Differentiation and Functionalization of Adjacent, Remote C–H Bonds

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TABLE OF CONTENTS

GENERAL INFORMATION

Solvents

Dry acetonitrile (MeCN), tetrahydrofuran (THF), dichloromethane (DCM), and toluene were purchased from Sigma-Aldrich. 1,1,1,3,3,3-Hexafluoro-2-propanol (HFIP) was purchased from Oakwood. Chloroform-d_1 and acetonitrile-d_3 were purchased from Cambridge Isotope Laboratories.

Chromatography

Analytical thin layer chromatography was performed on 0.25 mm silica gel 60-F254. Visualization was carried out with UV light and Vogel's permanganate. Preparative TLC was used to purify reactions run at 0.1 mmol scale out of convenience and was conducted using silica gel plates, unless otherwise stated.

Spectroscopy and Instruments

^{1}H NMR was recorded on Bruker DRX-600 instrument (600 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to 7.26 ppm of chloroform-*d*, or the center peak of the pentet at 1.94 ppm of acetonitrile-d_3. ^{13}C NMR spectra were recorded on Bruker DRX-600 instrument (151 MHz), and were fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center peak of a triplet at 77.16 ppm of chloroform-*d*, or the center peak of a septet at 1.32 ppm of acetonitrile-d_3. ^{19}F NMR spectra were recorded on Bruker AMX-400 instrument (376 MHz), and were fully decoupled by broad band proton decoupling. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, p = pentet, sext = sextet, sep = septet, m = multiplet, br = broad. Coupling constants, *J*, were reported in Hertz unit (Hz). High-resolution mass spectra (HRMS) were recorded on a Waters mass spectrometer using ESI-TOF (electrospray ionization-time of flight). The single crystal X-ray diffraction studies were carried out on a Bruker Kappa APEX-II CCD diffractometer equipped with Mo Kα radiation (λ = 0.71073 Å).

Starting materials

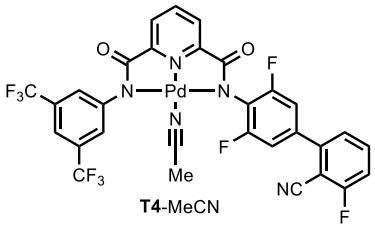
All substrates were used as received from commercial suppliers, unless otherwise stated. $Pd(OAc)_2$, AgOAc, Ag_2CO_3, and Ac-Gly-OH were purchased from Sigma-Aldrich. Methyl bicyclo[2.2.1]hept-2-ene-2-carboxylate (NBE-CO_2Me) was reported in the previous literature[1]. Templates (**T1**-MeCN, **T2**-MeCN, **T3**-MeCN,) were reported in the previous literature[2]. Compounds **1u**[3], **1v**[4], **3a**[5], and **5b**[6] were reported in the previous literatures.

EXPERIMENTAL SECTION

I. Preparation of Templates and Substrates

A. Preparation of Templates

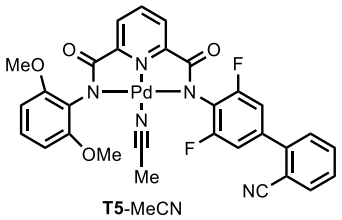
Templates were synthesized following the literature procedures[2].



T4-MeCN

Palladium-N^2-(3,5-bis(trifluoromethyl)phenyl)-N^6-(2'-cyano-3,3',5-trifluoro-[1,1'-biphenyl]-4-yl)pyridine-2,6-dicarboxamide complex (T4-MeCN)

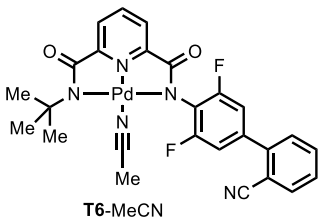
^{1}H NMR (600 MHz, CD_3CN) δ 8.33 (t, *J* = 7.8 Hz, 1H), 7.92 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.90–7.86 (m, 3H), 7.80–7.74 (m, 1H), 7.69 (s, 1H), 7.45 (d, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 8.8 Hz, 1H), 7.27 (d, *J* = 8.2 Hz, 2H); ^{13}C NMR (151 MHz, CD_3CN) δ 170.08, 169.56, 164.86 (d, *J* = 255.8 Hz), 158.71 (dd, *J* = 248.1, 6.6 Hz), 152.92, 151.08, 149.65, 145.52, 143.81, 136.39, 136.32, 131.73 (q, *J* = 32.7 Hz), 127.85, 127.82–127.68 (m), 127.43, 126.95 (d, *J* = 3.3 Hz), 125.50 (t, J = 16.8 Hz), 124.65 (q, *J* = 272.3 Hz), 116.63 (d, *J* = 19.8 Hz), 114.51, 113.27 (dd, *J* = 19.6, 6.0 Hz), 101.34 (d, *J* = 16.0 Hz); ^{19}F NMR (376 MHz, CD_3CN) δ -63.50, -108.24, -117.02. HRMS (ESI-TOF) *m/z* calc'd for $C_{30}H_{14}F_9N_5O_2Pd$ $[M+H]^+$: 754.0111; found: 754.0103.



T5-MeCN

Palladium-N^2-(2'-cyano-3,5-difluoro-[1,1'-biphenyl]-4-yl)-N^6-(2,6-dimethoxyphenyl)pyridine-2,6-dicarboxamide complex (T5-MeCN)

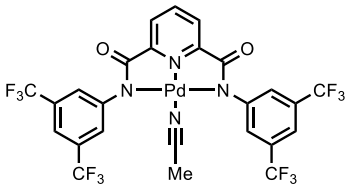
^{1}H NMR (600 MHz, CD_3CN) δ 8.27 (t, *J* = 7.8 Hz, 1H), 7.87–7.81 (m, 2H), 7.78 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.73 (td, *J* = 7.7, 1.3 Hz, 1H), 7.61 (d, *J* = 7.9 Hz, 1H), 7.55 (td, *J* = 7.7, 1.2 Hz, 1H), 7.21 (d, *J* = 8.3 Hz, 2H), 7.14 (t, *J* = 8.4 Hz, 1H), 6.63 (d, *J* = 8.5 Hz, 2H), 3.82 (s, 6H); ^{13}C NMR (151 MHz, CD_3CN) δ 169.29, 168.88, 159.34, 159.30, 157.70, 157.66, 156.15, 152.90, 151.51, 143.81, 143.79, 143.33, 136.87, 136.81, 136.74, 134.72, 134.32, 130.98, 129.61, 127.10, 126.92, 126.74, 125.71, 125.49, 119.27, 113.21, 113.17, 113.07, 113.03, 111.89, 105.23, 56.58; ^{19}F NMR (376 MHz, CD_3CN) δ -117.57. HRMS (ESI-TOF) *m/z* calc'd for $C_{30}H_{22}F_2N_5O_4Pd$ $[M+H]^+$: 660.0669; found: 660.0659.



T6-MeCN

Palladium-N^2-(*tert*-butyl)-N^6-(2'-cyano-3,5-difluoro-[1,1'-biphenyl]-4-yl)pyridine-2,6-dicarboxamide complex (T6-MeCN)

^{1}H NMR (600 MHz, CD_3CN) δ 8.17 (t, *J* = 7.8 Hz, 1H), 7.86 (dd, *J* = 7.8, 0.9 Hz, 1H), 7.76 (td, *J* = 7.7, 1.4 Hz, 1H), 7.70 (d, *J* = 7.8 Hz, 2H), 7.63 (d, *J* = 7.8 Hz, 1H), 7.58 (td, *J* = 7.6, 1.2 Hz, 1H), 7.29 (d, *J* = 8.2 Hz, 2H), 1.40 (s, 9H); ^{13}C NMR (151 MHz, CD_3CN) δ 169.29, 168.88, 158.50 (dd, J = 247.6, 6.6 Hz), 156.15, 152.90, 151.51, 143.81, 143.79, 143.33, 136.81 (t, *J* = 9.9 Hz), 134.72, 134.32, 130.98, 129.61, 127.10, 126.92, 126.74, 125.71 (t, *J* = 16.7 Hz), 125.49, 119.27, 113.12 (dd, *J* = 21.1, 6.0 Hz), 111.89, 105.23, 56.58; ^{19}F NMR (376 MHz, CD_3CN) δ -118.18. HRMS (ESI-TOF) *m/z* calc'd for $C_{26}H_{22}F_2N_5O_2Pd$ $[M+H]^+$: 580.0771; found: 580.0762.



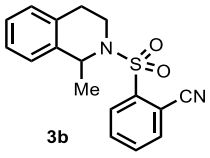
T7-MeCN

Palladium-N^2,N^6-bis(3,5-bis(trifluoromethyl)phenyl)pyridine-2,6-dicarboxamide complex (T7-MeCN)

^{1}H NMR (600 MHz, CD_3CN) δ 8.30 (t, *J* = 7.8 Hz, 1H), 7.90 (s, 4H), 7.88 (d, *J* = 7.8 Hz, 2H), 7.72 (s, 2H); ^{13}C NMR (151 MHz, CD_3CN) δ 170.08, 152.51, 149.42, 143.76, 131.76 (q, *J* = 33.0 Hz), 128.15–127.98 (m), 127.67, 124.63 (q, *J* = 271.8 Hz); ^{19}F NMR (376 MHz, CD_3CN) δ -63.43. HRMS (ESI-TOF) *m/z* calc'd for $C_{25}H_{13}F_{12}N_4O_2Pd$ $[M+H]^+$: 734.9876; found: 734.9883.

B. Preparation of Substrates

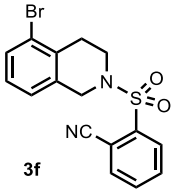
Substrates (**3b, 3f**) were synthesized following the literature procedures[5].



3b

2-((1-Methyl-3,4-dihydroisoquinolin-2(1*H*)-yl)sulfonyl)benzonitrile (3b)

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (ddd, *J* = 8.0, 1.3, 0.4 Hz, 1H), 7.78 (ddd, *J* = 7.6, 1.4, 0.4 Hz, 1H), 7.69 (td, *J* = 7.8, 1.4 Hz, 1H), 7.62 (td, *J* = 7.6, 1.3 Hz, 1H), 7.19–7.10 (m, 2H), 7.07 (d, *J* = 7.7 Hz, 1H), 7.03 (d, *J* = 7.4 Hz, 1H), 5.19 (q, *J* = 6.9 Hz, 1H), 4.14–4.04 (m, 1H), 3.55 (ddd, *J* = 14.0, 11.9, 4.2 Hz, 1H), 2.94–2.82 (m, 1H), 2.77–2.66 (m, 1H), 1.49 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 143.69, 137.29, 135.52, 132.90, 132.48, 132.41, 129.98, 129.19, 126.93, 126.90, 126.50, 116.16, 110.42, 52.39, 39.02, 28.27, 23.31. HRMS (ESI-TOF) *m/z* calc'd for $C_{17}H_{17}N_2O_2S$ $[M+H]^+$: 313.1005; found: 313.1012.

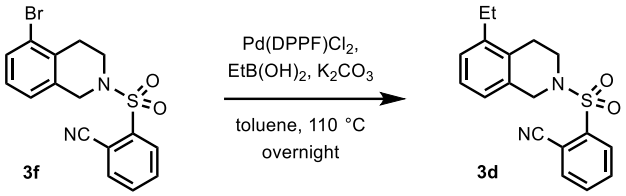


3f

2-((5-Bromo-3,4-dihydroisoquinolin-2(1*H*)-yl)sulfonyl)benzonitrile (3f)

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.85 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.76 (td, *J* = 7.8, 1.4 Hz, 1H), 7.69 (td, *J* = 7.6, 1.3 Hz, 1H), 7.43 (dd, *J* = 6.6, 2.6 Hz, 1H), 7.09–7.00 (m, 2H), 4.50 (s, 2H), 3.64 (t, *J* = 6.1 Hz, 2H), 2.93 (t, *J* = 6.1 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 141.02, 135.69, 133.97, 133.04,

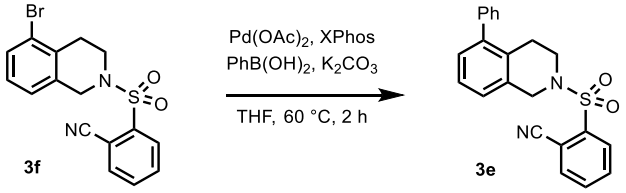
132.95, 132.93, 131.19, 130.40, 127.79, 125.62, 125.40, 116.21, 110.93, 47.45, 43.65, 29.51. HRMS (ESI-TOF) *m/z* calc'd for $C_{16}H_{14}BrN_2O_2S$ $[M+H]^+$: 376.9954; found: 376.9950.



2-((5-Ethyl-3,4-dihydroisoquinolin-2(1*H*)-yl)sulfonyl)benzonitrile (3d)

Aryl bromide **3f** (0.19 g, 0.5 mmol, 1.0 equiv), $Pd(DPPF)Cl_2$ (36.6 mg, 0.05 mmol, 10 mol%), $EtB(OH)_2$ (73.9 mg, 1.0 mmol, 2.0 equiv.), and K_2CO_3 (0.21 g, 1.5 mmol, 3.0 equiv.) were added to a flame-dried Schlenk tube. The Schlenk tube was evacuated and back-filled with nitrogen, and then toluene (5 mL) was added to the mixture. The Schlenk tube was immersed into a pre-heated oil bath at 110 °C overnight. The oil bath was removed, and the Schlenk tube was allowed to cool to room temperature. Water was added into the reaction mixture, which was then extracted with EtOAc. The combined organic layers were dried with Na_2SO_4. After the organic solvent was concentrated by rotary evaporation, the residue was purified by silica gel chromatography (hexanes/EtOAc = 2:1 v/v) to afford 0.14 g compound **3d** as a white solid (85% yield).

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.0 Hz, 1H), 7.85 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.75 (td, *J* = 7.8, 1.3 Hz, 1H), 7.67 (td, *J* = 7.6, 1.1 Hz, 1H), 7.13 (t, *J* = 7.6 Hz, 1H), 7.06 (d, *J* = 7.4 Hz, 1H), 6.91 (d, *J* = 7.6 Hz, 1H), 4.45 (s, 2H), 3.68 (t, *J* = 6.0 Hz, 2H), 2.91 (t, *J* = 6.0 Hz, 2H), 2.56 (q, *J* = 7.6 Hz, 2H), 1.17 (t, *J* = 7.6 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.51, 141.00, 135.69, 132.95, 132.77, 131.41, 131.05, 130.46, 126.69, 126.49, 124.17, 116.34, 111.05, 47.74, 43.78, 25.67, 25.52, 14.33. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{19}N_2O_2S$ $[M+H]^+$: 327.1162; found: 327.1171.

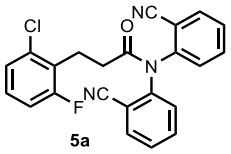


2-((5-Phenyl-3,4-dihydroisoquinolin-2(1*H*)-yl)sulfonyl)benzonitrile (3e)

Aryl bromide **3f** (0.19 g, 0.5 mmol, 1.0 equiv.), $Pd(OAc)_2$ (2.2 mg, 0.1 mmol, 20 mol%), XPhos (95.3 mg, 0.2 mmol, 40 mol%), $PhB(OH)_2$ (0.12 g, 1.0 mmol, 2.0 equiv.), and K_2CO_3 (0.14 g, 1.0 mmol, 2.0 equiv.) were added to a flame-dried Schlenk tube. The Schlenk tube was evacuated and back-filled with nitrogen, and then THF (3 mL) were added to the mixture. The Schlenk tube was immersed into a pre-heated oil bath at 60 °C. After 2 h, the oil bath was removed, and the Schlenk tube was allowed to cool to room temperature. Water was added into the reaction mixture, which was then extracted with EtOAc. The combined organic layers were dried with Na_2SO_4. After the organic solvent was concentrated by rotary evaporation, the residue was purified by silica gel chromatography (hexanes/EtOAc = 2:1 v/v) to afford 0.14 g compound **3e** as a white solid (75% yield).

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (d, *J* = 1.4 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.76 (t, *J* = 7.8 Hz, 1H), 7.69 (t, *J* = 7.6 Hz, 1H), 7.40 (t, *J* = 7.4 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.26–7.21 (m, 3H), 7.13 (d, *J* = 7.4 Hz, 1H), 7.09 (d, *J* = 7.7 Hz, 1H), 4.56 (s, 2H), 3.54 (t, *J* = 6.0 Hz, 2H), 2.83 (t, *J* = 5.9 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 142.26, 141.01, 140.60, 135.70, 132.98, 132.81, 131.86, 131.10, 130.48, 129.12, 128.51, 128.35, 127.33, 126.43, 125.66, 116.31, 111.01, 47.51, 43.78, 27.74. HRMS (ESI-TOF) *m/z* calc'd for $C_{22}H_{19}N_2O_2S$ $[M+H]^+$: 375.1162; found: 375.1165.

Substrate (**5a**) was synthesized following the literature procedures[9].



5a

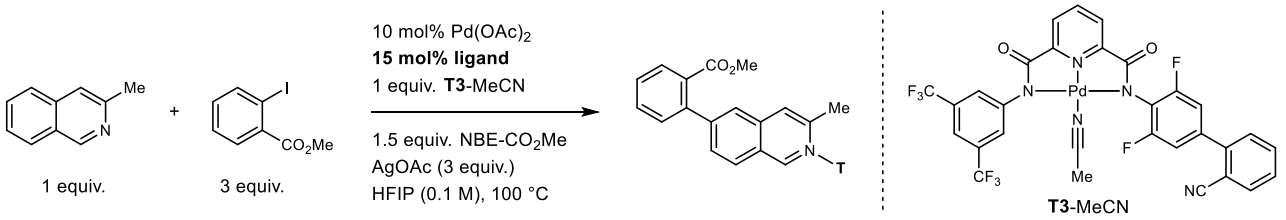
3-(2-Chloro-6-fluorophenyl)-*N*,*N*-bis(2-cyanophenyl)propanamide (5a)

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.91–7.31 (m, 8H), 7.13–7.05 (m, 2H), 6.94–6.86 (m, 1H), 3.25 (t, *J* = 8.5 Hz, 2H), 2.58 (br, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.60, 161.53 (d, *J* = 248.1 Hz), 144.13, 135.37 (d, *J* = 6.1 Hz), 134.96, 134.68, 134.37, 134.01, 130.75, 129.65, 129.42, 128.47, 128.34 (d, *J* = 9.4 Hz), 126.25 (d, *J* = 18.7 Hz), 125.36 (d, *J* = 3.3 Hz), 117.21, 116.50, 114.19 (d, *J* = 23.1 Hz), 113.34, 113.13, 33.59, 22.49 (d, *J* = 3.3 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -113.77. HRMS (ESI-TOF) *m/z* calc'd for $C_{23}H_{16}ClFN_3O$ $[M+H]^+$: 404.0960; found: 404.0967.

II. Remote Site-Selective Arylation

A. Optimization of the Reaction Conditions

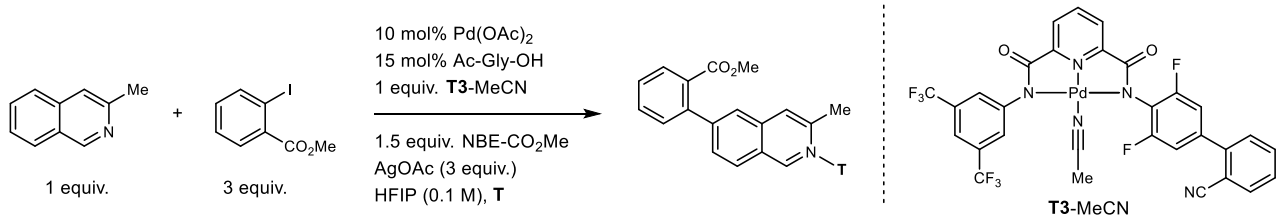
Table 1. Ligand screening[a]



Ac-Gly-OH	Ac-Ala-OH	Ac-Val-OH	TFA-Gly-OH	Fmoc-Gly-OH	AcHN, NMe2	AcHN, SPh
41%, 38% SM	36%, 55% SM	21%, 67% SM	7%, 85% SM	10%, 80% SM	<5%, 90% SM	<5%, 90% SM

[a]The yields were determined by ^{1}H-NMR using $CHCl_2CHCl_2$ as the standard.

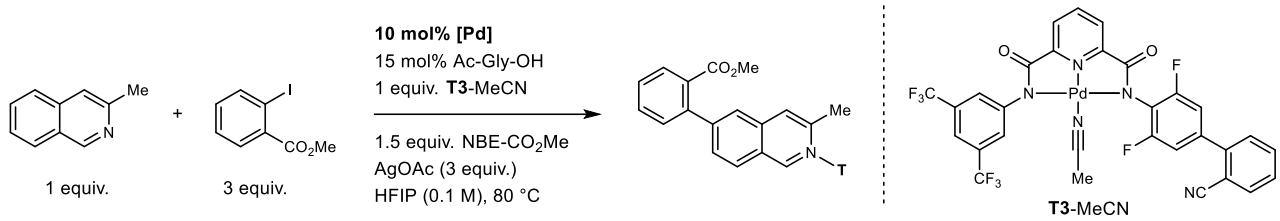
Table 2. Temperatures screening[a]



T	yield
120 °C	33%, 38% SM
100 °C	41%, 38% SM
80 °C	45%, 41% SM
60 °C	30%, 55% SM

[a]The yields were determined by ^{1}H-NMR using $CHCl_2CHCl_2$ as the standard.

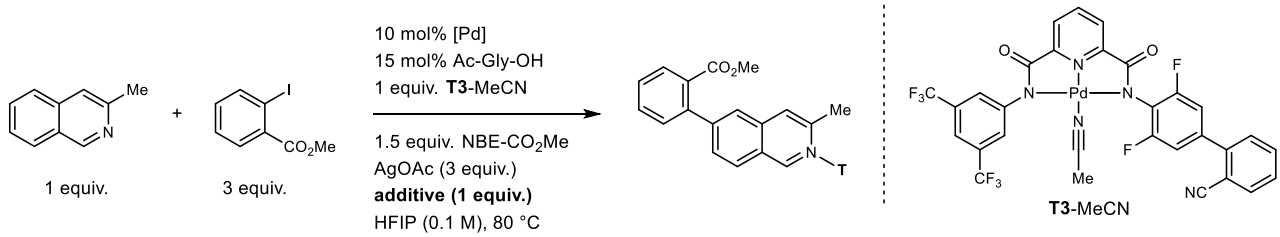
Table 3. Palladium screening[a]



[Pd]	yield
$Pd(OAc)_2$	45%, 41% SM
$Pd(MeCN)_2Cl_2$	44%, 46% SM
$Pd(PhCN)_2Cl_2$	41%, 50% SM
$Pd(TFA)_2$	36%, 43% SM

[a]The yields were determined by ^{1}H-NMR using $CHCl_2CHCl_2$ as the standard.

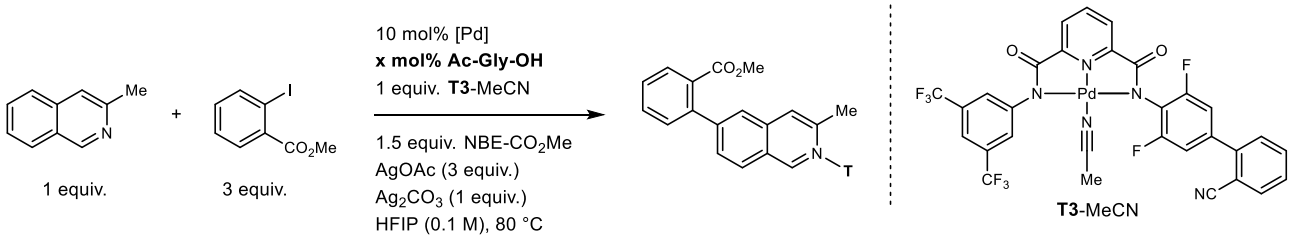
Table 4. Additive screening[a]



additive	yield
none	45%, 41% SM
Ag_2CO_3	52%, 38% SM
Li_2CO_3	40%, 50% SM
Na_2CO_3	29%, 65% SM
K_2CO_3	10%, 82% SM
Cs_2CO_3	16%, 77% SM
K_2HPO_4	12%, 81% SM

[a]The yields were determined by ^{1}H-NMR using $CHCl_2CHCl_2$ as the standard.

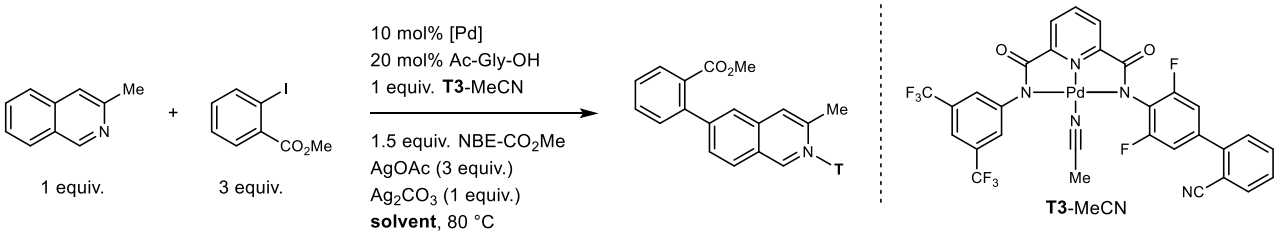
Table 5. Catalyst loading screening[a]



x mol%	yield
10 mol%	48%, 44% SM
15 mol%	52%, 38% SM
20 mol%	55%, 36% SM

[a]The yields were determined by ^{1}H-NMR using $CHCl_2CHCl_2$ as the standard.

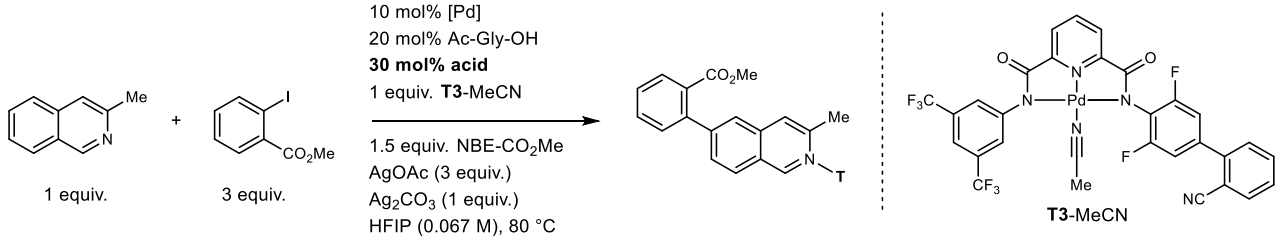
Table 6. Solvent screening[a]



solvent	yield
HFIP (0.1 M)	55%, 36% SM
HFIP (0.067 M)	63%, 24% SM
HFIP (0.05 M)	61%, 25% SM
DCM (0.067 M)	<5%, 90% SM
toluene (0.067 M)	<5%, 92% SM
THF (0.067 M)	<5%, 90% SM
MeCN (0.067 M)	<5%, 85% SM

[a]The yields were determined by ^{1}H-NMR using $CHCl_2CHCl_2$ as the standard.

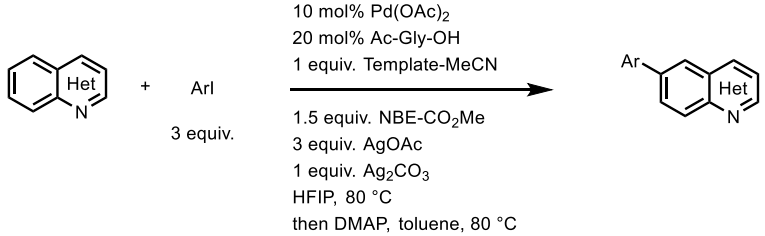
Table 7. Acid screening[a]



acid	yield
none	63%, 24% SM
AcOH	50%, 35% SM
$(PhO)_2PO_2H$	28%, 64% SM
Ad-CO_2H	53%, 30% SM
(±)-BNDHP	46%, 38% SM

[a]The yields were determined by ^{1}H-NMR using $CHCl_2CHCl_2$ as the standard.

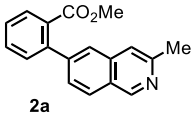
B. Pd-Catalyzed Remote Arylation of Benzoazines



General procedure A: A reaction vial (8 mL) was charged with benzoazine (0.10 mmol, 1.0 equiv.), template-MeCN (0.10 mmol, 1.0 equiv.) and 0.2 mL DCM. The mixture was stirred for 5 min at room temperature, and

then concentrated *in vacuo*. $Pd(OAc)_2$ (2.2 mg, 10 μmol, 10 mol%), Ac-Gly-OH (2.3 mg, 20 μmol, 20 mol%), aryl iodide (0.3 mmol, 3 equiv.), AgOAc (50 mg, 0.30 mmol, 3.0 equiv.), Ag_2CO_3 (27.6 mg, 0.1 mmol, 1.0 equiv.), NBE-CO_2Me (22.8 mg, 0.15 mmol, 1.5 equiv.) and HFIP (1.5 ml) were added. The reaction vial was sealed and allowed to stir at 80 °C for 18 h. The reaction mixture was cooled to room temperature. Then a solution of DMAP (36.7 mg, 0.3 mmol, 3 equiv.) in toluene (1.5 mL) was added. The mixture was stirred at 80 °C for 15 min. The reaction mixture was cooled to room temperature, diluted with EtOAc. The mixture was filtered through a short pad of celite and eluted with EtOAc (2 × 2 mL). The filtrate was evaporated under reduced pressure. (If the product release is not complete, a solution of DMAP (18.4 mg, 0.15 mmol, 1.5 equiv.) in toluene (1.5 mL) was added. The solution was stirred at 80 °C for 15 min., and then concentrated.) Purification by preparative TLC afforded the title compound and template-DMAP complex.

Template recovery: The template-DMAP complex was dissolved in acetonitrile (3 mL). To this mixture was added methanesulfonic acid (6.5 μl, 0.1 mmol) and the resulting mixture was heated at 60 °C for 2 h. Upon completion, the reaction mixture was cooled to room temperature. The solvent was removed *in vacuo*. Water was added to the reaction mixture and extracted with DCM three times. The organic layer was dried with Na_2SO_4 and concentrated *in vacuo.* This crude mixture was dissolved in acetonitrile (3 mL). To this mixture was added methanesulfonic acid (3.0 μl, 0.046 mmol) and the resulting mixture was heated at 60 °C for 30 min. Upon completion, the reaction mixture was cooled to room temperature. The solvent was removed *in vacuo*. Water was added to the reaction mixture and extracted with DCM three times. The organic layer was dried with Na_2SO_4 and concentrated *in vacuo* to give the template.

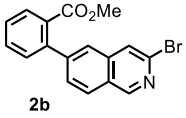


2a

Methyl 2-(3-methylisoquinolin-6-yl)benzoate (2a)

Substrate isoquinoline was arylated following the general procedure by using **T3**-MeCN (73.6 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 1:1 v/v), compound **2a** (16.9 mg) was obtained in 61% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.20 (s, 1H), 7.93 (dd, *J* = 7.8, 0.8 Hz, 2H), 7.65 (s, 1H), 7.59 (td, *J* = 7.6, 1.4 Hz, 1H), 7.51–7.41 (m, 4H), 3.60 (s, 3H), 2.71 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.58, 152.18, 151.83, 143.78, 142.14, 136.59, 131.71, 130.99, 130.65, 130.31, 127.93, 127.74, 126.96, 125.89, 124.84, 118.70, 52.14, 24.33. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{16}N_1O_2$ $[M+H]^+$: 278.1176; found: 278.1182.



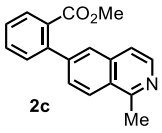
2b

Methyl 2-(3-bromoisoquinolin-6-yl)benzoate (2b)

Substrate isoquinoline was arylated following the general procedure by using **T3**-MeCN (73.6 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 4:1 v/v), compound **2b** (13 mg) was obtained in 38% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.06 (s, 1H), 8.00–7.93 (m, 2H), 7.91 (s, 1H), 7.67 (s, 1H), 7.61 (td, *J* = 7.6, 1.4 Hz, 1H), 7.55 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.51 (td, *J* = 7.6, 1.3 Hz, 1H), 7.41 (dd, *J* = 7.6, 0.9 Hz, 1H), 3.63 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.13, 152.54, 145.07, 141.69, 137.92, 136.39, 131.93, 131.00, 130.56,

130.34, 129.33, 128.31, 126.99, 126.61, 124.42, 123.91, 52.22. HRMS (ESI-TOF) *m/z* calc'd for $C_{17}H_{13}BrN_1O_2$ $[M+H]^+$: 342.0124; found: 342.0132.

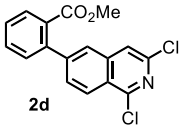


Methyl 2-(1-methylisoquinolin-6-yl)benzoate (2c)

Substrate isoquinoline was arylated following the general procedure by using **T3**-MeCN (73.6 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2c** (13.8 mg) was obtained in 50% yield as a yellow oil.

The position of C–H arylation on **2c** was determined by NOESY.

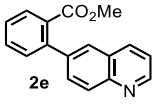
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.41 (d, *J* = 5.7 Hz, 1H), 8.13 (d, *J* = 8.6 Hz, 1H), 7.95 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.74 (d, *J* = 1.9 Hz, 1H), 7.60 (td, *J* = 7.6, 1.4 Hz, 1H), 7.57 – 7.50 (m, 2H), 7.49 (td, *J* = 7.6, 1.3 Hz, 1H), 7.44 (dd, *J* = 7.6, 1.4 Hz, 1H), 3.63 (s, 3H), 2.99 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.48, 158.60, 143.44, 142.30, 142.02, 135.97, 131.77, 131.08, 130.53, 130.36, 128.40, 127.98, 126.56, 126.08, 125.16, 119.52, 52.18, 22.51. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{16}N_1O_2$ $[M+H]^+$: 278.1176; found: 278.1184.



Methyl 2-(1,3-dichloroisoquinolin-6-yl)benzoate (2d)

Substrate isoquinoline was arylated following the general procedure by using **T3**-MeCN (73.6 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 9:1 v/v), compound **2d** (13.4 mg) was obtained in 40% yield as a white solid.

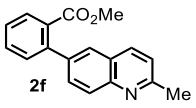
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.30 (d, *J* = 8.7 Hz, 1H), 8.00 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.69 (d, *J* = 1.7 Hz, 1H), 7.67 (s, 1H), 7.64–7.58 (m, 2H), 7.53 (td, *J* = 7.6, 1.3 Hz, 1H), 7.40 (dd, *J* = 7.6, 1.4 Hz, 1H), 3.65 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.89, 150.97, 146.07, 143.58, 141.27, 139.32, 132.05, 130.97, 130.69, 130.30, 130.17, 128.53, 125.93, 125.01, 124.82, 119.93, 52.28. HRMS (ESI-TOF) *m/z* calc'd for $C_{17}H_{12}Cl_2N_1O_2$ $[M+H]^+$: 332.0240; found: 332.0247.



Methyl 2-(quinolin-6-yl)benzoate (2e)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2e** (18.7 mg) was obtained in 71% yield as a yellow oil.

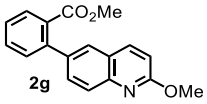
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 4.3, 1.7 Hz, 1H), 8.21–8.15 (m, 2H), 8.12 (d, *J* = 8.6 Hz, 1H), 7.93 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.76 (d, *J* = 2.1 Hz, 1H), 7.67 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.59 (td, *J* = 7.5, 1.5 Hz, 1H), 7.51–7.39 (m, 2H), 3.61 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.83, 150.56, 147.61, 141.98, 140.04, 136.35, 131.70, 131.21, 130.90, 130.83, 130.33, 128.93, 128.20, 127.81, 126.69, 121.58, 52.18. HRMS (ESI-TOF) *m/z* calc'd for $C_{17}H_{14}N_1O_2$ $[M+H]^+$: 264.1019; found: 264.1029.



Methyl 2-(2-methylquinolin-6-yl)benzoate (2f)

Substrate quinoline was arylated following the general procedure by using **T2**-MeCN (73.2 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2f** (19.4 mg) was obtained in 70% yield as a colorless oil.

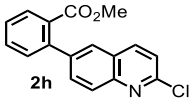
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.4 Hz, 1H), 8.02 (d, *J* = 8.7 Hz, 1H), 7.89 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.71 (d, *J* = 2.1 Hz, 1H), 7.62 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.57 (td, *J* = 7.4, 1.4 Hz, 1H), 7.50–7.41 (m, 2H), 7.31 (d, *J* = 8.5 Hz, 1H), 3.58 (s, 3H), 2.77 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.04, 159.23, 147.20, 141.96, 139.01, 136.38, 131.56, 131.10, 130.95, 130.69, 130.18, 128.17, 127.61, 126.44, 126.34, 122.46, 52.10, 25.50. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{16}N_1O_2$ $[M+H]^+$: 278.1176; found: 278.1185.



Methyl 2-(2-methoxyquinolin-6-yl)benzoate (2g)

Substrate quinoline was arylated following the general procedure by using **T2**-MeCN (73.2 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 4:1 v/v), compound **2g** (17.9 mg) was obtained in 61% yield as a colorless oil.

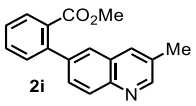
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.7 Hz, 1H), 7.89–7.83 (m, 2H), 7.67 (d, *J* = 2.2 Hz, 1H), 7.60–7.52 (m, 2H), 7.47–7.41 (m, 2H), 6.93 (d, *J* = 8.7 Hz, 1H), 4.10 (s, 3H), 3.60 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.23, 162.70, 145.95, 142.05, 138.85, 137.25, 131.48, 131.08, 131.02, 130.54, 130.08, 127.40, 126.84, 126.55, 124.91, 113.51, 53.55, 52.09. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{16}N_1O_3$ $[M+H]^+$: 294.1135; found: 294.1136.



Methyl 2-(2-chloroquinolin-6-yl)benzoate (2h)

Substrate quinoline was arylated following the general procedure by using **T2**-MeCN (73.2 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (DCM/Et_2O = 30:1 v/v), compound **2h** (18.7 mg) was obtained in 62% yield as a white solid.

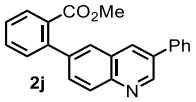
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.5 Hz, 1H), 8.03 (d, *J* = 8.6 Hz, 1H), 7.94 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.75 (d, *J* = 2.0 Hz, 1H), 7.68 (dd, *J* = 8.6, 2.0 Hz, 1H), 7.59 (td, *J* = 7.5, 1.4 Hz, 1H), 7.49 (td, *J* = 7.6, 1.3 Hz, 1H), 7.46–7.38 (m, 2H), 3.61 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.56, 150.80, 147.19, 141.64, 140.54, 139.04, 131.94, 131.75, 131.11, 130.65, 130.40, 128.03, 127.96, 126.70, 126.44, 122.79, 52.15. HRMS (ESI-TOF) *m/z* calc'd for $C_{17}H_{13}ClN_1O_2$ $[M+H]^+$: 298.0629; found: 298.0639.



Methyl 2-(3-methylquinolin-6-yl)benzoate (2i)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2i** (23.8 mg) was obtained in 86% yield as a yellow oil.

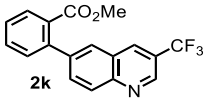
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.78 (d, *J* = 2.3 Hz, 1H), 8.07 (d, *J* = 8.6 Hz, 1H), 7.96–7.84 (m, 2H), 7.67 (d, *J* = 2.1 Hz, 1H), 7.61–7.54 (m, 2H), 7.49–7.42 (m, 2H), 3.59 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.91, 152.52, 145.84, 142.04, 139.90, 134.89, 131.57, 131.09, 130.96, 130.87, 130.18, 129.77, 128.64, 127.99, 127.65, 126.06, 52.10, 18.88. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{16}N_1O_2$ $[M+H]^+$: 278.1176; found: 278.1184.



Methyl 2-(3-phenylquinolin-6-yl)benzoate (2j)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 4:1 v/v), compound **2j** (23.1 mg) was obtained in 68% yield as a colorless oil.

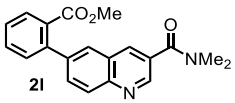
^{1}H NMR (600 MHz, $CDCl_3$) δ 9.20 (d, *J* = 2.3 Hz, 1H), 8.32 (d, *J* = 2.3 Hz, 1H), 8.15 (d, *J* = 8.6 Hz, 1H), 7.94 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.83 (d, *J* = 2.1 Hz, 1H), 7.73 (dd, *J* = 8.3, 1.2 Hz, 2H), 7.67 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.62–7.58 (m, 1H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.51–7.42 (m, 3H), 3.63 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.78, 150.10, 146.68, 141.98, 140.46, 137.99, 134.34, 133.42, 131.69, 131.15, 130.78, 130.31, 129.31, 128.73, 128.26, 127.92, 127.81, 127.55, 126.86, 52.17. HRMS (ESI-TOF) *m/z* calc'd for $C_{23}H_{18}N_1O_2$ $[M+H]^+$: 340.1332; found: 340.1336.



Methyl 2-(3-(trifluoromethyl)quinolin-6-yl)benzoate (2k)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2k** (18.2 mg) was obtained in 55% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.11 (d, *J* = 2.7 Hz, 1H), 8.46 (s, 1H), 8.20 (d, *J* = 8.7 Hz, 1H), 7.98 (dd, *J* = 7.8, 1.2 Hz, 1H), 7.86 (d, *J* = 1.9 Hz, 1H), 7.80 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.62 (td, *J* = 7.6, 1.4 Hz, 1H), 7.51 (td, *J* = 7.6, 1.3 Hz, 1H), 7.44 (dd, *J* = 7.6, 1.0 Hz, 1H), 3.64 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.25, 148.68, 146.12 (q, *J* = 3.1 Hz), 141.71, 141.50, 134.11 (q, *J* = 4.1 Hz), 133.31, 131.92, 131.18, 130.58, 130.43, 128.97, 128.19, 127.30, 126.18, 124.05 (q, *J* = 33.0 Hz), 123.79 (q, *J* = 272.3 Hz), 52.21; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.09. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{13}F_3N_1O_2$ $[M+H]^+$: 332.0893; found: 332.0903.

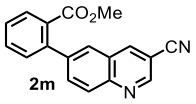


Methyl 2-(3-(dimethylcarbamoyl)quinolin-6-yl)benzoate (2l)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (EtOAc), compound **2l** (13.2 mg) was obtained in 40% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.98 (d, *J* = 2.2 Hz, 1H), 8.26 (d, *J* = 2.1 Hz, 1H), 8.13 (d, *J* = 8.6 Hz, 1H), 7.95 (dd, *J* = 7.8, 1.3 Hz, 1H), 7.79 (d, *J* = 1.9 Hz, 1H), 7.71 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.60 (td, *J* = 7.5, 1.4 Hz, 1H), 7.49 (td, *J* = 7.6, 1.3 Hz, 1H), 7.44 (dd, *J* = 7.6, 0.9 Hz, 1H), 3.62 (s, 3H), 3.19 (s, 3H), 3.10 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.19, 168.50, 148.63, 147.55, 141.71, 141.00, 135.22, 132.10, 131.80, 131.18, 130.58,

130.42, 129.66, 128.81, 127.98, 126.99, 126.93, 52.19, 39.79, 35.69. HRMS (ESI-TOF) *m/z* calc'd for $C_{20}H_{19}N_2O_3$ $[M+H]^+$: 335.1390; found: 335.1398.

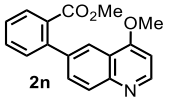


2m

Methyl 2-(3-cyanoquinolin-6-yl)benzoate (2m)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2m** (10.7 mg) was obtained in 37% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.06 (d, *J* = 2.1 Hz, 1H), 8.55 (d, *J* = 2.4 Hz, 1H), 8.18 (d, *J* = 8.5 Hz, 1H), 8.00 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.84–7.82 (m, 2H), 7.62 (td, *J* = 7.4, 1.4 Hz, 1H), 7.52 (td, *J* = 7.6, 1.3 Hz, 1H), 7.42 (dd, *J* = 7.6, 1.2 Hz, 1H), 3.65 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.02, 149.82, 148.15, 142.32, 141.54, 141.29, 134.37, 132.04, 131.20, 130.70, 130.24, 129.12, 128.38, 126.85, 126.14, 117.24, 106.98, 52.25. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{13}N_2O_2$ $[M+H]^+$: 289.0972; found: 289.0980.

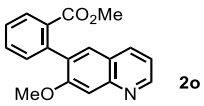


2n

Methyl 2-(4-methoxyquinolin-6-yl)benzoate (2n)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, and 40 mol% Ac-Gly-OH. After purification by preparative TLC (hexanes/EtOAc = 1:2 v/v), compound **2n** (10.5 mg) was obtained in 36% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.76 (d, *J* = 5.1 Hz, 1H), 8.16 (d, *J* = 2.0 Hz, 1H), 8.04 (d, *J* = 8.6 Hz, 1H), 7.91 (dd, *J* = 7.5, 1.0 Hz, 1H), 7.63 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.57 (td, *J* = 7.6, 1.4 Hz, 1H), 7.49–7.42 (m, 2H), 6.77 (d, *J* = 5.3 Hz, 1H), 4.04 (s, 3H), 3.60 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.94, 162.59, 151.44, 148.36, 142.27, 139.02, 131.58, 131.25, 131.00, 130.83, 130.21, 128.32, 127.60, 121.23, 120.94, 100.48, 55.82, 52.09. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{16}N_1O_3$ $[M+H]^+$: 294.1125; found: 294.1131.

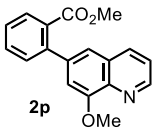


2o

Methyl 2-(7-methoxyquinolin-6-yl)benzoate (2o)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 1:1 v/v), compound **2o** (17.5 mg) was obtained in 60% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.83 (dd, *J* = 4.4, 1.8 Hz, 1H), 8.10 (dd, *J* = 8.1, 1.7 Hz, 1H), 7.95 (dd, *J* = 7.8, 1.1 Hz, 1H), 7.66 (s, 1H), 7.60 (td, *J* = 7.5, 1.4 Hz, 1H), 7.47 (td, *J* = 7.6, 1.3 Hz, 1H), 7.45 (s, 1H), 7.40 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.29 (dd, *J* = 8.1, 4.4 Hz, 1H), 3.86 (s, 3H), 3.62 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.32, 158.10, 150.42, 149.68, 138.02, 135.84, 133.77, 131.99, 131.70, 131.55, 129.70, 128.06, 127.90, 123.69, 119.35, 106.53, 55.66, 51.87. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{16}N_1O_3$ $[M+H]^+$: 294.1125; found: 294.1133.

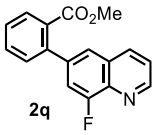


2p

Methyl 2-(8-methoxyquinolin-6-yl)benzoate (2p)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 1:1 v/v), compound **2p** (23.8 mg) was obtained in 81% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.13 (dd, *J* = 8.3, 1.7 Hz, 1H), 7.87 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.57 (td, *J* = 7.6, 1.4 Hz, 1H), 7.50–7.41 (m, 3H), 7.33 (d, *J* = 1.7 Hz, 1H), 7.00 (d, *J* = 1.8 Hz, 1H), 4.07 (s, 3H), 3.59 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.09, 154.90, 149.36, 141.97, 140.15, 139.54, 136.11, 131.47, 131.12, 130.86, 129.97, 129.13, 127.75, 122.14, 118.61, 109.13, 56.16, 52.17. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{16}N_1O_3$ $[M+H]^+$: 294.1125; found: 294.1131.

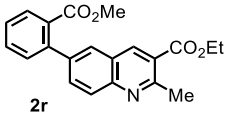


2q

Methyl 2-(8-fluoroquinolin-6-yl)benzoate (2q)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 4:1 v/v), compound **2q** (19 mg) was obtained in 68% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.98 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.19 (d, *J* = 8.6 Hz, 1H), 7.94 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.59 (td, *J* = 7.6, 1.4 Hz, 1H), 7.55 (d, *J* = 1.5 Hz, 1H), 7.51–7.46 (m, 2H), 7.43 (dd, *J* = 7.6, 1.2 Hz, 1H), 7.40 (dd, *J* = 11.0, 1.8 Hz, 1H), 3.64 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.37, 157.37 (d, *J* = 256.9 Hz), 150.62 (d, *J* = 1.7 Hz), 141.08 (d, *J* = 1.7 Hz), 140.28 (d, *J* = 8.3 Hz), 137.81 (d, *J* = 12.1 Hz), 135.99 (d, *J* = 3.3 Hz), 131.78, 131.05, 130.60, 130.40, 129.59 (d, *J* = 2.8 Hz), 128.14, 122.50, 122.35 (d, *J* = 3.9 Hz), 115.08 (d, *J* = 19.8 Hz), 52.25; ^{19}F NMR (376 MHz, $CDCl_3$) δ -126.65. HRMS (ESI-TOF) *m/z* calc'd for $C_{17}H_{13}F_1N_1O_2$ $[M+H]^+$: 282.0925; found: 282.0933.

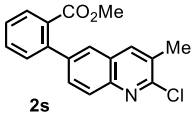


2r

Ethyl 6-(2-(methoxycarbonyl)phenyl)-2-methylquinoline-3-carboxylate (2r)

Substrate quinoline was arylated following the general procedure by using **T2**-MeCN (73.2 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 4:1 v/v), compound **2r** (19.9 mg) was obtained in 57% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.74 (s, 1H), 8.04 (d, *J* = 8.7 Hz, 1H), 7.93 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.80 (d, *J* = 2.1 Hz, 1H), 7.72 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.59 (td, *J* = 7.6, 1.4 Hz, 1H), 7.48 (td, *J* = 7.7, 1.4 Hz, 1H), 7.45 (dd, *J* = 7.6, 0.8 Hz, 1H), 4.45 (q, *J* = 7.2 Hz, 2H), 3.59 (s, 3H), 3.01 (s, 3H), 1.45 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.73, 166.65, 158.67, 147.93, 141.62, 140.03, 139.98, 133.01, 131.71, 131.09, 130.76, 130.37, 128.01, 127.88, 127.25, 125.65, 124.41, 61.53, 52.14, 25.80, 14.44. HRMS (ESI-TOF) *m/z* calc'd for $C_{21}H_{20}N_1O_4$ $[M+H]^+$: 350.1387; found: 350.1396.

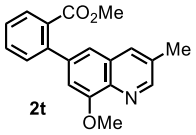


2s

Methyl 2-(2-chloro-3-methylquinolin-6-yl)benzoate (2s)

Substrate quinoline was arylated following the general procedure by using **T2**-MeCN (73.2 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 4:1 v/v), compound **2s** (19.5 mg) was obtained in 63% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.02–7.95 (m, 2H), 7.91 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.68 (d, *J* = 2.1 Hz, 1H), 7.62–7.55 (m, 2H), 7.47 (td, *J* = 7.6, 1.3 Hz, 1H), 7.43 (dd, *J* = 7.6, 1.2 Hz, 1H), 3.59 (s, 3H), 2.55 (d, *J* = 1.0 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.71, 152.12, 145.76, 141.77, 140.37, 137.96, 131.67, 131.04, 130.83, 130.77, 130.69, 130.30, 127.83, 127.69, 127.45, 125.70, 52.12, 20.23. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{15}ClN_1O_2$ $[M+H]^+$: 312.0786; found: 312.0796.

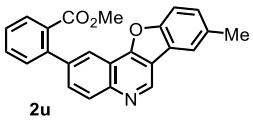


2t

Methyl 2-(8-methoxy-3-methylquinolin-6-yl)benzoate (2t)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 1:1 v/v), compound **2t** (25.3 mg) was obtained in 82% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.77 (dd, *J* = 2.2, 0.5 Hz, 1H), 7.89–7.85 (m, 1H), 7.85 (ddd, *J* = 7.7, 1.4, 0.6 Hz, 1H), 7.56 (td, *J* = 7.6, 1.5 Hz, 1H), 7.49–7.42 (m, 2H), 7.24 (d, *J* = 1.7 Hz, 1H), 6.93 (d, *J* = 1.7 Hz, 1H), 4.06 (s, 3H), 3.57 (s, 3H), 2.51 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.20, 154.94, 151.21, 142.07, 140.10, 137.79, 134.84, 131.64, 131.39, 131.20, 130.78, 129.88, 129.04, 127.64, 118.10, 108.19, 56.08, 52.15, 18.78. HRMS (ESI-TOF) *m/z* calc'd for $C_{19}H_{18}N_1O_3$ $[M+H]^+$: 308.1281; found: 308.1293.

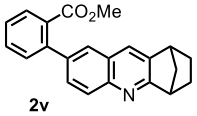


2u

Methyl 2-(8-methylbenzofuro[3,2-*c*]quinolin-2-yl)benzoate (2u)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, and 40 mol% Ac-Gly-OH. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2u** (27.8 mg) was obtained in 76% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 9.47 (s, 1H), 8.35 (d, *J* = 2.1 Hz, 1H), 8.26 (d, *J* = 8.6 Hz, 1H), 7.96 (d, *J* = 7.7 Hz, 1H), 7.90 (s, 1H), 7.71 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.66–7.57 (m, 2H), 7.54 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.50 (td, *J* = 7.5, 1.4 Hz, 1H), 7.34 (dd, *J* = 8.4, 1.9 Hz, 1H), 3.63 (s, 3H), 2.56 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.73, 157.87, 154.49, 146.58, 144.48, 141.98, 140.42, 133.90, 131.71, 131.28, 130.76, 130.47, 130.37, 129.31, 128.51, 127.87, 122.78, 120.69, 119.81, 117.13, 116.75, 111.70, 52.16, 21.54. HRMS (ESI-TOF) *m/z* calc'd for $C_{24}H_{18}N_1O_3$ $[M+H]^+$: 368.1281; found:368.1288.

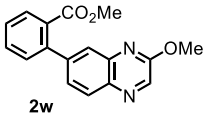


2v

Methyl 2-(1,2,3,4-tetrahydro-1,4-methanoacridin-7-yl)benzoate (2v)

Substrate quinoline was arylated following the general procedure by using **T2**-MeCN (73.2 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 3:1 v/v), compound **2v** (18.1 mg) was obtained in 55% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.6 Hz, 1H), 7.88 (dd, *J* = 8.1, 1.4 Hz, 1H), 7.74 (s, 1H), 7.66 (d, *J* = 2.2 Hz, 1H), 7.60–7.52 (m, 2H), 7.49–7.41 (m, 2H), 3.60 (s, 3H), 3.55 (s, 2H), 2.14–2.02 (m, 2H), 1.96 (dt, *J* = 9.3, 1.8 Hz, 1H), 1.75 (dt, *J* = 9.3, 1.4 Hz, 1H), 1.50–1.44 (m, 1H), 1.39–1.32 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.79, 169.10, 146.01, 142.23, 140.47, 138.64, 131.48, 131.14, 130.97, 130.07, 129.07, 128.25, 127.64, 127.44, 126.75, 125.85, 52.13, 46.87, 45.53, 42.31, 27.56, 25.82. HRMS (ESI-TOF) *m/z* calc'd for $C_{22}H_{20}N_1O_2$ $[M+H]^+$: 330.1489; found: 330.1496.

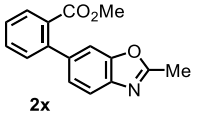


2w

Methyl 2-(3-methoxyquinoxalin-6-yl)benzoate (2w)

Substrate quinoxaline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 4:1 v/v), compound **2w** (12.6 mg) was obtained in 43% yield as a white solid.

^{1}H NMR (600 MHz, Chloroform-*d*) δ 8.48 (s, 1H), 8.01 (d, *J* = 8.5 Hz, 1H), 7.93 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.82 (dd, *J* = 2.1, 0.6 Hz, 1H), 7.59 (td, *J* = 7.5, 1.4 Hz, 1H), 7.52–7.44 (m, 3H), 4.10 (s, 3H), 3.63 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.67, 158.14, 143.74, 141.87, 140.31, 139.61, 138.10, 131.67, 131.09, 130.65, 130.32, 128.33, 127.88, 127.78, 126.34, 53.86, 52.15. HRMS (ESI-TOF) *m/z* calc'd for $C_{17}H_{15}N_2O_3$ $[M+H]^+$: 295.1077; found: 295.1083.

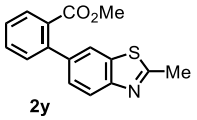


2x

Methyl 2-(2-methylbenzo[*d*]oxazol-6-yl)benzoate (2x)

Substrate benzo[*d*]oxazole was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2x** (14.9 mg) was obtained in 56% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.54 (td, *J* = 7.6, 1.4 Hz, 1H), 7.45–7.41 (m, 2H), 7.40 (dd, *J* = 7.7, 0.9 Hz, 1H), 7.24 (dd, *J* = 8.1, 1.7 Hz, 1H), 3.63 (s, 3H), 2.66 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.00, 164.36, 151.00, 142.15, 140.87, 138.29, 131.43, 131.13, 131.07, 130.02, 127.48, 125.01, 118.82, 110.18, 52.13, 14.72. HRMS (ESI-TOF) *m/z* calc'd for $C_{16}H_{14}N_1O_3$ $[M+H]^+$: 268.0968; found: 268.0976.

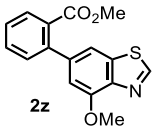


2y

Methyl 2-(2-methylbenzo[*d*]thiazol-6-yl)benzoate (2y)

Substrate benzo[*d*]thiazole was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 4:1 v/v), compound **2y** (11.6 mg) was obtained in 41% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.3 Hz, 1H), 7.86 (ddd, *J* = 7.8, 1.4, 0.4 Hz, 1H), 7.77 (dd, *J* = 1.8, 0.6 Hz, 1H), 7.55 (td, *J* = 7.4, 1.4 Hz, 1H), 7.46–7.39 (m, 2H), 7.37 (dd, *J* = 8.3, 1.8 Hz, 1H), 3.61 (s, 3H), 2.86 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.05, 167.36, 152.66, 141.97, 138.29, 135.78, 131.45, 131.06, 131.04, 130.06, 127.52, 126.96, 121.81, 120.95, 52.14, 20.29. HRMS (ESI-TOF) *m/z* calc'd for $C_{16}H_{14}N_1O_2S_1$ $[M+H]^+$: 284.0740; found: 284.0750.

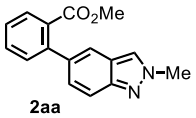


2z

Methyl 2-(4-methoxybenzo[d]thiazol-6-yl)benzoate (2z)

Substrate benzo[*d*]thiazole was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2z** (21.8 mg) was obtained in 73% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.92 (s, 1H), 7.85 (ddd, *J* = 7.8, 1.5, 0.6 Hz, 1H), 7.56 (td, *J* = 7.4, 1.4 Hz, 1H), 7.49–7.41 (m, 3H), 6.87 (d, *J* = 1.4 Hz, 1H), 4.05 (s, 3H), 3.62 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.10, 153.23, 152.59, 142.95, 141.87, 140.41, 135.60, 131.40, 131.21, 130.87, 129.92, 127.72, 113.37, 107.91, 56.17, 52.23. HRMS (ESI-TOF) *m/z* calc'd for $C_{16}H_{14}N_1O_3S_1$ $[M+H]^+$: 300.0689; found: 300.0695.

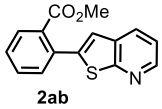


2aa

Methyl 2-(2-methyl-*2H*-indazol-5-yl)benzoate (2aa)

Substrate *2H*-indazole was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 1:1 v/v), compound **2aa** (8.2 mg) was obtained in 31% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.92 (s, 1H), 7.83 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.70 (d, *J* = 8.9 Hz, 1H), 7.58 (dd, *J* = 1.7, 1.0 Hz, 1H), 7.53 (td, *J* = 7.6, 1.5 Hz, 1H), 7.44 (dd, *J* = 7.7, 0.9 Hz, 1H), 7.41 (td, *J* = 7.5, 1.3 Hz, 1H), 7.23 (dd, *J* = 8.9, 1.7 Hz, 1H), 4.24 (s, 3H), 3.60 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 169.51, 148.45, 142.93, 135.09, 131.33, 131.17, 131.02, 129.88, 127.84, 127.05, 124.09, 122.20, 118.84, 116.78, 52.09, 40.49. HRMS (ESI-TOF) *m/z* calc'd for $C_{16}H_{15}N_2O_2$ $[M+H]^+$: 267.1128; found: 267.1137.



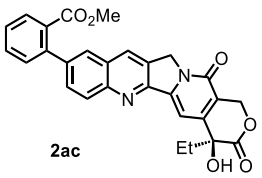
2ab

Methyl 2-(thieno[2,3-*b*]pyridin-2-yl)benzoate (2ab)

Substrate thieno[2,3-*b*]pyridine was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 4:1 v/v), compound **2ab** (14.8 mg) was obtained in 55% yield as a colorless oil.

The position of C–H arylation on **2ab** was determined by NOESY.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.55 (dd, *J* = 4.6, 1.7 Hz, 1H), 8.03 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.83 (d, *J* = 7.6 Hz, 1H), 7.59–7.53 (m, 2H), 7.48 (dt, *J* = 7.7, 4.5 Hz, 1H), 7.31 (dd, *J* = 8.0, 4.6 Hz, 1H), 7.17 (s, 1H), 3.74 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.52, 162.36, 146.47, 143.19, 134.20, 133.55, 131.80, 131.57, 131.44, 131.00, 129.97, 128.82, 120.20, 119.82, 52.49. HRMS (ESI-TOF) *m/z* calc'd for $C_{15}H_{12}N_1O_2S_1$ $[M+H]^+$: 270.0583; found: 270.0593.

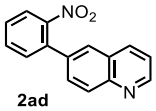


2ac

Methyl 2-(4-ethyl-4-hydroxy-3,14-dioxo-3,4,12,14-tetrahydro-1*H*-pyrano[3',4':6,7]indolizino[1,2-*b*]quinolin-9-yl)benzoate (2ac)

A reaction vial (8 mL) was charged with camptothecin (34.8 mg, 0.10 mmol, 1.0 equiv), **T2**-MeCN (73.2 mg, 0.10 mmol, 1.0 equiv.), and 0.2 mL HFIP. The mixture was stirred for 5 min at room temperature, and then concentrated. $Pd(OAc)_2$ (2.2 mg, 10 μmol, 10 mol%), Ac-Gly-OH (2.3 mg, 20 μmol, 20 mol%), aryl iodide (0.3 mmol, 3 equiv.), NBE-CO_2Me (22.8 mg, 0.15 mmol, 1.5 equiv.), AgOAc (50 mg, 0.30 mmol, 3.0 equiv.), Ag_2CO_3 (27.6 mg, 0.1 mmol, 1.0 equiv.), and HFIP (1.5 ml) were added. The reaction vial was sealed and allowed to stir at 80 °C for 24 h. The reaction mixture was cooled to room temperature. Then a solution of DMAP (36.7 mg, 0.3 mmol, 3 equiv.) in toluene (1.5 mL) was added. The mixture was stirred at 80 °C for 15 min. The reaction mixture was cooled to room temperature, diluted with EtOAc. The mixture was filtered through a short pad of celite and eluted with EtOAc (5 × 2 mL). The filtrate was evaporated under reduced pressure. After purification by preparative TLC (DCM/acetone = 5:1 v/v), compound **2ac** (22.7 mg) was obtained in 47% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.38 (s, 1H), 8.24 (d, *J* = 8.7 Hz, 1H), 7.97 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.85 (d, *J* = 2.1 Hz, 1H), 7.76 (dd, *J* = 8.7, 2.0 Hz, 1H), 7.71 (s, 1H), 7.62 (td, *J* = 7.6, 1.4 Hz, 1H), 7.51 (td, *J* = 7.6, 1.3 Hz, 1H), 7.47 (dd, *J* = 7.6, 0.9 Hz, 1H), 5.76 (d, *J* = 16.2 Hz, 1H), 5.36–5.25 (m, 3H), 3.84 (s, 1H), 3.63 (s, 3H), 1.98–1.82 (m, 2H), 1.05 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 174.03, 168.44, 157.77, 152.57, 150.26, 148.34, 146.56, 141.60, 141.56, 132.15, 131.87, 131.15, 131.13, 130.58, 130.54, 129.19, 129.02, 128.14, 128.07, 126.89, 118.79, 98.22, 72.89, 66.48, 52.20, 50.20, 31.75, 7.95. HRMS (ESI-TOF) *m/z* calc'd for $C_{28}H_{23}N_2O_6$ $[M+H]^+$: 483.1551; found: 483.1558.

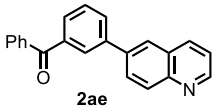


2ad

6-(2-Nitrophenyl)quinoline (2ad)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2ad** (16.9 mg) was obtained in 68% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_{3k}$) δ 8.96 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.21–8.13 (m, 2H), 7.96 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.78 (d, *J* = 2.0 Hz, 1H), 7.72–7.63 (m, 2H), 7.58–7.51 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.08, 149.25, 147.82, 136.36, 135.99, 135.86, 132.70, 132.34, 129.96, 129.65, 128.76, 128.22, 126.87, 124.50, 121.81. HRMS (ESI-TOF) *m/z* calc'd for $C_{15}H_{11}N_2O_2$ $[M+H]^+$: 251.0815; found: 251.0824.



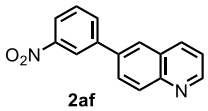
2ae

Phenyl(3-(quinolin-6-yl)phenyl)methanone (2ae)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH, and 1 equiv. NBE-CO_2Me (no Ag_2CO_3). The reaction mixture was stirred at 100 °C for 18 h. After purification by preparative TLC (hexanes/EtOAc = 4:1 v/v), compound **2ae** (14.5 mg) was obtained in 47% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.22 (dd, *J* = 8.4, 1.3 Hz, 1H), 8.20 (d, *J* = 8.7 Hz, 1H), 8.17 (t, *J* = 1.6 Hz, 1H), 8.05 (d, *J* = 2.1 Hz, 1H), 8.00 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.95 (ddd, *J* = 7.7, 2.0, 1.1

Hz, 1H), 7.87 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.81 (dt, *J* = 7.7, 1.3 Hz, 1H), 7.65–7.59 (m, 2H), 7.52 (t, *J* = 7.8 Hz, 2H), 7.45 (dd, *J* = 8.2, 4.2 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 196.66, 150.78, 147.90, 140.68, 138.50, 138.33, 137.57, 136.43, 132.75, 131.37, 130.25, 130.22, 129.50, 129.07, 129.03, 128.91, 128.54, 128.51, 125.95, 121.75. HRMS (ESI-TOF) *m/z* calc'd for $C_{22}H_{16}N_1O_1$ $[M+H]^+$: 310.1226; found: 310.1236.

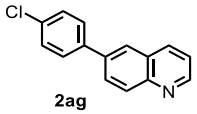


2af

6-(3-Nitrophenyl)quinoline (2af)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH, and 1 equiv. NBE-CO_2Me (no Ag_2CO_3). The reaction mixture was stirred at 100 °C for 18 h. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2af** (9.6 mg) was obtained in 38% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.97 (d, *J* = 2.8 Hz, 1H), 8.59 (s, 1H), 8.30–8.19 (m, 3H), 8.08 (d, *J* = 2.1 Hz, 1H), 8.05 (d, *J* = 7.8 Hz, 1H), 7.99 (dd, *J* = 8.8, 2.2 Hz, 1H), 7.68 (t, *J* = 8.0 Hz, 1H), 7.49 (dd, *J* = 8.3, 4.2 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.19, 148.95, 148.05, 142.11, 136.85, 136.55, 133.40, 130.60, 130.08, 128.66, 128.52, 126.28, 122.59, 122.38, 122.03. HRMS (ESI-TOF) *m/z* calc'd for $C_{15}H_{11}N_2O_2$ $[M+H]^+$: 251.0815; found: 251.0821.

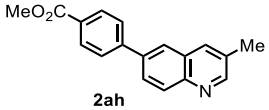


2ag

6-(4-Chlorophenyl)quinoline (2ag)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH, and 1 equiv. NBE-CO_2Me (no Ag_2CO_3). The reaction mixture was stirred at 100 °C for 18 h. After purification by preparative TLC (DCM/EtOAc = 5:1 v/v), compound **2ag** (9.1 mg) was obtained in 38% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.93 (dd, *J* = 4.2, 1.8 Hz, 1H), 8.21 (dd, *J* = 8.3, 1.6 Hz, 1H), 8.18 (d, *J* = 8.6 Hz, 1H), 7.97 (d, *J* = 2.1 Hz, 1H), 7.94 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.65 (d, *J* = 8.7 Hz, 2H), 7.47 (d, *J* = 8.7 Hz, 2H), 7.44 (dd, *J* = 8.2, 4.2 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.68, 147.81, 138.88, 138.21, 136.36, 134.08, 130.19, 129.25, 129.00, 128.80, 128.55, 125.57, 121.74. HRMS (ESI-TOF) *m/z* calc'd for $C_{15}H_{11}Cl_1N_1$ $[M+H]^+$: 240.0575; found: 240.0584.

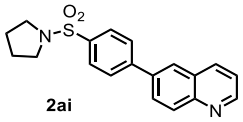


2ah

Methyl 4-(3-methylquinolin-6-yl)benzoate (2ah)

Substrate 3-methyl-quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH, and 1 equiv. NBE-CO_2Me (no Ag_2CO_3). The reaction mixture was stirred at 100 °C for 18 h. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2ah** (14.8 mg) was obtained in 53% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.79 (d, *J* = 2.2 Hz, 1H), 8.19–8.13 (m, 3H), 8.00–7.95 (m, 2H), 7.92 (dd, *J* = 8.7, 2.1 Hz, 1H), 7.78 (d, *J* = 8.7 Hz, 2H), 3.96 (s, 3H), 2.55 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.02, 152.94, 146.31, 145.01, 138.19, 135.09, 131.29, 130.34, 129.94, 129.34, 128.37, 128.02, 127.45, 125.56, 52.31, 18.93. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{16}N_1O_2$ $[M+H]^+$: 278.1176; found: 278.1187.

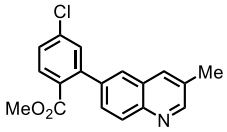


2ai

6-(4-(Pyrrolidin-1-ylsulfonyl)phenyl)quinoline (2ai)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH, and 1 equiv. NBE-CO_2Me (no Ag_2CO_3). The reaction mixture was stirred at 100 °C for 18 h. After purification by preparative TLC (hexanes/EtOAc = 1:2 v/v), compound **2ai** (13.8 mg) was obtained in 41% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.97 (dd, *J* = 4.2, 1.8 Hz, 1H), 8.28–8.18 (m, 2H), 8.06 (d, *J* = 2.1 Hz, 1H), 8.01–7.93 (m, 3H), 7.87 (d, *J* = 8.7 Hz, 2H), 7.48 (dd, *J* = 8.2, 4.2 Hz, 1H), 3.35–3.29 (m, 4H), 1.83–1.79 (m, 4H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.11, 148.08, 144.62, 137.58, 136.55, 136.24, 130.44, 128.90, 128.51, 128.30, 128.07, 126.39, 121.95, 48.10, 25.41. HRMS (ESI-TOF) *m/z* calc'd for $C_{19}H_{19}N_2O_2S_1$ $[M+H]^+$: 339.1162; found: 339.1172.

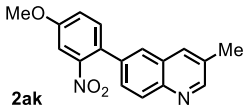


2aj

Methyl 4-chloro-2-(3-methylquinolin-6-yl)benzoate (2aj)

Substrate 3-methyl-quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2aj** (14.6 mg) was obtained in 47% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.79 (d, *J* = 2.2 Hz, 1H), 8.07 (d, *J* = 8.6 Hz, 1H), 7.92 (s, 1H), 7.89 (d, *J* = 2.3 Hz, 1H), 7.65 (d, *J* = 2.1 Hz, 1H), 7.56–7.51 (m, 2H), 7.39 (d, *J* = 8.1 Hz, 1H), 3.61 (s, 3H), 2.53 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 167.57, 152.73, 145.90, 140.52, 138.69, 134.90, 133.81, 132.43, 132.18, 131.59, 131.16, 130.18, 129.53, 128.83, 127.98, 126.17, 52.40, 18.90. HRMS (ESI-TOF) *m/z* calc'd for $C_{18}H_{15}Cl_1N_1O_2$ $[M+H]^+$: 312.0786; found: 312.0796.

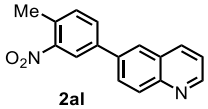


2ak

6-(4-Methoxy-2-nitrophenyl)-3-methylquinoline (2ak)

Substrate 3-methyl-quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv). After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2ak** (21.2 mg) was obtained in 72% yield as a yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.79 (d, *J* = 2.3 Hz, 1H), 8.08 (d, *J* = 8.7 Hz, 1H), 7.90 (s, 1H), 7.64 (d, *J* = 2.1 Hz, 1H), 7.54 (dd, *J* = 8.6, 2.1 Hz, 1H), 7.45 (d, *J* = 2.7 Hz, 1H), 7.42 (d, *J* = 8.5 Hz, 1H), 7.20 (dd, *J* = 8.5, 2.7 Hz, 1H), 3.92 (s, 3H), 2.52 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 159.49, 152.89, 149.71, 145.95, 135.85, 134.89, 133.13, 131.23, 129.54, 128.94, 128.25, 128.13, 126.19, 119.02, 109.36, 56.09, 18.88. HRMS (ESI-TOF) *m/z* calc'd for $C_{17}H_{15}N_2O_3$ $[M+H]^+$: 295.1077; found: 295.1081.

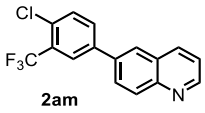


2al

6-(4-Methyl-3-nitrophenyl)quinoline (2al)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH, and 1 equiv. NBE-CO_2Me (no Ag_2CO_3). The reaction mixture was stirred at 100 °C for 18 h. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2al** (14.7 mg) was obtained in 52% yield as a yellow solid.

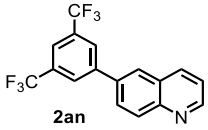
^1H NMR (600 MHz, $CDCl_3$) δ 8.95 (dd, *J* = 4.1, 1.5 Hz, 1H), 8.34 (d, *J* = 2.1 Hz, 1H), 8.25 (d, *J* = 7.8 Hz, 1H), 8.21 (d, *J* = 8.7 Hz, 1H), 8.04 (d, *J* = 2.2 Hz, 1H), 7.97 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.86 (dd, *J* = 7.9, 2.0 Hz, 1H), 7.51–7.44 (m, 2H), 2.68 (d, *J* = 0.5 Hz, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 150.97, 149.81, 147.84, 139.51, 136.77, 136.61, 133.60, 132.98, 131.66, 130.37, 128.65, 128.56, 125.85, 123.42, 121.96, 20.34. HRMS (ESI-TOF) *m/z* calc'd for $C_{16}H_{13}N_2O_2$ $[M+H]^+$: 265.0972; found: 265.0978.



6-(4-Chloro-3-(trifluoromethyl)phenyl)quinoline (2am)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH, and 1 equiv. NBE-CO_2Me (no Ag_2CO_3). The reaction mixture was stirred at 100 °C for 18 h. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2am** (12.7 mg) was obtained in 41% yield as a white solid.

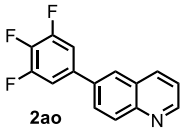
^1H NMR (600 MHz, $CDCl_3$) δ 8.96 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.27–8.18 (m, 2H), 8.02 (d, *J* = 2.3 Hz, 1H), 8.00 (d, *J* = 2.2 Hz, 1H), 7.93 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.81 (dd, *J* = 8.3, 2.1 Hz, 1H), 7.64 (d, *J* = 8.3 Hz, 1H), 7.47 (dd, *J* = 8.3, 4.2 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.14, 148.03, 139.41, 136.84, 136.42, 132.19, 131.86 (q, *J* = 1.9 Hz), 131.63, 130.62, 129.10 (q, *J* = 31.4 Hz), 128.60, 128.51, 126.56 (q, *J* = 5.2 Hz), 125.99, 122.93 (q, *J* = 273.4 Hz), 121.99; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.89. HRMS (ESI-TOF) *m/z* calc'd for $C_{16}H_{10}Cl_1F_3N_1$ $[M+H]^+$: 308.0448; found: 308.0448.



6-(3,5-Bis(trifluoromethyl)phenyl)quinoline (2an)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH, and 1 equiv. NBE-CO_2Me (no Ag_2CO_3). The reaction mixture was stirred at 100 °C for 18 h. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2an** (12.6 mg) was obtained in 37% yield as a white solid.

^1H NMR (600 MHz, $CDCl_3$) δ 8.99 (dd, *J* = 4.2, 1.8 Hz, 1H), 8.30–8.24 (m, 2H), 8.15 (s, 2H), 8.06 (d, *J* = 2.1 Hz, 1H), 7.98 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.92 (s, 1H), 7.50 (dd, *J* = 8.2, 4.2 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.47, 148.21, 142.61, 136.52, 136.38, 132.49 (q, *J* = 33.3 Hz), 130.88, 128.55, 128.51, 127.70–127.57 (m), 126.52, 123.42 (q, *J* = 272.6 Hz), 122.16, 121.57–121.41 (m); ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.10. HRMS (ESI-TOF) *m/z* calc'd for $C_{17}H_{10}F_6N_1$ $[M+H]^+$: 342.0712; found: 342.0724.



6-(3,4,5-Trifluorophenyl)quinoline (2ao)

Substrate quinoline was arylated following the general procedure by using **T1**-MeCN (67.0 mg, 0.10 mmol, 1.0 equiv.), 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH, and 1 equiv. NBE-CO_2Me (no Ag_2CO_3). The reaction mixture was stirred at 100 °C for 18 h. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **2ao** (8 mg) was obtained in 31% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.96 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.25–8.16 (m, 3H), 7.94 (d, *J* = 2.2 Hz, 1H), 7.87 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.47 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.36–7.29 (m, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 151.68 (ddd, *J* = 250.2, 9.9, 4.2 Hz), 151.18, 148.05, 136.72–136.48 (m), 136.41, 130.60, 128.43, 128.42, 125.87, 122.02, 111.57 (dd, *J* = 17.1, 5.0 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -133.89 (d, *J* = 20.7 Hz), -162.04 (t, *J* = 20.4 Hz). HRMS (ESI-TOF) *m/z* calc'd for $C_{15}H_9F_3N_1$ $[M+H]^+$: 260.0682; found: 260.0689.

Investigation of regioselectivity: In the representative examples (**2a**, **2e**, **2af**), either less than 5% of the over-arylated product (eq. 1) or none regio-isomer (eq. 2, eq. 3) was isolated.

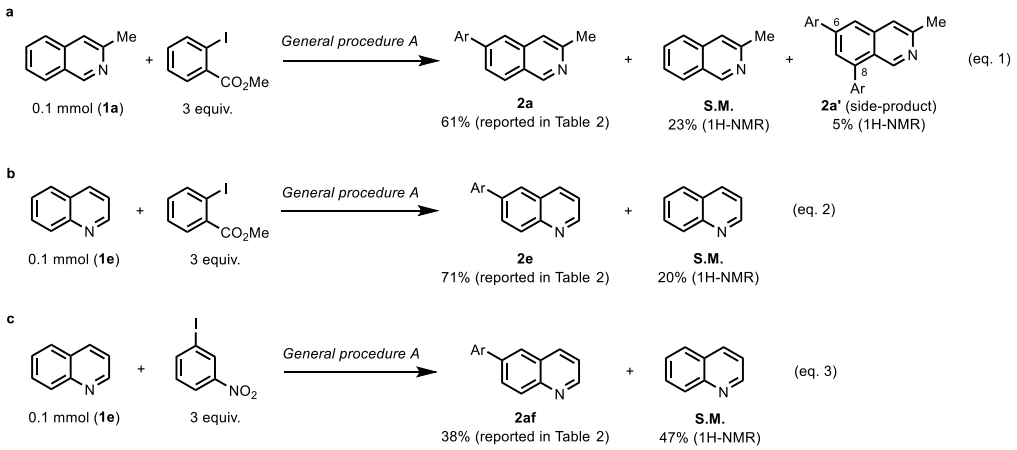
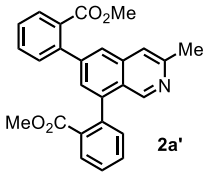


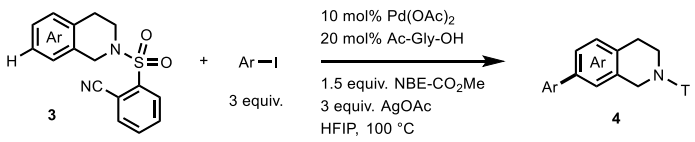
Figure 1 Investigation of regioselectivity



Dimethyl 2,2'-(3-methylisoquinoline-6,8-diyl)dibenzoate (2a')

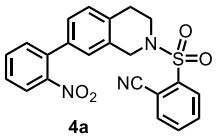
^{1}H NMR (600 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.08 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.90 (dd, *J* = 7.7, 0.9 Hz, 1H), 7.67 (s, 1H), 7.62 (td, *J* = 7.5, 1.4 Hz, 1H), 7.58 (td, *J* = 7.6, 1.4 Hz, 1H), 7.56–7.52 (m, 2H), 7.50–7.45 (m, 2H), 7.40 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.25 (d, *J* = 1.7 Hz, 1H), 3.64 (s, 3H), 3.51 (s, 3H), 2.69 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 168.72, 167.32, 151.74, 150.17, 143.08, 141.84, 140.16, 139.59, 136.55, 131.98, 131.86, 131.63, 131.28, 131.08, 130.89, 130.55, 130.26, 128.32, 127.94, 127.74, 124.72, 124.27, 118.98, 52.24, 52.03, 24.12. HRMS (ESI-TOF) *m/z* calc'd for $C_{26}H_{22}N_1O_4$ $[M+H]^+$: 412.1543; found: 412.1549.

C. Pd-Catalyzed C7 Arylation of Tetrahydroisoquinolines



General procedure B: Tetrahydroisoquinoline **3** (0.10 mmol, 1.0 equiv.), $Pd(OAc)_2$ (2.2 mg, 10 μmol, 10

mol%), Ac-Gly-OH (2.3 mg, 20 μmol, 20 mol%), aryl iodide (0.3 mmol, 3 equiv.), NBE-CO_2Me (22.8 mg, 0.15 mmol, 1.5 equiv.), AgOAc (50 mg, 0.30 mmol, 3.0 equiv.), and HFIP (1 ml) were added to a reaction vial (8 mL). The reaction vial was sealed and allowed to stir at 100 °C for 18 h. The reaction mixture was cooled to room temperature, and then diluted with EtOAc. The mixture was filtered through a short pad of celite and eluted with EtOAc (2 × 2 mL). The filtrate was evaporated under reduced pressure. Purification by preparative TLC afforded the title compound.

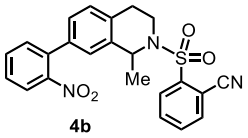


4a

2-((7-(2-Nitrophenyl)-3,4-dihydroisoquinolin-2(1*H*)-yl)sulfonyl)benzonitrile (4a)

Substrate arene was arylated following the general procedure. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **4a** (23.2 mg) was obtained in 55% yield as a yellow solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 8.0, 1.3 Hz, 1H), 7.87 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.84 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.77 (td, *J* = 7.8, 1.3 Hz, 1H), 7.69 (td, *J* = 7.6, 1.3 Hz, 1H), 7.61 (td, *J* = 7.6, 1.3 Hz, 1H), 7.48 (td, *J* = 7.8, 1.4 Hz, 1H), 7.39 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.14 (d, *J* = 8.0 Hz, 1H), 7.12–7.08 (m, 1H), 7.04 (s, 1H), 4.51 (s, 2H), 3.69 (t, *J* = 6.0 Hz, 2H), 3.00 (t, *J* = 6.0 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.20, 140.90, 135.87, 135.77, 135.73, 133.32, 133.07, 132.91, 132.51, 131.99, 131.91, 130.42, 129.42, 128.42, 126.67, 125.86, 124.24, 116.35, 110.94, 47.29, 43.61, 28.47. HRMS (ESI-TOF) *m/z* calc'd for $C_{22}H_{18}N_3O_4S$ $[M+H]^+$: 420.1013; found: 420.1011.

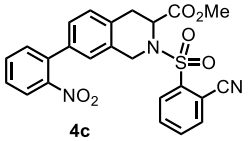


4b

2-((1-Methyl-7-(2-nitrophenyl)-3,4-dihydroisoquinolin-2(1*H*)-yl)sulfonyl)benzonitrile (4b)

Substrate arene was arylated following the general procedure. After purification by preparative TLC (hexanes/EtOAc = 1:1 v/v), compound **4b** (19.1 mg) was obtained in 44% yield as a colorless oil.

^{1}H NMR (600 MHz, CD_3CN) δ 8.10 (dd, *J* = 8.0, 0.6 Hz, 1H), 7.90–7.85 (m, 2H), 7.78 (td, *J* = 7.8, 1.4 Hz, 1H), 7.70 (dtd, *J* = 10.1, 7.6, 1.2 Hz, 2H), 7.56 (ddd, *J* = 8.1, 7.4, 1.4 Hz, 1H), 7.50–7.47 (m, 1H), 7.15 (s, 1H), 7.12–7.08 (m, 2H), 5.20 (q, *J* = 7.1 Hz, 1H), 4.10–3.97 (m, 1H), 3.64–3.53 (m, 1H), 2.87–2.71 (m, 2H), 1.46 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (151 MHz, CD_3CN) δ 150.22, 143.60, 138.81, 136.91, 136.42, 136.14, 134.47, 134.01, 133.90, 133.65, 132.90, 130.90, 130.50, 129.62, 127.41, 127.28, 125.07, 117.24, 110.71, 53.00, 39.35, 28.08, 23.33. HRMS (ESI-TOF) *m/z* calc'd for $C_{23}H_{20}N_3O_4S_1$ $[M+H]^+$: 434.1169; found: 434.1170.

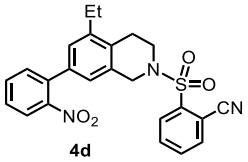


4c

Methyl 2-((2-cyanophenyl)sulfonyl)-7-(2-nitrophenyl)-1,2,3,4-tetrahydroisoquinoline-3-carboxylate (4c)

Substrate arene was arylated following the general procedure by using 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH. After purification by preparative TLC (hexanes/EtOAc = 1:2 v/v), compound **4c** (22.4 mg) was obtained in 47% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.17 (d, *J* = 7.9 Hz, 1H), 7.86 (d, *J* = 7.6 Hz, 1H), 7.84 (d, *J* = 8.1 Hz, 1H), 7.76 (t, *J* = 7.8 Hz, 1H), 7.69 (t, *J* = 7.4 Hz, 1H), 7.60 (t, *J* = 7.6 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.37 (d, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 7.9 Hz, 1H), 7.11 (d, *J* = 8.9 Hz, 1H), 6.99 (s, 1H), 5.33 (dd, *J* = 6.6, 2.2 Hz, 1H), 4.63 (d, *J* = 4.9 Hz, 2H), 3.62 (s, 3H), 3.48 (dd, *J* = 16.5, 6.6 Hz, 1H), 3.38 (d, *J* = 16.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 170.68, 149.17, 141.98, 136.21, 135.61, 135.52, 132.91, 132.85, 132.49, 131.99, 131.19, 130.90, 130.56, 129.45, 128.47, 126.79, 125.72, 124.26, 116.40, 110.92, 54.64, 52.86, 44.41, 31.33. HRMS (ESI-TOF) *m/z* calc'd for $C_{24}H_{20}N_3O_6S$ $[M+H]^+$: 478.1067; found: 478.1069.

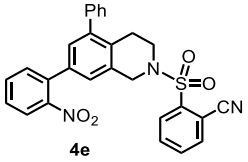


4d

2-((5-Ethyl-7-(2-nitrophenyl)-3,4-dihydroisoquinolin-2(1*H*)-yl)sulfonyl)benzonitrile (4d)

Substrate arene was arylated following the general procedure. After purification by preparative TLC (hexanes/EtOAc = 1:1 v/v), compound **4d** (21.5 mg) was obtained in 48% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (d, *J* = 7.9 Hz, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.76 (t, *J* = 7.8 Hz, 1H), 7.68 (t, *J* = 7.6 Hz, 1H), 7.60 (t, *J* = 7.5 Hz, 1H), 7.47 (t, *J* = 7.7 Hz, 1H), 7.41 (d, *J* = 7.7 Hz, 1H), 6.99 (s, 1H), 6.89 (s, 1H), 4.49 (s, 2H), 3.72 (t, *J* = 6.0 Hz, 2H), 2.92 (t, *J* = 6.0 Hz, 2H), 2.57 (q, *J* = 7.5 Hz, 2H), 1.16 (t, *J* = 7.5 Hz, 3H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.27, 142.95, 140.81, 135.93, 135.73, 135.65, 133.05, 132.87, 132.42, 131.98, 131.90, 131.26, 130.42, 128.28, 126.20, 124.15, 123.55, 116.37, 111.00, 47.77, 43.74, 29.35, 25.48, 14.14. HRMS (ESI-TOF) *m/z* calc'd for $C_{24}H_{22}N_3O_4S$ $[M+H]^+$: 448.1326; found: 448.1328.

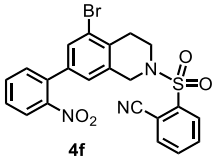


4e

2-((7-(2-Nitrophenyl)-5-phenyl-3,4-dihydroisoquinolin-2(1*H*)-yl)sulfonyl)benzonitrile (4e)

Substrate arene was arylated following the general procedure by using 20 mol% $Pd(OAc)_2$, 40 mol% Ac-Gly-OH. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **4e** (23.2 mg) was obtained in 45% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.0 Hz, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.86 (d, *J* = 7.9 Hz, 1H), 7.77 (t, *J* = 7.8 Hz, 1H), 7.70 (t, *J* = 7.6 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.48 (t, *J* = 7.1 Hz, 1H), 7.44 (d, *J* = 7.7 Hz, 1H), 7.40 (t, *J* = 7.3 Hz, 2H), 7.35 (t, *J* = 7.4 Hz, 1H), 7.24 (d, *J* = 6.9 Hz, 2H), 7.07 (d, *J* = 7.2 Hz, 2H), 4.59 (s, 2H), 3.59 (t, *J* = 5.9 Hz, 2H), 2.86 (t, *J* = 5.9 Hz, 2H). ^{13}C NMR (151 MHz, $CDCl_3$) δ 149.15, 142.63, 140.89, 139.93, 135.78, 135.73, 135.61, 133.06, 132.90, 132.57, 132.40, 132.08, 131.27, 130.47, 129.14, 128.49, 128.44, 128.12, 127.62, 125.00, 124.34, 116.35, 111.05, 47.58, 43.77, 27.60. HRMS (ESI-TOF) *m/z* calc'd for $C_{28}H_{22}N_3O_4S$ $[M+H]^+$: 496.1326; found: 496.1326.



4f

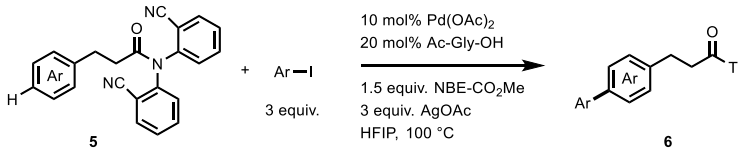
2-((5-Bromo-7-(2-nitrophenyl)-3,4-dihydroisoquinolin-2(1*H*)-yl)sulfonyl)benzonitrile (4f)

Substrate arene was arylated following the general procedure. After purification by preparative TLC (hexanes/EtOAc = 1:1 v/v), compound **4f** (15.2 mg) was obtained in 31% yield as a yellow oil.

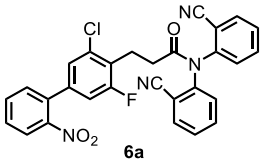
The position of C–H arylation on **4f** was determined by NOESY.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.12 (dd, *J* = 7.9, 0.9 Hz, 1H), 7.91 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.87 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.77 (td, *J* = 7.8, 1.4 Hz, 1H), 7.70 (td, *J* = 7.6, 1.3 Hz, 1H), 7.63 (td, *J* = 7.6, 1.3 Hz, 1H), 7.52 (ddd, *J* = 8.1, 7.6, 1.4 Hz, 1H), 7.40 (d, *J* = 1.8 Hz, 1H), 7.38 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.00 (d, *J* = 1.6 Hz, 1H), 4.53 (s, 2H), 3.70 (t, *J* = 6.1 Hz, 2H), 2.96 (t, *J* = 6.2 Hz, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 148.87, 140.96, 137.41, 135.78, 134.47, 134.16, 133.12, 133.05, 133.03, 132.78, 132.02, 130.51, 130.40, 128.99, 125.51, 125.17, 124.49, 116.26, 110.98, 47.53, 43.66, 29.30. HRMS (ESI-TOF) *m/z* calc'd for $C_{22}H_{17}BrN_3O_4S_1$ $[M+H]^+$: 498.0118; found: 498.0116.

D. Pd-Catalyzed *para*-Arylation of Phenylpropanoic Acid Derivatives



General procedure C: Phenylpropanoic acid derivative **5** (0.10 mmol, 1.0 equiv.), $Pd(OAc)_2$ (2.2 mg, 10 μmol, 10 mol%), Ac-Gly-OH (2.3 mg, 20 μmol, 20 mol%), aryl iodide (0.3 mmol, 3 equiv.), NBE-CO_2Me (22.8 mg, 0.15 mmol, 1.5 equiv.), AgOAc (50 mg, 0.30 mmol, 3.0 equiv.), and HFIP (1 ml) were added to a reaction vial (8 mL). The reaction vial was sealed and allowed to stir at 100 °C for 18 h. The reaction mixture was cooled to room temperature, and then diluted with EtOAc. The mixture was filtered through a short pad of celite and eluted with EtOAc (2 × 2 mL). The filtrate was evaporated under reduced pressure. Purification by preparative TLC afforded the title compound.

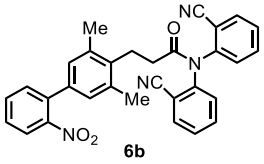


3-(3-Chloro-5-fluoro-2'-nitro-[1,1'-biphenyl]-4-yl)-*N*,*N*-bis(2-cyanophenyl)propanamide (6a)

Substrate arene was arylated following the general procedure. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **6a** (40.2 mg) was obtained in 77% yield as a colorless oil.

The position of C–H arylation on **6a** was determined by NOESY.

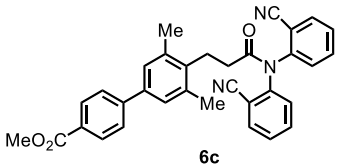
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.89 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.85–7.39 (m, 8H), 7.63 (td, *J* = 7.6, 1.3 Hz, 1H), 7.53 (td, *J* = 7.8, 1.4 Hz, 1H), 7.36 (dd, *J* = 7.6, 1.5 Hz, 1H), 7.07 (s, 1H), 6.89 (dd, *J* = 9.4, 1.7 Hz, 1H), 3.31–3.25 (m, 2H), 2.63 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.41, 161.12 (d, *J* = 249.8 Hz), 148.75, 144.06, 143.92, 138.03 (d, *J* = 9.9 Hz), 135.54 (d, *J* = 6.6 Hz), 134.92, 134.64, 134.23, 133.94 (d, *J* = 2.2 Hz), 133.89, 132.80, 131.83, 130.60, 129.64, 129.32, 129.19, 128.34, 126.02 (d, *J* = 18.7 Hz), 124.75 (d, *J* = 3.3 Hz), 124.45, 117.06, 116.39, 114.01 (d, *J* = 24.2 Hz), 113.19, 112.99, 33.30, 22.31 (d, *J* = 2.8 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -112.91. HRMS (ESI-TOF) *m/z* calc'd for $C_{29}H_{19}ClFN_4O_3$ $[M+H]^+$: 525.1124; found: 525.1140.



***N*,*N*-Bis(2-cyanophenyl)-3-(3,5-dimethyl-2'-nitro-[1,1'-biphenyl]-4-yl)propanamide (6b)**

Substrate arene was arylated following the general procedure. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **6b** (23.2 mg) was obtained in 46% yield as a yellow oil.

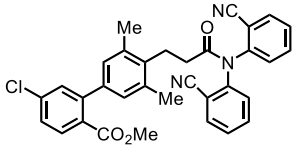
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.84–7.34 (m, 9H), 7.57 (td, *J* = 7.6, 1.3 Hz, 1H), 7.43 (ddd, *J* = 8.1, 7.4, 1.4 Hz, 1H), 7.39 (dd, *J* = 7.7, 1.4 Hz, 1H), 6.92 (s, 2H), 3.15 (dd, *J* = 9.0, 7.9 Hz, 2H), 2.49 (d, *J* = 24.9 Hz, 2H), 2.25 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.13, 149.37, 144.33, 144.11, 137.37, 137.02, 136.20, 135.22, 135.02, 134.66, 134.30, 133.85, 132.22, 132.04, 130.45, 129.57, 129.18, 128.36, 127.95, 127.65, 124.02, 117.18, 116.44, 113.25, 33.66, 25.23, 19.87. HRMS (ESI-TOF) *m/z* calc'd for $C_{31}H_{25}N_4O_3$ $[M+H]^+$: 501.1921; found: 501.1925.



6c

Methyl 4'-(3-(bis(2-cyanophenyl)amino)-3-oxopropyl)-3',5'-dimethyl-[1,1'-biphenyl]-4-carboxylate (6c)

Substrate arene was arylated following the general procedure by using 0.5 ml HFIP. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **6c** (20 mg) was obtained in 39% yield as a white solid. ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.06 (d, *J* = 8.7 Hz, 2H), 7.78 (d, *J* = 7.8 Hz, 2H), 7.74–7.38 (m, 6H), 7.60 (d, *J* = 8.7 Hz, 2H), 7.23 (s, 2H), 3.93 (s, 3H), 3.17 (t, *J* = 8.6 Hz, 2H), 2.67–2.37 (m,2H), 2.32 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.14, 167.28, 145.58, 144.48, 144.32, 138.05, 137.54, 137.34, 135.09, 134.71, 134.50, 133.99, 130.54, 130.23, 129.67, 129.30, 128.87, 128.57, 127.27, 127.04, 117.35, 116.54, 113.42, 113.25, 52.33, 33.95, 25.34, 20.08. HRMS (ESI-TOF) *m/z* calc'd for $C_{33}H_{28}N_3O_3$ $[M+H]^+$: 514.2125; found: 514.2137.

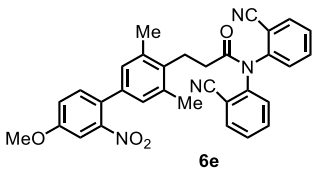


6d

Methyl 4'-(3-(bis(2-cyanophenyl)amino)-3-oxopropyl)-5-chloro-3',5'-dimethyl-[1,1'-biphenyl]-2-carboxylate (6d)

Substrate arene was arylated following the general procedure. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **6d** (27.1 mg) was obtained in 49% yield as a colorless oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.7 Hz, 2H), 7.73 (d, *J* = 2.3 Hz, 1H), 7.72–7.38 (m, 6H), 7.44 (dd, *J* = 8.2, 2.3 Hz, 1H), 7.26 (d, *J* = 8.2 Hz, 1H), 6.88 (s, 2H), 3.67 (s, 3H), 3.14 (t, *J* = 8.5 Hz, 2H), 2.48 (d, *J* = 29.5 Hz, 2H), 2.25 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.29, 168.18, 144.49, 144.36, 140.79, 137.95, 136.72, 136.55, 135.10, 134.73, 134.47, 133.99, 133.15, 132.31, 132.23, 131.34, 130.59, 129.76, 129.67, 129.32, 128.54, 128.25, 117.34, 116.56, 113.42, 113.30, 52.49, 33.93, 25.44, 19.96. HRMS (ESI-TOF) *m/z* calc'd for $C_{33}H_{27}Cl_1N_3O_3$ $[M+H]^+$: 548.1741; found: 548.1740.

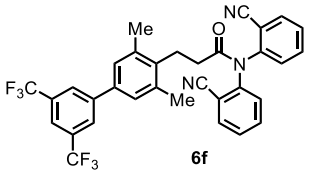


6e

***N,N*-Bis(2-cyanophenyl)-3-(4'-methoxy-3,5-dimethyl-2'-nitro-[1,1'-biphenyl]-4-yl)propanamide (6e)**

Substrate arene was arylated following the general procedure. After purification by preparative TLC (hexanes/EtOAc = 2:1 v/v), compound **6e** (24.3 mg) was obtained in 46% yield as a yellow oil.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (brs, 2H), 7.73–7.36 (m, 6H), 7.30 (d, *J* = 2.7 Hz, 1H), 7.28 (d, *J* = 8.6 Hz, 1H), 7.10 (dd, *J* = 8.6, 2.7 Hz, 1H), 6.88 (s, 2H), 3.88 (s, 3H), 3.14 (t, *J* = 8.6 Hz, 2H), 2.62–2.36 (m, 2H), 2.24 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.31, 159.10, 149.80, 144.46, 144.26, 137.05, 135.25, 135.13, 134.77, 134.43, 133.99, 133.00, 130.58, 129.72, 129.30, 128.63, 128.48, 127.90, 118.78, 117.29, 116.55, 113.37, 113.26, 109.13, 56.14, 33.83, 25.34, 19.99. HRMS (ESI-TOF) *m/z* calc'd for $C_{32}H_{27}N_4O_4$ $[M+H]^+$: 531.2032; found: 531.2025.



6f

***N*,*N*-Bis(2-cyanophenyl)-3-(3,5-dimethyl-3',5'-bis(trifluoromethyl)-[1,1'-biphenyl]-4-yl)propanamide (6f)**

Substrate arene was arylated following the general procedure by using 0.5 ml HFIP. After purification by preparative TLC (DCM), compound **6f** (25.5 mg) was obtained in 43% yield as a white solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.94 (s, 2H), 7.82–7.76 (m, 3H), 7.75–7.60 (m, 3H), 7.56–7.39 (m, 3H), 7.20 (s, 2H), 3.19 (t, *J* = 7.6 Hz, 2H), 2.62–2.38 (m, 2H), 2.34 (s, 6H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.00, 144.47, 144.35, 143.31, 138.38, 137.80, 136.29, 135.13, 134.72, 134.53, 134.00, 132.18 (q, *J* = 33.0 Hz), 130.53, 129.70, 129.29, 128.61, 127.23, 127.18, 123.64 (q, *J* = 272.8 Hz), 120.91–120.76 (m), 117.36, 116.54, 113.43, 113.26, 33.87, 25.36, 20.06. ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.11. HRMS (ESI-TOF) *m/z* calc'd for $C_{33}H_{24}F_6N_3O_1$ $[M+H]^+$: 592.1818; found: 592.1829.

X-RAY CRYSTALLOGRAPHIC DATA

X-ray structure of **2ah**:

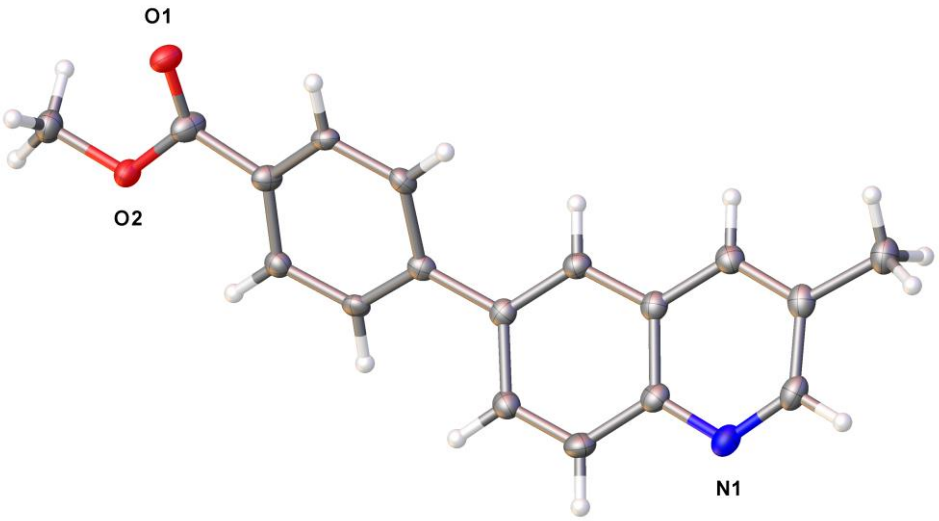


Table 8. Crystal data and structure refinement for **2ah**.

CCDC: 1890836

Report date	2018-08-07	
Identification code	VI-154-3	
Empirical formula	C18.50 H16 Cl N O2	
Molecular formula	C18 H15 N O2, 0.5(C H2 Cl2)	
Formula weight	319.77	
Temperature	100.0 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 18.1630(13) Å	□= 90°.
	b = 4.7535(4) Å	□= 100.305(4)°.
	c = 36.125(3) Å	□ = 90°.
Volume	3068.7(4) $Å^3$	
Z	8	
Density (calculated)	1.384 Mg/m^3	
Absorption coefficient	0.257 mm^{-1}	
F(000)	1336	
Crystal size	0.368 x 0.276 x 0.142 mm^3	
Crystal color, habit	Colorless Block	
Theta range for data collection	3.439 to 25.408°.	
Index ranges	-21<=h<=21, -5<=k<=5, -43<=l<=43	
Reflections collected	30644	
Independent reflections	2813 [R(int) = 0.0635, R(sigma) = 0.0307]	
Completeness to theta = 25.000°	99.8 %	

Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.2590 and 0.2217
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2813 / 0 / 271
Goodness-of-fit on F^2	1.040
Final R indices [I>2sigma(I)]	R1 = 0.0390, wR2 = 0.0952
R indices (all data)	R1 = 0.0584, wR2 = 0.1051
Extinction coefficient	n/a
Largest diff. peak and hole	0.185 and -0.297 e.$Å^{-3}$

COMPUTATIONAL STUDY

I. Mechanistic Study

Proposed Catalytic Cycle

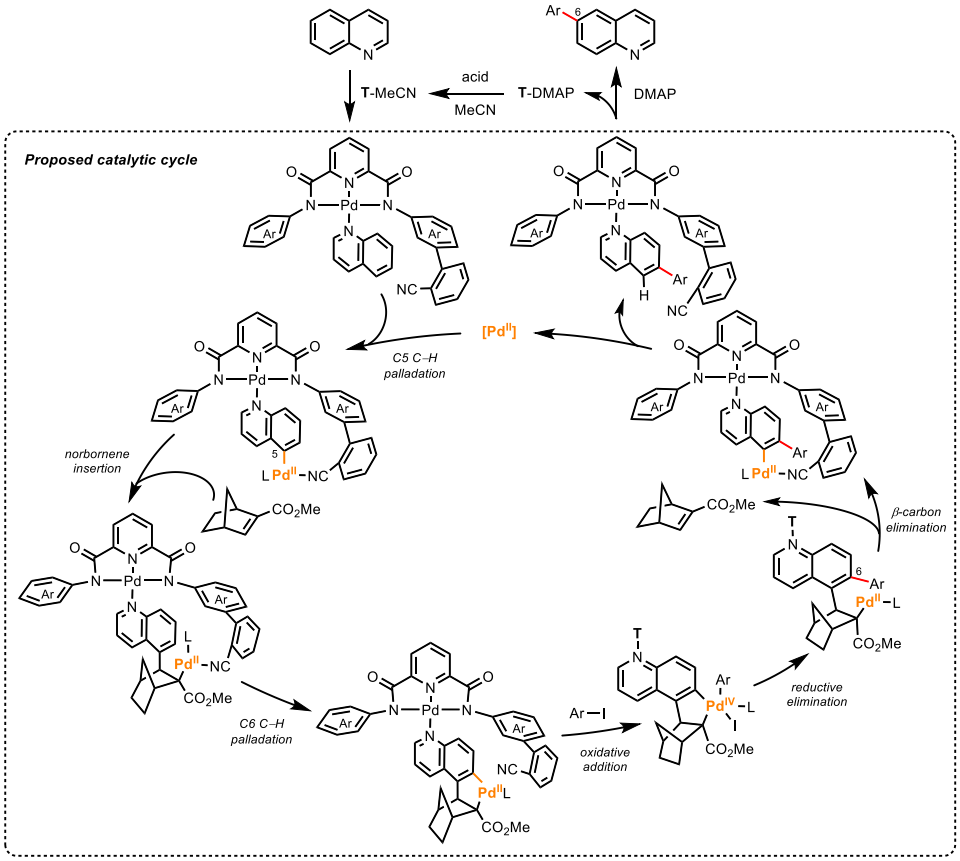


Figure 2 Proposed Catalytic Cycle

Computational Methods

Quantum mechanical calculations were performed with Gaussian 09.[7] Ground state and transition state geometries were optimized in the gas phase using the B3LYP[8-11] functional with the 6-31G(d)[12-13] basis set for all nonmetal atoms and the LANL2DZ[14-15] basis set with effective core potential (ECP) for Pd. Single-point corrections were calculated using Truhlar's M06[16] functional with the 6-311++G(d,p)[17] basis set for all nonmetal atoms and the SDD[18-19] effective core potential for Pd. Single-point solvation energies were calculated by using SMD solvation model (solvent = generic, eps = 16.7, epsinf = 1.625625) to model HFIP. Vibrational frequencies were computed to determine if the optimized structures are minima or saddle points on the potential energy surface corresponding to minima and transition state geometries, respectively. The reported free energies include zero-point energies and thermal corrections calculated at 298.15 K and 1 atm. Molecular structures were illustrated with CYLview.[20]

Additional Computational Discussion

Acknowledging that the Pd template T1 has many degrees of freedom, we conducted a full conformational search using MMFF in Spartan 16 to find the lowest energy conformer. Supplementary Table 9 below shows the conformers within 3 kcal mol^{-1} of the lowest energy conformer T1_conf_1.

Table 9. Conformers of Pd Template T1

Template conformer	Relative free energy (ΔΔG)
T1_conf_1	0.0
T1_conf_2	0.4
T1_conf_3	0.5
T1_conf_4	1.1
T1_conf_5	2.3
T1_conf_6	2.5
T1_conf_7	2.8

For the C5 CMD step with MPAA ligand bound bidentate, the transition state structures with and without nitrile coordination to the second Pd metal center were analyzed. The Pd template with nitrile coordination creates a pocket that positions the quinoline substrate such that the C5 position is easily accessible for CMD to take place. Without nitrile coordination, the chelation of the quinoline group is not as perpendicular to the square planar geometry of the Pd template. This causes the conformer to be 3.6 kcal mol^{-1} higher in energy than the C5 CMD TS conformer with nitrile coordination.

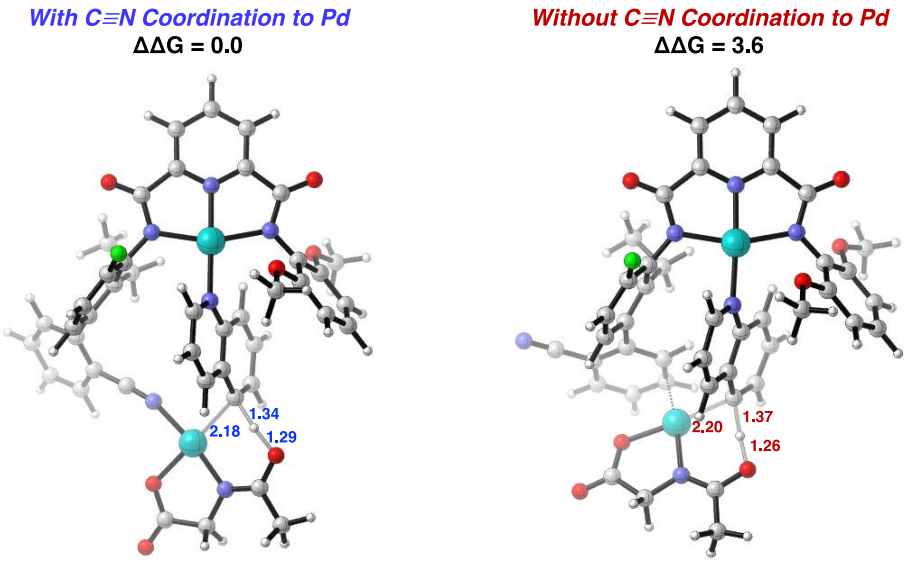


Figure 3. C5-CMD TS Structures.

The norbornene insertion step was lowest in energy when the nitrile group of the Pd template was coordinated to the second Pd metal center, but acetate rather than MPAA ligand was involved. The large size of the MPAA ligand destabilizes the TS due to a steric clash once the norbornene inserts itself.

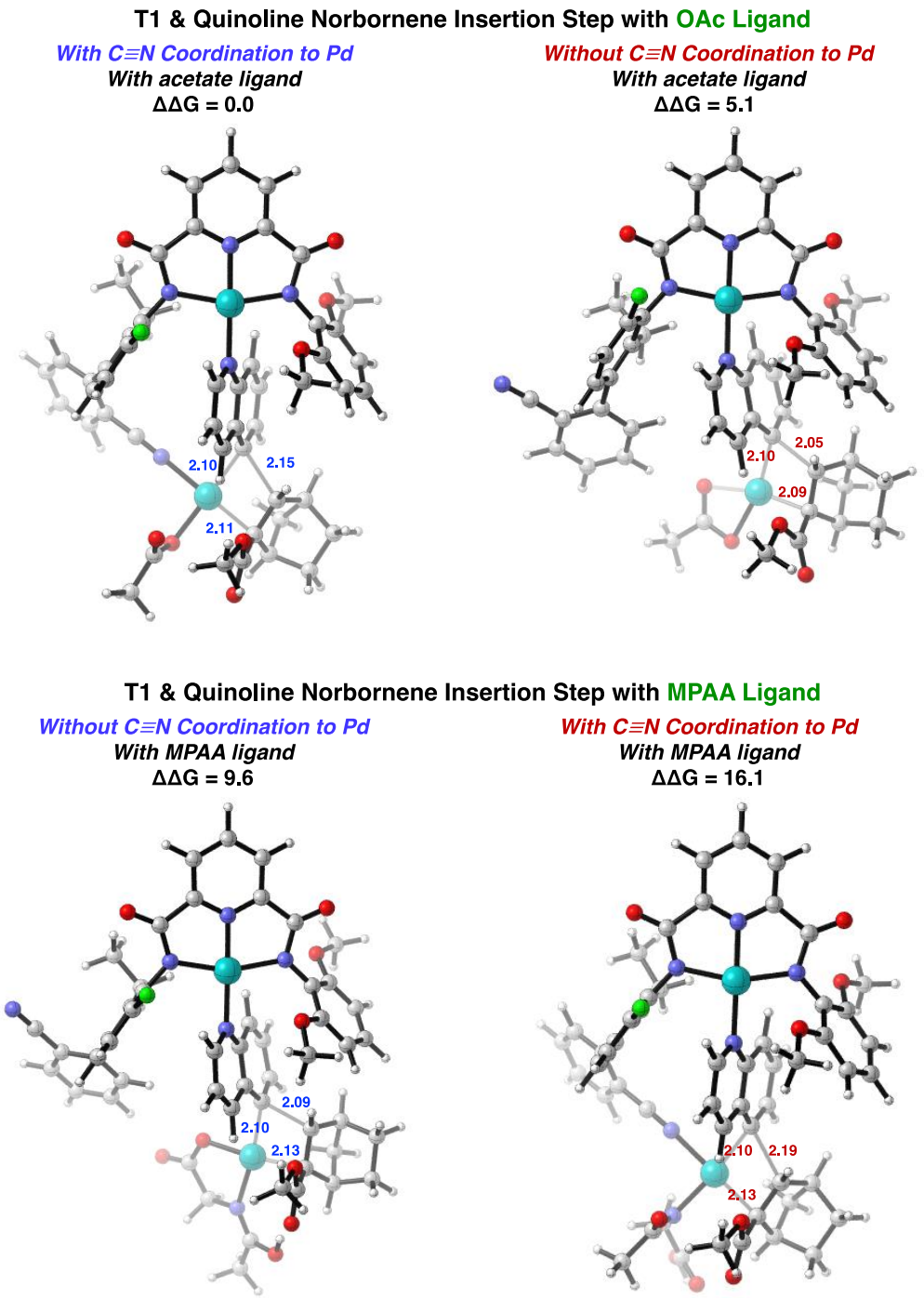


Figure 4. Norbornene Insertion TS Structures.

We then performed the analysis for C6-CMD step, taking into consideration if the MPAA ligand or acetate ligand acts as a base to deprotonate quinoline at the C6 position. When acetate is involved in this step, there is an open coordination site at the second Pd metal center. The nitrile coordination, which stabilized the C5 CMD step, does not assist in C6 CMD. Rather, the vacancy created when the nitrile group is rotated away from the palladacycle stabilizes this TS by a surprisingly large amount of 9.3 kcal mol^{-1}.

If MPAA ligand is involved, both possibilities of nitrile coordinated or not coordinated to Pd are energetically higher than if acetate participates. We explored various binding modes of the MPAA ligand and the ones shown in Fig. S4 where the deprotonated NHAc is coordinated bidentate to the second Pd metal center were lowest in energy. With that, we protonated the carboxylic position to maintain the overall neutrality of the TS structures. Regardless, the involvement of MPAA destabilized the overall TS at this particular step. Overall, the lowest energy TS system for C6 CMD included an acetate ligand and did not have nitrile coordination of the Pd template.

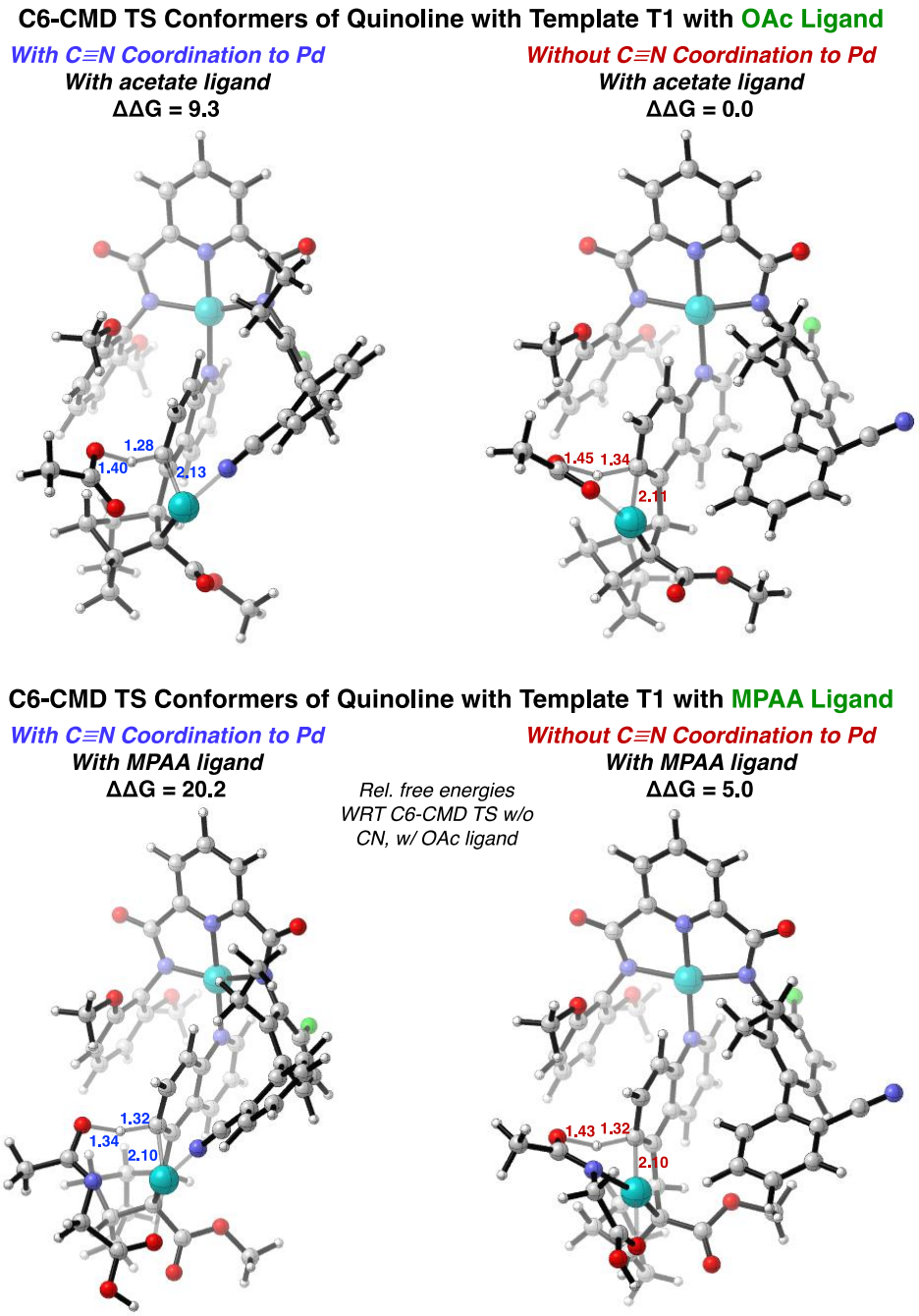


Figure 5. C6 CMD TS Structures.

Then, we analyzed the β-carbon elimination step and found that the nitrile group of the Pd template swings back to coordinate and stabilize this step. Furthermore, an acetate ligand prefers to coordinate in a monodentate fashion at the same Pd center, rather than a more bulky MPAA ligand. If the nitrile group is not coordinated to Pd, the ligand (either acetate or MPAA) must chelate in a bidentate way to compensate for the open coordination site. Both these conformers were higher in energy than the TS with both acetate and nitrile coordination.

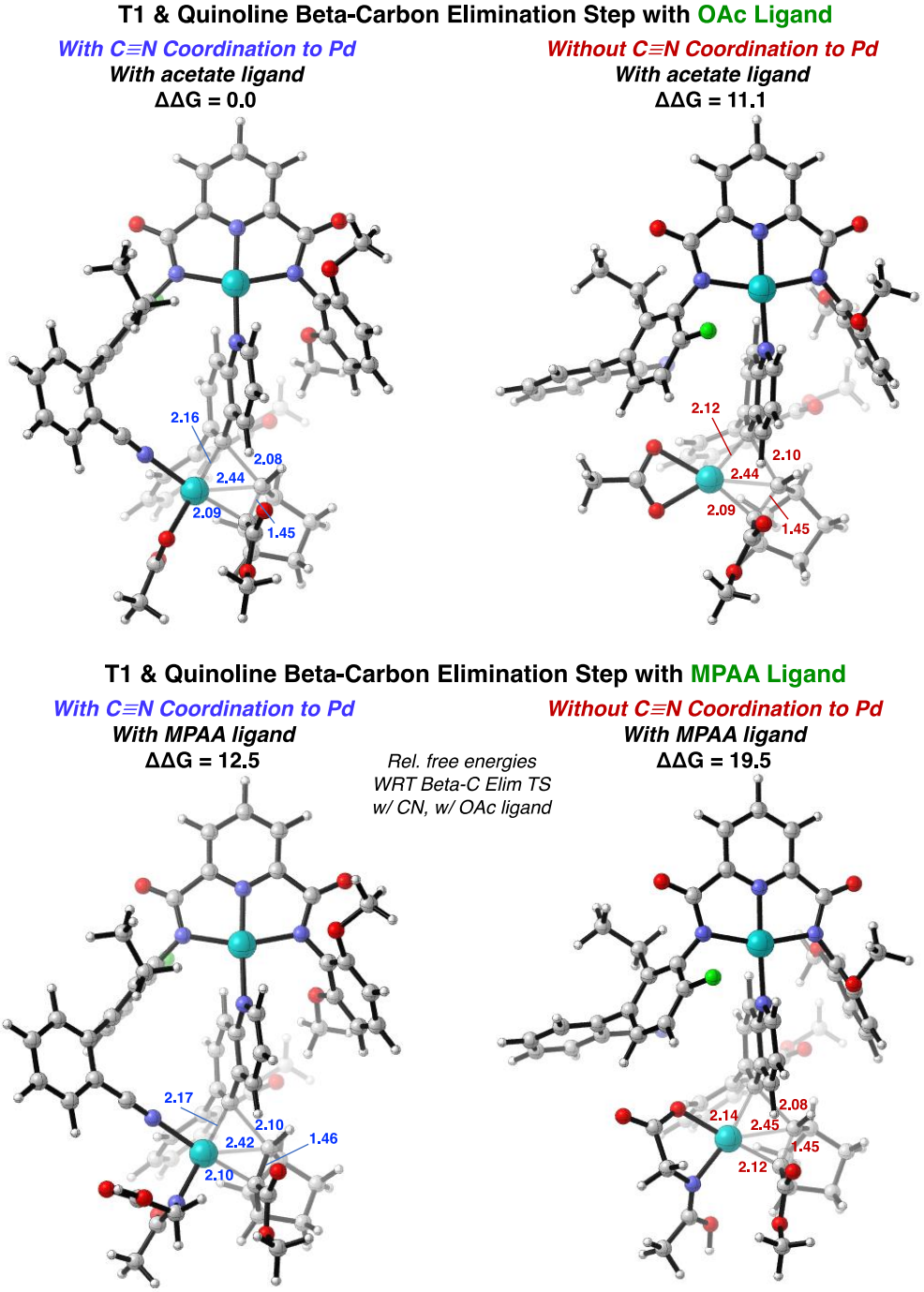


Figure 6. β-Carbon Elimination TS Structures.

Then, the catalytic cycle excluding well-established steps of oxidative addition and reductive elimination was

calculated. The free energy profile consists of the following steps: C5 CMD, norbornene insertion, C6 CMD, and *β*-carbon elimination.

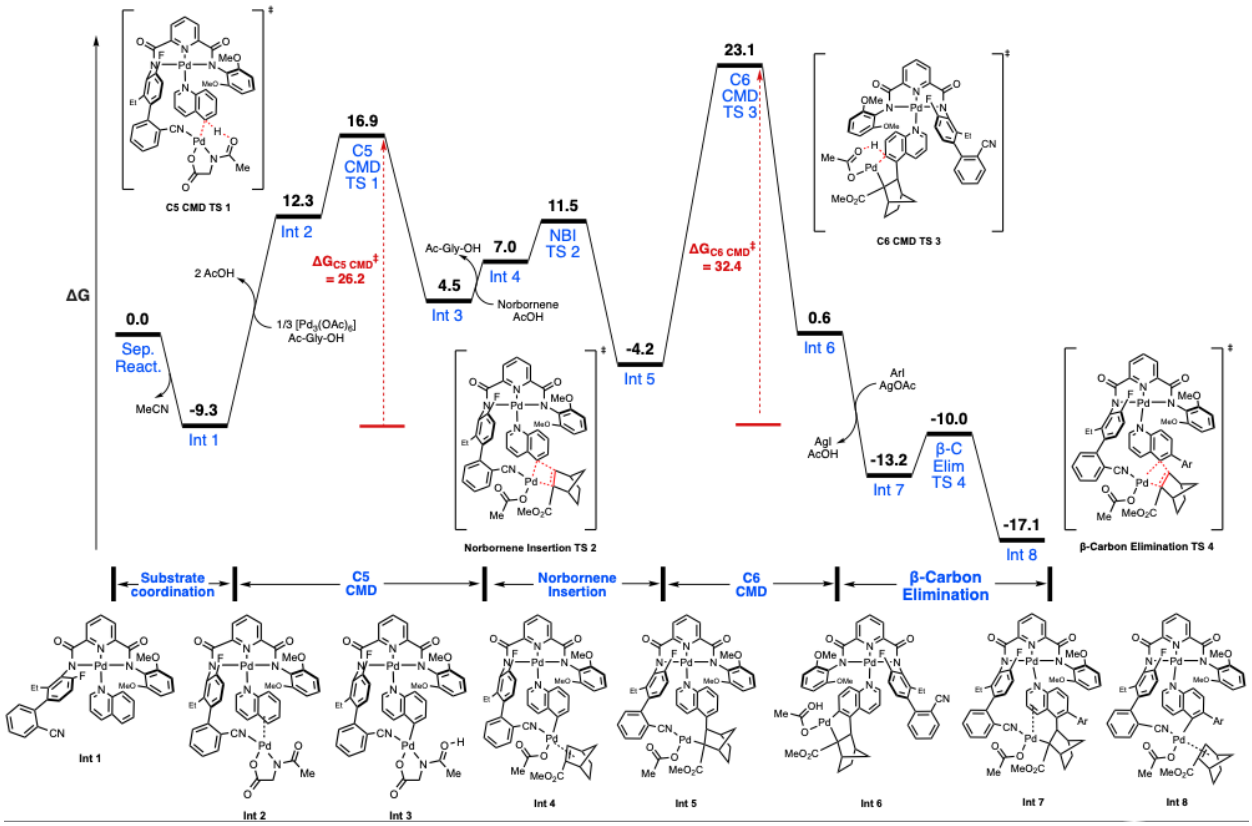


Figure 7. Free Energy Profile of Pd-catalyzed C6-Arylation of Quinoline.

Table 10. Energies, and vibrational frequencies

Filename	E(sol)	ZPVE	TCE	TCH	TCG	Negative Freq (cm^{-1})
Ac-Gly-OH	-874.02003	0.237203	0.256576	0.25752	0.181019	
AcOH	-229.04167	0.062031	0.066592	0.067536	0.034811	
AgOAc2	-750.96935	0.103425	0.11704	0.117985	0.056858	
AgI	-158.45942	0.000427	0.003368	0.004312	-0.025826	
C5_CMD_with_CN_TS	-2869.5246	0.707651	0.760858	0.761802	0.61667	-1229.267
C5_CMD_without_CN_TS	-2869.5314	0.707461	0.760764	0.761708	0.617752	-1425.236
Norbornene_Ins_with_CN_OAc_TS	-3162.0219	0.855883	0.915885	0.91683	0.75848	-184.593
Norbornene_Ins_no_CN_OAc_TS	-3162.0108	0.855082	0.91577	0.916714	0.755537	-242.133
Norbornene_Ins_with_CN_MPAA_TS	-3369.9552	0.91192	0.975987	0.976931	0.809409	-146.811
Norbornene_Ins_no_CN_MPAA_TS	-3369.9612	0.912023	0.976113	0.977058	0.808693	-213.709

C6_CMD_with_CN_with_MPAA_TS	-3369.9263	0.908548	0.971855	0.972799	0.808906	-1217.375
C6_CMD_with_CN_with_OAc_TS	-3161.9858	0.852392	0.912238	0.913182	0.755579	-964.686
C6_CMD_without_CN_with_MPAA_TS	-3369.9557	0.908135	0.972009	0.972953	0.806081	-1146.339
C6_CMD_without_CN_with_OAc_TS	-3161.9978	0.851537	0.911815	0.91276	0.752827	-1165.361
Beta_C_elim_no_CN_OAc_TS	-3620.7563	0.980013	1.049413	1.050357	0.873205	-209.079
Beta_C_elim_with_CN_MPAA_TS	-3828.7182	1.036564	1.109813	1.110757	0.92453	-204.501
Beta_C_elim_with_CN_OAc_TS	-3620.7735	0.980156	1.049552	1.050496	0.872615	-216.119
Beta_C_elim_without_CN_MPAA_TS	-3828.7049	1.035579	1.109324	1.110268	0.922473	-207.065
Cat_3Pd	-1754.4707	0.316132	0.350767	0.351712	0.24407	
Int_1	-2305.8326	0.614953	0.658603	0.659548	0.534769	
Int_2	-2869.5384	0.713205	0.766733	0.767677	0.623288	
Int_3	-2869.549	0.713138	0.766674	0.767618	0.621448	
Int_4	-3162.0264	0.855896	0.916816	0.917761	0.755845	
Int_5	-3162.0501	0.858244	0.918262	0.919206	0.761626	
Int_6	-3162.0438	0.859058	0.918799	0.919743	0.762945	
Int_7	-3620.7787	0.982205	1.051914	1.052858	0.872689	
Int_8	-3620.7829	0.980116	1.050412	1.051356	0.870748	
MeCN	-132.70646	0.045592	0.049187	0.050131	0.022612	
Methyl-2-iodobenzoate	-470.73375	0.13335	0.143785	0.144729	0.09483	
NBE-CO2_Me	-500.42135	0.197253	0.206944	0.207888	0.161713	
Quinoline	-401.73246	0.136138	0.142786	0.14373	0.105017	
T1_conf_1	-2036.7872	0.524204	0.564401	0.565345	0.447737	
T1_conf_2	-2036.787	0.524258	0.564495	0.565439	0.448142	
T1_conf_3	-2036.7884	0.524442	0.564453	0.565397	0.44982	
T1_conf_4	-2036.7877	0.524483	0.564495	0.565439	0.449915	
T1_conf_5	-2036.783	0.524091	0.564395	0.56534	0.44714	
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T1_conf_7	-2036.7826	0.524175	0.564424	0.565369	0.44753	

E(sol)= Single-point solvation energies; ZPVE = zero-point vibrational energy; TCE = thermal correction to energy; TCH = thermal correction to enthalpy; TCG = thermal correction to Gibbs free energy.

Cartesian Coordinates

Ac-Gly-OH

C 3.298605 0.952855 -0.006715
C 1.849710 0.524035 -0.004498
O 1.019646 1.545079 -0.003457
O 1.511892 -0.661185 -0.004338
H 3.479272 1.592226 0.867442
H 3.475846 1.592272 -0.881637
N 4.168430 -0.197639 -0.007571
H 3.731995 -1.109127 -0.010600
C 5.524575 -0.035926 0.003195

O 6.038450 1.076450 0.011158
C 6.344675 -1.316639 0.004022
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H 6.997437 -1.314531 -0.874308
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C -1.849696 -0.524064 0.000522
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O -1.511850 0.661149 0.000195
H -3.476431 -1.592414 0.876779
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H -3.731948 1.109158 0.003975
C -5.524583 0.035957 0.001557
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AgI
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C 6.330762 2.069254 -0.392518
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H 8.218896 1.336410 -1.131066
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C -0.715263 -1.469303 -2.217645
H 1.269411 -0.886144 -1.637576
C -2.404164 -1.613399 -0.449023
C -1.662575 -1.177922 1.888979
H -0.847559 -0.700371 3.826135
C -2.035545 -1.724856 -1.787567
H -0.454460 -1.574422 -3.267119
H -2.660985 -1.420925 2.241192
H -2.783404 -2.020375 -2.519393
N 0.898844 -0.560036 0.954970
Pd -4.246061 -0.469822 -0.201064
H -3.232082 -2.581562 -0.044853

C -7.053782 -0.014470 0.043973
O -8.155900 0.501511 0.086776
O -5.928977 0.656292 -0.068007
N -5.532928 -1.980786 0.082680
C -5.168504 -3.227826 0.297813
C -6.208173 -4.293667 0.578763
H -5.718002 -5.265773 0.635302
H -6.717124 -4.089571 1.527820
H -6.972121 -4.310583 -0.205488
O -3.943742 -3.601700 0.286041
C -6.929049 -1.549004 0.122000
H -7.424884 -1.870682 1.046001
H -7.498767 -1.969524 -0.717100

C5_CMD_without_CN_TS

Pd 2.797750 0.431934 0.452641
C 4.310731 2.822395 0.186003
C 5.506743 0.826631 -0.277274
C 5.441335 3.594829 -0.060717
C 6.668215 1.547550 -0.540334
H 5.364747 4.672579 0.031541
H 7.561916 1.004356 -0.826998
N 4.399392 1.491519 0.069463
H 7.521353 3.525174 -0.622191
C 6.626430 2.942115 -0.424176
N 4.106514 -1.088765 0.009755
N 2.031361 2.347930 0.694704
C 5.356380 -0.682950 -0.365352
C 2.930657 3.355838 0.539116
O 6.301720 -1.377845 -0.729554
O 2.732283 4.568958 0.610130
C 3.700590 -2.422900 -0.121361
C 3.626077 -3.041009 -1.386950
C 3.218851 -3.124276 1.003478
C 3.149464 -4.350844 -1.518377
C 2.714324 -4.424086 0.872645
C 2.699626 -5.026701 -0.385220
H 3.107575 -4.833380 -2.487553
H 2.349525 -4.970197 1.733900
H 2.321977 -6.040528 -0.484403
C 0.657801 2.564560 0.912182
C -0.264935 2.502219 -0.157132
C 0.169354 2.633278 2.220082
C -1.645320 2.437061 0.138238
C -1.186578 2.643279 2.515927
C -2.092480 2.527217 1.467042
H -1.509925 2.701131 3.549632
H -3.156826 2.477533 1.674372
O 3.985015 -2.247005 -2.436051
O 3.272484 -2.438049 2.183300
C 4.154836 -2.848103 -3.708718
H 4.878401 -3.672109 -3.667451
H 3.203633 -3.222733 -4.114055
H 4.537917 -2.061717 -4.361655
C 2.734733 -3.052783 3.340696
H 2.870893 -2.333165 4.150707
H 1.663130 -3.268242 3.221371
H 3.263766 -3.981411 3.593007
C -2.652132 2.163349 -0.920761
C -2.518612 0.989118 -1.707992
C -3.763026 2.985144 -1.168132
C -3.439513 0.680377 -2.727079
H -1.602464 0.421083 -1.617539
C -4.697379 2.656572 -2.176171
C -4.535893 1.524417 -2.957883
H -3.261312 -0.179922 -3.365377
H -5.547541 3.312337 -2.330723
H -5.258991 1.286891 -3.730774
C 0.273285 2.598886 -1.569853
H 1.222229 2.057008 -1.633181
H -0.406422 2.137453 -2.288881
C 0.490230 4.072723 -1.971817
H -0.462781 4.614475 -1.966275
H 1.167576 4.573235 -1.274498
H 0.913290 4.134687 -2.981406
F 1.057761 2.626993 3.236654
C -3.962405 4.195220 -0.423883
N -4.144051 5.187491 0.154269
C 0.195666 -1.166039 0.020316
C 0.646135 -0.507666 2.212637
C 0.639303 -1.366541 -1.313459
C -1.138380 -1.531391 0.373662
C -0.620355 -0.934026 2.656687
H 1.344200 -0.041300 2.898601
C -0.216073 -1.911494 -2.250786
H 1.659954 -1.105295 -1.573538
C -2.058826 -1.979309 -0.636930
C -1.518486 -1.417713 1.735215
H -0.876446 -0.832129 3.705420
C -1.560589 -2.197579 -1.918834
H 0.145319 -2.094743 -3.258769
H -2.521536 -1.710320 2.028102
H -2.227828 -2.573406 -2.691215
N 1.040892 -0.608232 0.950330
Pd -3.870289 -0.734983 -0.509461
H -2.955145 -2.899637 -0.173365
C -6.398438 0.086810 0.549766
O -7.380302 0.744843 0.834649
O -5.421625 0.524687 -0.217616
N -5.005506 -1.966101 0.626468
C -4.723801 -3.235754 0.826288
C -5.679954 -4.123215 1.595901
H -5.222615 -5.102093 1.740492
H -5.928349 -3.683422 2.567355
H -6.616744 -4.240716 1.039317
O -3.647315 -3.782936 0.394790
C -6.247139 -1.347082 1.089869
H -6.280540 -1.294981 2.185877
H -7.125987 -1.916065 0.762510

C6_CMD_with_CN_with_MPAA_TS

Pd 3.638022 -0.539706 0.422506
C 5.839268 1.034724 -0.423605
C 5.696064 -1.113678 -1.426135
C 7.021657 1.308699 -1.104262
C 6.868809 -0.889923 -2.142934
H 7.494841 2.273801 -0.961190
H 7.216675 -1.659189 -2.823528
N 5.253216 -0.154694 -0.606301
H 8.455280 0.522042 -2.508667
C 7.535913 0.327965 -1.963351
N 3.764611 -2.293365 -0.641724
N 3.898471 1.473448 0.906597
C 4.780847 -2.325851 -1.552641
C 5.059541 2.015559 0.441015
O 4.997178 -3.167720 -2.420541
O 5.484229 3.161213 0.602160
C 2.606933 -3.079557 -0.797222

C	1.631506	-2.728618	-1.759354
C	2.302736	-4.090208	0.134545
C	0.398814	-3.393331	-1.806740
C	1.076444	-4.767053	0.084416
C	0.142354	-4.409175	-0.887819
H	-0.366314	-3.101201	-2.515734
H	0.842907	-5.552869	0.792195
H	-0.811853	-4.927353	-0.926218
C	2.822953	2.244703	1.374365
C	2.087365	3.136996	0.550608
C	2.319067	1.957625	2.653163
C	0.926085	3.749445	1.078155
C	1.149033	2.506438	3.148923
C	0.457873	3.421288	2.356298
H	0.808517	2.230423	4.141117
H	-0.439622	3.899228	2.738087
O	1.960615	-1.682266	-2.565124
O	3.260629	-4.311670	1.084212
C	1.052437	-1.323744	-3.602172
H	0.922462	-2.149847	-4.313549
H	0.070992	-1.029772	-3.211189
H	1.513062	-0.475760	-4.112879
C	3.027575	-5.329106	2.040767
H	3.912148	-5.345917	2.680974
H	2.139882	-5.113530	2.652682
H	2.905634	-6.312523	1.566908
C	0.230098	4.848682	0.337664
C	0.829594	6.116899	0.319169
C	-1.026476	4.720996	-0.298686
C	0.231898	7.205854	-0.313337
H	1.782394	6.237441	0.824087
C	-1.631864	5.820710	-0.942022
C	-1.002106	7.058409	-0.952294
H	0.728928	8.171742	-0.303617
H	-2.593673	5.684773	-1.426530
H	-1.471730	7.901742	-1.449251
C	2.456473	3.306556	-0.913394
H	2.960253	2.387909	-1.235500
H	1.527543	3.368539	-1.495158
C	3.351279	4.508574	-1.274041
H	2.805676	5.451437	-1.181533
H	4.232707	4.542195	-0.631851
H	3.684156	4.420833	-2.315169
F	2.987637	1.067287	3.418385
C	-1.765120	3.494835	-0.330029
N	-2.463512	2.571633	-0.424193
C	0.723326	-0.878705	0.958777
C	2.062710	-1.838209	2.616568
C	0.642142	-0.014995	-0.163096
C	-0.447658	-1.515711	1.477528
C	0.954097	-2.461839	3.214229
H	3.062755	-1.958235	3.015394
C	-0.564665	0.192765	-0.758342
H	1.548232	0.446268	-0.536300
C	-1.692439	-1.323189	0.799788
C	-0.288798	-2.317566	2.633868
H	1.095607	-3.059882	4.108015
C	-1.746861	-0.483027	-0.322865
H	-0.644893	0.846556	-1.620742
H	-1.148546	-2.820870	3.062851
H	-2.329826	-0.749566	-1.481808
N	1.949588	-1.094005	1.523690
Pd	-3.542798	0.599782	-0.151452
C	-5.669393	-3.200998	0.897138
C	-4.987306	-2.195373	-0.076379
C	-3.241090	-3.387348	0.748718
C	-4.453630	-3.968584	1.516222
H	-6.300779	-2.710884	1.639263
H	-6.309266	-3.880135	0.321744
H	-4.369572	-3.814242	2.598762
H	-4.535105	-5.048022	1.348363
C	-3.859081	-3.094170	-0.632841
H	-3.177297	-2.604314	-1.323941
H	-4.253682	-3.996857	-1.115548
C	-4.215879	-1.155025	0.768834
C	-2.973240	-1.952363	1.286966
H	-5.673219	-1.753684	-0.800893
H	-2.348973	-4.019592	0.754692
H	-2.975719	-1.950000	2.380773
C	-5.045235	-0.460597	1.806458
O	-6.246418	-0.266981	1.729301
O	-4.308015	-0.017417	2.865037
C	-5.034439	0.758100	3.826897
H	-5.855979	0.176561	4.255896
H	-4.309399	1.025134	4.597032
H	-5.446867	1.657686	3.359636
C	-6.310688	1.228488	-1.453926
O	-7.622510	1.485094	-1.574330
O	-5.702048	1.534812	-0.438877
N	-4.344411	0.335562	-2.575731
C	-3.775440	-0.724443	-3.077973
C	-4.476143	-1.745658	-3.964958
H	-3.724831	-2.314949	-4.515838
H	-5.044077	-2.451157	-3.344250
H	-5.170275	-1.281350	-4.672688
O	-2.536919	-1.004332	-2.784032
C	-5.756701	0.544138	-2.698835
H	-6.371273	-0.363112	-2.832341
H	-6.017060	1.205231	-3.542170
H	-7.913368	1.867823	-0.724101

C6_CMD_with_CN_with_OAc_TS

Pd	-3.219051	-0.677599	-0.567476
C	-5.534451	0.802526	0.133310
C	-5.365248	-1.339050	1.145947
C	-6.769614	1.024370	0.734659
C	-6.590538	-1.166659	1.784728
H	-7.273753	1.968247	0.559391
H	-6.948483	-1.950712	2.442853
N	-4.911131	-0.360971	0.355219
H	-8.256742	0.175272	2.043757
C	-7.296288	0.021497	1.559913
N	-3.338035	-2.434836	0.490930
N	-3.527453	1.330704	-1.059797
C	-4.408754	-2.510206	1.334932
C	-4.743036	1.817625	-0.679067
O	-4.642778	-3.359580	2.190505
O	-5.208469	2.941666	-0.874662
C	-2.159744	-3.168801	0.728384
C	-1.259805	-2.763381	1.741808
C	-1.759632	-4.182674	-0.162744
C	-0.008066	-3.378607	1.878044
C	-0.513876	-4.809689	-0.023740
C	0.343585	-4.399599	0.997102
H	0.697336	-3.048365	2.630933
H	-0.206945	-5.597417	-0.700611
H	1.311690	-4.881388	1.104808
C	-2.460440	2.154313	-1.451712

C	-1.830102	3.082766	-0.580843
C	-1.852323	1.891924	-2.689911
C	-0.666778	3.753564	-1.027733
C	-0.679277	2.499248	-3.103855
C	-0.093478	3.448871	-2.268497
H	-0.256786	2.241225	-4.069047
H	0.802470	3.972832	-2.588700
O	-1.677227	-1.717793	2.506251
O	-2.645797	-4.457800	-1.166495
C	-0.858959	-1.320529	3.603564
H	-0.755012	-2.136987	4.329989
H	0.138800	-0.995252	3.284627
H	-1.385028	-0.485684	4.070958
C	-2.322556	-5.494359	-2.075370
H	-3.165970	-5.560217	-2.765897
H	-1.407021	-5.267503	-2.640832
H	-2.197419	-6.458381	-1.564245
C	-0.082184	4.888263	-0.245483
C	-0.763637	6.114452	-0.249777
C	1.148040	4.839027	0.451659
C	-0.271797	7.233955	0.419589
H	-1.694705	6.178202	-0.803176
C	1.646848	5.969720	1.132130
C	0.935525	7.162430	1.119530
H	-0.830494	8.165103	0.390309
H	2.590949	5.893383	1.662320
H	1.322560	8.029909	1.645102
C	-2.304231	3.226826	0.855770
H	-2.770089	2.277607	1.145289
H	-1.420594	3.344062	1.496521
C	-3.293184	4.369458	1.159914
H	-2.800126	5.344028	1.114132
H	-4.127527	4.358572	0.457072
H	-3.692768	4.249734	2.173994
F	-2.417838	0.967591	-3.496334
C	1.966363	3.666334	0.505724
N	2.721172	2.790390	0.617074
C	-0.266771	-0.885643	-0.901717
C	-1.437502	-1.947838	-2.623042
C	-0.311131	0.007869	0.197311
C	0.967260	-1.480985	-1.315423
C	-0.261611	-2.540312	-3.116823
H	-2.398621	-2.124145	-3.090879
C	0.836594	0.289049	0.874012
H	-1.263635	0.430953	0.490301
C	2.151015	-1.198573	-0.564755
C	0.927004	-2.325841	-2.452137
H	-0.311709	-3.171565	-3.997435
C	2.078435	-0.322767	0.530968
H	0.821542	0.960379	1.726210
H	1.835389	-2.807258	-2.798526
H	2.657118	-0.500856	1.657091
N	-1.438102	-1.171437	-1.547777
Pd	3.825238	0.892050	0.376731
O	4.596620	0.541982	2.859702
O	2.735063	-0.719533	3.040751
C	3.782568	-0.130062	3.521323
C	3.993327	-0.329176	5.018483
H	4.190438	-1.388634	5.219313
H	4.833184	0.272730	5.371789
H	3.081297	-0.061475	5.562506
C	6.288294	-2.658507	-0.407120
C	5.462094	-1.716099	0.516562
C	3.890481	-3.123985	-0.334954
C	5.195694	-3.598659	-1.022718
H	6.861796	-2.122878	-1.170298
H	7.004328	-3.224526	0.198699
H	5.144436	-3.515571	-2.114280
H	5.395839	-4.648380	-0.782954
C	4.410847	-2.710257	1.056971
H	3.662225	-2.262031	1.707442
H	4.878629	-3.545509	1.592021
C	4.618702	-0.817293	-0.414514
C	3.504344	-1.752644	-0.959770
H	6.043138	-1.161425	1.253756
H	3.073148	-3.850057	-0.351606
H	3.569019	-1.801332	-2.050733
C	5.379067	0.038769	-1.367692
O	5.933828	1.070100	-0.968051
O	5.375315	-0.326883	-2.657337
C	6.024227	0.583742	-3.569256
H	7.078524	0.699877	-3.305593
H	5.919403	0.129987	-4.554810
H	5.536732	1.561730	-3.537232

C6_CMD_without_CN_with_MPAA_TS

Pd	3.586518	-0.166353	0.228969
C	5.504460	1.210929	-1.334530
C	5.537031	-1.155297	-1.560816
C	6.548805	1.343585	-2.244408
C	6.581281	-1.081950	-2.478726
H	6.894773	2.339097	-2.499832
H	6.950918	-2.001211	-2.919559
N	5.073075	-0.019161	-1.027884
H	7.908559	0.260376	-3.518436
C	7.092443	0.180268	-2.805819
N	3.834800	-2.158824	-0.212301
N	3.746528	1.886553	0.130807
C	4.783534	-2.418641	-1.157873
C	4.708606	2.352716	-0.710588
O	5.057197	-3.492667	-1.687707
O	4.949029	3.518267	-1.026188
C	2.820827	-3.071053	0.119182
C	1.807280	-3.397512	-0.808164
C	2.667626	-3.486849	1.457895
C	0.685195	-4.139555	-0.415849
C	1.548050	-4.227668	1.856733
C	0.570165	-4.543516	0.912935
H	-0.114079	-4.353870	-1.114955
H	1.428399	-4.548813	2.884143
H	-0.304517	-5.110269	1.221010
C	2.714274	2.674967	0.673161
C	1.549911	2.999838	-0.060986
C	2.736796	2.941608	2.047136
C	0.454730	3.577841	0.617335
C	1.684327	3.547194	2.713936
C	0.539834	3.864344	1.986906
H	1.764280	3.742453	3.777936
H	-0.304052	4.329569	2.487642
O	1.974615	-2.875065	-2.055331
O	3.650067	-3.067528	2.311533
C	1.055878	-3.258481	-3.068525
H	1.070691	-4.345297	-3.225752
H	0.030965	-2.947029	-2.830793
H	1.394491	-2.757875	-3.978159
C	3.580082	-3.480995	3.664244
H	4.464889	-3.064301	4.149953
H	2.677578	-3.094120	4.159118

H	3.598137	-4.575275	3.756100
C	-0.844693	3.832387	-0.074081
C	-1.648127	2.757094	-0.478485
C	-1.332776	5.139904	-0.292449
C	-2.883174	2.964058	-1.090366
H	-1.304703	1.747313	-0.287236
C	-2.583156	5.349069	-0.903367
C	-3.354648	4.262609	-1.304092
H	-3.489960	2.105926	-1.369425
H	-2.933515	6.364829	-1.057173
H	-4.322232	4.427629	-1.769034
C	1.516594	2.762722	-1.555225
H	2.221610	1.965727	-1.810013
H	0.524164	2.417715	-1.860948
C	1.882557	4.039862	-2.335730
H	1.172165	4.845156	-2.116870
H	2.884825	4.376311	-2.057224
H	1.862091	3.849765	-3.415480
F	3.814350	2.543622	2.760382
C	-0.561974	6.283600	0.104543
N	0.032714	7.232985	0.417444
C	0.703478	-0.582765	1.011090
C	2.139412	-0.361002	2.841366
C	0.518607	-0.499588	-0.391617
C	-0.402302	-0.887492	1.864924
C	1.102849	-0.647929	3.749220
H	3.141720	-0.133642	3.185552
C	-0.709689	-0.768392	-0.926283
H	1.368393	-0.255329	-1.018555
C	-1.687244	-1.134155	1.287053
C	-0.155777	-0.918168	3.261393
H	1.311865	-0.652133	4.813422
C	-1.827537	-1.138382	-0.112220
H	-0.848738	-0.743417	-2.001748
H	-0.961103	-1.158851	3.946538
H	-2.342968	-2.108561	-0.845275
N	1.951316	-0.349557	1.529194
Pd	-3.764764	-0.583864	-0.687629
C	-5.632790	-1.585741	3.108648
C	-5.271263	-1.578425	1.593323
C	-3.481678	-2.586843	2.561990
C	-4.422396	-2.333088	3.764157
H	-5.775989	-0.572347	3.493989
H	-6.570088	-2.129361	3.269893
H	-3.941802	-1.747229	4.556259
H	-4.737535	-3.284058	4.207616
C	-4.513441	-2.921628	1.461998
H	-4.074268	-3.095840	0.475876
H	-5.132987	-3.787063	1.726235
C	-4.132969	-0.565923	1.363753
C	-2.928433	-1.190868	2.130496
H	-6.136326	-1.427493	0.943889
H	-2.700761	-3.331271	2.741821
H	-2.745210	-0.597654	3.030631
C	-4.437177	0.863328	1.636232
O	-5.530838	1.385781	1.498052
O	-3.337602	1.557073	2.042414
C	-3.551339	2.949378	2.318564
H	-4.267185	3.071548	3.137111
H	-2.572967	3.340910	2.598326
H	-3.925776	3.467118	1.433049
C	-5.621295	0.062758	-2.979589
O	-6.554213	0.540565	-3.806453
O	-5.719140	0.171016	-1.762036
N	-3.565600	-1.191311	-2.765685
C	-3.047866	-2.395804	-2.927010
C	-3.182121	-3.175365	-4.225385
H	-2.534622	-4.051786	-4.182053
H	-4.215744	-3.515939	-4.363621
H	-2.910937	-2.564150	-5.092562
O	-2.392087	-2.970768	-1.986254
C	-4.456924	-0.582695	-3.719401
H	-4.883880	-1.268094	-4.463881
H	-3.969361	0.225512	-4.288356
H	-7.248104	0.958804	-3.259240

C6_CMD_without_CN_with_OAc_TS

Pd	3.248961	-0.292201	0.404424
C	5.479083	0.812497	-0.946513
C	5.283617	-1.552668	-1.096587
C	6.631810	0.797805	-1.725458
C	6.431355	-1.626379	-1.881249
H	7.112004	1.740309	-1.964412
H	6.752327	-2.597183	-2.242560
N	4.883808	-0.352705	-0.660606
H	8.007340	-0.473075	-2.792464
C	7.109106	-0.438256	-2.182411
N	3.339737	-2.317640	0.068881
N	3.650053	1.723285	0.282046
C	4.367812	-2.717652	-0.734414
C	4.749448	2.055817	-0.445868
O	4.602606	-3.842674	-1.167716
O	5.153408	3.177777	-0.750383
C	2.231999	-3.130046	0.354697
C	1.307645	-3.483909	-0.652390
C	1.902721	-3.407167	1.698268
C	0.101943	-4.121700	-0.329215
C	0.697391	-4.039402	2.027973
C	-0.187753	-4.389420	1.007300
H	-0.626330	-4.357347	-1.095626
H	0.443744	-4.254994	3.058719
H	-1.126949	-4.874995	1.259238
C	2.664162	2.627280	0.719511
C	1.563026	2.974657	-0.097138
C	2.633744	2.981317	2.072533
C	0.463235	3.638491	0.486991
C	1.580977	3.679559	2.643859
C	0.489570	4.000893	1.840917
H	1.617275	3.936943	3.697073
H	-0.360232	4.523918	2.269302
O	1.643426	-3.087377	-1.911180
O	2.812771	-2.969033	2.620120
C	0.817247	-3.509839	-2.987516
H	0.783666	-4.605128	-3.055423
H	-0.206652	-3.128624	-2.889313
H	1.280064	-3.105720	-3.890240
C	2.570349	-3.251941	3.986428
H	3.427476	-2.850192	4.530776
H	1.652012	-2.764277	4.344850
H	2.498217	-4.332103	4.170979
C	-0.779160	3.905724	-0.298001
C	-1.622665	2.845435	-0.660499
C	-1.156646	5.211172	-0.681566
C	-2.783550	3.063385	-1.400621
H	-1.352914	1.836959	-0.365905
C	-2.336049	5.433447	-1.416323
C	-3.143309	4.360503	-1.781217
H	-3.409731	2.220069	-1.680038

H	-2.598408	6.447039	-1.702652
H	-4.045878	4.531206	-2.360784
C	1.610308	2.667060	-1.577684
H	2.231181	1.781485	-1.744640
H	0.609569	2.430703	-1.950618
C	2.191667	3.853984	-2.371185
H	1.575082	4.749978	-2.236092
H	3.205227	4.078912	-2.026993
H	2.226468	3.620073	-3.441734
F	3.646461	2.568782	2.867520
C	-0.335895	6.336840	-0.336435
N	0.303387	7.270787	-0.068502
C	0.261492	-0.436525	0.853161
C	1.490203	-0.093374	2.810141
C	0.240060	-0.496695	-0.561710
C	-0.954463	-0.567874	1.593070
C	0.335055	-0.195700	3.609702
H	2.461057	0.108983	3.248288
C	-0.936806	-0.747410	-1.212514
H	1.169979	-0.373252	-1.104540
C	-2.175388	-0.819626	0.894784
C	-0.875863	-0.441422	3.004877
H	0.419450	-0.080735	4.684804
C	-2.153535	-0.976727	-0.501924
H	-0.949545	-0.815944	-2.294053
H	-1.771501	-0.541404	3.608264
H	-2.699997	-1.955728	-1.228015
N	1.456659	-0.228816	1.492858
Pd	-4.036199	-0.500907	-1.321696
O	-3.517282	-1.088396	-3.378786
O	-2.676692	-2.902986	-2.327529
C	-3.034435	-2.262231	-3.375076
C	-2.807108	-2.942614	-4.710398
H	-2.939060	-4.022677	-4.613440
H	-3.476914	-2.534574	-5.469529
H	-1.772532	-2.755678	-5.023633
C	-6.288411	-1.488847	2.224870
C	-5.632156	-1.673132	0.822933
C	-3.943038	-2.146293	2.262101
C	-5.124095	-1.836532	3.211692
H	-6.681241	-0.477658	2.371660
H	-7.127641	-2.183772	2.334718
H	-4.899057	-1.015220	3.901036
H	-5.369008	-2.715289	3.817419
C	-4.669467	-2.849774	1.094616
H	-4.023450	-3.100601	0.249498
H	-5.194428	-3.756762	1.414851
C	-4.645178	-0.503485	0.626644
C	-3.496409	-0.797217	1.619456
H	-6.356701	-1.790504	0.013376
H	-3.118639	-2.699021	2.720735
H	-3.465358	-0.010125	2.379916
C	-5.229349	0.844842	0.467950
O	-5.919786	1.093293	-0.531695
O	-4.911351	1.755717	1.391200
C	-5.387190	3.101692	1.159337
H	-6.471531	3.101654	1.025960
H	-5.103898	3.662202	2.049894
H	-4.904716	3.519914	0.273830

Beta_C_elim_no_CN_OAc_TS

Pd	-3.599644	-0.081727	-0.507199
C	-5.790874	1.539206	0.288733
C	-6.156761	-0.798964	0.469008
C	-7.076403	1.807019	0.751367
C	-7.449775	-0.592250	0.940035
H	-7.390582	2.840653	0.844589
H	-8.058367	-1.455822	1.184764
N	-5.401498	0.265244	0.170743
H	-8.910827	0.911182	1.442207
C	-7.904493	0.725614	1.077341
N	-4.235241	-2.009653	-0.255065
N	-3.567716	2.005140	-0.448572
C	-5.484266	-2.148941	0.259609
C	-4.746960	2.579947	-0.089927
O	-6.086556	-3.191986	0.520530
O	-5.031467	3.778408	-0.032808
C	-3.322715	-3.069633	-0.405751
C	-2.521443	-3.476491	0.684940
C	-3.010489	-3.554698	-1.685830
C	-1.433985	-4.334424	0.487474
C	-1.934028	-4.421351	-1.887499
C	-1.147609	-4.795443	-0.800587
H	-0.775135	-4.596193	1.305913
H	-1.721383	-4.762644	-2.895387
H	-0.294570	-5.452092	-0.949437
C	-2.411958	2.740198	-0.778660
C	-1.637405	3.471926	0.155008
C	-1.925018	2.598646	-2.085229
C	-0.380584	3.973292	-0.258242
C	-0.688249	3.064270	-2.492260
C	0.085088	3.751022	-1.562971
H	-0.352887	2.885015	-3.507914
H	1.069327	4.112369	-1.841022
O	-2.852393	-2.916203	1.885160
O	-3.707247	-3.093675	-2.779692
C	-2.088824	-3.282967	3.022692
H	-2.169316	-4.360405	3.226300
H	-1.031937	-3.018909	2.899377
H	-2.514521	-2.725284	3.859544
C	-5.039021	-3.607977	-2.903262
H	-5.543706	-2.985962	-3.646758
H	-5.012862	-4.648942	-3.255578
H	-5.582562	-3.567796	-1.954307
C	0.498131	4.819417	0.604370
C	0.769877	6.131374	0.184794
C	1.144536	4.370453	1.777683
C	1.633457	6.968600	0.889761
H	0.279792	6.491777	-0.714490
C	2.013063	5.215121	2.492860
C	2.259997	6.510864	2.051246
H	1.813745	7.979156	0.533766
H	2.492256	4.837163	3.390676
H	2.932208	7.156363	2.608684
C	-2.189672	3.758714	1.536379
H	-2.991628	3.049727	1.755832
H	-1.422759	3.589640	2.295373
C	-2.728185	5.196485	1.659750
H	-1.931034	5.928984	1.489263
H	-3.526269	5.359154	0.932418
H	-3.132815	5.365278	2.664759
F	-2.690173	1.934479	-2.985131
C	0.954214	3.050686	2.300075
N	0.817354	2.020551	2.821807
C	3.890337	2.882199	-0.712612
C	4.133250	4.370244	-0.732936
H	3.595094	4.804900	-1.583887
H	3.737819	4.827789	0.177106

H	5.197697	4.586090	-0.849448
O	4.728904	2.087816	-1.260924
C	-0.600320	-0.602769	-0.473427
C	-1.567204	-0.618042	-2.603060
C	-0.785806	-0.614792	0.927604
C	0.717486	-0.715263	-1.016170
C	-0.309606	-0.739939	-3.212173
H	-2.478505	-0.600079	-3.185611
C	0.296958	-0.746452	1.750358
H	-1.791352	-0.550054	1.327822
C	1.850350	-0.783295	-0.122735
C	0.824102	-0.753280	-2.429688
H	-0.242504	-0.807796	-4.292452
C	1.628608	-0.829188	1.255062
H	0.157894	-0.735085	2.824997
H	1.794069	-0.815878	-2.908055
N	-1.700565	-0.507566	-1.287499
Pd	3.493576	0.374385	-0.784962
C	5.860077	-3.309223	-1.375118
C	5.673101	-1.863809	-0.815249
C	3.902824	-2.968975	0.076002
C	4.621114	-4.061282	-0.792526
H	5.904731	-3.333632	-2.468113
H	6.797816	-3.732522	-0.999499
H	3.967395	-4.473736	-1.567979
H	4.920366	-4.890680	-0.143633
C	5.125214	-2.176528	0.586714
H	4.876343	-1.288554	1.162653
H	5.805864	-2.800903	1.175673
C	4.428147	-1.334243	-1.538740
C	3.301604	-2.047071	-0.969895
H	6.551164	-1.223524	-0.887975
H	3.193356	-3.364369	0.796944
H	2.535190	-2.445736	-1.623402
C	2.689614	-0.807153	2.305863
C	2.867738	-1.846296	3.250364
C	3.467232	0.353567	2.439100
C	3.857513	-1.726995	4.240534
C	4.449097	0.457683	3.423120
H	3.273776	1.189347	1.778049
C	4.658680	-0.592051	4.318039
H	3.994496	-2.538834	4.945220
H	5.042954	1.365027	3.491830
H	5.426443	-0.521597	5.083103
C	2.040893	-3.086644	3.203201
O	1.414981	-3.490161	2.236472
O	2.052247	-3.753596	4.378887
C	1.313170	-4.985731	4.395532
H	1.473971	-5.407731	5.387834
H	0.249086	-4.797470	4.227320
H	1.678035	-5.665634	3.620500
O	2.834508	2.421040	-0.173978
C	4.511102	-1.039806	-2.999129
O	3.605876	-1.152462	-3.810093
O	5.744238	-0.614485	-3.329933
C	5.914069	-0.214730	-4.700281
H	6.956066	0.093576	-4.785478
H	5.698659	-1.048695	-5.374213
H	5.245591	0.618081	-4.935152

Beta_C_elim_with_CN_MPAA_TS

Pd	-3.907243	0.128796	-0.140189
C	-6.120514	1.328158	1.192756
C	-6.643498	-0.611615	-0.061282
C	-7.450568	1.481831	1.572797
C	-7.989122	-0.506535	0.278886
H	-7.713729	2.312948	2.217550
H	-8.680071	-1.247639	-0.107299
N	-5.783570	0.300248	0.407252
H	-9.431094	0.651434	1.386466
C	-8.386560	0.551396	1.105183
N	-4.686590	-1.545614	-1.053599
N	-3.792118	1.865525	1.026913
C	-6.034361	-1.688799	-0.939647
C	-4.972797	2.226452	1.609885
O	-6.755054	-2.562751	-1.427036
O	-5.172184	3.168170	2.377978
C	-3.925948	-2.383733	-1.882308
C	-2.851123	-3.125668	-1.331230
C	-4.099750	-2.386093	-3.276885
C	-2.002043	-3.862956	-2.162848
C	-3.258948	-3.137280	-4.106651
C	-2.217862	-3.868447	-3.544177
H	-1.177899	-4.429471	-1.746551
H	-3.410786	-3.110419	-5.181043
H	-1.553578	-4.443537	-4.183496
C	-2.601900	2.472883	1.471311
C	-1.824560	3.294134	0.628581
C	-2.113529	2.167402	2.747713
C	-0.579569	3.766661	1.098341
C	-0.890483	2.616038	3.215846
C	-0.119742	3.415184	2.377137
H	-0.555321	2.327892	4.206280
H	0.839131	3.791270	2.721699
O	-2.708501	-3.037886	0.020453
O	-5.057958	-1.556455	-3.804747
C	-1.592586	-3.680011	0.625561
H	-1.632942	-4.768529	0.487174
H	-0.643762	-3.294994	0.231648
H	-1.639704	-3.443722	1.687039
C	-6.133648	-2.215311	-4.482112
H	-6.811543	-1.424171	-4.811475
H	-5.777314	-2.770364	-5.360763
H	-6.654847	-2.885845	-3.793135
C	0.252181	4.718466	0.308251
C	-0.195397	6.027779	0.089437
C	1.535887	4.379012	-0.179649
C	0.593162	6.964196	-0.577870
H	-1.169884	6.310071	0.473278
C	2.344383	5.325162	-0.840413
C	1.866712	6.615999	-1.036738
H	0.217586	7.972848	-0.726582
H	3.328811	5.030081	-1.187035
H	2.487506	7.349095	-1.543221
C	-2.356514	3.618513	-0.750999
H	-1.544984	3.982087	-1.389862
F	-2.837128	1.330370	3.522809
C	2.039266	3.044656	-0.058723
N	2.490346	1.976591	-0.027778
C	5.010222	2.862190	-2.521294
O	4.814031	3.175640	-3.826155
O	4.975045	3.693113	-1.638415
N	5.128594	0.879781	-1.022884
C	6.058964	1.014859	-0.054706
C	7.392520	1.677143	-0.407049
H	8.009389	1.700083	0.492517
H	7.925145	1.116397	-1.186129
H	7.239557	2.699174	-0.768472

O	5.864638	0.603664	1.102833
C	5.298683	1.374465	-2.356531
H	4.622015	0.848324	-3.037710
H	6.310846	1.211410	-2.761352
H	4.678894	4.141204	-3.865905
H	-2.728330	2.692801	-1.203707
C	-3.501912	4.647538	-0.728108
H	-4.290361	4.339644	-0.036275
H	-3.144499	5.631435	-0.405210
H	-3.937684	4.758898	-1.727727
C	-0.906329	-0.389051	-0.022909
C	-1.769973	-0.065132	-2.171685
C	-1.134636	-0.464727	1.369310
C	0.408531	-0.619832	-0.535157
C	-0.517421	-0.304667	-2.755285
H	-2.645046	0.135782	-2.780189
C	-0.082451	-0.688296	2.210819
H	-2.138778	-0.331464	1.753083
C	1.507806	-0.853310	0.370612
C	0.563020	-0.580097	-1.944906
H	-0.418331	-0.286172	-3.834797
C	1.250490	-0.871877	1.744107
H	-0.257263	-0.699700	3.282160
H	1.529030	-0.782520	-2.393651
N	-1.957389	-0.104932	-0.856705
Pd	3.352526	0.019484	-0.369681
C	5.106063	-4.041819	-0.666670
C	5.157096	-2.549753	-0.219925
C	3.214030	-3.269267	0.702743
C	3.745456	-4.526022	-0.071015
H	5.169244	-4.162272	-1.751820
H	5.948355	-4.587414	-0.227596
H	3.042338	-4.874149	-0.835898
H	3.882899	-5.347817	0.639429
C	4.547700	-2.654115	1.183778
H	4.467286	-1.685986	1.668896
H	5.103542	-3.336232	1.836445
C	4.030831	-1.859758	-1.000082
C	2.783773	-2.329518	-0.412602
H	6.126279	-2.062914	-0.304172
H	2.443486	-3.495866	1.433953
H	1.977035	-2.636108	-1.069344
C	2.286843	-0.953744	2.815399
C	2.263969	-1.937771	3.836148
C	3.266077	0.045690	2.883075
C	3.231933	-1.910147	4.852133
C	4.243755	0.045511	3.877533
H	3.287990	0.822029	2.130402
C	4.228087	-0.936041	4.866792
H	3.206558	-2.675477	5.619398
H	5.022634	0.799885	3.846139
H	4.985699	-0.948214	5.645040
C	1.264650	-3.044813	3.828968
O	0.680024	-3.473866	2.847455
O	1.065864	-3.560452	5.062461
C	0.147078	-4.663569	5.124363
H	0.121066	-4.962190	6.172632
H	-0.846167	-4.353635	4.787328
H	0.492147	-5.488511	4.494451
C	4.157767	-1.721324	-2.476451
O	3.244551	-1.563661	-3.274062
O	5.448265	-1.789500	-2.869332
C	5.673386	-1.689437	-4.284172
H	5.351823	-0.713552	-4.658596
H	6.748778	-1.812995	-4.415528
H	5.125843	-2.471152	-4.817908

Beta_C_elim_with_CN_OAc_TS

Pd	-3.671483	-0.067073	-0.003950
C	-5.896662	0.980220	1.430866
C	-6.306502	-1.066297	0.310097
C	-7.203915	1.019874	1.906769
C	-7.627178	-1.078133	0.749596
H	-7.504711	1.854140	2.530661
H	-8.264588	-1.903449	0.452343
N	-5.514158	-0.049346	0.668275
H	-9.095683	-0.013563	1.914271
C	-8.069947	-0.023286	1.556603
N	-4.337746	-1.854711	-0.780319
N	-3.658288	1.739277	1.051639
C	-5.653656	-2.121795	-0.563874
C	-4.823806	2.016811	1.705136
O	-6.314750	-3.084107	-0.960616
O	-5.067250	2.985395	2.425403
C	-3.552144	-2.652288	-1.625469
C	-2.378058	-3.261836	-1.116651
C	-3.809801	-2.734858	-3.004353
C	-1.514471	-3.955141	-1.970708
C	-2.951429	-3.440120	-3.856254
C	-1.812783	-4.044447	-3.333806
H	-0.616259	-4.423387	-1.586804
H	-3.170417	-3.476997	-4.918679
H	-1.136378	-4.583577	-3.991439
C	-2.515812	2.515526	1.320738
C	-1.927681	3.331773	0.331485
C	-1.874390	2.389085	2.558670
C	-0.702379	3.973497	0.618659
C	-0.676336	3.017545	2.854160
C	-0.088641	3.806488	1.870553
H	-0.217742	2.870619	3.825927
H	0.849733	4.312898	2.077112
O	-2.162533	-3.094370	0.217477
O	-4.876870	-2.028574	-3.502175
C	-0.968946	-3.622468	0.782303
H	-0.931636	-4.715947	0.689354
H	-0.074817	-3.185477	0.320822
H	-0.977504	-3.343651	1.834203
C	-5.925601	-2.822840	-4.067921
H	-6.693439	-2.118219	-4.396336
H	-5.572447	-3.397798	-4.934899
H	-6.338243	-3.493100	-3.308616
C	-0.029836	4.865195	-0.367383
C	-0.620032	6.066111	-0.782088
C	1.248973	4.558008	-0.888260
C	0.023784	6.923157	-1.674022
H	-1.593058	6.328567	-0.381409
C	1.906170	5.423362	-1.784022
C	1.289808	6.605562	-2.176097
H	-0.461395	7.848197	-1.972527
H	2.885714	5.150991	-2.164487
H	1.791868	7.274747	-2.867912
C	-2.636171	3.464375	-0.999906
H	-1.944754	3.839041	-1.761270
F	-2.415466	1.558571	3.475258
C	1.903547	3.332378	-0.554890
N	2.488447	2.351615	-0.351489
C	6.174701	1.519277	-0.734215
C	7.403278	2.117854	-1.414049

H	8.200227	2.282242	-0.685766
H	7.753485	1.415773	-2.180261
H	7.151012	3.055224	-1.919292
O	6.237374	1.059532	0.411758
H	-2.955751	2.467989	-1.322991
C	-3.877483	4.373458	-0.928581
H	-4.553693	4.051433	-0.132089
H	-3.598980	5.412791	-0.721998
H	-4.422345	4.353072	-1.879409
C	-0.632410	-0.296365	-0.049332
C	-1.644854	-0.143689	-2.151876
C	-0.770430	-0.320711	1.357621
C	0.664920	-0.437212	-0.633218
C	-0.410080	-0.282695	-2.802065
H	-2.569216	-0.054705	-2.712262
C	0.343280	-0.432991	2.141416
H	-1.756501	-0.235529	1.798668
C	1.831164	-0.554794	0.212228
C	0.736103	-0.428538	-2.050550
H	-0.373772	-0.289191	-3.885622
C	1.655737	-0.541964	1.600547
H	0.233525	-0.409829	3.221307
H	1.691125	-0.547281	-2.551643
N	-1.752162	-0.145602	-0.827479
Pd	3.532852	0.479366	-0.612332
C	5.577101	-3.447644	-0.990175
C	5.533915	-1.970263	-0.492179
C	3.679279	-2.865011	0.463393
C	4.279758	-4.054888	-0.364442
H	5.607377	-3.526377	-2.081010
H	6.474426	-3.941018	-0.601262
H	3.580153	-4.436477	-1.116238
H	4.507088	-4.881673	0.316576
C	4.977625	-2.165566	0.922574
H	4.837330	-1.223255	1.440947
H	5.603439	-2.821734	1.537339
C	4.335518	-1.352734	-1.221392
C	3.148064	-1.934434	-0.615634
H	6.459416	-1.407905	-0.583232
H	2.950224	-3.161860	1.212723
H	2.353850	-2.294329	-1.260306
C	2.760894	-0.498817	2.603231
C	2.905205	-1.453531	3.641082
C	3.646361	0.587832	2.578144
C	3.946879	-1.317489	4.572132
C	4.695380	0.698371	3.489966
H	3.528834	1.349372	1.818316
C	4.850457	-0.260599	4.489234
H	4.052846	-2.063316	5.351456
H	5.394084	1.522994	3.394170
H	5.667075	-0.188965	5.201627
C	2.008118	-2.641036	3.737473
O	1.366916	-3.128477	2.821231
O	1.977542	-3.156384	4.986033
C	1.167340	-4.332856	5.144139
H	1.271243	-4.618926	6.191026
H	0.122762	-4.112784	4.906428
H	1.518325	-5.133328	4.486588
O	5.118180	1.520887	-1.493738
C	4.417877	-1.123861	-2.693037
O	3.473659	-1.077723	-3.467913
O	5.694137	-0.956061	-3.082582
C	5.874295	-0.527031	-4.440967
H	6.953502	-0.473305	-4.587867
H	5.423275	-1.238197	-5.138274
H	5.419159	0.457635	-4.578124

Beta_C_elim_without_CN_MPAA_TS

Pd	-3.800143	-0.270264	-0.684454
C	-6.255176	0.933404	0.074342
C	-6.255979	-1.440649	0.096981
C	-7.585242	0.968457	0.483951
C	-7.584551	-1.467195	0.510653
H	-8.060587	1.933056	0.623539
H	-8.058645	-2.428469	0.675556
N	-5.666930	-0.255053	-0.100407
H	-9.284140	-0.243788	1.022279
C	-8.246490	-0.247175	0.700232
N	-4.129531	-2.293553	-0.574718
N	-4.104898	1.776641	-0.521445
C	-5.365262	-2.654205	-0.133816
C	-5.368511	2.144347	-0.183588
O	-5.801742	-3.790214	0.054230
O	-5.833429	3.280028	-0.061305
C	-3.042614	-3.182977	-0.640998
C	-2.382407	-3.589308	0.540950
C	-2.440967	-3.473348	-1.876630
C	-1.155554	-4.258378	0.478202
C	-1.209552	-4.129570	-1.945945
C	-0.572520	-4.510131	-0.766853
H	-0.620287	-4.521797	1.380313
H	-0.772601	-4.312696	-2.922205
H	0.391217	-5.012011	-0.807672
C	-3.062145	2.691515	-0.774540
C	-2.383363	3.413981	0.235227
C	-2.569630	2.745993	-2.084129
C	-1.211451	4.122301	-0.115742
C	-1.411977	3.417305	-2.432075
C	-0.728207	4.103688	-1.433155
H	-1.062347	3.390123	-3.458806
H	0.206509	4.606785	-1.652875
O	-2.994506	-3.207743	1.698555
O	-3.009518	-3.016791	-3.044466
C	-2.369265	-3.541872	2.926504
H	-2.294446	-4.631229	3.054831
H	-1.366428	-3.105303	2.998275
H	-3.011799	-3.130652	3.707996
C	-4.236271	-3.657955	-3.409077
H	-4.665229	-3.064486	-4.220379
H	-4.040795	-4.678872	-3.766384
H	-4.939642	-3.701022	-2.572336
C	-0.458600	4.994752	0.836113
C	-0.422973	6.372523	0.574687
C	0.280712	4.527864	1.944376
C	0.304770	7.255561	1.369878
H	-0.984360	6.745681	-0.276355
C	1.015188	5.418349	2.748624
C	1.029385	6.778477	2.463831
H	0.304815	8.316522	1.134901
H	1.573794	5.024478	3.592121
H	1.599765	7.459045	3.089310
C	-2.952172	3.461238	1.638059
H	-3.623887	2.609817	1.779339
H	-2.153599	3.343725	2.374439
C	-3.717627	4.769854	1.909534
H	-3.053495	5.635966	1.811039
H	-4.545121	4.871761	1.203451
H	-4.124914	4.769376	2.927840

F	-3.238721	2.064331	-3.049284
C	0.314468	3.147702	2.325636
N	0.351092	2.068935	2.758696
N	4.821154	1.686608	-1.314448
C	6.093208	1.690578	-1.212519
C	7.060940	2.714986	-1.747739
H	7.813277	2.212122	-2.368883
H	6.575007	3.475316	-2.357234
H	7.581977	3.209279	-0.919347
O	6.652387	0.667170	-0.527476
C	4.036751	2.814079	-1.818287
H	3.598294	2.528738	-2.783186
H	4.616455	3.729679	-1.953479
C	2.856880	3.122388	-0.846543
O	2.410770	2.109574	-0.176193
O	2.429087	4.270797	-0.816620
C	-0.776472	-0.532138	-0.454659
C	-1.574635	-0.316939	-2.643045
C	-1.054031	-0.619111	0.929564
C	0.573782	-0.626931	-0.907032
C	-0.278415	-0.424890	-3.167218
H	-2.432629	-0.187116	-3.287071
C	-0.025676	-0.748574	1.820851
H	-2.084554	-0.574127	1.264850
C	1.645290	-0.753562	0.050744
C	0.786589	-0.572194	-2.307330
H	-0.131418	-0.391731	-4.241172
C	1.336515	-0.794039	1.413468
H	-0.238350	-0.753292	2.883390
H	1.787979	-0.655990	-2.711731
N	-1.812390	-0.361174	-1.338425
Pd	3.407303	0.279660	-0.579234
C	5.406832	-3.721588	-0.867213
C	5.361643	-2.252198	-0.347770
C	3.394475	-3.099087	0.396753
C	4.036644	-4.294991	-0.384750
H	5.541118	-3.779216	-1.951870
H	6.246057	-4.254031	-0.405569
H	3.402720	-4.641128	-1.208155
H	4.169574	-5.139190	0.299772
C	4.657404	-2.447704	1.002710
H	4.470678	-1.511924	1.525435
H	5.195802	-3.128539	1.671349
C	4.263746	-1.568988	-1.176519
C	3.009770	-2.131138	-0.707234
H	6.316210	-1.733891	-0.345508
H	2.582993	-3.379115	1.062257
H	2.265100	-2.449807	-1.427222
C	2.344924	-0.690970	2.510081
C	2.504066	-1.637360	3.552414
C	3.108772	0.487687	2.564522
C	3.467699	-1.419525	4.552242
C	4.065981	0.686309	3.558157
H	2.909061	1.269172	1.841726
C	4.262270	-0.277890	4.546943
H	3.591032	-2.162763	5.331019
H	4.644487	1.606305	3.564426
H	5.009407	-0.133531	5.322216
C	1.698689	-2.888644	3.605539
O	1.093157	-3.389477	2.672279
O	1.699992	-3.450003	4.835864
C	0.973256	-4.683697	4.949474
H	1.118730	-5.013195	5.978558
H	-0.089231	-4.523807	4.745222
H	1.359466	-5.426635	4.245741
H	7.614313	0.668502	-0.650463
C	4.491201	-1.324780	-2.623800
O	5.810847	-1.150597	-2.893778
O	3.641128	-1.263575	-3.497251
C	6.112425	-0.847804	-4.263820
H	5.656648	0.104217	-4.553861
H	7.200550	-0.785142	-4.317923
H	5.740488	-1.631557	-4.929086

Cat_3Pd

Pd	0.019796	-1.845612	-0.008271
C	2.310494	-1.203712	-1.860105
O	1.642569	-2.081213	-1.238427
O	2.324914	0.047206	-1.654719
C	0.008915	2.582633	1.891056
O	-1.061050	2.442258	1.228673
O	1.115802	1.994938	1.702942
C	-0.052611	3.570024	3.038212
H	0.918297	3.658771	3.527167
H	-0.370059	4.544034	2.652999
H	-0.809311	3.235866	3.754932
C	3.223525	-1.715642	-2.955337
H	2.734815	-2.526118	-3.500713
H	3.503676	-0.904516	-3.629525
H	4.130820	-2.116535	-2.488927
Pd	-1.619371	0.911634	-0.014149
C	-0.071423	2.596800	-1.871646
O	1.001585	2.478793	-1.209709
O	-1.163223	1.980152	-1.688453
C	2.237830	-1.330373	1.871280
O	1.170822	-1.984818	1.668386
O	2.648733	-0.309502	1.245145
C	3.143729	-1.850145	2.968674
H	3.638059	-1.017563	3.473593
H	2.574181	-2.454411	3.677077
H	3.913825	-2.481532	2.510435
C	-0.033983	3.592869	-3.012334
H	0.723132	3.275450	-3.736272
H	-1.009350	3.668411	-3.494573
H	0.270356	4.569397	-2.623104
Pd	1.595686	0.951263	0.020049
C	-2.279674	-1.272898	1.852562
O	-1.596699	-2.130646	1.218798
O	-2.328316	-0.022274	1.653352
C	-3.148615	-1.817587	2.967741
H	-2.536209	-2.423496	3.641512
H	-3.632127	-1.006166	3.513269
H	-3.910033	-2.472789	2.531352
C	-2.209055	-1.367605	-1.884616
O	-1.128145	-1.999886	-1.685533
O	-2.642780	-0.360565	-1.251439
C	-3.102499	-1.897490	-2.987341
H	-3.872622	-2.531614	-2.533038
H	-3.598478	-1.069460	-3.498303
H	-2.523524	-2.499627	-3.689780

Int_1

Pd	1.176210	0.904590	0.281290
C	1.267798	3.641876	-0.472147
C	3.317639	2.472972	-0.714384
C	1.846101	4.817743	-0.939631
C	3.949404	3.618310	-1.190995
H	1.228611	5.705928	-1.015380

H	4.996492	3.556091	-1.466065
N	2.025027	2.541707	-0.378374
H	3.673154	5.702693	-1.664566
C	3.200522	4.796383	-1.296628
N	3.084322	0.194711	-0.031931
N	-0.447129	2.185002	0.308949
C	3.959133	1.104971	-0.553457
C	-0.190335	3.463095	-0.078725
O	5.133363	0.932841	-0.872779
O	-0.981467	4.401607	-0.170053
C	3.429369	-1.157519	0.087196
C	3.703088	-1.943734	-1.050910
C	3.362524	-1.789885	1.345772
C	3.969174	-3.312890	-0.929019
C	3.598558	-3.164747	1.469274
C	3.913141	-3.906650	0.330847
H	4.194284	-3.916485	-1.800044
H	3.555751	-3.653674	2.434884
H	4.112047	-4.970446	0.427724
C	-1.723709	1.746452	0.703354
C	-2.520766	0.962538	-0.160151
C	-2.131050	1.919680	2.028850
C	-3.681109	0.347672	0.354980
C	-3.298262	1.364063	2.532251
C	-4.066368	0.569359	1.686675
H	-3.573294	1.538184	3.567042
H	-4.970011	0.100151	2.063600
O	3.621290	-1.281861	-2.240168
O	3.039752	-0.970758	2.390282
C	4.061048	-1.945880	-3.411919
H	5.101619	-2.281470	-3.315561
H	3.424678	-2.809452	-3.655127
H	3.991094	-1.210985	-4.216059
C	2.865969	-1.552228	3.669848
H	2.597565	-0.730036	4.336525
H	2.057255	-2.297194	3.667323
H	3.789148	-2.022732	4.033917
C	-4.487587	-0.601282	-0.464816
C	-3.919143	-1.808413	-0.897205
C	-5.838680	-0.353678	-0.794515
C	-4.654468	-2.737308	-1.630048
H	-2.884169	-2.014460	-0.646243
C	-6.582579	-1.293844	-1.531364
C	-5.991695	-2.481922	-1.948461
H	-4.181645	-3.663019	-1.946830
H	-7.617975	-1.075848	-1.773391
H	-6.569954	-3.203103	-2.518433
C	-2.138781	0.889380	-1.622983
H	-1.048902	0.849305	-1.714590
H	-2.533975	-0.018985	-2.083797
C	-2.668231	2.122409	-2.382960
H	-3.763654	2.150783	-2.353756
H	-2.297569	3.047381	-1.930397
H	-2.353871	2.092087	-3.432958
F	-1.321298	2.606827	2.863649
C	-6.479177	0.867673	-0.397026
N	-7.031303	1.844466	-0.090537
C	-0.051167	-1.918302	0.252280
C	-0.253954	-0.748582	2.263100
C	0.407194	-1.978241	-1.087791
C	-0.789278	-3.018822	0.792533
C	-0.983678	-1.794349	2.863483
H	-0.047851	0.165858	2.808135
C	0.132086	-3.085110	-1.858937
H	0.985387	-1.150662	-1.484605
C	-1.055057	-4.143465	-0.033600
C	-1.250506	-2.925475	2.128285
H	-1.333474	-1.678644	3.883220
C	-0.606826	-4.174434	-1.334520
H	0.491221	-3.123598	-2.882970
H	-1.820648	-3.747864	2.552659
H	-0.813152	-5.036520	-1.962142
N	0.196916	-0.803713	1.017248
H	-1.622529	-4.972618	0.380776

Int_2

Pd	2.749256	0.069668	0.101493
C	4.727561	1.748249	-1.070119
C	5.082476	-0.572726	-1.382906
C	5.882216	2.055105	-1.782758
C	6.246104	-0.328167	-2.107110
H	6.151303	3.097518	-1.912154
H	6.801744	-1.175199	-2.494052
N	4.388034	0.464453	-0.903305
H	7.548436	1.214419	-2.862147
C	6.643007	0.999714	-2.301665
N	3.365520	-1.851576	-0.325383
N	2.719711	2.143292	0.153141
C	4.502075	-1.941162	-1.076710
C	3.772786	2.754345	-0.455281
O	5.063882	-2.955196	-1.484486
O	3.990119	3.963132	-0.558133
C	2.637254	-3.000688	0.014188
C	1.986784	-3.770055	-0.972185
C	2.434041	-3.326434	1.371321
C	1.189188	-4.864002	-0.615189
C	1.612476	-4.400696	1.734126
C	1.007594	-5.162400	0.734326
H	0.693725	-5.462726	-1.369650
H	1.451125	-4.654314	2.774608
H	0.377651	-6.002250	1.013498
C	1.709358	2.892815	0.781071
C	0.553121	3.318059	0.092810
C	1.793782	3.118114	2.159120
C	-0.471472	3.958427	0.821754
C	0.802114	3.761641	2.881944
C	-0.334657	4.186083	2.198868
H	0.925496	3.912616	3.949065
H	-1.136829	4.681304	2.738052
O	2.148715	-3.324902	-2.249735
O	3.068015	-2.511390	2.265632
C	1.654433	-4.125665	-3.309441
H	2.086888	-5.134163	-3.286045
H	0.557748	-4.203066	-3.284097
H	1.957999	-3.623375	-4.229832
C	2.900063	-2.771628	3.648372
H	3.495020	-2.016941	4.166836
H	1.847975	-2.675374	3.951544
H	3.265765	-3.770387	3.921048
C	-1.740604	4.394615	0.171438
C	-2.040554	5.747006	-0.012735
C	-2.713818	3.452104	-0.228792
C	-3.255996	6.143186	-0.577765
H	-1.306884	6.488601	0.288393
C	-3.945602	3.837807	-0.792376
C	-4.206324	5.194179	-0.965049
H	-3.461910	7.201287	-0.713786
H	-4.673411	3.075763	-1.058700

H	-5.152133	5.506962	-1.396280
C	0.481072	3.140481	-1.408596
H	1.087854	2.275606	-1.692847
H	-0.544573	2.927688	-1.724257
C	0.990386	4.393006	-2.148479
H	0.354267	5.257318	-1.924357
H	2.013400	4.628160	-1.841518
H	0.973318	4.231388	-3.232530
F	2.876868	2.645090	2.820515
C	-2.496361	2.052846	-0.063305
N	-2.437715	0.894523	0.006067
C	-0.053759	-1.054006	0.662303
C	1.006226	-0.072709	2.494399
C	-0.072618	-1.351159	-0.734720
C	-1.133535	-1.478819	1.487278
C	-0.028963	-0.452034	3.364415
H	1.860852	0.486282	2.856822
C	-1.110709	-2.052842	-1.281128
H	0.772472	-1.040804	-1.340093
C	-2.214235	-2.221897	0.899897
C	-1.096368	-1.167951	2.859911
H	0.030716	-0.178788	4.412239
C	-2.193769	-2.514596	-0.466246
H	-1.103834	-2.293755	-2.339210
H	-1.914801	-1.486784	3.499552
H	-2.912559	-3.228297	-0.851143
N	1.005018	-0.369839	1.196165
Pd	-3.774478	-0.737679	-0.164055
H	-2.952886	-2.714704	1.524463
C	-6.244183	0.310330	-1.109123
O	-7.059698	1.090297	-1.564033
O	-5.072302	0.710143	-0.646024
N	-5.389064	-1.906890	-0.409775
C	-5.519723	-3.174738	0.048347
C	-6.869408	-3.860294	-0.190844
H	-6.762775	-4.906007	0.100400
H	-7.656183	-3.400620	0.419416
H	-7.187424	-3.800864	-1.237352
O	-4.623408	-3.801214	0.630728
C	-6.500917	-1.195005	-1.033971
H	-7.437581	-1.325476	-0.478650
H	-6.687913	-1.543638	-2.060342

Int_3

Pd	2.877252	-0.053265	0.357195
C	4.974128	1.790955	-0.161583
C	5.509262	-0.476996	-0.602584
C	6.245930	2.200642	-0.550118
C	6.793822	-0.126713	-1.009224
H	6.486213	3.257386	-0.514245
H	7.464985	-0.911486	-1.340357
N	4.674854	0.487484	-0.200337
H	8.155586	1.521097	-1.284080
C	7.157330	1.224823	-0.974453
N	3.655751	-1.896173	-0.099092
N	2.704993	2.009979	0.551532
C	4.928569	-1.881917	-0.592890
C	3.847920	2.703153	0.295174
O	5.599246	-2.830450	-0.993122
O	4.029543	3.920626	0.370299
C	2.867565	-3.054669	-0.123172
C	2.460389	-3.633560	-1.342676
C	2.332787	-3.560533	1.078975
C	1.588903	-4.729297	-1.359068
C	1.440873	-4.639975	1.066436
C	1.089665	-5.218521	-0.153040
H	1.282927	-5.184848	-2.292916
H	1.030708	-5.036302	1.987232
H	0.406508	-6.063291	-0.163384
C	1.535202	2.662232	0.983773
C	0.568072	3.159025	0.082163
C	1.252981	2.699014	2.354546
C	-0.619342	3.719921	0.600347
C	0.070423	3.204617	2.870207
C	-0.865732	3.726429	1.980336
H	-0.094840	3.196689	3.942224
H	-1.786745	4.160948	2.358125
O	2.927682	-3.007033	-2.460646
O	2.732118	-2.908829	2.211166
C	2.615548	-3.565750	-3.724492
H	2.995906	-4.591499	-3.816542
H	1.531943	-3.564840	-3.911548
H	3.109920	-2.930497	-4.461861
C	2.163413	-3.305216	3.446311
H	2.600891	-2.647549	4.200434
H	1.070895	-3.181351	3.444420
H	2.408113	-4.347123	3.692906
C	-1.594370	4.425145	-0.286774
C	-1.316362	5.733884	-0.702740
C	-2.827251	3.866460	-0.690128
C	-2.215739	6.457162	-1.486165
H	-0.381040	6.185165	-0.388230
C	-3.743065	4.594813	-1.476795
C	-3.432941	5.889397	-1.874000
H	-1.968750	7.470869	-1.788470
H	-4.682907	4.133705	-1.763595
H	-4.136580	6.452457	-2.479127
C	0.811527	3.037662	-1.407627
H	1.342526	2.095829	-1.585016
H	-0.151208	2.962409	-1.926816
C	1.629470	4.195565	-2.010168
H	1.058765	5.129922	-1.990022
H	2.555881	4.354050	-1.452582
H	1.878329	3.979059	-3.055685
F	2.160783	2.173561	3.208197
C	-3.198600	2.529257	-0.353675
N	-3.604388	1.459063	-0.174045
C	-0.041802	-0.820104	0.034536
C	0.629375	-0.422003	2.240650
C	0.306451	-1.040415	-1.322043
C	-1.417775	-0.846833	0.428201
C	-0.692314	-0.507005	2.714283
H	1.448880	-0.198829	2.913385
C	-0.686727	-1.255297	-2.249429
H	1.353300	-1.060049	-1.605238
C	-2.441305	-0.996930	-0.564012
C	-1.709799	-0.693171	1.806915
H	-0.887462	-0.386668	3.774294
C	-2.054113	-1.212541	-1.876998
H	-0.419987	-1.441295	-3.286549
H	-2.747722	-0.716487	2.126670
H	-2.809474	-1.338848	-2.649175
N	0.941820	-0.558523	0.958652
Pd	-4.362879	-0.439783	-0.135839
H	-3.026850	-2.812627	-0.332666
C	-7.215298	-0.635094	0.236436
O	-8.409324	-0.428778	0.387612
O	-6.275105	0.263161	0.215278

N	-5.307068	-2.263207	-0.081263
C	-4.801187	-3.453073	-0.102332
C	-5.611812	-4.715993	0.005429
H	-4.959504	-5.581889	-0.112030
H	-6.108876	-4.768002	0.980428
H	-6.393701	-4.738765	-0.760387
O	-3.500927	-3.676328	-0.218190
C	-6.768330	-2.103605	0.046227
H	-7.148850	-2.673473	0.901127
H	-7.268057	-2.484723	-0.852676

Int_4

Pd	3.346436	-0.319737	0.421748
C	5.706993	1.227320	0.117054
C	5.975623	-1.093273	-0.295260
C	7.053885	1.462301	-0.142005
C	7.328875	-0.918705	-0.572098
H	7.428411	2.477329	-0.070148
H	7.918685	-1.786585	-0.845826
N	5.242473	-0.024593	0.034094
H	8.918139	0.532033	-0.695296
C	7.863863	0.372397	-0.487239
N	3.909329	-2.250302	0.015285
N	3.429611	1.749812	0.615409
C	5.211980	-2.406723	-0.361889
C	4.673380	2.283153	0.475898
O	5.782425	-3.434781	-0.719653
O	5.009262	3.465555	0.580661
C	2.968167	-3.278272	-0.131594
C	2.610803	-3.758370	-1.408474
C	2.238800	-3.726347	0.988363
C	1.595370	-4.710799	-1.557623
C	1.206108	-4.661077	0.841830
C	0.905788	-5.150871	-0.428846
H	1.327584	-5.092216	-2.535463
H	0.646905	-5.013940	1.699735
H	0.113919	-5.886456	-0.541665
C	2.317787	2.548872	0.943306
C	1.507196	3.159471	-0.039040
C	1.914614	2.620016	2.282243
C	0.349306	3.855956	0.372866
C	0.755177	3.259247	2.690510
C	-0.026309	3.886228	1.723273
H	0.486199	3.265797	3.741198
H	-0.924467	4.420730	2.018610
O	3.281183	-3.181603	-2.447026
O	2.602009	-3.167636	2.180751
C	3.011811	-3.640290	-3.759371
H	3.233835	-4.710251	-3.866646
H	1.965631	-3.458342	-4.045464
H	3.670253	-3.068641	-4.416259
C	1.837682	-3.488674	3.328885
H	2.278304	-2.918084	4.149224
H	0.785245	-3.195172	3.205707
H	1.889339	-4.559406	3.568302
C	-0.446318	4.675396	-0.590626
C	0.064557	5.905478	-1.027660
C	-1.732580	4.311852	-1.048963
C	-0.658633	6.735115	-1.883953
H	1.041119	6.212101	-0.668175
C	-2.470196	5.149742	-1.910051
C	-1.930221	6.359355	-2.327428
H	-0.231554	7.682862	-2.199293
H	-3.455756	4.837109	-2.240590
H	-2.496801	7.005611	-2.990598
C	1.869521	2.999317	-1.501163
H	2.272741	1.989554	-1.635245
H	0.958201	3.058663	-2.107785
C	2.901179	4.018940	-2.019597
H	2.472128	5.025291	-2.064534
H	3.779068	4.056318	-1.369941
H	3.222795	3.749145	-3.032460
F	2.669753	1.990766	3.210150
C	-2.335419	3.065164	-0.698436
N	-2.908926	2.076461	-0.508006
C	0.386573	-0.628025	-0.149380
C	0.933826	-0.399640	2.115322
C	0.803875	-0.845194	-1.486155
C	-1.003372	-0.446475	0.145322
C	-0.414447	-0.250575	2.482728
H	1.723194	-0.337465	2.855069
C	-0.132103	-0.845024	-2.495443
H	1.853914	-1.023343	-1.692487
C	-1.941209	-0.425402	-0.930710
C	-1.378525	-0.240449	1.500074
H	-0.669094	-0.091523	3.525036
C	-1.505113	-0.619645	-2.223393
H	0.186700	-1.014801	-3.520969
H	-2.417764	-0.049034	1.749520
H	-2.210772	-0.600394	-3.049710
N	1.321498	-0.556134	0.855797
Pd	-3.805356	0.182807	-0.430043
O	-4.532267	0.923471	2.239861
O	-5.624521	1.054852	0.275042
C	-5.536167	1.203497	1.560261
C	-6.810139	1.689500	2.233338
H	-7.413030	0.804488	2.470553
H	-6.572140	2.206370	3.166150
H	-7.392623	2.335676	1.571654
C	-6.759795	-3.084354	-1.203218
C	-6.393856	-1.584421	-0.945457
C	-4.762471	-2.264279	-2.366240
C	-5.629285	-3.561264	-2.172294
H	-6.805174	-3.657936	-0.273530
H	-7.744006	-3.145855	-1.678495
H	-5.043206	-4.393691	-1.770178
H	-6.032306	-3.878888	-3.139585
C	-5.868308	-1.185575	-2.340592
H	-5.485722	-0.161032	-2.384332
H	-6.615464	-1.326386	-3.129152
C	-5.105645	-1.659919	-0.140010
C	-4.107963	-2.074835	-1.011143
H	-7.171865	-0.972805	-0.496191
H	-4.086078	-2.290460	-3.222136
H	-3.206614	-2.591939	-0.708033
C	-5.146499	-1.872657	1.333550
O	-6.181257	-1.866004	1.968373
O	-3.927602	-2.091851	1.859084
C	-3.869319	-2.052849	3.298043
H	-4.492235	-2.840338	3.730195
H	-2.818566	-2.210384	3.544362
H	-4.209401	-1.070565	3.635216

Int_5

Pd	3.094727	0.145965	0.388018
C	5.024686	2.201196	0.003707
C	5.743199	0.029972	-0.617400
C	6.255459	2.745236	-0.350943

C	6.990982	0.517284	-0.995664
H	6.405421	3.812348	-0.230252
H	7.722405	-0.181120	-1.387102
N	4.831216	0.885544	-0.141910
H	8.209448	2.289665	-1.139305
C	7.241659	1.887237	-0.853610
N	4.036694	-1.585212	-0.199408
N	2.754773	2.172364	0.739363
C	5.291392	-1.417679	-0.708126
C	3.827798	2.979708	0.519777
O	6.036871	-2.270232	-1.185457
O	3.906686	4.201235	0.668053
C	3.374878	-2.818634	-0.281777
C	2.939022	-3.326057	-1.522599
C	3.002257	-3.496574	0.896573
C	2.181197	-4.502067	-1.588290
C	2.228203	-4.662462	0.837724
C	1.834090	-5.154527	-0.406332
H	1.848891	-4.899021	-2.539734
H	1.940739	-5.188168	1.739920
H	1.241655	-6.064146	-0.454999
C	1.493749	2.691889	1.090803
C	0.639658	3.331637	0.163698
C	1.008329	2.437047	2.378873
C	-0.668521	3.668718	0.573467
C	-0.284632	2.732959	2.775646
C	-1.129398	3.351385	1.857832
H	-0.611222	2.477704	3.778164
H	-2.165036	3.548333	2.111006
O	3.263312	-2.561241	-2.603416
O	3.425823	-2.917143	2.058855
C	2.924855	-3.042180	-3.892110
H	3.389990	-4.015893	-4.094199
H	1.835982	-3.129580	-4.018330
H	3.311501	-2.304123	-4.597372
C	3.104064	-3.555709	3.282067
H	3.550382	-2.939778	4.065514
H	2.016975	-3.607402	3.436134
H	3.525204	-4.568485	3.334357
C	-1.617740	4.380173	-0.331707
C	-1.935920	5.724166	-0.109611
C	-2.272018	3.725488	-1.397929
C	-2.857975	6.393772	-0.916364
H	-1.446868	6.242891	0.709170
C	-3.202388	4.392890	-2.213921
C	-3.491758	5.731122	-1.971391
H	-3.083514	7.438144	-0.719383
H	-3.697563	3.849923	-3.012583
H	-4.211387	6.251889	-2.595501
C	1.140274	3.659896	-1.228061
H	1.988769	3.009999	-1.460656
H	0.365776	3.429946	-1.967413
C	1.563497	5.133330	-1.378109
H	0.712135	5.802482	-1.211797
H	2.348032	5.373240	-0.657053
H	1.945895	5.318540	-2.388970
F	1.838303	1.836975	3.269677
C	-2.055183	2.335245	-1.614265
N	-1.943433	1.192494	-1.801233
C	0.344996	-1.222711	0.143694
C	1.116481	-0.881193	2.322503
C	0.590133	-1.115488	-1.254166
C	-0.845725	-1.852341	0.623042
C	0.006702	-1.542651	2.865306
H	1.882139	-0.457573	2.957239
C	-0.323083	-1.603621	-2.143921
H	1.525555	-0.677837	-1.585919
C	-1.842793	-2.308005	-0.330986
C	-0.970524	-2.022438	2.020680
H	-0.073658	-1.655019	3.941159
C	-1.543175	-2.182731	-1.694130
H	-0.132681	-1.542269	-3.210468
H	-1.844595	-2.501242	2.434788
H	-2.189727	-2.639520	-2.430804
N	1.283320	-0.729439	1.013379
Pd	-3.161949	-0.450749	-0.896861
O	-3.813535	1.917822	0.861294
O	-4.785362	0.829064	-0.861532
C	-4.747435	1.737530	0.069363
C	-6.014638	2.576948	0.146930
H	-6.727899	2.036166	0.780008
H	-5.794167	3.544222	0.604782
H	-6.469090	2.711540	-0.837940
C	-5.989704	-3.679054	0.137985
C	-5.406323	-2.510312	-0.712212
C	-3.764359	-4.077674	-0.787487
C	-4.868576	-4.769576	0.054242
H	-6.218113	-3.368535	1.160165
H	-6.924266	-4.033735	-0.310148
H	-4.504330	-5.083238	1.038957
H	-5.225556	-5.667831	-0.460913
C	-4.652181	-3.301256	-1.795749
H	-4.127682	-2.659794	-2.506380
H	-5.306530	-3.974667	-2.360984
C	-4.262116	-1.891803	0.094887
C	-3.151709	-2.978702	0.129323
H	-6.142775	-1.777387	-1.040268
H	-3.021190	-4.762482	-1.206654
H	-3.006424	-3.391364	1.129979
C	-4.684211	-1.196909	1.349377
O	-5.807814	-0.785460	1.565446
O	-3.660782	-1.042429	2.224890
C	-3.905329	-0.138536	3.317196
H	-4.762558	-0.470902	3.909073
H	-2.991749	-0.157454	3.914442
H	-4.081293	0.862023	2.916604

Int_6

Pd	-3.382246	0.224533	-0.152658
C	-4.939870	2.612451	-0.077250
C	-6.033030	0.690116	0.758655
C	-6.077798	3.388720	0.122803
C	-7.199667	1.414174	0.988136
H	-6.046965	4.435606	-0.157400
H	-8.058886	0.893373	1.395859
N	-4.962688	1.319155	0.259754
H	-8.111913	3.361646	0.836729
C	-7.211981	2.776678	0.669175
N	-4.625117	-1.230526	0.626990
N	-2.671182	2.144682	-0.685716
C	-5.863695	-0.796997	0.990343
C	-3.637156	3.107788	-0.667351
O	-6.793861	-1.452305	1.465442
O	-3.553076	4.275223	-1.058441
C	-4.305508	-2.595416	0.659089
C	-3.172796	-3.035395	1.386497
C	-5.000435	-3.528986	-0.131003
C	-2.777994	-4.375907	1.341890

C	-4.616437	-4.874668	-0.159918
C	-3.510653	-5.287404	0.576229
H	-1.912145	-4.715911	1.897032
H	-5.164998	-5.572393	-0.784412
H	-3.200816	-6.328551	0.548659
C	-1.364006	2.487778	-1.076428
C	-0.532248	3.355132	-0.324106
C	-0.812121	1.834881	-2.188625
C	0.784646	3.593886	-0.781745
C	0.503080	1.999307	-2.588650
C	1.297519	2.902571	-1.887465
H	0.875896	1.445076	-3.442916
H	2.318316	3.086868	-2.209465
O	-2.514841	-2.068217	2.086460
O	-6.001622	-3.054472	-0.939392
C	-1.283621	-2.407675	2.706139
H	-1.424374	-3.147852	3.505292
H	-0.558795	-2.789399	1.974643
H	-0.899192	-1.479435	3.130691
C	-7.301057	-3.606289	-0.707721
H	-7.975685	-3.081483	-1.388170
H	-7.332046	-4.681047	-0.933156
H	-7.606069	-3.423878	0.326471
C	1.638247	4.654156	-0.165430
C	1.307013	6.001534	-0.369074
C	2.823838	4.386062	0.558732
C	2.095857	7.034423	0.135521
H	0.417619	6.227227	-0.947832
C	3.624411	5.426624	1.070283
C	3.256168	6.749543	0.861971
H	1.807810	8.066129	-0.045308
H	4.525250	5.181483	1.624136
H	3.871597	7.552475	1.255840
C	-0.992397	3.856363	1.036813
H	-1.746218	3.148294	1.399325
H	-0.140919	3.781591	1.726822
C	-1.580344	5.278589	1.132396
H	-0.801796	6.040544	1.042899
H	-2.329605	5.441764	0.356695
H	-2.057473	5.411245	2.110900
F	-1.591039	0.973893	-2.877340
C	3.256094	3.044494	0.784553
N	3.648166	1.969870	0.984279
C	-0.558435	-0.963134	-0.320346
C	-2.194087	-2.032261	-1.602549
C	-0.211608	0.047123	0.606056
C	0.450759	-1.859576	-0.800060
C	-1.268253	-2.969744	-2.093596
H	-3.235469	-2.071890	-1.900756
C	1.106615	0.247820	0.939258
H	-0.998387	0.669712	1.017485
C	1.803790	-1.667149	-0.383532
C	0.046189	-2.883283	-1.693594
H	-1.607345	-3.740038	-2.777300
C	2.135674	-0.574634	0.406779
H	1.356986	1.058227	1.614188
H	0.779797	-3.589795	-2.067512
H	5.673124	-0.772634	2.387949
N	-1.855763	-1.072989	-0.748955
Pd	4.054717	-0.122480	0.565037
O	6.264361	0.449138	0.541293
O	6.656360	-0.828025	2.350128
C	7.048663	-0.166401	1.257350
C	8.510515	-0.289997	0.962791
H	8.605652	-1.141076	0.278054
H	8.859375	0.606858	0.448229
H	9.093449	-0.480786	1.865642
C	5.133744	-4.460409	0.063521
C	4.742859	-3.163696	0.827720
C	2.755559	-3.962294	0.100874
C	3.761541	-4.991302	-0.460803
H	5.860695	-4.271364	-0.728415
H	5.590270	-5.172706	0.760903
H	3.720471	-5.048496	-1.555043
H	3.546124	-5.993889	-0.074307
C	3.401890	-3.591929	1.452916
H	2.884292	-2.780106	1.972546
H	3.497558	-4.451221	2.127363
C	4.288900	-2.084355	-0.190555
C	2.904439	-2.632199	-0.705939
H	5.524749	-2.836761	1.512131
H	1.723701	-4.323018	0.144896
H	2.944672	-2.842085	-1.781272
C	5.312512	-1.786221	-1.230920
O	6.522836	-1.897677	-1.082921
O	4.776935	-1.320265	-2.392287
C	5.730209	-0.891265	-3.371812
H	6.385088	-1.716494	-3.667720
H	5.141942	-0.545317	-4.223167
H	6.346517	-0.078278	-2.975413

Int_7

Pd	-3.629284	-0.332900	-0.146380
C	-6.243368	0.552560	0.559549
C	-6.174942	-1.477078	-0.658953
C	-7.633883	0.519133	0.603228
C	-7.564259	-1.564021	-0.650728
H	-8.157163	1.320809	1.112373
H	-8.032117	-2.412747	-1.137145
N	-5.587333	-0.436160	-0.057138
H	-9.376831	-0.602275	0.009886
C	-8.291749	-0.553561	-0.010941
N	-3.930902	-2.128488	-1.121376
N	-4.040779	1.412954	0.921786
C	-5.229092	-2.487109	-1.284429
C	-5.364081	1.621631	1.177728
O	-5.684826	-3.496452	-1.829701
O	-5.867938	2.550211	1.812347
C	-2.865824	-2.933437	-1.560463
C	-1.993824	-3.497534	-0.595401
C	-2.528300	-3.045190	-2.917215
C	-0.816040	-4.140868	-0.989555
C	-1.369831	-3.722373	-3.316833
C	-0.519499	-4.253682	-2.351755
H	-0.116914	-4.516472	-0.251761
H	-1.135647	-3.783188	-4.375396
H	0.398487	-4.750760	-2.653616
C	-3.086268	2.203070	1.586916
C	-2.324034	3.174604	0.910617
C	-2.821999	1.966144	2.941163
C	-1.336819	3.881742	1.625808
C	-1.844320	2.644472	3.649784
C	-1.100974	3.613923	2.980789
H	-1.678251	2.407556	4.695123
H	-0.334771	4.171824	3.511334
O	-2.378037	-3.325477	0.698035
O	-3.307858	-2.396063	-3.847621
C	-1.617300	-3.966207	1.718124

H	-1.597181	-5.053720	1.565242
H	-0.592947	-3.587050	1.765757
H	-2.135550	-3.739792	2.651945
C	-4.148387	-3.259780	-4.623804
H	-4.717413	-2.609139	-5.292966
H	-3.549463	-3.959402	-5.224046
H	-4.830171	-3.810517	-3.969241
C	-0.557405	4.974521	0.974699
C	-1.004978	6.299115	1.026515
C	0.657335	4.719887	0.305116
C	-0.277246	7.331907	0.432886
H	-1.937046	6.510407	1.541311
C	1.397134	5.757251	-0.296221
C	0.924358	7.062892	-0.229638
H	-0.649242	8.351124	0.487574
H	2.326494	5.524320	-0.806806
H	1.489714	7.866136	-0.691970
C	-2.639152	3.468112	-0.538536
H	-1.760663	3.888003	-1.040809
F	-3.522481	0.994198	3.564901
C	1.181525	3.396368	0.190459
N	1.724470	2.384864	0.007464
C	-0.637827	-0.471475	0.570763
C	-1.156210	-0.375157	-1.708279
C	-1.106782	-0.583558	1.895210
C	0.759512	-0.640504	0.292563
C	0.155160	-0.711255	-2.058884
H	-1.925828	-0.263938	-2.464581
C	-0.221367	-0.949914	2.873665
H	-2.163203	-0.472513	2.104121
C	1.704069	-0.757331	1.368651
C	1.110451	-0.845066	-1.071554
H	0.379139	-0.921796	-3.098062
C	1.169681	-1.083625	2.625236
H	-0.588584	-1.161495	3.873514
H	2.079589	-1.264672	-1.305315
N	-1.551606	-0.294608	-0.441720
Pd	2.944124	1.255246	-1.294101
C	6.094765	-0.017905	1.511241
C	5.122713	0.874583	0.671219
C	3.875848	0.213388	2.430082
C	5.241826	-0.429400	2.751435
H	6.474775	-0.872355	0.949980
H	6.962361	0.584908	1.801855
H	5.172687	-1.513350	2.884827
H	5.650092	-0.010900	3.678515
C	4.321887	1.540869	1.798494
H	3.500247	2.169392	1.458745
H	4.953427	2.124017	2.479930
C	4.031865	0.001205	0.004820
C	3.238948	-0.610322	1.238220
H	5.632596	1.513519	-0.047702
H	3.223715	0.321010	3.290630
H	3.629106	-1.631269	1.300048
C	4.544894	-1.071927	-0.921881
O	3.912382	-2.066390	-1.264152
O	5.812466	-0.870067	-1.321594
C	6.296556	-1.772012	-2.320818
H	5.663076	-1.716999	-3.210987
H	7.308560	-1.436335	-2.549447
H	6.303864	-2.801343	-1.950149
C	1.959536	-1.665266	3.752132
C	2.716775	-2.847725	3.602864
C	1.925496	-1.060476	5.018035
C	3.456547	-3.352611	4.681249
C	2.641036	-1.581013	6.094422
H	1.349522	-0.147192	5.140607
C	3.419068	-2.728014	5.925317
H	4.049187	-4.249746	4.535607
H	2.599933	-1.084756	7.060116
H	3.988644	-3.134909	6.755686
C	2.705749	-3.619704	2.320466
O	1.725509	-3.833597	1.634468
O	3.938924	-4.069486	2.005431
C	4.030505	-4.783423	0.753262
H	5.065518	-5.121694	0.693503
H	3.343973	-5.634181	0.748114
H	3.794499	-4.108211	-0.072592
C	1.943837	1.194787	-4.091184
O	1.198226	0.998314	-5.185969
O	1.685026	2.060010	-3.265031
N	4.011971	0.661725	-2.931573
C	5.139266	1.378499	-3.220860
C	5.709602	1.286254	-4.642523
H	6.700455	1.742188	-4.628596
H	5.792849	0.252184	-4.996612
H	5.085461	1.836107	-5.358199
O	5.730861	2.057041	-2.380352
C	3.104354	0.213548	-3.955712
H	2.668460	-0.757777	-3.678401
H	3.563378	0.070556	-4.940445
H	0.454244	1.631420	-5.154630
H	-2.883314	2.528470	-1.044011
C	-3.828506	4.438023	-0.672305
H	-4.696394	4.063830	-0.120352
H	-3.572332	5.422992	-0.264721
H	-4.108138	4.567850	-1.724288

Int_8

Pd	-3.671633	-0.168825	0.263560
C	-5.850374	0.927797	1.726809
C	-6.256101	-1.211731	0.790386
C	-7.128415	0.966079	2.275915
C	-7.547637	-1.227381	1.309617
H	-7.421969	1.840000	2.846859
H	-8.174302	-2.090165	1.112944
N	-5.478552	-0.148166	1.023564
H	-8.980257	-0.118625	2.477722
C	-7.977194	-0.126751	2.060597
N	-4.335748	-2.018115	-0.370848
N	-3.676502	1.715965	1.139852
C	-5.625449	-2.306699	-0.051127
C	-4.808023	2.026942	1.831729
O	-6.281380	-3.310234	-0.340704
O	-5.053133	3.062124	2.450392
C	-3.584138	-2.826718	-1.234057
C	-2.338885	-3.337993	-0.789791
C	-3.945321	-3.006580	-2.581071
C	-1.498757	-4.026636	-1.671339
C	-3.115719	-3.715004	-3.458288
C	-1.901407	-4.215812	-2.996933
H	-0.530559	-4.382644	-1.346614
H	-3.417612	-3.833647	-4.494267
H	-1.248437	-4.758148	-3.676523
C	-2.552511	2.559777	1.150685
C	-2.099452	3.169727	-0.039388
C	-1.782101	2.678926	2.310855
C	-0.838359	3.806515	-0.040961

C	-0.582793	3.371657	2.341201
C	-0.105911	3.920671	1.155178
H	-0.021408	3.434056	3.267194
H	0.854571	4.424188	1.148260
O	-2.039611	-3.079942	0.510679
O	-5.089483	-2.393274	-3.029700
C	-0.790227	-3.533004	1.027338
H	-0.719214	-4.628133	0.989212
H	-0.758597	-3.200256	2.063530
C	-6.129801	-3.279523	-3.456640
H	-6.968187	-2.642127	-3.747834
H	-5.817585	-3.879133	-4.322918
H	-6.429998	-3.930221	-2.630730
C	-0.191298	4.269863	-1.298744
C	-0.026645	3.368064	-2.363922
C	0.375177	5.557519	-1.442300
C	0.670575	3.714161	-3.518391
H	-0.423765	2.364929	-2.257209
C	1.094251	5.902035	-2.601976
C	1.244311	4.984767	-3.637521
H	0.784429	2.984927	-4.316026
H	1.523034	6.896145	-2.678014
H	1.797140	5.259998	-4.530936
C	-3.046755	3.195876	-1.221750
H	-2.516475	3.437375	-2.145162
F	-2.196056	2.033810	3.422195
C	0.220444	6.559565	-0.426777
N	0.104894	7.408931	0.358935
C	-0.599706	-0.212935	0.113818
C	-1.709436	-0.288137	-1.943937
C	-0.662714	-0.167791	1.525306
C	0.680582	-0.270909	-0.532511
C	-0.494689	-0.332057	-2.652847
H	-2.659353	-0.326209	-2.465541
C	0.495748	-0.188586	2.257205
H	-1.629123	-0.106451	2.011966
C	1.869758	-0.299789	0.261904
C	0.688952	-0.317759	-1.950715
H	-0.513209	-0.384048	-3.735917
C	1.780014	-0.262726	1.644894
H	0.439951	-0.137079	3.341270
H	1.640302	-0.352544	-2.472558
N	-1.762646	-0.214888	-0.620153
C	5.551993	-4.299542	-1.072973
C	5.341553	-2.819045	-1.548318
C	5.432966	-2.618619	0.711387
C	5.595976	-4.166092	0.484630
H	4.756165	-4.966127	-1.420137
H	6.498662	-4.680845	-1.468906
H	4.810386	-4.741735	0.983618
H	6.558968	-4.494785	0.889275
C	6.210439	-2.077081	-0.506721
H	6.192449	-0.990975	-0.613388
H	7.252053	-2.416395	-0.523197
C	3.925404	-2.499620	-1.068650
C	3.992373	-2.380586	0.311722
H	5.540545	-2.630418	-2.602016
H	5.716467	-2.262220	1.702389
H	3.149032	-2.554651	0.970526
C	2.691917	-2.961523	-1.764695
O	1.712691	-3.410938	-1.203557
O	2.793110	-2.839759	-3.103242
C	1.647058	-3.309105	-3.842053
H	0.734175	-2.825951	-3.485908
H	1.849588	-3.056827	-4.882992
H	1.539540	-4.391422	-3.722831
C	2.982158	-0.276336	2.528777
C	3.173038	-1.245584	3.539769
C	3.940699	0.737707	2.399721
C	4.287242	-1.171180	4.389190
C	5.062558	0.789078	3.225542
H	3.803500	1.498680	1.643903
C	5.238063	-0.165453	4.228856
H	4.408557	-1.922850	5.161807
H	5.790144	1.583841	3.086392
H	6.104440	-0.127206	4.882723
C	2.267041	-2.426042	3.652260
O	1.751694	-2.999230	2.708630
O	2.104362	-2.825967	4.928871
C	1.289386	-3.999834	5.105424
H	1.284935	-4.191645	6.178405
H	0.274538	-3.816101	4.742107
H	1.713323	-4.847318	4.559687
C	3.590737	3.845792	0.210968
O	3.087102	4.880130	0.589555
O	4.827432	3.452842	0.608910
N	3.628389	1.706689	-1.143337
C	4.716453	1.696399	-1.907133
C	5.279779	2.933418	-2.561629
H	5.988792	2.635307	-3.336244
H	4.488523	3.549741	-3.003201
H	5.800701	3.540548	-1.813435
O	5.281555	0.564675	-2.066200
C	2.904605	2.885308	-0.754310
H	1.969306	2.586027	-0.271728
H	2.609274	3.498870	-1.614430
H	-3.498509	2.207258	-1.355967
C	-4.162852	4.236549	-1.000291
H	-4.696140	4.052916	-0.062873
H	-3.739808	5.246231	-0.949026
H	-4.883779	4.208004	-1.825882
Pd	3.634497	-0.311188	-0.692650
H	0.057554	-3.099384	0.490690
H	5.144944	4.153035	1.211587

MeCN

C	0.000000	0.000000	0.280813
N	0.000000	0.000000	1.441048
C	0.000000	0.000000	-1.181446
H	0.000000	1.026922	-1.561180
H	0.889341	-0.513461	-1.561180
H	-0.889341	-0.513461	-1.561180

methyl_2-iodobenzoate

C	-2.229576	-2.430241	-0.211411
C	-0.864446	-2.144915	-0.184435
C	-0.421021	-0.824429	-0.064619
C	-1.346635	0.228500	0.034302
C	-2.716866	-0.089659	0.037866
C	-3.162033	-1.399505	-0.093210
H	-2.556163	-3.461543	-0.312781
H	-0.145236	-2.953687	-0.249571
H	-3.420056	0.729494	0.145773
H	-4.226482	-1.614044	-0.098796
I	1.717785	-0.591500	0.085515
C	-1.049908	1.694351	0.150122
O	-1.767002	2.472654	0.748289
O	0.047419	2.066118	-0.526284

C	0.391533	3.457825	-0.428515
H	-0.405312	4.078365	-0.848122
H	0.548788	3.740279	0.616184
H	1.312193	3.568880	-1.001641

NBE-CO2Me

C	-2.430656	-0.305266	-1.098666
C	-2.003679	-1.101535	0.188337
C	-1.060908	0.928238	0.506289
C	-1.781136	1.096530	-0.873530
H	-2.086732	-0.794966	-2.014379
H	-3.523102	-0.238067	-1.147166
H	-1.077959	1.376891	-1.662669
H	-2.542306	1.881670	-0.810246
C	-2.074722	0.026867	1.249120
H	-1.723719	-0.291421	2.236039
H	-3.072512	0.472723	1.340480
C	-0.502090	-1.281082	0.082167
C	0.061013	-0.072295	0.273365
H	-2.586608	-2.006991	0.370485
H	-0.757448	1.862949	0.978319
H	0.009425	-2.189412	-0.216182
C	1.466780	0.321145	0.111650
O	1.863116	1.472610	0.134171
O	2.287498	-0.745078	-0.066469
C	3.674114	-0.419706	-0.235525
H	4.056914	0.112034	0.640896
H	4.187384	-1.374409	-0.358743
H	3.819457	0.211364	-1.117699

quinoline

C	2.398979	-0.716999	-0.000001
C	1.206140	-1.405629	-0.000002
C	-0.029306	-0.704849	0.000007
C	-0.014350	0.727490	0.000005
C	1.231511	1.408578	0.000000
C	2.412988	0.701198	0.000000
H	3.340163	-1.260096	-0.000001
H	1.169965	-2.490532	-0.000004
C	-1.266192	1.395231	0.000000
H	1.235485	2.496254	-0.000006
H	3.363299	1.227898	-0.000001
C	-2.424053	0.653723	-0.000002
C	-2.325509	-0.762186	0.000005
H	-1.292159	2.482647	-0.000001
H	-3.401115	1.127389	-0.000011
H	-3.235731	-1.362045	-0.000010
N	-1.188736	-1.428693	-0.000004

T1_conf_1

Pd	1.064459	0.500673	0.307788
C	0.782789	3.320746	0.148877
C	2.969834	2.515258	-0.278252
C	1.189765	4.633722	-0.064145
C	3.435345	3.808502	-0.499435
H	0.454375	5.425225	0.028072
H	4.481236	3.943305	-0.752069
N	1.683138	2.335390	0.039483
H	2.872481	5.888212	-0.557054
C	2.531575	4.870704	-0.387919
N	3.047994	0.137350	-0.127722
N	0.353150	-1.425047	0.486571
N	-0.707051	1.529481	0.644444
C	-0.083595	-2.492862	0.536413
C	-0.635008	-3.838310	0.590362
H	-0.818417	-4.119967	1.632271
H	-1.581872	-3.863995	0.037513
H	0.076728	-4.542309	0.147441
C	3.800892	1.250140	-0.367613
C	-0.624989	2.879942	0.500578
O	5.002922	1.318173	-0.616101
O	-1.527473	3.711765	0.616288
C	3.604615	-1.145917	-0.209796
C	4.150855	-1.641240	-1.412640
C	3.530054	-2.004856	0.906358
C	4.650955	-2.949108	-1.479824
C	3.997258	-3.322460	0.832442
C	4.564715	-3.774199	-0.359620
H	5.086118	-3.329237	-2.396312
H	3.950518	-3.979050	1.693117
H	4.947030	-4.789897	-0.416044
C	-1.900271	0.890711	1.026540
C	-3.013550	0.754713	0.170154
C	-1.923095	0.243841	2.269453
C	-4.107018	-0.024275	0.602082
C	-2.994128	-0.522302	2.700872
C	-4.092391	-0.652256	1.855101
H	-2.956375	-0.994927	3.676688
H	-4.944903	-1.250817	2.162784
O	4.115591	-0.780957	-2.464599
O	2.970151	-1.451081	2.022310
C	4.830583	-1.121157	-3.638971
H	5.890397	-1.308417	-3.421624
H	4.402055	-2.002005	-4.138104
H	4.744402	-0.257544	-4.301076
C	2.644457	-2.298865	3.106515
H	2.113674	-1.672368	3.825886
H	1.989122	-3.123660	2.789270
H	3.540827	-2.720075	3.582030
C	-5.290135	-0.250501	-0.280276
C	-6.312073	0.698593	-0.393464
C	-5.417093	-1.450315	-1.015705
C	-7.423516	0.467373	-1.205095
H	-6.223172	1.625586	0.165059
C	-6.536803	-1.687032	-1.832125
C	-7.538373	-0.726031	-1.924435
H	-8.203904	1.219963	-1.275082
H	-6.607150	-2.617532	-2.386590
H	-8.403802	-0.905448	-2.555165
C	-2.961899	1.353062	-1.219615
H	-3.977894	1.471938	-1.608159
H	-2.531621	2.356030	-1.164307
C	-2.150684	0.475604	-2.192300
H	-1.120517	0.355585	-1.842822
H	-2.593795	-0.522594	-2.283664
H	-2.123095	0.930110	-3.189323
F	-0.837860	0.345658	3.066416
C	-4.380749	-2.439022	-0.939606
N	-3.543842	-3.244950	-0.891542

T1_conf_2

Pd	1.000364	0.555311	0.238032
C	0.842104	3.357175	-0.208318
C	2.984003	2.414080	-0.572779
C	1.305691	4.623995	-0.547116
C	3.503992	3.656348	-0.924785
H	0.608858	5.454354	-0.520169
H	4.551008	3.716961	-1.200414

N	1.693302	2.324413	-0.232081
H	3.036471	5.745671	-1.175278
C	2.651623	4.765981	-0.906553
N	2.973936	0.071620	-0.135727
N	0.343151	-1.349296	0.661011
N	-0.729636	1.681521	0.424951
C	0.215599	-2.484906	0.826401
C	0.118852	-3.923112	1.020328
H	1.058187	-4.381523	0.693158
H	-0.039303	-4.144754	2.080674
H	-0.729790	-4.300107	0.443291
C	3.759315	1.111099	-0.538261
C	-0.577952	3.014107	0.195322
O	4.951867	1.092364	-0.835901
O	-1.438038	3.894487	0.259775
C	3.470072	-1.238034	-0.092401
C	3.852883	-1.919305	-1.266483
C	3.472276	-1.937443	1.131650
C	4.252751	-3.262300	-1.211371
C	3.845463	-3.287352	1.187320
C	4.240309	-3.930209	0.012285
H	4.559035	-3.787334	-2.108114
H	3.860761	-3.823983	2.128590
H	4.550326	-4.971029	0.053537
C	-1.959144	1.180369	0.894124
C	-2.884081	0.559084	0.032247
C	-2.235299	1.232759	2.264960
C	-4.065429	0.018317	0.581297
C	-3.395540	0.708747	2.813249
C	-4.313089	0.101939	1.958213
H	-3.563026	0.780043	3.882647
H	-5.229869	-0.319335	2.360767
O	3.765016	-1.192115	-2.410957
O	3.067550	-1.207621	2.210855
C	4.274438	-1.752025	-3.608641
H	5.335444	-2.016487	-3.507895
H	3.706942	-2.641634	-3.916802
H	4.166143	-0.976609	-4.369184
C	2.914084	-1.866823	3.453351
H	2.534233	-1.113492	4.145752
H	2.191562	-2.693874	3.386681
H	3.868907	-2.258351	3.830186
C	-5.097903	-0.625884	-0.282127
C	-6.295173	0.039663	-0.569521
C	-4.922170	-1.923742	-0.814325
C	-7.280299	-0.550344	-1.363358
H	-6.441363	1.037282	-0.166433
C	-5.911266	-2.518815	-1.616320
C	-7.088718	-1.829746	-1.890942
H	-8.197747	-0.007772	-1.573758
H	-5.747720	-3.516418	-2.011743
H	-7.852432	-2.288976	-2.511289
C	-2.622938	0.579196	-1.457552
H	-1.544823	0.517834	-1.632668
H	-3.075275	-0.292664	-1.939366
C	-3.174783	1.865900	-2.101867
H	-4.266684	1.904480	-2.008396
H	-2.763391	2.752504	-1.609632
H	-2.923313	1.903484	-3.168308
F	-1.329166	1.808886	3.078592
C	-3.724933	-2.661234	-0.532899
N	-2.767468	-3.286030	-0.321523

T1_conf_3

Pd	-1.040005	0.597432	0.273279
C	-0.945336	3.371250	-0.318692
C	-2.979832	2.297249	-0.895177
C	-1.422302	4.593636	-0.780032
C	-3.512410	3.494613	-1.364929
H	-0.770279	5.458419	-0.726232
H	-4.517469	3.487462	-1.772031
N	-1.739458	2.295458	-0.393325
H	-3.117005	5.592340	-1.662254
C	-2.721938	4.647619	-1.299500
N	-2.871702	-0.037577	-0.427215
N	-0.337057	-1.211818	0.966472
N	0.583003	1.824038	0.647054
C	-0.060992	-2.295480	1.252836
C	0.251506	-3.680064	1.570152
H	1.209873	-3.936748	1.106975
H	0.315589	-3.814195	2.654415
H	-0.546236	-4.315570	1.170580
C	-3.666603	0.943530	-0.942454
C	0.442441	3.113806	0.241907
O	-4.784646	0.835188	-1.441544
O	1.285135	4.012349	0.263433
C	-3.270481	-1.381076	-0.417036
C	-4.370805	-1.822922	0.346029
C	-2.482480	-2.337363	-1.093134
C	-4.688887	-3.187513	0.410299
C	-2.776538	-3.704137	-1.002229
C	-3.885911	-4.110333	-0.257956
H	-5.540128	-3.531588	0.985476
H	-2.178674	-4.438487	-1.529233
H	-4.131311	-5.167593	-0.202569
C	1.794834	1.308630	1.140340
C	2.864168	0.951147	0.292381
C	1.869880	0.981932	2.499668
C	3.957878	0.253142	0.842942
C	2.952065	0.313706	3.051522
C	3.997504	-0.056124	2.209460
H	2.957544	0.088394	4.112695
H	4.850638	-0.595649	2.610645
O	-5.039442	-0.847843	1.015075
O	-1.433162	-1.825615	-1.801332
C	-6.254029	-1.182608	1.662563
H	-6.977229	-1.615528	0.958701
H	-6.094237	-1.883444	2.494422
H	-6.649838	-0.244516	2.055889
C	-0.471600	-2.718373	-2.336011
H	0.298637	-2.089952	-2.785625
H	-0.012137	-3.336540	-1.552000
H	-0.904433	-3.372329	-3.104960
C	5.077256	-0.226578	-0.020981
C	6.169213	0.592823	-0.326681
C	5.068852	-1.539888	-0.542896
C	7.218231	0.129868	-1.122494
H	6.184655	1.604495	0.067543
C	6.125397	-2.009415	-1.343068
C	7.198228	-1.171981	-1.631333
H	8.054574	0.786507	-1.345302
H	6.092708	-3.022748	-1.730863
H	8.014543	-1.532174	-2.250097
C	2.779775	1.260096	-1.188525
H	2.328689	2.247119	-1.321004
H	3.790680	1.324773	-1.604101
C	1.980177	0.207218	-1.979799
H	2.438942	-0.783500	-1.894177
H	0.953017	0.132415	-1.610404

H 1.941774 0.476165 -3.041984
F 0.829586 1.300812 3.294574
C 3.963108 -2.411637 -0.266552
N 3.073185 -3.134100 -0.069454

T1_conf_4

Pd 1.010450 0.578728 0.196705
C 1.011829 3.345942 -0.438221
C 3.027299 2.206414 -0.948173
C 1.541678 4.551459 -0.885977
C 3.610594 3.383844 -1.407889
H 0.919054 5.438256 -0.844257
H 4.628362 3.343715 -1.779995
N 1.769345 2.243261 -0.493130
H 3.290835 5.491540 -1.725251
C 2.855218 4.561288 -1.371659
N 2.858918 -0.109619 -0.413082
N 0.331488 -1.188280 1.010076
N -0.603766 1.846454 0.464562
C 0.201756 -2.261257 1.416116
C 0.092775 -3.632517 1.888106
H 0.083710 -3.658391 2.982055
H -0.832765 -4.062127 1.495080
H 0.956791 -4.192728 1.513768
C 3.685743 0.838666 -0.939154
C -0.390961 3.140124 0.101644
O 4.815190 0.693177 -1.401993
O -1.192359 4.075357 0.133118
C 3.234925 -1.457632 -0.341609
C 2.440462 -2.426404 -0.992367
C 4.310434 -1.888365 0.462350
C 2.705445 -3.793675 -0.838980
C 4.599767 -3.254997 0.589874
C 3.792033 -4.189961 -0.056407
H 2.100380 -4.536627 -1.345317
H 5.432748 -3.590884 1.195777
H 4.016398 -5.248422 0.046228
C -1.849947 1.434904 0.971285
C -2.756537 0.704665 0.174467
C -2.163740 1.679155 2.312169
C -3.951194 0.237144 0.760981
C -3.342415 1.236274 2.893385
C -4.235503 0.513202 2.106764
H -3.539903 1.455264 3.937309
H -5.162751 0.148498 2.539441
O 1.414056 -1.925166 -1.737956
O 4.982443 -0.899912 1.108154
C 0.403399 -2.811103 -2.192447
H 0.791179 -3.528357 -2.928480
H -0.064329 -3.353467 -1.360614
H -0.350327 -2.180015 -2.666867
C 6.181892 -1.228450 1.786352
H 6.587279 -0.282224 2.149234
H 5.999014 -1.893985 2.642196
H 6.907889 -1.699627 1.110587
C -4.969167 -0.519798 -0.023469
C -6.202951 0.071228 -0.322980
C -4.756758 -1.849254 -0.458155
C -7.186066 -0.617402 -1.035002
H -6.378367 1.091305 0.005117
C -5.744672 -2.543496 -1.178543
C -6.957488 -1.925962 -1.467615
H -8.130885 -0.129076 -1.256773
H -5.552156 -3.562661 -1.498892
H -7.719285 -2.462835 -2.024695
C -2.461879 0.548100 -1.302144
H -1.387086 0.397641 -1.443492
H -2.961662 -0.336269 -1.706168
C -2.915100 1.791351 -2.092269
H -4.004880 1.901765 -2.040961
H -2.468373 2.701711 -1.681193
H -2.630948 1.703920 -3.147516
F -1.279317 2.360270 3.063656
C -3.528132 -2.527085 -0.162701
N -2.548536 -3.115511 0.053773

T1_conf_5

Pd -1.127887 0.389009 0.026886
C -0.493945 3.141906 -0.251617
C -2.745201 2.591137 -0.737816
C -0.733435 4.488219 -0.507790
C -3.044756 3.923210 -1.006941
H 0.085430 5.189744 -0.393389
H -4.060570 4.175999 -1.290010
N -1.495960 2.265605 -0.385866
H -2.234469 5.918783 -1.097310
C -2.023340 4.873087 -0.892498
N -3.129356 0.253645 -0.475668
N -0.894880 -1.595830 0.533488
N 0.756688 1.200694 0.348611
C -1.083833 -2.696563 0.826925
C -1.398510 -4.074602 1.175370
H -0.701442 -4.760824 0.684631
H -1.334811 -4.213369 2.258997
H -2.419525 -4.285813 0.837057
C -3.728800 1.438865 -0.787451
C 0.826246 2.553990 0.204705
O -4.902411 1.637328 -1.093327
O 1.791266 3.292642 0.402254
C -3.879388 -0.925853 -0.378388
C -4.853017 -1.095094 0.628905
C -3.581086 -2.012814 -1.224997
C -5.529144 -2.316003 0.768376
C -4.239647 -3.242317 -1.075536
C -5.213898 -3.373835 -0.083117
H -6.286016 -2.447098 1.532178
H -4.028602 -4.073296 -1.738233
H -5.742514 -4.317605 0.021833
C 1.861304 0.455580 0.807749
C 2.997599 0.175939 0.016663
C 1.767430 -0.120641 2.082529
C 4.001402 -0.664733 0.550286
C 2.750715 -0.935627 2.615732
C 3.875565 -1.199838 1.838938
H 2.629899 -1.340230 3.614946
H 4.664929 -1.834169 2.230965
O -5.038627 -0.020682 1.437798
O -2.610110 -1.771332 -2.152315
C -6.109715 -0.046682 2.366187
H -7.071667 -0.209585 1.862744
H -5.965802 -0.820338 3.133685
H -6.112642 0.934715 2.843521
C -2.208595 -2.831570 -2.999334
H -1.420632 -2.423784 -3.635052
H -1.807232 -3.680098 -2.425223
H -3.035365 -3.187077 -3.629127
C 5.210926 -1.038115 -0.241288
C 5.105350 -1.881283 -1.355191
C 6.500959 -0.594129 0.127991
C 6.228464 -2.263445 -2.088045

H	4.121876	-2.244885	-1.638515
C	7.634760	-0.982288	-0.608133
C	7.497640	-1.812502	-1.715665
H	6.114087	-2.918946	-2.947038
H	8.612244	-0.622312	-0.303095
H	8.374995	-2.107938	-2.283329
C	3.142992	0.804705	-1.354556
H	3.473146	0.049890	-2.076496
H	2.162422	1.151940	-1.691863
C	4.138213	1.980901	-1.364033
H	3.822387	2.743387	-0.649352
H	5.146230	1.645337	-1.098545
H	4.184020	2.430311	-2.363121
F	0.656430	0.118844	2.813408
C	6.681828	0.270860	1.259084
N	6.871097	0.966860	2.171456

T1_conf_6

Pd	1.098941	0.403561	0.261451
C	0.455998	3.165041	0.363725
C	2.739851	2.694601	-0.053467
C	0.693799	4.534650	0.304826
C	3.037400	4.052031	-0.127325
H	-0.140577	5.211008	0.453635
H	4.062941	4.345081	-0.322947
N	1.478253	2.319776	0.188699
H	2.209417	6.038000	0.005432
C	1.999911	4.973342	0.056515
N	3.137240	0.345251	-0.071526
N	0.805125	-1.637466	0.243151
N	-0.816076	1.156982	0.563224
C	0.921674	-2.784306	0.179401
C	1.148007	-4.220214	0.097732
H	2.228580	-4.390391	0.028035
H	0.757487	-4.716324	0.991670
H	0.653255	-4.633640	-0.786425
C	3.735572	1.562785	-0.215918
C	-0.890648	2.516181	0.611782
O	4.921935	1.804746	-0.426178
O	-1.883553	3.218093	0.812014
C	3.873870	-0.840034	-0.197669
C	4.449685	-1.225101	-1.426163
C	3.952115	-1.724912	0.897692
C	5.110635	-2.456577	-1.547443
C	4.590265	-2.967459	0.774205
C	5.170630	-3.312562	-0.448801
H	5.566160	-2.751483	-2.485072
H	4.671051	-3.639584	1.620621
H	5.686835	-4.264290	-0.542988
C	-1.941676	0.339670	0.788684
C	-3.047783	0.267829	-0.089743
C	-1.905487	-0.512456	1.900567
C	-4.086727	-0.645096	0.205734
C	-2.919234	-1.407349	2.197767
C	-4.016672	-1.460983	1.345284
H	-2.844062	-2.029548	3.083174
H	-4.828491	-2.149568	1.558068
O	4.278523	-0.344235	-2.445527
O	3.348514	-1.282264	2.037358
C	4.979192	-0.566242	-3.657460
H	6.062271	-0.626956	-3.488193
H	4.639357	-1.480863	-4.163932
H	4.759803	0.295791	-4.289887
C	3.276952	-2.153175	3.150842
H	2.710681	-1.615659	3.913122
H	2.751098	-3.086977	2.901614
H	4.273443	-2.399538	3.541772
C	-5.277706	-0.801349	-0.679210
C	-5.139646	-1.258088	-1.997460
C	-6.586279	-0.537707	-0.210978
C	-6.245009	-1.439362	-2.827203
H	-4.143222	-1.477718	-2.366985
C	-7.702125	-0.725044	-1.046719
C	-7.531863	-1.172647	-2.352448
H	-6.102036	-1.794520	-3.844081
H	-8.693295	-0.510138	-0.659992
H	-8.396227	-1.313218	-2.994610
C	-3.086224	1.168281	-1.308649
H	-4.093227	1.166608	-1.734241
H	-2.890593	2.194532	-0.985462
C	-2.075945	0.768565	-2.400768
H	-1.052279	0.779038	-2.015364
H	-2.278516	-0.238471	-2.784507
H	-2.131223	1.466024	-3.244634
F	-0.825584	-0.465599	2.713150
C	-6.813807	-0.064148	1.124982
N	-7.046737	0.311128	2.201004

T1_conf_7

Pd	1.129932	0.398971	0.211223
C	0.466526	3.158145	0.241561
C	2.749574	2.694037	-0.184965
C	0.692499	4.527341	0.144128
C	3.035025	4.051291	-0.300315
H	-0.144920	5.201152	0.287281
H	4.056352	4.346817	-0.513497
N	1.493137	2.315961	0.077750
H	2.192462	6.033650	-0.214259
C	1.992115	4.969207	-0.131641
N	3.169721	0.349387	-0.126829
N	0.857179	-1.643749	0.268994
N	-0.787677	1.144513	0.493725
C	0.991762	-2.790351	0.247792
C	1.241655	-4.224424	0.218731
H	2.324409	-4.378957	0.145848
H	0.867501	-4.692468	1.134557
H	0.746623	-4.679841	-0.644395
C	3.754739	1.566905	-0.317595
C	-0.869534	2.504269	0.532179
O	4.937283	1.813358	-0.544331
O	-1.857480	3.201628	0.763159
C	3.919174	-0.831136	-0.216355
C	4.496078	-1.250116	-1.433281
C	4.013042	-1.677423	0.907959
C	5.172922	-2.476190	-1.515491
C	4.667758	-2.914701	0.824094
C	5.248488	-3.293466	-0.388728
H	5.629171	-2.796546	-2.444397
H	4.761138	-3.556329	1.692601
H	5.777286	-4.240794	-0.452493
C	-1.904323	0.334173	0.780797
C	-2.987044	0.153595	-0.108072
C	-1.875526	-0.407751	1.970140
C	-4.005189	-0.761654	0.245527
C	-2.874291	-1.295897	2.329085
C	-3.946246	-1.463747	1.456541
H	-2.805971	-1.830376	3.270566
H	-4.745730	-2.152995	1.711287
O	4.310393	-0.406648	-2.481271
O	3.407427	-1.204890	2.034637

C	5.016763	-0.655723	-3.684585
H	6.100229	-0.695167	-3.511613
H	4.691556	-1.590425	-4.163277
H	4.786107	0.183014	-4.343772
C	3.357442	-2.036677	3.178721
H	2.788297	-1.481213	3.925881
H	2.844623	-2.986908	2.966880
H	4.360427	-2.253667	3.570481
C	-5.157353	-1.040787	-0.661883
C	-4.965480	-1.717212	-1.873770
C	-6.478002	-0.677599	-0.312960
C	-6.034150	-2.014944	-2.718606
H	-3.957799	-2.018388	-2.144998
C	-7.556895	-0.980655	-1.162785
C	-7.334365	-1.644957	-2.364370
H	-5.853078	-2.541785	-3.651482
H	-8.559631	-0.685758	-0.870097
H	-8.169648	-1.874899	-3.019101
C	-3.063184	0.962462	-1.387160
H	-2.072007	1.366224	-1.611674
H	-3.332377	0.310247	-2.224951
C	-4.081901	2.114929	-1.296252
H	-5.095337	1.731935	-1.136159
H	-3.822424	2.777976	-0.468565
H	-4.082752	2.694876	-2.226785
F	-0.813497	-0.258219	2.792969
C	-6.747317	0.016119	0.914452
N	-7.007992	0.572744	1.901827

Norbornene_Ins_no_CN_MPAA_TS

Pd	3.306889	-0.870301	0.258565
C	6.111569	-0.477476	0.061684
C	5.381255	-2.668549	-0.469418
C	7.437077	-0.825436	-0.178535
C	6.687731	-3.074691	-0.726840
H	8.203341	-0.068871	-0.050395
H	6.860386	-4.099842	-1.035060
N	5.159489	-1.405176	-0.092526
H	8.745146	-2.433530	-0.770004
C	7.717765	-2.138721	-0.575810
N	3.006066	-2.864945	-0.241738
N	4.260521	0.923719	0.604984
C	4.145142	-3.539993	-0.585975
C	5.616928	0.894838	0.485730
O	4.251509	-4.711868	-0.943679
O	6.410838	1.819304	0.651481
C	1.762965	-3.494997	-0.384990
C	1.307405	-3.926449	-1.650075
C	0.897902	-3.628874	0.721469
C	0.066548	-4.561696	-1.789753
C	-0.359536	-4.233944	0.580969
C	-0.748249	-4.715836	-0.670249
H	-0.266231	-4.924827	-2.754742
H	-1.009228	-4.373409	1.437284
H	-1.700699	-5.227439	-0.771598
C	3.574501	2.074002	1.038330
C	2.828087	2.863462	0.138321
C	3.492740	2.350011	2.405870
C	2.016494	3.895913	0.647924
C	2.722510	3.382639	2.918241
C	1.982220	4.154428	2.025508
H	2.702826	3.558193	3.988697
H	1.362216	4.964769	2.397213
O	2.136123	-3.637944	-2.688802
O	1.375750	-3.134726	1.900655
C	1.879724	-4.237881	-3.947210
H	1.840796	-5.331639	-3.866831
H	0.941683	-3.872404	-4.389798
H	2.713980	-3.951170	-4.589782
C	0.532244	-3.177105	3.037408
H	1.095234	-2.701637	3.843027
H	-0.400512	-2.619175	2.869800
H	0.290897	-4.208907	3.326943
C	1.165022	4.722585	-0.259019
C	-0.065312	4.239014	-0.720755
C	1.571960	6.012183	-0.666660
C	-0.875169	5.002128	-1.564398
H	-0.397473	3.249430	-0.417070
C	0.757665	6.785142	-1.513641
C	-0.458811	6.277843	-1.958296
H	-1.829748	4.604386	-1.899797
H	1.093064	7.773373	-1.813383
H	-1.087415	6.875650	-2.612198
C	2.973503	2.615348	-1.345927
H	3.054508	1.538499	-1.528443
H	2.085242	2.969779	-1.876446
C	4.228000	3.318525	-1.901892
H	4.149452	4.404183	-1.779734
H	5.125800	2.991267	-1.368006
H	4.351799	3.099738	-2.969176
F	4.139351	1.526244	3.264655
C	2.828493	6.549256	-0.230119
N	3.843320	7.009463	0.105121
C	0.304621	-0.398575	-0.171598
C	1.124774	0.119581	1.955380
C	0.565363	-0.724341	-1.527867
C	-1.042787	-0.212072	0.267330
C	-0.164305	0.407541	2.435596
H	1.992299	0.208972	2.598561
C	-0.480062	-0.868348	-2.410636
H	1.592398	-0.875607	-1.842755
C	-2.121386	-0.472713	-0.646959
C	-1.241914	0.224712	1.597896
H	-0.285759	0.763708	3.452616
C	-1.816777	-0.770625	-1.966348
H	-0.277396	-1.104982	-3.450751
H	-2.249733	0.428149	1.937248
H	-2.617314	-0.969405	-2.671601
N	1.351256	-0.270173	0.707506
Pd	-3.986905	0.398368	-0.260739
C	-5.685554	-3.645384	0.323752
C	-5.687832	-2.169108	-0.166805
C	-3.752945	-2.970384	-1.042442
C	-4.330479	-4.185017	-0.232827
H	-5.761764	-3.722154	1.413115
H	-6.536836	-4.186327	-0.102676
H	-3.647124	-4.517103	0.554896
H	-4.477694	-5.029326	-0.913913
C	-5.055339	-2.331984	-1.567086
H	-4.902411	-1.382975	-2.090288
H	-5.626982	-3.008859	-2.210525
C	-4.543608	-1.472585	0.594912
C	-3.324846	-2.016925	0.053945
H	-6.653059	-1.668229	-0.113657
H	-2.975388	-3.239744	-1.755036
H	-2.499714	-2.307633	0.692010
C	-4.668541	-1.206188	2.042002
O	-5.677333	-0.750975	2.577779
O	-3.565832	-1.499656	2.751177

C	-3.588243	-1.129759	4.144493
H	-4.371454	-1.679215	4.671838
H	-2.602386	-1.394860	4.526510
H	-3.769890	-0.056508	4.248582
N	-5.825328	1.541953	-0.331777
C	-7.039740	1.358177	0.074571
C	-8.227019	2.152589	-0.412691
H	-8.177795	3.179464	-0.031969
H	-8.247353	2.210283	-1.504995
H	-9.145729	1.689907	-0.050149
O	-7.397512	0.447443	0.968096
C	-5.599263	2.652762	-1.274098
H	-6.065333	3.578686	-0.922532
H	-6.042716	2.417853	-2.251593
C	-4.117198	2.975886	-1.533447
O	-3.231695	2.131169	-1.099897
O	-3.874735	4.004188	-2.156704
H	-6.645259	0.025390	1.469018

Norbornene_Ins_no_CN_OAc_TS

Pd	3.022005	-0.852985	0.053858
C	5.817562	-0.704558	-0.451332
C	4.907903	-2.891491	-0.530332
C	7.085131	-1.184531	-0.765842
C	6.150864	-3.429195	-0.852398
H	7.904565	-0.477938	-0.837983
H	6.229080	-4.501044	-0.996854
N	4.802487	-1.570557	-0.347190
H	8.222824	-2.959185	-1.216527
C	7.242941	-2.561037	-0.968822
N	2.572997	-2.874543	-0.017064
N	4.120011	0.903024	0.032522
C	3.627164	-3.683063	-0.335476
C	5.460097	0.743753	-0.173866
O	3.637637	-4.907921	-0.441348
O	6.328404	1.613346	-0.169751
C	1.312061	-3.429041	0.243948
C	0.575621	-4.087621	-0.762645
C	0.714205	-3.247218	1.509076
C	-0.696848	-4.609053	-0.493160
C	-0.571535	-3.738946	1.774225
C	-1.252546	-4.432262	0.773473
H	-1.252998	-5.142194	-1.254951
H	-1.023818	-3.619034	2.751169
H	-2.232565	-4.848766	0.986967
C	3.597265	2.090323	0.569836
C	2.602619	2.818115	-0.119230
C	3.938364	2.471012	1.873943
C	1.936162	3.866695	0.551013
C	3.325386	3.532178	2.523049
C	2.313446	4.218316	1.856892
H	3.629698	3.791125	3.531539
H	1.801374	5.035098	2.355948
O	1.175509	-4.127729	-1.982894
O	1.470871	-2.564221	2.417098
C	0.551455	-4.866745	-3.017222
H	0.422447	-5.920577	-2.738240
H	-0.426559	-4.441132	-3.285993
H	1.220973	-4.800878	-3.876771
C	0.925551	-2.318666	3.701642
H	1.690215	-1.761480	4.246422
H	0.009627	-1.713994	3.641067
H	0.709298	-3.253122	4.236392
C	0.790683	4.585970	-0.074086
C	-0.368713	3.883994	-0.434196
C	0.811441	5.981602	-0.299393
C	-1.463012	4.524509	-1.013190
H	-0.406015	2.812625	-0.258561
C	-0.297722	6.633406	-0.869527
C	-1.427077	5.905585	-1.228907
H	-2.326775	3.934524	-1.303304
H	-0.252047	7.705359	-1.034794
H	-2.274961	6.412282	-1.681467
C	2.369218	2.486006	-1.577742
H	2.307635	1.399957	-1.701423
H	1.421947	2.902141	-1.925933
C	3.515722	3.032395	-2.451128
H	3.550518	4.126383	-2.398289
H	4.483941	2.651150	-2.112232
H	3.372403	2.744009	-3.499159
F	4.864979	1.746281	2.532875
C	1.967789	6.765679	0.028397
N	2.883924	7.435756	0.283531
C	0.016205	-0.430049	-0.361839
C	0.879195	0.496022	1.602826
C	0.252758	-0.985909	-1.642924
C	-1.326460	-0.207689	0.082400
C	-0.408236	0.796117	2.083146
H	1.761193	0.754252	2.177498
C	-0.809452	-1.330777	-2.445450
H	1.275396	-1.163743	-1.955851
C	-2.419865	-0.625485	-0.754216
C	-1.505131	0.418921	1.340299
H	-0.514902	1.305469	3.034618
C	-2.138605	-1.180336	-1.993767
H	-0.625354	-1.756286	-3.427306
H	-2.509538	0.598112	1.704938
H	-2.944016	-1.520080	-2.634520
N	1.086088	-0.113458	0.443938
Pd	-4.191074	0.501472	-0.646864
O	-3.747922	2.337174	-1.815512
O	-5.692583	2.025361	-0.820508
C	-4.915040	2.755641	-1.522838
C	-5.361480	4.123714	-1.968596
H	-4.906380	4.873946	-1.310312
H	-5.013341	4.316476	-2.986958
H	-6.447749	4.215052	-1.908762
C	-6.329249	-3.116845	0.605260
C	-6.126582	-1.832544	-0.253074
C	-4.161515	-2.929676	-0.539404
C	-4.956812	-3.844923	0.453207
H	-6.587959	-2.883177	1.640532
H	-7.146134	-3.714418	0.187485
H	-4.432232	-3.968445	1.406152
H	-5.068870	-4.840827	0.012691
C	-5.311387	-2.406428	-1.429167
H	-5.011005	-1.647493	-2.157508
H	-5.835221	-3.212337	-1.953599
C	-5.065670	-1.015377	0.492454
C	-3.807460	-1.708003	0.297640
H	-7.038329	-1.282369	-0.482134
H	-3.311693	-3.415697	-1.016175
H	-3.108943	-1.822218	1.120057
C	-5.481291	-0.387533	1.779158
O	-6.637705	-0.236486	2.111089
O	-4.431723	-0.009161	2.554300
C	-4.787565	0.653176	3.781764
H	-5.397203	-0.003713	4.407610

H	-3.841484	0.884432	4.272651
H	-5.348470	1.567584	3.571033

Norbornene_Ins_with_CN_OAc_TS

Pd	3.285114	-0.339512	0.489469
C	5.747151	1.056583	0.285086
C	5.875028	-1.266420	-0.183775
C	7.113297	1.208248	0.068880
C	7.244164	-1.174379	-0.418991
H	7.551343	2.194254	0.176922
H	7.783864	-2.071696	-0.700995
N	5.204636	-0.159751	0.154522
H	8.927639	0.170702	-0.458577
C	7.859615	0.075989	-0.283703
N	3.731160	-2.295532	0.048267
N	3.495909	1.707348	0.738084
C	5.028891	-2.524971	-0.308101
C	4.770862	2.169579	0.635732
O	5.538931	-3.576614	-0.687123
O	5.172805	3.328324	0.762930
C	2.724734	-3.249061	-0.157670
C	2.354996	-3.644326	-1.459974
C	1.944360	-3.690875	0.930453
C	1.265271	-4.499079	-1.667879
C	0.837700	-4.525229	0.725500
C	0.518138	-4.926849	-0.571540
H	0.984979	-4.811841	-2.666352
H	0.237838	-4.870567	1.558676
H	-0.331269	-5.585965	-0.730194
C	2.402882	2.552224	1.005366
C	1.671661	3.186393	-0.023467
C	1.915781	2.625064	2.315727
C	0.499699	3.897207	0.315146
C	0.745131	3.285769	2.651699
C	0.038474	3.929576	1.638477
H	0.408041	3.293256	3.682538
H	-0.871382	4.472682	1.876295
O	3.091375	-3.083750	-2.461109
O	2.333939	-3.223765	2.152770
C	2.839144	-3.494116	-3.793074
H	2.984843	-4.575364	-3.915804
H	1.821271	-3.228781	-4.114166
H	3.562781	-2.960260	-4.411934
C	1.563827	-3.588289	3.284902
H	2.042831	-3.104414	4.138566
H	0.528207	-3.230308	3.198789
H	1.560384	-4.675294	3.441803
C	-0.238781	4.697960	-0.707374
C	0.278032	5.931861	-1.124352
C	-1.478135	4.295895	-1.253229
C	-0.396049	6.731058	-2.047416
H	1.218538	6.265594	-0.698622
C	-2.165152	5.102322	-2.182314
C	-1.620891	6.317526	-2.579288
H	0.032564	7.683359	-2.346578
H	-3.116742	4.762904	-2.579298
H	-2.149498	6.939462	-3.295061
C	2.127585	3.033022	-1.459708
H	2.527540	2.019662	-1.578018
H	1.260589	3.112591	-2.125604
C	3.203621	4.045475	-1.895355
H	2.793703	5.059895	-1.937691
H	4.044734	4.050106	-1.197739
H	3.576133	3.794638	-2.895618
F	2.595342	1.971636	3.286331
C	-2.086150	3.047602	-0.909994
N	-2.664300	2.061189	-0.720310
C	0.314958	-0.677220	-0.105127
C	0.852480	-0.416887	2.156915
C	0.741842	-0.776130	-1.453435
C	-1.080400	-0.720151	0.205718
C	-0.497932	-0.481020	2.538948
H	1.633580	-0.259215	2.890861
C	-0.193375	-0.878645	-2.457458
H	1.804562	-0.789192	-1.670680
C	-2.031214	-0.791581	-0.863738
C	-1.462819	-0.625114	1.567216
H	-0.761193	-0.388777	3.587053
C	-1.577413	-0.880719	-2.166886
H	0.134580	-0.952913	-3.490895
H	-2.514208	-0.647523	1.831165
H	-2.284116	-0.940730	-2.987771
N	1.244437	-0.512909	0.892495
Pd	-3.799436	0.260172	-0.458952
O	-4.796490	1.398803	2.027013
O	-5.536992	1.370428	-0.100230
C	-5.641278	1.668565	1.159014
C	-6.955071	2.338840	1.535444
H	-7.680778	1.543935	1.745786
H	-6.826700	2.941993	2.437610
H	-7.344846	2.948770	0.716459
C	-6.222965	-3.345829	-1.098651
C	-5.864752	-1.841829	-1.287398
C	-3.915536	-2.879497	-1.810541
C	-4.867301	-4.059119	-1.403698
H	-6.607673	-3.552272	-0.096924
H	-6.995882	-3.638846	-1.817079
H	-4.478115	-4.624143	-0.550249
H	-4.952945	-4.756195	-2.243611
C	-4.919344	-1.929595	-2.503756
H	-4.493177	-0.963258	-2.790419
H	-5.394332	-2.386248	-3.378541
C	-4.885759	-1.519137	-0.155423
C	-3.648929	-2.165342	-0.497855
H	-6.712317	-1.161191	-1.346734
H	-3.026689	-3.187544	-2.361711
H	-3.029325	-2.623817	0.264350
C	-5.426527	-1.463488	1.233710
O	-6.602652	-1.298109	1.484399
O	-4.474406	-1.649752	2.175124
C	-4.890880	-1.362539	3.526024
H	-5.738002	-1.993581	3.806452
H	-4.022510	-1.585965	4.147949
H	-5.159120	-0.305856	3.590487

Norbornene_Ins_with_CN_MPAA_TS

Pd	3.719231	-0.183527	0.395467
C	6.038401	1.428640	0.105159
C	6.341272	-0.861799	-0.434781
C	7.372215	1.705568	-0.178436
C	7.682204	-0.643862	-0.739568
H	7.728227	2.723575	-0.065719
H	8.281333	-1.483270	-1.074901
N	5.596951	0.172771	-0.029794
H	9.237957	0.845033	-0.830778
C	8.193547	0.652351	-0.602037
N	4.311029	-2.079958	-0.120335
N	3.766654	1.870886	0.689275

C	5.602522	-2.186899	-0.548575
C	4.991148	2.442976	0.537835
O	6.181157	-3.181330	-0.980135
O	5.300759	3.627991	0.683038
C	3.383201	-3.117436	-0.286549
C	2.966827	-3.519142	-1.572424
C	2.717068	-3.647941	0.837334
C	1.946259	-4.464653	-1.732381
C	1.679688	-4.576252	0.681849
C	1.314340	-4.980551	-0.602122
H	1.630170	-4.782591	-2.718401
H	1.167252	-4.989633	1.541874
H	0.518668	-5.710720	-0.723516
C	2.626727	2.616625	1.040667
C	1.807230	3.243575	0.075992
C	2.196494	2.595647	2.372860
C	0.607767	3.855412	0.499645
C	1.000958	3.157306	2.790782
C	0.206852	3.796544	1.841492
H	0.712391	3.094205	3.834353
H	-0.725862	4.263345	2.144176
O	3.584455	-2.875379	-2.603936
O	3.140942	-3.169141	2.043590
C	3.265785	-3.266747	-3.927197
H	3.489765	-4.327821	-4.098798
H	2.207895	-3.079047	-4.161783
H	3.893789	-2.656010	-4.578651
C	2.484158	-3.624933	3.213565
H	2.973205	-3.115421	4.046393
H	1.416649	-3.363302	3.204224
H	2.590180	-4.710435	3.342853
C	-0.232588	4.643536	-0.451449
C	0.156493	5.940306	-0.812037
C	-1.448736	4.160057	-0.982523
C	-0.618058	6.722793	-1.668241
H	1.077672	6.335199	-0.396410
C	-2.237160	4.948591	-1.843852
C	-1.818145	6.228019	-2.187255
H	-0.287317	7.724979	-1.925626
H	-3.167149	4.545550	-2.232810
H	-2.424123	6.836436	-2.851481
C	2.205040	3.190007	-1.384526
H	2.690935	2.224795	-1.564945
H	1.302643	3.212807	-2.006699
C	3.158986	4.317134	-1.823671
H	2.654619	5.288873	-1.803927
H	4.028797	4.372911	-1.164524
H	3.504134	4.142009	-2.849558
F	2.964323	1.951542	3.281589
C	-1.927141	2.845654	-0.685774
N	-2.402710	1.801232	-0.523487
C	0.767135	-0.749826	-0.084985
C	1.376574	-0.524334	2.162673
C	1.144036	-0.788495	-1.450953
C	-0.609729	-0.889641	0.278173
C	0.050379	-0.694271	2.594503
H	2.174772	-0.336716	2.870514
C	0.175669	-0.921483	-2.419561
H	2.195718	-0.733202	-1.710883
C	-1.596396	-0.981452	-0.754460
C	-0.943082	-0.866349	1.656139
H	-0.174277	-0.658874	3.655003
C	-1.194267	-1.008374	-2.075764
H	0.465654	-0.950579	-3.466730
H	-1.979648	-0.969371	1.960109
H	-1.931707	-1.080557	-2.869132
N	1.722866	-0.550364	0.881419
Pd	-3.418322	-0.074270	-0.242189
C	-5.655982	-3.819806	-0.881541
C	-5.436037	-2.283489	-1.021429
C	-3.443580	-3.136597	-1.698602
C	-4.271328	-4.407387	-1.298510
H	-5.961484	-4.095867	0.130383
H	-6.447091	-4.145579	-1.565341
H	-3.787021	-4.976688	-0.498112
H	-4.352511	-5.070246	-2.166331
C	-4.557459	-2.243574	-2.290990
H	-4.217335	-1.236452	-2.555535
H	-5.044137	-2.699156	-3.160145
C	-4.420405	-1.923734	0.068302
C	-3.163982	-2.461484	-0.369291
H	-6.343791	-1.686297	-0.996990
H	-2.566801	-3.347079	-2.311440
H	-2.470362	-2.900317	0.338119
C	-4.871521	-1.998498	1.490608
O	-6.035596	-1.973080	1.824904
O	-3.841319	-2.173801	2.351886
C	-4.192395	-2.056642	3.743825
H	-4.940528	-2.807090	4.013187
H	-3.263461	-2.227880	4.290918
H	-4.576676	-1.051006	3.924174
C	-7.183332	1.073997	-1.122052
O	-7.681585	1.662153	-2.244135
O	-7.745648	0.161150	-0.562679
N	-5.106800	1.044888	0.278728
C	-5.278019	1.206415	1.604617
C	-6.487175	1.995548	2.104682
H	-6.515113	1.922198	3.192754
H	-6.420413	3.055992	1.828280
H	-7.414018	1.590285	1.686083
O	-4.480408	0.718107	2.428408
C	-5.883428	1.752234	-0.699163
H	-5.289405	1.899910	-1.609406
H	-6.168223	2.766580	-0.375848
H	-8.526869	1.212039	-2.432276

II. Fukui Indices

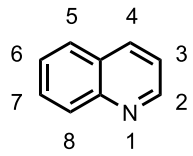
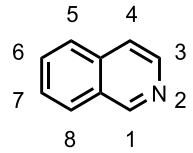
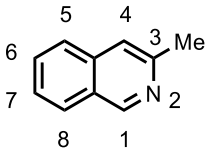
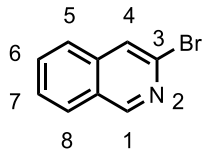
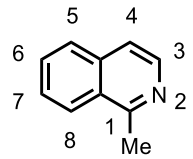
Computational Methods

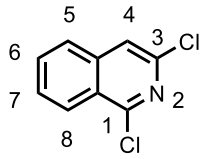
All calculations were carried out using the Gaussian 09 suite of quantum chemical programs[7]. Gas phase geometry optimizations were performed at the B3LYP level of theory[8-11] using 6-311++G** basis set[12-13,21] for all atoms. Natural population analysis was performed to calculate condensed Fukui indices using 'pop=nbo' keyword.

Discussion

Condensed Fukui Indices
$f_A^- = P_A(N) - P_A(N-1)$
where,
f_A^- = Nucleophilic Fukui function of Atom A
$P_A(N)$ = Electron density at atom A in a neutral molecule with N electrons
$P_A(N-1)$ = Electron density at atom A in a cationic molecule with (N-1) electrons

Table 11. Condensed Fukui indices calculated at the B3LYP/6-311++G** level of theory.

	Atom (A)	**$P_A(N)$**	**$P_A(N-1)$**	**f_A^-**
 **1e(Quinoline)**	C5	-0.17787	0.15622	-0.33409
	C6	-0.19750	-0.03425	-0.16325
	C7	-0.19446	-0.04110	-0.15336
	C8	-0.18032	0.15942	-0.33974
 **isoquinoline**	C5	-0.18248	0.11687	-0.29935
	C6	-0.18325	-0.08775	-0.0955
	C7	-0.20380	0.01115	-0.21495
	C8	-0.16291	0.07910	-0.24201
 **1a**	C5	-0.16968	0.10546	-0.27514
	C6	-0.19160	-0.10357	-0.08803
	C7	-0.20772	0.02309	-0.23081
	C8	-0.16284	0.02309	-0.18593
 **1b**	C5	-0.16692	0.08583	-0.25275
	C6	-0.18513	-0.10589	-0.07924
	C7	-0.20123	0.02198	-0.22321
	C8	-0.16074	0.02224	-0.18298
 **1c**	C5	-0.16478	0.09517	-0.25995
	C6	-0.19440	-0.09673	-0.09767
	C7	-0.20034	0.01437	-0.21471
	C8	-0.17061	0.04923	-0.21984

 **1d**	C5	-0.16619	-0.06993	-0.09626
	C6	-0.18111	-0.10470	-0.07641
	C7	-0.19380	0.02318	-0.21698
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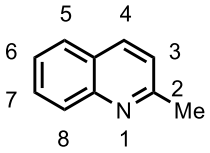 **1f**	C5	-0.17697	0.13274	-0.30971
	C6	-0.20221	0.00556	-0.20777
	C7	-0.19480	-0.08036	-0.11444
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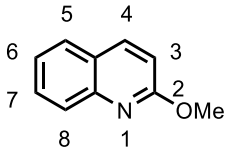 **1g**	C5	-0.17259	0.00624	-0.17883
	C6	-0.21094	0.08094	-0.29188
	C7	-0.18947	-0.13911	-0.05036
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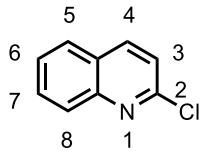 **1h**	C5	-0.17402	0.10371	-0.27773
	C6	-0.19683	0.04152	-0.23835
	C7	-0.18766	-0.10972	-0.07794
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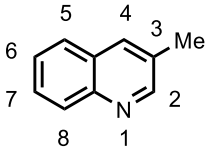 **1i**	C5	-0.16559	0.15746	-0.32305
	C6	-0.20561	-0.08778	-0.11783
	C7	-0.19885	0.00719	-0.20604
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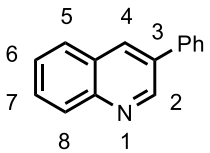 **1j**	C5	-0.17783	0.05937	-0.2372
	C6	-0.19638	-0.11872	-0.07766
	C7	-0.20492	0.01902	-0.22394
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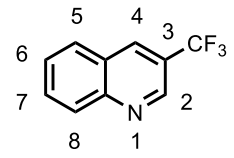 **1k**	C5	-0.15577	0.17022	-0.32599
	C6	-0.20083	-0.02856	-0.17227
	C7	-0.18195	-0.04610	-0.13585
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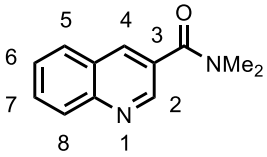 **1l**	C5	-0.16105	0.08985	-0.2509
	C6	-0.20536	-0.07248	-0.13288
	C7	-0.18997	-0.03258	-0.15739
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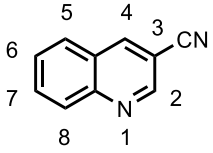
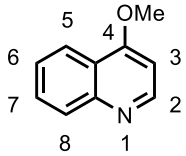
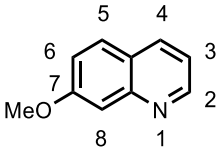
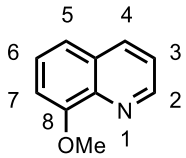
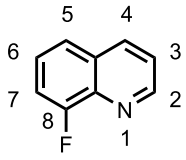
 **1m**	C5	-0.16895	0.15754	-0.32649
	C6	-0.19124	-0.07038	-0.12086
	C7	-0.17933	-0.00375	-0.17558
	C8	-0.18063	0.13338	-0.31401
 **1n**	C5	-0.17429	0.07087	-0.24516
	C6	-0.20051	0.00011	-0.20062
	C7	-0.19359	-0.09034	-0.10325
	C8	-0.18301	0.10271	-0.28572
 **1o**	C5	-0.15705	0.04488	-0.20193
	C6	-0.27009	-0.16048	-0.10961
	C8	-0.23084	0.13953	-0.37037
 **1p**	C5	-0.21336	0.14832	-0.36168
	C6	-0.18358	-0.06525	-0.11833
	C7	-0.28741	-0.02037	-0.26704

 **1q**	C5	-0.19403	0.16070	-0.35473
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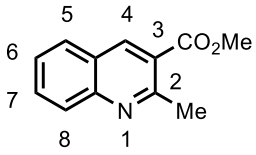 **1r**	C5	-0.18897	0.13020	-0.31917
	C6	-0.18882	0.00257	-0.19139
	C7	-0.19180	-0.08044	-0.11136
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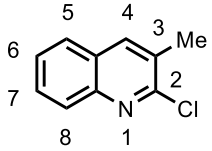 **1s**	C5	-0.16139	0.14673	-0.30812
	C6	-0.20498	-0.03010	-0.17488
	C7	-0.19226	-0.05257	-0.13969
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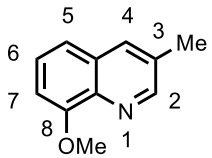 **1t**	C5	-0.21533	0.15261	-0.36794
	C6	-0.18286	-0.07547	-0.10739
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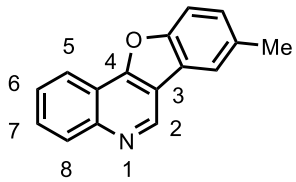 **1u**	C5	-0.18230	0.04825	-0.23055
	C6	-0.19330	-0.11423	-0.07907
	C7	-0.19767	0.01657	-0.21424
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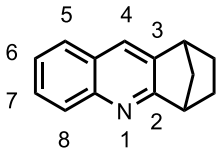 **1v**	C5	-0.17637	0.14828	-0.32465
	C6	-0.21201	-0.08683	-0.12518
	C7	-0.19974	-0.00116	-0.19858
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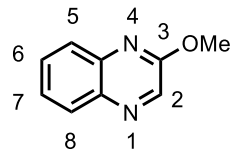
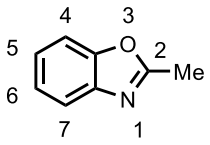
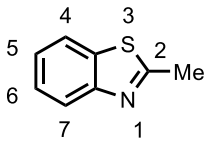
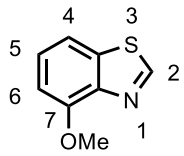
 **1w**	C5	-0.19745	0.04256	-0.24001
	C6	-0.18784	-0.13588	-0.05196
	C7	-0.20669	0.12848	-0.33517
	C8	-0.17510	-0.04467	-0.13043
 **1x**	C4	-0.23965	-0.13103	-0.10862
	C5	-0.19916	0.18280	-0.38196
	C6	-0.21161	-0.08396	-0.12765
	C7	-0.19386	-0.02768	-0.16618
 **1y**	C4	-0.21427	0.13467	-0.34894
	C5	-0.19789	-0.05377	-0.14412
	C6	-0.20689	-0.04013	-0.16676
	C7	-0.18468	0.14517	-0.32985
 **1z**	C4	-0.24873	0.12658	-0.37531
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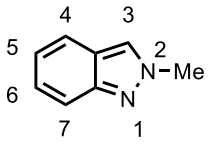 **1aa**	C4	-0.18333	0.07838	-0.26171
	C5	-0.21868	-0.01340	-0.20528
	C6	-0.20621	-0.06594	-0.14027
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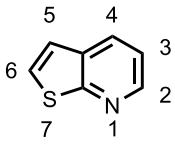 **1ab**	C5	-0.24418	0.12611	-0.37029
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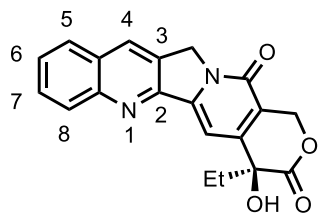 **1ac**	C5	-0.17946	-0.08973	-0.08973
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Cartesian Coordinate

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H 0.345779 2.780056 -0.000182
H -1.068367 -2.573177 0.000157
C 2.022116 -0.190954 0.000005
H 2.663517 1.887741 -0.000121
N 1.026871 -1.053688 0.000068
C 3.426403 -0.738186 0.000064
H 3.979415 -0.397107 -0.881261
H 3.979388 -0.396995 0.881363
H 3.398538 -1.827142 0.000134

1g

E= -516.593324084 H= -516.415881 G= -516.461000
C 3.062524 -1.038400 -0.000084
C 1.769213 -1.504876 -0.000047
C 0.678278 -0.597368 0.000027
C 0.953519 0.804976 0.000045
C 2.297787 1.254723 0.000032
C 3.333671 0.351124 -0.000033
H 3.888472 -1.741130 -0.000171
C -0.164042 1.673529 0.000011
H 2.495392 2.321979 0.000080
H 4.360605 0.697955 -0.000026
C -1.435994 1.162469 0.000008
H -0.007688 2.747595 -0.000001
H 1.545550 -2.564829 -0.000069
C -1.591531 -0.255059 0.000074
H -2.291138 1.823352 -0.000085
N -0.587104 -1.093137 0.000067
O -2.810281 -0.853964 0.000213
C -3.985281 -0.051308 -0.000193
H -4.045086 0.576279 -0.895556
H -4.817478 -0.752958 -0.000309
H -4.045514 0.576568 0.894933

1h

E= -861.657735421 H= -861.523572 G= -861.565780
C 2.907314 -1.209737 -0.000059
C 1.575914 -1.555870 -0.000092
C 0.579538 -0.550328 -0.000021
C 0.972769 0.822148 0.000059
C 2.352114 1.145635 0.000089
C 3.299968 0.149020 0.000035
H 3.666320 -1.983815 -0.000104
C -0.059842 1.794957 0.000113
H 2.648830 2.189324 0.000160
H 4.353981 0.401747 0.000059
C -1.371738 1.401015 0.000071
H 0.196486 2.849306 0.000188
H 1.253827 -2.590046 -0.000163
C -1.632533 0.006727 -0.000044
H -2.188395 2.109693 0.000119
N -0.735206 -0.925947 -0.000076
Cl -3.325036 -0.500940 -0.000037

1i

E= -441.359521397 H= -441.187804 G= -441.230922
C 2.921964 0.386690 0.000039
C 1.861596 1.262056 0.000030
C 0.530354 0.775619 0.000160
C 0.304347 -0.633962 -0.000016
C 1.418599 -1.511256 -0.000025
C 2.699448 -1.010963 0.000037
H 3.937973 0.765199 0.000169
C -1.040352 -1.082831 -0.000128
H 1.245100 -2.582629 -0.000219
H 3.546537 -1.687664 -0.000044
C -2.074198 -0.177959 -0.000131
H -1.241329 -2.150555 -0.000055
H 2.007245 2.335751 -0.000027
C -1.724472 1.203705 -0.000271
N -0.499173 1.672210 -0.000010
H -2.521500 1.946288 0.000115
C -3.524108 -0.587607 0.000227
H -3.628452 -1.674317 -0.000061
H -4.045132 -0.199387 0.881012
H -4.045288 -0.199118 -0.880352

1j

E= -633.142939639 H= -632.915097 G= -632.965690
C 4.538145 -0.030396 0.017469
C 3.625217 -1.033688 -0.206261
C 2.235145 -0.761032 -0.158456
C 1.795710 0.568811 0.122149
C 2.763076 1.582153 0.350193
C 4.104460 1.287956 0.298121
H 5.600157 -0.245490 -0.019702
C 0.401833 0.803448 0.169491
H 2.427204 2.591346 0.565689
H 4.838356 2.066667 0.472432
C -0.485999 -0.228061 -0.053889
H 0.040699 1.799282 0.406275
H 3.934208 -2.049401 -0.422373
C 0.072019 -1.512484 -0.331177

N 1.355337 -1.778883 -0.383732
H -0.599105 -2.343175 -0.536369
C -1.955101 -0.034952 -0.017346
C -2.791957 -0.989527 0.580136
C -2.544410 1.108304 -0.577720
C -4.171300 -0.803387 0.620782
H -2.358497 -1.871307 1.038299
C -3.923331 1.294388 -0.536209
H -1.918896 1.844628 -1.069982
C -4.742834 0.339134 0.063416
H -4.799459 -1.549071 1.095188
H -4.359226 2.181727 -0.981677
H -5.816839 0.482979 0.094150

1k

E= -739.178225219 H= -739.028522 G= -739.074310
C 3.904536 0.177950 0.000457
C 2.943613 1.159755 0.000360
C 1.568153 0.814270 -0.000045
C 1.201806 -0.568469 -0.000271
C 2.218663 -1.559069 -0.000226
C 3.541596 -1.191688 0.000131
H 4.954212 0.449104 0.000764
C -0.175452 -0.877425 -0.000729
H 1.934602 -2.606069 -0.000497
H 4.316089 -1.949915 0.000163
C -1.093413 0.146511 -0.001064
H -0.495820 -1.914077 -0.001070
H 3.200632 2.211980 0.000575
C -0.629846 1.486749 -0.000687
N 0.642087 1.813745 -0.000243
H -1.345756 2.302072 -0.000935
C -2.563123 -0.168421 -0.000038
F -2.924915 -0.882124 1.095141
F -3.329105 0.941529 -0.019256
F -2.919066 -0.916104 -1.074178

1l

E= -649.416633495 H= -649.185182 G= -649.239770
C -4.221138 -0.159320 0.094140
C -3.379664 0.892426 0.370497
C -1.978738 0.750489 0.210532
C -1.455588 -0.501317 -0.237226
C -2.349637 -1.566440 -0.517885
C -3.703980 -1.398325 -0.354357
H -5.292012 -0.042522 0.216974
C -0.050880 -0.611653 -0.374511
H -1.948476 -2.514138 -0.862536
H -4.383061 -2.215446 -0.569507
C 0.749519 0.469999 -0.091608
H 0.377209 -1.547990 -0.718846
H -3.754772 1.850109 0.710753
C 0.118837 1.680053 0.316924
N -1.174576 1.820288 0.481155
H 0.739085 2.550936 0.508584
C 2.233397 0.496410 -0.335814
O 2.710604 1.416966 -0.989295
N 2.998174 -0.537612 0.142957
C 4.415170 -0.562189 -0.205064
H 5.027721 -0.124042 0.592205
H 4.730589 -1.597826 -0.357997
H 4.571576 0.009892 -1.116015
C 2.610526 -1.435556 1.224635
H 2.666774 -2.481334 0.903401
H 3.288951 -1.304663 2.075578
H 1.599448 -1.224901 1.561397

1m

E= -494.295920662 H= -494.152912 G= -494.196239
C 3.177861 0.259532 0.000132
C 2.169417 1.193893 0.000156
C 0.814396 0.781855 0.000076
C 0.514687 -0.617111 -0.000020
C 1.578415 -1.556909 -0.000041
C 2.882284 -1.125486 0.000033
H 4.212878 0.581935 0.000191
C -0.844434 -0.996177 -0.000094
H 1.345458 -2.616406 -0.000119
H 3.692706 -1.845029 0.000017
C -1.817726 -0.016641 -0.000066
H -1.118211 -2.045303 -0.000174
H 2.374782 2.257390 0.000231
C -1.411783 1.352360 0.000042
N -0.161113 1.736964 0.000108
H -2.171550 2.128927 0.000061
C -3.207177 -0.346040 -0.000142
N -4.334845 -0.599417 -0.000202

1n

E= -516.591290921 H= -516.413442 G= -516.458300
C 3.012820 -0.590298 0.000089
C 2.465865 0.671124 0.000107
C 1.059557 0.850606 -0.000004
C 0.224655 -0.307071 -0.000081
C 0.811698 -1.595660 -0.000079
C 2.180703 -1.732853 -0.000002
H 4.090202 -0.713451 0.000152
C -1.188144 -0.094656 -0.000166
H 0.166419 -2.464605 -0.000145
H 2.626023 -2.721270 -0.000009
C -1.668672 1.198031 -0.000124
H 3.083876 1.560945 0.000187
C -0.737707 2.263445 -0.000009
N 0.567417 2.125714 0.000041
H -1.115674 3.283619 0.000020
H -2.726372 1.421086 -0.000183
O -1.953985 -1.210105 -0.000238
C -3.371648 -1.065335 0.000308
H -3.713830 -0.536500 -0.894699
H -3.772410 -2.077214 0.000878
H -3.713047 -0.535766 0.895175

1o

E= -516.586441849 H= -516.409112 G= -516.454339
C -1.636444 -0.254883 0.000027
C -0.558692 -1.118731 0.000052
C 0.760026 -0.620195 0.000104
C 0.977225 0.795646 0.000005
C -0.147361 1.652836 -0.000047
C -1.427602 1.148927 -0.000050
C 2.315134 1.257634 0.000020
H 0.007623 2.726916 -0.000158
H -2.267427 1.830280 -0.000188
C 3.340787 0.346355 0.000051
H -0.717218 -2.189406 -0.000058
C 3.019553 -1.034436 -0.000127
N 1.796050 -1.513008 -0.000032
H 3.822293 -1.768704 0.000018
H 4.378114 0.658869 0.000242
H 2.512111 2.325186 0.000103
O -2.873449 -0.829168 -0.000073
C -4.026755 0.002302 0.000058

H -4.068748 0.632260 -0.894960
H -4.878189 -0.676176 0.000295
H -4.068555 0.632451 0.894959

1p

E= -516.583303209 H= -516.405761 G= -516.450648
N 0.435625 1.683847 0.000000
C -0.462913 2.644674 0.000000
C -1.859032 2.420202 0.000000
C -2.314515 1.125761 0.000000
C -1.786288 -1.307049 0.000000
C -0.833221 -2.292256 0.000000
C 0.546376 -1.978444 0.000000
C 0.970330 -0.663404 0.000000
C 0.000000 0.398640 0.000000
C -1.386883 0.055283 0.000000
H -0.080180 3.662721 0.000000
H -2.542923 3.260900 0.000000
H -3.377218 0.905664 0.000000
H -2.842820 -1.550998 0.000000
H -1.128738 -3.335494 0.000000
H 1.264306 -2.787154 0.000000
O 2.264647 -0.273842 0.000000
C 3.274696 -1.272373 0.000000
H 4.220638 -0.733693 0.000000
H 3.214541 -1.902173 0.894448
H 3.214541 -1.902173 -0.894448

1q

E= -501.295186166 H= -501.159806 G= -501.200707
N 1.002361 -1.425192 0.000000
C 2.264808 -1.058888 -0.000002
C 2.699413 0.288983 0.000001
C 1.758204 1.286610 0.000000
C -0.655853 1.915718 -0.000001
C -1.970756 1.518178 -0.000002
C -2.309870 0.145811 0.000001
C -1.315744 -0.795553 0.000004
C 0.061450 -0.445040 0.000000
C 0.381761 0.948937 -0.000001
H 2.998806 -1.860968 0.000004
H 3.759474 0.512835 0.000003
H 2.049161 2.331899 0.000000
H -0.396271 2.968543 -0.000001
H -2.764471 2.255831 -0.000004
H -3.343712 -0.176556 0.000000
F -1.644444 -2.098198 0.000000

1r

E= -708.633969212 H= -708.385750 G= -708.443686
N -1.581186 1.666497 0.000014
C -0.263265 1.714428 0.000057
C 0.532199 0.510475 0.000079
C -0.116256 -0.707768 0.000053
C -2.251812 -1.991198 -0.000043
C -3.625677 -1.975398 -0.000104
C -4.323601 -0.742896 -0.000128
C -3.643560 0.452546 -0.000090
C -2.226116 0.467542 -0.000026
C -1.524245 -0.772681 -0.000003
H 0.462552 -1.622838 0.000074
H -1.707892 -2.930191 -0.000025
H -4.181892 -2.905770 -0.000135
H -5.407995 -0.746778 -0.000177
H -4.161417 1.404077 -0.000105
C 0.336479 3.096168 0.000108
H 0.974334 3.254393 0.872300
H 0.974209 3.254497 -0.872158
H -0.477572 3.819718 0.000206
C 2.024119 0.556686 0.000098
O 2.698021 1.562188 -0.000391
O 2.570772 -0.681826 0.000174
C 4.018104 -0.744994 -0.000116
C 4.413219 -2.207545 0.000311
H 4.390482 -0.219134 0.881915
H 4.390096 -0.219760 -0.882686
H 5.503284 -2.292320 0.000081
H 4.031335 -2.717913 0.887471
H 4.030913 -2.718550 -0.886302

1s

E= -900.986263116 H= -900.822923 G= -900.868605
N -0.338734 -1.195018 0.000017
C -1.358977 -0.399517 -0.000016
C -1.316524 1.029383 -0.000023
C -0.054809 1.576899 -0.000071
C 2.425274 1.278694 -0.000131
C 3.503842 0.425079 -0.000126
C 3.307728 -0.975930 -0.000071
C 2.038442 -1.506164 -0.000018
C 0.911934 -0.648820 -0.000019
C 1.105208 0.763090 -0.000080
H 0.058847 2.656797 -0.000095
H 2.572037 2.353723 -0.000170
H 4.511701 0.824000 -0.000163
H 4.168701 -1.634684 -0.000068
H 1.865210 -2.575382 0.000023
Cl -2.951020 -1.178853 0.000200
C -2.559280 1.874865 0.000027
H -3.177983 1.670515 -0.877876
H -3.177936 1.670489 0.877957
H -2.299130 2.934695 0.000035

1t

E= -555.911655517 H= -555.705051 G= -555.754294
N -0.488408 -1.438337 0.000000
C -1.801396 -1.462867 0.000000
C -2.637133 -0.312628 0.000000
C -2.008648 0.910101 0.000000
C 0.099744 2.234617 0.000000
C 1.471108 2.242951 0.000000
C 2.212926 1.038755 0.000000
C 1.568477 -0.183956 0.000000
C 0.131942 -0.231166 0.000000
C -0.594250 0.996470 0.000000
H -2.261355 -2.450341 0.000000
H -2.589798 1.827985 0.000000
H -0.464370 3.160750 0.000000
H 2.009235 3.184370 0.000000
H 3.292959 1.091616 0.000000
O 2.194371 -1.382714 0.000000
C 3.614452 -1.407734 0.000000
H 3.890159 -2.460889 0.000000
H 4.023341 -0.924558 -0.894298
H 4.023341 -0.924558 0.894298
C -4.135818 -0.465203 0.000000
H -4.477234 -1.018496 -0.880730
H -4.477234 -1.018490 0.880734
H -4.633588 0.506640 -0.000003

1u

E= -746.510183201 H= -746.270632 G= -746.325189

N -1.849888 2.089395 -0.000007
C -0.538619 2.015508 -0.000005
C 0.158870 0.783604 0.000000
C -0.590315 -0.384510 0.000004
C -2.822209 -1.529302 0.000008
C -4.190949 -1.389050 0.000006
C -4.778773 -0.103402 0.000001
C -3.994636 1.027901 -0.000004
C -2.581982 0.929848 -0.000004
C -1.997677 -0.379655 0.000004
H 0.004897 2.957217 -0.000010
H -2.361695 -2.509968 0.000013
H -4.824987 -2.268249 0.000009
H -5.858995 -0.011169 -0.000001
H -4.428577 2.020451 -0.000008
C 1.546005 0.363000 0.000001
C 1.501183 -1.038954 0.000007
C 2.635589 -1.832378 -0.000012
C 3.860075 -1.169826 -0.000031
C 3.956464 0.236962 -0.000025
C 2.790849 1.002338 -0.000017
H 2.569474 -2.913071 -0.000026
H 4.772322 -1.757175 -0.000056
H 2.852994 2.085031 -0.000032
O 0.197115 -1.498909 0.000008
C 5.316363 0.895524 0.000045
H 5.897124 0.607222 0.881610
H 5.897897 0.605842 -0.880548
H 5.230413 1.983735 -0.000831

1v

E= -596.222024588 H= -595.976419 G= -596.023277
N 0.251753 -1.383768 -0.143397
C -0.833708 -0.667466 -0.236847
C -0.893287 0.764162 -0.228610
C 0.265221 1.473177 -0.119463
C 2.751478 1.379485 0.060184
C 3.909522 0.639246 0.141796
C 3.852575 -0.771708 0.128212
C 2.641310 -1.419774 0.033432
C 1.433735 -0.686901 -0.049620
C 1.489334 0.744144 -0.035914
H 0.284624 2.559257 -0.102275
H 2.791614 2.464249 0.069123
H 4.869079 1.138278 0.217120
H 4.770256 -1.345605 0.193134
H 2.575312 -2.501307 0.020361
C -2.264094 -1.154997 -0.332513
C -2.359501 1.125643 -0.317835
C -2.869138 -0.033869 -1.218902
H -3.959956 -0.078093 -1.280118
H -2.449572 -0.009194 -2.227102
C -2.932111 -0.830374 1.041469
H -3.929809 -1.274163 1.083810
H -2.355972 -1.231665 1.876696
C -3.006053 0.731437 1.048549
H -4.041727 1.078945 1.086114
H -2.476397 1.175587 1.892945
H -2.374515 -2.185427 -0.664601
H -2.576880 2.142286 -0.645058

1w

E= -532.640943632 H= -532.475337 G= -532.520181
N 0.153712 1.895136 0.000038
C -1.124377 1.648617 0.000039
C -1.632323 0.305577 0.000115
C 1.391474 -1.597496 0.000065
C 2.749857 -1.364859 0.000071
C 3.258570 -0.046871 0.000064
C 2.398662 1.028942 0.000057
C 1.002013 0.817719 0.000051
C 0.488934 -0.510808 0.000050
H -1.821966 2.481091 -0.000029
H 0.985920 -2.602294 0.000076
H 3.438766 -2.202130 0.000079
H 4.330418 0.113815 0.000068
H 2.759185 2.050797 0.000052
N -0.861219 -0.743060 0.000094
O -2.972830 0.194003 -0.000016
C -3.523324 -1.131611 -0.000425
H -3.206520 -1.680190 0.888465
H -4.602370 -0.992669 -0.001234
H -3.205151 -1.680235 -0.888787

1x

E= -439.164526796 H= -439.023361 G= -439.064268
C 0.189731 0.735972 -0.000007
C 0.187063 -0.661888 0.000002
C 1.334832 -1.435026 0.000014
C 2.539364 -0.729892 0.000022
C 2.569527 0.674392 0.000014
C 1.399079 1.429783 -0.000001
H 1.299914 -2.516907 0.000020
H 3.473037 -1.279930 0.000034
H 3.528505 1.179205 0.000020
H 1.418428 2.512553 -0.000008
N -1.134584 1.182949 -0.000023
O -1.124397 -1.070072 -0.000008
C -1.845150 0.105797 -0.000016
C -3.322986 -0.024869 -0.000004
H -3.661181 -0.574046 0.882846
H -3.769031 0.967855 -0.000202
H -3.661166 -0.574403 -0.882635

1y

E= -762.141629920 H= -762.003119 G= -762.045901
C -0.349241 0.757835 -0.000017
C -0.422487 -0.653211 -0.000004
C -1.648091 -1.319103 0.000015
C -2.808980 -0.553298 0.000012
C -2.749766 0.848895 0.000004
C -1.529366 1.510248 -0.000009
H -1.698739 -2.401213 0.000017
H -3.772747 -1.049287 0.000017
H -3.670151 1.421210 0.000007
H -1.468645 2.591820 -0.000012
N 0.934165 1.285129 -0.000008
C 1.832341 0.360501 -0.000005
C 3.306748 0.608776 0.000078
H 3.780825 0.171317 -0.882962
H 3.481315 1.684418 0.000060
H 3.780727 0.171363 0.883195
S 1.202582 -1.309337 -0.000044

1z

E= -837.359750466 H= -837.215554 G= -837.260962
C -0.080147 -0.248907 -0.033695
C 1.070190 0.580143 0.024706
C 1.003007 1.970607 0.051219
C -0.263716 2.543335 0.019601
C -1.416448 1.758151 -0.030797
C -1.355993 0.363529 -0.056372

H 1.895747 2.581046 0.091992
H -0.362650 3.622652 0.038345
H -2.397145 2.217132 -0.051371
N 0.185365 -1.611293 -0.081061
C 1.451910 -1.840322 -0.056548
S 2.502798 -0.431140 0.027584
H 1.885825 -2.831730 -0.083402
O -2.553010 -0.269150 -0.131840
C -2.691593 -1.664968 0.160937
H -3.766834 -1.838919 0.184515
H -2.223264 -2.282027 -0.605032
H -2.253186 -1.907074 1.131448

1aa

E= -419.259094586 H= -419.105093 G= -419.146967
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C -0.217851 0.761393 -0.000082
C -1.470067 1.422859 0.000033
C -2.608150 0.652956 0.000216
C -2.543357 -0.771823 0.000216
C -1.344510 -1.442536 0.000037
H -1.529359 2.505424 0.000011
H -3.580898 1.131266 0.000348
H -3.470496 -1.334002 0.000361
H -1.293999 -2.524648 0.000016
N 1.119026 -1.109705 -0.000398
C 3.301380 -0.090876 0.000747
H 3.628705 -0.625058 0.893635
H 3.628596 -0.639171 -0.883479
H 3.731852 0.909461 -0.007194
C 1.122051 1.156473 -0.000403
H 1.589054 2.127902 -0.000560
N 1.852013 0.017196 -0.000623

1ab

E= -722.799897991 H= -722.690803 G= -722.729065
C -0.128130 0.871607 0.000013
C 0.028110 -0.537463 -0.000004
C -2.192059 -0.935828 0.000260
C -2.482108 0.437216 0.000312
C -1.443174 1.355860 0.000178
H -2.996557 -1.664799 0.000366
H -3.514511 0.765111 0.000452
H -1.639735 2.422626 0.000210
C 2.189424 0.701024 -0.000371
S 1.731735 -0.986721 -0.000160
H 3.238500 0.957360 -0.000573
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C 1.134971 1.555716 -0.000139
H 1.238758 2.632950 -0.000157

1ac

E= -1182.51831128 H= -1182.171553 G= -1182.241753
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C 6.566790 -0.739291 -0.159226
O -1.491182 3.347091 0.279009
N -0.030052 1.596466 0.123866
C 5.904917 -1.985949 -0.265646
H 6.489710 -2.894281 -0.355478
C 4.532760 -2.051963 -0.256675
H 4.006262 -2.995147 -0.337985
O -4.631784 0.759668 -0.772249
C 3.755275 -0.870930 -0.140468
O -5.011727 -1.219488 -1.689625
C 4.426059 0.394938 -0.032482
O -2.862978 -2.389732 -0.676869
H -3.567312 -2.615370 -1.305198
C 5.843564 0.423888 -0.045315
H 6.348895 1.380614 0.036408
C -3.828224 -1.452309 1.346465
H -4.168200 -0.516570 1.800877
H -4.715704 -2.075702 1.199161
C -3.776999 1.599914 0.049032
H -4.220495 1.649075 1.049190
H -3.839101 2.594005 -0.390300
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C -1.317592 2.134003 0.169180
C -2.357343 1.127452 0.073792
C -2.070438 -0.211361 -0.027381
C -0.732866 -0.678105 -0.085359
H -0.500785 -1.724937 -0.206111
C 0.259501 0.256394 -0.004012
C 1.169786 2.447457 0.190490
H 1.173397 3.011070 1.127733
H 1.154354 3.173073 -0.627699
C 1.719567 0.131568 -0.027953
C 2.277822 1.436609 0.086012
C 3.637920 1.571072 0.083607
C -2.844562 -2.161345 2.278616
H -1.978205 -1.535646 2.506461
H -2.488178 -3.090468 1.830835
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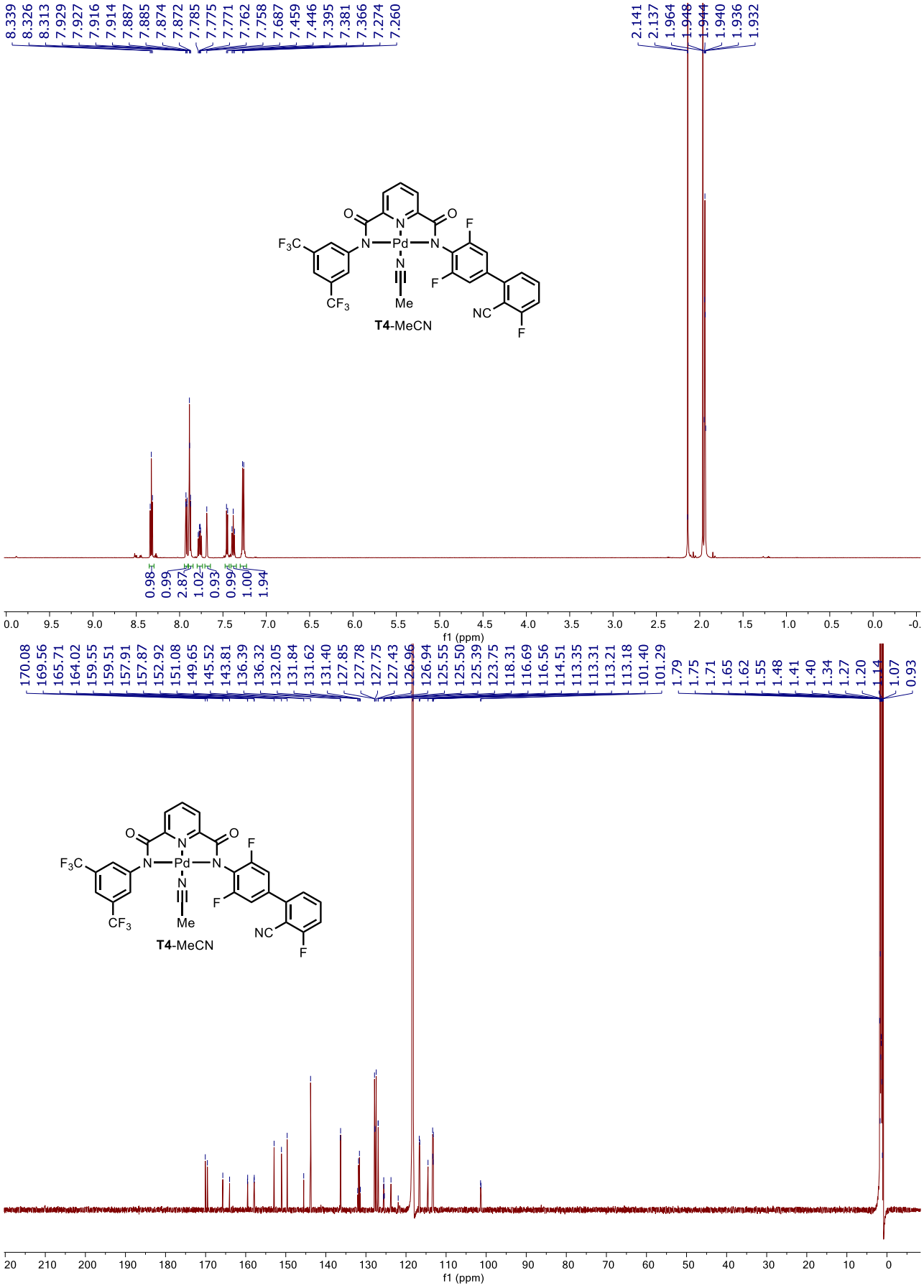
H 7.650079 -0.705956 -0.168297

NMR SPECTRA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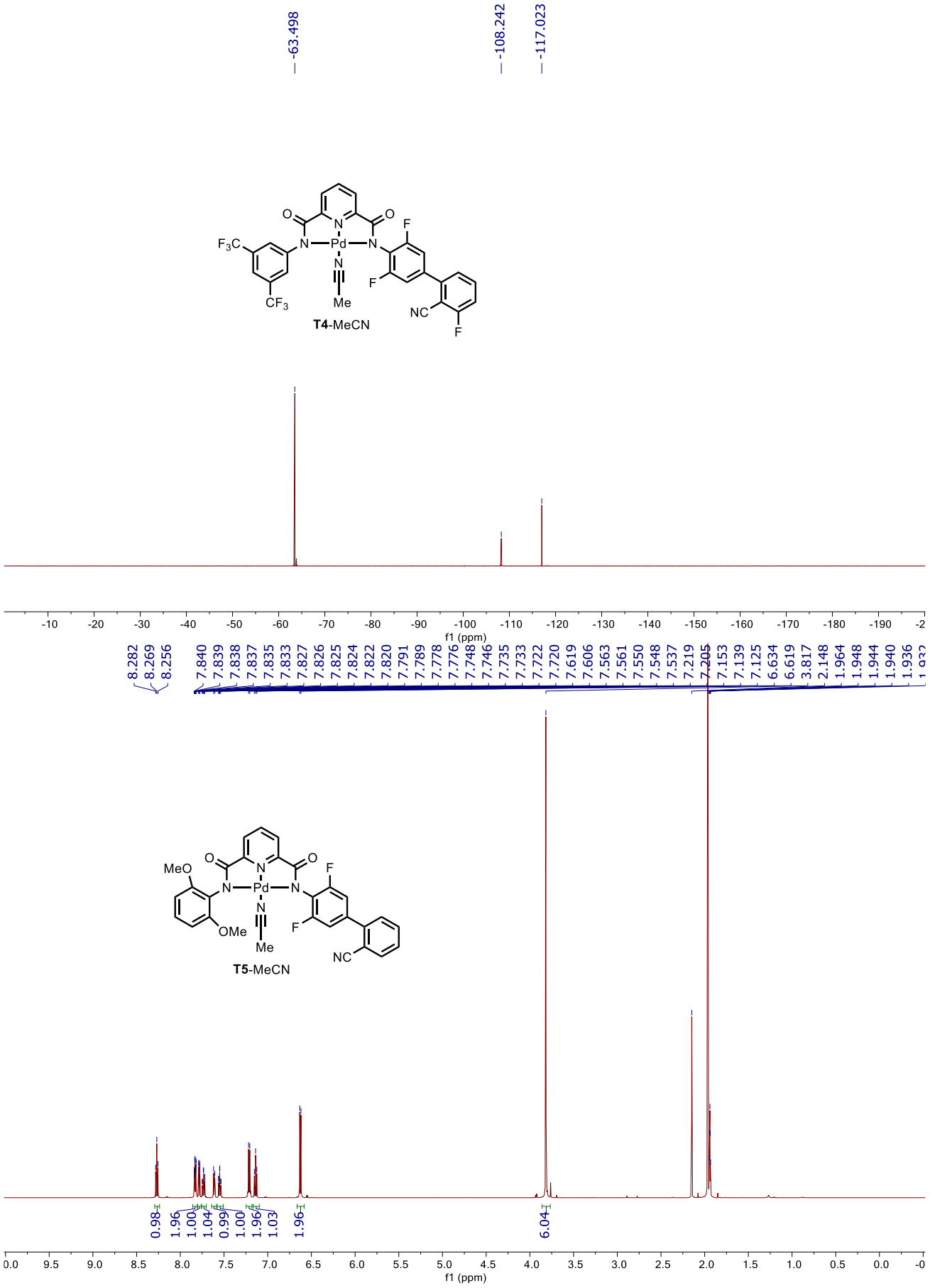
7.872
7.785
7.775
7.771
7.762
7.758
7.687
7.459
7.446
7.395
7.381
7.366
7.274
7.260
2.141
2.137
1.964
1.948
1.944
1.940
1.936
1.932
T4-MeCN
0.98
0.99
2.87
1.02
0.93
0.99
1.00
1.94
f1 (ppm)
170.08
169.56
165.71
164.02
159.55
159.51
157.91
157.87
152.92
151.08
149.65
145.52
143.81
136.39
136.32
132.05
131.84
131.62
131.40
127.85
127.78
127.75
127.43
126.96
126.94
125.55
125.50
125.39
123.75
118.31
116.69
116.56
114.51
113.35
113.31
113.21
113.18
101.40
101.29
1.79
1.75
1.71
1.65
1.62
1.55
1.48
1.41
1.40
1.34
1.27
1.20
1.14
1.07
0.93
T4-MeCN
f1 (ppm)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-108.242
-117.023
T4-MeCN
f1 (ppm)
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8.269
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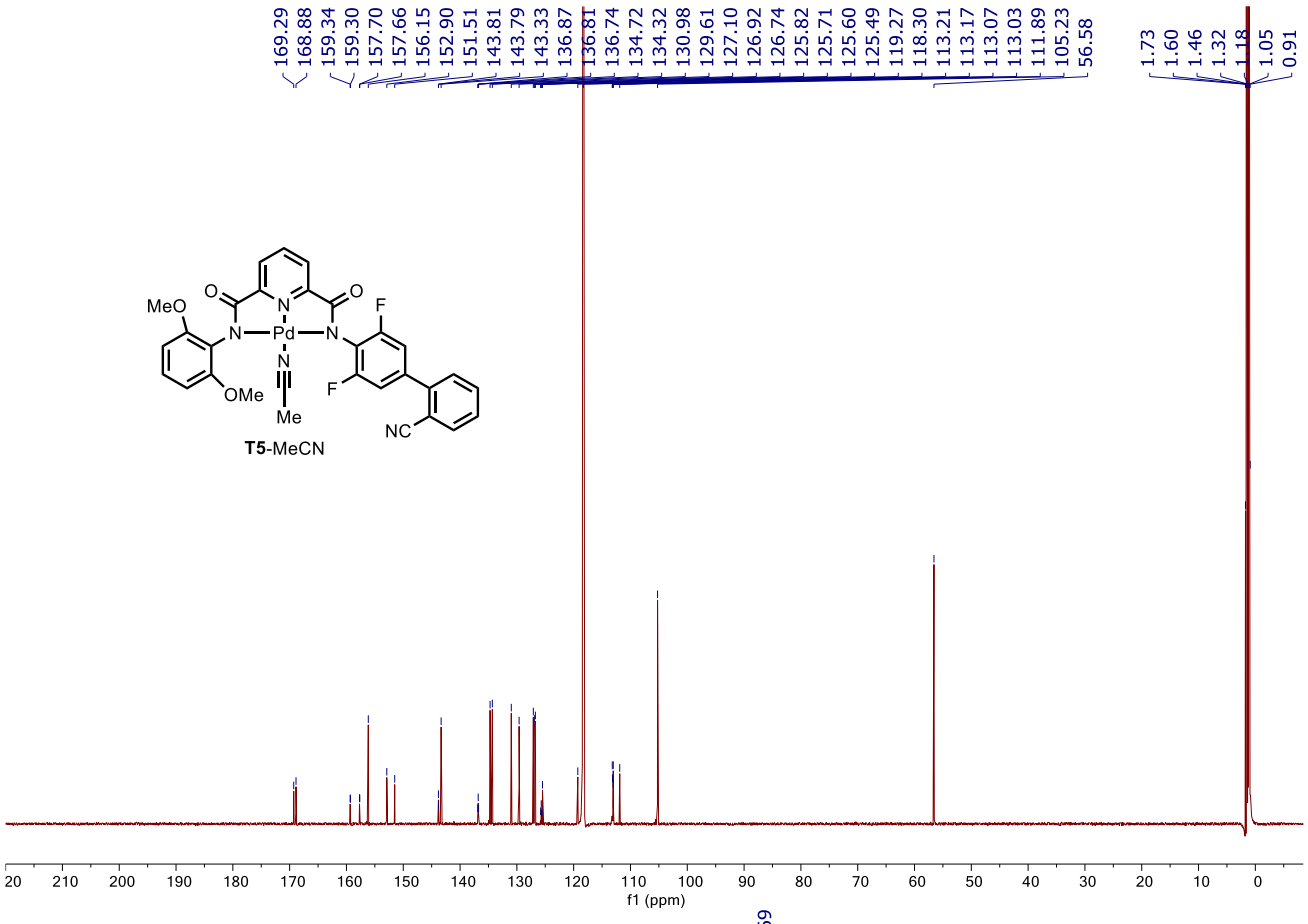
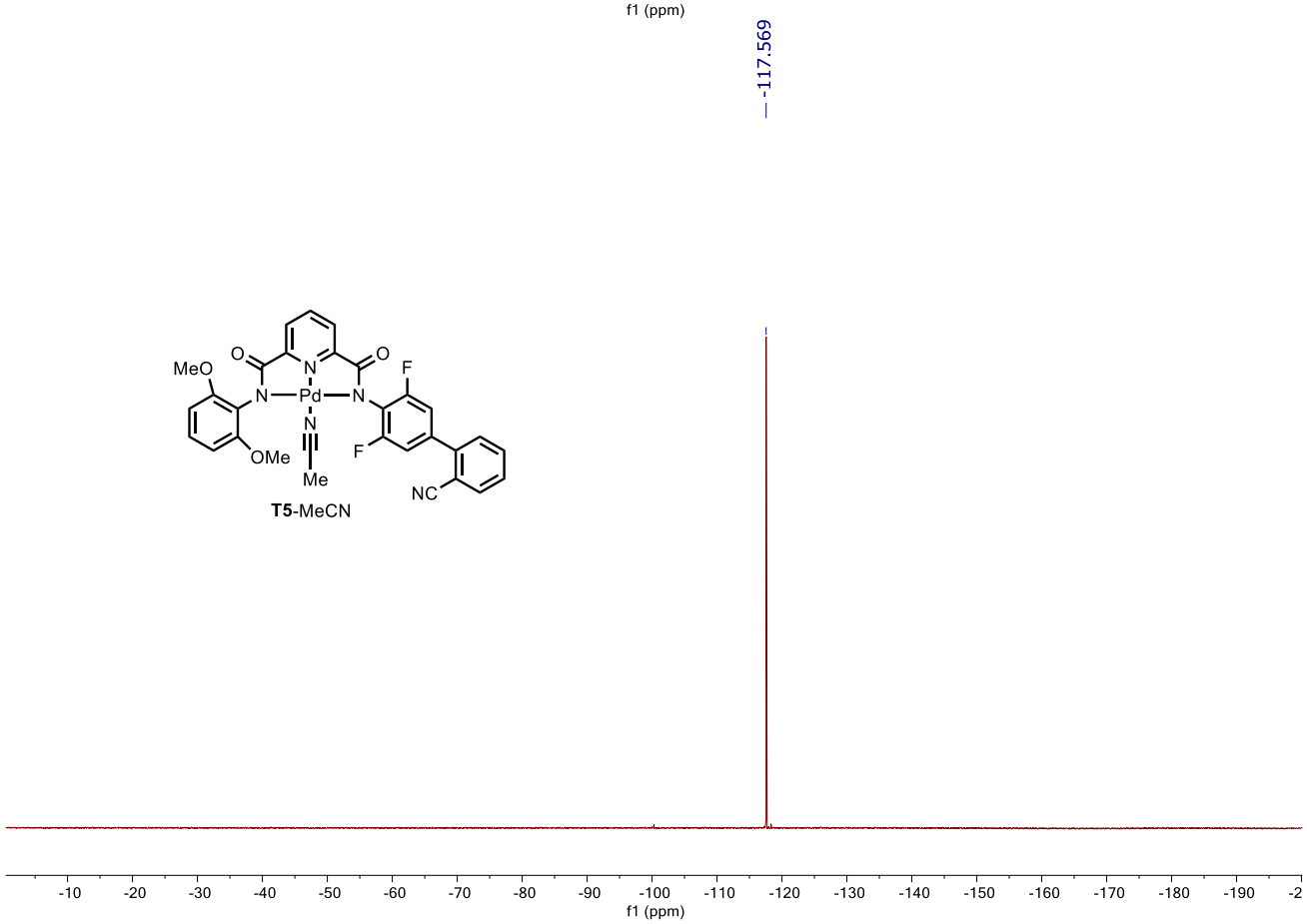
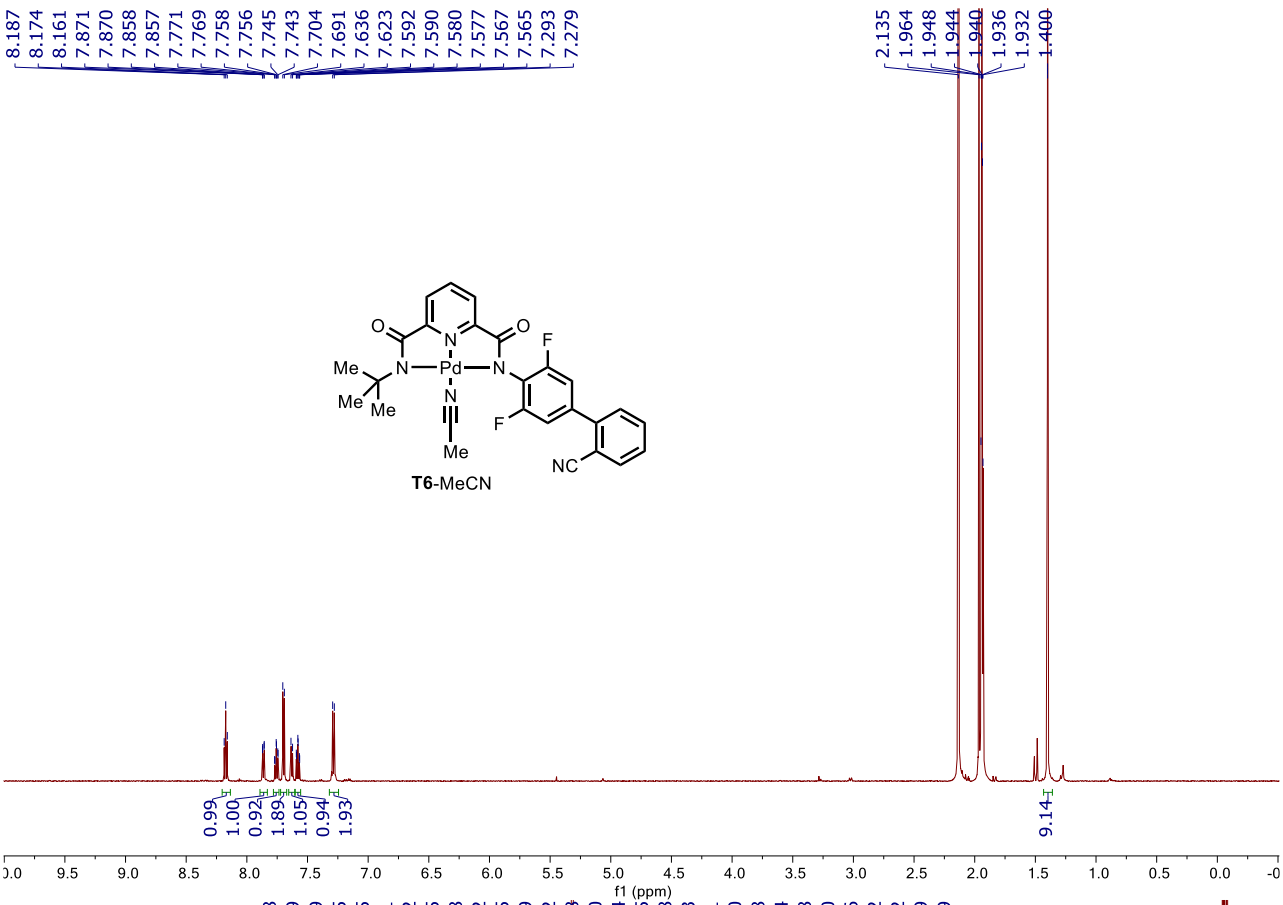
7.840
7.839
7.838
7.837
7.835
7.833
7.827
7.826
7.825
7.824
7.822
7.820
7.791
7.789
7.778
7.776
7.748
7.746
7.735
7.733
7.722
7.720
7.619
7.606
7.563
7.561
7.550
7.548
7.537
7.219
7.205
7.153
7.139
7.125
6.634
6.619
3.817
2.148
1.964
1.948
1.944
1.940
1.936
T5-MeCN
0.98
1.96
1.00
1.04
0.99
1.00
1.96
1.03
1.96
6.04
f1 (ppm)


169.29
168.88
159.34
159.30
157.70
157.66
156.15
152.90
151.51
143.81
143.79
143.33
136.87
136.81
136.74
134.72
134.32
130.98
129.61
127.10
126.92
126.74
125.82
125.71
125.60
125.49
119.27
118.30
113.21
113.17
113.07
113.03
111.89
105.23
56.58
1.73
1.60
1.46
1.32
1.18
1.05
0.91
MeO
OMe
F
F
NC
Me
T5-MeCN
f1 (ppm)


-117.569
MeO
OMe
F
F
NC
Me
T5-MeCN
f1 (ppm)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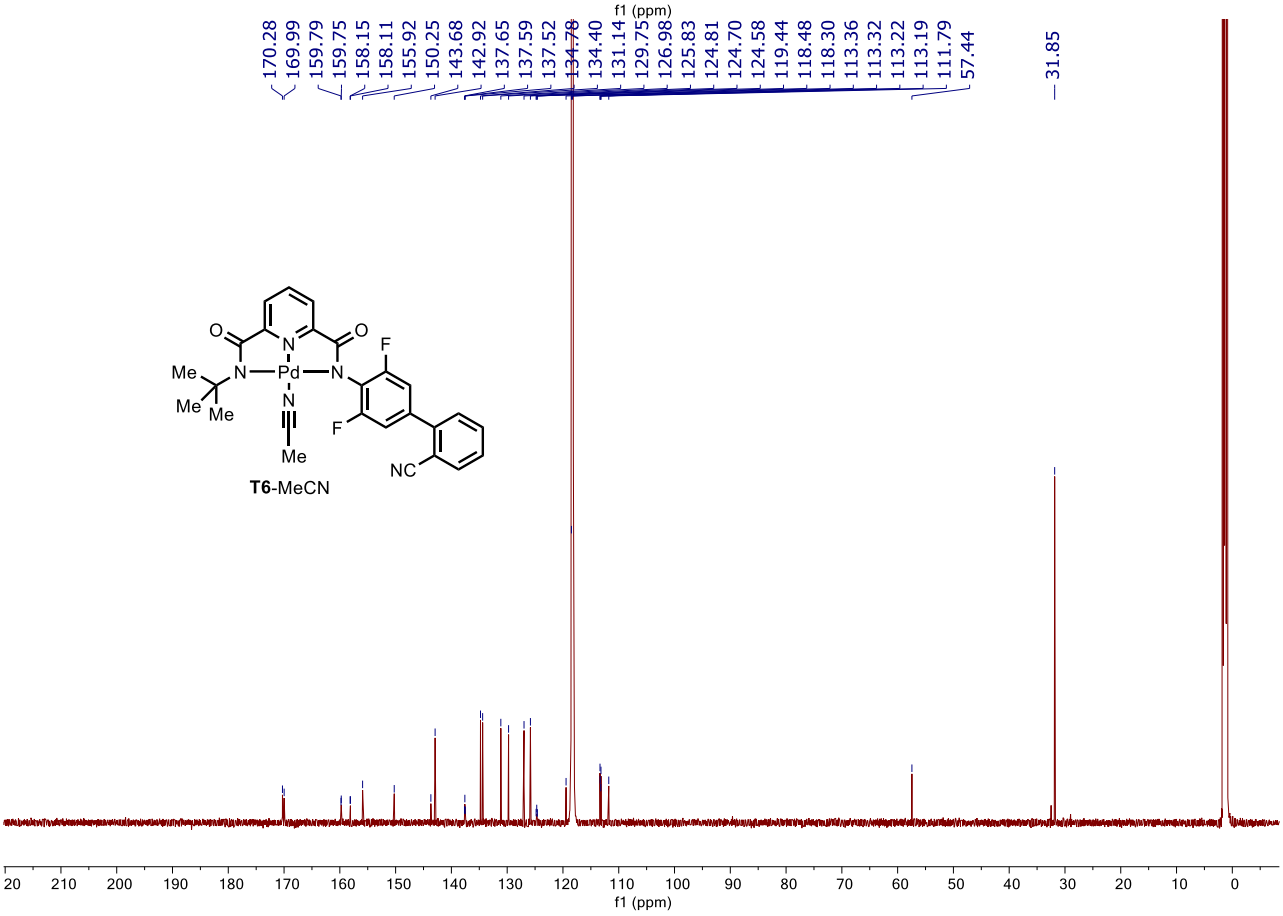
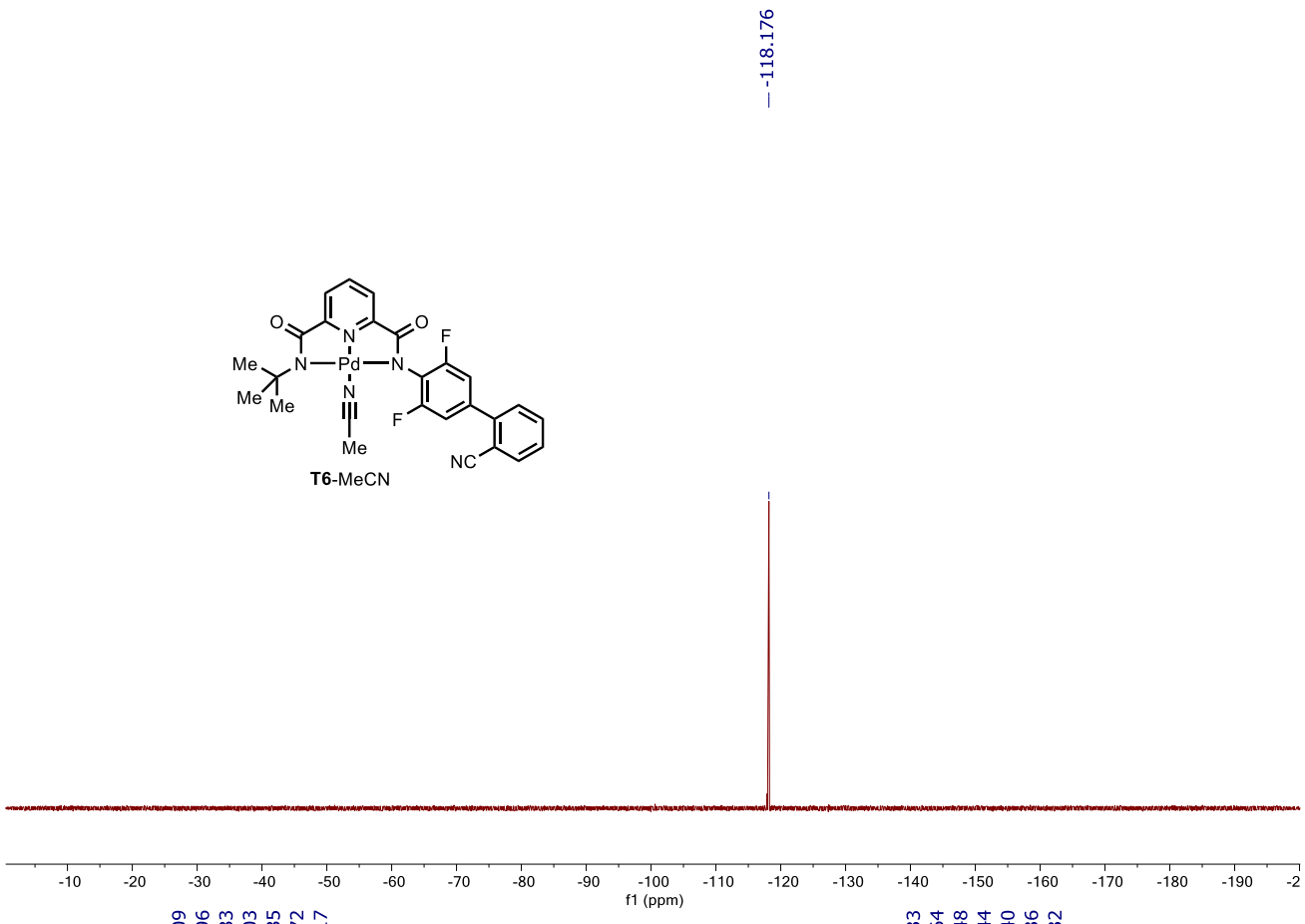
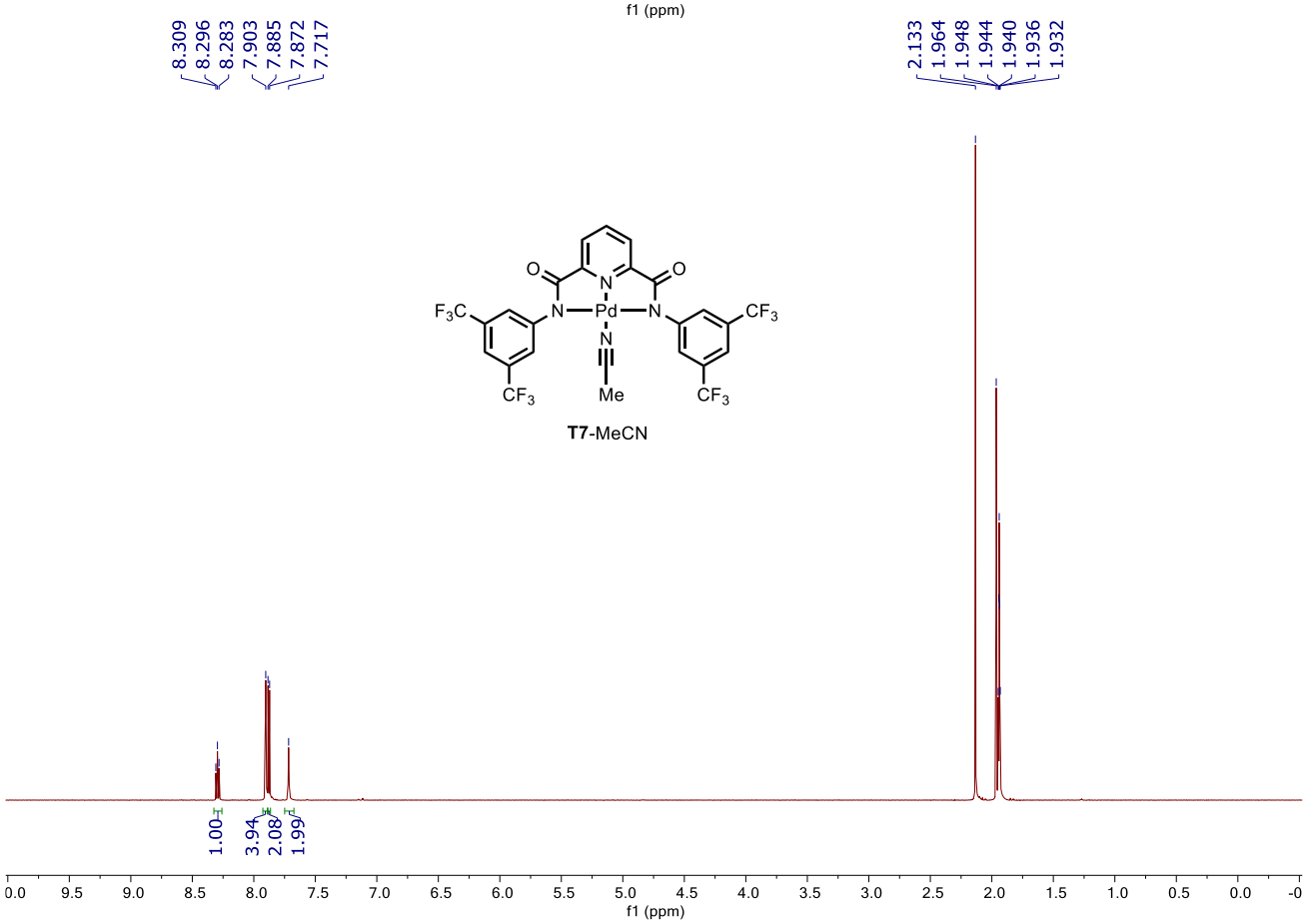
8.174
8.161
7.871
7.870
7.858
7.857
7.771
7.769
7.758
7.756
7.745
7.743
7.704
7.691
7.636
7.623
7.592
7.590
7.580
7.577
7.567
7.565
7.293
7.279
2.135
1.964
1.948
1.944
1.940
1.936
1.932
1.400
0.99
1.00
0.92
1.89
1.05
0.94
1.93
9.14
f1 (ppm)
T6-MeCN

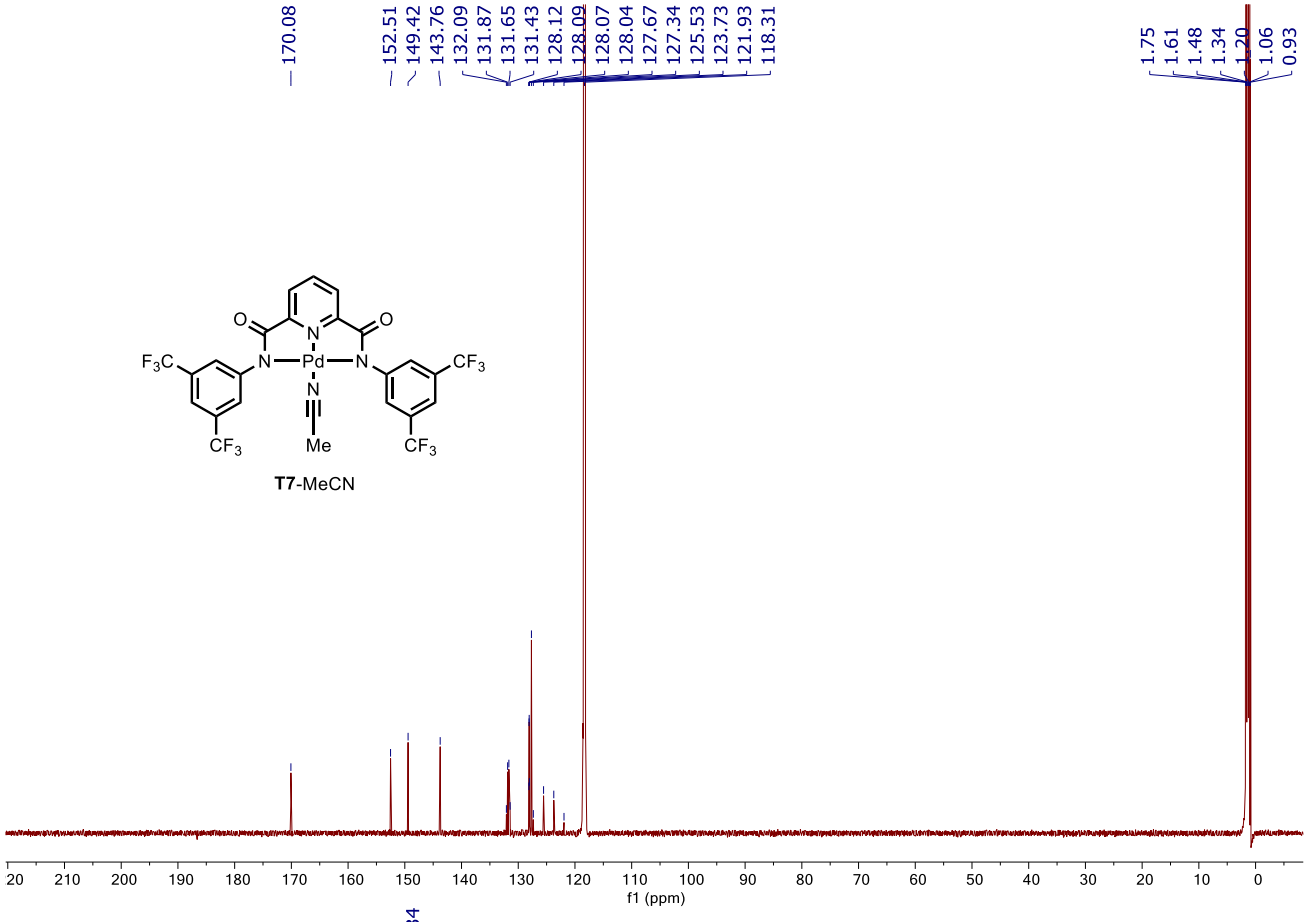

170.28
169.99
159.79
159.75
158.15
158.11
155.92
150.25
143.68
142.92
137.65
137.59
137.52
134.78
134.40
131.14
129.75
126.98
125.83
124.81
124.70
124.58
119.44
118.48
118.30
113.36
113.32
113.22
113.19
111.79
57.44
31.85
f1 (ppm)
T6-MeCN

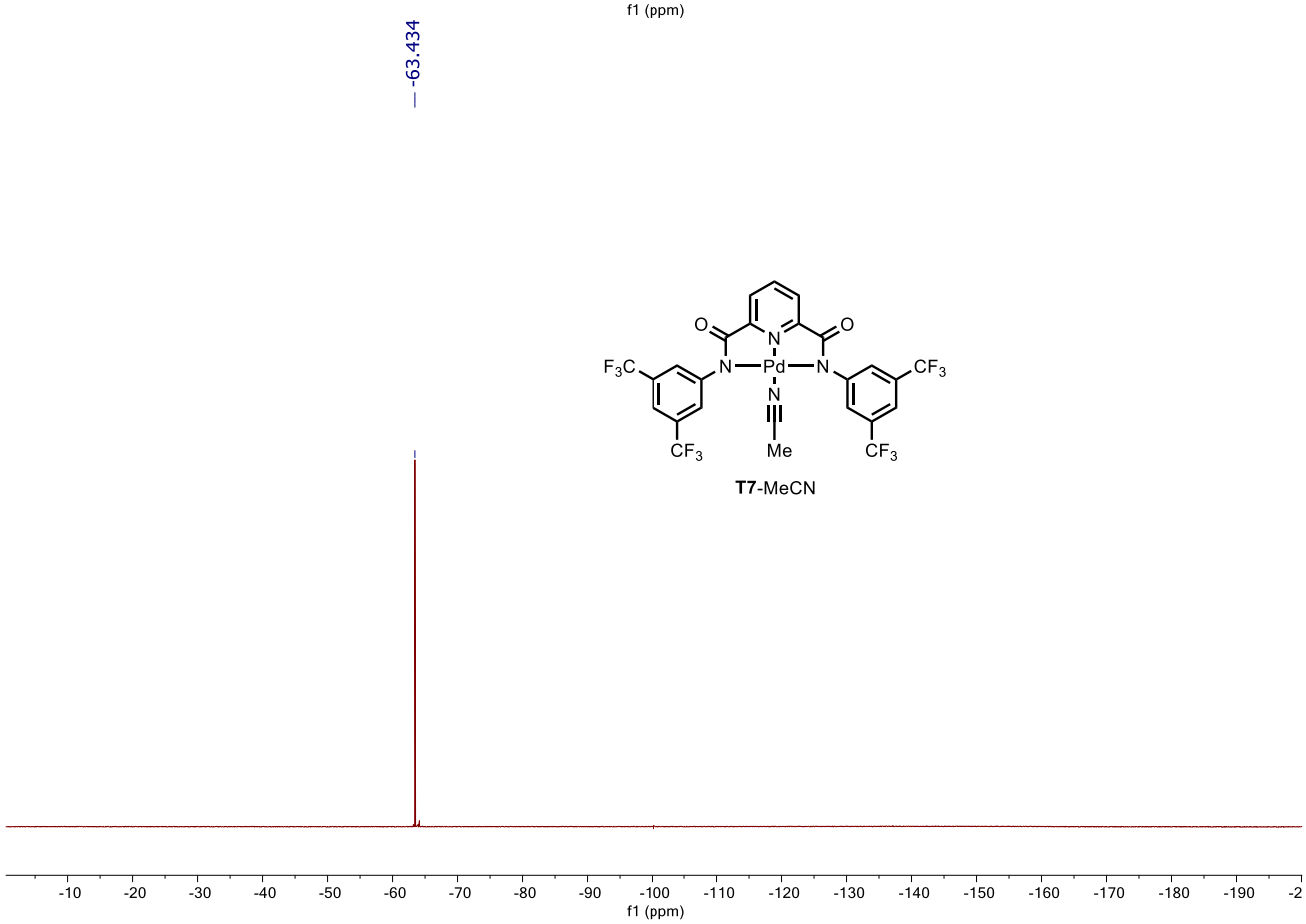


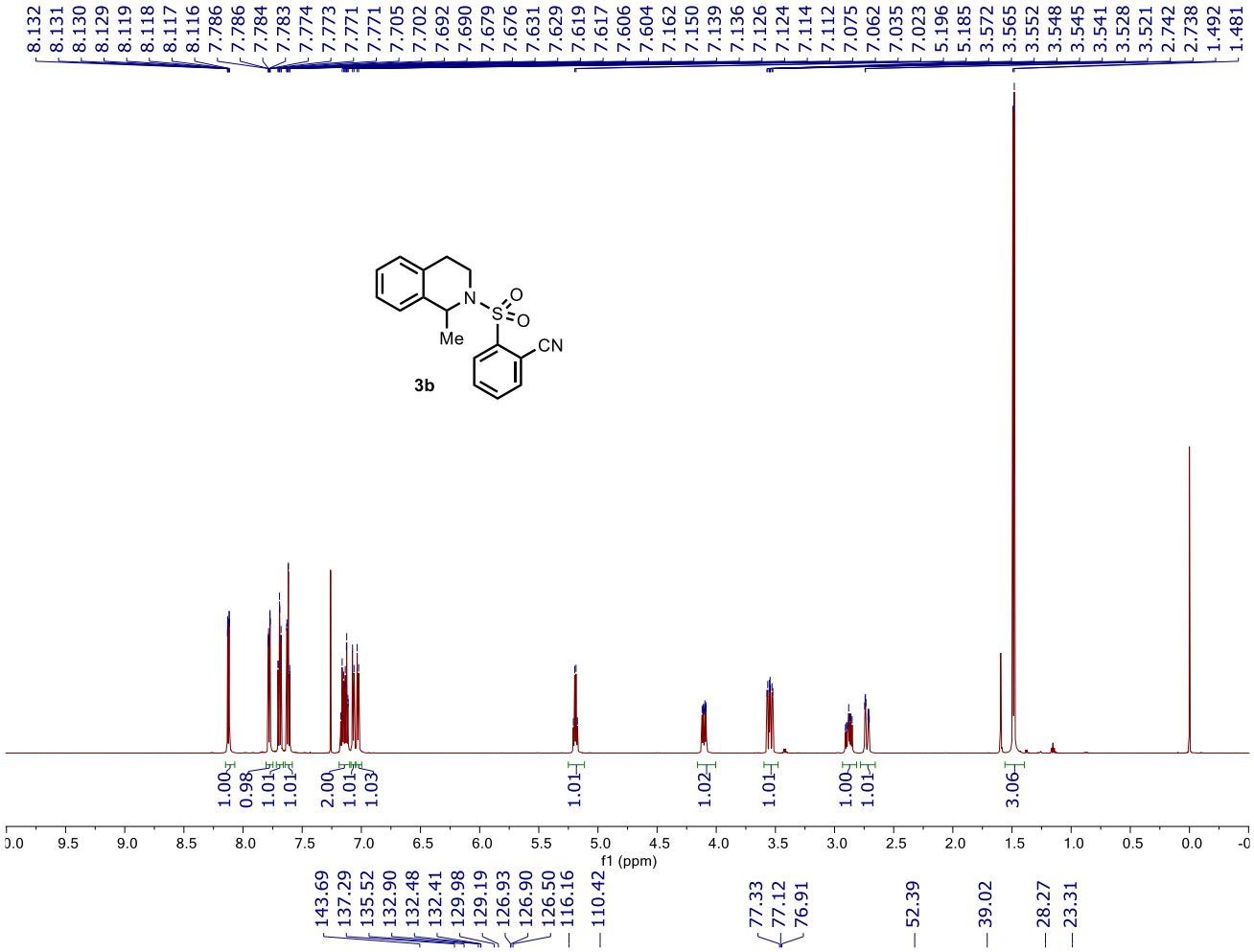
T6-MeCN



T7-MeCN


170.08
152.51
149.42
143.76
132.09
131.87
131.65
131.43
128.12
128.09
128.07
128.04
127.67
127.34
125.53
123.73
121.93
118.31
1.75
1.61
1.48
1.34
1.20
1.06
0.93
T7-MeCN
f1 (ppm)


-63.434
T7-MeCN
f1 (ppm)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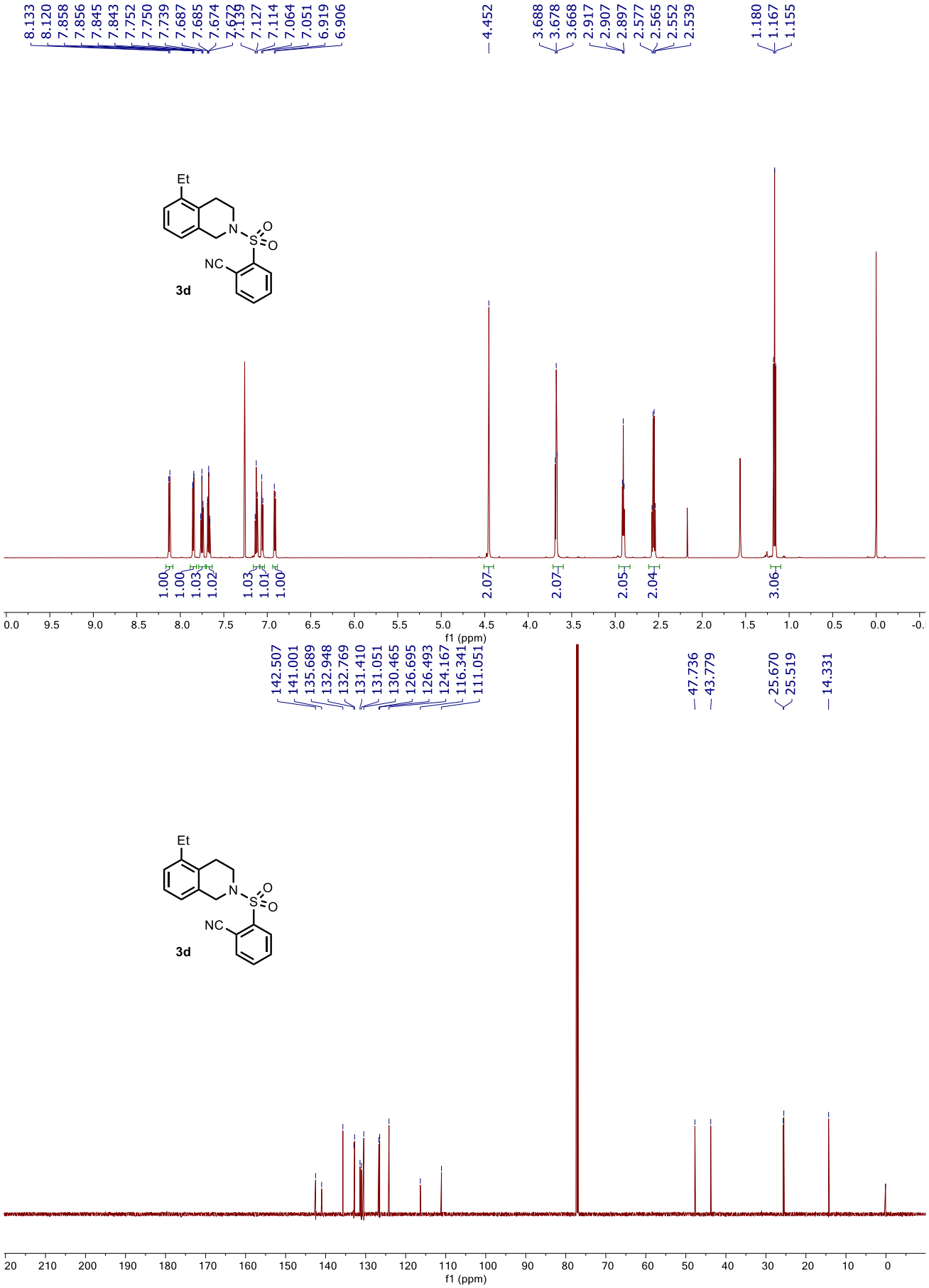
8.131
8.130
8.129
8.119
8.118
8.117
8.116
7.786
7.786
7.784
7.783
7.774
7.773
7.771
7.771
7.705
7.702
7.692
7.690
7.679
7.676
7.631
7.629
7.619
7.617
7.606
7.604
7.162
7.150
7.139
7.136
7.126
7.124
7.114
7.112
7.075
7.062
7.035
7.023
5.196
5.185
3.572
3.565
3.552
3.548
3.545
3.541
3.528
3.521
2.742
2.738
1.492
1.481
N
S
O
O
Me
CN
3b
1.00
0.98
1.01
1.01
2.00
1.01
1.03
1.01
1.02
1.01
1.00
1.01
3.06
f1 (ppm)
143.69
137.29
135.52
132.90
132.48
132.41
129.98
129.19
126.93
126.90
126.50
116.16
110.42
77.33
77.12
76.91
52.39
39.02
28.27
23.31
N
S
O
O
Me
CN
3b
f1 (ppm)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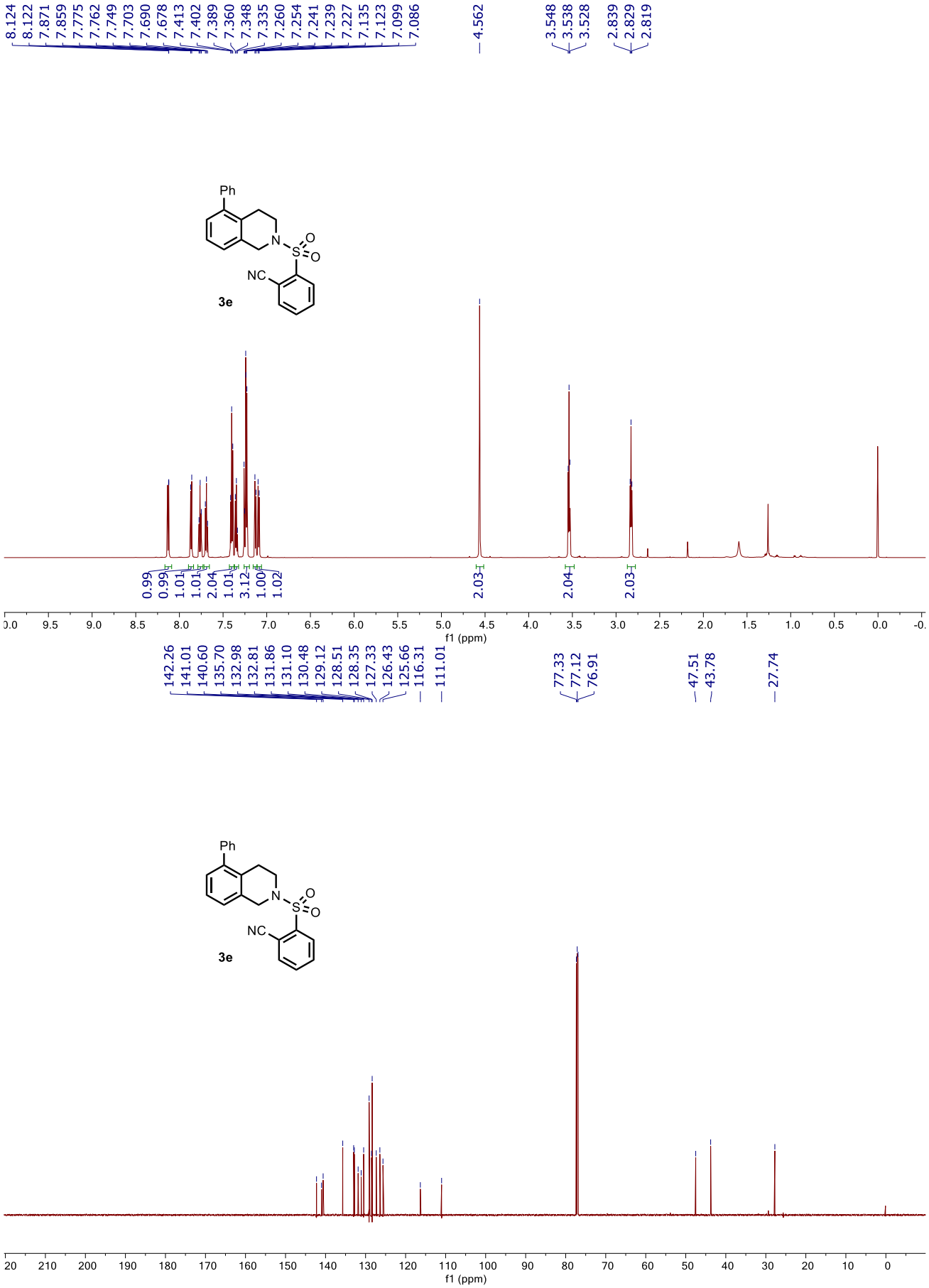
7.856
7.845
7.843
7.752
7.750
7.739
7.687
7.685
7.674
7.672
7.139
7.127
7.114
7.064
7.051
6.919
6.906
4.452
3.688
3.678
3.668
2.917
2.907
2.897
2.577
2.565
2.552
2.539
1.180
1.167
1.155
Et
N
S
O
O
NC
3d
1.00
1.00
1.03
1.02
1.03
1.01
1.00
2.07
2.07
2.05
2.04
3.06
f1 (ppm)
142.507
141.001
135.689
132.948
132.769
131.410
131.051
130.465
126.695
126.493
124.167
116.341
111.051
47.736
43.779
25.670
25.519
14.331
Et
N
S
O
O
NC
3d
f1 (ppm)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7.859
7.775
7.762
7.749
7.703
7.690
7.678
7.413
7.402
7.389
7.360
7.348
7.335
7.260
7.254
7.241
7.239
7.227
7.135
7.123
7.099
7.086
4.562
3.548
3.538
3.528
2.839
2.829
2.819
Ph
N
S
O
O
NC
3e
0.99
0.99
1.01
1.01
2.04
1.01
3.12
1.00
1.02
2.03
2.04
2.03
f1 (ppm)
142.26
141.01
140.60
135.70
132.98
132.81
131.86
131.10
130.48
129.12
128.51
128.35
127.33
126.43
125.66
116.31
111.01
77.33
77.12
76.91
47.51
43.78
27.74
f1 (ppm)


8.134
8.132
8.121
8.118
7.858
7.856
7.845
7.843
7.776
7.774
7.763
7.761
7.750
7.748
7.702
7.700
7.690
7.688
7.677
7.675
7.436
7.431
7.425
7.420
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7.046
7.043
4.498
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3.632
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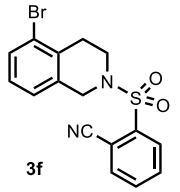
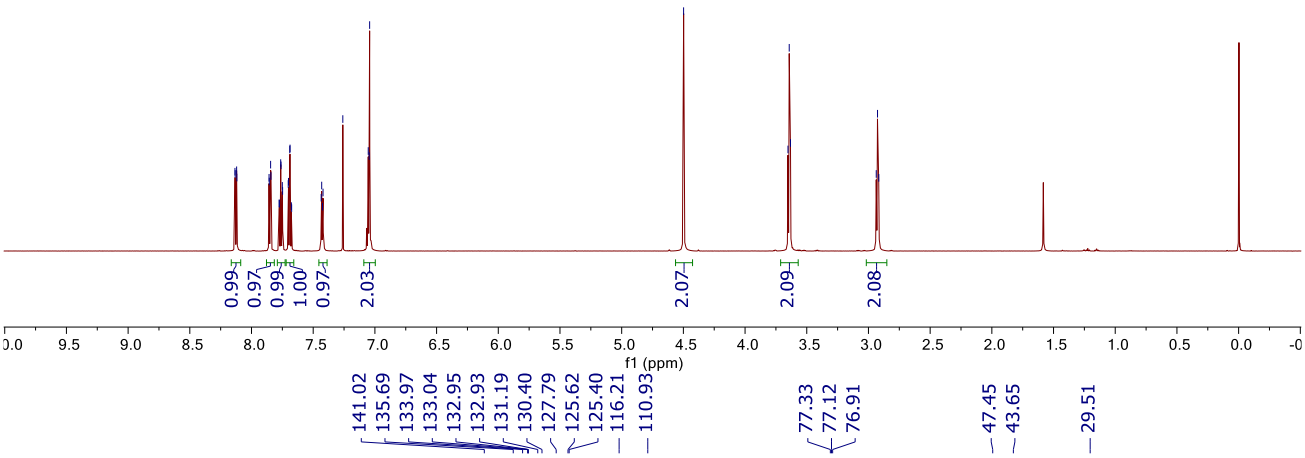
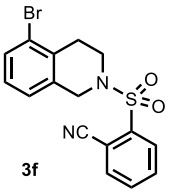
2.927
2.917


Br
N
S
O
O
NC

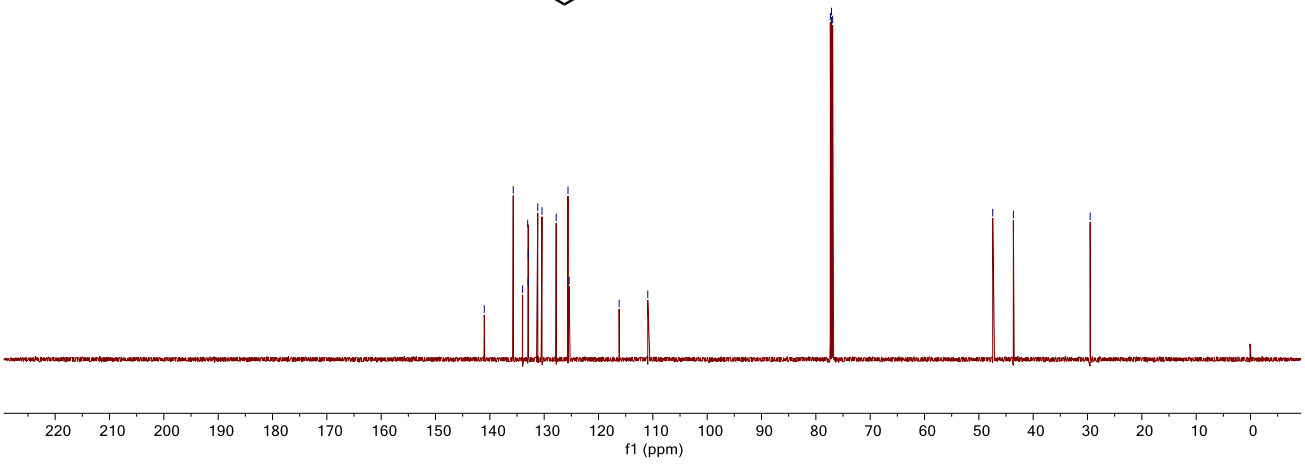
3f

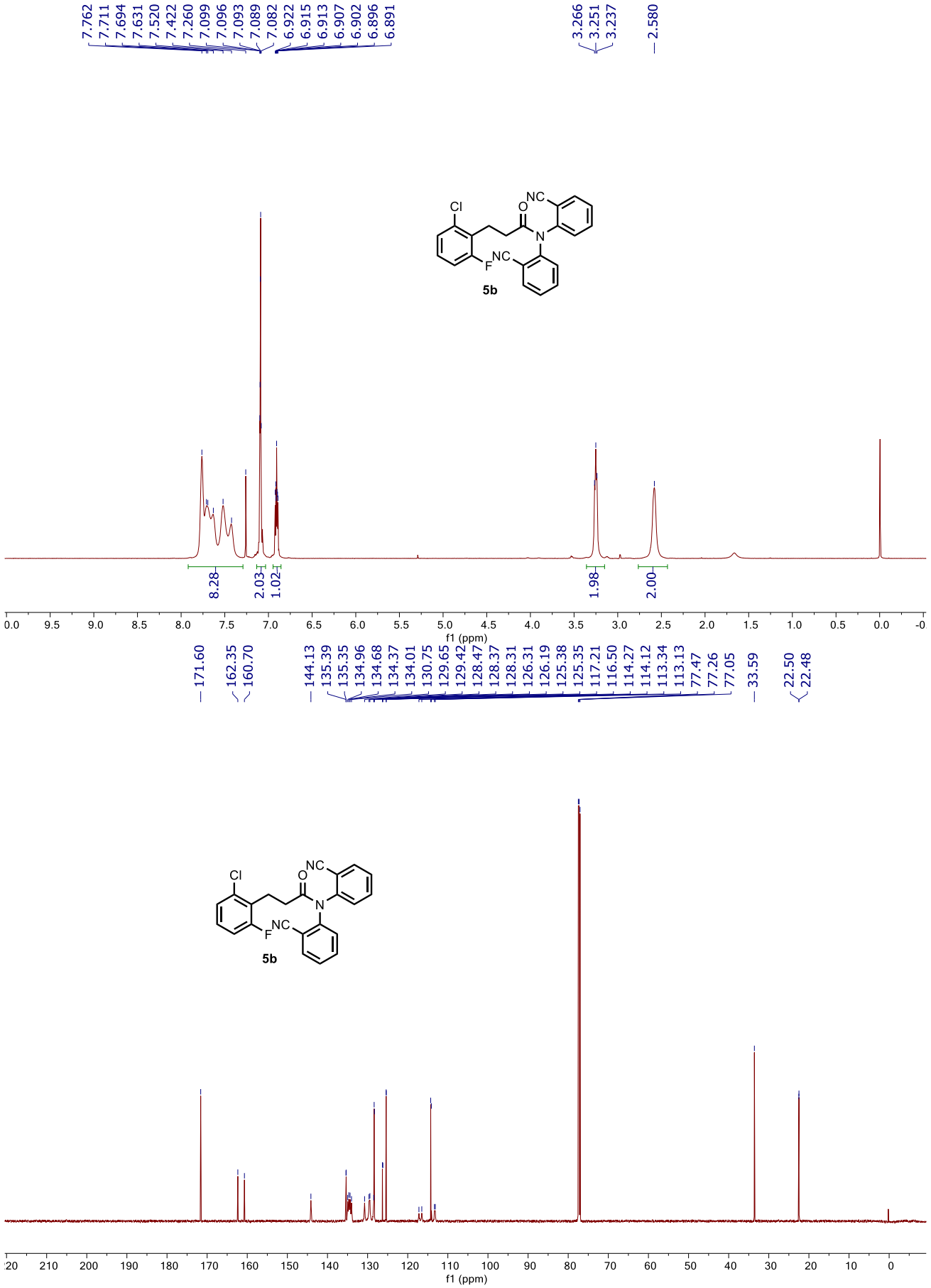

0.99
0.97
0.99
1.00
0.97
2.03
2.07
2.09
2.08
f1 (ppm)

141.02
135.69
133.97
133.04
132.95
132.93
131.19
130.40
127.79
125.62
125.40
116.21
110.93
77.33
77.12
76.91
47.45
43.65
29.51


Br
N
S
O
O
NC

3f


f1 (ppm)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7.260
7.099
7.096
7.093
7.089
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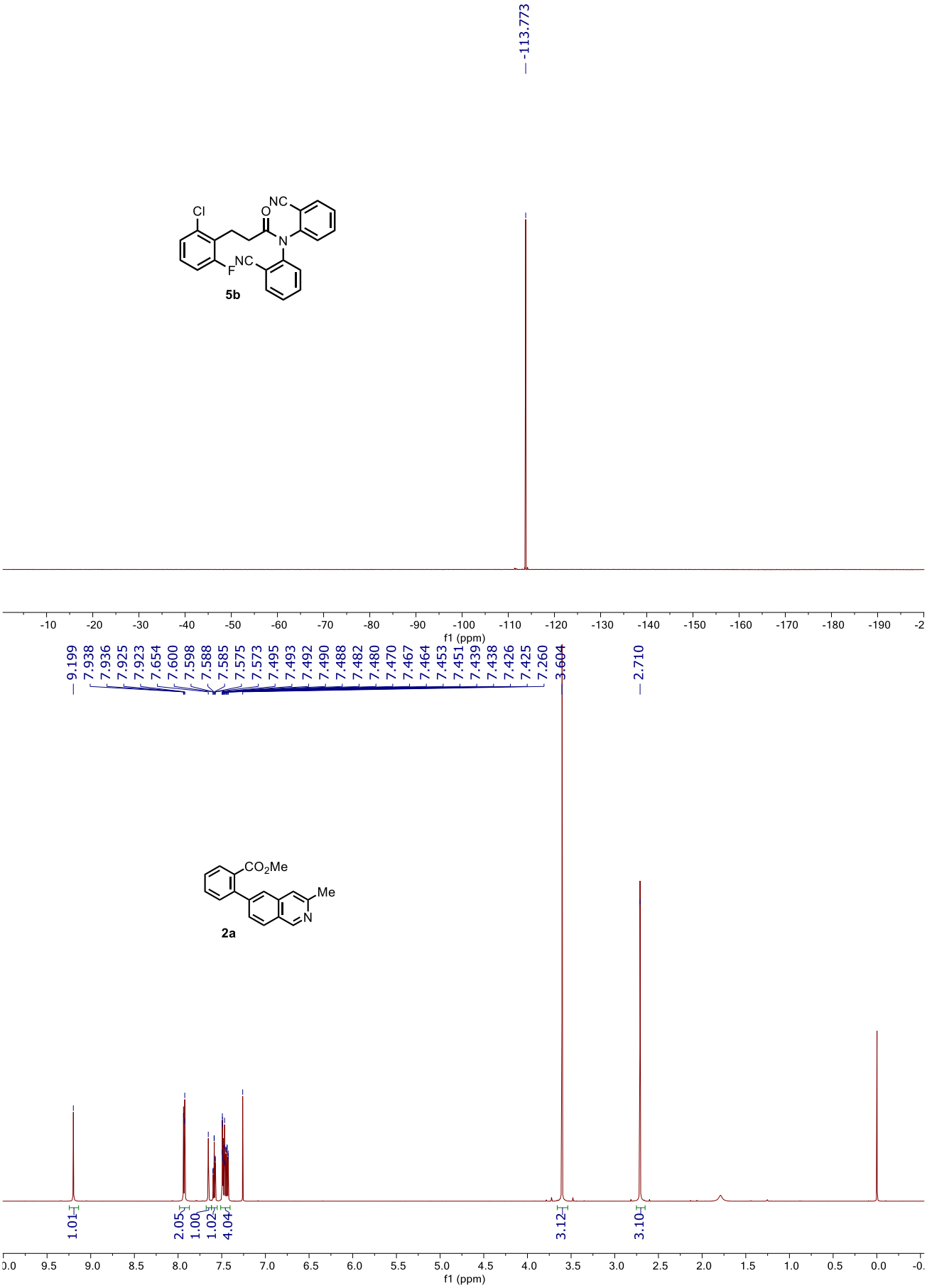
6.922
6.915
6.913
6.907
6.902
6.896
6.891
3.266
3.251
3.237
2.580
Cl
O
NC
N
F
NC
5b
8.28
2.03
1.02
1.98
2.00
f1 (ppm)
171.60
162.35
160.70
144.13
135.39
135.35
134.96
134.68
134.37
134.01
130.75
129.65
129.42
128.47
128.37
128.31
126.31
126.19
125.38
125.35
117.21
116.50
114.27
114.12
113.34
113.13
77.47
77.26
77.05
33.59
22.50
22.48
Cl
O
NC
N
F
NC
5b
f1 (ppm)


-113.773
Cl
O
NC
N
F
NC
5b
f1 (ppm)
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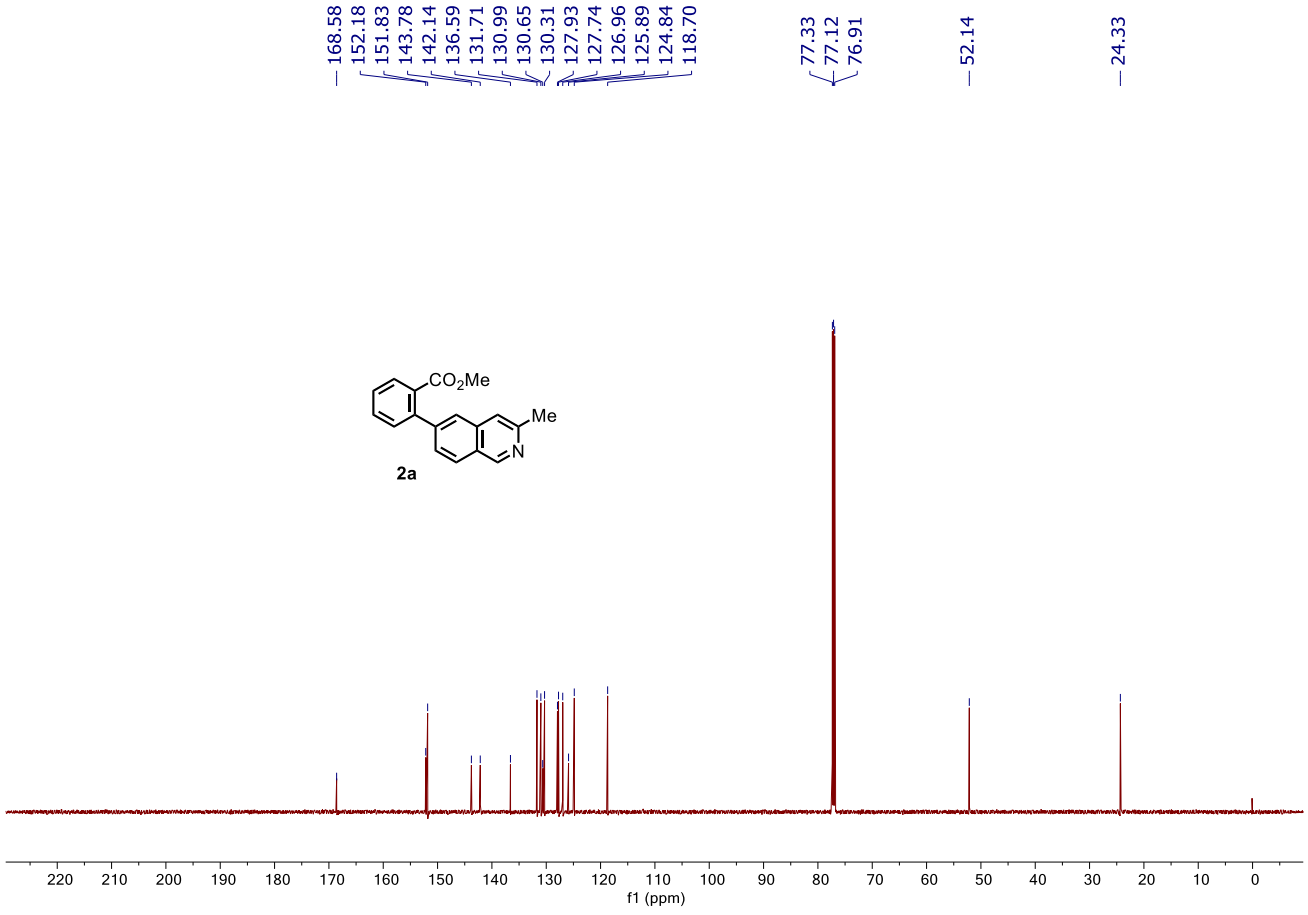
7.938
7.936
7.925
7.923
7.654
7.600
7.598
7.588
7.585
7.575
7.573
7.495
7.493
7.492
7.490
7.488
7.482
7.480
7.470
7.467
7.464
7.453
7.451
7.439
7.438
7.426
7.425
7.260
3.604
2.710
CO2Me
Me
N
2a
1.01
2.05
1.00
1.02
4.04
3.12
3.10
f1 (ppm)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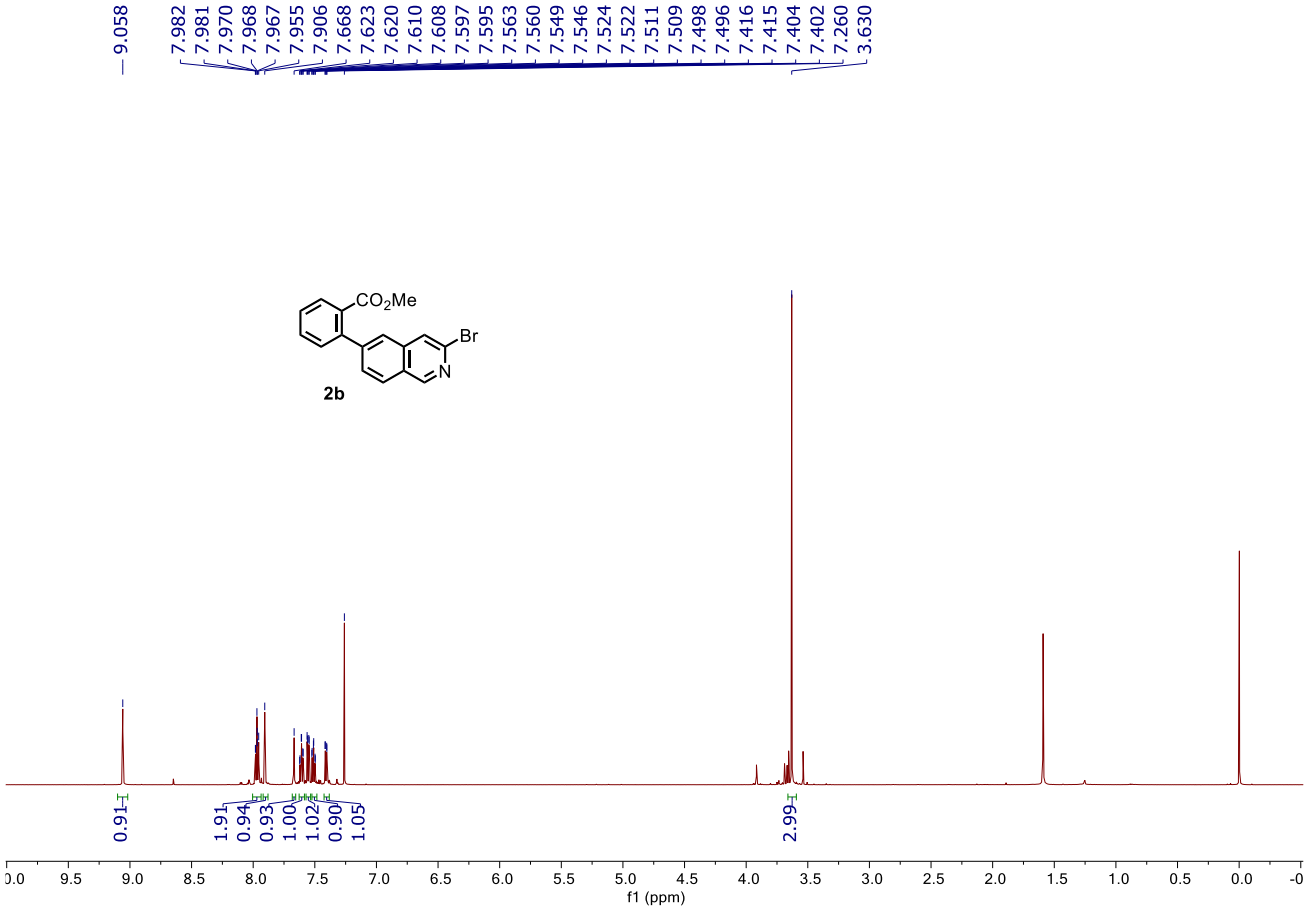
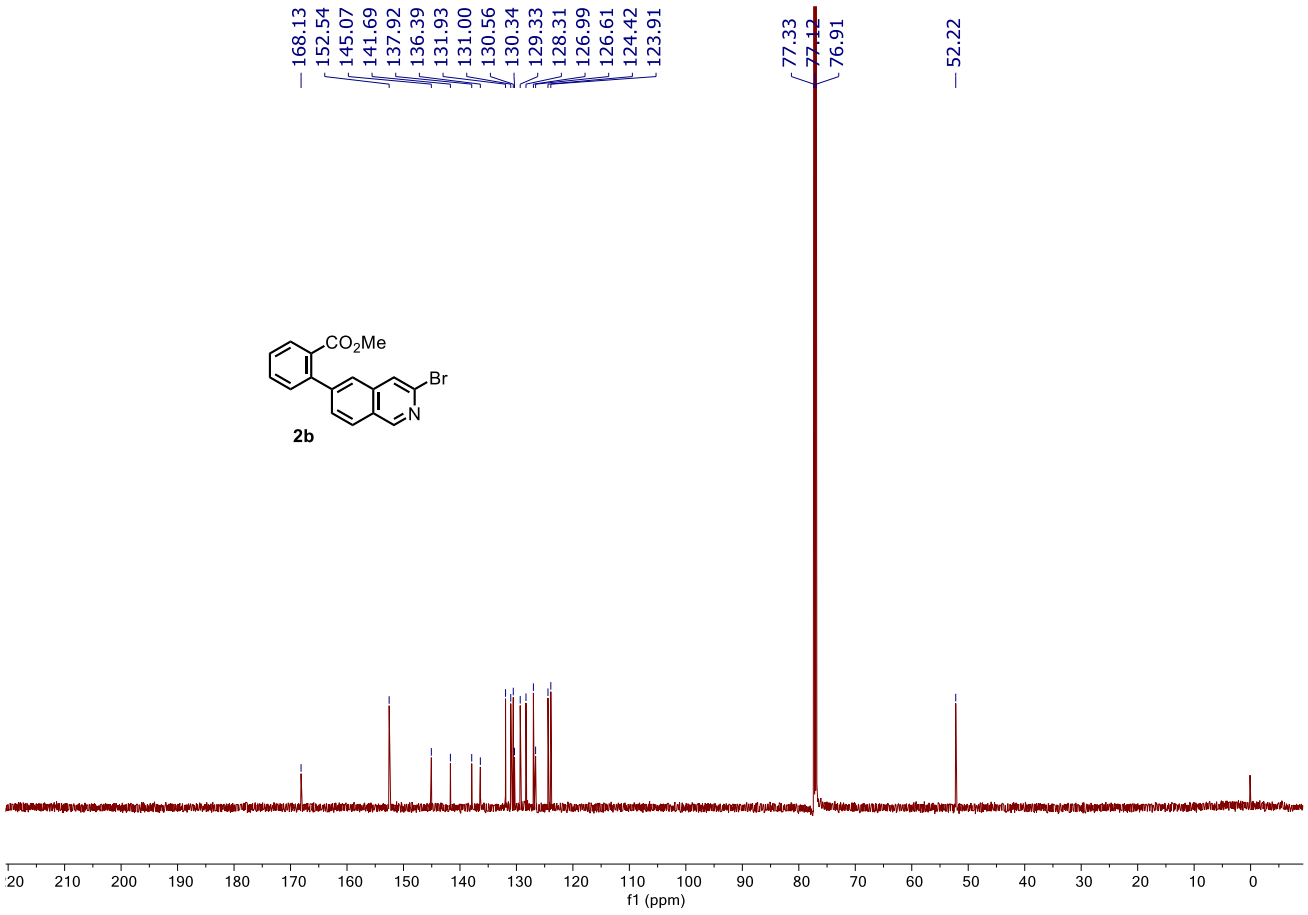
152.18
151.83
143.78
142.14
136.59
131.71
130.99
130.65
130.31
127.93
127.74
126.96
125.89
124.84
118.70
77.33
77.12
76.91
52.14
24.33
CO2Me
Me
N
2a
f1 (ppm)


9.058
7.982
7.981
7.970
7.968
7.967
7.955
7.906
7.668
7.623
7.620
7.610
7.608
7.597
7.595
7.563
7.560
7.549
7.546
7.524
7.522
7.511
7.509
7.498
7.496
7.416
7.415
7.404
7.402
7.260
3.630
CO2Me
Br
N
2b
0.91
1.91
0.94
0.93
1.00
1.02
0.90
1.05
2.99
f1 (ppm)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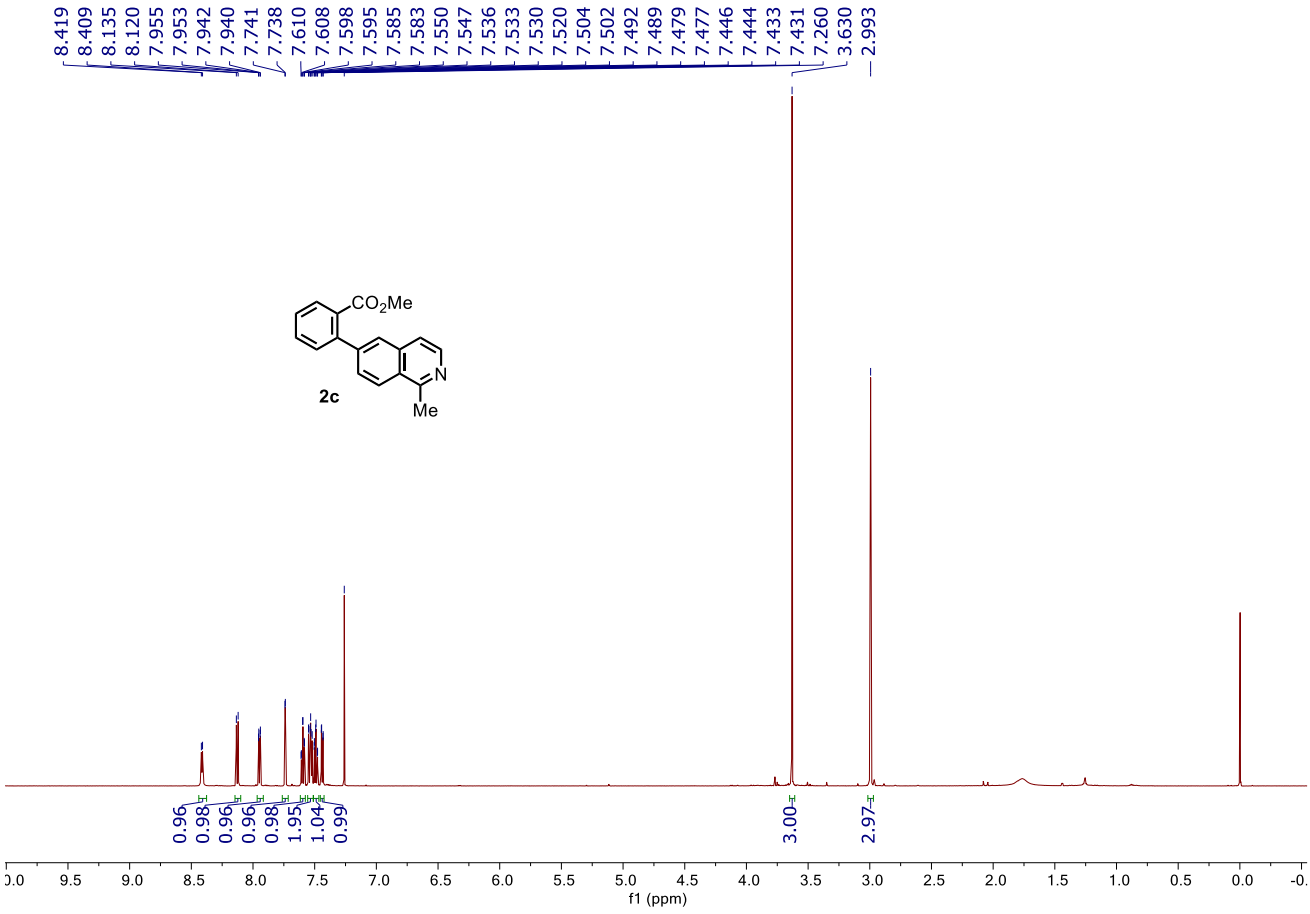
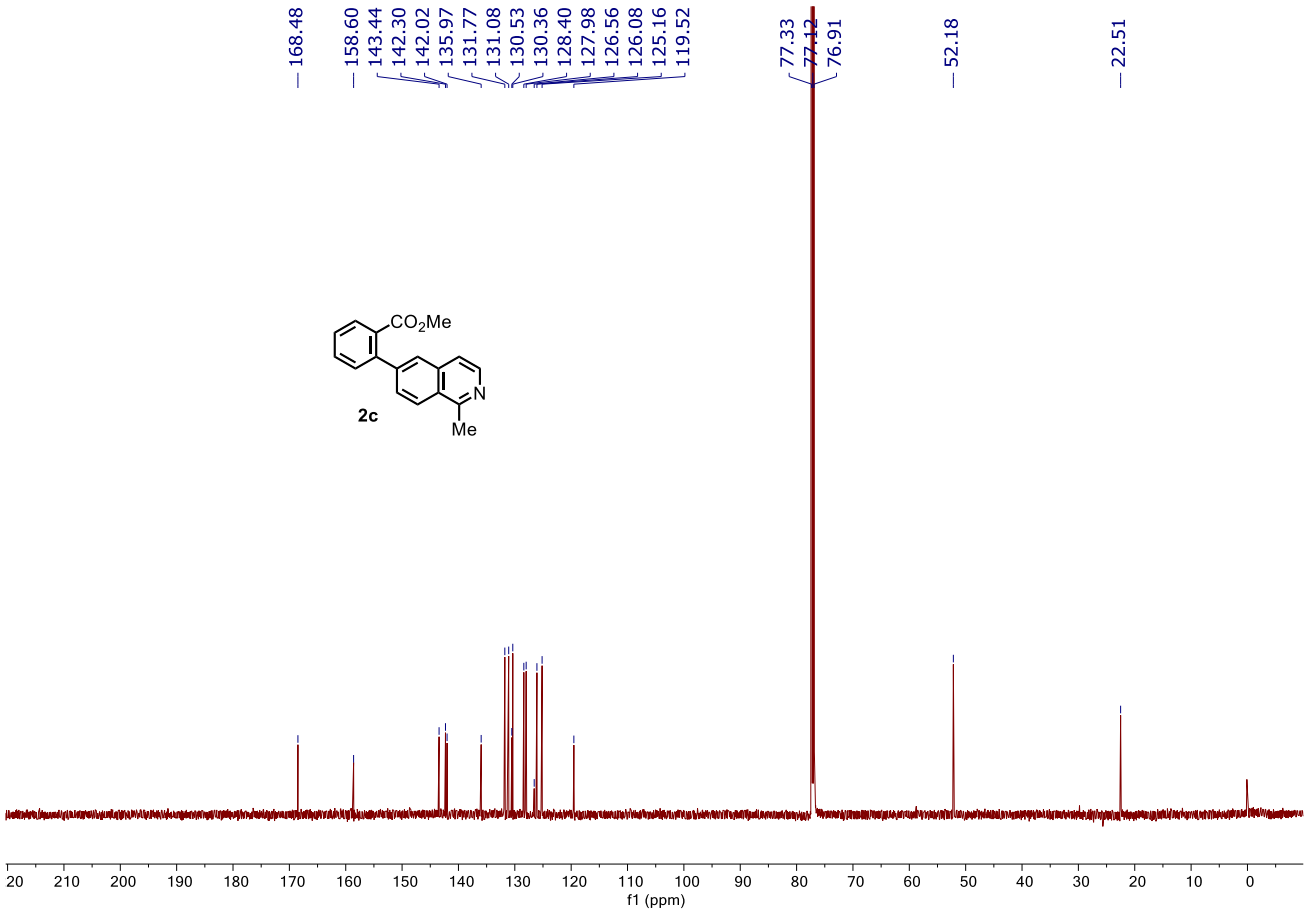
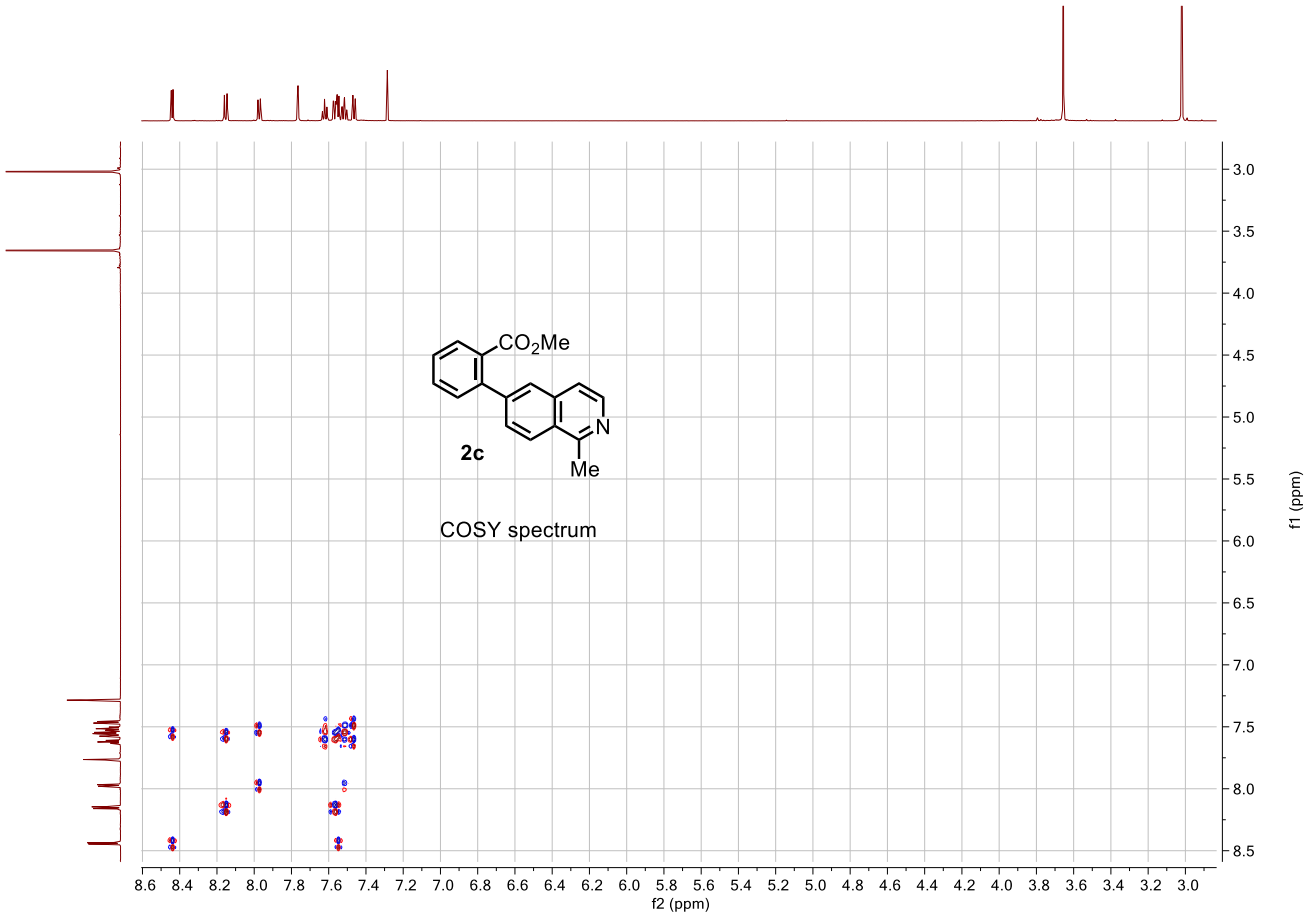
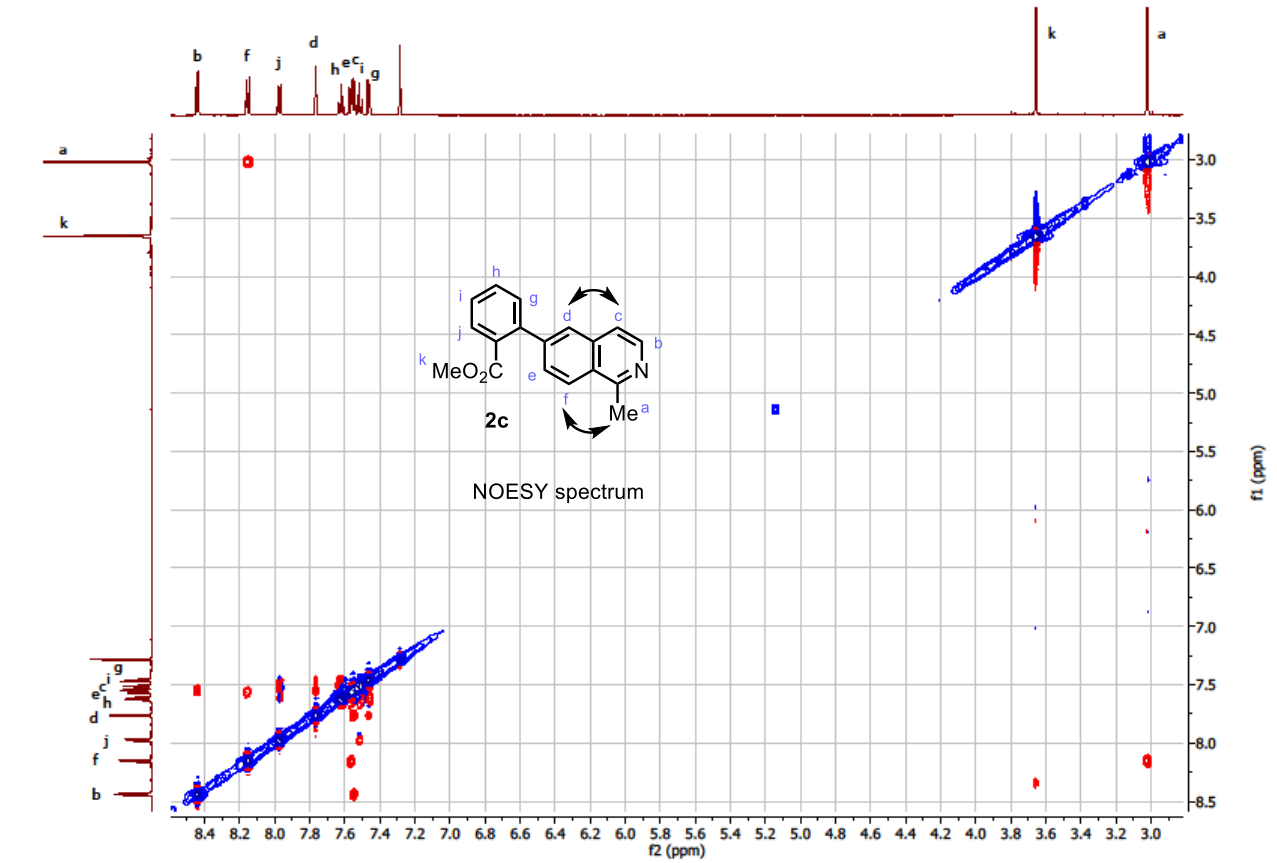
152.54
145.07
141.69
137.92
136.39
131.93
131.00
130.56
130.34
129.33
128.31
126.99
126.61
124.42
123.91
77.33
77.12
76.91
52.22
CO2Me
Br
N
2b
f1 (ppm)

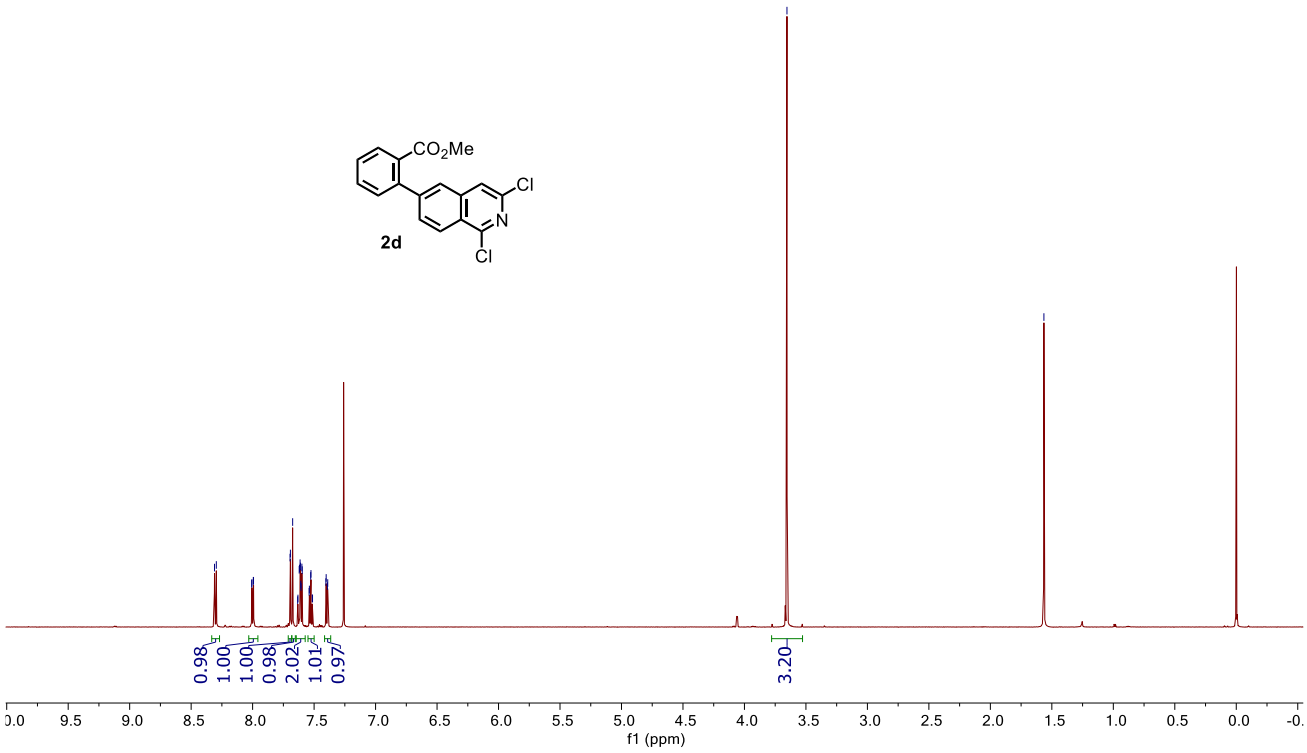

8.419
8.409
8.135
8.120
7.955
7.953
7.942
7.940
7.741
7.738
7.610
7.608
7.598
7.595
7.585
7.583
7.550
7.547
7.536
7.533
7.530
7.520
7.504
7.502
7.492
7.489
7.479
7.477
7.446
7.444
7.433
7.431
7.260
3.630
2.993
CO2Me
N
Me
2c
0.96
0.98
0.96
0.96
0.98
1.95
1.04
0.99
3.00
2.97
f1 (ppm)


168.48
158.60
143.44
142.30
142.02
135.97
131.77
131.08
130.53
130.36
128.40
127.98
126.56
126.08
125.16
119.52
77.33
77.12
76.91
52.18
22.51
CO2Me
N
Me
2c
f1 (ppm)

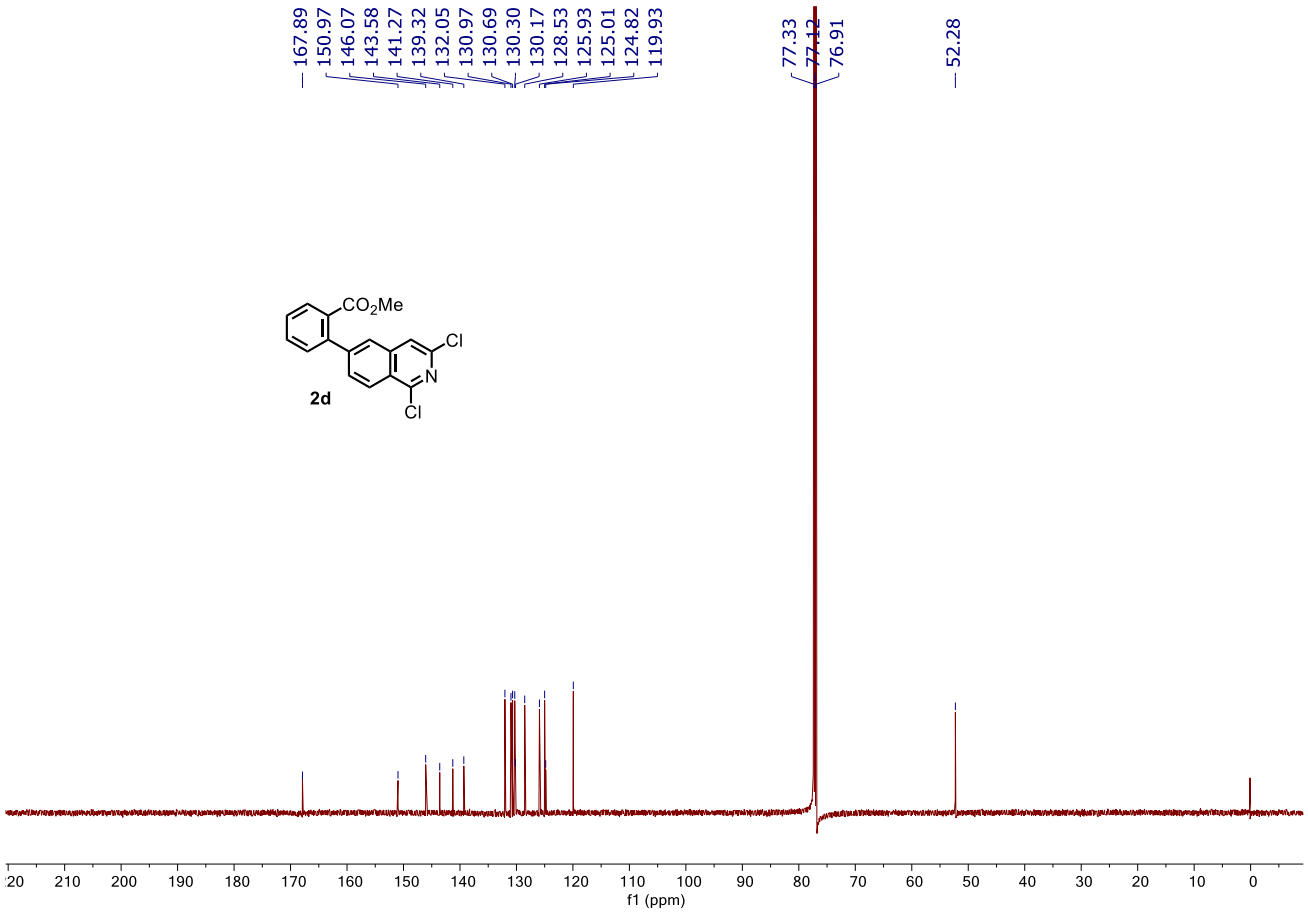

CO2Me
N
Me
2c
COSY spectrum
f1 (ppm)
f2 (ppm)

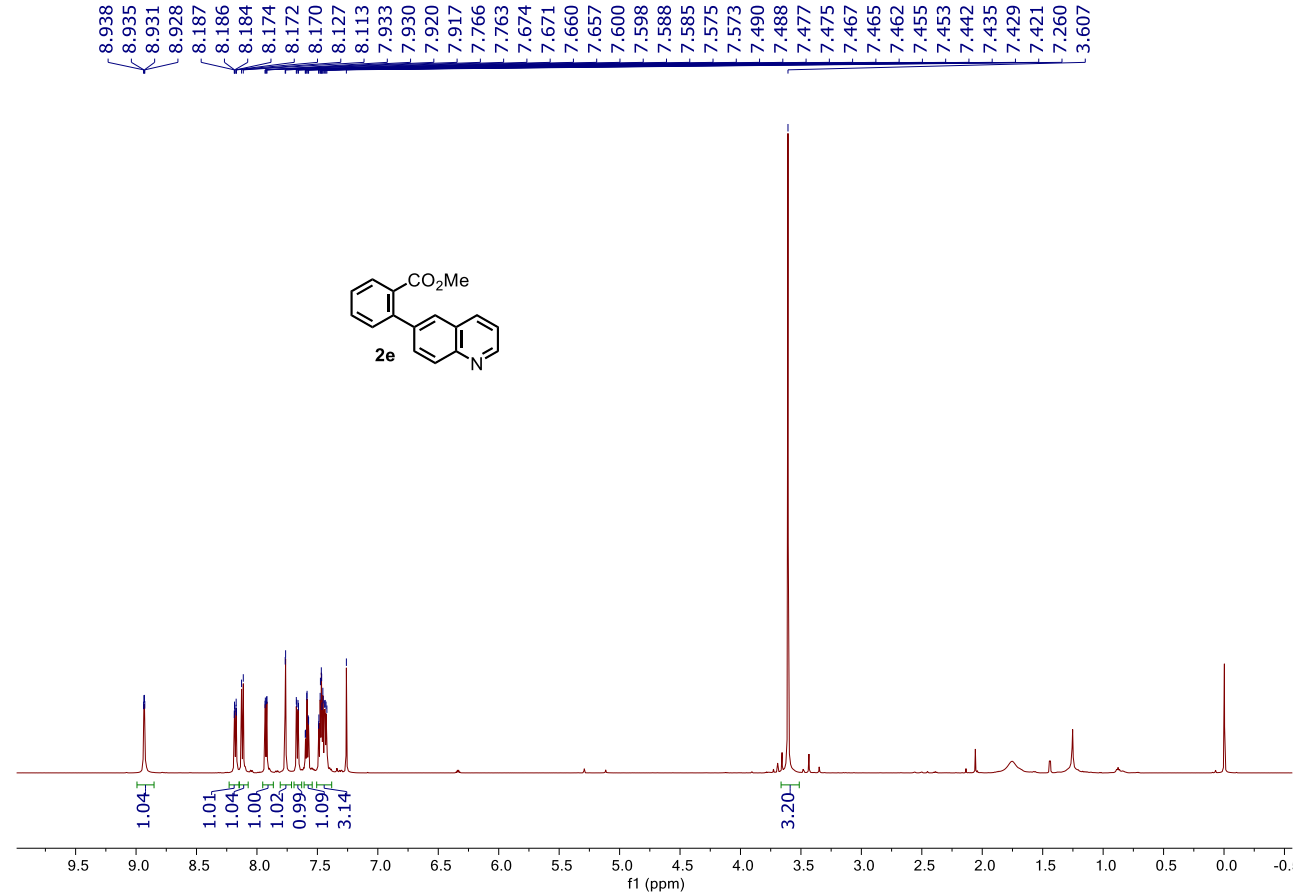


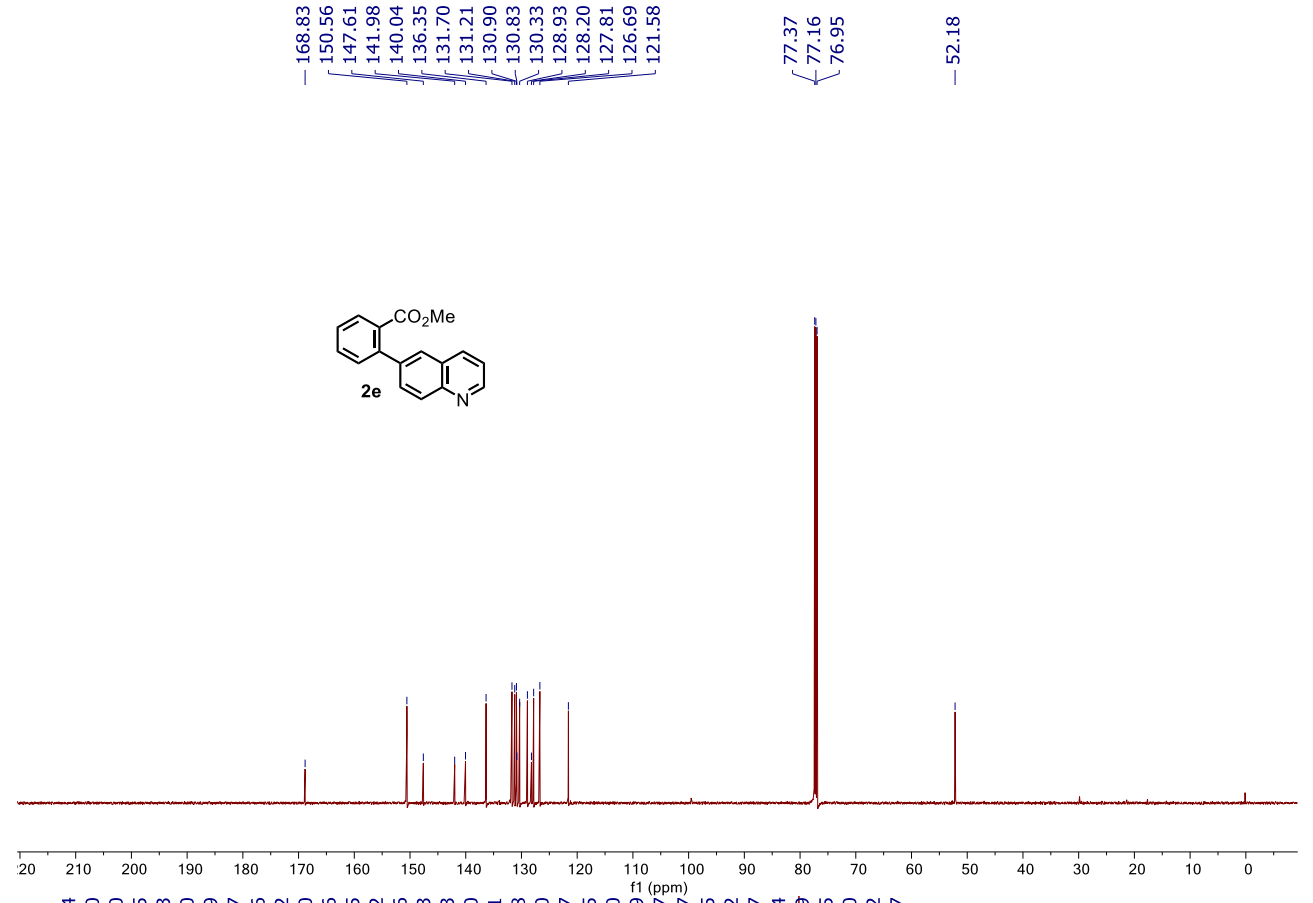
8.310 8.295 8.007 8.006 7.994 7.993 7.695 7.693 7.674 7.634 7.631 7.621 7.619 7.614 7.611 7.609 7.606 7.599 7.597 7.540 7.538 7.528 7.526 7.515 7.513 7.404 7.402 7.392 7.389 — 3.654 — 1.564



0.98 1.00 1.00 0.98 2.02 1.01 0.97 — 3.20


167.89
150.97
146.07
143.58
141.27
139.32
132.05
130.97
130.69
130.30
130.17
128.53
125.93
125.01
124.82
119.93
77.33
77.12
76.91
52.28
CO2Me
Cl
N
Cl
2d
f1 (ppm)


8.938
8.935
8.931
8.928
8.187
8.186
8.184
8.174
8.172
8.170
8.127
8.113
7.933
7.930
7.920
7.917
7.766
7.763
7.674
7.671
7.660
7.657
7.600
7.598
7.588
7.585
7.575
7.573
7.490
7.488
7.477
7.475
7.467
7.465
7.462
7.455
7.453
7.442
7.435
7.429
7.421
7.260
3.607
CO2Me
N
2e
1.04
1.01
1.04
1.00
1.02
0.99
1.09
3.14
3.20
f1 (ppm)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150.56
147.61
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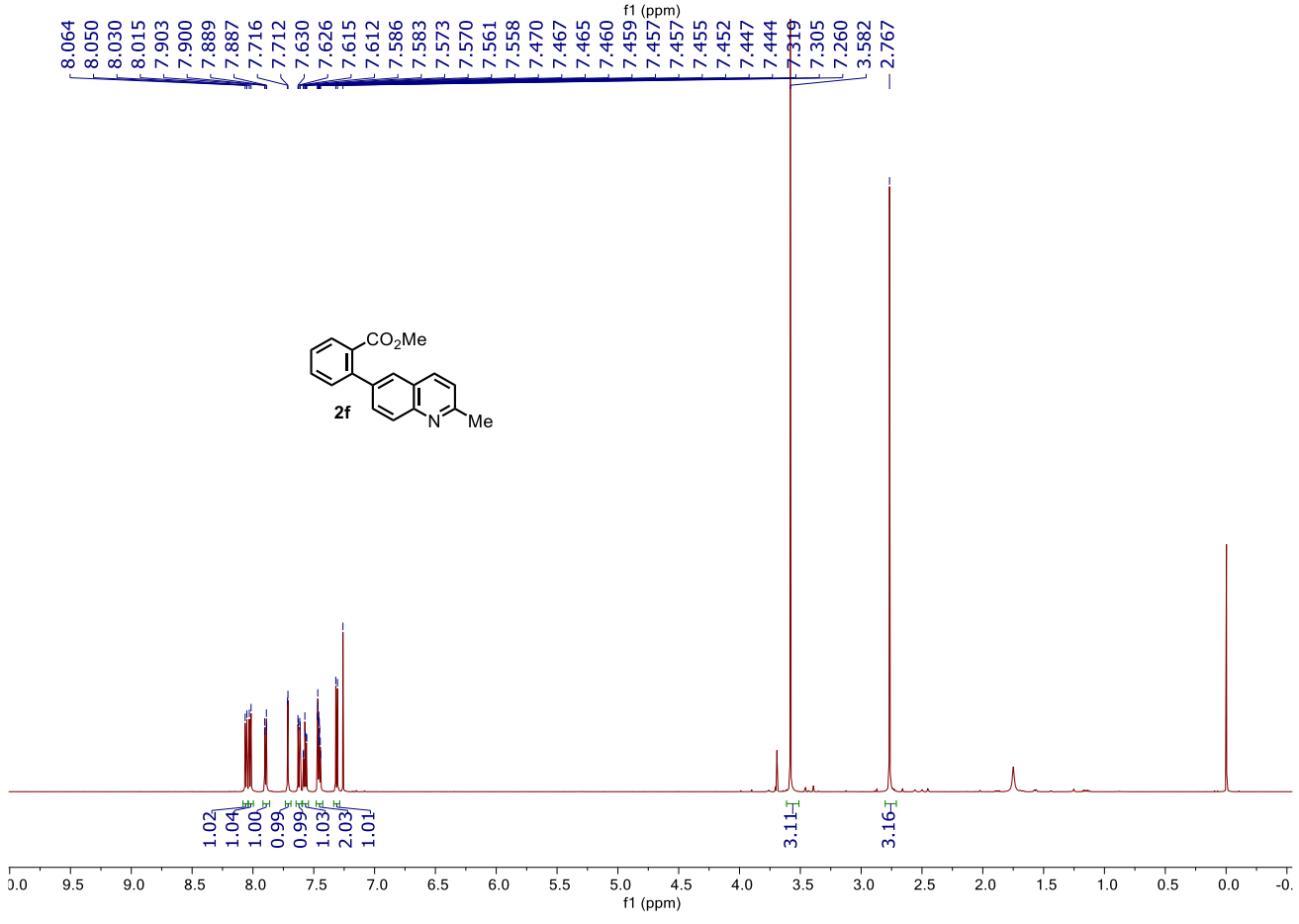
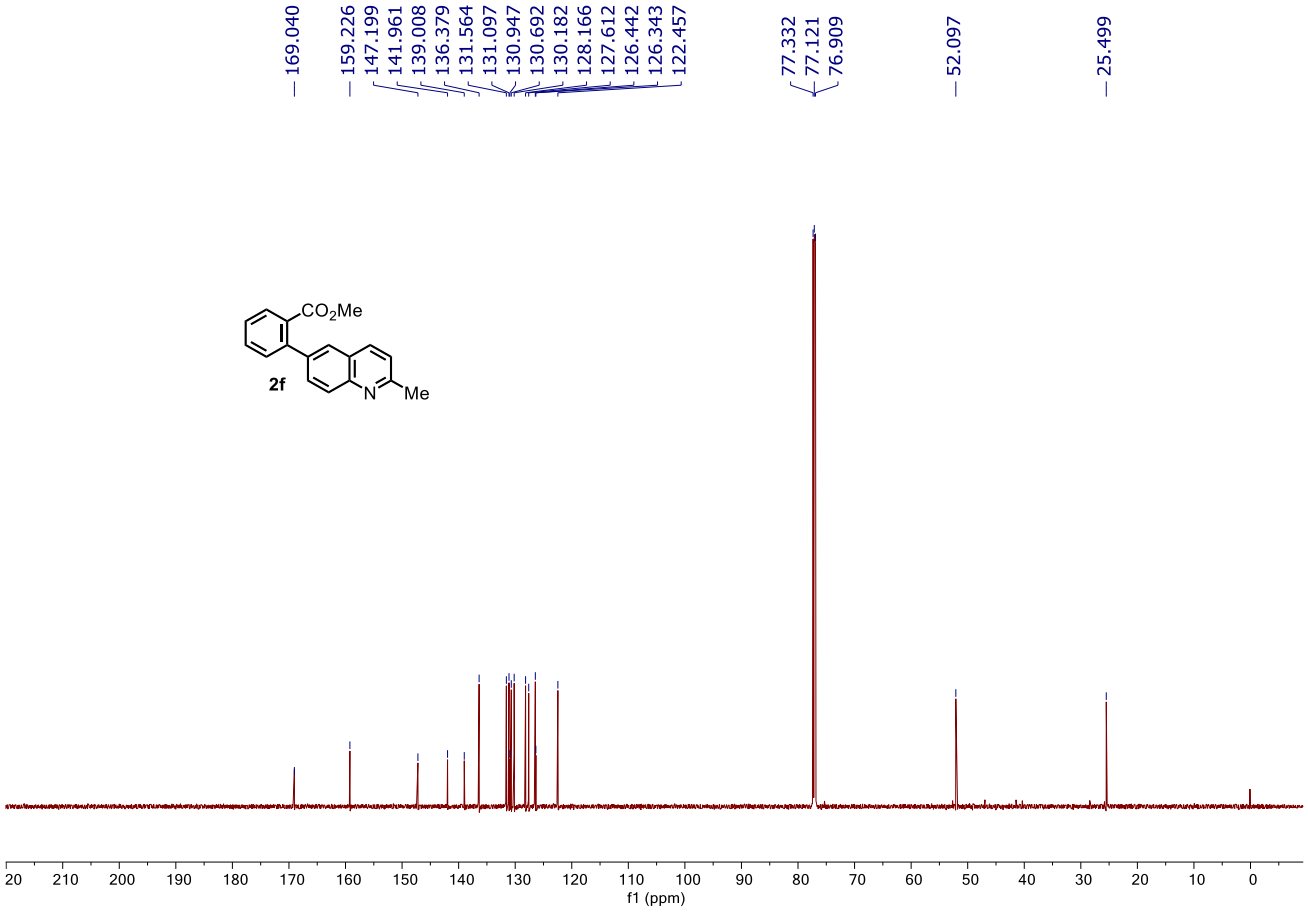
140.04
136.35
131.70
131.21
130.90
130.83
130.33
128.93
128.20
127.81
126.69
121.58
77.37
77.16
76.95
52.18
CO2Me
2e
N
f1 (ppm)


8.064
8.050
8.030
8.015
7.903
7.900
7.889
7.887
7.716
7.712
7.630
7.626
7.615
7.612
7.586
7.583
7.573
7.570
7.561
7.558
7.470
7.467
7.465
7.460
7.459
7.457
7.457
7.455
7.452
7.447
7.444
7.319
7.305
7.260
3.582
2.767
CO2Me
2f
N
Me
1.02
1.04
1.00
0.99
0.99
1.03
2.03
1.01
3.11
3.16
f1 (ppm)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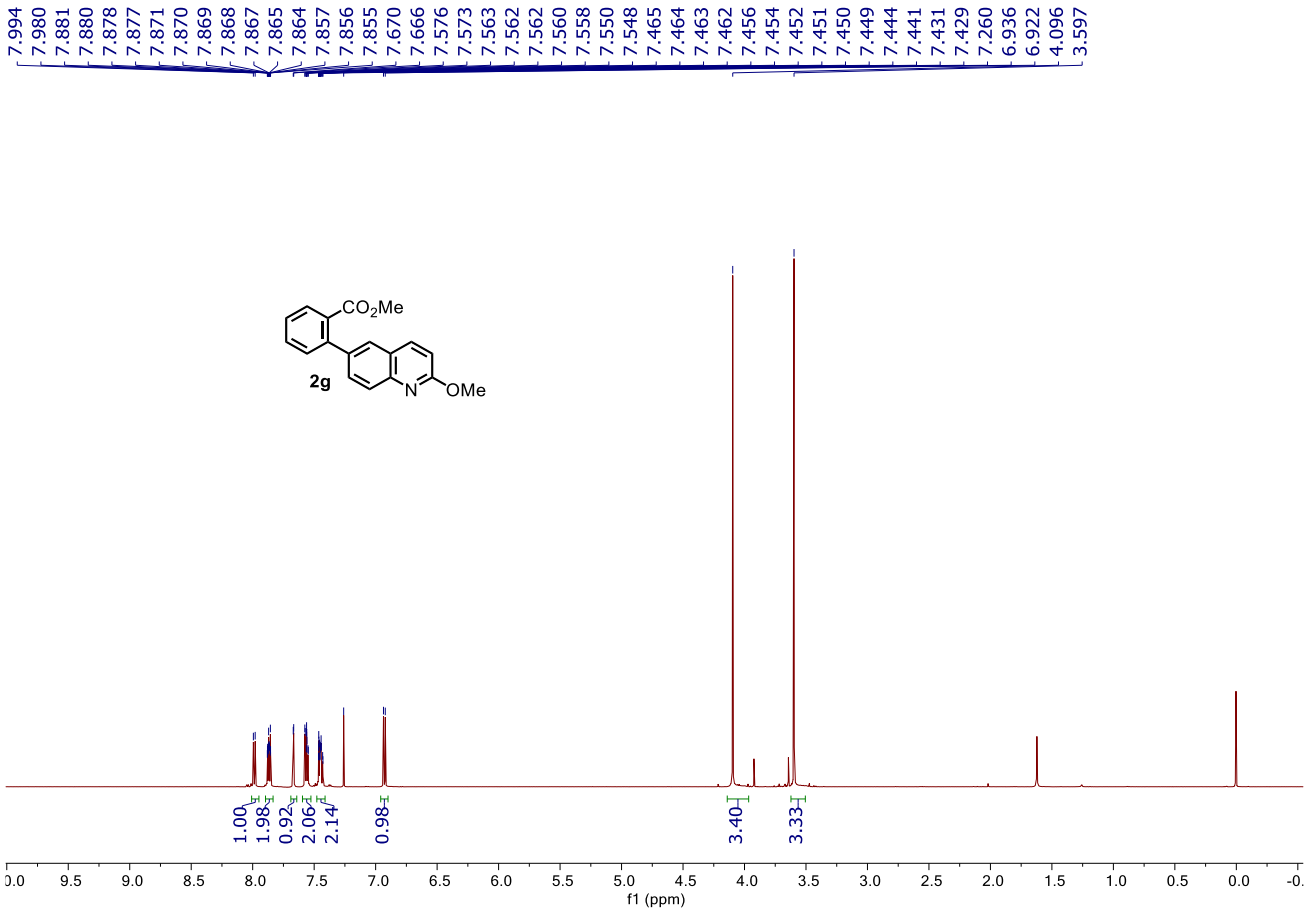
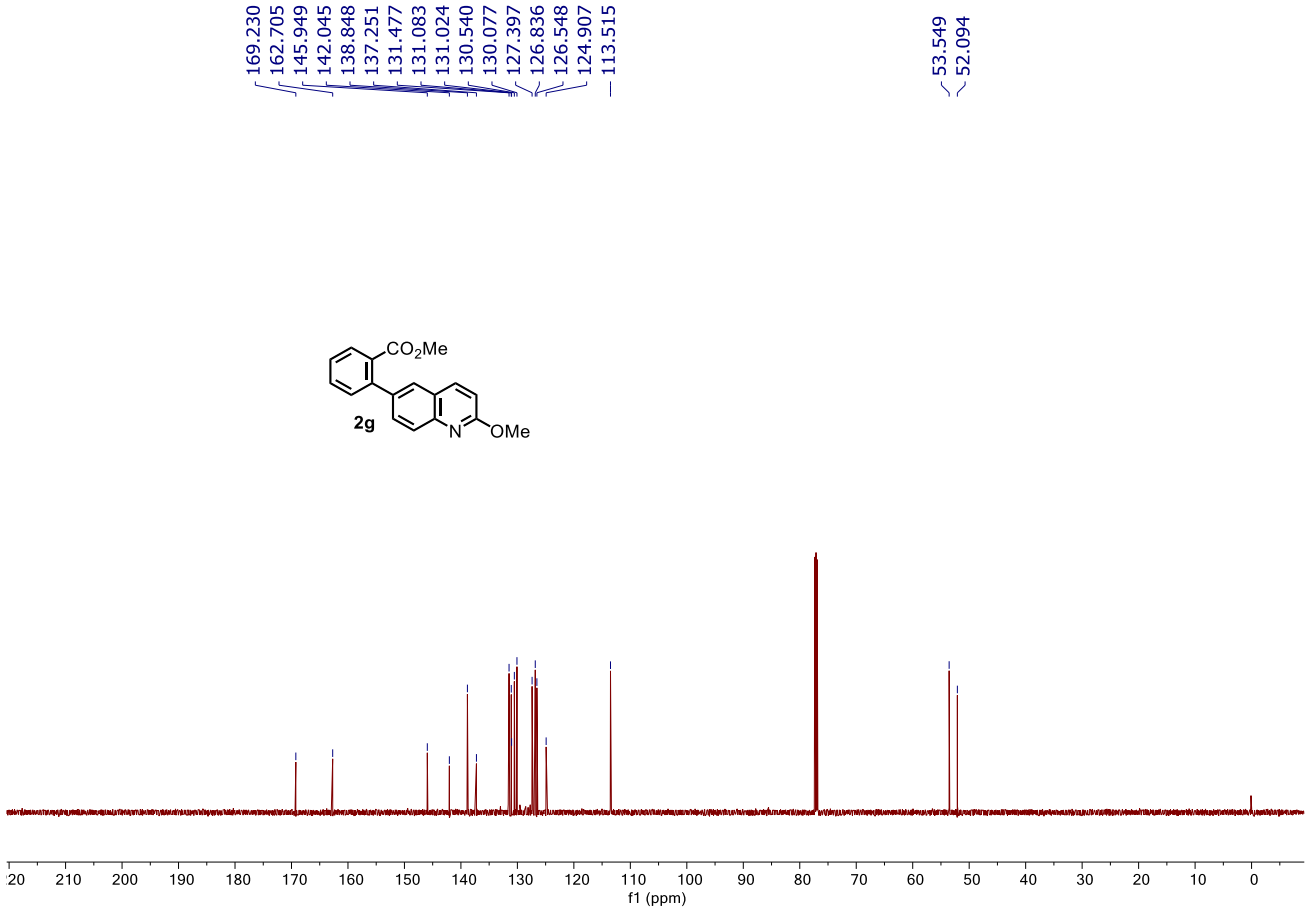
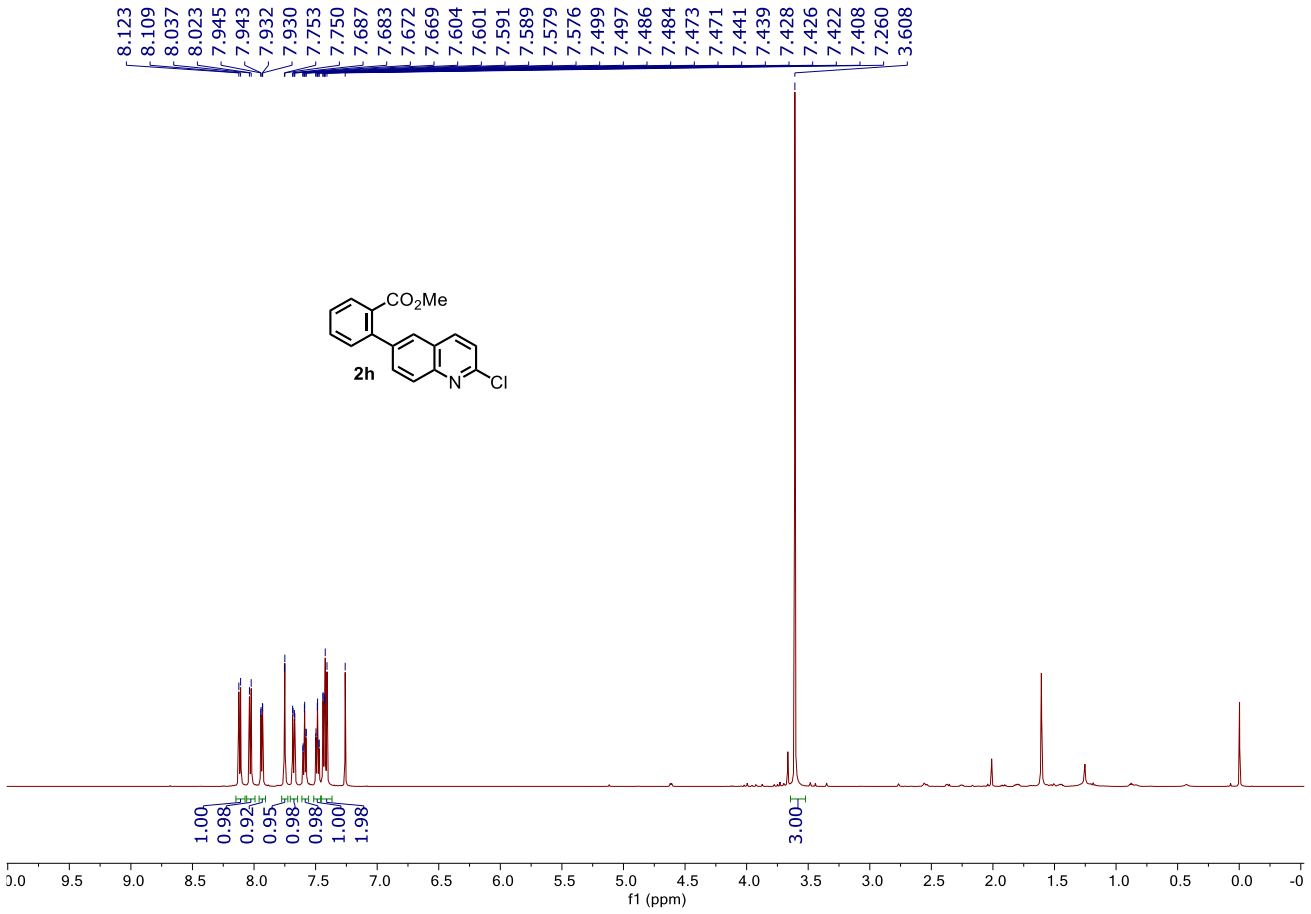
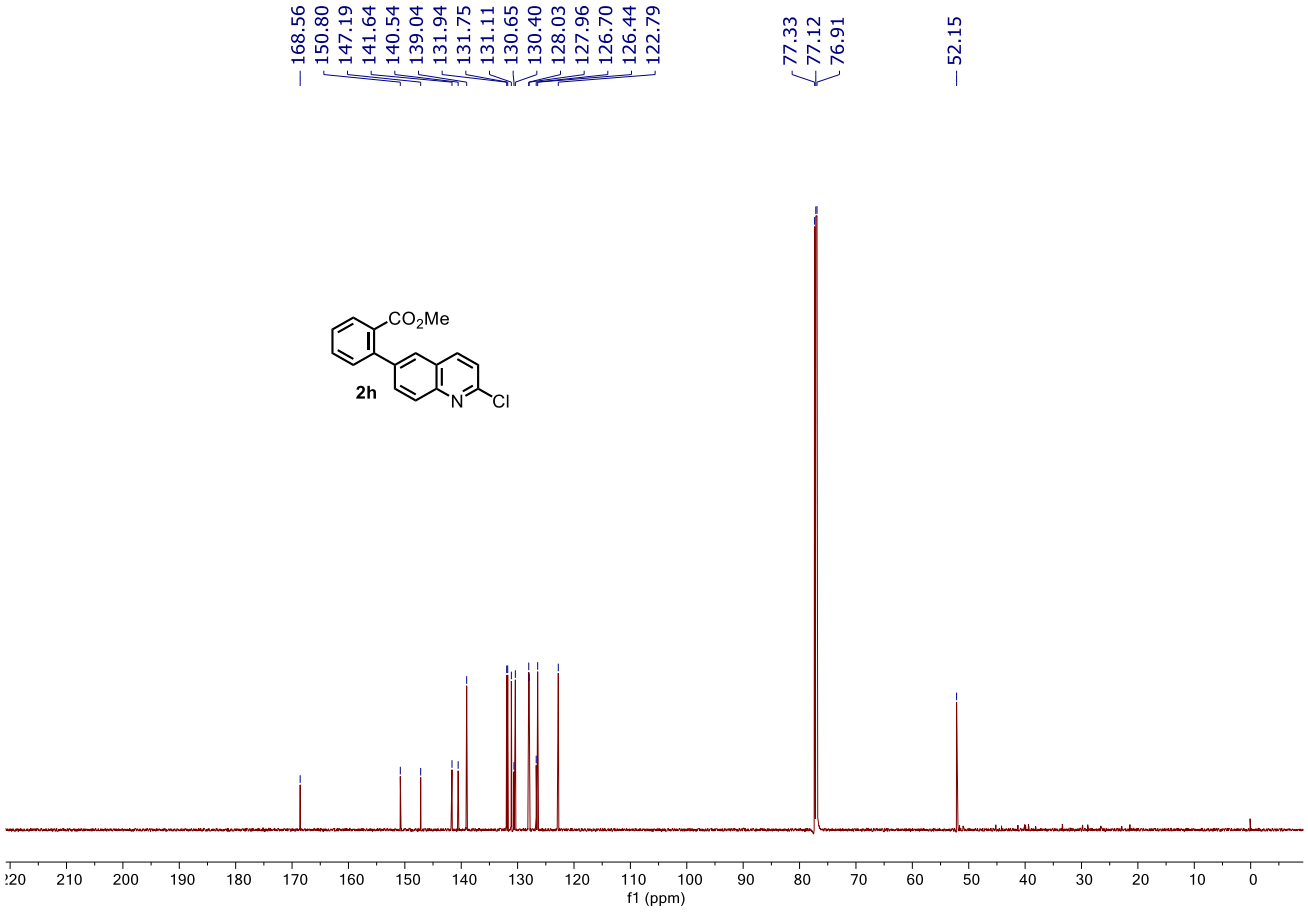
159.226
147.199
141.961
139.008
136.379
131.564
131.097
130.947
130.692
130.182
128.166
127.612
126.442
126.343
122.457
77.332
77.121
76.909
52.097
25.499
CO2Me
2f
N
Me
f1 (ppm)


7.994
7.980
7.881
7.880
7.878
7.877
7.871
7.870
7.869
7.868
7.867
7.865
7.864
7.857
7.856
7.855
7.670
7.666
7.576
7.573
7.563
7.562
7.562
7.560
7.558
7.550
7.548
7.465
7.464
7.463
7.462
7.456
7.454
7.452
7.451
7.450
7.449
7.444
7.441
7.431
7.429
7.260
6.936
6.922
4.096
3.597
CO2Me
2g
N
OMe
1.00
1.98
0.92
2.06
2.14
0.98
3.40
3.33
f1 (ppm)


169.230
162.705
145.949
142.045
138.848
137.251
131.477
131.083
131.024
130.540
130.077
127.397
126.836
126.548
124.907
113.515
53.549
52.094
CO2Me
2g
N
OMe
f1 (ppm)


8.123
8.109
8.037
8.023
7.945
7.943
7.932
7.930
7.753
7.750
7.687
7.683
7.672
7.669
7.604
7.601
7.591
7.589
7.579
7.576
7.499
7.497
7.486
7.484
7.473
7.471
7.441
7.439
7.428
7.426
7.422
7.408
7.260
3.608
CO2Me
2h
N
Cl
1.00
0.98
0.92
0.95
0.98
0.98
1.00
1.98
3.00
f1 (ppm)


168.56
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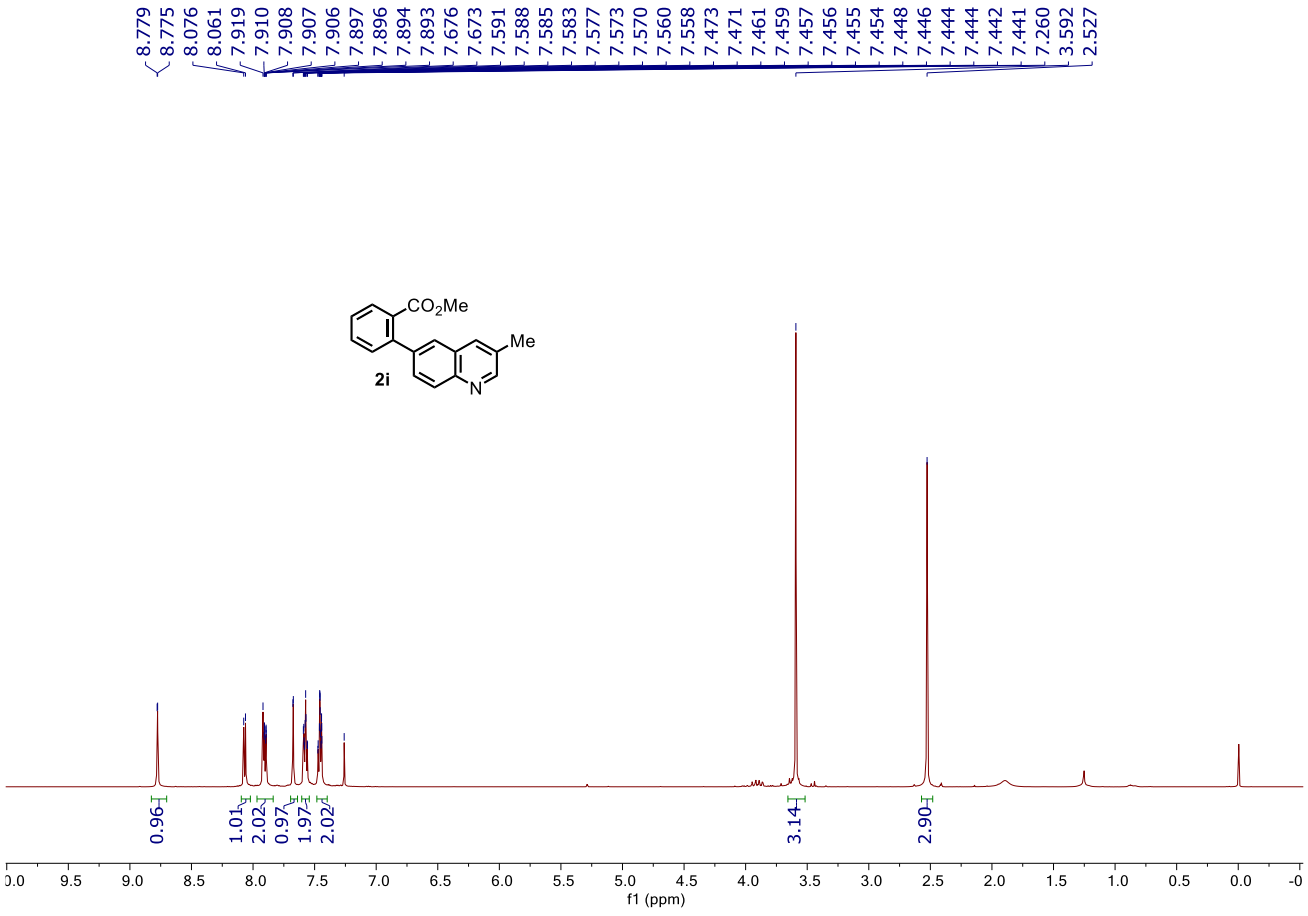
131.75
131.11
130.65
130.40
128.03
127.96
126.70
126.44
122.79
77.33
77.12
76.91
52.15
CO2Me
2h
N
Cl
f1 (ppm)


8.779
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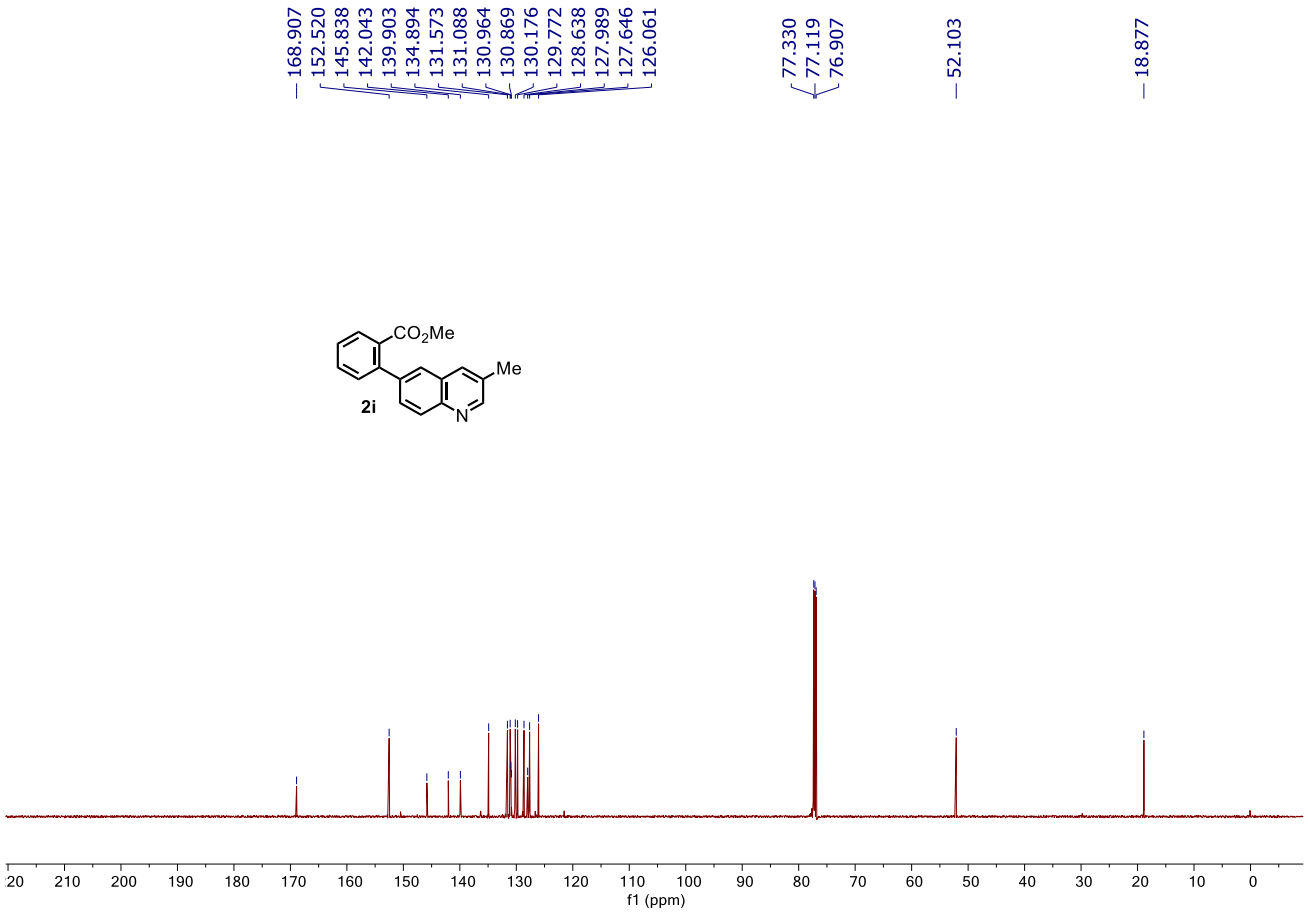
7.908
7.907
7.906
7.897
7.896
7.894
7.893
7.676
7.673
7.591
7.588
7.585
7.583
7.577
7.573
7.570
7.560
7.558
7.473
7.471
7.461
7.459
7.457
7.456
7.455
7.454
7.448
7.446
7.444
7.444
7.442
7.441
7.260
3.592
2.527
CO2Me
Me
2i
N
0.96
1.01
2.02
0.97
1.97
2.02
3.14
2.90
f1 (ppm)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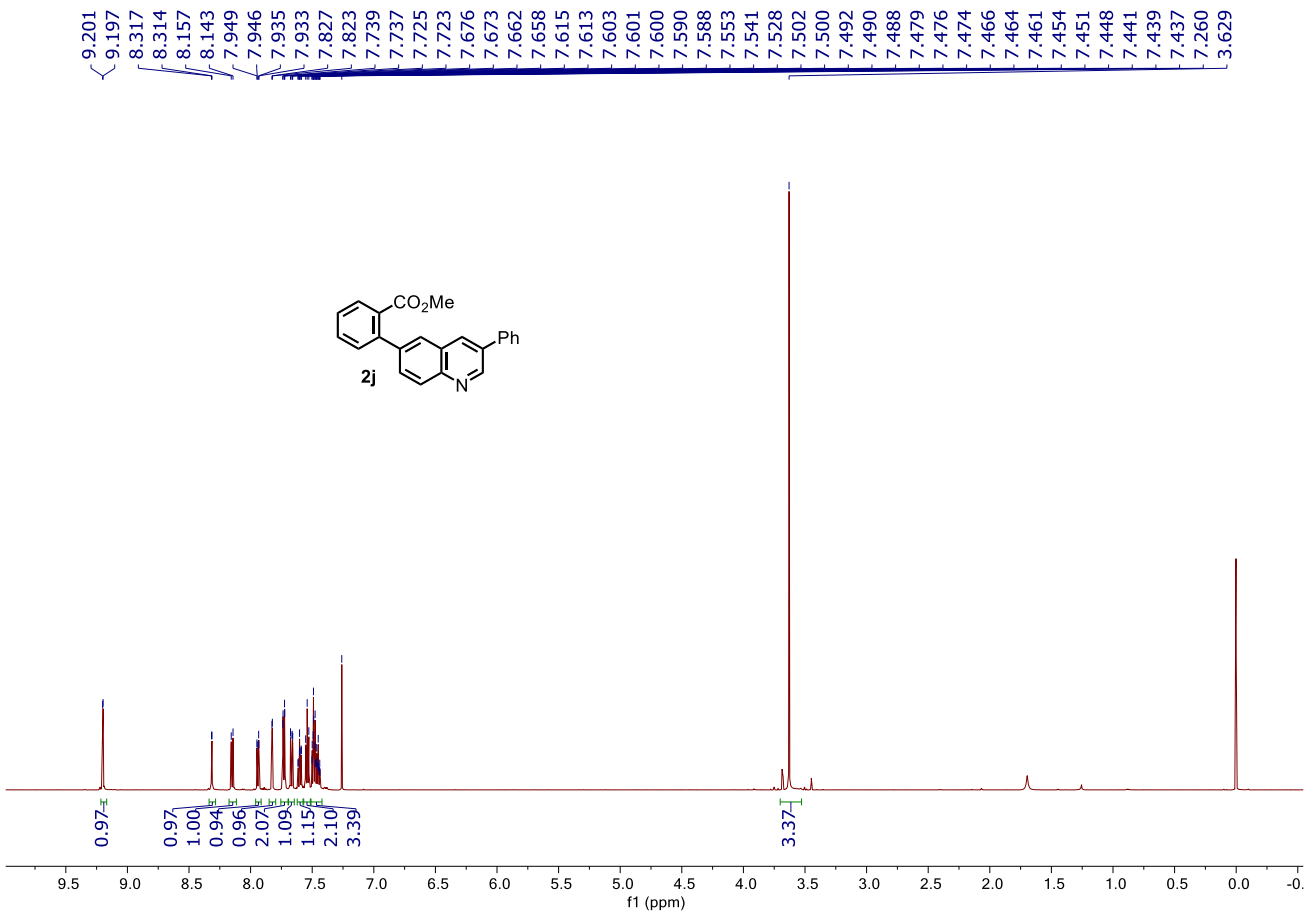
152.520
145.838
142.043
139.903
134.894
131.573
131.088
130.964
130.869
130.176
129.772
128.638
127.989
127.646
126.061
77.330
77.119
76.907
52.103
18.877
CO2Me
Me
N
2i
f1 (ppm)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9.197
8.317
8.314
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8.143
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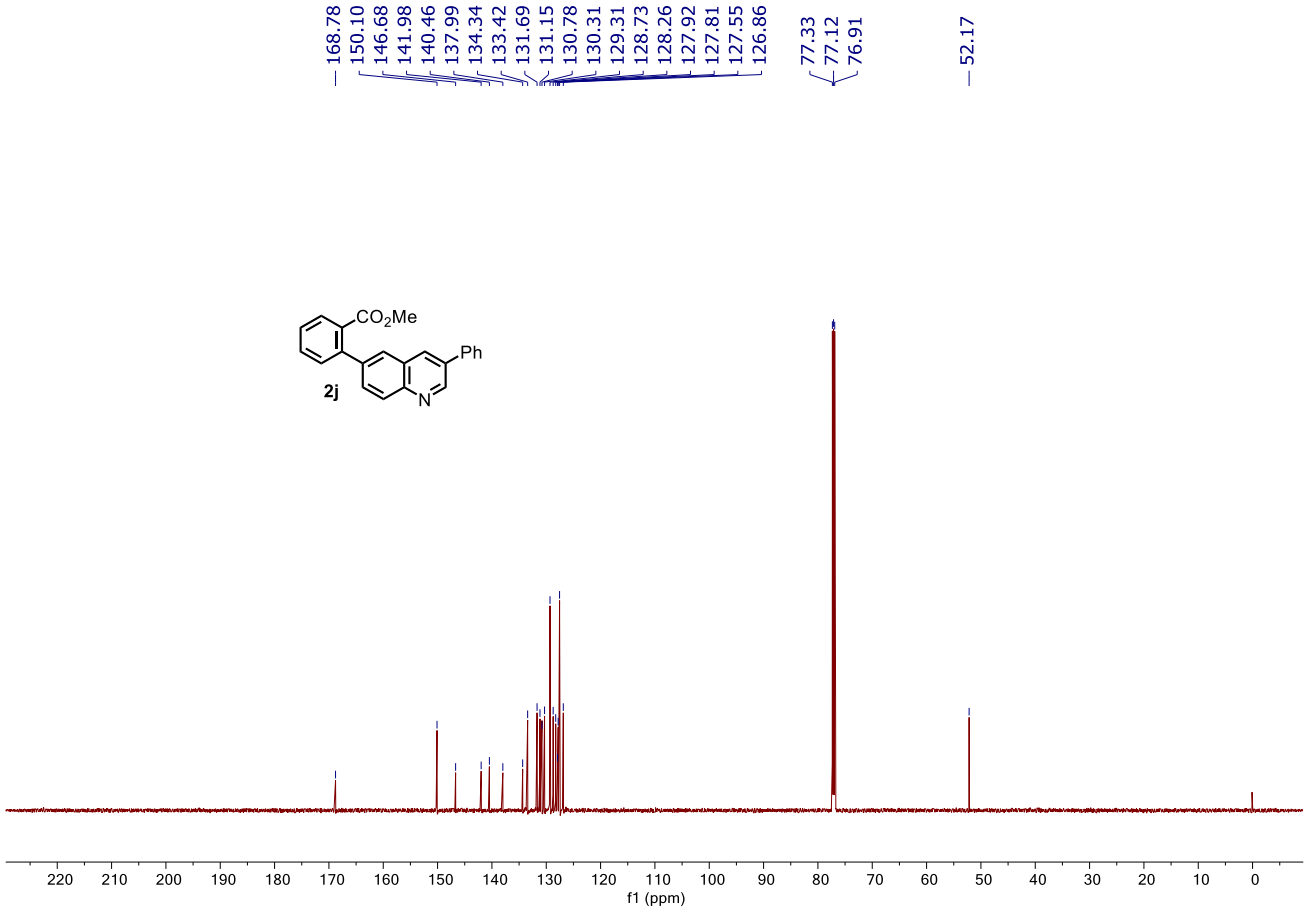
7.946
7.935
7.933
7.827
7.823
7.739
7.737
7.725
7.723
7.676
7.673
7.662
7.658
7.615
7.613
7.603
7.601
7.600
7.590
7.588
7.553
7.541
7.528
7.502
7.500
7.492
7.490
7.488
7.479
7.476
7.474
7.466
7.464
7.461
7.454
7.451
7.448
7.441
7.439
7.437
7.260
3.629
CO2Me
Ph
N
2j
0.97
0.97
1.00
0.94
0.96
2.07
1.09
1.15
2.10
3.39
3.37
f1 (ppm)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133.42
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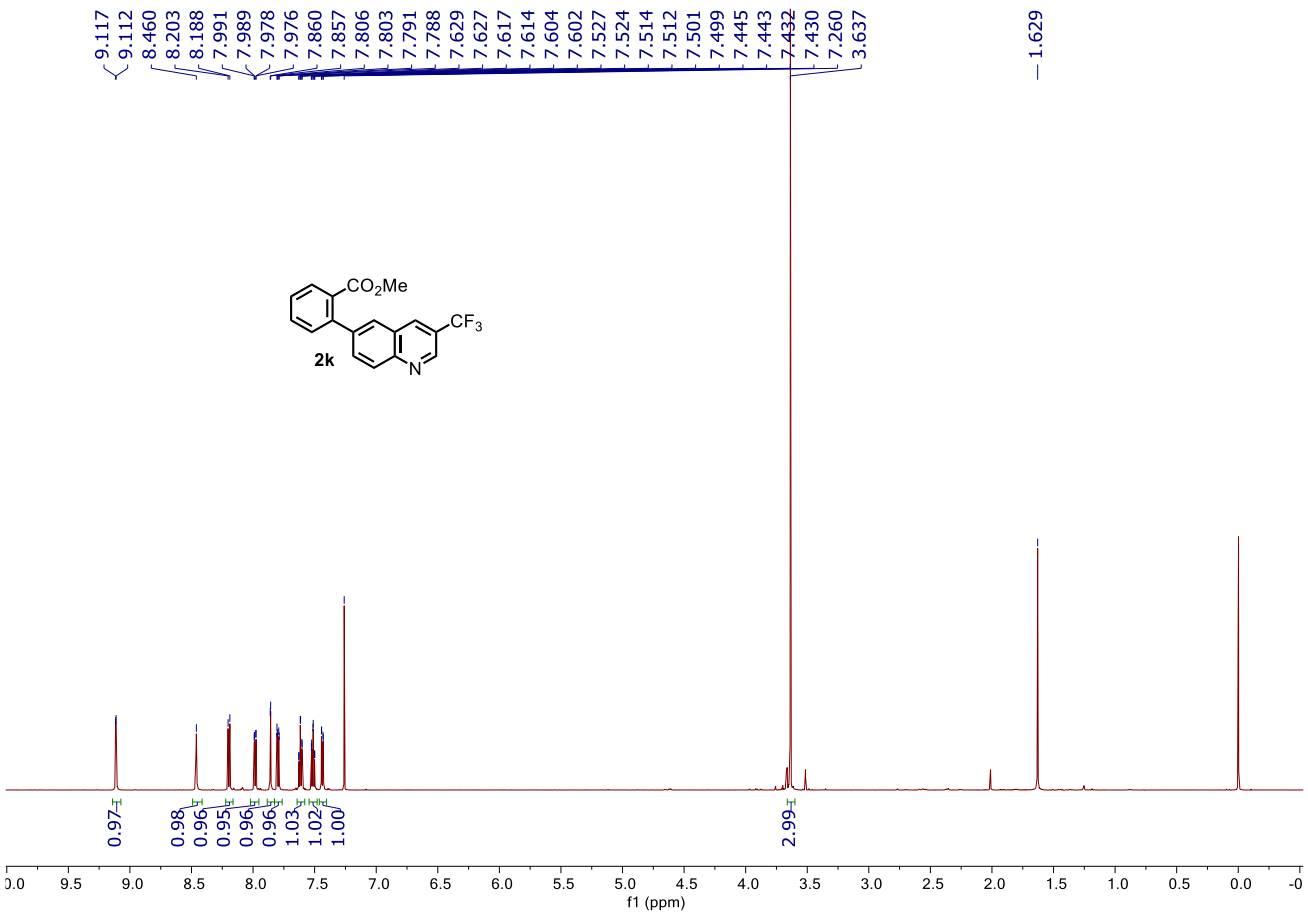
131.15
130.78
130.31
129.31
128.73
128.26
127.92
127.81
127.55
126.86
77.33
77.12
76.91
52.17
CO2Me
Ph
2j
N
f1 (ppm)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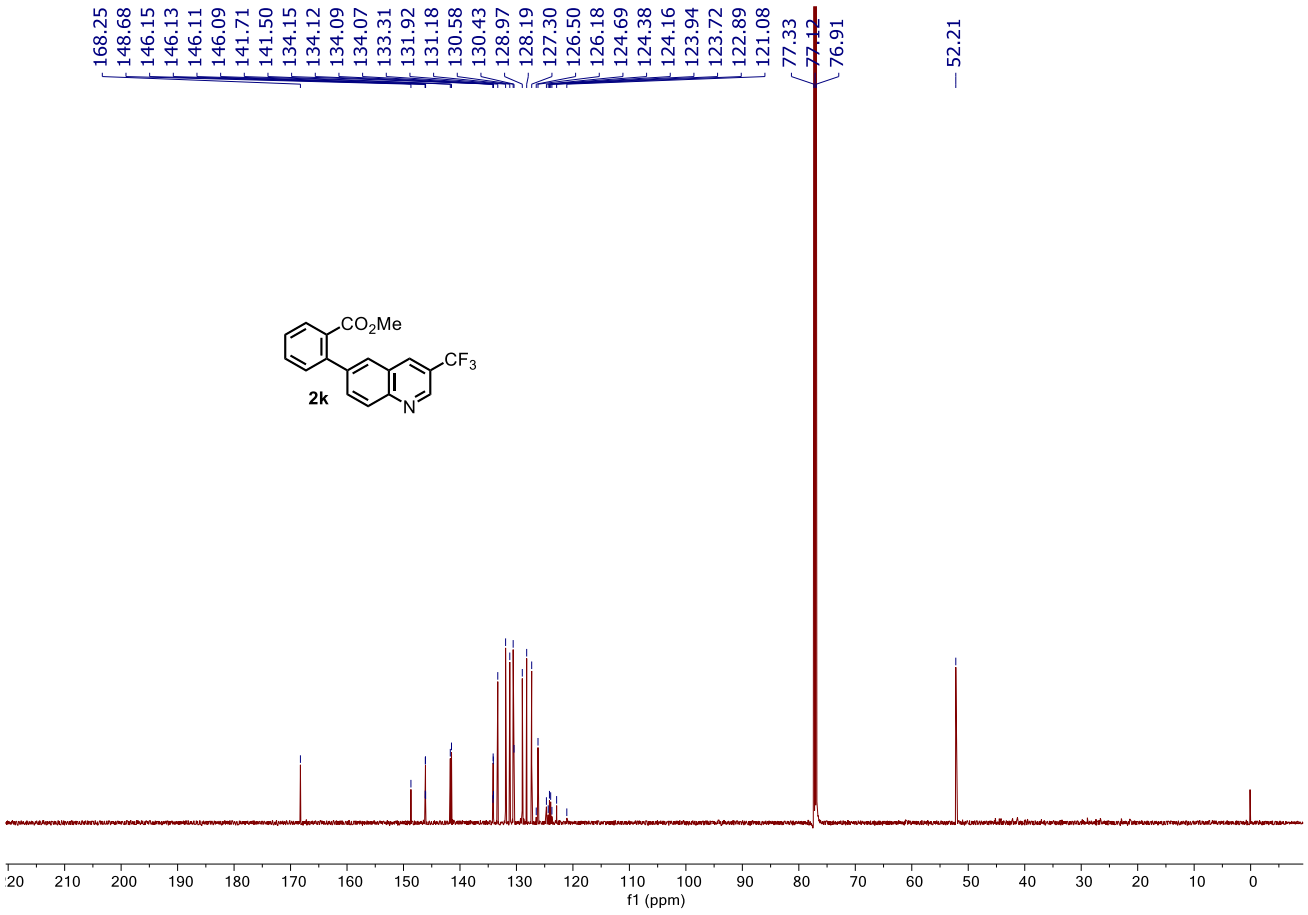
8.203
8.188
7.991
7.989
7.978
7.976
7.860
7.857
7.806
7.803
7.791
7.788
7.629
7.627
7.617
7.614
7.604
7.602
7.527
7.524
7.514
7.512
7.501
7.499
7.445
7.443
7.432
7.430
7.260
3.637
1.629
CO2Me
CF3
2k
N
0.97
0.98
0.96
0.95
0.96
0.96
1.03
1.02
1.00
2.99
f1 (ppm)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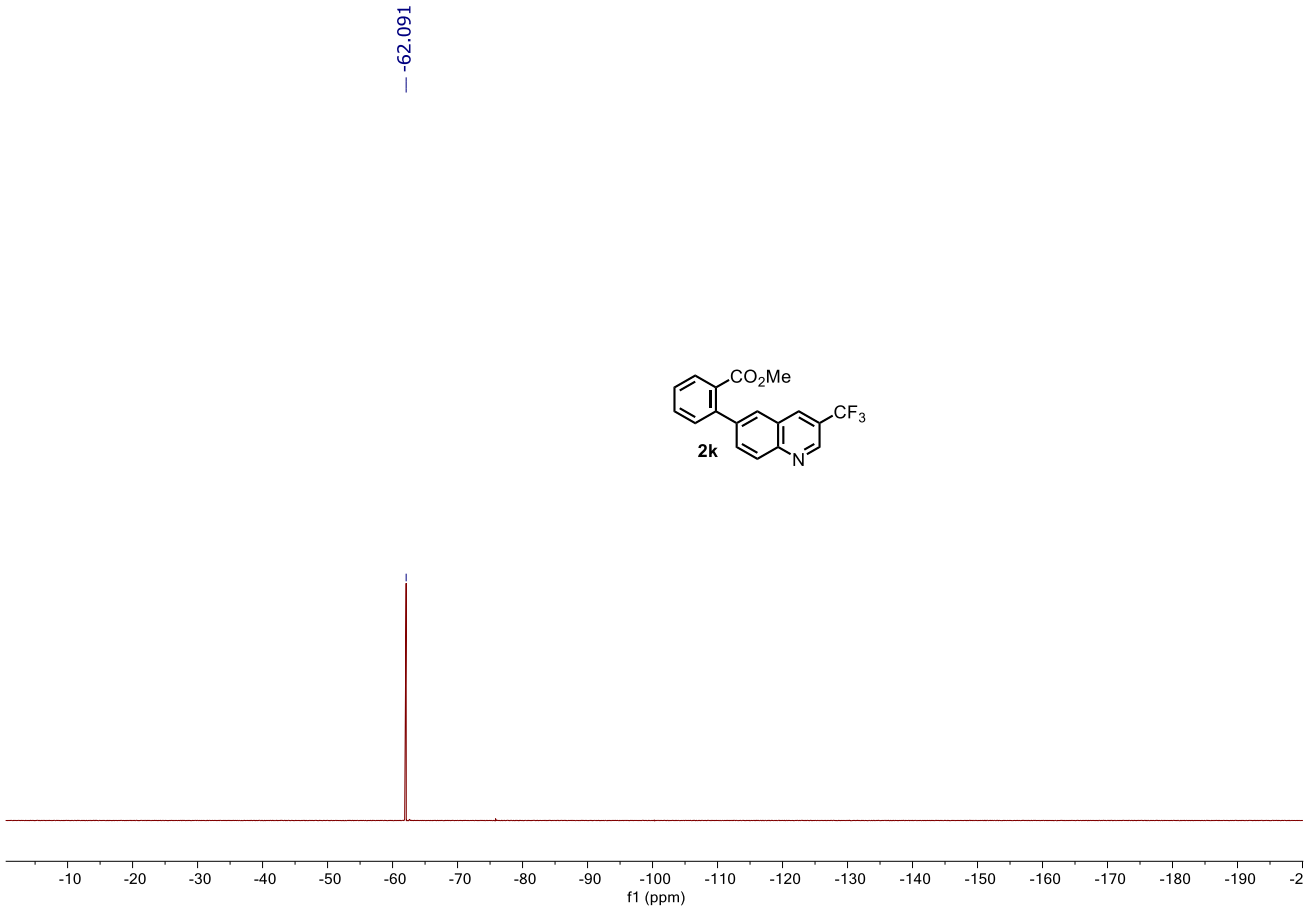
146.13
146.11
146.09
141.71
141.50
134.15
134.12
134.09
134.07
133.31
131.92
131.18
130.58
130.43
128.97
128.19
127.30
126.50
126.18
124.69
124.38
124.16
123.94
123.72
122.89
121.08
77.33
77.12
76.91
52.21
CO2Me
CF3
N
2k
f1 (ppm)


-62.091
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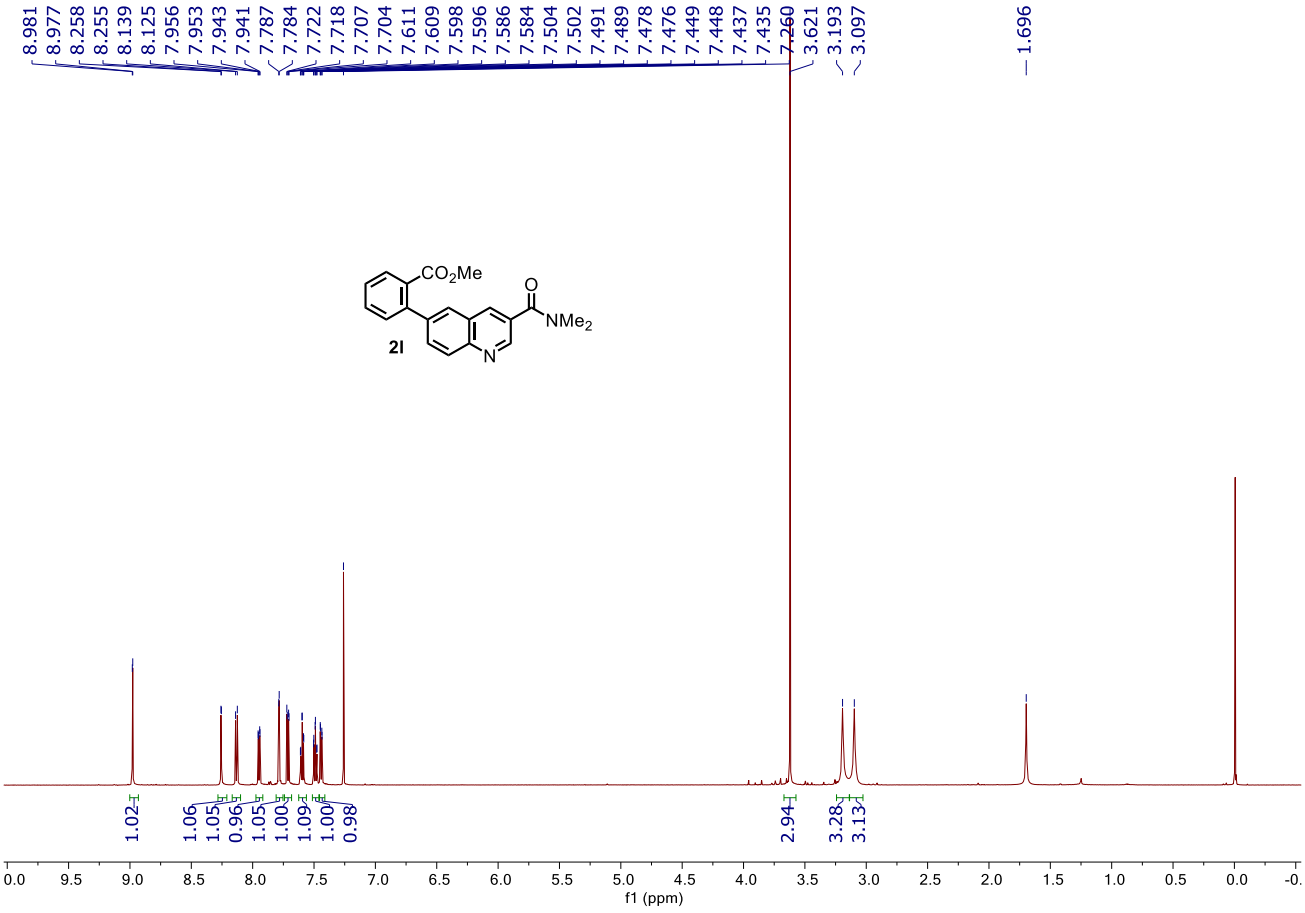
CF3
N
2k
f1 (ppm)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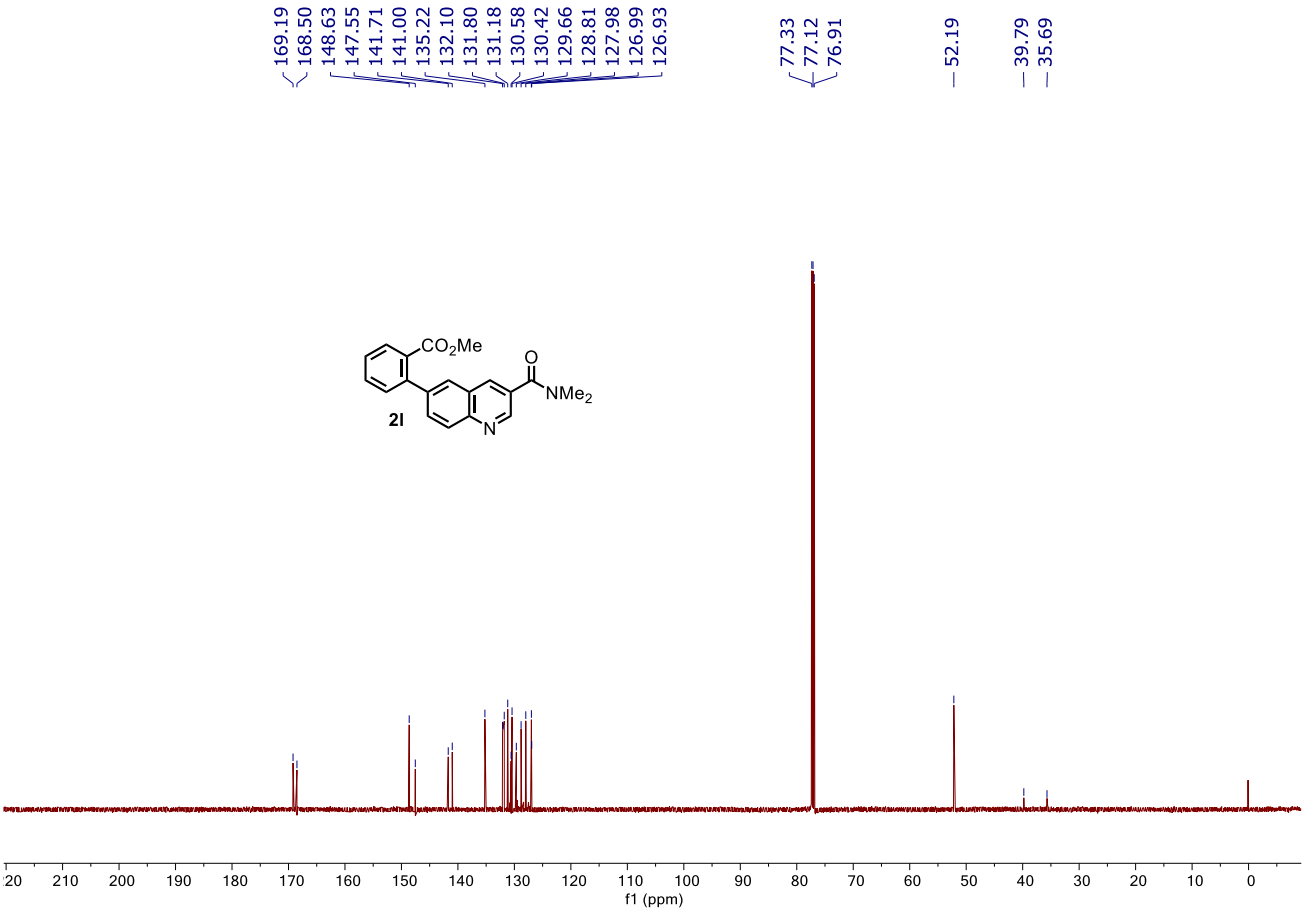
7.784
7.722
7.718
7.707
7.704
7.611
7.609
7.598
7.596
7.586
7.584
7.504
7.502
7.491
7.489
7.478
7.476
7.449
7.448
7.437
7.435
7.260
3.621
3.193
3.097
1.696
CO2Me
O
NMe2
N
2l
1.02
1.06
1.05
0.96
1.05
1.00
1.09
1.00
0.98
2.94
3.28
3.13
f1 (ppm)


169.19
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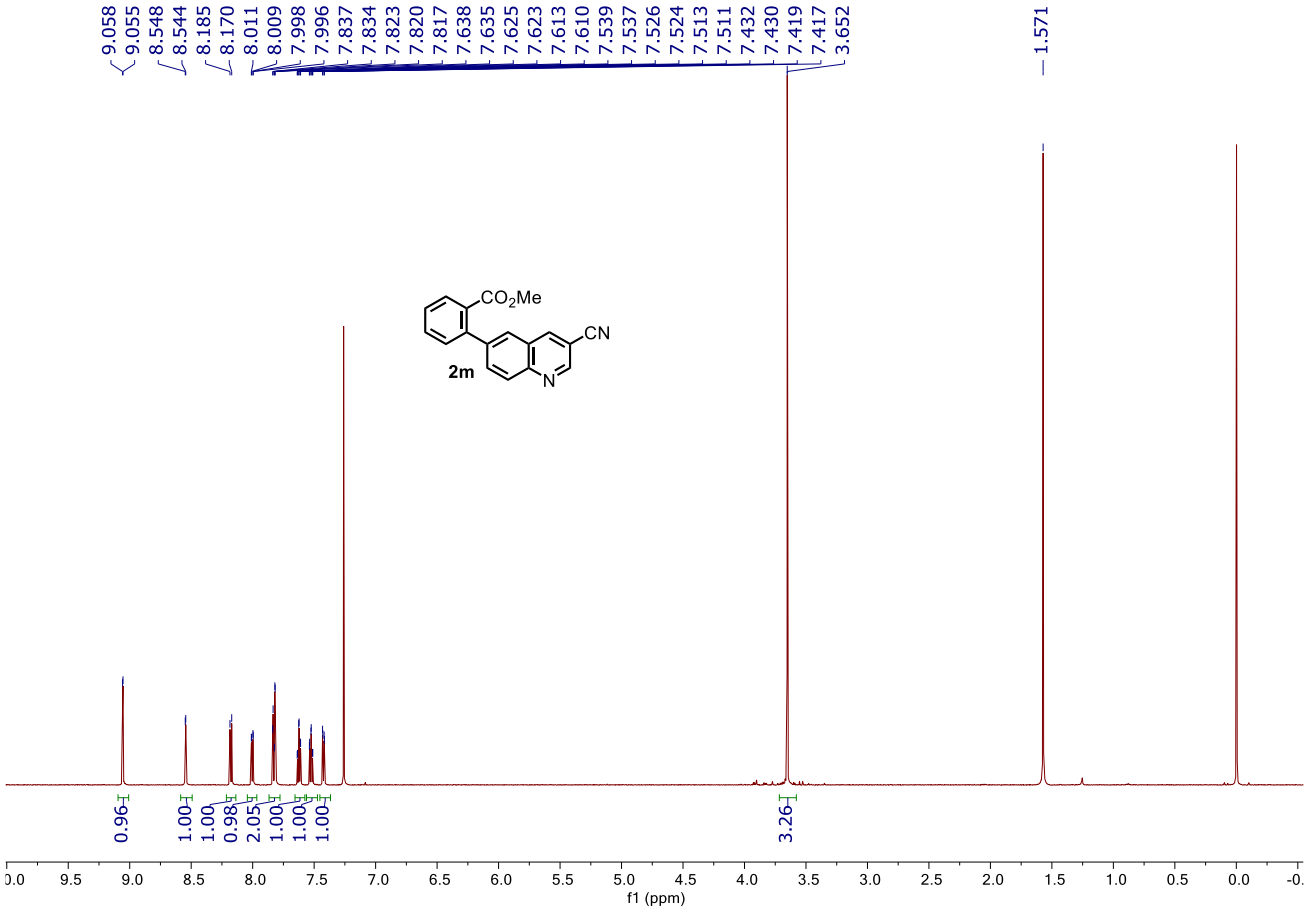
147.55
141.71
141.00
135.22
132.10
131.80
131.18
130.58
130.42
129.66
128.81
127.98
126.99
126.93
77.33
77.12
76.91
52.19
39.79
35.69
CO2Me
O
NMe2
N
2l
f1 (ppm)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8.544
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8.170
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7.996
7.837
7.834
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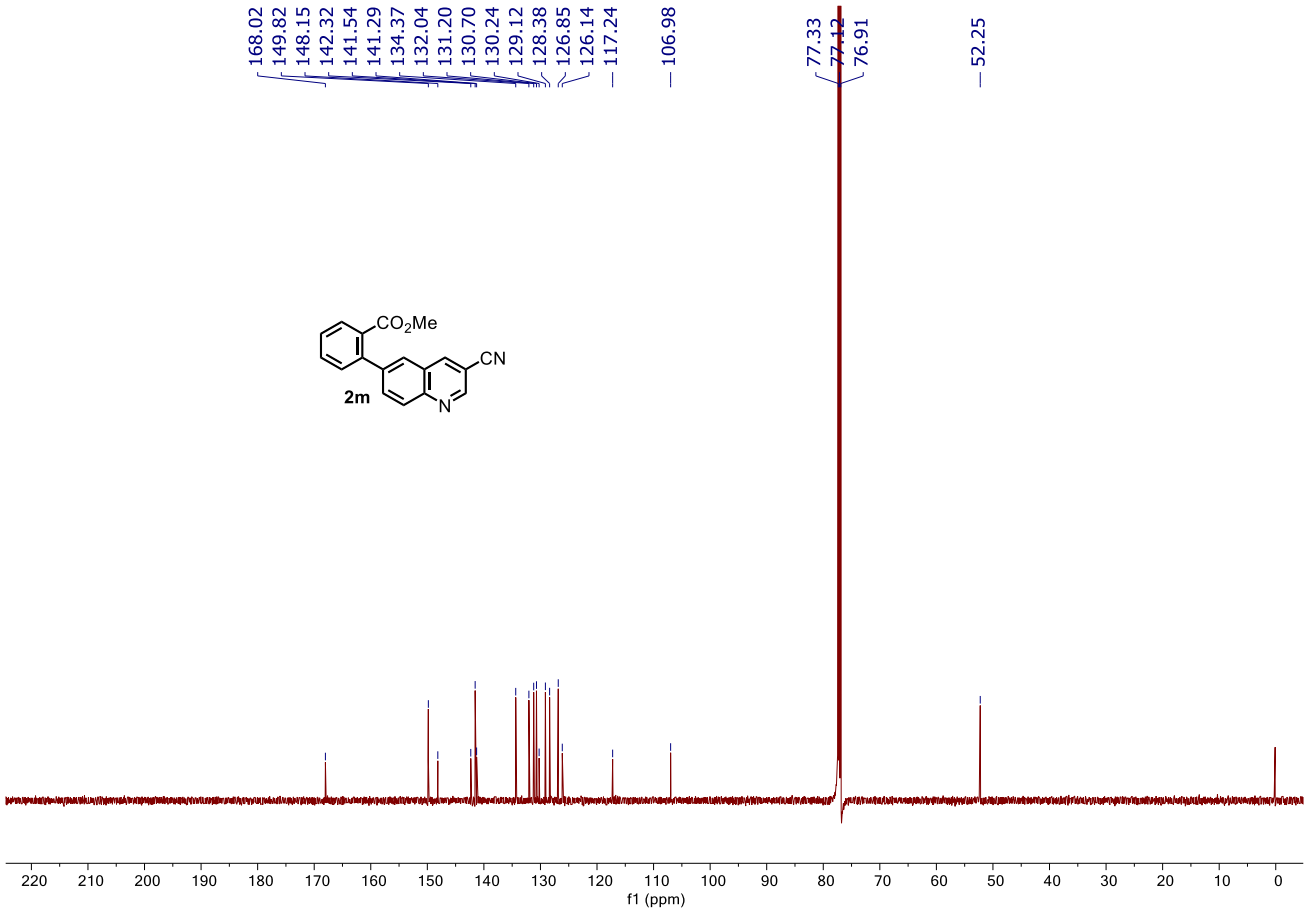
7.817
7.638
7.635
7.625
7.623
7.613
7.610
7.539
7.537
7.526
7.524
7.513
7.511
7.432
7.430
7.419
7.417
3.652
1.571
CO2Me
CN
N
2m
0.96
1.00
1.00
0.98
2.05
1.00
1.00
1.00
3.26
f1 (ppm)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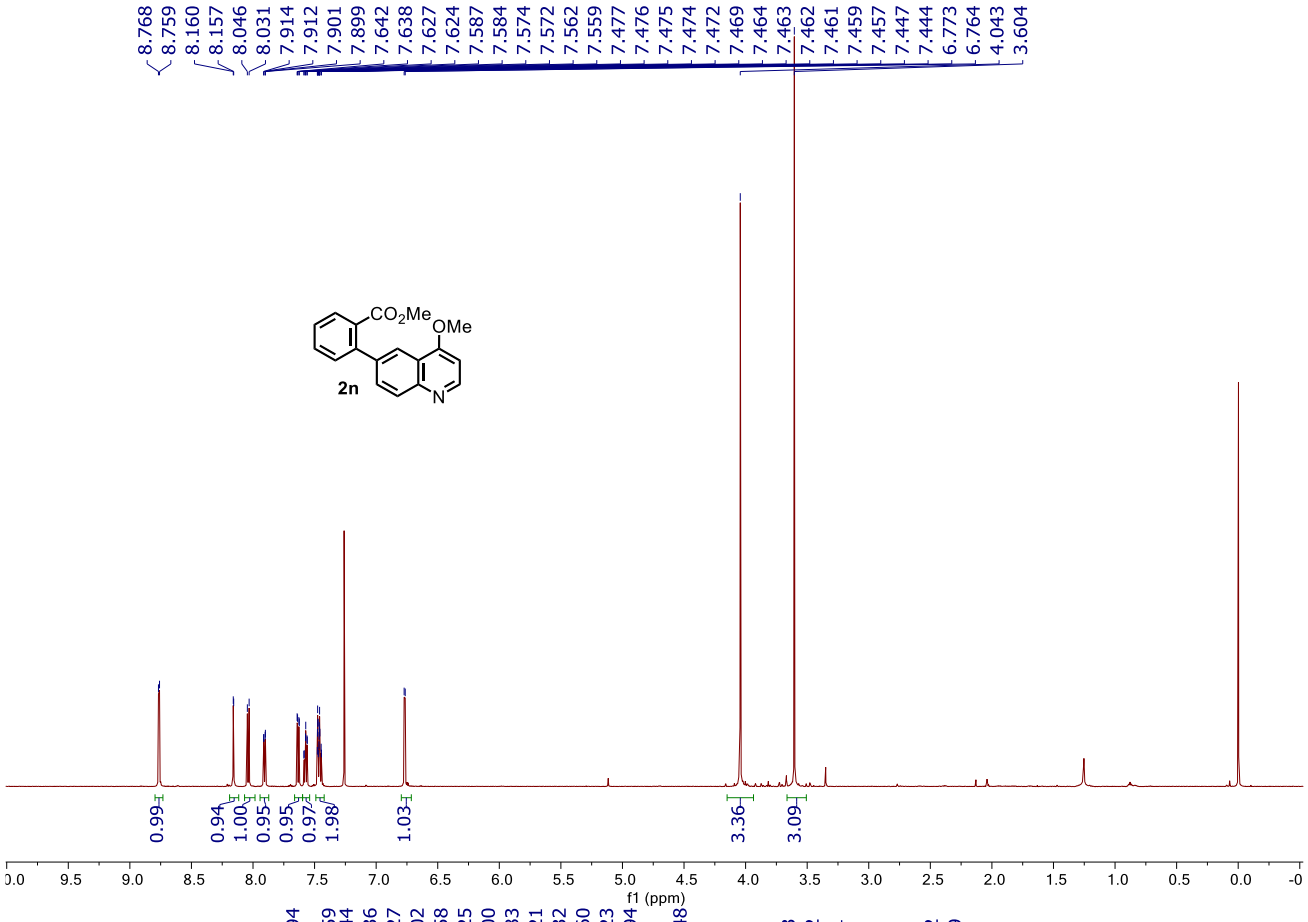
148.15
142.32
141.54
141.29
134.37
132.04
131.20
130.70
130.24
129.12
128.38
126.85
126.14
117.24
106.98
77.33
77.12
76.91
52.25
CO2Me
CN
N
2m
f1 (ppm)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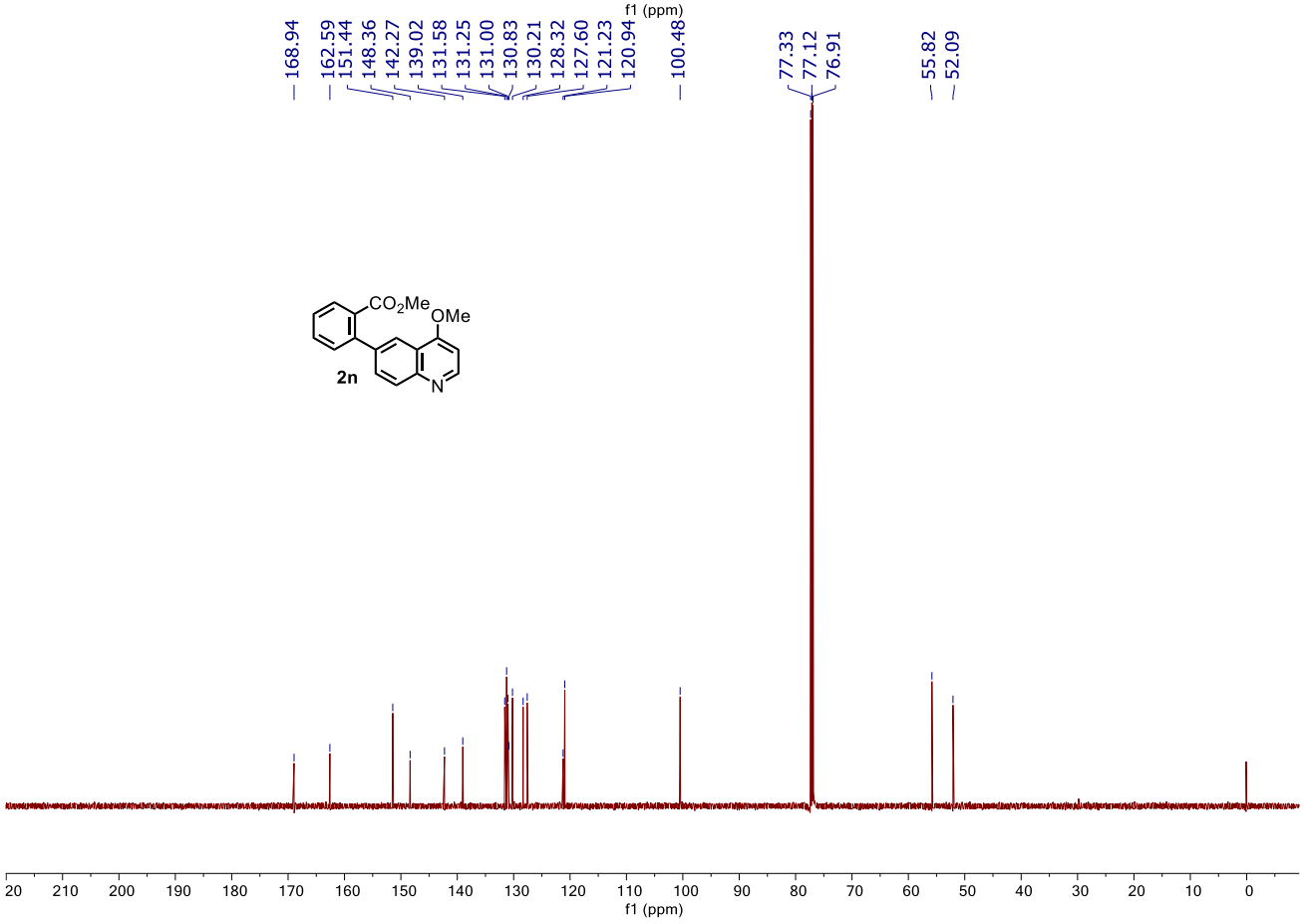
7.899
7.642
7.638
7.627
7.624
7.587
7.584
7.574
7.572
7.562
7.559
7.477
7.476
7.475
7.474
7.472
7.469
7.464
7.463
7.462
7.461
7.459
7.457
7.447
7.444
6.773
6.764
4.043
3.604
CO2Me
OMe
N
2n
0.99
0.94
1.00
0.95
0.95
0.97
1.98
1.03
3.36
3.09
f1 (ppm)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131.58
131.25
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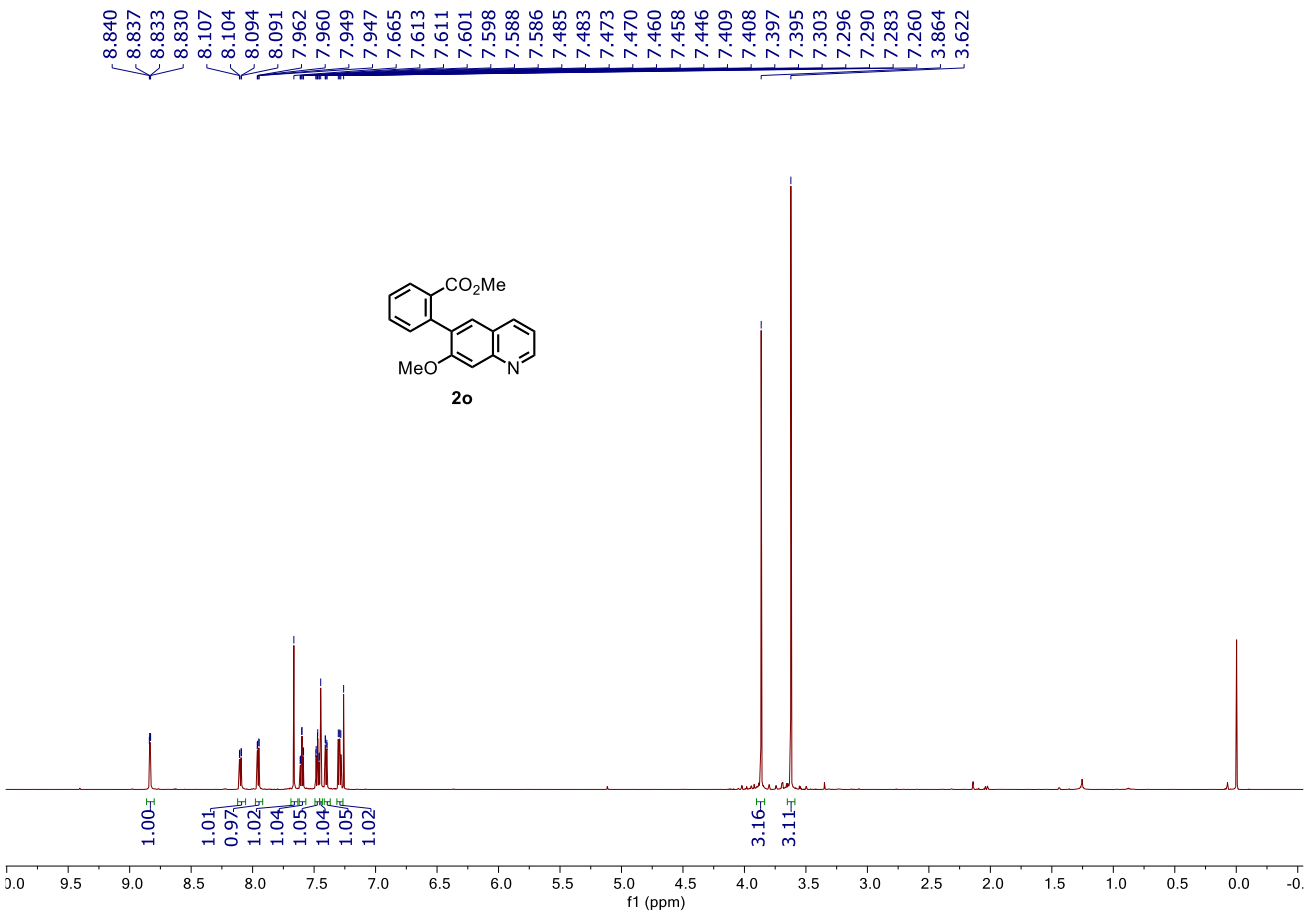
130.83
130.21
128.32
127.60
121.23
120.94
100.48
77.33
77.12
76.91
55.82
52.09
CO2Me
OMe
N
2n
f1 (ppm)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8.094
8.091
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7.960
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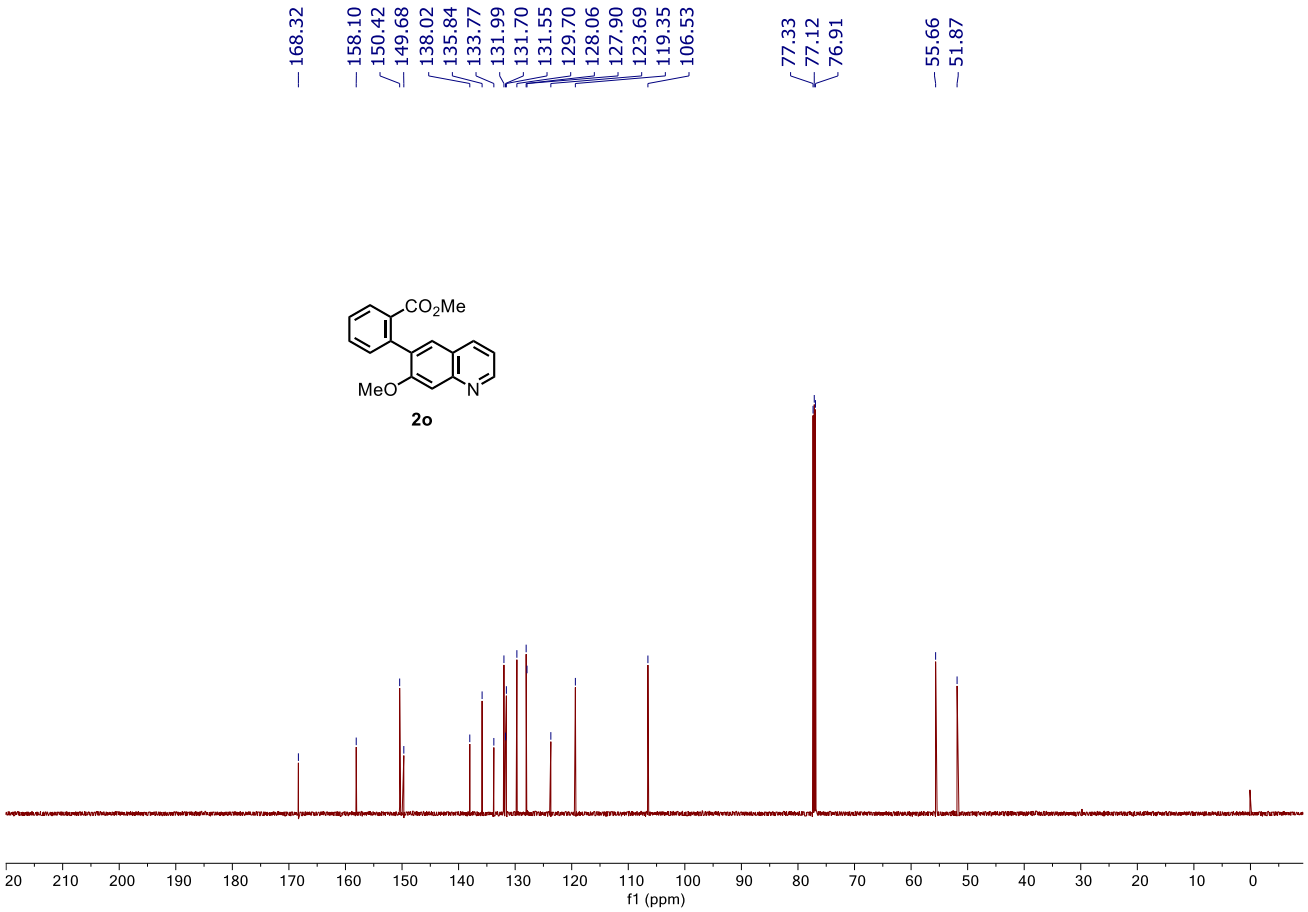
7.947
7.665
7.613
7.611
7.601
7.598
7.588
7.586
7.485
7.483
7.473
7.470
7.460
7.458
7.446
7.409
7.408
7.397
7.395
7.303
7.296
7.290
7.283
7.260
3.864
3.622
CO2Me
MeO
N
2o
1.00
1.01
0.97
1.02
1.04
1.05
1.04
1.05
1.02
3.16
3.11
f1 (ppm)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135.84
133.77
131.99
131.70
131.55
129.70
128.06
127.90
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119.35
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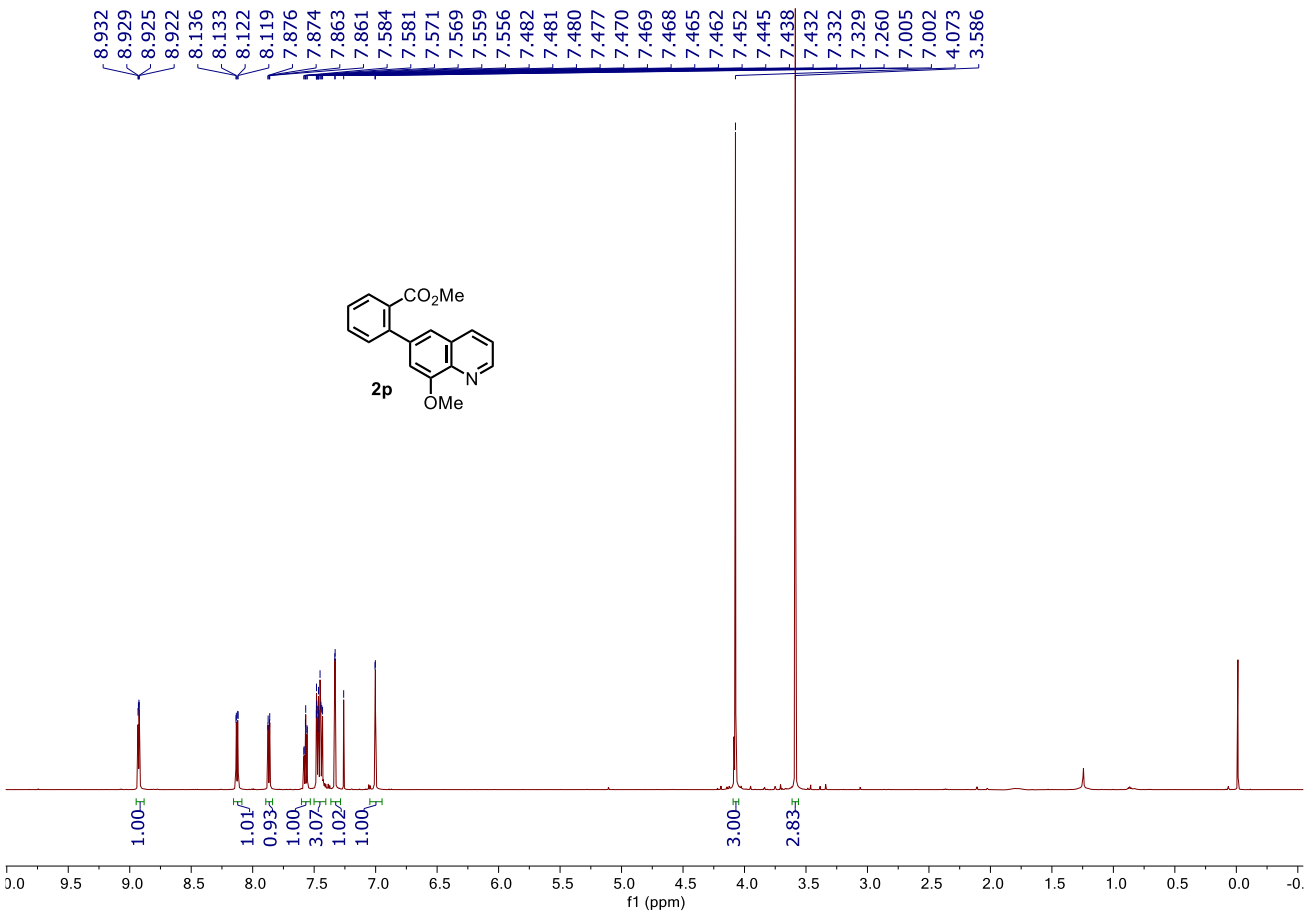
77.33
77.12
76.91
55.66
51.87
CO2Me
MeO
N
2o
f1 (ppm)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8.133
8.122
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7.874
7.863
7.861
7.584
7.581
7.571
7.569
7.559
7.556
7.482
7.481
7.480
7.477
7.470
7.469
7.468
7.465
7.462
7.452
7.445
7.438
7.432
7.332
7.329
7.260
7.005
7.002
4.073
3.586
CO2Me
N
OMe
2p
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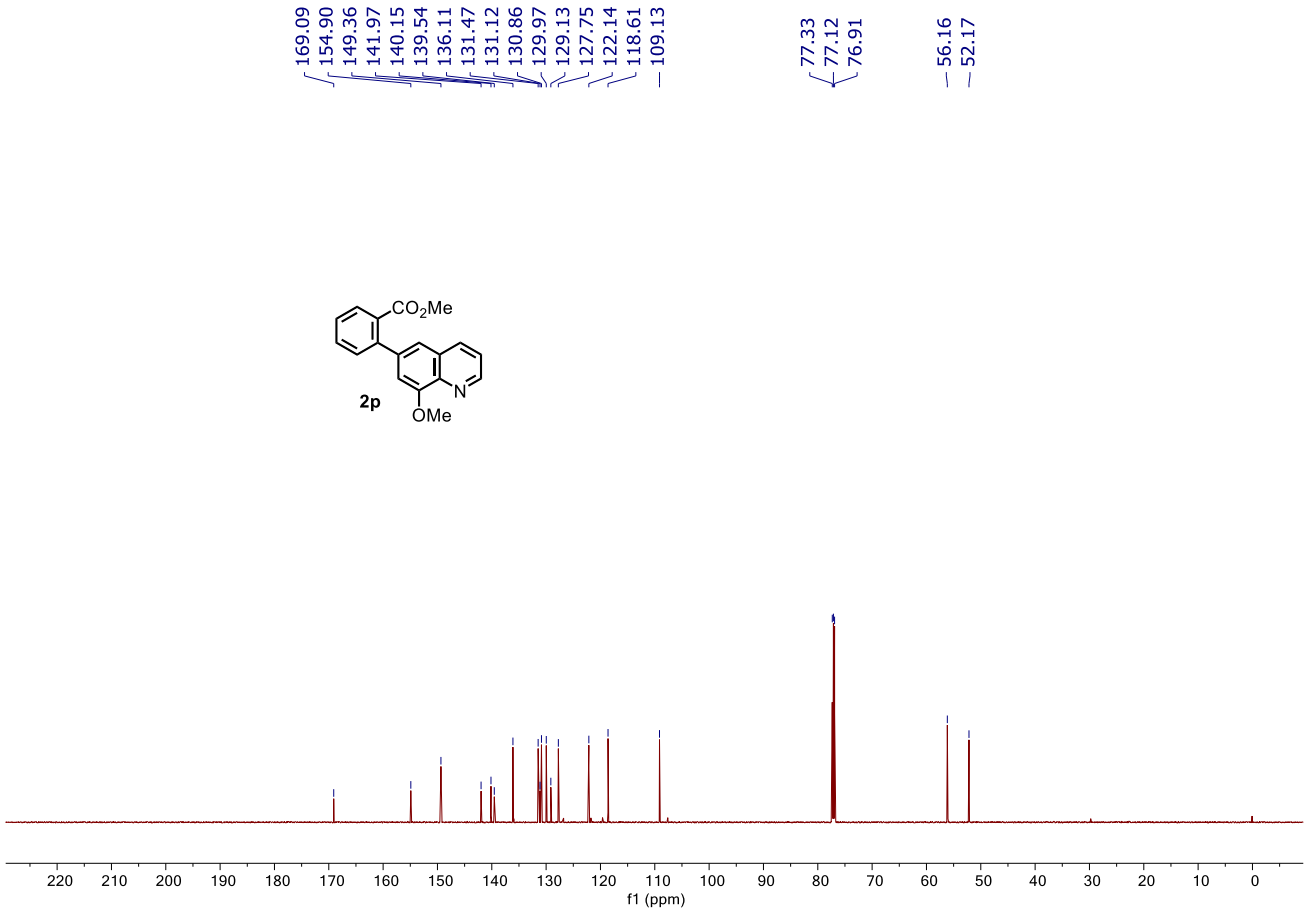
1.01
0.93
1.00
3.07
1.02
1.00
3.00
2.83
f1 (ppm)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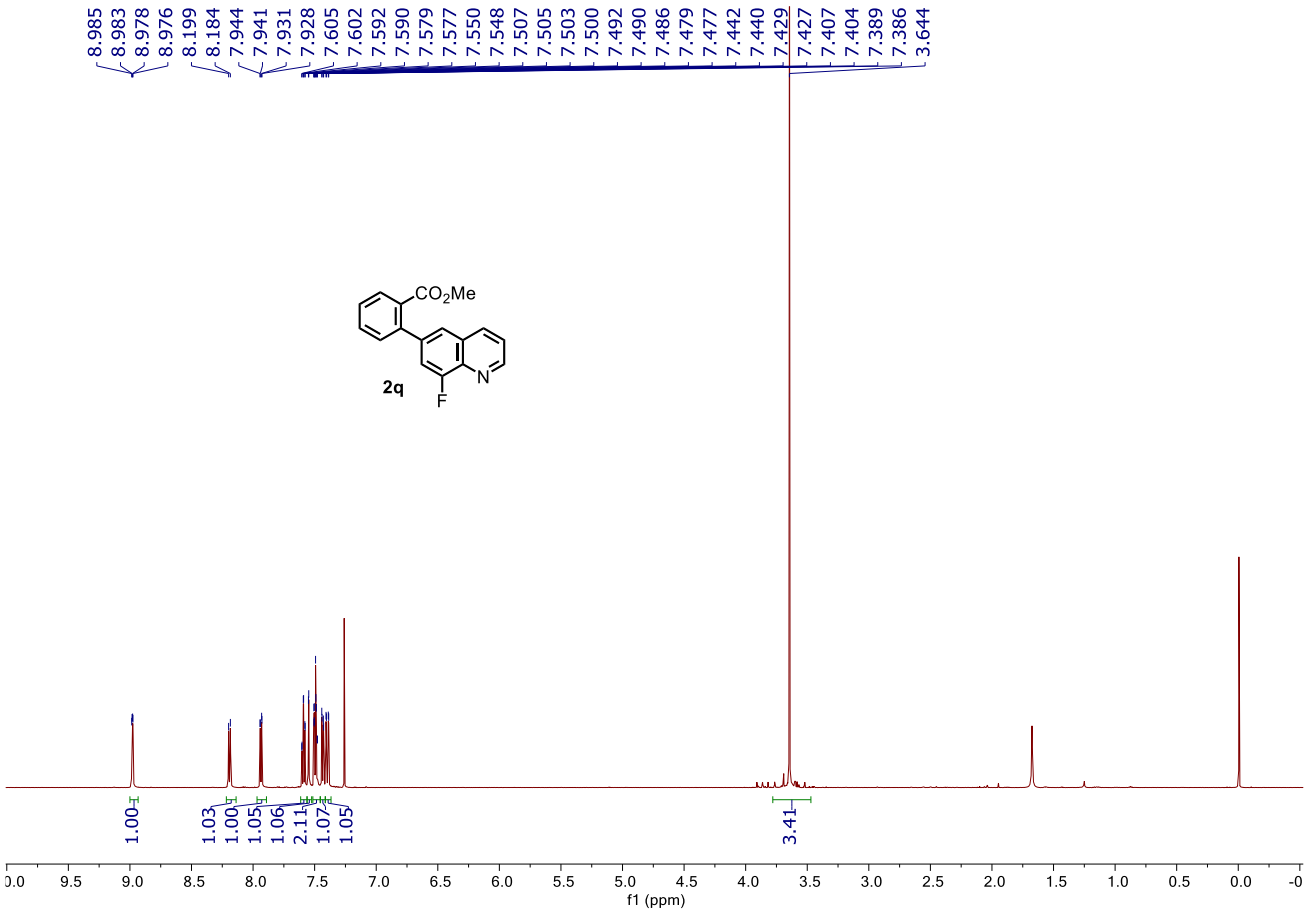
139.54
136.11
131.47
131.12
130.86
129.97
129.13
127.75
122.14
118.61
109.13
77.33
77.12
76.91
56.16
52.17
CO2Me
N
OMe
2p
f1 (ppm)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8.184
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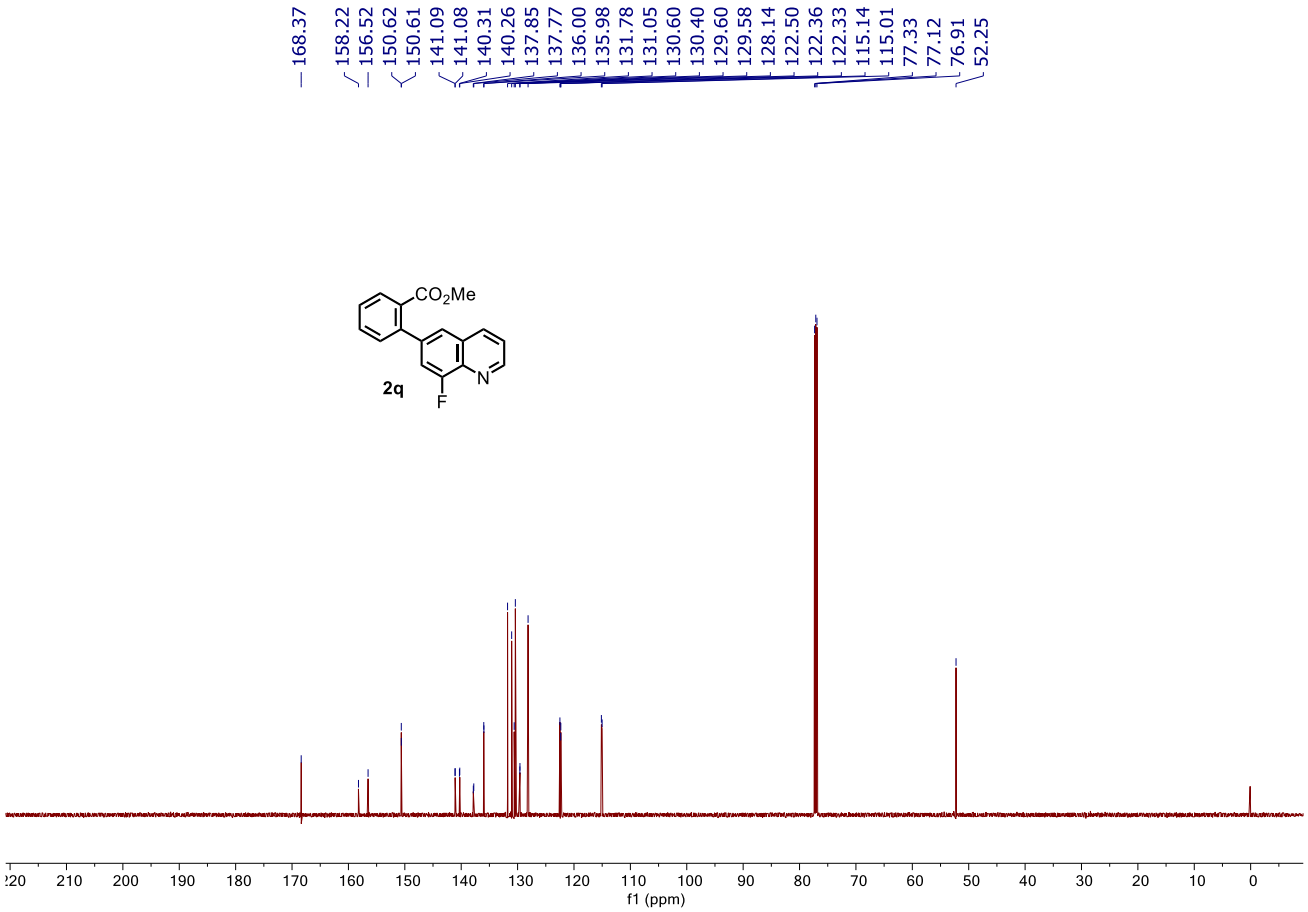
7.931
7.928
7.605
7.602
7.592
7.590
7.579
7.577
7.550
7.548
7.507
7.505
7.503
7.500
7.492
7.490
7.486
7.479
7.477
7.442
7.440
7.429
7.427
7.407
7.404
7.389
7.386
3.644
CO2Me
N
F
2q
1.00
1.03
1.00
1.05
1.06
2.11
1.07
1.05
3.41
f1 (ppm)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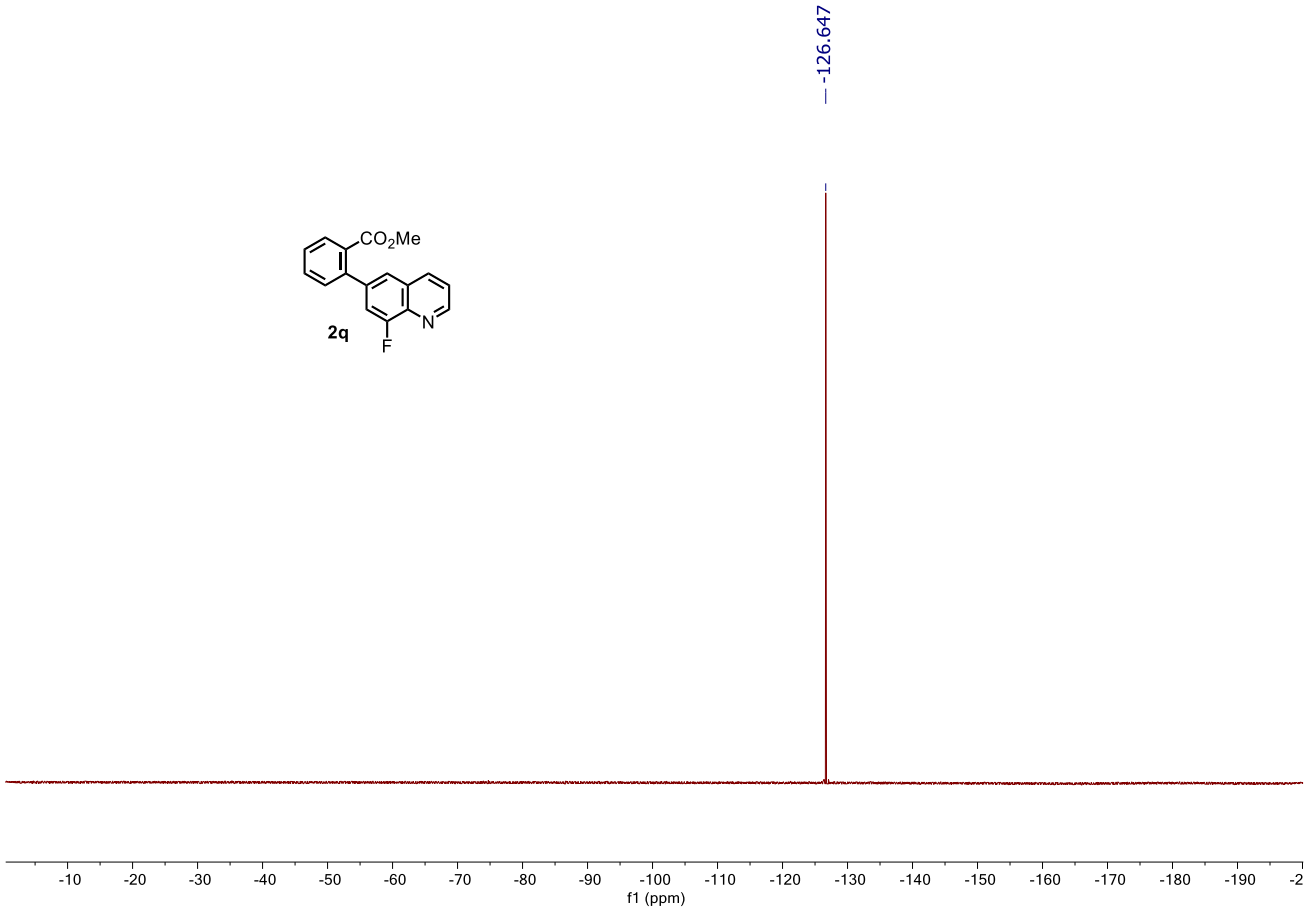
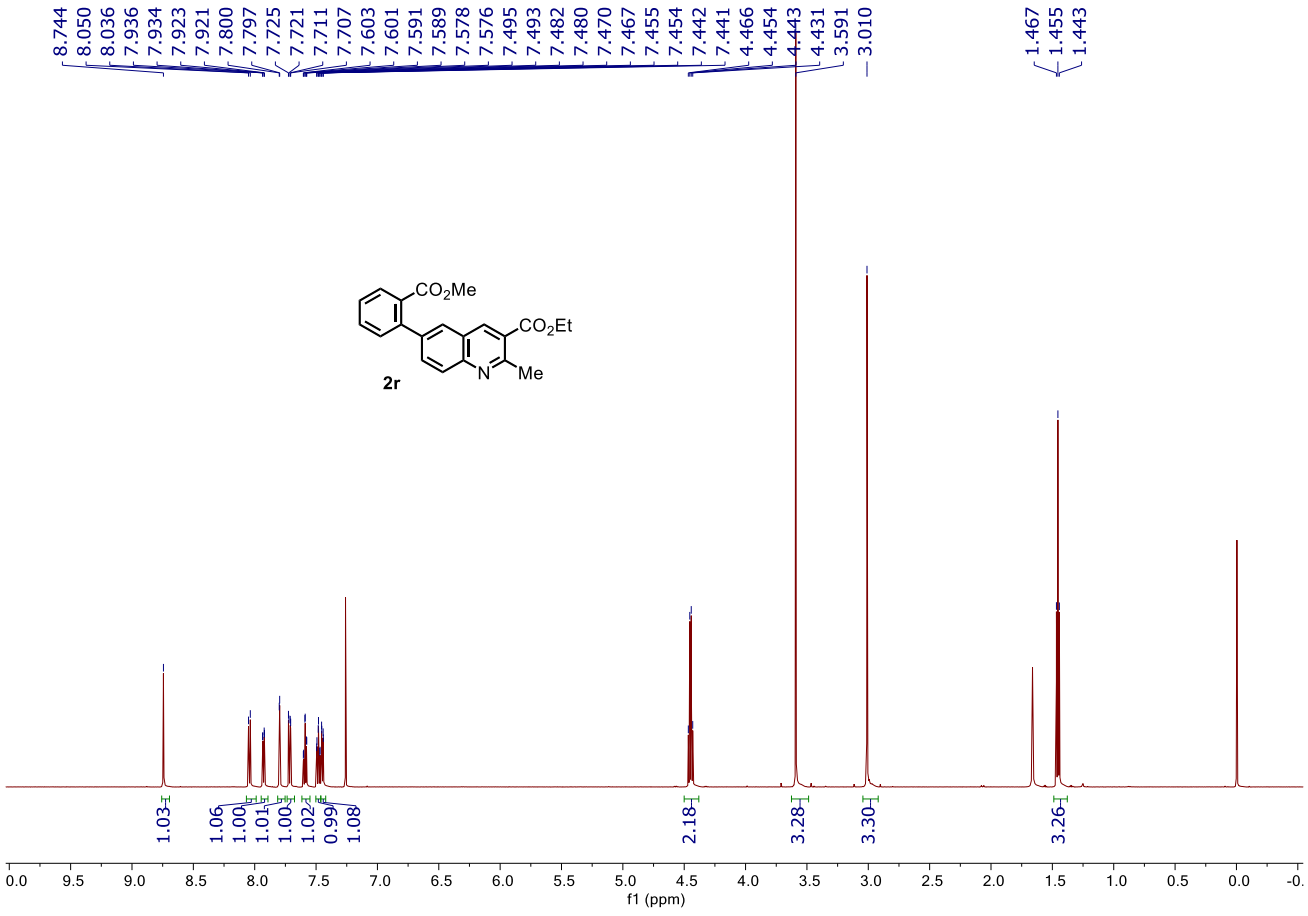
158.22
156.52
150.62
150.61
141.09
141.08
140.31
140.26
137.85
137.77
136.00
135.98
131.78
131.05
130.60
130.40
129.60
129.58
128.14
122.50
122.36
122.33
115.14
115.01
77.33
77.12
76.91
52.25
CO2Me
N
F
2q
f1 (ppm)


-126.647
CO2Me
2q
F
N
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
f1 (ppm)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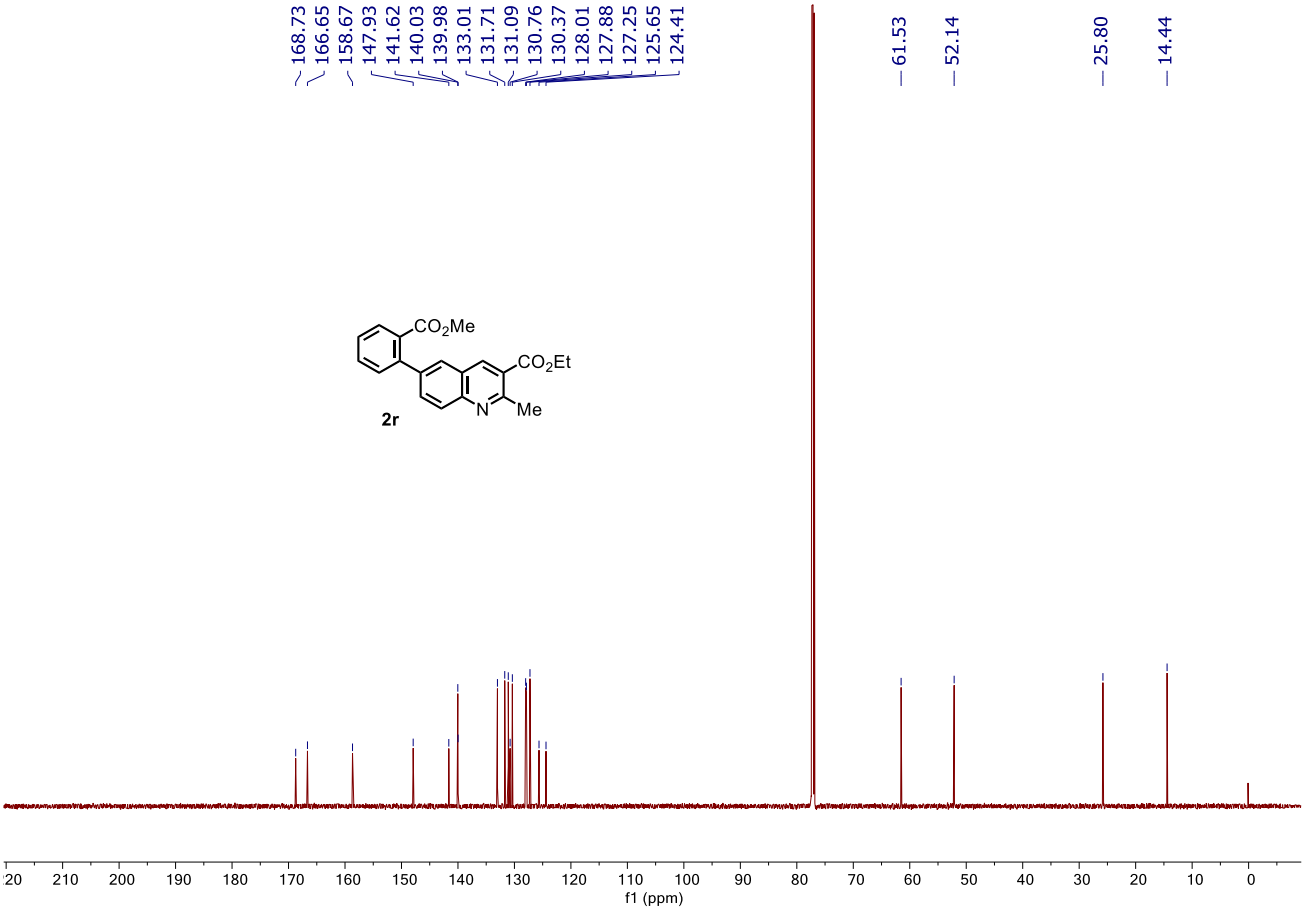
7.797
7.725
7.721
7.711
7.707
7.603
7.601
7.591
7.589
7.578
7.576
7.495
7.493
7.482
7.480
7.470
7.467
7.455
7.454
7.442
7.441
4.466
4.454
4.443
4.431
3.591
3.010
1.467
1.455
1.443
CO2Me
CO2Et
N
Me
2r
1.03
1.06
1.00
1.01
1.00
1.02
0.99
1.08
2.18
3.28
3.30
3.26
0.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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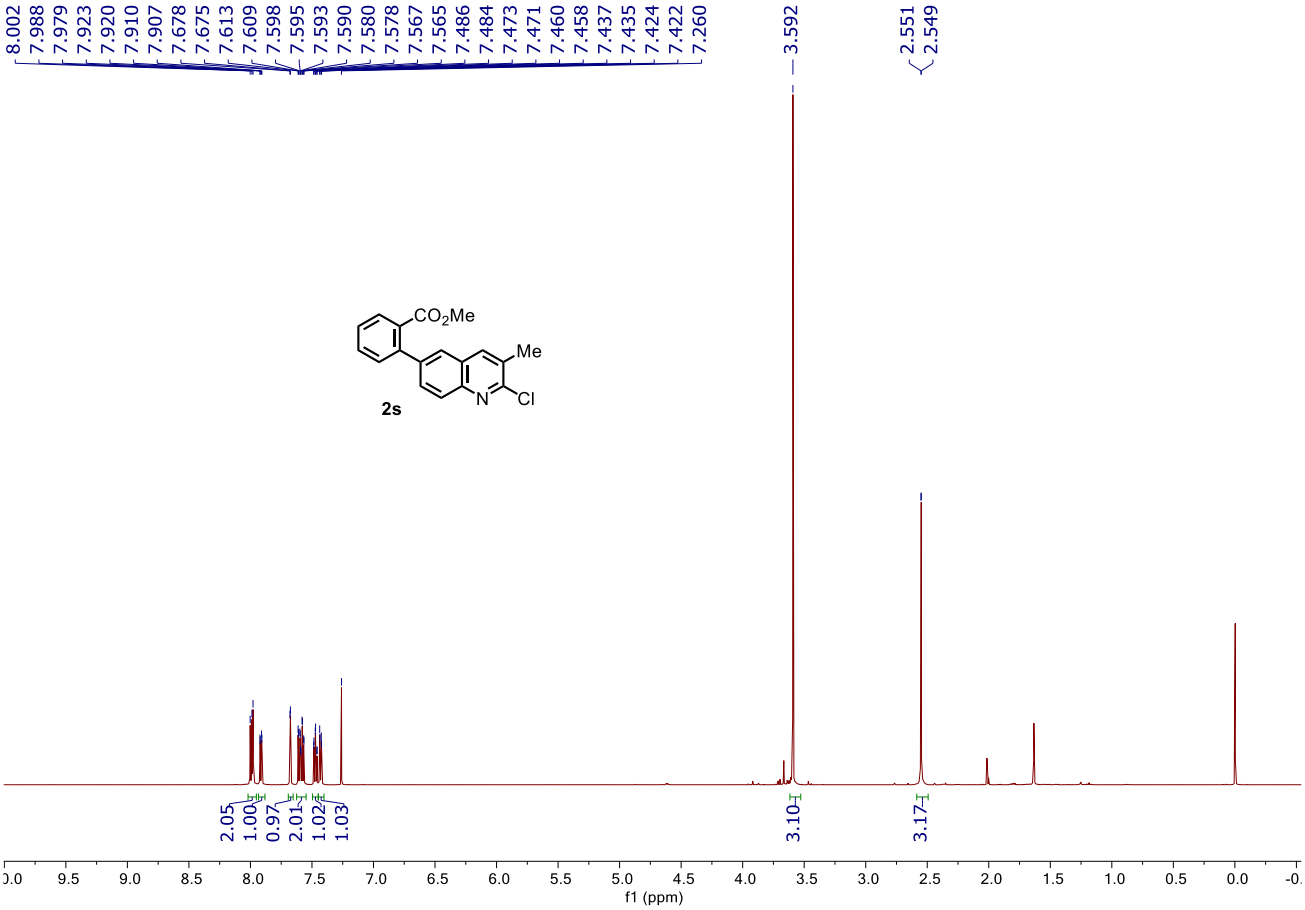
158.67
147.93
141.62
140.03
139.98
133.01
131.71
131.09
130.76
130.37
128.01
127.88
127.25
125.65
124.41
61.53
52.14
25.80
14.44
CO2Me
CO2Et
N
Me
2r
f1 (ppm)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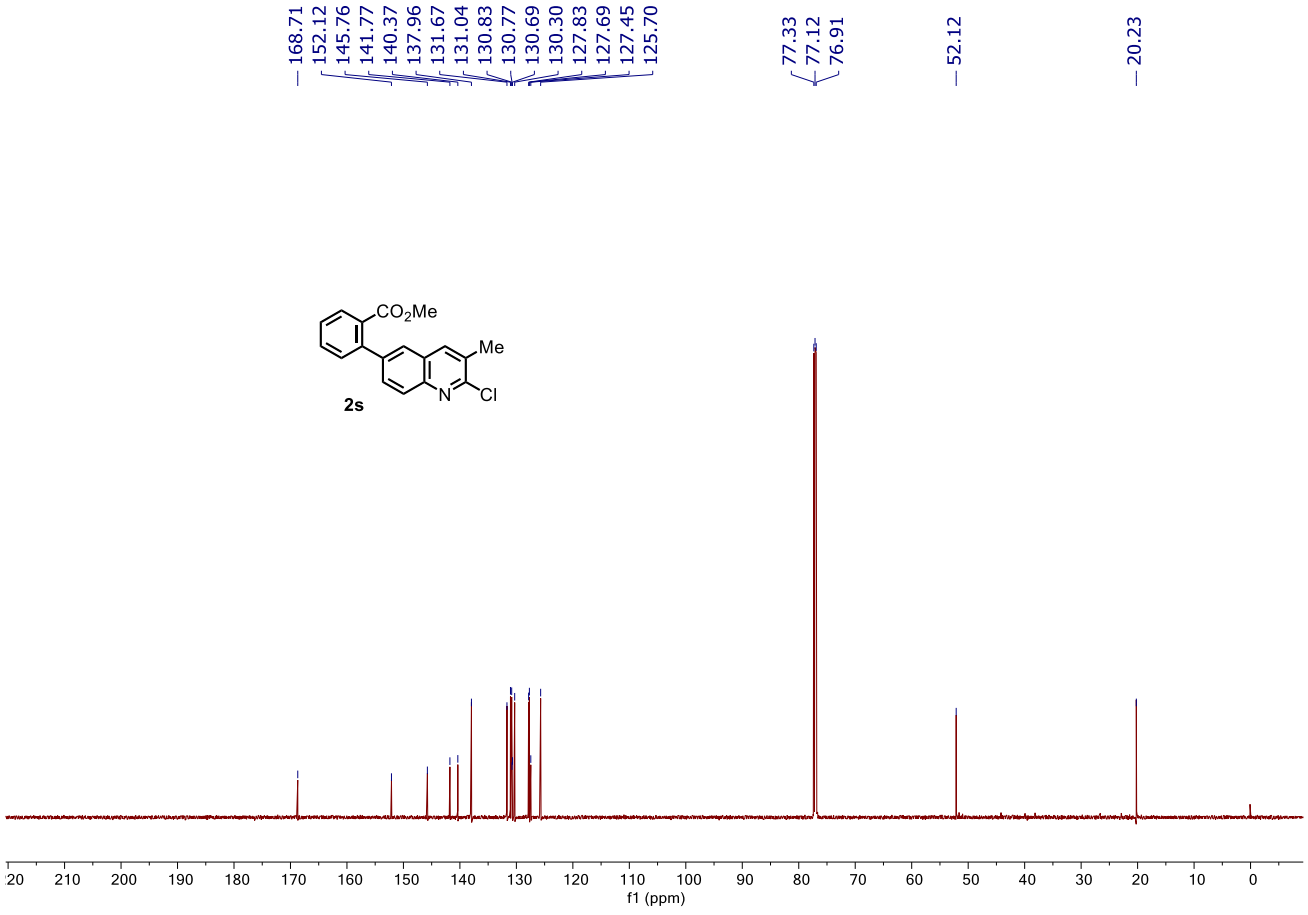
7.910
7.907
7.678
7.675
7.613
7.609
7.598
7.595
7.593
7.590
7.580
7.578
7.567
7.565
7.486
7.484
7.473
7.471
7.460
7.458
7.437
7.435
7.424
7.422
7.260
3.592
2.551
2.549
CO2Me
Me
N
Cl
2s
2.05
1.00
0.97
2.01
1.02
1.03
3.10
3.17
f1 (ppm)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152.12
145.76
141.77
140.37
137.96
131.67
131.04
130.83
130.77
130.69
130.30
127.83
127.69
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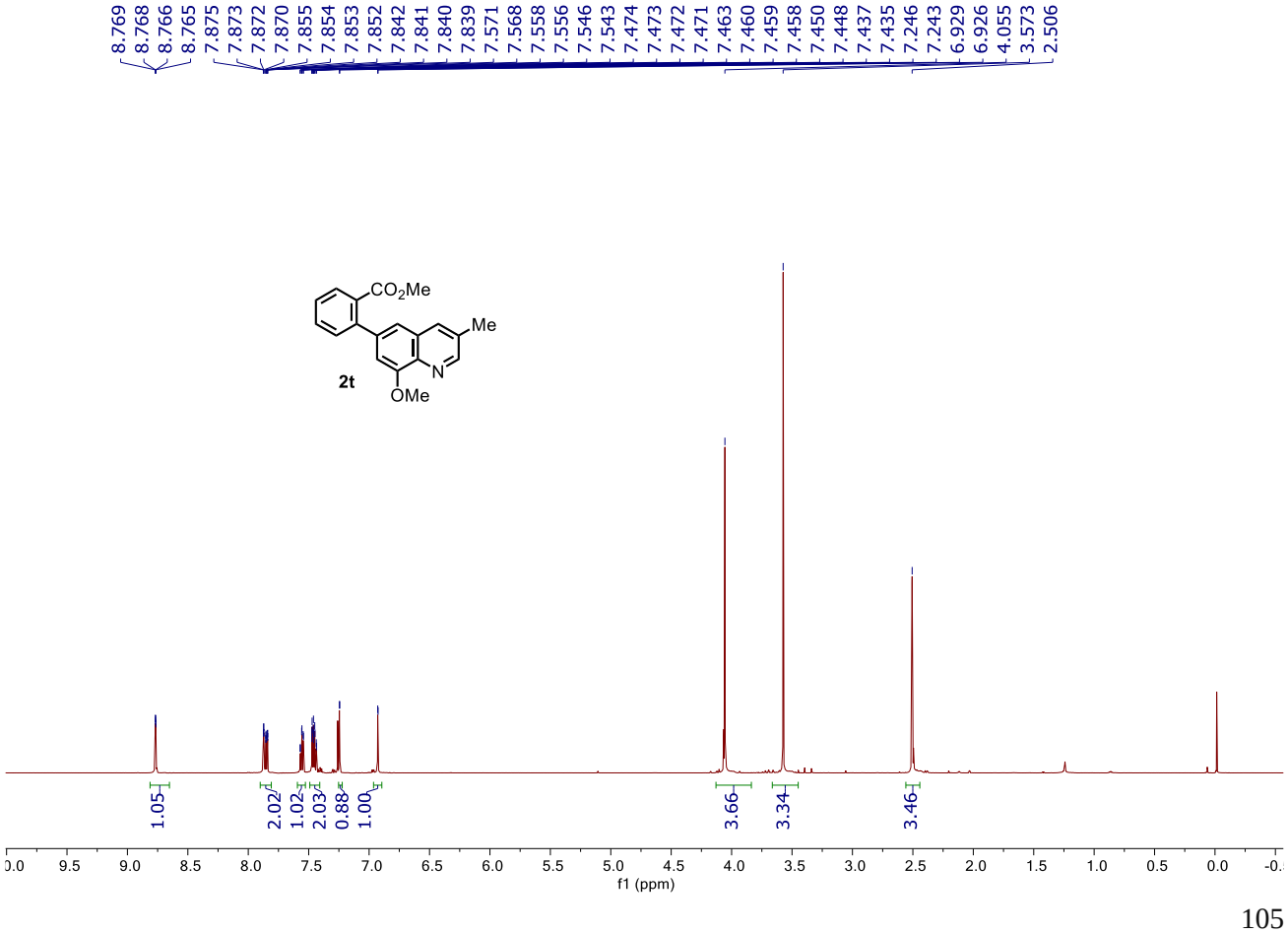
125.70
77.33
77.12
76.91
52.12
20.23
CO2Me
Me
N
Cl
2s
f1 (ppm)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8.765
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7.870
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7.854
7.853
7.852
7.842
7.841
7.840
7.839
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7.568
7.558
7.556
7.546
7.543
7.474
7.473
7.472
7.471
7.463
7.460
7.459
7.458
7.450
7.448
7.437
7.435
7.246
7.243
6.929
6.926
4.055
3.573
2.506
CO2Me
Me
N
OMe
2t
1.05
2.02
1.02
2.03
0.88
1.00
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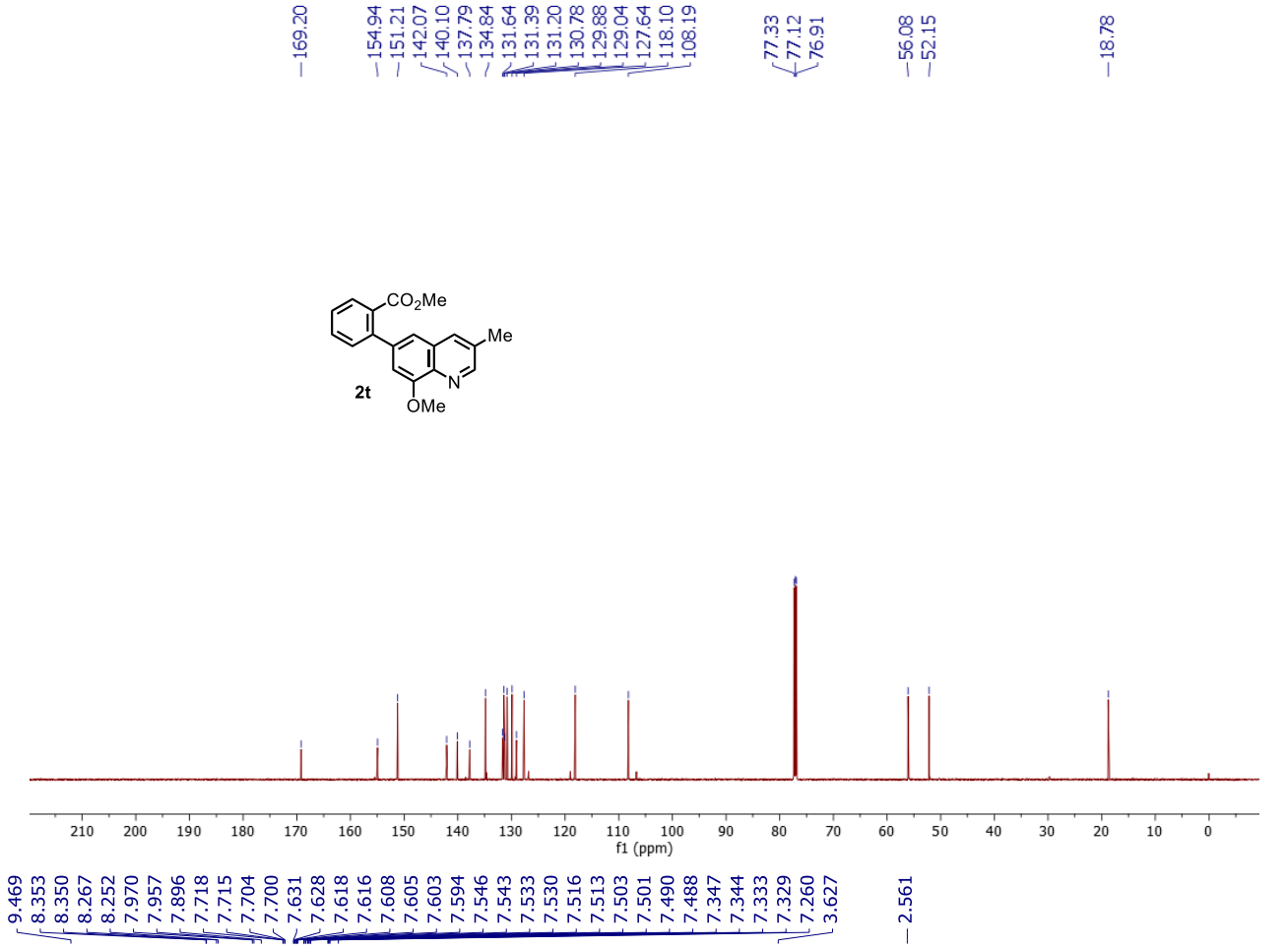
3.34
3.46
f1 (ppm)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131.64
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131.20
130.78
129.88
129.04
127.64
118.10
108.19
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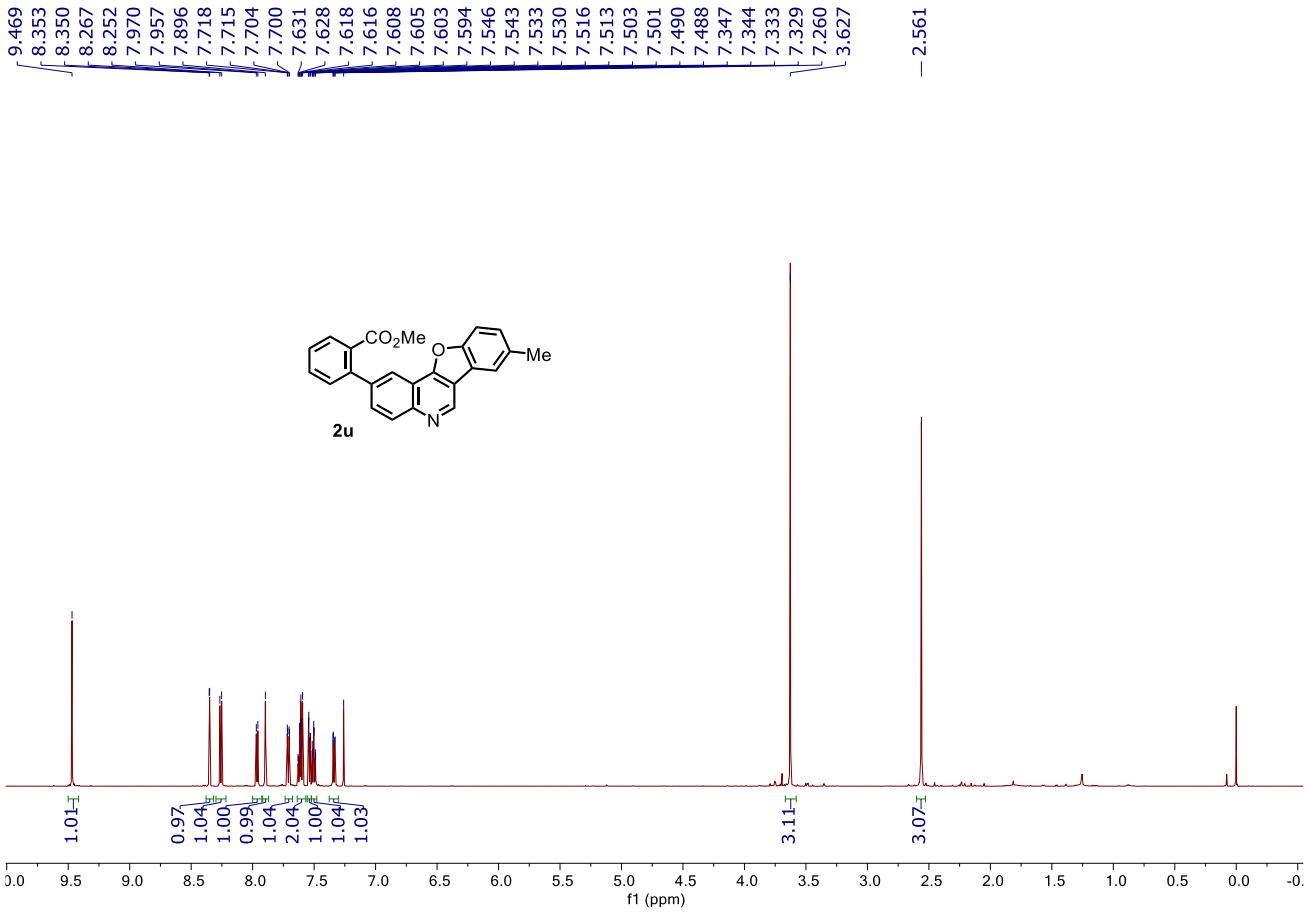
77.12
76.91
56.08
52.15
18.78
CO2Me
Me
N
OMe
2t
f1 (ppm)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7.700
7.631
7.628
7.618
7.616
7.608
7.605
7.603
7.594
7.546
7.543
7.533
7.530
7.516
7.513
7.503
7.501
7.490
7.488
7.347
7.344
7.333
7.329
7.260
3.627
2.561
CO2Me
O
Me
N
2u
1.01
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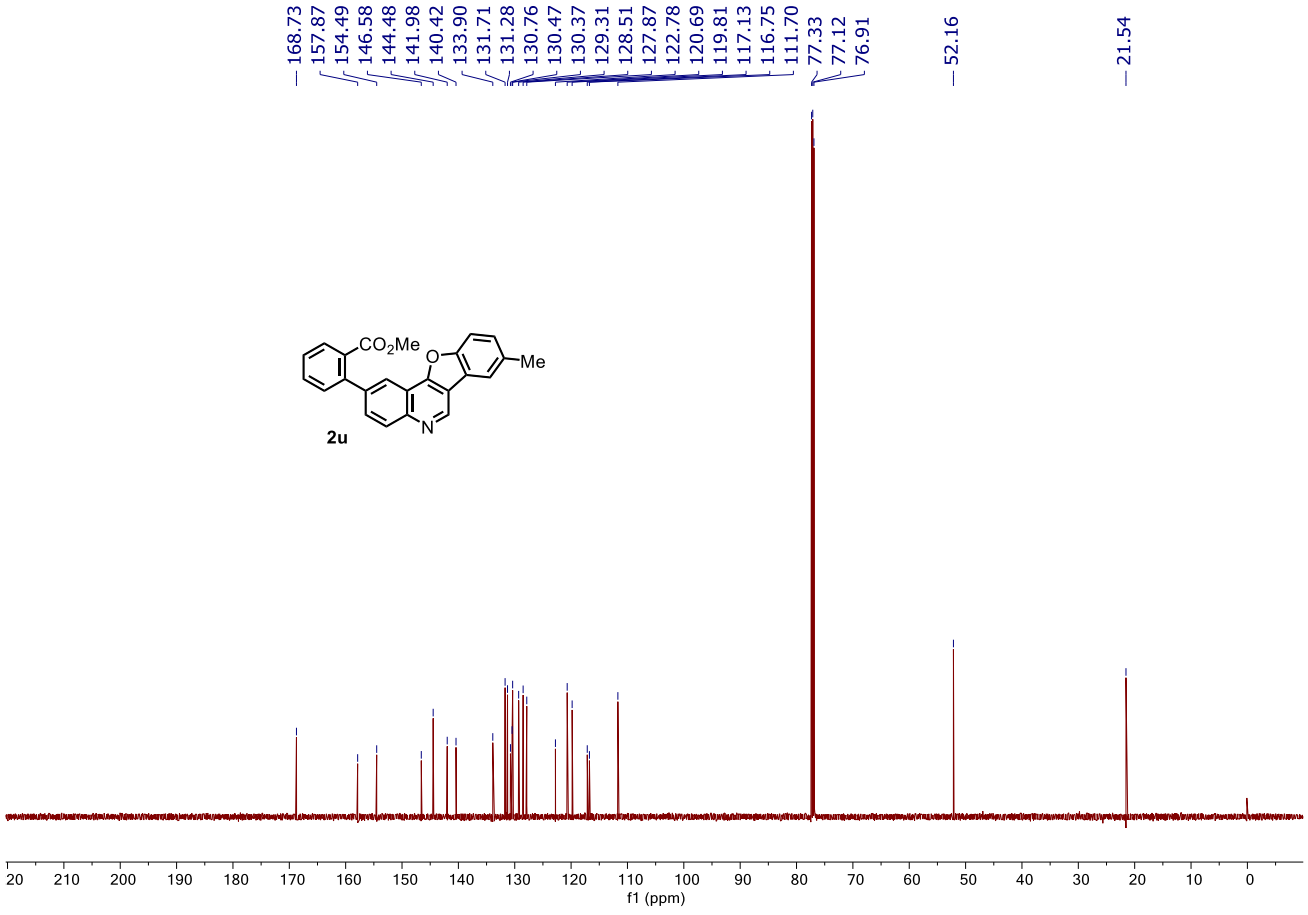
1.04
1.00
0.99
1.04
2.04
1.00
1.04
1.03
3.11
3.07
f1 (ppm)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130.76
130.47
130.37
129.31
128.51
127.87
122.78
120.69
119.81
117.13
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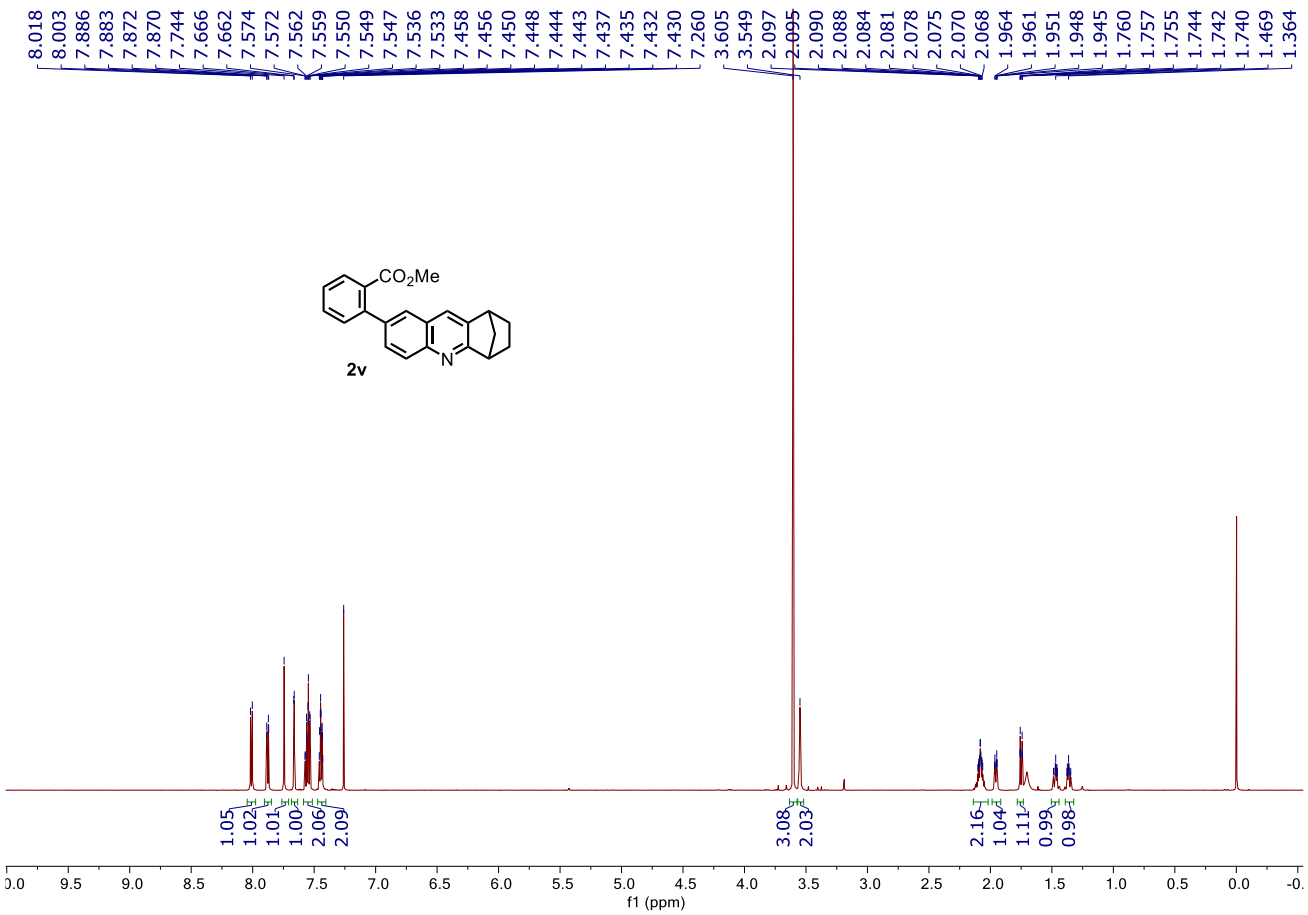
77.12
76.91
52.16
21.54
CO2Me
O
Me
N
2u
f1 (ppm)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7.549
7.547
7.536
7.533
7.458
7.456
7.450
7.448
7.444
7.443
7.437
7.435
7.432
7.430
7.260
3.605
3.549
2.097
2.095
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2.084
2.081
2.078
2.075
2.070
2.068
1.964
1.961
1.951
1.948
1.945
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1.757
1.755
1.744
1.742
1.740
1.469
1.364
CO2Me
N
2v
1.05
1.02
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2.09
3.08
2.03
2.16
1.04
1.11
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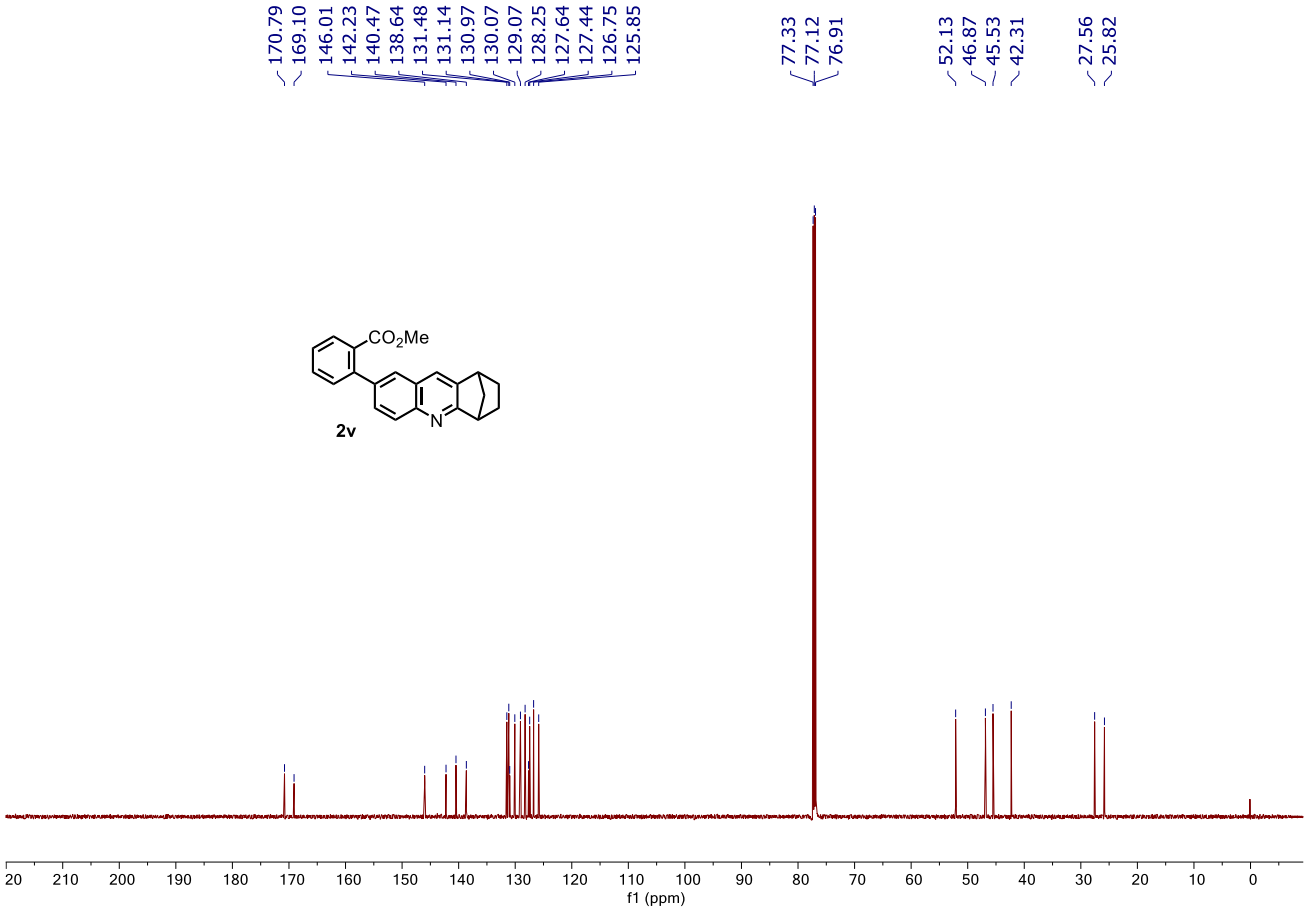
0.98
f1 (ppm)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129.07
128.25
127.64
127.44
126.75
125.85
77.33
77.12
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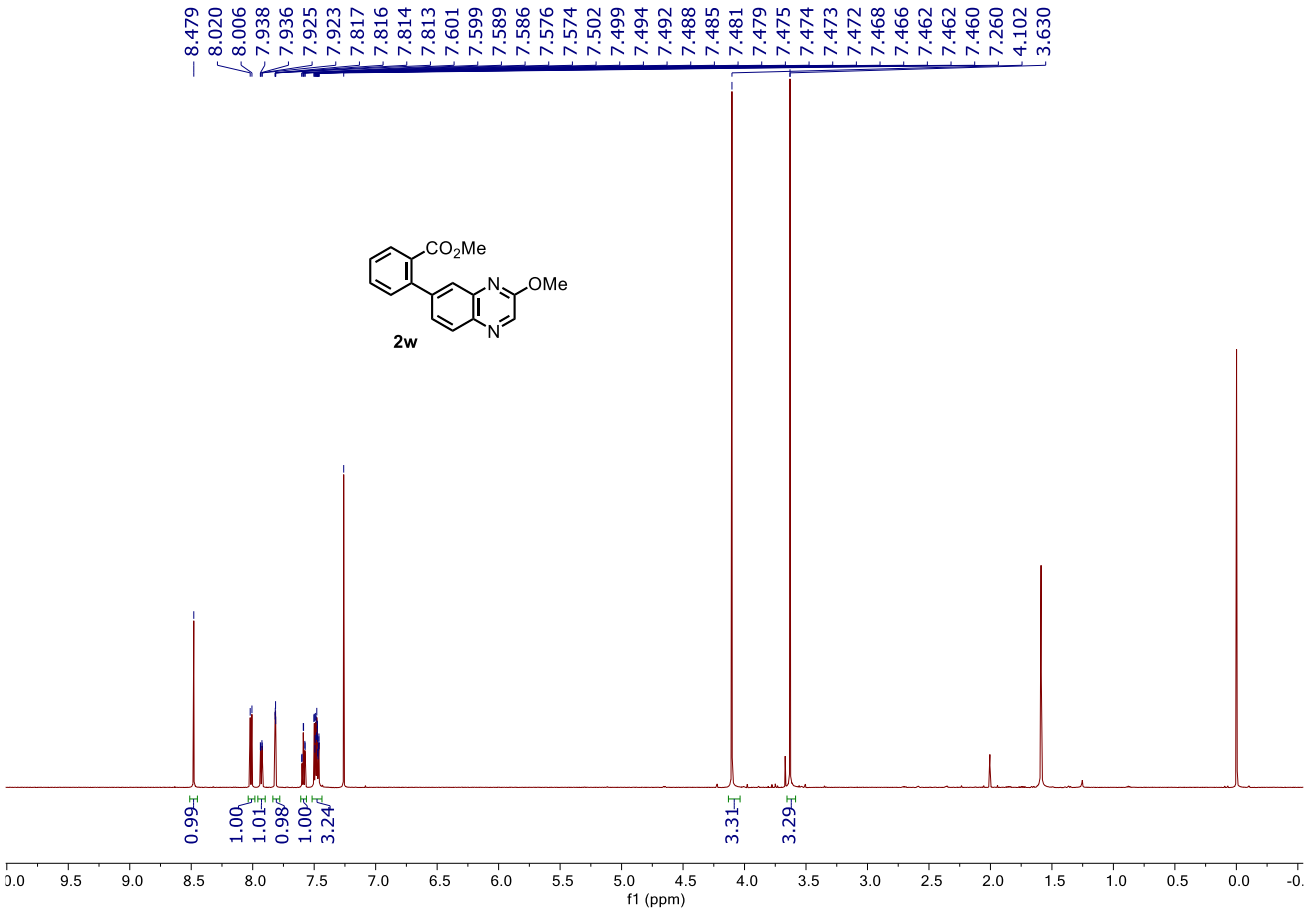
52.13
46.87
45.53
42.31
27.56
25.82
CO2Me
N
2v
f1 (ppm)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7.599
7.589
7.586
7.576
7.574
7.502
7.499
7.494
7.492
7.488
7.485
7.481
7.479
7.475
7.474
7.473
7.472
7.468
7.466
7.462
7.462
7.460
7.260
4.102
3.630
CO2Me
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OMe
N
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1.01
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1.00
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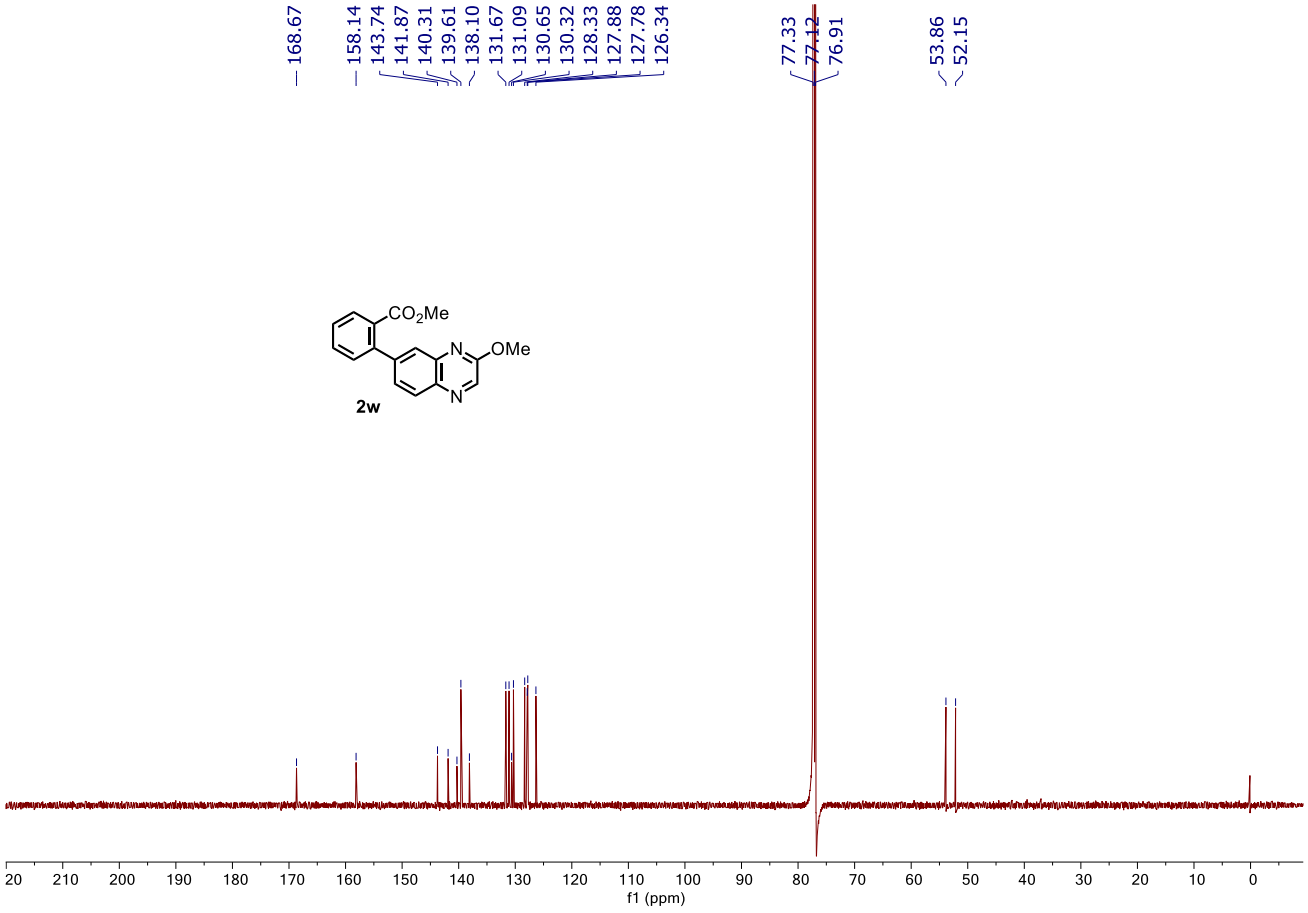
3.31
3.29
f1 (ppm)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131.09
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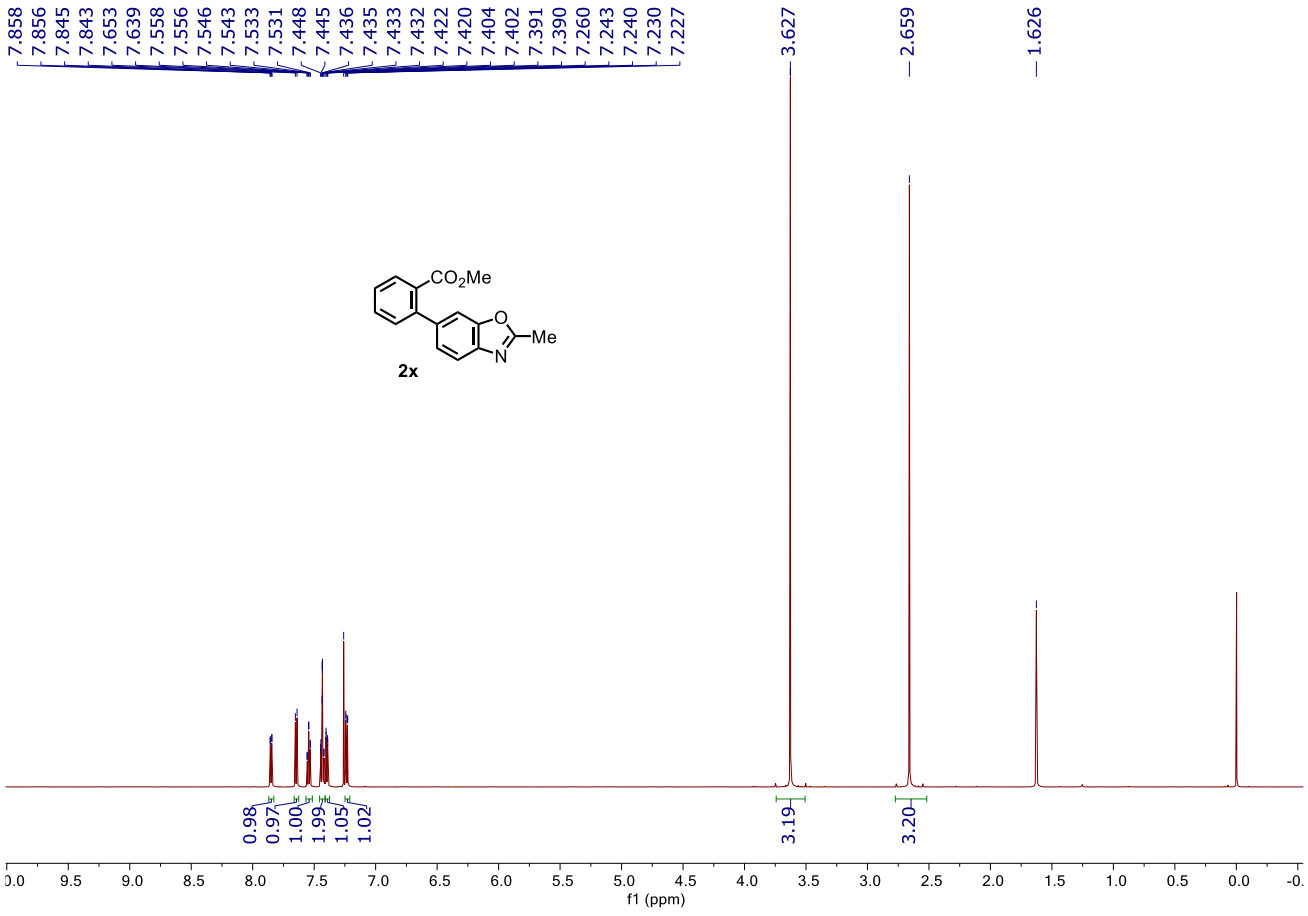
130.32
128.33
127.88
127.78
126.34
77.33
77.12
76.91
53.86
52.15
CO2Me
N
OMe
N
2w
f1 (ppm)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7.445
7.436
7.435
7.433
7.432
7.422
7.420
7.404
7.402
7.391
7.390
7.260
7.243
7.240
7.230
7.227
3.627
2.659
1.626
CO2Me
O
Me
N
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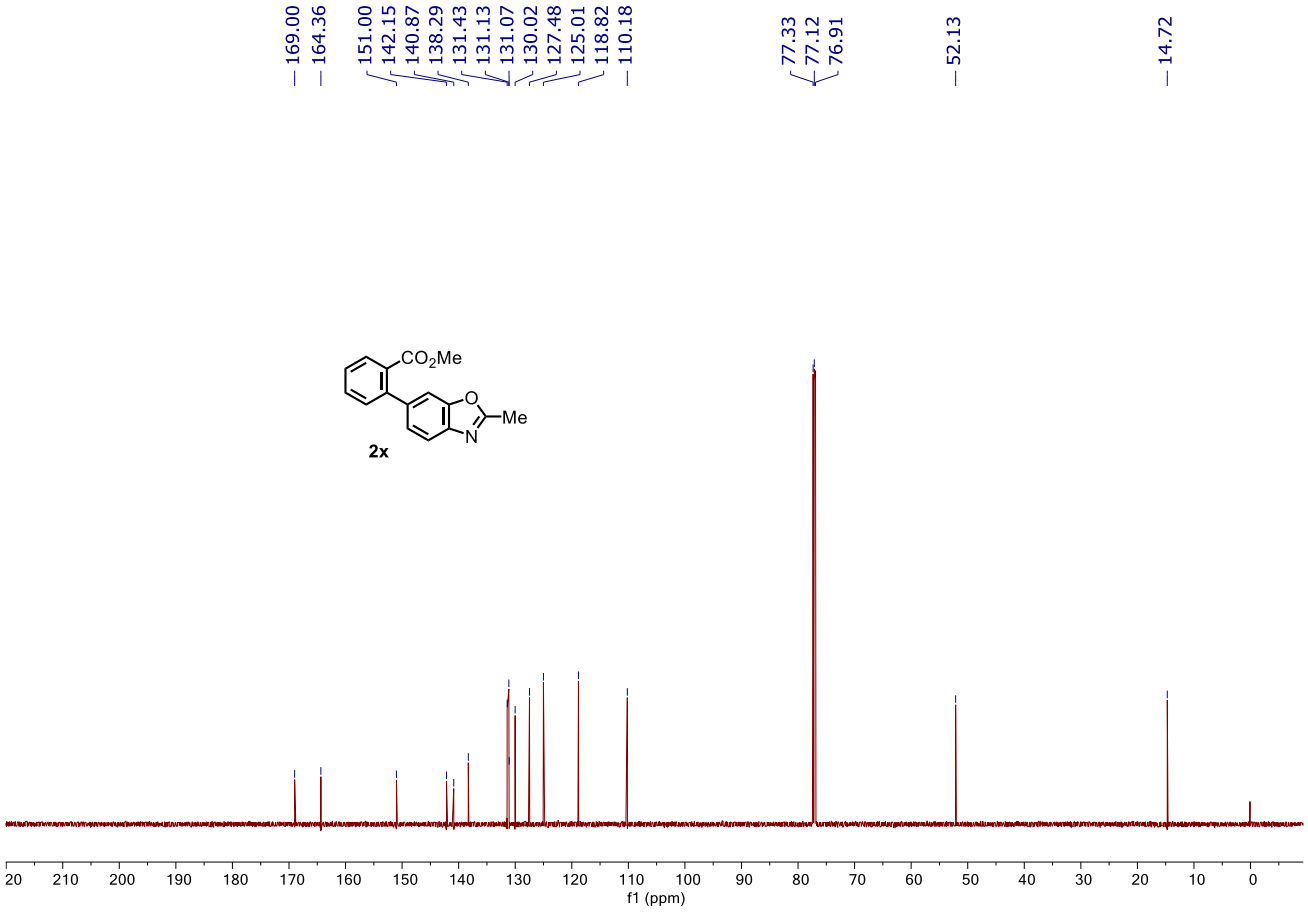
0.98
0.97
1.00
1.99
1.05
1.02
3.19
3.20
f1 (ppm)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138.29
131.43
131.13
131.07
130.02
127.48
125.01
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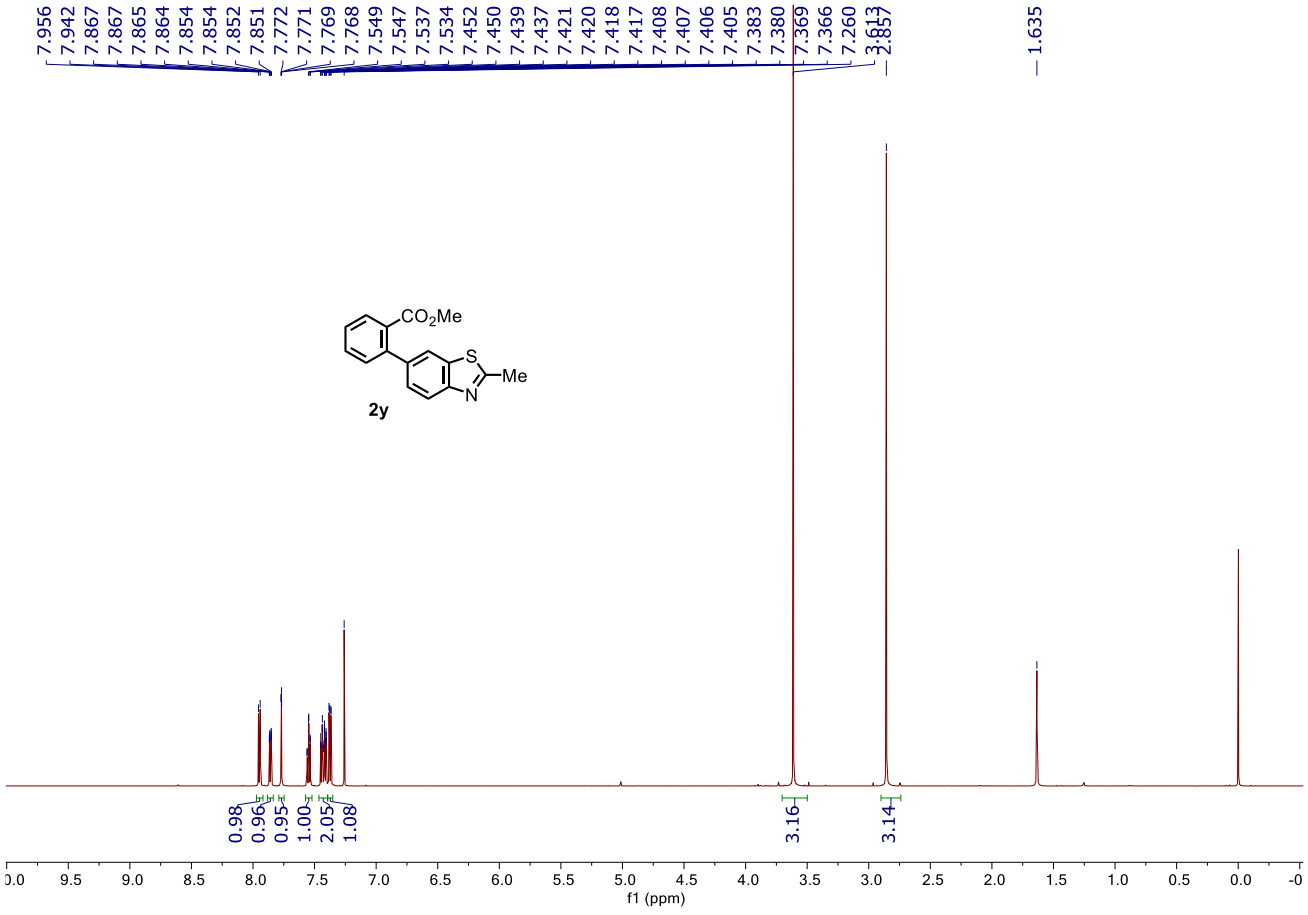
110.18
77.33
77.12
76.91
52.13
14.72
CO2Me
O
Me
N
2x
f1 (ppm)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7.450
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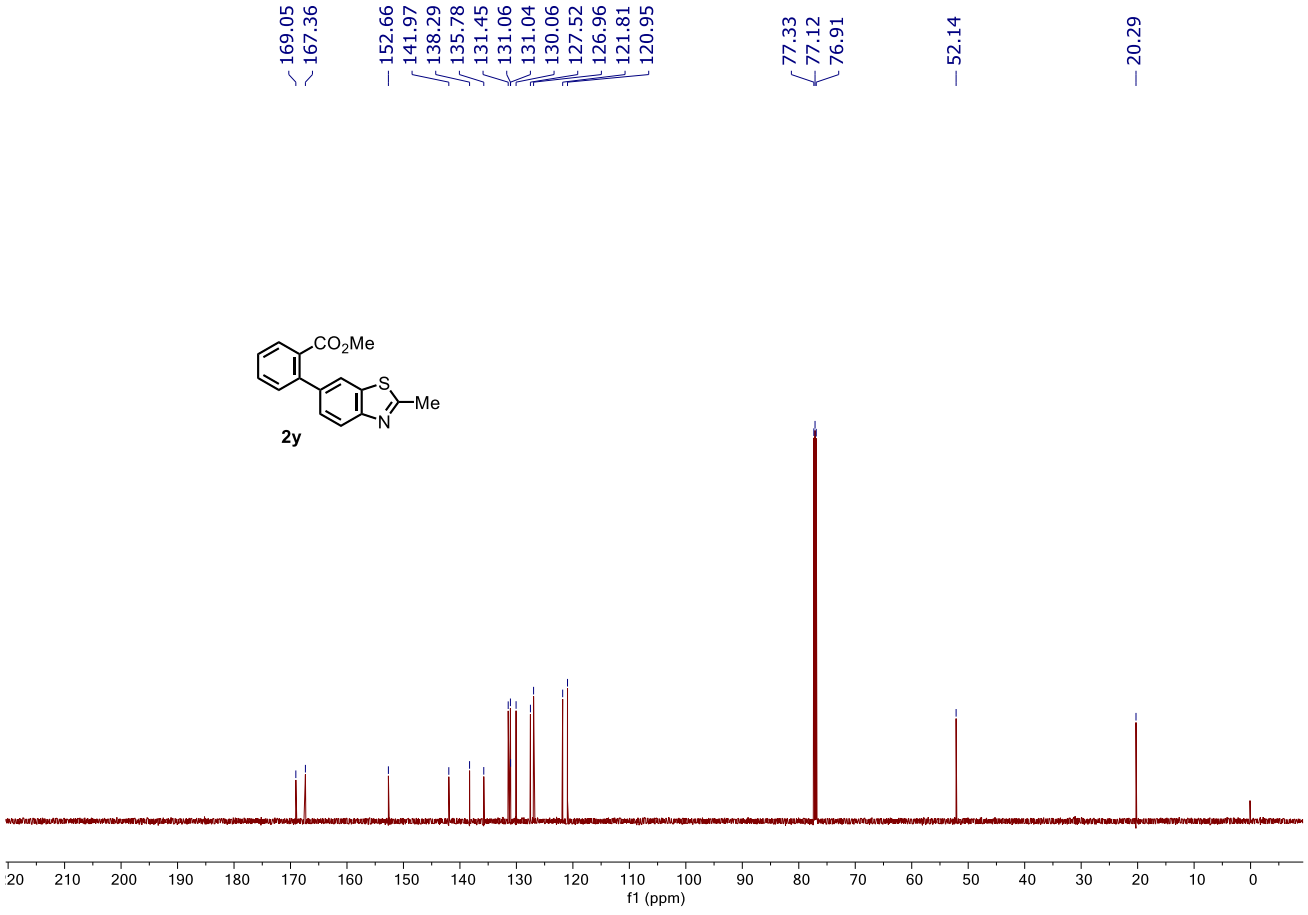
7.407
7.406
7.405
7.383
7.380
7.369
7.366
7.260
3.613
2.857
1.635
CO2Me
S
Me
N
2y
0.98
0.96
0.95
1.00
2.05
1.08
3.16
3.14
f1 (ppm)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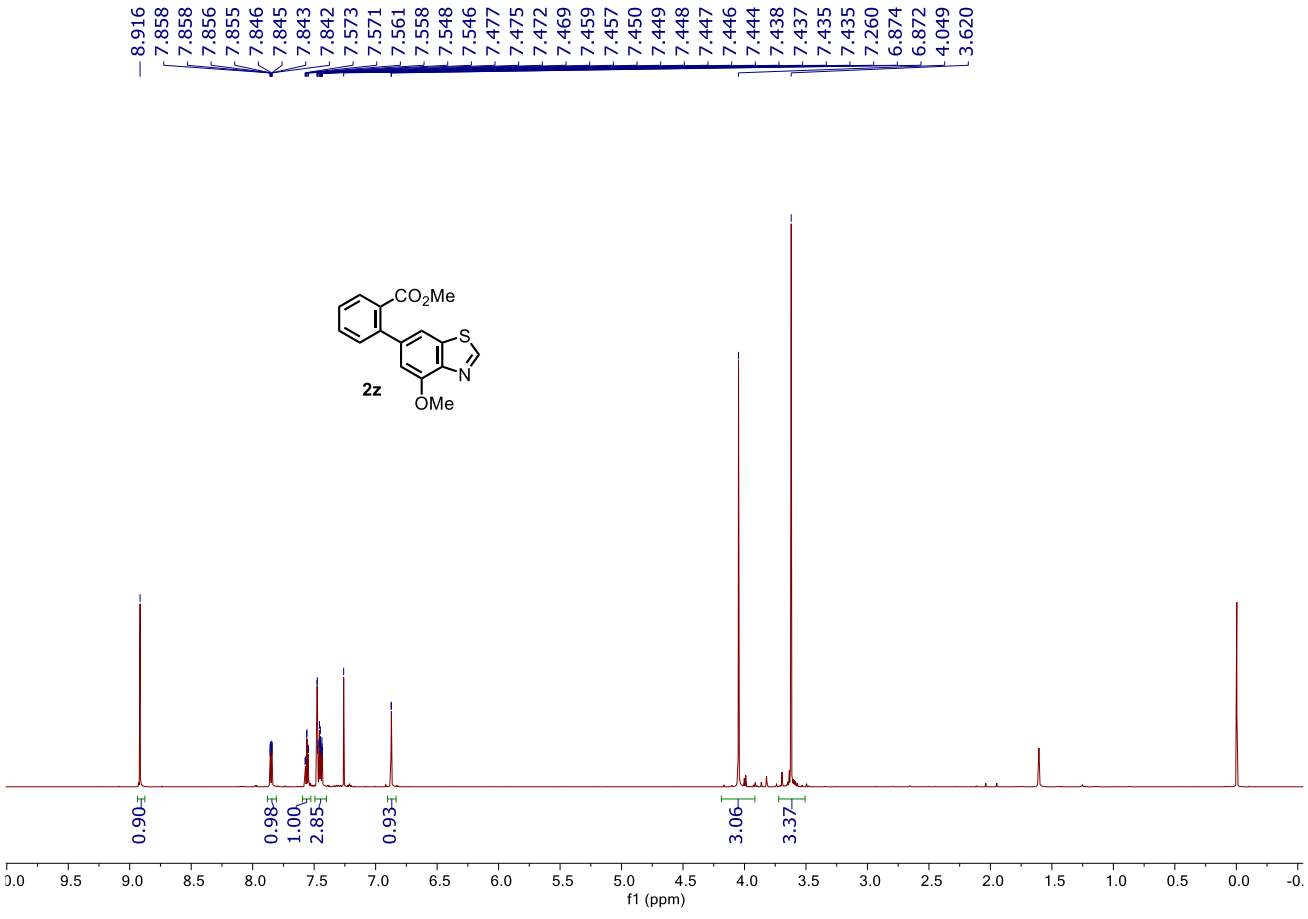
167.36
152.66
141.97
138.29
135.78
131.45
131.06
131.04
130.06
127.52
126.96
121.81
120.95
77.33
77.12
76.91
52.14
20.29
CO2Me
S
N
Me
2y
f1 (ppm)


8.916
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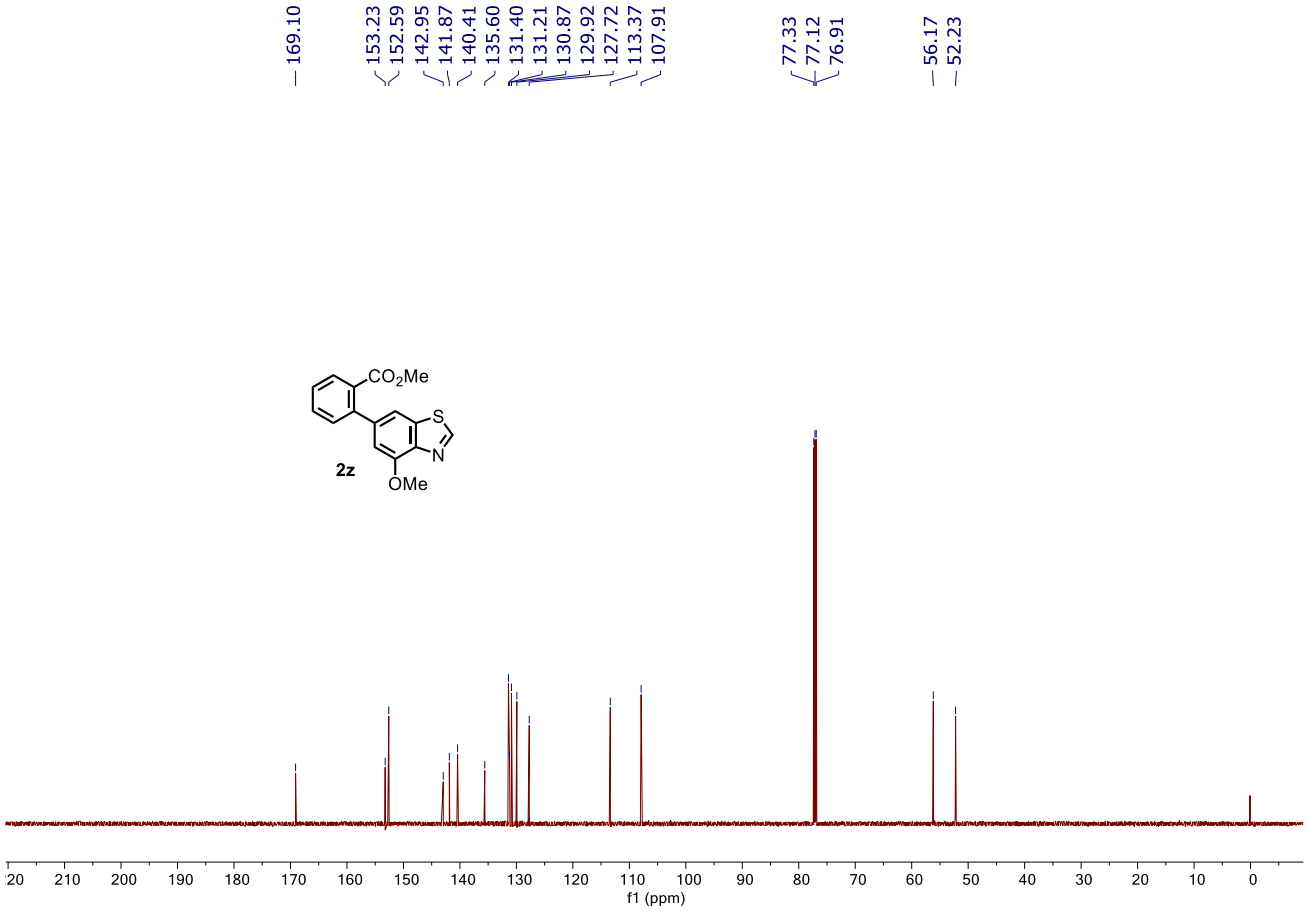
7.858
7.856
7.855
7.846
7.845
7.843
7.842
7.573
7.571
7.561
7.558
7.548
7.546
7.477
7.475
7.472
7.469
7.459
7.457
7.450
7.449
7.448
7.447
7.446
7.444
7.438
7.437
7.435
7.435
7.260
6.874
6.872
4.049
3.620
CO2Me
S
N
OMe
2z
0.90
0.98
1.00
2.85
0.93
3.06
3.37
f1 (ppm)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153.23
152.59
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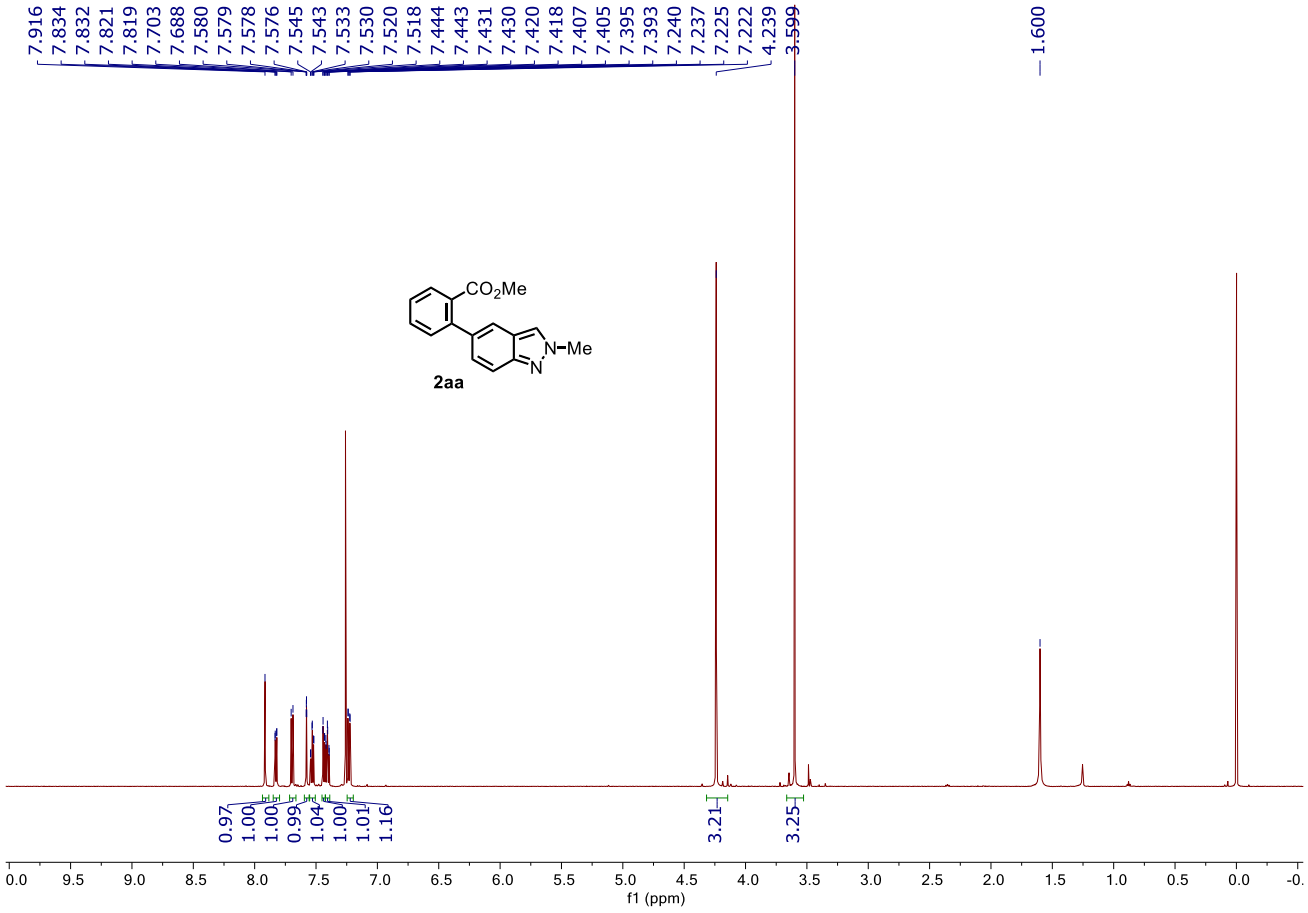
140.41
135.60
131.40
131.21
130.87
129.92
127.72
113.37
107.91
77.33
77.12
76.91
56.17
52.23
CO2Me
S
N
OMe
2z
f1 (ppm)


7.916
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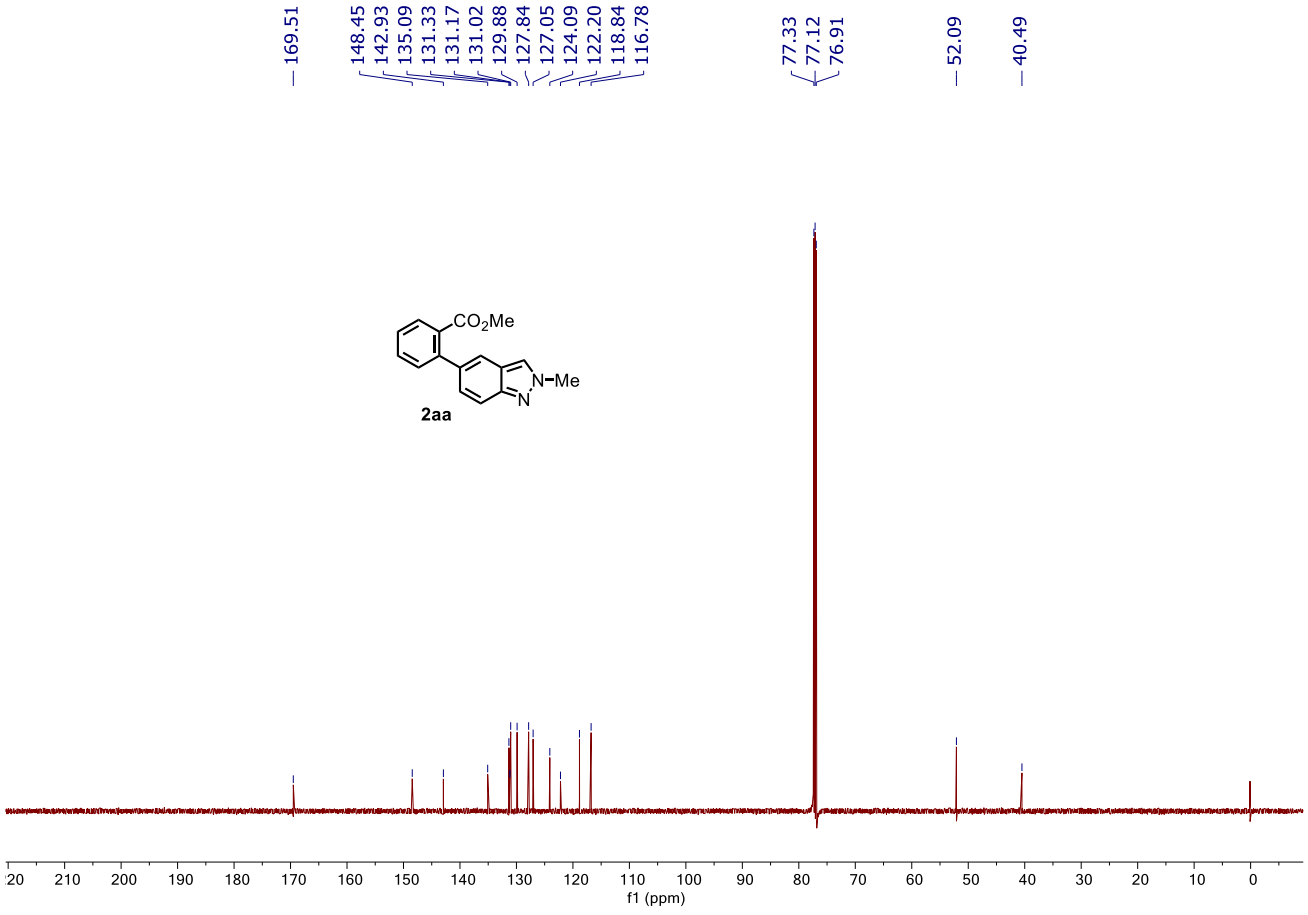
7.821
7.819
7.703
7.688
7.580
7.579
7.578
7.576
7.545
7.543
7.533
7.530
7.520
7.518
7.444
7.443
7.431
7.430
7.420
7.418
7.407
7.405
7.395
7.393
7.240
7.237
7.225
7.222
4.239
3.599
1.600
CO2Me
N-Me
N
2aa
0.97
1.00
1.00
0.99
1.04
1.00
1.01
1.16
3.21
3.25
f1 (ppm)


169.51
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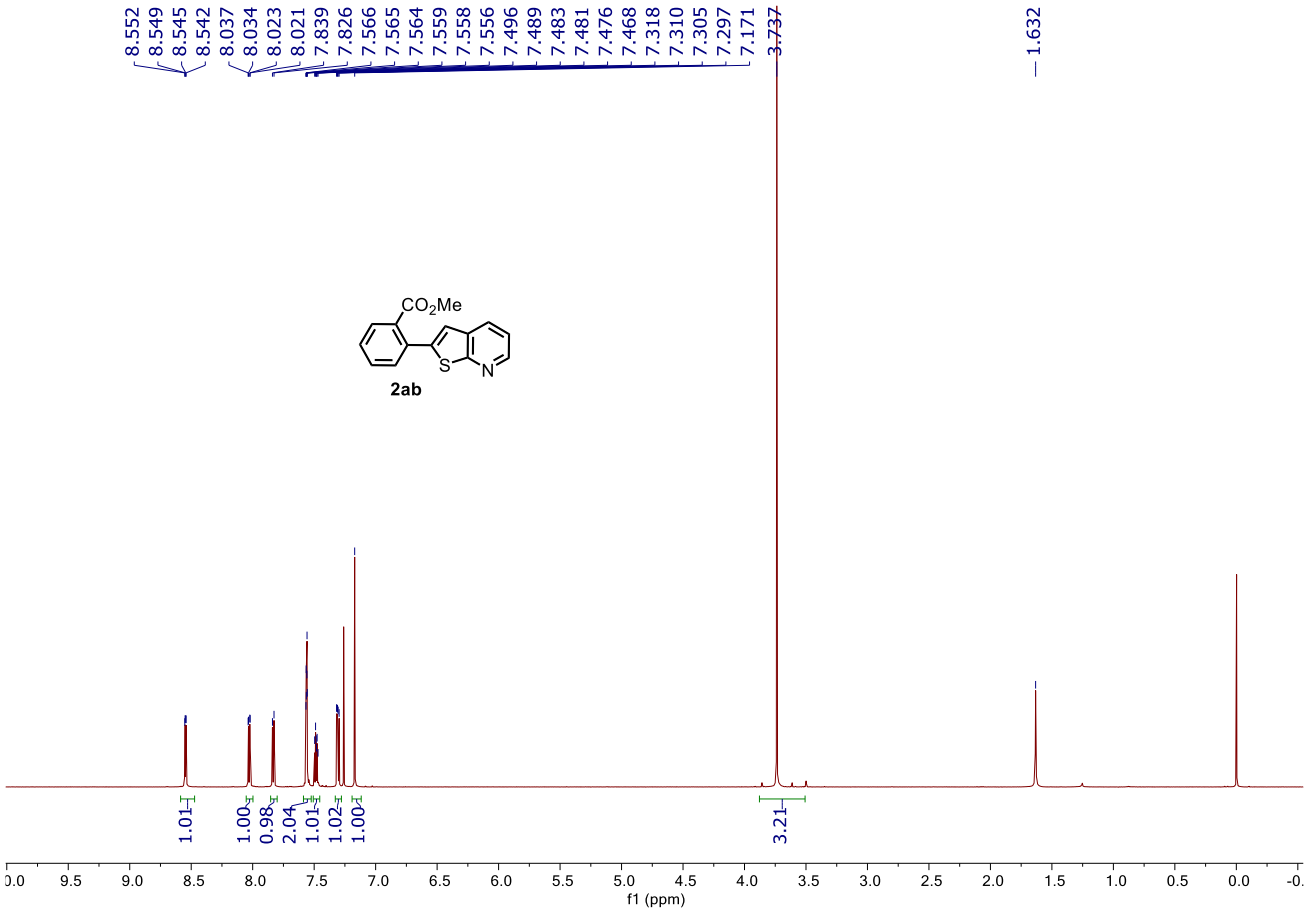
131.33
131.17
131.02
129.88
127.84
127.05
124.09
122.20
118.84
116.78
77.33
77.12
76.91
52.09
40.49
CO2Me
N-Me
N
2aa
f1 (ppm)


8.552
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8.023
8.021
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7.826
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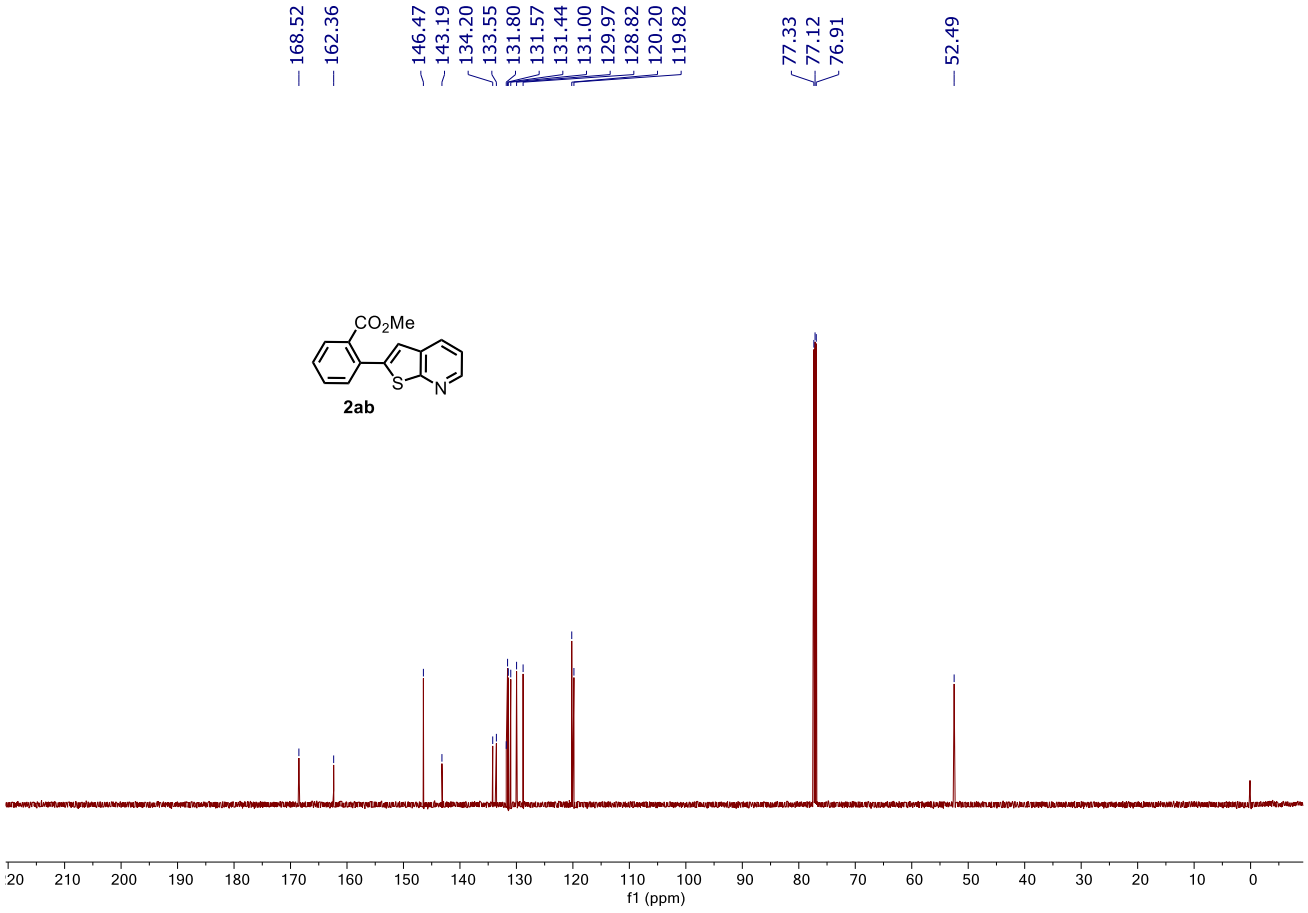
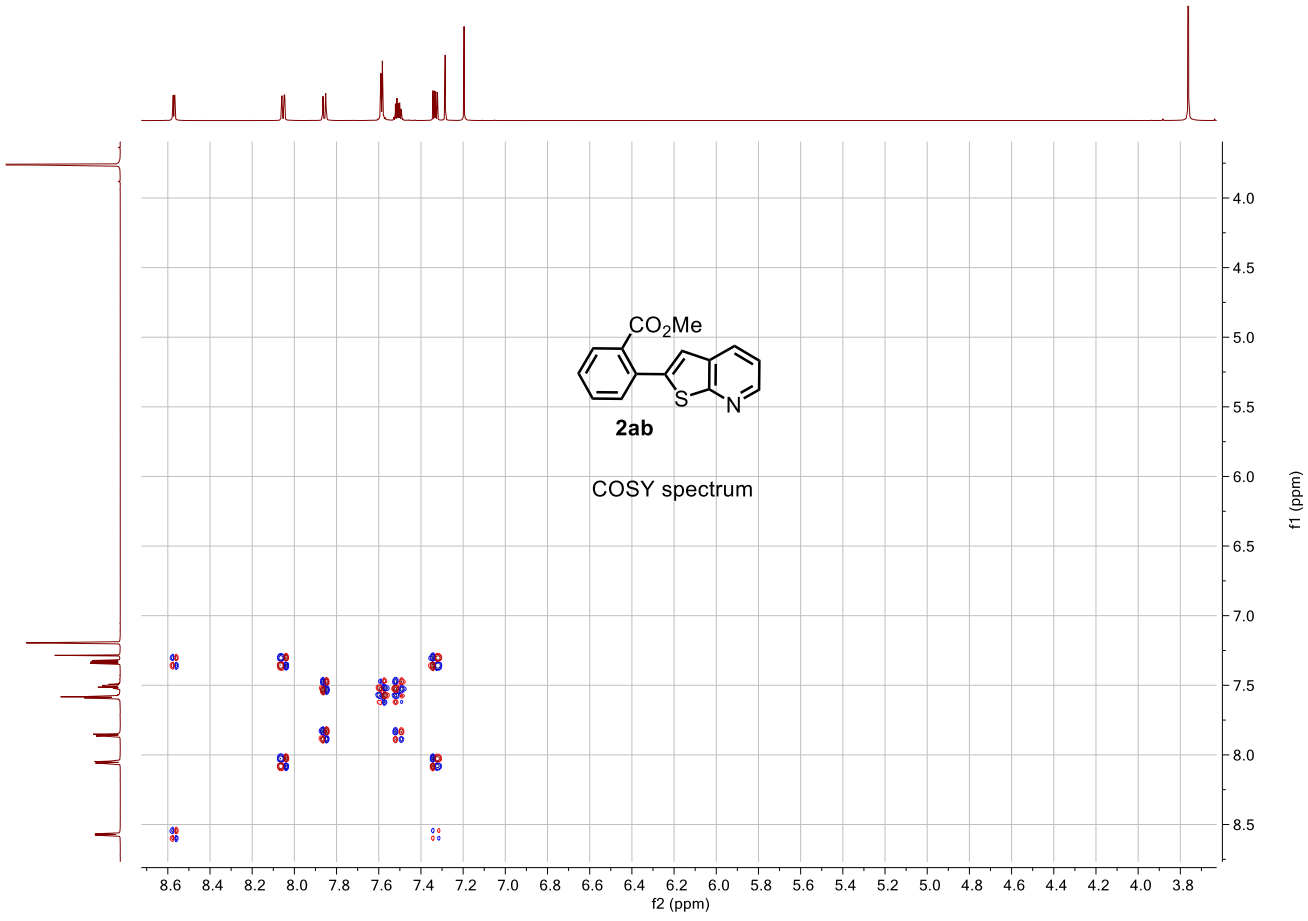
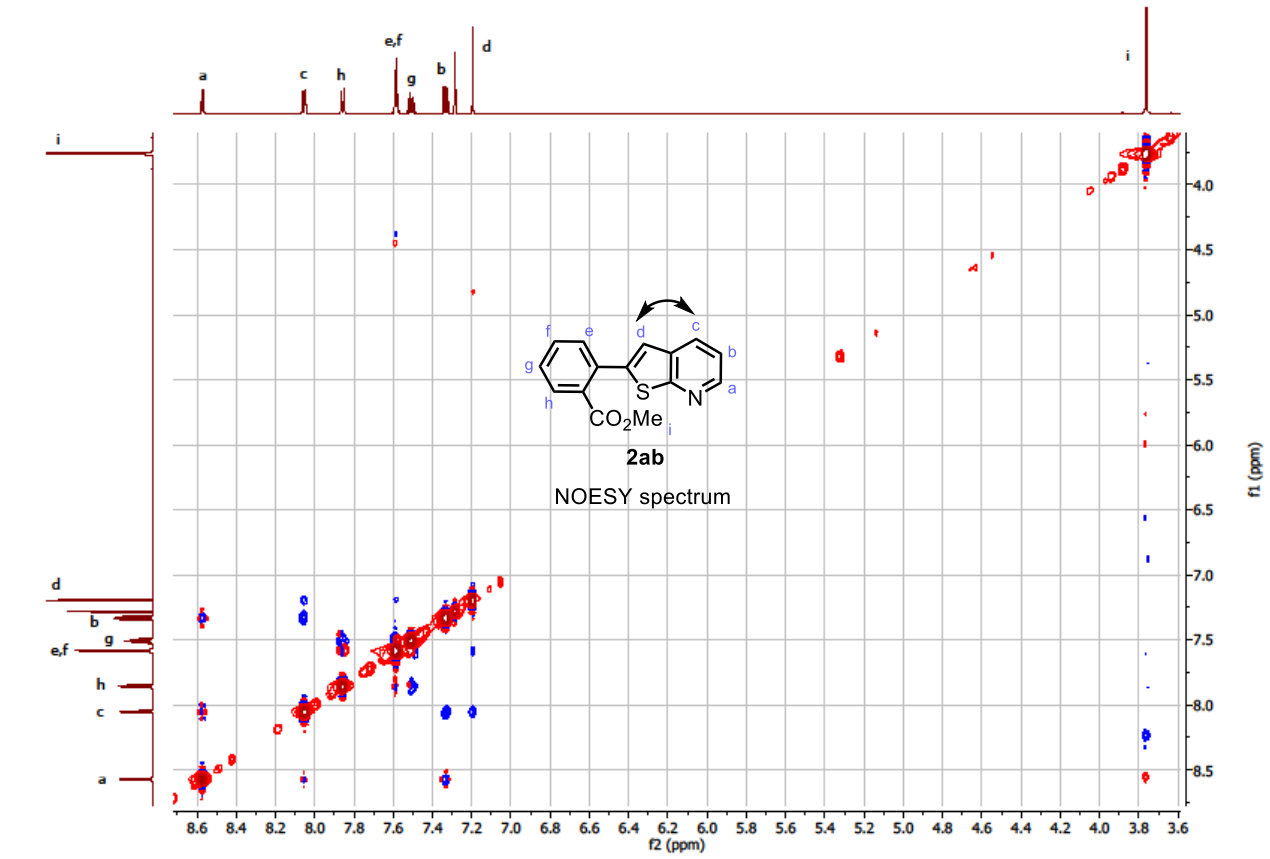
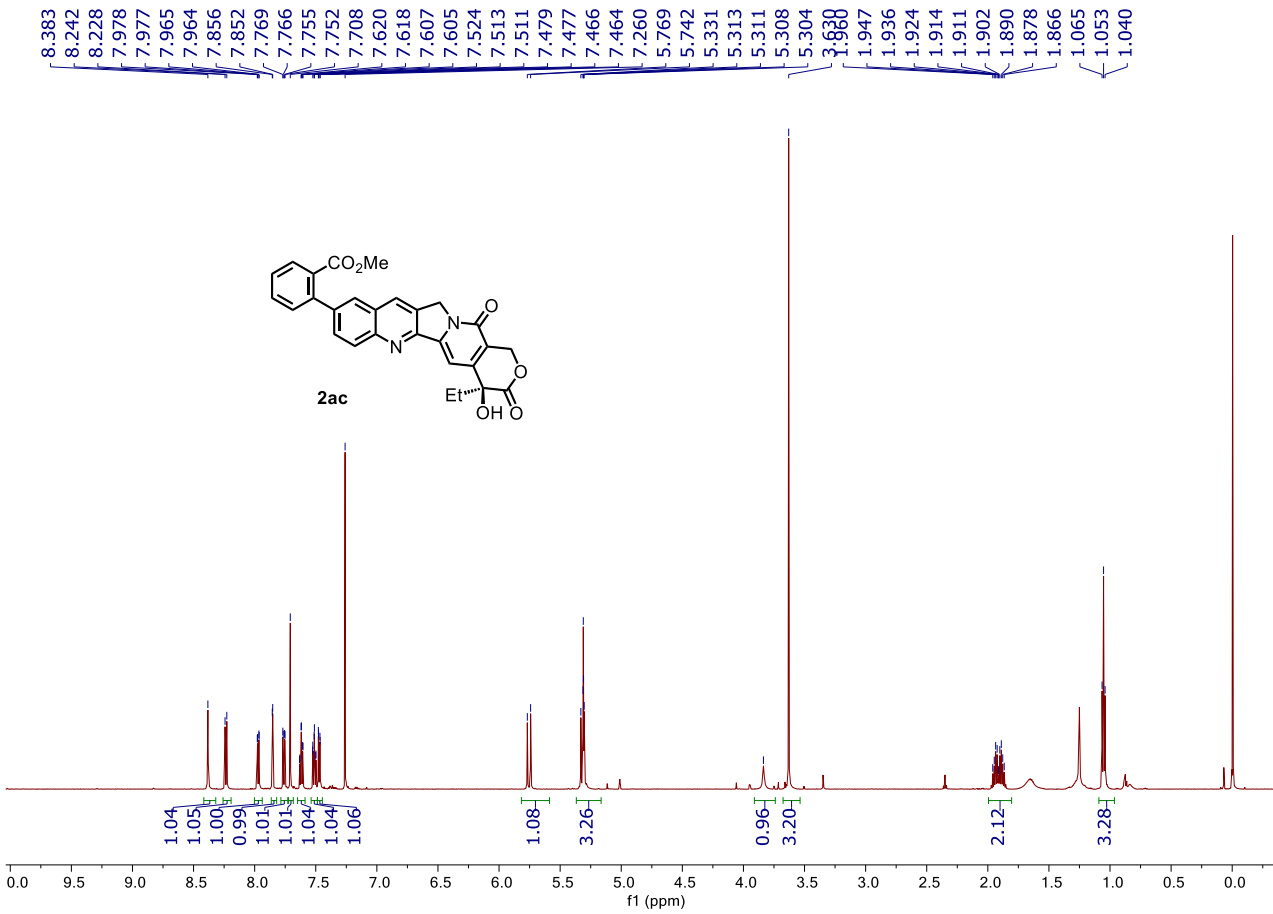
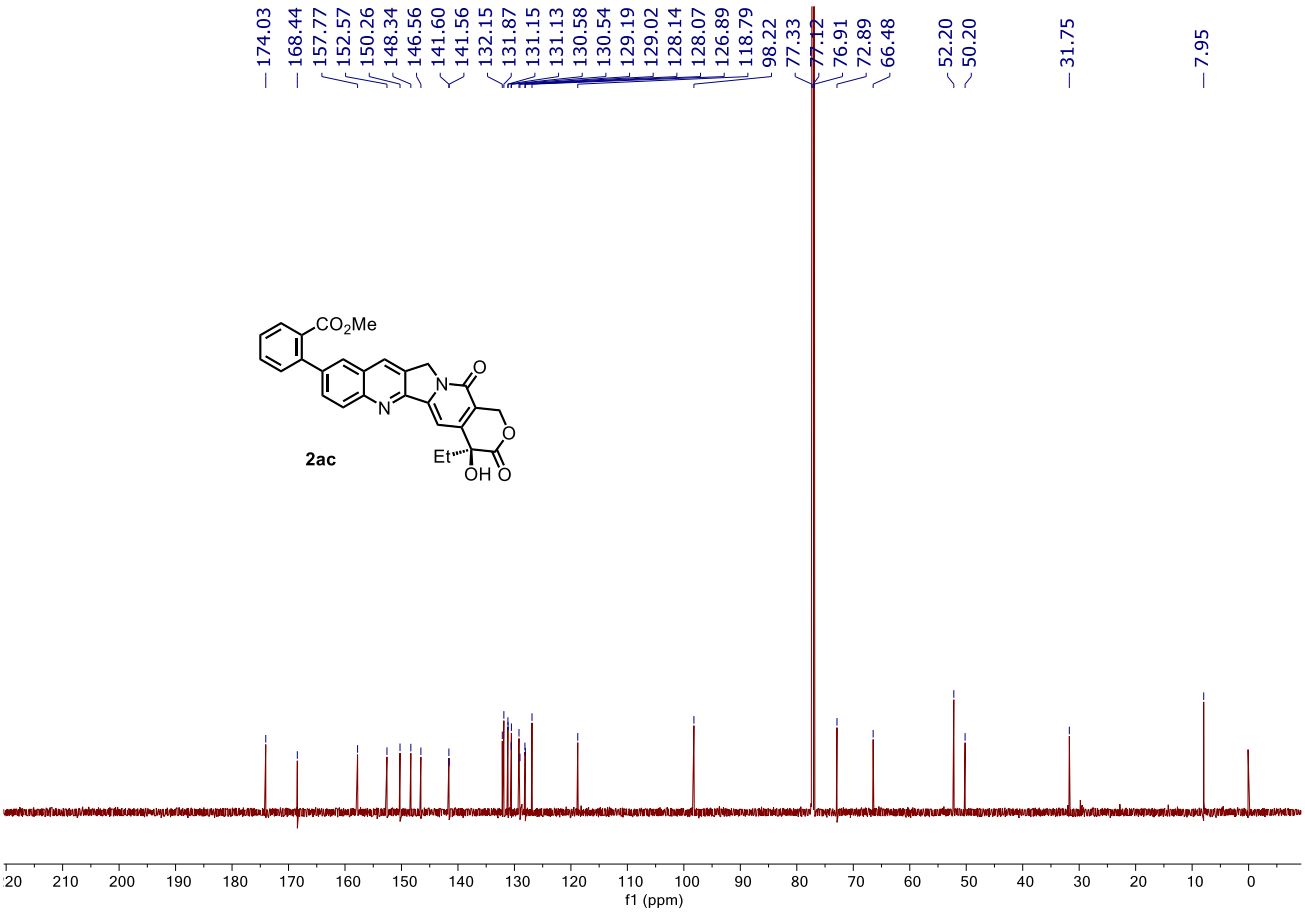
7.565
7.564
7.559
7.558
7.556
7.496
7.489
7.483
7.481
7.476
7.468
7.318
7.310
7.305
7.297
7.171
3.737
1.632
CO2Me
S
N
2ab
1.01
1.00
0.98
2.04
1.01
1.02
1.00
3.21
f1 (ppm)


168.52
162.36
146.47
143.19
134.20
133.55
131.80
131.57
131.44
131.00
129.97
128.82
120.20
119.82
77.33
77.12
76.91
52.49
CO2Me
S
N
2ab
f1 (ppm)

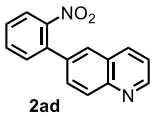

CO2Me
S
N
2ab
COSY spectrum
f1 (ppm)
f2 (ppm)

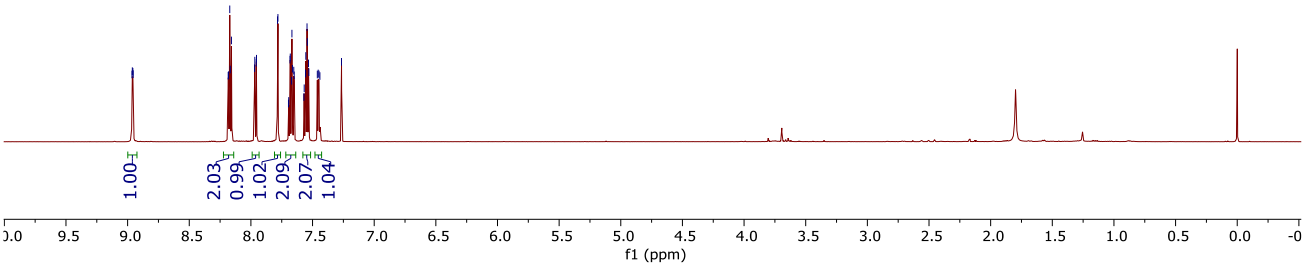

a
c
h
e,f
g
b
d
i
f
e
d
c
g
b
h
a
S
N
CO2Me
i
2ab
NOESY spectrum
f2 (ppm)
f1 (ppm)

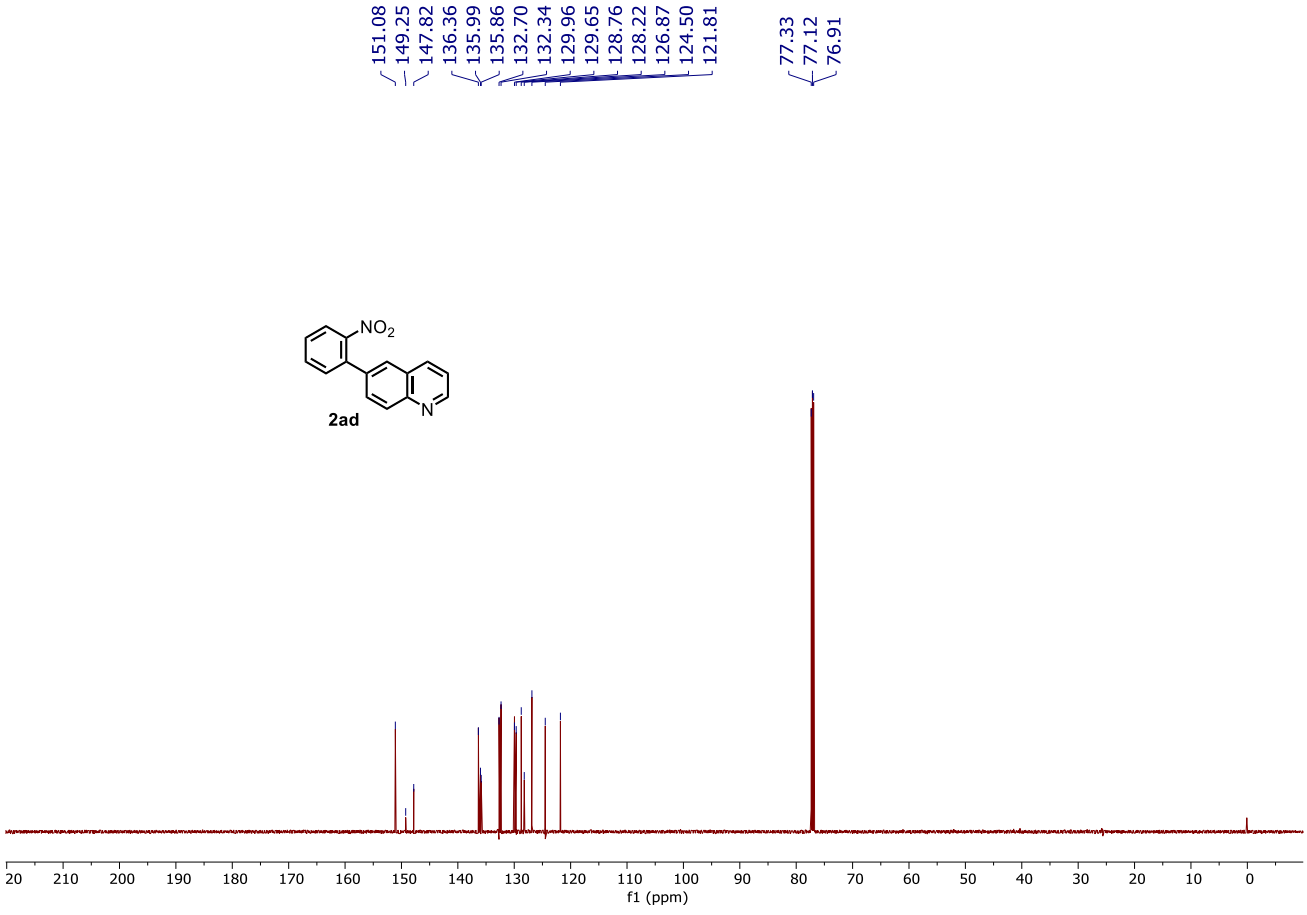

CO2Me
N
O
N
O
Et
OH
O
2ac
f1 (ppm)

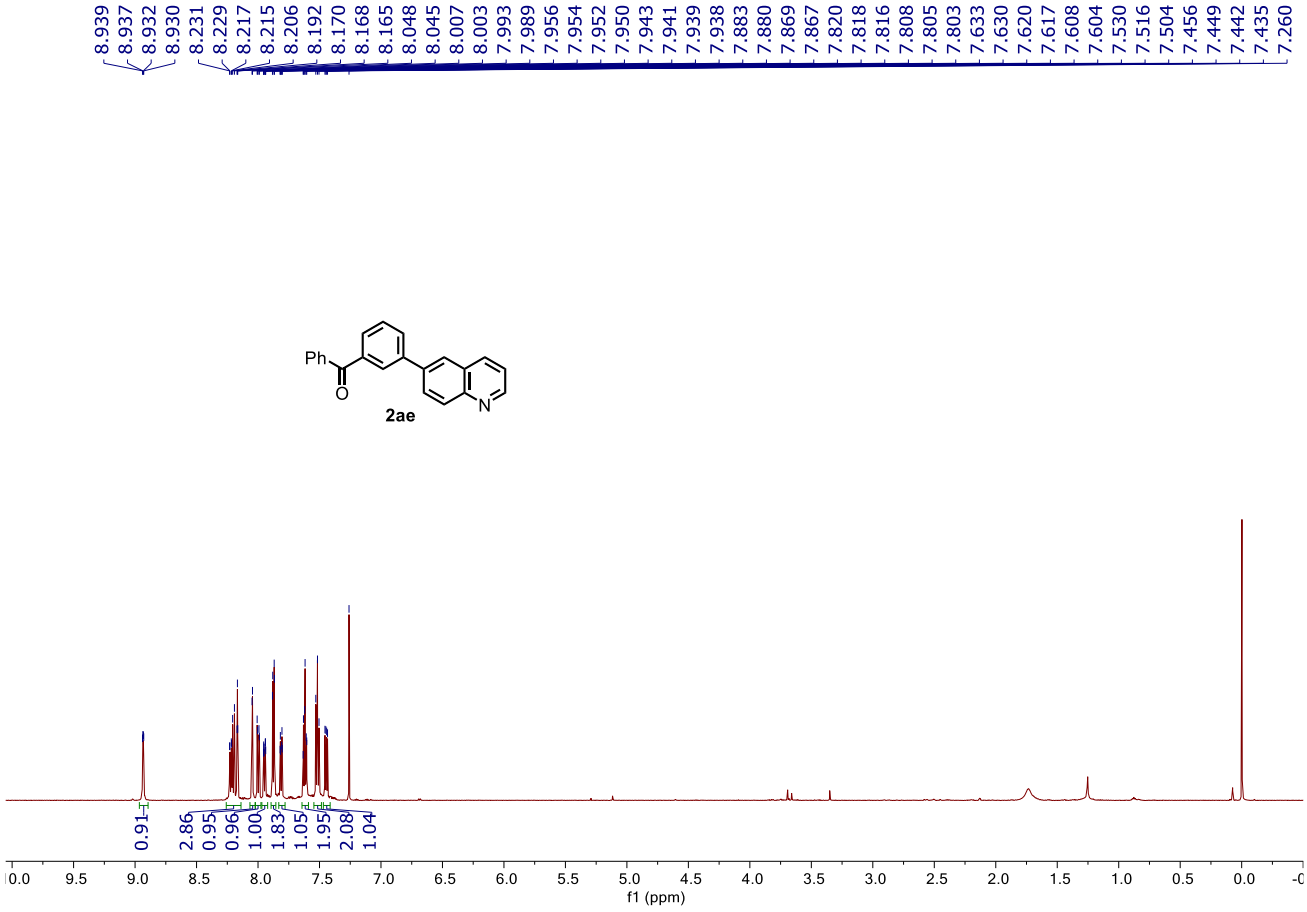

174.03
168.44
157.77
152.57
150.26
148.34
146.56
141.60
141.56
132.15
131.87
131.15
131.13
130.58
130.54
129.19
129.02
128.14
128.07
126.89
118.79
98.22
77.33
77.12
76.91
72.89
66.48
52.20
50.20
31.75
7.95
CO2Me
N
O
O
Et
OH
O
2ac
f1 (ppm)


8.965
8.962
8.957
8.955
8.184
8.181
8.172
8.167
8.158
7.970
7.968
7.957
7.955
7.784
7.781
7.695
7.693
7.683
7.681
7.670
7.667
7.663
7.652
7.649
7.570
7.568
7.557
7.555
7.545
7.542
7.533
7.530
7.461
7.454
7.448
7.440
7.265


NO2
N
2ad


1.00
2.03
0.99
1.02
2.09
2.07
1.04
f1 (ppm)


151.08
149.25
147.82
136.36
135.99
135.86
132.70
132.34
129.96
129.65
128.76
128.22
126.87
124.50
121.81
77.33
77.12
76.91
NO2
N
2ad
f1 (ppm)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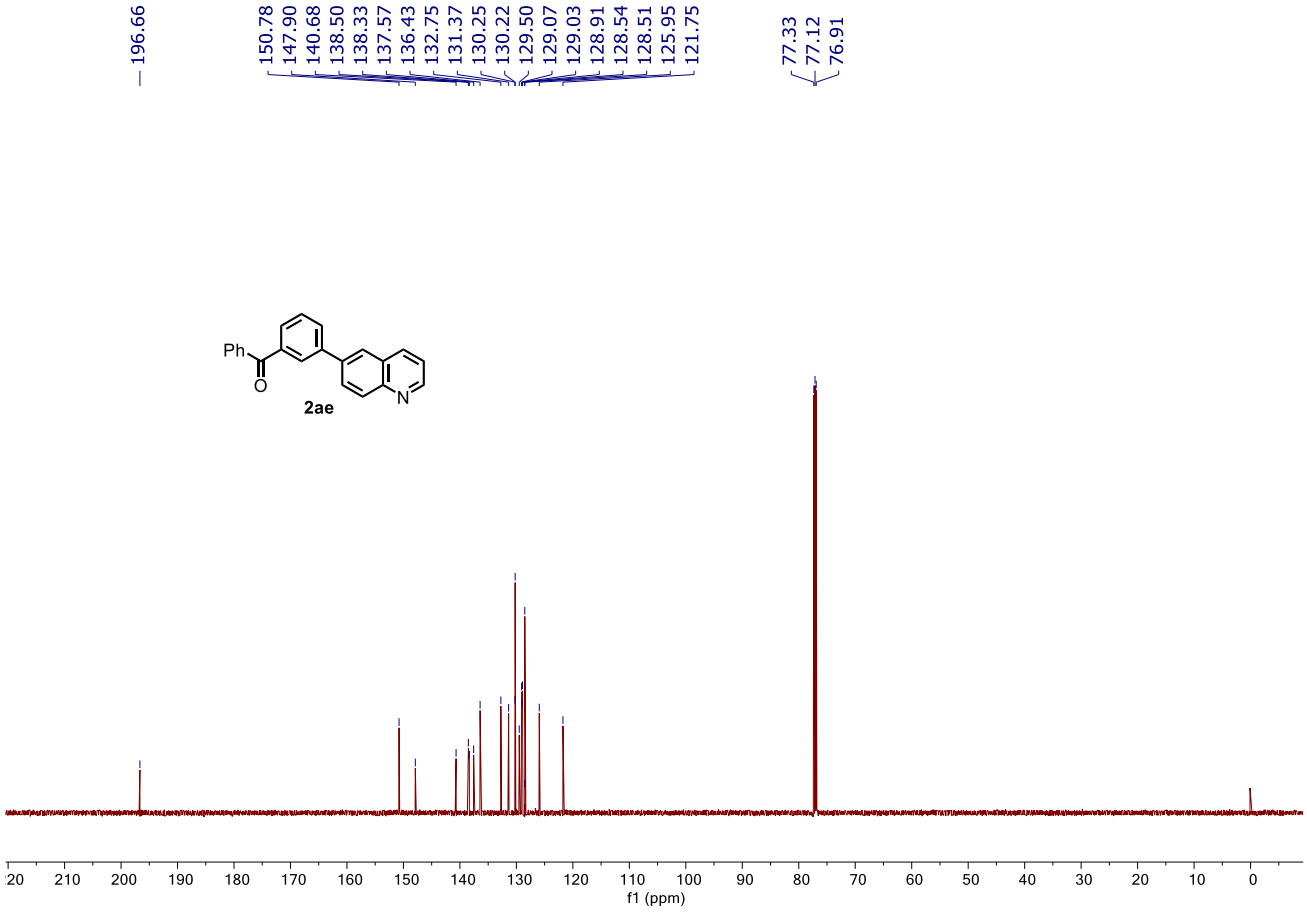
8.937
8.932
8.930
8.231
8.229
8.217
8.215
8.206
8.192
8.170
8.168
8.165
8.048
8.045
8.007
8.003
7.993
7.989
7.956
7.954
7.952
7.950
7.943
7.941
7.939
7.938
7.883
7.880
7.869
7.867
7.820
7.818
7.816
7.808
7.805
7.803
7.633
7.630
7.620
7.617
7.608
7.604
7.530
7.516
7.504
7.456
7.449
7.442
7.435
7.260
Ph
O
N
2ae
0.91
2.86
0.95
0.96
1.00
1.83
1.05
1.95
2.08
1.04
f1 (ppm)


196.66
150.78
147.90
140.68
138.50
138.33
137.57
136.43
132.75
131.37
130.25
130.22
129.50
129.07
129.03
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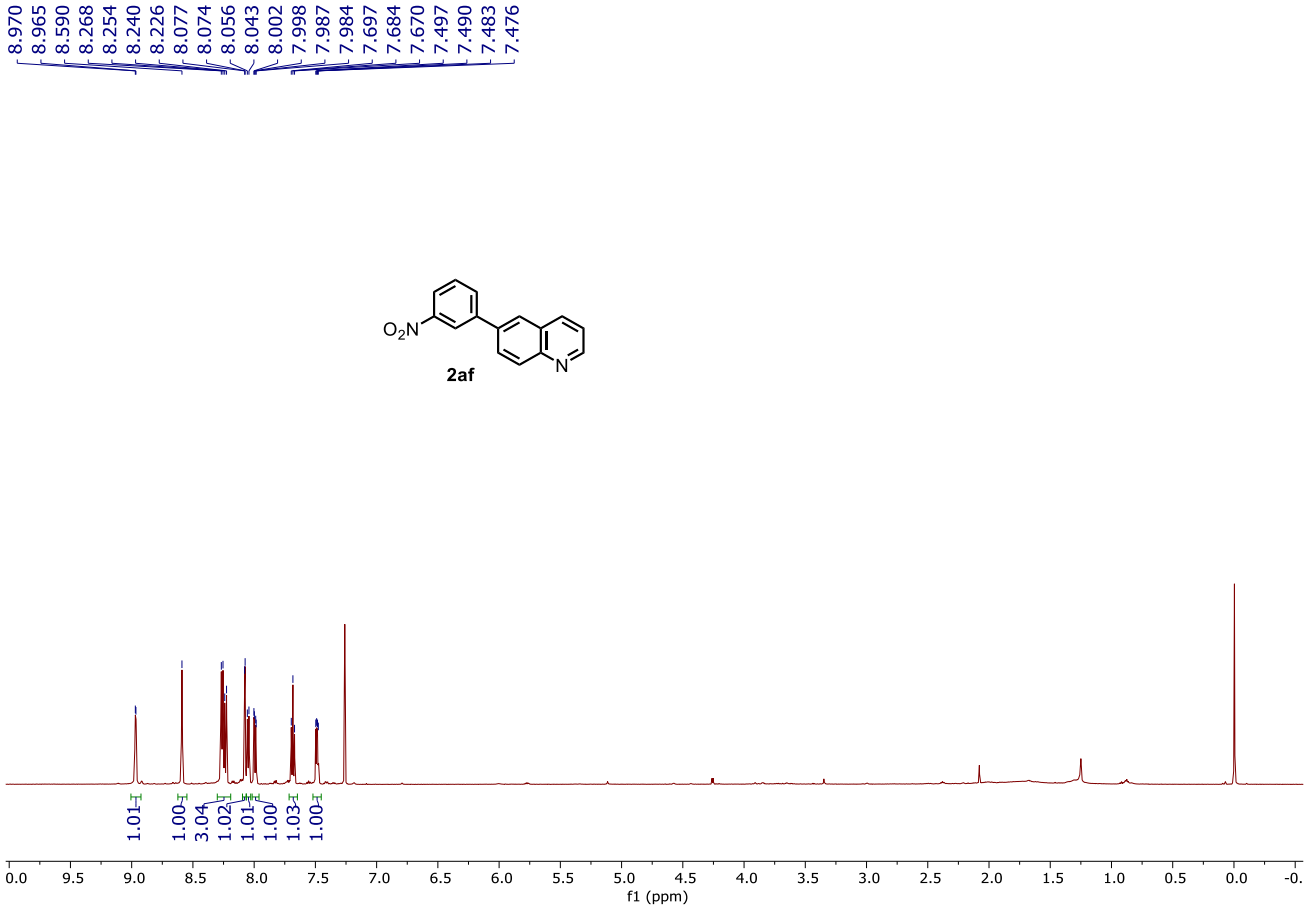
77.12
76.91
Ph
O
N
2ae
f1 (ppm)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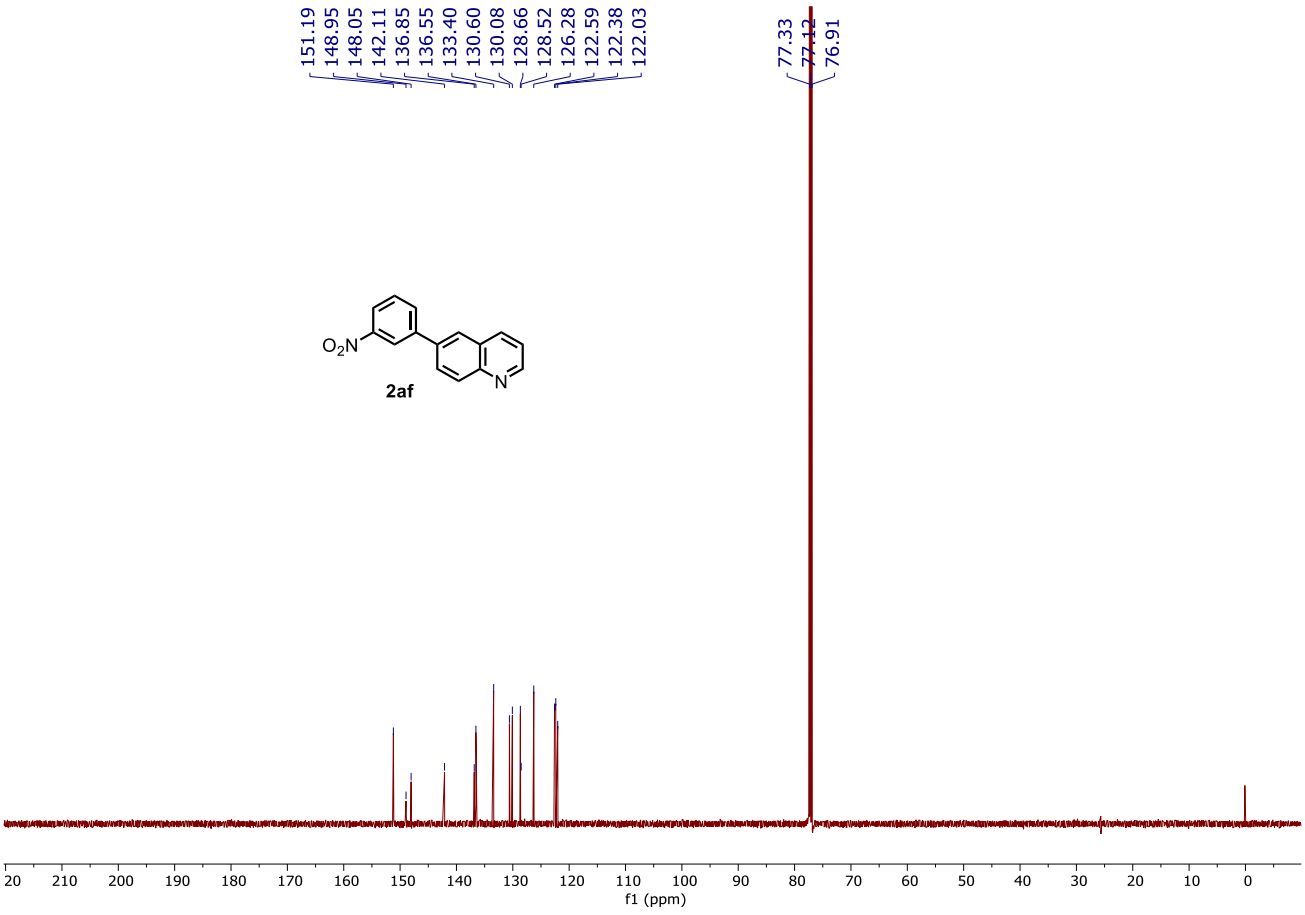
8.254
8.240
8.226
8.077
8.074
8.056
8.043
8.002
7.998
7.987
7.984
7.697
7.684
7.670
7.497
7.490
7.483
7.476
O2N
N
2af
1.01
1.00
3.04
1.02
1.01
1.00
1.03
1.00
f1 (ppm)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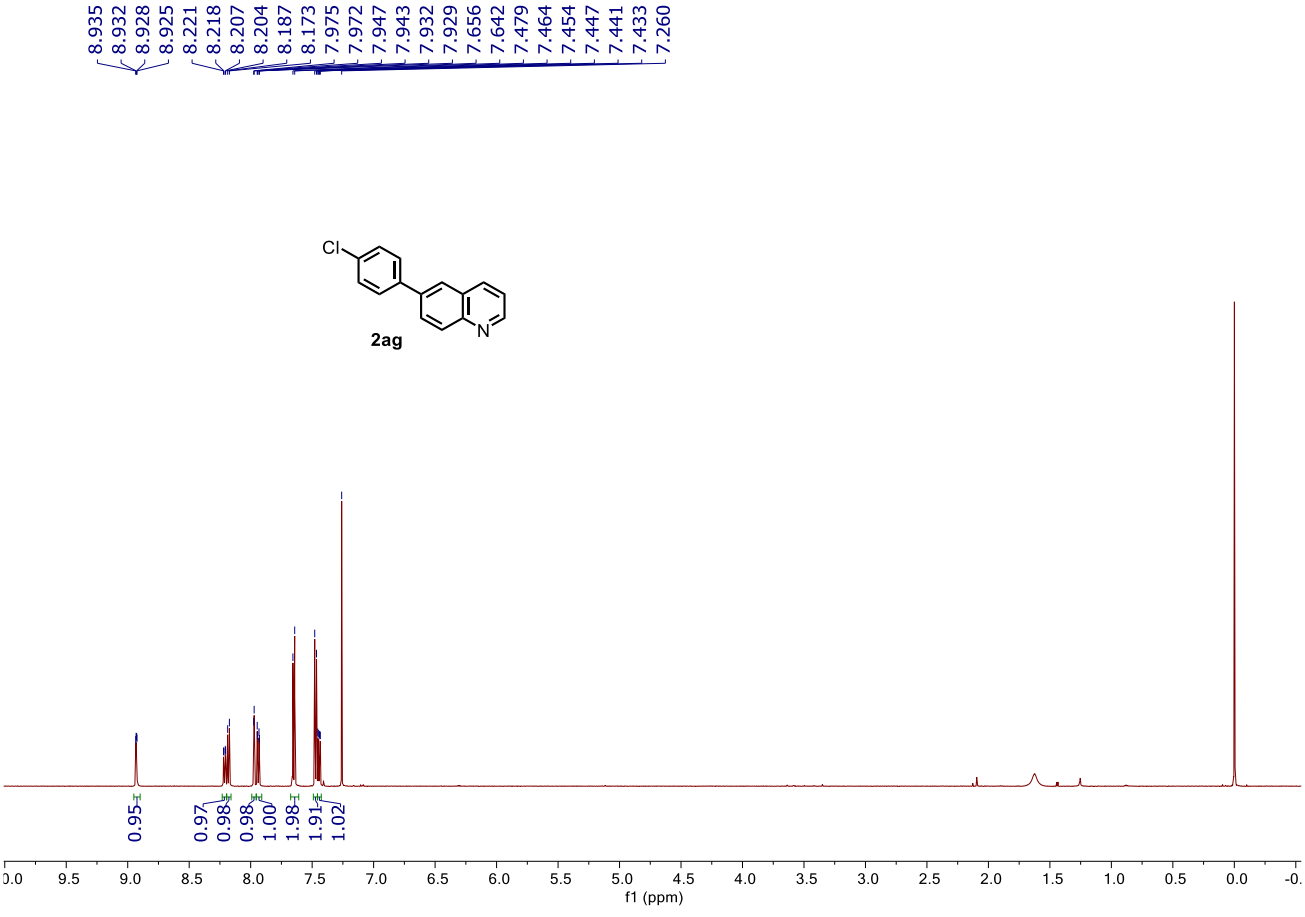
148.95
148.05
142.11
136.85
136.55
133.40
130.60
130.08
128.66
128.52
126.28
122.59
122.38
122.03
77.33
77.12
76.91
O2N
N
2af
f1 (ppm)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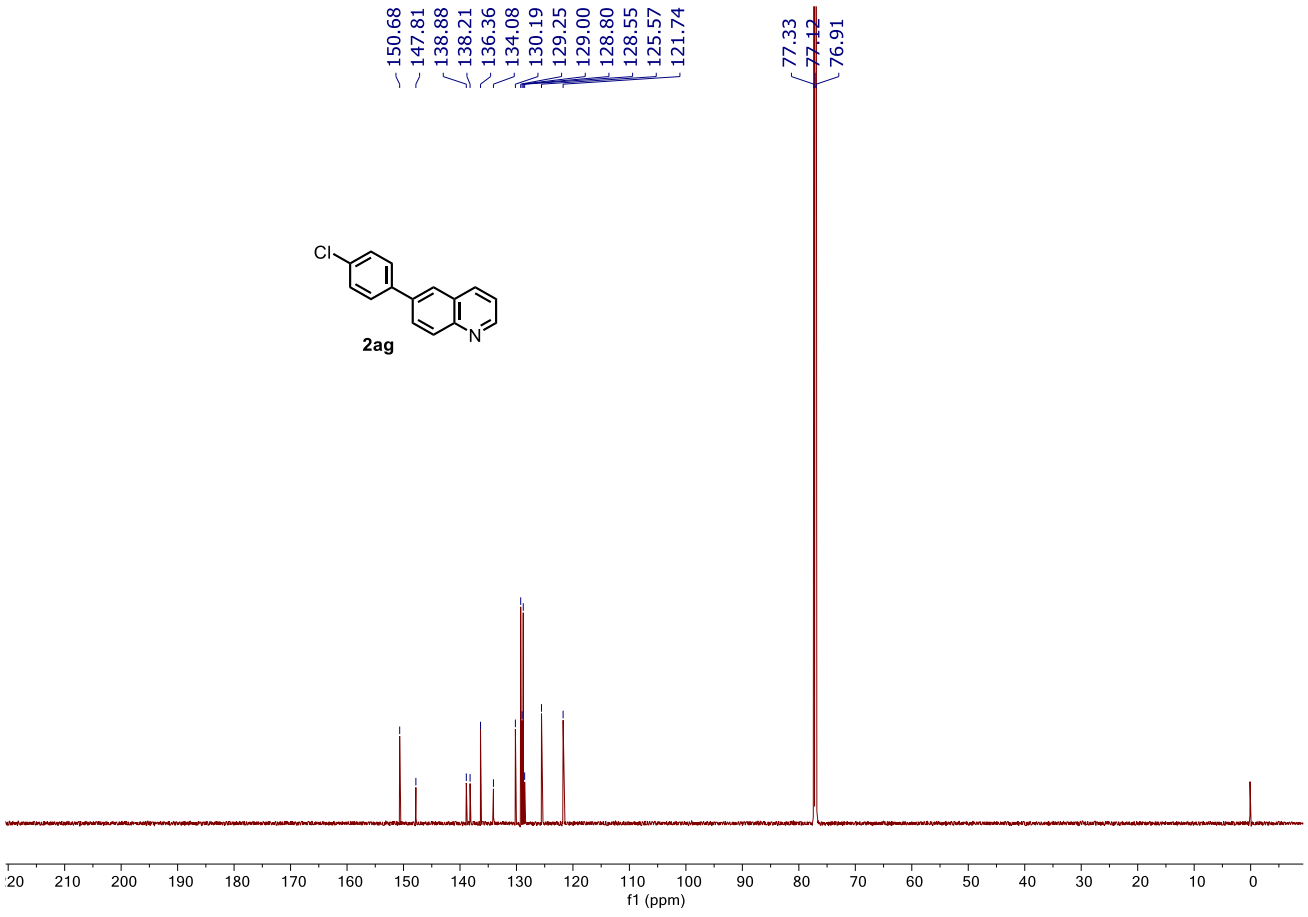
8.932
8.928
8.925
8.221
8.218
8.207
8.204
8.187
8.173
7.975
7.972
7.947
7.943
7.932
7.929
7.656
7.642
7.479
7.464
7.454
7.447
7.441
7.433
7.260
Cl
N
2ag
0.95
0.97
0.98
0.98
1.00
1.98
1.91
1.02
f1 (ppm)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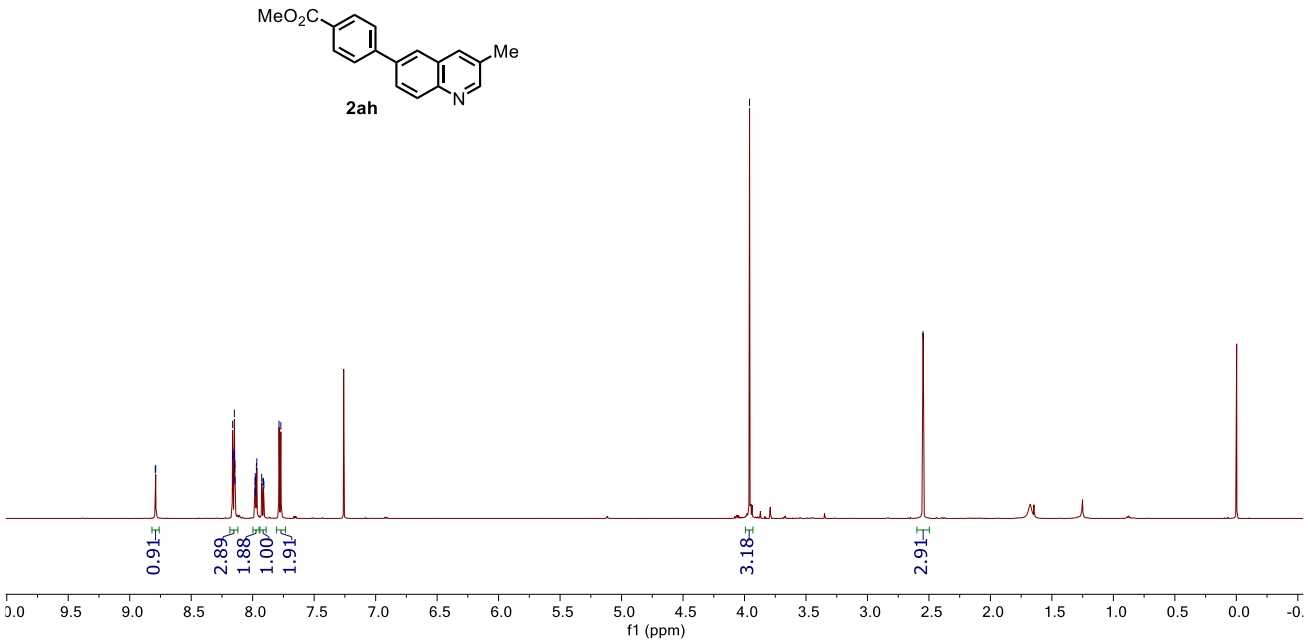
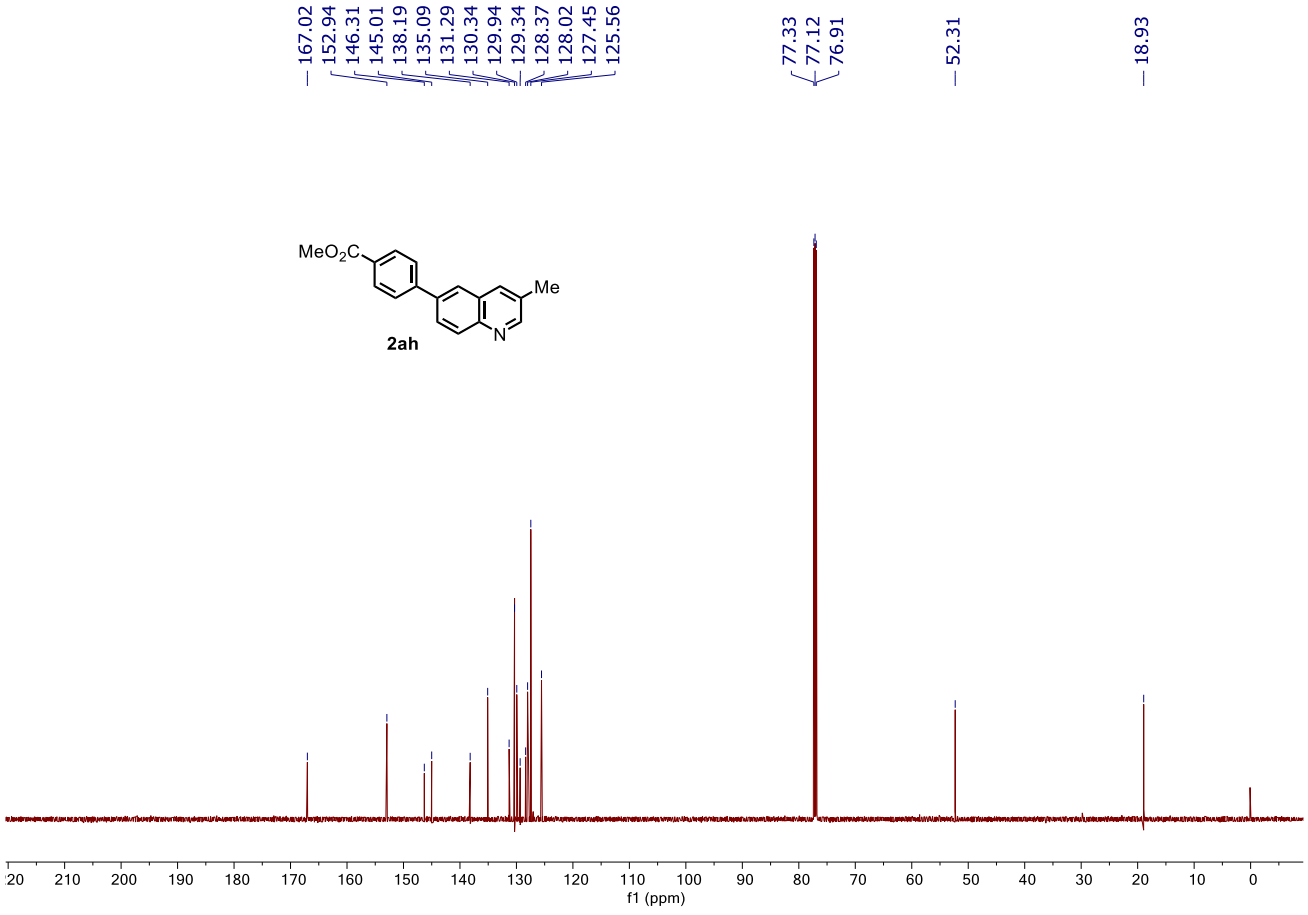
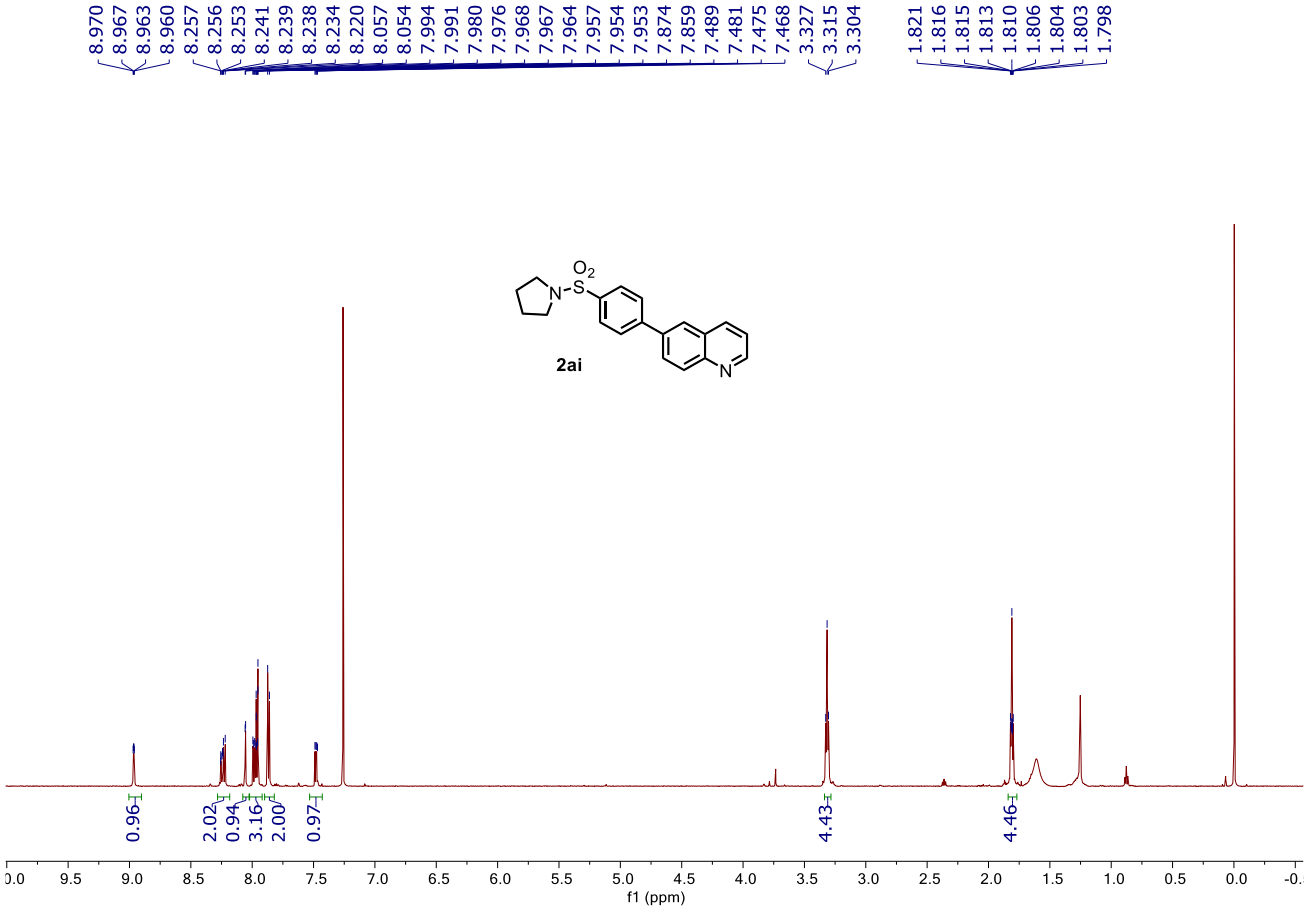
138.21
136.36
134.08
130.19
129.25
129.00
128.80
128.55
125.57
121.74
77.33
77.12
76.91
Cl
N
2ag
f1 (ppm)


8.792
8.789
8.163
8.162
8.160
8.152
8.150
8.149
8.146
8.145
8.144
7.983
7.981
7.979
7.977
7.975
7.970
7.966
7.927
7.923
7.912
7.909
7.786
7.771
3.959
2.548


MeO2C
Me
N
2ah
0.91
2.89
1.88
1.00
1.91
3.18
2.91
f1 (ppm)


167.02
152.94
146.31
145.01
138.19
135.09
131.29
130.34
129.94
129.34
128.37
128.02
127.45
125.56
77.33
77.12
76.91
52.31
18.93
MeO2C
Me
N
2ah
f1 (ppm)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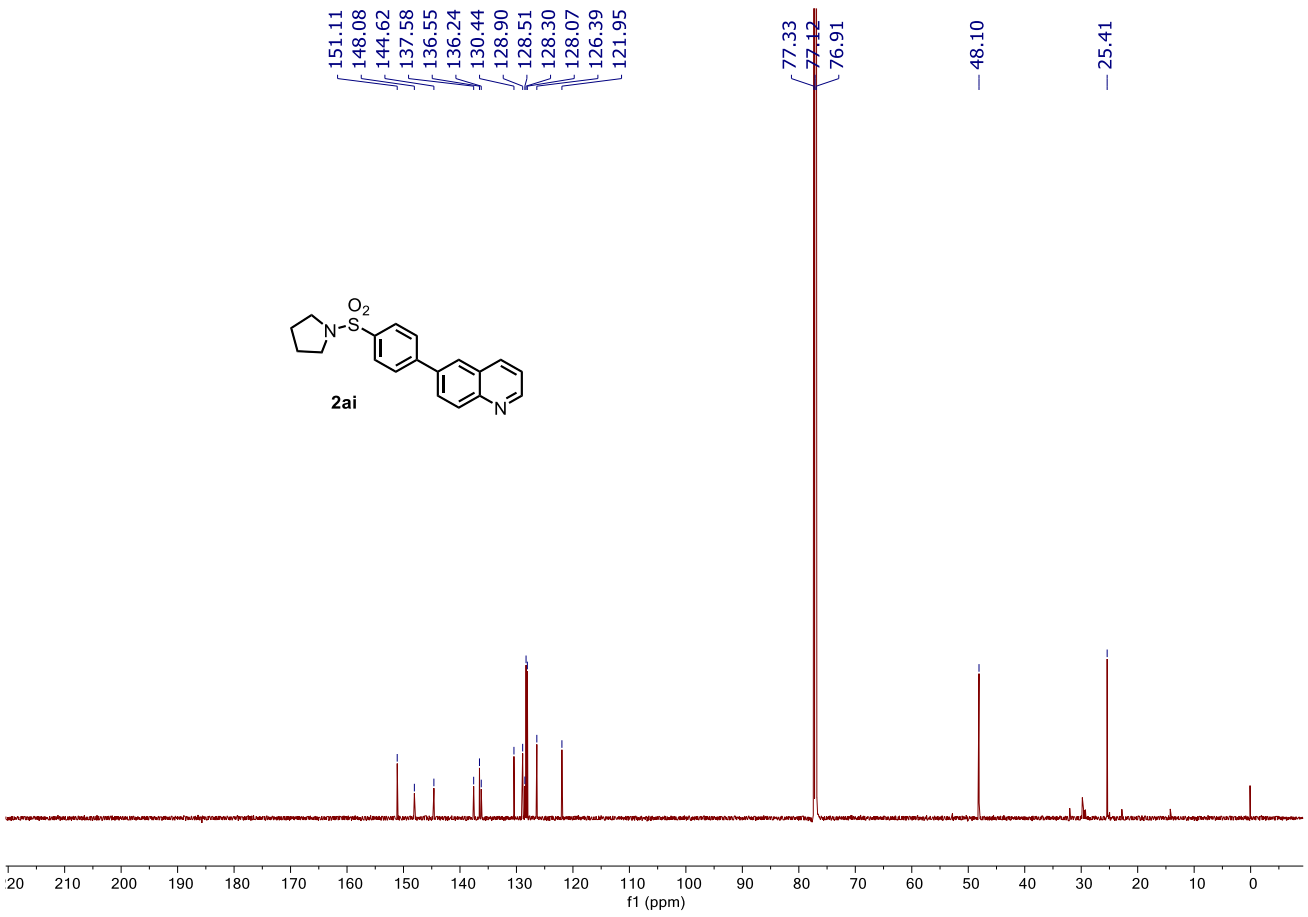
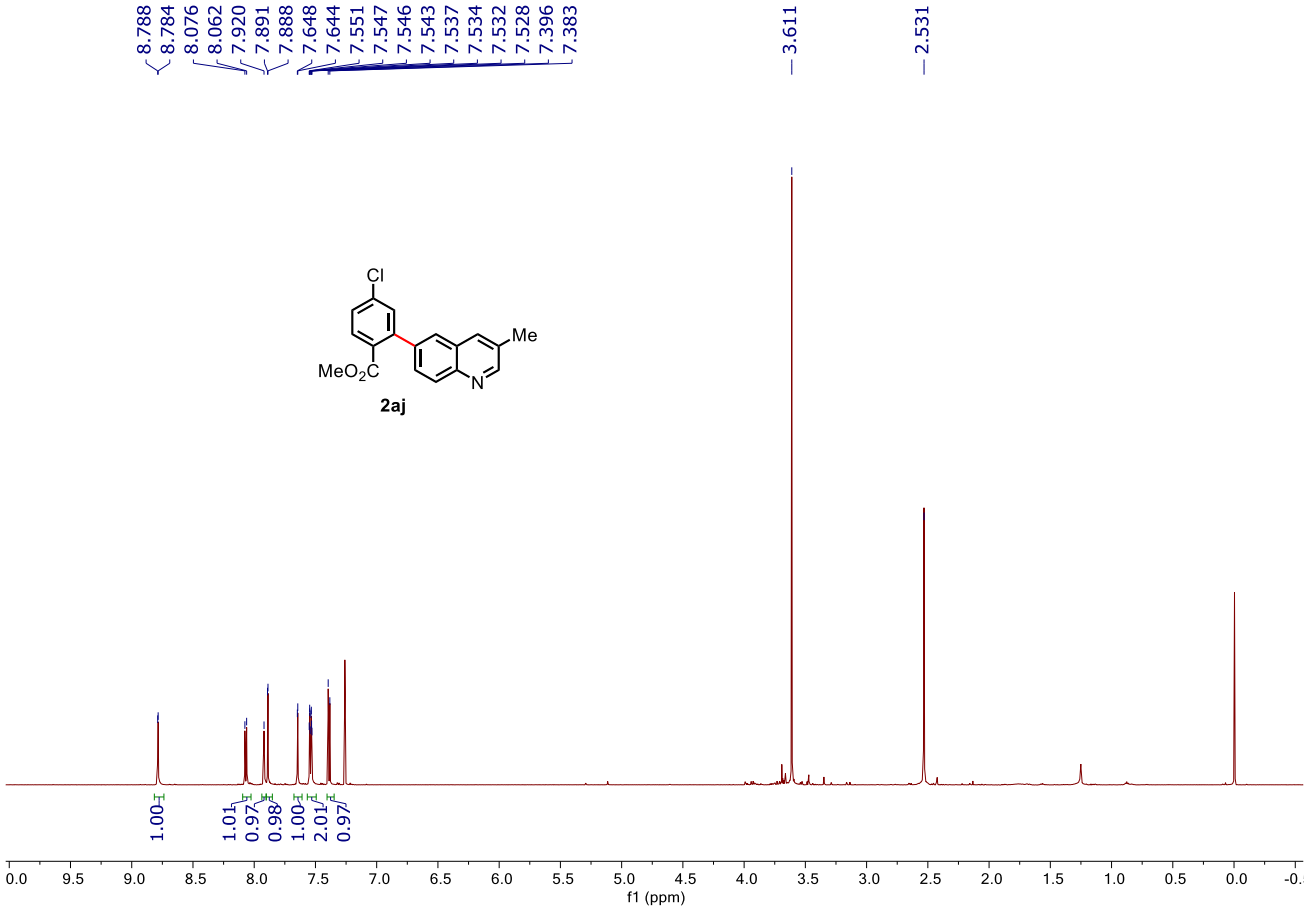
8.967
8.963
8.960
8.257
8.256
8.253
8.241
8.239
8.238
8.234
8.220
8.057
8.054
7.994
7.991
7.980
7.976
7.968
7.967
7.964
7.957
7.954
7.953
7.874
7.859
7.489
7.481
7.475
7.468
3.327
3.315
3.304
1.821
1.816
1.815
1.813
1.810
1.806
1.804
1.803
1.798
O2
N
S
N
2ai
0.96
2.02
0.94
3.16
2.00
0.97
4.43
4.46
f1 (ppm)


151.11
148.08
144.62
137.58
136.55
136.24
130.44
128.90
128.51
128.30
128.07
126.39
121.95
77.33
77.12
76.91
48.10
25.41
O2
N
S
N
2ai
f1 (ppm)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8.062
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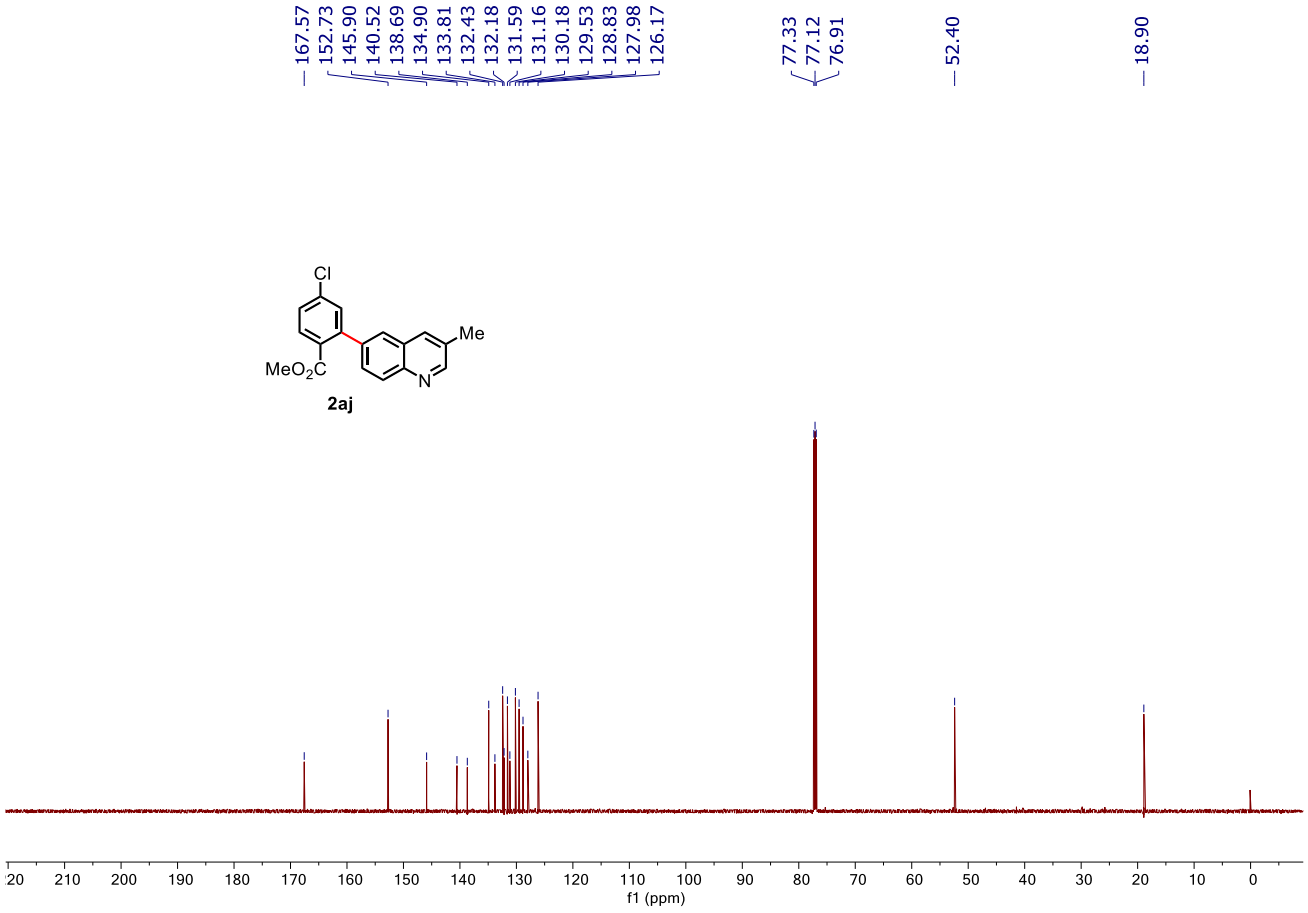
7.891
7.888
7.648
7.644
7.551
7.547
7.546
7.543
7.537
7.534
7.532
7.528
7.396
7.383
3.611
2.531
Cl
Me
MeO2C
N
2aj
1.00
1.01
0.97
0.98
1.00
2.01
0.97
f1 (ppm)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138.69
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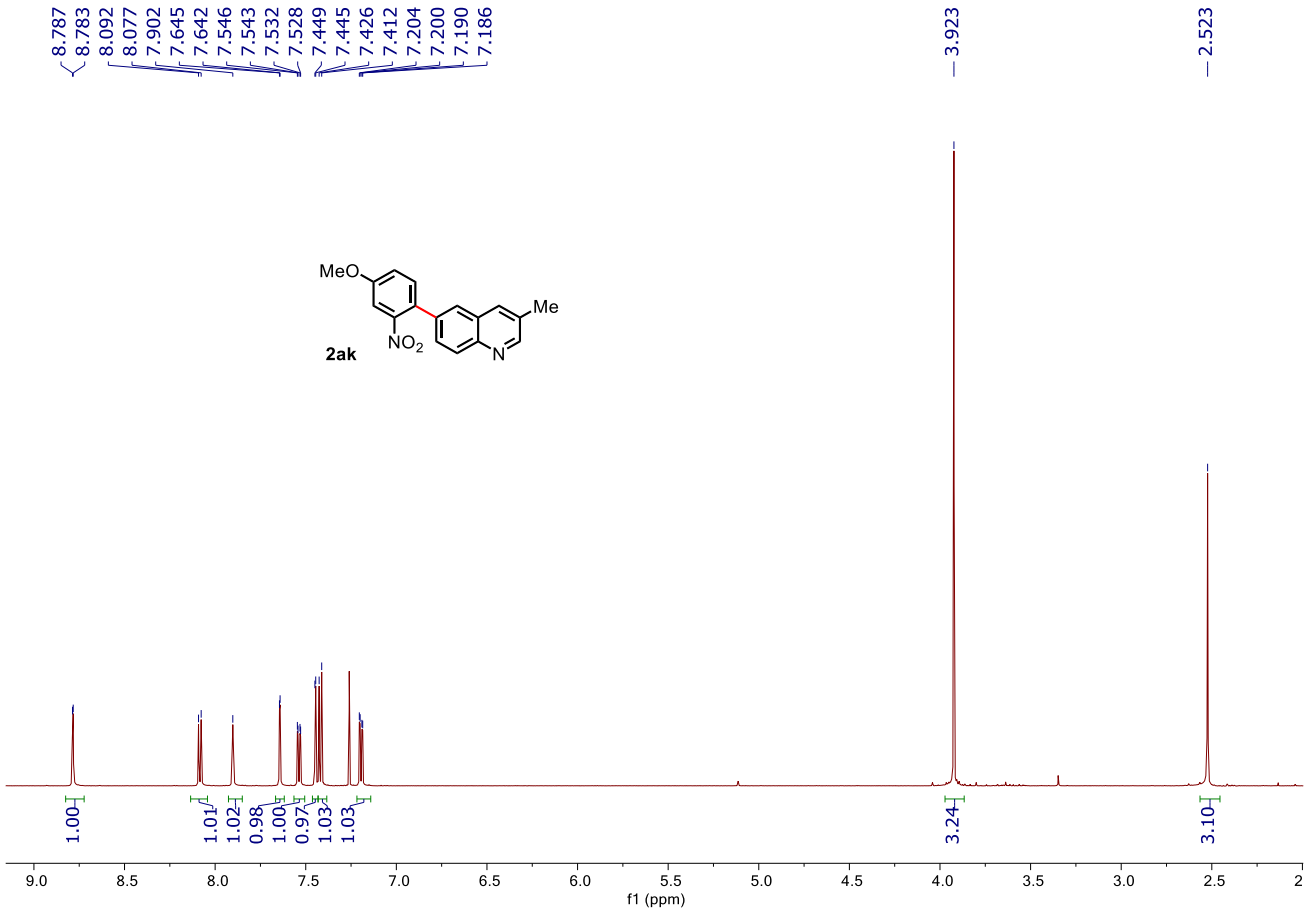
133.81
132.43
132.18
131.59
131.16
130.18
129.53
128.83
127.98
126.17
77.33
77.12
76.91
52.40
18.90
Cl
MeO2C
Me
N
2aj
f1 (ppm)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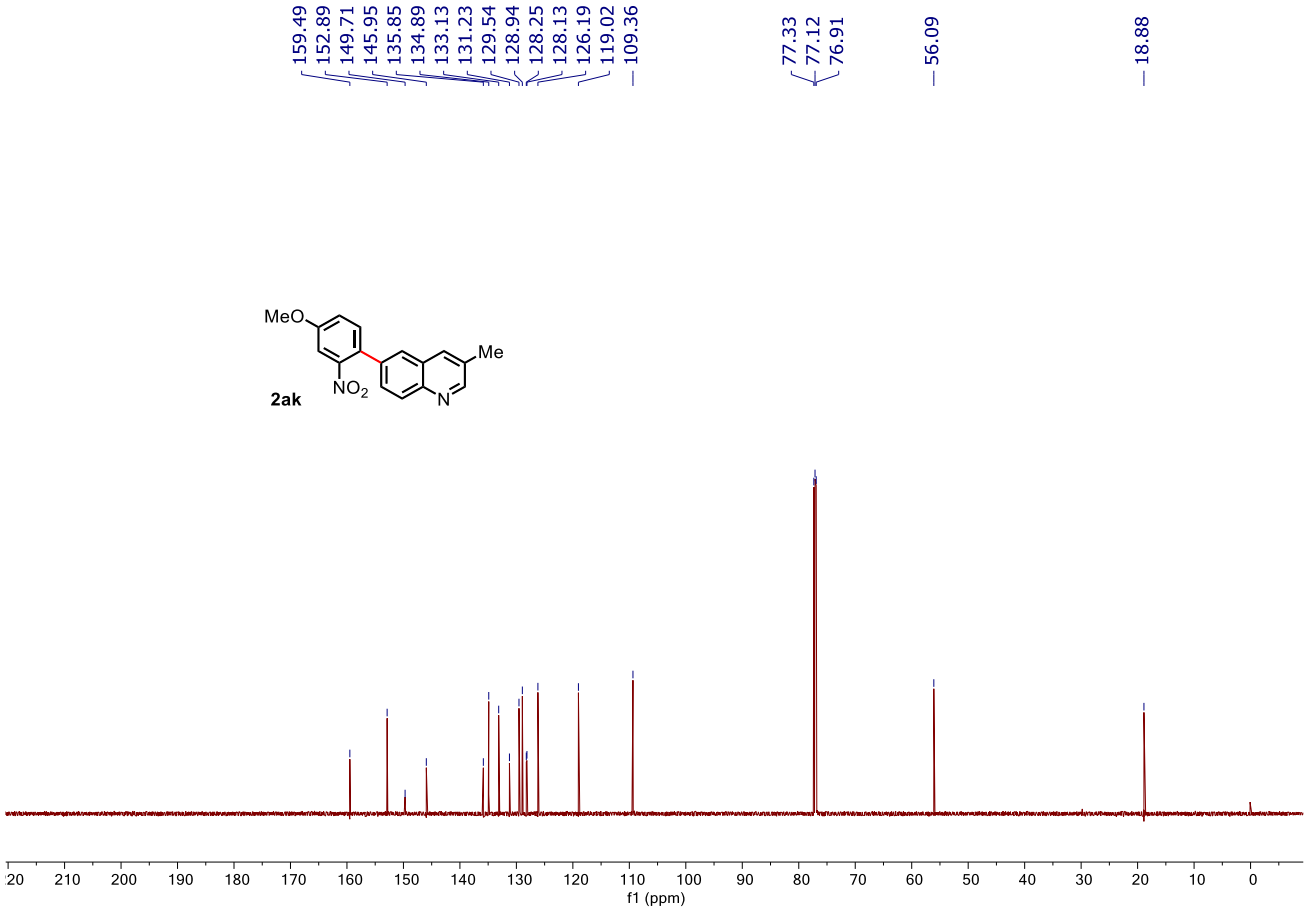
7.546
7.543
7.532
7.528
7.449
7.445
7.426
7.412
7.204
7.200
7.190
7.186
3.923
2.523
MeO
NO2
Me
N
2ak
1.00
1.01
1.02
0.98
1.00
0.97
1.03
1.03
3.24
3.10
f1 (ppm)


159.49
152.89
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134.89
133.13
131.23
129.54
128.94
128.25
128.13
126.19
119.02
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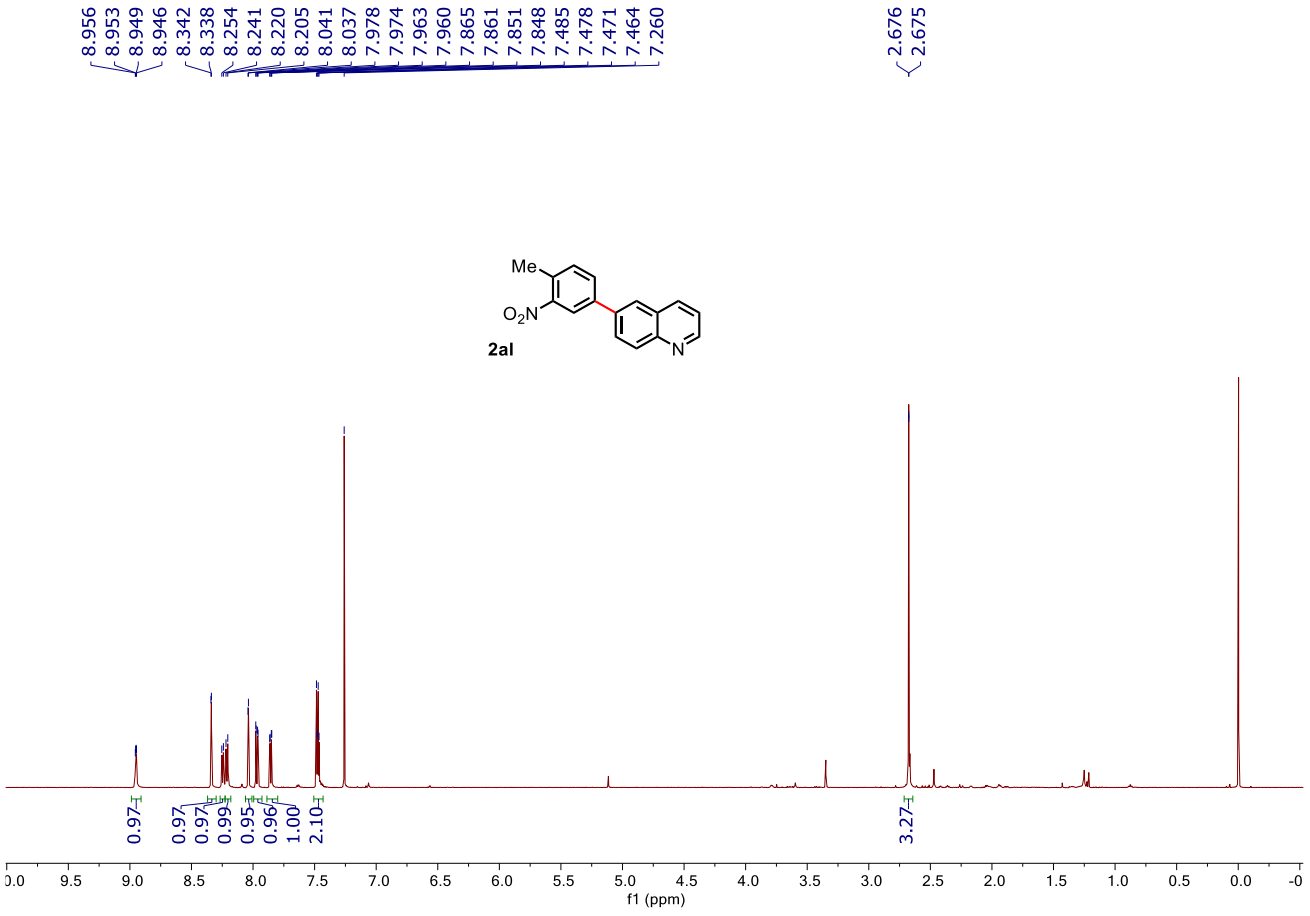
77.33
77.12
76.91
56.09
18.88
MeO
Me
NO2
N
2ak
f1 (ppm)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8.241
8.220
8.205
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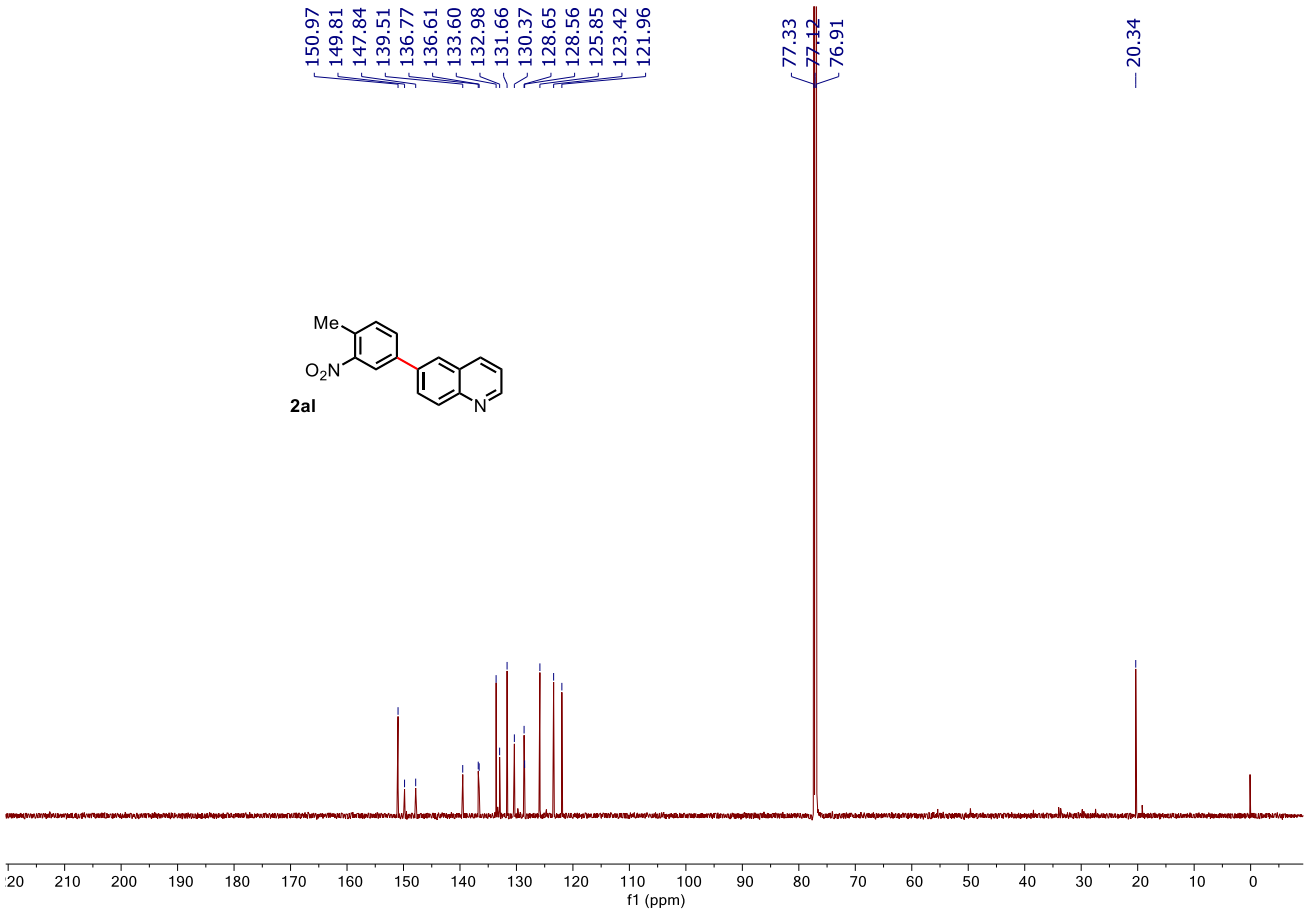
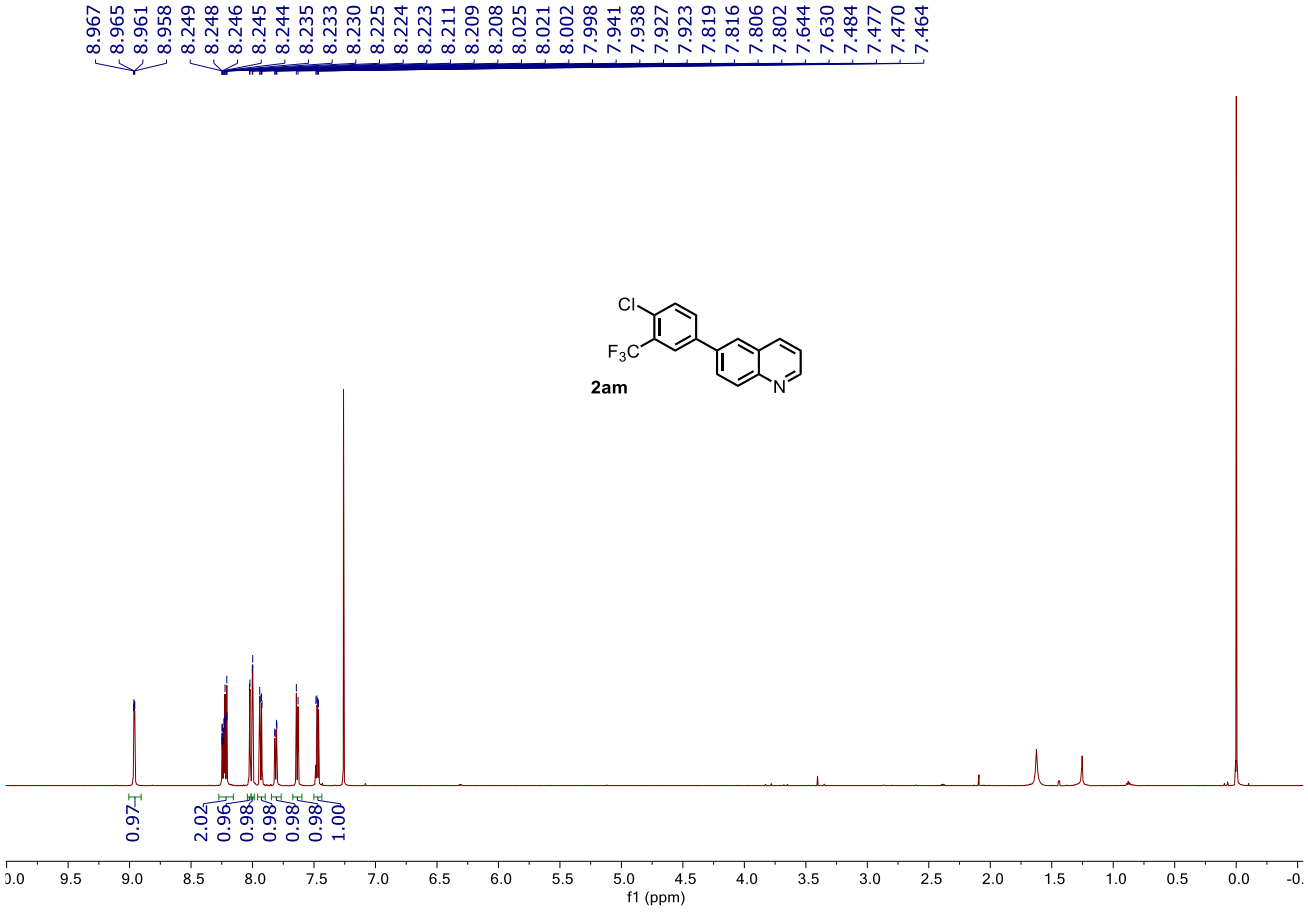
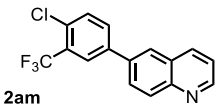
8.037
7.978
7.974
7.963
7.960
7.865
7.861
7.851
7.848
7.485
7.478
7.471
7.464
7.260
2.676
2.675
Me
O2N
N
2al
0.97
0.97
0.97
0.99
0.95
0.96
1.00
2.10
3.27
f1 (ppm)


150.97
149.81
147.84
139.51
136.77
136.61
133.60
132.98
131.66
130.37
128.65
128.56
125.85
123.42
121.96
77.33
77.12
76.91
20.34
Me
O2N
2al
f1 (ppm)


8.967
8.965
8.961
8.958
8.249
8.248
8.246
8.245
8.244
8.235
8.233
8.230
8.225
8.224
8.223
8.211
8.209
8.208
8.025
8.021
8.002
7.998
7.941
7.938
7.927
7.923
7.819
7.816
7.806
7.802
7.644
7.630
7.484
7.477
7.470
7.464
Cl
F3C
2am
0.97
2.02
0.96
0.98
0.98
0.98
0.98
1.00
f1 (ppm)

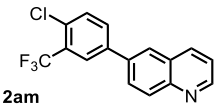

151.14
148.03
139.41
136.84
136.42
132.19
131.88
131.87
131.85
131.84
131.63
130.62
129.41
129.21
129.00
128.79
128.60
128.51
126.61
126.58
126.54
126.51
125.99
125.64
123.83
122.02
121.99
120.21
77.33
77.12
76.91


Cl
F3C
N

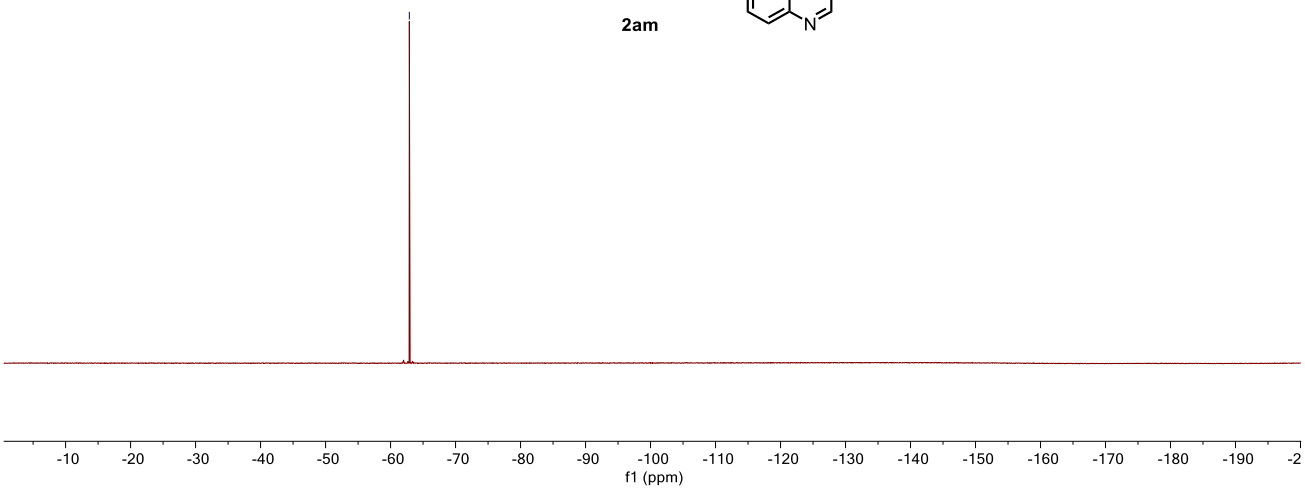
2am

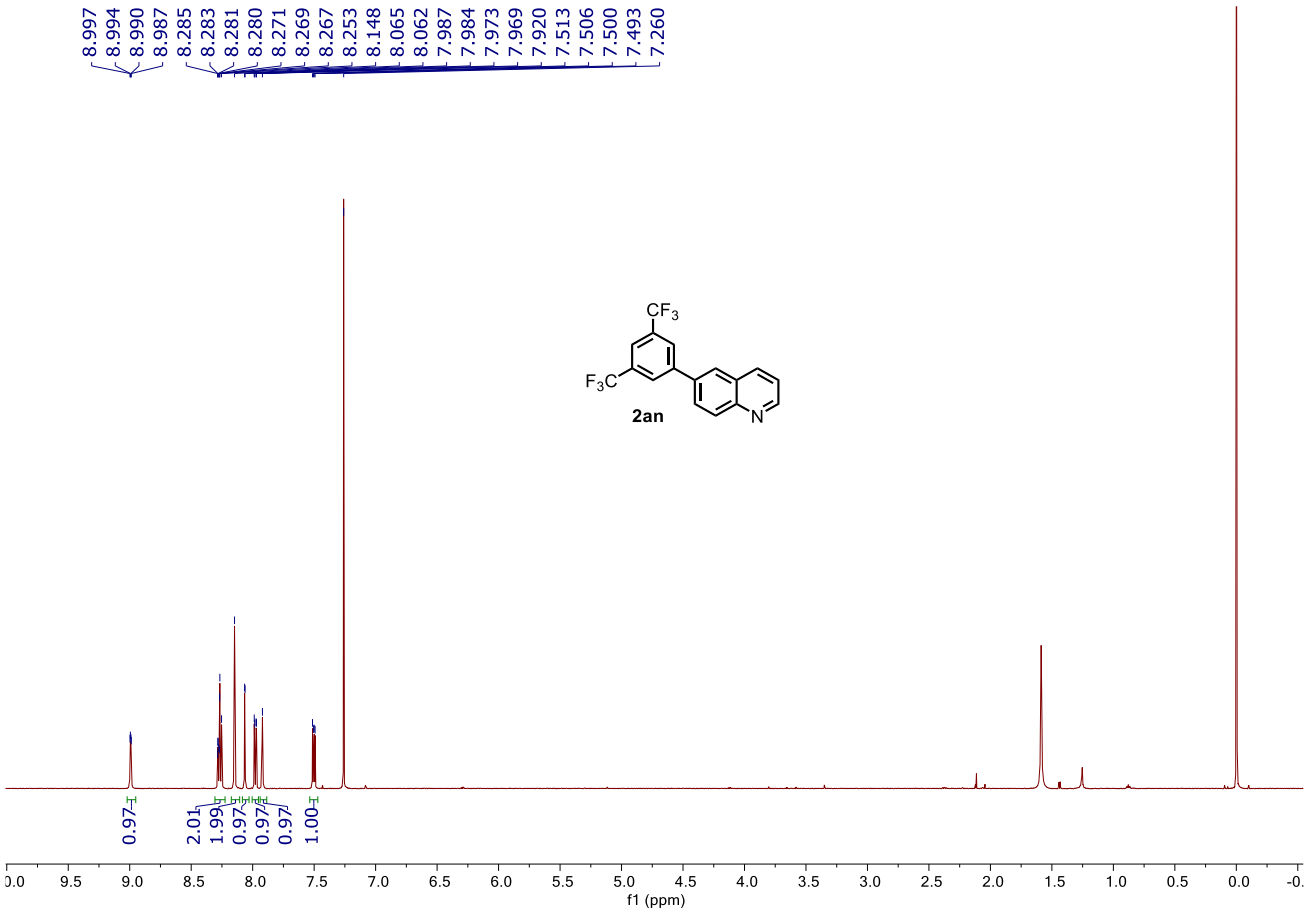
20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

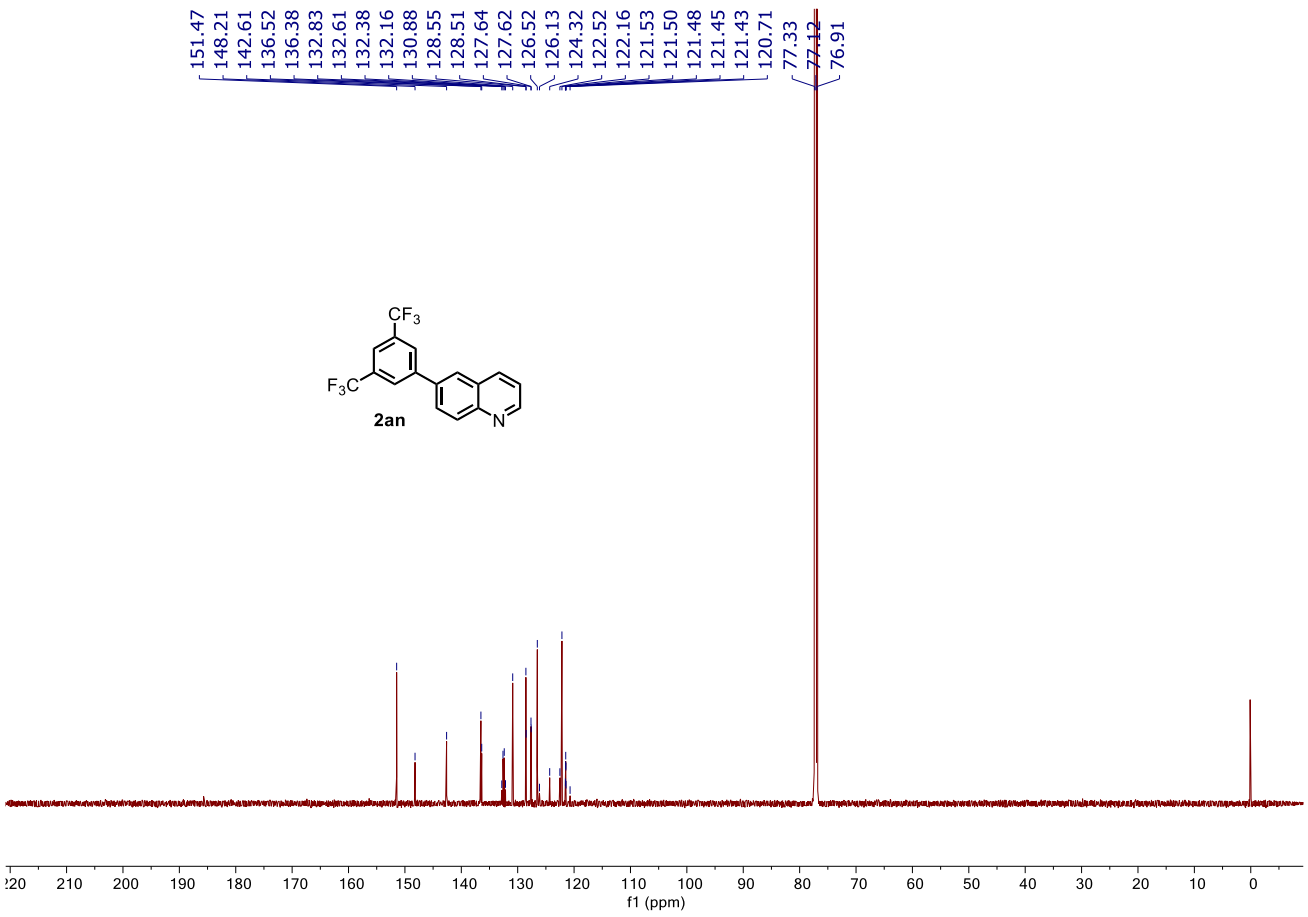

-62.885

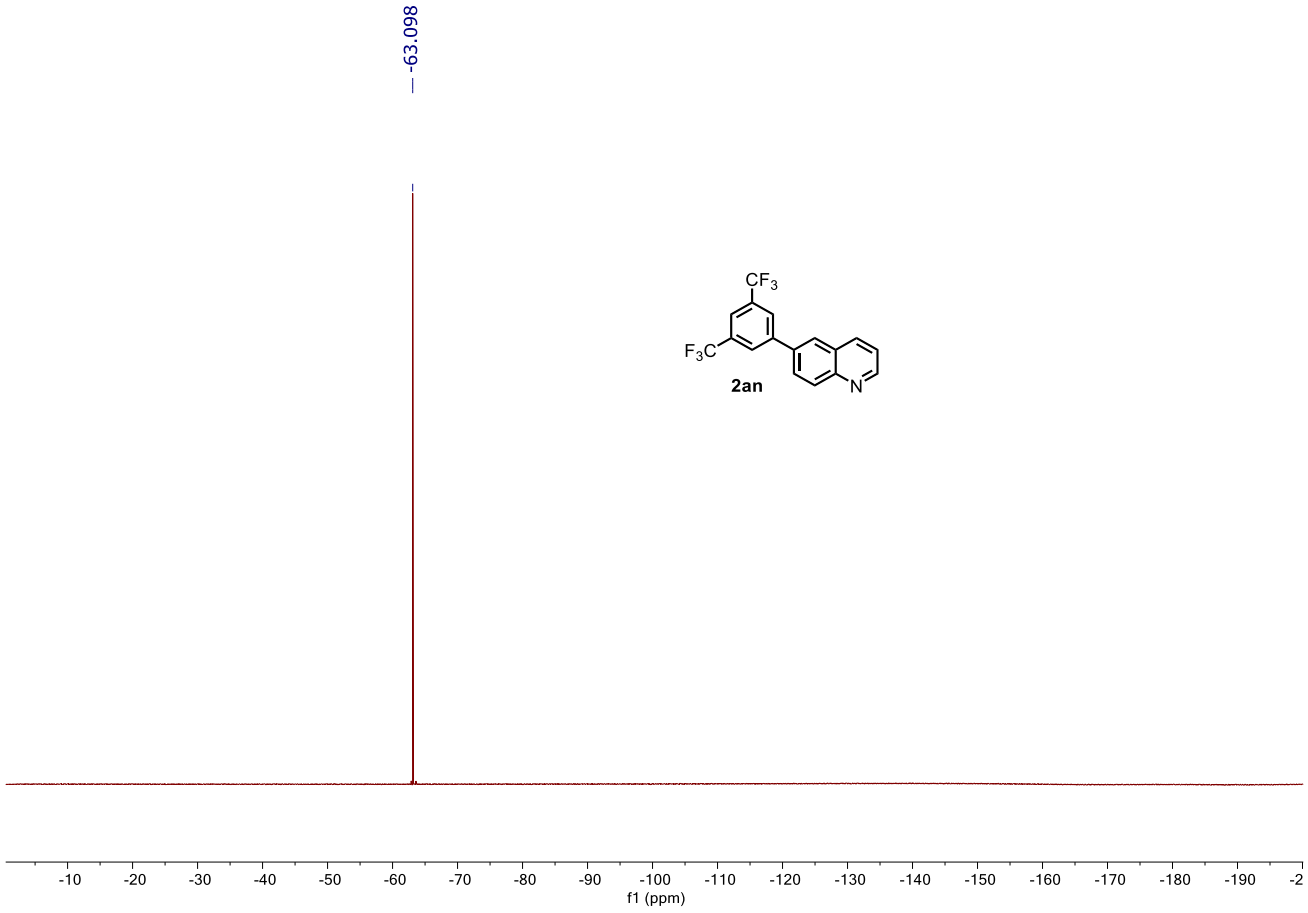

Cl
F3C
N

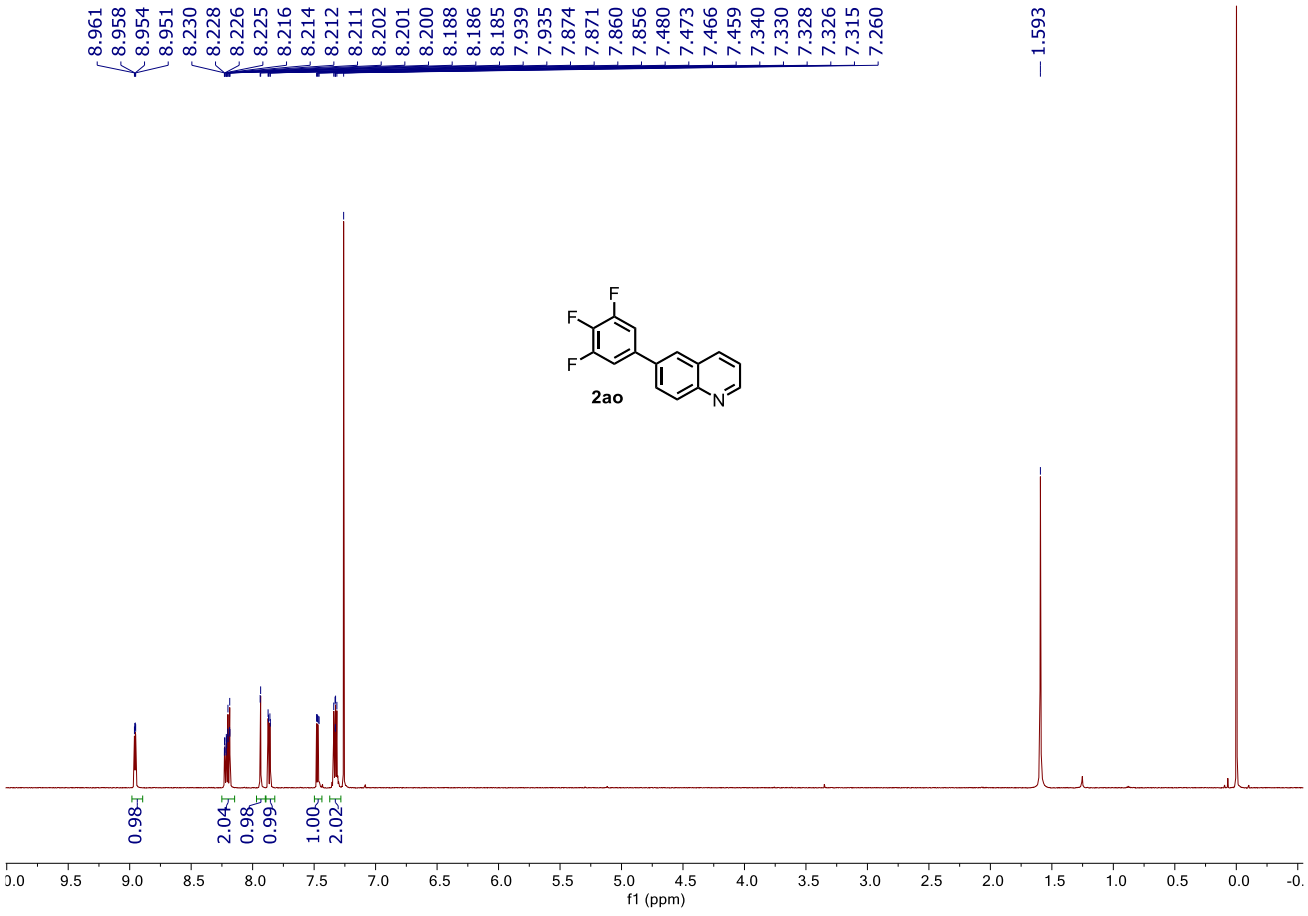
2am

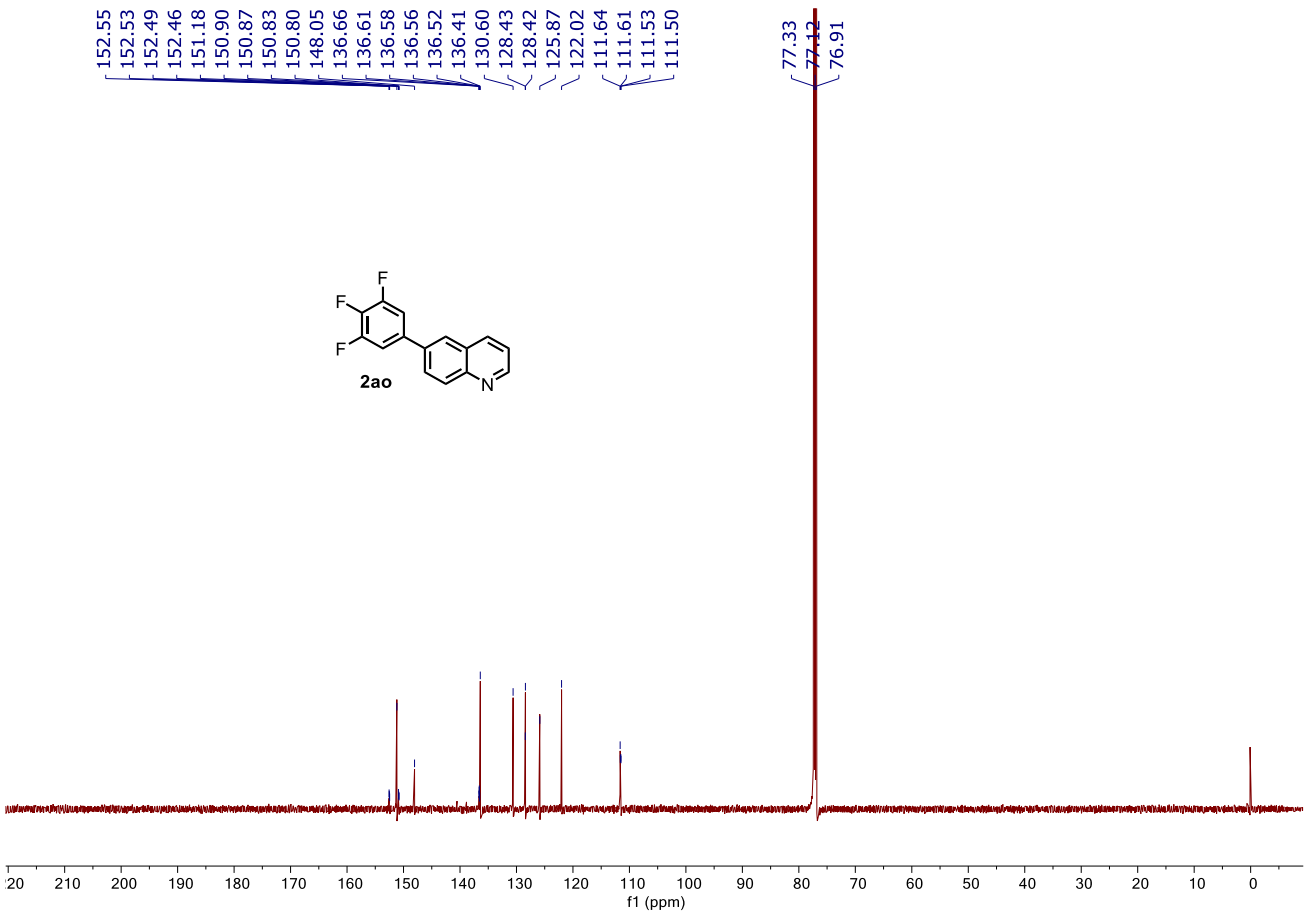

-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-2
f1 (ppm)

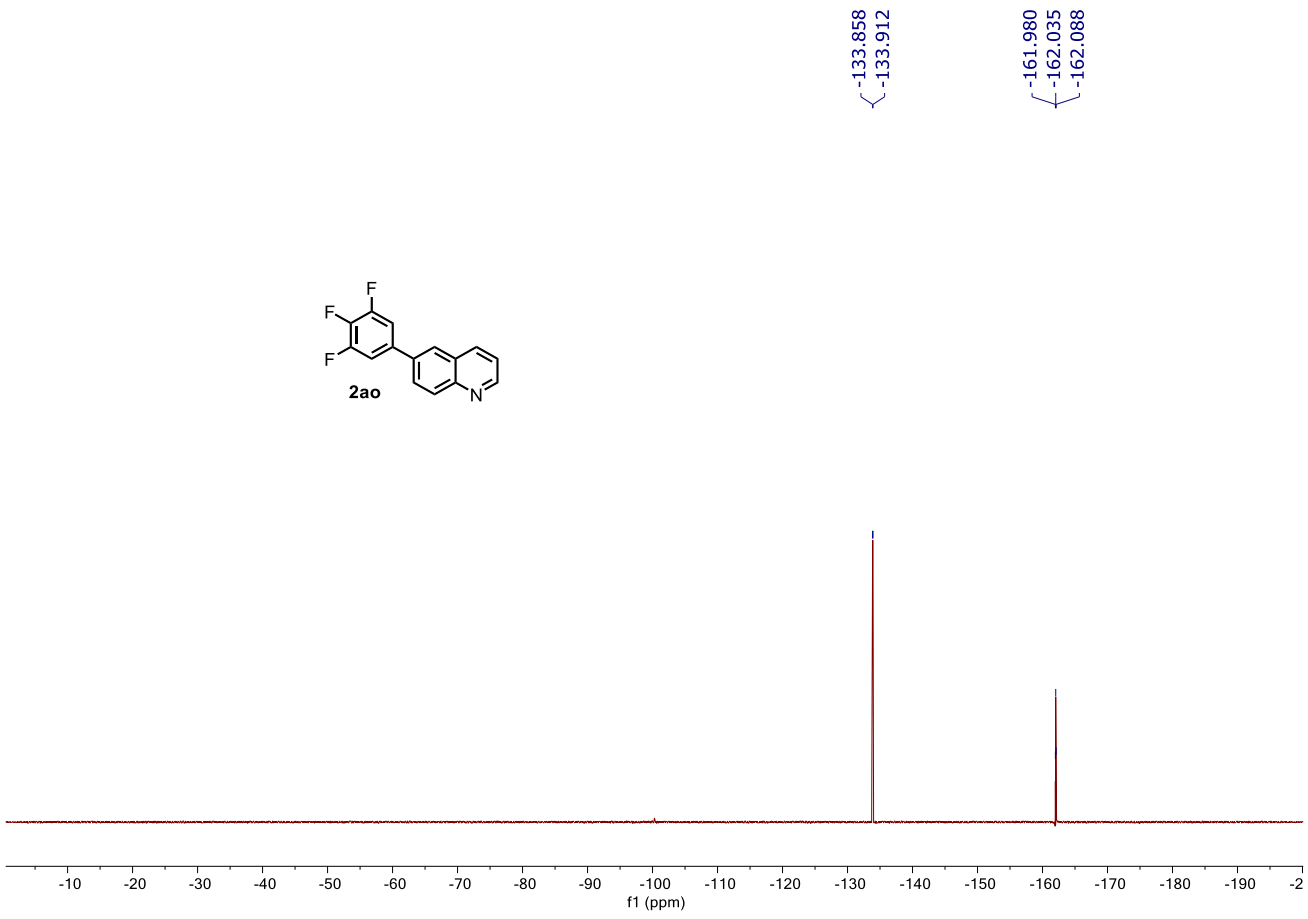

8.997
8.994
8.990
8.987
8.285
8.283
8.281
8.280
8.271
8.269
8.267
8.253
8.148
8.065
8.062
7.987
7.984
7.973
7.969
7.920
7.513
7.506
7.500
7.493
7.260
CF3
F3C
N
2an
0.97
2.01
1.99
0.97
0.97
0.97
1.00
f1 (ppm)

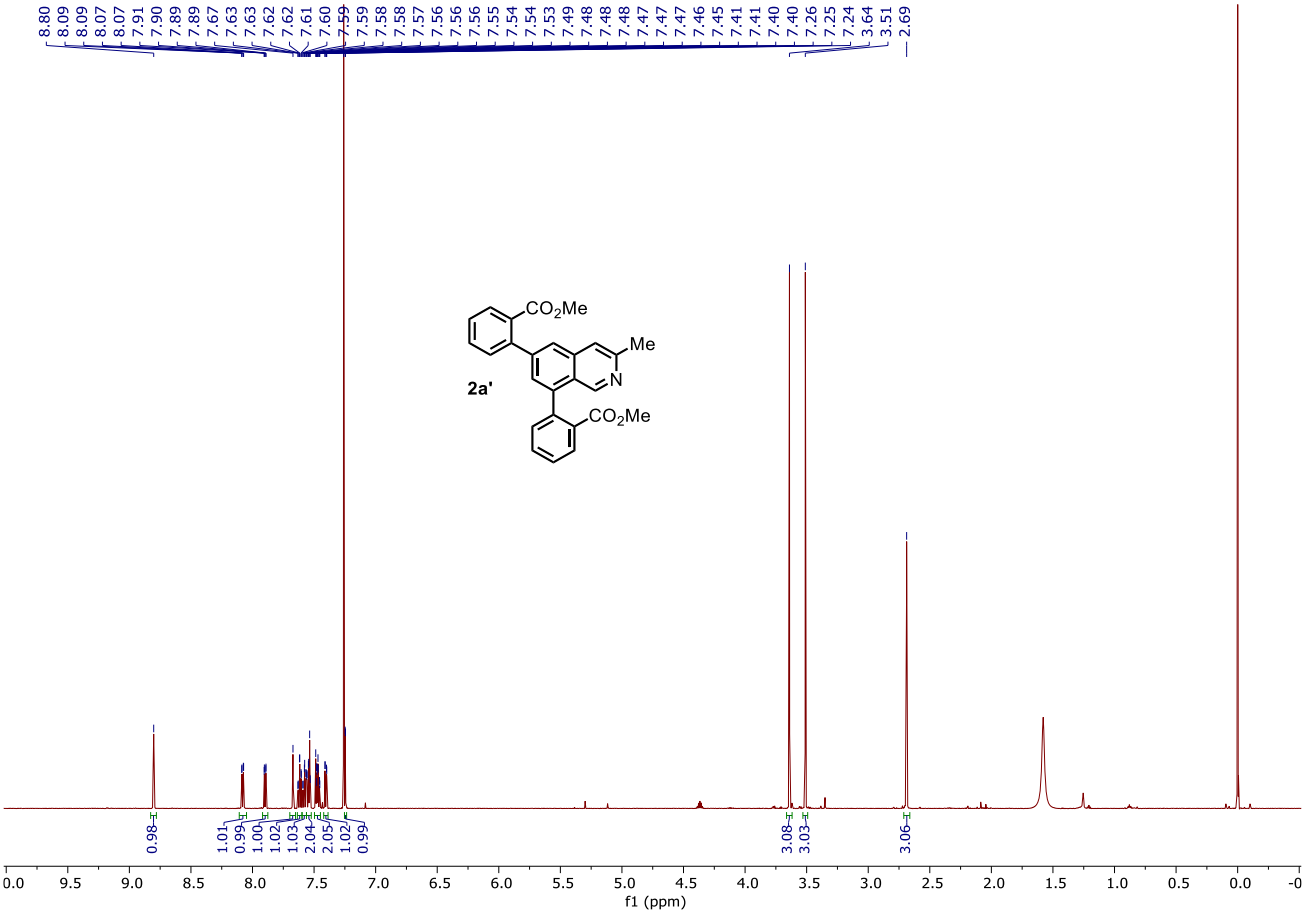

151.47
148.21
142.61
136.52
136.38
132.83
132.61
132.38
132.16
130.88
128.55
128.51
127.64
127.62
126.52
126.13
124.32
122.52
122.16
121.53
121.50
121.48
121.45
121.43
120.71
77.33
77.12
76.91
CF3
F3C
N
2an
f1 (ppm)

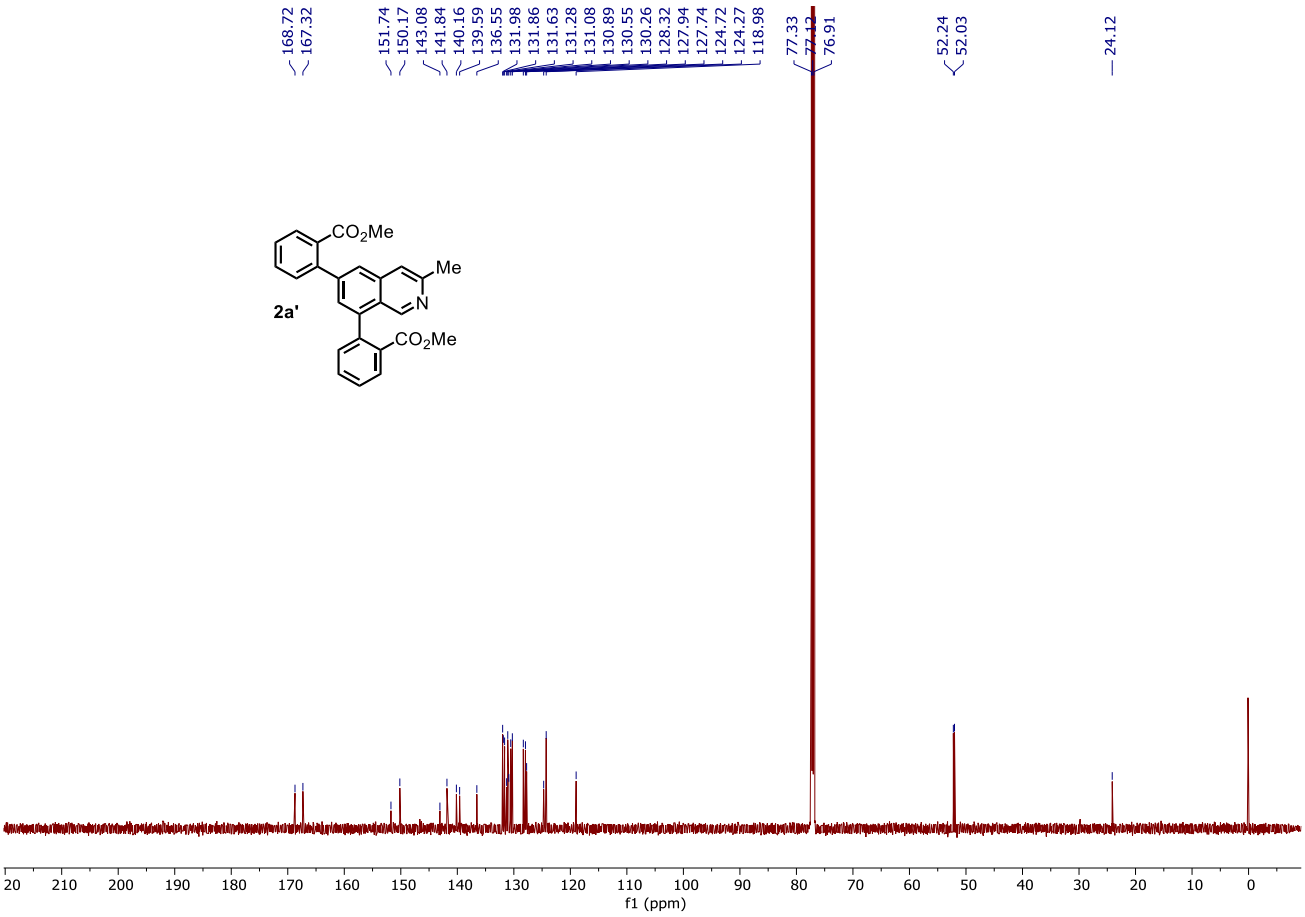

-63.098
CF3
F3C
N
2an
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
f1 (ppm)

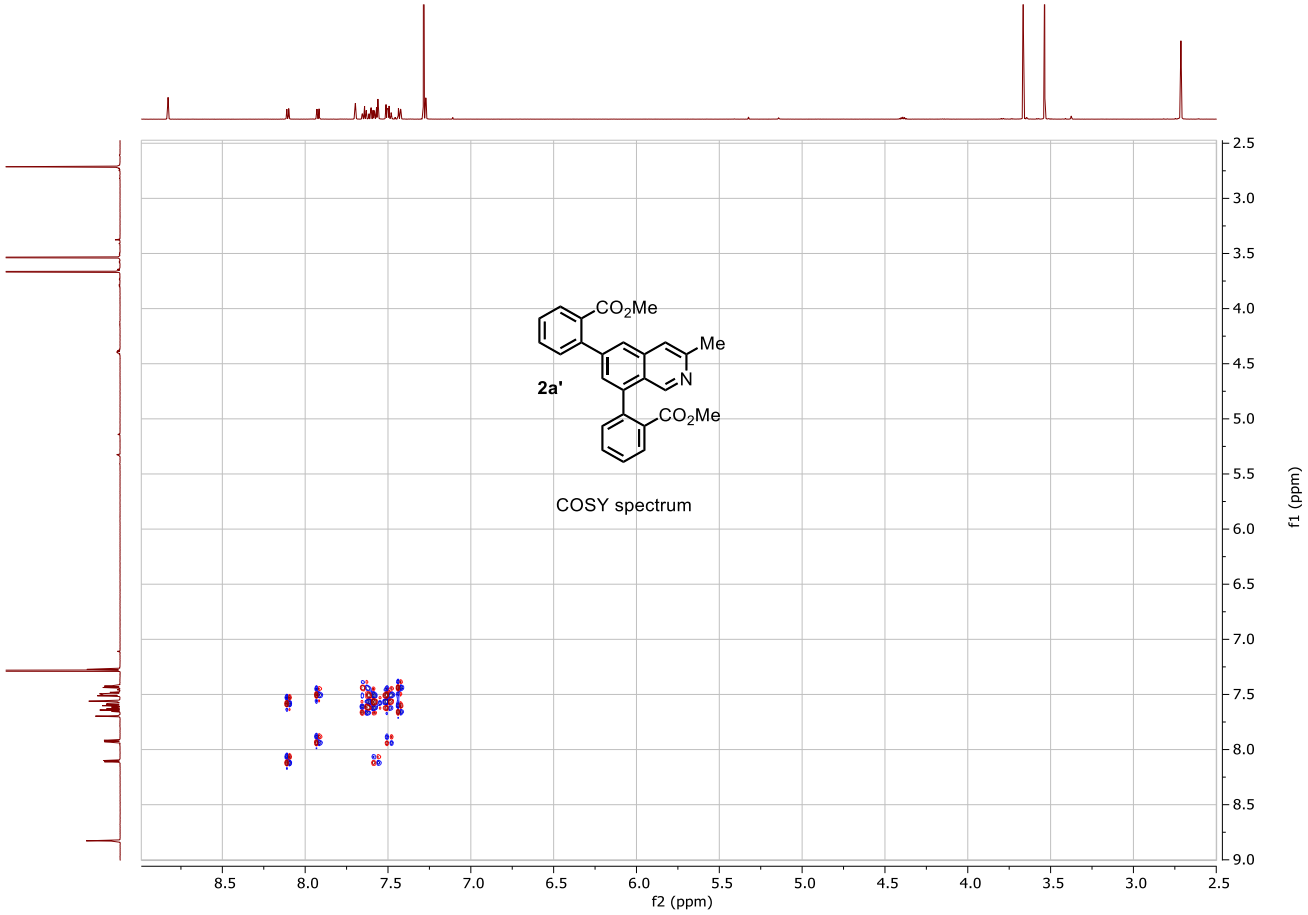

8.961
8.958
8.954
8.951
8.230
8.228
8.226
8.225
8.216
8.214
8.212
8.211
8.202
8.201
8.200
8.188
8.186
8.185
7.939
7.935
7.874
7.871
7.860
7.856
7.480
7.473
7.466
7.459
7.340
7.330
7.328
7.326
7.315
7.260
1.593
F
F
F
N
2ao
0.98
2.04
0.98
0.99
1.00
2.02
f1 (ppm)

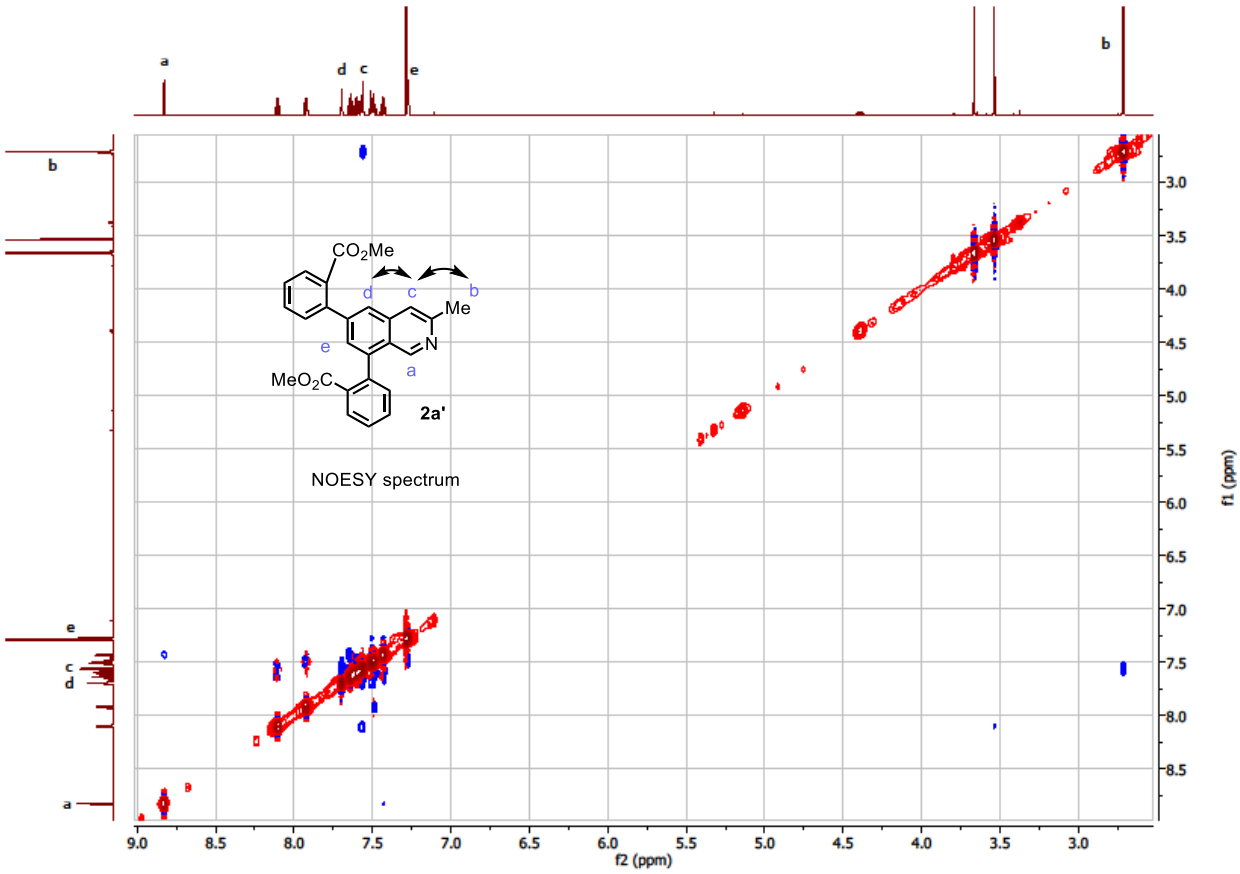

152.55
152.53
152.49
152.46
151.18
150.90
150.87
150.83
150.80
148.05
136.66
136.61
136.58
136.56
136.52
136.41
130.60
128.43
128.42
125.87
122.02
111.64
111.61
111.53
111.50
77.33
77.12
76.91
F
F
F
N
2ao
f1 (ppm)


-133.858
-133.912
-161.980
-162.035
-162.088
F
F
F
N
2ao
f1 (ppm)

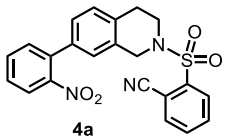

8.80 8.09 8.09 8.07 8.07 7.91 7.90 7.89 7.89 7.67 7.63 7.63 7.62 7.62 7.61 7.60 7.59 7.59 7.58 7.58 7.57 7.56 7.56 7.56 7.55 7.54 7.54 7.53 7.49 7.48 7.48 7.48 7.47 7.47 7.47 7.46 7.45 7.41 7.41 7.40 7.40 7.26 7.25 7.24 3.64 3.51 2.69
CO2Me
Me
N
CO2Me
2a'
0.98 1.01 0.99 1.00 1.02 1.03 2.04 2.05 1.02 0.99 3.08 3.03 3.06
f1 (ppm)


168.72 167.32 151.74 150.17 143.08 141.84 140.16 139.59 136.55 131.98 131.86 131.63 131.28 131.08 130.89 130.55 130.26 128.32 127.94 127.74 124.72 124.27 118.98 77.33 77.12 76.91 52.24 52.03 24.12
CO2Me
Me
N
CO2Me
2a'
f1 (ppm)

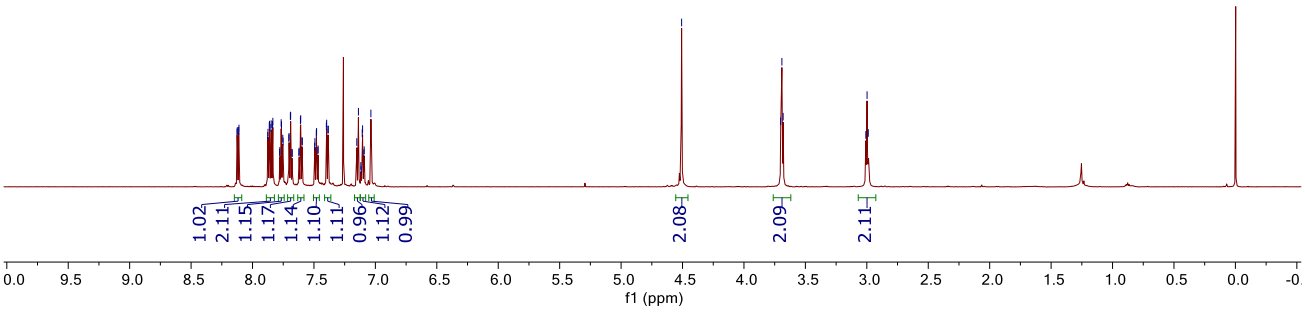

CO2Me
Me
N
CO2Me
2a'
COSY spectrum
f2 (ppm)
f1 (ppm)


a
d
c
e
b
CO2Me
Me
N
MeO2C
2a'
NOESY spectrum
f2 (ppm)
f1 (ppm)

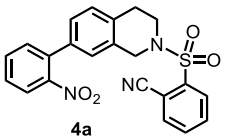

8.126
8.124
8.113
8.110
7.876
7.874
7.864
7.861
7.850
7.848
7.837
7.835
7.780
7.777
7.767
7.764
7.754
7.751
7.704
7.702
7.692
7.690
7.679
7.677
7.623
7.620
7.610
7.608
7.597
7.595
7.494
7.492
7.481
7.479
7.468
7.466
7.399
7.397
7.386
7.384
7.151
7.138
7.107
7.104
7.094
7.091
7.036
4.508
3.701
3.691
3.681
3.008
2.998
2.988


O
N
S
O
NO2
NC

4a

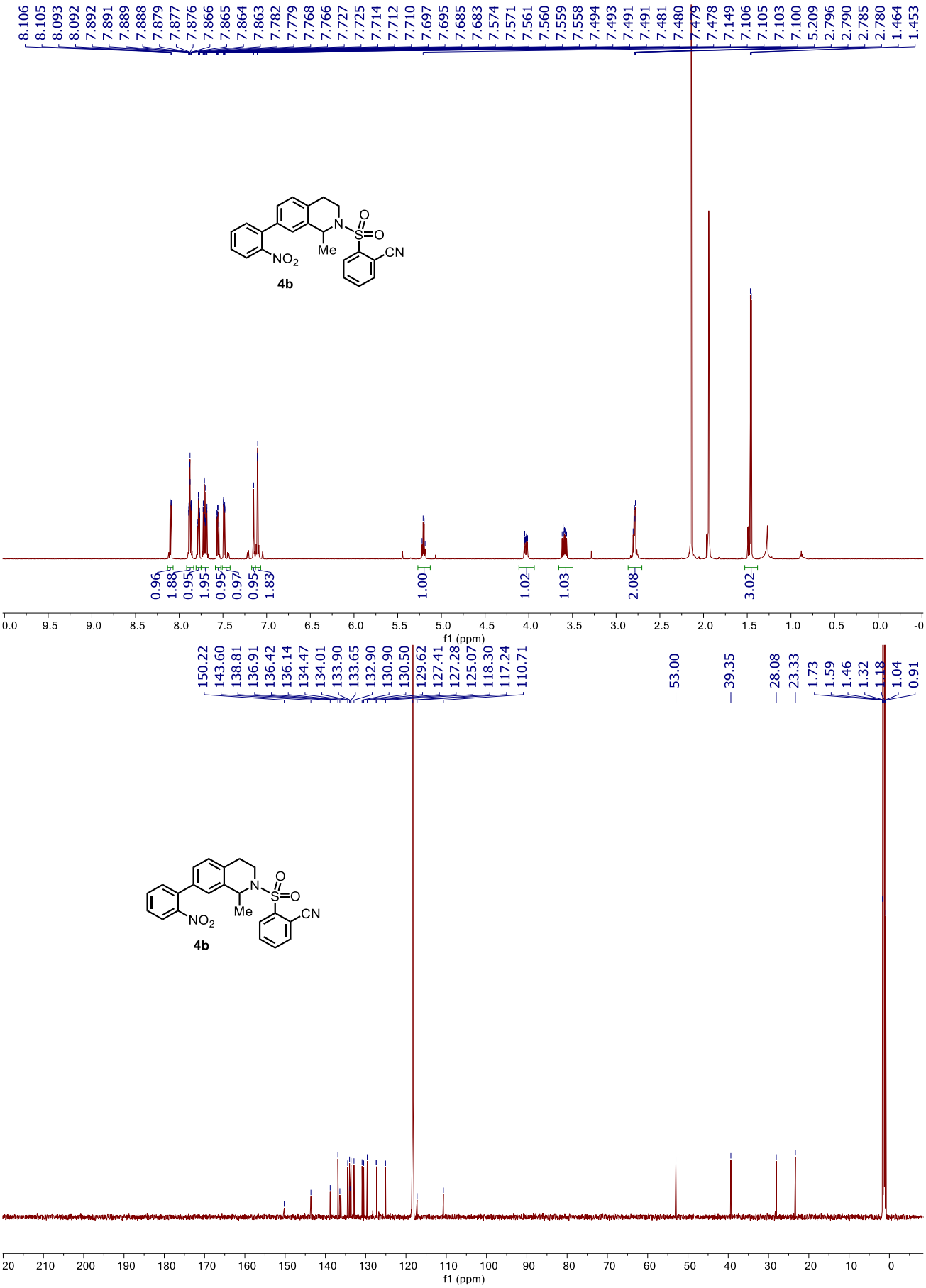

1.02
2.11
1.15
1.17
1.14
1.10
1.11
0.96
1.12
0.99
2.08
2.09
2.11
f1 (ppm)


149.20
140.90
135.87
135.77
135.73
133.32
133.07
132.91
132.51
131.99
131.91
130.42
129.42
128.42
126.67
125.86
124.24
116.35
110.94
77.33
77.12
76.91
47.29
43.61
28.47


O
N
S
O
NO2
NC

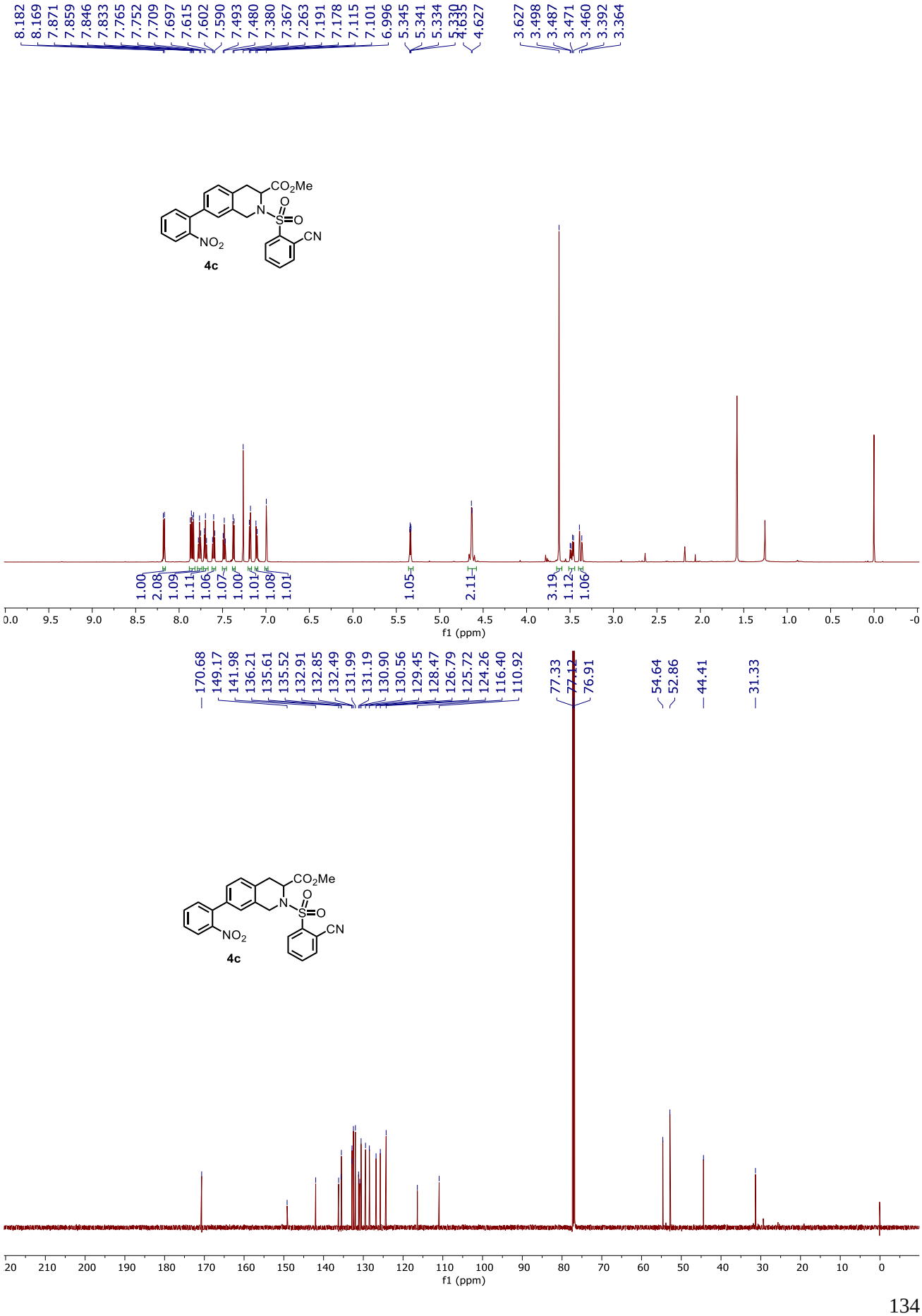
4a

f1 (ppm)

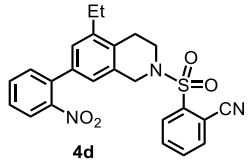

8.106 8.105 8.093 8.092 7.892 7.891 7.889 7.888 7.879 7.877 7.876 7.866 7.865 7.864 7.863 7.782 7.779 7.768 7.766 7.727 7.725 7.714 7.712 7.710 7.697 7.695 7.685 7.683 7.574 7.571 7.561 7.560 7.559 7.558 7.494 7.493 7.491 7.491 7.481 7.480 7.479 7.478 7.149 7.106 7.105 7.103 7.100 5.209 2.796 2.790 2.785 2.780 1.464 1.453
0.96 1.88 0.95 1.95 0.95 0.97 0.95 1.83 1.00 1.02 1.03 2.08 3.02
f1 (ppm)
150.22 143.60 138.81 136.91 136.42 136.14 134.47 134.01 133.90 133.65 132.90 130.90 130.50 129.62 127.41 127.28 125.07 118.30 117.24 110.71 53.00 39.35 28.08 23.33 1.73 1.59 1.46 1.32 1.18 1.04 0.91
f1 (ppm)

4b

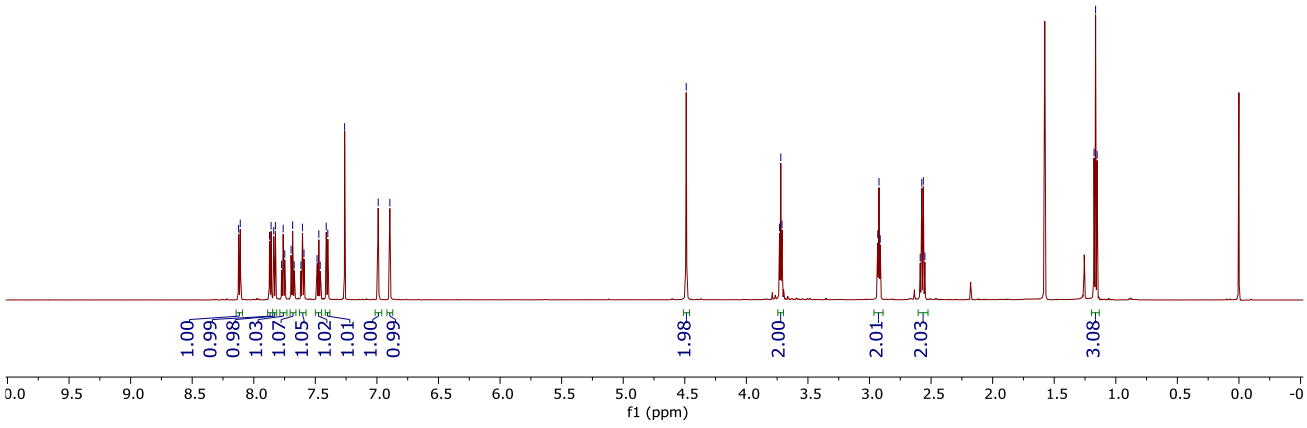
4b


8.182
8.169
7.871
7.859
7.846
7.833
7.765
7.752
7.709
7.697
7.615
7.602
7.590
7.493
7.480
7.380
7.367
7.263
7.191
7.178
7.115
7.101
6.996
5.345
5.341
5.334
5.330
4.635
4.627
3.627
3.498
3.487
3.471
3.460
3.392
3.364
CO2Me
N
O
S
O
CN
NO2
4c
1.00
2.08
1.09
1.11
1.06
1.07
1.00
1.01
1.08
1.01
1.05
2.11
3.19
1.12
1.06
f1 (ppm)
170.68
149.17
141.98
136.21
135.61
135.52
132.91
132.85
132.49
131.99
131.19
130.90
130.56
129.45
128.47
126.79
125.72
124.26
116.40
110.92
77.33
77.12
76.91
54.64
52.86
44.41
31.33
CO2Me
N
O
S
O
CN
NO2
4c
f1 (ppm)

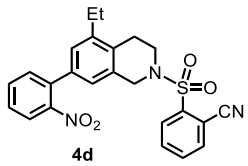

8.123
8.110
7.872
7.859
7.838
7.824
7.774
7.761
7.748
7.697
7.684
7.672
7.617
7.605
7.592
7.486
7.472
7.460
7.412
7.399
7.262
6.990
6.895
4.488
3.730
3.720
3.710
2.933
2.923
2.913
2.588
2.576
2.563
2.551
1.177
1.164
1.152


Et
N
O
S
O
CN
NO2

4d


1.00
0.99
0.98
1.03
1.07
1.05
1.02
1.01
1.00
0.99
1.98
2.00
2.01
2.03
3.08
f1 (ppm)

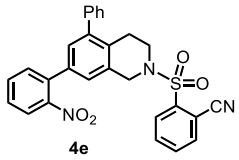

149.27
142.95
140.81
135.93
135.73
135.65
133.05
132.87
132.42
131.98
131.90
131.26
130.42
128.28
126.20
124.15
123.55
116.37
111.00
77.33
77.12
76.91
47.77
43.74
29.35
25.48
14.14


Et
N
O
S
O
CN
NO2

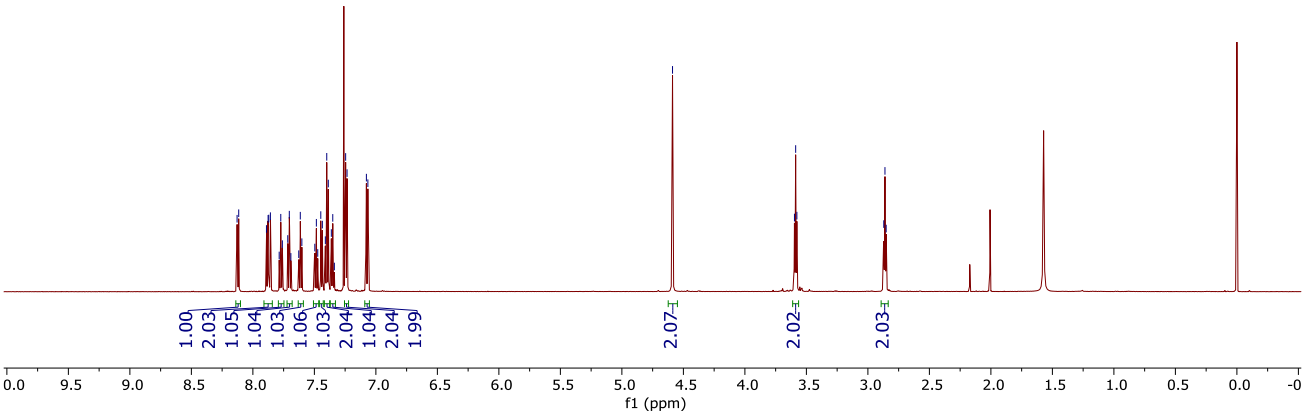
4d

f1 (ppm)

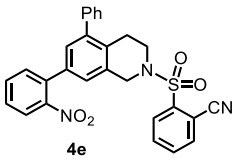

8.128
8.115
7.890
7.876
7.871
7.858
7.786
7.773
7.760
7.716
7.704
7.691
7.627
7.614
7.602
7.496
7.484
7.473
7.448
7.435
7.411
7.399
7.387
7.362
7.350
7.338
7.246
7.234
7.077
7.065
4.588
3.597
3.587
3.577
2.871
2.861
2.851


Ph
O
N
S
O
NO2
CN

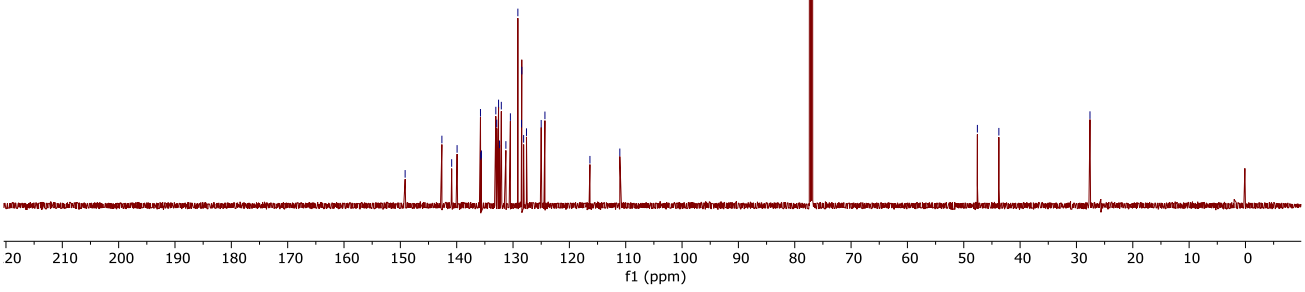
4e

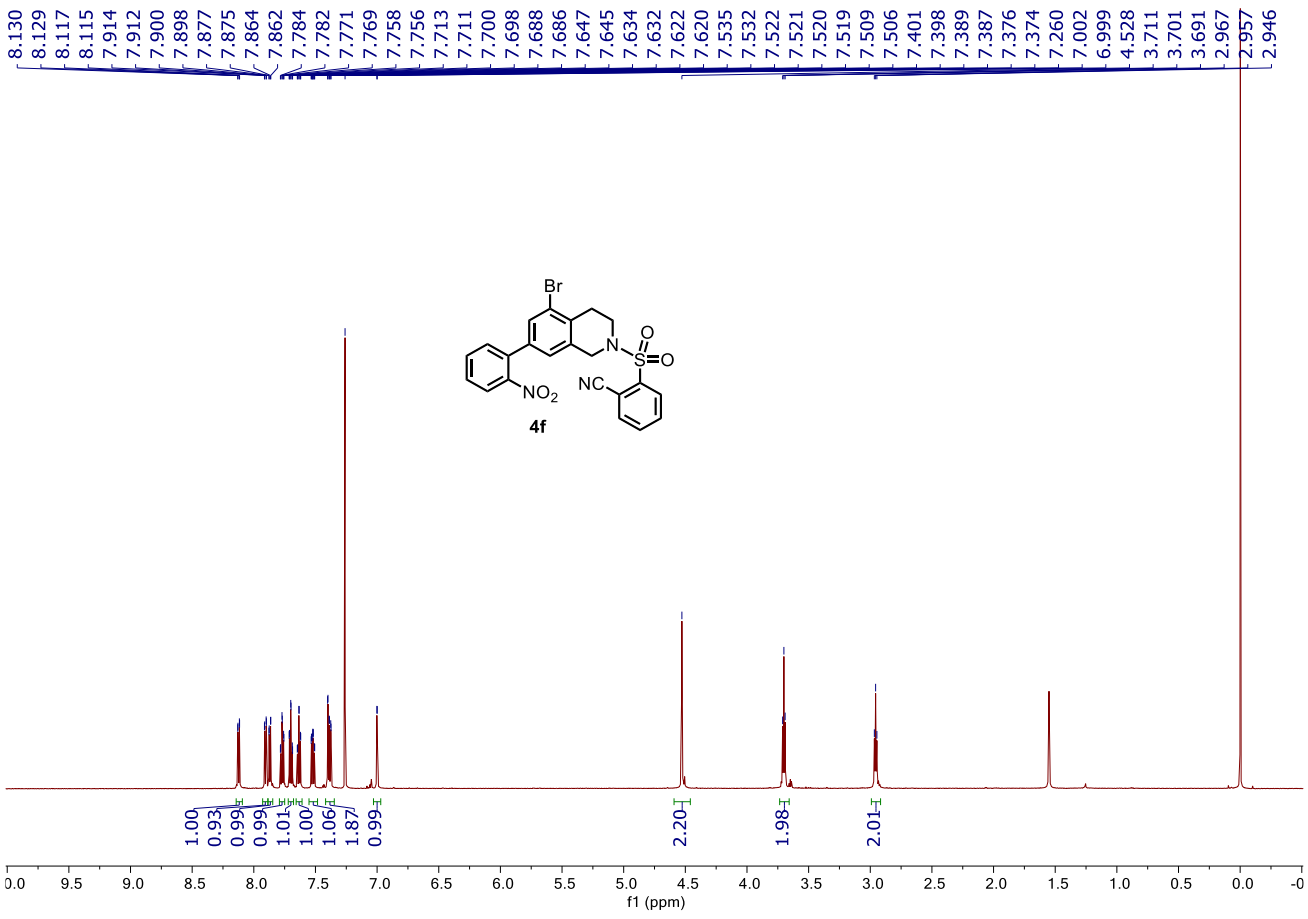

1.00
2.03
1.05
1.04
1.03
1.06
1.03
2.04
1.04
2.04
1.99
2.07
2.02
2.03
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0
f1 (ppm)

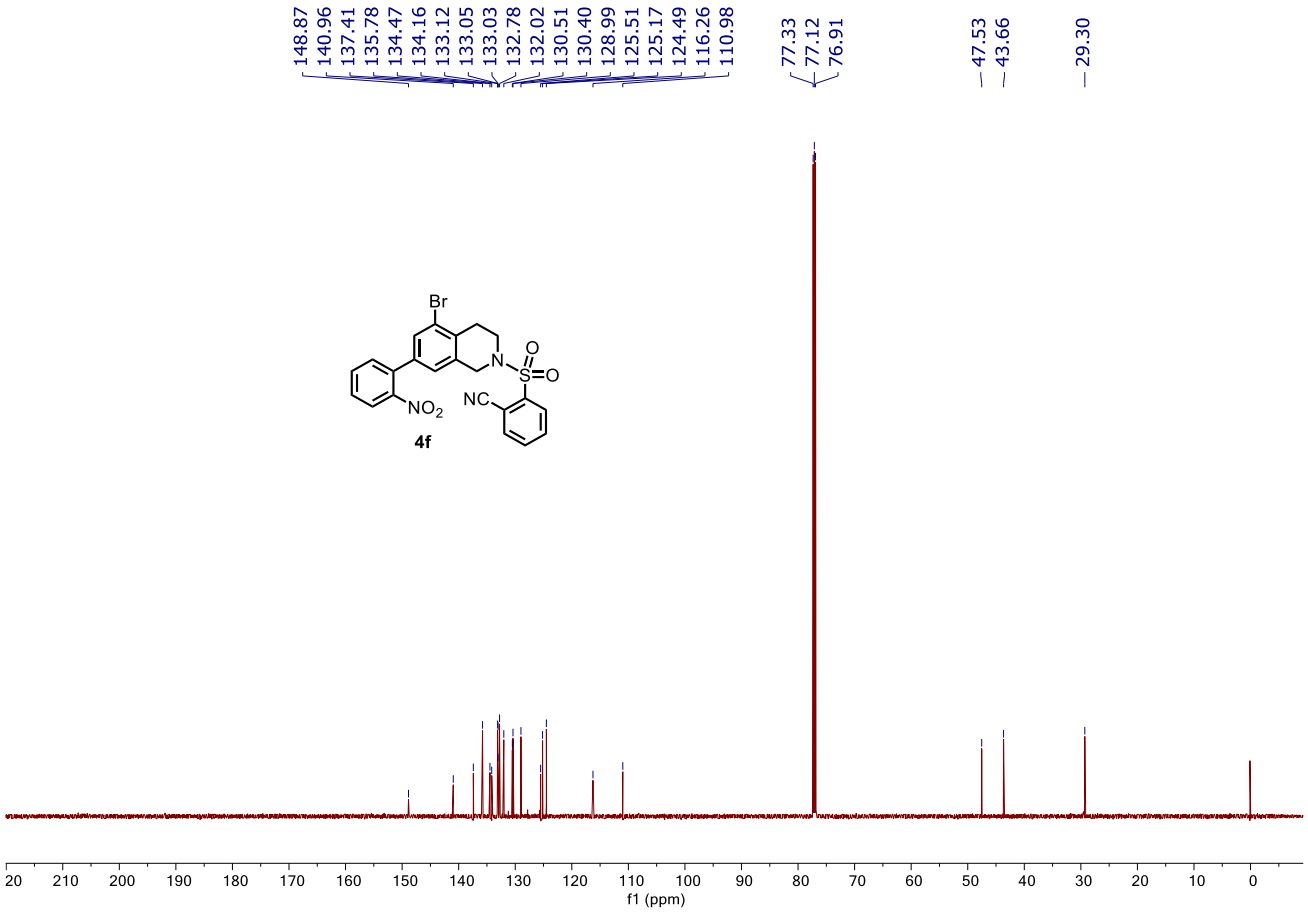

149.15
142.63
140.89
139.93
135.78
135.73
135.61
133.06
132.90
132.57
132.40
132.08
131.27
130.47
129.14
128.49
128.44
128.12
127.62
125.00
124.34
116.35
111.05
77.33
77.12
76.91
47.58
43.77
27.60


Ph
O
N
S
O
NO2
CN

4e


20
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.130
8.129
8.117
8.115
7.914
7.912
7.900
7.898
7.877
7.875
7.864
7.862
7.784
7.782
7.771
7.769
7.758
7.756
7.713
7.711
7.700
7.698
7.688
7.686
7.647
7.645
7.634
7.632
7.622
7.620
7.535
7.532
7.522
7.521
7.520
7.519
7.509
7.506
7.401
7.398
7.389
7.387
7.376
7.374
7.260
7.002
6.999
4.528
3.711
3.701
3.691
2.967
2.957
2.946
Br
O
N
S
O
NC
NO2
4f
1.00
0.93
0.99
0.99
1.01
1.00
1.06
1.87
0.99
2.20
1.98
2.01
f1 (ppm)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140.96
137.41
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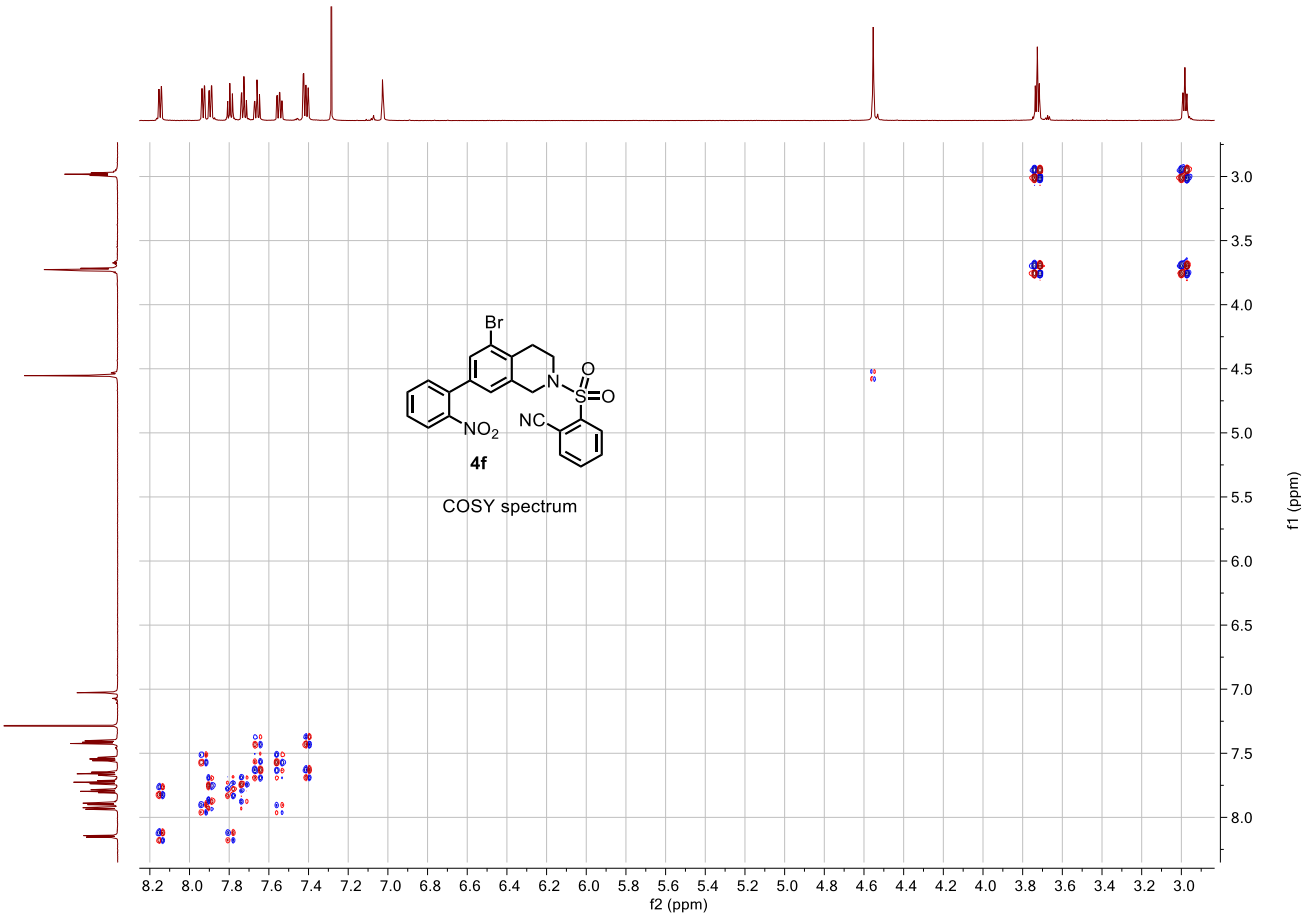
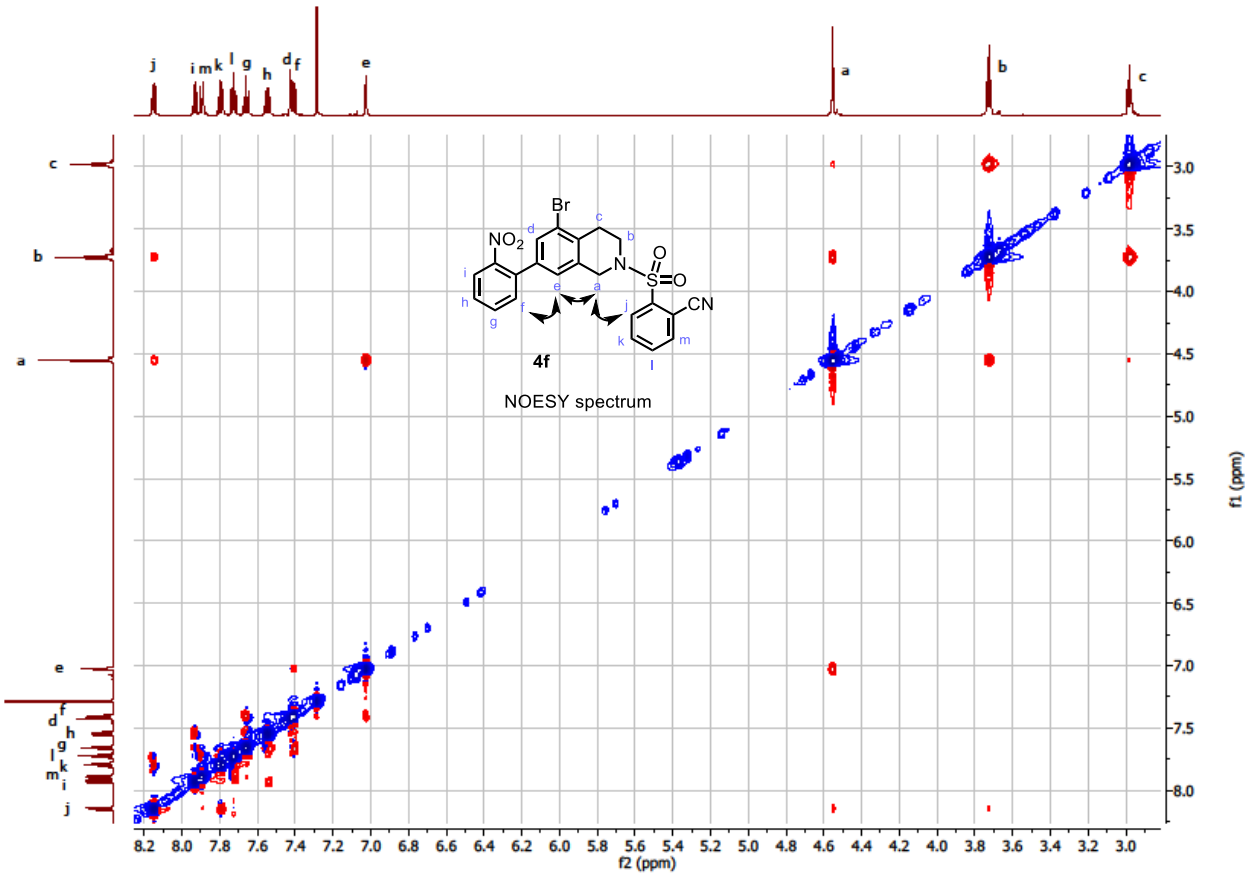
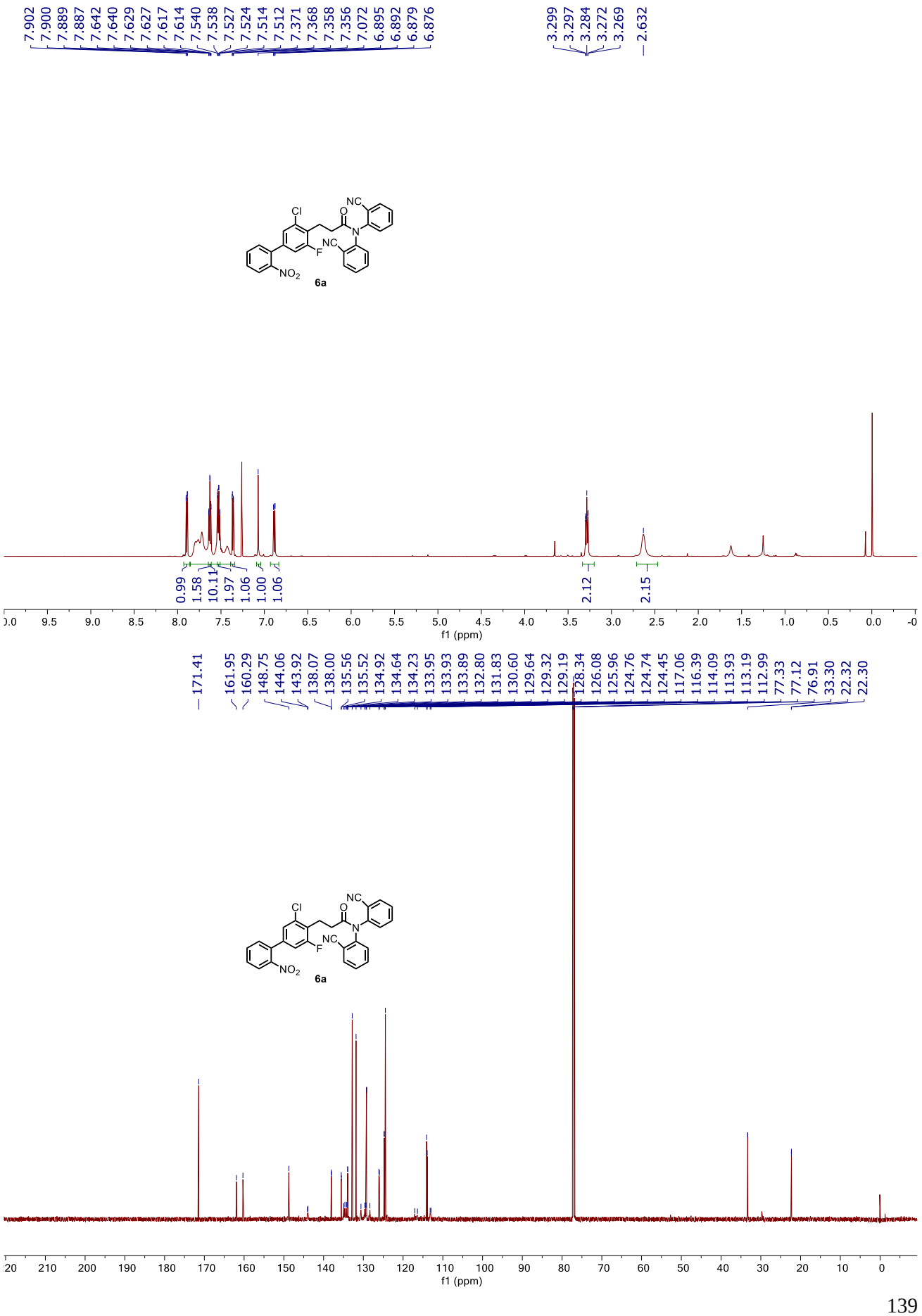
133.12
133.05
133.03
132.78
132.02
130.51
130.40
128.99
125.51
125.17
124.49
116.26
110.98
77.33
77.12
76.91
47.53
43.66
29.30
Br
O
N
S
O
NC
NO2
4f
f1 (ppm)


Br
NO2
NC
N
S
O
4f
COSY spectrum
f2 (ppm)
f1 (ppm)


j
i m k l g h d f
e
a
b
c
Br
NO2
NC
N
S
O
4f
NOESY spectrum
f2 (ppm)
f1 (ppm)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7.900
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7.887
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7.640
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7.627
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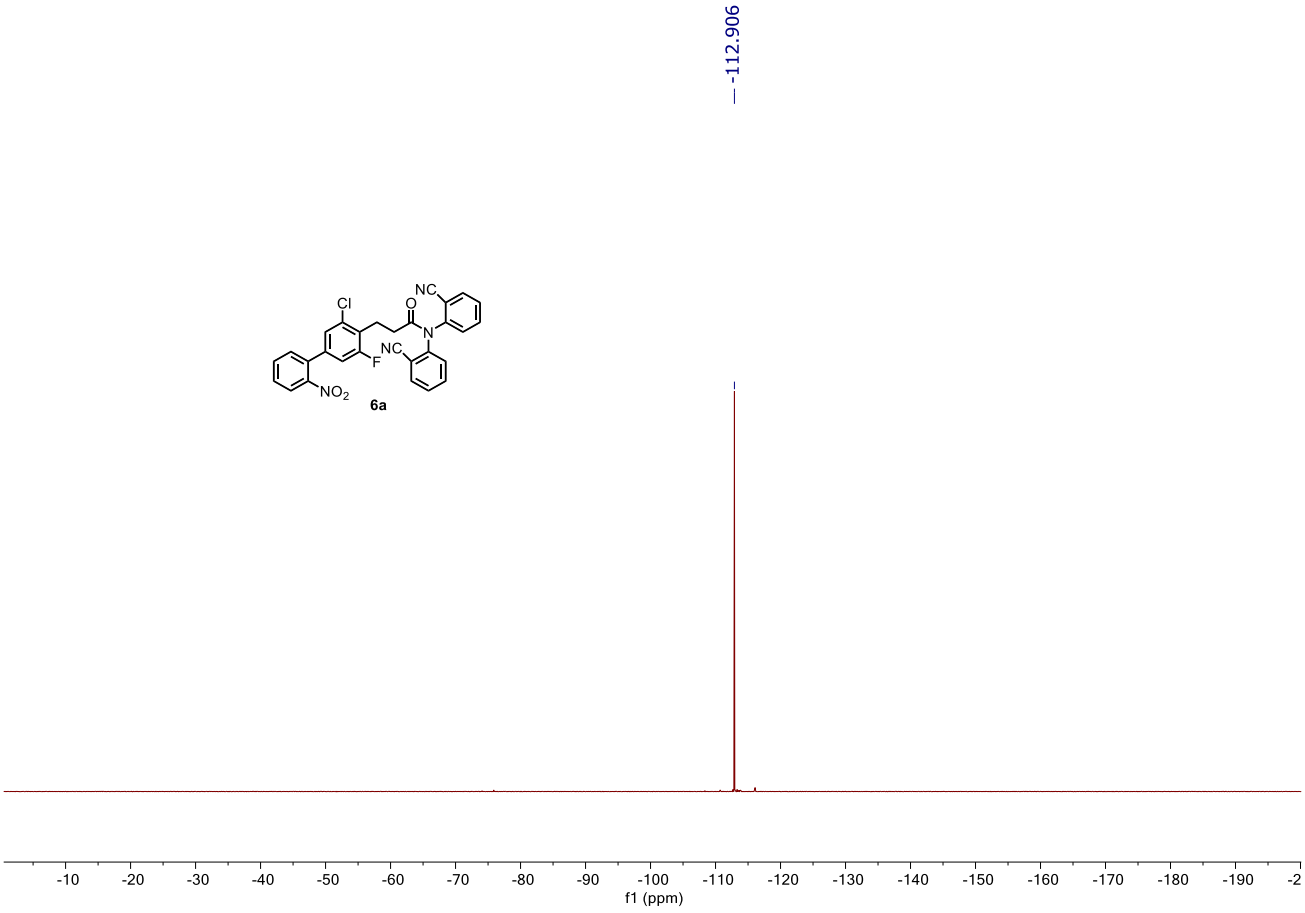
7.614
7.540
7.538
7.527
7.524
7.514
7.512
7.371
7.368
7.358
7.356
7.072
6.895
6.892
6.879
6.876
3.299
3.297
3.284
3.272
3.269
2.632
Cl
O
NC
N
NC
F
NO2
6a
0.99
1.58
10.11
1.97
1.06
1.00
1.06
2.12
2.15
f1 (ppm)
171.41
161.95
160.29
148.75
144.06
143.92
138.07
138.00
135.56
135.52
134.92
134.64
134.23
133.95
133.93
133.89
132.80
131.83
130.60
129.64
129.32
129.19
128.34
126.08
125.96
124.76
124.74
124.45
117.06
116.39
114.09
113.93
113.19
112.99
77.33
77.12
76.91
33.30
22.32
22.30
Cl
O
NC
N
NC
F
NO2
6a
f1 (ppm)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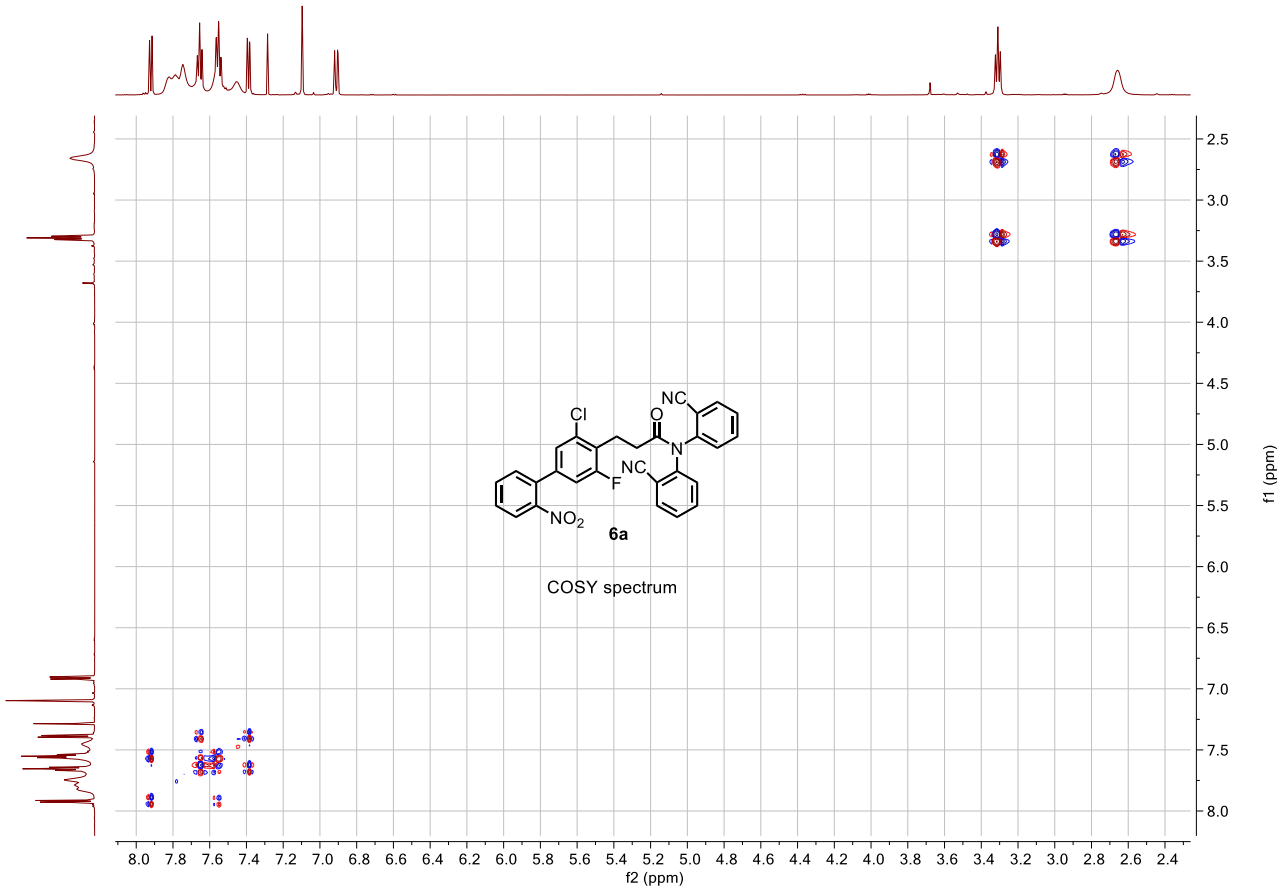
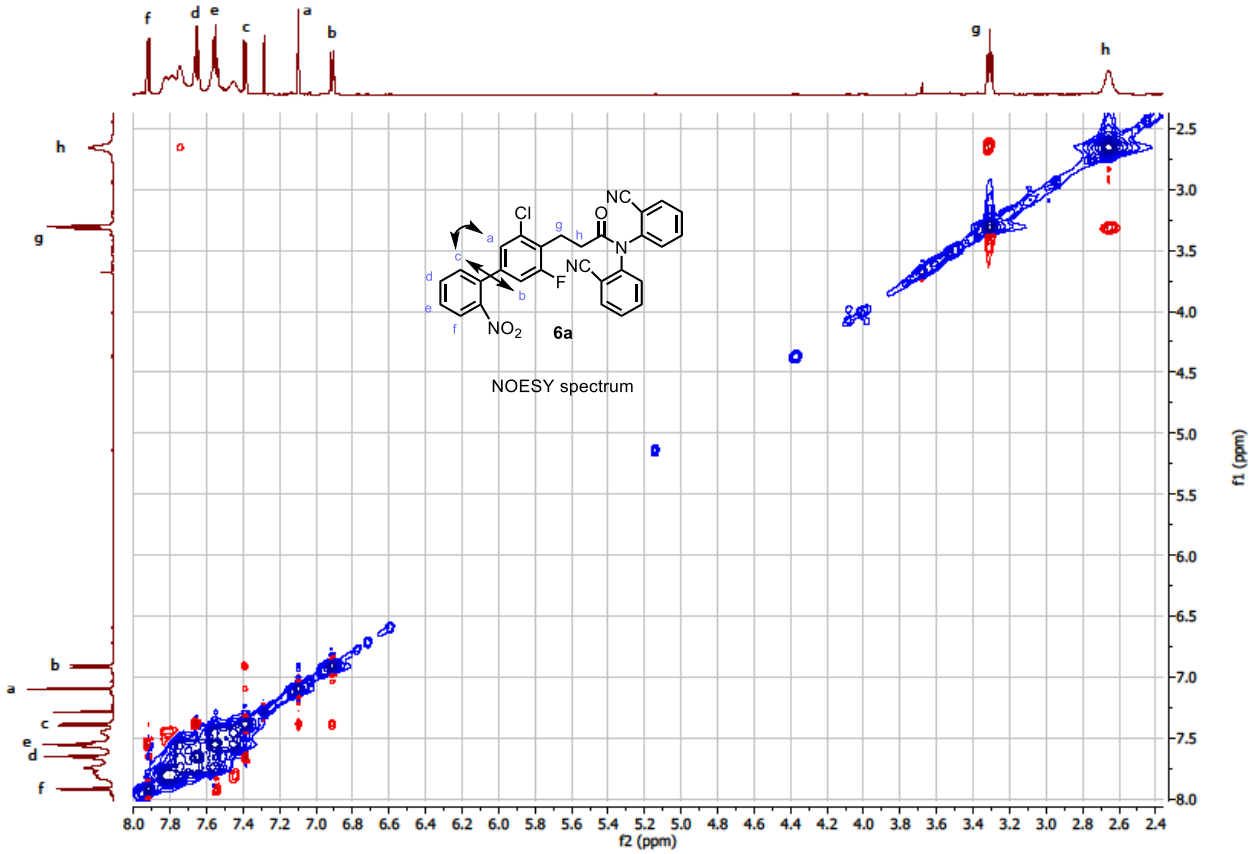
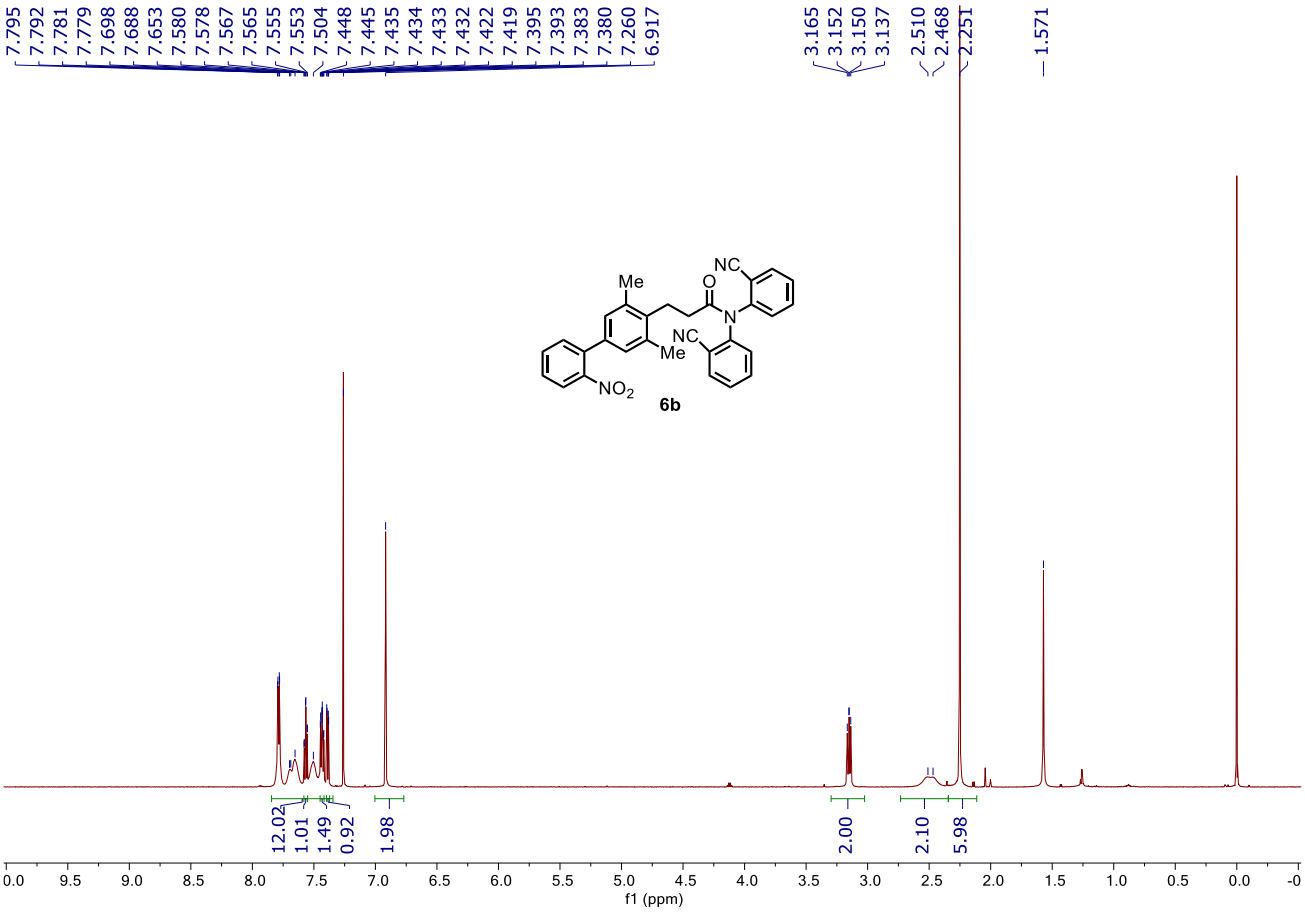
Cl
NC
O
N
F
NC
NO2
6a
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
f1 (ppm)


Cl
NC
O
N
F
NC
NO2
6a
COSY spectrum
8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4
f2 (ppm)
2.5 3.0 3.5 4.0 4.5 5.0 5.5 6.0 6.5 7.0 7.5 8.0
f1 (ppm)


f
d
e
c
a
b
g
h
NC
Cl
O
N
NC
F
NO2
6a
NOESY spectrum
f2 (ppm)
f1 (ppm)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7.781
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7.688
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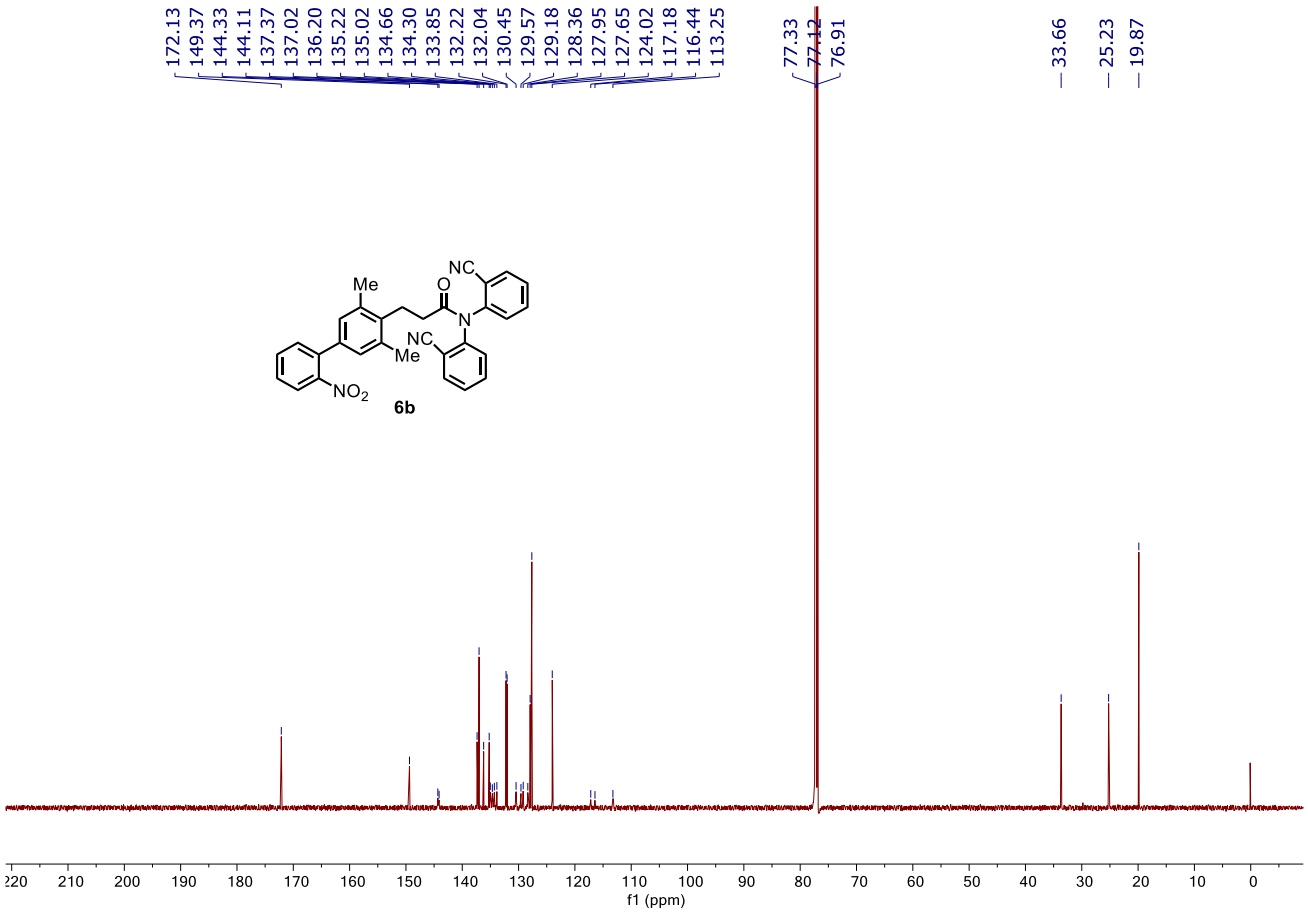
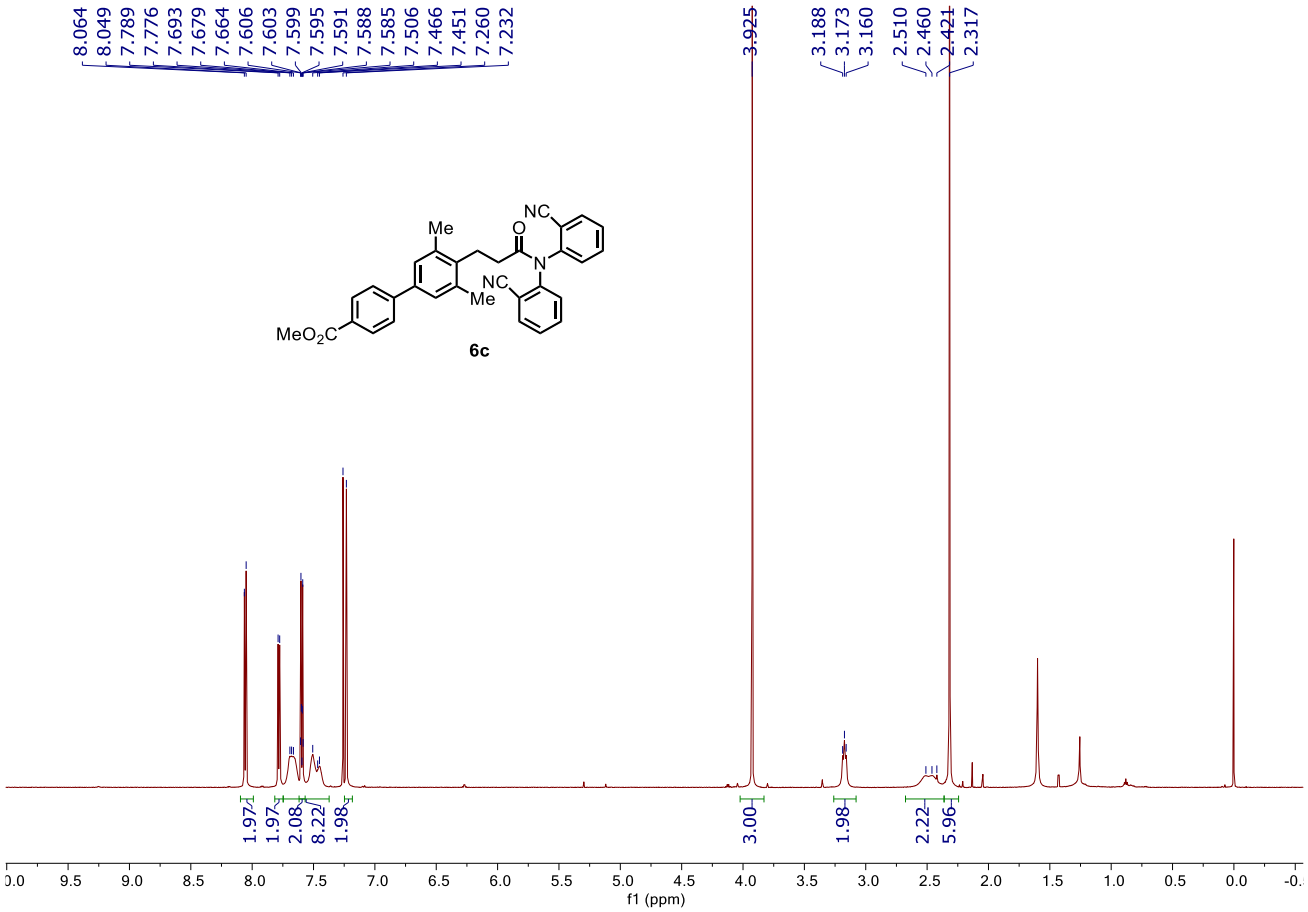
7.580
7.578
7.567
7.565
7.555
7.553
7.504
7.448
7.445
7.435
7.434
7.433
7.432
7.422
7.419
7.395
7.393
7.383
7.380
7.260
6.917
3.165
3.152
3.150
3.137
2.510
2.468
2.251
1.571
Me
NC
O
N
NC
Me
NO2
6b
12.02
1.01
1.49
0.92
1.98
2.00
2.10
5.98
f1 (ppm)


172.13
149.37
144.33
144.11
137.37
137.02
136.20
135.22
135.02
134.66
134.30
133.85
132.22
132.04
130.45
129.57
129.18
128.36
127.95
127.65
124.02
117.18
116.44
113.25
77.33
77.12
76.91
33.66
25.23
19.87
Me
O
NC
N
NC
Me
NO2
6b
f1 (ppm)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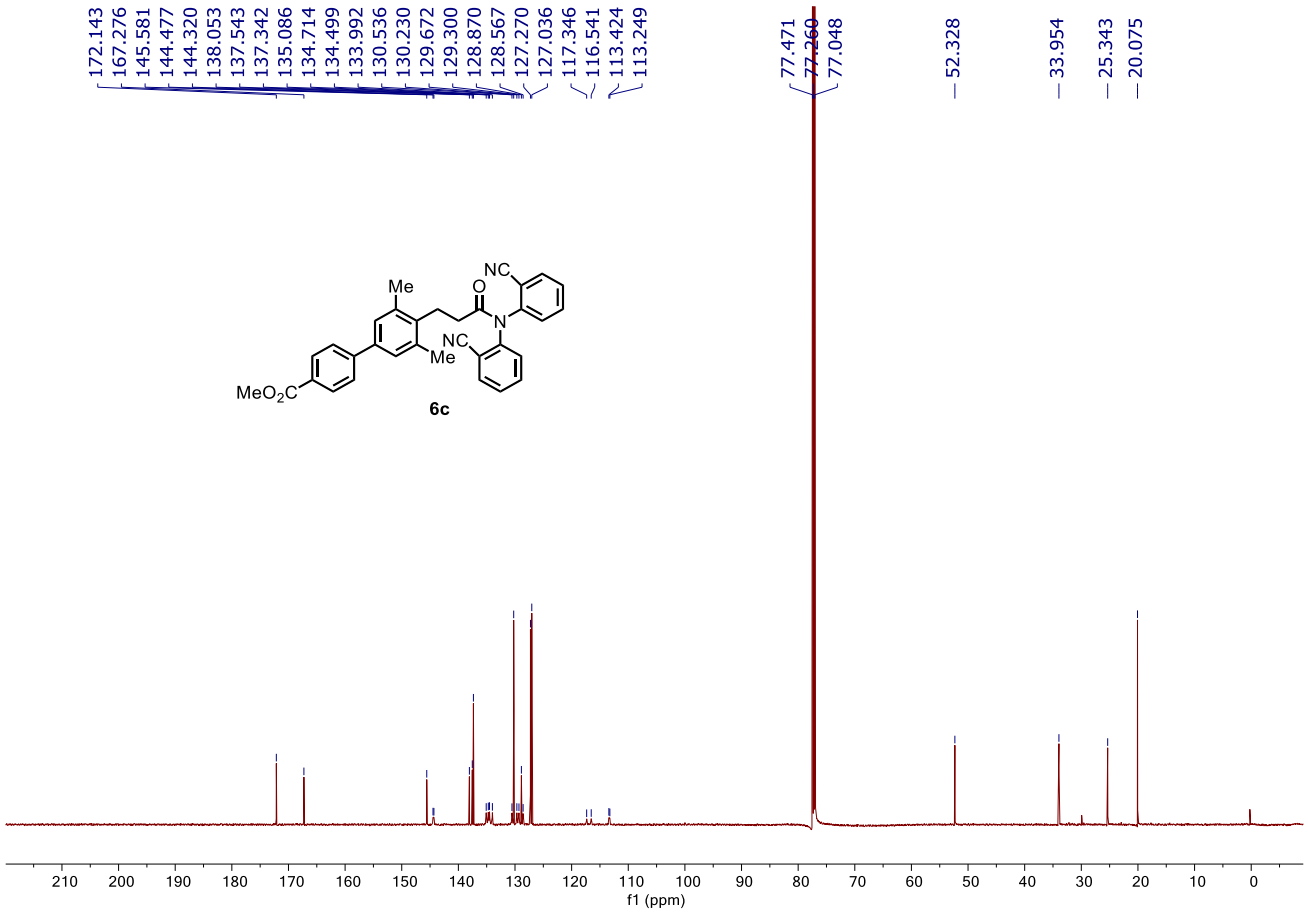
8.049
7.789
7.776
7.693
7.679
7.664
7.606
7.603
7.599
7.595
7.591
7.588
7.585
7.506
7.466
7.451
7.260
7.232
3.925
3.188
3.173
3.160
2.510
2.460
2.421
2.317
Me
O
NC
N
NC
Me
MeO2C
6c
1.97
1.97
2.08
8.22
1.98
3.00
1.98
2.22
5.96
f1 (ppm)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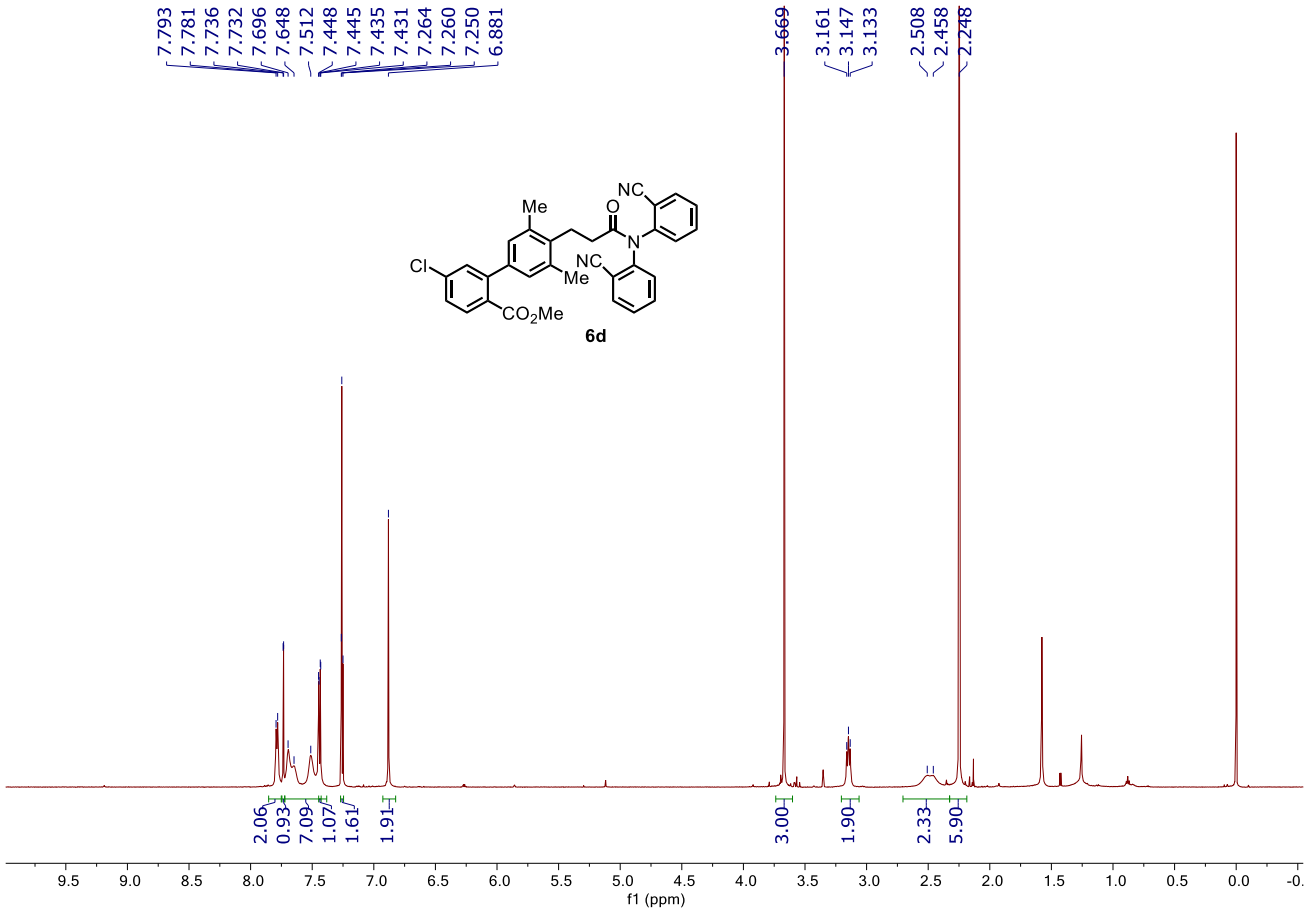
167.276
145.581
144.477
144.320
138.053
137.543
137.342
135.086
134.714
134.499
133.992
130.536
130.230
129.672
129.300
128.870
128.567
127.270
127.036
117.346
116.541
113.424
113.249
77.471
77.260
77.048
52.328
33.954
25.343
20.075
Me
NC
O
N
NC
Me
MeO2C
6c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.736
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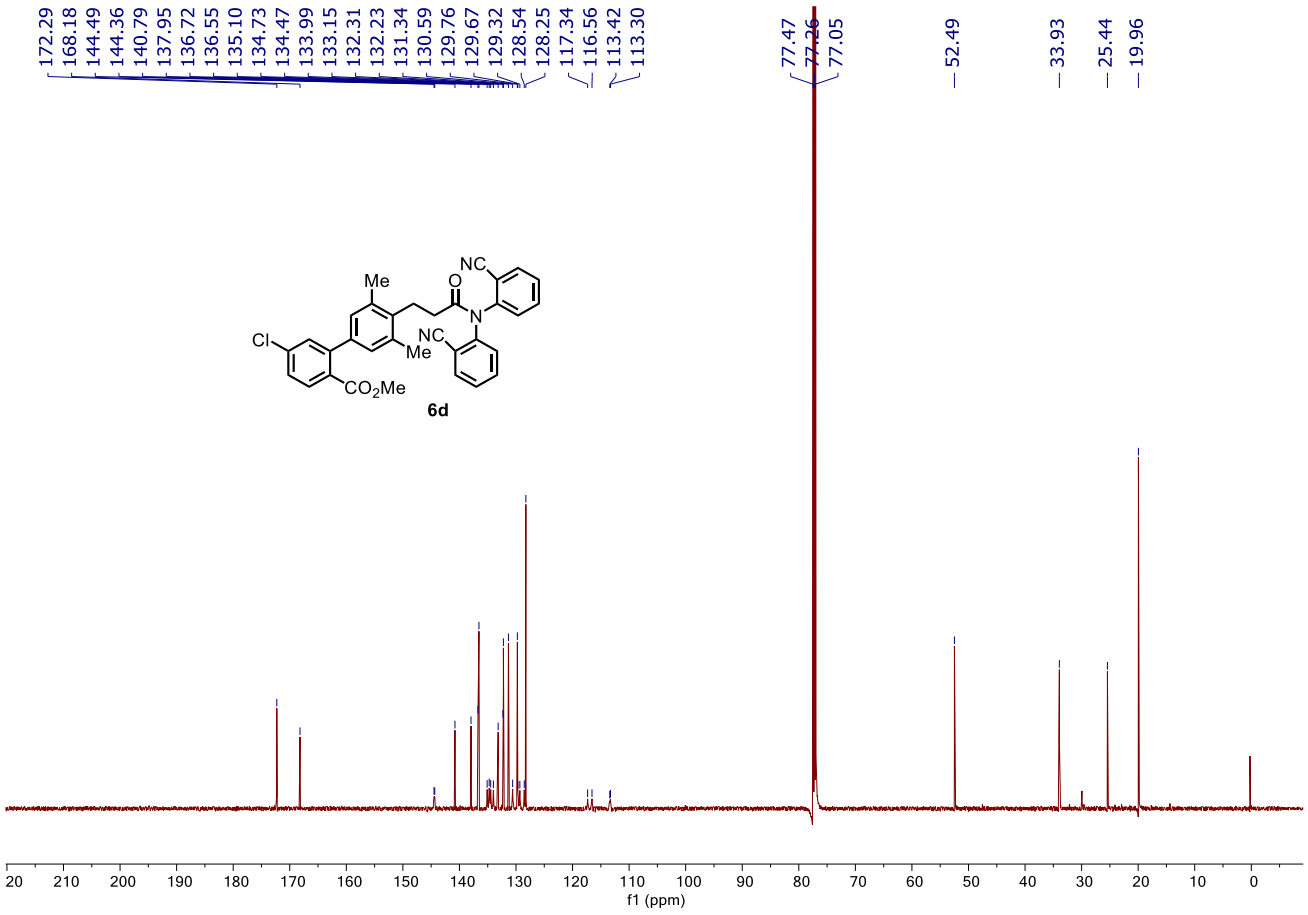
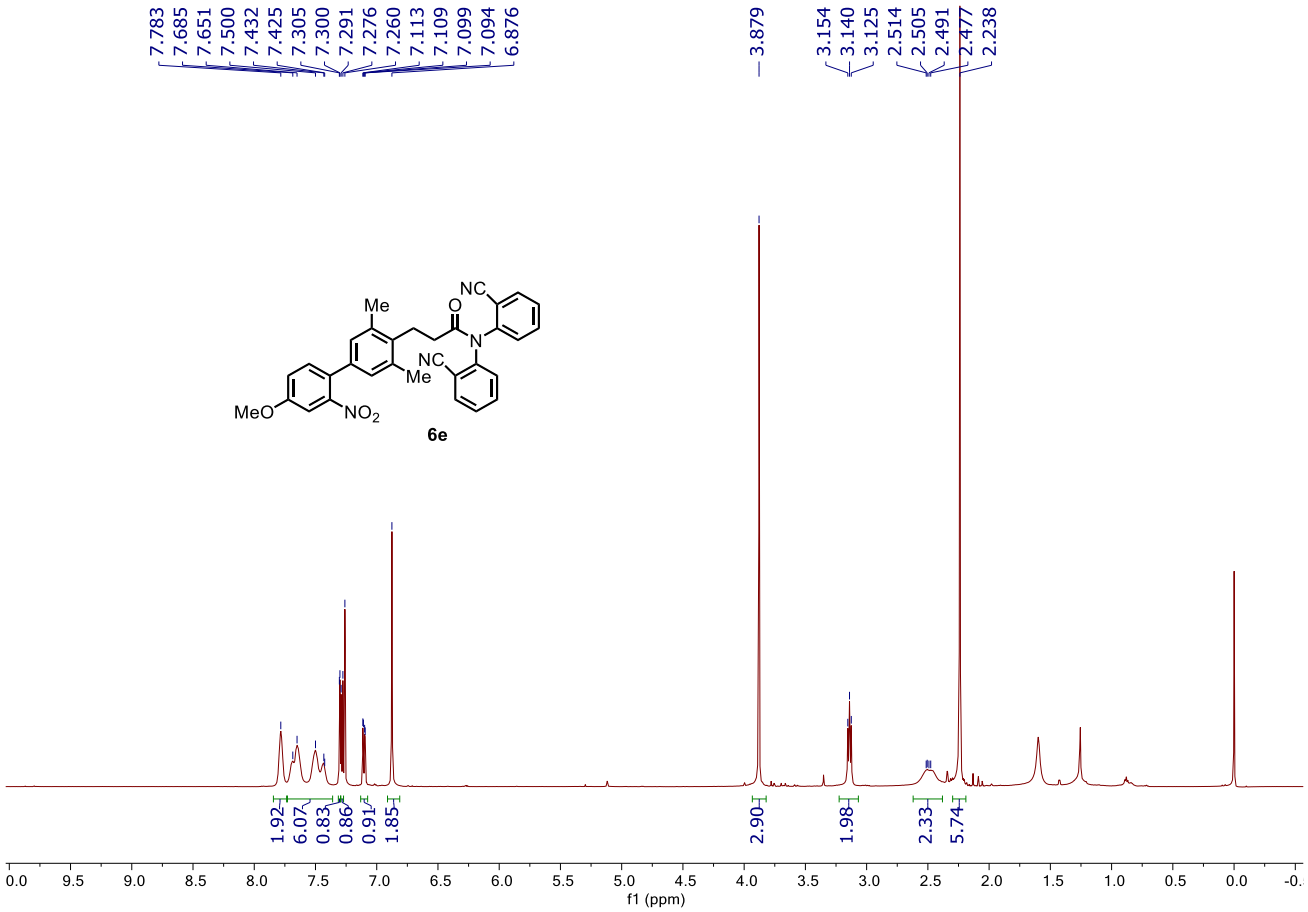
7.448
7.445
7.435
7.431
7.264
7.260
7.250
6.881
3.669
3.161
3.147
3.133
2.508
2.458
2.248
Me
NC
O
N
Cl
NC
Me
CO2Me
6d
2.06
0.93
7.09
1.07
1.61
1.91
3.00
1.90
2.33
5.90
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


172.29
168.18
144.49
144.36
140.79
137.95
136.72
136.55
135.10
134.73
134.47
133.99
133.15
132.31
132.23
131.34
130.59
129.76
129.67
129.32
128.54
128.25
117.34
116.56
113.42
113.30
77.47
77.26
77.05
52.49
33.93
25.44
19.96
Me
O
NC
N
NC
Me
Cl
CO2Me
6d
f1 (ppm)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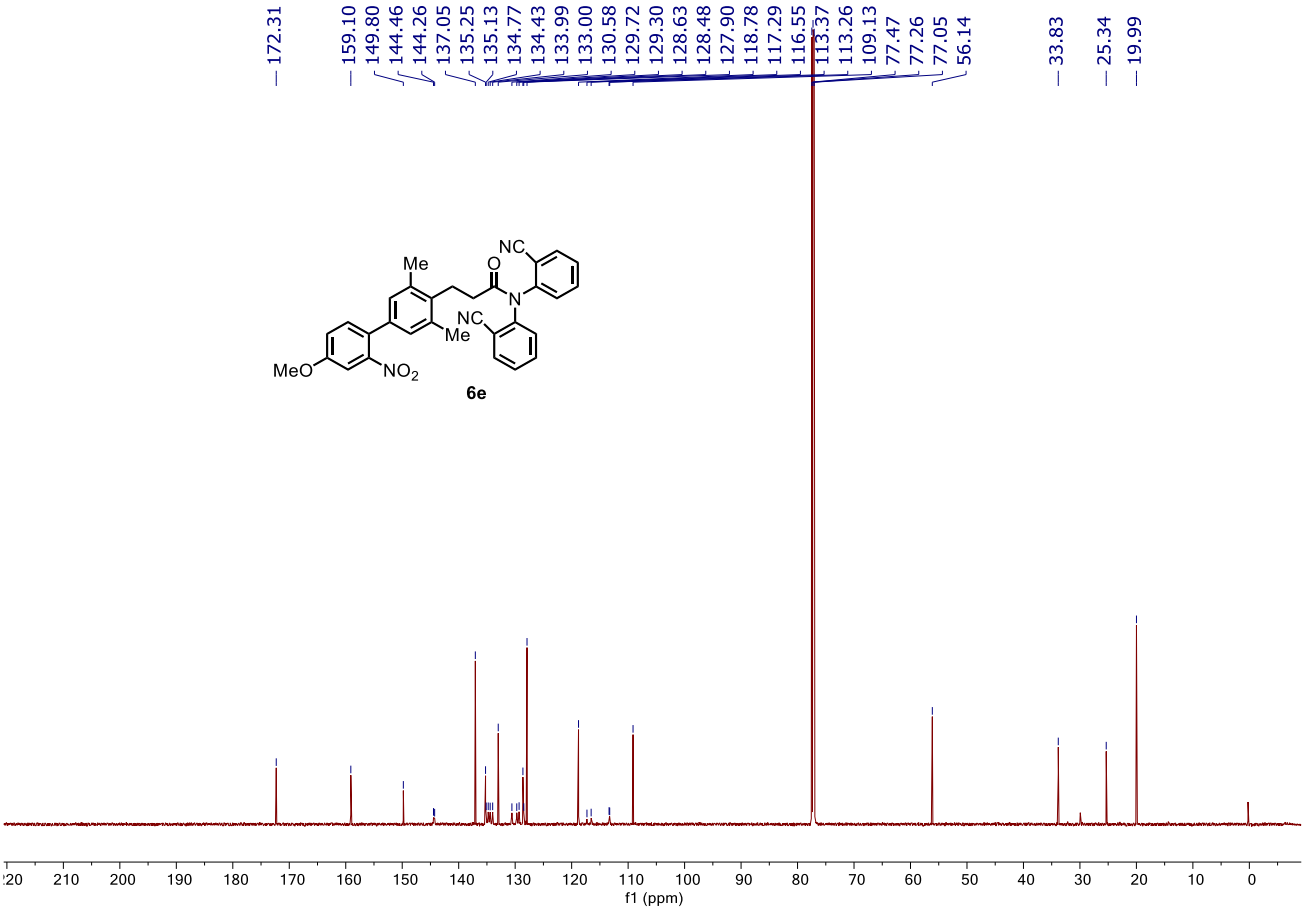
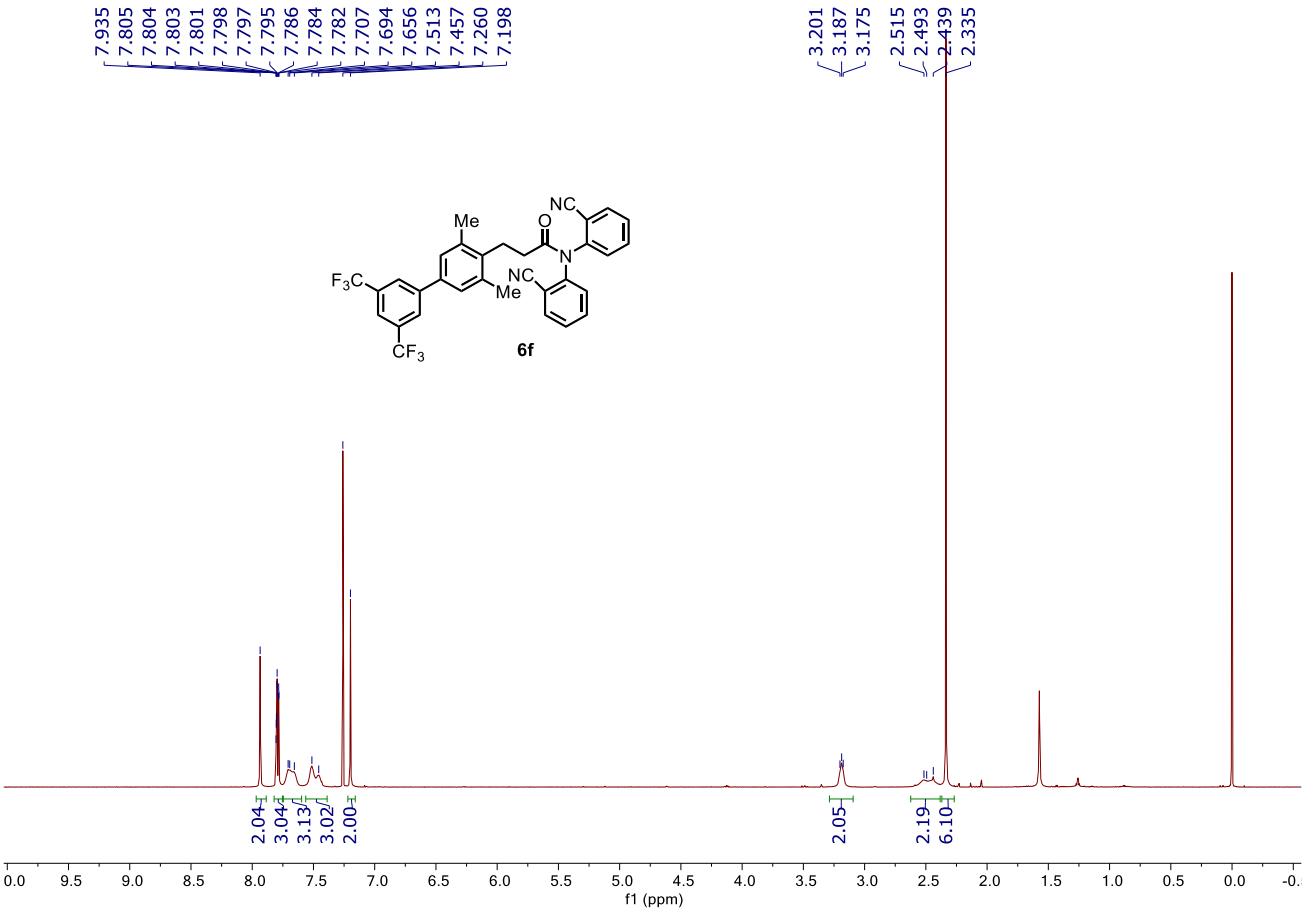
7.685
7.651
7.500
7.432
7.425
7.305
7.300
7.291
7.276
7.260
7.113
7.109
7.099
7.094
6.876
3.879
3.154
3.140
3.125
2.514
2.505
2.491
2.477
2.238
Me
O
NC
N
NC
Me
MeO
NO2
6e
1.92
6.07
0.83
0.86
0.91
1.85
2.90
1.98
2.33
5.74
f1 (ppm)


172.31
159.10
149.80
144.46
144.26
137.05
135.25
135.13
134.77
134.43
133.99
133.00
130.58
129.72
129.30
128.63
128.48
127.90
118.78
117.29
116.55
113.37
113.26
109.13
77.47
77.26
77.05
56.14
33.83
25.34
19.99
NC
Me
O
N
NC
Me
MeO
NO2
6e
f1 (ppm)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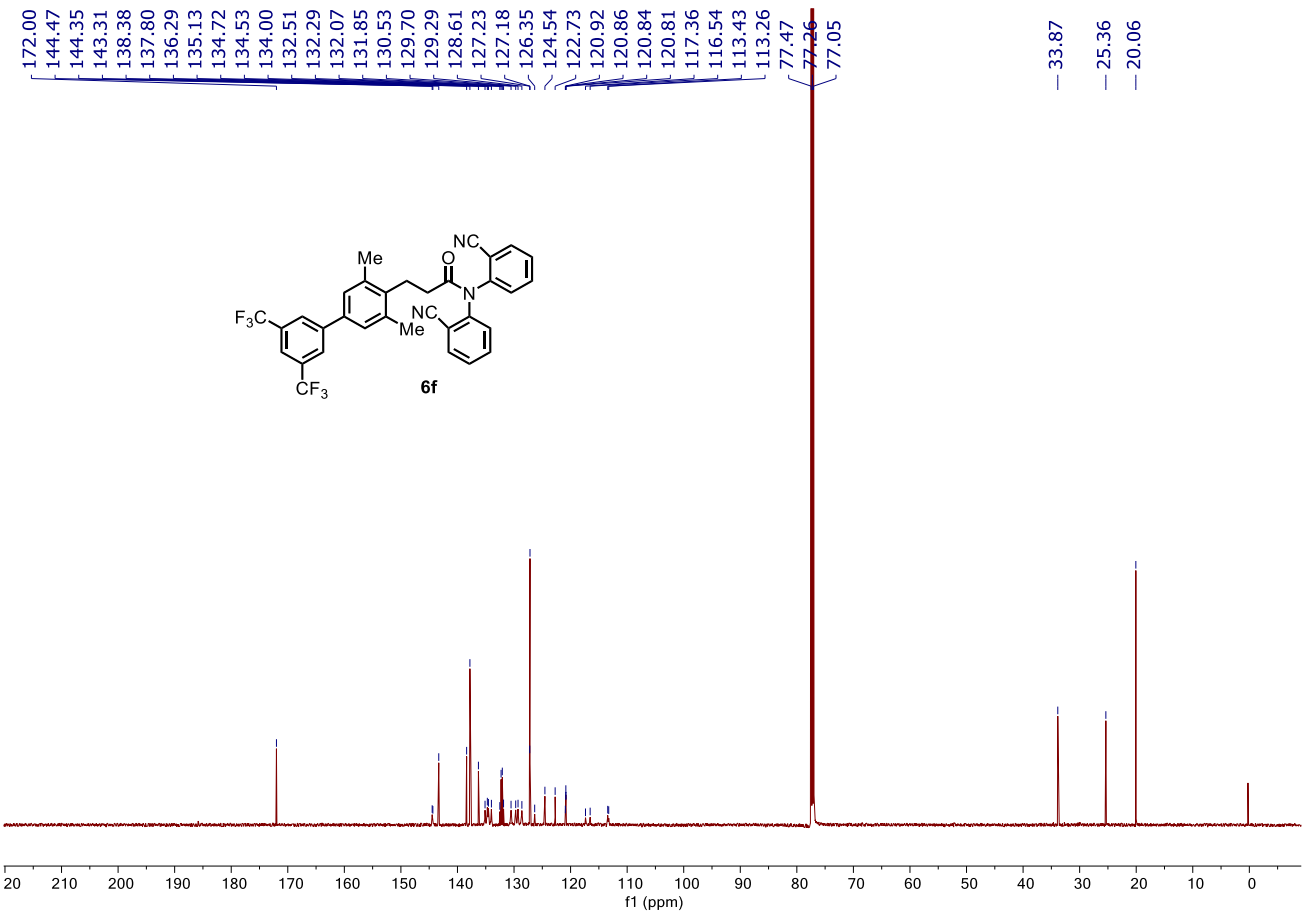
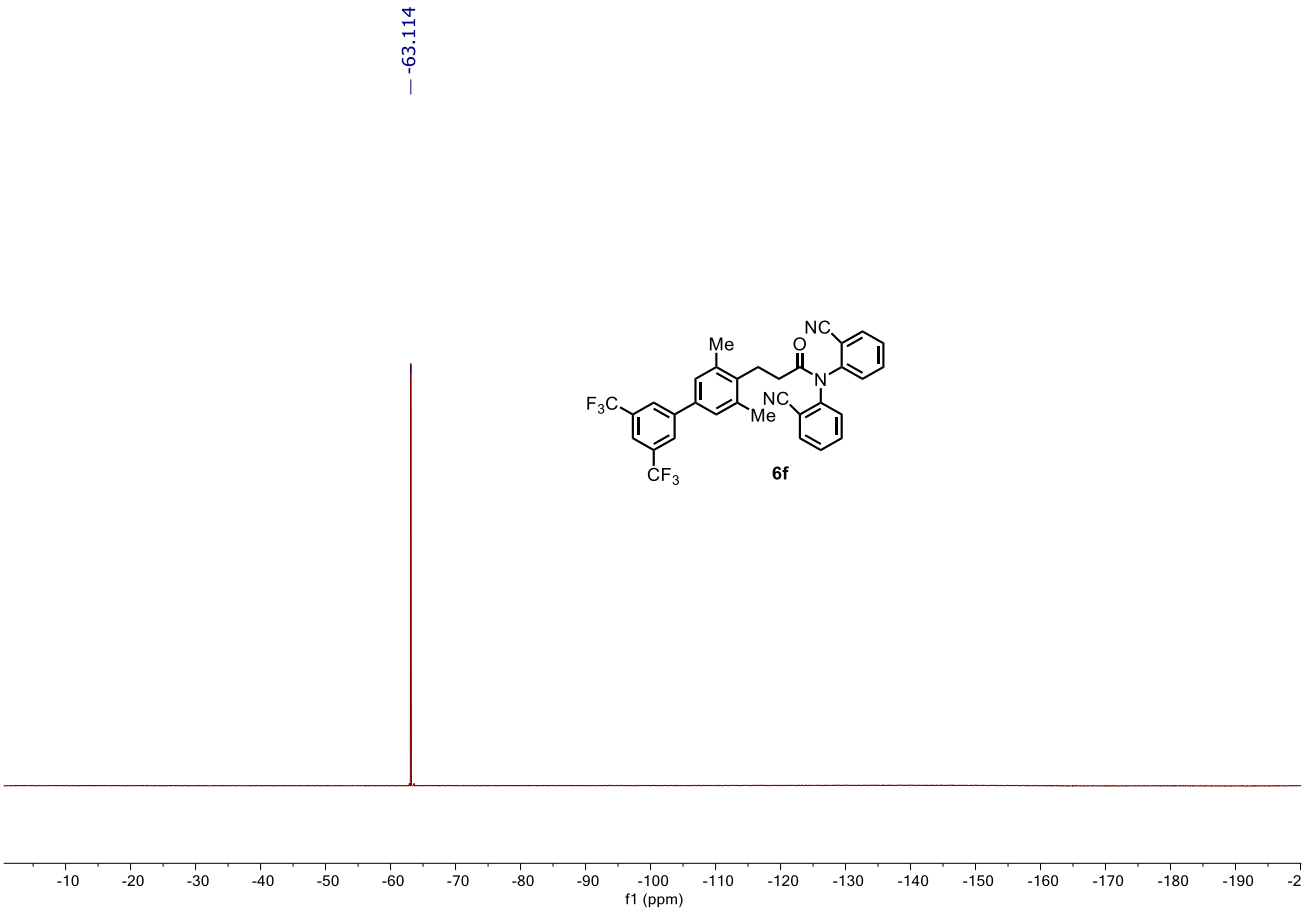
7.805
7.804
7.803
7.801
7.798
7.797
7.795
7.786
7.784
7.782
7.707
7.694
7.656
7.513
7.457
7.260
7.198
3.201
3.187
3.175
2.515
2.493
2.439
2.335
NC
Me
O
N
NC
Me
F3C
CF3
6f
2.04
3.04
3.13
3.02
2.00
2.05
2.19
6.10
f1 (ppm)


172.00
144.47
144.35
143.31
138.38
137.80
136.29
135.13
134.72
134.53
134.00
132.51
132.29
132.07
131.85
130.53
129.70
129.29
128.61
127.23
127.18
126.35
124.54
122.73
120.92
120.86
120.84
120.81
117.36
116.54
113.43
113.26
77.47
77.26
77.05
33.87
25.36
20.06
Me
O
NC
N
NC
Me
F3C
CF3
6f
20 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


-63.114
Me
O
NC
N
NC
Me
F3C
CF3
6f
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -2
f1 (ppm)

REFERENCES

1. Shen, P.-X., Wang, X.-C., Wang, P., Zhu, R.-Y. & Yu, J.-Q. Ligand-enabled *meta*-C–H alkylation and arylation using a modified norbornene. *J. Am. Chem. Soc.* **137**, 11574−11577 (2015).
2. Zhang, Z., Tanaka, K. & Yu, J.-Q. Remote site-selective C–H activation directed by a catalytic bifunctional template nature. *Nature* **543**, 538−542 (2017).
3. Hong, F., Chen, Y., Lu, B. & Cheng, J. One-pot assembly of fused heterocycles *via* oxidative palladium-catalyzed cyclization of arylols and iodoarenes. *Adv. Synth. Catal.* **358**, 353−357 (2016).
4. Fu, H., et al. Ligand-enabled alkynylation of C(sp^3)−H bonds with palladium(II) catalysts. *Angew. Chem., Int. Ed.* **56**, 1873−1876 (2017).
5. Yang, G., Zhu, D., Wang, P., Tang, R.-Y. & Yu, J.-Q. Remote C−H activation of various *N*-heterocycles using a single template. *Chem. Eur. J.* **24**, 3434−3438 (2018).
6. Leow, D., Li, G., Mei, T.-S. & Yu, J.-Q. Activation of remote *meta*-C–H bonds assisted by an end-on template. *Nature* **486**, 518−522 (2012).
7. *Gaussian 09, Revision A.02*, Frisch, M. J., et al. Gaussian, Inc., Wallingford CT, **2009**.
8. Becke, A. D. Density-functional thermochemistry. III. The role of exact exchange. *J. Chem. Phys.* **98**, 5648−5652 (1993).
9. Lee, C., Yang, W. & Parr, R. G. Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. *Phys. Rev. B* **37**, 785−789 (1988).
10. Becke, A. D. A new mixing of Hartree–Fock and local density-functional theories. *J. Chem. Phys.* **98**, 1372−1377 (1993).
11. Stephens, P. J., Devlin, F. J., Chabalowski, C. F. & Frisch, M. J. *Ab initio* calculation of vibrational absorption and circular dichroism spectra using density functional force fields. *J. Phys. Chem.* **98**, 11623−11627 (1994).
12. Ditchfield, R., Hehre, W. J. & Pople, J. A. Self-consistent molecular-orbital methods. IX. An extended Gaussian-type basis for molecular-orbital studies of organic molecules. *J. Chem. Phys.* **54**, 724−728 (1971).
13. Hehre, W. J., Ditchfield, R. & Pople, J. A. Self-consistent molecular orbital methods. XII. Further extensions of Gaussian-type basis sets for use in molecular orbital studies of organic molecules. *J. Chem. Phys.* **56**, 2257−2261 (1972).
14. Hay, P. J. & Wadt, W. R. *Ab initio* effective core potentials for molecular calculations. Potentials for K to Au including the outermost core orbitals. *J. Chem. Phys.* **82**, 299−310 (1985).
15. Roy, L. E., Hay, P. J. & Martin, R. L. Revised basis sets for the LANL effective core potentials. *J. Chem. Theory Comput.* **4**, 1029−1031 (2008).
16. Zhao, Y. & Truhlar, D. G. The M06 suite of density functionals for main group thermochemistry, thermochemical kinetics, noncovalent interactions, excited states, and transition elements: two new

functionals and systematic testing of four M06-class functionals and 12 other functionals. *Theor. Chem. Acc.* **120**, 215−241 (2008).

17. Marenich, A. V., Cramer, C. J. & Truhlar, D. G. Universal solvation model based on solute electron density and on a continuum model of the solvent defined by the bulk dielectric constant and atomic surface tensions. *J. Phys. Chem. B* **113**, 6378−6396 (2009).
18. Dolg, M., Wedig, U., Stoll, H. & Preuss, H. Energy-adjusted *ab initio* pseudopotentials for the first row transition elements. *J. Chem. Phys.* **86**, 866−872 (1987).
19. Andrae, D., Haußermann, U., Dolg, M., Stoll, H. & Preu, H. *Ab initio* energy-adjusted pseudopotentials for the noble gases Ne through Xe: Calculation of atomic dipole and quadrupole polarizabilities. *Theor. Chem. Acc.* **77**, 123−141 (1990).
20. Legault, C. Y. CYLview, 1.0b; Universitéde Sherbrooke, 2009 (http://www.cylview.org).
21. Hariharan, P. C. & Pople, J. A. The influence of polarization functions on molecular orbital hydrogenation energies. *Theor. Chim. Acta* **28**, 213−222 (1973).