The Supporting Information for

Chelation-Assisted Palladium-Catalyzed High Regioselective Heck Diarylation Reaction of 9-Allyl-9*H*-Purine: Synthesis of 9-(3,3-Diaryl-allyl)-9*H*-Purines

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General Information: NMR spectra were recorded with a 400 MHz spectrometer for ^{1}H NMR, 100 MHz for ^{13}C NMR. Chemical shifts δ are given in ppm relative to the residual signals of tetramethylsilane in $CDCl_3$ or deuterated solvent $CDCl_3$ 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 silica gel (200-300 mesh) was used as the stationary phase. All reactions were monitored by thin layer chromatography (TLC). All reagents and solvents were obtained from commercial suppliers and used without further purification unless otherwise noted. Starting materials 9-allyl-6-methoxylpurine (**1**)[1] and 9-allyl-6-methylpurine (**2**)[2] were prepared according to literature methods.

General procedure of chelation-assisted Pd-catalyzed diarylation reactions:

A 25 mL tube, containing a Teflon stirbar, was charged with 9-allyl-6-methoxylpurine or 9-allyl-6-methylpurine (0.2 mmol), $Pd(OAc)_2$ (0.01 mmol, 2.3 mg, 5 mol %), Ar_1I (0.204 mmol) and Ar_2I (0.204 mmol) (for double arylation) or ArI (0.6 mmol) (for diarylation), and AgOAc (0.4 mmol, 66.8 mg), then AcOH (0.8 mL) was added and the tube was sealed with a Teflon lined cap. The resulting mixture was stirred at 120 ^oC for 4.5 hours. TLC showed no starting material remained, and then reaction mixture was cooled down to room temperature, filtered through a plug of celite, and the celite was rinsed with copious EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by column chromatography on a silica gel (eluent: petroleum ether/EtOAc) affording the corresponding double arylated product.

General procedure of chelation-assisted Pd-catalyzed phenylation of 1 under classical Heck reaction conditions:

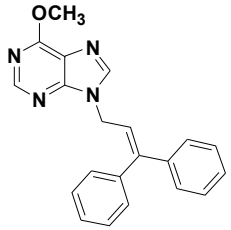
A 25 mL Schlenk tube containing a stir bar was charged with 0.3 mmol **1**, 3 equiv of PhI (for diphenylation) or 1.2 equiv of PhI (for monophenylation), 5 mol % $Pd(OAc)_2$, 10 mol % Ph_3P or 5 mol % bidentate ligand (dppp, dppf), and 0.9 mmol NaOAc, then DMF (1.5 mL) was added and the reaction mixture was heated at 120 ^oC for eight hours under N_2 atmosphere via several vacuum-N_2 exchanges. The resulting mixture was cooled down to room temperature, filtered through a plug of celite, and the celite was rinsed with copious EtOAc. The filtrate was extracted with 1 N *aq* HCl (3×10 mL). The combined aqueous phase was neutralized by adding $NaHCO_3$ and then was extracted with EtOAc (3×20 mL). After combining the organic phase and drying over $MgSO_4$, the solvent was removed under reduced pressure. The residue was purified by column chromatography on a silica gel (eluent: petroleum ether/EtOAc) affording the corresponding product.

For diphenylation: **1aa** was obtained in respectively 78%, 77%, 44% isolated yield with Ph_3P, dppp, dppf respectively as the ligand.

For monophenylation: **1a** was obtained in 88 % isolated yiled with Ph_3P as the ligand.

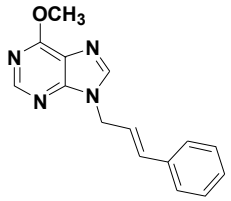
Characterization of compounds

9-(3,3-Diphenyl-allyl)-6-methoxy-9*H*-purine (1aa)



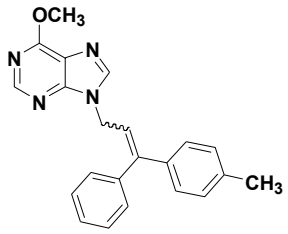
White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 7.84 (s, 1H), 7.48-7.40 (m, 3H), 7.29-7.22 (m, 7H), 6.33 (t, *J* = 7.2 Hz, 1H), 4.90 (d, *J* = 7.2 Hz, 2H), 4.19 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 152.0, 151.8, 147.0, 141.6, 140.6, 138.2, 129.4, 128.7, 128.3, 128.2, 128.1, 127.4, 121.4, 120.8, 54.1, 43.0; HRMS: calcd for $C_{21}H_{18}N_4NaO$ $[M + Na]^+$ 365.1378, found 365.1375.

6-Methoxy-9-(3-phenyl-allyl)-9*H*-purine (1a)



Pale white crystal. ^{1}H NMR (400 MHz, $CDCl_3$) (mingled with a trace of Ph_3PO) δ 8.58 (s, 1H), 7.99 (s, 1H), 7.37-7.27 (m, 5H), 6.62 (d, *J* = 16.0 Hz, 1H), 6.41-6.34 (m, 1H), 5.02 (d, *J* = 6.4 Hz, 2H), 4.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 152.4, 151.6, 141.9, 135.4, 134.7, 128.6, 128.4, 126.6, 122.0, 120.6, 54.3, 45.8; HRMS: calcd for $C_{15}H_{15}N_4O$ $[M + H]^+$ 267.1246, found 267.1248.

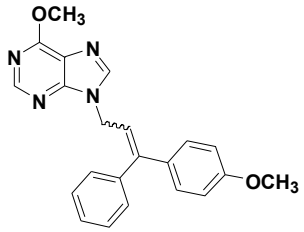
6-Methoxy-9-(3-phenyl-3-*p*-tolyl-allyl)-9*H*-purine (1ab)



White crystal. ^{1}H NMR (400 MHz, $CDCl_3$) (E/Z *isomers*) δ 8.55-8.54 (m, 1H), 7.84 (s, 1H), 7.46-7.38 (m, 1H), 7.27-7.23 (m, 5H), 7.14-7.06 (m, 3H), 6.34-6.24 (m, 1H), 4.92-4.88 (m, 2H),

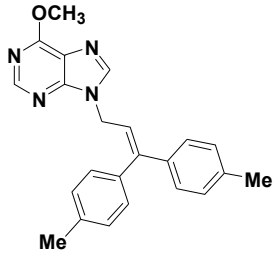
4.18 (s, 3H), 2.40-2.32 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 152.0, 151.8, 147.1, 147.0, 141.7, 140.8, 138.2, 138.1, 138.0, 137.8, 129.55, 129.4, 129.3, 129.0, 128.9, 128.8, 128.7, 128.3, 128.27, 128.2, 128.1, 128.0, 127.5, 127.45, 127.4, 127.3, 121.5, 120.8, 120.6, 119.6, 54.2, 43.0, 21.3, 21.1; HRMS: calcd for $C_{22}H_{20}N_4NaO$ $[M + Na]^+$ 379.1535, found 379.1533.

6-Methoxy-9-[3-(4-methoxy-phenyl)-3-phenyl-allyl]-9*H*-purine (1ac)



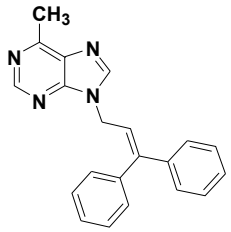
Light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) (E/Z *isomers*) δ 8.56-8.55 (m, 1H), 7.86-7.83 (m, 1H), 7.45-7.41 (m, 1H), 7.40-7.23 (m, 4H), 7.18-7.15 (m, 2H), 6.98-6.96 (m, 1H), 6.82-6.80 (m, 1H), 6.28-6.23 (m, 1H), 4.95-4.86 (m, 2H), 4.19 (s, 3H), 3.86-3.79 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.3, 169.6, 169.3, 159.4, 158.7, 152.5, 151.0, 142.6, 140.7, 134.8, 134.5, 132.8, 132.1, 130.8, 129.5, 129.2, 128.7, 128.3, 127.9, 127.6, 126.2, 116.2, 115.9, 114.1, 113.7, 86.6, 80.2, 73.1, 70.4, 62.9, 55.5, 20.8, 20.6, 20.5; HRMS: calcd for $C_{22}H_{20}N_4NaO_2$ $[M + Na]^+$ 395.1484, found 395.1485.

9-(3,3-Di-*p*-tolylallyl)-6-methoxy-9*H*-purine (1bb)



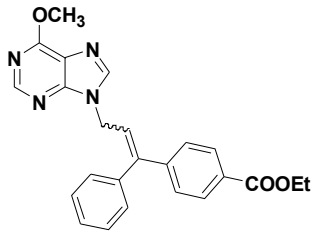
Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 7.84 (s, 1H), 7.24 (d, J = 8.0 Hz, 1H), 7.12 (d, J = 6.8 Hz, 4H), 7.08 (d, J = 8.4 Hz, 2H), 6.26 (t, J = 7.2 Hz, 1H), 4.90 (d, J = 7.2 Hz, 2H), 4.19 (s, 3H), 2.40 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 152.0, 151.9, 147.1, 141.7, 138.1, 138.0, 137.8, 135.3, 129.4, 129.3, 128.9, 127.4, 121.5, 119.7, 54.2, 43.0, 21.3, 21.1; HRMS: calcd for $C_{23}H_{23}N_4O$ $[M + H]^+$ 371.1872, found 371.1867.

9-(3,3-Diphenylallyl)-6-methyl-9*H*-purine (2aa)



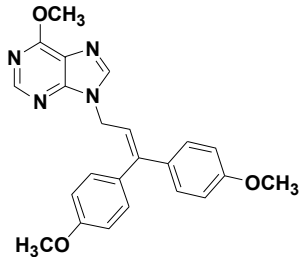
Light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.85 (s, 1H), 7.93 (s, 1H), 7.47-7.39 (m, 3H), 7.28-7.26 (m, 7H), 6.36-6.32 (m, 1H), 4.94-4.92 (m, 2H), 2.87 (d, *J* = 2.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.2, 152.3, 150.3, 147.3, 144.9, 143.2, 140.5, 138.7, 129.5, 128.8, 128.4, 128.3, 128.2, 127.5, 120.7, 42.8, 19.5; HRMS: calcd for $C_{21}H_{18}N_4Na$ $[M + Na]^+$ 349.1429, found 349.1436.

Ethyl 4-(3-(6-methoxy-9*H*-purin-9-yl)-1-phenylprop-1-en-1-yl)benzoate (1ad)



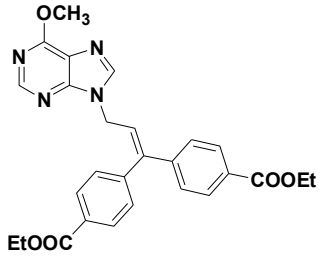
Light yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) (E/Z *isomers*) δ 8.56 (s, 0.5H), 8.55 (s, 0.5H), 8.13 (d, *J* = 7.6 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 7.84 (s, 0.5H), 7.83 (s, 0.5H), 7.48-7.42 (m, 1.7H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.29-7.24 (m, 3.3H), 7.20 (d, *J* = 3.6 Hz, 1H), 6.40 (t, *J* = 7.2 Hz, 0.5H), 6.36 (t, *J* = 6.8 Hz, 0.5H), 4.93 (d, *J* = 7.2 Hz, 1H), 4.89 (d, *J* = 6.8 Hz, 1H), 4.41 (q, *J* = 7.2 Hz, 1H), 4.35 (q, *J* = 6.8 Hz, 1H), 4.19 (s, 3H), 1.41 (t, *J* = 7.2 Hz, 1.5H), 1.37 (t, *J* = 6.8 Hz, 1.5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.2, 166.1, 161.1, 152.2, 151.8, 146.1, 144.8, 142.9, 141.6, 141.5, 139.9, 137.6, 130.3, 129.9, 129.6, 129.5, 129.4, 128.9, 128.5, 128.4, 127.4, 127.3, 122.9, 121.6, 121.5, 61.2, 61.0, 54.2, 42.9, 14.4, 14.3; HRMS: calcd for $C_{24}H_{22}N_4NaO_3$ $[M + Na]^+$ 437.1590, found 437.1591.

9-(3,3-Bis(4-methoxyphenyl)allyl)-6-methoxy-9*H*-purine (1cc)



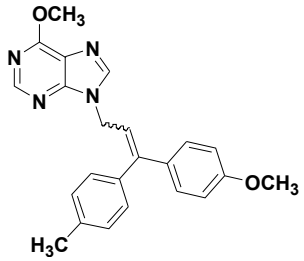
Yellow oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (s, 1H), 7.85 (s, 1H), 7.16 (d, *J* = 2.8 Hz, 2H), 7.14 (d, *J* = 2.8 Hz, 2H), 6.95 (d, *J* = 8.8 Hz, 2H), 6.79 (d, *J* = 8.4 Hz, 2H), 6.18 (t, *J* = 7.2 Hz, 1H), 4.89 (d, *J* = 7.2 Hz, 2H), 4.18 (s, 3H), 3.84 (s, 3H), 3.77 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 159.6, 159.3, 152.0, 146.4, 141.7, 133.6, 132.2, 130.8, 130.5, 128.8, 121.3, 118.6, 114.0, 113.6, 113.4, 55.3, 54.2, 43.1; HRMS: calcd for $C_{23}H_{22}N_4NaO_3$ $[M + Na]^+$ 425.1590, found 425.1591.

Diethyl 4,4'-(3-(6-methoxy-9*H*-purin-9-yl)prop-1-ene-1,1-diyl)dibenzoate (1dd)



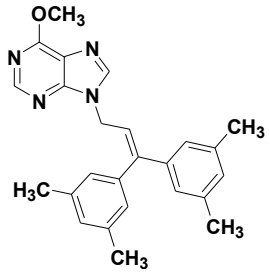
Brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 8.15 (d, *J* = 6.8 Hz, 2H), 7.94 (d, *J* = 7.2 Hz, 2H), 7.84 (s, 1H), 7.35 (d, *J* = 7.2 Hz, 2H), 7.25 (d, *J* = 6.8 Hz, 2H), 6.44 (t, *J* = 6.4 Hz, 1H), 4.91 (d, *J* = 6.8 Hz, 2H), 4.41 (q, *J* = 7.2 Hz, 2H), 4.35 (q, *J* = 7.2 Hz, 2H), 4.19 (s, 3H), 1.42 (t, *J* = 7.2 Hz, 3H), 1.37 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.1, 166.0, 161.1, 152.3, 151.8, 145.1, 144.1, 142.2, 141.5, 130.6, 130.3, 130.2, 129.7, 129.6, 127.3, 123.7, 121.5, 61.3, 61.1, 54.3, 42.9, 14.4, 14.3; HRMS: calcd for $C_{27}H_{26}N_4NaO_5$ $[M + Na]^+$ 509.1801, found 509.1806.

6-Methoxy-9-(3-(4-methoxyphenyl)-3-(*p*-tolyl)allyl)-9*H*-purine (1bc)



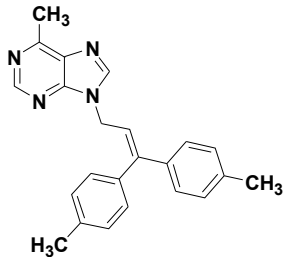
Brown oil. ^{1}H NMR (400 MHz, $CDCl_3$) (E/Z *isomers*) δ 8.55 (s, 1H), 7.85 (s, 0.5H), 7.84 (s, 0.5H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.18-7.07 (m, 5H), 6.95 (d, *J* = 8.4 Hz, 1H), 6.80 (d, *J* = 8.8 Hz, 1H), 6.22 (q, *J* = 7.2 Hz, 1H), 4.92 (d, *J* = 6.8 Hz, 1H), 4.88 (d, *J* = 7.2 Hz, 1H), 4.19 (s, 3H), 3.85 (s, 1.5H), 3.78 (s, 1.5H), 2.40 (s, 1.5H), 2.32 (s, 1.5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.0, 159.6, 159.3, 152.1, 152.0, 151.8, 146.7, 146.6, 141.8, 141.7, 138.2, 138.1, 137.8, 135.4, 133.4, 130.8, 130.5, 129.4, 128.9, 128.7, 127.5, 121.5, 119.6, 118.7, 114.0, 113.6, 55.3, 55.2, 54.2, 43.1, 21.3, 21.1; HRMS: calcd for $C_{23}H_{22}N_4NaO_2$ $[M + Na]^+$ 409.1640, found 409.1638.

9-(3,3-Bis(3,5-dimethylphenyl)allyl)-6-methoxy-9*H*-purine (1ee)



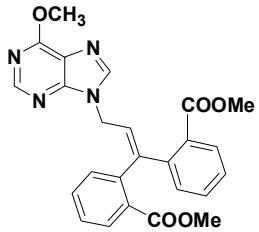
Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 7.85 (s, 1H), 7.01 (s, 1H), 6.92 (s, 1H), 6.85 (s, 2H) 6.83 (s, 2H), 6.22 (t, *J* = 7.2 Hz, 1H), 4.88 (d, *J* = 7.2 Hz, 2H), 4.19 (s, 3H), 2.33 (s, 6H), 2.25 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.9, 151.9, 151.8, 147.7, 141.7, 140.8, 138.2, 138.1, 137.7, 129.8, 129.6, 127.1, 125.3, 121.4, 120.3, 54.2, 42.9, 21.3, 21.2; HRMS: calcd for $C_{25}H_{27}N_4O$ $[M + H]^+$ 339.2185, found 339.2182.

9-(3,3-Di-*p*-tolylallyl)-6-methyl-9*H*-purine (2bb)



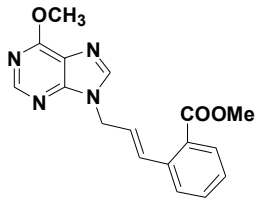
White power. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (s, 1H), 7.84 (s, 1H), 7.24 (d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 6.8 Hz, 4H), 7.08 (d, *J* = 8.4 Hz, 2H), 6.26 (t, *J* = 7.2 Hz, 1H), 4.90 (d, *J* = 7.2 Hz, 2H), 4.19 (s, 3H), 2.40 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.1, 152.2, 150.3, 147.2, 143.3, 138.1, 138.0, 137.9, 135.3, 132.9, 129.3, 129.0, 127.4, 119.4, 42.8, 21.3, 21.1, 19.5; HRMS: calcd for $C_{23}H_{23}N_4O$ $[M + H]^+$ 355.1923, found 355.1921.

Dimethyl 2,2'-(3-(6-methoxy-9*H*-purin-9-yl)prop-1-ene-1,1-diyl)dibenzoate (1ff)



Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.50 (s, 1H), 8.01 (s, 1H), 7.84 (dd, *J* = 7.6, 0.8 Hz, 1H), 7.59-7.52 (m, 3H), 7.43-7.35 (m, 3H), 7.31-7.27 (m, 1H), 5.95 (t, *J* = 7.2 Hz, 1H), 4.80 (d, *J* = 7.2 Hz, 2H), 4.16 (s, 3H), 3.74 (s, 3H), 3.62 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.0, 167.7, 160.9, 151.9, 151.7, 144.1, 142.4, 140.8, 138.1, 132.0, 131.6, 131.4, 131.0, 130.9, 130.6, 129.9, 129.1, 128.2, 127.6, 124.4, 121.2, 54.1, 52.3, 52.2, 42.3; HRMS: calcd for $C_{25}H_{23}N_4O_5$ $[M + H]^+$ 459.1668, found 459.1669.

(*E*)-Methyl 2-(3-(6-methoxy-9*H*-purin-9-yl)prop-1-en-1-yl)benzoate (1f)



White solid. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.58 (s, 1H), 8.06 (s, 1H), 7.97-7.91 (m, 1H), 7.49-7.45 (m, 3H), 7.38-7.33 (m, 1H), 6.23 (dt, *J* = 14.6, 6.4 Hz, 1H), 5.06 (dd, *J* = 6.4, 1.6 Hz,

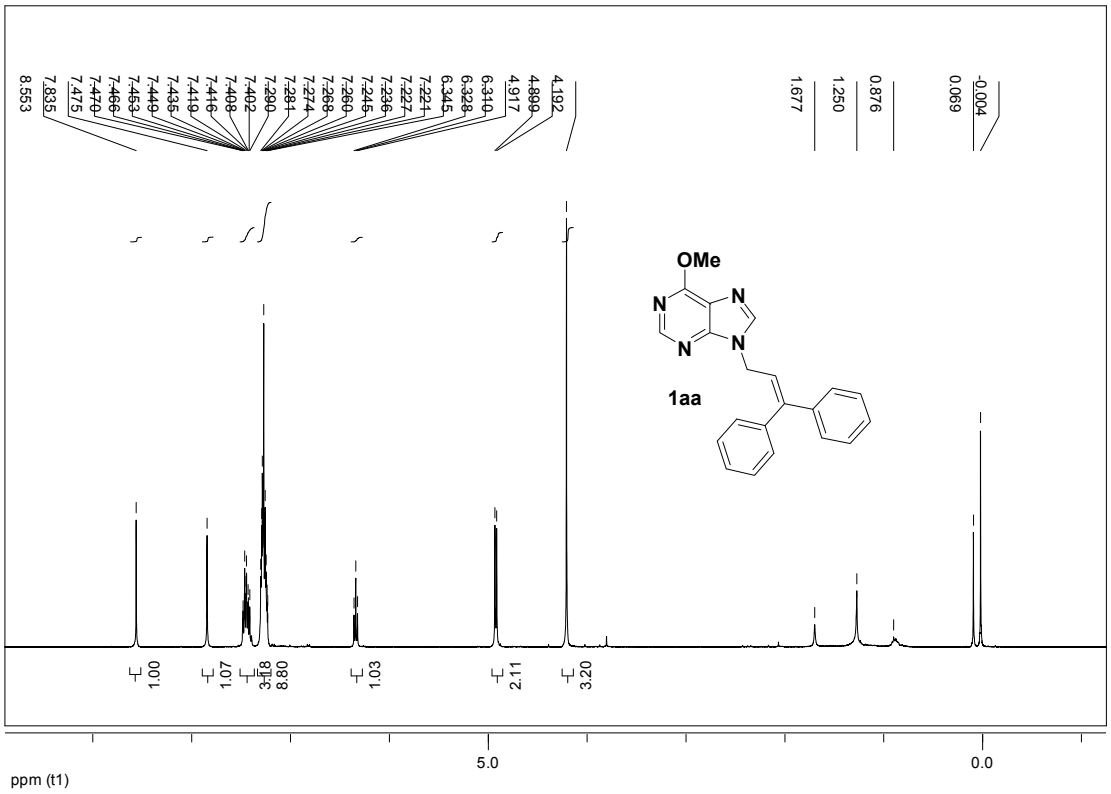
2H), 4.20 (s, 3H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.4, 161.1, 152.1, 151.8, 142.0, 137.7, 134.1, 132.3, 130.6, 128.4, 127.9, 127.7, 124.8, 121.4, 54.2, 52.2, 45.6; HRMS: calcd for $C_{17}H_{17}N_4O_3$ $[M + H]^+$ 325.1301, found 325.1301.

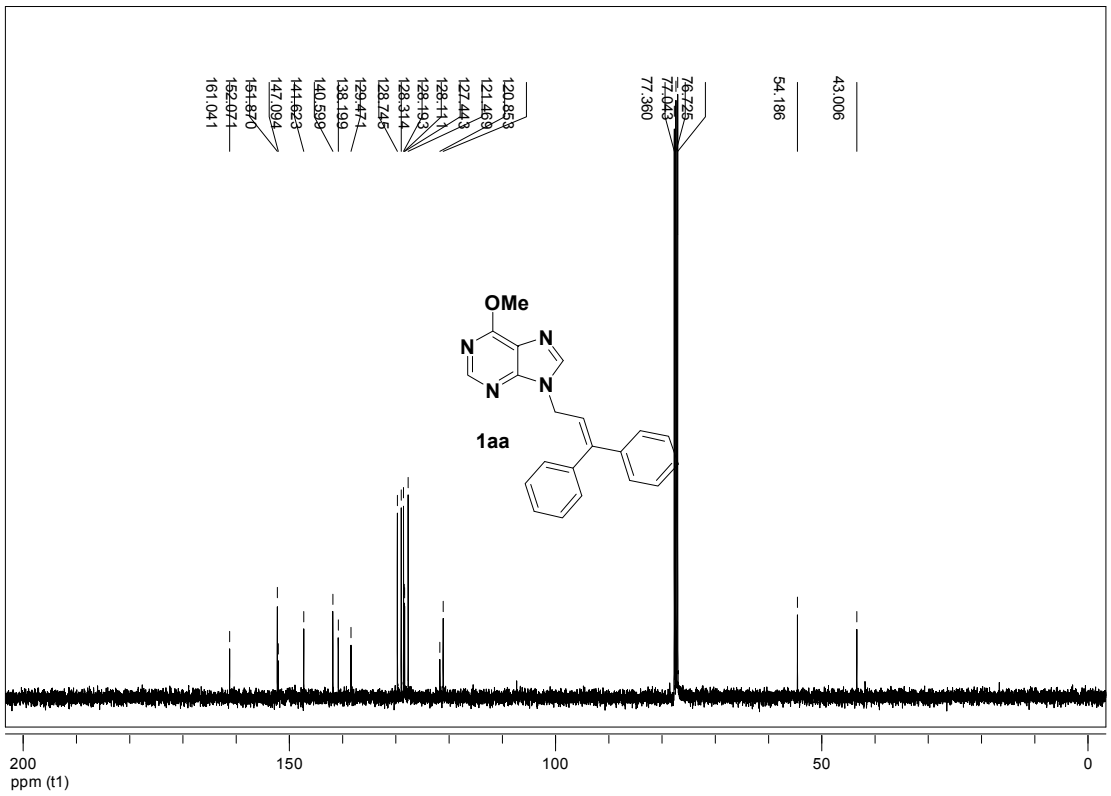
References:

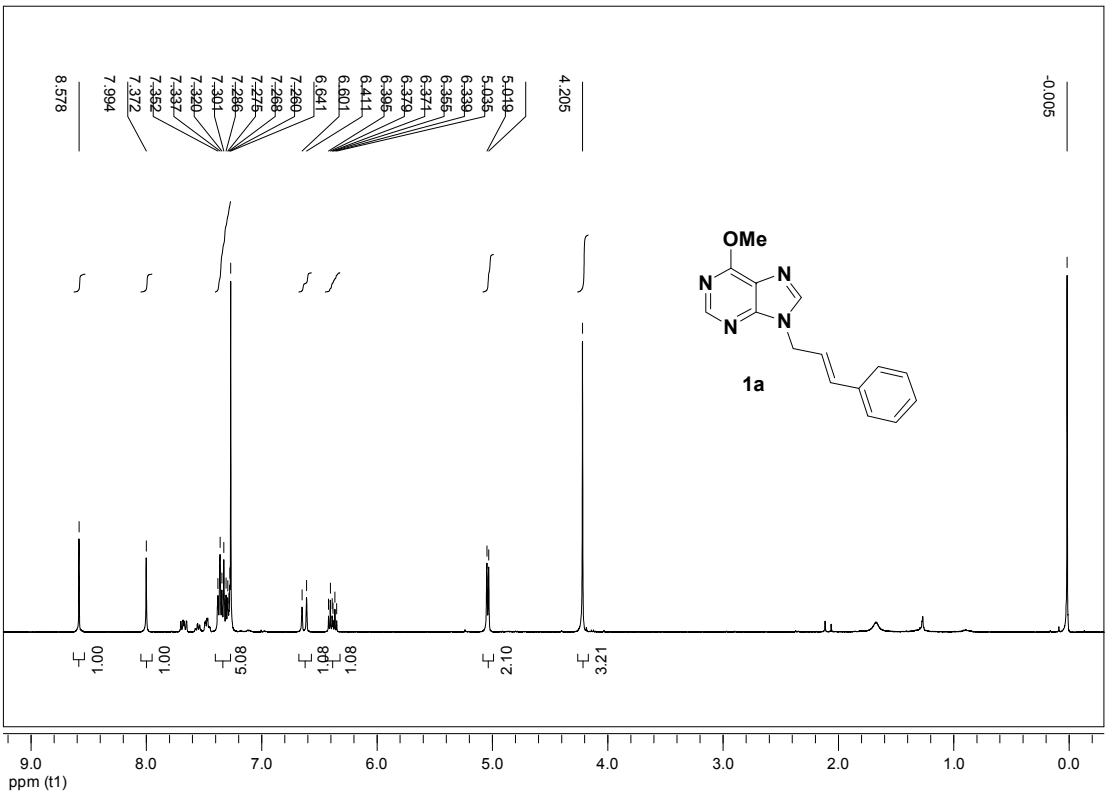
(1) Huang, L.-K.; Cherng, Y.-C.; Cheng, Y.-R.; Jang, J.-P.; Chao, Y.-L.; Cherng, Y.-J. *Tetrahedron* **2007**, *63*, 532.

(2) Qu, G.-R.; Mao, Z.-J.; Niu, H.-Y.; Wang, D.-C.; Xia, C.; Guo. H.-M. *Org. Lett.* **2009**, *11*, 1745.

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



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7.301
7.286
7.275
7.268
7.260
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6.601
6.411
6.395
6.379
6.371
6.355
6.339
5.035
5.019
4.205
-0.005
OMe
N
N
N
N
1a
1.00
1.00
5.08
1.08
1.01
2.10
3.21
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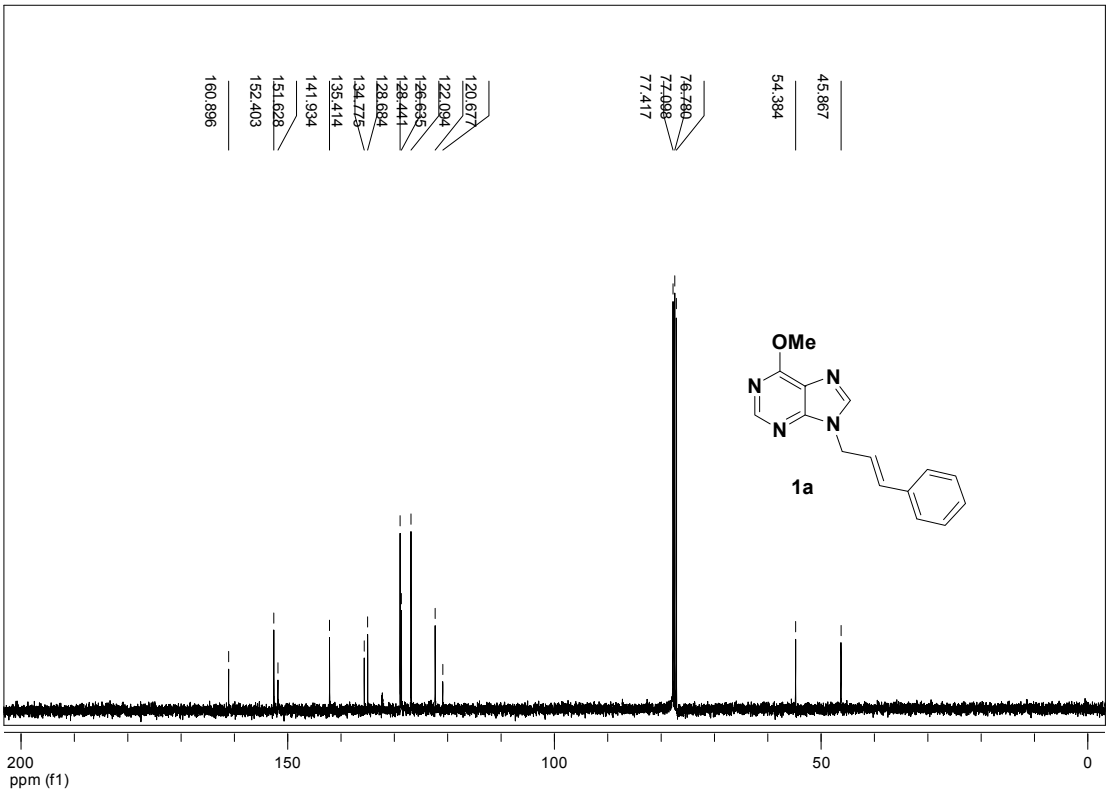
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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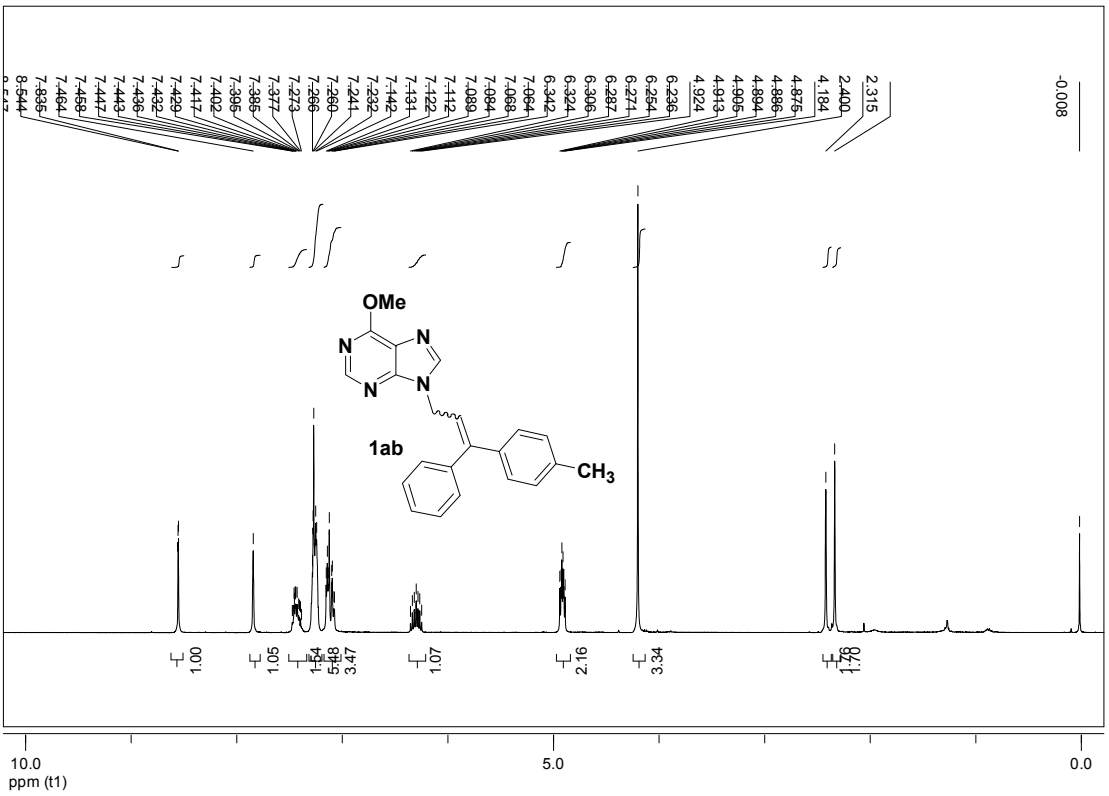
151.628
141.934
135.414
134.775
128.684
128.441
126.635
122.094
120.677
77.417
77.008
76.780
54.384
45.867
OMe
N
N
N
N
1a
200
150
100
50
0
ppm (f1)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N
N
1ab
CH3
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ppm (t1)
5.0
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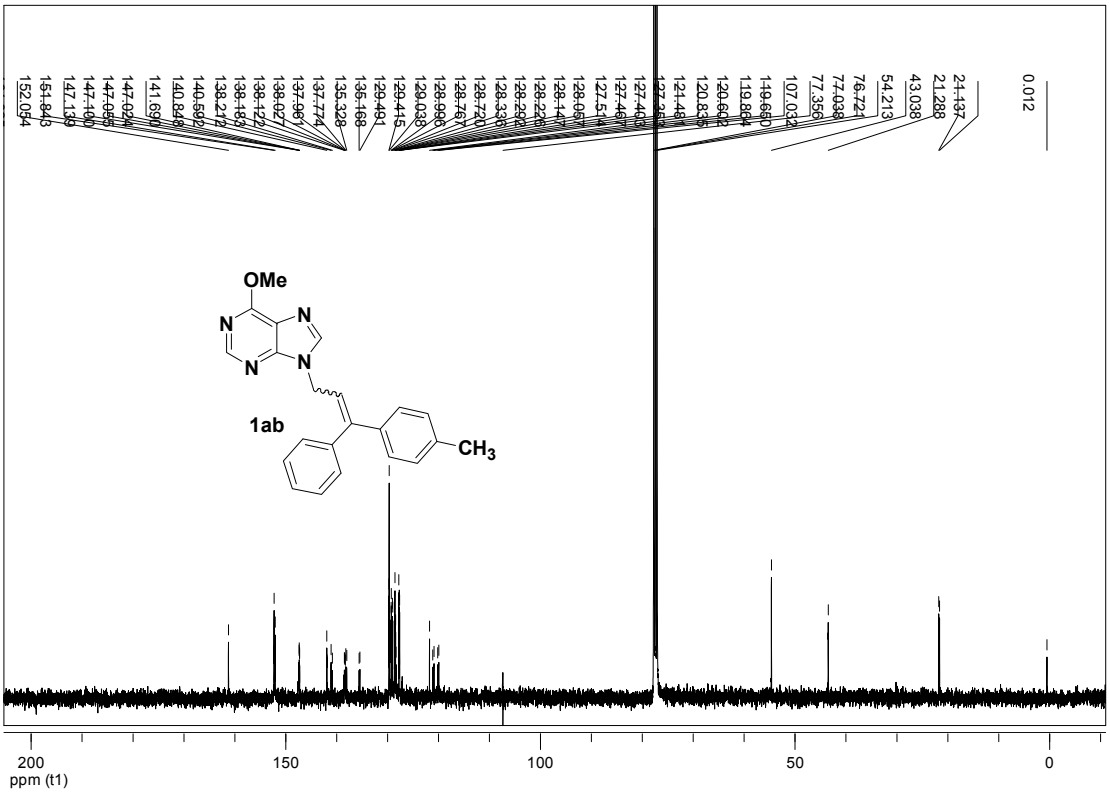
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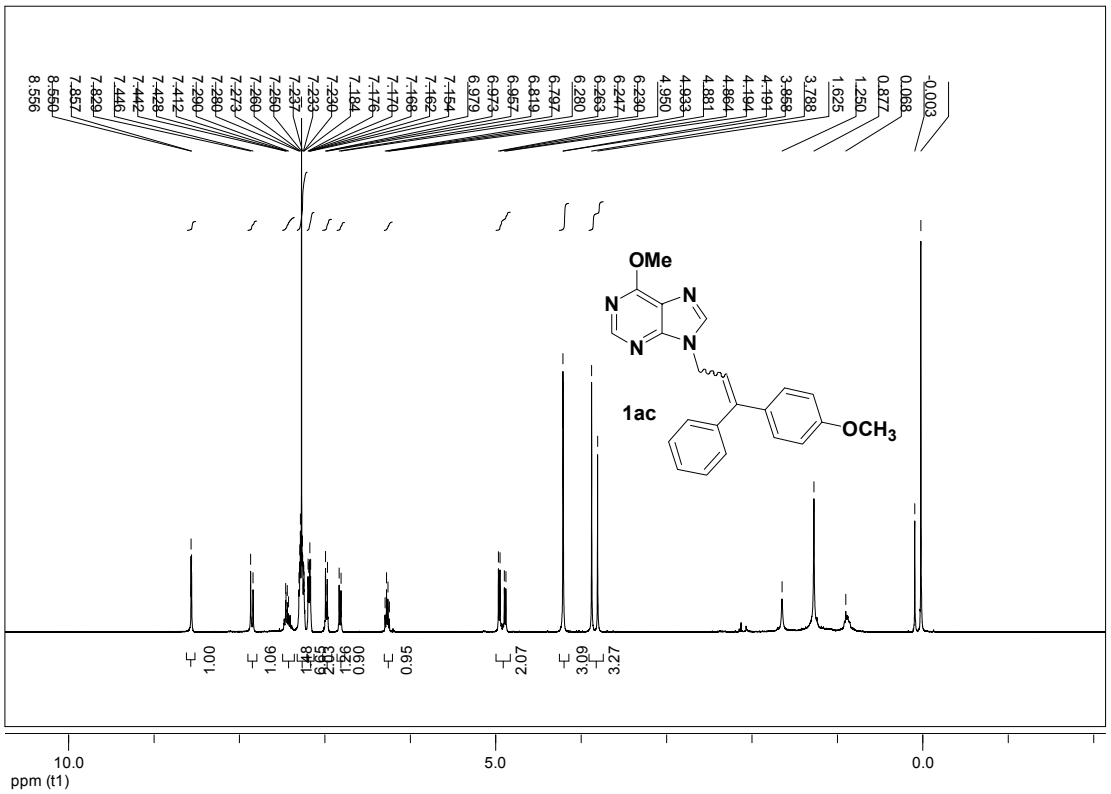
N
N
N
1ab
CH3
200
ppm (t1)
150
100
50
0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7.857
7.829
7.446
7.442
7.428
7.412
7.290
7.280
7.273
7.260
7.237
7.233
7.230
7.184
7.176
7.170
7.168
7.162
7.154
6.979
6.973
6.967
6.819
6.797
6.280
6.263
6.247
6.230
4.950
4.933
4.881
4.864
4.194
4.191
3.858
3.788
1.625
1.250
0.877
0.068
-0.003
OMe
N
N
N
N
1ac
OCH3
1.00
1.06
1.48
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2.03
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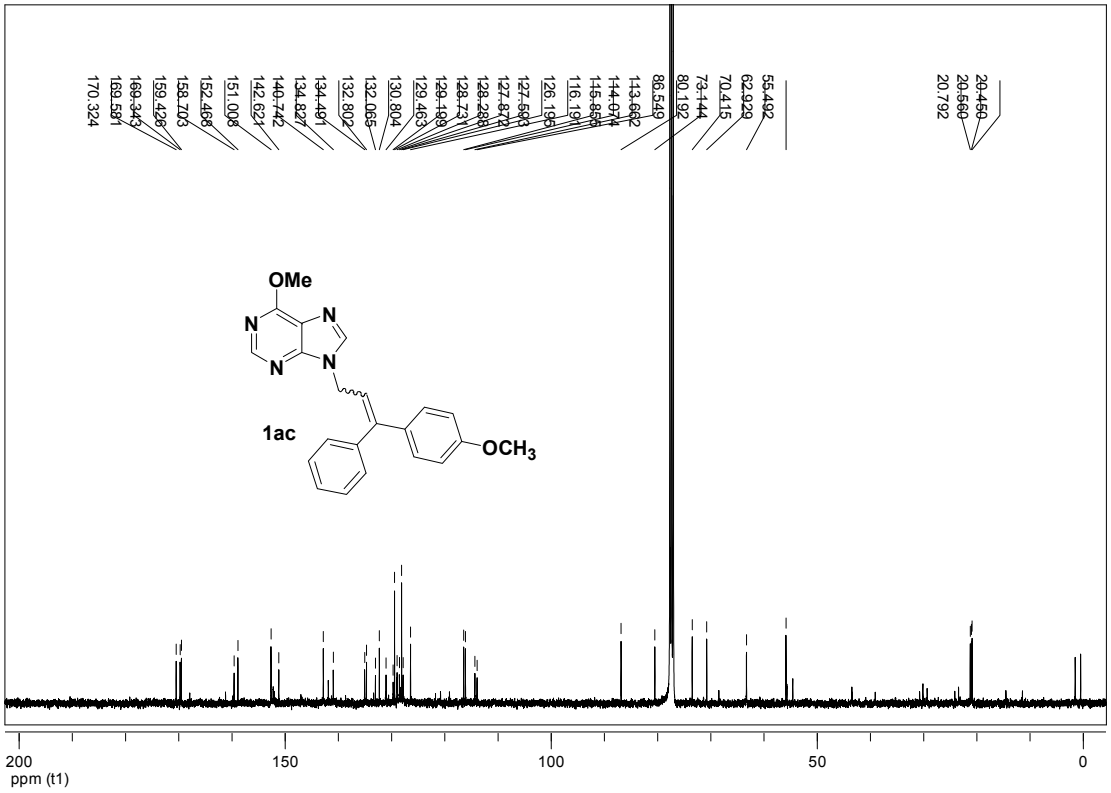
0.60
0.96
2.07
3.09
3.27
10.0
5.0
0.0
ppm (t1)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158.703
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142.621
140.742
134.827
134.491
132.802
132.065
130.804
129.463
129.198
128.731
128.288
127.871
127.590
126.195
116.191
115.856
114.671
113.662
86.549
80.192
78.144
70.415
62.929
55.492
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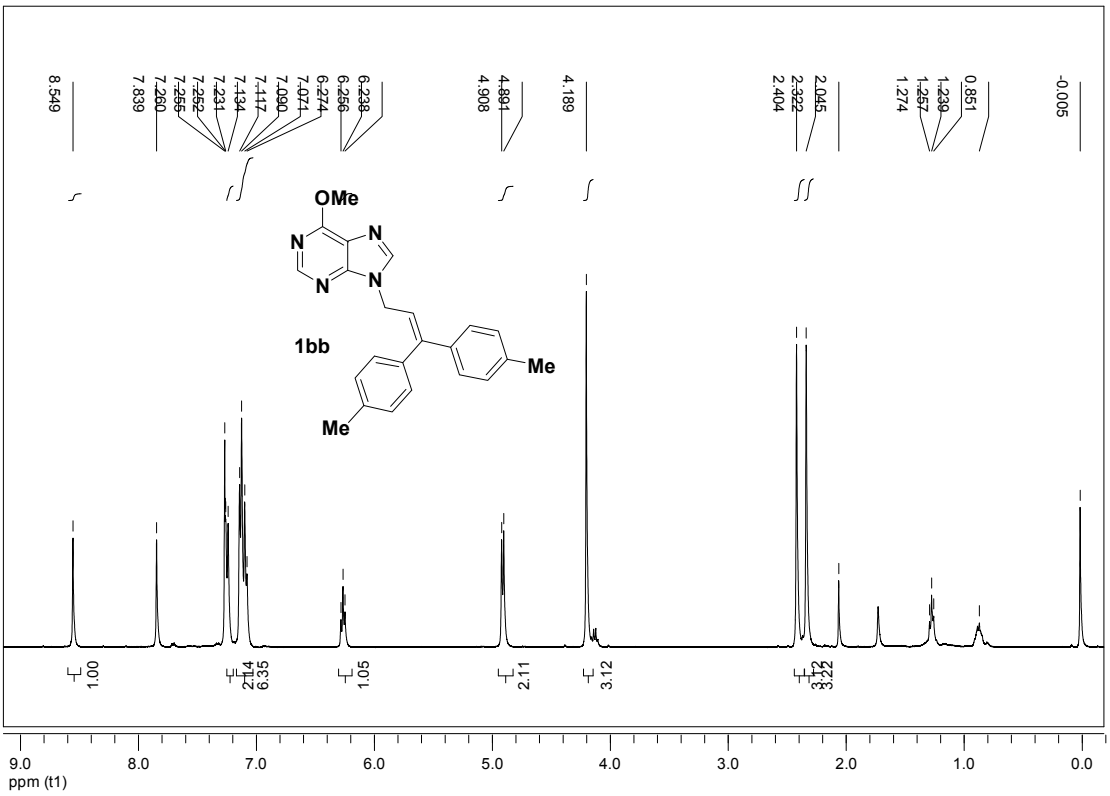
20.660
20.450
OMe
N
N
N
N
1ac
OCH3
200
150
100
50
0
ppm (t1)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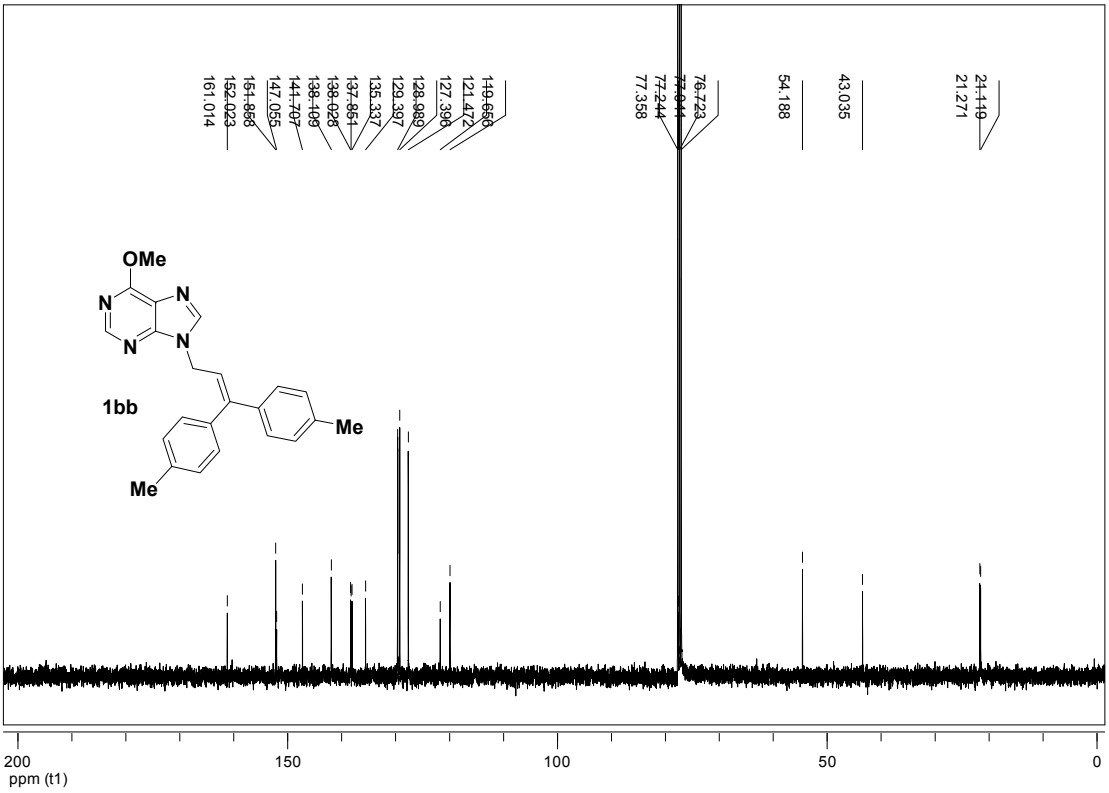
7.260
7.255
7.252
7.231
7.134
7.117
7.090
7.071
6.274
6.256
6.238
4.908
4.891
4.189
2.404
2.322
2.045
1.274
1.257
1.239
0.851
-0.005
OMe
N
N
N
N
1bb
Me
Me
1.00
2.14
6.35
1.05
2.11
3.12
3.12
3.22
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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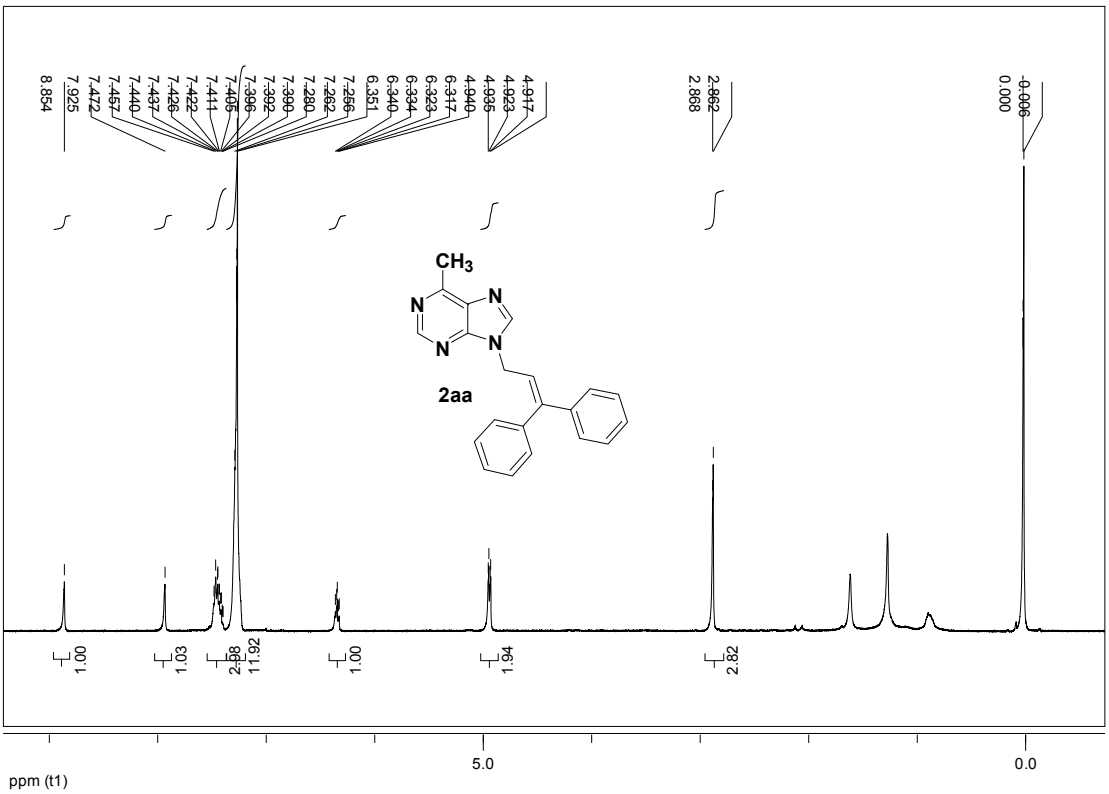
151.868
147.055
141.707
138.109
138.026
137.851
135.337
129.397
128.980
127.396
121.472
119.650
77.358
77.244
77.011
76.723
54.188
43.035
24.119
21.271
OMe
N
N
N
N
1bb
Me
Me
200
150
100
50
0
ppm (t1)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7.472
7.457
7.440
7.437
7.426
7.422
7.411
7.405
7.396
7.392
7.390
7.280
7.262
7.256
6.351
6.340
6.334
6.323
6.317
4.940
4.936
4.923
4.917
2.862
2.868
0.006
0.000
CH3
N
N
N
N
2aa
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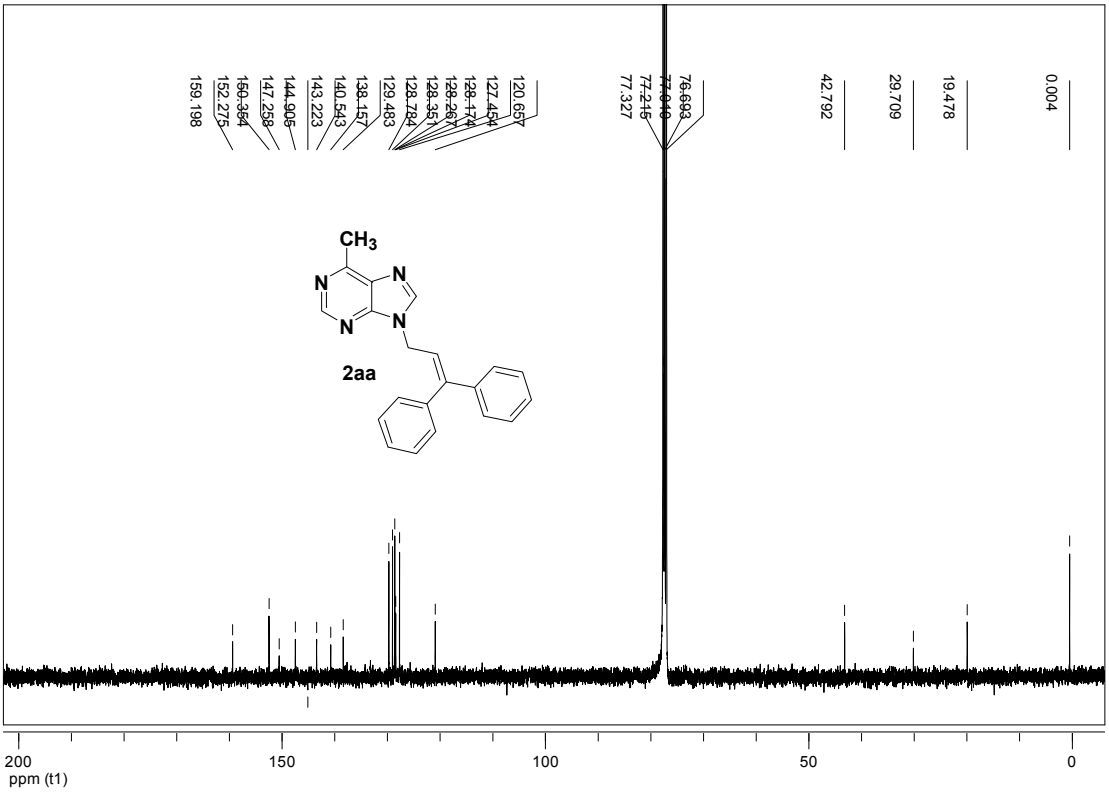
1.03
2.88
11.26
1.00
1.94
2.82
5.0
0.0
ppm (t1)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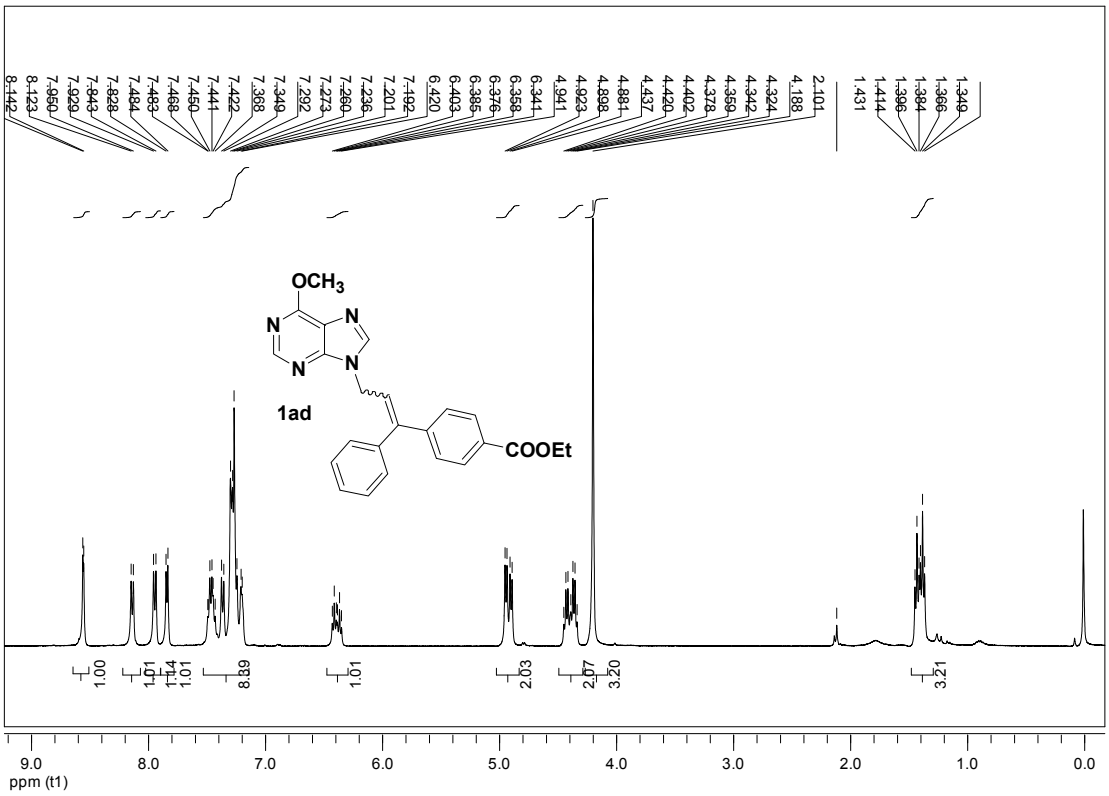
143.223
140.543
138.157
129.483
128.784
128.351
128.267
128.174
127.454
120.657
77.327
77.215
77.010
76.693
42.792
29.709
19.478
0.004
CH3
N
N
N
N
2aa
200
150
100
50
0
ppm (t1)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8.123
7.960
7.929
7.843
7.828
7.484
7.463
7.468
7.450
7.441
7.422
7.368
7.349
7.292
7.273
7.260
7.236
7.201
7.192
6.420
6.403
6.385
6.376
6.358
6.341
4.941
4.923
4.898
4.881
4.437
4.420
4.402
4.378
4.359
4.342
4.324
4.188
2.101
1.431
1.414
1.396
1.384
1.366
1.349
OCH3
N
N
N
N
1ad
COOEt
1.00
1.01
1.14
1.01
8.89
1.01
2.03
2.07
3.20
3.71
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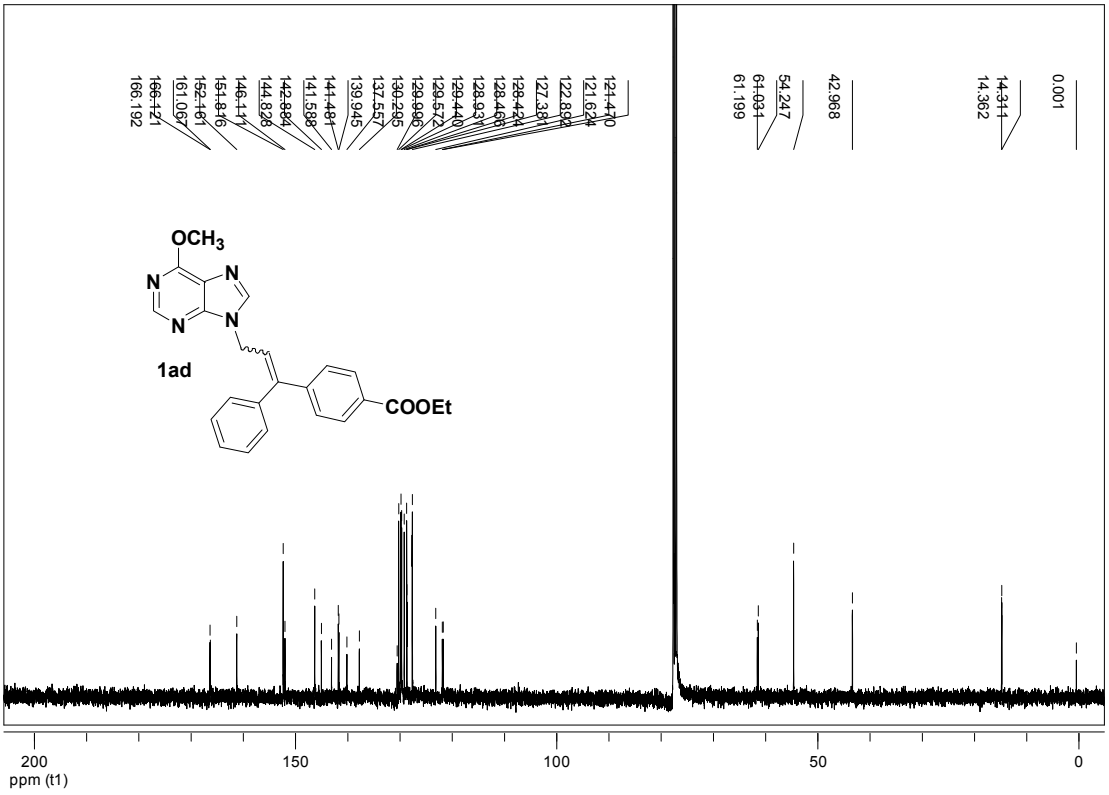
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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161.067
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146.111
144.826
142.884
141.588
141.481
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137.557
130.295
129.990
129.572
129.440
128.931
128.466
128.424
127.381
122.899
121.624
121.470
61.199
61.031
54.247
42.968
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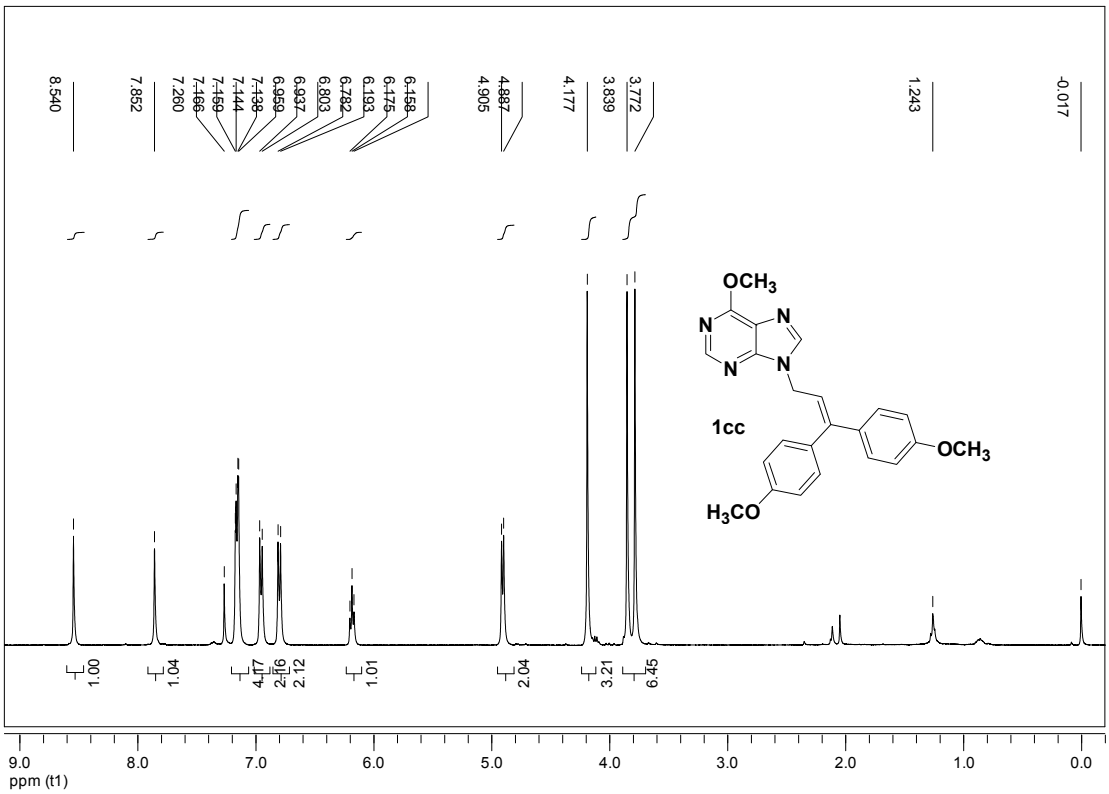
OCH3
N
N
N
N
1ad
COOEt
200
150
100
50
0
ppm (t1)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7.144
7.138
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6.937
6.803
6.782
6.193
6.175
6.158
4.905
4.887
4.177
3.839
3.772
1.243
-0.017
1.00
1.04
4.17
2.16
2.12
1.01
2.04
3.21
9.45
OCH3
N
N
N
N
1cc
OCH3
H3CO
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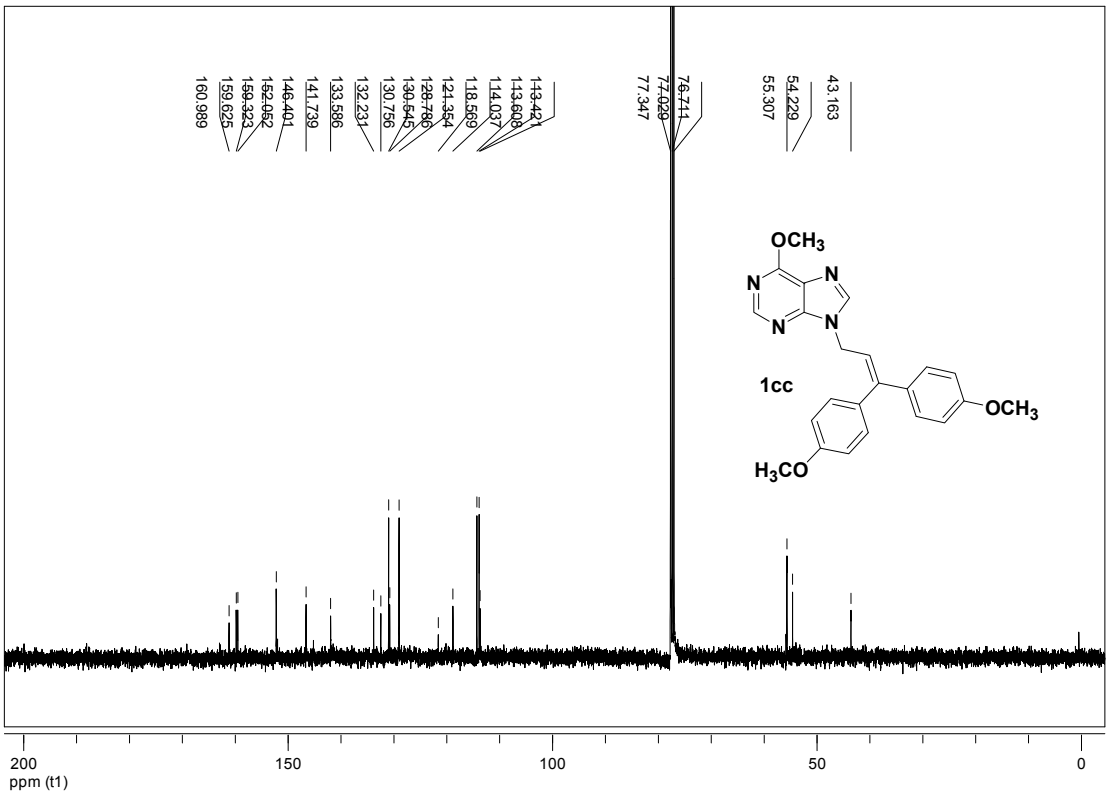
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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132.231
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128.786
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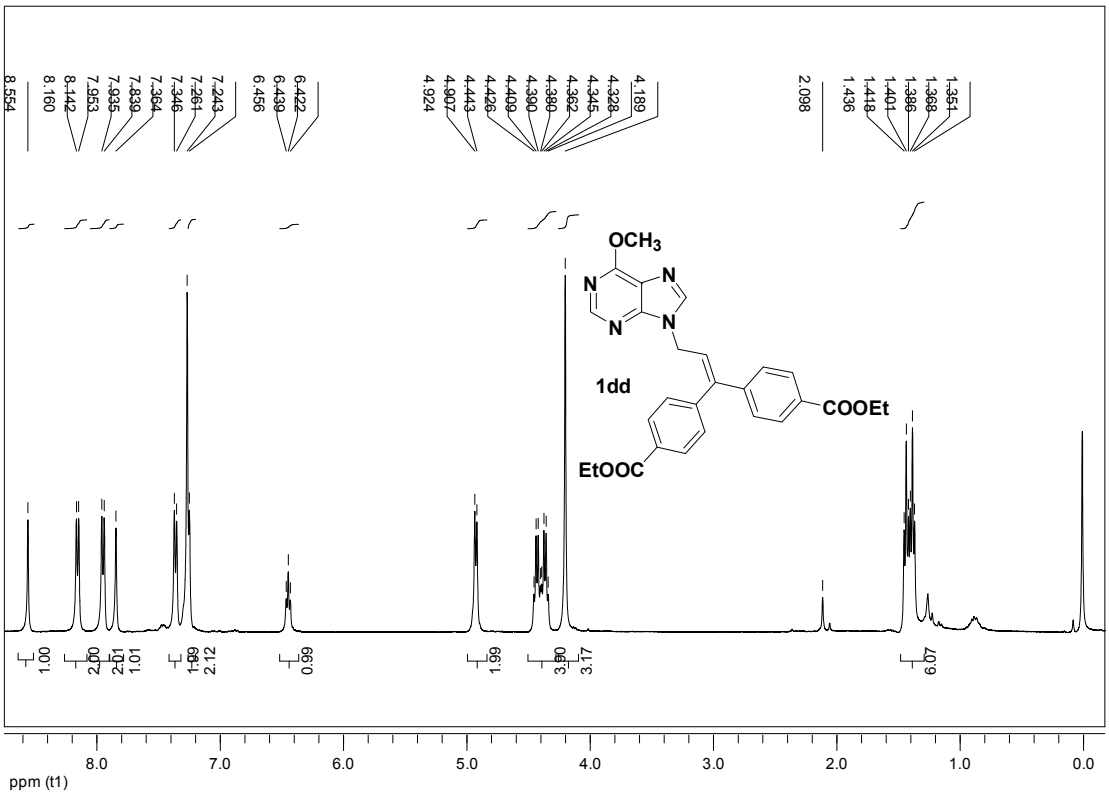
118.569
114.037
113.608
113.421
77.347
77.029
76.711
55.307
54.229
43.163
OCH3
N
N
N
N
1cc
OCH3
H3CO
200
150
100
50
0
ppm (t1)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7.953
7.935
7.839
7.364
7.346
7.261
7.243
6.456
6.439
6.422
4.924
4.907
4.443
4.426
4.409
4.390
4.380
4.362
4.345
4.328
4.189
2.098
1.436
1.418
1.401
1.386
1.368
1.351
OCH3
N
N
N
N
1dd
COOEt
EtOOC
1.00
2.00
2.01
1.01
1.89
2.12
0.99
1.99
3.60
3.17
4.07
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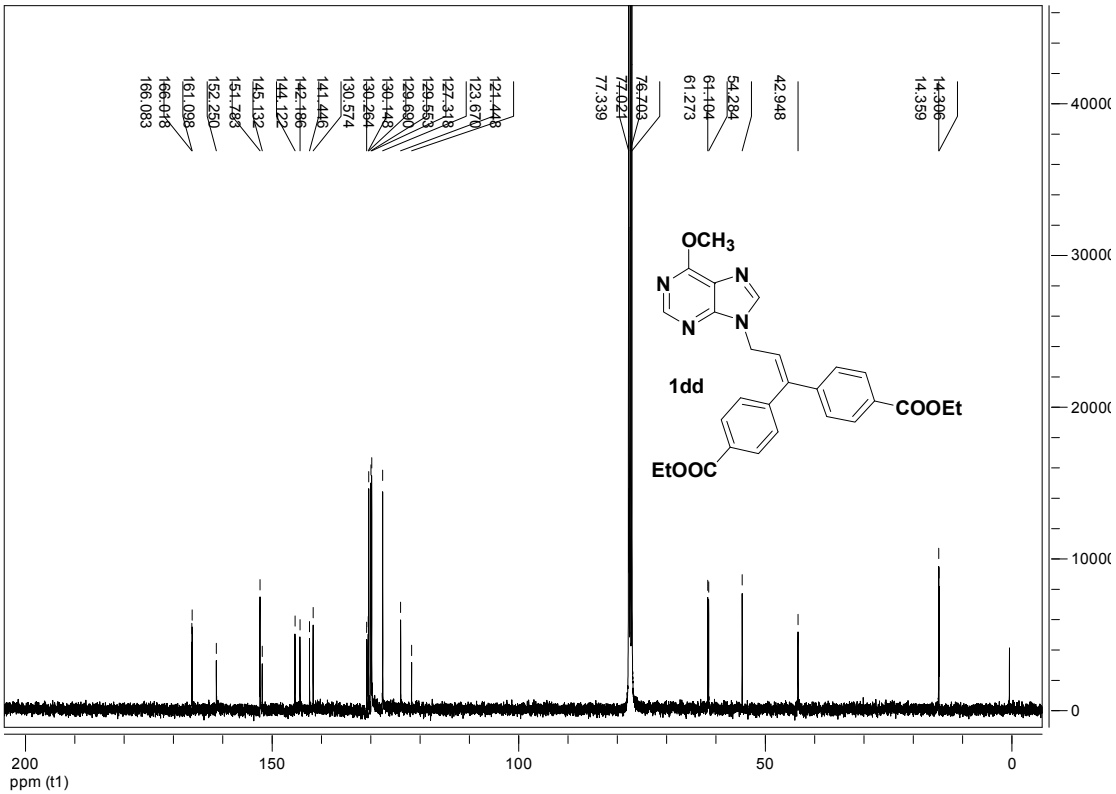
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)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142.186
141.446
130.574
130.264
130.148
129.690
129.553
127.318
123.670
121.448
77.339
77.021
76.703
61.273
61.104
54.284
42.948
14.359
14.306
OCH3
N
N
N
N
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COOEt
EtOOC
40000
30000
20000
10000
0
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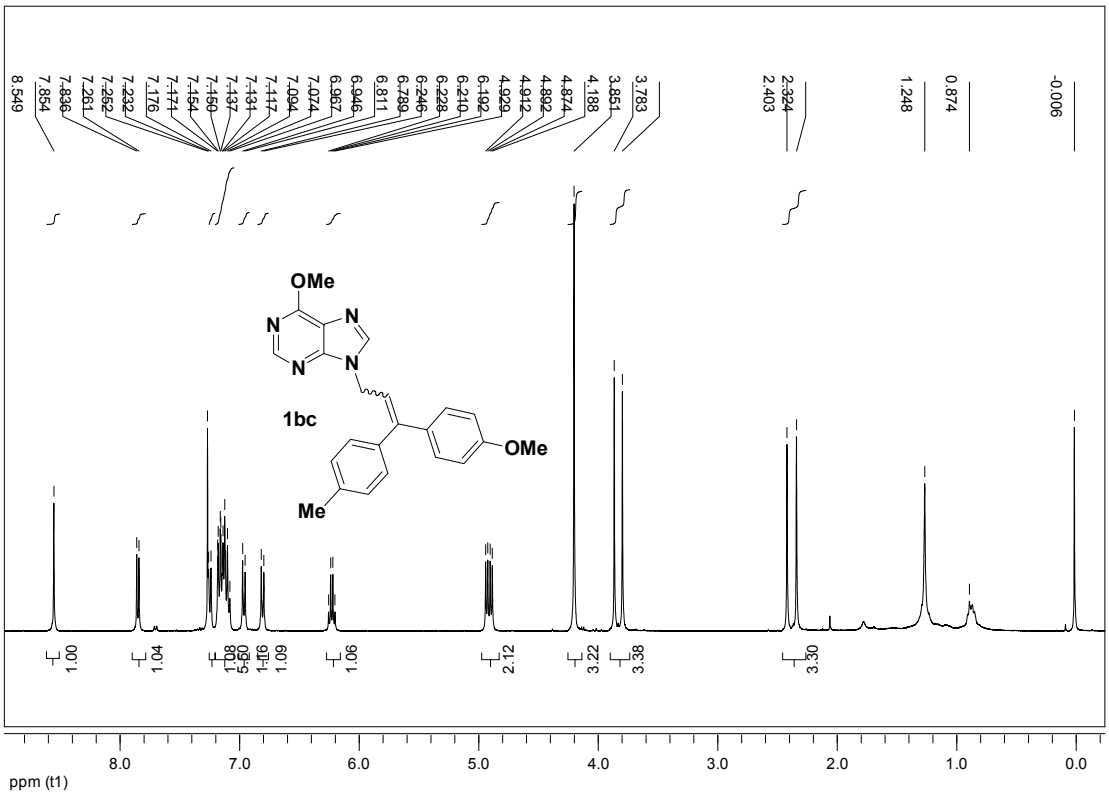
150
100
50
0
ppm (t1)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7.154
7.150
7.137
7.131
7.117
7.094
7.074
6.967
6.946
6.811
6.789
6.246
6.228
6.210
6.192
4.929
4.912
4.892
4.874
4.188
3.851
3.783
2.403
2.324
1.248
0.874
-0.006
OMe
N
N
N
N
1bc
OMe
Me
1.00
1.04
1.08
5.50
1.16
1.09
1.06
2.12
3.22
3.38
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7.0
6.0
5.0
4.0
3.0
2.0
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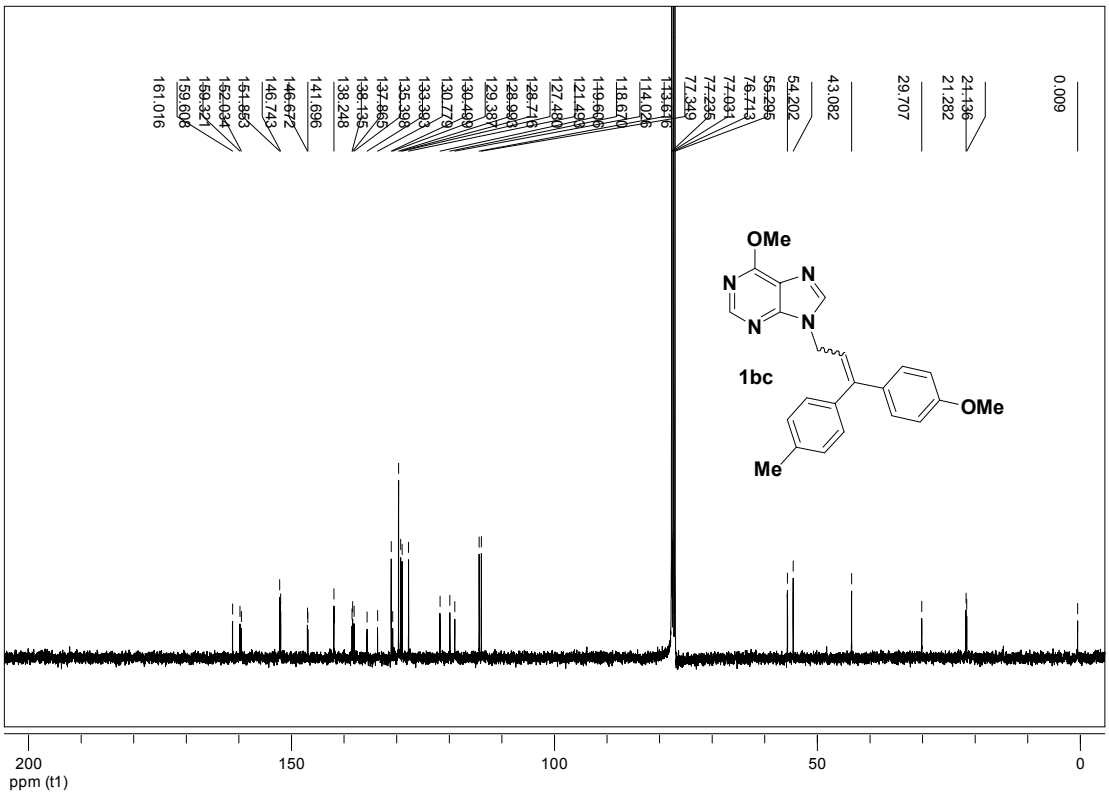
0.0
ppm (t1)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138.135
137.866
135.396
133.393
130.779
130.499
129.387
128.990
128.718
127.480
121.498
119.606
118.670
114.026
113.616
77.349
77.235
77.031
76.713
55.295
54.202
43.082
29.707
21.282
21.136
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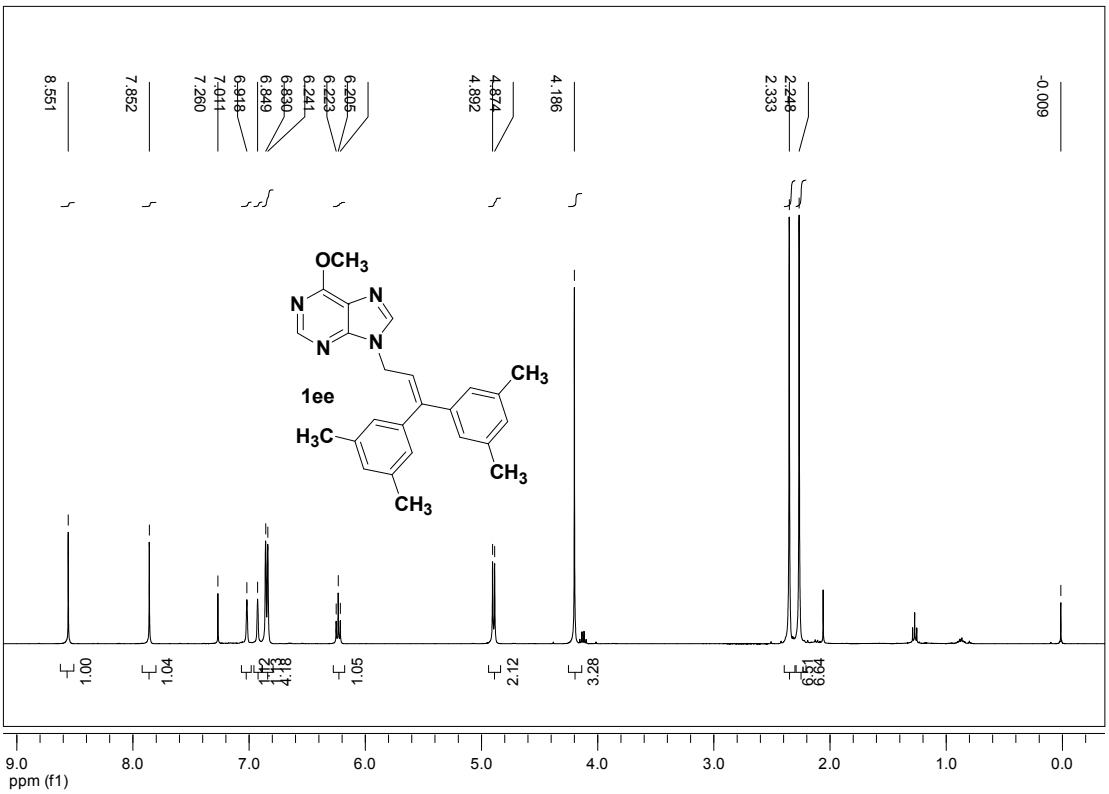
OMe
N
N
N
N
1bc
OMe
Me
200
150
100
50
0
ppm (t1)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7.011
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6.830
6.241
6.223
6.205
4.892
4.874
4.186
2.333
2.248
-0.009
OCH3
N
N
N
N
1ee
CH3
H3C
CH3
CH3
1.00
1.04
1.12
1.13
4.18
1.05
2.12
3.28
6.11
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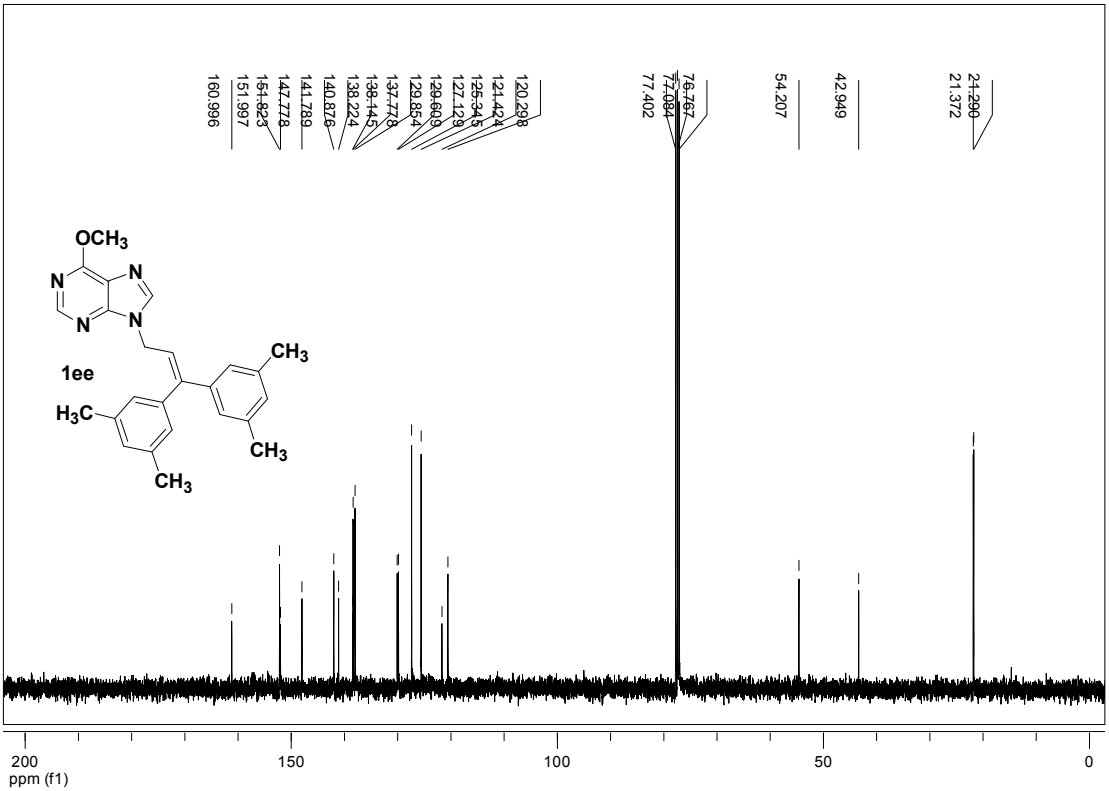
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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127.129
125.345
121.424
120.298
77.402
77.084
76.767
54.207
42.949
21.372
21.290
OCH3
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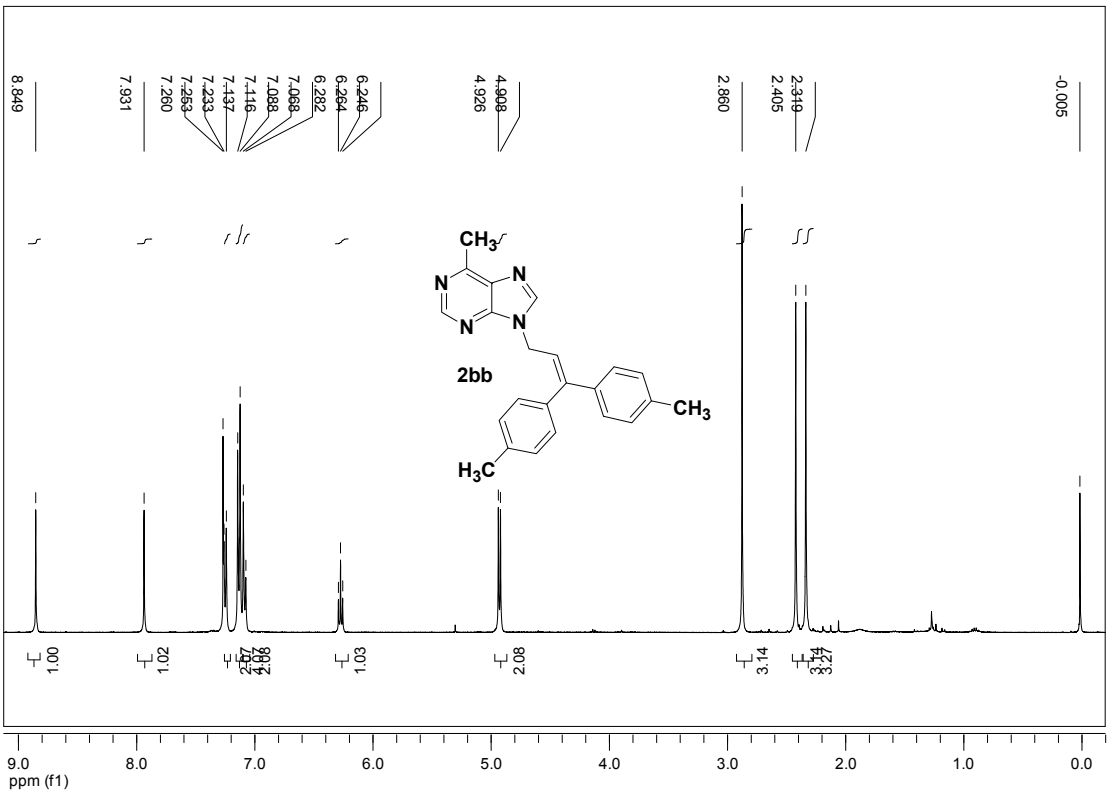
N
N
N
1ee
CH3
H3C
CH3
CH3
200
150
100
50
0
ppm (f1)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7.088
7.068
6.282
6.264
6.246
4.926
4.908
2.860
2.405
2.319
-0.005
1.00
1.02
2.08
1.03
2.08
3.14
3.14
3.27
2bb
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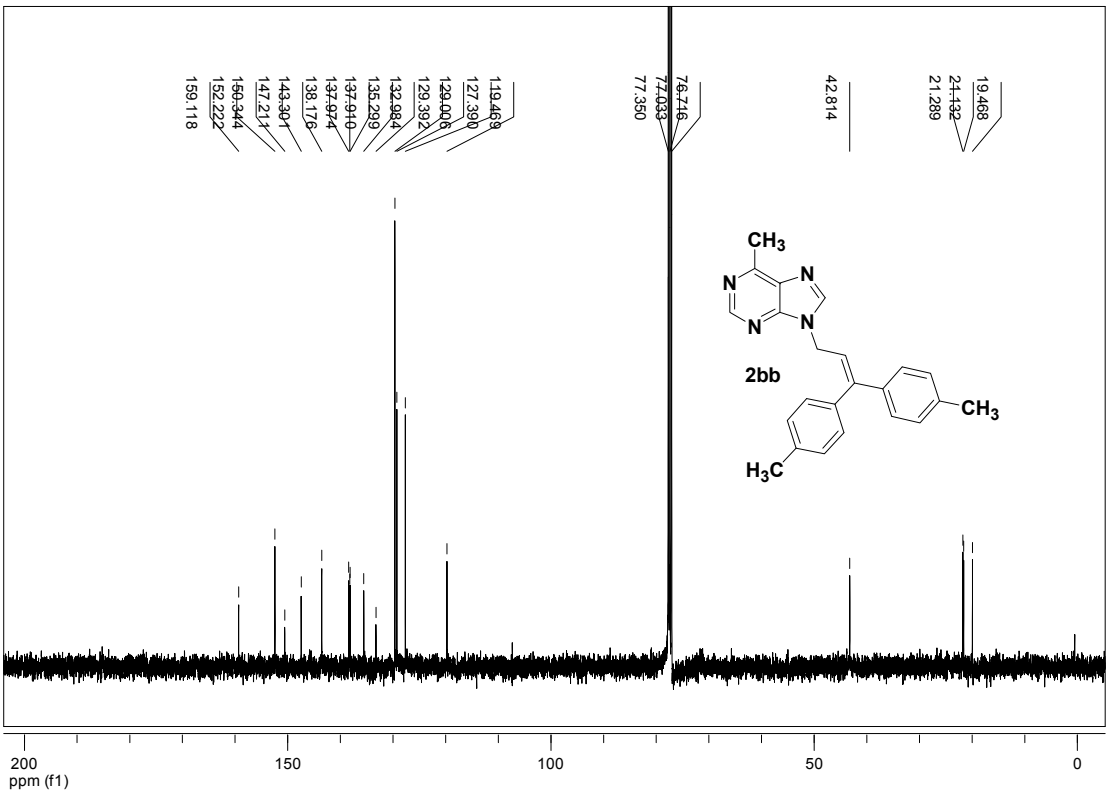
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)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132.984
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129.008
127.390
119.469
77.350
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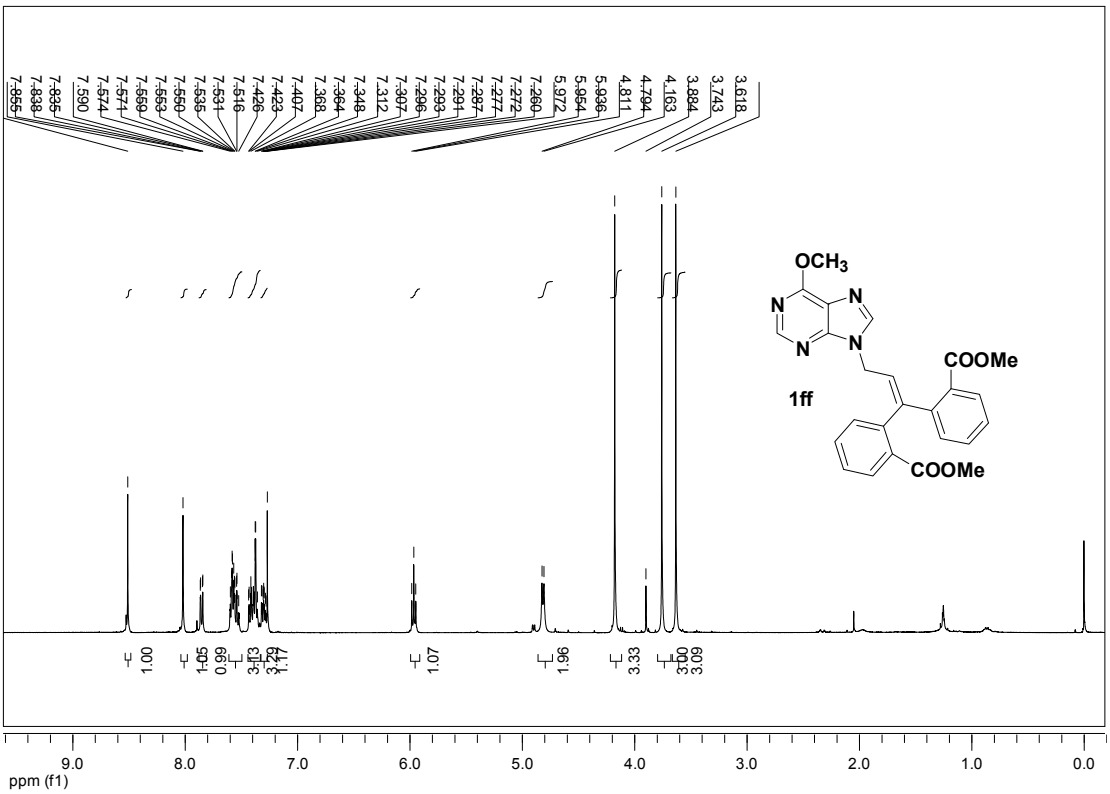
21.289
21.132
19.468
2bb
200
150
100
50
0
ppm (f1)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7.426
7.423
7.407
7.368
7.364
7.348
7.312
7.307
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7.291
7.287
7.277
7.272
7.260
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5.964
5.936
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4.794
4.163
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3.743
3.618
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1.05
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3.13
2.42
1.17
1.07
1.96
3.33
3.00
3.03
OCH3
N
N
N
N
COOMe
COOMe
1ff
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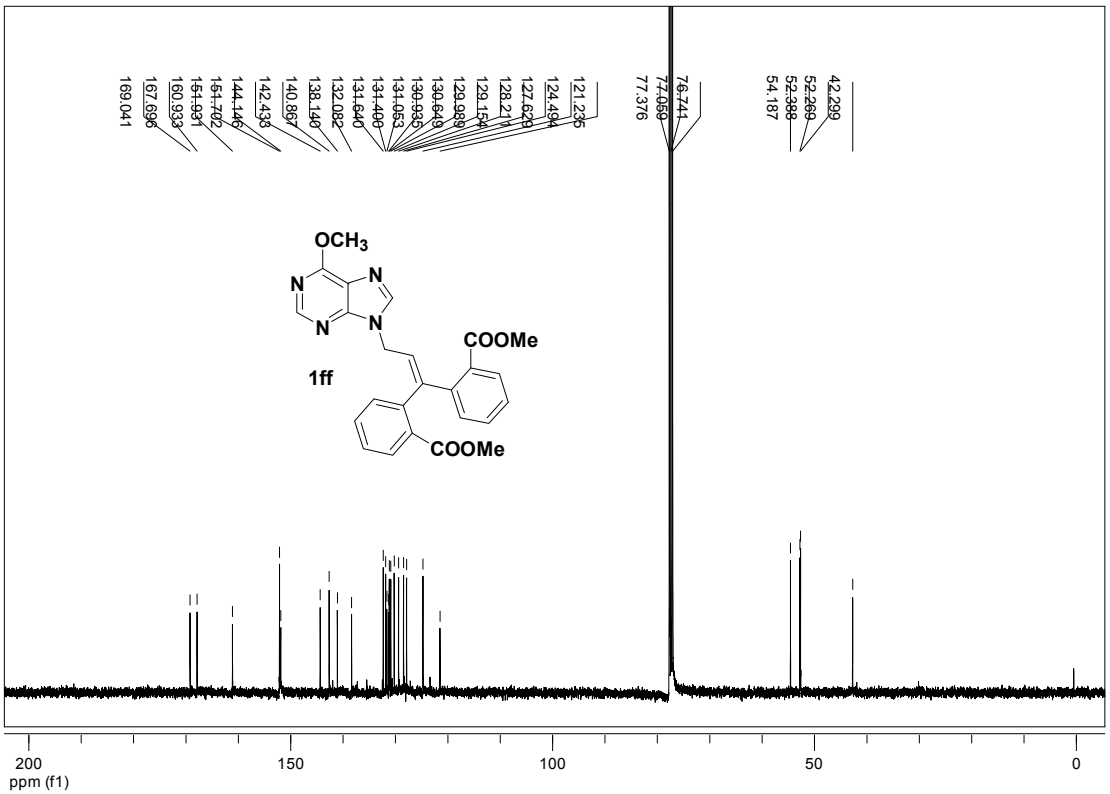
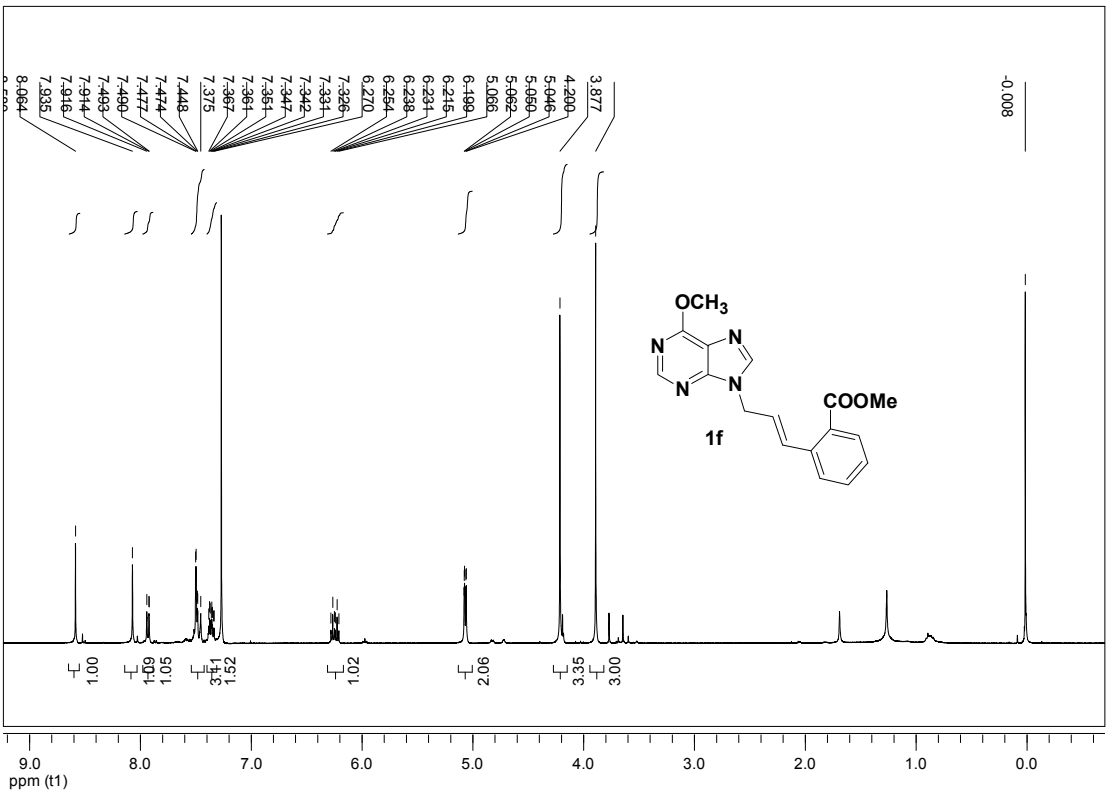
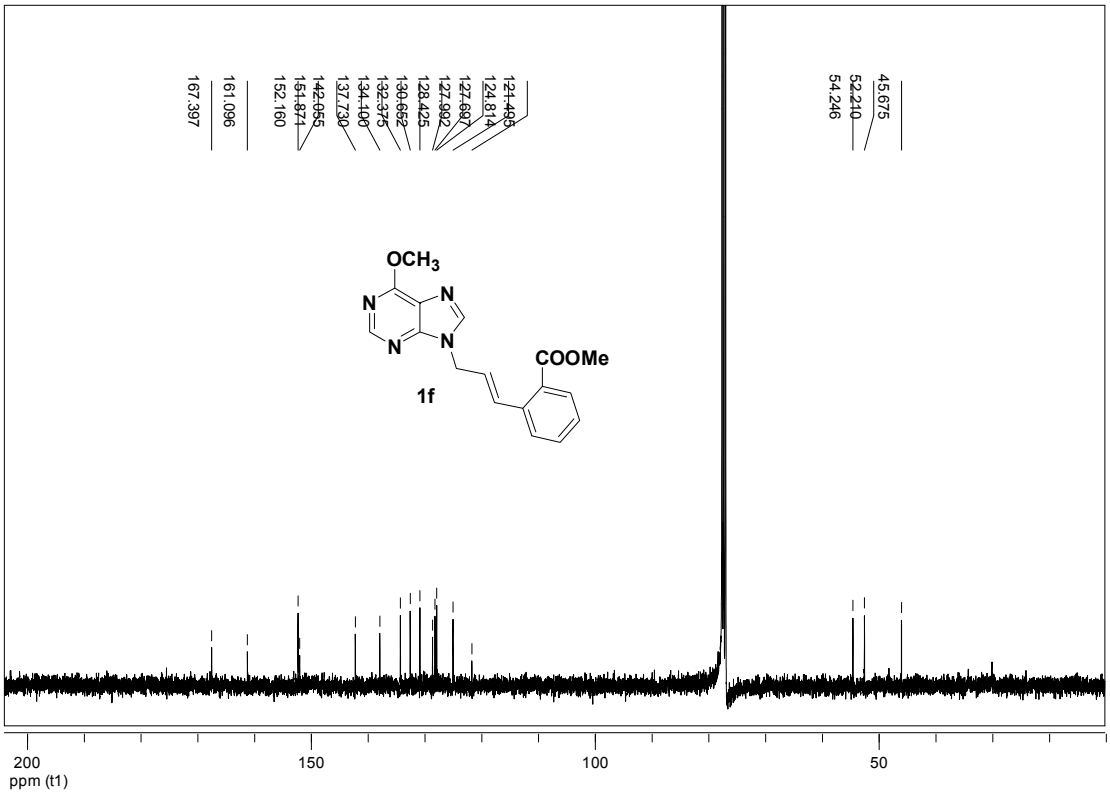
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (f1)


169.041
167.696
160.933
154.931
154.702
144.146
142.436
140.867
138.146
132.082
131.640
131.406
131.053
130.933
130.648
129.988
129.154
128.211
127.628
124.494
121.235
77.376
77.059
76.741
54.187
52.388
52.269
42.239
OCH3
N
N
N
N
COOMe
COOMe
1ff
200
150
100
50
0
ppm (f1)


8.064
7.935
7.916
7.914
7.493
7.490
7.477
7.474
7.448
7.375
7.367
7.361
7.351
7.347
7.342
7.331
7.326
6.270
6.254
6.238
6.231
6.215
6.199
5.066
5.062
5.050
5.046
4.200
3.877
-0.008
1.00
1.09
1.05
3.11
1.52
1.02
2.06
3.35
3.00
OCH3
N
N
N
N
COOMe
1f
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
ppm (t1)


167.397
161.096
152.160
142.055
137.730
134.106
132.375
130.662
128.425
127.992
127.697
124.814
121.498
54.246
52.210
45.675
OCH3
N
N
N
N
COOMe
1f
200
150
100
50
ppm (t1)