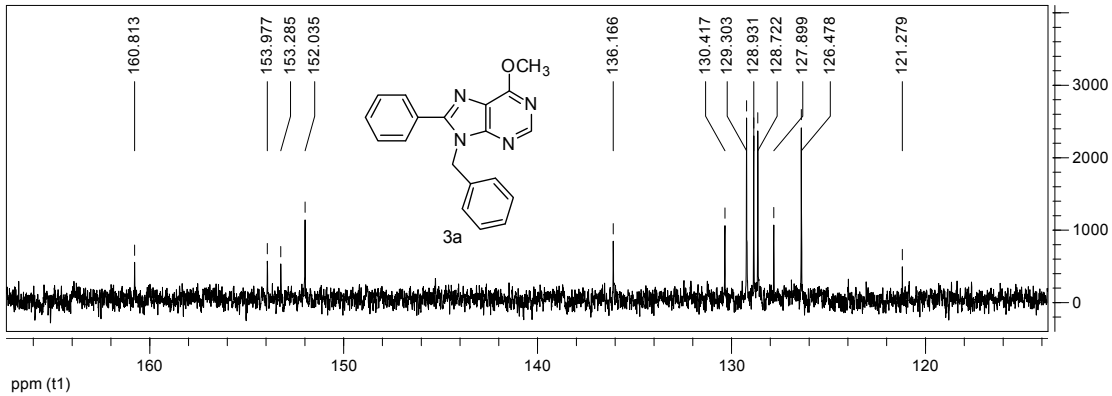


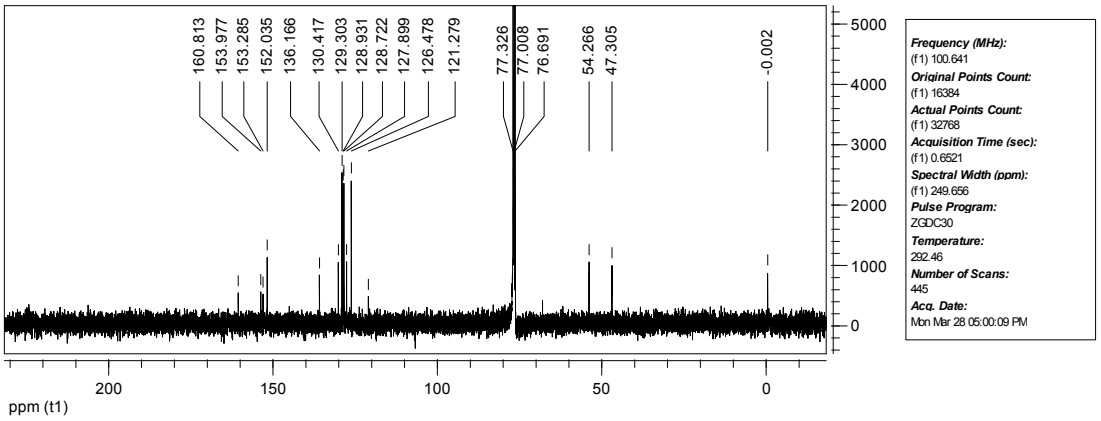
Yellow solid. M.p. 154-156 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 7.76 (d, *J* = 8.4 Hz, 2H), 7.62-7.56 (m, 4H), 7.29 (t, *J* = 6.8 Hz, 3H), 7.13 (q, *J* = 8.6 Hz, 4H), 5.60 (d, *J* = 6 Hz, 2H), 4.24 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 154.3, 153.1, 152.3, 142.3, 136.4, 136.2, 130.0, 129.2, 129.0, 128.9, 128.3, 128.2, 127.4, 126.6, 121.6, 116.2, 116.0, 54.5, 47.6. HRMS: calcd for $C_{25}H_{20}FN_4O$ $[M+H]^+$ 411.1621, found 411.1624.

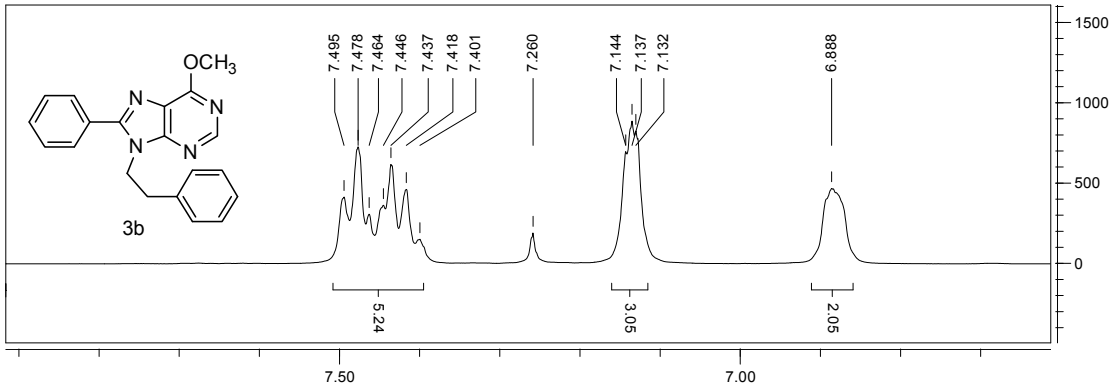
Copies of ^{1}H and ^{13}C NMR spectra







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N
N
3b
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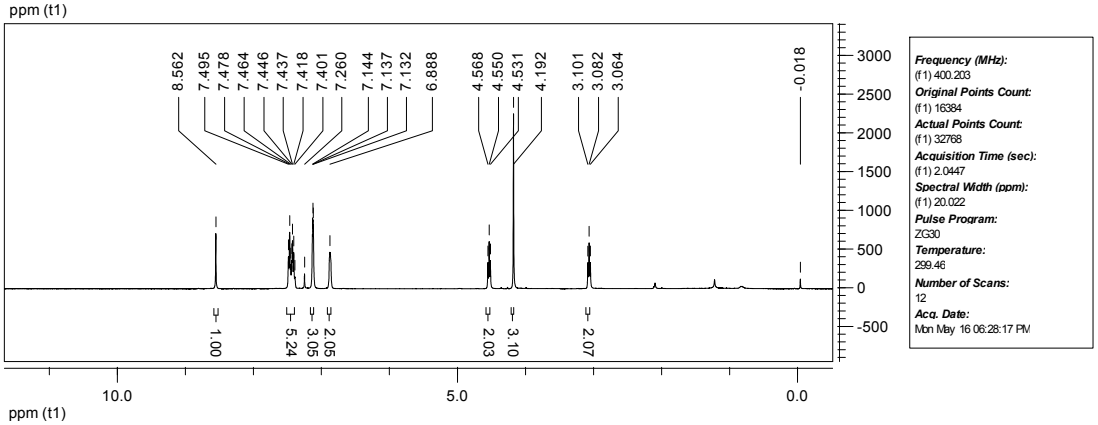
7.478
7.464
7.446
7.437
7.418
7.401
7.260
7.144
7.137
7.132
6.888
5.24
3.05
2.05
7.50
7.00
ppm (t1)


8.562
7.495
7.478
7.464
7.446
7.437
7.418
7.401
7.260
7.144
7.137
7.132
6.888
4.568
4.550
4.531
4.192
3.101
3.082
3.064
-0.018
1.00
5.24
3.05
2.05
2.03
3.10
2.07
10.0
5.0
0.0
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Actual Points Count:
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Spectral Width (ppm):
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Pulse Program:
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Temperature:
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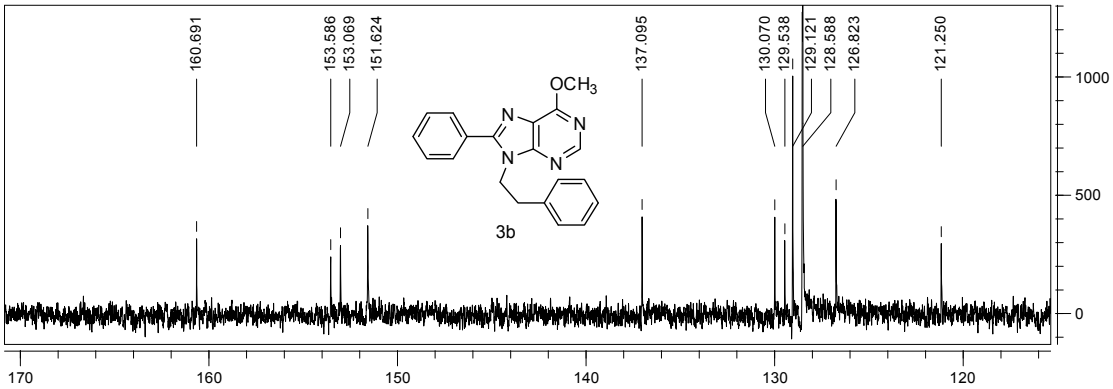
Acq. Date:
Mon May 16 06:28:17 PM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153.586
153.069
151.624
137.095
130.070
129.538
129.121
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OCH3
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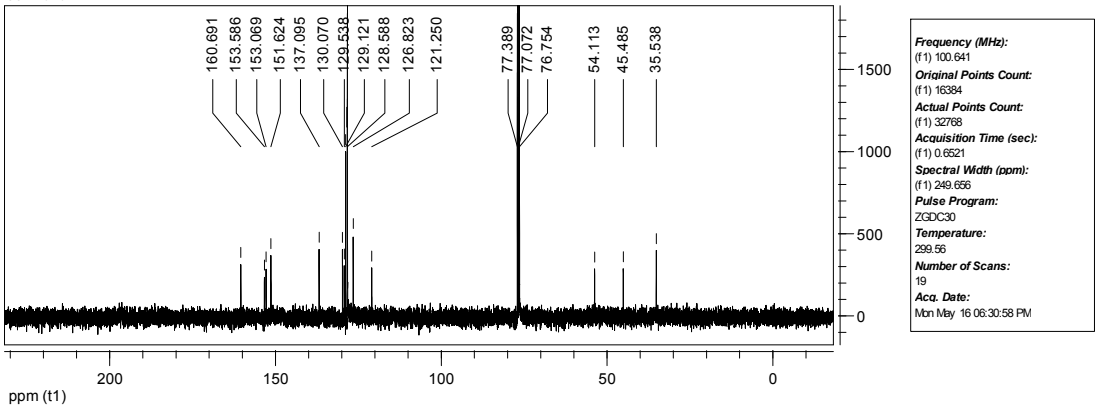
N
N
N
3b
170
160
150
140
130
120
ppm (t1)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153.069
151.624
137.095
130.070
129.538
129.121
128.588
126.823
121.250
77.389
77.072
76.754
54.113
45.485
35.538
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150
100
50
0
ppm (t1)
Frequency (MHz):
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Original Points Count:
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Actual Points Count:
(f1) 32768
Acquisition Time (sec):
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Spectral Width (ppm):
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Pulse Program:
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Temperature:
299.56
Number of Scans:
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Acq. Date:
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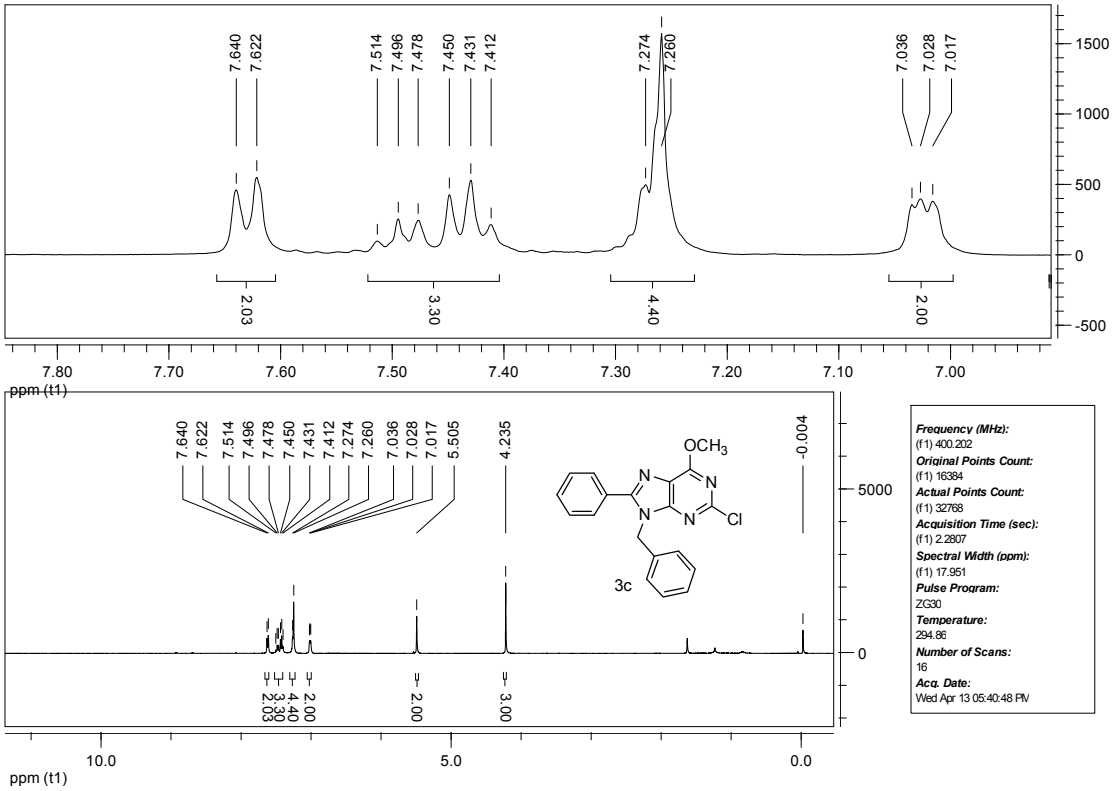
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7.514
7.496
7.478
7.450
7.431
7.412
7.274
7.260
7.036
7.028
7.017
2.03
3.30
4.40
2.00
ppm (t1)
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4.235
-0.004
OCH3
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Cl
3c
2.00
3.00
Frequency (MHz):
(f1) 400.202
Original Points Count:
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Actual Points Count:
(f1) 32768
Acquisition Time (sec):
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Spectral Width (ppm):
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Pulse Program:
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Temperature:
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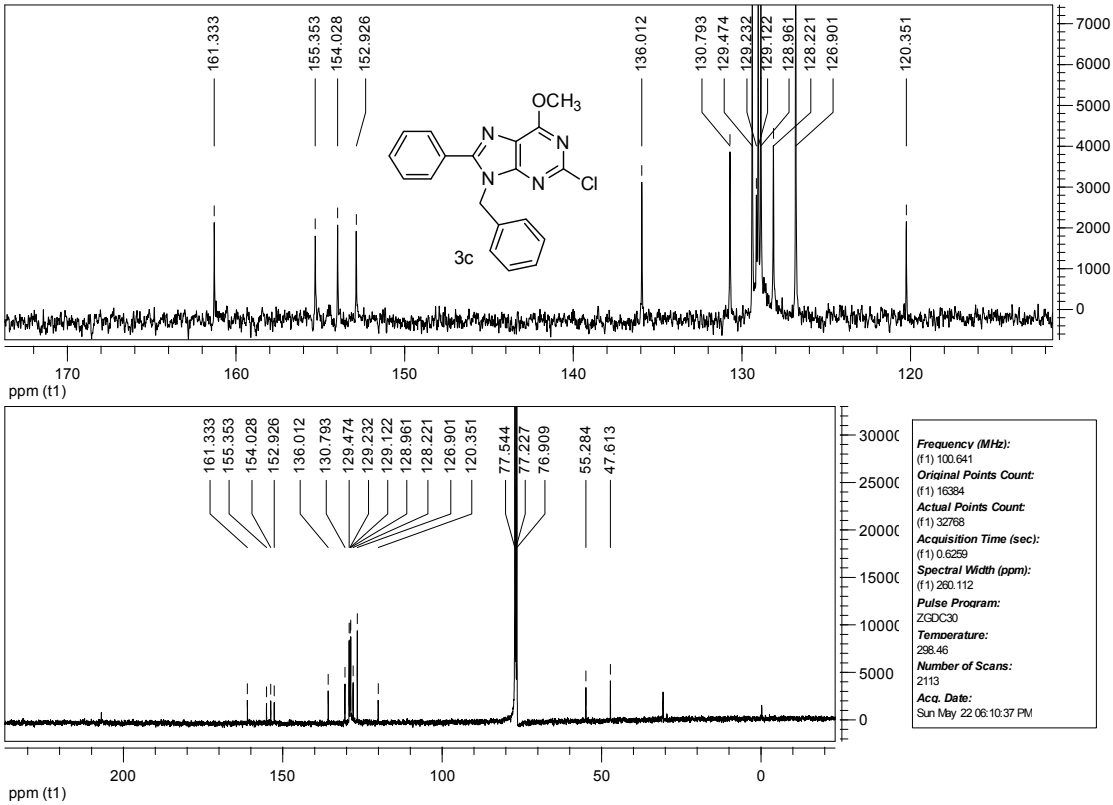
Acq. Date:
Wed Apr 13 05:40:48 PM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152.926
136.012
130.793
129.474
129.232
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126.901
120.351
OCH3
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Cl
3c
ppm (t1)
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77.227
76.909
55.284
47.613
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Actual Points Count:
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Spectral Width (ppm):
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Temperature:
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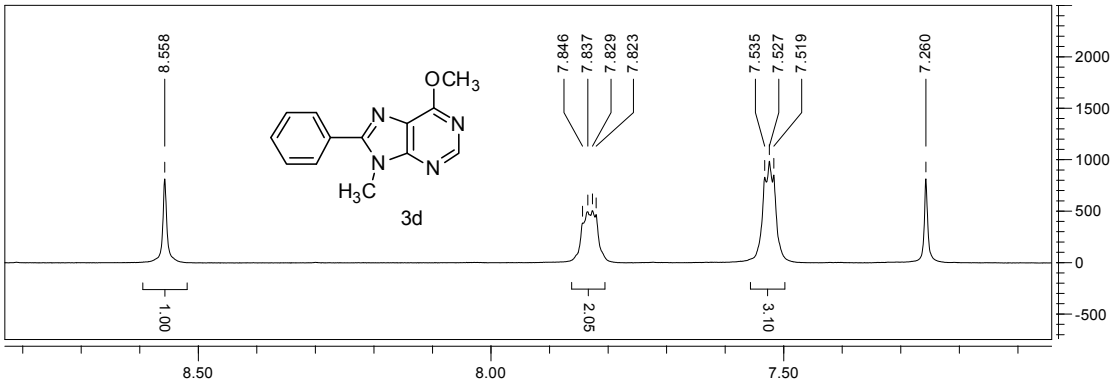
Acq. Date:
Sun May 22 06:10:37 PM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7.846
7.837
7.829
7.823
7.535
7.527
7.519
7.260
OCH3
N
N
N
N
H3C
3d
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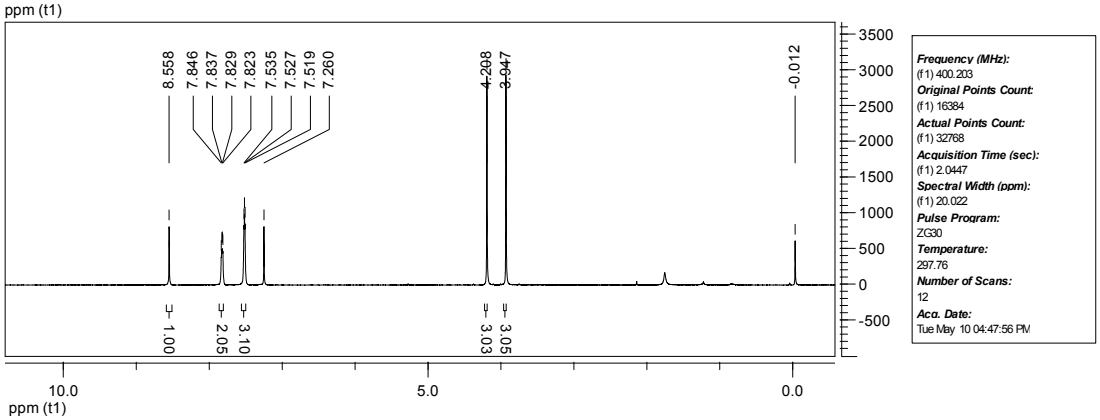
2.05
3.10
2000
1500
1000
500
0
-500
8.50
8.00
7.50
ppm (t1)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7.846
7.837
7.829
7.823
7.535
7.527
7.519
7.260
4.298
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-0.012
1.00
2.05
3.10
3.03
3.05
3500
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2500
2000
1500
1000
500
0
-500
10.0
5.0
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ppm (t1)
Frequency (MHz):
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Original Points Count:
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Actual Points Count:
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Acquisition Time (sec):
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Spectral Width (ppm):
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Pulse Program:
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Temperature:
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Number of Scans:
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Acq. Date:
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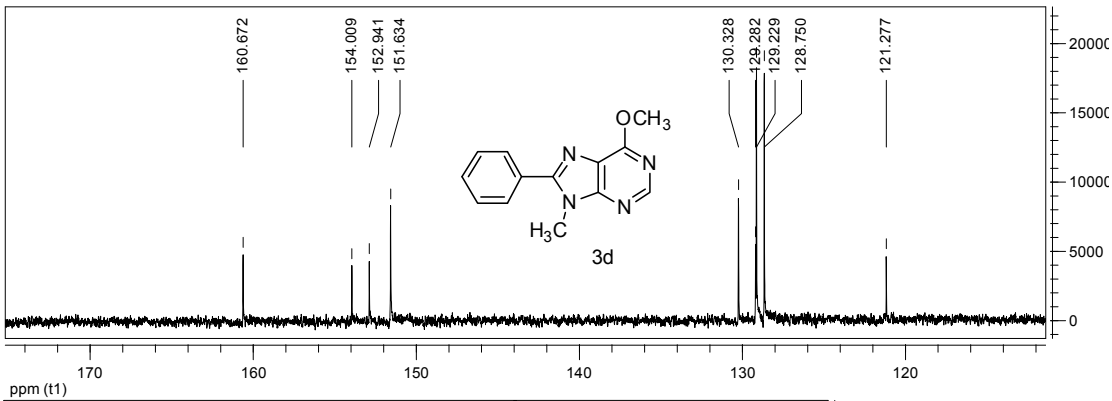
160.672
154.009
152.941
151.634
130.328
129.282
129.229
128.750
121.277
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N
N
H3C
3d
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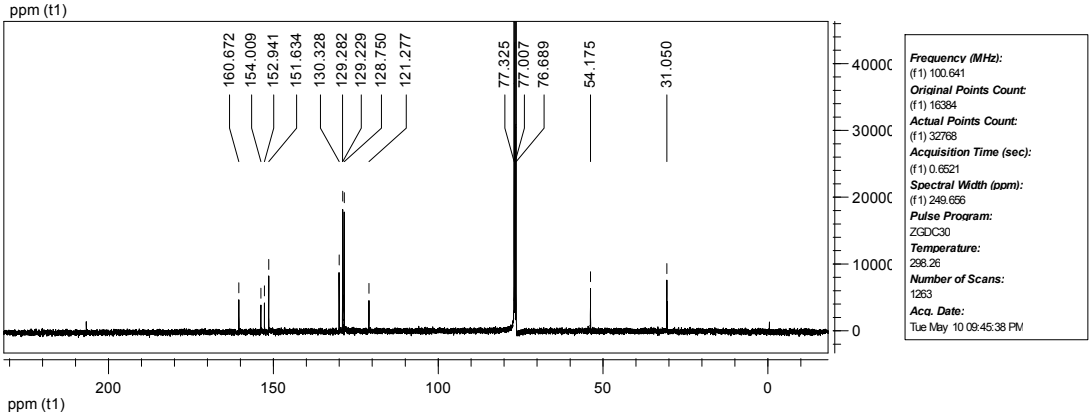
170
160
150
140
130
120
ppm (t1)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152.941
151.634
130.328
129.282
129.229
128.750
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77.325
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54.175
31.050
40000
30000
20000
10000
0
200
150
100
50
0
ppm (t1)
Frequency (MHz):
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Original Points Count:
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Actual Points Count:
(f1) 32768
Acquisition Time (sec):
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Spectral Width (ppm):
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Pulse Program:
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Temperature:
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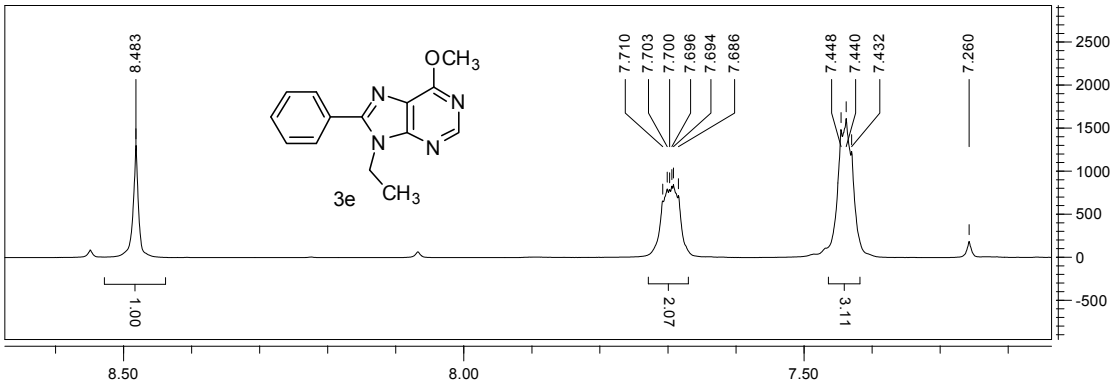
Number of Scans:
1263
Acq. Date:
Tue May 10 09:45:38 PM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7.700
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7.694
7.686
7.448
7.440
7.432
7.260
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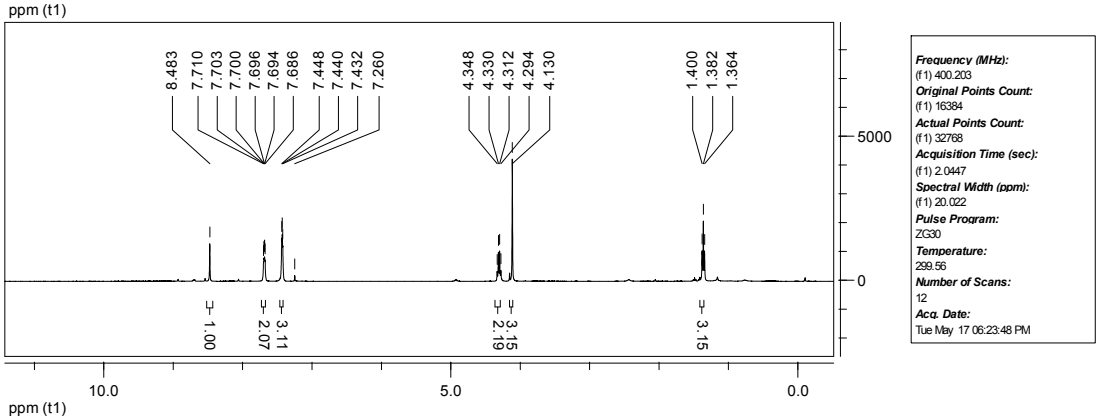
N
N
N
CH3
3e
1.00
2.07
3.11
ppm (t1)


8.483
7.710
7.703
7.700
7.696
7.694
7.686
7.448
7.440
7.432
7.260
4.348
4.330
4.312
4.294
4.130
1.400
1.382
1.364
1.00
2.07
3.11
2.19
3.15
3.15
ppm (t1)
Frequency (MHz):
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Original Points Count:
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Actual Points Count:
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Acquisition Time (sec):
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Spectral Width (ppm):
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Temperature:
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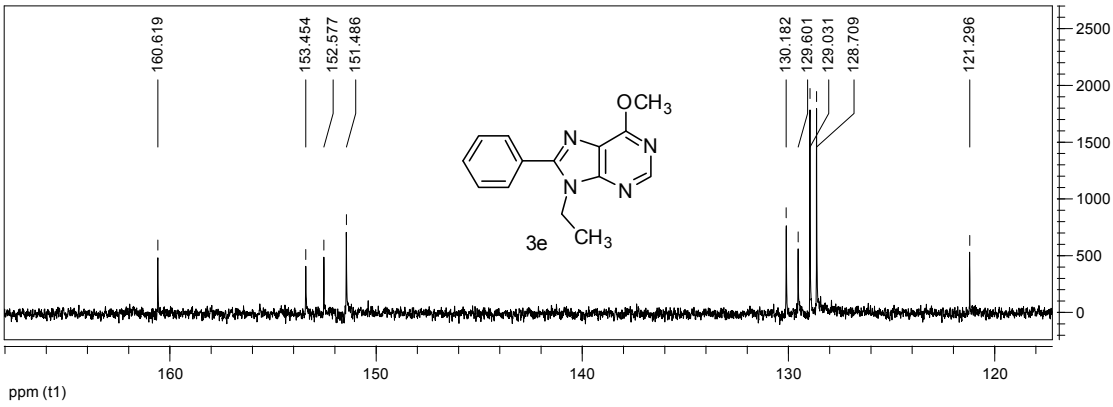
Acq. Date:
Tue May 17 06:23:48 PM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129.031
128.709
121.296
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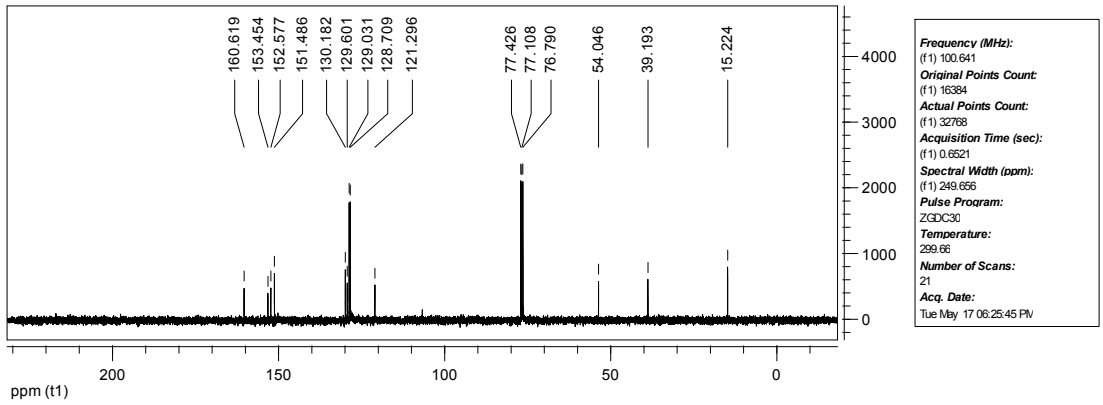
N
N
N
N
CH3
3e
ppm (t1)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153.454
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129.601
129.031
128.709
121.296
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77.108
76.790
54.046
39.193
15.224
ppm (t1)
Frequency (MHz):
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Original Points Count:
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Actual Points Count:
(f1) 32768
Acquisition Time (sec):
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Spectral Width (ppm):
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Pulse Program:
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Temperature:
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Acq. Date:
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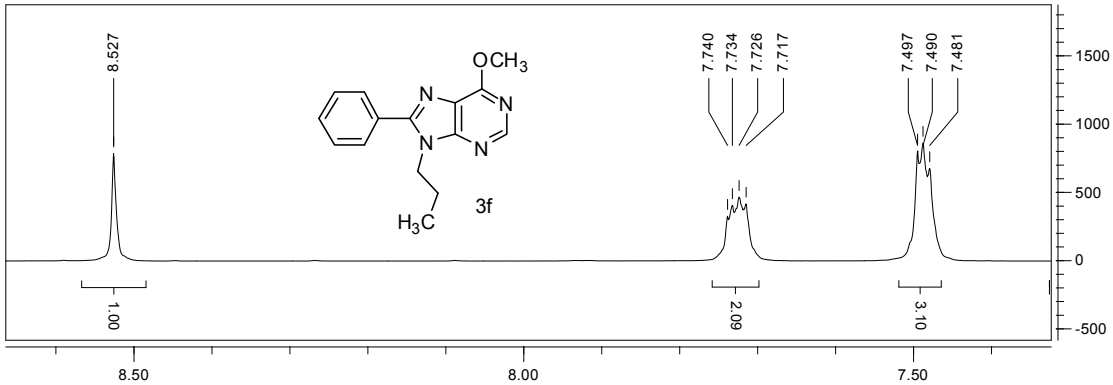
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7.490
7.481
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N
N
N
H3C
3f
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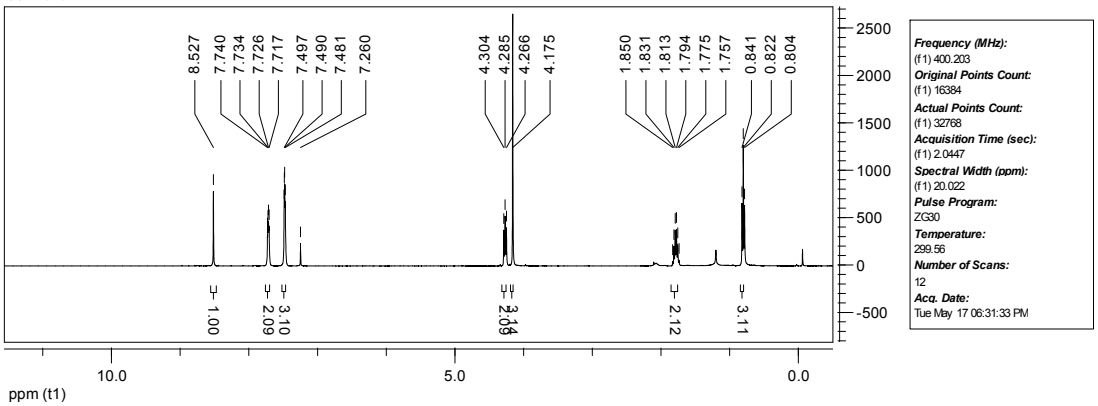
2.09
3.10
ppm (t1)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7.490
7.481
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4.175
1.850
1.831
1.813
1.794
1.775
1.757
0.841
0.822
0.804
1.00
2.09
3.10
2.12
3.11
ppm (t1)
Frequency (MHz):
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Original Points Count:
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Actual Points Count:
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Acquisition Time (sec):
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Spectral Width (ppm):
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Pulse Program:
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Temperature:
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Acq. Date:
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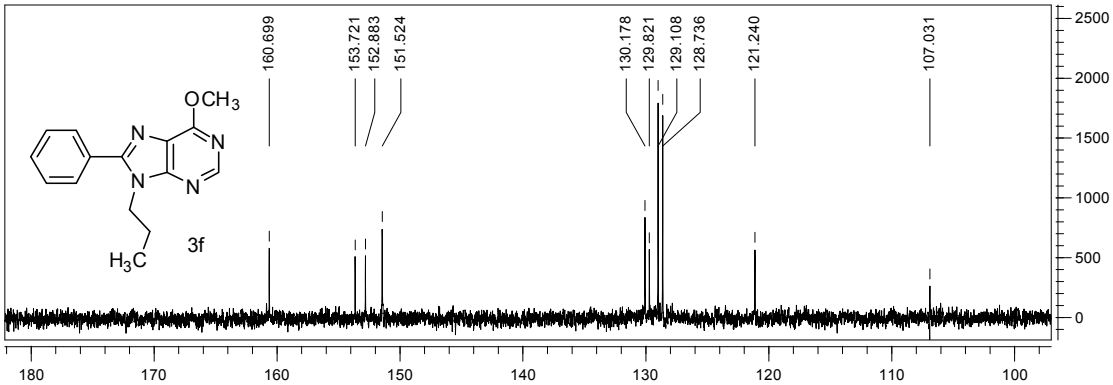
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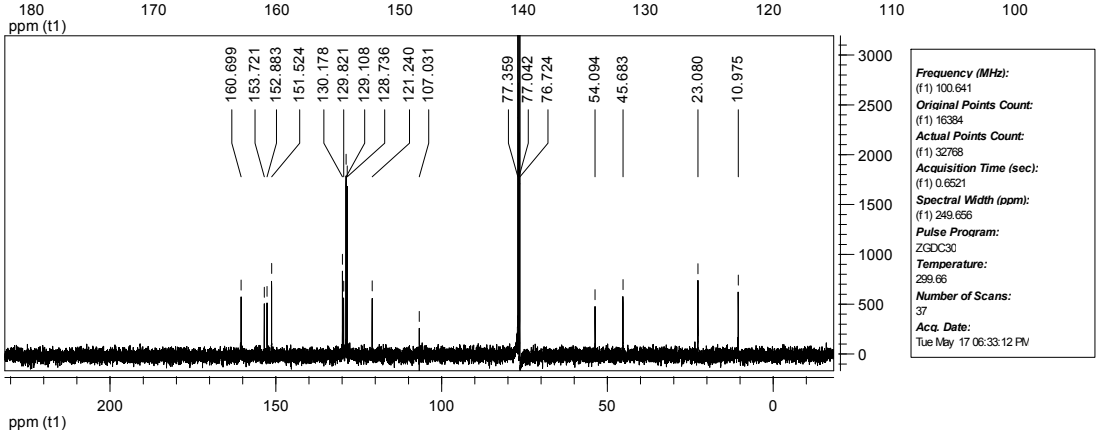
N
N
N
H3C
3f
ppm (t1)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107.031
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76.724
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45.683
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ppm (t1)
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Original Points Count:
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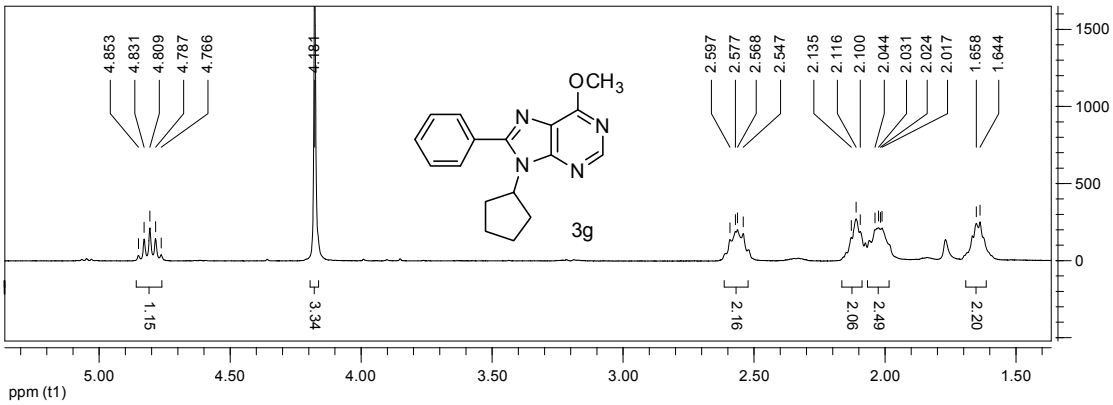
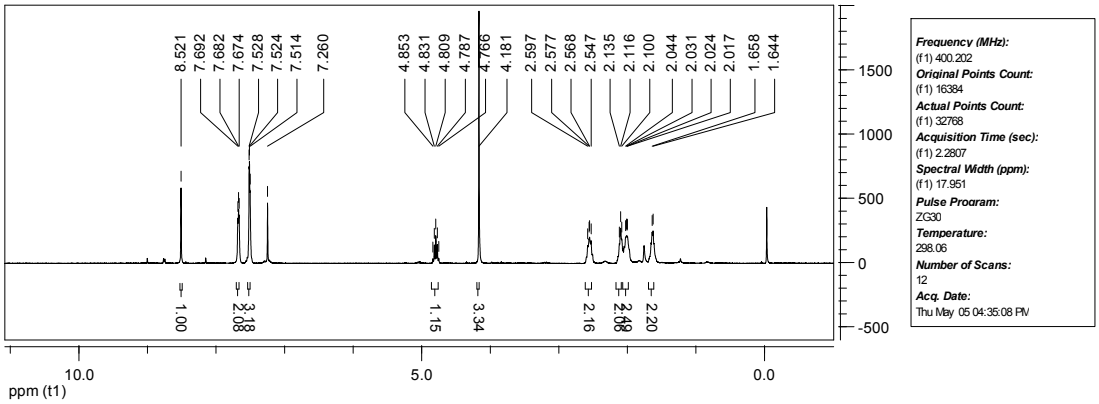
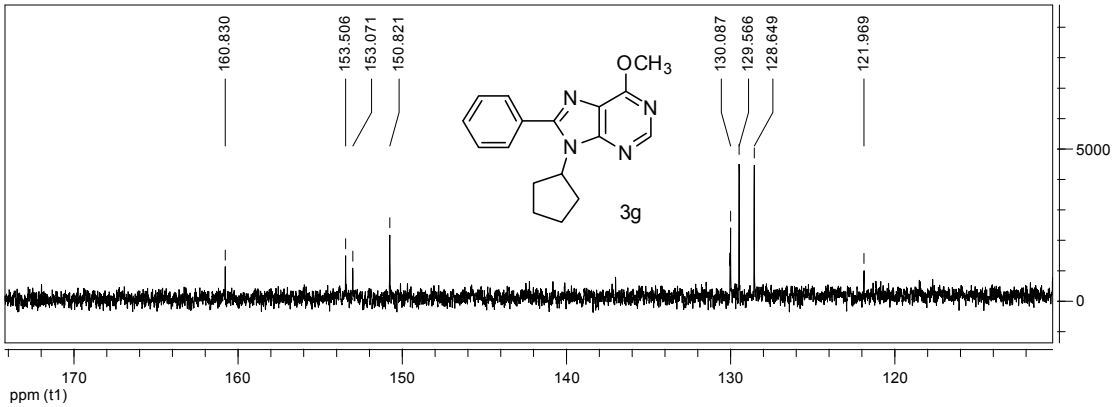
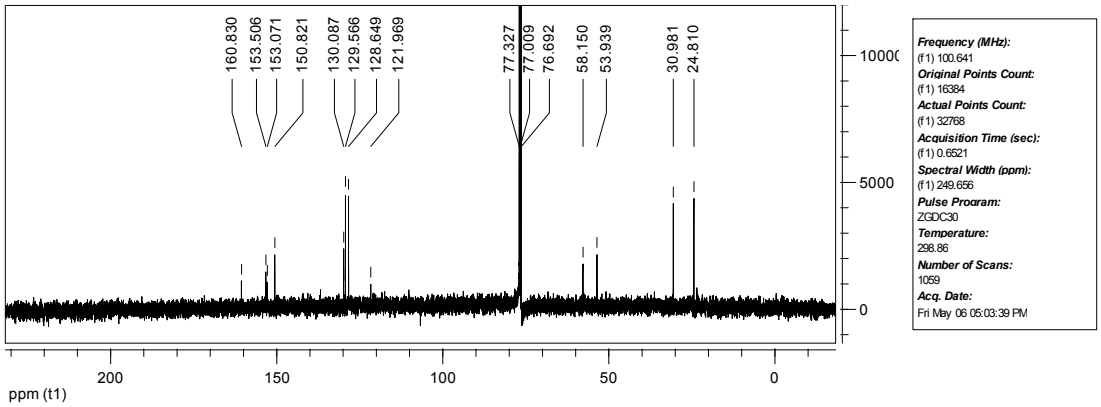
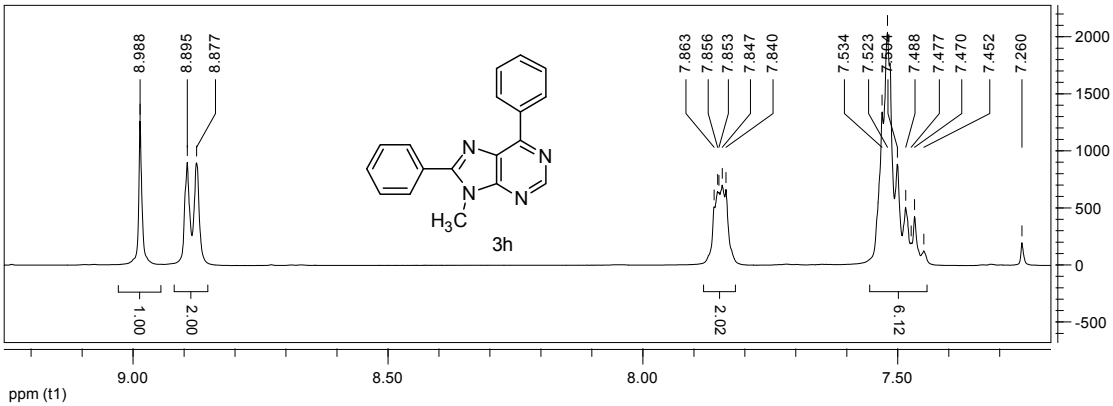
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
299.66
Number of Scans:
37
Acq. Date:
Tue May 17 06:33:12 PM

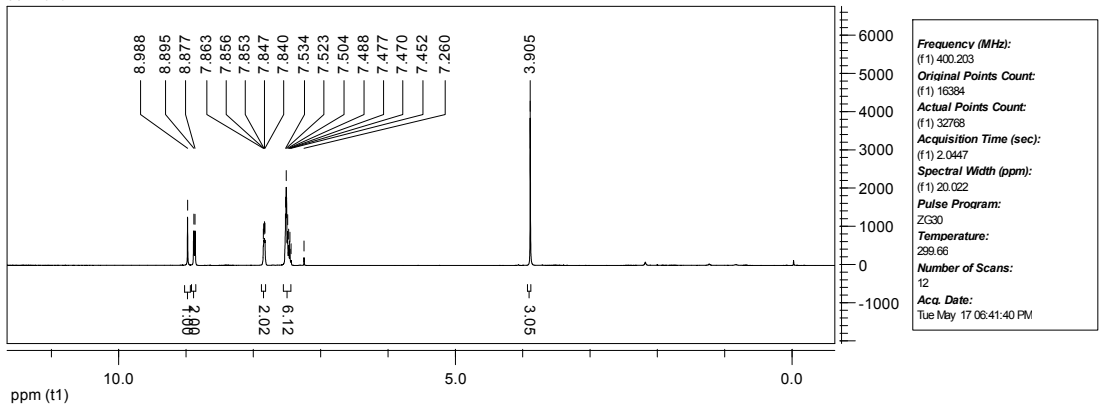

4.853
4.831
4.809
4.787
4.766
4.181
2.597
2.577
2.568
2.547
2.135
2.116
2.100
2.044
2.031
2.024
2.017
1.658
1.644
OCH3
N
N
N
N
3g
1.15
3.34
2.16
2.06
2.49
2.20
1500
1000
500
0
5.00
4.50
4.00
3.50
3.00
2.50
2.00
1.50
ppm (t1)

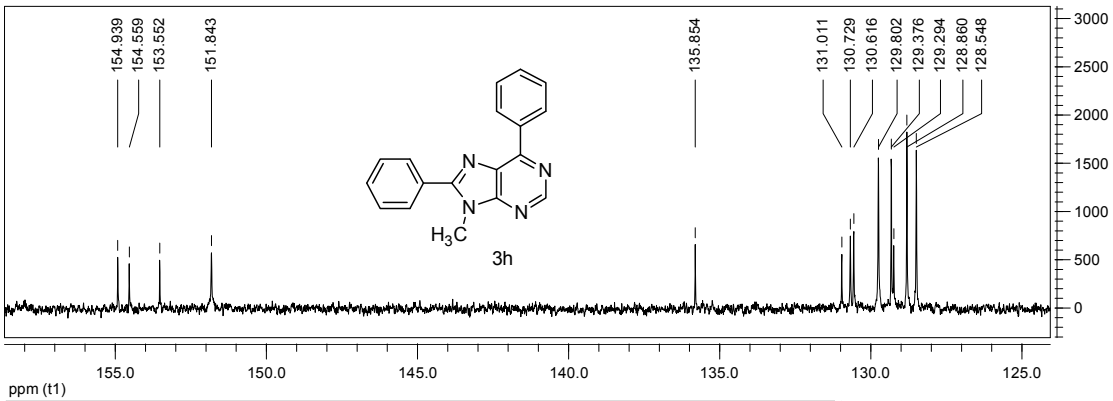

8.521
7.692
7.682
7.674
7.528
7.524
7.514
7.260
4.853
4.831
4.809
4.787
4.766
4.181
2.597
2.577
2.568
2.547
2.135
2.116
2.100
2.044
2.031
2.024
2.017
1.658
1.644
1.00
2.08
3.18
1.15
3.34
2.16
2.08
2.20
1500
1000
500
0
-500
10.0
5.0
0.0
ppm (t1)
Frequency (MHz):
(f1) 400.202
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.2807
Spectral Width (ppm):
(f1) 17.951
Pulse Program:
ZG30
Temperature:
298.06
Number of Scans:
12
Acq. Date:
Thu May 05 04:35:08 PM

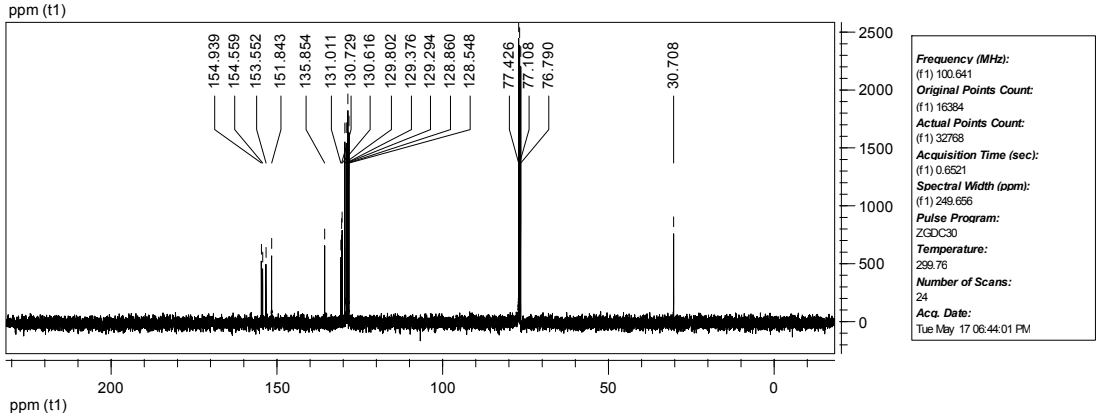

160.830
153.506
153.071
150.821
130.087
129.566
128.649
121.969
OCH3
N
N
N
N
3g
5000
0
170
160
150
140
130
120
ppm (t1)

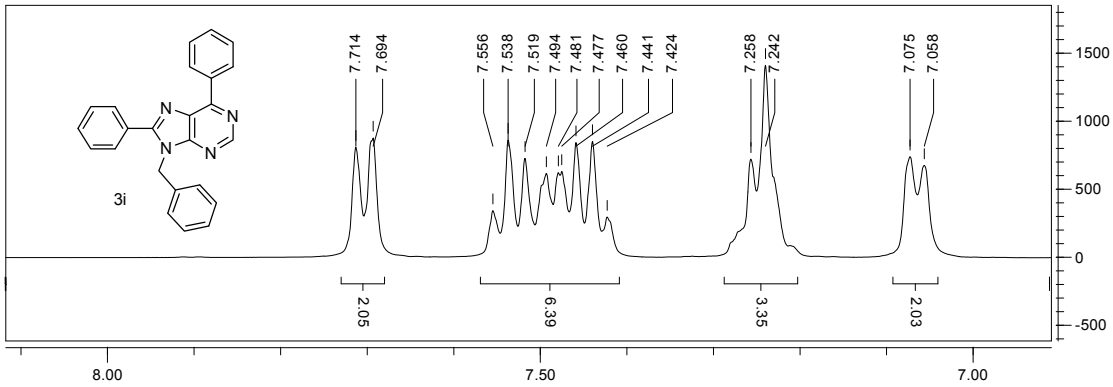

160.830
153.506
153.071
150.821
130.087
129.566
128.649
121.969
77.327
77.009
76.692
58.150
53.939
30.981
24.810
10000
5000
0
200
150
100
50
0
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
298.86
Number of Scans:
1059
Acq. Date:
Fri May 06 05:03:39 PM

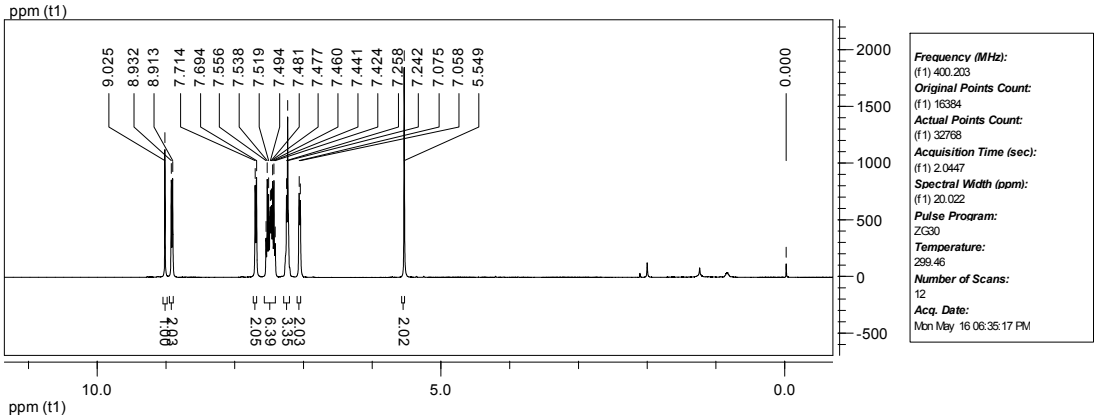

8.988
8.895
8.877
7.863
7.856
7.853
7.847
7.840
7.534
7.523
7.504
7.488
7.477
7.470
7.452
7.260
N
N
N
N
H3C
3h
1.00
2.00
2.02
6.12
9.00
8.50
8.00
7.50
ppm (t1)

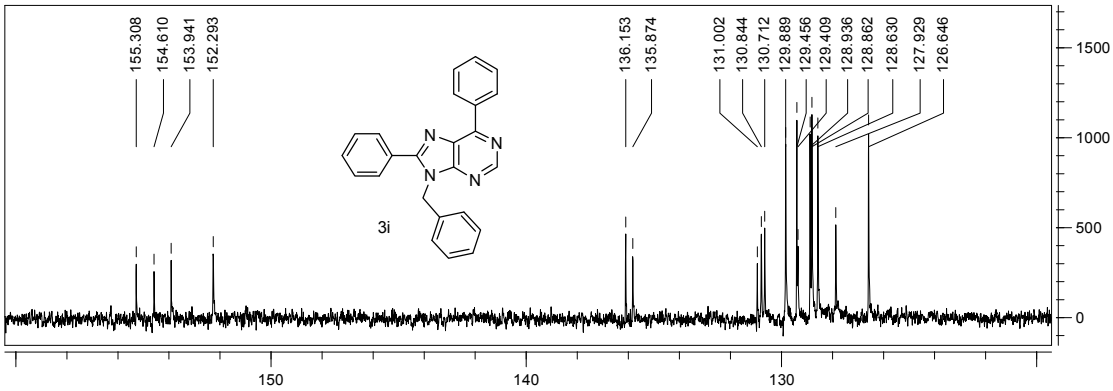

8.988
8.895
8.877
7.863
7.856
7.853
7.847
7.840
7.534
7.523
7.504
7.488
7.477
7.470
7.452
7.260
3.905
2.00
2.02
6.12
3.05
10.0
5.0
0.0
ppm (t1)
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
299.66
Number of Scans:
12
Acq. Date:
Tue May 17 06:41:40 PM

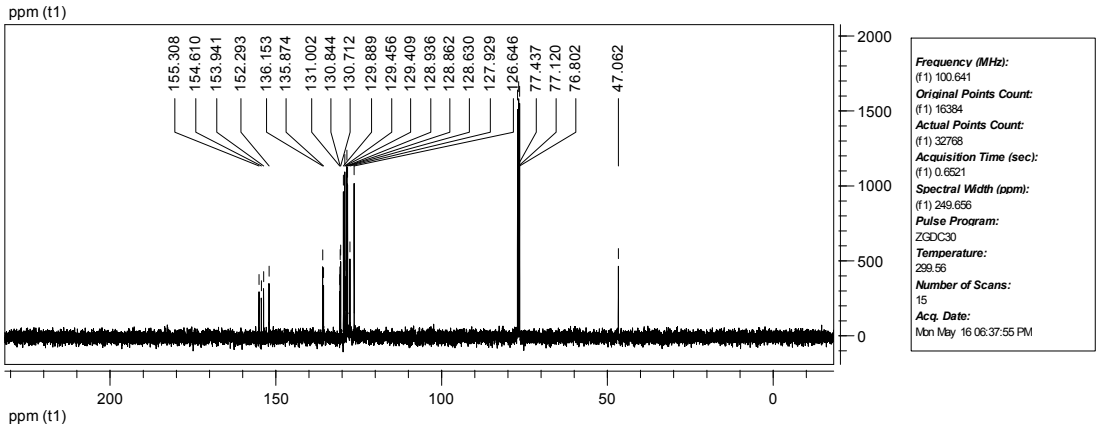

154.939
154.559
153.552
151.843
135.854
131.011
130.729
130.616
129.802
129.376
129.294
128.860
128.548
N
N
N
N
H3C
3h
155.0
150.0
145.0
140.0
135.0
130.0
125.0
ppm (t1)

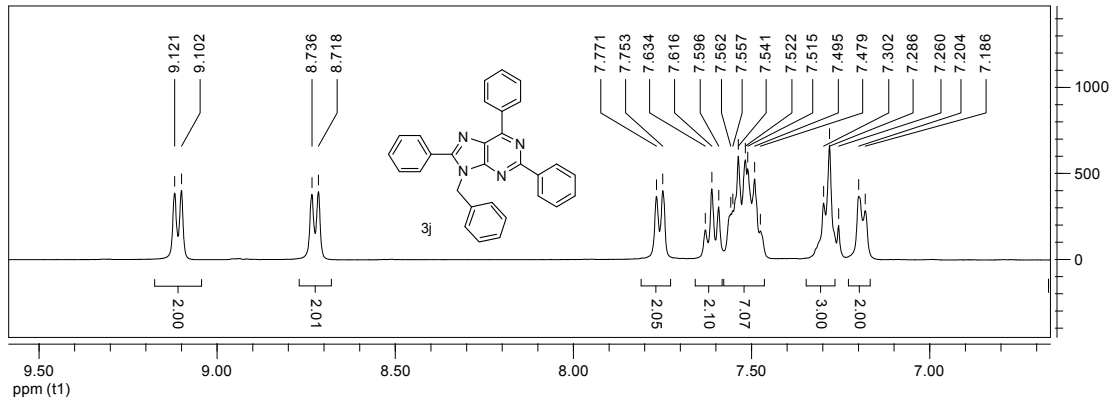

154.939
154.559
153.552
151.843
135.854
131.011
130.729
130.616
129.802
129.376
129.294
128.860
128.548
77.426
77.108
76.790
30.708
200
150
100
50
0
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
299.76
Number of Scans:
24
Acq. Date:
Tue May 17 06:44:01 PM

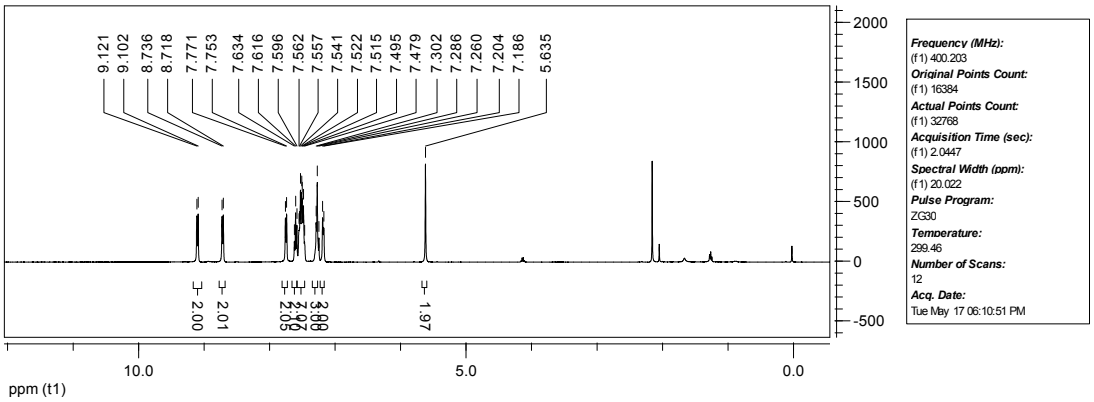

3i
7.714
7.694
7.556
7.538
7.519
7.494
7.481
7.477
7.460
7.441
7.424
7.258
7.242
7.075
7.058
2.05
6.39
3.35
2.03
8.00
7.50
7.00
ppm (t1)

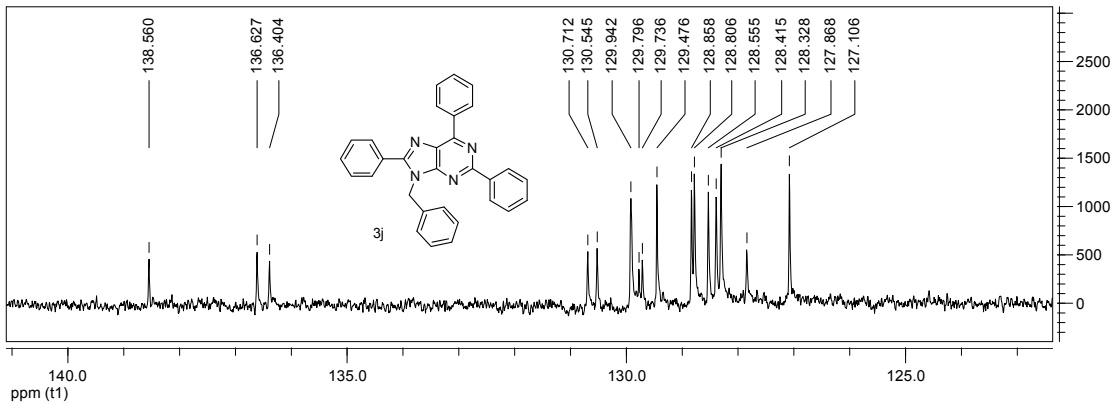

9.025
8.932
8.913
7.714
7.694
7.556
7.538
7.519
7.494
7.481
7.477
7.460
7.441
7.424
7.258
7.242
7.075
7.058
5.549
0.000
10.0
5.0
0.0
ppm (t1)
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
299.46
Number of Scans:
12
Acq. Date:
Mon May 16 06:35:17 PM

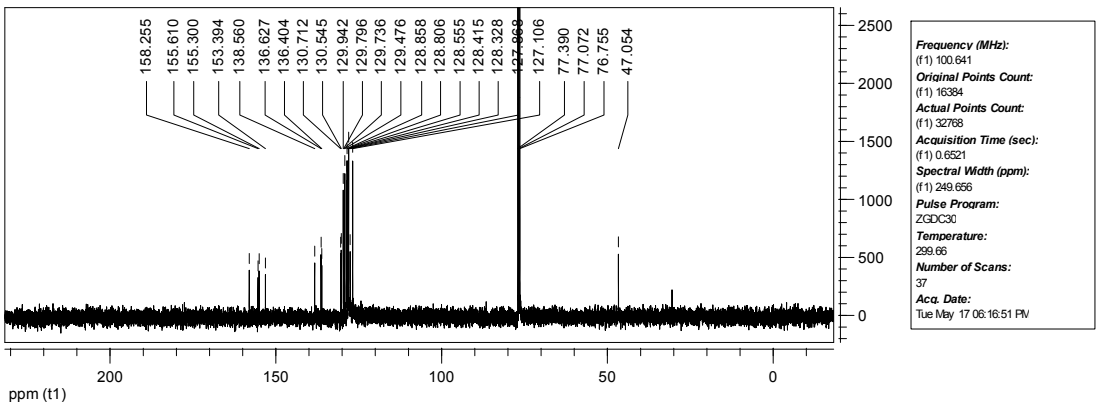

3i
155.308
154.610
153.941
152.293
136.153
135.874
131.002
130.844
130.712
129.889
129.456
129.409
128.936
128.862
128.630
127.929
126.646
150
140
130
ppm (t1)

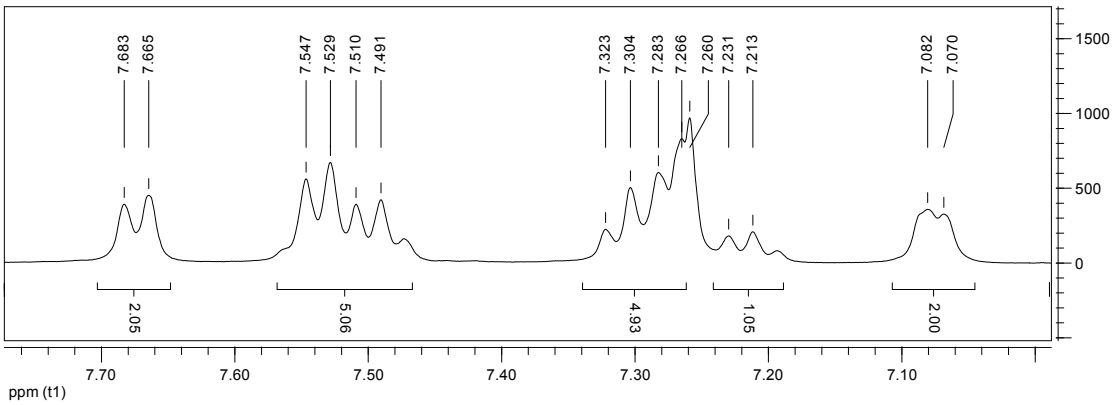

155.308
154.610
153.941
152.293
136.153
135.874
131.002
130.844
130.712
129.889
129.456
129.409
128.936
128.862
128.630
127.929
126.646
77.437
77.120
76.802
47.062
200
150
100
50
0
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
299.56
Number of Scans:
15
Acq. Date:
Mon May 16 06:37:55 PM

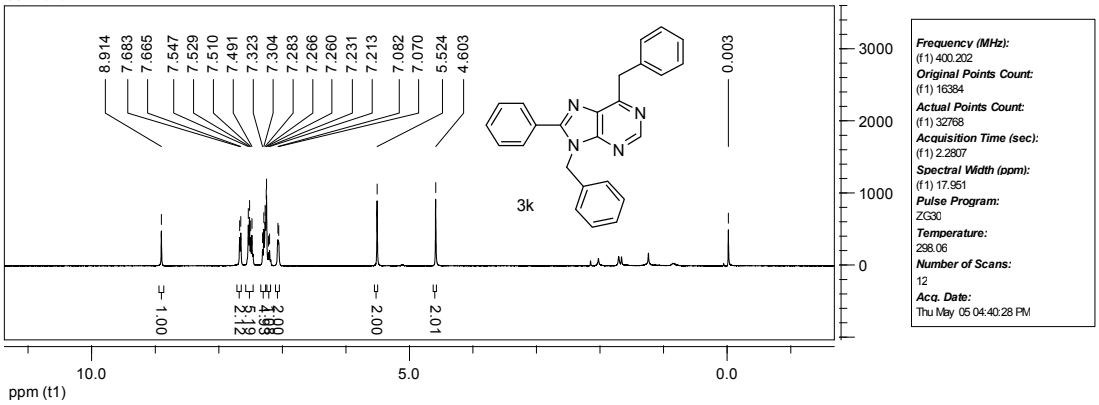

9.121
9.102
8.736
8.718
7.771
7.753
7.634
7.616
7.596
7.562
7.557
7.541
7.522
7.515
7.495
7.479
7.302
7.286
7.260
7.204
7.186
3j
2.00
2.01
2.05
2.10
7.07
3.00
2.00
9.50
9.00
8.50
8.00
7.50
7.00
ppm (t1)

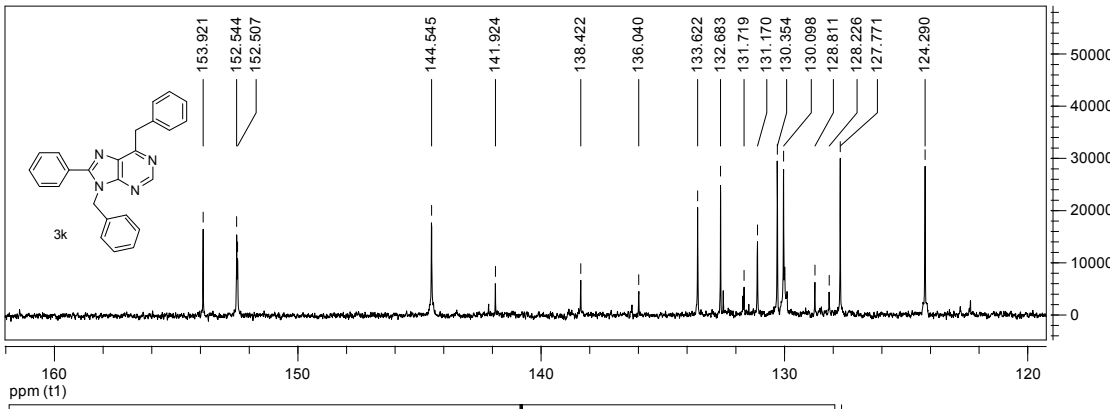

9.121
9.102
8.736
8.718
7.771
7.753
7.634
7.616
7.596
7.562
7.557
7.541
7.522
7.515
7.495
7.479
7.302
7.286
7.260
7.204
7.186
5.635
2.00
2.01
1.97
10.0
5.0
0.0
ppm (t1)
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
299.46
Number of Scans:
12
Acq. Date:
Tue May 17 06:10:51 PM

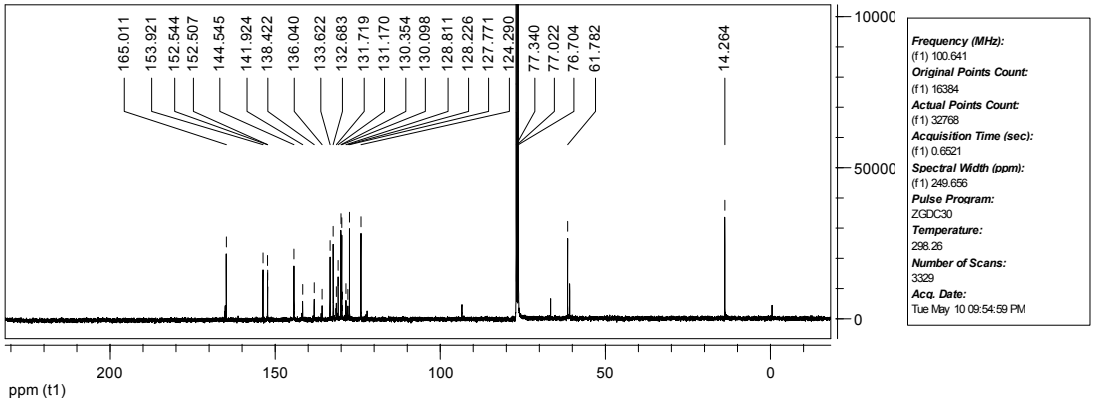

138.560
136.627
136.404
130.712
130.545
129.942
129.796
129.736
129.476
128.858
128.806
128.555
128.415
128.328
127.868
127.106
3j
140.0
135.0
130.0
125.0
ppm (t1)

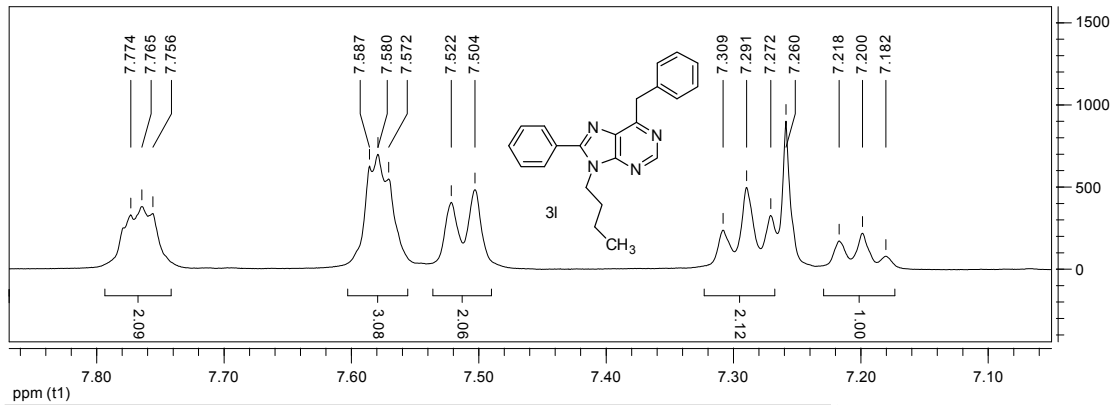

158.255
155.610
155.300
153.394
138.560
136.627
136.404
130.712
130.545
129.942
129.796
129.736
129.476
128.858
128.806
128.555
128.415
128.328
127.868
127.106
77.390
77.072
76.755
47.054
200
150
100
50
0
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
299.66
Number of Scans:
37
Acq. Date:
Tue May 17 06:16:51 PM

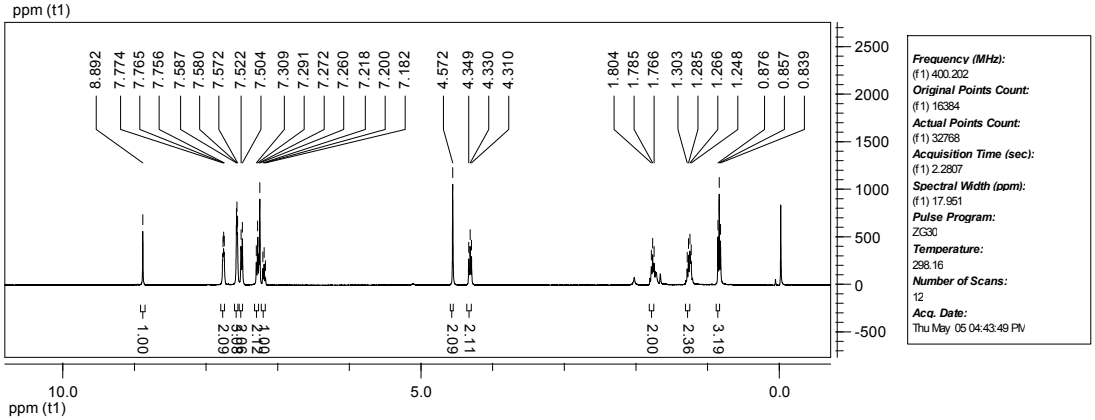

7.683
7.665
7.547
7.529
7.510
7.491
7.323
7.304
7.283
7.266
7.260
7.231
7.213
7.082
7.070
2.05
5.06
4.93
1.05
2.00
ppm (t1)

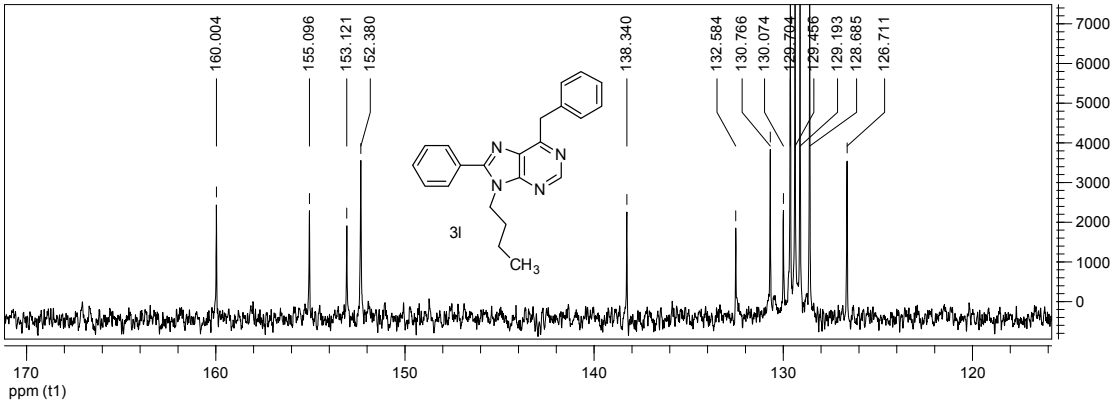

8.914
7.683
7.665
7.547
7.529
7.510
7.491
7.323
7.304
7.283
7.266
7.260
7.231
7.213
7.082
7.070
5.524
4.603
0.003
3k
1.00
2.00
2.01
ppm (t1)
Frequency (MHz):
(f1) 400.202
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.2807
Spectral Width (ppm):
(f1) 17.951
Pulse Program:
ZG30
Temperature:
298.06
Number of Scans:
12
Acq. Date:
Thu May 05 04:40:28 PM

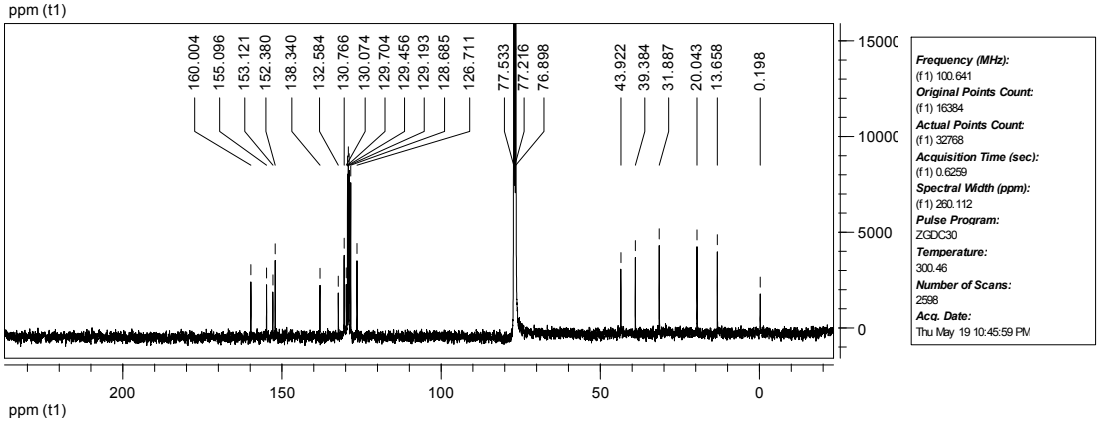

153.921
152.544
152.507
144.545
141.924
138.422
136.040
133.622
132.683
131.719
131.170
130.354
130.098
128.811
128.226
127.771
124.290
3k
ppm (t1)

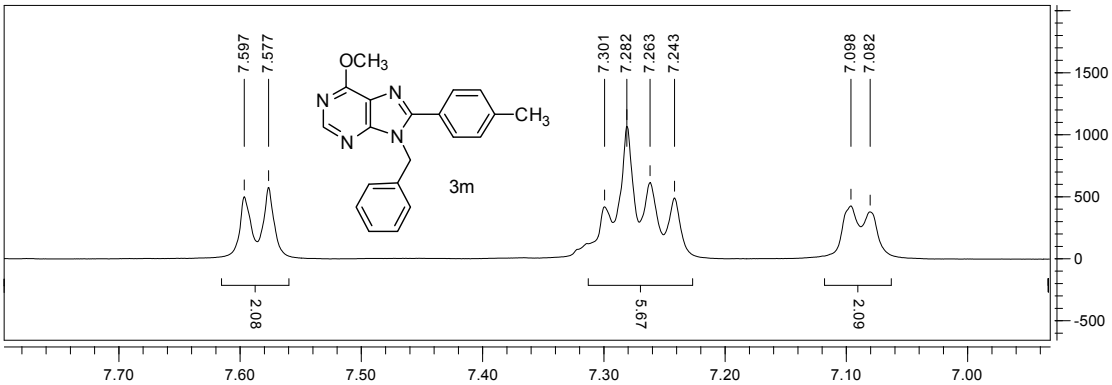

165.011
153.921
152.544
152.507
144.545
141.924
138.422
136.040
133.622
132.683
131.719
131.170
130.354
130.098
128.811
128.226
127.771
124.290
77.340
77.022
76.704
61.782
14.264
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
298.26
Number of Scans:
3329
Acq. Date:
Tue May 10 09:54:59 PM

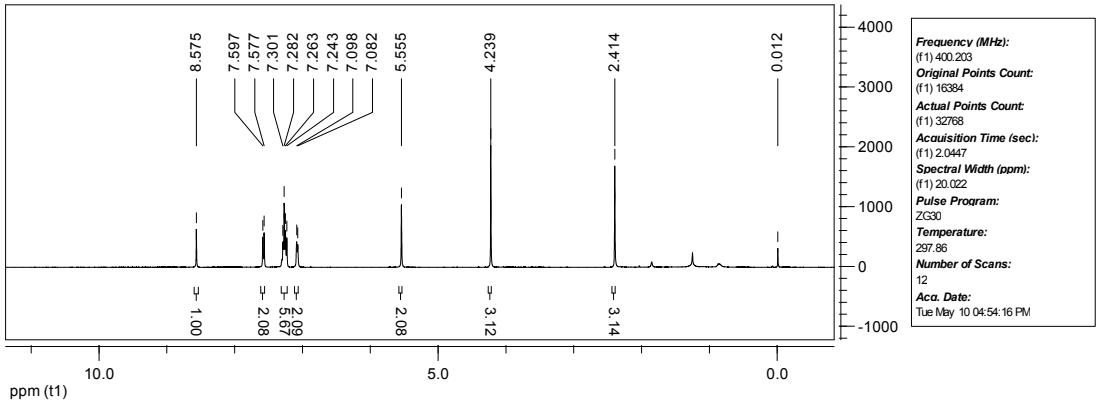

7.774
7.765
7.756
7.587
7.580
7.572
7.522
7.504
7.309
7.291
7.272
7.260
7.218
7.200
7.182
3l
CH3
2.09
3.08
2.06
2.12
1.00
ppm (t1)

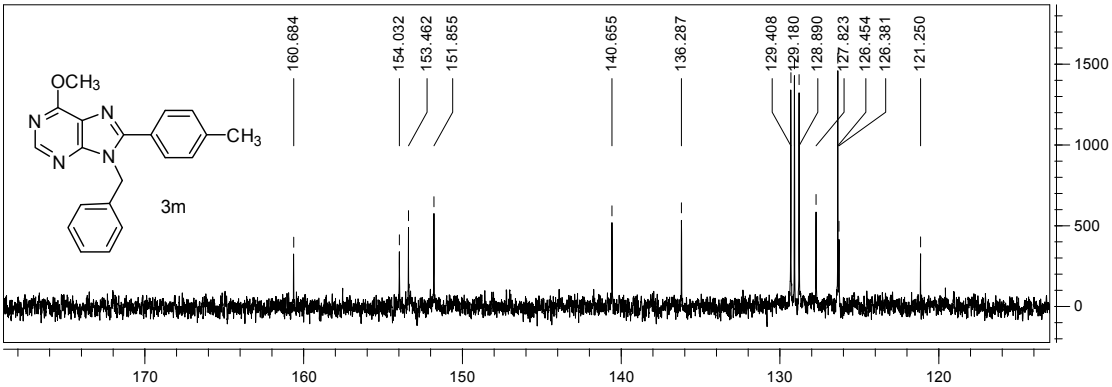

8.892
7.774
7.765
7.756
7.587
7.580
7.572
7.522
7.504
7.309
7.291
7.272
7.260
7.218
7.200
7.182
4.572
4.349
4.330
4.310
1.804
1.785
1.766
1.303
1.285
1.266
1.248
0.876
0.857
0.839
1.00
2.09
2.11
2.00
2.36
3.19
ppm (t1)
Frequency (MHz):
(f1) 400.202
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.2807
Spectral Width (ppm):
(f1) 17.951
Pulse Program:
ZG30
Temperature:
298.16
Number of Scans:
12
Acq. Date:
Thu May 05 04:43:49 PM

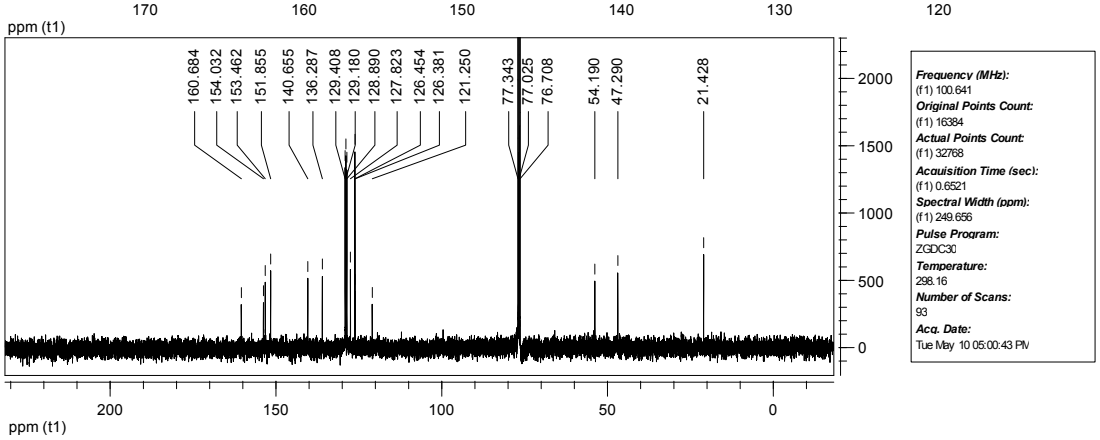

160.004
155.096
153.121
152.380
138.340
132.584
130.766
130.074
129.704
129.456
129.193
128.685
126.711
3l
CH3
ppm (t1)

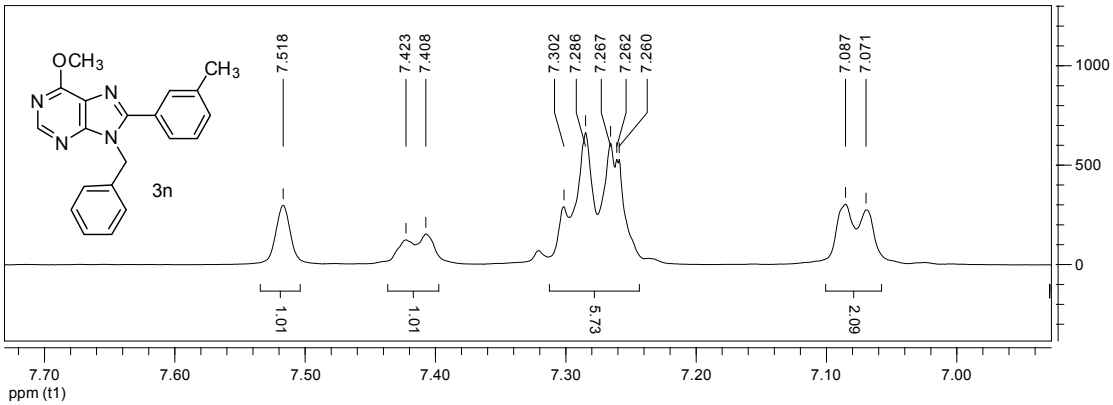

160.004
155.096
153.121
152.380
138.340
132.584
130.766
130.074
129.704
129.456
129.193
128.685
126.711
77.533
77.216
76.898
43.922
39.384
31.887
20.043
13.658
0.198
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6259
Spectral Width (ppm):
(f1) 260.112
Pulse Program:
ZGDC30
Temperature:
300.46
Number of Scans:
2598
Acq. Date:
Thu May 19 10:45:59 PM

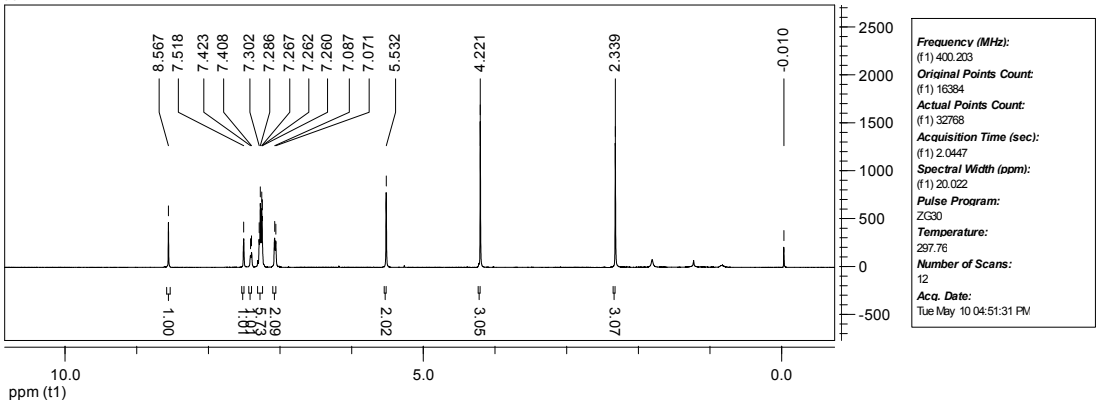

7.597
7.577
7.301
7.282
7.263
7.243
7.098
7.082
OCH3
CH3
3m
2.08
5.67
2.09
ppm (t1)

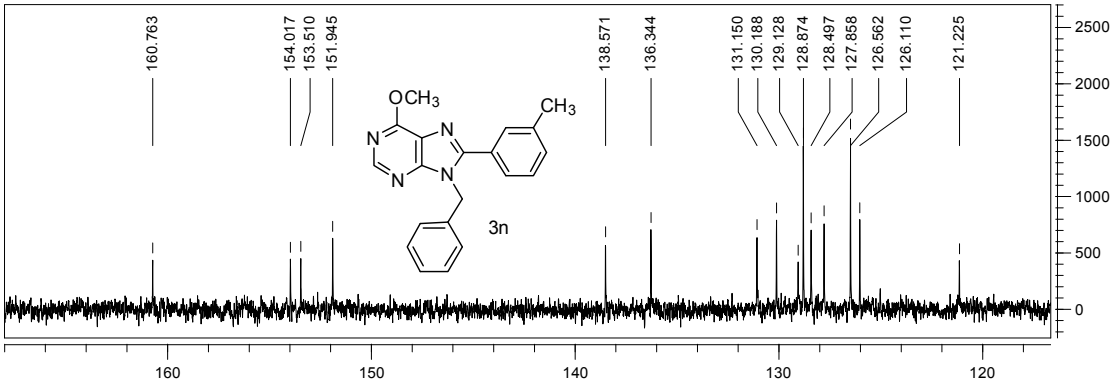

8.575
7.597
7.577
7.301
7.282
7.263
7.243
7.098
7.082
5.555
4.239
2.414
0.012
1.00
2.08
5.67
2.09
2.08
3.12
3.14
ppm (t1)
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
297.86
Number of Scans:
12
Acq. Date:
Tue May 10 04:54:16 PM

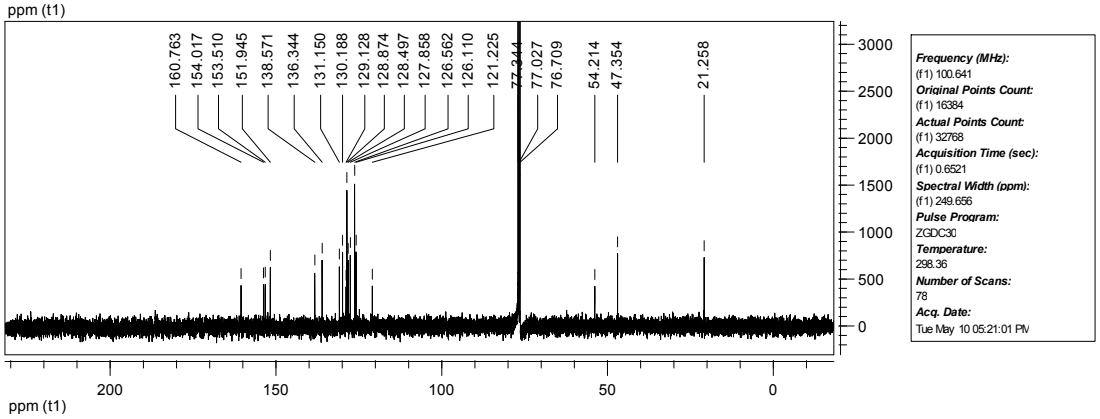

160.684
154.032
153.462
151.855
140.655
136.287
129.408
129.180
128.890
127.823
126.454
126.381
121.250
OCH3
CH3
3m
ppm (t1)

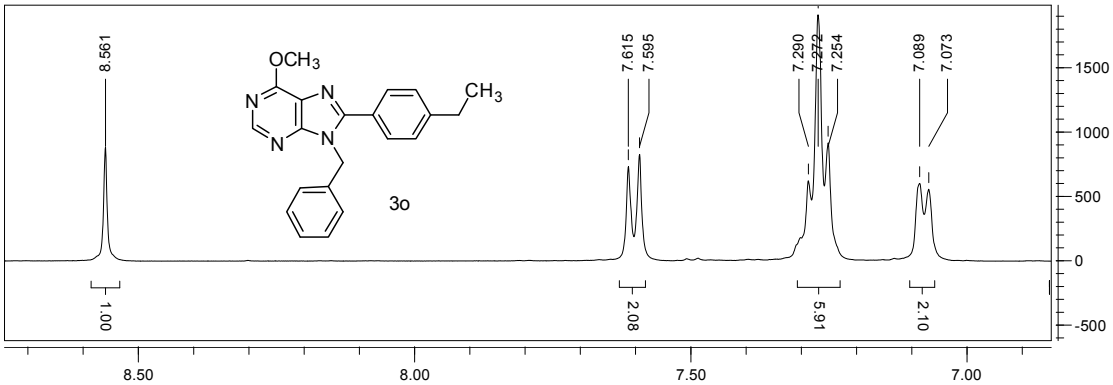

160.684
154.032
153.462
151.855
140.655
136.287
129.408
129.180
128.890
127.823
126.454
126.381
121.250
77.343
77.025
76.708
54.190
47.290
21.428
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
298.16
Number of Scans:
93
Acq. Date:
Tue May 10 05:00:43 PM

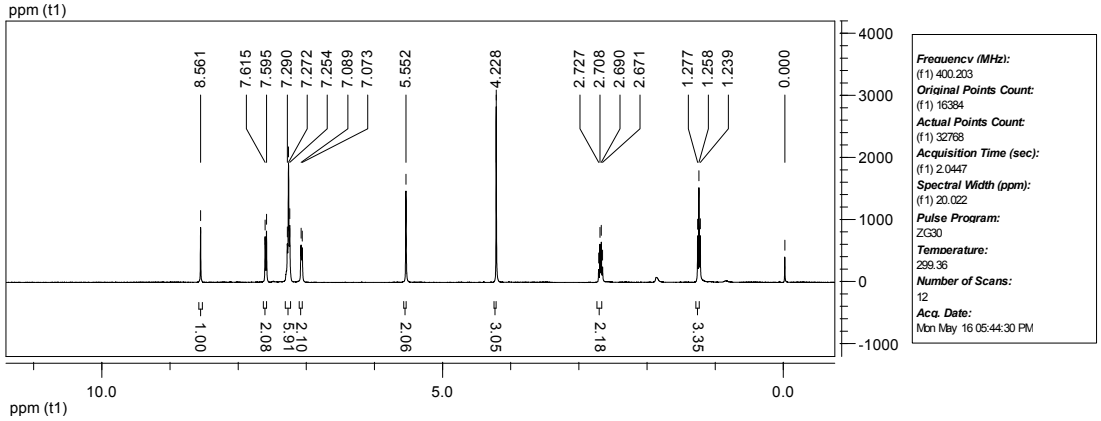

OCH3
CH3
N
N
N
N
3n
7.518
7.423
7.408
7.302
7.286
7.267
7.262
7.260
7.087
7.071
1.01
1.01
5.73
2.09
7.70
7.60
7.50
7.40
7.30
7.20
7.10
7.00
ppm (t1)

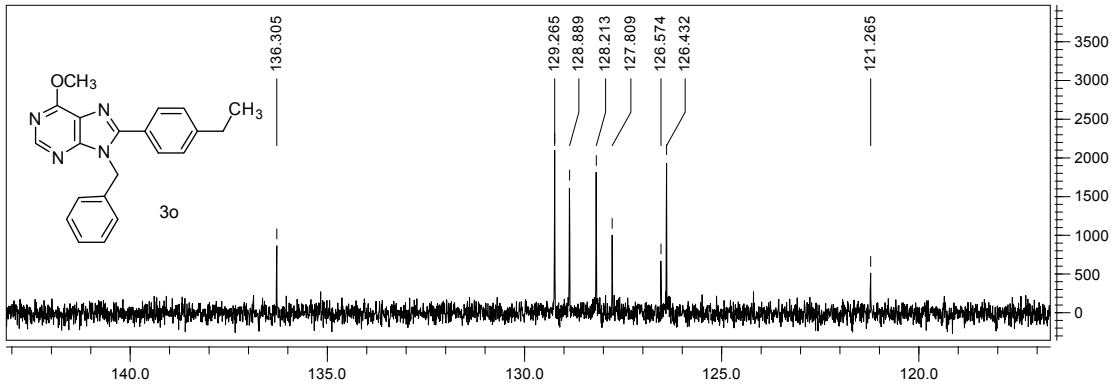

8.567
7.518
7.423
7.408
7.302
7.286
7.267
7.262
7.260
7.087
7.071
5.532
4.221
2.339
-0.010
1.00
2.09
2.02
3.05
3.07
10.0
5.0
0.0
ppm (t1)
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
297.76
Number of Scans:
12
Acq. Date:
Tue May 10 04:51:31 PM

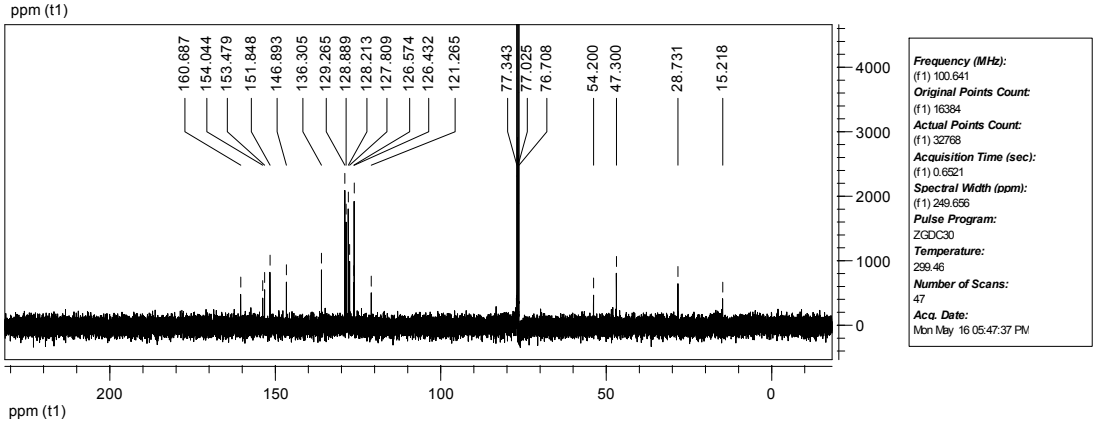

160.763
154.017
153.510
151.945
138.571
136.344
131.150
130.188
129.128
128.874
128.497
127.858
126.562
126.110
121.225
OCH3
CH3
N
N
N
N
3n
160
150
140
130
120
ppm (t1)

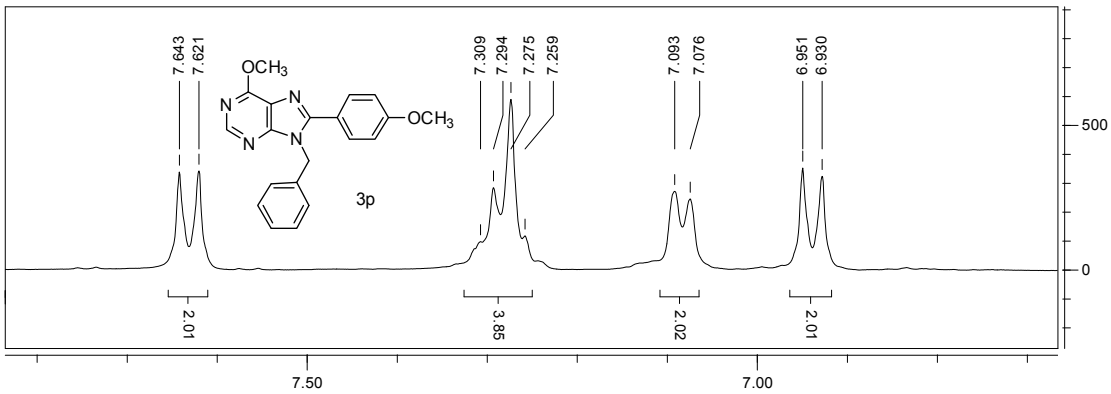

160.763
154.017
153.510
151.945
138.571
136.344
131.150
130.188
129.128
128.874
128.497
127.858
126.562
126.110
121.225
77.344
77.027
76.709
54.214
47.354
21.258
200
150
100
50
0
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
298.36
Number of Scans:
78
Acq. Date:
Tue May 10 05:21:01 PM

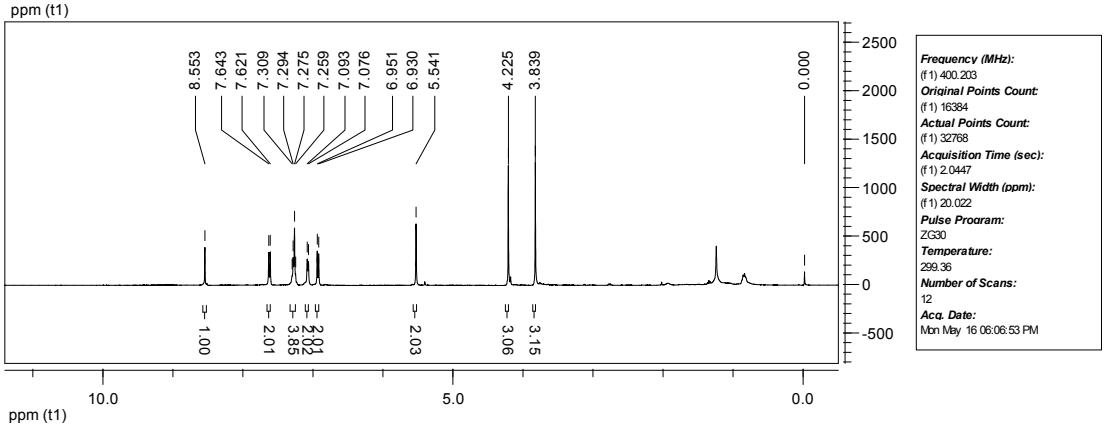

8.561
7.615
7.595
7.290
7.272
7.254
7.089
7.073
OCH3
CH3
3o
1.00
2.08
5.91
2.10
ppm (t1)

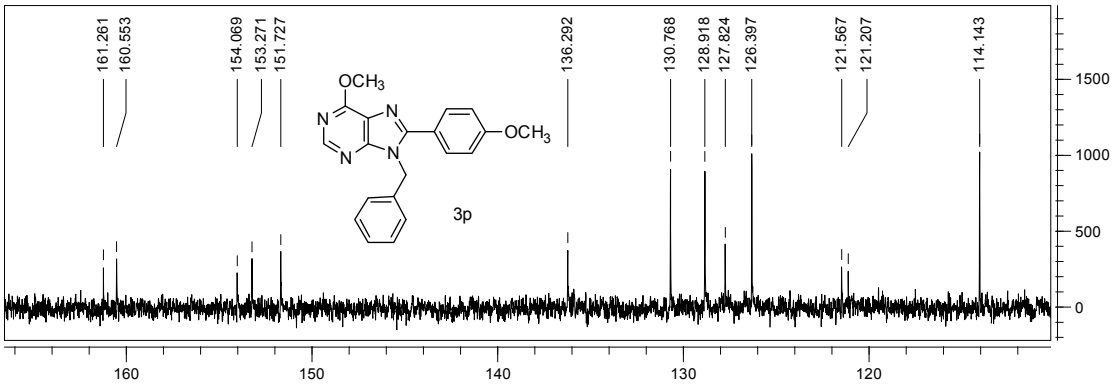

8.561
7.615
7.595
7.290
7.272
7.254
7.089
7.073
5.552
4.228
2.727
2.708
2.690
2.671
1.277
1.258
1.239
0.000
1.00
2.08
5.91
2.10
2.06
3.05
2.18
3.35
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
299.36
Number of Scans:
12
Acq. Date:
Mon May 16 05:44:30 PM
ppm (t1)

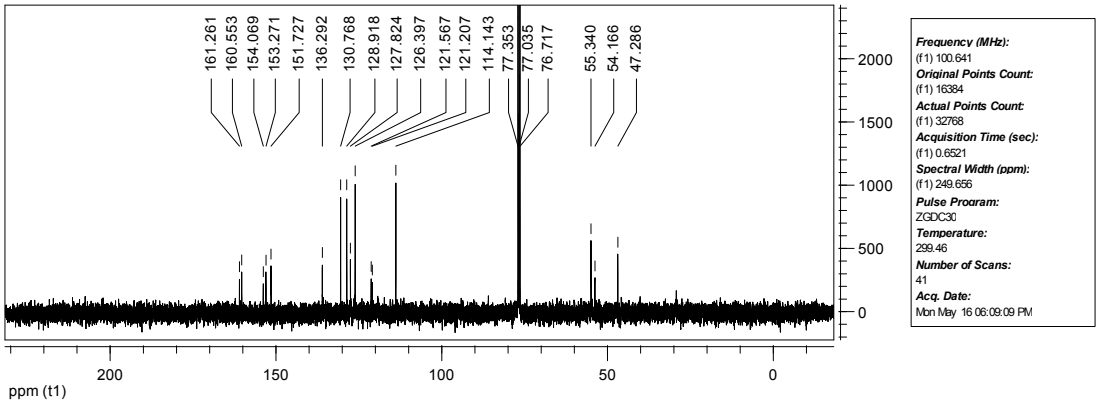

136.305
129.265
128.889
128.213
127.809
126.574
126.432
121.265
OCH3
CH3
3o
ppm (t1)

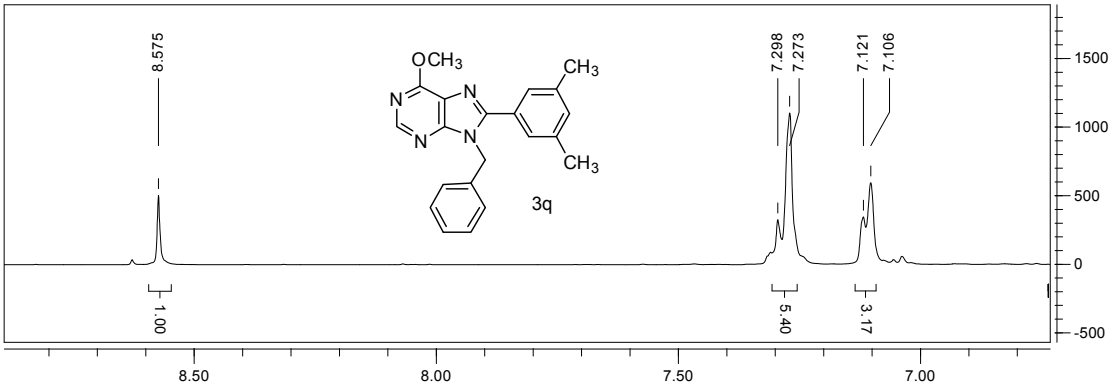

160.687
154.044
153.479
151.848
146.893
136.305
129.265
128.889
128.213
127.809
126.574
126.432
121.265
77.343
77.025
76.708
54.200
47.300
28.731
15.218
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
299.46
Number of Scans:
47
Acq. Date:
Mon May 16 05:47:37 PM
ppm (t1)

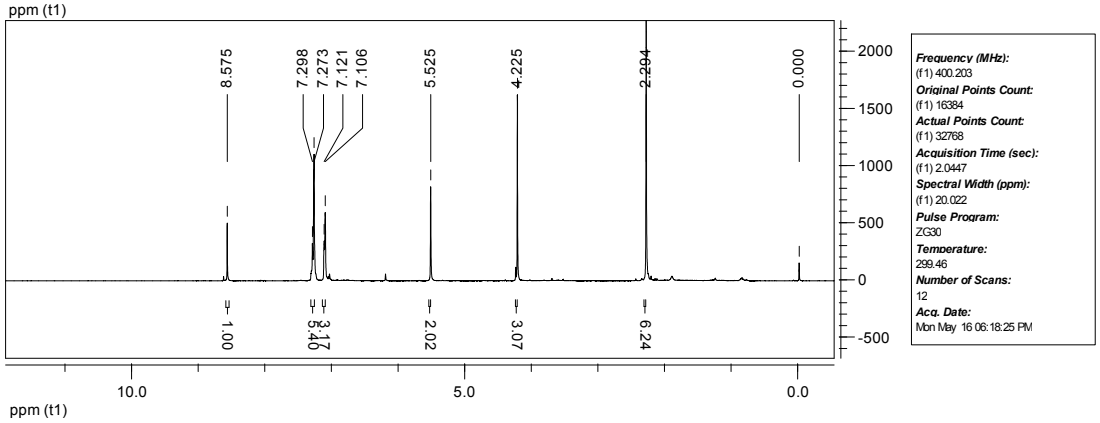

7.643
7.621
7.309
7.294
7.275
7.259
7.093
7.076
6.951
6.930
OCH3
OCH3
3p
2.01
3.85
2.02
2.01
7.50
7.00
ppm (t1)

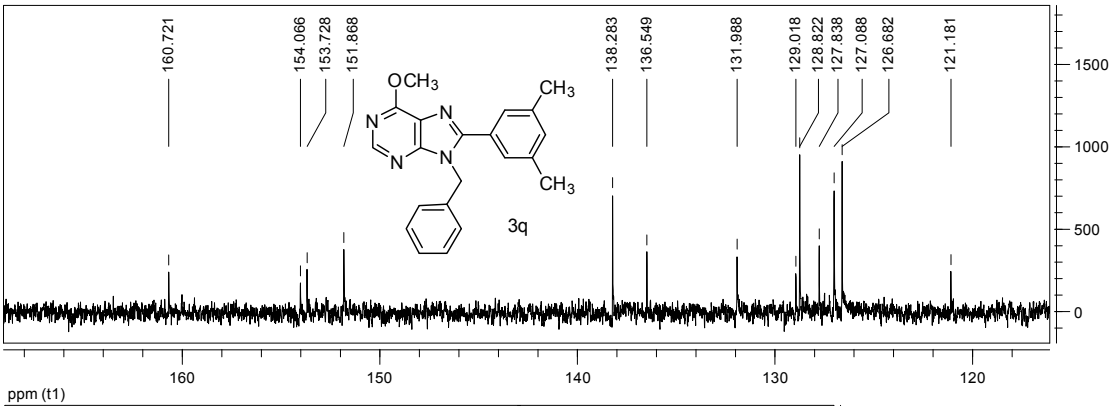

8.553
7.643
7.621
7.309
7.294
7.275
7.259
7.093
7.076
6.951
6.930
5.541
4.225
3.839
0.000
1.00
2.01
3.85
2.03
3.06
3.15
10.0
5.0
0.0
ppm (t1)
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
299.36
Number of Scans:
12
Acq. Date:
Mon May 16 06:06:53 PM

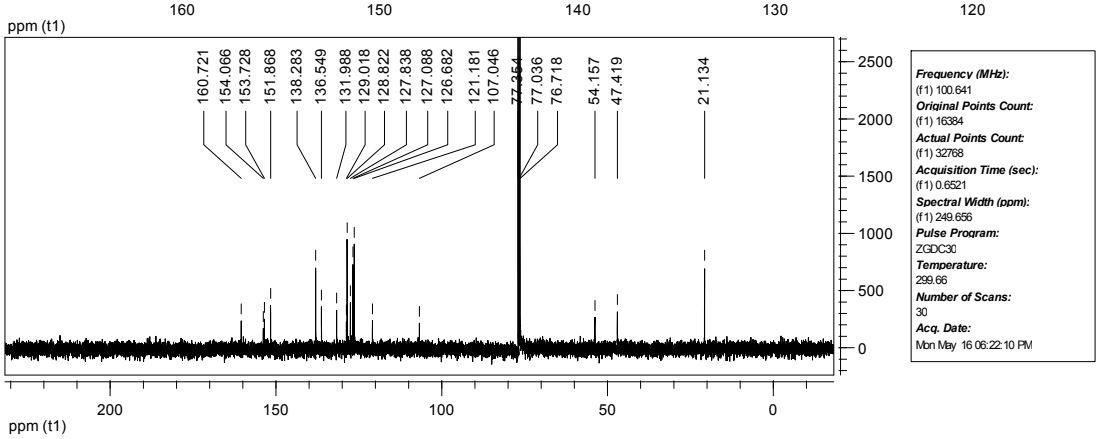

161.261
160.553
154.069
153.271
151.727
136.292
130.768
128.918
127.824
126.397
121.567
121.207
114.143
OCH3
OCH3
3p
160
150
140
130
120
ppm (t1)

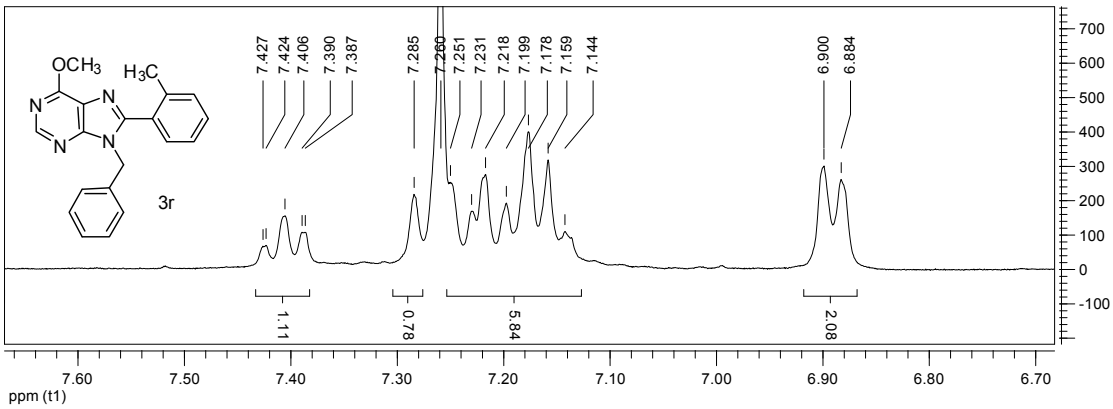

161.261
160.553
154.069
153.271
151.727
136.292
130.768
128.918
127.824
126.397
121.567
121.207
114.143
77.353
77.035
76.717
55.340
54.166
47.286
200
150
100
50
0
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
299.46
Number of Scans:
41
Acq. Date:
Mon May 16 06:09:09 PM

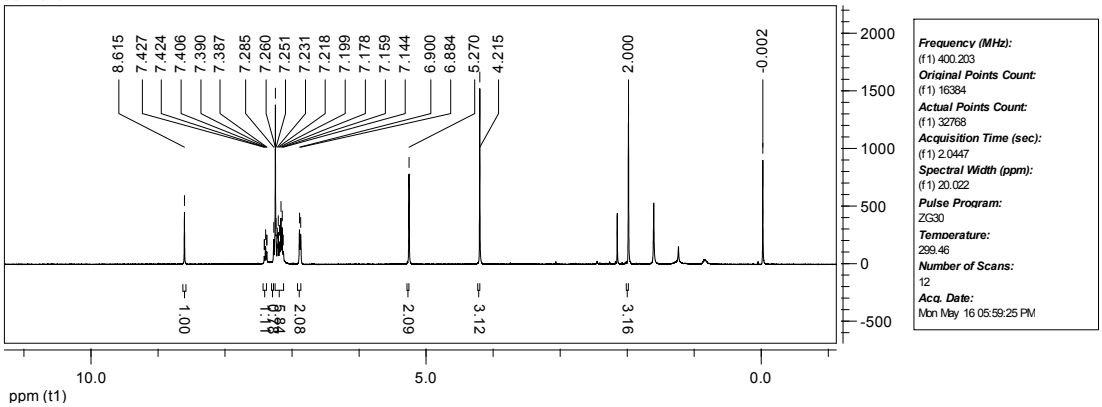

8.575
7.298
7.273
7.121
7.106
OCH3
CH3
CH3
N
N
N
N
3q
1.00
5.40
3.17
1500
1000
500
0
-500
8.50
8.00
7.50
7.00
ppm (t1)

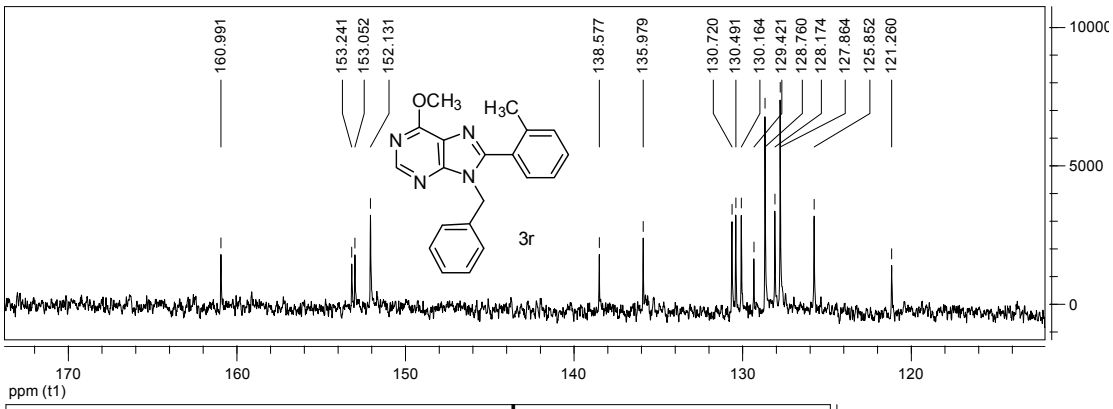

8.575
7.298
7.273
7.121
7.106
5.525
4.225
2.294
0.000
1.00
3.17
5.40
2.02
3.07
6.24
2000
1500
1000
500
0
-500
10.0
5.0
0.0
ppm (t1)
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
299.46
Number of Scans:
12
Acq. Date:
Mon May 16 06:18:25 PM

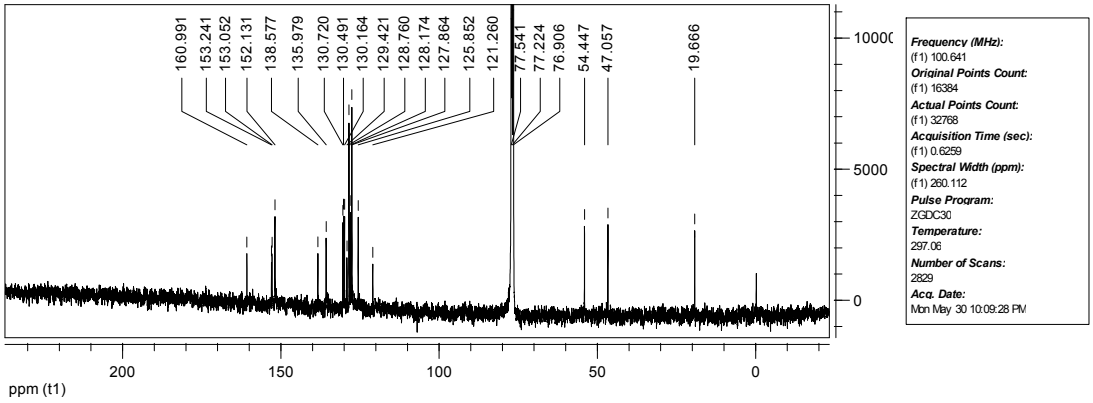

160.721
154.066
153.728
151.868
138.283
136.549
131.988
129.018
128.822
127.838
127.088
126.682
121.181
OCH3
CH3
CH3
N
N
N
N
3q
1500
1000
500
0
160
150
140
130
120
ppm (t1)

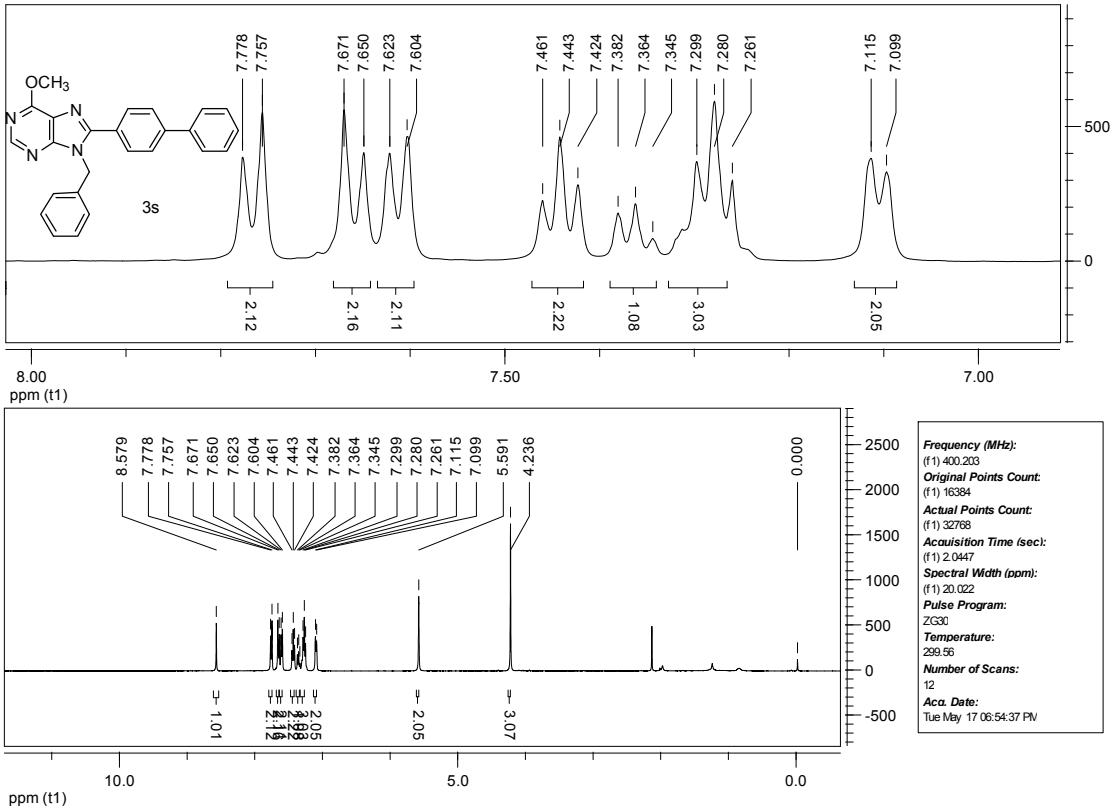

160.721
154.066
153.728
151.868
138.283
136.549
131.988
129.018
128.822
127.838
127.088
126.682
121.181
107.046
77.354
77.036
76.718
54.157
47.419
21.134
2500
2000
1500
1000
500
0
200
150
100
50
0
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
299.66
Number of Scans:
30
Acq. Date:
Mon May 16 06:22:10 PM

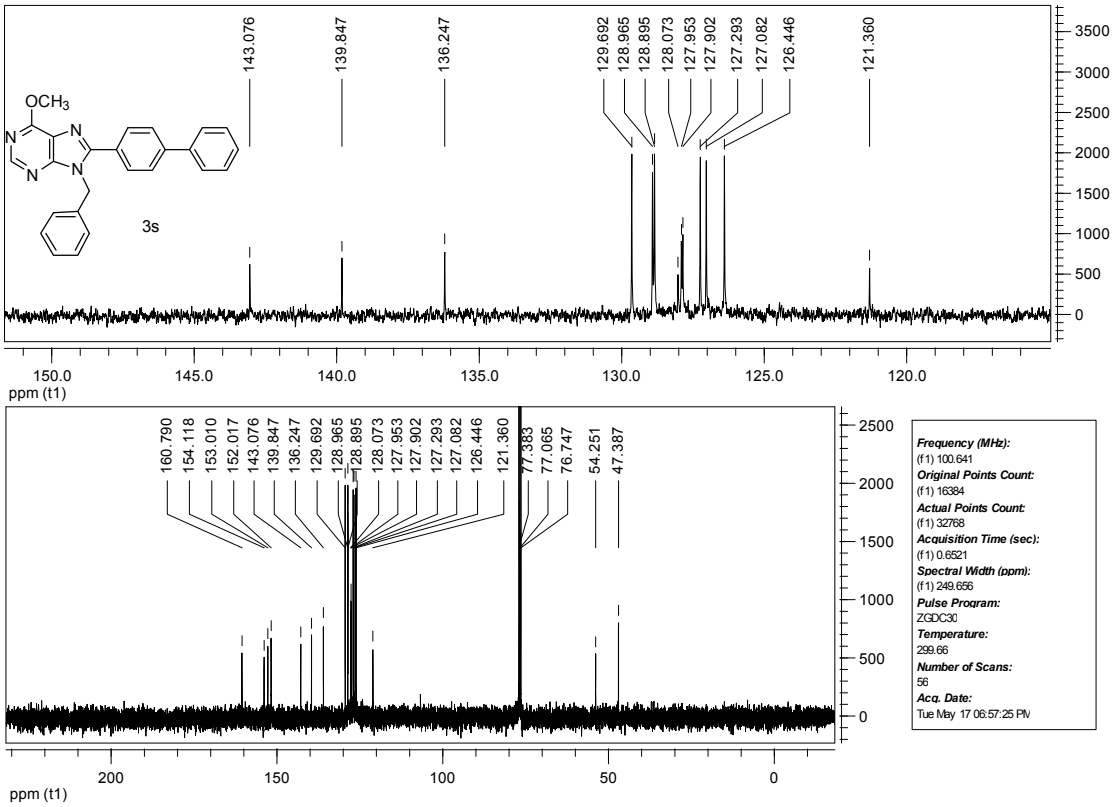

OCH3
H3C
N
N
N
N
3r
7.427
7.424
7.406
7.390
7.387
7.285
7.260
7.251
7.231
7.218
7.199
7.178
7.159
7.144
6.900
6.884
1.11
0.78
5.84
2.08
ppm (t1)

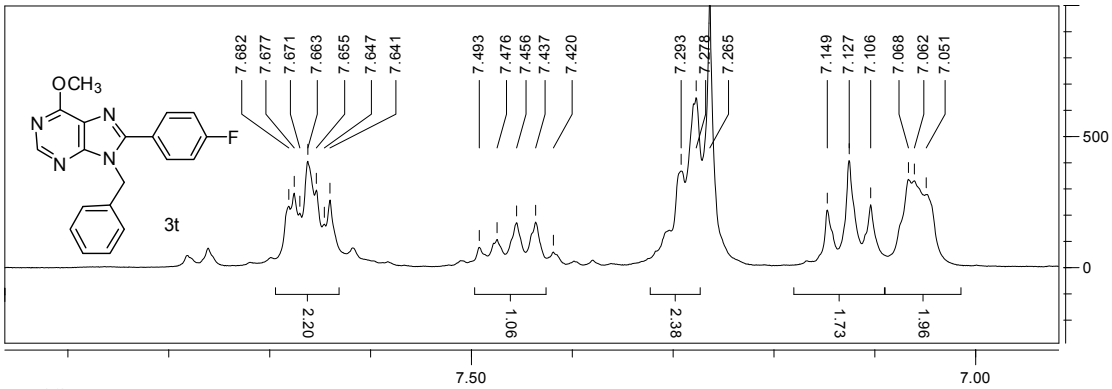

8.615
7.427
7.424
7.406
7.390
7.387
7.285
7.260
7.251
7.231
7.218
7.199
7.178
7.159
7.144
6.900
6.884
5.270
4.215
2.000
-0.002
1.00
2.08
2.09
3.12
3.16
ppm (t1)
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
299.46
Number of Scans:
12
Acq. Date:
Mon May 16 05:59:25 PM

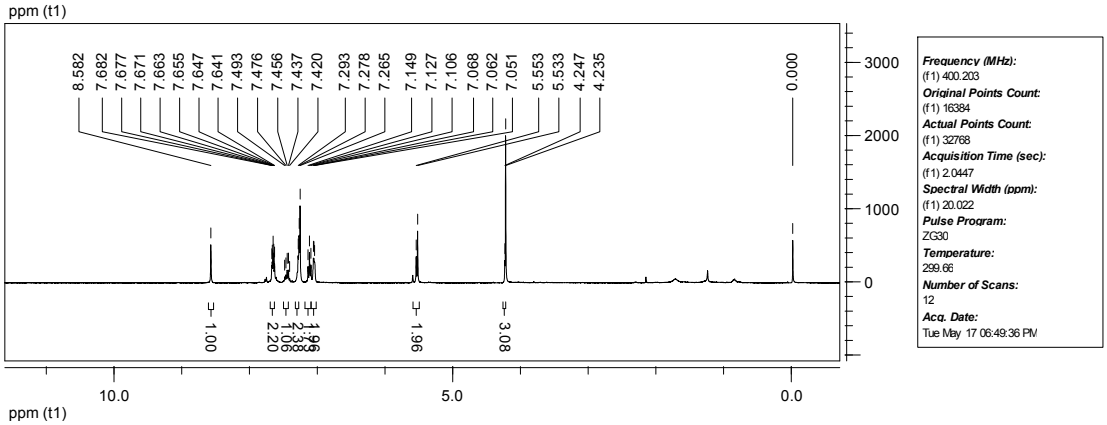

160.991
153.241
153.052
152.131
138.577
135.979
130.720
130.491
130.164
129.421
128.760
128.174
127.864
125.852
121.260
OCH3
H3C
N
N
N
N
3r
ppm (t1)

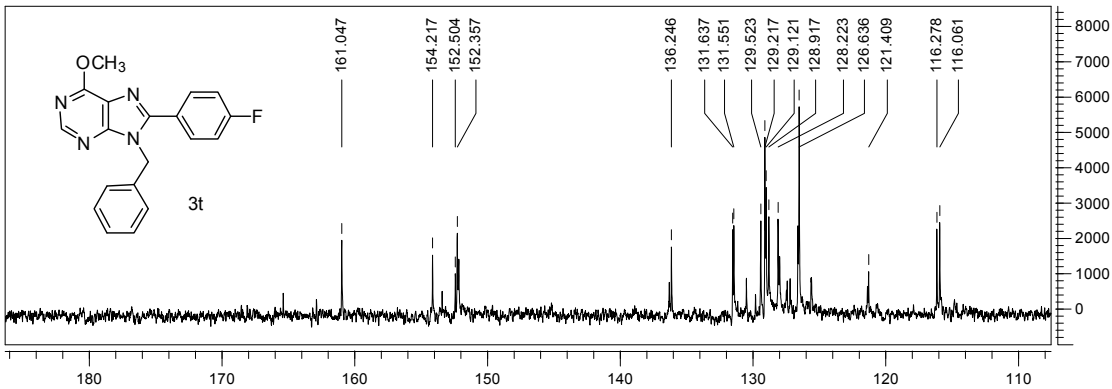

160.991
153.241
153.052
152.131
138.577
135.979
130.720
130.491
130.164
129.421
128.760
128.174
127.864
125.852
121.260
77.541
77.224
76.906
54.447
47.057
19.666
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6259
Spectral Width (ppm):
(f1) 260.112
Pulse Program:
ZGDC30
Temperature:
297.06
Number of Scans:
2829
Acq. Date:
Mon May 30 10:09:28 PM

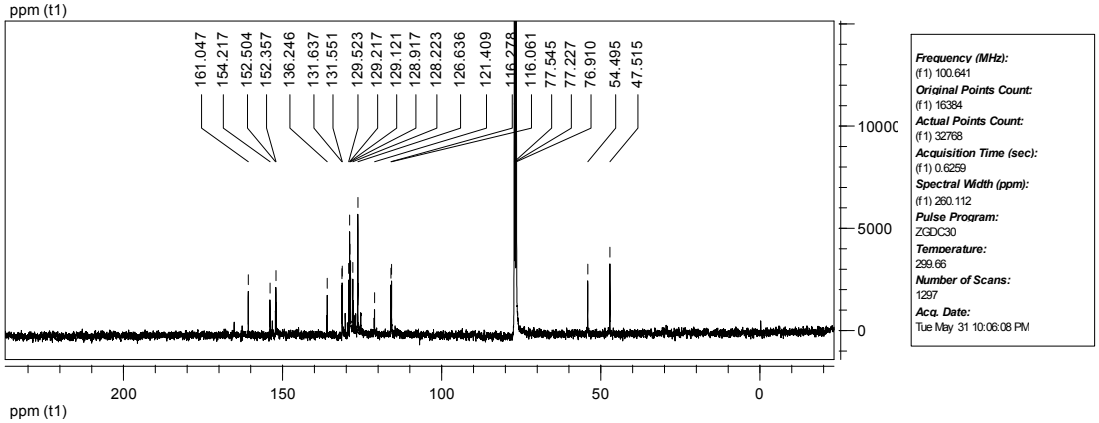

OCH3
N
N
N
N
3s
7.778
7.757
7.671
7.650
7.623
7.604
7.461
7.443
7.424
7.382
7.364
7.345
7.299
7.280
7.261
7.115
7.099
2.12
2.16
2.11
2.22
1.08
3.03
2.05
8.00
7.50
7.00
ppm (t1)
8.579
5.591
4.236
0.000
1.01
2.05
3.07
10.0
5.0
0.0
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
299.56
Number of Scans:
12
Acq. Date:
Tue May 17 06:54:37 PM

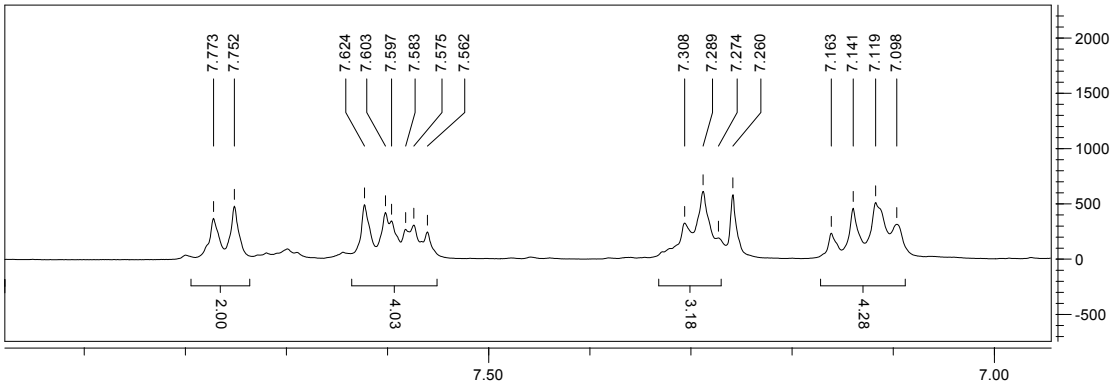

OCH3
N
N
N
N
3s
143.076
139.847
136.247
129.692
128.965
128.895
128.073
127.953
127.902
127.293
127.082
126.446
121.360
150.0
145.0
140.0
135.0
130.0
125.0
120.0
ppm (t1)
160.790
154.118
153.010
152.017
143.076
139.847
136.247
129.692
128.965
128.895
128.073
127.953
127.902
127.293
127.082
126.446
121.360
77.383
77.065
76.747
54.251
47.387
200
150
100
50
0
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6521
Spectral Width (ppm):
(f1) 249.656
Pulse Program:
ZGDC30
Temperature:
299.66
Number of Scans:
56
Acq. Date:
Tue May 17 06:57:25 PM

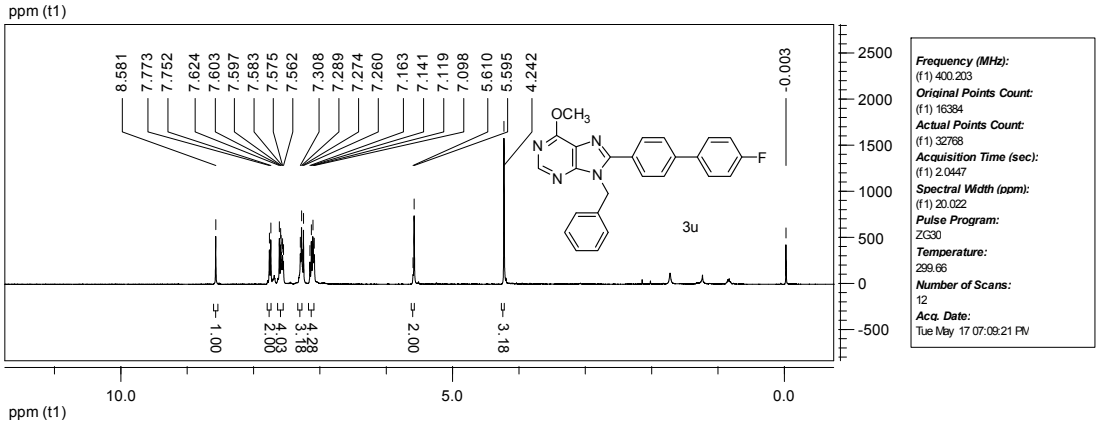

OCH3
N
N
N
N
F
3t
7.682
7.677
7.671
7.663
7.655
7.647
7.641
7.493
7.476
7.456
7.437
7.420
7.293
7.278
7.265
7.149
7.127
7.106
7.068
7.062
7.051
2.20
1.09
2.38
1.73
1.96
500
0
7.50
7.00
ppm (t1)

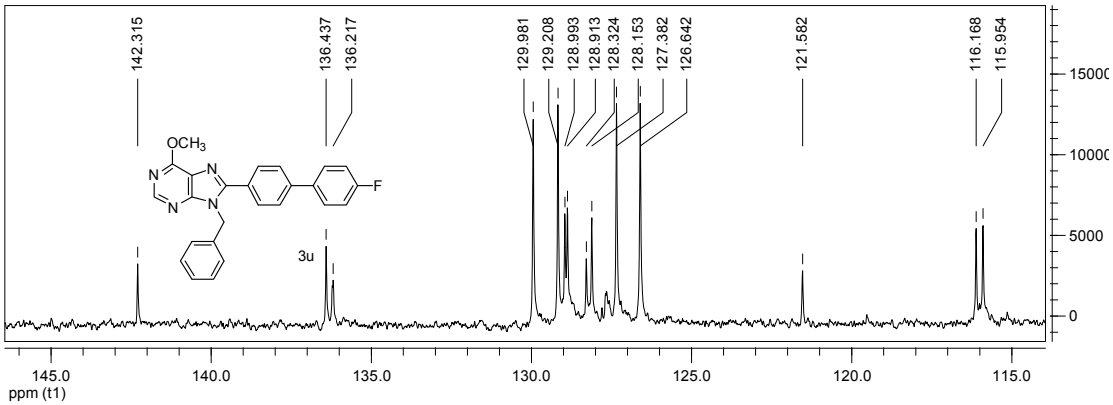

8.582
7.682
7.677
7.671
7.663
7.655
7.647
7.641
7.493
7.476
7.456
7.437
7.420
7.293
7.278
7.265
7.149
7.127
7.106
7.068
7.062
7.051
5.553
5.533
4.247
4.235
0.000
1.00
2.20
1.96
3.08
3000
2000
1000
0
10.0
5.0
0.0
ppm (t1)
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
299.66
Number of Scans:
12
Acq. Date:
Tue May 17 06:49:36 PM

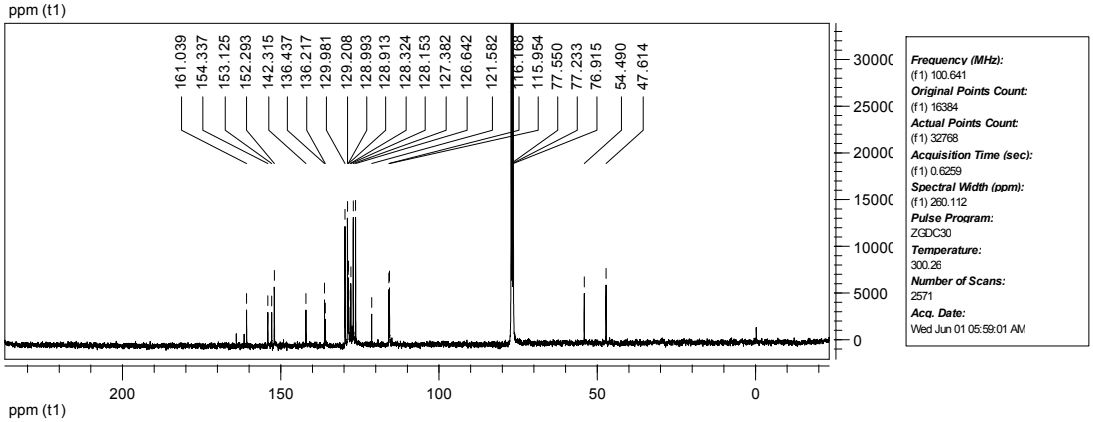

OCH3
N
N
N
N
F
3t
161.047
154.217
152.504
152.357
136.246
131.637
131.551
129.523
129.217
129.121
128.917
128.223
126.636
121.409
116.278
116.061
8000
7000
6000
5000
4000
3000
2000
1000
0
180
170
160
150
140
130
120
110
ppm (t1)


161.047
154.217
152.504
152.357
136.246
131.637
131.551
129.523
129.217
129.121
128.917
128.223
126.636
121.409
116.278
116.061
77.545
77.227
76.910
54.495
47.515
10000
5000
0
200
150
100
50
0
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6259
Spectral Width (ppm):
(f1) 260.112
Pulse Program:
ZGDC30
Temperature:
299.66
Number of Scans:
1297
Acq. Date:
Tue May 31 10:06:08 PM


7.773
7.752
7.624
7.603
7.597
7.583
7.575
7.562
7.308
7.289
7.274
7.260
7.163
7.141
7.119
7.098
2.00
4.03
3.18
4.28
7.50
7.00
ppm (t1)


8.581
7.773
7.752
7.624
7.603
7.597
7.583
7.575
7.562
7.308
7.289
7.274
7.260
7.163
7.141
7.119
7.098
5.610
5.595
4.242
-0.003
OCH3
N
N
N
N
F
3u
1.00
2.00
4.03
3.18
4.28
2.00
3.18
10.0
5.0
0.0
ppm (t1)
Frequency (MHz):
(f1) 400.203
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 2.0447
Spectral Width (ppm):
(f1) 20.022
Pulse Program:
ZG30
Temperature:
299.66
Number of Scans:
12
Acq. Date:
Tue May 17 07:09:21 PM


142.315
136.437
136.217
129.981
129.208
128.993
128.913
128.324
128.153
127.382
126.642
121.582
116.168
115.954
OCH3
N
N
N
N
F
3u
145.0
140.0
135.0
130.0
125.0
120.0
115.0
ppm (t1)


161.039
154.337
153.125
152.293
142.315
136.437
136.217
129.981
129.208
128.993
128.913
128.324
128.153
127.382
126.642
121.582
116.168
115.954
77.550
77.233
76.915
54.490
47.614
200
150
100
50
0
ppm (t1)
Frequency (MHz):
(f1) 100.641
Original Points Count:
(f1) 16384
Actual Points Count:
(f1) 32768
Acquisition Time (sec):
(f1) 0.6259
Spectral Width (ppm):
(f1) 260.112
Pulse Program:
ZGDC30
Temperature:
300.26
Number of Scans:
2571
Acq. Date:
Wed Jun 01 05:59:01 AM