Supporting Information

Palladium-Catalyzed Chemoselective Direct α-Arylation of Carbonyl Compounds with Chloroaryl Triflates at the C−Cl Site

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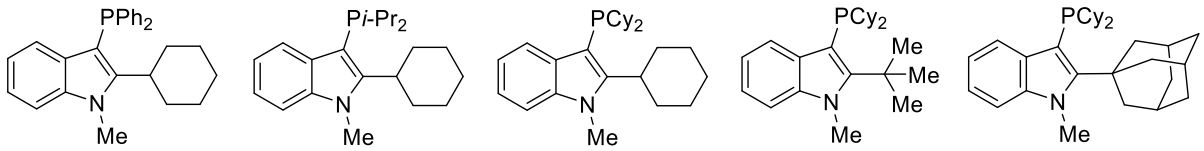
1. General considerations

Unless otherwise noted, all reagents were purchased from commercial suppliers and used without purification. All Pd-catalyzed cross-coupling reactions were performed in resealable screw cap Schlenk tube (approx. 20 mL volume) in the presence of Teflon-coated magnetic stir bar (5 mm x 10 mm). Solvents were distillated following the standard procedures under nitrogen.[1] Thin layer chromatography was performed on pre-coated silica gel 60 F_{254} plates. Silica gel (Merck, 70-230 and 230-400 mesh) was used for column chromatography. Melting points were recorded on an uncorrected Stuart Melting Point SMP30 instrument. NMR spectra were recorded on a Brüker spectrometer (400 MHz for ^{1}H, 100 MHz for ^{13}C, 376 MHz for ^{19}F and 162 MHz for ^{31}P) or JEOL JMN-ECZ500R/S1 spectrometer (465.89 MHz for ^{19}F and 200.43 MHz for ^{31}P). Spectra were referenced internally to the residual proton resonance in $CDCl_3$ (δ 7.26 ppm) as the internal standard. Chemical shifts (δ) were reported as part per million (ppm) in δ scale downfield from TMS. ^{13}C NMR spectra were referenced to $CDCl_3$ (δ 77.0 ppm, the middle peak). ^{31}P NMR spectra were referenced to 85% H_3PO_4 externally. Coupling constants (*J*) were reported in Hertz (Hz). Mass spectra (EI-MS) was recorded on a HP5977A MSD Mass Spectrometer. High-resolution mass spectra (HRMS) were obtained on Agilent 6540 ESI-QTOF-MS (ESI-MS), Agilent 6540 APPI-QTOF-MS (APPI-MS) or Waters GCT Premier mass spectrometer (EI-MS). GC-MS analysis was conducted on a HP 7890B GC system using a HP5MS column (30 m × 0.25 mm). The products described in GC yield were accorded to the authentic samples/dodecane calibration standard from HP 7890B GC-FID system. All yields reported refer to isolated yield of compounds estimated to be greater than 95% purity as determined by capillary gas chromatography (GC) or ^{1}H NMR. Compounds described in the literature were characterized by comparison of their ^{1}H, ^{13}C and/or ^{19}F NMR spectra to the previously reported data.

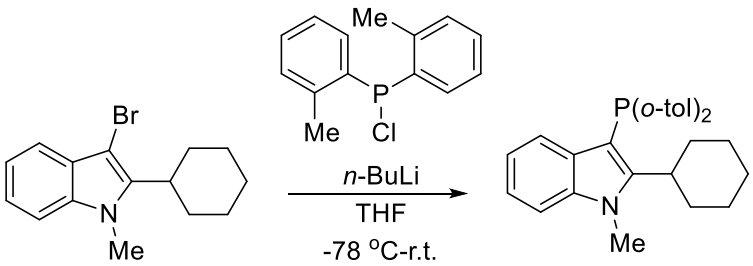
2. The preparation of ligands

The following alkyl-indole phosphine ligands (**L13**, **L15**, **L16**, **L21** and **L22**) were prepared according to the reported procedures.[2]



L13 **L15** **L16** **L21** **L22**

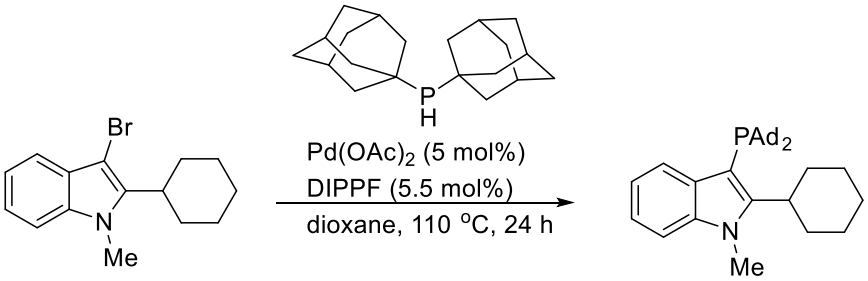
2-Cyclohexyl-3-(di-*o*-tolylphosphaneyl)-1-methyl-1*H*-indole (L14)



A 50 mL Schlenk flask was added 3-bromo-2-cyclohexyl-1-methyl-1*H*-indole (877 mg, 3.0 mmol). The flask was then evacuated and flushed with nitrogen (3 cycles) followed by the addition of freshly distilled THF (30 mL). The reaction mixture was cooled to -78 °C. *n*-BuLi (3.3 mmol) was added dropwise while stirring. The solution was stirred at -78 °C for 20 min. Di(*o*-tolyl)chlorophosphine (821 mg, 3.3 mmol) was dissolved in freshly distilled THF (5.0 mL) and the solution was then added dropwise. The resulting solution was allowed to stir at room temperature overnight. After completion of the reaction, solvent was removed under vacuum and distilled MeOH was added to precipitate the product. After solvent was removed by filtration, the crude product was further washed with distilled MeOH to give the product as a white solid (252.0 mg, 20%).

M.P.: 175.8-176.8 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, J = 8.1 Hz, 1H), 7.27–7.07 (m, 9H), 6.95 (d, J = 7.7 Hz, 1H), 6.85–6.81 (m, 1H), 3.90 (s, 3H), 3.61 (s, 1H), 2.39 (s, 6H), 2.14–2.10 (m, 2H), 1.90–1.79 (m, 5H), 1.46–1.32 (m, 3H); ^{31}P NMR (200.43 MHz, $CDCl_3$) δ -43.5; ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.5, 152.2, 141.9, 141.7, 138.5, 135.9, 135.8, 132.3, 131.0, 129.94, 129.9, 127.8, 125.5, 120.9, 120.8, 119.6, 108.8, 98.6, 37.9, 37.8, 31.4, 27.0, 26.0, 21.4, 21.2. HRMS (APPI): calculated for $C_{29}H_{33}NP^{+}$: 426.2345, found: 426.2340.

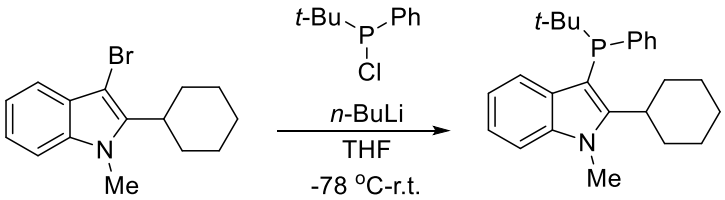
2-Cyclohexyl-3-(di-adamantan-1-yl)phosphaneyl)-1-methyl-1*H*-indole (L17)



A Schlenk flask was added $Pd(OAc)_2$ (28.1 mg, 5 mol%) and DIPPF (57.5 mg, 5.5 mol%). The flask was then evacuated and flushed with nitrogen (3 cycles) followed by the addition of freshly distilled dioxane (5.0 mL). The mixture was stirred at room temperature for 5 min. Another Schlenk flask was added di-1-adamantylphosphine (756.1 mg, 2.5 mmol), 3-bromo-2-cyclohexyl-1-methyl-1*H*-indole (730 mg, 2.5 mmol) and NaO*t*Bu (360 mg, 3.75 mmol). The flask was then evacuated and flushed with nitrogen (3 cycles) followed by the addition of freshly distilled dioxane (7.5 mL) and the freshly prepared catalyst stock solution. The mixture was stirred at 110 °C for 24 h. After completion of the reaction, the mixture was filtered over celite. The filtrate was concentrated and washed with distilled MeOH to give the product as a white solid (553.8 mg, 43%).

M.P.: 248.0-249.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (d, J = 8.0 Hz, 1H), 7.28 (d, J = 8.0 Hz, 1H), 7.20–7.16 (m, 1H), 7.13–7.09 (m, 1H), 3.88 (s, 3H), 2.07–1.53 (m, 41H); ^{31}P NMR (200.43 MHz, *d*-benzene) δ 19.2; ^{13}C NMR (100 MHz, $CDCl_3$) δ 155.5 (d, J = 40.1 Hz), 138.5, 130.5 (d, J = 4.7 Hz), 124.5, 120.5, 119.0, 108.5, 101.6 (d, J = 17.4 Hz), 42.8 (d, J = 12.8 Hz), 36.88, 36.85 (d, J = 19.1 Hz), 32.3, 30.7, 29.0 (d, J = 8.9 Hz), 26.8, 26.3. HRMS (ESI): calculated for $C_{35}H_{49}NP^{+}$: 514.3597, found: 514.3604.

3-(*tert*-Butyl(phenyl)phosphaneyl)-2-cyclohexyl-1-methyl-1*H*-indole (L18)

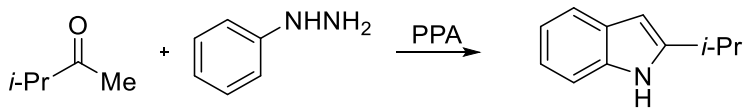


A 100 mL Schlenk flask was added 3-bromo-2-cyclohexyl-1-methyl-1*H*-indole (1.27 g, 4.35 mmol). The flask was then evacuated and flushed with nitrogen (3 cycles) followed by the addition of freshly distilled THF (30 mL). The reaction mixture was cooled to -78 °C. *n*-BuLi (4.73 mmol) was added dropwise while stirring. The solution was stirred at -78 °C for 20 min. Chloro(*tert*-butyl)phenylphosphine (863 mg, 4.30 mmol) was added dropwise. The resulting

solution was allowed to stir at room temperature overnight. After completion of the reaction, solvent was removed under vacuum and distilled MeOH was added to precipitate the product. After solvent was removed by filtration, the crude product was further washed with distilled anhydrous MeOH to give the product as a white solid (1.22 g, 74%).

M.P.: 176.0-178.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54–7.51 (m, 2H), 7.31 (d, J = 8.1 Hz, 1H), 7.25–7.10 (m, 5H), 6.91–6.88 (m, 1H), 3.92 (s, 3H), 2.05–1.82 (m, 7H), 1.57–1.32 (13H); ^{31}P NMR (162 MHz, $CDCl_3$) δ -7.7; ^{13}C NMR (100 MHz, $CDCl_3$) δ 154.4 (d, J = 37.2 Hz), 139.5 (d, J = 15.2 Hz), 138.9 (d, J = 2.8 Hz), 131.5 (d, J = 14.4 Hz), 129.3 (d, J = 4.3 Hz), 127.7 (d, J = 4.0 Hz), 126.0, 123.3, 120.8, 119.1, 108.7, 102.3 (d, J = 6.7 Hz), 37.8, 37.6, 32.4, 32.2, 32.0, 31.8, 30.9, 30.2, 30.1, 26.94, 26.9, 26.2. HRMS (ESI): calculated for $C_{25}H_{33}NP^{+}$: 378.2345, found: 378.2349.

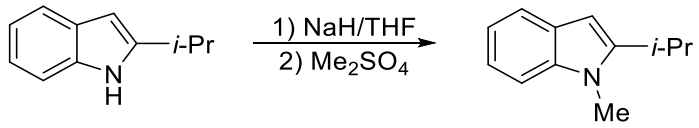
2-Isopropyl-1*H*-indole



3-Methyl-2-butanone (2.1 mL, 20 mmol) was mixed with phenylhydrazine (2.4 ml, 24 mmol), and stirring was started. About 25 g of polyphosphoric acid was added to the mixture. An exothermic reaction ensured whereupon the mixture was heated to 85 °C. The temperature was then increased from 85 ºC to 110 °C gradually. This process was conducted around 30 min. The mixture was then kept at 110 ºC for another 1 h. The mixture was poured into ice water and stirred for 1 h. The mixture was then extracted with Et_2O. The organic phase was combined and dried over Na_2SO_4. The concentrated organic phase was filtered through a short silica pad and eluted with ethyl acetate/hexane (1:9) mixture. The solution was evaporated to yield a solid product. The product was further washed with hexane. The white solid was filtered and dried under vacuum to yield 2-isopropyl-1*H*-indole (1.59 g, 50%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (br s, 1H), 7.60 (d, J = 7.6 Hz, 1H), 7.33 (d, J = 7.8 Hz, 1H), 7.20–7.12 (m, 2H), 6.30 (s, 1H), 3.13–3.03 (m, 1H), 1.39 (d, J = 6.9 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.9, 135.6, 128.5, 120.9, 119.8, 119.5, 110.3, 97.3, 27.6, 22.4. The data are in agreement with those previously reported in the literature.[3]

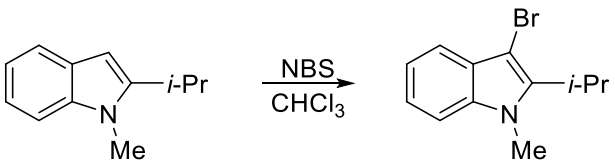
2-Isopropyl-1-methyl-1*H*-indole



2-Isopropyl-1*H*-indole (1.27 g, 8.0 mmol) was placed in the dropping funnel and dissolved with 25 mL tetrahydrofuran. The solution was added dropwise to the 2.5 equivalent sodium hydride (0.8 g, 20 mmol, 60% dispersion in mineral oil) which suspended in 25 mL tetrahydrofuran at room temperature. Sodium hydride was washed with anhydrous hexane (5 mL x 3) to remove mineral oil prior to usage. Additional 5 mL tetrahydrofuran was added to rinse out the dropping funnel, after completion of the addition of 25 mL tetrahydrofuran solution. The reaction mixture was refluxed for 15 minutes and then stirred at room temperature for 1 hour. Dimethyl sulfate (1.89 mL, 20 mmol) was added to the reaction mixture and the reaction mixture was allowed to stir for overnight. Methanol was added to the reaction mixture which was then concentrated under reduced pressure. The concentrated mixture was diluted with ethyl acetate and washed with water and brine. The organic layer was dried over Na_2SO_4, and then concentrated. The concentrated mixture was applied to a short silica pad and eluted with ethyl acetate/hexane (1:20) mixture. The solution was evaporated to yield 2-isopropyl-1-methyl-1*H*-indole as yellow liquid (1.26 g, 91%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 8.1 Hz, 1H), 7.23 (t, *J* = 8.1 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 6.34 (s, 1H), 3.75 (s, 3H), 3.19–3.09 (m, 1H), 1.41 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.6, 137.3, 127.8, 120.5, 119.8, 119.2, 108.7, 96.1, 29.4, 25.9, 22.5. The data are in agreement with those previously reported in the literature.[4]

3-Bromo-2-isopropyl-1-methyl-1*H*-indole

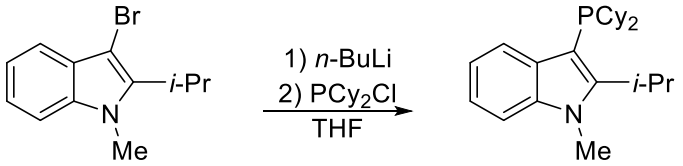


N-Bromosuccinimide (1.24 g, 7.0 mmol) was added to a solution of 2-isopropyl-1-methyl-1*H*-indole (1.21 g, 7.0 mmol) in anhydrous chloroform (50 mL) in portion at 0 °C. After stirring for 30 min, DCM and water were added to the mixture and the organic phase was separated. The organic layer was washed with water and then with brine. The organic layer was dried over Na_2SO_4, and then concentrated. The concentrated mixture was applied to a short silica pad and

eluted with ethyl acetate/hexane (1:20) mixture. The eluent was evaporated to yield 3-bromo-2-isopropyl-1-methyl-1*H*-indole as yellow liquid product (1.69 g, 96%).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 7.7 Hz, 1H), 7.34–7.22 (m, 3H), 3.81 (s, 3H), 3.58–3.47 (m, 1H), 1.55 (d, *J* = 7.2 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 136.2, 127.3, 121.9, 120.0, 118.5, 109.0, 87.7, 30.7, 26.3, 20.8; HRMS (ESI): calcd. for $C_{12}H_{15}BrN^{+}$: 252.0382, found 252.0385.

3-(Dicyclohexylphosphaneyl)-2-isopropyl-1-methyl-1*H*-indole (L19)



3-Bromo-2-isopropyl-1-methyl-1*H*-indole (1.25 g, 5.00 mmol) was dissolved in freshly distilled THF (15 mL) at room temperature under nitrogen atmosphere. The solution was cooled to -78 ^{o}C. Titrated *n*-BuLi (5.25 mmol) was added dropwise with a syringe. After the reaction mixture was stirred for 30 min at -78 ^{o}C, chlorodicyclohexylphosphine (1.16 mL, 5.25 mmol) was added. The reaction was allowed to warm to room temperature and stirred for overnight. The solvent was removed under reduced pressure. The solid product was washed with methanol successively. The white solid was collected by filtration and dried over vacuum to afford 3-(dicyclohexylphosphaneyl)-2-isopropyl-1-methyl-1*H*-indole (1.43 g, 77%).

M.P.: 144.5–146.0 °C. ^{1}H NMR (400 MHz, C_6D_6) δ 7.93 (d, *J* = 4.7 Hz, 1H), 7.25–7.20 (m, 2H), 7.04–7.02 (m, 1H), 4.36–4.23 (m, 1H), 3.12 (s, 3H), 2.56–2.45 (m, 2H), 2.16–2.07 (m, 2H), 1.81–1.68 (m, 4H), 1.59–1.07 (m, 20H); ^{13}C NMR (100 MHz, C_6D_6) δ 154.3, 153.9, 138.60, 138.58, 130.5, 121.0, 120.8, 119.6, 109.1, 101.8, 101.7, 34.1, 34.0, 32.6, 32.4, 30.64, 30.56, 30.48, 27.03, 27.01, 27.0, 26.9, 26.4, 26.1, 25.9, 21.5; ^{31}P NMR (162 MHz, C_6D_6) δ -19.9. HRMS (ESI): calcd. for $C_{24}H_{37}NP^{+}$: 370.2658, found 370.2662.

3. General procedures for condition optimization and scope

3.1 General procedures for condition optimization (GP1)

A Schlenk tube with Teflon-coated magnetic stir bar was added palladium source (4.0 mol% of Pd), **L15** (Pd/L ratio was indicated), 1-methylindolin-2-one (0.20 mmol), and base (0.40 mmol). It was evacuated and flushed with nitrogen (3 cycles). 3-Chlorophenyl trifluoromethanesulfonate (0.20 mmol) and solvent (1.0 mL) were then added by syringes. The Schlenk tube was sealed and stirred at room temperature for 1 min. Then it was stirred at 110 ^{o}C for indicated time. Water, ethyl acetate, and dodecane (45.2 μL, internal standard) were added. The organic layer after extraction was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.

3.2 General procedures for ligand screening (GP2)

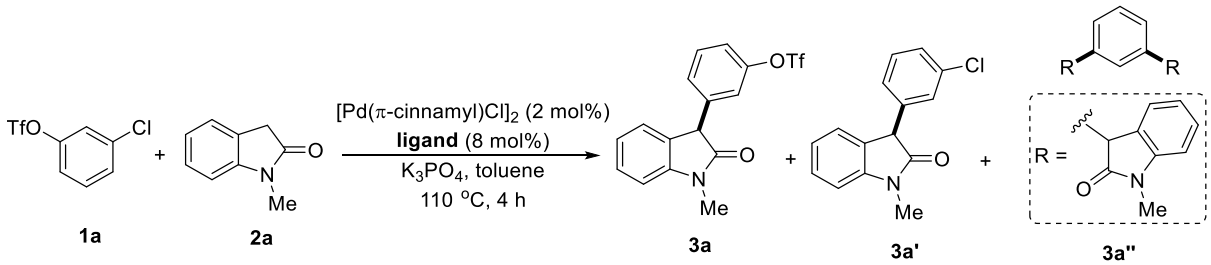
A Schlenk tube with Teflon-coated magnetic stir bar was added palladium(π-cinnamyl) chloride dimer (2.0 mol%), ligand (4.0-8.0 mol%, if solid), 1-methylindolin-2-one (0.20 mmol), and K_3PO_4 (0.40 mmol). It was evacuated and flushed with nitrogen (3 cycles). 3-Chlorophenyl trifluoromethanesulfonate (0.20 mmol) and toluene (1.0 mL) were then added by syringes. The Schlenk tube was sealed and stirred at room temperature for 1 min. Then it was stirred at 110 ^{o}C for 4 h. Water, ethyl acetate, and dodecane (45.2 μL, internal standard) were added. The organic layer after extraction was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.

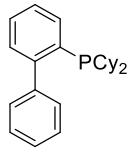
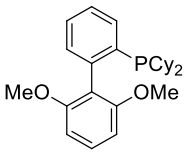
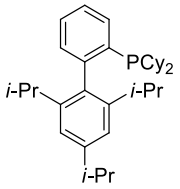
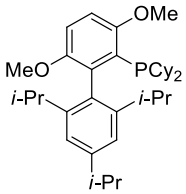
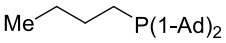
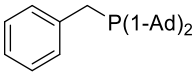
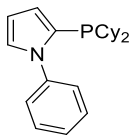
3.3 General procedures for the entries of the scope (GP3)

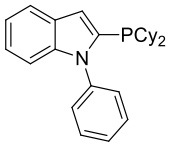
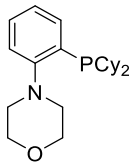
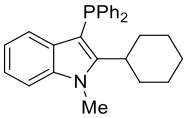
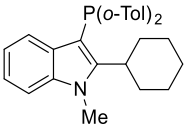
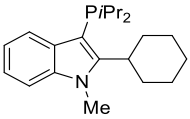
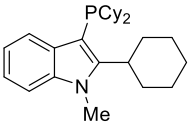
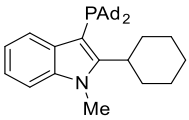
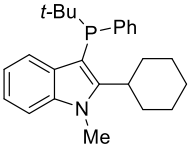
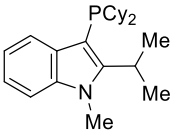
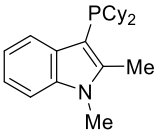
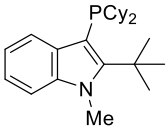
A Schlenk tube with Teflon-coated magnetic stir bar was added palladium(π-cinnamyl) chloride dimer (2.0 mol%), **L15** or **L18** (8.0 mol%), substrates (0.20 mmol, if solid), and K_3PO_4 (amount was indicated). It was evacuated and flushed with nitrogen (3 cycles). Substrates (0.20 mmol, if liquid) and toluene (1.0 mL) were then added by syringes. The Schlenk tube was sealed and stirred at room temperature for 1 min. Then it was stirred at indicated temperature for indicated time. Water and ethyl acetate were added. The organic layer after extraction was collected and subjected to column chromatography (on silica gel) to afford the product.

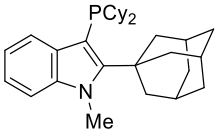
4. Data of screening and scope

Table S1 Screening of ligands[a]



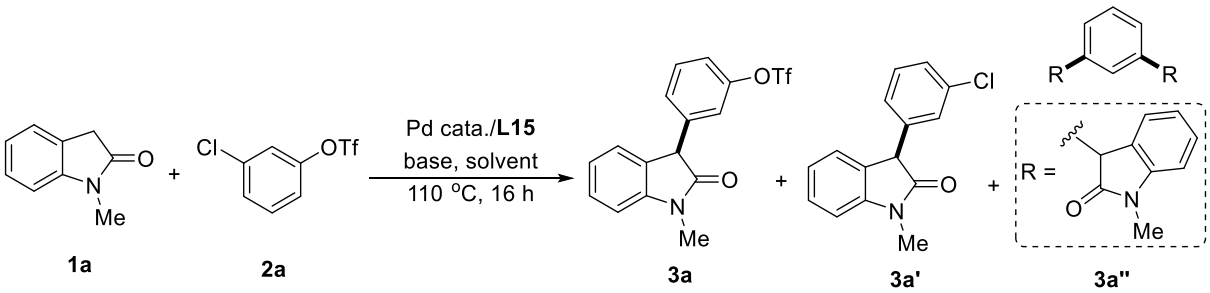
code	ligand	yield of 3a (%)	yield of 3a' (%)	yield of 3a'' (%)	ratio (%) of products (3a : 3a' : 3a'')
L1	PPh_3	n.d.	42	n.d.	0 : 100 : 0
L2	PCy_3	12	17	n.d.	41 : 59 : 0
L3	P^tBu_3	5 <	n.d.	n.d.	100 : 0 : 0
L4		5 <	38	n.d.	10 : 90 : 0
L5		n.d.	63	n.d.	0 : 100 : 0
L6		n.d.	85	n.d.	0 : 100 : 0
L7		n.d.	94	n.d.	0 : 100 : 0
L8		17	n.d.	n.d.	100 : 0 : 0
L9		19	n.d.	n.d.	100 : 0 : 0
L10		33	10	n.d.	77 : 23 : 0

L11		22	22	n.d.	50 : 50 : 0
L12		n.d.[b]	15[b]	n.d. [b]	0 : 100 : 0
L13		n.d. 13[b]	65 18[b]	n.d. n.d.[b]	0 : 100 : 0 42 : 58 : 0
L14		32 30[b]	n.d. n.d.[b]	n.d. n.d.[b]	100 : 0 : 0 100 : 0 : 0
L15		86	n.d.	n.d.	100 : 0 : 0
L16		80	n.d.	n.d.	100 : 0 : 0
L17		30	n.d.	n.d.	100 : 0 : 0
L18		74	n.d.	n.d.	100 : 0 : 0
L19		51	n.d.	n.d.	100 : 0 : 0
L20		12	< 5	n.d.	75 : 25 : 0
L21		6	n.d.	n.d.	100 : 0 : 0

L22		8	n.d.	n.d.	100 : 0 : 0

[a]Reaction condition: **1a** (0.20 mmol), **2a** (0.20 mmol), Pd:L = 1:2, K_3PO_4 (0.40 mmol), toluene (1.0 mL), under N_2 for 4 h. The yield was calibrated by GC-FID using dodecane as internal standard; [b]Ligand (4.0 mol%) was used.

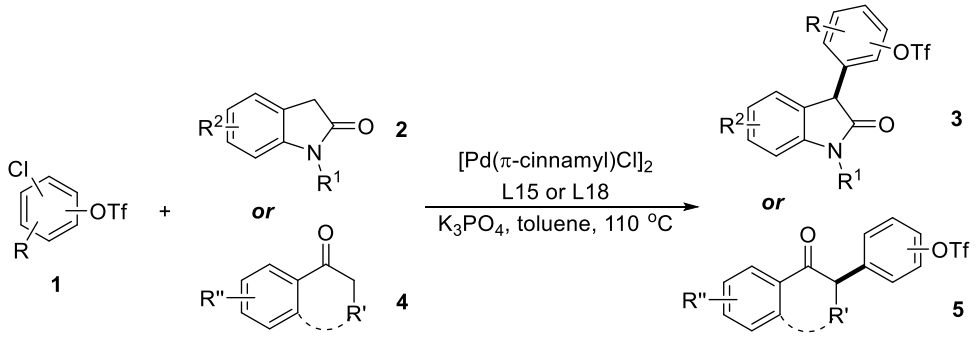
Table S2 Condition screening[a]

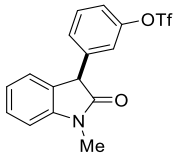
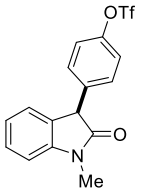
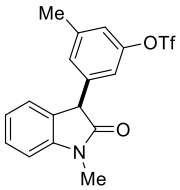
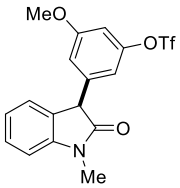
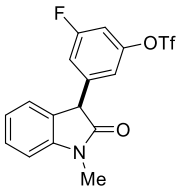
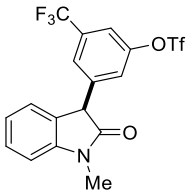


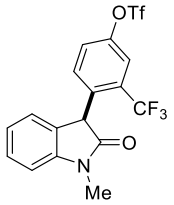
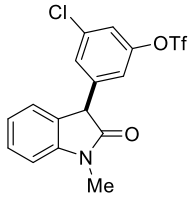
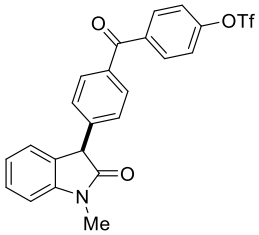
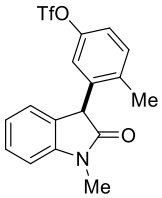
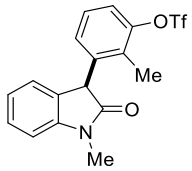
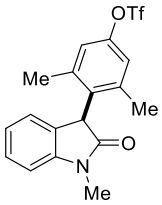
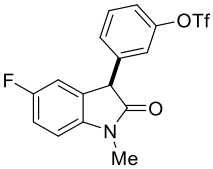
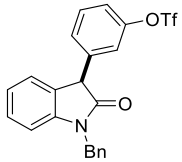
entry	catalyst (mol%)	base	solvent	3a (%)	3a' (%)	3a'' (%)
1	$Pd(OAc)_2$ (4)	K_3PO_4	toluene	62	n.d.	n.d.
2	$Pd(dba)_2$ (4)	K_3PO_4	toluene	81	n.d.	n.d.
3	[Pd(π-cinnamyl)Cl]$_2$ (2)	K_3PO_4	toluene	90 (88[b])	n.d.	n.d.
4	[Pd(π-cinnamyl)Cl]$_2$ (2)	K_2CO_3	toluene	19	n.d.	n.d.
5	[Pd(π-cinnamyl)Cl]$_2$ (2)	Cs_2CO_3	toluene	2<	n.d.	n.d.
6	[Pd(π-cinnamyl)Cl]$_2$ (2)	NaO*t*Bu	toluene	2 <	n.d.	n.d.
7	[Pd(π-cinnamyl)Cl]$_2$ (2)	K_3PO_4	THF	81	n.d.	n.d.
8	[Pd(π-cinnamyl)Cl]$_2$ (2)	K_3PO_4	dioxane	83	n.d.	n.d.
9[c]	[Pd(π-cinnamyl)Cl]$_2$ (2)	K_3PO_4	toluene	84	n.d.	n.d.
10[d]	[Pd(π-cinnamyl)Cl]$_2$ (2)	K_3PO_4	toluene	78	n.d.	n.d.

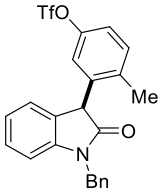
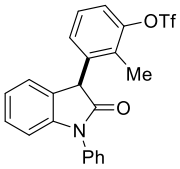
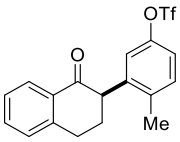
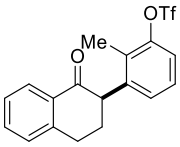
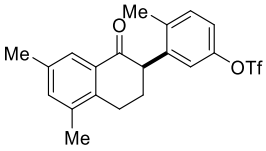
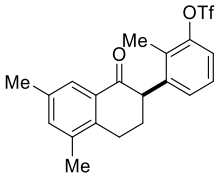
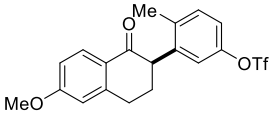
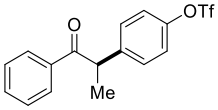
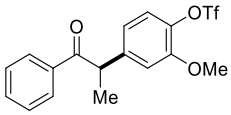
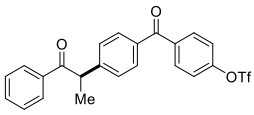
[a]Reaction condition: **1b** (0.20 mmol), **2a** (0.20 mmol), Pd:L = 1:2, base (0.40 mmol), solvent (1.0 mL), under N_2. The yield was calibrated by GC-FID using dodecane as internal standard. n.d. = not detected; [b]Isolated yield; [c]Reaction time: 12 h; [d]Pd:ligand = 1:1.

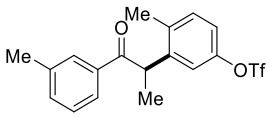
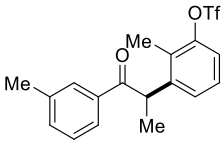
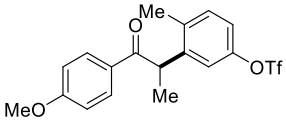
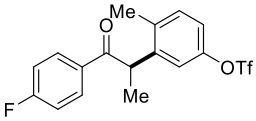
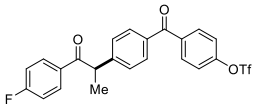
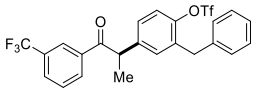
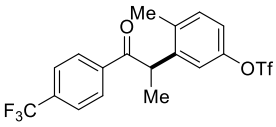
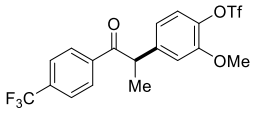
Table S3 Chemoselectivity data of the scope[a]



entry	product (reacting at C–Cl bond)	major product (%) (reacting at C–Cl bond)	minor product (%)[b] (reacting at C–OTf bond)	difunctionalized product (%)[b] (reacting at both C–Cl & C–OTf)
Scheme 5, 3a		88 63[c]	n.d. n.d.	n.d. n.d.
Scheme 5, 3b		80[d] 56[c,d]	n.d. n.d.	n.d. n.d.
Scheme 5, 3c		91 70[c]	n.d. n.d.	n.d. n.d.
Scheme 5, 3d		79 68[c]	n.d. n.d.	n.d. n.d.
Scheme 5, 3e		84 70[c]	n.d. n.d.	n.d. n.d.
Scheme 5, 3f		81 71[c]	n.d. n.d.	n.d. n.d.

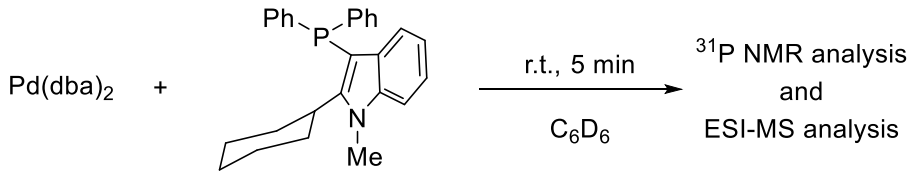
Scheme 5, 3g		80[c]	n.d.	n.d.
Scheme 5, 3h		54 48[c]	n.d. n.d.	n.d. n.d.
Scheme 5, 3i		71 57[c]	n.d. n.d.	n.d. n.d.
Scheme 5, 3j		81 92[c]	n.d. n.d.	n.d. n.d.
Scheme 5, 3k		88[c]	n.d.	n.d.
Scheme 5, 3l		73 84[c]	n.d. n.d.	n.d. n.d.
Scheme 5, 3m		88 64[c]	n.d. n.d.	n.d. n.d.
Scheme 5, 3n		79 73[c]	n.d. n.d.	n.d. n.d.

Scheme 5, 3o		78[c]	n.d.	n.d.
Scheme 5, 3p		93[c]	n.d.	n.d.
Scheme 8, 5a		81[c]	n.d.	n.d.
Scheme 8, 5b		79[c]	n.d.	n.d.
Scheme 8, 5c		64[c]	n.d.	n.d.
Scheme 8, 5d		75[c]	n.d.	n.d.
Scheme 8, 5e		53[c]	n.d.	n.d.
Scheme 8, 5f		62[c,e]	n.d.	n.d.
Scheme 8, 5g		66[c,e]	n.d.	n.d.
Scheme 8, 5h		68[c,e]	n.d.	n.d.

Scheme 8, 5i		74[c,e]	n.d.	n.d.
Scheme 8, 5j		53[c,e]	n.d.	n.d.
Scheme 8, 5k		60[c,e]	n.d.	n.d.
Scheme 8, 5l		71[c,e]	n.d.	n.d.
Scheme 8, 5m		66[c,e]	n.d.	n.d.
Scheme 8, 5n		60[c,e]	n.d.	n.d.
Scheme 8, 5o		72[c,e]	n.d.	< 3
Scheme 8, 5p		65[c,e]	n.d.	n.d.

[a]Reaction condition: **1** (0.20 mmol), **2** (0.20 mmol) or **4** (0.20 mmol), [Pd(π-cinnamyl)Cl]$_2$ (2.0 mol%), **L15** (8.0 mol%), Pd:L = 1:2, K_3PO_4 (0.4 mmol), toluene (1.0 mL), 110 °C, 16 h. Isolated yields were reported. n.d. = not detected; [b]GC-MS yields were reported; [c]**L18** (8.0 mol%) was used; [d]Reaction condition: 80 °C, 14 h; [e]K_3PO_4 (0.50 mmol) was used.

5. ^{31}P NMR and HRMS analysis for Pd/L13 species



L13

To an NMR tube was charged Pd(dba)$_2$ (4.6 mg, 0.0080 mmol), ligand **L13** (3.2 mg, 0.080 mmol, if Pd:L=1:1; 6.3 mg, 0.016 mmol, if Pd:L=1:2), and *d*-benzene. The tube was placed at room temperature and shook for 3 minutes. The mixture in the tube was subjected to ^{31}P NMR analysis. The ^{31}P signal located at -30.7 ppm was due to the free phosphine of **L13** (Fig. S1a). A new species with ^{31}P signal located at 9.05 ppm was observed in both cases of Pd:**L13**=1:1 (Fig. S1b) and 1:2 (Fig. S1c).

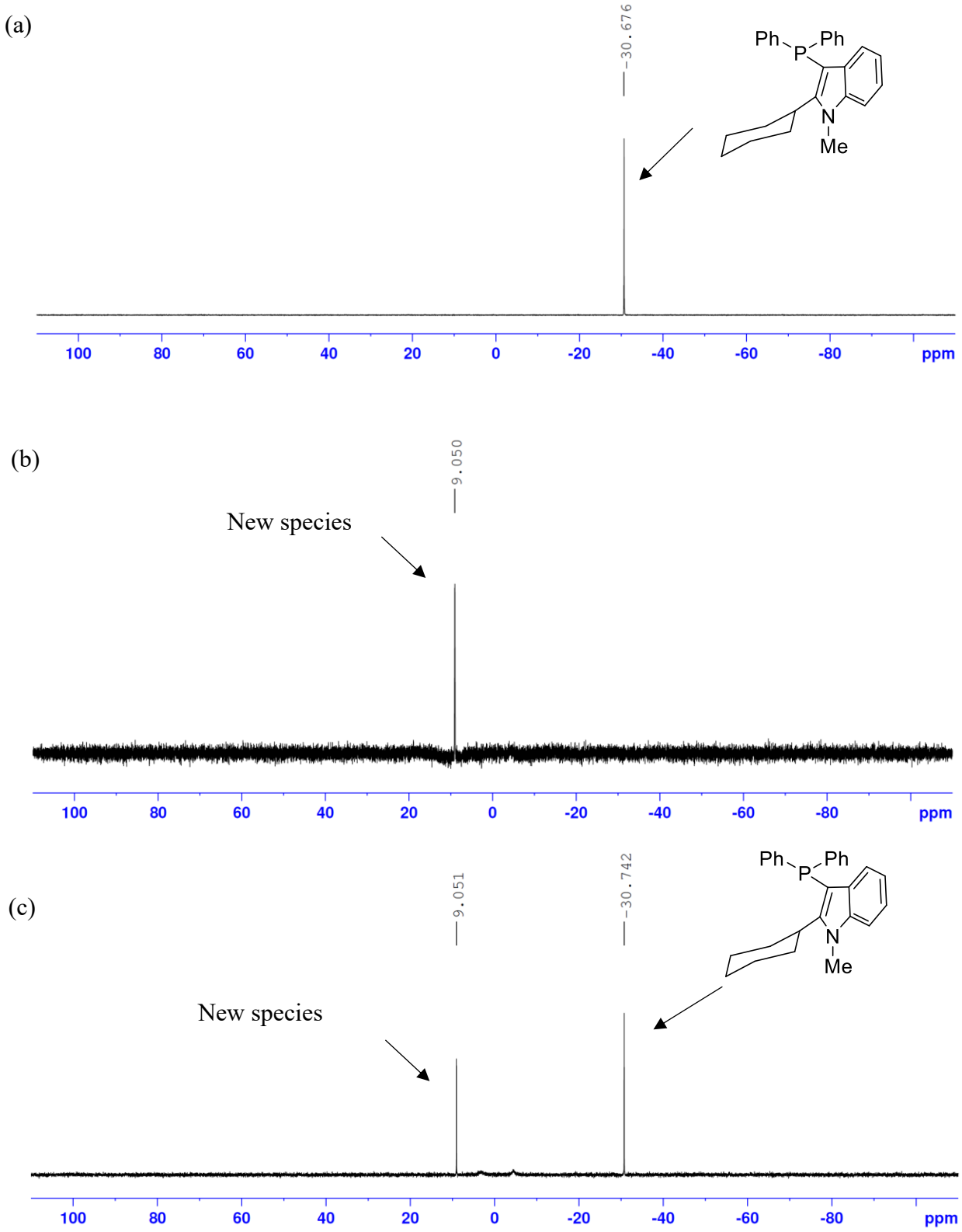
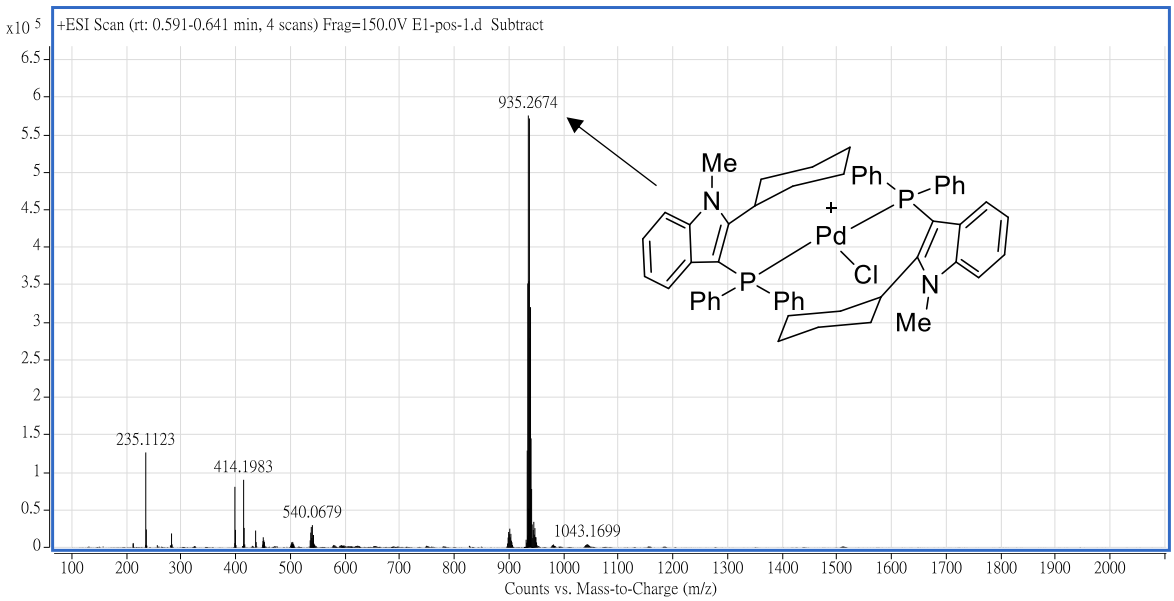


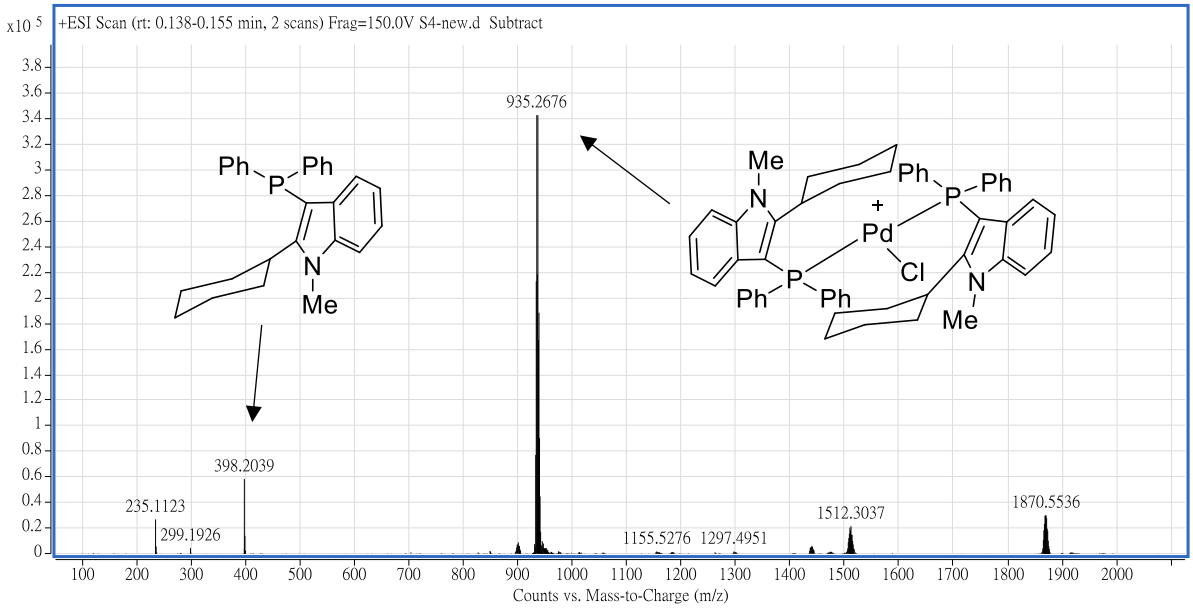
Fig. S1 ^{31}P NMR spectrum of (a) L13. (b) 4 mol% Pddba$_2$ and 4 mol% **L13** (Pd:L=1:1). (c) 4 mol% Pddba$_2$ and 8 mol% **L13** (Pd:L=1:2).

To confirm the coordination mode of the newly formed species, the mixtures were directly subjected to HRMS analysis. Fig. S2 depicts the ESI-MS spectrum showing one major cluster peak at m/z 935 in both cases of Pd:**L13**=1:1 (Fig. S2a) and 1:2 (Fig. S2b). This intense peak is assignable to the putative bisligated complex formulated as [$C_{54}H_{56}ClN_2P_2Pd$]. This formulation is supported by the observed agreement of the simulated isotopic pattern with the experiment pattern. These results might further support the readily formation of Pd(L13)$_2$.

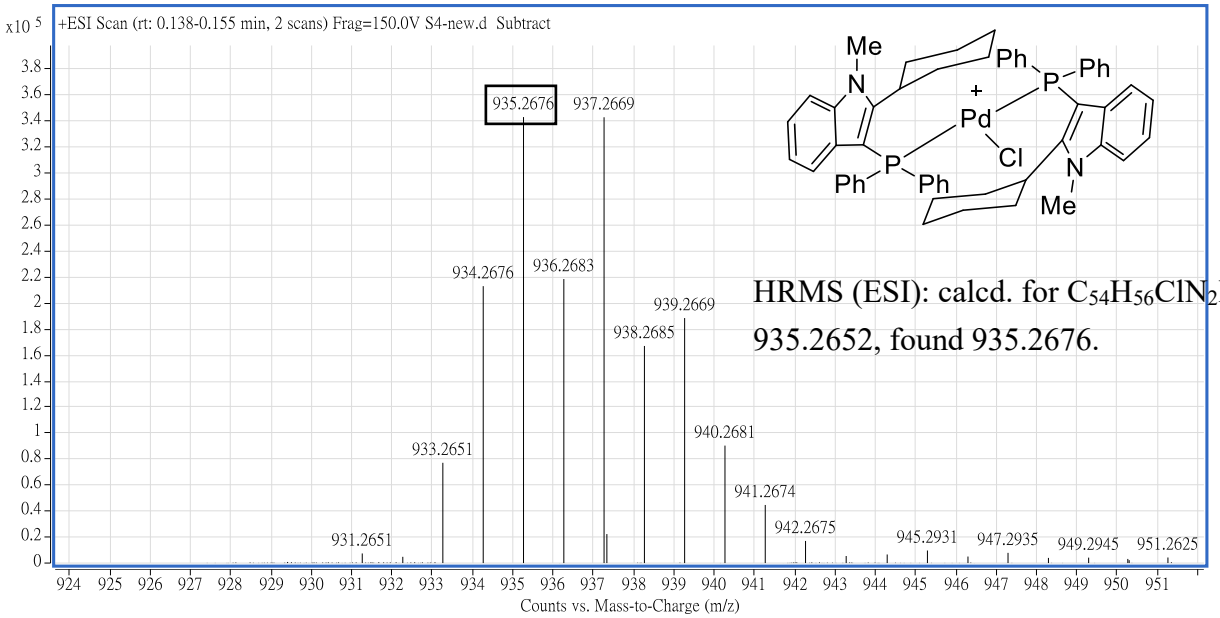
(a)



(b)



(c)



HRMS (ESI): calcd. for $C_{54}H_{56}ClN_2P_2Pd^+$: 935.2652, found 935.2676.

(d)

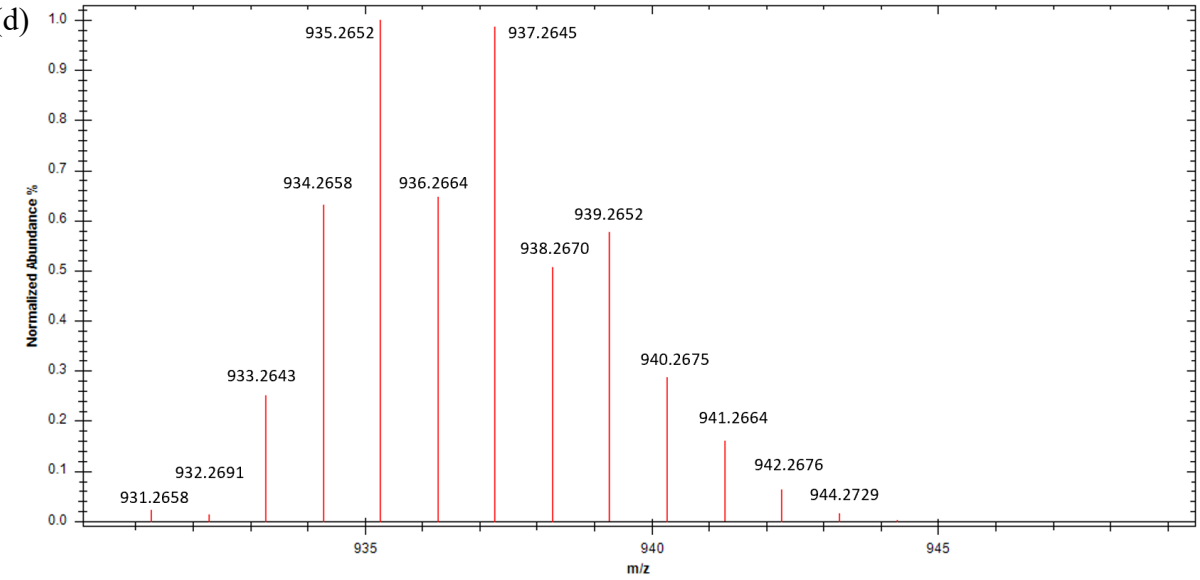
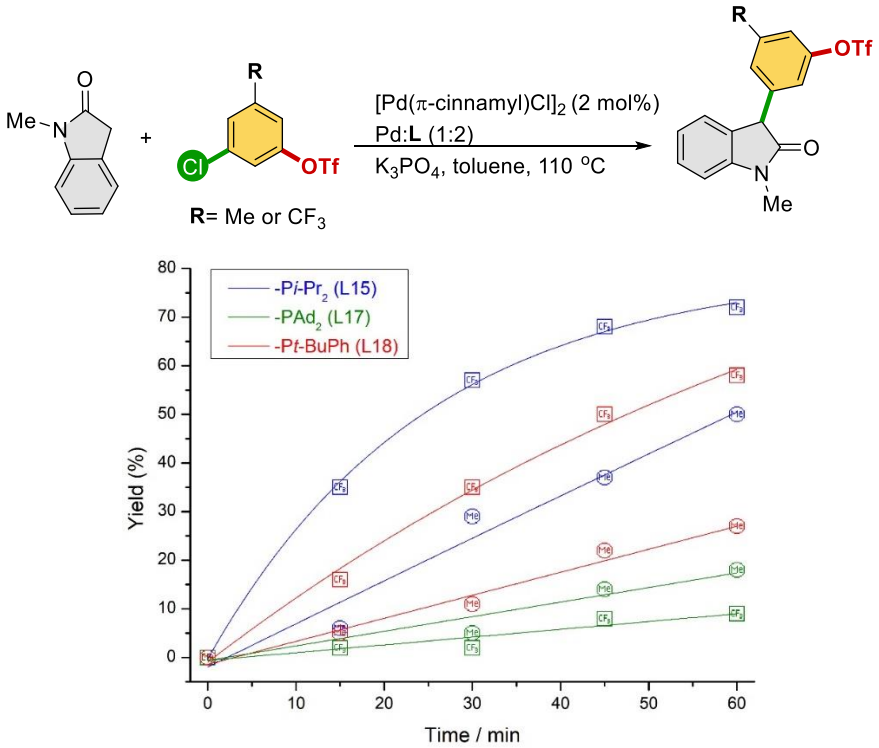


Fig. S2 Full scan ESI-MS spectrum of (a) 4 mol% $Pddba_2$ and 4 mol% **L13** (Pd:L=1:1). (b) 4 mol% $Pddba_2$ and 8 mol% **L13** (Pd:L=1:2). (c) The experimental isotopic pattern and (d) the simulated isotopic pattern of the cluster peak at m/z 935 based on the molecular formula of $C_{54}H_{56}ClN_2P_2Pd$ cationic complex

6. Reaction rate study of electronically different Cl-Ar-OTf in α-arylation reaction

General procedure for reaction rate study:

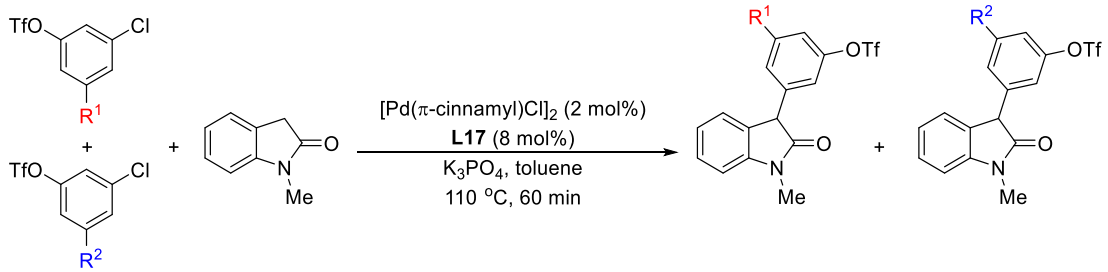
Palladium(π-cinnamyl) chloride dimer (41.4 mg, 0.080 mmol) and ligand (**L15** or **L18** or **L17,** 0.32 mmol) in 20.0 mL freshly distilled toluene (4.00 mol% Pd per 1.00 mL stock solution) was prepared was then prepared under N_2 with stirring up to dissolve all the solids (around 10 min). 1-Methylindolin-2-one (29.4 mg, 0.20 mmol) and K_3PO_4 (0.40 mmol) was added into a Schlenk tube with Teflon-coated magnetic stir bar. It was evacuated and backfilled with nitrogen (3 cycles). 3-Chloro-5-(trifluoromethyl)phenyl triflate (0.20 mmol) or 3-chloro-5-methylphenyl triflate (0.20 mmol) was then added by syringes followed by the addition of and stock solution (1.0 mL). The Schlenk tube was sealed and stirred at room temperature for 5 min before stirring in oil bath. An array of Schlenk tubes those were prepared in parallel according to above procedure were placed into a preheated oil bath (110 °C) and stirred for the time indicated. After completion of reaction, the reaction tube was immediately cooled with ice bath, and water (~2 mL) were added to quench the reaction. Dodecane (45.2 μL, internal standard) and EA (~4 mL) was added for extraction. The organic layer was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.



General procedure for competition experiments:

Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L15** or **L18** or **L17** (8.0 mol%), 1-methylindolin-2-one (29.4 mg, 0.20 mmol) and K_3PO_4 (0.40 mmol) was added into a Schlenk tube with Teflon-coated magnetic stir bar. It was evacuated and backfilled with nitrogen (3 cycles). R^1-chloroaryl triflate (0.10 mmol) and R^1-chloroaryl triflate (0.10 mmol) was then added by syringes followed by the addition of freshly distilled toluene (1.0 mL). The Schlenk tube was sealed and stirred at room temperature for 5 min before stirring in oil bath. The Schlenk tube was then placed into a preheated oil bath (110 °C) and stirred for 60 min. After reacting for indicated time, the reaction tube was immediately cooled with ice bath, and water (~2 mL) were added to quench the reaction. Dodecane (45.2 μL, internal standard) and EA (~4 mL) was added for extraction. The organic layer was subjected to GC analysis. The GC yield was previously calibrated by authentic sample/dodecane calibration curve.

Table S4 Competition experiment of different chloroaryl triflates[a]



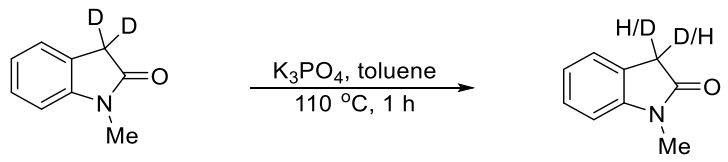
entry	Ligand	substrate 1	yield (%)[b]	substrate 2	yield (%)[b]
1	**L15**	R^1 = Me	22%	R^2 = CF_3	35%
2	**L18**	R^1 = Me	20%	R^2 = CF_3	30%
3	**L17**	R^1 = Me	4%	R^2 = CF_3	10%
4	**L17**	R^1 = H	10%	R^2 = Me	10%
5	**L17**	R^1 = H	6%	R^2= CF_3	9%

[a]Reaction condition: R^1-chloroaryl triflate (0.10 mmol), R^2-chloroaryl triflate (0.10 mmol), 1-methylindolin-2-one (0.20 mmol), [Pd(π-cinnamyl)Cl]$_2$ (2.0 mol%), **L15** or **L18** or **L17** (8.0 mol%), Pd:L = 1:2, K_3PO_4 (0.40 mmol), toluene (1.0 mL), 110 ºC, 60 min. [b]Calibrated GC yields were reported using dodecane as the internal standard. Maximum yield for each substrate in the reaction mixture is 50%.

General procedure for isotope experiments:

A Schlenk tube with Teflon-coated magnetic stir bar was charged with deuterated 1-methylindolin-2-one (0.10 mmol) and K_3PO_4 (0.20 mmol). The tube was evacuated and backfilled with nitrogen (3 cycles). Freshly distilled toluene (0.50 mL) was then added by syringe. The Schlenk tube was sealed and stirred at a preheated oil bath (110 °C) for 60 min. After reacting for indicated time, the reaction tube was immediately cooled with ice bath, and the reaction mixture was filtered on celite. After removing the solvent, the resulting product was dissolved with $CDCl_3$ to perform ^{1}H NMR analysis.

Table S5 Isotope experiments[a]



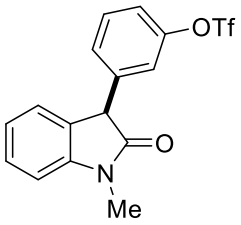
(0.1H, 1.9D)

entry	catalyst	base	H/D ratio[b]
1[c]	[Pd(π-cinnamyl)Cl]$_2$ /**L18**	K_3PO_4	>99% H (2.00 H)
2	-	K_3PO_4	>99% H (2.00 H)
3	-	K_3PO_4[d]	68% H (1.36 H, 0.64 D)

[a]Reaction condition: deuterated 1-methylindolin-2-one (0.10 mmol), K_3PO_4 (0.20 mmol), toluene (0.5 mL), 110 °C, 60 min; [b]The ratio of H was determined by ^{1}H NMR analysis; [c][Pd(π-cinnamyl)Cl]$_2$ (1.0 mol%), **L18** (4.0 mol%), Pd:L = 1:2; The product was isolated before ^{1}H NMR analysis; [d]K_3PO_4 was further dried under vacuum with heat gun.

7. Characterization of products

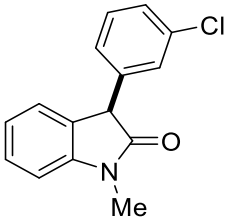
3-(1-Methyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3a)



Compound **3a** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 3-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.20 mmol), and K_3PO_4 (85 mg, 0.40 mmol) were used.

Yellow liquid, R_f = 0.4 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.44–7.36 (m, 2H), 7.29 (d, *J* = 7.8 Hz, 1H), 7.23–7.17 (m, 3H), 7.13–7.10 (m, 1H), 6.93 (d, *J* = 7.8 Hz, 1H), 4.65 (s, 1H), 3.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.7, 149.7, 144.4, 139.3, 130.5, 129.0, 128.5, 127.1, 125.0, 123.0, 121.4, 120.4, 118.7 (q, *J* = 319.1 Hz), 108.5, 51.2, 26.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.8. HRMS (EI): calcd. for $C_{16}H_{12}F_3NO_4S^+$: 371.0434, found 371.0437.

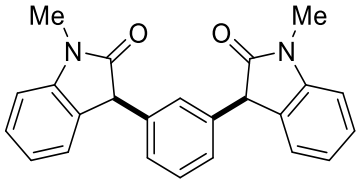
3-(3-Chlorophenyl)-1-methylindolin-2-one (3a')



Compound **3a'** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **SPhos** (6.6 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 3-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.20 mmol), and K_3PO_4 (85 mg, 0.40 mmol) were used.

Yellow liquid, R_f = 0.4 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37–7.33 (m, 1H), 7.27–7.26 (m, 2H), 7.17–7.12 (m, 3H), 7.10–7.06 (m, 1H), 6.91 (d, *J* = 7.8 Hz, 1H), 4.57 (s, 1H), 3.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.2, 144.4, 138.4, 134.6, 130.0, 128.7, 128.4, 127.9, 127.7, 126.8, 125.0, 122.8, 108.3, 51.5, 26.5.

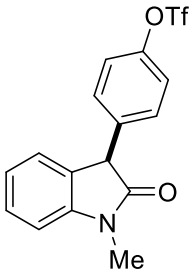
3,3'-(1,3-Phenylene)bis(1-methylindolin-2-one) (3a'')



A Schlenk tube with Teflon-coated magnetic stir bar was added $Pd(OAc)_2$ (1.8 mg, 4.0 mol%), **SPhos** (6.6 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (58.9 mg, 0.40 mmol), and K_3PO_4 (127.2 mg, 0.60 mmol). It was evacuated and flushed with nitrogen (3 cycles). 1,3-Dibromobenzene (47.2 mg, 0.20 mmol) and toluene (1.0 mL) was then added by syringes. The Schlenk tube was sealed and stirred at room temperature for 1 min. Then it was stirred at indicated temperature for 12 h. Water and ethyl acetate were added. The organic layer after extraction was collected and subjected to column chromatography (on silica gel) to afford the product **3a''** as a white solid (63.6 mg, 86%).

M.P: 200.0-202.5 °C. R_f = 0.1 (hexane/EA = 2/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.40–7.28 (m, 3H), 7.22–7.05 (m, 6H), 6.96 (dd, *J* = 7.7, 1.5 Hz, 1H), 6.90–6.88 (m, 2H), 4.64 (s, 1H), 4.57 (s, 1H), 3.25 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.72, 175.66, 144.4, 144.3, 136.99, 136.97, 130.2, 129.3, 129.2, 128.6, 128.4 (overlapped), 128.38, 128.37, 127.6, 126.8, 125.1, 122.73, 122.68, 108.11, 108.10, 51.8, 26.4. HRMS (APPI): calcd. for $C_{24}H_{21}N_2O_2^+$: 369.1598, found 369.1602.

4-(1-Methyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3b)

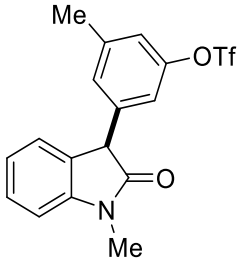


Compound **3b** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.4 mmol) were used.

Yellow solid, R_f = 0.4 (hexane/EA = 4/1). M.P.: 60.5-62.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.35 (m, 1H), 7.33–7.31 (m, 2H), 7.25–7.23 (m, 2H), 7.19–7.17 (m, 1H), 7.12–7.08 (m, 1H), 6.93 (d, *J* = 7.8 Hz, 1H), 4.64 (s, 1H), 3.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 148.9, 144.4, 137.0, 130.3, 128.9, 127.6, 125.1, 122.9, 121.6, 118.7 (q, *J* = 318.8 Hz), 108.4,

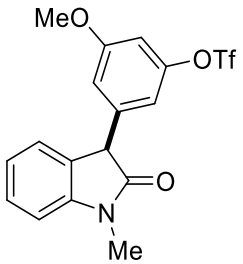
51.0, 26.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.8. HRMS (ESI): calcd. for $C_{16}H_{13}F_3NO_4S^+$: 372.0512, found 372.0517.

3-Methyl-5-(1-methyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3c)



Compound **3c** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 3-chloro-5-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Yellow liquid, R_f = 0.4 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (t, *J* = 7.7 Hz, 1H), 7.18–7.16 (m, 1H), 7.12–7.08 (m, 2H), 7.02 (s, 1H), 6.94–6.92 (m, 2H), 4.60 (s, 1H), 3.26 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 149.6, 144.4, 141.3, 138.9, 129.2, 128.9, 127.3, 125.0, 122.9, 120.9, 118.6 (q, *J* = 318.7 Hz), 118.4, 108.4, 51.2, 26.5, 21.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.9. HRMS (EI): calcd. for $C_{17}H_{14}F_3NO_4S^+$: 385.0590, found 385.0596.

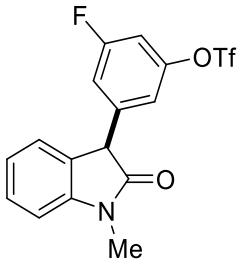
3-Methoxy-5-(1-methyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3d)



Compound **3d** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 3-chloro-5-methoxyphenyl trifluoromethanesulfonate (58.1 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Yellow liquid, R_f = 0.3 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.35 (m, 1H), 7.19–7.17 (m, 1H), 7.12–7.08 (m, 1H), 6.92 (d, *J* = 7.8 Hz, 1H), 6.83–6.82 (m, 1H), 6.74–6.73 (m, 2H), 4.59 (s, 1H), 3.79 (s, 3H), 3.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.6, 160.9,

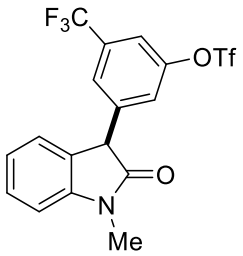
150.2, 144.4, 139.7, 128.9, 127.0, 125.0, 123.0, 118.6 (q, J = 318.8 Hz), 114.5, 113.4, 108.5, 106.5, 55.7, 51.3, 26.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.9. HRMS (EI): calcd. for $C_{17}H_{14}F_3NO_5S^+$: 401.0539, found 401.0537.

3-Fluoro-5-(1-methyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3e)



Compound **3e** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 3-chloro-5-fluorophenyl trifluoromethanesulfonate (55.7 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Yellow liquid, R_f = 0.4 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42–7.37 (m, 1H), 7.21–7.19 (m, 1H), 7.15–7.11 (m, 1H), 7.04–7.02 (m, 2H), 6.99–6.96 (m, 1H), 6.94 (d, J = 7.8 Hz, 1H), 4.63 (s, 1H), 3.25 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.0, 162.7 (d, J = 250.2 Hz), 149.6 (d, J = 11.6 Hz), 144.4, 140.7 (d, J = 8.7 Hz), 129.3, 126.3, 125.1, 123.1, 118.6 (q, J = 318.8 Hz), 117.5 (d, J = 3.2 Hz), 115.8 (d, J = 22.0 Hz), 108.5 (d, J = 25.9 Hz), 108.7, 51.0, 50.9, 26.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.7 (s, 3F), -107.6 (s, 1F); HRMS (EI): calcd. for $C_{16}H_{11}F_4NO_4S^+$: 389.0339, found 389.0338.

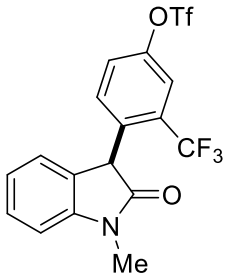
3-(1-Methyl-2-oxoindolin-3-yl)-5-(trifluoromethyl)phenyl trifluoromethanesulfonate (3f)



Compound **3f** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 3-chloro-5-(trifluoromethyl)phenyl trifluoromethanesulfonate (65.7 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Yellow liquid, R_f = 0.5 (hexane/EA = 4/1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39 (s, 1H), 7.29 (s, 1H), 7.26–7.22 (m, 2H), 7.03–6.95 (m, 2H), 6.79 (d, *J* = 7.9 Hz, 1H), 4.54 (s, 1H), 3.09 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.8, 149.4, 144.5, 140.6, 133.2 (q, *J* = 33.7 Hz), 129.5, 125.9, 125.2 (d, *J* = 3.5 Hz), 125.1, 125.0, 123.3, 122.7 (q, *J* = 271.4 Hz), 118.6 (q, *J* = 319.1 Hz), 117.9 (d, *J* = 3.7 Hz), 108.9, 50.9, 26.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.7, -72.6. HRMS (EI): calcd. for $C_{17}H_{11}F_6NO_4S^+$: 439.0307, found 439.0316.

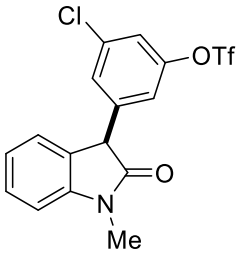
4-(1-Methyl-2-oxoindolin-3-yl)-3-(trifluoromethyl)phenyl trifluoromethanesulfonate (3g)



Compound **3g** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 4-chloro-3-(trifluoromethyl)phenyl trifluoro methanesulfonate (65.7 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used.

Yellow solid, R_f = 0.3 (hexane/EA = 4/1). M.P.: 80.5-82.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 2.5 Hz, 1H), 7.38–7.32 (m, 2H), 7.07–6.93 (m, 4H), 5.04 (s, 1H), 3.31 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.7, 148.0, 144.1, 137.0, 132.1, 129.1, 128.8, 125.4, 124.8, 123.3, 123.0 (q, *J* = 272.9 Hz), 119.6, 119.5, 118.6 (q, *J* = 318.9 Hz), 108.5, 48.0, 26.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -58.5, -72.7. HRMS (ESI): calcd. for $C_{17}H_{12}F_6NO_4S^+$: 440.0386, found 440.0387.

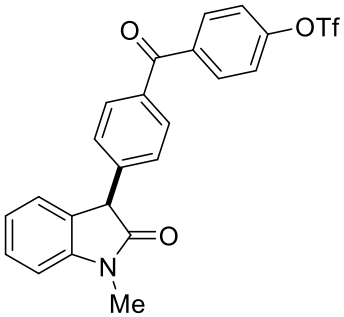
3-Chloro-5-(1-methyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3h)



Compound **3h** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 3,5-dichlorophenyl

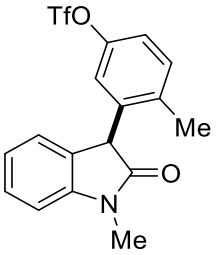
trifluoromethanesulfonate (59.0 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Yellow liquid, R_f = 0.5 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42–7.38 (m, 1H), 7.27–7.26 (m, 1H), 7.24–7.23 (m, 1H), 7.20–7.18 (m, 1H), 7.14 (d, *J* = 7.5 Hz, 1H), 7.12–7.11 (m, 1H), 6.94 (d, *J* = 7.8 Hz, 1H), 4.62 (s, 1H), 3.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.0, 149.5, 144.4, 140.4, 135.8, 129.3, 128.6, 126.3, 125.1, 123.2, 121.1, 120.1, 118.6 (q, *J* = 318.7 Hz), 108.7, 50.9, 26.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.7. HRMS (EI): calcd. for $C_{16}H_{11}ClF_3NO_4S^+$: 405.0044, found 405.0029.

4-(4-(1-Methyl-2-oxoindolin-3-yl)benzoyl)phenyl trifluoromethanesulfonate (3i)



Compound **3i** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 4-(4-chlorobenzoyl)phenyl trifluoromethanesulfonate (72.9 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Colorless liquid, R_f = 0.2 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91–7.87 (m, 2H), 7.77–7.74 (m, 2H), 7.40–7.35 (m, 5H), 7.18–7.17 (m, 1H), 7.11–7.08 (m, 1H), 6.94 (d, *J* = 7.8 Hz, 1H), 4.71 (s, 1H), 3.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 194.1, 175.0, 151.9, 144.4, 141.9, 137.5, 135.9, 132.1, 130.5, 128.8, 128.7, 127.8, 125.0, 122.9, 121.3, 118.7 (q, *J* = 319.0 Hz), 108.4, 51.9, 26.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.7. HRMS (ESI): calcd. for $C_{23}H_{17}F_3NO_5S^+$: 476.0774, found 476.0778.

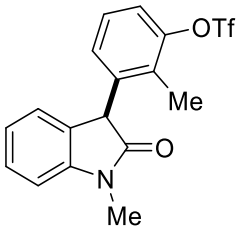
4-Methyl-3-(1-methyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3j)



Compound **3j** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl)

chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Colorless liquid, R_f = 0.5 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.39–7.35 (m, 1H), 7.30 (d, *J* = 8.4 Hz, 1H), 7.12–7.05 (m, 3H), 6.93 (d, *J* = 7.8 Hz, 1H), 6.77 (s, 1H), 4.84 (s, 1H), 3.27 (s, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 147.7, 144.4, 138.2, 137.8, 132.4, 128.8, 127.6, 124.5, 123.0, 120.1, 118.6 (q, *J* = 318.9 Hz), 108.4, 49.7 (low signal), 26.4, 19.3; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.9. HRMS (EI): calcd. for $C_{17}H_{14}F_3NO_4S^+$: 385.0590, found 385.0608.

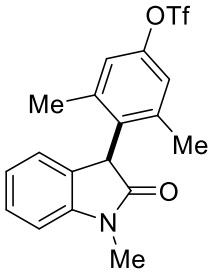
2-Methyl-3-(1-methyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3k)



Compound **3k** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 3-chloro-2-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.2 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used.

Yellow liquid, R_f = 0.5 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38–7.34 (m, 1H), 7.26–7.17 (m, 2H), 7.08–7.07 (m, 2H), 6.93 (d, *J* = 7.8 Hz, 1H), 6.87 (s, 1H), 4.90 (s, 1H), 3.27 (s, 3H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.0, 148.9, 144.2, 138.7, 130.8, 128.7, 128.1, 127.3, 124.6, 123.0, 120.7, 118.6 (q, *J* = 318.3 Hz), 108.4, 48.9 (low signal), 26.4, 13.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.8. HRMS (EI): calcd. for $C_{17}H_{14}F_3NO_4S^+$: 385.0590, found 385.0602.

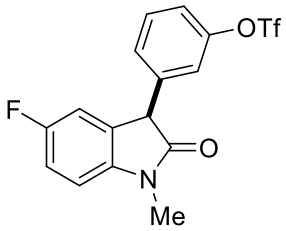
3,5-Dimethyl-4-(1-methyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3l)



Compound **3l** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl)

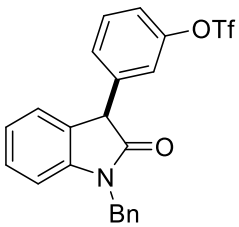
chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-methylindolin-2-one (29.4 mg, 0.20 mmol), 4-chloro-3,5-dimethylphenyl trifluoromethanesulfonate (57.7 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.4 mmol) were used. Colorless liquid, R_f = 0.4 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35–7.31 (m, 1H), 7.06 (d, *J* = 2.5 Hz, 1H), 7.05–7.01 (m, 1H), 6.93–6.91 (m, 2H), 6.85 (d, *J* = 2.4 Hz, 1H), 5.02 (s, 1H), 3.32 (s, 3H), 2.58 (s, 3H), 1.69 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 148.3, 143.8, 140.7, 140.1, 134.2, 128.4, 127.2, 123.5, 122.9, 121.7, 120.5, 118.7 (q, *J* = 319.3 Hz), 108.2, 47.8, 26.5, 21.5, 19.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.0. HRMS (EI): calcd. for $C_{18}H_{16}F_3NO_4S^+$: 399.0747, found 399.0766.

3-(5-Fluoro-1-methyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3m)



Compound **3m** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 5-fluoro-1-methylindolin-2-one (33.0 mg, 0.20 mmol), 3-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Yellow liquid, R_f = 0.3 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) 7.45–7.41 (m, 1H), 7.26–7.21 (m, 2H), 7.16–7.15 (m, 1H), 7.10–7.05 (m, 1H), 6.94 (dd, *J* = 7.7, 1.7 Hz, 1H), 6.87–6.84 (m, 1H), 4.64 (s, 1H), 3.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 159.3 (d, *J* = 240.3 Hz), 149.7, 140.4, 138.6, 130.7, 128.6 (d, *J* = 8.5 Hz), 128.3, 121.4, 120.6, 118.7 (q, *J* = 318.8 Hz), 115.3 (d, *J* = 23.4 Hz), 113.1 (d, *J* = 24.9 Hz), 109.0 (d, *J* = 8.1 Hz), 51.4, 26.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.8 (s, 3F), -119.8 (s, 1F). HRMS (EI): calcd. for $C_{16}H_{11}F_4NO_4S^+$: 389.0339, found 389.0340.

3-(1-Benzyl-2-oxoindolin-3-yl)phenyl trifluoromethanesulfonate (3n)

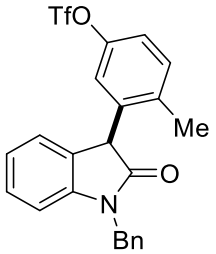


Compound **3n** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl)

chloride dimer (2.0 mg, 2.0 mol%), **L15** (5.3 mg, 8.0 mol%) or **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-benzylindolin-2-one (44.7 mg, 0.20 mmol), 3-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used.

Yellow liquid, R_f = 0.5 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48–7.44 (m, 1H), 7.36–7.23 (m, 8H), 7.20–7.18 (m, 2H), 7.10–7.06 (m, 1H), 6.84 (d, *J* = 7.8 Hz, 1H), 5.01 (d, *J* = 15.6 Hz, A part of AB system, 1H), 4.90 (d, *J* = 15.6 Hz, B part of AB system, 1H), 4.76 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.8, 149.7, 143.5, 139.4, 135.5, 130.6, 128.9, 128.8, 128.5, 127.7, 127.23, 127.18, 125.1, 123.0, 121.3, 120.4, 118.7 (q, *J* = 319.0 Hz), 109.5, 51.2, 44.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.8. HRMS (EI): calcd. for $C_{22}H_{16}F_3NO_4S^+$: 447.0747, found 447.0747.

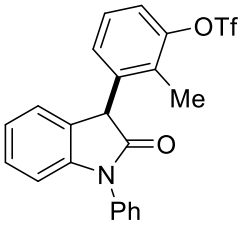
3-(1-Benzyl-2-oxoindolin-3-yl)-4-methylphenyl trifluoromethanesulfonate (3o)



Compound **3o** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-benzylindolin-2-one (44.7 mg, 0.20 mmol), 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used.

Yellow liquid, R_f = 0.5 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34–7.24 (m, 7H), 7.14–7.11 (m, 1H), 7.09–7.03 (m, 2H), 6.85 (d, *J* = 7.9 Hz, 1H), 6.75 (s, 1H), 5.01 (d, *J* = 15.6 Hz, A part of AB system, 1H), 4.96 (s, 1H), 4.90 (d, *J* = 15.6 Hz, B part of AB system, 1H), 2.53 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.9, 147.8, 143.5, 138.3, 138.0, 135.6, 132.5, 128.83, 128.77, 127.77, 127.69, 127.4, 124.7, 123.1, 120.2, 118.6 (q, *J* = 316.9 Hz), 109.4, 49.2, 44.0, 19.5; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.9. HRMS (EI): calcd. for $C_{23}H_{18}F_3NO_4S^+$: 461.0903, found 461.0903.

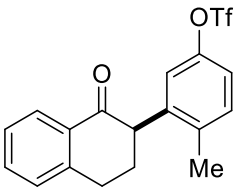
2-Methyl-3-(2-oxo-1-phenylindolin-3-yl)phenyl trifluoromethanesulfonate (3p)



Compound **3p** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-phenylindolin-2-one (41.8 mg, 0.20 mmol), 3-chloro-2-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used.

Yellow solid, R_f = 0.5 (hexane/EA = 4/1). M.P.: 139.5-140.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57–7.53 (m, 2H), 7.47–7.42 (m, 3H), 7.31–7.10 (m, 6H), 6.92 (d, *J* = 7.9 Hz, 1H), 5.12 (s, 1H), 2.64 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.3, 148.9, 144.2, 138.8, 134.2, 130.9, 129.6, 128.6, 128.2, 127.8, 127.4, 126.4, 124.8, 123.4, 120.8, 118.6 (q, *J* = 318.0 Hz), 109.7, 49.0 (low signal), 13.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.7. HRMS (EI): calcd. for $C_{22}H_{16}F_3NO_4S^+$: 447.0747, found 447.0756.

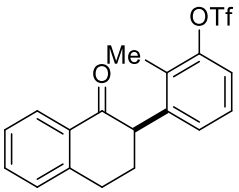
4-Methyl-3-(1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl)phenyl trifluoromethanesulfonate (5a)



Compound **5a** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 3,4-dihydronaphthalen-1(2*H*)-one (29.2 mg, 0.20 mmol), 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used.

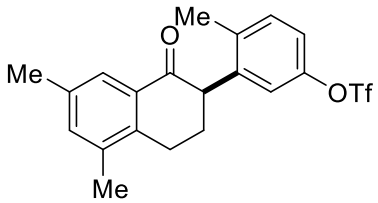
Yellow liquid, R_f = 0.7 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 (d, *J* = 7.6 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.38–7.28 (m, 3H), 7.11 (dd, *J* = 8.5, 2.6 Hz, 1H), 7.01 (s, 1H), 3.99 (dd, *J* = 12.4, 4.7 Hz, 1H), 3.22 (ddd, *J* = 16.7, 11.6, 4.8 Hz, 1H), 3.11 (dt, *J* = 16.8, 3.8 Hz, 1H), 2.44 (ddd, *J* = 24.9, 12.9, 4.2 Hz, 1H), 2.40–2.34 (m, 1H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.6, 147.8, 143.7, 141.0, 137.4, 133.7, 132.6, 131.8, 128.8, 127.8, 126.9, 120.3, 119.4, 118.7 (q, *J* = 319.2 Hz), 51.4, 30.1, 29.5, 19.4; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.9. HRMS (EI): calcd. for $C_{18}H_{15}F_3O_4S^+$: 384.0638, found 384.0634.

2-Methyl-3-(1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl)phenyl trifluoromethanesulfonate (5b)



Compound **5b** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 3,4-dihydronaphthalen-1(2*H*)-one (29.2 mg, 0.20 mmol), 3-chloro-2-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Orange liquid, R_f = 0.7 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.09 (d, *J* = 7.7 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 1H), 7.36 (t, *J* = 7.6 Hz, 1H), 7.33 (d, *J* = 7.7 Hz, 1H), 7.27–7.20 (m, 2H), 7.14 (d, *J* = 7.4 Hz, 1H), 4.04 (dd, *J* = 12.3, 4.7 Hz, 1H), 3.21 (ddd, *J* = Hz, 16.7, 11.5, 4.6 Hz, 1H), 3.10 (dt, *J* = 16.7, 3.9 Hz, 1H), 2.47 (ddd, *J* = 25.0, 12.8, 4.3 Hz, 1H), 2.42–2.36 (m, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 196.8, 148.7, 143.8, 141.9, 133.7, 132.6, 130.1, 128.8, 127.8, 127.6, 127.1, 126.9, 119.9, 118.7 (q, *J* = 318.1 Hz), 51.6, 30.3, 29.5, 12.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.8. HRMS (EI): calcd. for $C_{18}H_{15}F_3O_4S^+$: 384.0638, found 384.0641.

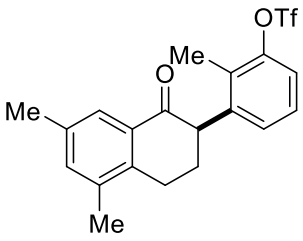
3-(5,7-Dimethyl-1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl)-4-methylphenyl trifluoromethanesulfonate (5c)



Compound **5c** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 5,7-dimethyl-3,4-dihydronaphthalen-1(2*H*)-one (34.8 mg, 0.20 mmol), 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Colorless liquid, R_f = 0.7 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (s, 1H), 7.29 (d, *J* = 8.5 Hz, 1H), 7.26 (s, 1H), 7.10 (d, *J* = 8.4 Hz, 1H), 7.02 (s, 1H), 3.97 (t, *J* = 8.6 Hz, 1H), 3.08 (dt, *J* = 17.1, 3.8 Hz, 1H), 2.99–2.90 (m, 1H), 2.43–2.38 (m, 2H), 2.36 (s, 3H), 2.33 (s, 3H), 2.32 (s, 3H); ^{19}F NMR (465.89 MHz, $CDCl_3$) δ -72.8; ^{13}C NMR (100 MHz, $CDCl_3$) δ

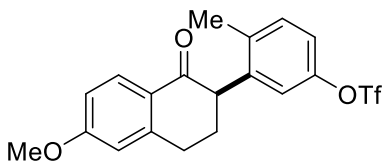
197.0, 147.9, 141.0, 139.1, 137.4, 136.3, 136.13, 136.06, 132.7, 131.7, 125.7, 120.2, 119.3, 118.7 (q, *J* = 318.9 Hz), 50.6, 29.4, 26.2, 20.8, 19.3, 19.2. HRMS (APPI): calcd. For $C_{20}H_{20}F_3O_4S^+$: 413.1029, found 413.1031.

3-(5,7-Dimethyl-1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl)-2-methylphenyl trifluoromethanesulfonate (5d)



Compound **5d** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2 mol%), **L18** (6.0 mg, 8 mol%), Pd:L = 1:2, 5,7-dimethyl-3,4-dihydronaphthalen-1(2*H*)-one (34.8 mg, 0.2 mmol), 3-chloro-2-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.2 mmol), and K_3PO_4 (85.0 mg, 0.4 mmol) were used. White solid, R_f = 0.8 (hexane/EA = 4/1). M.P.: 103.0-104.3 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.76 (s, 1H), 7.25–7.17 (m, 3H), 7.12 (d, *J* = 7.4 Hz, 1H), 3.99 (dd, J = 10.8, 6.2 Hz, 1H), 3.04 (dt, *J* = 17.1, 4.0 Hz, 1H), 2.96–2.88 (m, 1H), 2.42–2.37 (m, 2H), 2.34 (s, 3H), 2.31 (s, 3H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.3, 148.7, 141.9, 139.2, 136.3, 136.1, 136.06, 132.7, 130.1, 127.4, 127.1, 125.7, 119.8, 118.6 (q, *J* = 318.3 Hz), 50.8, 29.6, 26.2, 20.8, 19.2, 12.9; ^{19}F NMR (465.89 MHz, $CDCl_3$) δ -73.7. HRMS (APPI): calcd. For $C_{20}H_{20}F_3O_4S^+$: 413.1029, found: 413.1025.

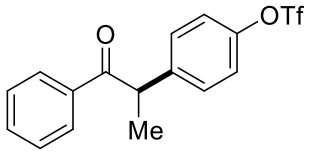
3-(6-Methoxy-1-oxo-1,2,3,4-tetrahydronaphthalen-2-yl)-4-methylphenyl trifluoromethanesulfonate (5e)



Compound **5e** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 6-methoxy-3,4-dihydronaphthalen-1(2*H*)-one (35.2 mg, 0.20 mmol), 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (85.0 mg, 0.40 mmol) were used. Colorless liquid, R_f = 0.5 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, *J* = 8.7 Hz, 1H), 7.27 (d, *J* = 8.8 Hz, 1H), 7.09 (d, *J* = 8.4, 1H), 6.99 (s, 1H), 6.87 (d, *J* = 8.7 Hz, 1H),

6.76 (s, 1H), 3.94 (dd, *J* = 11.9, 4.9 Hz, 1H), 3.88 (s, 3H), 3.16 (ddd, *J* = 16.6, 11.2, 4.9 Hz, 1H), 3.04 (dt, *J* = 16.7, 3.8 Hz, 1H), 2.44–2.31 (m, 5H); ^{19}F NMR (465.89 MHz, $CDCl_3$) δ -72.8; ^{13}C NMR (100 MHz, $CDCl_3$) δ 195.3, 163.8, 147.8, 146.2, 141.3, 137.4, 131.8, 130.3, 126.2, 120.4, 119.3, 118.7 (q, *J* = 319.0 Hz), 113.4, 112.6, 55.4, 51.1, 30.2, 29.7, 19.4. HRMS (APPI): calcd. For $C_{19}H_{18}F_3O_5S^+$: 415.0822, found 415.0817.

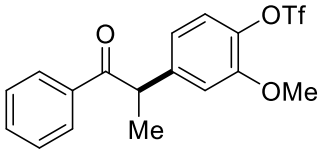
4-(1-Oxo-1-phenylpropan-2-yl)phenyl trifluoromethanesulfonate (5f)



Compound **5f** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2 mol%), **L18** (6.0 mg, 8 mol%), Pd:L = 1:2, propiophenone (26.8 mg, 0.2 mmol), 4-chlorophenyl trifluoromethanesulfonate (52.1 mg, 0.2 mmol), and K_3PO_4 (106.0 mg, 0.5 mmol) were used.

Pale-yellow liquid, R_f = 0.8 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.95–7.93 (m, 2H), 7.55–7.51 (m, 1H), 7.44–7.37 (m, 4H), 7.22–7.19 (m, 2H), 4.76 (q, *J* = 6.9 Hz, 1H), 1.55 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.7, 148.4, 141.8, 136.0, 133.2, 129.6, 128.7, 128.6, 121.7, 118.7 (q, *J* = 318.8 Hz), 46.8, 19.5; ^{19}F NMR (465.89 MHz, $CDCl_3$) δ -72.8. HRMS (APPI): calcd. For $C_{16}H_{17}F_3NO_4S^+$ $[M + NH_4]^+$: 376.0825, found: 376.0828.

2-Methoxy-4-(1-oxo-1-phenylpropan-2-yl)phenyl trifluoromethanesulfonate (5g)



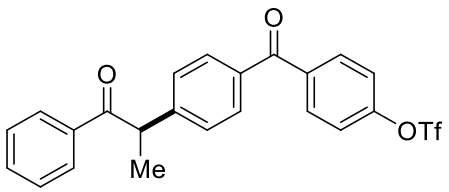
Compound **5g** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2 mol%), **L18** (6.0 mg, 8 mol%), Pd:L = 1:2, propiophenone (26.8 mg, 0.2 mmol), 4-chloro-2-methoxyphenyl trifluoromethanesulfonate (58.0 mg, 0.2 mmol), and K_3PO_4 (106.0 mg, 0.5 mmol) were used.

Pale-yellow liquid, R_f = 0.6 (hexane/EA = 4/1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96–7.94 (m, 2H), 7.55–7.51 (m, 1H), 7.44–7.41 (m, 2H), 7.14 (d, *J* = 8.2 Hz, 1H), 6.95–6.91 (m, 2H), 4.72 (q, *J* = 6.9 Hz, 1H), 3.87 (s, 3H), 1.54 (d, *J* = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.8, 151.6, 142.8, 137.6, 136.1, 133.2, 128.7, 128.6,

122.6, 120.3, 118.6 (q, *J* = 318.7 Hz), 112.2, 56.2, 47.3, 19.6; ^{19}F NMR (465.89 MHz, $CDCl_3$) δ -73.8. HRMS (APPI): calcd. For $C_{17}H_{19}F_3NO_5S^+$ $[M + NH_4]^+$: 406.0931, found: 406.0930.

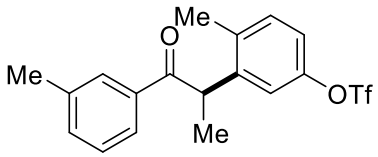
4-(4-(1-Oxo-1-phenylpropan-2-yl)benzoyl)phenyl trifluoromethanesulfonate (5h)



Compound **5h** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2 mol%), **L18** (6.0 mg, 8 mol%), Pd:L = 1:2, propiophenone (26.8 mg, 0.2 mmol), 4-(4-chlorobenzoyl)phenyl trifluoromethanesulfonate (72.8 mg, 0.2 mmol), and K_3PO_4 (106.0 mg, 0.5 mmol) were used.

Pale-yellow liquid, R_f = 0.6 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97–7.95 (m, 2H), 7.87–7.85 (m, 2H), 7.74–7.72 (m, 2H), 7.53–7.49 (m, 1H), 7.45–7.36 (m, 6H), 4.81 (q, *J* = 6.9 Hz, 1H), 1.58 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 199.5, 194.1, 151.8, 146.8, 137.5, 136.1, 135.3, 133.1, 132.0, 130.7, 128.7, 128.6, 128.0, 121.3, 118.6 (q, *J* = 319.0 Hz), 47.6, 19.3; ^{19}F NMR (465.89 MHz, $CDCl_3$) δ -72.6. HRMS (APPI): calcd. For $C_{23}H_{18}F_3O_5S^+$: 463.0822, found: 463.0823.

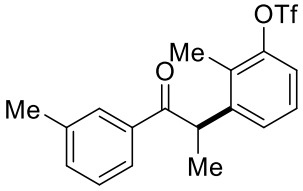
4-Methyl-3-(1-oxo-1-(*m*-tolyl)propan-2-yl)phenyl trifluoromethanesulfonate (5i)



Compound **5i** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-(*m*-tolyl)propan-1-one (29.6 mg, 0.20 mmol), 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (106 mg, 0.50 mmol) were used.

Yellow liquid, R_f = 0.7 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (s, 1H), 7.61 (d, *J* = 7.6 Hz, 1H), 7.33–7.24 (m, 3H), 7.05–7.03 (m, 2H), 4.81 (q, *J* = 6.9 Hz, 1H), 2.45 (s, 3H), 2.36 (s, 3H), 1.50 (d, *J* = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.3, 148.2, 142.5, 138.5, 136.2, 135.4, 133.9, 132.2, 128.9, 128.5, 125.5, 120.0, 119.5, 118.6 (q, *J* = 318.9 Hz), 44.1, 21.3, 19.2, 17.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.9. HRMS (ESI): calcd. For $C_{18}H_{18}F_3O_4S^+$: 387.0872, found: 387.0876.

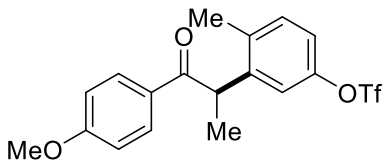
2-Methyl-3-(1-oxo-1-(*m*-tolyl)propan-2-yl)phenyl trifluoromethanesulfonate (5j)



Compound **5j** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2 mol%), **L18** (6.0 mg, 8 mol%), Pd:L = 1:2, 1-(*m*-tolyl)propan-1-one (29.6 mg, 0.2 mmol), 3-chloro-2-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.2 mmol), and K_3PO_4 (106.0 mg, 0.5 mmol) were used.

Colorless liquid, R_f = 0.85 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (s, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.29–7.22 (m, 2H), 7.17–7.06 (m, 3H), 4.77 (q, *J* = 6.8 Hz, 1H), 2.47 (s, 3H), 2.31 (s, 3H), 1.47 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.1, 148.8, 143.4, 138.5, 136.0, 133.9, 129.0, 128.5, 128.1, 127.7, 127.1, 125.5, 119.8, 118.6 (q, *J* = 318.2 Hz), 44.4, 21.3, 18.0, 12.6; ^{19}F NMR (465.89 MHz, $CDCl_3$) δ -73.6. HRMS (APPI): calcd. For $C_{18}H_{18}F_3O_4S^+$: 387.0872, found: 387.0871.

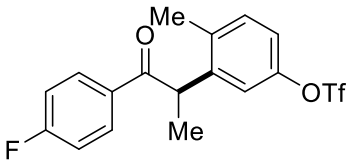
3-(1-(4-Methoxyphenyl)-1-oxopropan-2-yl)-4-methylphenyl trifluoromethanesulfonate (5k)



Compound **5k** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-(4-methoxyphenyl)propan-1-one (32.8 mg, 0.20 mmol), 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (106 mg, 0.50 mmol) were used.

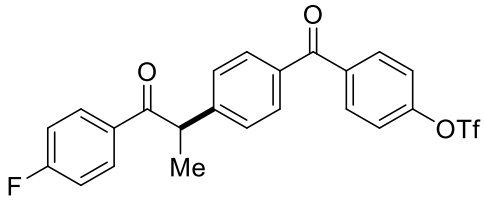
Yellow liquid, R_f = 0.6 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85–7.81 (m, 2H), 7.25–7.23 (m, 1H), 7.05–7.02 (m, 2H), 6.89–6.85 (m, 2H), 4.76 (q, *J* = 6.9 Hz, 1H), 3.82 (s, 3H), 2.45 (s, 3H), 1.48 (d, *J* = 6.9 Hz, 3H) ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.5, 163.5, 148.2, 142.8, 135.3, 132.2, 130.7, 129.0, 120.0, 119.4, 118.6 (q, *J* = 319.1 Hz), 113.8, 55.4, 43.8, 19.2, 18.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.9. HRMS (ESI): calcd. For $C_{18}H_{18}F_3O_5S^+$: 403.0822, found: 403.0823.

3-(1-(4-Fluorophenyl)-1-oxopropan-2-yl)-4-methylphenyl trifluoromethanesulfonate (5l)



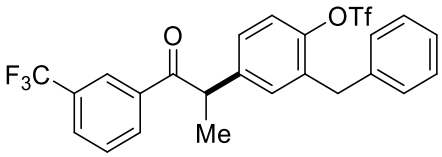
Compound **5l** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-(4-fluorophenyl)propan-1-one (30.4 mg, 0.20 mmol), 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (106 mg, 0.50 mmol) were used. Yellow liquid, R_f = 0.7 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87–7.82 (m, 2H), 7.26 (d, *J* = 8.4 Hz, 1H), 7.09–7.04 (m, 3H), 6.96 (d, *J* = 2.6 Hz, 1H), 4.74 (q, *J* = 6.8 Hz, 1H), 2.46 (s, 3H), 1.49 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.4, 165.6 (d, *J* = 253.8 Hz), 148.2, 142.3, 135.3, 132.43, 132.41, 131.0 (d, *J* = 9.1 Hz), 120.0, 119.7, 118.6 (q, *J* = 318.9 Hz), 115.8 (d, *J* = 21.8 Hz), 44.2, 19.1, 17.8; ^{19}F NMR (376 MHz, $CDCl_3$) δ -72.9 (s, 3F), -104.8 (s, 1F). HRMS (EI): calcd. For $C_{17}H_{14}F_4O_4S^+$: 390.0543, found 390.0543.

4-(4-(1-(4-Fluorophenyl)-1-oxopropan-2-yl)benzoyl)phenyl trifluoromethanesulfonate (5m)



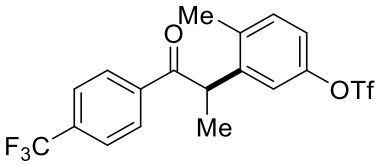
Compound **5m** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2 mol%), **L18** (6.0 mg, 8 mol%), Pd:L = 1:2, 1-(4-fluorophenyl)propan-1-one (30.4 mg, 0.2 mmol), 4-(4-chlorobenzoyl)phenyl trifluoromethanesulfonate (72.8 mg, 0.2 mmol), and K_3PO_4 (106.0 mg, 0.5 mmol) were used. Pale-yellow liquid, R_f = 0.6 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00–7.96 (m, 2H), 7.88–7.84 (m, 2H), 7.74–7.73 (m, 2H), 7.43–7.36 (m, 4H), 7.10–7.05 (m, 2H), 4.75 (q, *J* = 6.8 Hz, 1H), 1.57 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 197.9, 194.1, 165.6 (d, *J* = 254.1 Hz), 151.9, 146.6, 137.4, 135.4, 132.5 (d, *J* = 2.9 Hz), 132.0, 131.4 (d, *J* = 9.3 Hz), 130.8, 127.9, 121.4, 118.7 (q, *J* = 318.9 Hz), 115.8 (d, *J* = 21.8 Hz), 47.7, 19.3; ^{19}F NMR (465.89 MHz, $CDCl_3$) δ -72.6, -104.5. HRMS (APPI): calcd. For $C_{23}H_{17}F_4O_5S^+$: 481.0727, found: 481.0727.

2-Benzyl-4-(1-oxo-1-(3-(trifluoromethyl)phenyl)propan-2-yl)phenyl trifluoromethanesulfonate (5n)



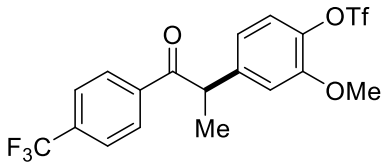
Compound **5n** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2 mol%), **L18** (6.0 mg, 8 mol%), Pd:L = 1:2, 1-(3-(trifluoromethyl)phenyl)propan-1-one (40.4 mg, 0.2 mmol), 2-benzyl-4-chlorophenyl trifluoromethanesulfonate (70.1 mg, 0.2 mmol), and K_3PO_4 (106.0 mg, 0.5 mmol) were used. Colorless liquid, R_f = 0.8 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 8.02 (d, *J* = 7.9 Hz, 1H), 7.76 (d, *J* = 7.8 Hz, 1H), 7.54–7.50 (m, 1H), 7.31–7.19 (m, 5H), 7.11–7.09 (m, 3H), 4.63 (q, *J* = 6.8 Hz, 1H), 4.04 (s, 2H), 1.52 (d, *J* = Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.2, 146.9, 141.0, 138.8, 136.5, 134.8, 131.7, 131.4, 131.2 (q, *J* = 32.2 Hz), 129.5 (q, *J* = 3.7 Hz), 129.3, 128.9, 128.7, 127.3, 126.7, 125.5 (q, *J* = 3.7 Hz), 123.5 (q, *J* = 270.9 Hz), 122.0, 118.5 (q, *J* = 318.3 Hz), 47.3, 35.8, 19.2; ^{19}F NMR (465.89 MHz, $CDCl_3$) δ -62.8, -73.7. HRMS (APPI): calcd. For $C_{24}H_{22}F_6NO_4S^+$ $[M + NH_4]^+$: 534.1168, found: 534.1173.

4-Methyl-3-(1-oxo-1-(4-(trifluoromethyl)phenyl)propan-2-yl)phenyl trifluoromethanesulfonate (5o)



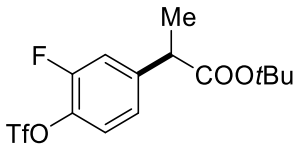
Compound **5o** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2.0 mol%), **L18** (6.0 mg, 8.0 mol%), Pd:L = 1:2, 1-(4-(trifluoromethyl)phenyl)propan-1-one (40.4 mg, 0.20 mmol), 3-chloro-4-methylphenyl trifluoromethanesulfonate (54.9 mg, 0.20 mmol), and K_3PO_4 (106 mg, 0.50 mmol) were used. Colorless liquid, R_f = 0.8 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89–7.87 (m, 2H), 7.65–7.63 (m, 2H), 7.21–7.14 (m, 2H), 7.06–7.04 (m, 1H), 4.78 (q, *J* = 6.8 Hz, 1H), 2.50 (s, 3H), 1.52 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.9, 149.0, 142.6, 138.7, 134.3 (q, *J* = 32.7 Hz), 128.7, 128.2, 128.0, 127.0, 125.8 (q, *J* = 3.8 Hz), 123.4 (q, *J* = 271.0 Hz), 120.3, 118.5 (q, *J* = 318.2 Hz), 45.0, 17.8, 12.6; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.3, -73.7. HRMS (EI): calcd. For $C_{18}H_{14}F_6O_4S^+$: 440.0512, found 440.0529.

2-Methoxy-4-(1-oxo-1-(4-(trifluoromethyl)phenyl)propan-2-yl)phenyl trifluoromethanesulfonate (5p)



Compound **5p** was synthesized according to general procedure (**GP3**). Palladium(π-cinnamyl) chloride dimer (2.0 mg, 2 mol%), **L18** (6.0 mg, 8 mol%), Pd:L = 1:2, 1-(4-(trifluoromethyl)phenyl)propan-1-one (40.4 mg, 0.2 mmol), 4-chloro-2-methoxyphenyl trifluoromethanesulfonate (58.0 mg, 0.2 mmol), and K_3PO_4 (106.0 mg, 0.5 mmol) were used. Pale-yellow liquid, R_f = 0.65 (hexane/EA = 4/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04–8.02 (m, 2H), 7.69–7.67 (m, 2H), 7.15 (d, *J* = 8.0 Hz, 1H), 6.91–6.89 (m, 2H), 4.69 (q, *J* = 6.8 Hz, 1H), 3.87 (s, 3H), 1.56 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 198.8, 151.8, 142.1, 138.8, 137.8, 134.4 (q, *J* = 32.2 Hz), 129.0, 125.7 (q, *J* = 3.7 Hz), 123.4 (q, *J* = 271.3 Hz), 122.9, 120.3, 118.7 (q, *J* = 318.6Hz), 112.1, 56.2, 47.9, 19.4; ^{19}F NMR (465.89 MHz, $CDCl_3$) δ -63.1, -73.8. HRMS (APPI): calcd. For $C_{18}H_{18}F_6NO_5S^+$ $[M + NH_4]^+$: 474.0804, found: 474.0802.

***tert*-Butyl 2-(3-fluoro-4-(((trifluoromethyl)sulfonyl)oxy)phenyl)propanoate (7a)**

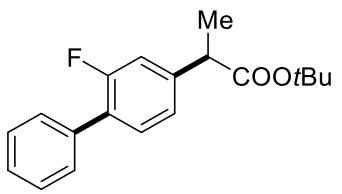


A Schlenk tube with Teflon-coated magnetic stir bar was added $Pd(dba)_2$ (4.6 mg, 4.0 mol%), **L15** (5.3 mg, 8.0 mol%), Pd:L = 1:2, and ZnF (10.3 mg, 0.10 mmol). It was evacuated and flushed with nitrogen (3 cycles). 4-Chloro-2-fluorophenyl trifluoromethanesulfonate (57.7 mg, 0.20 mmol), (*E*)-((1-(*tert*-butoxy)prop-1-en-1-yl)oxy)trimethylsilane and (101 mg, 0.50 mmol), and THF (1.0 mL) was then added by syringes. The Schlenk tube was sealed and stirred at room temperature for 1 min. Then it was stirred at 110 °C for 18 h. Water and ethyl acetate were added for extraction. After removing the solvent, the resulting residue was subjected to column chromatography (on silica gel) to afford the product.

Colorless liquid (52.1 mg, 70%). R_f = 0.6 (hexane/EA = 9/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.29–7.22 (m, 2H), 7.15–7.12 (m, 1H), 3.63 (q, *J* = 7.2 Hz, 1H), 1.45 (d, *J* = 7.2 Hz, 3H), 1.40 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -73.3 (d, *J* = 4.9 Hz, 3F), -127.2 (q, *J* = 5.1 Hz, 1F);

^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 153.4 (d, *J* = 251.8 Hz), 143.5 (d, *J* = 6.7 Hz), 135.5 (d, *J* = 13.8 Hz), 124.1 (d, *J* = 3.6 Hz), 123.3, 118.7 (d, *J* = 318.6 Hz), 116.7 (d, *J* = 18.6 Hz), 81.4, 45.9, 27.8, 18.4. HRMS (APPI): calcd. For $C_{14}H_{20}F_4NO_5S^+$ $[M+NH_4]^+$: 390.0993, found: 390.0999.

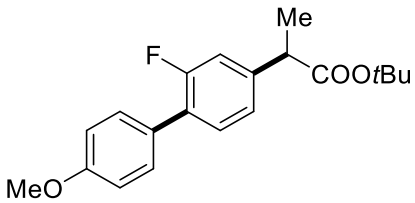
***tert*-Butyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (8a)**[5]



A Schlenk tube with Teflon-coated magnetic stir bar was added $Pd(dba)_2$ (4.6 mg, 4.0 mol%), **L13** (6.4 mg, 8.0 mol%), Pd:L = 1:2, phenylboronic acid (36.6 mg, 0.30 mmol)), and K_3PO_4 (85.0 mg, 0.40 mmol). It was evacuated and flushed with nitrogen (3 cycles). *Tert*-Butyl 2-(3-fluoro-4 (((trifluoromethyl)sulfonyl)oxy)phenyl)propanoate (74.5mg, 0.20 mmol) and dioxane (1.0 mL) was then added by syringes. The Schlenk tube was sealed and stirred at room temperature for 1 min. Then it was stirred at 110 °C for 6 h. Water and ethyl acetate were added for extraction. After removing the solvent, the resulting residue was subjected to column chromatography (on silica gel) to afford the product.

Pale-yellow solid (58.0 mg, 97%). R_f = 0.8 (hexane/EA = 9/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56–7.54 (m, 2H), 7.46–7.34 (m, 4H), 7.16–7.10 (m, 2H), 3.65 (q, *J* = 7.2 Hz, 1H), 1.49 (d, *J* = 7.2 Hz, 3H), 1.43 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.0; ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3, 159.4 (d, *J* = 246.3 Hz), 142.5 (d, *J* = 7.8 Hz), 135.6, 130.6 (d, *J* = 4.0 Hz), 128.9 (d, *J* = 2.9 Hz), 128.4, 127.6, 127.4 (d, *J* = 13.6 Hz), 123.4 (d, *J* = 3.2 Hz), 115.1 (d, *J* = 23.4 Hz), 80.9, 46.0, 27.9, 18.4.

***tert*-Butyl 2-(2-fluoro-4'-methoxy-[1,1'-biphenyl]-4-yl)propanoate (8b)**

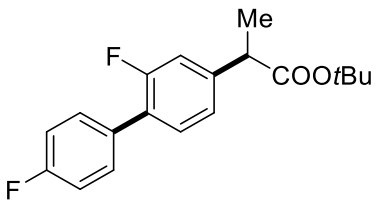


A Schlenk tube with Teflon-coated magnetic stir bar was added $Pd(dba)_2$ (4.6 mg, 4.0 mol%), **L13** (6.4 mg, 8.0 mol%), Pd:L = 1:2, 4-methoxyphenylboronic acid (47.4 mg, 0.30 mmol)), and K_3PO_4 (85.0 mg, 0.40 mmol). It was evacuated and flushed with nitrogen (3 cycles). *Tert*-

Butyl 2-(3-fluoro-4 (((trifluoromethyl)sulfonyl)oxy)phenyl)propanoate (74.5mg, 0.20 mmol) and dioxane (1.0 mL) was then added by syringes. The Schlenk tube was sealed and stirred at room temperature for 1 min. Then it was stirred at 110 °C for 12 h. Water and ethyl acetate were added for extraction. After removing the solvent, the resulting residue was subjected to column chromatography (on silica gel) to afford the product.

Colorless liquid (58.5 mg, 89%). R_f = 0.7 (hexane/EA = 9/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51–7.49 (m, 2H), 7.39–7.35 (m, 1H), 7.14–7.09 (m, 2H), 7.00–6.97 (m, 2H), 3.85 (s, 3H), 3.65 (q, *J* = 7.2 Hz, 1H), 1.49 (d, *J* = 7.2 Hz, 3H), 1.44 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -118.3; ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.3, 159.5 (d, *J* = 245.6 Hz), 159.1, 141.8 (d, *J* = 7.8 Hz), 130.3 (d, *J* = 3.9 Hz), 130.0 (d, *J* = 3.1 Hz), 127.9, 127.0 (d, *J* = 13.3 Hz), 123.4 (d, *J* = 3.3 Hz), 115.0 (d, *J* = 23.6 Hz), 113.8, 80.8, 55.2, 45.8, 27.9, 18.4. HRMS (APPI): calcd. For $C_{20}H_{23}FO_3^+$: 330.1626, found: 330.1627.

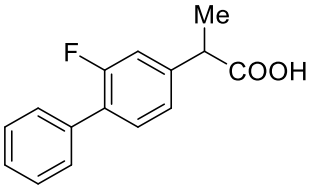
***tert*-Butyl 2-(2,4'-difluoro-[1,1'-biphenyl]-4-yl)propanoate (8c)**



A Schlenk tube with Teflon-coated magnetic stir bar was added $Pd(dba)_2$ (6.9 mg, 4.0 mol%), **L13** (9.5 mg, 8.0 mol%), Pd:L = 1:2, 4-fluorobenzeneboronic acid (63.0 mg, 0.45 mmol)), and K_3PO_4 (127.0 mg, 0.6 mmol). It was evacuated and flushed with nitrogen (3 cycles). *Tert*-Butyl 2-(3-fluoro-4 (((trifluoromethyl)sulfonyl)oxy)phenyl)propanoate (111.0 mg, 0.30 mmol) and dioxane (1.0 mL) was then added by syringes. The Schlenk tube was sealed and stirred at room temperature for 1 min. Then it was stirred at 110 °C for 12 h. Water and ethyl acetate were added for extraction. After removing the solvent, the resulting residue was subjected to column chromatography (on silica gel) to afford the product.

Pale-yellow solid (88.1 mg, 97%). R_f = 0.85 (hexane/EA = 9/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53–7.49 (m, 2H), 7.37–7.33 (m, 1H), 7.16–7.10 (m, 4H), 3.65 (q, *J* = 7.2 Hz, 1H), 1.49 (d, *J* = 7.2 Hz, 3H), 1.44 (s, 9H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.7, -118.1; ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.2, 162.3 (d, *J* = 245.4 Hz), 159.5 (d, *J* = 246.2 Hz), 142.6 (d, *J* = 7.5 Hz), 131.5 (d, *J* = 3.3 Hz), 130.6–130.4 (m), 126.4 (d, *J* = 13.2 Hz), 123.5 (d, *J* = 3.4 Hz), 115.3 (d, *J* = 21.3 Hz), 115.2 (d, *J* = 23.3 Hz), 80.9, 45.9, 27.9, 18.4. HRMS (APPI): calcd. For $C_{19}H_{20}F_2O_2^+$: 318.1426, found: 318.1420.

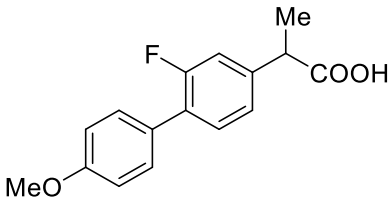
2-(2-Fluoro-[1,1'-biphenyl]-4-yl)propanoic acid (9a, Flurbiprofen)[6]



A 25 mL flask with Teflon-coated magnetic stir bar was added *tert*-Butyl 2-(2-fluoro-[1,1'-biphenyl]-4-yl)propanoate (60.1 mg, 0.20 mmol). The flask was evacuated and flushed with nitrogen (3 cycles). Anhydrous DCM (10 mL) was added to dissolve the solid. The flask was put in an ice bath and stirred at for a few minutes. Trifluoromethanesulfonic acid (0.50 mmol) was added under N_2 atmosphere. Then the solution was allowed to stir at room temperature and use TLC to confirm the completion of the reaction. The reaction mixture was subjected to column chromatography (on silica gel) to afford the product.

Pale-yellow solid (52.1 mg, 88%). R_f = 0.5 (hexane/EA = 3/1). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56–7.54 (m, 2H), 7.49–7.36 (m, 4H), 7.20–7.15 (m,2H), 3.80 (q, *J* = 7.2 Hz, 1H), 1.58 (d, *J* = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.4; ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.2, 159.6 (d, *J* = 247.1 Hz), 140.9 (d, *J* = 7.7 Hz), 135.4, 130.8 (d, *J* = 3.8 Hz), 128.9 (d, *J* = 2.8 Hz), 128.4, 128.2, 128.0, 127.7, 123.7 (d, *J* = 3.4 Hz), 115.3 (d, *J* = 23.8 Hz), 44.8, 18.0.

2-(2-Fluoro-4'-methoxy-[1,1'-biphenyl]-4-yl)propanoic acid (9b)

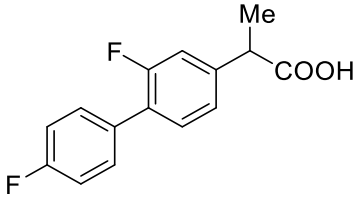


A 25 mL flask with Teflon-coated magnetic stir bar was added *ter*t-butyl 2-(2-fluoro-4'-methoxy-[1,1'-biphenyl]-4-yl)propanoate (50.8 mg, 0.154 mmol). The flask was evacuated and flushed with nitrogen (3 cycles). Anhydrous DCM (10 mL) was added to dissolve the solid. The flask was put in an ice bath and stirred at for a few minutes. Trifluoromethanesulfonic acid (0.39 mmol) was added under N_2 atmosphere. Then the solution was allowed to stir at room temperature and use TLC to confirm the completion of the reaction. The reaction mixture was subjected to column chromatography (on silica gel) to afford the product.

White solid (38.0 mg, 90%). R_f = 0.5 (hexane/EA = 3/1). M.P.: 115.0-116.0 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.48–7.46 (m, 2H), 7.39–7.35 (m, 1H), 7.16–7.11 (m, 2H), 7.00–6.96 (m, 2H), 3.85 (s, 3H), 3.77 (q, *J* = 7.2 Hz, 1H), 1.55 (d, *J* = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ

-117.5; ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.1, 159.6 (d, *J* = 246.4 Hz), 159.2, 141.3 (d, *J* = 7.8 Hz), 130.6 (d, *J* = 4.1 Hz), 130.0 (d, *J* = 3.0 Hz), 127.76, 127.75 (d, *J* = 13.2 Hz), 123.6 (d, *J* = 3.3 Hz), 115.3 (d, *J* = 23.7 Hz), 113.9, 55.3, 44.8, 18.0. HRMS (APPI): calcd. For $C_{16}H_{15}FO_3^+$: 274.1000, found: 274.1001.

2-(2,4'-Difluoro-[1,1'-biphenyl]-4-yl)propanoic acid (9c)



A 25 mL flask with Teflon-coated magnetic stir bar was added *tert*-butyl 2-(2,4'-difluoro-[1,1'-biphenyl]-4-yl)propanoate (63.6 mg, 0.20 mmol). The flask was evacuated and flushed with nitrogen (3 cycles). Anhydrous DCM (10 mL) was added to dissolve the solid. The flask was put in an ice bath and stirred at for a few minutes. Trifluoromethanesulfonic acid (0.50 mmol) was added under N_2 atmosphere. Then the solution was allowed to stir at room temperature and use TLC to confirm the completion of the reaction. The reaction mixture was subjected to column chromatography (on silica gel) to afford the product.

White solid (52.1 mg, 75%). R_f = 0.6 (hexane/EA = 3/1). M.P.: 118.5-119.5 °C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.52–7.48 (m, 2H), 7.39–7.35 (m, 1H), 7.19–7.10 (m, 4H), 3.79 (q, *J* = 7.2 Hz, 1H), 1.56 (d, *J* = 7.2 Hz, 3H); ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.7, -117.9; ^{13}C NMR (100 MHz, $CDCl_3$) δ 180.3, 162.4 (d, *J* = 245.7 Hz), 159.6 (d, *J* = 246.8 Hz), 141.0 (d, *J* = 7.6 Hz), 131.3 (d, *J* = 3.6 Hz), 130.7–130.5 (m), 127.1 (d, *J* = 13.5 Hz), 123.7 (d, *J* = 3.4 Hz), 115.41 (d, *J* = 21.4 Hz), 115.40 (d, *J* = 23.4 Hz), 44.8, 17.9. HRMS (APPI): calcd. For $C_{15}H_{11}F_2O_2$ [M – H]$^-$: 261.0733, found: 261.0727.

8. X-ray crystallography data of L17

Table S6 Crystal data and structure refinement for L17. (CCDC 2117109)

Identification code	exp_6910
Empirical formula	C35 H48 N P
Formula weight	513.71
Temperature	293(2) K
Wavelength	0.71073 A
Crystal system, space group	Triclinic, P -1
Unit cell dimensions	a = 10.6770(8) A alpha = 96.831(6) deg.
	B = 11.8045(10) A beta = 101.037(6) deg.
	C = 12.4452(9) A gamma = 111.157(7) deg.
Volume	1405.1(2) A^3
Z, Calculated density	2, 1.214 Mg/m^3
Absorption coefficient	0.123 mm^-1
F(000)	560
Crystal size	0.3 x 0.29 x 0.27 mm
Theta range for data collection	2.702 to 26.000 deg.
Limiting indices	-13<=h<=13, -14<=k<=14, -15<=l<=14
Reflections collected / unique	11455 / 5514 [R(int) = 0.0225]
Completeness to theta = 25.242	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.89425
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5514 / 0 / 335
Goodness-of-fit on F^2	1.051
Final R indices [I>2sigma(I)]	R1 = 0.0450, wR2 = 0.1007
R indices (all data)	R1 = 0.0624, wR2 = 0.1127
Extinction coefficient	n/a
Largest diff. peak and hole	0.275 and -0.217 e.A^-3

Table S7 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for L17. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
P(1)	4478(1)	6264(1)	6609(1)	28(1)
N(1)	2506(2)	5095(2)	8919(1)	39(1)
C(11)	3503(2)	6979(2)	5650(1)	28(1)
C(12)	4000(2)	8397(2)	5815(2)	32(1)
C(21)	3763(2)	6163(2)	7827(1)	30(1)
C(1)	6369(2)	7316(2)	7141(1)	29(1)
C(13)	3080(2)	8753(2)	4918(2)	36(1)
C(28)	3215(2)	5017(2)	8110(1)	31(1)
C(2)	7001(2)	7539(2)	6134(2)	37(1)
C(17)	1974(2)	6446(2)	5715(2)	34(1)
C(29)	3409(2)	3852(2)	7716(1)	32(1)
C(16)	3534(2)	6465(2)	4458(1)	36(1)
C(22)	3406(2)	7008(2)	8537(1)	34(1)
C(18)	1064(2)	6809(2)	4824(2)	38(1)
C(6)	7029(2)	6546(2)	7788(2)	36(1)
C(27)	2613(2)	6295(2)	9187(2)	39(1)
C(15)	2631(2)	6832(2)	3571(2)	41(1)
C(19)	1586(2)	8218(2)	5017(2)	40(1)
C(9)	6774(2)	8563(2)	7933(2)	41(1)
C(5)	8613(2)	7224(2)	8172(2)	40(1)
C(3)	8583(2)	8219(2)	6518(2)	46(1)
C(34)	4208(2)	3462(2)	8665(2)	43(1)
C(20)	1125(2)	6298(2)	3661(2)	47(1)
C(23)	3674(2)	8275(2)	8714(2)	44(1)
C(4)	9202(2)	7441(2)	7156(2)	44(1)
C(14)	3157(2)	8244(2)	3760(2)	43(1)
C(30)	2089(2)	2764(2)	7022(2)	44(1)
C(8)	8365(2)	9242(2)	8301(2)	52(1)
C(31)	2384(2)	1641(2)	6626(2)	50(1)
C(33)	4455(2)	2319(2)	8241(2)	51(1)
C(26)	2084(2)	6802(2)	9972(2)	54(1)

C(35)	1680(2)	4119(2)	9406(2)	57(1)
C(24)	3152(2)	8775(2)	9494(2)	54(1)
C(32)	3117(2)	1259(2)	7594(2)	52(1)
C(10)	8993(2)	8464(2)	8936(2)	51(1)
C(25)	2364(3)	8037(3)	10109(2)	60(1)
C(7)	8939(2)	9455(2)	7282(2)	57(1)

Table S8 Bond lengths [A] and angles [deg] for L17.

P(1)-C(11)	1.9023(17)
P(1)-C(21)	1.8203(17)
P(1)-C(1)	1.8822(18)
N(1)-C(28)	1.384(2)
N(1)-C(27)	1.374(2)
N(1)-C(35)	1.452(2)
C(11)-C(12)	1.536(2)
C(11)-C(17)	1.545(2)
C(11)-C(16)	1.545(2)
C(12)-H(12A)	0.9700
C(12)-H(12B)	0.9700
C(12)-C(13)	1.542(2)
C(21)-C(28)	1.385(2)
C(21)-C(22)	1.454(2)
C(1)-C(2)	1.540(2)
C(1)-C(6)	1.545(2)
C(1)-C(9)	1.535(2)
C(13)-H(13)	0.9800
C(13)-C(19)	1.524(3)
C(13)-C(14)	1.523(3)
C(28)-C(29)	1.503(2)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(2)-C(3)	1.531(3)
C(17)-H(17A)	0.9700
C(17)-H(17B)	0.9700
C(17)-C(18)	1.535(2)

C(29)-H(29)	0.9800
C(29)-C(34)	1.537(2)
C(29)-C(30)	1.532(3)
C(16)-H(16A)	0.9700
C(16)-H(16B)	0.9700
C(16)-C(15)	1.531(2)
C(22)-C(27)	1.411(3)
C(22)-C(23)	1.399(3)
C(18)-H(18)	0.9800
C(18)-C(19)	1.523(3)
C(18)-C(20)	1.523(3)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(6)-C(5)	1.533(3)
C(27)-C(26)	1.395(3)
C(15)-H(15)	0.9800
C(15)-C(20)	1.532(3)
C(15)-C(14)	1.526(3)
C(19)-H(19A)	0.9700
C(19)-H(19B)	0.9700
C(9)-H(9A)	0.9700
C(9)-H(9B)	0.9700
C(9)-C(8)	1.540(3)
C(5)-H(5)	0.9800
C(5)-C(4)	1.526(3)
C(5)-C(10)	1.518(3)
C(3)-H(3)	0.9800
C(3)-C(4)	1.523(3)
C(3)-C(7)	1.519(3)
C(34)-H(34A)	0.9700
C(34)-H(34B)	0.9700
C(34)-C(33)	1.520(3)
C(20)-H(20A)	0.9700
C(20)-H(20B)	0.9700
C(23)-H(23)	0.9300
C(23)-C(24)	1.382(3)
C(4)-H(4A)	0.9700
C(4)-H(4B)	0.9700

C(14)-H(14A)	0.9700
C(14)-H(14B)	0.9700
C(30)-H(30A)	0.9700
C(30)-H(30B)	0.9700
C(30)-C(31)	1.518(3)
C(8)-H(8)	0.9800
C(8)-C(10)	1.527(3)
C(8)-C(7)	1.519(3)
C(31)-H(31A)	0.9700
C(31)-H(31B)	0.9700
C(31)-C(32)	1.513(3)
C(33)-H(33A)	0.9700
C(33)-H(33B)	0.9700
C(33)-C(32)	1.512(3)
C(26)-H(26)	0.9300
C(26)-C(25)	1.361(3)
C(35)-H(35A)	0.9600
C(35)-H(35B)	0.9600
C(35)-H(35C)	0.9600
C(24)-H(24)	0.9300
C(24)-C(25)	1.389(3)
C(32)-H(32A)	0.9700
C(32)-H(32B)	0.9700
C(10)-H(10A)	0.9700
C(10)-H(10B)	0.9700
C(25)-H(25)	0.9300
C(7)-H(7A)	0.9700
C(7)-H(7B)	0.9700

C(21)-P(1)-C(11)	106.24(7)
C(21)-P(1)-C(1)	106.24(8)
C(1)-P(1)-C(11)	111.12(8)
C(28)-N(1)-C(35)	129.37(17)
C(27)-N(1)-C(28)	108.92(15)
C(27)-N(1)-C(35)	121.59(17)
C(12)-C(11)-P(1)	120.03(12)
C(12)-C(11)-C(17)	108.18(14)
C(12)-C(11)-C(16)	108.33(14)

C(17)-C(11)-P(1)	107.40(11)
C(17)-C(11)-C(16)	107.32(14)
C(16)-C(11)-P(1)	104.96(11)
C(11)-C(12)-H(12A)	109.6
C(11)-C(12)-H(12B)	109.6
C(11)-C(12)-C(13)	110.48(14)
H(12A)-C(12)-H(12B)	108.1
C(13)-C(12)-H(12A)	109.6
C(13)-C(12)-H(12B)	109.6
C(28)-C(21)-P(1)	118.79(13)
C(28)-C(21)-C(22)	106.29(15)
C(22)-C(21)-P(1)	134.10(13)
C(2)-C(1)-P(1)	108.67(12)
C(2)-C(1)-C(6)	107.47(14)
C(6)-C(1)-P(1)	104.47(12)
C(9)-C(1)-P(1)	118.74(12)
C(9)-C(1)-C(2)	109.53(15)
C(9)-C(1)-C(6)	107.35(14)
C(12)-C(13)-H(13)	109.3
C(19)-C(13)-C(12)	109.26(15)
C(19)-C(13)-H(13)	109.3
C(14)-C(13)-C(12)	109.63(15)
C(14)-C(13)-H(13)	109.3
C(14)-C(13)-C(19)	110.12(16)
N(1)-C(28)-C(21)	109.67(15)
N(1)-C(28)-C(29)	121.95(15)
C(21)-C(28)-C(29)	128.20(16)
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.0
C(3)-C(2)-C(1)	110.93(15)
C(3)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2B)	109.5
C(11)-C(17)-H(17A)	109.5
C(11)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	108.1
C(18)-C(17)-C(11)	110.73(14)
C(18)-C(17)-H(17A)	109.5

C(18)-C(17)-H(17B)	109.5
C(28)-C(29)-H(29)	105.4
C(28)-C(29)-C(34)	112.66(14)
C(28)-C(29)-C(30)	115.19(15)
C(34)-C(29)-H(29)	105.4
C(30)-C(29)-H(29)	105.4
C(30)-C(29)-C(34)	111.89(15)
C(11)-C(16)-H(16A)	109.4
C(11)-C(16)-H(16B)	109.4
H(16A)-C(16)-H(16B)	108.0
C(15)-C(16)-C(11)	111.21(14)
C(15)-C(16)-H(16A)	109.4
C(15)-C(16)-H(16B)	109.4
C(27)-C(22)-C(21)	106.51(16)
C(23)-C(22)-C(21)	136.07(18)
C(23)-C(22)-C(27)	117.41(17)
C(17)-C(18)-H(18)	109.3
C(19)-C(18)-C(17)	109.24(15)
C(19)-C(18)-H(18)	109.3
C(20)-C(18)-C(17)	110.04(15)
C(20)-C(18)-H(18)	109.3
C(20)-C(18)-C(19)	109.61(16)
C(1)-C(6)-H(6A)	109.4
C(1)-C(6)-H(6B)	109.4
H(6A)-C(6)-H(6B)	108.0
C(5)-C(6)-C(1)	111.01(15)
C(5)-C(6)-H(6A)	109.4
C(5)-C(6)-H(6B)	109.4
N(1)-C(27)-C(22)	108.57(16)
N(1)-C(27)-C(26)	128.7(2)
C(26)-C(27)-C(22)	122.7(2)
C(16)-C(15)-H(15)	109.5
C(16)-C(15)-C(20)	109.39(16)
C(20)-C(15)-H(15)	109.5
C(14)-C(15)-C(16)	109.54(16)
C(14)-C(15)-H(15)	109.5
C(14)-C(15)-C(20)	109.44(16)
C(13)-C(19)-H(19A)	109.8

C(13)-C(19)-H(19B)	109.8
C(18)-C(19)-C(13)	109.37(15)
C(18)-C(19)-H(19A)	109.8
C(18)-C(19)-H(19B)	109.8
H(19A)-C(19)-H(19B)	108.2
C(1)-C(9)-H(9A)	109.7
C(1)-C(9)-H(9B)	109.7
C(1)-C(9)-C(8)	109.88(15)
H(9A)-C(9)-H(9B)	108.2
C(8)-C(9)-H(9A)	109.7
C(8)-C(9)-H(9B)	109.7
C(6)-C(5)-H(5)	109.4
C(4)-C(5)-C(6)	109.56(15)
C(4)-C(5)-H(5)	109.4
C(10)-C(5)-C(6)	109.70(16)
C(10)-C(5)-H(5)	109.4
C(10)-C(5)-C(4)	109.36(18)
C(2)-C(3)-H(3)	109.6
C(4)-C(3)-C(2)	109.70(16)
C(4)-C(3)-H(3)	109.6
C(7)-C(3)-C(2)	108.91(17)
C(7)-C(3)-H(3)	109.6
C(7)-C(3)-C(4)	109.40(17)
C(29)-C(34)-H(34A)	109.2
C(29)-C(34)-H(34B)	109.2
H(34A)-C(34)-H(34B)	107.9
C(33)-C(34)-C(29)	111.87(16)
C(33)-C(34)-H(34A)	109.2
C(33)-C(34)-H(34B)	109.2
C(18)-C(20)-C(15)	109.20(15)
C(18)-C(20)-H(20A)	109.8
C(18)-C(20)-H(20B)	109.8
C(15)-C(20)-H(20A)	109.8
C(15)-C(20)-H(20B)	109.8
H(20A)-C(20)-H(20B)	108.3
C(22)-C(23)-H(23)	120.1
C(24)-C(23)-C(22)	119.8(2)
C(24)-C(23)-H(23)	120.1

C(5)-C(4)-H(4A)	109.8
C(5)-C(4)-H(4B)	109.8
C(3)-C(4)-C(5)	109.40(15)
C(3)-C(4)-H(4A)	109.8
C(3)-C(4)-H(4B)	109.8
H(4A)-C(4)-H(4B)	108.2
C(13)-C(14)-C(15)	109.27(15)
C(13)-C(14)-H(14A)	109.8
C(13)-C(14)-H(14B)	109.8
C(15)-C(14)-H(14A)	109.8
C(15)-C(14)-H(14B)	109.8
H(14A)-C(14)-H(14B)	108.3
C(29)-C(30)-H(30A)	109.3
C(29)-C(30)-H(30B)	109.3
H(30A)-C(30)-H(30B)	107.9
C(31)-C(30)-C(29)	111.78(16)
C(31)-C(30)-H(30A)	109.3
C(31)-C(30)-H(30B)	109.3
C(9)-C(8)-H(8)	109.2
C(10)-C(8)-C(9)	109.75(18)
C(10)-C(8)-H(8)	109.2
C(7)-C(8)-C(9)	109.91(17)
C(7)-C(8)-H(8)	109.2
C(7)-C(8)-C(10)	109.46(17)
C(30)-C(31)-H(31A)	109.3
C(30)-C(31)-H(31B)	109.3
H(31A)-C(31)-H(31B)	108.0
C(32)-C(31)-C(30)	111.50(17)
C(32)-C(31)-H(31A)	109.3
C(32)-C(31)-H(31B)	109.3
C(34)-C(33)-H(33A)	109.3
C(34)-C(33)-H(33B)	109.3
H(33A)-C(33)-H(33B)	107.9
C(32)-C(33)-C(34)	111.66(17)
C(32)-C(33)-H(33A)	109.3
C(32)-C(33)-H(33B)	109.3
C(27)-C(26)-H(26)	121.1
C(25)-C(26)-C(27)	117.7(2)

C(25)-C(26)-H(26)	121.1
N(1)-C(35)-H(35A)	109.5
N(1)-C(35)-H(35B)	109.5
N(1)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(23)-C(24)-H(24)	119.5
C(23)-C(24)-C(25)	120.9(2)
C(25)-C(24)-H(24)	119.5
C(31)-C(32)-H(32A)	109.5
C(31)-C(32)-H(32B)	109.5
C(33)-C(32)-C(31)	110.91(17)
C(33)-C(32)-H(32A)	109.5
C(33)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	108.0
C(5)-C(10)-C(8)	109.04(16)
C(5)-C(10)-H(10A)	109.9
C(5)-C(10)-H(10B)	109.9
C(8)-C(10)-H(10A)	109.9
C(8)-C(10)-H(10B)	109.9
H(10A)-C(10)-H(10B)	108.3
C(26)-C(25)-C(24)	121.5(2)
C(26)-C(25)-H(25)	119.3
C(24)-C(25)-H(25)	119.3
C(3)-C(7)-H(7A)	109.7
C(3)-C(7)-H(7B)	109.7
C(8)-C(7)-C(3)	109.98(17)
C(8)-C(7)-H(7A)	109.7
C(8)-C(7)-H(7B)	109.7
H(7A)-C(7)-H(7B)	108.2

Symmetry transformations used to generate equivalent atoms:

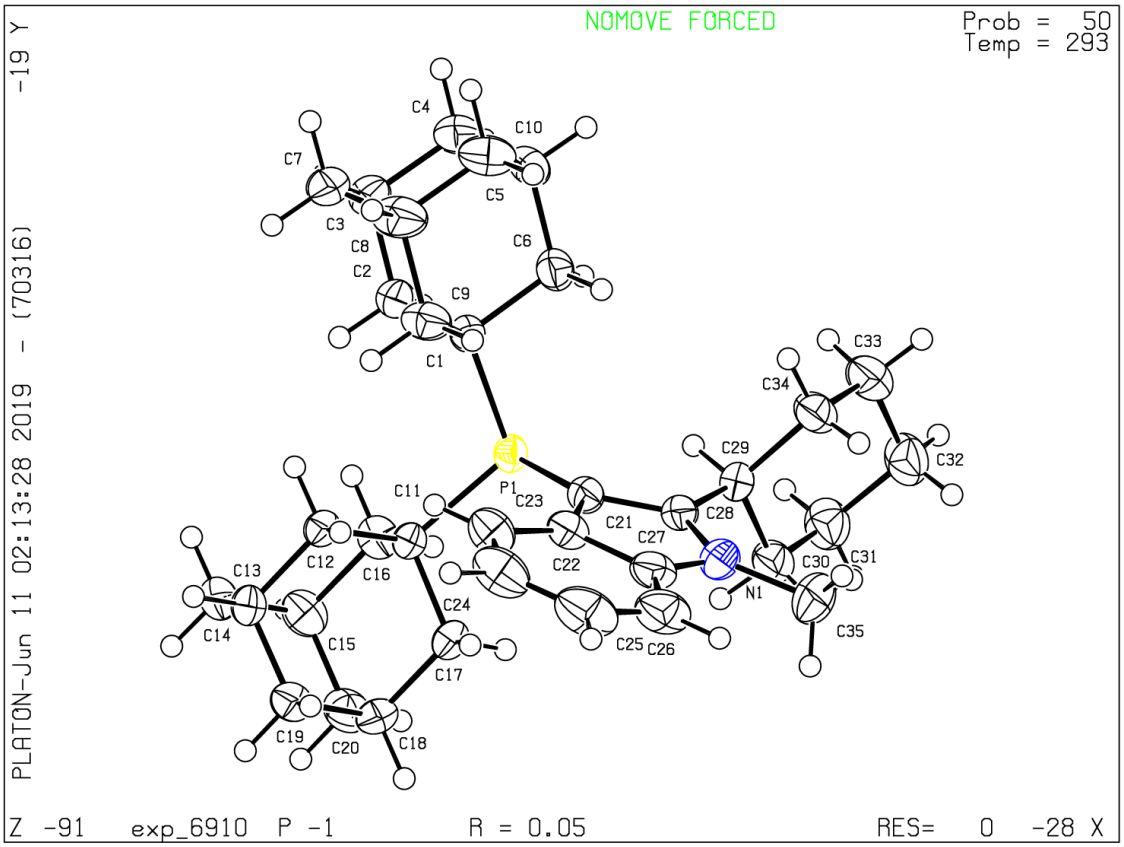


Fig. S3 ORTEP drawing of **L17** (50% probability for the thermal ellipsoid).

9. Computational Details

All density functional theory (DFT) calculations were performed using the Gaussian 16 software.[7] The B3PW91[8] functional has been used in this study. This hybrid functional has been shown to perform well in modelling a range of reactions involving transition metals.[9] Geometry optimizations of all the minima and transition states were fully optimized at the B3PW91-D3(BJ) level of theory, with the SDD[10] pseudopotential for Pd and K and the 6-31G(d) for other atoms in toluene solvent employing the Solvation Model Based on Density (SMD)[11]. Dispersion corrections according to Grimmes's DFT-D3 scheme[12] including Becke–Johnson damping was employed[13]. Vibrational frequencies were computed at the same level of theory to evaluate its zero-point vibrational energy and thermal corrections at 383.15K, and to check whether each optimized structure is an energy minimum or a transition state. Intrinsic reaction coordinates (IRC) calculations were performed to confirm whether the located transition state connect the correct reactant and product.[14] On the basis of the optimized structures, the single point energies were calculated at the B3PW91-D3(BJ)/Def2-TZVP[15] level and solvation energy corrections were calculated using the SMD model with Toluene as the solvent. For the rotational energy barrier study, geometries of the complexes were optimized at various fixed indole-PR_2 dihedral angles, using relaxed dihedral scans at the SMD(toluene)/B3PW91/6-31G* level in 30° increments and the rotation was performed from 0° to 360°. The reported Gibbs free energies were corrected using the quasi-harmonic model[16] with a cut-off frequency of 100 cm^{-1}. The Gibbs free energies were further corrected to standard state from 1 atm to 1 mol/L, a correction of $RTLn(c_s/c_g)$ (1.89 kcal/mol) is added to energies of all species. C_s is the standard molar concentration in solution (1 mol/L), c_g is the standard molar concentration in the gas phase (0.0446 mol/L), and R is the gas constant. Conformational searches are conducted to ensure that the most stable conformers are located. The images of computed species were generated using CYLView.[17]

Table S9 Table of energies of minimum energy structures[a]

Structure	*ZPE*	*tcH*	*E caled*	*H*	*G*	*qh-G*	*Imaginary frequency (cm^{-1})*
7A	0.974468	1.062675	-3012.07704510	-3011.01437010	-3011.24193310	-3011.21956910	
7B-TS-Cl	1.085657	1.196051	-4664.81866110	-4663.62261010	-4663.89859210	-4663.87090710	-225.07
7C-TS-Otf	1.085354	1.195682	-4664.83348410	-4663.63780210	-4663.91268010	-4663.88513210	-172.65
7D	0.597107	0.665525	-3222.79959110	-3222.13406610	-3222.32395310	-3222.30454010	
7E-TS-Cl	0.596568	0.664282	-3222.78685710	-3222.12257510	-3222.31283610	-3222.29279010	-95.17
7F	0.597091	0.665545	-3222.79775410	-3222.13220910	-3222.32074910	-3222.30211410	
7G-TS-Otf	0.595802	0.663535	-3222.77037610	-3222.10684110	-3222.29117110	-3222.27490210	-339.48
8A	0.773763	0.829488	-1887.04797010	-1886.21848210	-1886.36895410	-1886.35892010	
8B	0.885238	0.964288	-3539.83233410	-3538.86804610	-3539.07185310	-3539.05452110	
8C-TS	0.884643	0.963037	-3539.81639510	-3538.85335810	-3539.05706410	-3539.03929710	-120.06
8D	0.887689	0.966349	-3539.85739910	-3538.89105010	-3539.09293610	-3539.07694810	
8E	1.038819	1.130671	-3557.46499310	-3556.33432210	-3556.56446710	-3556.54474310	
8F-TS	1.036701	1.128224	-3557.44169410	-3556.31347010	-3556.54434810	-3556.52372510	-360.40
8G	1.039295	1.131279	-3557.49163910	-3556.36036010	-3556.59196410	-3556.57129510	
8H	0.885405	0.964422	-3539.83451810	-3538.87009610	-3539.07427010	-3539.05650410	
8I-TS	0.883951	0.962424	-3539.81147910	-3538.84905510	-3539.05136110	-3539.03428510	-164.47
8J	0.886216	0.965241	-3539.83495810	-3538.86971710	-3539.07474410	-3539.05675010	
8K	1.010779	1.092344	-3056.15034110	-3055.05799710	-3055.26164110	-3055.24725710	
8L-TS	1.007641	1.08904	-3056.12631610	-3055.03727610	-3055.24361110	-3055.22715010	-344.23
8M	1.010389	1.092124	-3056.17650370	-3055.08437970	-3055.29065870	-3055.27444470	
8N	1.039386	1.131199	-3557.42747810	-3556.29627910	-3556.52579310	-3556.50646210	
8O-TS	1.035525	1.127608	-3557.39768810	-3556.27008010	-3556.50441810	-3556.48247610	-140.19
8P	1.038596	1.13097	-3557.48581010	-3556.35484010	-3556.58983310	-3556.56739510	
8Q	1.039033	1.13093	-3557.46781152	-3556.33688152	-3556.56691552	-3556.54728452	
8R-TS	1.037152	1.128697	-3557.42861510	-3556.29991810	-3556.53196310	-3556.51065010	-293.47
8S	1.038738	1.130904	-3557.48616310	-3556.35525910	-3556.58959010	-3556.56745810	
$(KCl)_4$	0.005088	0.027124	-4240.77074210	-4240.74361810	-4240.82834110	-4240.82600210	
KOTf	0.028611	0.043311	-1561.49609110	-1561.45278010	-1561.51800510	-1561.51590310	
S1	0.110654	0.132468	-1652.73603310	-1652.60356510	-1652.68428910	-1652.68101310	
S2	0.150761	0.168839	-1077.73688910	-1077.56805010	-1077.63895610	-1077.63774010	
PPh-1	0.486576	0.531467	-1570.01889910	-1569.48743210	-1569.62062810	-1569.61029710	
PPh-2	0.486509	0.531542	-1570.01993210	-1569.48839010	-1569.62292310	-1569.61183310	

PPh-3	0.486972	0.531871	-1570.01744710	-1569.48557610	-1569.61796510	-1569.60812010	
PPh-4	0.487189	0.532046	-1570.01528010	-1569.48323410	-1569.61613410	-1569.60602210	
PPh-5	0.486909	0.531982	-1570.01571010	-1569.48372810	-1569.61917510	-1569.60769110	
PPh-6	0.487081	0.531841	-1570.01710510	-1569.48526410	-1569.61673310	-1569.60754610	
PPh-7	0.487149	0.531836	-1570.01657110	-1569.48473510	-1569.61534710	-1569.60660710	
PPh-8	0.486987	0.531894	-1570.01634610	-1569.48445210	-1569.61822510	-1569.60765910	
PPh-9	0.486916	0.531937	-1570.01552810	-1569.48359110	-1569.61884710	-1569.60753910	
PPh-10	0.487066	0.531935	-1570.01649510	-1569.48456010	-1569.61730210	-1569.60733910	
PPh-11	0.48671	0.531694	-1570.01875710	-1569.48706310	-1569.62070510	-1569.61019810	
PPh-12	0.486539	0.531506	-1570.02045510	-1569.48894910	-1569.62289810	-1569.61206210	
PiPr-1	0.493865	0.536673	-1343.79295710	-1343.25628410	-1343.38234310	-1343.37466610	
PiPr-2	0.494602	0.537294	-1343.78358310	-1343.24628910	-1343.37109610	-1343.36442810	
PiPr-3	0.495535	0.537898	-1343.77371010	-1343.23581210	-1343.35870310	-1343.35274110	
PiPr-4	0.494906	0.537808	-1343.77270210	-1343.23489410	-1343.36038110	-1343.35355310	
PiPr-5	0.494726	0.537474	-1343.77626510	-1343.23879110	-1343.36407610	-1343.35739510	
PiPr-6	0.494654	0.537273	-1343.77620510	-1343.23893210	-1343.36247210	-1343.35662910	
PiPr-7	0.494815	0.537277	-1343.77518110	-1343.23790410	-1343.36097110	-1343.35516610	
PiPr-8	0.494728	0.537407	-1343.77681510	-1343.23940810	-1343.36326510	-1343.35733110	
PiPr-9	0.495013	0.537859	-1343.77394710	-1343.23608810	-1343.36290210	-1343.35526810	
PiPr-10	0.495221	0.537686	-1343.77862810	-1343.24094210	-1343.36522910	-1343.35843710	
PiPr-11	0.494365	0.537119	-1343.79165310	-1343.25453410	-1343.37934110	-1343.37255810	
PiPr-12	0.494039	0.536828	-1343.79622510	-1343.25939710	-1343.38459910	-1343.37739810	

[a]Zero-point correction(ZPE), thermal correction to enthalpy (tcH), energies€, enthalpies (H), Gibbs free energies (G) (in Hartree), and quasi-harmonic corrected Gibbs free energy of the structures calculated at the B3PW91-D3(BJ)/Def2-TZVP-SMD(toluene)//B3PW91-D3(BJ)/6-31G(d)-SDD(Pd,K)-SMD(toluene) level of theory.

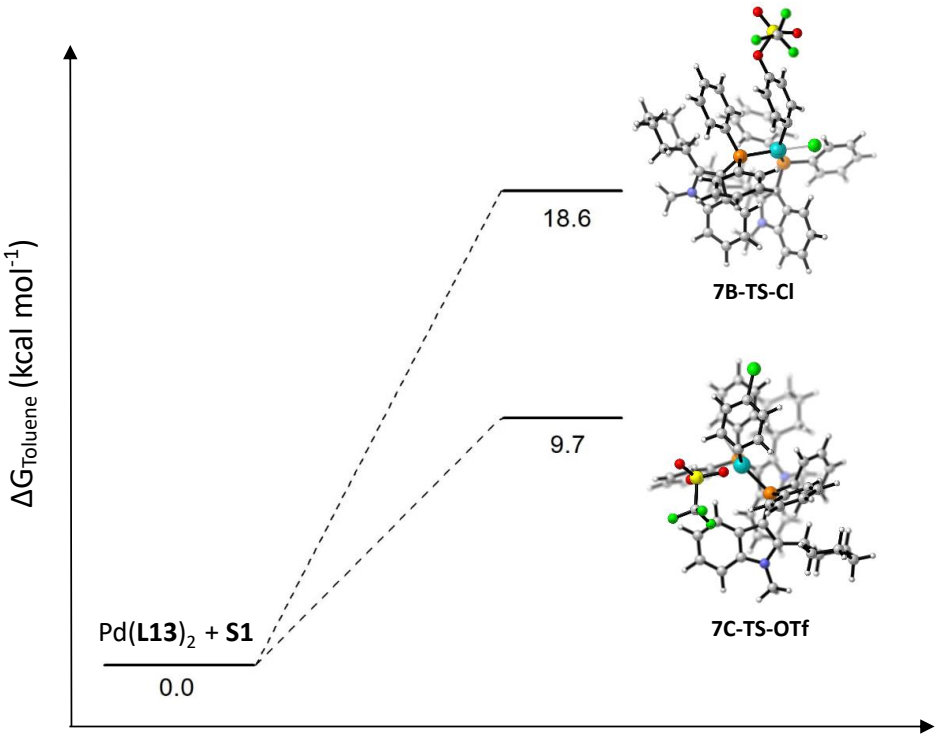


Fig. S4 Free energy profiles calculated for the chemoselective Pd(**L13**)$_2$ cross-coupling reaction of 4-chlorophenyltriflate.

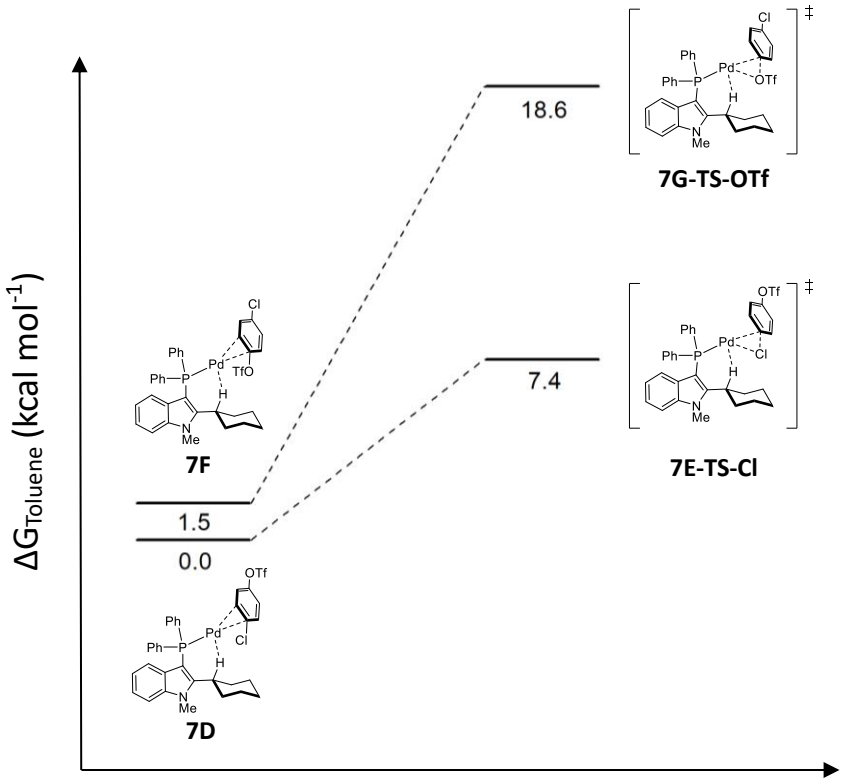


Fig. S5 Free energy profiles calculated for the chemoselective Pd(**L13**) cross-coupling reaction of 4-chlorophenyltriflate.

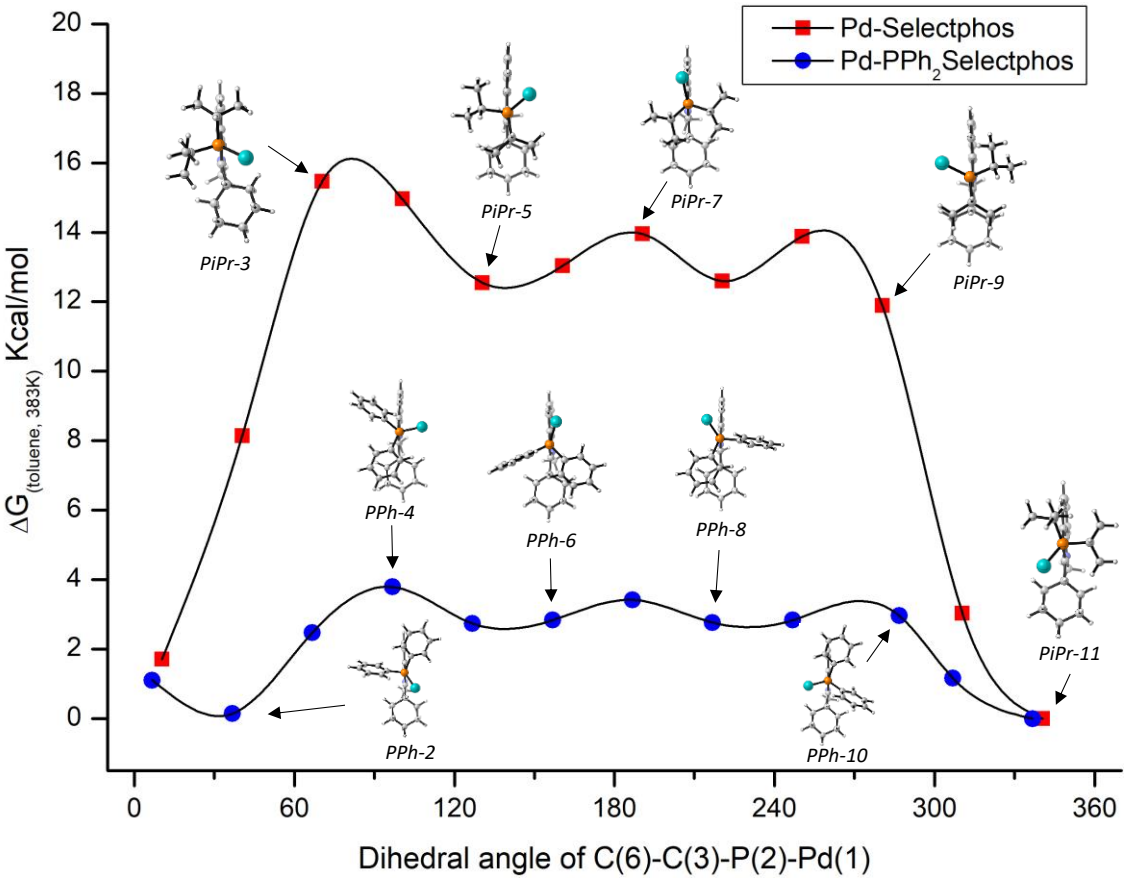


Fig. S6 Relative energy of SelectPhos (**L15**) and PhSelectPhos (**L13**) with different dihedral angles (PR_2-indole) in constrained-relaxation dihedral scans.

A preliminary investigation of the possible pathways for the reductive elimination step was also attempted (Figure S7). The calculated results suggested that the C-bound Pd-enolate (**8F-TS**) with an energy barrier of 13.2 kcal mol^{-1} may be a more facial pathway than the O-bound (**8O-TS**, 15.1 kcal mol^{-1}) and η^3-bound Pd-enolate (**8R-TS**, 23.0 kcal mol^{-1}) pathway for this *α*-arylation reaction.

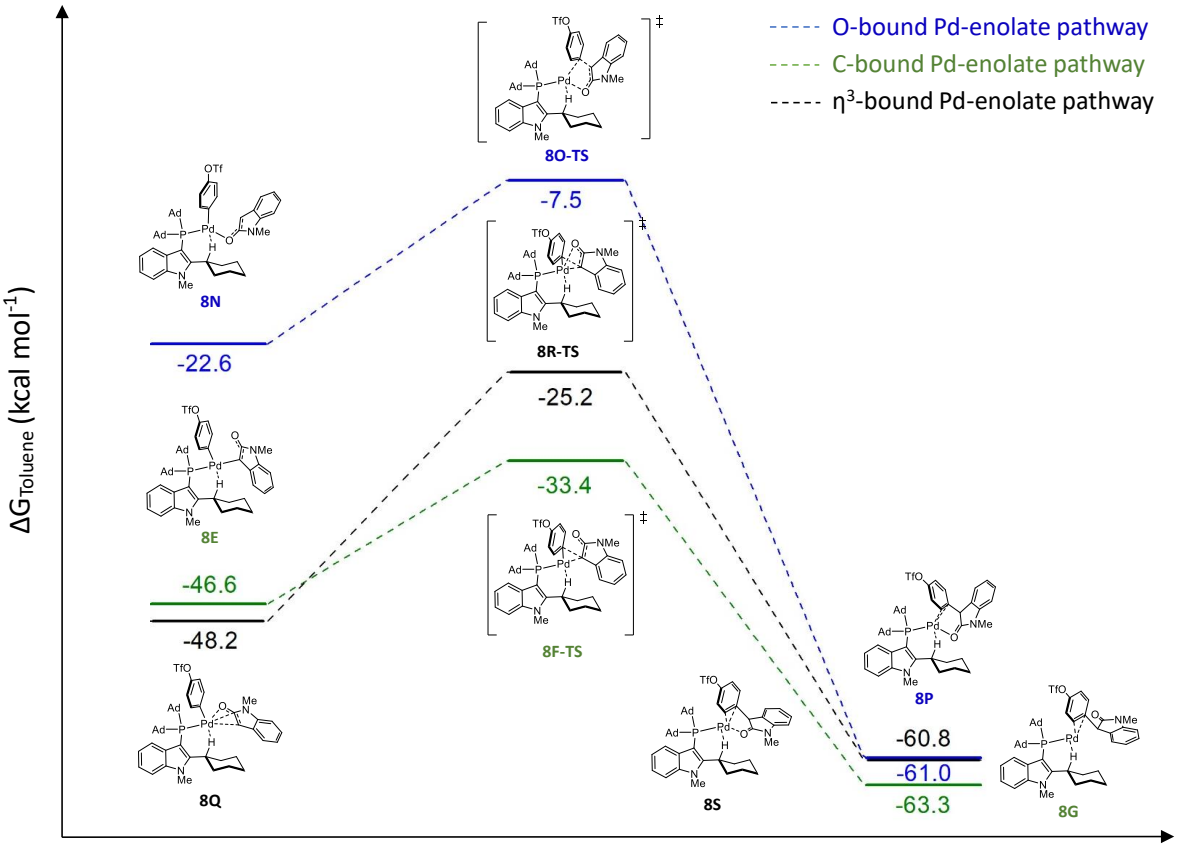


Fig. S7 Free energy profiles calculated for the chemoselective Pd-**L17** cross-coupling reaction of different reductive elimination mode.

Cartesian Coordinates of Minimum Energy Calculated Structures

7A

Charge: 0 Multiplicity: 1

0 1

P	-1.66893200	-0.13996300	1.49248100
C	-2.48691400	0.96906800	0.32536400
C	-2.12620300	2.36406800	0.22067700
N	-3.68982800	1.89534600	-1.34648900
C	-3.45029000	0.72217600	-0.65055500
C	-4.12617700	-0.57749800	-0.95599100
H	-3.69475900	-1.28439700	-0.24184500
C	-2.89048000	2.90369100	-0.84163400
C	-1.21086600	3.19263000	0.88529300
H	-0.59927100	2.78539200	1.68976600
C	-3.78966800	-1.13549300	-2.35025200
H	-4.22378800	-0.50224600	-3.13454100
H	-2.70489700	-1.11534600	-2.49427900
C	-2.74943900	4.22591500	-1.27014700
H	-3.32697800	4.61989500	-2.10153700
C	-1.82353300	5.01981300	-0.60248500
H	-1.68144000	6.05095900	-0.91504300
C	-5.64184400	-0.61113500	-0.68852700
H	-5.84590300	-0.23786400	0.32124700
H	-6.18493800	0.04486400	-1.38134100
C	-4.32707400	-2.55781900	-2.49400400
H	-4.10846000	-2.94159200	-3.49895900
H	-3.79743700	-3.20826900	-1.78514900
C	-1.06420000	4.50803200	0.46512000
H	-0.33898200	5.14869700	0.95751900
C	-5.82930800	-2.61830500	-2.21507100
H	-6.18895500	-3.65263100	-2.28828500
H	-6.36546400	-2.04380000	-2.98585000
C	-4.52686600	2.09605500	-2.50678400
H	-5.07715500	3.03604500	-2.40071200
H	-5.25010900	1.29018700	-2.59806300
H	-3.92599200	2.13688200	-3.42309100
C	-6.16228300	-2.04130300	-0.83845500

H	-7.24552200	-2.06683200	-0.66409300
H	-5.70071500	-2.66889500	-0.06235300
C	-2.85888700	-0.36820100	2.86660200
C	-2.40857500	-1.01883300	4.02423200
C	-4.17401200	0.10173300	2.81795100
C	-3.27213200	-1.23088100	5.09556300
H	-1.37506300	-1.35616800	4.07758500
C	-5.03404900	-0.09646000	3.89732100
H	-4.51459500	0.63520600	1.93575600
C	-4.58851300	-0.77014800	5.03349300
H	-2.91491900	-1.74343100	5.98519000
H	-6.05404500	0.27694200	3.84986800
H	-5.26008800	-0.92556900	5.87389300
C	-1.64572800	-1.79154600	0.68126400
C	-0.94290100	-1.90197900	-0.52737100
C	-2.22771300	-2.93515300	1.23788700
C	-0.84364700	-3.12888200	-1.17289500
H	-0.48151100	-1.01882700	-0.95755900
C	-2.10606400	-4.16929500	0.59738000
H	-2.78480300	-2.86479300	2.16713600
C	-1.41705000	-4.27107600	-0.60954800
H	-0.31110100	-3.19204900	-2.11686800
H	-2.56102100	-5.05088700	1.04228500
H	-1.32898200	-5.23189500	-1.11010400
Pd	0.50001900	0.49189100	1.70150600
P	2.35140500	0.92796600	0.50594800
C	2.11060900	0.10015000	-1.09147200
C	4.03981700	0.46287400	1.06835700
C	2.64383600	2.67851700	0.03821700
C	1.10785200	0.53723300	-2.03778700
C	2.54254200	-1.15320800	-1.50674500
C	4.16429100	-0.18001600	2.30414500
C	5.18708900	0.72229700	0.30844800
C	2.45158800	3.64646900	1.03105600
C	3.07006900	3.07835500	-1.23263500
C	1.01861900	-0.46985000	-3.03398500
C	0.24191600	1.63939800	-2.10352800
N	1.88563600	-1.48824000	-2.68534200

C	3.43746300	-2.09839700	-0.76875300
C	5.41780200	-0.57963600	2.76764600
H	3.26573600	-0.37636000	2.88580500
C	6.43724600	0.32218200	0.77035500
H	5.09714800	1.22853700	-0.64858200
C	2.69770200	4.99070900	0.76371700
H	2.09943000	3.33574600	2.01252800
C	3.29843500	4.42591900	-1.50475400
H	3.20601600	2.33495100	-2.01265800
C	0.13219200	-0.37537600	-4.11014300
H	0.25561300	2.40369100	-1.33502500
C	-0.65223300	1.72706600	-3.16235300
C	2.11171700	-2.64639100	-3.51856400
H	3.81029600	-1.52234500	0.07924900
C	4.69647700	-2.55914500	-1.51970000
C	2.66899500	-3.27476100	-0.13904000
C	6.55412700	-0.33232500	1.99943800
H	5.50559400	-1.08390000	3.72648500
H	7.32395700	0.52074600	0.17372000
C	3.11588200	5.38362300	-0.50782800
H	2.55009200	5.73326400	1.54392800
H	3.61787800	4.72807300	-2.49901700
H	0.08517900	-1.13857700	-4.88133900
C	-0.70195000	0.73642200	-4.15852300
H	-1.32205000	2.57940600	-3.21546400
H	1.19251500	-2.88018900	-4.06133400
H	2.36749000	-3.51142700	-2.90875200
H	2.91246700	-2.47220000	-4.24744300
H	4.43855300	-3.17883200	-2.38709600
H	5.22971700	-1.68063000	-1.90326400
C	5.59883700	-3.36264000	-0.58271200
H	1.81419700	-2.88019200	0.42199100
H	2.25631500	-3.93755000	-0.91130200
C	3.59381000	-4.07564000	0.77668100
H	7.53192500	-0.64431700	2.35717000
H	3.29348000	6.43428800	-0.72264100
H	-1.40614200	0.83574200	-4.98062300
H	6.48498000	-3.71557300	-1.12587900

H	5.95863200	-2.70057400	0.21720500
C	4.84901700	-4.54217000	0.03826900
H	3.05382100	-4.93329700	1.19763700
H	3.89029300	-3.44003100	1.62346900
H	5.50875100	-5.09289100	0.72094200
H	4.56039300	-5.24695300	-0.75660300

7B-TS-Cl

Charge: 0 Multiplicity: 1

P	-1.53496000	-1.92257700	-0.63155400
C	-3.20333100	-1.51873500	-0.08328900
C	3.33442100	-0.87773400	1.55125800
C	-3.67511700	-2.07982700	1.15957500
N	-5.31232800	-0.80263900	0.26929300
C	-4.23706800	-0.75429600	-0.60905200
C	-4.27059300	-0.02026400	-1.91380300
H	-3.36706700	-0.34076900	-2.43647600
C	-5.00560700	-1.63067900	1.33032400
C	-3.09706200	-2.90450200	2.13329800
H	-2.07150100	-3.24828400	2.02860500
C	3.75851900	-1.48319000	-1.16057300
C	-4.13949400	1.50651600	-1.77627900
H	-4.99135400	1.92442400	-1.22408800
H	-3.24730500	1.72776000	-1.18128900
C	4.42239700	-0.34685400	0.88380400
H	5.10704500	0.32444200	1.39071500
C	4.61467900	-0.64504500	-0.46558200
C	2.67333900	-2.04611200	-0.49027900
H	2.03928400	-2.76707300	-0.99622000
C	-5.78122600	-2.00586300	2.42832300
H	-6.80673600	-1.66710400	2.54390700
C	-5.18804800	-2.82939800	3.37943700
H	-5.76373400	-3.14082200	4.24718000
C	-5.43313500	-0.42665300	-2.83597900
H	-5.44191300	-1.51830200	-2.94454100
H	-6.40068400	-0.14526300	-2.40407200
C	2.40945900	-1.67535200	0.84640000
C	-4.04456800	2.16697400	-3.15116300

H	-4.00200400	3.25829100	-3.04268900
H	-3.10183000	1.86061700	-3.62457600
C	-3.85777000	-3.26600600	3.23873000
H	-3.42215500	-3.90386900	4.00323700
C	-5.20624100	1.76520500	-4.05907800
H	-5.09578200	2.23439100	-5.04494800
H	-6.15012800	2.14053900	-3.63498700
C	-6.56775100	-0.09246400	0.18912100
H	-7.37065100	-0.73206900	-0.19686900
H	-6.46831200	0.78171700	-0.45011300
H	-6.84008200	0.25782000	1.18836500
C	-5.28813900	0.24548000	-4.20094600
H	-6.12856300	-0.03529000	-4.84836600
H	-4.37352200	-0.12132800	-4.68871300
H	3.16416700	-0.63453300	2.59318300
H	3.94719300	-1.71988800	-2.20227100
Cl	1.57227000	-3.17921400	1.90064400
C	-1.71164900	-3.71079300	-1.00952800
C	-0.59182200	-4.53880500	-0.88363400
C	-2.92900700	-4.26567900	-1.42211000
C	-0.67810800	-5.89618900	-1.18718300
H	0.34227600	-4.11819500	-0.52214200
C	-3.01674800	-5.62249000	-1.72242000
H	-3.80659200	-3.62962700	-1.49816300
C	-1.89058400	-6.43933800	-1.60900500
H	0.19835600	-6.52997000	-1.08040900
H	-3.96646000	-6.04510500	-2.04062600
H	-1.96228800	-7.49944900	-1.83819100
C	-1.26589200	-1.18679100	-2.29134800
C	-0.85797800	0.15442800	-2.36520500
C	-1.35866400	-1.93455500	-3.47058400
C	-0.54801700	0.72965900	-3.59350100
H	-0.79994600	0.74330100	-1.45414700
C	-1.05282500	-1.35233700	-4.70082900
H	-1.66956800	-2.97353600	-3.42950700
C	-0.64377800	-0.02207300	-4.76613500
H	-0.21806300	1.76311200	-3.63730900
H	-1.12872100	-1.94512200	-5.60875300

H	-0.39553600	0.42778400	-5.72372700
Pd	0.34278700	-1.30930600	0.66037100
P	0.37908600	0.91334200	1.28388500
C	-1.09514800	1.94128000	1.04398100
C	1.78083600	1.78054000	0.48059700
C	0.63865600	1.18678200	3.08298800
C	-2.28820900	1.61215400	1.78943000
C	-1.36185100	3.11411800	0.34365900
C	2.07294800	1.42956200	-0.84497200
C	2.59443000	2.71393800	1.13022500
C	0.95665400	0.09234200	3.89260300
C	0.45923200	2.44374300	3.67372600
C	-3.24103000	2.61965100	1.50870600
C	-2.61144200	0.59300900	2.69390900
N	-2.65942800	3.52022900	0.63586400
C	-0.45446000	3.87553000	-0.57116000
C	3.13162800	2.02840500	-1.51940300
H	1.47976100	0.66597400	-1.33750000
C	3.67069000	3.29524900	0.46022900
H	2.40339400	2.97452200	2.16597600
C	1.13594400	0.25699000	5.26521500
H	1.03468300	-0.89462200	3.44300200
C	0.63951600	2.60933600	5.04426500
H	0.15355300	3.28647100	3.05906400
C	-4.51556800	2.61586000	2.08102800
H	-1.90113800	-0.19649400	2.91561900
C	-3.86330200	0.60166200	3.29070500
C	-3.37699500	4.65950000	0.11322000
H	0.42246200	3.23618800	-0.68806000
C	0.07758300	5.19091600	0.02411200
C	-0.99982400	4.08188400	-1.99352900
C	3.93801400	2.96067800	-0.86660800
H	3.34964500	1.73941900	-2.54363500
H	4.30341600	4.01055300	0.97944900
C	0.98522300	1.51700600	5.84144800
H	1.37903200	-0.60296900	5.88386100
H	0.49732100	3.58884800	5.49374400
H	-5.25148300	3.37897100	1.84462400

C	-4.80639700	1.59778200	2.98327600
H	-4.12719400	-0.19146800	3.98215600
H	-3.98398900	4.39056700	-0.75937300
H	-2.68530400	5.45189800	-0.16519000
H	-4.03561600	5.05183700	0.89297000
H	-0.73820400	5.91138400	0.17251200
H	0.50444300	4.98979300	1.01399000
C	1.13845000	5.79901800	-0.89357100
H	-1.36185800	3.12579100	-2.38431300
H	-1.85834300	4.76325800	-1.99606100
C	0.09128200	4.66428600	-2.89086900
H	4.78174200	3.40871200	-1.38394600
H	1.11841400	1.64622400	6.91242000
H	-5.78383400	1.57126900	3.45826900
H	1.48059900	6.75882700	-0.48593700
H	2.01031200	5.13169300	-0.90928700
C	0.62089500	5.98105200	-2.32092800
H	-0.29567800	4.81349500	-3.90698900
H	0.92052800	3.94579400	-2.96517400
H	1.41676000	6.38032900	-2.96209000
H	-0.18959700	6.72559200	-2.32424800
O	5.68200600	-0.01056100	-1.13638100
S	7.02828600	-0.84857500	-1.47901400
O	6.73243400	-2.23342900	-1.79138300
O	7.79660500	0.00939800	-2.35718900
C	7.88038500	-0.83558100	0.17542000
F	9.13693000	-1.22705700	-0.00368700
F	7.86405600	0.39503400	0.67719700
F	7.26864100	-1.66619400	1.00916700

7C-Ts-OTf

Charge: 0 Multiplicity: 1

P	-1.28598700	0.41949800	-0.77240600
C	-2.31631200	1.22514000	0.44868800
C	-2.53272100	0.73137400	1.78502500
N	-3.82887000	2.55970800	1.45078300
C	-3.13789900	2.33838000	0.27741000
C	-3.29683500	3.15052700	-0.97090000

H	-2.51890900	2.77620200	-1.64610100
C	-3.46774100	1.60562700	2.39002400
C	-2.02340100	-0.34201900	2.52658700
H	-1.33589300	-1.04700800	2.06963200
C	-3.02288500	4.65628200	-0.81408100
H	-3.80104900	5.12973700	-0.20359300
H	-2.07438700	4.81243800	-0.28854500
C	-3.87475700	1.45594200	3.71857300
H	-4.57643600	2.14334900	4.18200800
C	-3.33855300	0.39252600	4.43617900
H	-3.63351500	0.24829800	5.47210600
C	-4.62752800	2.90078700	-1.70484700
H	-4.77428600	1.82301600	-1.83045700
H	-5.47197200	3.27225400	-1.10860200
C	-2.99603200	5.32491300	-2.18763300
H	-2.80619900	6.40021400	-2.07815800
H	-2.15860600	4.91240900	-2.76898500
C	-2.42686900	-0.50006400	3.84394200
H	-2.03142400	-1.32895600	4.42337400
C	-4.30639800	5.08885000	-2.94021200
H	-4.26278700	5.55149700	-3.93434800
H	-5.12539700	5.58542300	-2.39824600
C	-4.76330100	3.62357500	1.74564600
H	-5.53182600	3.24285300	2.42307100
H	-5.25808000	3.95804300	0.83589500
H	-4.26251700	4.47575400	2.21951700
C	-4.61593800	3.59694200	-3.06557600
H	-5.57799800	3.44486300	-3.57057700
H	-3.85276800	3.11912100	-3.69503300
C	-2.47304200	0.06706400	-2.12439400
C	-3.55914200	-0.75773400	-1.80029000
C	-2.34998600	0.54919900	-3.43075000
C	-4.49921500	-1.09871300	-2.76613800
H	-3.65928000	-1.13884300	-0.79159100
C	-3.29642300	0.20682000	-4.39799900
H	-1.52699200	1.20414900	-3.69740300
C	-4.37027000	-0.61803400	-4.07084500
H	-5.32820400	-1.74841100	-2.49906700

H	-3.19264300	0.59328600	-5.40869900
H	-5.10302100	-0.88660600	-4.82703700
C	-0.13170800	1.63091500	-1.50172300
C	0.01597300	2.93051100	-1.01804200
C	0.68103700	1.19471600	-2.56136600
C	0.92339200	3.80279700	-1.61889000
H	-0.56408400	3.25328800	-0.16092500
C	1.57947500	2.06882600	-3.16285400
H	0.59918400	0.16935200	-2.91525900
C	1.69643100	3.38093200	-2.69677300
H	1.02217700	4.81297600	-1.23260900
H	2.19299500	1.72609900	-3.99197600
H	2.39876600	4.06367100	-3.16743200
Pd	0.07225400	-1.30201600	-0.11897900
P	1.91622600	-0.35387200	1.03926900
C	2.36757800	1.39255900	1.07702200
C	3.32569300	-1.26901700	0.31520200
C	1.91755600	-0.83974000	2.79935100
C	1.46144700	2.34836400	1.66642800
C	3.43642900	2.11417500	0.54900300
C	3.35382300	-1.42247900	-1.07895200
C	4.33660400	-1.84315400	1.09215900
C	1.16940300	-1.96337400	3.17260900
C	2.61909100	-0.12215300	3.77383000
C	2.00950500	3.63222200	1.43719900
C	0.25129100	2.23080000	2.35609700
N	3.21025200	3.46586600	0.77537400
C	4.69722600	1.59569300	-0.07135300
C	4.39887300	-2.10755100	-1.68869900
H	2.55120400	-0.99958600	-1.67787400
C	5.37259800	-2.54693500	0.47831500
H	4.31524500	-1.73822700	2.17282000
C	1.13861400	-2.37440700	4.50260700
H	0.59153200	-2.50451500	2.42728200
C	2.58088900	-0.53202700	5.10496800
H	3.18213300	0.76173000	3.48773100
C	1.34274800	4.79940800	1.81519300
H	-0.16617600	1.25710300	2.58022300

C	-0.41607100	3.38657800	2.74159800
C	3.99658400	4.59002900	0.32184100
H	4.55945200	0.51651100	-0.12670000
C	5.93318200	1.78901600	0.82815900
C	4.95270500	2.04082800	-1.52023600
C	5.40988600	-2.67406800	-0.91016700
H	4.41283800	-2.22114700	-2.76826100
H	6.15298000	-2.99550700	1.08745000
C	1.84322500	-1.65825100	5.47035700
H	0.55078200	-3.24477600	4.78134600
H	3.12306800	0.03260300	5.85911700
H	1.75399500	5.78377400	1.61125000
C	0.11862200	4.65699600	2.46372600
H	-1.36380800	3.30079000	3.26439600
H	3.61409100	4.98661200	-0.62596300
H	5.03713100	4.30397400	0.18906800
H	3.96049600	5.37984000	1.07730700
H	6.16663000	2.85311800	0.96356000
H	5.71236300	1.38891200	1.82521600
C	7.14533100	1.07850600	0.22660200
H	4.06475900	1.81304700	-2.11852700
H	5.10474000	3.12504800	-1.58476000
C	6.17962800	1.32708200	-2.08740000
H	6.21819300	-3.22296400	-1.38553200
H	1.81005400	-1.97190000	6.51048800
H	-0.42488100	5.54651400	2.77172800
H	8.02863800	1.24856200	0.85524100
H	6.95697500	-0.00423100	0.22628000
C	7.41023100	1.54015100	-1.20627500
H	6.37459200	1.67460200	-3.11010200
H	5.96708700	0.25096200	-2.15111100
H	8.27275400	1.00503900	-1.62316000
H	7.67468400	2.60867200	-1.20148300
C	-0.52807900	-2.84767500	-1.23351400
C	0.50878900	-3.60321800	-0.62253700
C	-0.64064000	-2.77270800	-2.63856000
C	1.52905900	-4.13442400	-1.44055700
H	0.46321900	-3.88312000	0.42492100

C	0.38083300	-3.28319300	-3.41307700
H	-1.48599300	-2.26277200	-3.08758500
H	2.33464200	-4.70654400	-0.99264500
C	1.46454000	-3.95177800	-2.80569500
H	0.35718700	-3.16438200	-4.49220800
Cl	2.72646000	-4.60211100	-3.83233900
F	-4.16794200	-2.14121600	1.28409500
C	-4.10391000	-3.47289900	1.19357800
S	-2.40507000	-4.02623500	0.70490300
F	-5.00113000	-3.87877900	0.29252600
F	-4.41614200	-3.99379900	2.38094200
O	-2.48910900	-5.48324100	0.61506800
O	-1.50839000	-3.46110900	1.72346100
O	-2.28999700	-3.33486500	-0.64924700

7D

Charge: 0 Multiplicity: 1

P	-1.17202800	-0.60004300	0.47232200
N	-4.84672800	-0.36647000	-1.04208400
C	-3.42011900	-2.08224500	-0.64244900
C	-3.68716700	0.18352100	-0.53592800
C	-3.44122100	1.64828500	-0.36928600
H	-2.35885900	1.70439600	-0.14032400
C	-4.70514600	-1.74147600	-1.13417900
C	-2.78927500	-0.84509000	-0.25324800
C	-1.22070000	-1.35535400	2.13945200
C	-0.07803600	-1.70685500	-0.49754300
C	-5.59805900	-2.70282500	-1.61196000
H	-6.57593600	-2.43101200	-1.99859000
C	-2.23551200	-2.21893100	2.56487200
H	-3.04912700	-2.47181700	1.89331200
C	0.98978500	-2.38655200	0.09641100
H	1.10535000	-2.38087600	1.17597000
C	-5.18379400	-4.02994000	-1.58740600
H	-5.85377600	-4.80264100	-1.95475500
C	-3.02703500	-3.42835200	-0.63090700
H	-2.04543800	-3.71054500	-0.26261900
C	-0.18940800	-1.02026100	3.02884800

H	0.57942400	-0.31838800	2.70994200
C	-4.13471500	2.28709400	0.84324300
H	-5.22286100	2.33333000	0.69292900
H	-3.96093900	1.66446700	1.72911700
C	-2.20712100	-2.75202300	3.85240800
H	-3.00237900	-3.41943500	4.17447700
C	-6.05311700	0.32606800	-1.43848600
H	-6.92105600	-0.27460300	-1.15243300
H	-6.08105600	0.49815400	-2.52056100
H	-6.12233100	1.28138300	-0.92133300
C	-3.62085400	2.49077000	-1.64069700
H	-3.09335500	2.01046000	-2.47410800
H	-4.67791100	2.55780500	-1.92732000
C	-0.20765400	-1.72203300	-1.89276400
H	-1.03693300	-1.19738400	-2.36033800
C	-3.91306000	-4.38825100	-1.10267400
H	-3.61912500	-5.43442500	-1.10167300
C	-0.15445600	-1.56761300	4.30887700
H	0.65411500	-1.30617500	4.98663000
C	0.71980200	-2.40108900	-2.67745500
H	0.60513400	-2.41119200	-3.75852900
C	-1.16516300	-2.43508900	4.72319000
H	-1.14566000	-2.85506800	5.72543200
C	1.92098500	-3.06039100	-0.69239500
H	2.75352200	-3.57273200	-0.21828900
C	1.79204500	-3.06741700	-2.08016100
H	2.52061500	-3.59025500	-2.69385300
C	-3.07346900	3.89847700	-1.40403400
H	-1.98940500	3.83251100	-1.23590000
H	-3.21953400	4.51487600	-2.30006900
C	-3.73033400	4.55860900	-0.19102700
H	-3.29387900	5.55047600	-0.01975100
H	-4.79961400	4.71629300	-0.39891900
C	-3.58514000	3.69647900	1.06359000
H	-4.08859200	4.17054400	1.91544300
H	-2.51898300	3.61821900	1.32613300
Pd	-0.15787900	1.43978400	0.40500000
C	1.45372300	2.81735800	0.05946400

C	2.16786000	2.62987100	1.27346700
C	1.53442100	1.83088200	-0.97217900
C	2.98485000	1.51965400	1.43292100
H	2.10016400	3.38136600	2.05330700
C	2.39965100	0.72580700	-0.79748900
H	1.11990700	2.03434200	-1.95465500
H	3.53403800	1.36403000	2.35472200
C	3.10385300	0.60253700	0.38139800
H	2.48824300	-0.02584900	-1.57358100
O	3.87200800	-0.56187400	0.57609600
S	5.48509400	-0.49480000	0.40459600
O	6.00326900	0.80147400	0.79628700
O	5.97796900	-1.74282000	0.94693500
C	5.63676200	-0.60980400	-1.44700000
F	6.90638900	-0.86282300	-1.74098700
F	4.86749300	-1.59263900	-1.89921900
F	5.27000600	0.53816000	-2.00332900
Cl	0.84144700	4.43182100	-0.31997400

7E-TS-Cl

Charge: 0 Multiplicity: 1

P	1.21708900	0.37354900	0.40539200
N	4.90952100	0.98168100	-0.97943400
C	3.14539200	2.33659300	-0.54114500
C	3.88305600	0.17455100	-0.53293000
C	3.97212500	-1.31050900	-0.39793200
H	2.93298200	-1.61417800	-0.15427400
C	4.48298700	2.29883100	-1.00897000
C	2.77863300	0.97349500	-0.24045100
C	1.14587600	0.94493500	2.14116500
C	-0.01897900	1.41108300	-0.46073300
C	5.16787900	3.44949700	-1.40501900
H	6.18772900	3.40693600	-1.77611000
C	2.08275700	1.82979100	2.68424300
H	2.88796800	2.21146600	2.06476700
C	-1.01375000	2.12771000	0.20924100
H	-1.04315800	2.13464600	1.29429300
C	4.49084700	4.66029500	-1.31375700

H	4.99420100	5.57511200	-1.61487800
C	2.48813400	3.57263400	-0.45514200
H	1.46608000	3.62842700	-0.09524900
C	0.11646500	0.45036100	2.95453100
H	-0.59940400	-0.25244500	2.53696500
C	4.81078400	-1.79460300	0.79473800
H	5.87677400	-1.57734700	0.63810100
H	4.50393200	-1.24933600	1.69525900
C	1.98356400	2.22158600	4.01848700
H	2.71763100	2.90817700	4.43238100
C	6.23666000	0.58318500	-1.39400900
H	6.96255700	1.31471900	-1.02776700
H	6.31241500	0.52295900	-2.48588200
H	6.48958200	-0.38394000	-0.96473700
C	4.30750100	-2.06858900	-1.69055700
H	3.65518000	-1.71353400	-2.49781900
H	5.34068800	-1.87718700	-2.00655000
C	0.00049200	1.41062900	-1.86192400
H	0.77120300	0.85129200	-2.38707300
C	3.16735900	4.72052100	-0.84195100
H	2.66672500	5.68318800	-0.78208100
C	0.01176000	0.85496100	4.28235100
H	-0.79445700	0.47115900	4.90234000
C	-0.95187900	2.12796600	-2.57846100
H	-0.92018700	2.12991600	-3.66513600
C	0.94753300	1.74081400	4.81790500
H	0.87190500	2.05087200	5.85682800
C	-1.97381000	2.83749500	-0.51178600
H	-2.74750800	3.38399900	0.01990700
C	-1.94506400	2.84183000	-1.90461600
H	-2.69338900	3.39723800	-2.46379100
C	4.11779400	-3.57017500	-1.47348400
H	3.05288500	-3.76722600	-1.28096700
H	4.38206800	-4.11809300	-2.38661000
C	4.94439100	-4.07363700	-0.28972700
H	4.77023600	-5.14593500	-0.13619900
H	6.01447000	-3.95827600	-0.52007700
C	4.61849000	-3.29862200	0.98741000

H	5.23694000	-3.65391400	1.82106600
H	3.57039500	-3.48469300	1.26619600
Pd	0.72557400	-1.81260200	0.09014800
C	-1.38909800	-2.24789500	-0.08351300
C	-2.01579700	-2.11862300	1.17021500
C	-1.86588800	-1.54569600	-1.20622400
C	-2.99965400	-1.15242900	1.33404800
H	-1.69123200	-2.72690700	2.00707400
C	-2.84942700	-0.58480000	-1.02689100
H	-1.42035600	-1.70520600	-2.18145400
H	-3.45836200	-0.99035800	2.30358700
C	-3.39037300	-0.38942500	0.23889100
H	-3.17546000	0.03160200	-1.85634100
O	-4.30540400	0.66615200	0.41278500
S	-5.89306300	0.34215800	0.53738400
O	-6.12341300	-0.93266100	1.18873800
O	-6.50064900	1.57867800	0.98099900
C	-6.33835300	0.12766200	-1.25680600
F	-7.66155200	0.14215200	-1.35987600
F	-5.82234200	1.12443900	-1.96730500
F	-5.86746500	-1.02991200	-1.70356700
Cl	-0.47787800	-3.87817300	-0.40306800

7F

Charge: 0 Multiplicity: 1

P	1.30642700	0.26828900	0.71971100
N	3.07547800	-2.57618100	-1.45073100
C	3.82876800	-0.73081900	-0.36878900
C	1.97458600	-1.96043400	-0.88786500
C	0.57620200	-2.47950500	-0.98591500
H	-0.03966700	-1.67640100	-0.53956400
C	4.21199700	-1.84012900	-1.16576900
C	2.39667300	-0.82100700	-0.20566600
C	1.56616500	-0.16852000	2.47880300
C	2.11977200	1.90087700	0.55971300
C	5.53688500	-2.06912400	-1.54285500
H	5.81343800	-2.91277100	-2.16834900
C	0.54602500	0.14734800	3.38491800

H	-0.36352900	0.61941000	3.01721300
C	2.47162100	2.67837400	1.66690300
H	2.30776700	2.29831300	2.67103600
C	6.49665400	-1.17062000	-1.09159100
H	7.53729500	-1.31982500	-1.36693600
C	4.82147000	0.15587400	0.07752400
H	4.56178600	1.00804600	0.69585600
C	2.72543000	-0.79911500	2.94426200
H	3.51747600	-1.05615000	2.24766500
C	0.31669600	-3.72295700	-0.11893200
H	0.88914300	-4.58461400	-0.49006100
H	0.66846800	-3.52515800	0.90072300
C	0.68885700	-0.14509500	4.73958500
H	-0.10877600	0.10462300	5.43444500
C	3.11058600	-3.78410300	-2.24531700
H	4.00457300	-4.35817600	-1.98559600
H	3.13337600	-3.55791000	-3.31780200
H	2.24205300	-4.40259500	-2.02902100
C	0.03896800	-2.64300500	-2.41547000
H	0.20644300	-1.71080200	-2.96999900
H	0.57489300	-3.43183800	-2.95719200
C	2.34332800	2.40150500	-0.72976100
H	2.06714100	1.80096300	-1.59205100
C	6.14182200	-0.07354500	-0.28710400
H	6.91515500	0.61023200	0.05279300
C	2.86225800	-1.10086800	4.29749600
H	3.76415300	-1.59439900	4.65063500
C	2.92766400	3.65051100	-0.90712900
H	3.10377600	4.02479300	-1.91171500
C	1.84772200	-0.77174600	5.19698400
H	1.95760200	-1.00979500	6.25185200
C	3.04744500	3.93596200	1.48513200
H	3.32054900	4.53163900	2.35263100
C	3.28001900	4.42338400	0.20067000
H	3.73253400	5.40158800	0.06122600
C	-1.44941800	-2.98815100	-2.37803000
H	-2.00331000	-2.14434400	-1.94523000
H	-1.83139500	-3.12583500	-3.39750500

C	-1.71734700	-4.23239200	-1.53217800
H	-2.79354500	-4.43700200	-1.49980800
H	-1.23946400	-5.10325800	-2.00645500
C	-1.17281300	-4.06361600	-0.11410600
H	-1.34785200	-4.97309700	0.47427100
H	-1.71916300	-3.25308800	0.38568400
Pd	-0.87003500	0.41561600	0.04479700
C	-2.61093500	1.08227000	-1.00397700
C	-2.84989700	2.36335700	-0.44088400
C	-1.59617300	0.91728300	-1.99193100
O	-3.69804900	0.14653300	-1.02507300
C	-2.11232800	3.45248200	-0.86758700
H	-3.63834800	2.48802700	0.29225600
C	-0.89269200	2.05815400	-2.44660200
H	-1.55779100	0.00142100	-2.57350300
S	-3.93999100	-0.91524700	0.16916300
H	-2.28422200	4.43112900	-0.43281400
C	-1.15940000	3.29357500	-1.88967500
H	-0.16485600	1.95281700	-3.24386600
O	-4.39428800	-2.14914700	-0.43818900
O	-2.86364700	-0.87491300	1.14885100
C	-5.42686200	-0.13942600	0.97121500
Cl	-0.29991100	4.70186700	-2.46062800
F	-5.07710600	1.00360100	1.55573300
F	-6.36293000	0.09002200	0.06289100
F	-5.88008900	-0.98402100	1.88814300

7G-Ts-OTf

Charge: 0 Multiplicity: 1

P	1.24362000	0.26849600	0.70932800
N	2.97845700	-2.44210200	-1.65605800
C	3.69864600	-0.60599600	-0.54068900
C	1.86721700	-1.86362400	-1.07775300
C	0.49203300	-2.44437200	-1.14641500
H	-0.15068500	-1.67186900	-0.68953200
C	4.10209200	-1.68842200	-1.36022700
C	2.26691600	-0.72196000	-0.38236100
C	2.05939100	0.02987300	2.33828700

C	1.56887200	2.00929100	0.29224800
C	5.43028600	-1.87652200	-1.74845700
H	5.72525800	-2.69593700	-2.39709300
C	1.79669500	-1.17459100	3.00537400
H	1.11571400	-1.89672100	2.55804200
C	1.05244300	2.99319700	1.14605400
H	0.48694400	2.69816000	2.02689100
C	6.37076800	-0.96817000	-1.27701500
H	7.41354100	-1.08754700	-1.55835100
C	4.66993000	0.29223400	-0.07627400
H	4.39090000	1.12762300	0.55563000
C	2.91700900	0.96246500	2.92867000
H	3.12258900	1.90470300	2.43011500
C	0.31578900	-3.68440300	-0.25221400
H	0.90155000	-4.52924000	-0.63957000
H	0.70649400	-3.46261700	0.74821200
C	2.39317900	-1.44825900	4.23196700
H	2.18135900	-2.38647700	4.73809200
C	3.03522400	-3.63472900	-2.47368300
H	3.98374000	-4.14514800	-2.28880500
H	2.96264400	-3.39495800	-3.54057600
H	2.23288800	-4.31827700	-2.20350600
C	-0.07259500	-2.68445900	-2.55442300
H	0.06656400	-1.78637400	-3.16931300
H	0.46450100	-3.49399100	-3.06300800
C	2.25532300	2.39397300	-0.86316500
H	2.63654700	1.63738100	-1.54085300
C	5.99452000	0.10167700	-0.44634200
H	6.75359800	0.79346700	-0.09120600
C	3.50716600	0.69031100	4.16247100
H	4.17321600	1.42267200	4.61141300
C	2.45472300	3.74441700	-1.14023900
H	2.98674900	4.03532700	-2.04170100
C	3.25035200	-0.51373300	4.81495500
H	3.71193200	-0.72250700	5.77637100
C	1.26148500	4.34102300	0.87090700
H	0.86280700	5.09723000	1.54194400
C	1.96743500	4.71835600	-0.27117900

H	2.12047900	5.77070600	-0.49318800
C	-1.55267900	-3.05562500	-2.45770100
H	-2.11318800	-2.20958900	-2.03961800
H	-1.95969000	-3.23961400	-3.45979300
C	-1.76255900	-4.27929700	-1.56533200
H	-2.83252600	-4.49858000	-1.47812100
H	-1.29241300	-5.15611100	-2.03646500
C	-1.15988800	-4.06975800	-0.17660500
H	-1.28294000	-4.97255400	0.43479200
H	-1.70729400	-3.26674200	0.33503300
Pd	-0.99136200	-0.16079400	0.92229400
C	-1.87840500	0.94204000	-0.62651900
C	-2.25464800	2.18611300	-0.07999400
C	-1.19005000	0.88424100	-1.85247900
O	-3.20317200	-0.10204100	-0.78864200
C	-1.79710200	3.35378100	-0.67867100
H	-2.87319600	2.23451600	0.80846000
C	-0.74430100	2.05927900	-2.43851500
H	-0.99614800	-0.07487000	-2.31574100
S	-3.82772900	-0.95295300	0.34944400
H	-2.04603400	4.31548200	-0.24202600
C	-1.05661000	3.28931100	-1.85765700
H	-0.17623200	2.01997700	-3.36231900
O	-4.22057300	-2.27832300	-0.09761900
O	-3.02246300	-0.81270800	1.58752100
C	-5.39926800	-0.03777000	0.71393200
Cl	-0.58448600	4.76542600	-2.66377500
F	-5.12054000	1.19548100	1.12704300
F	-6.14389400	0.01865800	-0.38249200
F	-6.05526100	-0.68564000	1.66989300

8A

Charge: 0 Multiplicity: 1

Pd	-0.69713400	-0.47615300	-2.31879800
P	0.32544600	-0.13666000	-0.35354400
C	-0.73488300	0.52420400	0.98363700
C	-0.39404300	0.99212700	2.31700300
N	-2.61883600	1.27349500	2.00853200

C	-2.11731400	0.71939200	0.84703100
C	-2.98889400	0.40142500	-0.32152000
H	-2.27096700	0.01487300	-1.07700700
C	-1.59564700	1.46136300	2.91031800
C	0.77481200	1.07637000	3.09139400
H	1.71431900	0.69971200	2.71385100
C	-3.64513300	1.61025600	-1.00346300
H	-4.43013000	2.05683400	-0.37851800
H	-2.88759900	2.38649900	-1.16557600
C	-1.65717000	2.01004900	4.19297700
H	-2.59472200	2.36704800	4.60910200
C	-0.47607400	2.08751900	4.91877800
H	-0.48605500	2.50977800	5.91996200
C	-3.97464300	-0.75644000	-0.10674200
H	-3.44425000	-1.60114200	0.34833800
H	-4.78434600	-0.48254400	0.58408800
C	-4.25065700	1.17516900	-2.33841100
H	-4.74463100	2.02453100	-2.82718900
H	-3.43195600	0.85623000	-3.00298200
C	0.72800300	1.61846000	4.36906000
H	1.64197700	1.67472800	4.95452100
C	-5.23262500	0.01687000	-2.15811100
H	-5.63285300	-0.29613900	-3.13087800
H	-6.09125600	0.36206900	-1.56205100
C	-3.97958800	1.65854100	2.30743300
H	-4.28294700	1.23059500	3.26871100
H	-4.65381400	1.28703800	1.54164900
H	-4.07188300	2.74971000	2.36001500
C	-4.57608300	-1.16910800	-1.45029800
H	-5.30102900	-1.98088300	-1.30934200
H	-3.76861000	-1.56772900	-2.08397500
C	1.74112200	1.10372500	-0.62072200
C	2.20862600	0.94783800	-2.08674000
C	1.13042700	2.50963400	-0.46238000
C	2.98630100	0.98901800	0.27354900
H	1.33166200	1.01274200	-2.74751400
H	2.63879700	-0.04950400	-2.23964600
C	3.23627900	2.02469500	-2.45604600

H	0.79343100	2.65755800	0.56922900
H	0.24419100	2.59466800	-1.10698400
C	2.15843300	3.58734200	-0.82929200
H	3.44792600	0.00205300	0.15630800
H	2.71960300	1.10296600	1.32460300
C	4.01220200	2.07640000	-0.08646100
H	3.53810200	1.88043200	-3.50184600
C	2.60084200	3.40898600	-2.28572500
C	4.45887100	1.90355200	-1.54071600
H	1.69742600	4.57524000	-0.69891800
C	3.37430100	3.45883100	0.09672400
H	4.87675800	1.97625200	0.58312500
H	1.73616100	3.50967800	-2.95610900
H	3.31957400	4.19309600	-2.56200000
H	4.93510200	0.92222700	-1.67499800
H	5.20697000	2.66532300	-1.80083400
H	4.10801400	4.24484900	-0.12980200
H	3.06473800	3.59471700	1.14219300
C	0.93123300	-1.79989300	0.28644900
C	1.91559200	-2.39768900	-0.73465300
C	1.56932200	-1.81686800	1.68359200
C	-0.32437700	-2.69788100	0.33170200
H	2.82345900	-1.78505500	-0.79229600
H	1.45183200	-2.38179700	-1.73155500
C	2.29278300	-3.83070000	-0.33738700
H	0.85983700	-1.42064000	2.41675800
H	2.46057500	-1.18206900	1.70951100
C	1.95853800	-3.25138600	2.07585400
H	-0.80820800	-2.68699800	-0.65592100
H	-1.04503300	-2.28033700	1.04715500
C	0.04783900	-4.13121500	0.72837500
H	2.99855200	-4.23163400	-1.07679700
C	2.94744200	-3.81675800	1.04971400
C	1.03106000	-4.70097400	-0.30131500
H	2.42621800	-3.23001900	3.06902800
C	0.70189800	-4.12705900	2.11464800
H	-0.86384900	-4.74288900	0.74867200
H	3.85969900	-3.20393200	1.02824600

H	3.24857400	-4.83397300	1.33625300
H	0.56285600	-4.72364400	-1.29506400
H	1.29348200	-5.73604200	-0.04172300
H	0.96274200	-5.15180200	2.41403900
H	-0.00289400	-3.73898600	2.86277900

8B

Charge: 0 Multiplicity: 1

Pd	-0.00021200	1.41142500	0.68273200
P	-1.31692400	-0.46418700	0.15011400
C	-2.85024000	-0.15165900	-0.77799200
C	1.71026700	1.70550700	2.13223000
C	-3.88335600	-1.05816200	-1.24631300
N	-4.42608400	1.04522400	-1.88872400
C	-3.23987700	1.12973100	-1.18553000
C	-2.56802100	2.43625900	-0.91009500
H	-1.73086500	2.17419600	-0.22976000
C	-4.84752800	-0.26707200	-1.92362900
C	-4.12397200	-2.43950700	-1.16694600
H	-3.41334500	-3.09652500	-0.68567400
C	3.18941400	1.65967200	-0.27209900
C	-3.42439000	3.43251600	-0.11265800
H	-4.27719800	3.78621200	-0.70508800
H	-3.83950200	2.92592700	0.76707300
C	2.67017600	0.69564900	1.90493900
H	2.83616600	-0.08139100	2.64342900
C	3.38107500	0.69427700	0.72398700
C	2.29290000	2.69188000	-0.04889300
H	2.17745300	3.48778200	-0.77711900
C	-6.00744700	-0.79637600	-2.49409400
H	-6.73269600	-0.16155800	-2.99455500
C	-6.21095200	-2.16573300	-2.38854100
H	-7.10443200	-2.61064600	-2.81800200
C	-1.89431500	3.08864700	-2.12707600
H	-1.25961900	2.34633900	-2.62519900
H	-2.63759300	3.41698600	-2.86609900
C	1.56005500	2.75086600	1.17149600
C	-2.57622000	4.62926400	0.31283200

H	-3.19706000	5.35669500	0.85109200
H	-1.80636800	4.28391800	1.01507300
C	-5.27291700	-2.97790100	-1.73059000
H	-5.44664600	-4.04849300	-1.66165100
C	-1.89711400	5.29231300	-0.88576700
H	-1.26525000	6.12299400	-0.54799800
H	-2.66409700	5.72692700	-1.54507600
C	-5.18843600	2.10770700	-2.50682200
H	-5.52246700	1.78339600	-3.49709500
H	-4.57166000	2.99262200	-2.63605800
H	-6.06639300	2.36809800	-1.90416200
C	-1.06122900	4.28774800	-1.67857800
H	-0.59756900	4.77237200	-2.54728400
H	-0.24501100	3.92115100	-1.04078200
H	1.27795800	1.81582300	3.12160100
H	3.74375000	1.60659200	-1.20119400
Cl	0.93809900	4.32344600	1.70183000
O	4.22323500	-0.40804100	0.48244500
S	5.84051600	-0.22220300	0.50937700
O	6.20201800	1.17894400	0.60142200
O	6.39579400	-1.23440900	1.38469700
C	6.15206100	-0.78831800	-1.23101900
F	7.46366000	-0.79672000	-1.43474600
F	5.66256200	-2.00910600	-1.39942900
F	5.57504300	0.04871000	-2.08763800
C	-1.78705400	-1.38137900	1.73858300
C	-0.71309800	-1.04019800	2.79527200
C	-3.12518500	-0.78217400	2.21357500
C	-1.91383100	-2.91119900	1.67177500
H	-0.60986500	0.05052000	2.85691000
H	0.26358000	-1.42698900	2.47975100
C	-1.09104400	-1.61068000	4.16731100
H	-3.91406000	-1.00559300	1.48712600
H	-3.03736900	0.31225100	2.26751000
C	-3.50871500	-1.34907000	3.58684300
H	-0.96545300	-3.35770900	1.35275400
H	-2.67354400	-3.20164400	0.94431700
C	-2.30705500	-3.47865700	3.04506700

H	-0.30423100	-1.35003100	4.88766200
C	-2.42503200	-1.00202800	4.61366300
C	-1.22495900	-3.13394900	4.07266200
H	-4.46705600	-0.91129700	3.89507800
C	-3.64647800	-2.87299700	3.48159300
H	-2.40435000	-4.56884200	2.95891200
H	-2.32809300	0.08879600	4.70425700
H	-2.70518200	-1.38650700	5.60408100
H	-0.26574100	-3.57927000	3.77369600
H	-1.48563000	-3.55457100	5.05361100
H	-3.95198200	-3.29283700	4.44985400
H	-4.42964800	-3.12920800	2.75485100
C	-0.24163700	-1.49025700	-1.00361000
C	1.05473100	-1.86147900	-0.26290000
C	-0.86417200	-2.75451000	-1.61271800
C	0.12240300	-0.53689500	-2.16311200
H	0.83852900	-2.53823700	0.57259600
H	1.49363400	-0.95313100	0.16336600
C	2.04659000	-2.53364100	-1.21987900
H	-1.76706100	-2.48907500	-2.17113900
H	-1.15613300	-3.45872400	-0.82720900
C	0.13586700	-3.43621600	-2.56110800
H	0.56352200	0.38185700	-1.74970500
H	-0.79089900	-0.24698300	-2.69893700
C	1.11177700	-1.20642300	-3.12422600
H	2.95912100	-2.78465000	-0.66612200
C	1.41188500	-3.80505100	-1.79475800
C	2.38951400	-1.56767700	-2.35889700
H	-0.32877600	-4.34417600	-2.96738800
C	0.48337300	-2.47765600	-3.70528100
H	1.34935700	-0.50414000	-3.93443600
H	1.17444600	-4.50663800	-0.98261600
H	2.11995100	-4.31349000	-2.46372200
H	2.84847000	-0.66017600	-1.94923700
H	3.12282400	-2.02609400	-3.03613200
H	1.18099900	-2.95898000	-4.40472200
H	-0.42329800	-2.22541800	-4.27225300

8C-TS

Charge: 0 Multiplicity: 1

Pd	0.24928200	1.32437400	-1.01706200
P	1.48438600	-0.39049500	-0.02126700
C	3.14308400	0.08599400	0.56705900
C	-2.36623400	0.32470700	-2.02508400
C	4.22924500	-0.72782900	1.08565400
N	4.90303200	1.43370200	1.05668700
C	3.61436800	1.40632300	0.56260300
C	2.91227400	2.64444500	0.11196700
H	1.95885900	2.27147900	-0.31247700
C	5.30770800	0.15231200	1.36226000
C	4.43120300	-2.09262600	1.34774900
H	3.63581500	-2.80714300	1.19231100
C	-3.47715500	1.09824600	0.43141200
C	3.58375800	3.39419800	-1.04853700
H	4.52899900	3.85606700	-0.73664300
H	3.82665700	2.67978500	-1.84470800
C	-3.35421200	-0.45199900	-1.43999000
H	-3.71048100	-1.35254700	-1.92791800
C	-3.89152100	-0.05943400	-0.21628100
C	-2.47271800	1.87382300	-0.13404900
H	-2.14361200	2.78758900	0.34752900
C	6.54228000	-0.27849300	1.85278400
H	7.35166300	0.42134000	2.03839900
C	6.70478600	-1.63725500	2.08686500
H	7.65315700	-2.00774000	2.46627400
C	2.47453600	3.58684500	1.24369600
H	1.96753200	3.00276300	2.02042600
H	3.33811600	4.06844000	1.72277900
C	-1.87082900	1.44721400	-1.33371300
C	2.64310600	4.47724900	-1.57779600
H	3.13277700	5.03899100	-2.38327300
H	1.76096400	3.99139500	-2.01782200
C	5.65269100	-2.53373500	1.83859000
H	5.79363100	-3.59300600	2.03650500
C	2.19019600	5.42446300	-0.46621500
H	1.49126200	6.16901700	-0.86753100

H	3.06013300	5.98152300	-0.08591000
C	5.77572300	2.57414300	1.22792400
H	6.29827200	2.48723600	2.18525200
H	5.19822600	3.49439000	1.24398200
H	6.51737300	2.63026500	0.42250000
C	1.54007500	4.66009400	0.68734200
H	1.23896600	5.35066300	1.48529400
H	0.62476200	4.16984400	0.32349000
H	-1.94645500	0.05090900	-2.98574700
H	-3.93742900	1.38793400	1.36979800
Cl	-1.07749000	2.81935400	-2.38746100
C	1.70094300	-1.74632900	-1.33028200
C	0.48627300	-1.64914100	-2.27920000
C	2.96281300	-1.38703600	-2.13852000
C	1.80207700	-3.20325000	-0.85191500
H	0.39865100	-0.61245900	-2.63288200
H	-0.43784700	-1.87164800	-1.73349600
C	0.63832800	-2.59862500	-3.47270800
H	3.84889900	-1.44814300	-1.49746500
H	2.88847200	-0.34726700	-2.48777600
C	3.12040000	-2.33643800	-3.33388400
H	0.90207300	-3.48201200	-0.29261800
H	2.65561800	-3.33304300	-0.18559500
C	1.97091700	-4.15275700	-2.04907200
H	-0.24386500	-2.49758200	-4.11894000
C	1.90084500	-2.22104000	-4.25520300
C	0.75326000	-4.04119400	-2.97079600
H	4.02946800	-2.06227800	-3.88475900
C	3.24124100	-3.77690700	-2.82135200
H	2.05797700	-5.17953600	-1.67025600
H	1.81265800	-1.19408000	-4.63583500
H	2.02024500	-2.88131700	-5.12526200
H	-0.15837100	-4.32548200	-2.42681900
H	0.85397300	-4.73289400	-3.81845600
H	3.38799400	-4.46708500	-3.66351200
H	4.11978000	-3.86997200	-2.16813500
C	0.56967400	-0.98720400	1.50483300
C	-0.82546100	-1.48038700	1.08605200

C	1.26863300	-2.06629000	2.34504600
C	0.39297100	0.26463400	2.39108700
H	-0.74214200	-2.36999300	0.45047500
H	-1.32013800	-0.70520500	0.49145600
C	-1.66415700	-1.81833500	2.32551200
H	2.24839100	-1.70257100	2.67007800
H	1.43153500	-2.97202300	1.75298500
C	0.42037500	-2.41361100	3.57827900
H	-0.09953500	1.05453200	1.80674900
H	1.37937800	0.64521800	2.68643600
C	-0.44040500	-0.06993600	3.63498400
H	-2.65196500	-2.16777300	2.00020400
C	-0.95855400	-2.91514800	3.13207000
C	-1.82185200	-0.56744900	3.19679500
H	0.93413900	-3.19860400	4.14846900
C	0.26074400	-1.16278100	4.44875900
H	-0.54790500	0.83743600	4.24417000
H	-0.84914000	-3.82141700	2.51987300
H	-1.56277100	-3.18854100	4.00799300
H	-2.33695000	0.21693800	2.63057900
H	-2.43994000	-0.79595600	4.07600800
H	-0.32500000	-1.39781900	5.34821300
H	1.24618700	-0.81173600	4.78472100
O	-4.84103900	-0.87347400	0.42870400
S	-6.38028600	-0.88687800	-0.10337500
O	-6.44204800	-0.69797600	-1.53948900
O	-7.00853200	-1.99829300	0.57741800
C	-7.02280100	0.67459800	0.68091400
F	-8.34614000	0.67245400	0.58392700
F	-6.66636000	0.71121300	1.95970600
F	-6.52860600	1.73167200	0.04879400

8D

Charge: 0 Multiplicity: 1

Pd	0.17334100	0.28595100	-1.61898500
P	1.55478100	-0.40216100	0.09682900
C	2.84422600	0.88513500	0.16959200
C	-2.12458500	-1.40523200	-0.93872400

C	4.25302800	0.76986600	0.50167700
N	3.81553900	2.92357900	-0.04284300
C	2.61928200	2.24324000	-0.12624600
C	1.32450500	2.95945800	-0.37817200
H	0.54842400	2.18532000	-0.28543500
C	4.81860800	2.05867800	0.33997800
C	5.10224200	-0.25374800	0.94841700
H	4.71693900	-1.24408300	1.13679200
C	-3.43249900	0.56936600	0.54426500
C	1.15227100	3.52573600	-1.79987200
H	1.89210900	4.30717900	-2.01202600
H	1.31957400	2.72615700	-2.53193800
C	-3.35832800	-1.68577400	-0.35184200
H	-3.82542100	-2.65704000	-0.47295400
C	-3.98690200	-0.69327900	0.38721700
C	-2.19510600	0.83571800	-0.03948200
H	-1.76624800	1.82614900	0.06812900
C	6.16719200	2.33846200	0.57020300
H	6.56700100	3.33944700	0.44037200
C	6.97926900	1.29328200	0.98841500
H	8.03319600	1.47487500	1.17937400
C	1.00170000	4.01430900	0.69839800
H	1.09427100	3.56458400	1.69330000
H	1.72142500	4.84032300	0.66283600
C	-1.52482400	-0.15644000	-0.75867900
C	-0.25383100	4.09626900	-1.97514300
H	-0.35692700	4.51822500	-2.98172000
H	-0.97597700	3.27185200	-1.91455500
C	6.44450200	0.00956900	1.18321100
H	7.08929100	-0.79251200	1.53200800
C	-0.57532300	5.14717900	-0.91386400
H	-1.59783000	5.52091500	-1.04892300
H	0.09462400	6.01163600	-1.03822600
C	4.08937000	4.32730700	-0.27183300
H	4.30090800	4.84103000	0.67267400
H	3.24749400	4.80920800	-0.75788700
H	4.95862200	4.42063600	-0.93001800
C	-0.40215700	4.58151400	0.49526100

H	-0.60139000	5.35392500	1.24873500
H	-1.14182400	3.78546400	0.66130400
H	-1.63801000	-2.17427800	-1.52686200
H	-3.95987900	1.32885400	1.11247500
Cl	-0.78700200	0.84048200	-3.67109500
O	-5.19822600	-0.96367800	1.05830900
S	-6.57645800	-1.08167000	0.20481000
O	-6.35831200	-1.74191700	-1.06694100
O	-7.57292200	-1.51740600	1.15945400
C	-6.90976500	0.71329000	-0.16359400
F	-8.15713600	0.81678700	-0.60521900
F	-6.76745200	1.42995400	0.94654600
F	-6.06782000	1.14948100	-1.08962100
C	2.24897100	-2.00334900	-0.65960400
C	1.06188000	-2.74702600	-1.31951600
C	3.21624900	-1.57202600	-1.78065800
C	2.92879200	-3.01636300	0.27853900
H	0.54347700	-2.06562400	-2.00570100
H	0.33577000	-3.04772900	-0.55542600
C	1.54559200	-3.97175300	-2.10604100
H	4.07292400	-1.03492400	-1.36354000
H	2.70097100	-0.87582200	-2.46062700
C	3.70321600	-2.79672100	-2.56402000
H	2.21305300	-3.36564400	1.03046700
H	3.76454400	-2.57468500	0.81879100
C	3.44555000	-4.22409700	-0.52030300
H	0.67172700	-4.45815700	-2.55780300
C	2.50865400	-3.51058700	-3.20528100
C	2.26228300	-4.94626600	-1.16878400
H	4.39864900	-2.45964800	-3.34280000
C	4.42320200	-3.75027600	-1.60270900
H	3.96067200	-4.90028900	0.17405000
H	1.99179100	-2.83189500	-3.89698900
H	2.85321400	-4.37301000	-3.79163600
H	1.57102700	-5.30749300	-0.39479500
H	2.61156200	-5.82474000	-1.72791000
H	4.81783300	-4.61450500	-2.15362800
H	5.28049500	-3.24108800	-1.14132600

C	0.99319800	-0.62795700	1.86385600
C	-0.06243200	-1.74057100	1.97762200
C	2.16326500	-0.91905200	2.82261400
C	0.36152000	0.71081600	2.29010000
H	0.36599300	-2.70567800	1.68449400
H	-0.89684100	-1.53716900	1.30151500
C	-0.57193200	-1.82671300	3.42301400
H	2.90976200	-0.12013000	2.74816200
H	2.65925700	-1.85626100	2.55722100
C	1.64314900	-1.01533800	4.26589800
H	-0.45871400	0.96605000	1.61452200
H	1.11536600	1.50254900	2.21630400
C	-0.16305400	0.62293400	3.72802700
H	-1.31989800	-2.62727400	3.48327400
C	0.60057300	-2.13634300	4.36113800
C	-1.21264000	-0.49110000	3.81715900
H	2.49001600	-1.23804100	4.92758300
C	1.00238700	0.31545300	4.67363500
H	-0.61800000	1.58560000	3.99519000
H	1.05581800	-3.09906000	4.08960400
H	0.24222000	-2.22913200	5.39529000
H	-2.05460600	-0.26998500	3.14809400
H	-1.61342100	-0.55142600	4.83799800
H	0.64520400	0.26047400	5.71096400
H	1.74751100	1.12159800	4.62846300

8E

Charge: 0 Multiplicity: 1

Pd	0.30177700	-1.19381400	-0.23837100
P	1.92561300	0.52095000	0.20533900
C	3.51187200	0.17723600	-0.63101100
C	-2.06262800	-0.05225100	1.16082200
C	4.80323200	0.84047700	-0.51426200
N	4.96392300	-0.78051200	-2.09026900
C	3.67738300	-0.82976300	-1.58932500
C	2.71386200	-1.88620300	-2.04006500
H	1.85492700	-1.81965800	-1.34174000
C	5.67233800	0.20538300	-1.43751900

C	5.34501300	1.88440000	0.25503800
H	4.73259400	2.43390500	0.95376300
C	-3.18911100	1.02841300	-1.15492800
C	3.24927400	-3.32012100	-1.88033300
H	4.14446100	-3.46845100	-2.49172100
H	3.55773100	-3.47047300	-0.83826300
C	-3.23253100	0.70063100	1.25013400
H	-3.72350800	0.85759700	2.20479000
C	-3.76817800	1.23818500	0.08884600
C	-2.01030400	0.28744600	-1.22753100
H	-1.57025800	0.10069100	-2.20137000
C	7.01373600	0.55964300	-1.60201100
H	7.65270800	0.04048900	-2.30967100
C	7.51001600	1.58931200	-0.81590800
H	8.55021000	1.88745300	-0.91322400
C	2.09839500	-1.61558700	-3.42257000
H	1.64066700	-0.61982800	-3.40853600
H	2.88402400	-1.58850300	-4.18915400
C	-1.42031600	-0.23034600	-0.06844100
C	2.20726500	-4.35918500	-2.29069000
H	2.65425300	-5.36001400	-2.24363200
H	1.38306000	-4.35632500	-1.56753600
C	6.67643600	2.24519400	0.10385600
H	7.07703300	3.05446800	0.70829000
C	1.64907000	-4.08555700	-3.68671400
H	0.88172700	-4.82874300	-3.93420700
H	2.45454900	-4.20290000	-4.42807400
C	5.56201500	-1.54653100	-3.16472100
H	6.16079600	-0.87386700	-3.78551200
H	4.79667300	-1.98529000	-3.79915100
H	6.20985800	-2.34085200	-2.77710500
C	1.06372300	-2.67750900	-3.78598900
H	0.69153700	-2.49229600	-4.80132600
H	0.19397900	-2.59171600	-3.12082300
H	-1.66527700	-0.50158400	2.06304100
H	-3.64951900	1.43886400	-2.04788800
O	-4.90177200	2.08084600	0.16371000
S	-6.37156300	1.43601500	0.39357900

O	-6.29017300	0.14672500	1.05443700
O	-7.20452100	2.51603100	0.87769800
C	-6.87334900	1.11711400	-1.36744600
F	-8.15137600	0.75794700	-1.37580700
F	-6.71141500	2.22219600	-2.08354000
F	-6.13276700	0.14093500	-1.88086000
C	-1.39993800	-3.16893300	1.07217900
C	-2.08714000	-2.81493400	-1.14755700
C	-2.80113300	-2.99122800	1.02614100
C	-0.78489500	-3.40327800	2.29650900
N	-3.18524400	-2.77912200	-0.29063900
O	-2.17042400	-2.72750000	-2.37020600
C	-3.58506200	-3.01323600	2.17264400
C	-1.56283900	-3.44042600	3.46066500
H	0.29219000	-3.54373300	2.34901200
C	-4.52576300	-2.49611100	-0.72660400
C	-2.94334900	-3.23932300	3.39606200
H	-4.65755200	-2.85034000	2.12524600
H	-1.08725600	-3.62362400	4.42051100
H	-5.18399500	-3.36025000	-0.57186700
H	-4.93109100	-1.63738900	-0.18458200
H	-4.47867800	-2.26909600	-1.79285500
H	-3.53420000	-3.26140000	4.30813700
C	-0.87848400	-2.94143600	-0.28608100
H	-0.12924500	-3.63386100	-0.67460400
C	2.23738800	0.37535600	2.06417200
C	3.15560300	-0.84824900	2.25605500
C	2.85802800	1.58626600	2.77636700
C	0.88702700	0.06058400	2.73880700
H	4.12827200	-0.66605500	1.78568700
H	2.71324600	-1.72201900	1.75365000
C	3.34472600	-1.14326700	3.75054400
H	2.21822900	2.46761000	2.65710200
H	3.83172900	1.82098100	2.34598500
C	3.04981200	1.28841700	4.27197700
H	0.44177000	-0.81625900	2.25230300
H	0.18836400	0.89183100	2.59592300
C	1.06949500	-0.22618500	4.23270300

H	4.00784800	-2.01155400	3.85701800
C	3.97753600	0.07760700	4.42969100
C	1.98839500	-1.44069900	4.39871400
H	3.50536600	2.16725800	4.74649900
C	1.69360900	0.99218000	4.91901100
H	0.08615200	-0.44318200	4.66880400
H	4.95655700	0.29325800	3.98012100
H	4.14795200	-0.13092000	5.49464100
H	1.53009100	-2.32005100	3.92822800
H	2.12210000	-1.67430700	5.46376600
H	1.81962500	0.80155900	5.99355700
H	1.03017600	1.86250800	4.81966500
C	1.42823600	2.24801300	-0.34227100
C	0.20303900	2.72085600	0.46167700
C	2.52006700	3.32554400	-0.25781700
C	1.03341400	2.09288500	-1.82614100
H	0.47570800	2.85723500	1.51502300
H	-0.58805300	1.96975200	0.42625200
C	-0.31798200	4.05027200	-0.10215600
H	3.39245000	3.01669000	-0.83961500
H	2.84197900	3.46327100	0.77962500
C	1.99809200	4.66245000	-0.80725800
H	0.26835500	1.31632400	-1.92449100
H	1.90877000	1.76371400	-2.40173200
C	0.50815500	3.42282200	-2.38227900
H	-1.19598100	4.35563800	0.48104600
C	0.77887000	5.11445200	0.00367500
C	-0.71525300	3.86573200	-1.57114500
H	2.79914000	5.40847900	-0.72409100
C	1.60483200	4.48776700	-2.27815700
H	0.22529500	3.27855900	-3.43325700
H	1.05975800	5.26390900	1.05576300
H	0.41067700	6.07873700	-0.37267300
H	-1.51070200	3.11556100	-1.64824900
H	-1.11244600	4.80769500	-1.97376400
H	1.24682000	5.44140800	-2.68978400
H	2.48161200	4.18731300	-2.86827500

8F-TS

Charge: 0 Multiplicity: 1

Pd	-0.29496500	-1.07027700	0.30148400
P	-2.00708300	0.46310000	-0.20620300
C	-3.62007400	0.11758900	0.56791800
C	2.21066400	-0.23118500	-1.11326300
C	-4.91795300	0.74281700	0.37479600
N	-5.13449500	-0.90171300	1.91729200
C	-3.81305700	-0.89522700	1.51799200
C	-2.81775000	-1.86614300	2.06753100
H	-1.90346800	-1.68472100	1.47036400
C	-5.83030200	0.06590400	1.22492100
C	-5.42861200	1.79091000	-0.40872400
H	-4.77786300	2.37212000	-1.04587100
C	3.12985000	1.08026000	1.17501600
C	-3.15888600	-3.34656800	1.83520900
H	-4.05017900	-3.64357200	2.40049600
H	-3.39419600	-3.49875000	0.77442800
C	3.16873300	0.76908200	-1.23343900
H	3.57227600	1.04014100	-2.20302000
C	3.62116600	1.40310200	-0.08382800
C	2.16363400	0.08796400	1.28733900
H	1.81395400	-0.20368400	2.27083400
C	-7.19013200	0.37701000	1.29405500
H	-7.86296600	-0.17251200	1.94554200
C	-7.65687700	1.41001600	0.49297800
H	-8.70966100	1.67740500	0.51953500
C	-2.37928400	-1.58058200	3.51276600
H	-2.09617400	-0.52505200	3.59569600
H	-3.20545400	-1.74293200	4.21833300
C	1.67457100	-0.56955300	0.14129600
C	-1.98799100	-4.23658400	2.25350700
H	-2.26272500	-5.29230800	2.13590800
H	-1.14278700	-4.05825600	1.57439000
C	-6.77781800	2.11197100	-0.34757500
H	-7.15729400	2.92567500	-0.95984500
C	-1.54340600	-3.95660600	3.68912500
H	-0.67762300	-4.58045800	3.94266100

H	-2.35179900	-4.24102700	4.37992400
C	-5.78004000	-1.75323000	2.89266700
H	-6.45477400	-1.14857900	3.50584000
H	-5.04318300	-2.20285900	3.55242700
H	-6.35829500	-2.54712400	2.40591700
C	-1.20410200	-2.48010400	3.89174200
H	-0.90924700	-2.29496400	4.93209700
H	-0.33762200	-2.21698700	3.26822000
H	1.87473300	-0.74784100	-2.00463700
H	3.51350600	1.58711900	2.05435500
O	4.59331200	2.42485400	-0.17134800
S	6.13749800	2.00710300	-0.45253000
O	6.23085900	0.90987200	-1.39655700
O	6.84381300	3.25814800	-0.62801600
C	6.63498200	1.31959100	1.20594300
F	7.95883900	1.21416000	1.22233100
F	6.24052800	2.14027900	2.17237900
F	6.09155700	0.12168300	1.38448600
C	1.74830900	-3.08530400	-0.96959900
C	2.53534100	-2.72934200	1.22545200
C	3.12520000	-3.37298900	-0.89508900
C	1.06158100	-3.28555700	-2.15696500
N	3.57542800	-3.13128400	0.40139800
O	2.61117800	-2.58115600	2.43646200
C	3.83480900	-3.83413600	-1.99534300
C	1.76007300	-3.76297100	-3.27302700
H	-0.00020200	-3.06249500	-2.21624700
C	4.92694200	-3.31770900	0.86067600
C	3.12875800	-4.02183100	-3.19007500
H	4.89868700	-4.04288400	-1.93668200
H	1.23403000	-3.92597300	-4.20941900
H	5.24903300	-4.35710100	0.72747400
H	5.61055700	-2.65525400	0.31824700
H	4.94895300	-3.06864400	1.92314300
H	3.66163400	-4.38117000	-4.06641500
C	1.34688300	-2.50970100	0.32837900
H	0.43657100	-2.94406900	0.79468400
C	-2.23085500	0.38136100	-2.08336000

C	-3.17057800	-0.80957600	-2.35578700
C	-2.76847200	1.62468200	-2.80805600
C	-0.84932100	0.04706600	-2.68503400
H	-4.16424900	-0.60408300	-1.94215700
H	-2.78743100	-1.70316800	-1.84126300
C	-3.27722100	-1.07335600	-3.86340300
H	-2.10465000	2.47977800	-2.63841600
H	-3.75603700	1.89240600	-2.43039200
C	-2.88079800	1.35724800	-4.31834700
H	-0.44652600	-0.83727500	-2.17534500
H	-0.14327600	0.86191000	-2.49131500
C	-0.95046000	-0.21765100	-4.19039800
H	-3.95740500	-1.91929200	-4.02721400
C	-3.83157800	0.17779200	-4.55586500
C	-1.89223000	-1.40224100	-4.43132000
H	-3.28011600	2.25753700	-4.80331200
C	-1.49869900	1.02897200	-4.89166100
H	0.05070700	-0.45547100	-4.57316800
H	-4.82947800	0.41351200	-4.16131500
H	-3.94313700	-0.00515900	-5.63339200
H	-1.49293600	-2.30383400	-3.94674200
H	-1.96477900	-1.61775600	-5.50618100
H	-1.56864700	0.85824700	-5.97474300
H	-0.81620000	1.87673700	-4.74020400
C	-1.50585600	2.16519200	0.40498100
C	-0.21066300	2.60826400	-0.29963700
C	-2.56477000	3.26840900	0.26538300
C	-1.20533600	1.97814700	1.90769200
H	-0.39445100	2.75867800	-1.37010100
H	0.55033800	1.82706800	-0.20704100
C	0.30117600	3.91944300	0.31295600
H	-3.47985900	2.96920200	0.78535100
H	-2.81838200	3.42573000	-0.78819100
C	-2.04668800	4.58429700	0.86547800
H	-0.45484300	1.18618100	2.03208300
H	-2.11666500	1.64812400	2.42350700
C	-0.69610400	3.28838800	2.52093600
H	1.22392400	4.21179400	-0.20422800

C	-0.76264600	5.01007700	0.14361400
C	0.59017300	3.71328200	1.80388900
H	-2.81774200	5.35557400	0.73924400
C	-1.75864300	4.38044800	2.35688700
H	-0.49081600	3.12435200	3.58706400
H	-0.96769200	5.17435100	-0.92373300
H	-0.39731200	5.96220700	0.55242800
H	1.35994400	2.94296000	1.92808800
H	0.98025200	4.64149500	2.24384100
H	-1.40756300	5.31938000	2.80683700
H	-2.68072900	4.09344900	2.88100300

8G

Charge: 0 Multiplicity: 1

Pd	-0.21655400	-0.61112800	-0.31561200
P	1.62438800	0.71079800	0.20527800
C	3.15039200	0.48118400	-0.75796200
C	-2.44575200	-1.35424500	1.02456100
C	4.45236300	1.11518300	-0.64574800
N	4.51741700	-0.36235600	-2.36112900
C	3.24808400	-0.43128900	-1.81667000
C	2.22004300	-1.39203400	-2.32534300
H	1.36887600	-1.28921600	-1.62062000
C	5.27178400	0.55214800	-1.65820500
C	5.03572800	2.08205500	0.18952000
H	4.45534400	2.56772100	0.96112200
C	-2.85662900	0.52682800	-1.01386800
C	2.65110600	-2.86608200	-2.24375700
H	3.51498600	-3.06811400	-2.88813600
H	2.97037600	-3.08818900	-1.21790000
C	-3.03436900	-0.13352400	1.32269900
H	-3.31053300	0.12252500	2.33944200
C	-3.24286700	0.78114900	0.28871200
C	-2.27712200	-0.71947700	-1.32465900
H	-2.12751300	-0.98263100	-2.36723600
C	6.60995800	0.90543100	-1.84611500
H	7.21219400	0.44520500	-2.62390500
C	7.15057200	1.85962700	-0.99464300

H	8.18959600	2.15605400	-1.11002600
C	1.63105100	-1.01673000	-3.69494500
H	1.26447900	0.01540600	-3.64690200
H	2.39331100	-1.04393800	-4.48505000
C	-2.09574500	-1.69998500	-0.31319300
C	1.50550300	-3.79071400	-2.65152800
H	1.84434800	-4.83414400	-2.63569300
H	0.70562900	-3.71254600	-1.90539800
C	6.36505300	2.44228700	0.01317000
H	6.80277200	3.19178800	0.66723400
C	0.94641900	-3.42625900	-4.02595300
H	0.11103700	-4.09013500	-4.28284900
H	1.72089100	-3.58522200	-4.79161500
C	5.06555600	-1.09059600	-3.48442400
H	5.62545900	-0.39937500	-4.12205300
H	4.27040900	-1.52701200	-4.08210200
H	5.73957000	-1.88771800	-3.14919100
C	0.49323600	-1.96761400	-4.06067500
H	0.08655400	-1.71046200	-5.04680500
H	-0.31938000	-1.82914800	-3.33334300
H	-2.28972900	-2.08512900	1.81277400
H	-3.00431600	1.27159300	-1.78736100
O	-3.72632700	2.06908800	0.59753700
S	-5.32136700	2.30604900	0.78695800
O	-5.97114100	1.12500900	1.32015500
O	-5.44420300	3.61747500	1.38698900
C	-5.84581800	2.47114900	-0.99153900
F	-7.06552600	2.99439700	-1.01690000
F	-5.00157200	3.27268300	-1.63253600
F	-5.85816700	1.27888100	-1.57279400
C	-0.99881500	-3.92796300	0.29691800
C	-3.13841300	-3.95263300	-0.74642500
C	-1.73929100	-5.04247800	0.71487000
C	0.27657400	-3.71436200	0.79062600
N	-2.99148600	-5.03909600	0.09272900
O	-4.12641200	-3.69656500	-1.40857300
C	-1.22668500	-5.96258700	1.62094200
C	0.81468000	-4.63398700	1.70010400

H	0.83349000	-2.83187900	0.47614300
C	-4.02333400	-6.02144700	0.30761200
C	0.06753100	-5.73965100	2.10621200
H	-1.80379500	-6.82374300	1.94365100
H	1.81748200	-4.48470400	2.08930100
H	-3.67916900	-7.01864300	0.01058200
H	-4.32352600	-6.04433300	1.36146700
H	-4.88046400	-5.73732500	-0.30549600
H	0.49334300	-6.44508700	2.81485800
C	-1.82714100	-3.14252600	-0.68031900
H	-1.38696900	-3.16890300	-1.68525400
C	2.04508000	0.38393800	2.02482400
C	3.01843600	-0.81094800	2.04170400
C	2.65530200	1.53436700	2.83984500
C	0.74027500	-0.05782900	2.72537300
H	3.96035500	-0.53249600	1.55582600
H	2.59116500	-1.63956400	1.46033200
C	3.29023700	-1.26272500	3.48289500
H	1.97440600	2.39279400	2.85362800
H	3.59323600	1.86427600	2.38983800
C	2.93675500	1.08384700	4.28239500
H	0.29068600	-0.88548100	2.16133100
H	0.00610200	0.75559800	2.71135700
C	1.01122200	-0.49841300	4.16836000
H	3.98871200	-2.10986500	3.46219600
C	3.91263700	-0.09905400	4.26444900
C	1.97917900	-1.68588300	4.15496000
H	3.38383000	1.92332100	4.83096100
C	1.62685500	0.66268900	4.95518200
H	0.06092600	-0.79967300	4.62863100
H	4.86027200	0.20265500	3.79738100
H	4.14235500	-0.41373900	5.29181000
H	1.52684800	-2.52594400	3.61188200
H	2.17502100	-2.02889400	5.18044400
H	1.81430000	0.36122500	5.99508700
H	0.92869200	1.51089900	4.98429300
C	1.07493100	2.48516100	-0.10162000
C	-0.15008200	2.77047200	0.78588300

C	2.11695700	3.59505300	0.09639700
C	0.62489300	2.52141200	-1.57861600
H	0.13855400	2.76135700	1.84366200
H	-0.89065200	1.97338300	0.64537000
C	-0.75728000	4.13538600	0.43993700
H	2.97595400	3.41526100	-0.55750300
H	2.48249200	3.60348300	1.12828600
C	1.50532100	4.96633200	-0.23568000
H	-0.11074200	1.72409500	-1.74829100
H	1.48575100	2.31178600	-2.22769100
C	0.01785800	3.88571900	-1.92681100
H	-1.62720000	4.30976700	1.08502500
C	0.29475000	5.22727200	0.66860200
C	-1.19706900	4.14413900	-1.02779800
H	2.26687400	5.73960000	-0.06940300
C	1.06317300	4.98393100	-1.70288200
H	-0.29359500	3.87732800	-2.98002400
H	0.60624200	5.23426800	1.72274500
H	-0.13209600	6.21625300	0.45173500
H	-1.96136000	3.37423700	-1.18884700
H	-1.65466500	5.11125400	-1.27811800
H	0.64265400	5.96608100	-1.96006200
H	1.92973100	4.81927500	-2.35807600

8H

Charge: 0 Multiplicity: 1

C	2.03916100	-0.75761300	-1.20955300
C	3.33078400	-1.39921800	-1.39470500
N	2.22126700	-1.43011100	-3.37029300
C	1.40190000	-0.79661000	-2.45652100
C	0.08205000	-0.21371100	-2.84888800
H	-0.32515600	0.21016500	-1.90865400
C	3.38840900	-1.81928200	-2.74915200
C	4.45819100	-1.65777200	-0.59679500
H	4.50313100	-1.31257300	0.42605500
C	-0.97381000	-1.22519100	-3.31830800
H	-0.67716400	-1.70506800	-4.25916200
H	-1.06694600	-2.01835300	-2.56912500

C	4.47604500	-2.50387200	-3.29615300
H	4.47776300	-2.82524700	-4.33343900
C	5.55861700	-2.76210100	-2.46647200
H	6.42213300	-3.29276900	-2.85813300
C	0.20713800	0.99585500	-3.79166600
H	0.92316600	1.70719300	-3.36345600
H	0.60796100	0.69797100	-4.76935500
C	-2.31843300	-0.52697700	-3.51097800
H	-3.06429700	-1.24449800	-3.87486000
H	-2.66690300	-0.18023800	-2.53002900
C	5.54861500	-2.33220300	-1.12982500
H	6.41278200	-2.52382900	-0.49925100
C	-2.20736200	0.66447000	-4.46208100
H	-3.18101700	1.16196000	-4.56216600
H	-1.93758700	0.30482200	-5.46682000
C	1.97118100	-1.73349900	-4.76252000
H	2.83845600	-1.44025400	-5.36270000
H	1.10842300	-1.18435400	-5.12602100
H	1.79051700	-2.80610600	-4.89944200
C	-1.15310100	1.66246600	-3.98259600
H	-1.06504600	2.49802900	-4.68870800
H	-1.46728400	2.08798000	-3.02098000
C	1.22514900	-1.53267000	1.55625600
C	0.12089400	-1.22690800	2.59193800
C	0.80844200	-2.79872800	0.77958200
C	2.52956400	-1.81843900	2.31357100
H	-0.81936000	-1.02480300	2.06762800
H	0.36904000	-0.32212800	3.15823500
C	-0.06601500	-2.40454400	3.55555900
H	1.57229700	-3.04494000	0.03319600
H	-0.12738400	-2.60469000	0.23857700
C	0.62386200	-3.97919000	1.74197600
H	2.84832400	-0.93199900	2.87501300
H	3.32471700	-2.07170000	1.61159800
C	2.34155000	-3.00023300	3.27893000
H	-0.85750800	-2.14869100	4.27165700
C	-0.47275800	-3.64919700	2.75989300
C	1.24708600	-2.67091300	4.29864800

H	0.33761800	-4.86563800	1.16087600
C	1.94300700	-4.24569800	2.47737700
H	3.29183600	-3.18304800	3.79796700
H	-1.42396300	-3.46527900	2.24572300
H	-0.62600800	-4.49939700	3.43930400
H	1.53391800	-1.78802800	4.88745600
H	1.12384500	-3.50441900	5.00407800
H	1.83312800	-5.10748900	3.15024800
H	2.73283000	-4.49535700	1.75543100
C	2.21103200	1.36967200	0.83460000
C	1.72948000	1.82906300	2.22116200
C	3.73724800	1.21118100	0.86104100
C	1.85788800	2.46689400	-0.19392400
H	1.97868800	1.07360900	2.97561100
H	0.63775800	1.93447000	2.21052400
C	2.39248600	3.15980300	2.60078400
H	4.09343400	0.89744500	-0.12539000
H	4.02686300	0.43718400	1.58068700
C	4.40545200	2.53959900	1.24970700
H	0.76626400	2.58957100	-0.23181700
H	2.18309300	2.14695400	-1.19314300
C	2.52488000	3.79432300	0.18294400
H	2.03303700	3.46524700	3.59247400
C	3.91432000	2.97525200	2.63519100
C	2.02723100	4.22912300	1.56598000
H	5.49342100	2.39392000	1.27026400
C	4.04643500	3.61272300	0.21580100
H	2.25330600	4.55303400	-0.56240000
H	4.18537100	2.21944300	3.38584500
H	4.40228500	3.91416100	2.93104800
H	0.94026200	4.37272900	1.54051100
H	2.47506900	5.19314300	1.84405800
H	4.53610200	4.56266500	0.47129800
H	4.41254500	3.31502100	-0.77645500
P	1.22148600	-0.12984800	0.29220100
Pd	-1.01790600	0.55993900	0.02086500
C	-3.00313400	1.27713300	0.15780300
C	-2.34241000	1.68000900	1.36093700

C	-3.17567800	2.19633400	-0.90902400
C	-1.88738800	3.02209100	1.45479000
H	-2.44703300	1.09404300	2.26841000
C	-2.69454900	3.48449800	-0.79882500
H	-3.71823600	1.87506700	-1.79180100
H	-1.43465600	3.36553600	2.37860000
C	-2.06461500	3.88726400	0.39491000
H	-2.81018400	4.18572600	-1.61784800
Cl	-1.50929300	5.54064000	0.52256200
F	-5.27524200	-3.22105600	0.53491900
C	-5.29978100	-1.91664400	0.28128400
S	-3.57689300	-1.27684000	0.55066000
F	-6.14755900	-1.31650700	1.10462800
F	-5.66790500	-1.71270800	-0.97686100
O	-3.99161600	0.23816100	0.17167500
O	-2.73395400	-1.89795900	-0.45814000
O	-3.27829000	-1.40184500	1.96817600

8I-TS

Charge: 0 Multiplicity: 1

C	2.09780200	-0.61692100	-1.21255500
C	3.46359800	-1.06281200	-1.41900400
N	2.31316800	-1.33102600	-3.35338300
C	1.43854700	-0.78410400	-2.43649200
C	0.04335000	-0.38212700	-2.79667200
H	-0.35727400	0.07274900	-1.87200800
C	3.54652000	-1.51038200	-2.76289400
C	4.63542300	-1.11765400	-0.64708400
H	4.64812500	-0.73949900	0.36572900
C	-0.91798600	-1.53669400	-3.11788500
H	-0.62460000	-2.05844900	-4.03777900
H	-0.87969700	-2.27137100	-2.30678200
C	4.71665600	-2.01974100	-3.32971600
H	4.74615800	-2.35133800	-4.36344000
C	5.84797500	-2.07852900	-2.52670800
H	6.77651800	-2.46857700	-2.93441700
C	-0.01801800	0.74100700	-3.84592200
H	0.65209200	1.55413200	-3.54253500

H	0.33658100	0.38786200	-4.82253800
C	-2.34030100	-1.00166500	-3.26990800
H	-3.02269000	-1.81924200	-3.53026600
H	-2.66557500	-0.62356200	-2.29285400
C	5.80512000	-1.62335600	-1.19873300
H	6.70629000	-1.65733000	-0.59228100
C	-2.42160000	0.11829400	-4.30699900
H	-3.44778400	0.50371300	-4.36833200
H	-2.18270200	-0.28818900	-5.30140600
C	2.08769100	-1.66189300	-4.74350100
H	2.65792600	-0.99276200	-5.39814000
H	1.03381900	-1.57935000	-4.98995900
H	2.40174200	-2.69401800	-4.93040700
C	-1.44995900	1.25371600	-3.98313400
H	-1.49789500	2.03207700	-4.75521200
H	-1.74358200	1.72676700	-3.03612700
C	1.51251500	-1.30280600	1.65379200
C	0.36718300	-1.11042400	2.67541100
C	1.33471300	-2.68655300	0.99543000
C	2.84321400	-1.27335100	2.41883200
H	-0.59884500	-1.14335700	2.15579300
H	0.44360800	-0.12752800	3.15398200
C	0.39518500	-2.21209400	3.74176400
H	2.13329200	-2.85454400	0.26379500
H	0.38069900	-2.71483300	0.45300300
C	1.36413300	-3.78926300	2.06205000
H	2.98625300	-0.29855200	2.90012100
H	3.67721300	-1.42976900	1.73333700
C	2.87203200	-2.38211600	3.48380100
H	-0.43173200	-2.04100100	4.44242500
C	0.22179500	-3.57356400	3.06071200
C	1.73343800	-2.16788900	4.48581200
H	1.24521600	-4.76105100	1.56569200
C	2.70809900	-3.74503400	2.79947900
H	3.83825800	-2.34275700	4.00384600
H	-0.74612600	-3.60898300	2.54572500
H	0.22212500	-4.37424400	3.81315200
H	1.85356600	-1.19955100	4.99206600

H	1.76170900	-2.94457200	5.26233900
H	2.75550100	-4.54884100	3.54699700
H	3.53176100	-3.91085100	2.09130100
C	1.96048600	1.65256700	0.65735200
C	1.41927000	2.16125700	2.00434300
C	3.49154800	1.75773000	0.65309400
C	1.40828400	2.56325900	-0.46274600
H	1.79897800	1.54050300	2.82471800
H	0.32454200	2.08259700	2.01193600
C	1.84567600	3.61791500	2.23108600
H	3.88336700	1.41161600	-0.30903600
H	3.91853500	1.11691800	1.43270100
C	3.92289000	3.21349400	0.89180500
H	0.30993400	2.50042600	-0.47755300
H	1.76593500	2.20333300	-1.43639700
C	1.84129400	4.01595000	-0.23955800
H	1.44996000	3.95686600	3.19757300
C	3.37713600	3.69886000	2.24030300
C	1.28960600	4.49880000	1.10649600
H	5.01955300	3.26071100	0.89666100
C	3.37200800	4.09825700	-0.23238700
H	1.43663200	4.63629300	-1.04968600
H	3.78150800	3.08170000	3.05488000
H	3.69944200	4.73228000	2.42758700
H	0.19297400	4.45031500	1.09715000
H	1.56724100	5.54795200	1.27615000
H	3.69345200	5.13868200	-0.08653900
H	3.77183600	3.76736600	-1.20073800
P	1.24853600	-0.03872700	0.28162700
Pd	-1.11341300	0.27094600	0.15892000
C	-2.84129000	1.15022900	0.35931100
C	-2.47446200	1.82082400	1.54598500
C	-3.35506100	1.83078400	-0.75780300
C	-2.44832300	3.22433600	1.53146700
H	-2.29611300	1.27440700	2.46717500
C	-3.30866000	3.21805100	-0.75275900
H	-3.73075700	1.28390400	-1.61463300
H	-2.15173900	3.77383300	2.41890900

C	-2.84513700	3.89761400	0.38378200
H	-3.62407800	3.77706700	-1.62804700
Cl	-2.79756000	5.64367400	0.35799400
F	-4.11296000	-3.98466100	-0.18069800
C	-4.58891300	-2.74562900	-0.07297300
S	-3.36626300	-1.70420500	0.84555700
F	-5.74602900	-2.77649900	0.58166500
F	-4.78792500	-2.24674000	-1.29191900
O	-4.02027400	-0.33367200	0.72973400
O	-2.13603400	-1.82147700	0.01531900
O	-3.29172700	-2.22354300	2.20807800

8J

Charge: 0 Multiplicity: 1

C	2.35017000	0.28853400	-1.11047700
C	3.78921200	0.43548500	-1.23287600
N	2.94747900	-0.23237700	-3.22966800
C	1.87765000	-0.09655100	-2.37207800
C	0.45631400	-0.23168700	-2.82316200
H	-0.14206100	0.04006200	-1.94001700
C	4.11647000	0.08755900	-2.56788800
C	4.83402700	0.85975900	-0.39590100
H	4.63435500	1.18961500	0.61511900
C	-0.00418200	-1.65188500	-3.19006000
H	0.54436400	-2.03497300	-4.06048800
H	0.21215400	-2.32509700	-2.35398200
C	5.42114800	0.11216200	-3.06503700
H	5.64001500	-0.15893600	-4.09351600
C	6.43118600	0.51111800	-2.19978600
H	7.45804500	0.54417900	-2.55302800
C	0.08092200	0.80503900	-3.89806000
H	0.38884400	1.80266300	-3.55982000
H	0.61950400	0.61289000	-4.83394900
C	-1.50341700	-1.66073200	-3.48924100
H	-1.81215400	-2.66590000	-3.79971500
H	-2.04116800	-1.44457500	-2.55886900
C	6.13509300	0.88985800	-0.87996700
H	6.93734000	1.22176700	-0.22646300

C	-1.88204500	-0.63415700	-4.55623100
H	-2.96707500	-0.64455100	-4.71976100
H	-1.41866300	-0.91196600	-5.51514600
C	2.94864600	-0.60768000	-4.62762500
H	3.18895300	0.25295000	-5.26212500
H	1.97914500	-1.00195400	-4.91625200
H	3.69589300	-1.39006000	-4.79190000
C	-1.42086000	0.77104700	-4.16911800
H	-1.67521800	1.49085200	-4.95729400
H	-1.95153100	1.09538500	-3.26325900
C	1.90062300	-0.84025300	1.62638700
C	0.80492800	-1.00382300	2.70229300
C	2.03628900	-2.18199100	0.87472100
C	3.23530800	-0.51027500	2.30729200
H	-0.15368600	-1.24880700	2.23311000
H	0.67064200	-0.07144600	3.25755000
C	1.18946600	-2.11665600	3.68617500
H	2.80097300	-2.09460300	0.09341500
H	1.08663900	-2.42620800	0.38399600
C	2.42040700	-3.29542700	1.85980000
H	3.17178500	0.45460300	2.82787500
H	4.02455700	-0.43514600	1.55641500
C	3.60838500	-1.62293500	3.29960700
H	0.39421300	-2.20396300	4.43674800
C	1.33116900	-3.43916100	2.92848200
C	2.51610300	-1.76035200	4.36517300
H	2.52137000	-4.23533400	1.30228200
C	3.75313800	-2.94432900	2.53295400
H	4.56391300	-1.36412400	3.77425700
H	0.37534500	-3.70324400	2.46452000
H	1.59314500	-4.24768700	3.62480000
H	2.41459900	-0.81959000	4.92486500
H	2.79237000	-2.53869900	5.08952000
H	4.04913200	-3.74745600	3.22148900
H	4.54667700	-2.85432700	1.77826700
C	1.24565200	2.17769900	0.89154600
C	0.66972800	2.32413000	2.30971700
C	2.54727300	2.98071900	0.79446900

C	0.22454700	2.77871800	-0.10103900
H	1.37609800	1.91762700	3.04187000
H	-0.26154600	1.74619400	2.39774100
C	0.39836700	3.80236800	2.62300900
H	2.97784300	2.87921100	-0.20743400
H	3.27614200	2.57817300	1.50803900
C	2.27995800	4.46049800	1.10737800
H	-0.79671700	2.28374800	-0.01600800
H	0.55417600	2.63733900	-1.13597200
C	-0.05131300	4.25379900	0.20327300
H	-0.00609400	3.87711300	3.64005100
C	1.71098500	4.58938100	2.52564200
C	-0.61536700	4.36938900	1.62260600
H	3.22356100	5.01514700	1.03302100
C	1.27399100	5.02159500	0.09490100
H	-0.77352600	4.64114000	-0.52505400
H	2.43500400	4.20562900	3.25726400
H	1.53513500	5.64579100	2.76838800
H	-1.56639900	3.82384100	1.69066900
H	-0.82865300	5.42051400	1.85544400
H	1.09436900	6.08750200	0.28715200
H	1.67581600	4.93846200	-0.92373700
P	1.29492500	0.37853700	0.34759400
Pd	-1.09083400	0.37127400	0.08555900
C	-3.03219000	0.80881300	0.08318200
C	-3.53525900	1.35771200	1.26523800
C	-3.85206900	0.72000400	-1.04088600
C	-4.83393800	1.86769400	1.31308800
H	-2.92666700	1.38814100	2.16748300
C	-5.15022700	1.22879000	-1.00878600
H	-3.49842800	0.23702900	-1.94595200
H	-5.22756700	2.29830900	2.22858400
C	-5.62244500	1.80346900	0.16816800
H	-5.79122200	1.16507100	-1.88267700
Cl	-7.25134900	2.44630800	0.21408900
F	-0.66809900	-4.34974900	0.32060200
C	-1.95273000	-4.12867600	0.02122300
S	-2.49940400	-2.45041400	0.58607400

F	-2.69525800	-5.06056900	0.61898900
F	-2.10113700	-4.24040800	-1.30071900
O	-3.86136500	-2.31753200	0.07671800
O	-1.45055600	-1.65072500	-0.18722100
O	-2.29238600	-2.41287100	2.03617800

8K

Charge: 0 Multiplicity: 1

Pd	1.08976300	-0.58846500	0.66569900
P	-0.87055600	0.18175200	-0.45063900
C	-2.35732200	-0.10614900	0.57776600
C	3.11370800	0.94286700	-0.81019300
C	-3.75274600	-0.17619500	0.17732700
N	-3.66346600	-0.10367800	2.43629800
C	-2.35668000	-0.08808400	1.98376100
C	-1.20693000	-0.13559000	2.94769500
H	-0.31266200	-0.29510100	2.31842300
C	-4.52557400	-0.17992800	1.36504500
C	-4.44912500	-0.24534600	-1.03929500
H	-3.91590500	-0.24195800	-1.97706600
C	3.31243300	3.06989400	0.97565700
C	-1.27527700	-1.33959400	3.90652000
H	-2.11368700	-1.23698000	4.60347200
H	-1.46935600	-2.25321500	3.33237500
C	3.95859900	2.01187900	-1.10389400
H	4.54829700	2.01575800	-2.01566800
C	4.03933600	3.07474100	-0.20960500
C	2.46560900	1.99426200	1.25002600
H	1.90329000	2.00745700	2.17839300
C	-5.92060600	-0.25600900	1.37323700
H	-6.48132100	-0.27239300	2.30284500
C	-6.56991900	-0.32539300	0.14871400
H	-7.65405100	-0.38987800	0.11779900
C	-0.91472000	1.16598200	3.71543700
H	-0.81659700	1.99253500	3.00701800
H	-1.74451200	1.42451700	4.38653100
C	2.33023000	0.93214700	0.35145000
C	0.01053100	-1.46017400	4.72317900

H	-0.06397200	-2.31177800	5.41080700
H	0.85517100	-1.66841300	4.05322900
C	-5.83461600	-0.31932400	-1.04762500
H	-6.35720900	-0.37447200	-1.99880800
C	0.29681700	-0.17055300	5.49072400
H	1.23540800	-0.26311700	6.05071800
H	-0.49907800	-0.00171700	6.23163000
C	-4.16102300	-0.02607700	3.79347900
H	-5.02364100	0.64630000	3.81487400
H	-3.40551800	0.38466400	4.45690700
H	-4.47033800	-1.01036200	4.16315600
C	0.36599900	1.02075700	4.53755100
H	0.56140900	1.94806200	5.09030000
H	1.21242400	0.87397800	3.85235100
H	3.06003600	0.11664500	-1.51310600
H	3.39952200	3.89536500	1.67587700
C	1.96571100	-2.84262500	1.25244100
C	3.94893700	-1.63523000	0.94259000
C	2.71141900	-3.41762700	0.17903900
C	0.72699300	-3.39234400	1.59522500
N	3.86128700	-2.67649300	-0.00481200
O	4.93597600	-0.92754700	1.07218300
C	2.26578600	-4.54334300	-0.48997600
C	0.26699000	-4.52845100	0.90835800
H	0.15746200	-2.98275900	2.42030400
C	4.88615600	-2.94593700	-0.97556200
C	1.03049400	-5.09596100	-0.10524100
H	2.84732400	-4.99064700	-1.29070600
H	-0.68620600	-4.97077300	1.18337600
H	5.33089000	-3.93687700	-0.82252200
H	4.48489600	-2.88945400	-1.99484200
H	5.65829300	-2.18431700	-0.84747200
H	0.66785800	-5.98108900	-0.62088300
C	2.65868100	-1.62829600	1.67153800
H	2.67524200	-1.27857600	2.70024300
C	-0.91301600	-0.90304400	-2.01296000
C	-1.52092500	-2.26107800	-1.61483000
C	-1.62954000	-0.34292200	-3.25650300

C	0.55862200	-1.14736200	-2.42940000
H	-2.56324600	-2.13742700	-1.30303600
H	-0.97343600	-2.66926800	-0.75452500
C	-1.44492500	-3.24351500	-2.79165400
H	-1.15575900	0.59129300	-3.57222800
H	-2.67333600	-0.10811000	-3.05349700
C	-1.57238000	-1.34591800	-4.41787300
H	1.11994900	-1.55433100	-1.57681900
H	1.03478300	-0.19630000	-2.69568900
C	0.64289500	-2.13108800	-3.60439100
H	-1.89309800	-4.19612900	-2.48117400
C	-2.21558800	-2.66895200	-3.98557000
C	0.01753400	-3.46579500	-3.18883300
H	-2.12669700	-0.92394300	-5.26633100
C	-0.11100500	-1.57234100	-4.81325600
H	1.70131300	-2.27946900	-3.85668200
H	-3.26747100	-2.50432300	-3.71326800
H	-2.20554600	-3.38248000	-4.82085000
H	0.57023700	-3.88688300	-2.34349800
H	0.07898500	-4.18541600	-4.01730600
H	-0.04693800	-2.27286200	-5.65714900
H	0.33967700	-0.62537200	-5.14143100
C	-1.01293700	2.00902800	-0.89316500
C	0.12520900	2.42442800	-1.84192000
C	-2.36725100	2.42019200	-1.49875600
C	-0.85017800	2.77501100	0.43308100
H	0.04049600	1.90011300	-2.79969600
H	1.08903900	2.15121600	-1.40901900
C	0.08323600	3.93847600	-2.08931500
H	-3.17752800	2.14610600	-0.81593800
H	-2.54781400	1.90089300	-2.44298800
C	-2.39552600	3.93698300	-1.74940900
H	0.09000100	2.48588200	0.91069200
H	-1.66910600	2.49924400	1.10771000
C	-0.86992000	4.28977200	0.19407000
H	0.90037100	4.20279700	-2.77257600
C	-1.26442800	4.32060000	-2.71107100
C	0.26796900	4.67394600	-0.75807600

H	-3.36534400	4.19802100	-2.19286600
C	-2.21535800	4.68338700	-0.42315900
H	-0.73656400	4.79910700	1.15775900
H	-1.39624100	3.80431500	-3.67253500
H	-1.29441900	5.39941400	-2.91722400
H	1.23600100	4.40542100	-0.31782000
H	0.27154300	5.76026200	-0.92271100
H	-2.25378200	5.76855000	-0.59141600
H	-3.03494600	4.43115200	0.26403600
Cl	5.07810800	4.43924600	-0.57977700

8L-TS

Charge: 0 Multiplicity: 1

Pd	0.79712200	0.72826400	0.08336100
P	-1.31945900	-0.29913000	0.16843600
C	-2.73092100	0.81115300	-0.13353400
C	2.91471600	-1.34453500	0.30484800
C	-4.15395900	0.61485600	0.08235300
N	-3.82662700	2.72086300	-0.68409700
C	-2.58401500	2.12139700	-0.61233900
C	-1.34015800	2.82785600	-1.05167900
H	-0.52307000	2.10973900	-0.84812500
C	-4.79186800	1.83701300	-0.25270800
C	-4.97600700	-0.44431700	0.50067100
H	-4.55757000	-1.41772900	0.71293200
C	3.15364400	-1.48246100	-2.47313500
C	-0.98705300	4.08071400	-0.23211900
H	-1.76107200	4.85202000	-0.32433500
H	-0.94746200	3.80619800	0.83015000
C	3.41079200	-2.50183700	-0.28873600
H	3.71028600	-3.34693900	0.32343200
C	3.51435100	-2.56598600	-1.67613100
C	2.65285100	-0.32996200	-1.87291800
H	2.40507700	0.52716400	-2.48956200
C	-6.16961200	2.03845000	-0.14423500
H	-6.62262700	2.99301400	-0.39507200
C	-6.94380800	0.97367900	0.29664300
H	-8.01929800	1.09461400	0.39320400

C	-1.26426700	3.06003400	-2.57098800
H	-1.44050100	2.10599000	-3.08110200
H	-2.04990100	3.74650700	-2.91366900
C	2.48314700	-0.26520700	-0.48018600
C	0.35401200	4.66492000	-0.67833800
H	0.55799700	5.59013500	-0.12460800
H	1.15814200	3.96166900	-0.42709200
C	-6.34797300	-0.25939700	0.60731900
H	-6.97116400	-1.08890200	0.93083800
C	0.39740800	4.91481000	-2.18469600
H	1.38122500	5.30628200	-2.46946100
H	-0.34327700	5.68371000	-2.45416400
C	-4.16781000	4.06258700	-1.10443600
H	-5.00563800	4.02240400	-1.80778600
H	-3.32800900	4.53212800	-1.60684500
H	-4.45545400	4.67842300	-0.24427600
C	0.10084600	3.62826900	-2.95337800
H	0.14151700	3.80670600	-4.03536300
H	0.88159400	2.89139900	-2.71908200
H	2.84384500	-1.29651000	1.38586200
H	3.26513800	-1.53381700	-3.55177200
C	3.59481200	1.22709800	1.56270100
C	3.75857500	2.03831400	-0.64627400
C	4.94763900	1.36381400	1.19536600
C	3.26316900	0.82736800	2.84789300
N	5.02244600	1.82134600	-0.11903200
O	3.52895200	2.54247400	-1.73781100
C	5.97730900	1.08391100	2.08294300
C	4.29033600	0.54940900	3.75857300
H	2.22006900	0.72725300	3.13582600
C	6.24023100	2.11620100	-0.82706500
C	5.62602600	0.66895600	3.37375500
H	7.01877100	1.18597800	1.79294800
H	4.04414800	0.23585900	4.76921100
H	6.81678900	2.89332400	-0.31142400
H	6.85739800	1.21609200	-0.92550200
H	5.96342600	2.47430000	-1.82034600
H	6.41352800	0.44363400	4.08800700

C	2.77816900	1.53223200	0.37302300
H	1.98299500	2.29954100	0.54706700
C	-1.44285200	-0.96359400	1.93750800
C	-1.87769200	0.22777800	2.81325700
C	-2.36742100	-2.15891600	2.21278200
C	-0.01410400	-1.37143200	2.36289200
H	-2.89078100	0.54293800	2.53941800
H	-1.21196100	1.08264000	2.62234200
C	-1.83357100	-0.15424500	4.29819300
H	-2.06219600	-3.02117700	1.60922600
H	-3.39671400	-1.91722800	1.94743200
C	-2.32784600	-2.53648900	3.70310400
H	0.66484100	-0.52999400	2.16807600
H	0.34390600	-2.20377400	1.74736100
C	0.03509200	-1.75278000	3.84578700
H	-2.15606100	0.70860200	4.89526600
C	-2.78032800	-1.33588200	4.54305900
C	-0.40575500	-0.55163700	4.68910200
H	-3.01034700	-3.38058900	3.86720900
C	-0.90377400	-2.93597800	4.10046000
H	1.06611500	-2.02996600	4.10281700
H	-3.80771100	-1.05448100	4.27420100
H	-2.78454400	-1.60209400	5.60898100
H	0.27685200	0.29386800	4.52424300
H	-0.36060400	-0.80035900	5.75829400
H	-0.87300100	-3.22686200	5.15953900
H	-0.57882800	-3.80726100	3.51499800
C	-1.45528000	-1.64424200	-1.12961300
C	-0.37585000	-2.71261500	-0.88625900
C	-2.83021000	-2.31837200	-1.24430300
C	-1.15101200	-0.94273700	-2.47038500
H	-0.56498400	-3.23402100	0.05982500
H	0.60684700	-2.23619200	-0.80475600
C	-0.37524900	-3.73330400	-2.03271400
H	-3.59704700	-1.56170300	-1.43925400
H	-3.09113300	-2.81897100	-0.30602500
C	-2.82354100	-3.34724000	-2.38543600
H	-0.17496100	-0.44468500	-2.40687600

H	-1.90439500	-0.16573200	-2.65418400
C	-1.15045600	-1.95943300	-3.61906200
H	0.40030700	-4.48409800	-1.83549100
C	-1.74963100	-4.40799900	-2.11457400
C	-0.07549600	-3.01961900	-3.35500500
H	-3.81172000	-3.82299400	-2.43670800
C	-2.52393500	-2.63354600	-3.70843900
H	-0.93115500	-1.43325200	-4.55756700
H	-1.96903400	-4.93336700	-1.17417400
H	-1.75372700	-5.16180300	-2.91393300
H	0.91244900	-2.54810200	-3.30381300
H	-0.05013900	-3.74659800	-4.17848500
H	-2.53800300	-3.35327000	-4.53861600
H	-3.30105300	-1.88444000	-3.91430300
Cl	4.11786900	-4.02682400	-2.43017500

8M

Charge: 0 Multiplicity: 1

Pd	-0.86548400	0.43723400	-0.44526500
P	1.33379400	0.05729500	0.19120600
C	2.22171000	-1.35636400	-0.53461500
C	-2.93816100	1.71109000	0.68567800
C	3.56816800	-1.85308800	-0.31132800
N	2.57525200	-3.14926800	-1.88103200
C	1.64683500	-2.19955600	-1.49426400
C	0.25668000	-2.17817900	-2.04736900
H	-0.26895800	-1.40577600	-1.44897800
C	3.73964600	-2.97396800	-1.16467400
C	4.65087400	-1.49939500	0.51061600
H	4.59112100	-0.63922300	1.16222100
C	-1.93196600	3.03288700	-1.57095600
C	-0.52581800	-3.48377400	-1.82716100
H	-0.06483400	-4.32260400	-2.36153700
H	-0.49830700	-3.74191000	-0.76112600
C	-2.50514500	3.02625200	0.79071600
H	-2.52909400	3.53889200	1.74653400
C	-2.02394800	3.68130900	-0.34904400
C	-2.38663400	1.70399800	-1.68312900

H	-2.46057500	1.25926000	-2.67119900
C	4.91373500	-3.72926000	-1.21045100
H	5.00745000	-4.58931000	-1.86682300
C	5.95772000	-3.35052700	-0.37714100
H	6.88434000	-3.91806100	-0.38472300
C	0.16554300	-1.66663200	-3.49423700
H	0.67126500	-0.69594100	-3.55436100
H	0.68264100	-2.33684900	-4.19436200
C	-2.94580500	1.03133000	-0.56555000
C	-1.97279600	-3.33931100	-2.29659700
H	-2.49643000	-4.29735500	-2.18695700
H	-2.48869500	-2.62814400	-1.64072600
C	5.82343200	-2.24216100	0.47465500
H	6.65247400	-1.95652200	1.11675300
C	-2.05496300	-2.84442600	-3.74001700
H	-3.10415600	-2.72066200	-4.03763700
H	-1.62522300	-3.60191100	-4.41303600
C	2.44340500	-4.19730700	-2.86943100
H	3.36502400	-4.25335200	-3.45649400
H	1.62732900	-3.97797900	-3.55254800
H	2.26517100	-5.17077400	-2.39758200
C	-1.29664200	-1.52935200	-3.91200300
H	-1.36434300	-1.17453200	-4.94812700
H	-1.76203700	-0.76067500	-3.27855200
H	-3.33717500	1.20451000	1.56021900
H	-1.53691900	3.54510700	-2.44153600
C	-3.78194000	-1.20087000	0.37351200
C	-5.28680800	0.15736200	-0.87401300
C	-5.09788300	-1.38104100	0.82229800
C	-2.74362600	-1.89570700	0.96966400
N	-5.96606700	-0.57627500	0.07844600
O	-5.79061400	0.94370100	-1.65393200
C	-5.40404400	-2.24994300	1.86233600
C	-3.03161800	-2.78249800	2.01521200
H	-1.72186800	-1.73202000	0.62797300
C	-7.38981300	-0.49051700	0.28117200
C	-4.34542400	-2.95112500	2.45205300
H	-6.42412700	-2.38356700	2.20901500

H	-2.22736400	-3.33987800	2.48638500
H	-7.86522000	-1.46482200	0.12024100
H	-7.61724400	-0.14373100	1.29581000
H	-7.78227600	0.22690800	-0.44179100
H	-4.55725200	-3.63858700	3.26674400
C	-3.79275400	-0.20821000	-0.75535300
H	-3.50732700	-0.68117400	-1.70350800
C	1.34346100	-0.17227600	2.07436900
C	1.14197200	-1.67775700	2.33510600
C	2.57851300	0.30777400	2.85171600
C	0.11069500	0.57408700	2.63251300
H	2.00152900	-2.24146500	1.95536300
H	0.25912300	-2.02966800	1.78414700
C	0.96671400	-1.94491600	3.83603000
H	2.73300700	1.38107600	2.69326600
H	3.47424800	-0.20872600	2.50278100
C	2.41111200	0.03339700	4.35501100
H	-0.78530800	0.23995400	2.09392000
H	0.19802900	1.64980800	2.44163500
C	-0.05748400	0.31571500	4.13414700
H	0.83034600	-3.02370900	3.98984700
C	2.22172900	-1.47177300	4.57977900
C	-0.25643700	-1.18600300	4.36322700
H	3.31547400	0.37384900	4.87643200
C	1.19040400	0.79252700	4.88352200
H	-0.93956700	0.86497700	4.48920800
H	3.10226500	-2.01967500	4.21685100
H	2.12719200	-1.68340000	5.65386100
H	-1.16428200	-1.52257800	3.84579300
H	-0.39577000	-1.39277800	5.43355800
H	1.07542500	0.62164000	5.96294000
H	1.32756900	1.87332200	4.73897400
C	2.27799200	1.59047700	-0.35590300
C	1.63138900	2.81847100	0.31101100
C	3.79373300	1.61624800	-0.11460200
C	2.04287300	1.68435000	-1.87942400
H	1.78542300	2.78540700	1.39641900
H	0.54770500	2.79675600	0.13618500

C	2.23758800	4.11089900	-0.24854000
H	4.26128000	0.76320600	-0.61595000
H	4.01686100	1.53496800	0.95398500
C	4.39943000	2.91921700	-0.66236000
H	0.96274200	1.65339300	-2.07700300
H	2.48859400	0.80973700	-2.37186400
C	2.64681100	2.97622400	-2.44159100
H	1.75976900	4.96719800	0.24324600
C	3.74616700	4.12372100	0.02521200
C	1.98547600	4.17894500	-1.75847400
H	5.47885800	2.91652700	-0.46114300
C	4.15553600	2.99729700	-2.17337600
H	2.46020500	3.01420400	-3.52321800
H	3.93179200	4.08618600	1.10807000
H	4.19117100	5.05726600	-0.34635200
H	0.90522600	4.17573100	-1.95209400
H	2.38719700	5.11640100	-2.16747400
H	4.60090800	3.91514400	-2.58200700
H	4.63989600	2.14884300	-2.67619100
Cl	-1.48330200	5.33930800	-0.21044400

8N

Charge: 0 Multiplicity: 1

P	-2.57151800	0.28864200	0.20396100
C	-3.83991900	-0.77741800	-0.50093500
C	-5.27285500	-0.58921200	-0.59527500
N	-4.69328300	-2.42972400	-1.78681100
C	-3.53440400	-1.92745500	-1.23220200
C	-2.18871300	-2.55600100	-1.40905300
H	-1.52815500	-2.02753700	-0.71355700
C	-5.76503300	-1.64452000	-1.40603200
C	-6.19545000	0.34561700	-0.10145900
H	-5.87016100	1.15459500	0.53977000
C	-1.59005800	-2.31579400	-2.80626900
H	-2.19811700	-2.79725600	-3.58440600
H	-1.60410900	-1.23849000	-3.01570000
C	-7.11822600	-1.79069500	-1.71790300
H	-7.47490600	-2.61791100	-2.32421600

C	-8.00197400	-0.84389200	-1.21545000
H	-9.06176000	-0.92926000	-1.43926100
C	-2.11950700	-4.03596400	-0.99195600
H	-2.50356200	-4.13944500	0.03022400
H	-2.75242900	-4.66121300	-1.63222200
C	-0.15972700	-2.84634300	-2.86786900
H	0.25366800	-2.69978300	-3.87394900
H	0.45513300	-2.25806800	-2.17502800
C	-7.54201800	0.21439300	-0.41454500
H	-8.25260200	0.93867400	-0.02535000
C	-0.09231100	-4.31994100	-2.46690900
H	0.94552800	-4.67555000	-2.50196900
H	-0.65127500	-4.92259300	-3.19938800
C	-4.85375600	-3.58408300	-2.64526700
H	-5.16554600	-4.46716400	-2.07630000
H	-3.92415400	-3.80237200	-3.16586100
H	-5.61420000	-3.36100400	-3.39851300
C	-0.68017900	-4.54084000	-1.07267000
H	-0.64325600	-5.60501900	-0.80739800
H	-0.07538200	-4.00272600	-0.33352500
C	-2.80494300	2.01092400	-0.54329300
C	-3.27553700	1.83292100	-1.99976000
C	-3.71877800	3.02162200	0.16279900
C	-1.37945000	2.60131100	-0.57955300
H	-4.28836800	1.41861000	-2.01119800
H	-2.62714000	1.10930200	-2.51316300
C	-3.25073700	3.17827500	-2.73791100
H	-3.40150200	3.16630700	1.20132200
H	-4.74517900	2.64758400	0.18319200
C	-3.68935700	4.36809000	-0.57842600
H	-0.70175400	1.93362300	-1.20285600
H	-0.97091400	2.72357900	0.42826300
C	-1.33543800	3.94280000	-1.32429800
H	-3.60239100	3.02135000	-3.76524600
C	-4.17656000	4.16651600	-2.01834200
C	-1.82297800	3.73592100	-2.76066500
H	-4.35187700	5.07082300	-0.05751800
C	-2.25988900	4.92241900	-0.58958900

H	-0.30524900	4.31777800	-1.32231700
H	-5.20561500	3.78275400	-2.01588100
H	-4.18929000	5.12756000	-2.54987900
H	-1.15196700	3.04328200	-3.28730100
H	-1.79586400	4.68892300	-3.30488300
H	-2.23506900	5.89863400	-1.09151400
H	-1.90462700	5.07739600	0.43844900
C	-2.76599400	0.24247400	2.05715800
C	-1.76074300	1.21272800	2.70311800
C	-4.17188700	0.52544800	2.60324200
C	-2.37111200	-1.20232600	2.44069100
H	-2.01099600	2.24984600	2.44797400
H	-0.75558000	1.01758800	2.30633100
C	-1.77145200	1.04616700	4.22817600
H	-4.88746700	-0.17409100	2.15838700
H	-4.49081900	1.53977400	2.33778000
C	-4.18149500	0.36890600	4.13221000
H	-1.37565200	-1.43565100	2.04288300
H	-3.07937400	-1.90431600	1.98159300
C	-2.38713900	-1.36672500	3.96558200
H	-1.05071300	1.74834000	4.66709700
C	-3.17949600	1.34787100	4.75652900
C	-1.38206200	-0.39192600	4.59005900
H	-5.19165700	0.58603200	4.50272900
C	-3.79272000	-1.06782500	4.49940800
H	-2.10472800	-2.39787400	4.21286500
H	-3.45982600	2.38223400	4.51206100
H	-3.19771400	1.25883300	5.85116200
H	-0.37075100	-0.61261800	4.22473300
H	-1.36607100	-0.51237400	5.68178900
H	-3.81924400	-1.19847600	5.58994600
H	-4.51675900	-1.77373600	4.07023200
Pd	-0.18585900	0.30375500	-0.31612100
C	1.69418100	0.85820200	-0.71005100
C	2.17802900	2.02448200	-0.10410800
C	2.53775300	0.13770200	-1.55949800
C	3.49593900	2.43999500	-0.29766400
H	1.53864700	2.61372200	0.55022300

C	3.85422000	0.54201300	-1.77188800
H	2.19176700	-0.77747500	-2.03127100
H	3.88590400	3.32851200	0.18871700
C	4.31397100	1.67692100	-1.11783200
H	4.51911900	-0.02351600	-2.41538700
O	5.64458400	2.09271700	-1.34449500
S	6.75046300	1.85482500	-0.17257800
O	6.11668100	1.63685600	1.11274500
O	7.77464400	2.85758900	-0.38199200
C	7.46194700	0.23395800	-0.73979500
F	8.33596000	-0.17632500	0.17218500
F	8.07905900	0.41361100	-1.90205100
F	6.50011000	-0.66340800	-0.88096800
C	1.71126800	-1.81750200	0.57178200
N	2.55775600	-1.21123100	1.50647400
O	0.45405100	-1.48372500	0.46849500
C	2.43676800	-2.78501900	-0.11712300
C	3.80824300	-1.77748900	1.41760200
C	2.17266900	-0.20286100	2.45356000
C	3.76141000	-2.78685100	0.40893500
H	2.04774100	-3.40435300	-0.91069300
C	4.96639600	-1.49916000	2.14005700
H	2.79262200	0.69284600	2.34217900
H	2.25828300	-0.57537000	3.48207000
H	1.13358200	0.06280100	2.25905300
C	4.92659500	-3.52435300	0.14490300
C	6.10401300	-2.25043400	1.85457300
H	4.98679700	-0.71743000	2.89331900
C	6.08177300	-3.25315700	0.86947400
H	4.92215600	-4.30122800	-0.61641800
H	7.02401700	-2.05075200	2.39738000
H	6.98681400	-3.82128800	0.66804500

8O-TS

Charge: 0 Multiplicity: 1

P	-2.19830900	0.47318200	0.25622800
C	-3.31770000	0.34628800	-1.16133500
C	-4.59338900	0.98713900	-1.41669800

N	-4.07329600	-0.32443700	-3.18988800
C	-3.04001200	-0.44527500	-2.28140500
C	-1.85205400	-1.32203300	-2.52136400
H	-1.19475400	-1.14149100	-1.65245000
C	-5.01874100	0.55179900	-2.69790400
C	-5.42652800	1.87963600	-0.72418500
H	-5.16733600	2.21662500	0.27009500
C	-1.01293400	-0.93849000	-3.75135000
H	-1.57507600	-1.08619700	-4.68118000
H	-0.76749800	0.12983500	-3.70000600
C	-6.20319200	0.98648900	-3.29649700
H	-6.49572700	0.64588300	-4.28521900
C	-6.99518600	1.87790600	-2.58470200
H	-7.92310300	2.23751700	-3.02084000
C	-2.17038200	-2.82607100	-2.47461000
H	-2.71242400	-3.04504100	-1.54780900
H	-2.83214900	-3.11524200	-3.30170700
C	0.26239700	-1.77748400	-3.80129500
H	0.84485600	-1.52540600	-4.69644300
H	0.88627400	-1.51563600	-2.93645200
C	-6.60879400	2.31566700	-1.30724800
H	-7.24709700	3.00602600	-0.76230100
C	-0.03885200	-3.27584700	-3.76160700
H	0.89763800	-3.84683600	-3.75415300
H	-0.57565900	-3.55934800	-4.67962400
C	-4.21886600	-0.94391000	-4.48949800
H	-5.23831600	-1.32723800	-4.59595600
H	-3.53403800	-1.78026700	-4.59340100
H	-4.02525400	-0.22248100	-5.29190000
C	-0.88431600	-3.64624100	-2.54303300
H	-1.12350700	-4.71685100	-2.55780000
H	-0.29929000	-3.46843700	-1.63196500
C	-1.81677400	2.30741800	0.55027200
C	-1.72299000	2.96256900	-0.84183800
C	-2.77819600	3.11956400	1.43121000
C	-0.41639400	2.37730700	1.20188000
H	-2.70070000	2.93530000	-1.33465600
H	-1.02932100	2.38677800	-1.47203800

C	-1.24106000	4.41383500	-0.72026500
H	-2.83806500	2.67874300	2.43274800
H	-3.78470500	3.11273000	1.00935900
C	-2.30117200	4.57710000	1.54332300
H	0.31127800	1.82833200	0.57999300
H	-0.42153300	1.89340300	2.18489700
C	0.06901000	3.82617900	1.32635100
H	-1.19368500	4.85481400	-1.72434500
C	-2.23370300	5.20111700	0.14414400
C	0.14698300	4.44848400	-0.07143000
H	-3.01808400	5.13245100	2.16190700
C	-0.91486400	4.61754500	2.19381800
H	1.06367200	3.82278100	1.78915700
H	-3.22857200	5.18860600	-0.32180500
H	-1.92156300	6.25189800	0.21575800
H	0.86702400	3.89209100	-0.68691500
H	0.50891700	5.48336000	-0.00471900
H	-0.57501100	5.65678100	2.29929100
H	-0.95880200	4.18670200	3.20372700
C	-3.07393100	-0.34440900	1.68987200
C	-2.17992200	-0.23524100	2.93878400
C	-4.48483000	0.16753500	2.01457800
C	-3.18314300	-1.83406500	1.29398900
H	-2.08154800	0.81337600	3.24492200
H	-1.17402500	-0.60675500	2.70404500
C	-2.78686600	-1.04619600	4.09162200
H	-5.12505500	0.06301000	1.13255100
H	-4.46088900	1.22921700	2.28058600
C	-5.08352300	-0.63778100	3.17856300
H	-2.18974400	-2.22480600	1.04703800
H	-3.81333200	-1.92533400	0.39980700
C	-3.78865600	-2.64591900	2.44651500
H	-2.13872500	-0.95038900	4.97255400
C	-4.18479400	-0.50390200	4.41380600
C	-2.88754800	-2.51945700	3.68044500
H	-6.08323100	-0.24334000	3.40269200
C	-5.18711500	-2.11294000	2.77541700
H	-3.85224200	-3.69858200	2.14134200

H	-4.11834800	0.54989600	4.71931700
H	-4.61913300	-1.05763600	5.25749900
H	-1.88829500	-2.91096000	3.45214300
H	-3.29356100	-3.11585000	4.50917100
H	-5.63397400	-2.69760300	3.59152400
H	-5.84579900	-2.21761600	1.90233300
Pd	0.04245500	-0.38933800	0.08578000
C	2.00770400	-0.30978200	0.08897300
C	2.64948800	-0.12040300	1.32184300
C	2.37025100	0.45092700	-1.03477400
C	3.57246200	0.90779600	1.46343700
H	2.38790400	-0.74209500	2.17349700
C	3.30058100	1.48568800	-0.89204700
H	1.93724300	0.25246900	-2.01243400
H	4.05159300	1.10669700	2.41621300
C	3.87487200	1.69644400	0.35209100
H	3.58459700	2.10938400	-1.73390800
O	4.75429500	2.79174900	0.48692100
S	6.35058900	2.52466300	0.63941900
O	6.61763100	1.33312600	1.42057200
O	6.92154100	3.81744900	0.95072700
C	6.80564800	2.13072100	-1.12248900
F	8.12869200	2.16699000	-1.22323800
F	6.27025100	3.03483900	-1.93579900
F	6.36483200	0.92202200	-1.44470900
C	1.11533300	-2.98093700	0.67597700
N	1.54228700	-4.08511500	1.39473600
O	0.11806300	-2.28148700	1.08419800
C	1.98384800	-2.80148300	-0.42697500
C	2.69605500	-4.60016500	0.81262700
C	0.98000300	-4.51094700	2.64945000
C	2.98870900	-3.82116300	-0.34303600
H	1.70470300	-2.26732600	-1.32023200
C	3.48608400	-5.66733300	1.21370900
H	1.73556300	-4.48589500	3.44383100
H	0.57722400	-5.52768800	2.57432200
H	0.16920500	-3.82690700	2.90365900
C	4.10013400	-4.16742300	-1.11850900

C	4.59813200	-5.98289200	0.42531000
H	3.24630800	-6.24757000	2.10074200
C	4.89603400	-5.24415800	-0.72627200
H	4.34665000	-3.59462000	-2.00939600
H	5.23346000	-6.81723000	0.71041100
H	5.76437900	-5.51250600	-1.32286300

8P

Charge: 0 Multiplicity: 1

P	-1.96170600	0.40673500	0.24669200
C	-3.31798400	0.01018200	-0.90342900
C	-4.67102200	0.52926200	-1.00537900
N	-4.33216400	-0.93312200	-2.70207200
C	-3.16684200	-0.89889800	-1.95815200
C	-2.00291400	-1.78761200	-2.26301600
H	-1.25295400	-1.54008400	-1.48450500
C	-5.25644000	-0.07456600	-2.14883300
C	-5.47819200	1.40579400	-0.26129600
H	-5.11365000	1.84961400	0.65405900
C	-1.29470200	-1.49358700	-3.59520100
H	-1.95414700	-1.66233000	-4.45597300
H	-1.01586500	-0.43282100	-3.61650400
C	-6.56008600	0.18854200	-2.57497200
H	-6.97360200	-0.29222800	-3.45670400
C	-7.31530400	1.08078700	-1.82562900
H	-8.33416700	1.30891800	-2.12675700
C	-2.31251700	-3.28140500	-2.06502900
H	-2.73569000	-3.42412400	-1.06419500
H	-3.06820700	-3.63262100	-2.77972700
C	-0.05027100	-2.36801600	-3.73863600
H	0.43408300	-2.18161400	-4.70572800
H	0.66466100	-2.07246200	-2.95988600
C	-6.77662300	1.67580000	-0.67337700
H	-7.38920700	2.35350900	-0.08455400
C	-0.36909000	-3.85266500	-3.56945800
H	0.54860800	-4.44859600	-3.65929700
H	-1.03470700	-4.17853400	-4.38322800
C	-4.65314500	-1.73267000	-3.86353800

H	-5.47691200	-2.41988500	-3.63871300
H	-3.79275200	-2.31461900	-4.17726300
H	-4.95103300	-1.08294400	-4.69387300
C	-1.04434300	-4.11654900	-2.22408100
H	-1.28193300	-5.18248900	-2.11577800
H	-0.35783000	-3.86098300	-1.40648100
C	-1.73451100	2.28475600	0.26329300
C	-1.79213600	2.72938800	-1.21164100
C	-2.71202600	3.13704000	1.08478000
C	-0.30924300	2.56248600	0.78949400
H	-2.79462000	2.54804600	-1.61658700
H	-1.08929700	2.12207600	-1.79978800
C	-1.44028400	4.21714600	-1.33717700
H	-2.67736800	2.84311200	2.14065600
H	-3.73381300	2.99299400	0.73259300
C	-2.36280000	4.62951600	0.95533800
H	0.40069600	1.95436200	0.21902600
H	-0.22047900	2.24632300	1.83452200
C	0.04553200	4.04821700	0.66637400
H	-1.49832300	4.50731800	-2.39470200
C	-2.44222100	5.04240100	-0.51979200
C	-0.02254700	4.45977200	-0.80764700
H	-3.08799600	5.21039400	1.54068500
C	-0.94747500	4.88063400	1.48294600
H	1.06349100	4.19918800	1.04435100
H	-3.46010100	4.88125100	-0.90112500
H	-2.22233700	6.11410600	-0.62260500
H	0.70292500	3.87541100	-1.38969000
H	0.24898700	5.51859200	-0.91986700
H	-0.69999000	5.94893300	1.41169700
H	-0.88626100	4.60435100	2.54505600
C	-2.51098300	-0.28343700	1.90351400
C	-1.48257500	0.10493200	2.98044100
C	-3.91781500	0.09134700	2.38978900
C	-2.46329300	-1.81512500	1.71023600
H	-1.50645700	1.18833900	3.15001700
H	-0.47221300	-0.14747700	2.62942500
C	-1.79071900	-0.61931300	4.29681700

H	-4.65817900	-0.20292600	1.63872100
H	-4.00175300	1.17491100	2.52924000
C	-4.22723400	-0.62035600	3.71737800
H	-1.47001400	-2.11480500	1.35076400
H	-3.18897000	-2.10438400	0.93852800
C	-2.77736500	-2.53572500	3.02518600
H	-1.04478700	-0.32575000	5.04751100
C	-3.19198200	-0.21818700	4.77476000
C	-1.73447600	-2.13533000	4.07528700
H	-5.23108100	-0.32547200	4.05063000
C	-4.17698400	-2.13801200	3.50709900
H	-2.73321700	-3.61920400	2.85441200
H	-3.23259400	0.86632000	4.94938600
H	-3.42088200	-0.70806300	5.73146500
H	-0.73350900	-2.42911700	3.73245100
H	-1.92590000	-2.66165100	5.02105300
H	-4.41890500	-2.65730600	4.44516500
H	-4.92972500	-2.43930000	2.76553200
Pd	0.13393300	-0.55412200	-0.15498800
C	2.16593100	-1.18585500	-0.16089800
C	2.42966200	-0.64396700	1.13538000
C	2.16275700	-0.27703200	-1.26026600
C	2.82406000	0.67772700	1.29971000
H	2.40516200	-1.30317900	1.99881100
C	2.57794500	1.05721400	-1.09228900
H	2.03929400	-0.65783300	-2.26962500
H	3.04847700	1.07647500	2.28242300
C	2.93093700	1.49244700	0.17123400
H	2.62374400	1.73425600	-1.93818800
O	3.29505900	2.84817100	0.31941200
S	4.85297000	3.22608200	0.57055500
O	5.50836800	2.24819200	1.41701400
O	4.85878700	4.64525600	0.85383900
C	5.54313400	3.00397500	-1.14493500
F	6.74406300	3.56899000	-1.18315400
F	4.74490000	3.59118100	-2.02955400
F	5.65024700	1.71136800	-1.42839800
C	1.65267800	-3.54423200	0.67745500

N	2.62682300	-4.37225000	1.18714800
O	0.48497200	-3.53079200	1.03456600
C	2.30424000	-2.67436000	-0.40579900
C	3.86749000	-4.14429800	0.57951600
C	2.38650400	-5.33615300	2.23103300
C	3.73959900	-3.13827200	-0.38768300
H	1.81842300	-2.92469700	-1.35695000
C	5.08321700	-4.76003100	0.84248700
H	3.00374900	-5.11592300	3.10929400
H	2.60931900	-6.35014900	1.88063500
H	1.33208500	-5.27156800	2.50491600
C	4.84663800	-2.71416700	-1.09959400
C	6.19408100	-4.33157700	0.10596000
H	5.17567500	-5.53922100	1.59289900
C	6.08404500	-3.32226200	-0.84957400
H	4.75873100	-1.91551600	-1.83169200
H	7.16014500	-4.79338100	0.29121700
H	6.96352600	-3.00135800	-1.40030900

8Q

Charge: 0 Multiplicity: 1

Pd	-0.14357600	0.73993800	0.81726900
P	-1.87279700	-0.20109600	-0.49189500
C	-3.21055900	-0.73674400	0.62687500
C	2.04057900	-1.21238700	0.48545300
C	-4.64678900	-0.78068500	0.42771400
N	-4.19805700	-1.39280500	2.56079000
C	-2.98369200	-1.16040800	1.94704700
C	-1.68371300	-1.51168600	2.61112400
H	-0.91854000	-1.34101000	1.83955800
C	-5.22048200	-1.17412700	1.66335300
C	-5.52237200	-0.56830300	-0.64823800
H	-5.14051800	-0.31523700	-1.62594600
C	3.28670300	0.12117600	-1.62742800
C	-1.60320100	-3.00813700	2.97479800
H	-2.31711200	-3.24772000	3.77187000
H	-1.88873200	-3.61725500	2.11010100
C	3.23616700	-1.70886300	-0.03355500

H	3.69823600	-2.60372100	0.37172700
C	3.84008800	-1.02816500	-1.08131000
C	2.09949100	0.61039200	-1.08655400
H	1.68543700	1.52811000	-1.49159200
C	-6.59549600	-1.31921900	1.85845800
H	-7.00003900	-1.62405800	2.81895300
C	-7.42926000	-1.07741700	0.77503300
H	-8.50437800	-1.18454300	0.88952200
C	-1.25648300	-0.62450300	3.79353500
H	-1.27998600	0.42673500	3.48537100
H	-1.94830300	-0.72347000	4.63946800
C	1.45304500	-0.04944000	-0.03111800
C	-0.19905400	-3.37666500	3.44821700
H	-0.16598500	-4.43735700	3.72733400
H	0.50666600	-3.24940300	2.61456400
C	-6.89136200	-0.71392700	-0.47028300
H	-7.55651900	-0.55030500	-1.31398900
C	0.23723100	-2.49837300	4.62024900
H	1.25949600	-2.75312800	4.92707400
H	-0.41164900	-2.70160800	5.48537600
C	-4.46971900	-1.81356100	3.91860300
H	-5.24377000	-1.16881000	4.34632500
H	-3.58012100	-1.71955900	4.53339900
H	-4.81808500	-2.85237600	3.94532400
C	0.14739100	-1.01786300	4.25402800
H	0.45322100	-0.38979900	5.10004000
H	0.85411600	-0.81613800	3.43700000
H	1.57738000	-1.73929600	1.31456300
H	3.78614100	0.63627800	-2.44089300
O	5.03244400	-1.56841600	-1.61880500
S	6.44437000	-0.84399100	-1.28422700
O	7.42460800	-1.52499900	-2.10280400
O	6.31254600	0.59962800	-1.25045700
C	6.72251300	-1.39526700	0.47250600
F	7.98234600	-1.12403700	0.79142700
F	5.90675500	-0.74360600	1.29370300
F	6.50674000	-2.70188200	0.57406800
C	2.33529100	2.61248100	1.55246400

C	0.09635500	2.81516400	2.15209700
C	1.88540600	3.92880800	1.29696300
C	3.64743300	2.27132000	1.24127600
N	0.54269200	4.02950600	1.66784300
O	-1.10043800	2.53933800	2.41558000
C	2.70858500	4.89889300	0.74050800
C	4.48728800	3.23641300	0.67892500
H	4.00425900	1.25905700	1.40524800
C	-0.28327300	5.19611400	1.50344600
C	4.02296300	4.53090500	0.43181400
H	2.34960800	5.90652200	0.55051000
H	5.50543000	2.96796100	0.41313200
H	0.04266300	6.00169900	2.17232100
H	-0.24583200	5.55863000	0.47078600
H	-1.30883200	4.91707400	1.75236000
H	4.68957600	5.26661800	-0.01055100
C	1.20430200	1.85661700	2.08434300
H	1.33841500	1.15207900	2.90081500
C	-1.53150300	-1.69214300	-1.57299300
C	-0.95950800	-2.76754400	-0.62907400
C	-2.79329900	-2.27484800	-2.23404500
C	-0.47788100	-1.37207800	-2.64667200
H	-1.70820700	-3.00586900	0.13397200
H	-0.07373500	-2.37761000	-0.11947700
C	-0.59384200	-4.03564100	-1.40790600
H	-3.24836500	-1.54694000	-2.91074100
H	-3.53588200	-2.51379100	-1.46371400
C	-2.43180100	-3.54197600	-3.02582000
H	0.42172000	-0.96613800	-2.17587200
H	-0.85280800	-0.61177000	-3.34040700
C	-0.12762400	-2.64377100	-3.43162300
H	-0.18215300	-4.77338300	-0.70658200
C	-1.85267900	-4.59704000	-2.07705100
C	0.45215200	-3.69057300	-2.47357900
H	-3.34182800	-3.93031300	-3.50131000
C	-1.39249300	-3.19621200	-4.09990300
H	0.61764200	-2.39015700	-4.19631200
H	-2.59669200	-4.86592100	-1.31450700

H	-1.61110000	-5.51338700	-2.63302900
H	1.35962700	-3.29743700	-1.99663000
H	0.73909500	-4.59391200	-3.02908500
H	-1.14862000	-4.09109300	-4.68870100
H	-1.80418400	-2.45329000	-4.79750400
C	-2.42802800	1.29688600	-1.52160100
C	-1.14649600	2.08461600	-1.89318500
C	-3.17234400	1.02207400	-2.84094200
C	-3.28532900	2.19243600	-0.60536000
H	-0.49597900	1.46942700	-2.52558900
H	-0.57666200	2.31088000	-0.98155100
C	-1.49413400	3.39661900	-2.60790000
H	-4.08188700	0.44599400	-2.67680500
H	-2.54115500	0.43228300	-3.51316800
C	-3.54695800	2.33951000	-3.53693400
H	-2.73566000	2.40442900	0.32162400
H	-4.20543200	1.67458200	-0.31958400
C	-3.63670300	3.50261900	-1.32223000
H	-0.55897500	3.92101800	-2.84410100
C	-2.26952800	3.10324200	-3.89459300
C	-2.35313200	4.25901800	-1.67787000
H	-4.10625000	2.10053500	-4.45084400
C	-4.41854500	3.18672100	-2.60248900
H	-4.25413600	4.11335000	-0.65121900
H	-1.65369200	2.50655000	-4.58171500
H	-2.51704400	4.04064800	-4.41123200
H	-1.79444700	4.48865700	-0.76331100
H	-2.59580500	5.21446100	-2.16314100
H	-4.71366200	4.11737000	-3.10623800
H	-5.34189700	2.64567100	-2.35407800

8R-TS

Charge: 0 Multiplicity: 1

Pd	-0.24832400	1.09499200	0.45015400
P	-1.92623900	-0.34074500	-0.39974600
C	-3.35134900	-0.64353600	0.69535000
C	2.20309900	-0.29421700	1.36337400
C	-4.57479800	-1.39467700	0.45463300

N	-4.48737500	-0.84121500	2.65024800
C	-3.35357600	-0.31745600	2.05889600
C	-2.33934700	0.44838500	2.85000100
H	-1.62796500	0.83875900	2.10156100
C	-5.24972000	-1.48491400	1.69992700
C	-5.19000200	-2.01129900	-0.64889600
H	-4.74187200	-1.96865200	-1.63058300
C	3.22361200	-0.38384300	-1.24137400
C	-1.48514800	-0.44357800	3.76789200
H	-2.09784700	-0.92897800	4.53934100
H	-1.04852100	-1.24782000	3.16400500
C	3.15095300	-1.25773800	1.02571900
H	3.50713300	-1.97409500	1.75913700
C	3.64605500	-1.28812800	-0.26987800
C	2.29015600	0.57711300	-0.89454400
H	1.98292500	1.30984700	-1.63406700
C	-6.47624700	-2.13257800	1.86581000
H	-6.97284800	-2.16305100	2.83098600
C	-7.04691100	-2.73070300	0.75105200
H	-8.00014600	-3.24383700	0.84416700
C	-2.89429500	1.69195300	3.56612200
H	-3.38794600	2.33232000	2.82541800
H	-3.65586000	1.42143400	4.30624400
C	1.73245600	0.62076900	0.40380400
C	-0.38685000	0.37598400	4.44105200
H	0.20546900	-0.26375000	5.10792400
H	0.29597400	0.75034300	3.66452500
C	-6.40328000	-2.66887100	-0.49483900
H	-6.86452600	-3.13728100	-1.36027700
C	-0.96645600	1.56757800	5.20098100
H	-0.16105000	2.14358100	5.67447400
H	-1.61057600	1.20001200	6.01476700
C	-4.90360600	-0.77913100	4.03474100
H	-5.67481500	-0.01479100	4.18522700
H	-4.05758700	-0.56245000	4.68057400
H	-5.30826100	-1.75233500	4.32758400
C	-1.77462700	2.46417800	4.26423600
H	-2.20282300	3.30917000	4.81883200

H	-1.11417000	2.88555200	3.49746600
H	1.81713600	-0.26317100	2.37737800
H	3.63255000	-0.43140600	-2.24475900
O	4.58254000	-2.29195000	-0.60174900
S	6.14700700	-1.87810300	-0.74447600
O	6.80590000	-3.05055700	-1.27938500
O	6.29908300	-0.55475200	-1.31774000
C	6.64232500	-1.74170100	1.04576400
F	7.96866200	-1.72836400	1.10430900
F	6.16411300	-0.61779000	1.56842600
F	6.17511900	-2.78353400	1.72433100
C	2.74391200	2.97113200	0.51238400
C	0.45075100	3.38729900	0.79955800
C	2.32950500	4.00582500	-0.34224800
C	4.08206000	2.60742900	0.55967900
N	0.95307100	4.19434500	-0.21091500
O	-0.64777900	3.57096500	1.33794600
C	3.22510900	4.69085300	-1.15452500
C	4.99919000	3.29608700	-0.23843500
H	4.40415900	1.77816000	1.18292700
C	0.22023000	5.29959100	-0.77281500
C	4.57172700	4.31975800	-1.08684200
H	2.89559500	5.48784900	-1.81431800
H	6.04894100	3.01912100	-0.21141800
H	0.61918900	6.25727800	-0.41549000
H	0.26979500	5.27852900	-1.86604200
H	-0.81912800	5.20769500	-0.45477700
H	5.29532400	4.83893000	-1.70961200
C	1.53757600	2.37205500	1.14613600
H	1.58707700	2.16115300	2.21272200
C	-1.30435900	-2.06022000	-0.89937500
C	-1.34852400	-2.92633000	0.37537100
C	-2.07217700	-2.77724700	-2.01882100
C	0.17056700	-1.93301000	-1.32022100
H	-2.38314900	-3.04288400	0.71567500
H	-0.79680800	-2.41808800	1.17846500
C	-0.73361100	-4.30664100	0.10573400
H	-2.04279000	-2.18238300	-2.93939500

H	-3.11824900	-2.90727000	-1.73769400
C	-1.45931200	-4.16146300	-2.28668500
H	0.72564100	-1.45221800	-0.51499600
H	0.26851900	-1.28942600	-2.20081600
C	0.78376700	-3.30823100	-1.60721400
H	-0.78738300	-4.90178300	1.02691800
C	-1.52852000	-5.00249000	-1.00613100
C	0.72744400	-4.15107300	-0.32973300
H	-2.03636900	-4.65162400	-3.08199300
C	0.00039000	-4.00433800	-2.72344500
H	1.82847400	-3.16734600	-1.91095400
H	-2.57510400	-5.12989700	-0.69685700
H	-1.11961300	-6.00531700	-1.19146600
H	1.30863900	-3.66050600	0.46247700
H	1.17915700	-5.13765200	-0.50253100
H	0.43928500	-4.98764200	-2.94204700
H	0.05503300	-3.41284700	-3.64834700
C	-2.54510500	0.68472400	-1.85596200
C	-1.38205100	0.83671800	-2.85403300
C	-3.79581700	0.20903700	-2.60725100
C	-2.86697000	2.07250600	-1.25751100
H	-1.14388800	-0.13374600	-3.30535600
H	-0.48536200	1.17396500	-2.31522500
C	-1.74895300	1.83489300	-3.95815000
H	-4.63622300	0.13981000	-1.91029100
H	-3.63463200	-0.78415800	-3.03898300
C	-4.15678600	1.19670700	-3.72983400
H	-1.99666400	2.44915300	-0.70151100
H	-3.68847200	1.98001100	-0.53505000
C	-3.23294800	3.06945900	-2.36265100
H	-0.90251900	1.92429200	-4.65177800
C	-2.98434600	1.32425600	-4.70872400
C	-2.05001100	3.20000500	-3.32961800
H	-5.04142800	0.81753400	-4.25781900
C	-4.46630400	2.56802300	-3.12061400
H	-3.44684400	4.04310600	-1.90287500
H	-2.76744300	0.34975300	-5.16826600
H	-3.24618300	2.01419500	-5.52272700

H	-1.16466400	3.56012300	-2.78853600
H	-2.27852700	3.93634900	-4.11242500
H	-4.74293500	3.28010900	-3.91051600
H	-5.32261200	2.49163000	-2.43686800

8S

Charge: 0 Multiplicity: 1

Pd	0.09209300	0.61635800	0.24375400
P	-1.96552800	-0.38106100	-0.24465400
C	-3.41089200	0.19945300	0.69976300
C	2.40598400	0.37920500	1.54840100
C	-4.79331600	-0.24679700	0.70538000
N	-4.53853500	1.32743500	2.31511000
C	-3.31059900	1.17535800	1.69813700
C	-2.11592700	1.98270000	2.09602000
H	-1.32847900	1.68989100	1.37036000
C	-5.45570500	0.48279000	1.72741700
C	-5.56136600	-1.16782300	-0.02652700
H	-5.12363100	-1.73086900	-0.83856600
C	2.49234800	-0.79438500	-1.00143700
C	-1.54036300	1.61573700	3.47304600
H	-2.24525800	1.85356100	4.28061200
H	-1.37391600	0.53239200	3.50802100
C	2.78167300	-0.95065100	1.41086300
H	3.01516200	-1.56174400	2.27603700
C	2.85835500	-1.49863400	0.12790100
C	2.08940500	0.54825300	-0.86409400
H	1.96550600	1.14416000	-1.76413800
C	-6.81083000	0.32493000	2.02692500
H	-7.29016800	0.91028800	2.80604000
C	-7.53140300	-0.60268900	1.28658000
H	-8.58781600	-0.75150300	1.49310300
C	-2.28303600	3.49874800	1.90565500
H	-2.61702400	3.69312600	0.87981700
H	-3.05460200	3.90277900	2.57271900
C	2.13381300	1.19841600	0.41061400
C	-0.22841600	2.35992200	3.71092200
H	0.17074600	2.11658700	4.70396600

H	0.50206400	1.99956000	2.97349600
C	-6.90750800	-1.34003600	0.26738800
H	-7.48913700	-2.05381400	-0.31006500
C	-0.39798100	3.86997100	3.55015900
H	0.56259600	4.37848700	3.70642000
H	-1.07907600	4.24381700	4.32984700
C	-4.91413500	2.22774900	3.38285800
H	-5.51386600	3.06271200	3.00162700
H	-4.03217400	2.62415500	3.87713300
H	-5.50117400	1.68159100	4.12788400
C	-0.96144600	4.21692000	2.17246500
H	-1.10049500	5.30140900	2.07715000
H	-0.24948000	3.91939100	1.39318200
H	2.40638400	0.83359900	2.53546200
H	2.51568900	-1.26671100	-1.97669900
O	3.21411700	-2.86154800	0.02802400
S	4.67465000	-3.26295200	-0.55178100
O	4.64821100	-4.70444800	-0.67940000
O	5.08252700	-2.38262500	-1.62929100
C	5.75195500	-2.85787700	0.91115800
F	6.95117900	-3.38767100	0.69960500
F	5.86349300	-1.54176300	1.04349300
F	5.22347600	-3.37515000	2.01464400
C	3.80067900	3.08476600	0.40331900
C	1.68859400	3.50408200	-0.60528700
C	3.92893300	4.00512100	-0.64568400
C	4.92111200	2.66569400	1.09746000
N	2.67334800	4.24545300	-1.21578700
O	0.50842900	3.51240900	-0.91979100
C	5.15696900	4.53945200	-1.00987300
C	6.17133600	3.19183800	0.74582000
H	4.83441900	1.93102700	1.89342800
C	2.43090900	5.12795600	-2.32892300
C	6.28148900	4.11700400	-0.29117500
H	5.24785500	5.25272800	-1.82335000
H	7.06031100	2.87248700	1.28206600
H	2.72090600	6.15448500	-2.07874700
H	2.99312700	4.80060600	-3.21077400

H	1.36263100	5.09735300	-2.54961000
H	7.25726100	4.51584500	-0.55500100
C	2.34661200	2.69459100	0.52077100
H	1.91888000	3.04788600	1.46852800
C	-1.82504400	-2.24354900	0.05820900
C	-2.10707300	-2.46514400	1.55737500
C	-2.72362400	-3.17756200	-0.76475700
C	-0.35478200	-2.63213200	-0.20373000
H	-3.14528700	-2.19937700	1.78636700
H	-1.46325300	-1.79906000	2.14942100
C	-1.84805200	-3.92821800	1.94090200
H	-2.53109200	-3.04348400	-1.83569200
H	-3.77557900	-2.94884000	-0.58600500
C	-2.46837200	-4.64390500	-0.37865700
H	0.29147800	-1.97146800	0.38598300
H	-0.09568700	-2.46160900	-1.25457100
C	-0.09504800	-4.09571200	0.16773600
H	-2.06547500	-4.05785700	3.00945400
C	-2.76784200	-4.83508900	1.11338000
C	-0.38516300	-4.28891400	1.65940500
H	-3.13302200	-5.28429500	-0.97369900
C	-1.00722600	-5.00610300	-0.66034700
H	0.95577400	-4.32973400	-0.03924900
H	-3.81925900	-4.59160600	1.31992100
H	-2.61596300	-5.88605900	1.39597600
H	0.28251300	-3.64938600	2.25340300
H	-0.18767300	-5.32872600	1.95501800
H	-0.82251400	-6.06004500	-0.41015400
H	-0.78812600	-4.88492900	-1.73057900
C	-2.31547800	0.05300000	-2.03912800
C	-1.19459900	-0.53057400	-2.91816700
C	-3.67578700	-0.35502200	-2.62048000
C	-2.22236200	1.59437200	-2.08437700
H	-1.24386200	-1.62640100	-2.91519400
H	-0.22101800	-0.24846200	-2.49736700
C	-1.32483600	-0.02136300	-4.35875100
H	-4.47919400	0.07964400	-2.01740800
H	-3.79496200	-1.44370400	-2.59744600

C	-3.80610600	0.14044700	-4.07060100
H	-1.26512400	1.92160700	-1.65750300
H	-3.01582900	2.02397200	-1.45814100
C	-2.35628500	2.10141900	-3.52429800
H	-0.51523300	-0.45189200	-4.96320800
C	-2.68189700	-0.45609400	-4.92557700
C	-1.22537300	1.50858300	-4.37319900
H	-4.78028200	-0.17726100	-4.46515700
C	-3.71069500	1.66997500	-4.09765800
H	-2.28224700	3.19669800	-3.52205400
H	-2.75221300	-1.55301500	-4.92996100
H	-2.78260700	-0.12177800	-5.96752700
H	-0.25323100	1.82618600	-3.97191900
H	-1.28966800	1.88087800	-5.40528400
H	-3.82316600	2.03747400	-5.12741500
H	-4.52609200	2.10761300	-3.50546900

$(KCl)_4$

Charge: 0 Multiplicity: 1

K	0.01524500	-1.52627100	2.10297200
K	0.20729600	-1.46647900	-2.13536100
K	2.00321400	1.65237400	0.11420900
K	-2.22580500	1.34051000	-0.08180600
Cl	-2.09568500	-1.72895700	-0.11930300
Cl	-0.21663600	1.53362500	2.23428900
Cl	-0.01602000	1.59721800	-2.20023000
Cl	2.32839700	-1.40203600	0.08522900

KOTf

Charge: 0 Multiplicity: 1

O	1.24617000	1.96204200	-0.00007100
S	0.24418300	0.89878200	-0.00000400
O	-0.58198500	0.75307900	-1.22902100
C	1.20033100	-0.67947600	0.00000000
F	0.32985300	-1.71912500	-0.00003500
F	1.96891200	-0.79163700	-1.08341800
F	1.96884700	-0.79164600	1.08346000
O	-0.58187800	0.75314100	1.22909100

K	-2.64083600	-0.43832000	0.00000000

S1

Charge: 0 Multiplicity: 1

C	2.58736000	1.20405800	0.28281100
C	1.03960900	-0.75280700	-0.98655500
C	1.26612400	1.48104900	-0.05345500
H	0.82678200	2.44703200	0.16746500
C	0.51424400	0.49471900	-0.67751200
C	2.36295100	-1.02712800	-0.65750600
H	2.79864700	-1.99259400	-0.89061800
C	3.12151900	-0.04586600	-0.02279900
H	3.19639000	1.95538100	0.77348600
H	0.42061400	-1.49466800	-1.47950500
Cl	4.78004700	-0.38902500	0.39493500
O	-0.80128900	0.76778400	-1.08726200
S	-1.99201000	0.83527200	0.02603200
O	-1.50000300	1.36045200	1.28418000
O	-3.13121000	1.38572400	-0.67340200
C	-2.31428200	-0.98455300	0.27714200
F	-3.44953100	-1.11462000	0.94885800
F	-2.41524900	-1.58534500	-0.90205500
F	-1.31702200	-1.52165600	0.96851600

S2 ok

Charge: 0 Multiplicity: 1

C	-0.87247300	-0.81220200	0.41943300
C	-1.13304700	0.53172100	0.00322600
C	-2.37416100	0.93892000	-0.46978500
C	-3.40356200	-0.00864900	-0.52605000
C	-3.17819100	-1.32595800	-0.11016100
C	-1.92737100	-1.73310900	0.36044700
C	1.05717700	0.42566200	0.67013400
H	-2.54436900	1.96660500	-0.78248700
H	-4.38454000	0.28577000	-0.89079100
H	-3.99178800	-2.04715100	-0.15354100
H	-1.77366200	-2.76247700	0.67988300
N	0.03121100	1.25351600	0.16025000

C	0.22603500	2.63379700	-0.17429800
H	0.04922400	2.82131700	-1.24265800
H	-0.43877000	3.28642600	0.40623800
H	1.26396900	2.87658400	0.06733200
O	2.23751900	0.85858500	0.84032400
C	0.50152200	-0.87027300	0.80917100
H	0.97878600	-1.68013900	1.35298100
K	3.12352300	-1.00366700	-0.69336900

PPh-1

Charge: 0 Multiplicity: 1

P	-0.61480300	-0.78307900	-0.08005200
C	0.06671200	0.86401800	0.20120400
C	-1.81445800	-1.02301600	1.28552300
C	-1.67329700	-0.49154900	-1.55792600
C	-0.68616500	2.09584800	0.27543400
C	1.41772100	1.21203900	0.20852700
C	-1.84822900	-0.18919000	2.40756400
C	-2.66673000	-2.13727300	1.24020500
C	-1.01402700	-0.33361300	-2.78444800
C	-3.06804300	-0.40705900	-1.52246900
C	0.26120300	3.14652300	0.35041700
C	-2.05126500	2.41515300	0.29641500
N	1.52456100	2.58494900	0.31896400
C	2.58852500	0.28882000	0.12742900
C	-2.73037900	-0.45293500	3.45541000
H	-1.18569000	0.66863800	2.46051100
C	-3.55718200	-2.38899600	2.27879700
H	-2.62373400	-2.80939900	0.38600700
C	-1.73311700	-0.07920000	-3.94747500
H	0.07026400	-0.41537000	-2.81965600
C	-3.78930400	-0.16370400	-2.69144700
H	-3.59663000	-0.52816500	-0.58175400
C	-0.11178200	4.48909400	0.43736500
H	-2.80064100	1.63350100	0.24796200
C	-2.43000500	3.74860000	0.38308200
C	2.72578700	3.38848100	0.35765000
H	2.12051900	-0.70450300	-0.02245600

C	3.39066400	0.15304800	1.43113000
C	3.49725600	0.49098000	-1.09405400
C	-3.59119300	-1.54626500	3.39197500
H	-2.74563900	0.20419800	4.32129100
H	-4.21797400	-3.25057000	2.22593700
C	-3.12604600	0.00415600	-3.90472400
H	-1.20763300	0.04589200	-4.89088700
H	-4.87378700	-0.09997000	-2.64898800
H	0.62789400	5.28311800	0.48469900
C	-1.47207700	4.77542700	0.45274100
H	-3.48631000	4.00394500	0.39662000
H	2.89478500	3.89153100	-0.60175100
H	3.58773500	2.76782100	0.58877300
H	2.63261600	4.14533700	1.14278700
H	3.93257700	1.07937200	1.66687400
H	2.69764100	-0.02924200	2.26107500
C	4.38840100	-0.99850200	1.30742400
H	2.88077200	0.54522900	-1.99953900
H	4.05008700	1.43743600	-1.03027400
C	4.49097700	-0.66661300	-1.19518000
H	-4.28080600	-1.74748700	4.20758900
H	-3.68976500	0.19580700	-4.81399200
H	-1.79860500	5.80993200	0.51761700
H	4.98368800	-1.08336400	2.22525400
H	3.82601700	-1.93935800	1.20573400
C	5.30046500	-0.82290900	0.09273900
H	5.15965700	-0.51706500	-2.05226800
H	3.93152300	-1.59501700	-1.38672100
H	5.98778100	-1.67412000	0.00808900
H	5.92502300	0.07180800	0.23683800
Pd	0.76439700	-2.47753400	-0.22754800

PPh-2

Charge: 0 Multiplicity: 1

P	-0.54969300	-0.80259000	0.22282600
C	-0.05657300	0.93064800	0.07567500
C	-2.25485400	-0.67146700	0.88477700
C	-0.81954400	-1.33663400	-1.51159400

C	-0.88840000	2.09969800	-0.11278200
C	1.26913100	1.35569800	-0.00157200
C	-2.42256000	-0.09954500	2.15367200
C	-3.37680200	-1.12551200	0.18545100
C	-0.76206600	-2.70365200	-1.80746100
C	-1.09617300	-0.42420900	-2.53656500
C	-0.00290200	3.19880100	-0.27213000
C	-2.27069200	2.34178400	-0.18645600
N	1.29198400	2.71906400	-0.21748600
C	2.49009300	0.50305800	0.12022000
C	-3.69342900	0.04225100	2.69898600
H	-1.55021700	0.24699300	2.70294500
C	-4.65002600	-0.99343000	0.74112600
H	-3.26065000	-1.56659400	-0.79986100
C	-0.99182000	-3.15509300	-3.10531400
H	-0.52759100	-3.40478100	-1.00850500
C	-1.31581000	-0.87644600	-3.83603900
H	-1.13978600	0.63806300	-2.31582000
C	-0.45115700	4.50795600	-0.45978300
H	-2.98112900	1.52956900	-0.09199700
C	-2.72085800	3.64058600	-0.38465900
C	2.44663700	3.57879800	-0.34919800
H	2.08869600	-0.48489400	0.41387200
C	3.44874300	0.89154600	1.25614100
C	3.22995800	0.26177800	-1.20547100
C	-4.81304700	-0.40422800	1.99306700
H	-3.81279500	0.50157300	3.67690900
H	-5.51655800	-1.34602200	0.18727100
C	-1.26659900	-2.24093600	-4.12239000
H	-0.94584100	-4.21877900	-3.32471000
H	-1.52660000	-0.16090900	-4.62682200
H	0.24370300	5.33694600	-0.55803000
C	-1.82396200	4.71514100	-0.51326300
H	-3.78989400	3.82923700	-0.43835100
H	2.26082500	4.31433900	-1.13731600
H	3.31856800	2.99461300	-0.63492900
H	2.66025000	4.10787900	0.58706600
H	3.94292400	1.85061800	1.05541600

H	2.87720700	1.01487600	2.18420800
C	4.51398100	-0.19223200	1.42601700
H	2.50855600	-0.05156600	-1.96922700
H	3.69642200	1.18770000	-1.57085600
C	4.30446000	-0.80885800	-1.01500800
H	-5.80642700	-0.29553200	2.42038300
H	-1.43640500	-2.59046900	-5.13756800
H	-2.20729000	5.72174000	-0.65772400
H	5.21473600	0.08868700	2.22240100
H	4.02297700	-1.12324700	1.74795200
C	5.26487600	-0.44595200	0.11821700
H	4.85614800	-0.96047300	-1.95135300
H	3.81036100	-1.76315500	-0.77941400
H	6.00755500	-1.24209600	0.25536600
H	5.82408100	0.46102700	-0.15776800
Pd	0.70926200	-2.11189700	1.44531500

PPh-3

Charge: 0 Multiplicity: 1

P	-0.53666500	-0.84429900	0.31256200
C	-0.33501100	0.93977800	0.05195200
C	-2.32190400	-1.11817400	-0.02556300
C	0.25478900	-1.57882400	-1.17791300
C	-1.31272100	1.99638100	-0.06151700
C	0.92170300	1.52771700	-0.04307200
C	-3.18149100	-1.29662000	1.06409700
C	-2.85241700	-1.10260400	-1.32026000
C	0.73411000	-2.89071800	-1.09461500
C	0.38650800	-0.87783700	-2.38233200
C	-0.57398000	3.20122200	-0.23123300
C	-2.71594200	2.07807800	-0.03254600
N	0.77177900	2.89188700	-0.20287800
C	2.23346700	0.81728400	0.08324600
C	-4.55468100	-1.42631300	0.86664200
H	-2.75813400	-1.32225800	2.06635400
C	-4.22397900	-1.24126500	-1.51778800
H	-2.19669500	-0.97319000	-2.17551000
C	1.33034100	-3.49567800	-2.19874100

H	0.64676800	-3.42335800	-0.14947000
C	0.98473900	-1.48313000	-3.48630200
H	0.03146800	0.14691300	-2.44770200
C	-1.18632600	4.44549300	-0.39692000
H	-3.32143200	1.19210800	0.11023200
C	-3.32696500	3.31525700	-0.18619900
C	1.80632400	3.88657000	-0.37223300
H	1.96664700	-0.24569200	0.13804100
C	2.96217900	1.10150000	1.40822300
C	3.17601400	0.94052000	-1.12366100
C	-5.07824300	-1.39577900	-0.42556100
H	-5.21446000	-1.55543200	1.72070600
H	-4.62731900	-1.22381100	-2.52698800
C	1.45895500	-2.79162200	-3.39613400
H	1.70350000	-4.51372900	-2.12176900
H	1.08504400	-0.92959500	-4.41657600
H	-0.60207300	5.34929800	-0.54412400
C	-2.57427800	4.48811000	-0.37105800
H	-4.41200200	3.37638800	-0.16459500
H	1.92777100	4.16198600	-1.42681400
H	2.75362900	3.51022200	0.00711600
H	1.54583500	4.78198600	0.19983200
H	3.30987500	2.14275900	1.45087100
H	2.25604100	0.96252500	2.23629900
C	4.15363700	0.15559400	1.55862000
H	2.62627900	0.70727500	-2.04193700
H	3.54972200	1.96747400	-1.22513200
C	4.35934900	-0.01242200	-0.95654300
H	-6.14872100	-1.50002000	-0.58267300
H	1.93267600	-3.25952700	-4.25522100
H	-3.08271400	5.44058500	-0.49513000
H	4.69488300	0.37549600	2.48768700
H	3.77261000	-0.87263400	1.64801000
C	5.09792700	0.24236400	0.35848300
H	5.04672700	0.08849200	-1.80600000
H	3.98547900	-1.04631300	-0.97326800
H	5.92392900	-0.47073100	0.47439600
H	5.55069100	1.24512900	0.32827600

Pd	0.15149800	-1.57044200	2.25370400

PPh-4

Charge: 0 Multiplicity: 1

P	-0.74073900	-0.75806300	0.39932000
C	-0.24796100	0.92914700	-0.03785900
C	-2.11763400	-1.08509600	-0.77725300
C	0.55099300	-1.86511800	-0.30863100
C	-1.20321000	2.01323700	-0.02494600
C	1.01142400	1.49739200	-0.19629700
C	-3.03194100	-2.09351700	-0.45208500
C	-2.25974300	-0.39853000	-1.98862900
C	1.28632100	-2.68203900	0.55593400
C	0.81542200	-1.90874300	-1.68342200
C	-0.46892400	3.20645900	-0.23468100
C	-2.59255500	2.09045600	0.15477500
N	0.86856800	2.87301700	-0.32053900
C	2.34000800	0.80860300	-0.15283100
C	-4.06325700	-2.42115700	-1.32903000
H	-2.92914900	-2.61089000	0.49989700
C	-3.29742800	-0.72053900	-2.86106300
H	-1.56782200	0.40037300	-2.23886000
C	2.28754500	-3.51590400	0.05916100
H	1.06564200	-2.64537600	1.62109800
C	1.81423900	-2.74154500	-2.17913700
H	0.24317300	-1.28690700	-2.36531800
C	-1.08653200	4.45659800	-0.31776100
H	-3.17626500	1.19365900	0.33667600
C	-3.20873700	3.33392500	0.09398600
C	1.89022800	3.85650800	-0.59952900
H	2.10105900	-0.25207100	-0.05868500
C	3.16182600	1.14162200	1.10612200
C	3.17662600	0.92029600	-1.43847000
C	-4.19919100	-1.73298500	-2.53475300
H	-4.76697300	-3.20698000	-1.06654500
H	-3.40456000	-0.17486200	-3.79514800
C	2.55445200	-3.54460500	-1.30850900
H	2.85595700	-4.14414200	0.74003000

H	2.01619200	-2.76611500	-3.24686700
H	-0.51766800	5.36274400	-0.50447600
C	-2.46580700	4.50287200	-0.14902800
H	-4.28443700	3.40501400	0.23171400
H	1.92520000	4.10564600	-1.66725100
H	2.86608400	3.49072100	-0.28987500
H	1.67708900	4.76677700	-0.03152600
H	3.47138400	2.19490500	1.11336700
H	2.53118000	0.99289000	1.99104700
C	4.40240900	0.25109700	1.17519600
H	2.56079800	0.61723200	-2.29383800
H	3.48461000	1.95712800	-1.62211000
C	4.41977700	0.03622800	-1.33923400
H	-5.01041700	-1.97985000	-3.21480300
H	3.33338200	-4.19447700	-1.69868000
H	-2.97658900	5.46063800	-0.20344600
H	5.00114400	0.50874800	2.05802400
H	4.08326200	-0.79357700	1.30083600
C	5.24516700	0.36717700	-0.09539600
H	5.03048600	0.14574000	-2.24459300
H	4.10357100	-1.01496100	-1.29410500
H	6.11796600	-0.29513200	-0.03317900
H	5.63457800	1.39328200	-0.17930300
Pd	-1.18954000	-1.03437700	2.51282900

PPh-5

Charge: 0 Multiplicity: 1

P	-0.81945700	-0.79873400	0.35416700
C	-0.30045900	0.92001000	0.11320400
C	-1.58982800	-1.21401500	-1.26072100
C	0.69465600	-1.83814800	0.32137400
C	-1.30397500	1.96022600	0.12602100
C	0.93211600	1.54453700	-0.05670600
C	-2.35516800	-2.38416200	-1.34728900
C	-1.42019000	-0.42142500	-2.39971700
C	1.35341400	-2.08623900	1.53298100
C	1.20635100	-2.38682700	-0.86066100
C	-0.62323200	3.18879600	-0.04208600

C	-2.70142700	1.96351900	0.24125700
N	0.72683700	2.91664300	-0.13674900
C	2.28970900	0.91773900	-0.14057400
C	-2.92586600	-2.76449400	-2.55821900
H	-2.50122100	-2.98844300	-0.45405500
C	-2.00389100	-0.79651600	-3.60956600
H	-0.83361800	0.49032000	-2.33449400
C	2.52449500	-2.83838200	1.55753000
H	0.93572500	-1.68134100	2.45225900
C	2.37127800	-3.15186700	-0.83155600
H	0.70150900	-2.20559100	-1.80462000
C	-1.29396400	4.41291300	-0.09529300
H	-3.24195800	1.02865100	0.36769200
C	-3.37445200	3.17816000	0.19536300
C	1.69772900	3.96950000	-0.33417200
H	2.10649200	-0.15529700	-0.08300400
C	3.20169900	1.23272200	1.05943300
C	2.99953000	1.12882800	-1.49040900
C	-2.75344200	-1.96869300	-3.69233900
H	-3.51506800	-3.67618100	-2.61592400
H	-1.87246900	-0.17014400	-4.48836000
C	3.03658200	-3.37317400	0.37399900
H	3.03232800	-3.01743700	2.50165500
H	2.76044000	-3.57471700	-1.75420200
H	-0.76150600	5.34944200	-0.23356000
C	-2.67889400	4.38911000	0.02793700
H	-4.45747700	3.19423100	0.28547600
H	1.60563200	4.40256300	-1.33748700
H	2.70691300	3.58795300	-0.21033400
H	1.53935100	4.75956000	0.40744100
H	3.43827200	2.30306000	1.11131100
H	2.66534800	0.98757400	1.98412300
C	4.50170600	0.43409300	0.96941300
H	2.32553300	0.81869600	-2.29855600
H	3.22826700	2.18794800	-1.66225600
C	4.29699500	0.32193000	-1.54016200
H	-3.20902600	-2.25884000	-4.63561800
H	3.94577500	-3.96820200	0.39335200

H	-3.23260200	5.32356400	-0.00998000
H	5.16071600	0.69758200	1.80650800
H	4.26847300	-0.63459800	1.07066200
C	5.21188500	0.66478600	-0.36443500
H	4.81199000	0.49953200	-2.49288500
H	4.05228700	-0.74888100	-1.50360500
H	6.13077800	0.06678400	-0.41234000
H	5.51881900	1.71938300	-0.43761600
Pd	-2.08838800	-1.10413500	2.10142400

PPh-6

Charge: 0 Multiplicity: 1

P	-0.74293100	-0.96233800	0.02108800
C	-0.69099400	0.83561500	-0.15833500
C	0.02143000	-1.63551900	-1.50125500
C	0.51457900	-1.29250400	1.32920400
C	-1.87016000	1.66717300	-0.21277400
C	0.40920700	1.69033900	-0.08800700
C	0.15357800	-3.02624700	-1.62934700
C	0.43930500	-0.81400600	-2.55174900
C	0.22150500	-0.82586200	2.61962100
C	1.69737500	-2.00679300	1.12094400
C	-1.42223800	3.01035100	-0.17022600
C	-3.24734700	1.41723400	-0.29707100
N	-0.04192500	2.99742200	-0.08297900
C	1.85848700	1.30538600	-0.11805800
C	0.73506500	-3.57702700	-2.76708900
H	-0.20538100	-3.67205600	-0.83078400
C	1.00683200	-1.36801800	-3.69895000
H	0.30851800	0.26040800	-2.47024700
C	1.10000700	-1.05646200	3.67280800
H	-0.70473200	-0.28168100	2.79040300
C	2.57132200	-2.24924600	2.18212700
H	1.94626200	-2.36945700	0.12816900
C	-2.30033900	4.09594600	-0.21449600
H	-3.60475400	0.38775400	-0.32766100
C	-4.12702200	2.49061900	-0.33707200
C	0.73026300	4.21928900	-0.02854800

H	1.85451400	0.21993700	-0.26332800
C	2.62100300	1.54801000	1.19666800
C	2.62197500	1.88052400	-1.32632000
C	1.16541800	-2.74810300	-3.80547600
H	0.84175100	-4.65557500	-2.85053800
H	1.32492700	-0.71753900	-4.50982600
C	2.27996500	-1.77281900	3.45784600
H	0.86107700	-0.68336400	4.66550800
H	3.48749800	-2.80693700	2.00428700
H	-1.94025400	5.12045300	-0.19322500
C	-3.65944900	3.81697700	-0.29711800
H	-5.19596600	2.30502200	-0.40471500
H	0.78489900	4.69811200	-1.01325000
H	1.73799200	4.01686000	0.32482400
H	0.25909900	4.91196100	0.67556000
H	2.66869200	2.62111200	1.42522800
H	2.07898400	1.07193100	2.01943500
C	4.04063200	0.98787600	1.10567200
H	2.06949000	1.66311000	-2.24736900
H	2.69753700	2.97220300	-1.25618700
C	4.02931600	1.29004300	-1.39592600
H	1.61085600	-3.17953600	-4.69804700
H	2.96351900	-1.96086300	4.28146600
H	-4.37067400	4.63785700	-0.33606900
H	4.58378600	1.20026900	2.03513200
H	3.98070900	-0.10497700	1.02116200
C	4.79781100	1.54472800	-0.09914400
H	4.56975800	1.71237700	-2.25256200
H	3.95496800	0.20680700	-1.57084500
H	5.79944600	1.10003800	-0.15660700
H	4.94181500	2.62854600	0.02743300
Pd	-2.65330500	-1.83510200	0.61564400

PPh-7

Charge: 0 Multiplicity: 1

P	-0.70654500	-0.99214400	0.07945800
C	-0.71621400	0.80814600	-0.07809200
C	0.34056400	-1.60574000	-1.29743900

C	0.31021800	-1.22405500	1.59719900
C	-1.90769100	1.62048300	-0.11759200
C	0.37297500	1.67064200	-0.19023600
C	0.80426400	-2.93031500	-1.27079400
C	0.58056800	-0.83044900	-2.43680700
C	-0.28031100	-0.81965300	2.80354700
C	1.61313100	-1.72929000	1.61881800
C	-1.47716300	2.96540400	-0.24158000
C	-3.28313400	1.35485000	-0.05758600
N	-0.09384600	2.96993000	-0.26749400
C	1.82402500	1.29731900	-0.16866200
C	1.54082000	-3.44307300	-2.33425300
H	0.57843500	-3.56225200	-0.41540500
C	1.30469500	-1.35102700	-3.50827800
H	0.19364500	0.18286700	-2.48221200
C	0.42465600	-0.90060400	3.99966000
H	-1.29820200	-0.43589200	2.79580200
C	2.31324600	-1.82556900	2.82213900
H	2.09432700	-2.03752700	0.69600300
C	-2.37383800	4.03379400	-0.32249300
H	-3.62383400	0.32328400	0.04383200
C	-4.17982000	2.41168100	-0.13128800
C	0.66988700	4.19306500	-0.38306500
H	1.83157000	0.20393200	-0.23057000
C	2.52000900	1.64255600	1.16184100
C	2.63918600	1.78199700	-1.38015300
C	1.79839000	-2.65316700	-3.45619800
H	1.90497000	-4.46644700	-2.29227900
H	1.48360100	-0.73414200	-4.38536600
C	1.72600600	-1.40735800	4.01360700
H	-0.04445800	-0.57506800	4.92463600
H	3.32587100	-2.22096600	2.82234900
H	-2.03108200	5.05834600	-0.43416400
C	-3.73058500	3.73844100	-0.26358900
H	-5.24769600	2.21298900	-0.08795700
H	0.73776400	4.52640100	-1.42525100
H	1.67330500	4.05514700	0.01360500
H	0.18249900	4.97424200	0.20686600

H	2.54566200	2.72992800	1.31358900
H	1.93855900	1.22046700	1.98881800
C	3.94642200	1.09388100	1.18101600
H	2.13304300	1.48471200	-2.30482900
H	2.70811100	2.87592300	-1.39487400
C	4.05039200	1.19854000	-1.33557500
H	2.36841100	-3.05634000	-4.28897000
H	2.27515700	-1.47845300	4.94872300
H	-4.45478900	4.54662000	-0.32349700
H	4.44415900	1.38476700	2.11464900
H	3.90076100	-0.00336400	1.17948200
C	4.75516900	1.56187200	-0.02845400
H	4.62982300	1.55534700	-2.19643300
H	3.98885400	0.10439100	-1.42742000
H	5.76136200	1.12457400	-0.00338100
H	4.88552600	2.65366700	0.01908800
Pd	-2.63359700	-2.01019000	0.00286100

PPh-8

Charge: 0 Multiplicity: 1

P	-0.82761700	-0.84381700	-0.21439500
C	-0.49924000	0.92567100	-0.02815000
C	0.71738300	-1.58520800	-0.88406900
C	-0.87054000	-1.47933100	1.50509300
C	-1.57958600	1.88626800	-0.01988500
C	0.68916900	1.64850300	0.06981000
C	1.51663600	-2.47339800	-0.15606600
C	1.06692500	-1.28240700	-2.20847800
C	-1.35195600	-2.77672600	1.72647600
C	-0.43222600	-0.71869800	2.59256100
C	-0.98593500	3.16728200	0.07743800
C	-2.97750300	1.79027500	-0.07553100
N	0.38400900	2.99892500	0.13288500
C	2.08605900	1.11478800	0.15085800
C	2.64829900	-3.04287900	-0.74067700
H	1.26229600	-2.71448800	0.87131200
C	2.20445800	-1.83893300	-2.78311200
H	0.43548000	-0.60977900	-2.78449400

C	-1.36548900	-3.31330100	3.01071700
H	-1.71687300	-3.35733000	0.88143400
C	-0.46009000	-1.25140000	3.88087800
H	-0.07969300	0.29482900	2.42604700
C	-1.73884300	4.34366300	0.09929700
H	-3.44949900	0.81155800	-0.14724400
C	-3.73382100	2.95500800	-0.04914500
C	1.28221200	4.13078500	0.18788100
H	1.97157200	0.03074000	0.08766300
C	2.78302600	1.36396500	1.50186100
C	2.98355400	1.50124800	-1.03810900
C	2.99808000	-2.72619300	-2.05161600
H	3.25957900	-3.73297100	-0.16456100
H	2.46843500	-1.58894500	-3.80748300
C	-0.92011000	-2.55014100	4.09174600
H	-1.73564700	-4.32268000	3.17118800
H	-0.12285800	-0.64917300	4.72081700
H	-1.26734400	5.32017300	0.16296500
C	-3.12196400	4.21874500	0.03610100
H	-4.81795700	2.89051600	-0.09434400
H	1.25563700	4.69239000	-0.75341500
H	2.30132300	3.80209300	0.36824600
H	0.98725000	4.79681400	1.00563600
H	2.96257600	2.43364700	1.66901900
H	2.12858100	1.02606700	2.31380100
C	4.11617300	0.61714700	1.55019300
H	2.46540300	1.25303200	-1.97125300
H	3.16808800	2.58283300	-1.05736900
C	4.31885700	0.76273600	-0.95997500
H	3.88088000	-3.16935900	-2.50466400
H	-0.94175600	-2.96442400	5.09639400
H	-3.73910600	5.11322100	0.05344500
H	4.62095800	0.81377700	2.50457000
H	3.92025600	-0.46402000	1.51123100
C	5.01733000	1.00614600	0.37795100
H	4.96539800	1.07053300	-1.79168800
H	4.13484800	-0.31292200	-1.08274700
H	5.95905300	0.44449100	0.42175800

H	5.28209000	2.07113400	0.46315700
Pd	-2.52560700	-1.35345000	-1.48843400

PPh-9

Charge: 0 Multiplicity: 1

P	-0.79828800	-0.77809300	-0.39217200
C	-0.25347200	0.91512500	-0.04850000
C	0.64016900	-1.88168400	-0.08570800
C	-1.84615100	-1.15040600	1.07177800
C	-1.23351300	1.97682300	-0.03829200
C	0.99437900	1.51036600	0.10328700
C	1.04022500	-2.24865200	1.20486300
C	1.35689300	-2.36359500	-1.18790300
C	-2.73086300	-2.23267900	0.99241300
C	-1.76974500	-0.41437100	2.25886500
C	-0.52474800	3.18763000	0.14480200
C	-2.63014400	2.01159000	-0.15912700
N	0.81901900	2.88322300	0.23620900
C	2.34007200	0.85353000	0.12701100
C	2.15360900	-3.06592900	1.38752200
H	0.48204300	-1.89409200	2.06615800
C	2.47722800	-3.17066700	-1.00332900
H	1.02459900	-2.09230700	-2.18794000
C	-3.51561800	-2.58326400	2.08755700
H	-2.80121500	-2.79031800	0.06045300
C	-2.56372700	-0.76004100	3.35162300
H	-1.09215200	0.43232000	2.32185200
C	-1.16861400	4.42595300	0.20104900
H	-3.19362500	1.09330600	-0.29802500
C	-3.27607100	3.24038800	-0.10271800
C	1.82376300	3.91382700	0.37259700
H	2.14130400	-0.20201300	-0.06246900
C	3.02623100	0.89200800	1.50489400
C	3.27974300	1.29421600	-1.00962800
C	2.87816600	-3.52253500	0.28571000
H	2.45688200	-3.34627600	2.39295100
H	3.03027800	-3.53397400	-1.86557800
C	-3.43524900	-1.84503600	3.26926300

H	-4.19819200	-3.42631500	2.01637700
H	-2.50281100	-0.17784700	4.26769700
H	-0.61527500	5.35147100	0.33091400
C	-2.55368200	4.43366800	0.07655600
H	-4.35792800	3.28178900	-0.19805100
H	1.97115200	4.44999500	-0.57274100
H	2.77230400	3.48575900	0.68528500
H	1.50761000	4.62931000	1.13835800
H	3.25127600	1.92242200	1.80902100
H	2.33360700	0.49078800	2.25481200
C	4.31992500	0.07823700	1.48624100
H	2.75706700	1.18020100	-1.96725100
H	3.54501700	2.35465600	-0.92041300
C	4.55878800	0.45704900	-0.99425900
H	3.74711600	-4.15875100	0.43173500
H	-4.05597500	-2.11102800	4.12102600
H	-3.08579500	5.38051800	0.11593800
H	4.82224300	0.15289300	2.45925300
H	4.06894900	-0.98058800	1.33710900
C	5.25452200	0.53170000	0.36486700
H	5.23501800	0.79162600	-1.79116900
H	4.30373300	-0.59017400	-1.21056700
H	6.16445200	-0.08173700	0.36000200
H	5.57482000	1.56804900	0.55210700
Pd	-1.75865200	-1.01283400	-2.33448500

PPh-10

Charge: 0 Multiplicity: 1

P	0.55026300	-0.83549200	0.32380000
C	0.31668800	0.93981000	0.03657600
C	-0.32791900	-1.62841000	-1.08715600
C	2.30887100	-1.09971100	-0.14799600
C	1.29202600	2.00066600	-0.04976400
C	-0.93945500	1.52133600	-0.09645200
C	-0.53219800	-0.98262100	-2.31218000
C	-0.78854200	-2.93901100	-0.92091700
C	3.22830200	-1.42266700	0.85506800
C	2.76019000	-0.93889700	-1.46302800

C	0.55501100	3.20104400	-0.25135100
C	2.69256400	2.08603300	0.03411500
N	-0.78999100	2.88637500	-0.25866300
C	-2.25296400	0.81533600	0.04181900
C	-1.18291300	-1.64059900	-3.35409900
H	-0.19771400	0.04310200	-2.44026100
C	-1.43675100	-3.59724300	-1.96373900
H	-0.64432000	-3.42872700	0.04031700
C	4.58305300	-1.55850600	0.55544000
H	2.86571400	-1.55413700	1.87289900
C	4.11198000	-1.07957600	-1.76349400
H	2.05822700	-0.69219000	-2.25313000
C	1.17053800	4.44521500	-0.40751200
H	3.29288700	1.20199700	0.20969700
C	3.30581400	3.32358600	-0.10635000
C	-1.82577200	3.87398900	-0.45933200
H	-1.99188200	-0.24855200	0.08714700
C	-3.21998800	0.94761400	-1.14436500
C	-2.95436300	1.10225400	1.38169800
C	-1.63704700	-2.94815000	-3.18189600
H	-1.34048800	-1.12870200	-4.30015400
H	-1.79397700	-4.61407100	-1.82219200
C	5.02686600	-1.38363400	-0.75430800
H	5.28987100	-1.80245600	1.34432400
H	4.45362100	-0.94657500	-2.78674000
H	0.59093400	5.34665100	-0.58419200
C	2.55660900	4.49166000	-0.33176600
H	4.38890700	3.38909300	-0.04268800
H	-1.54991900	4.79586500	0.06026100
H	-2.76594300	3.52302900	-0.03897400
H	-1.97010700	4.09597600	-1.52360700
H	-3.59245900	1.97582500	-1.23344100
H	-2.69214000	0.71677900	-2.07592500
C	-4.40381200	-0.00071700	-0.95573600
H	-2.23332000	0.95801900	2.19577300
H	-3.29303300	2.14631400	1.43108000
C	-4.14941400	0.16483800	1.55505000
H	-2.15088100	-3.45733000	-3.99308200

H	6.08250900	-1.48914000	-0.99097200
H	3.06644000	5.44459200	-0.44633500
H	-5.10681600	0.10411300	-1.79184200
H	-4.03547100	-1.03638400	-0.98000200
C	-5.11600300	0.25719100	0.37322200
H	-4.67124400	0.38938000	2.49406200
H	-3.77467200	-0.86602600	1.63847300
H	-5.94329800	-0.45171400	0.50459700
H	-5.56405400	1.26228300	0.35190900
Pd	0.03587800	-1.50117900	2.33776900

PPh-11

Charge: 0 Multiplicity: 1

P	-0.52848700	-0.84744700	-0.28825900
C	-0.28398300	0.94236800	-0.12658700
C	-0.08054300	-1.45552900	1.38568800
C	-2.35194400	-1.02706000	-0.33395600
C	-1.22591100	2.02203700	0.06521700
C	0.99210600	1.49705500	-0.08406400
C	-0.20948500	-0.64505000	2.52055700
C	0.41376600	-2.75633400	1.52481600
C	-2.99240000	-0.82477400	-1.56407400
C	-3.11833300	-1.33159300	0.79494600
C	-0.44769200	3.20654300	0.19700700
C	-2.62458700	2.13713300	0.15247900
N	0.88668700	2.85856600	0.11931500
C	2.28087100	0.74901000	-0.21108700
C	0.14699400	-1.13401900	3.77568500
H	-0.58350800	0.36966700	2.41538000
C	0.76956500	-3.24490000	2.78043100
H	0.52839900	-3.37241300	0.63482700
C	-4.37916300	-0.88635200	-1.65460200
H	-2.39190500	-0.60904200	-2.44514700
C	-4.50754700	-1.40900600	0.69844900
H	-2.63429800	-1.49488500	1.75276500
C	-1.01643600	4.46894800	0.37933800
H	-3.26068900	1.26546600	0.07167300
C	-3.19250500	3.38954900	0.34450000

C	1.95334100	3.83033500	0.20221700
H	1.96882900	-0.27773400	-0.46476100
C	3.07639200	0.62936500	1.09925500
C	3.17005300	1.18173000	-1.38754200
C	0.63854600	-2.43347800	3.90702500
H	0.04531700	-0.49832400	4.65163900
H	1.15826100	-4.25535500	2.87803300
C	-5.14109100	-1.17760600	-0.52130400
H	-4.86674700	-0.71323000	-2.61045900
H	-5.09524300	-1.64478800	1.58202600
H	-0.40211500	5.36136900	0.45754400
C	-2.40122100	4.54606700	0.45318300
H	-4.27409600	3.47573900	0.40959300
H	2.07832400	4.36772200	-0.74538100
H	2.88935500	3.33881500	0.45799200
H	1.72534300	4.55250600	0.99172800
H	3.46605700	1.60894100	1.40986500
H	2.40996900	0.28468100	1.89745000
C	4.23964700	-0.34502700	0.91763800
H	2.56465500	1.21319400	-2.30174200
H	3.57147700	2.19153300	-1.23341700
C	4.32905100	0.19731400	-1.54916700
H	0.92431100	-2.81040200	4.88569200
H	-6.22425700	-1.23258400	-0.59218100
H	-2.87658600	5.51301900	0.59509400
H	4.82659700	-0.40708800	1.84274600
H	3.83104800	-1.34946700	0.73421000
C	5.13299100	0.06105200	-0.25528400
H	4.98073300	0.51382700	-2.37347200
H	3.91965800	-0.78589400	-1.82610700
H	5.94206200	-0.66858800	-0.38681600
H	5.61320500	1.02469800	-0.02660600
Pd	0.49703200	-1.81274600	-1.96169700

PPh-12

Charge: 0 Multiplicity: 1

P	-0.57652800	-0.77908900	-0.18796500
C	0.03034200	0.90694200	0.03078500

C	-1.18835900	-1.27062400	1.47190200
C	-2.12636500	-0.50158200	-1.13282900
C	-0.75196200	2.11098500	0.20350500
C	1.37267200	1.28026000	0.08868200
C	-1.42167000	-0.34609000	2.49569300
C	-1.43331500	-2.62967800	1.70966800
C	-2.03960100	0.18318400	-2.35267500
C	-3.37145700	-0.96499200	-0.69720400
C	0.17423600	3.17461200	0.35498600
C	-2.12441600	2.40125400	0.26186100
N	1.44942800	2.64344700	0.29638900
C	2.56049900	0.38405000	-0.03717900
C	-1.90050700	-0.77499500	3.73259600
H	-1.22901700	0.70829000	2.32610200
C	-1.92553700	-3.05483200	2.94107000
H	-1.22547700	-3.34856500	0.91918400
C	-3.18096900	0.41746300	-3.11135300
H	-1.07305400	0.54434900	-2.69589300
C	-4.51350500	-0.73653400	-1.46536200
H	-3.45442500	-1.49086000	0.24922200
C	-0.22611100	4.50018200	0.53558000
H	-2.85991500	1.61111200	0.16133700
C	-2.52806300	3.71680600	0.44923400
C	2.63586100	3.46131700	0.41333100
H	2.11763200	-0.59437400	-0.30723000
C	3.30844800	0.13338100	1.28183300
C	3.51425500	0.71830000	-1.19362100
C	-2.15787700	-2.12686800	3.95680400
H	-2.07419300	-0.04869400	4.52262400
H	-2.11532100	-4.11141100	3.11237500
C	-4.42358400	-0.04230600	-2.66994500
H	-3.10254000	0.96154600	-4.04916500
H	-5.47709500	-1.09726100	-1.11411700
H	0.49763900	5.30415000	0.63399300
C	-1.59125200	4.75697600	0.58051000
H	-3.58938300	3.94698700	0.49179800
H	2.84403400	3.99669900	-0.52057200
H	3.49464400	2.84450800	0.66802700

H	2.49416000	4.19118400	1.21600800
H	3.81378400	1.04483000	1.63121500
H	2.58419600	-0.14423900	2.05703300
C	4.33931800	-0.97927800	1.09186900
H	2.93283700	0.84599200	-2.11494300
H	4.04523300	1.66253900	-1.01809100
C	4.53660600	-0.40633300	-1.36067400
H	-2.53143500	-2.45795900	4.92239500
H	-5.31552400	0.14046200	-3.26345100
H	-1.93793400	5.77762400	0.71889400
H	4.89816500	-1.13922400	2.02253200
H	3.80610300	-1.91734200	0.87632400
C	5.29622900	-0.66815800	-0.05957500
H	5.23561500	-0.16404700	-2.17110400
H	4.00681100	-1.32323300	-1.66144200
H	6.00768600	-1.49261700	-0.19475100
H	5.89164000	0.22181300	0.19518100
Pd	0.75290300	-2.24240600	-1.13012300

PiPr-1

Charge: 0 Multiplicity: 1

Pd	1.87690200	-1.76603400	-0.02971300
P	-0.31244900	-1.43285500	0.00509400
C	-0.90133500	0.28089800	0.15933300
C	-2.26909000	0.76262900	0.07220500
N	-0.86860900	2.53977700	-0.04161500
C	-0.08183700	1.40912500	0.04778000
C	1.41097700	1.45409400	0.05991800
H	1.69868700	0.39121800	0.18973100
C	-2.19926700	2.17770000	-0.02316500
C	-0.94605300	-2.33743200	1.52376700
H	-0.49862900	-3.33310100	1.40602700
C	-3.54297300	0.17238400	0.02045800
H	-3.65994800	-0.90303200	0.05218300
C	2.03491900	2.18407900	1.25859600
H	1.85295100	3.26611600	1.21327200
H	1.56888200	1.82264600	2.18332700
C	-1.28281500	-2.10338900	-1.43270900

H	-2.34816700	-1.93734600	-1.23715000
C	-3.32837000	2.99524700	-0.09955500
H	-3.24111400	4.07688500	-0.14380500
C	-4.57129800	2.37556300	-0.12135000
H	-5.47197400	2.98041100	-0.18249500
C	2.05253900	1.86417400	-1.27430700
H	1.60108800	1.27562100	-2.08175000
H	1.86436700	2.92159700	-1.50646300
C	-0.89522000	-1.34209800	-2.69738300
H	-1.11295700	-0.27298400	-2.60562400
H	-1.45191100	-1.72895200	-3.56035800
H	0.17697600	-1.45550400	-2.90136800
C	3.54269100	1.93014200	1.28754100
H	4.00105100	2.46938100	2.12622100
H	3.71620100	0.85803000	1.46579700
C	-4.67263400	0.97564300	-0.07364700
H	-5.65386500	0.50966600	-0.11025500
C	-0.32749700	-1.68380600	2.75926100
H	0.76546200	-1.64056200	2.67747400
H	-0.58673300	-2.24918500	3.66349300
H	-0.69674700	-0.65857000	2.88307800
C	-2.45160800	-2.50270900	1.69793700
H	-2.92850800	-1.55215800	1.95387800
H	-2.65052900	-3.20092700	2.52173100
H	-2.93951900	-2.90822000	0.80459000
C	4.20345800	2.33349100	-0.03128900
H	5.27948800	2.12060400	0.00273100
H	4.10292500	3.42115100	-0.16725900
C	-1.02388500	-3.60056400	-1.57633500
H	0.04825700	-3.79289300	-1.71111000
H	-1.55669300	-3.99689600	-2.45014300
H	-1.35709800	-4.16491200	-0.69849400
C	-0.44884500	3.92190000	-0.09745100
H	-1.00193600	4.44106000	-0.88655000
H	0.61059300	3.98412400	-0.33009200
H	-0.63358000	4.42806100	0.85749200
C	3.56004100	1.61831700	-1.21960000
H	4.03052200	1.93423800	-2.15930400

H	3.73056400	0.53404900	-1.12714000

PiPr-2

Charge: 0 Multiplicity: 1

Pd	1.67951000	-1.75608500	0.86374800
P	-0.25265100	-1.42830100	-0.15437900
C	-0.94053700	0.25852200	0.01913600
C	-2.30378800	0.75522700	0.07891900
N	-0.89254300	2.52880300	-0.00116300
C	-0.11535900	1.38912000	-0.05184700
C	1.38135400	1.43453200	-0.09105400
H	1.67927600	0.38201500	-0.22638700
C	-2.22242300	2.17507200	0.06211400
C	-1.48400600	-2.66571900	0.53768900
H	-0.84098400	-3.54635300	0.65758300
C	-3.58916000	0.19251300	0.16832900
H	-3.72724900	-0.87729000	0.21714000
C	2.00764800	1.83311700	1.25788800
H	1.80360000	2.88593800	1.49734300
H	1.55015700	1.22804600	2.05013500
C	-0.29965800	-1.77764800	-1.98932900
H	-1.35618700	-1.78476200	-2.28731700
C	-3.34153900	3.00922000	0.10333100
H	-3.24094100	4.09008200	0.07118600
C	-4.59202600	2.41149900	0.17845000
H	-5.48396900	3.03120500	0.21189600
C	2.01636300	2.20367500	-1.25946200
H	1.56197500	1.88794500	-2.20480500
H	1.84152100	3.28316400	-1.17218700
C	0.42246700	-0.69478700	-2.78112200
H	-0.04284900	0.28467900	-2.63805700
H	0.39617300	-0.92942400	-3.85290700
H	1.47425100	-0.62724800	-2.47791800
C	3.51773900	1.60068400	1.21974400
H	3.97287000	1.90800300	2.16989100
H	3.69761200	0.51884400	1.11454500
C	-4.70862700	1.01313500	0.21464300

H	-5.69407900	0.55970200	0.28267500
C	-1.90207600	-2.25018800	1.94896600
H	-1.01488900	-2.06360400	2.56612400
H	-2.48258900	-3.05243400	2.42152100
H	-2.50889100	-1.34121200	1.96162600
C	-2.64080100	-3.09012000	-0.37298100
H	-3.38142300	-3.65737300	0.20537200
H	-2.28935700	-3.74411000	-1.17718800
H	-3.16048700	-2.25755500	-0.85111600
C	4.17273900	2.33398300	0.04923200
H	5.24911900	2.12204900	0.02267500
H	4.06978400	3.41940500	0.20022200
C	0.32341400	-3.14665900	-2.25665400
H	1.38362700	-3.13833100	-1.97478000
H	0.25052900	-3.39776100	-3.32269800
H	-0.15797800	-3.95062900	-1.69015500
C	-0.46040400	3.90868900	-0.01659200
H	-0.54707200	4.34407600	-1.01902300
H	0.57106500	3.98540000	0.31768100
H	-1.07957300	4.48675200	0.67513000
C	3.52439500	1.95018600	-1.28163600
H	3.98754200	2.50645200	-2.10645300
H	3.70522400	0.88281300	-1.47692900

PiPr-3

Charge: 0 Multiplicity: 1

Pd	1.26632900	-2.01105400	1.17709000
P	-0.21625200	-1.36805000	-0.31891100
C	-0.86165800	0.32157400	-0.01757400
C	-2.20282900	0.85406000	0.16070700
N	-0.76561700	2.59075800	-0.12527800
C	-0.02767600	1.42856000	-0.21967000
C	1.47600800	1.40537200	-0.18092200
H	1.74657300	0.36614400	-0.40381000
C	-2.09132200	2.27267800	0.08432400
C	-1.65349700	-2.55413300	-0.10329500
H	-1.16072700	-3.52036100	-0.26534900
C	-3.48699300	0.32943600	0.40493600

H	-3.64978300	-0.73350700	0.49941400
C	1.97896200	1.62889100	1.25981100
H	1.77562000	2.65937700	1.58378400
H	1.42337600	0.96048000	1.92928000
C	0.03764600	-1.52784100	-2.17178900
H	-0.95331600	-1.36893000	-2.61534800
C	-3.18647100	3.13222100	0.20547500
H	-3.07495300	4.20887000	0.12085700
C	-4.43344800	2.57114000	0.43695000
H	-5.30204400	3.21568200	0.54085900
C	2.25883900	2.28031600	-1.17059900
H	1.89339800	2.13238200	-2.19248500
H	2.12889800	3.34389400	-0.94195100
C	0.98729500	-0.50693200	-2.77735700
H	0.62838200	0.51241100	-2.61789500
H	1.05812400	-0.66856300	-3.86052800
H	1.99677700	-0.59792900	-2.36080900
C	3.47592900	1.33593900	1.34956400
H	3.83672000	1.52681600	2.36847600
H	3.62661400	0.26335900	1.15347800
C	-4.57596700	1.17874900	0.54046400
H	-5.55769300	0.75263600	0.73006600
C	-2.10423900	-2.57556800	1.36257000
H	-1.30365300	-2.99406500	1.98377500
H	-2.99600800	-3.20493300	1.47992600
H	-2.32997900	-1.58627500	1.76766600
C	-2.77295500	-2.45099700	-1.14772900
H	-3.66868500	-2.98104900	-0.79927800
H	-2.46812200	-2.92276300	-2.08791800
H	-3.06474000	-1.42436600	-1.38092900
C	4.27788500	2.15283100	0.33676800
H	5.34108200	1.88619600	0.38936800
H	4.20811500	3.22028100	0.59575900
C	0.51674900	-2.94676400	-2.47800700
H	1.46497500	-3.14873700	-1.96457300
H	0.67945300	-3.06266400	-3.55700200
H	-0.19895600	-3.71454800	-2.16852800
C	-0.27525400	3.94886900	-0.21602000

H	-0.07335200	4.23640300	-1.25324500
H	0.63256100	4.07175300	0.37579800
H	-1.02723900	4.62455300	0.19338300
C	3.74978900	1.94963600	-1.08380600
H	4.31285500	2.56987400	-1.79265000
H	3.90692300	0.90329700	-1.38390100

PiPr-4

Charge: 0 Multiplicity: 1

Pd	-2.07101800	-1.46228800	1.52969300
P	-1.02590800	-1.06584400	-0.35493100
C	-0.17361700	0.55258500	-0.28907100
C	-0.99188700	1.73892900	-0.11727900
N	1.16863400	2.32949400	0.15433300
C	1.14096600	0.95692400	-0.06984800
C	2.38179500	0.12221800	-0.01973600
H	2.04173200	-0.88783300	-0.24155200
C	-0.11601000	2.82553600	0.11435400
C	-2.02532600	-1.02710500	-1.97051500
H	-1.73561500	-1.97440100	-2.44336900
C	-2.37358900	1.97863100	-0.08818200
H	-3.07344000	1.15727800	-0.18692900
C	3.01008200	0.03429500	1.38500700
H	3.35739200	1.01733000	1.72564800
H	2.23843900	-0.28379800	2.09677400
C	0.11173900	-2.49009800	-0.81954300
H	-0.66473700	-3.23390800	-1.05471900
C	-0.57041900	4.13619100	0.28234100
H	0.11870700	4.96325300	0.42586800
C	-1.94398300	4.34681700	0.26843500
H	-2.33122300	5.35365900	0.40044000
C	3.42377500	0.44983900	-1.10543800
H	2.93529100	0.43504900	-2.08782200
H	3.82576000	1.46126000	-0.97615000
C	0.95357800	-2.31851800	-2.08535400
H	0.33071200	-2.09627700	-2.95751800
H	1.49430300	-3.24941100	-2.29986800
H	1.69370200	-1.51957000	-2.00813200

C	4.18716600	-0.94221800	1.39669600
H	4.65199700	-0.95167400	2.39048300
H	3.81502700	-1.96071700	1.21535000
C	-2.83712000	3.27432500	0.10149200
H	-3.90753300	3.46146500	0.12351200
C	-3.53255000	-1.11100300	-1.73969700
H	-3.78244700	-1.92570600	-1.05178500
H	-4.04637400	-1.29086700	-2.69361300
H	-3.94010300	-0.18726100	-1.31816800
C	-1.64936200	0.10071000	-2.92739200
H	-2.12927600	-0.06506300	-3.90089500
H	-0.56812200	0.16064000	-3.08771600
H	-1.98060000	1.07360500	-2.55340300
C	5.22001900	-0.59486700	0.32478900
H	6.04179200	-1.32170000	0.34097400
H	5.66342000	0.38693000	0.54970500
C	0.87532300	-3.07272800	0.36928500
H	1.61658500	-2.39119600	0.79217000
H	1.40068100	-3.98738500	0.06506100
H	0.17424300	-3.32305300	1.17373900
C	2.31180800	3.20134800	0.30427400
H	2.53950800	3.72480400	-0.63262300
H	3.18847800	2.64031900	0.61505700
H	2.09894800	3.94327800	1.07978300
C	4.57813000	-0.55113500	-1.06183300
H	5.32478800	-0.29427000	-1.82367400
H	4.19987800	-1.55237800	-1.31557700

PiPr-5

Charge: 0 Multiplicity: 1

Pd	-2.69094400	-1.25739100	1.11386800
P	-0.98476000	-1.11291300	-0.27143600
C	-0.14560800	0.50096100	-0.11534800
C	-0.97325900	1.69326600	-0.07309000
N	1.18824400	2.31700000	0.13409300
C	1.16863300	0.92997200	0.04296500
C	2.41669600	0.10774100	0.11022800
H	2.06538400	-0.92236100	0.06570200

C	-0.10169500	2.79904500	0.07287100
C	-1.34709300	-1.23859900	-2.11254200
H	-1.36812500	-2.32342500	-2.29002800
C	-2.35612400	1.93262500	-0.11818400
H	-3.04885400	1.09738400	-0.18657300
C	3.17373100	0.22390800	1.44648700
H	3.55705900	1.24006500	1.59409600
H	2.47607700	0.03313600	2.27112100
C	0.11327900	-2.61839500	-0.00755400
H	-0.67793800	-3.37959500	-0.06950200
C	-0.56276300	4.11565200	0.15799500
H	0.12075900	4.95079200	0.28054100
C	-1.93554600	4.32097500	0.09438600
H	-2.32728800	5.33282200	0.15760900
C	3.35287100	0.27679300	-1.10207500
H	2.77938000	0.10709300	-2.02127800
H	3.73488400	1.30310500	-1.16449100
C	1.14994100	-3.00695400	-1.06298400
H	0.68848800	-3.16548200	-2.04225700
H	1.61966800	-3.95494400	-0.76940700
H	1.95095300	-2.27638500	-1.19193200
C	4.34392500	-0.75813100	1.49099600
H	4.88796200	-0.64815900	2.43735800
H	3.95570300	-1.78702500	1.46828200
C	-2.82295600	3.23816400	-0.03529100
H	-3.89330400	3.42559400	-0.06410700
C	-2.72394900	-0.68383100	-2.47017800
H	-3.50275700	-1.11349900	-1.83049500
H	-2.96322200	-0.91479900	-3.51664700
H	-2.75305000	0.40481300	-2.35667200
C	-0.26623400	-0.59969700	-2.98150700
H	-0.46113200	-0.80769200	-4.04181400
H	0.73650400	-0.96692700	-2.74663800
H	-0.26044500	0.48710200	-2.84726400
C	5.28532400	-0.55144100	0.30463900
H	6.11478300	-1.26839300	0.34671600
H	5.73266600	0.45202400	0.36768100
C	0.64168300	-2.68165200	1.42506800

H	1.41337300	-1.93507500	1.62939500
H	1.07502400	-3.67025400	1.62240700
H	-0.17554300	-2.51322600	2.13653600
C	2.31278200	3.19811100	0.35683900
H	2.21611200	4.07585100	-0.28967800
H	3.24736000	2.70411200	0.10655900
H	2.35496700	3.53205100	1.40075700
C	4.53592100	-0.68920400	-1.02025100
H	5.21401100	-0.51822300	-1.86576400
H	4.17031100	-1.72165400	-1.11608200

PiPr-6

Charge: 0 Multiplicity: 1

Pd	-3.01009500	-1.19905900	0.61404400
P	-0.93099800	-1.12838500	-0.14288200
C	-0.15084500	0.51569100	0.03258000
C	-0.98619100	1.70533400	0.04928500
N	1.17917700	2.35327700	0.08075100
C	1.17077000	0.96863600	0.03848400
C	2.42769500	0.15593900	0.06670100
H	2.07195100	-0.87521700	0.02726200
C	-0.11736000	2.82252100	0.08816200
C	-0.83509600	-1.50090600	-1.97610300
H	-1.01958200	-2.58330300	-2.03200700
C	-2.36919000	1.94567500	0.01508900
H	-3.05892600	1.10045200	-0.02810700
C	3.23013100	0.28178600	1.37744600
H	3.68018700	1.27902500	1.45783700
H	2.55954200	0.17804900	2.23759700
C	0.02359700	-2.51917500	0.70326100
H	-0.79890500	-3.23894800	0.79994900
C	-0.57717300	4.14173300	0.12711700
H	0.11010300	4.98156200	0.17235300
C	-1.95133600	4.34268200	0.10601400
H	-2.34437300	5.35566700	0.13337200
C	3.36462600	0.32151600	-1.14587400
H	2.79446400	0.23661200	-2.07518300
H	3.82399200	1.31767000	-1.15361900

C	1.14005200	-3.26226200	-0.02891200
H	0.82300000	-3.60593700	-1.01838900
H	1.40723000	-4.15366800	0.55406500
H	2.05614400	-2.67857300	-0.15099300
C	4.33806700	-0.77017400	1.42391800
H	4.91480200	-0.66664700	2.35152200
H	3.88284500	-1.77108200	1.44734400
C	-2.83726000	3.25218900	0.04740400
H	-3.90860600	3.43578700	0.02661200
C	-1.96975000	-0.77768700	-2.70186400
H	-2.94514200	-1.06159000	-2.29193300
H	-1.95219000	-1.01739000	-3.77333400
H	-1.86757800	0.30934100	-2.59961900
C	0.50195400	-1.17063300	-2.62852000
H	0.50345100	-1.49656500	-3.67687500
H	1.34796200	-1.64979300	-2.13011100
H	0.66737200	-0.08854300	-2.61549600
C	5.26051500	-0.66006400	0.20934100
H	6.02240100	-1.44908600	0.23752700
H	5.79894100	0.29847300	0.25311300
C	0.41289400	-2.10098400	2.11753600
H	1.22470200	-1.36963900	2.11623700
H	0.74690200	-2.97341100	2.69304700
H	-0.44014200	-1.65251400	2.64024700
C	2.30306200	3.25411100	0.20879000
H	2.20597200	4.06544900	-0.51985200
H	3.23645800	2.73634200	0.01174100
H	2.34371200	3.68619000	1.21583300
C	4.47353700	-0.73046500	-1.09986100
H	5.14661900	-0.60194500	-1.95673700
H	4.02558200	-1.72997800	-1.20141700

PiPr-7

Charge: 0 Multiplicity: 1

Pd	-3.16895100	-1.02552100	-0.28860200
P	-0.97810800	-1.10696800	0.06771300
C	-0.13186700	0.51272900	-0.00642600
C	-0.90456500	1.74426600	-0.02574200

N	1.28998900	2.27872200	-0.10146200
C	1.21411000	0.89703200	-0.03098800
C	2.44445500	0.03930600	0.00362700
H	2.06884600	-0.97034500	0.17884100
C	0.01938500	2.81480400	-0.08056200
C	-0.27710000	-2.29174000	-1.21624200
H	-1.10106200	-3.01487800	-1.26452200
C	-2.27215700	2.05802000	0.01825800
H	-3.00464000	1.24822100	0.07038400
C	3.39410600	0.34113400	1.17990300
H	3.83917900	1.33687500	1.07687100
H	2.82967600	0.35116700	2.11819500
C	-0.64712400	-1.84355700	1.76084500
H	-0.95365900	-2.89229400	1.63576800
C	-0.37111800	4.15702800	-0.09558200
H	0.35807600	4.96134300	-0.12324800
C	-1.73206500	4.42996500	-0.05899000
H	-2.07136900	5.46251900	-0.06735400
C	3.21993400	-0.01779700	-1.32868700
H	2.53531200	-0.29615600	-2.13697600
H	3.61631800	0.97081400	-1.59078300
C	0.77907700	-1.78904400	2.29465300
H	1.50155700	-2.29816600	1.65302200
H	0.82416100	-2.26613600	3.28238800
H	1.09484000	-0.74916300	2.41852300
C	4.52053500	-0.68929100	1.24044200
H	5.18825000	-0.46237200	2.08092500
H	4.09473400	-1.68435100	1.43604800
C	-2.67274400	3.38642100	-0.00171700
H	-3.73295800	3.62460600	0.03260600
C	-0.22483200	-1.57119100	-2.56124000
H	-1.19151900	-1.10966200	-2.79461000
H	0.02334900	-2.27740600	-3.36348800
H	0.52816100	-0.77672800	-2.56091500
C	0.98981100	-3.09282900	-0.93654800
H	1.11149300	-3.85069000	-1.72192100
H	0.94098400	-3.62341400	0.01935200
H	1.89225600	-2.47917000	-0.94708900

C	5.30387100	-0.72174500	-0.07119700
H	6.10303100	-1.47186700	-0.02202100
H	5.79405800	0.25178000	-0.22206800
C	-1.59200100	-1.17836600	2.76488000
H	-1.37664900	-0.10586200	2.84883400
H	-1.46817600	-1.62548000	3.75998800
H	-2.63745900	-1.28406000	2.45484000
C	2.45963800	3.12847200	-0.15922700
H	2.27849000	3.93626400	-0.87439400
H	3.32706000	2.57230300	-0.50242100
H	2.68073300	3.56767700	0.82078700
C	4.38014800	-1.01233600	-1.25303700
H	4.94263900	-0.99447800	-2.19489800
H	3.98074700	-2.03116300	-1.14898000

PiPr-8

Charge: 0 Multiplicity: 1

Pd	-2.82162400	-1.22757900	-0.93935100
P	-0.95371100	-1.13039000	0.23229900
C	-0.14999300	0.50165400	0.07219800
C	-0.99080700	1.68566900	0.05272600
N	1.16399700	2.33606500	-0.14842800
C	1.16132600	0.94992700	-0.06685700
C	2.41892000	0.14092800	-0.11150200
H	2.07271600	-0.89167400	-0.06278800
C	-0.13202600	2.80254600	-0.08471700
C	0.10621100	-2.60250300	-0.28001400
H	-0.69482800	-3.35434500	-0.29371900
C	-2.37428800	1.91300700	0.13227900
H	-3.05587200	1.06849000	0.21936100
C	3.34047300	0.32909000	1.10968200
H	3.73661600	1.35149400	1.14676200
H	2.75777800	0.19121200	2.02703700
C	-1.12518800	-1.35543200	2.08678800
H	-1.21985700	-2.44400900	2.20878100
C	-0.60658200	4.11543900	-0.15262900
H	0.06756300	4.95839600	-0.27348400
C	-1.98009000	4.30699900	-0.06869600

H	-2.38236200	5.31555200	-0.11689800
C	3.20543000	0.25552600	-1.43071800
H	2.52764600	0.08554500	-2.27570700
H	3.60948500	1.26665900	-1.55782500
C	0.08096300	-0.85227800	2.87555700
H	1.02227900	-1.28951700	2.53303400
H	-0.03362800	-1.09646400	3.93983200
H	0.16618800	0.23600800	2.78795800
C	4.51108700	-0.65411700	1.06413900
H	5.17883300	-0.47636400	1.91650900
H	4.12916500	-1.67901700	1.17589300
C	-2.85449200	3.21457400	0.06987700
H	-3.92554500	3.39196400	0.12551100
C	0.58001700	-2.45714900	-1.72450300
H	-0.25297700	-2.15961000	-2.37244900
H	0.97556700	-3.41334700	-2.08941000
H	1.36828500	-1.70823800	-1.83364600
C	1.17905500	-3.15942400	0.65595900
H	1.56140100	-4.09806300	0.23347000
H	0.77427100	-3.39204100	1.64545100
H	2.03763600	-2.49845300	0.79440200
C	5.28425100	-0.55084600	-0.25055300
H	6.09667100	-1.28797800	-0.27105700
H	5.75724600	0.44055900	-0.31598100
C	-2.40943000	-0.70717900	2.60021100
H	-2.37288000	0.38181900	2.48565000
H	-2.54458700	-0.92608000	3.66768300
H	-3.28432600	-1.07549600	2.05338800
C	2.27793500	3.23059500	-0.37089200
H	2.31597100	3.56459300	-1.41490200
H	3.21783600	2.74704400	-0.12070200
H	2.17095200	4.10695000	0.27570600
C	4.36017300	-0.74537700	-1.45290600
H	4.92365600	-0.64606800	-2.38902600
H	3.95383900	-1.76737600	-1.43673900

PiPr-9

Charge: 0 Multiplicity: 1

Pd	-2.29584700	-1.35535100	-1.43710800
P	-1.01699300	-1.08186400	0.32572900
C	-0.14903800	0.52519600	0.24520200
C	-0.96945700	1.71700800	0.13241200
N	1.19120500	2.32069400	-0.11216300
C	1.16479800	0.93838800	0.04258200
C	2.40713700	0.10788000	-0.02859100
H	2.05740800	-0.91635400	0.09059200
C	-0.09473800	2.81130400	-0.06462900
C	0.11870500	-2.56317200	0.54601200
H	-0.66205400	-3.31677200	0.73112200
C	-2.35151600	1.95749700	0.13063300
H	-3.04932000	1.13096900	0.20622100
C	3.40034900	0.33758000	1.12670300
H	3.80379300	1.35707600	1.10833500
H	2.86933100	0.23674000	2.08137700
C	-1.82133100	-1.09987500	2.04163600
H	-1.60156900	-2.11765800	2.39086700
C	-0.55012400	4.12398800	-0.20993100
H	0.13833300	4.95076400	-0.35909800
C	-1.92367300	4.33428800	-0.17478600
H	-2.31254800	5.34299300	-0.28649000
C	3.09825000	0.14004900	-1.40501300
H	2.35945700	-0.10363100	-2.17837300
H	3.46951400	1.14543400	-1.63605900
C	-1.20128300	-0.10758600	3.02127000
H	-0.11211500	-0.20015400	3.07479600
H	-1.60636200	-0.27279900	4.02835500
H	-1.43012500	0.92317600	2.73271100
C	4.55946800	-0.65623800	1.04732400
H	5.27459700	-0.46129900	1.85629000
H	4.17445700	-1.67424600	1.20542700
C	-2.81526200	3.25875700	-0.01876700
H	-3.88572400	3.44721100	-0.02456100
C	0.79570300	-2.99120900	-0.75606700
H	0.04512700	-3.10039600	-1.54762800
H	1.30076000	-3.95573000	-0.61679700
H	1.54072500	-2.27709800	-1.11569900

C	1.04315000	-2.58755400	1.76461300
H	1.56637100	-3.55167200	1.80777800
H	0.48500600	-2.48059200	2.69966000
H	1.80352700	-1.80464300	1.75045900
C	5.25606400	-0.59261600	-0.31183700
H	6.07566100	-1.32091800	-0.35270100
H	5.71108000	0.40110800	-0.44064900
C	-3.34283100	-0.97383800	2.00334000
H	-3.66114600	0.04967300	1.78438600
H	-3.76351100	-1.24376000	2.98117500
H	-3.77746400	-1.63276200	1.24385500
C	2.31567800	3.19137200	-0.37125200
H	2.28271500	3.57532500	-1.39808400
H	3.25406800	2.66518700	-0.22663800
H	2.29205900	4.03867100	0.32238300
C	4.26579400	-0.84624600	-1.44830000
H	4.77114300	-0.78308300	-2.42008800
H	3.87719400	-1.87133300	-1.36209200

PiPr-10

Charge: 0 Multiplicity: 1

Pd	0.51105000	-2.46955000	-1.15773500
P	-0.49126600	-1.25939300	0.37750000
C	-0.73222100	0.50082800	-0.07370600
C	-1.93928600	1.30018900	-0.21967300
N	-0.14937800	2.69663800	-0.11623400
C	0.32231900	1.40826200	0.03660700
C	1.78019400	1.05453800	0.04125900
H	1.80946700	-0.01791500	0.26983500
C	-1.52113600	2.66196000	-0.24878100
C	0.01114600	-1.30122300	2.18662200
H	-0.41315600	-2.26435300	2.49123900
C	-3.32207200	1.05812800	-0.33555300
H	-3.72151600	0.05459900	-0.33237200
C	2.66283800	1.75239700	1.08697600
H	2.72618900	2.82827600	0.88916300
H	2.21686100	1.64967200	2.08401300
C	-2.25149800	-1.90127200	0.48606500

H	-2.85289700	-1.15156500	1.01265600
C	-2.40724800	3.73450400	-0.37478100
H	-2.05506400	4.76173800	-0.37573000
C	-3.76004700	3.44921100	-0.48726400
H	-4.47493600	4.26124700	-0.58862900
C	2.39060700	1.15799300	-1.37062900
H	1.75206400	0.60023400	-2.06602600
H	2.40589300	2.20211700	-1.71241600
C	-2.78817900	-2.11330800	-0.93310000
H	-2.58155300	-1.27344700	-1.60324200
H	-3.87383000	-2.28064400	-0.91277400
H	-2.31397000	-2.99895800	-1.37332500
C	4.07696200	1.17044200	1.06248400
H	4.70652300	1.68737700	1.79766800
H	4.04099900	0.11377400	1.36374900
C	-4.20770600	2.11902500	-0.46736500
H	-5.27079500	1.91082800	-0.55640200
C	1.51266500	-1.40609800	2.43579100
H	1.98286500	-2.10352500	1.73291300
H	1.69308700	-1.77225600	3.45463500
H	2.01224600	-0.43935700	2.34974300
C	-0.63969500	-0.19456800	3.00911600
H	-0.25399000	0.78841000	2.71847100
H	-0.42789800	-0.33936800	4.07642400
H	-1.72746800	-0.17111900	2.88237800
C	4.69350400	1.27107900	-0.33331400
H	5.69697800	0.82718800	-0.33670200
H	4.81791000	2.33212700	-0.59801800
C	-2.34393300	-3.21923500	1.25562600
H	-1.58886800	-3.93362600	0.90228200
H	-3.33153100	-3.66934600	1.09224700
H	-2.22420900	-3.09333000	2.33613000
C	0.61000500	3.92719000	-0.13846400
H	0.08138900	4.65851700	-0.75396100
H	1.58716400	3.76507500	-0.59034400
H	0.74121400	4.34110500	0.86799600
C	3.80964900	0.59167000	-1.37937400
H	4.24942100	0.69624000	-2.37938100

H	3.75653000	-0.48626900	-1.16652000

PiPr-11

Charge: 0 Multiplicity: 1

Pd	1.59734800	-1.95646300	-0.73142600
P	-0.26717900	-1.39950900	0.30119700
C	-0.88043100	0.27920700	-0.06394100
C	-2.23475800	0.77595300	-0.22002600
N	-0.81418800	2.54442000	-0.16357300
C	-0.05378400	1.40410700	0.00832300
C	1.44333300	1.41428100	0.08338300
H	1.70897400	0.37570100	0.33209300
C	-2.14318600	2.19414500	-0.28407000
C	-0.36501900	-1.54254200	2.16416100
H	-0.10961300	-2.59337700	2.35437100
C	-3.51740000	0.20573100	-0.31141400
H	-3.65907300	-0.86614800	-0.26850300
C	2.08639000	2.29334500	1.16615600
H	1.94125000	3.35884200	0.95075200
H	1.61485800	2.10378300	2.13684000
C	-1.62221800	-2.54468700	-0.27401500
H	-2.54935600	-2.27416600	0.23974900
C	-3.25776100	3.02355000	-0.42778900
H	-3.15944200	4.10468900	-0.45658900
C	-4.50519900	2.42145400	-0.51870900
H	-5.39229700	3.03879800	-0.63135300
C	2.09521500	1.65467000	-1.29149400
H	1.63088500	0.98125400	-2.02215000
H	1.91560900	2.68204100	-1.63763700
C	-1.81135200	-2.40685800	-1.78269600
H	-2.03655500	-1.37848700	-2.08139300
H	-2.63322900	-3.04931000	-2.12436300
H	-0.89571100	-2.71214200	-2.30450900
C	3.58703400	2.00785300	1.23851800
H	4.05342300	2.64027300	2.00449600
H	3.73882100	0.96480000	1.55235700
C	-4.62918600	1.02378900	-0.45996400

H	-5.61502900	0.57140500	-0.52898500
C	0.69551300	-0.66980300	2.82512600
H	1.69356300	-0.87543700	2.42259500
H	0.71647800	-0.84956800	3.90730400
H	0.47054200	0.39059200	2.66978200
C	-1.75162200	-1.24045300	2.72613200
H	-2.06477300	-0.22236800	2.46956900
H	-1.74038000	-1.32174800	3.82086900
H	-2.51424300	-1.93235900	2.35482700
C	4.26066700	2.22960000	-0.11647700
H	5.33037500	1.99344900	-0.05213400
H	4.18962200	3.29498300	-0.38363900
C	-1.28212200	-3.98646100	0.10027000
H	-0.31586100	-4.27755700	-0.33058500
H	-2.05219800	-4.66536600	-0.28814500
H	-1.22683400	-4.13544500	1.18392900
C	-0.36096100	3.91719200	-0.20748100
H	-1.00053300	4.48212900	-0.89022600
H	0.65605000	3.96917300	-0.59105400
H	-0.39745100	4.38657600	0.78249500
C	3.59863800	1.39277000	-1.21114700
H	4.06956500	1.58875200	-2.18289600
H	3.75080400	0.32419100	-0.99228000

PiPr-12

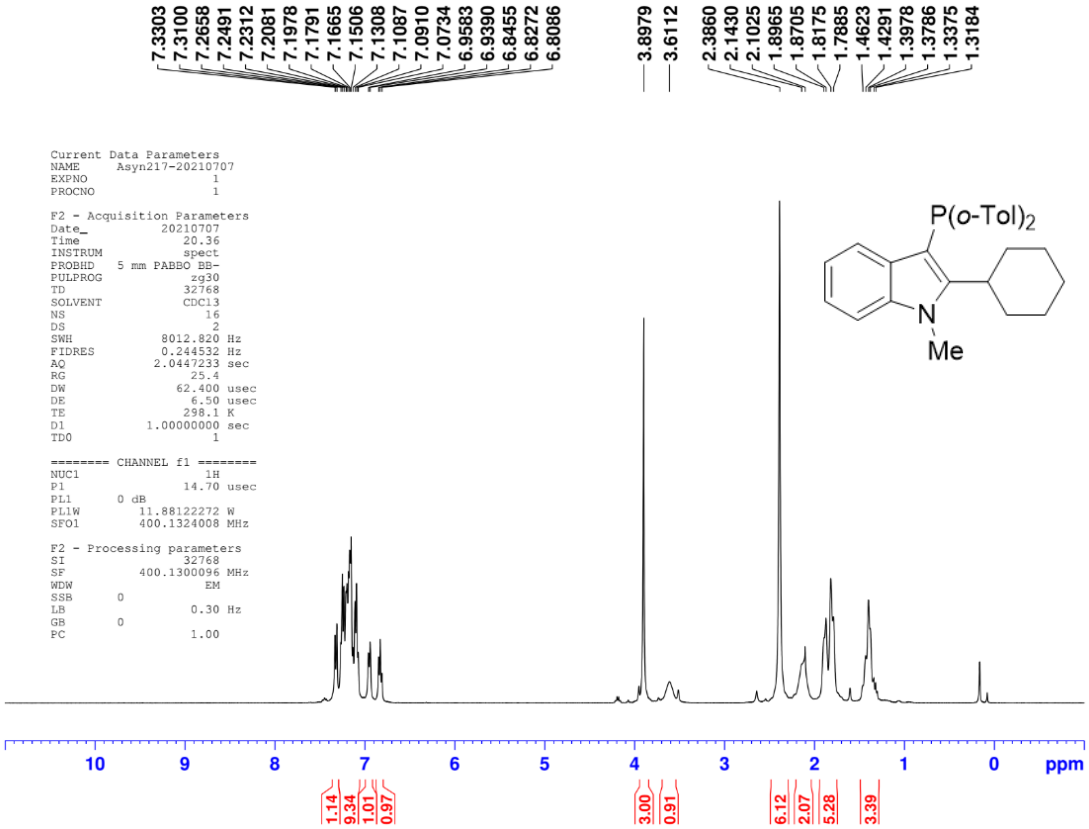
Charge: 0 Multiplicity: 1

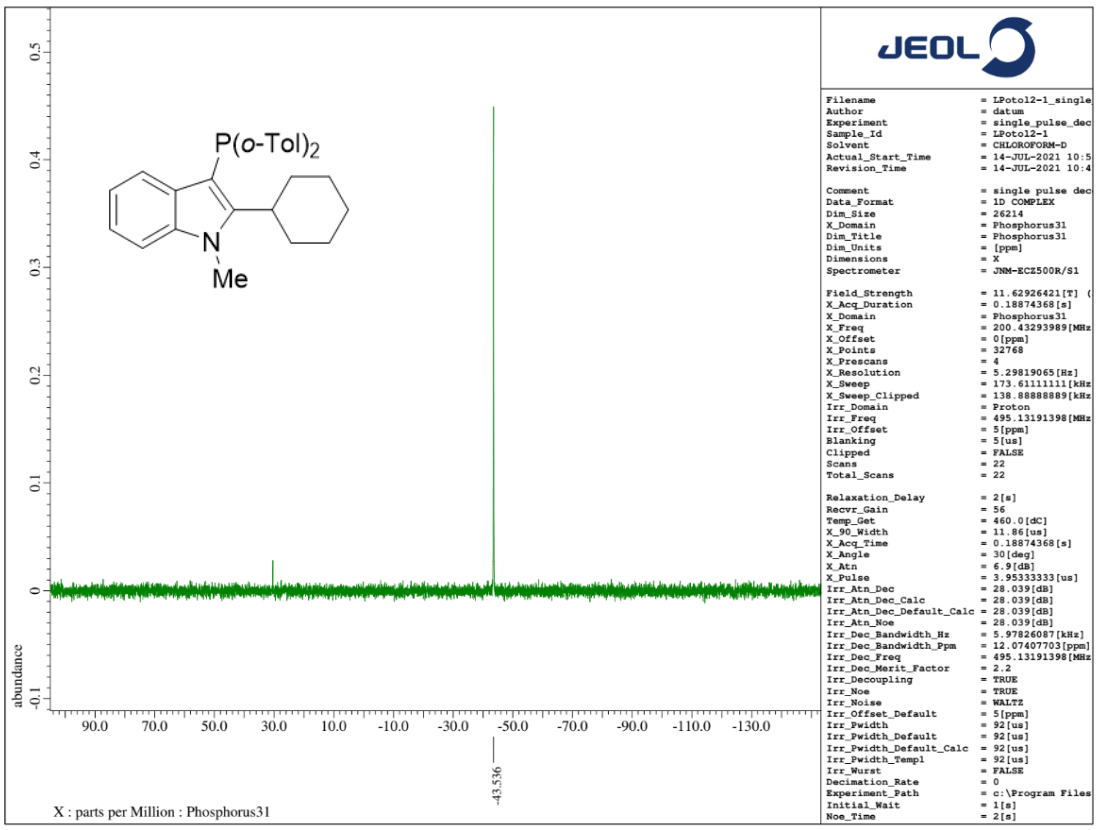
Pd	1.84265300	-1.76937200	-0.40372300
P	-0.27016700	-1.44449600	0.15350900
C	-0.91039200	0.25288800	0.01564600
C	-2.28295900	0.71010200	-0.08328700
N	-0.90994100	2.51156400	-0.16303900
C	-0.10675100	1.39529900	-0.02940100
C	1.38457400	1.46178500	0.03295100
H	1.68588600	0.40437700	0.15935700
C	-2.23295700	2.12533300	-0.19611400
C	-0.62720800	-1.93380000	1.92401900
H	-0.25373600	-2.96434300	1.98899400
C	-3.54979700	0.10191700	-0.09254500

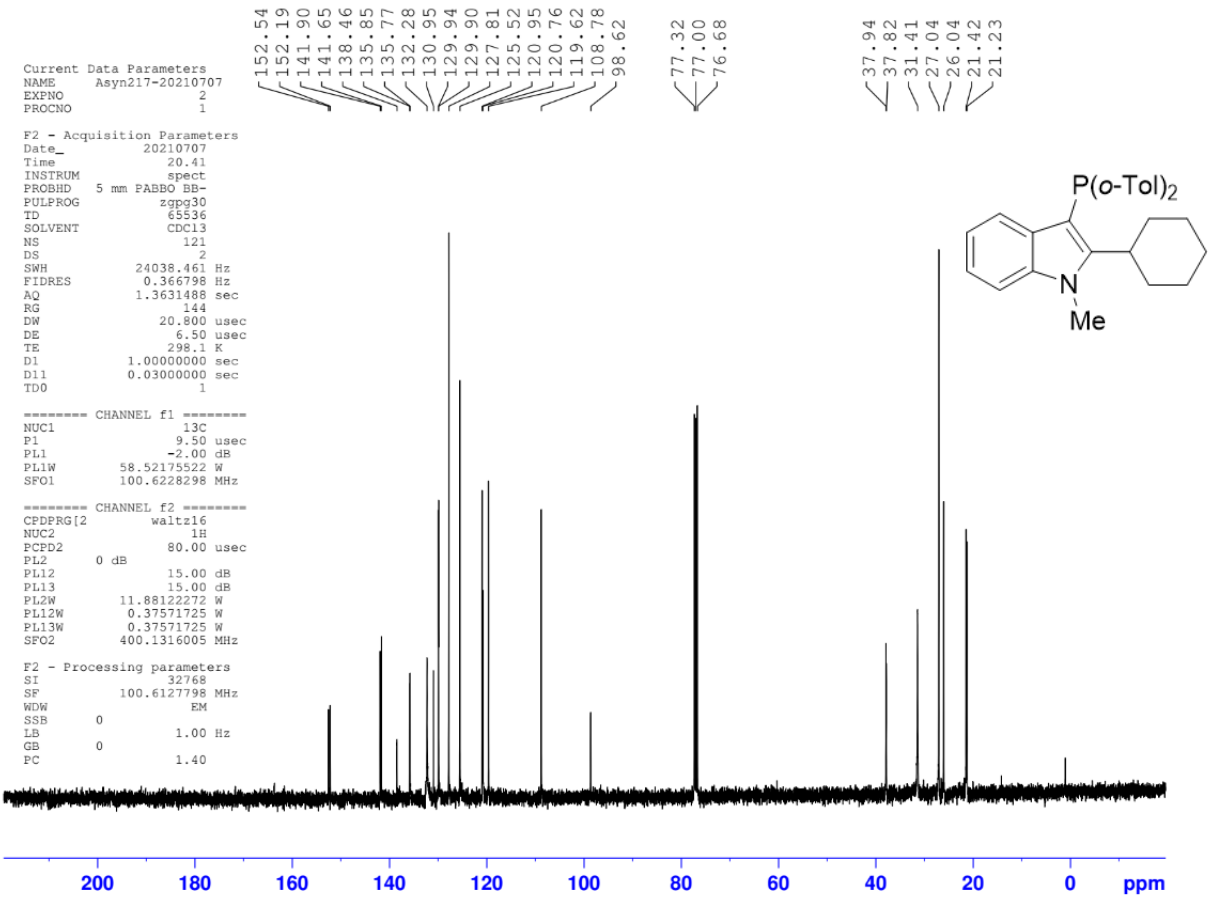
H	-3.65396600	-0.97127500	0.00788200
C	1.96409900	2.19634600	1.25095100
H	1.76577200	3.27544800	1.20303500
H	1.47950600	1.82757100	2.16258600
C	-1.43151800	-2.47410500	-0.87512500
H	-2.44841500	-2.35590500	-0.48972000
C	-3.37327900	2.92258000	-0.31170600
H	-3.30174600	4.00376600	-0.38668100
C	-4.60676500	2.28420900	-0.32212400
H	-5.51550300	2.87324600	-0.41156000
C	2.05602800	1.89372200	-1.28079700
H	1.63540300	1.30374100	-2.10400600
H	1.85720100	2.94964600	-1.50928800
C	-1.39273600	-1.99428800	-2.32306400
H	-1.70922100	-0.95014300	-2.41233100
H	-2.05784000	-2.60673200	-2.94508900
H	-0.37501000	-2.07545400	-2.72539400
C	3.47428600	1.96649200	1.32070300
H	3.89990400	2.50850100	2.17470900
H	3.66097100	0.89671800	1.49762200
C	-4.68979700	0.88610600	-0.21274700
H	-5.66555900	0.40744500	-0.21726200
C	0.21609200	-1.06043500	2.85081200
H	1.27851500	-1.11232600	2.58584500
H	0.10263200	-1.38498500	3.89290100
H	-0.10052600	-0.01248000	2.78904500
C	-2.09778000	-1.90344000	2.32695000
H	-2.50476900	-0.88930600	2.26001400
H	-2.20834400	-2.23846100	3.36671200
H	-2.71463600	-2.56161500	1.70573300
C	4.16494000	2.38882100	0.02325400
H	5.24270600	2.19197300	0.08576100
H	4.05141600	3.47564700	-0.10894900
C	-1.04423900	-3.94687300	-0.76236000
H	-0.01039200	-4.09862000	-1.09759700
H	-1.70521200	-4.56070400	-1.38773800
H	-1.12005900	-4.31750600	0.26599200
C	-0.51600300	3.90072300	-0.23107400

H	-0.97331400	4.37432300	-1.10622100
H	0.56291900	3.98181400	-0.32518900
H	-0.83305100	4.43904600	0.66981900
C	3.56549400	1.67196500	-1.18686900
H	4.05587500	2.00197100	-2.11142200
H	3.75264800	0.59012000	-1.09612600

10. ^{1}H, ^{13}C, ^{19}F, ^{31}P NMR and HRMS spectra



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PULPROG zgpg30
TD 65536
SOLVENT CDCl3
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DS 2
SWH 24038.461 Hz
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RG 144
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DE 6.50 usec
TE 298.1 K
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D11 0.03000000 sec
TD0 1
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P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
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PL12W 0.37571725 W
PL13W 0.37571725 W
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F2 - Processing parameters
SI 32768
SF 100.6127798 MHz
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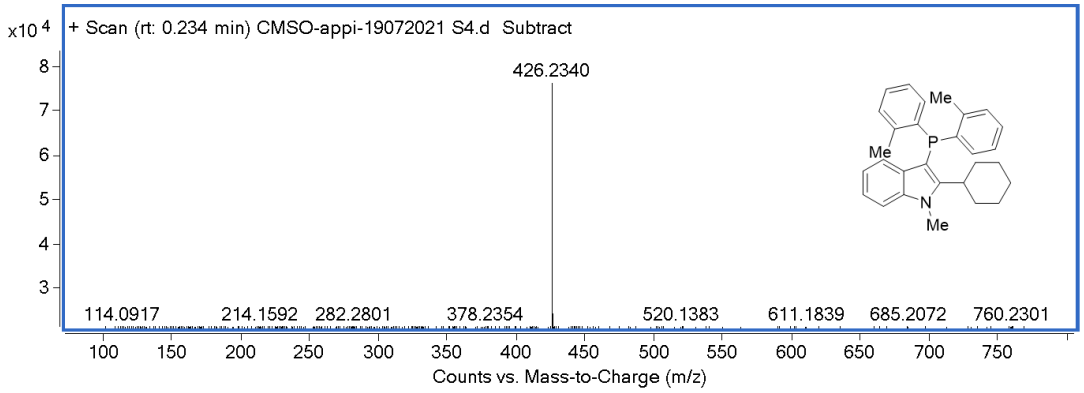
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Me
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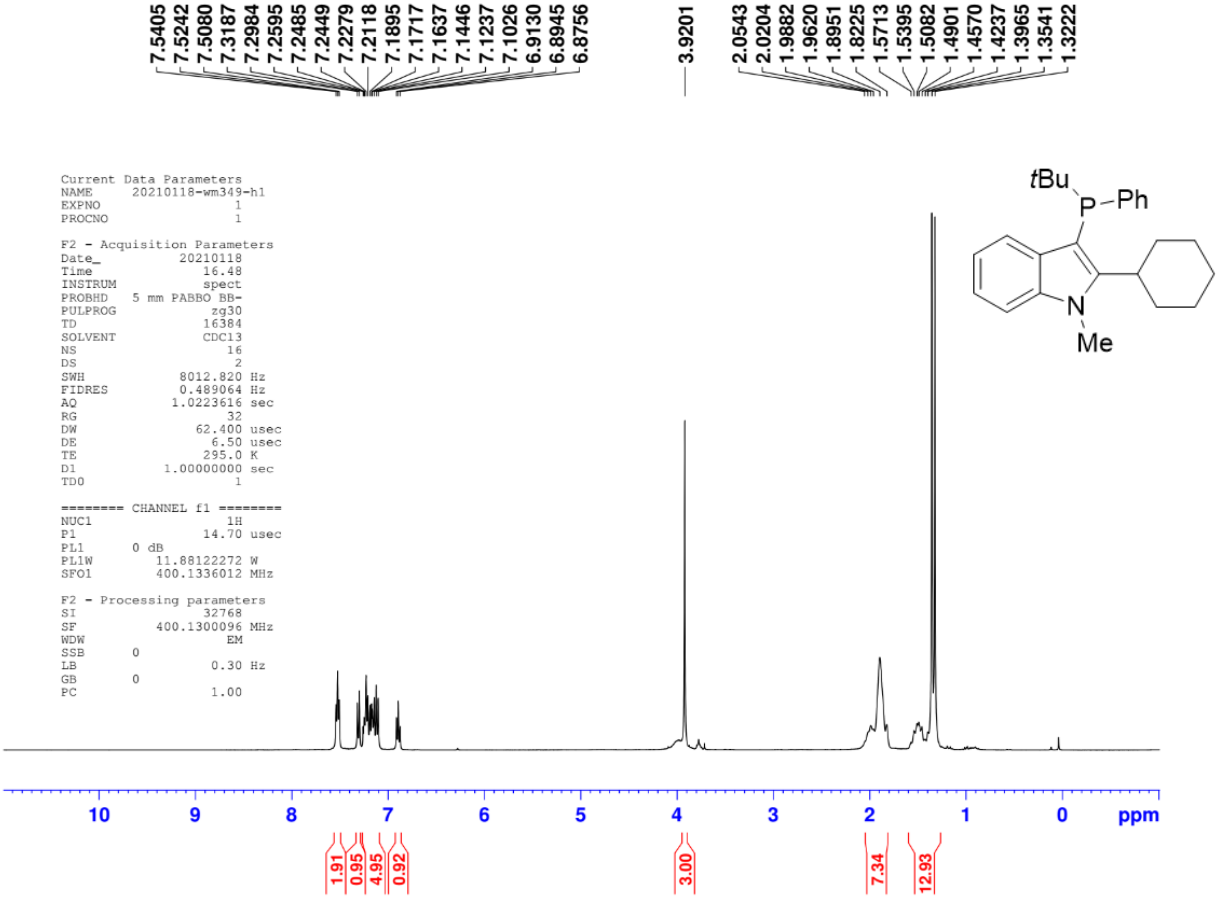
N
Me
Counts vs. Mass-to-Charge (m/z)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PULPROG zg30
TD 16384
SOLVENT CDCl3
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DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
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NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
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N
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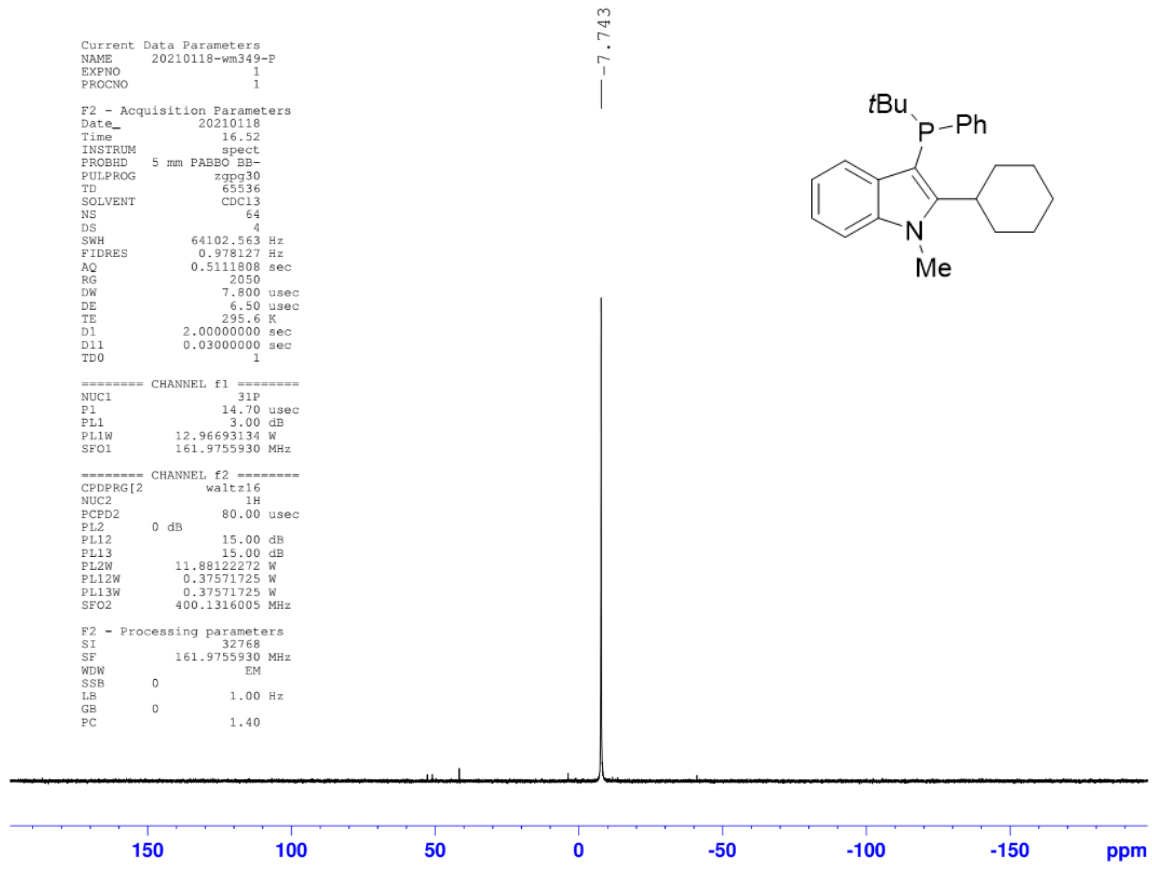
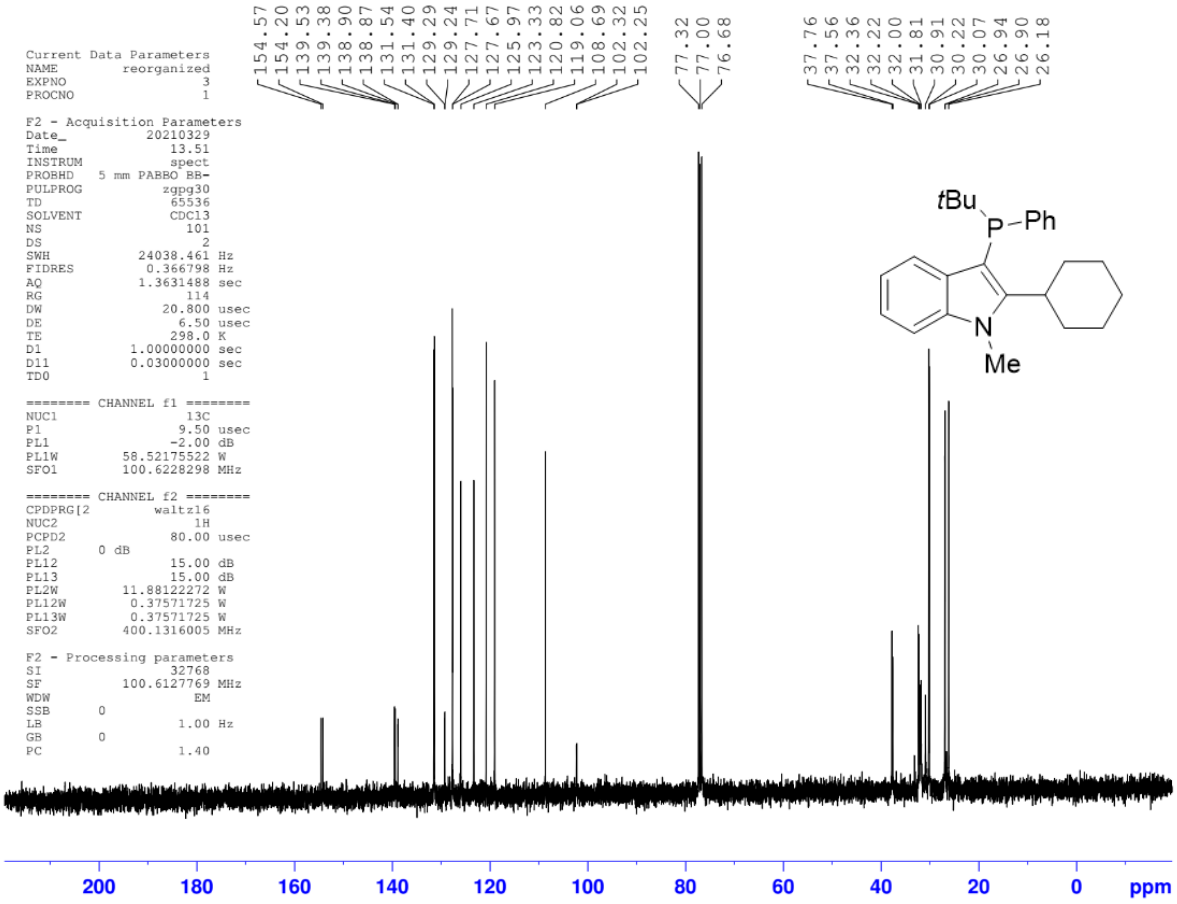
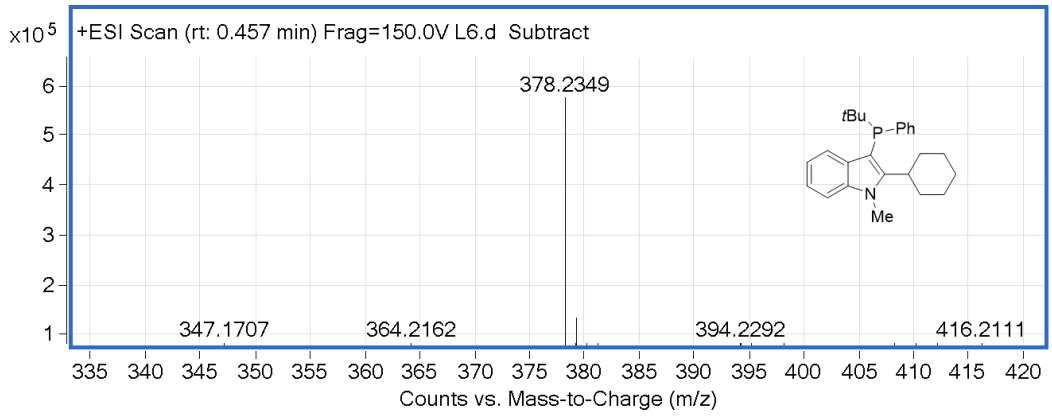
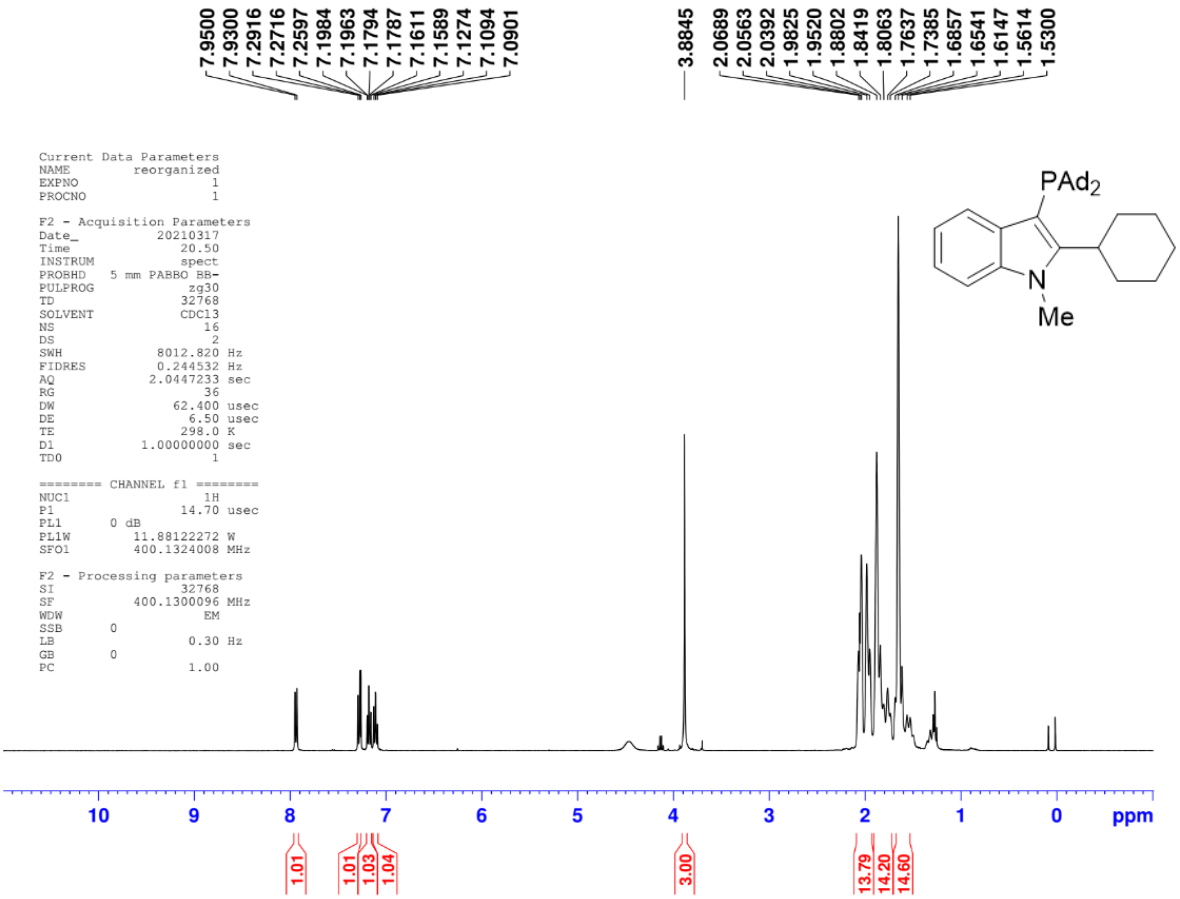
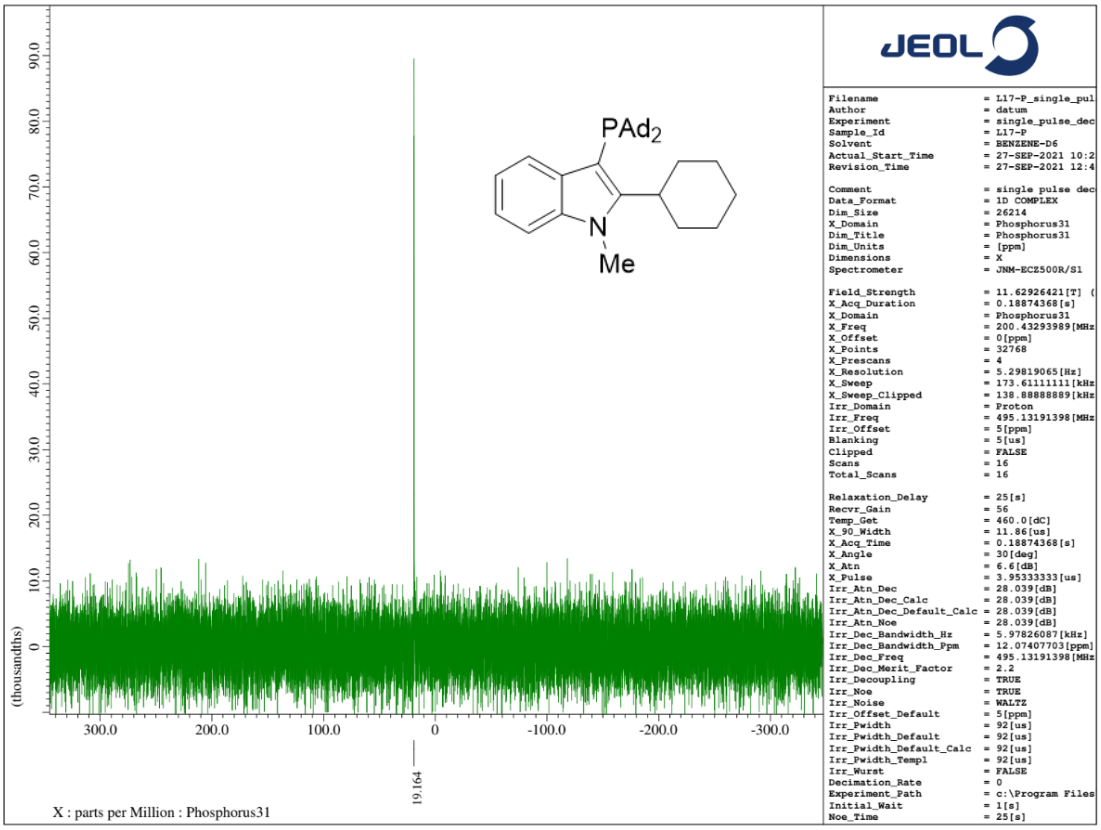
8
7
6
5
4
3
2
1
0
ppm
1.91
0.95
4.95
0.92
3.00
7.34
12.93

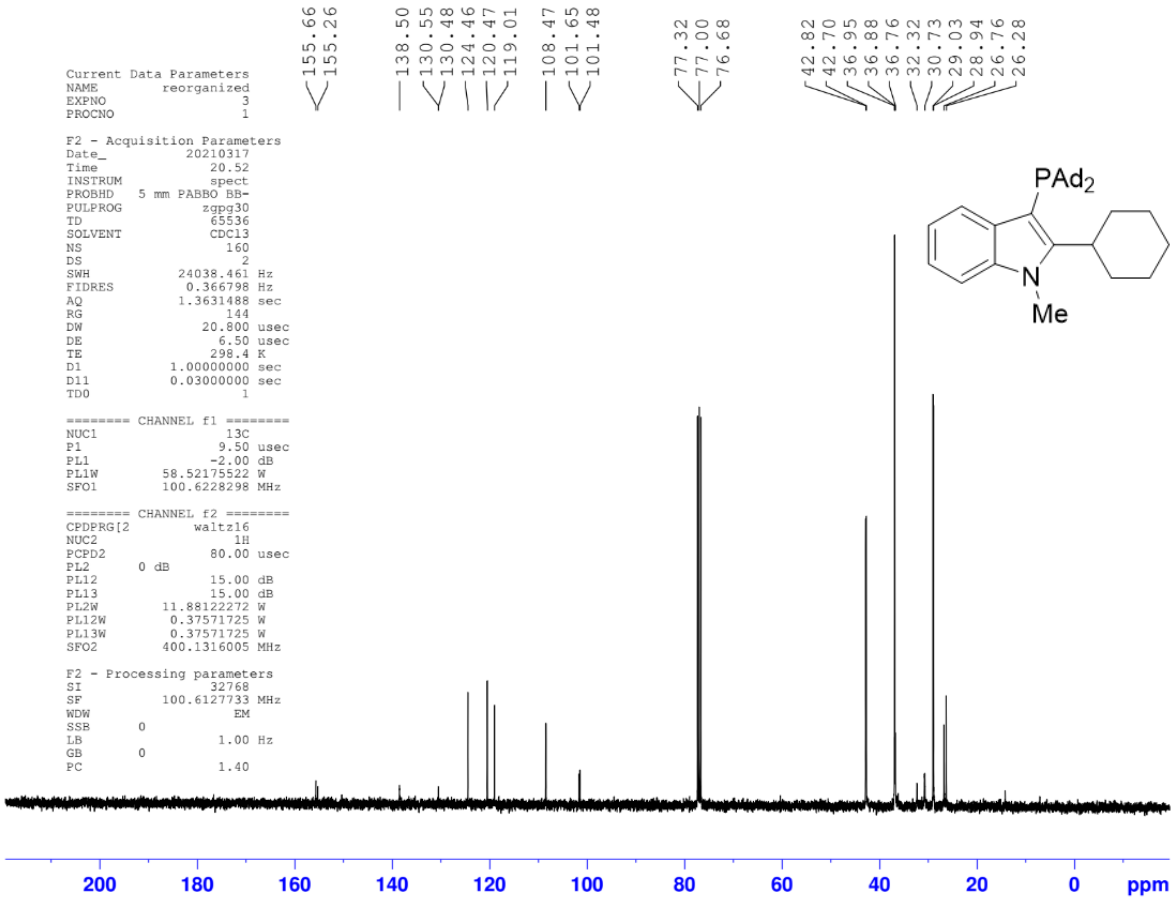

7.743
Current Data Parameters
NAME 20210118-wm349-P
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210118
Time 16.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 64
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 2050
DW 7.800 usec
DE 6.50 usec
TE 295.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 31P
P1 14.70 usec
PL1 3.00 dB
PL1W 12.96693134 W
SFO1 161.9755930 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 161.9755930 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
tBu
P
Ph
N
Me
150
100
50
0
-50
-100
-150
ppm

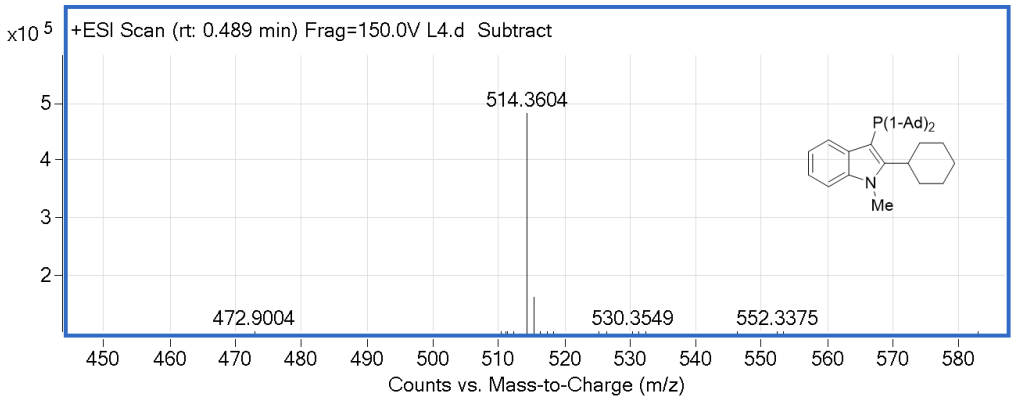

154.57
154.20
139.53
139.38
138.90
138.87
131.54
131.40
129.29
129.24
127.71
127.67
125.97
123.33
120.82
119.06
108.69
102.32
102.25
77.32
77.00
76.68
37.76
37.56
32.36
32.22
32.00
31.81
30.91
30.22
30.07
26.94
26.90
26.18
Current Data Parameters
NAME reorganized
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210329
Time 13.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 101
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127769 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
tBu
P
Ph
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

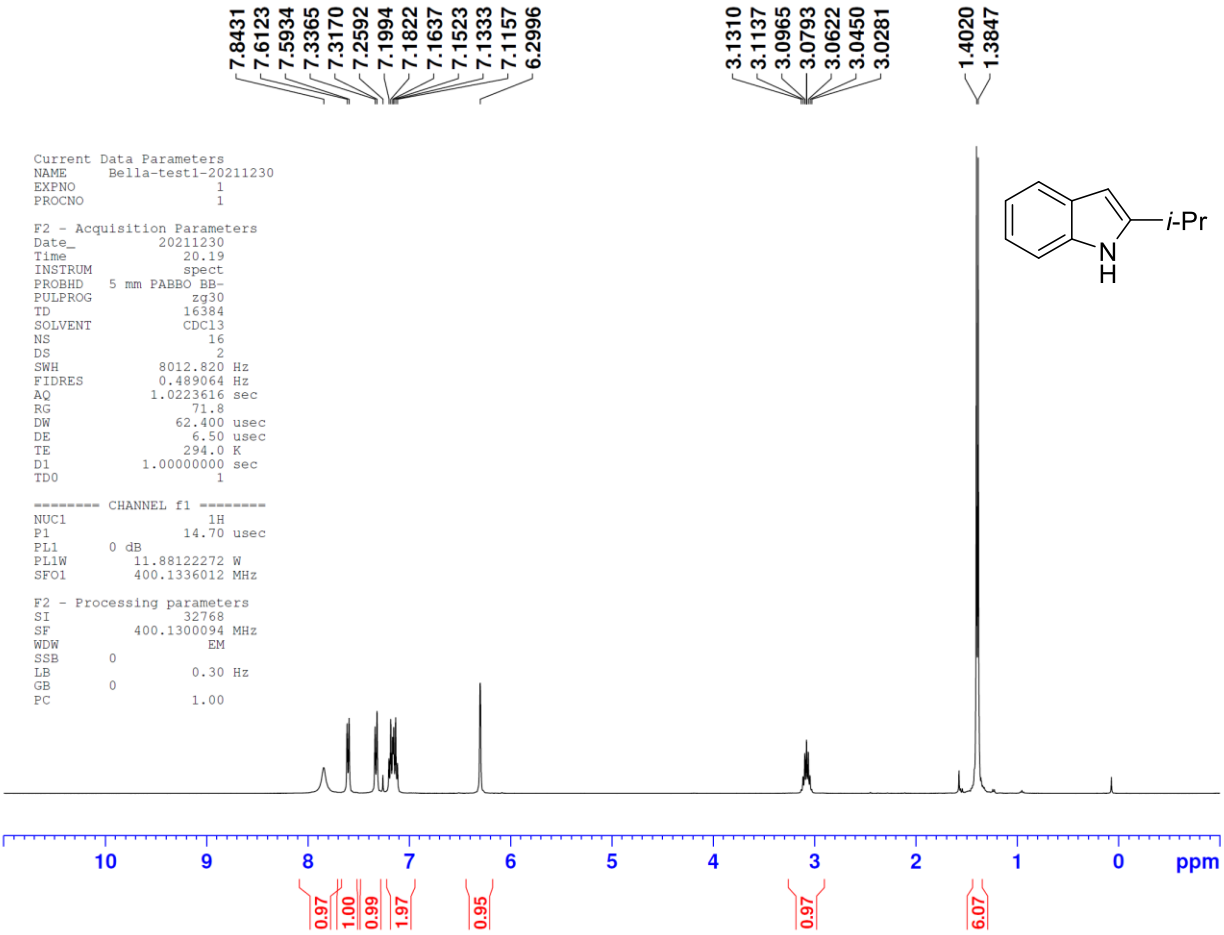

x10^5
+ESI Scan (rt: 0.457 min) Frag=150.0V L6.d Subtract
378.2349
347.1707
364.2162
394.2292
416.2111
tBu
P
Ph
N
Me
Counts vs. Mass-to-Charge (m/z)

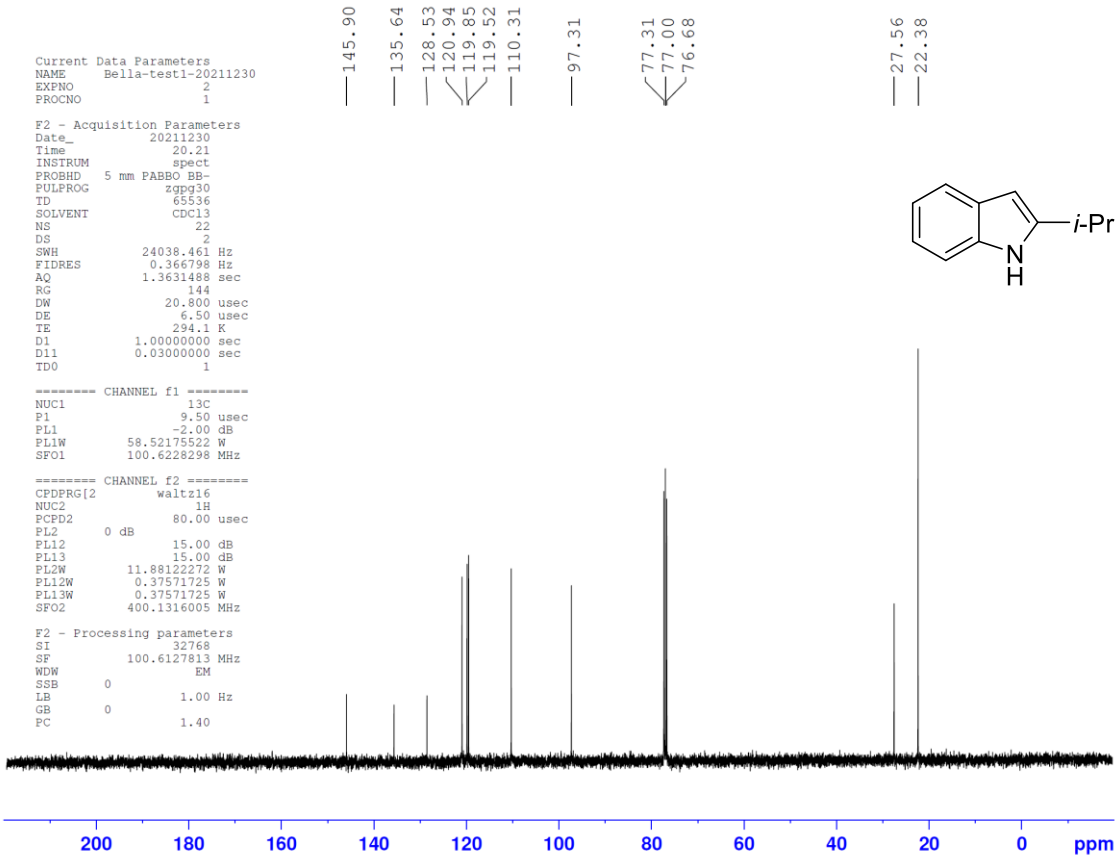

7.9500
7.9300
7.2916
7.2716
7.2597
7.1984
7.1963
7.1794
7.1787
7.1611
7.1589
7.1274
7.1094
7.0901
3.8845
2.0689
2.0563
2.0392
1.9825
1.9520
1.8802
1.8419
1.8063
1.7637
1.7385
1.6857
1.6541
1.6147
1.5614
1.5300
Current Data Parameters
NAME reorganized
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210317
Time 20.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 36
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
PAd2
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.01
1.01
1.03
1.04
3.00
13.79
14.20
14.60

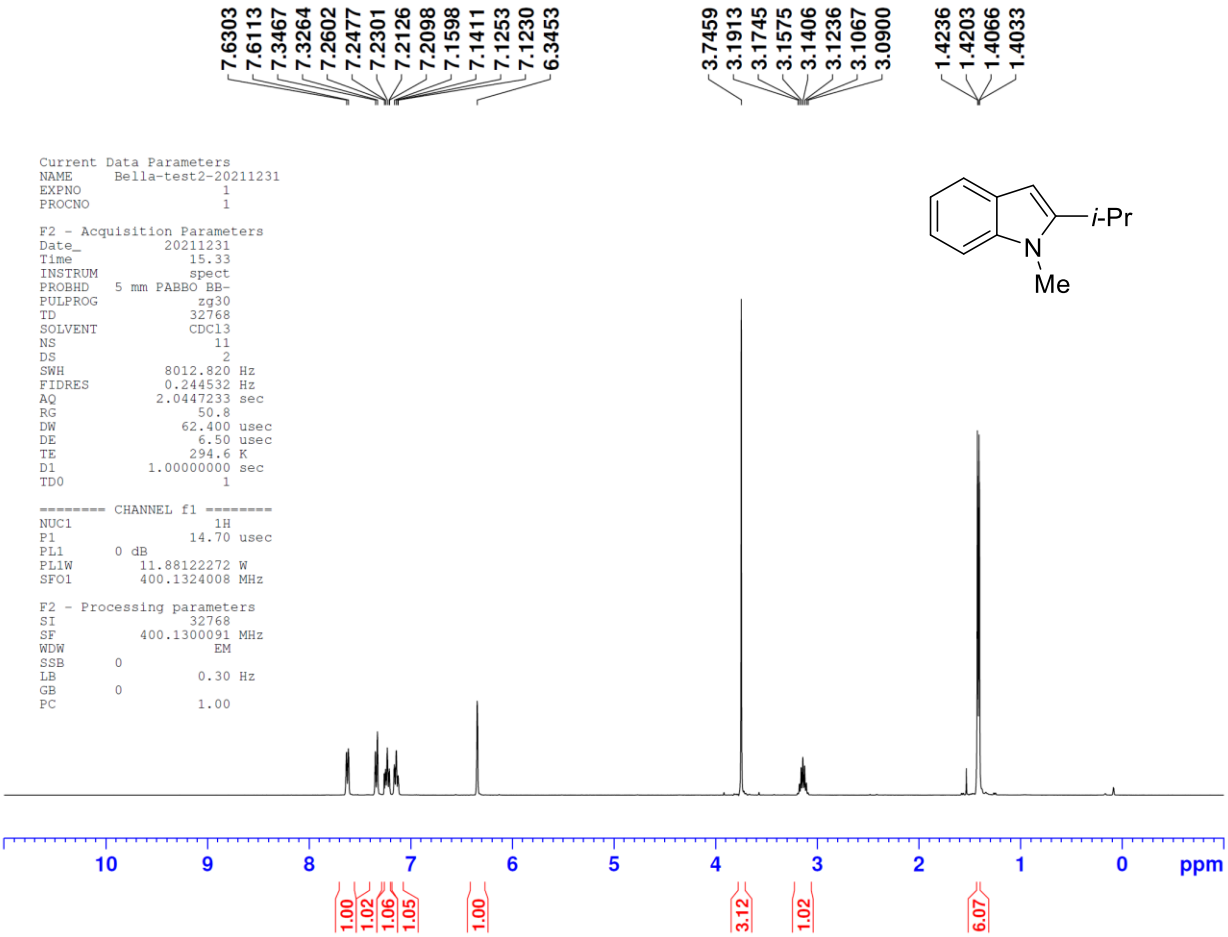

JEOL
PAd2
N
Me
(thousandths)
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
300.0
200.0
100.0
0
-100.0
-200.0
-300.0
19.164
X : parts per Million : Phosphorus31
Filename = L17-P_single_pul
Author = datum
Experiment = single_pulse_dec
Sample_Id = L17-P
Solvent = BENZENE-D6
Actual_Start_Time = 27-SEP-2021 10:2
Revision_Time = 27-SEP-2021 12:4
Comment = single pulse dec
Data_Format = 1D COMPLEX
Dim_Size = 26214
X_Domain = Phosphorus31
Dim_Title = Phosphorus31
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (
X_Acq_Duration = 0.18874368[s]
X_Domain = Phosphorus31
X_Freq = 200.43293989[MHz
X_Offset = 0[ppm]
X_Points = 32768
X_Prescans = 4
X_Resolution = 5.29819065[Hz]
X_Sweep = 173.61111111[kHz
X_Sweep_Clipped = 138.88888889[kHz
Irr_Domain = Proton
Irr_Freq = 495.13191398[MHz
Irr_Offset = 5[ppm]
Blanking = 5[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 25[s]
Recvr_Gain = 56
Temp_Get = 460.0[dC]
X_90_Width = 11.86[us]
X_Acq_Time = 0.18874368[s]
X_Angle = 30[deg]
X_Atn = 6.6[dB]
X_Pulse = 3.95333333[us]
Irr_Atn_Dec = 28.039[dB]
Irr_Atn_Dec_Calc = 28.039[dB]
Irr_Atn_Dec_Default_Calc = 28.039[dB]
Irr_Atn_Noe = 28.039[dB]
Irr_Dec_Bandwidth_Hz = 5.97826087[kHz]
Irr_Dec_Bandwidth_Ppm = 12.07407703[ppm]
Irr_Dec_Freq = 495.13191398[MHz
Irr_Dec_Merit_Factor = 2.2
Irr_Decoupling = TRUE
Irr_Noe = TRUE
Irr_Noise = WALTZ
Irr_Offset_Default = 5[ppm]
Irr_Pwidth = 92[us]
Irr_Pwidth_Default = 92[us]
Irr_Pwidth_Default_Calc = 92[us]
Irr_Pwidth_Templ = 92[us]
Irr_Wurst = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files
Initial_Wait = 1[s]
Noe_Time = 25[s]

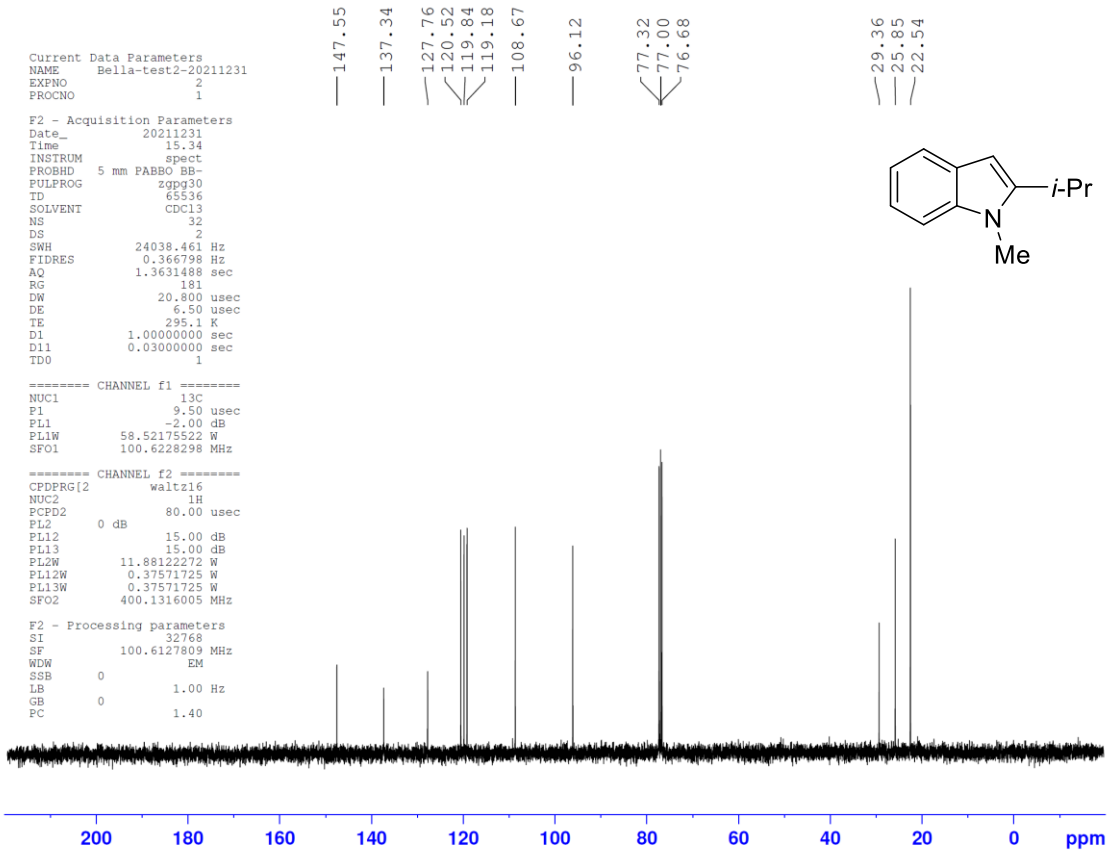

155.66
155.26
138.50
130.55
130.48
124.46
120.47
119.01
108.47
101.65
101.48
77.32
77.00
76.68
42.82
42.70
36.95
36.88
36.76
32.32
30.73
29.03
28.94
26.76
26.28
Current Data Parameters
NAME reorganized
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210317
Time 20.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 160
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127733 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
PAd2
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

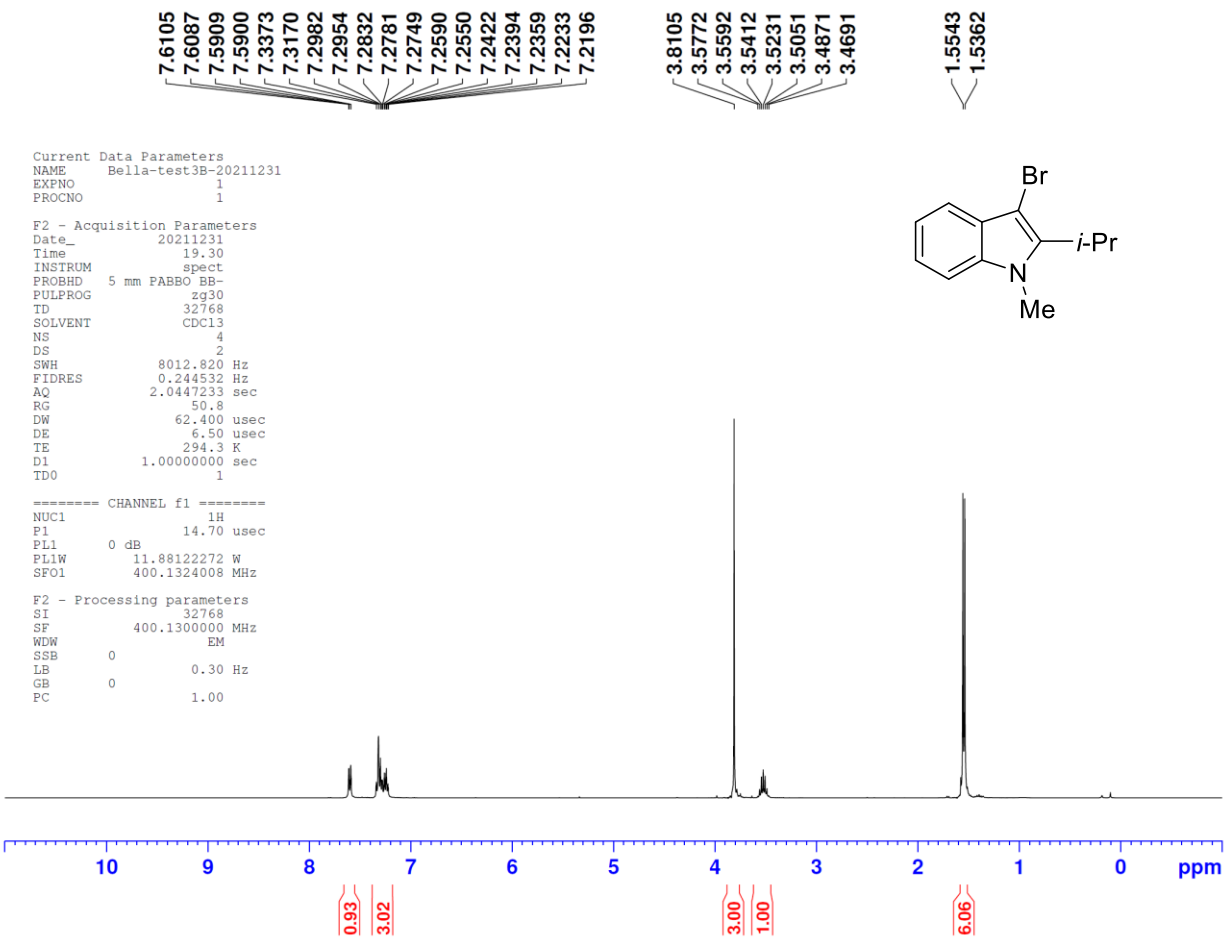

x10 5
+ESI Scan (rt: 0.489 min) Frag=150.0V L4.d Subtract
514.3604
472.9004
530.3549
552.3375
P(1-Ad)2
N
Me
5
4
3
2
450
460
470
480
490
500
510
520
530
540
550
560
570
580
Counts vs. Mass-to-Charge (m/z)

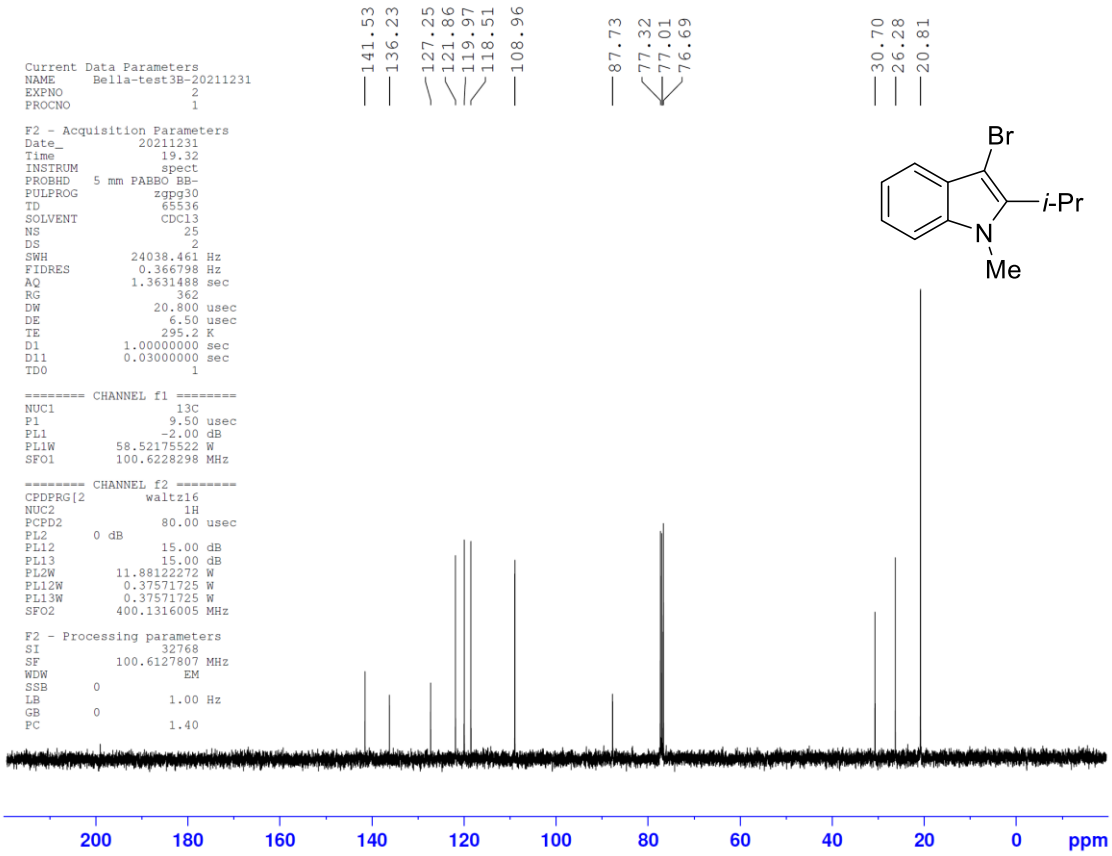

7.8431
7.6123
7.5934
7.3365
7.3170
7.2592
7.1994
7.1822
7.1637
7.1523
7.1333
7.1157
6.2996
3.1310
3.1137
3.0965
3.0793
3.0622
3.0450
3.0281
1.4020
1.3847
Current Data Parameters
NAME Bella-test1-20211230
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211230
Time 20.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 294.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
i-Pr
N
H
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
1.00
0.99
1.97
0.95
0.97
6.07

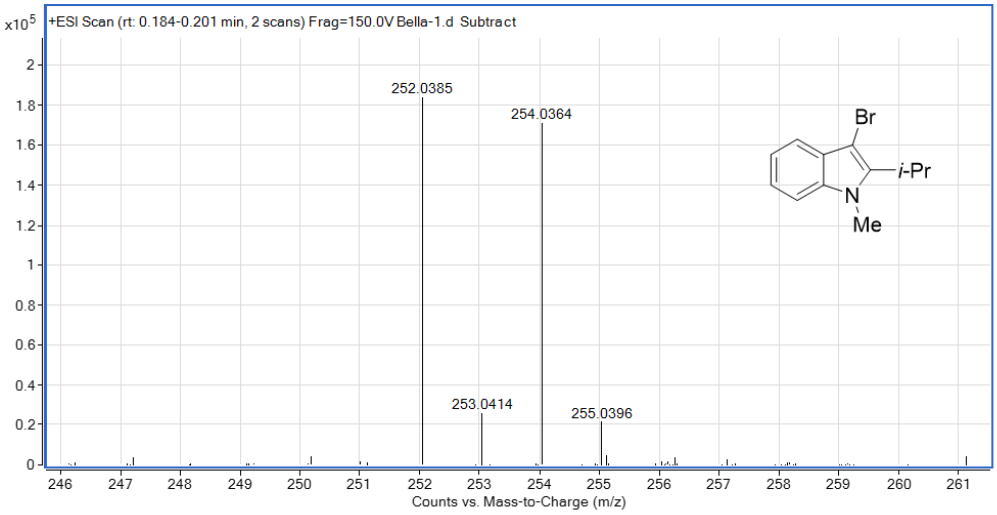

145.90
135.64
128.53
120.94
119.85
119.52
110.31
97.31
77.31
77.00
76.68
27.56
22.38
Current Data Parameters
NAME Bella-test1-20211230
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211230
Time 20.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 22
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 294.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127813 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
i-Pr
N
H
200
180
160
140
120
100
80
60
40
20
0
ppm

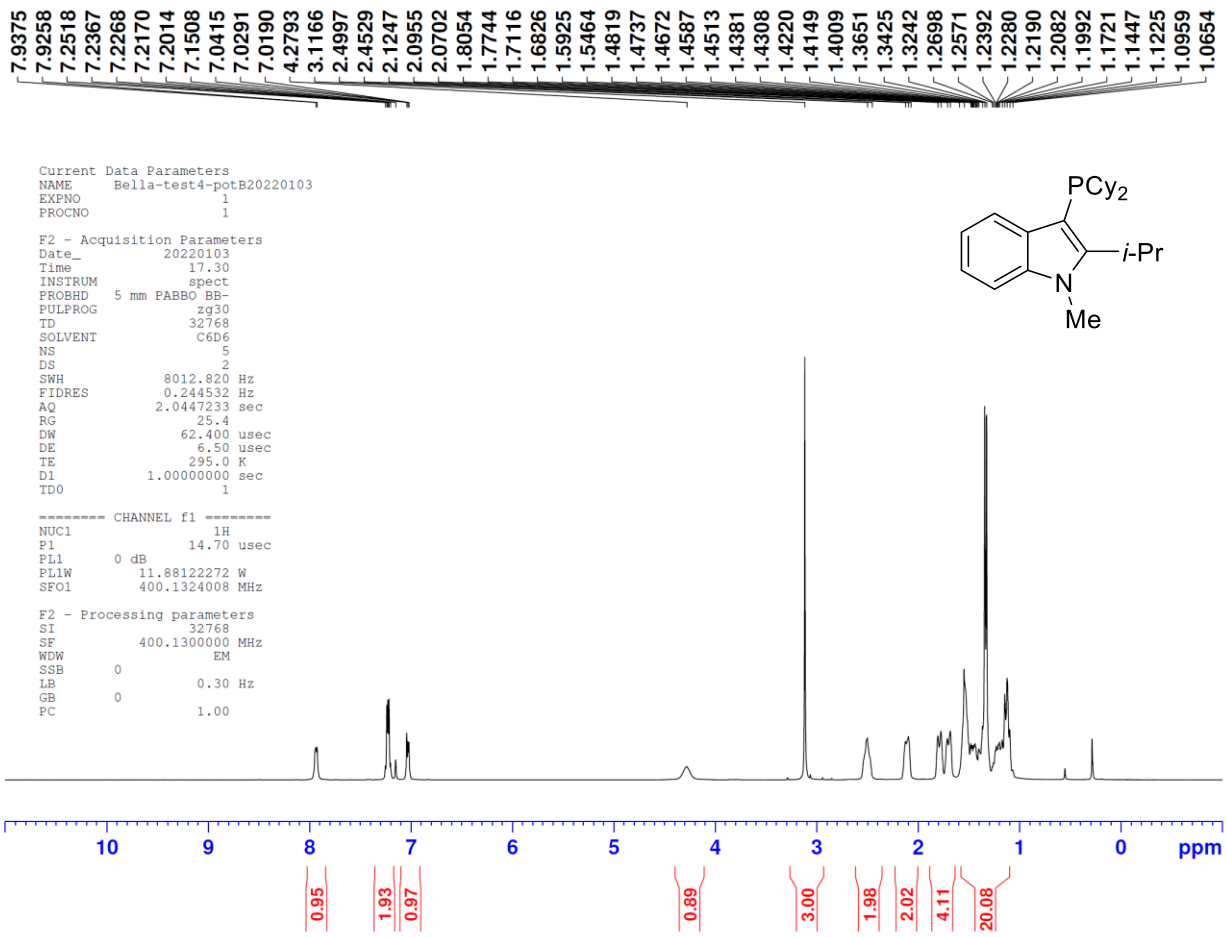

7.6303
7.6113
7.3467
7.3264
7.2602
7.2477
7.2301
7.2126
7.2098
7.1598
7.1411
7.1253
7.1230
6.3453
3.7459
3.1913
3.1745
3.1575
3.1406
3.1236
3.1067
3.0900
1.4236
1.4203
1.4066
1.4033
Current Data Parameters
NAME Bella-test2-20211231
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211231
Time 15.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 11
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 50.8
DW 62.400 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
i-Pr
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.02
1.06
1.05
1.00
3.12
1.02
6.07

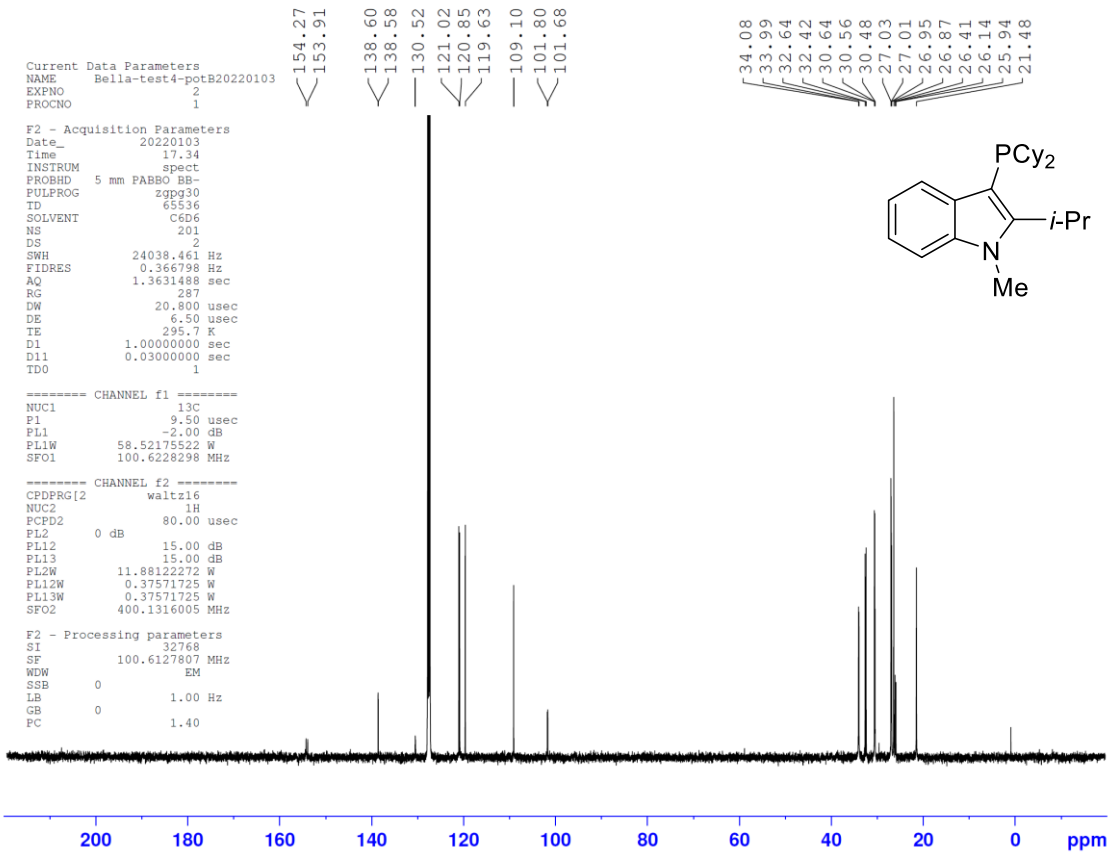

147.55
137.34
127.76
120.52
119.84
119.18
108.67
96.12
77.32
77.00
76.68
29.36
25.85
22.54
Current Data Parameters
NAME Bella-test2-20211231
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211231
Time 15.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 32
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127809 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
i-Pr
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

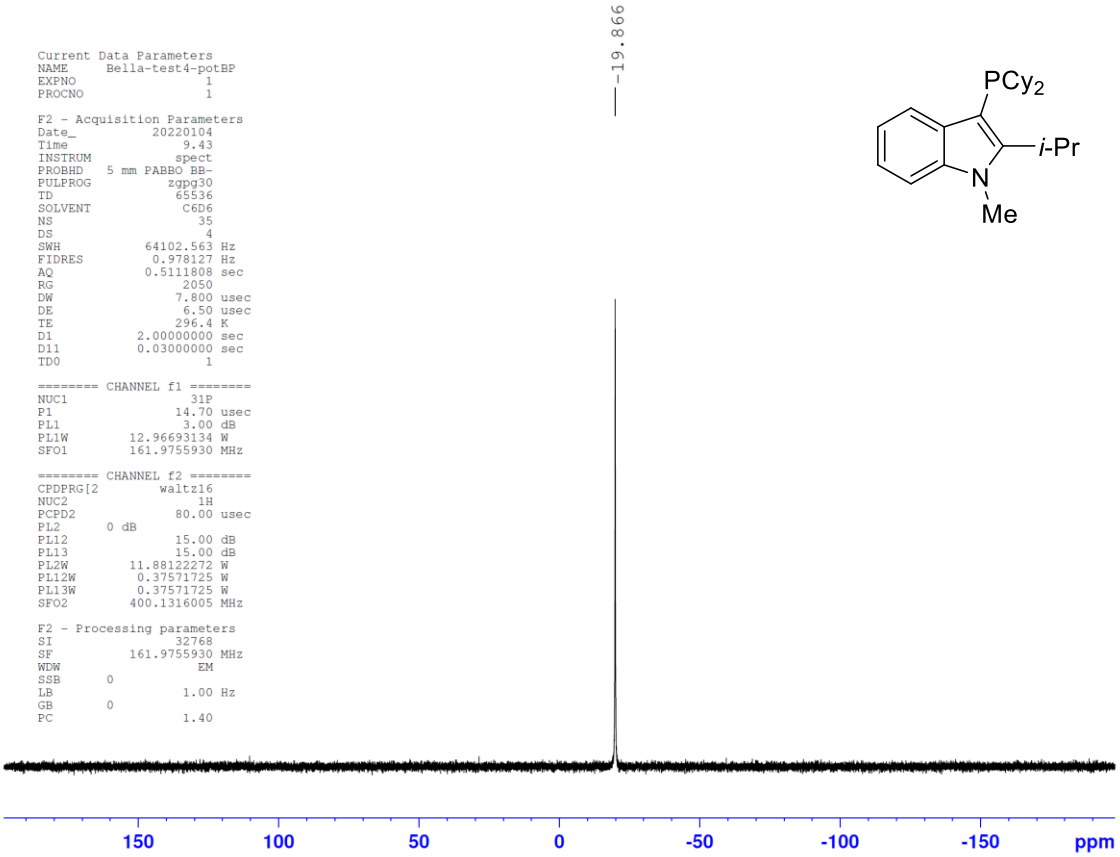

7.6105
7.6087
7.5909
7.5900
7.3373
7.3170
7.2982
7.2954
7.2832
7.2781
7.2749
7.2590
7.2550
7.2422
7.2394
7.2359
7.2233
7.2196
3.8105
3.5772
3.5592
3.5412
3.5231
3.5051
3.4871
3.4691
1.5543
1.5362
Current Data Parameters
NAME Bella-test3B-20211231
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211231
Time 19.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 50.8
DW 62.400 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Br
i-Pr
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
0.93
3.02
3.00
1.00
6.06

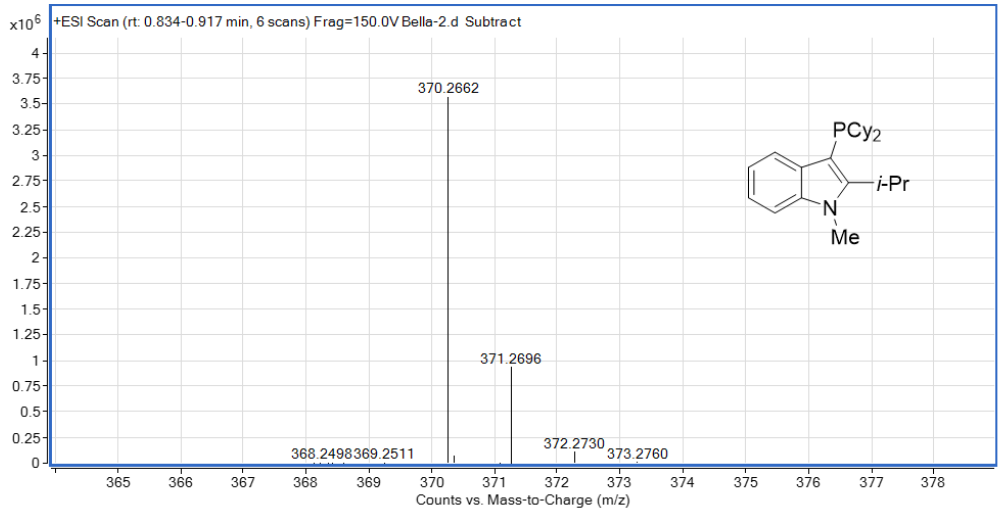

141.53
136.23
127.25
121.86
119.97
118.51
108.96
87.73
77.32
77.01
76.69
30.70
26.28
20.81
Current Data Parameters
NAME Bella-test3B-20211231
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211231
Time 19.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 25
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 362
DW 20.800 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127807 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Br
i-Pr
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

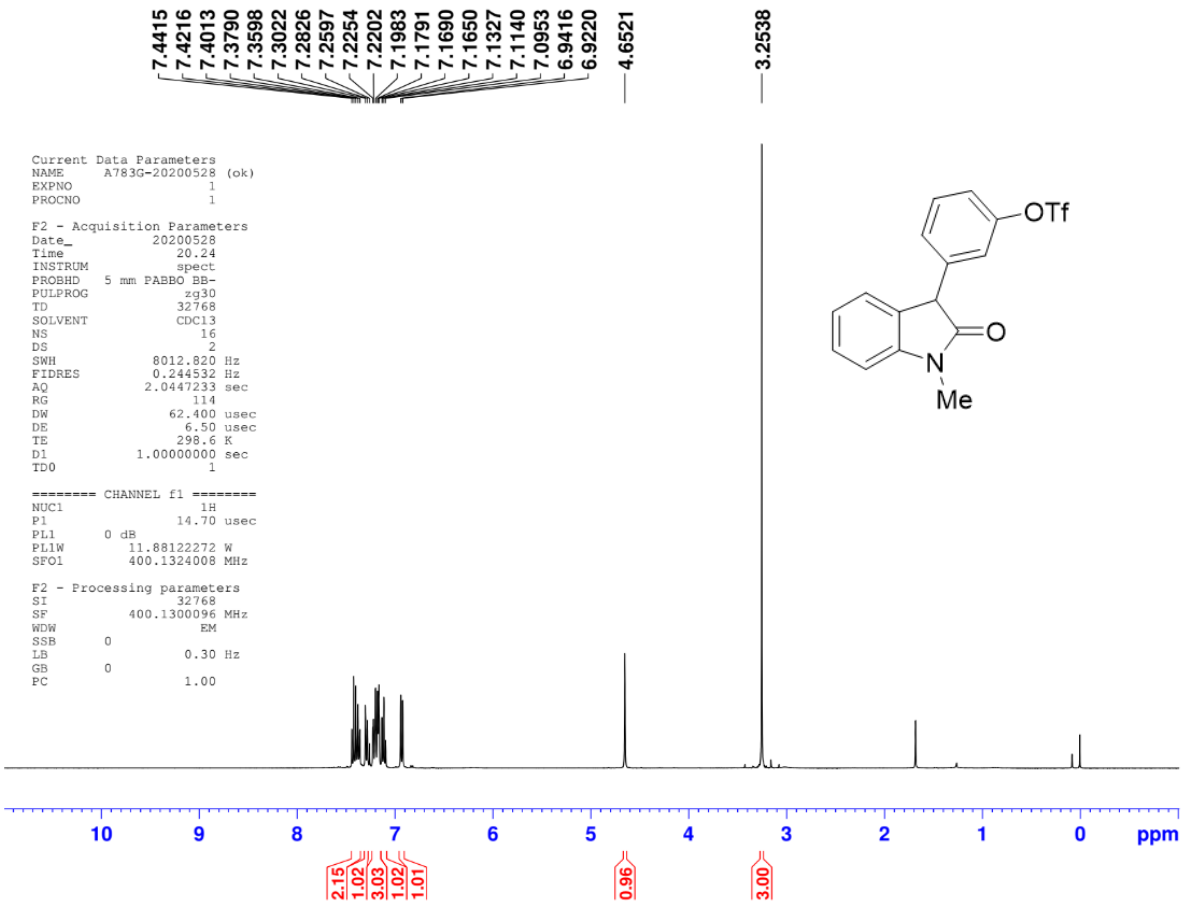

x10^5
+ESI Scan (rt: 0.184-0.201 min, 2 scans) Frag=150.0V Bella-1.d Subtract
252.0385
254.0364
253.0414
255.0396
Br
i-Pr
N
Me
Counts vs. Mass-to-Charge (m/z)

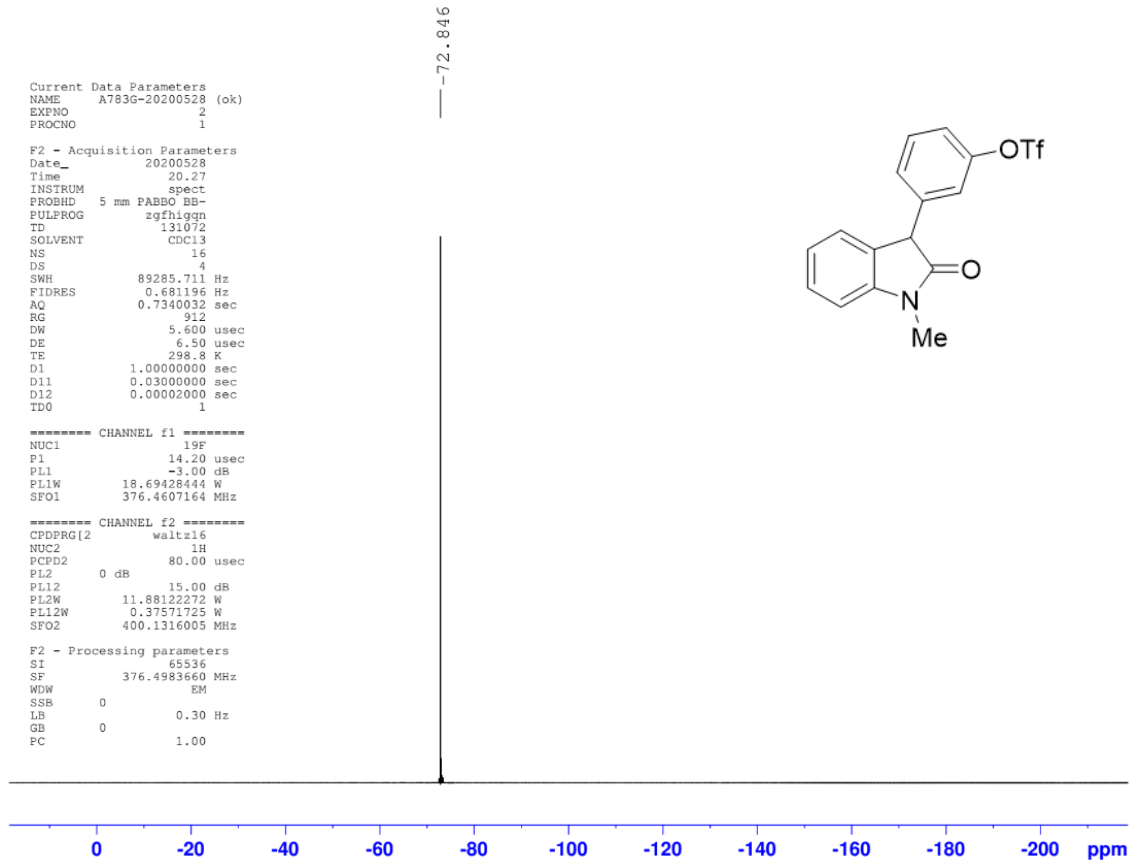

7.9375 7.9258 7.2518 7.2367 7.2268 7.2170 7.2014 7.1508 7.0415 7.0291 7.0190 4.2793 3.1166 2.4997 2.4529 2.1247 2.0955 2.0702 1.8054 1.7744 1.7116 1.6826 1.5925 1.5464 1.4819 1.4737 1.4672 1.4587 1.4513 1.4381 1.4308 1.4220 1.4149 1.4009 1.3651 1.3425 1.3242 1.2698 1.2571 1.2392 1.2280 1.2190 1.2082 1.1992 1.1721 1.1447 1.1225 1.0959 1.0654
Current Data Parameters
NAME Bella-test4-potB20220103
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220103
Time 17.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT C6D6
NS 5
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 25.4
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
PCy2
i-Pr
N
Me
10 9 8 7 6 5 4 3 2 1 0 ppm
0.95 1.93 0.97 0.89 3.00 1.98 2.02 4.11 20.08

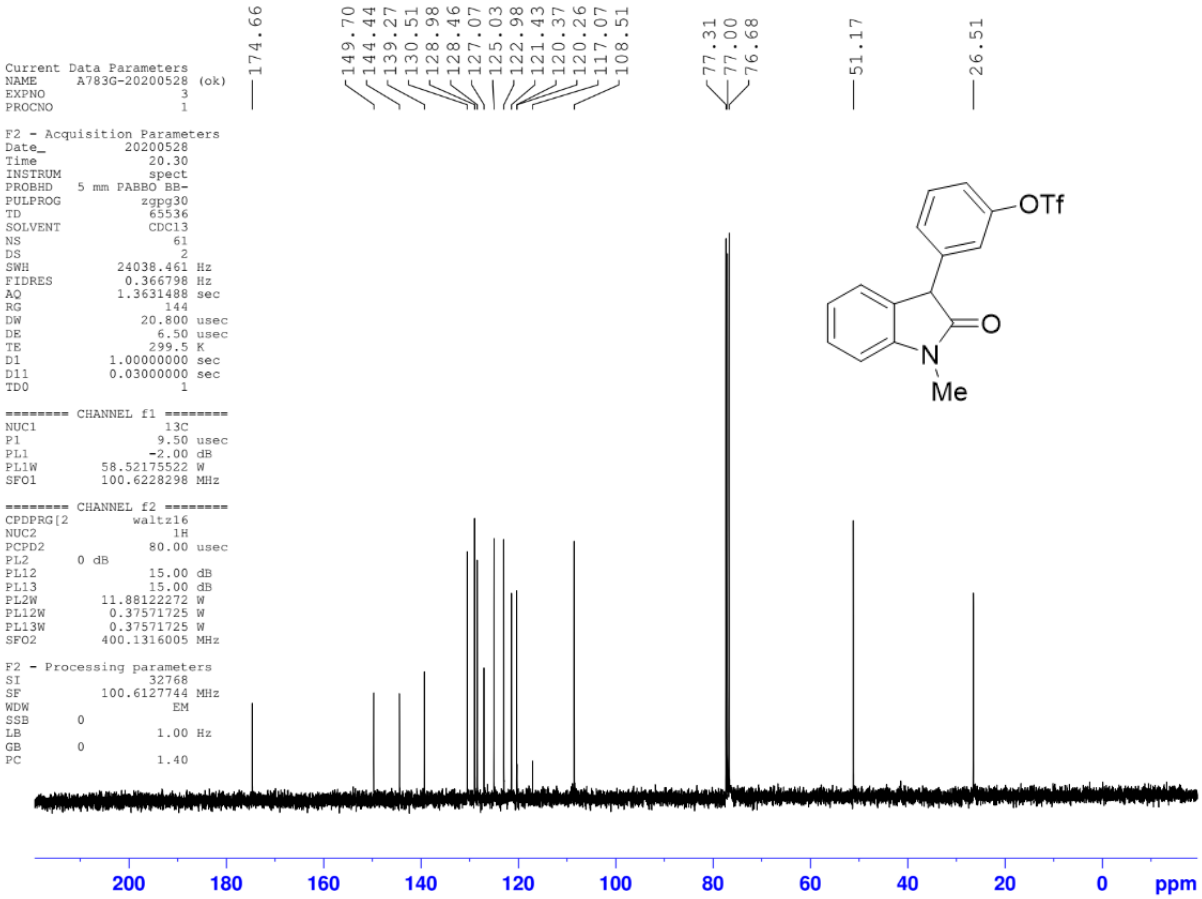

154.27 153.91 138.60 138.58 130.52 121.02 120.85 119.63 109.10 101.80 101.68
34.08 33.99 32.64 32.42 30.64 30.56 30.48 27.03 27.01 26.95 26.87 26.41 26.14 25.94 21.48
Current Data Parameters
NAME Bella-test4-potB20220103
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220103
Time 17.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 201
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 287
DW 20.800 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127807 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
PCy2
i-Pr
N
Me
200 180 160 140 120 100 80 60 40 20 0 ppm

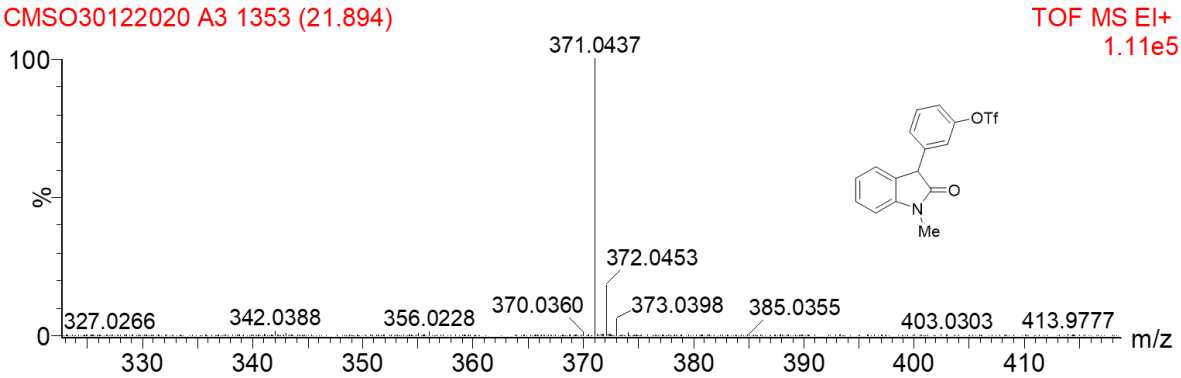

Current Data Parameters
NAME Bella-test4-potBP
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220104
Time 9.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT C6D6
NS 35
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 2050
DW 7.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 31P
P1 14.70 usec
PL1 3.00 dB
PL1W 12.96693134 W
SFO1 161.9755930 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 161.9755930 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
-19.866
PCy2
i-Pr
N
Me
150
100
50
0
-50
-100
-150
ppm

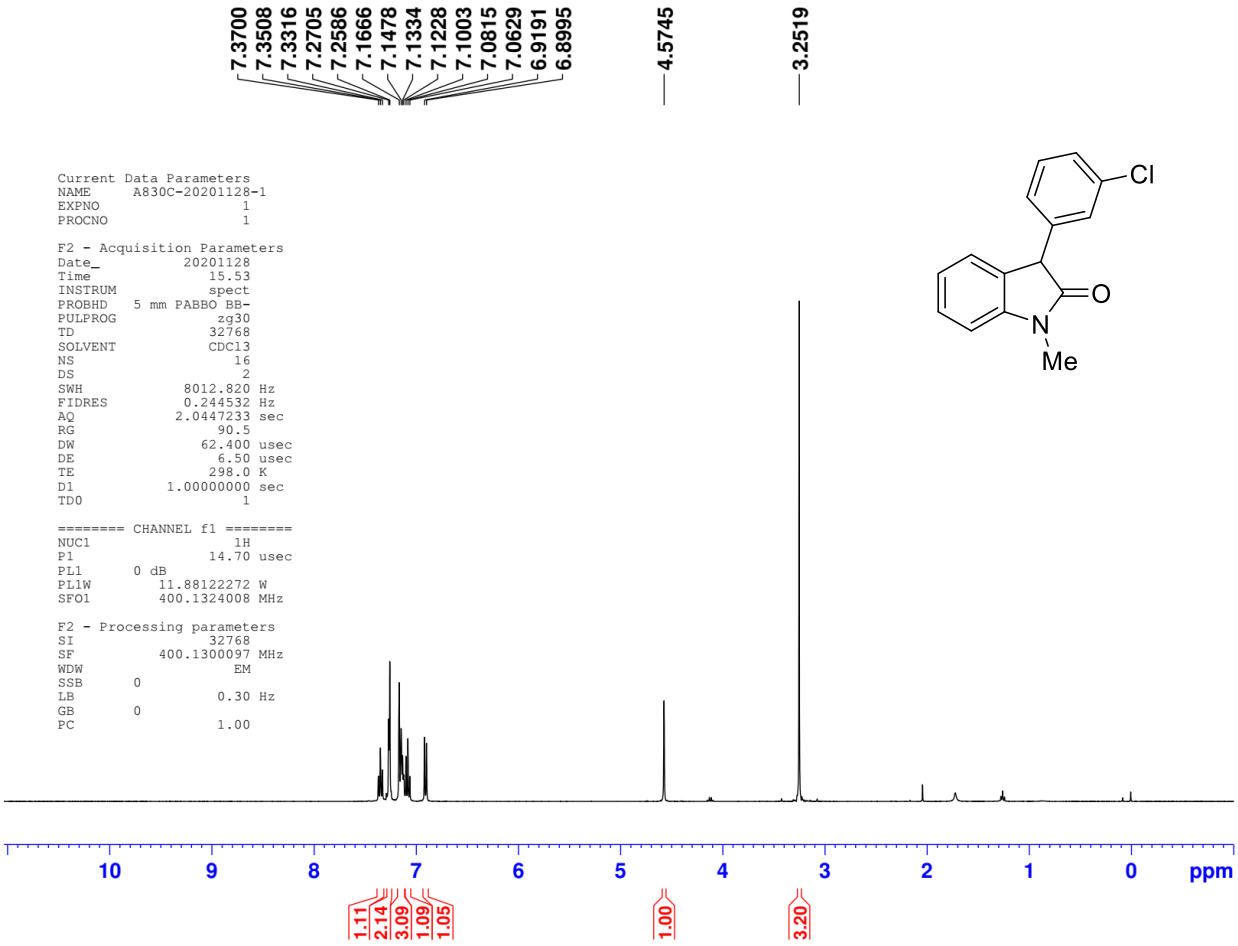

x10^6
+ESI Scan (rt: 0.834-0.917 min, 6 scans) Frag=150.0V Bella-2.d Subtract
370.2662
371.2696
372.2730
373.2760
368.2498
369.2511
PCy2
i-Pr
N
Me
Counts vs. Mass-to-Charge (m/z)

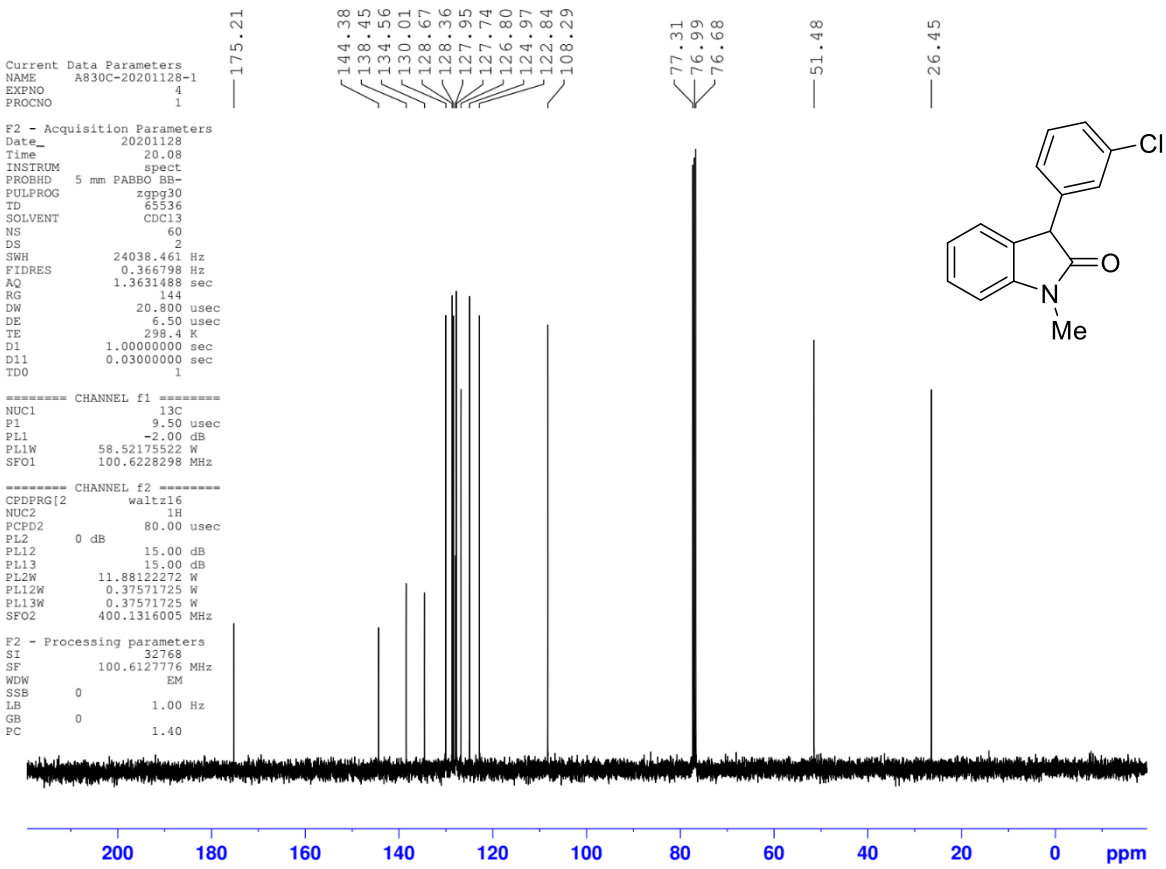

7.4415
7.4216
7.4013
7.3790
7.3598
7.3022
7.2826
7.2597
7.2254
7.2202
7.1983
7.1791
7.1690
7.1650
7.1327
7.1140
7.0953
6.9416
6.9220
4.6521
3.2538
Current Data Parameters
NAME A783G-20200528 (ok)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200528
Time 20.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
2.15
1.02
3.03
1.02
1.01
0.96
3.00

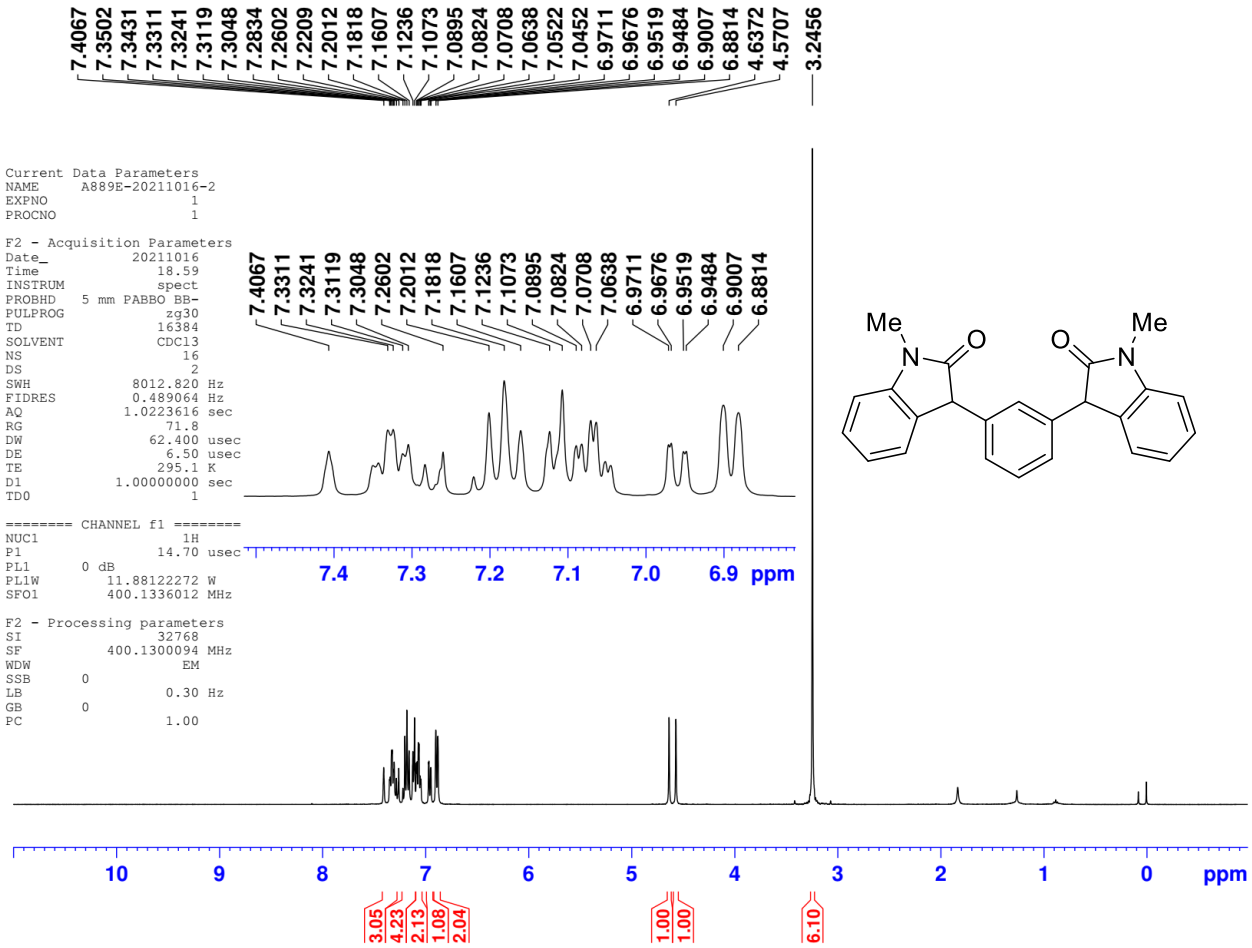

-72.846
Current Data Parameters
NAME A783G-20200528 (ok)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200528
Time 20.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.8 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

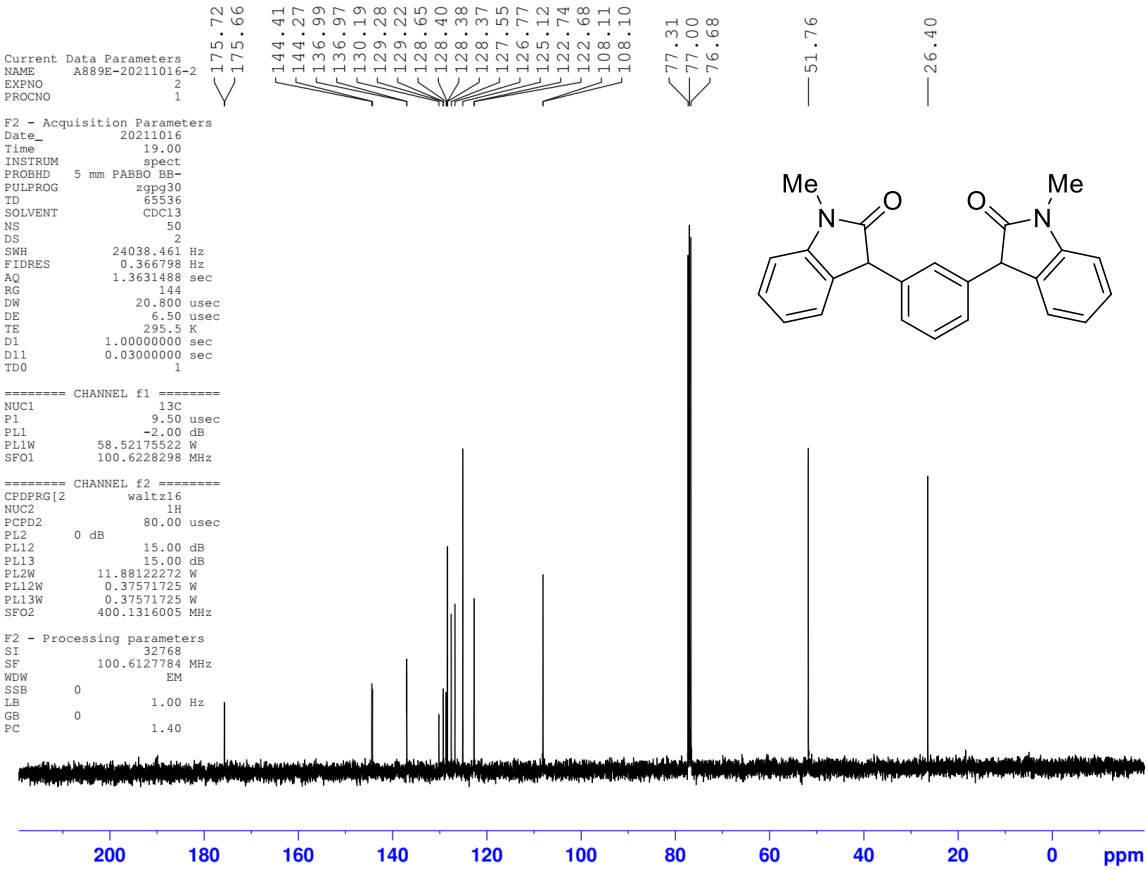

174.66
149.70
144.44
139.27
130.51
128.98
128.46
127.07
125.03
122.98
121.43
120.37
120.26
117.07
108.51
77.31
77.00
76.68
51.17
26.51
Current Data Parameters
NAME A783G-20200528 (ok)
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200528
Time 20.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 61
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127744 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OTf
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

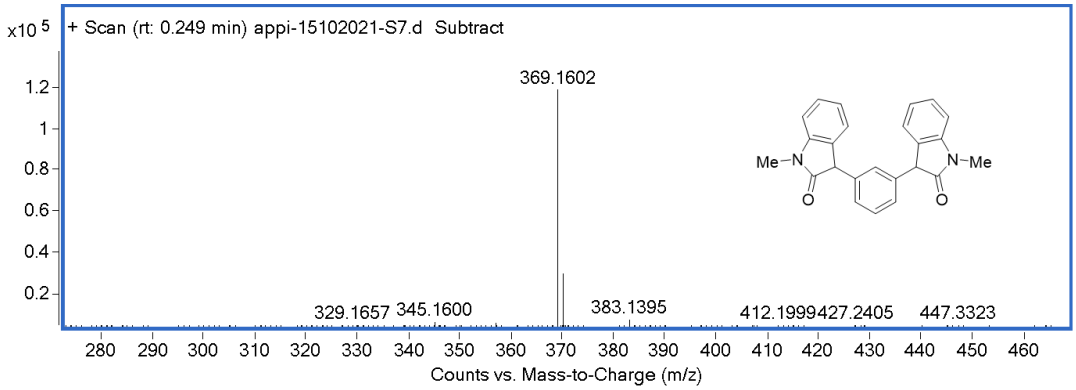

CMSO30122020 A3 1353 (21.894)
TOF MS EI+
1.11e5
100
%
0
371.0437
372.0453
327.0266
342.0388
356.0228
370.0360
373.0398
385.0355
403.0303
413.9777
330
340
350
360
370
380
390
400
410
m/z
OTf
O
N
Me

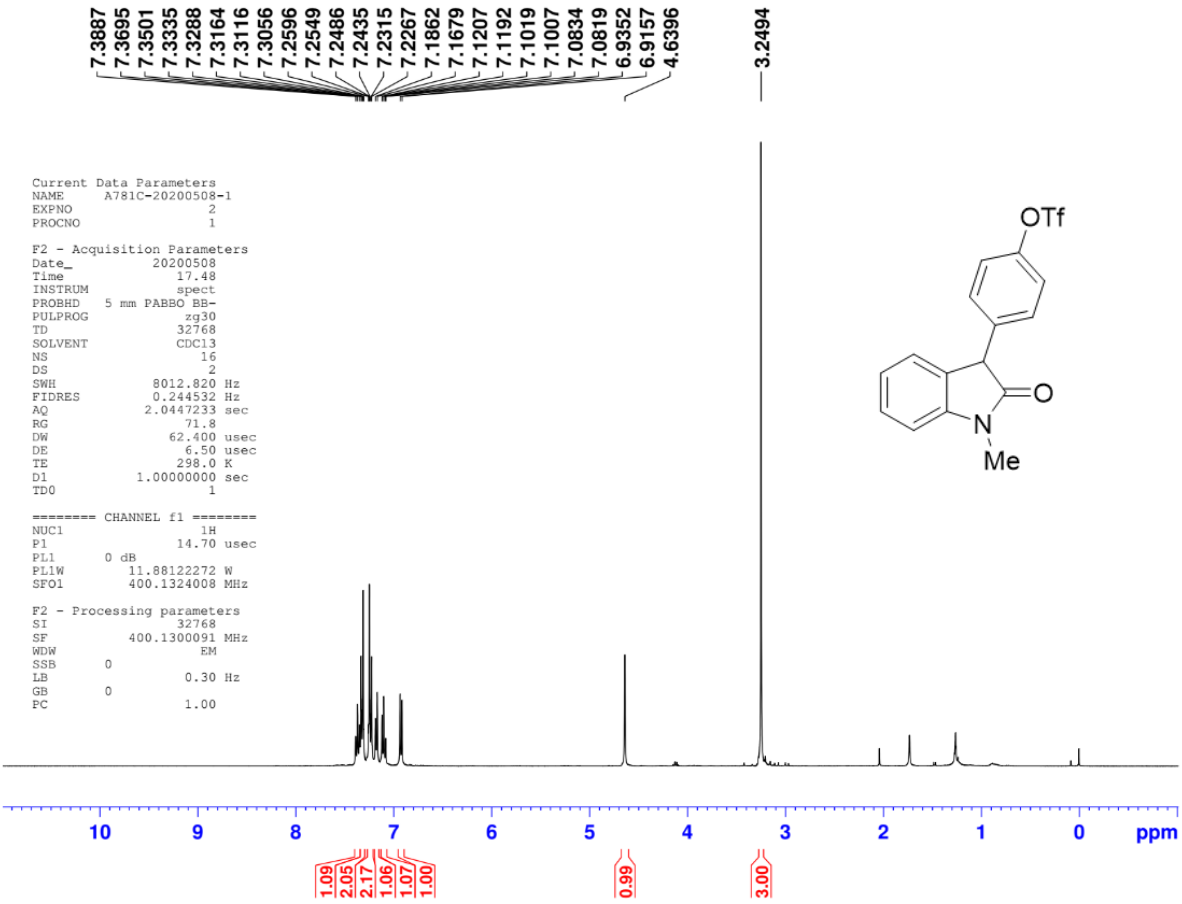

7.3700
7.3508
7.3316
7.2705
7.2586
7.1666
7.1478
7.1334
7.1228
7.1003
7.0815
7.0629
6.9191
6.8995
4.5745
3.2519
Current Data Parameters
NAME A830C-20201128-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201128
Time 15.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 90.5
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.11
2.14
3.09
1.09
1.05
1.00
3.20

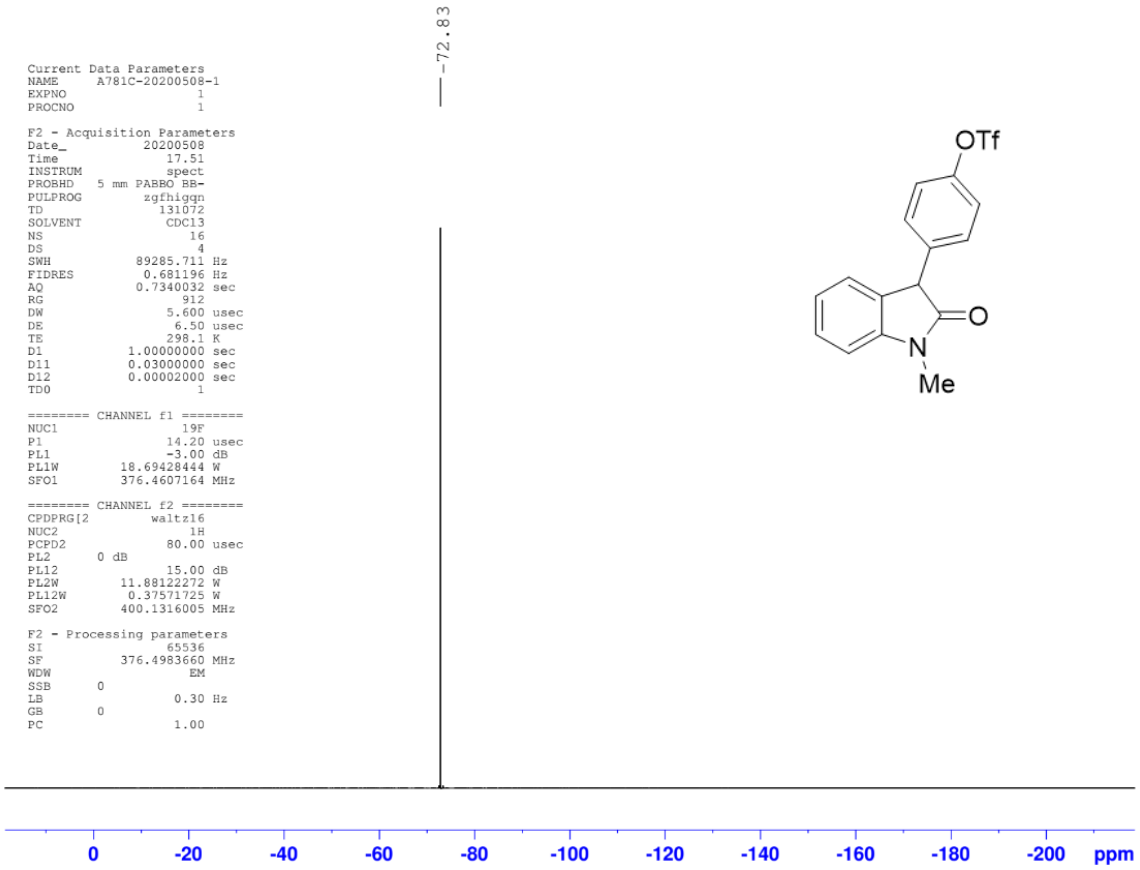

175.21
144.38
138.45
134.56
130.01
128.67
128.36
127.95
127.74
126.80
124.97
122.84
108.29
77.31
76.99
76.68
51.48
26.45
Current Data Parameters
NAME A830C-20201128-1
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201128
Time 20.08
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 60
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127776 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Cl
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

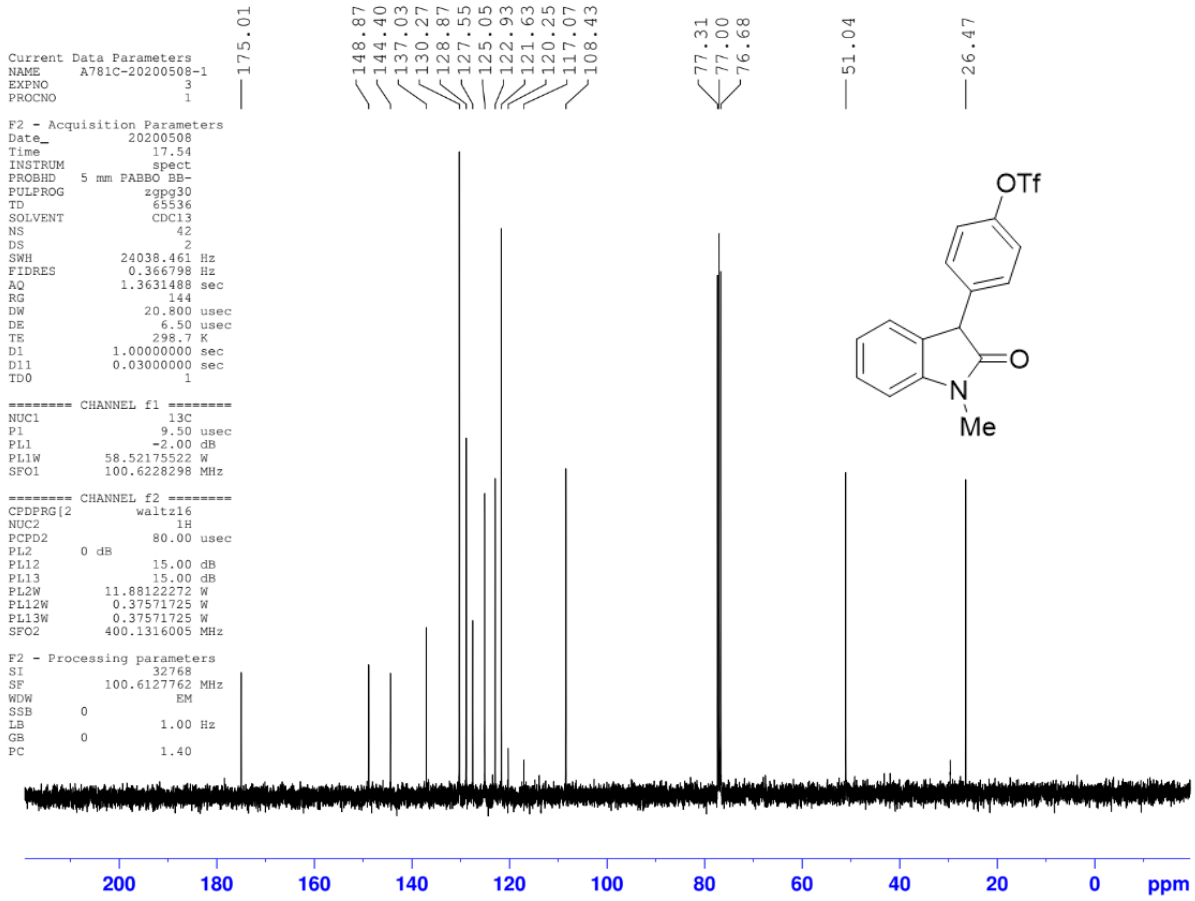

7.4067 7.3502 7.3431 7.3311 7.3241 7.3119 7.3048 7.2834 7.2602 7.2209 7.2012 7.1818 7.1607 7.1236 7.1073 7.0895 7.0824 7.0708 7.0638 7.0522 7.0452 6.9711 6.9676 6.9519 6.9484 6.9007 6.8814 4.6372 4.5707 3.2456
Current Data Parameters
NAME A889E-20211016-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211016
Time 18.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.4067 7.3311 7.3241 7.3119 7.3048 7.2602 7.2012 7.1818 7.1607 7.1236 7.1073 7.0895 7.0824 7.0708 7.0638 6.9711 6.9676 6.9519 6.9484 6.9007 6.8814
7.4 7.3 7.2 7.1 7.0 6.9 ppm
Me N O O N Me
10 9 8 7 6 5 4 3 2 1 0 ppm
3.05 4.23 2.13 1.08 2.04 1.00 1.00 6.10

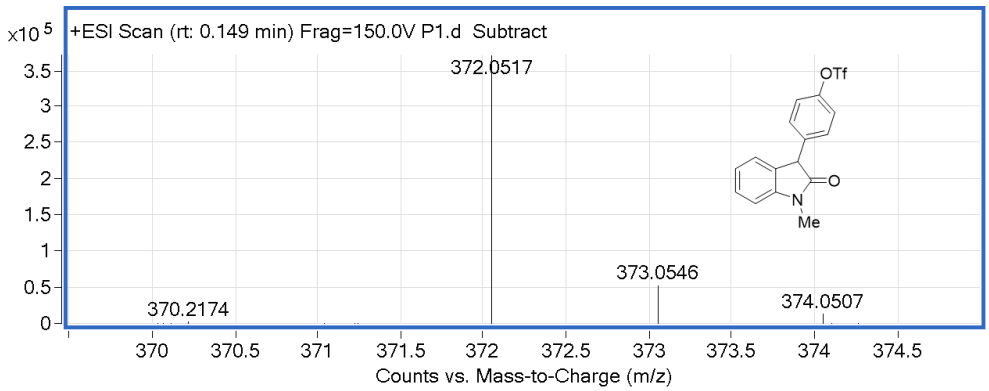

175.72 175.66 144.41 144.27 136.99 136.97 130.19 129.28 129.22 128.65 128.40 128.38 128.37 127.55 126.77 125.12 122.74 122.68 108.11 108.10 77.31 77.00 76.68 51.76 26.40
Current Data Parameters
NAME A889E-20211016-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211016
Time 19.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 50
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127784 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me N O O N Me
200 180 160 140 120 100 80 60 40 20 0 ppm

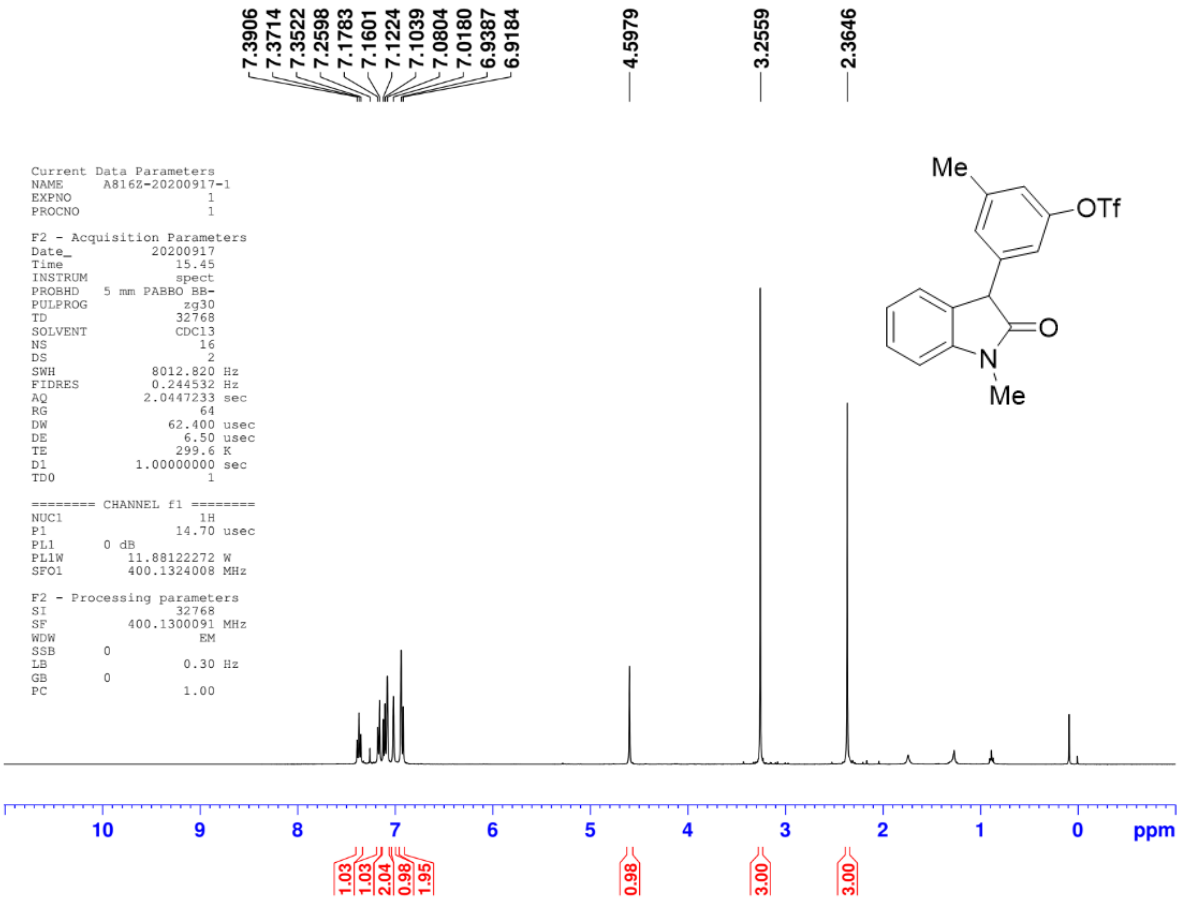

x10 5
+ Scan (rt: 0.249 min) appi-15102021-S7.d Subtract
369.1602
329.1657
345.1600
383.1395
412.1999
427.2405
447.3323
Counts vs. Mass-to-Charge (m/z)
Me
N
O
O
N
Me

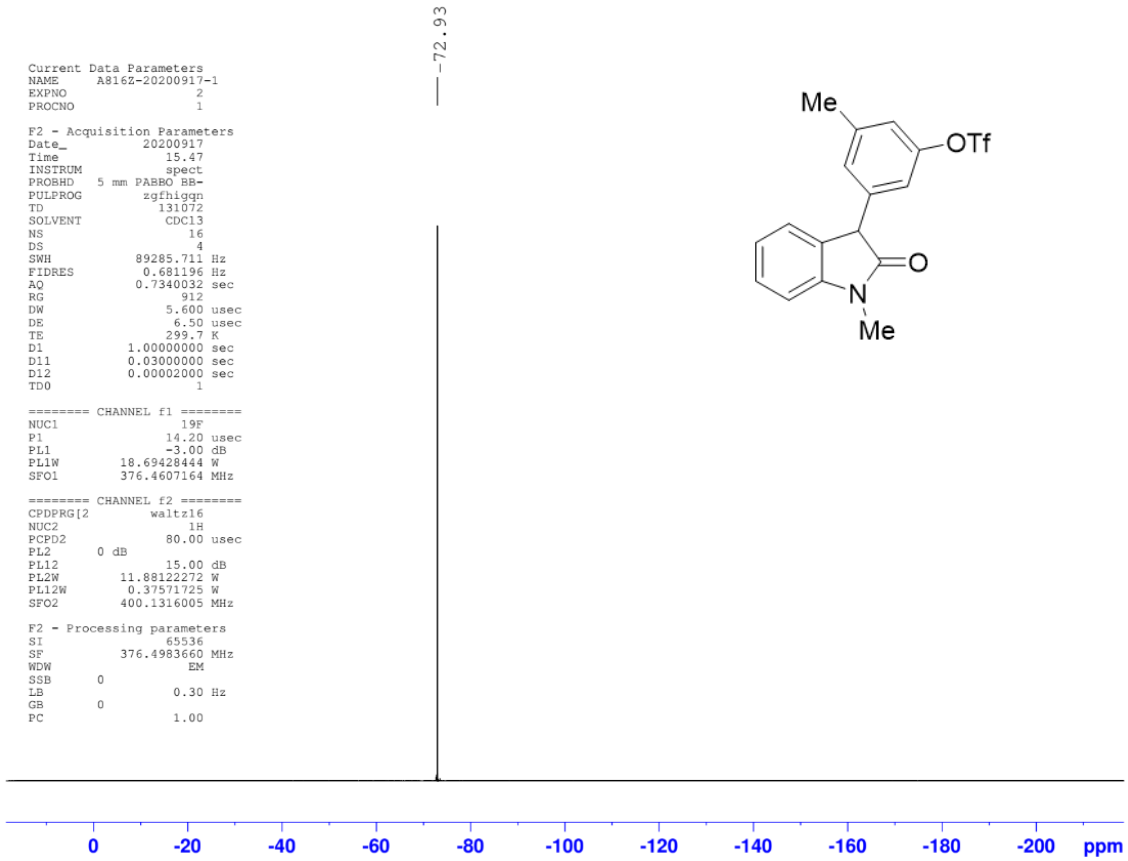

7.3887
7.3695
7.3501
7.3335
7.3288
7.3164
7.3116
7.3056
7.2596
7.2549
7.2486
7.2435
7.2315
7.2267
7.1862
7.1679
7.1207
7.1192
7.1019
7.1007
7.0834
7.0819
6.9352
6.9157
4.6396
3.2494
Current Data Parameters
NAME A781C-20200508-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200508
Time 17.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.09
2.05
2.17
1.06
1.07
1.00
0.99
3.00

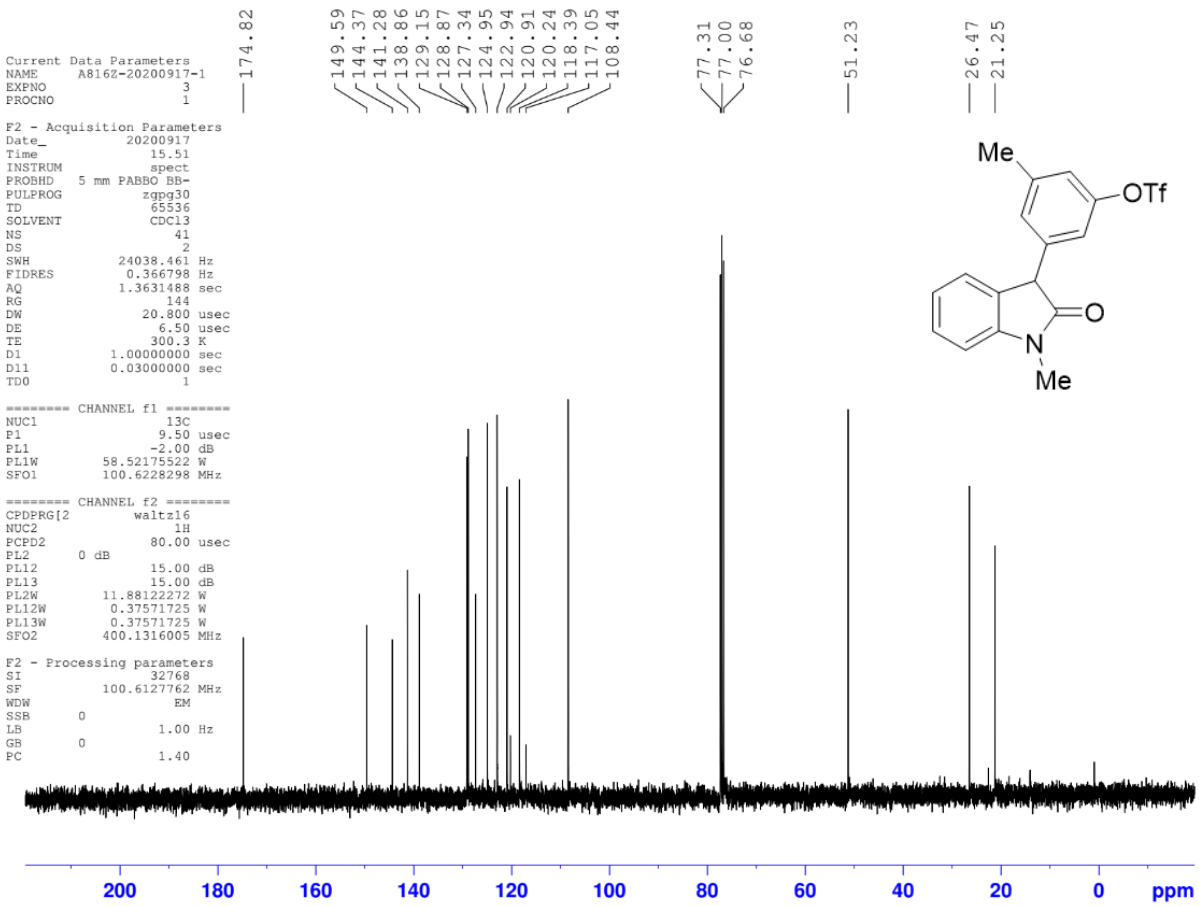

-72.83
Current Data Parameters
NAME A781C-20200508-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200508
Time 17.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

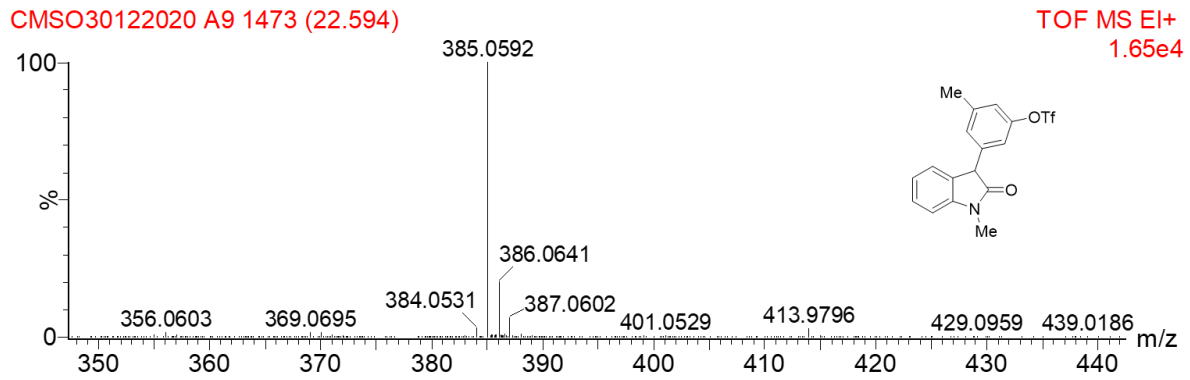

175.01
148.87
144.40
137.03
130.27
128.87
127.55
125.05
122.93
121.63
120.25
117.07
108.43
77.31
77.00
76.68
51.04
26.47
Current Data Parameters
NAME A781C-20200508-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200508
Time 17.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 42
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127762 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OTf
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

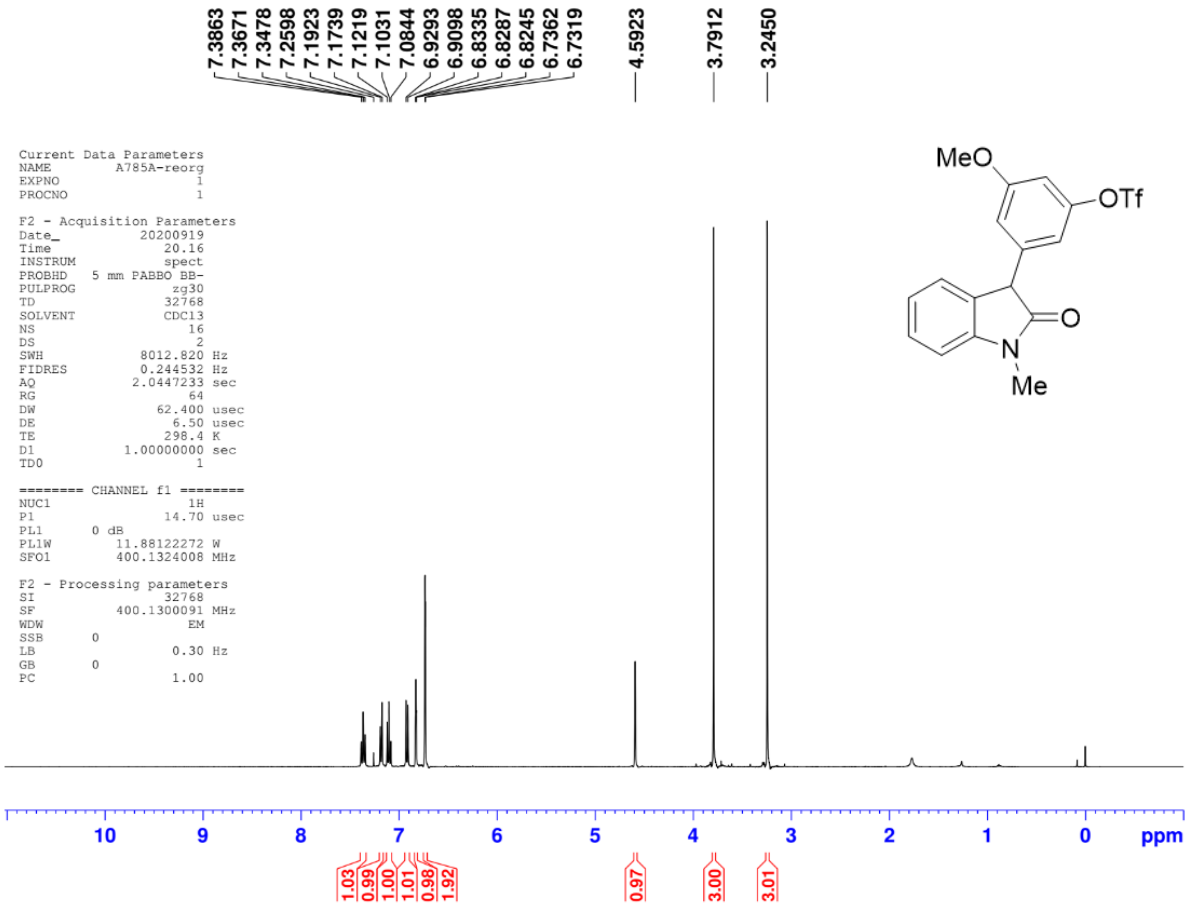

x10 5
+ESI Scan (rt: 0.149 min) Frag=150.0V P1.d Subtract
372.0517
373.0546
374.0507
370.2174
OTf
O
N
Me
3.5
3
2.5
2
1.5
1
0.5
0
370
370.5
371
371.5
372
372.5
373
373.5
374
374.5
Counts vs. Mass-to-Charge (m/z)

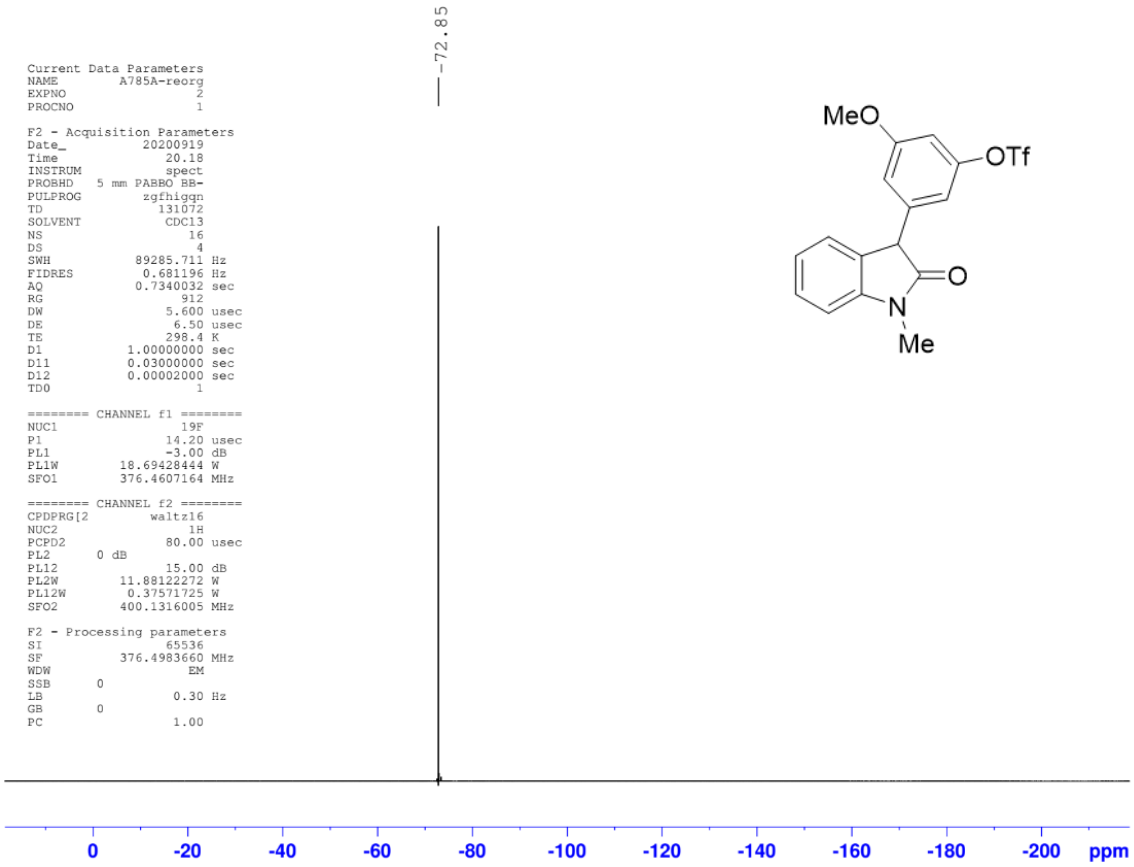

7.3906
7.3714
7.3522
7.2598
7.1783
7.1601
7.1224
7.1039
7.0804
7.0180
6.9387
6.9184
4.5979
3.2559
2.3646
Current Data Parameters
NAME A816Z-20200917-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200917
Time 15.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
OTf
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
1.03
2.04
0.98
1.95
0.98
3.00
3.00

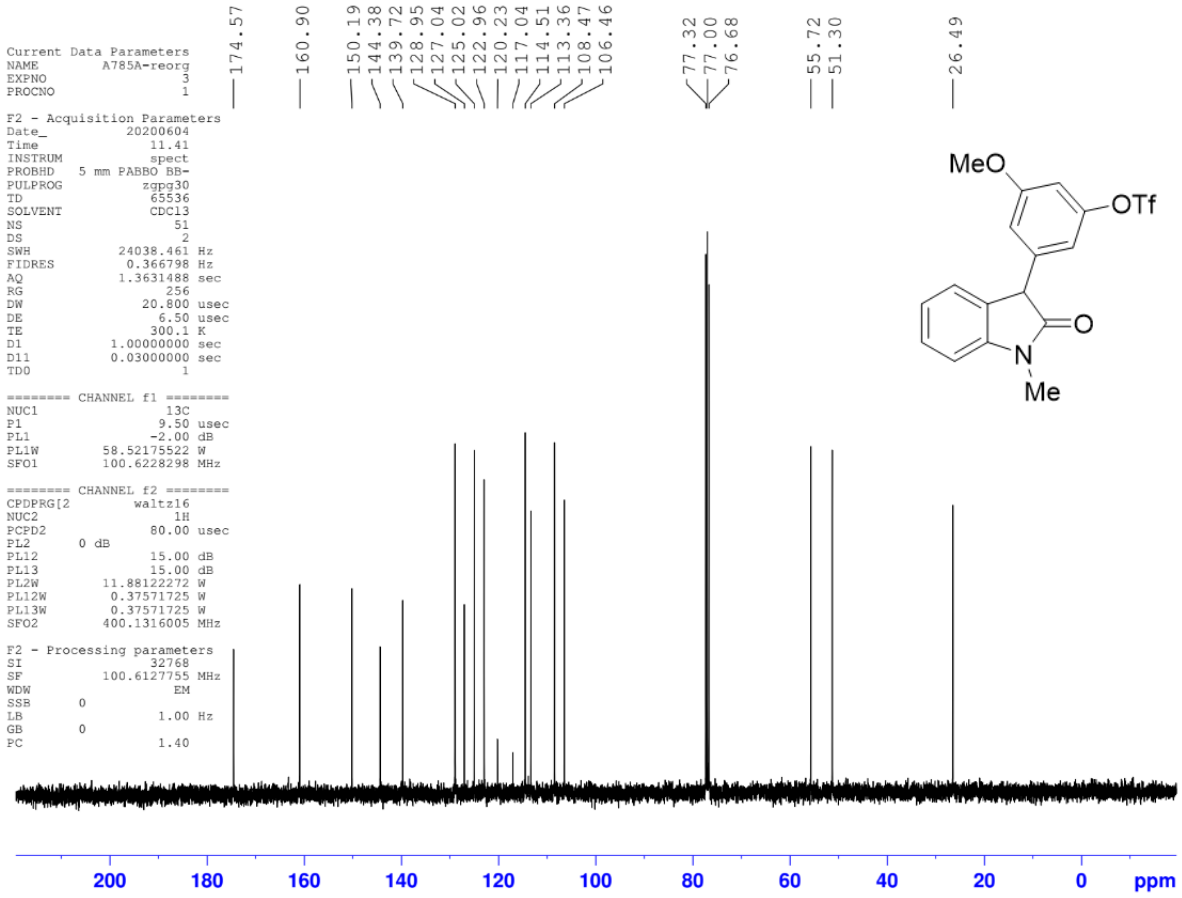

72.93
Current Data Parameters
NAME A816Z-20200917-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200917
Time 15.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
OTf
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

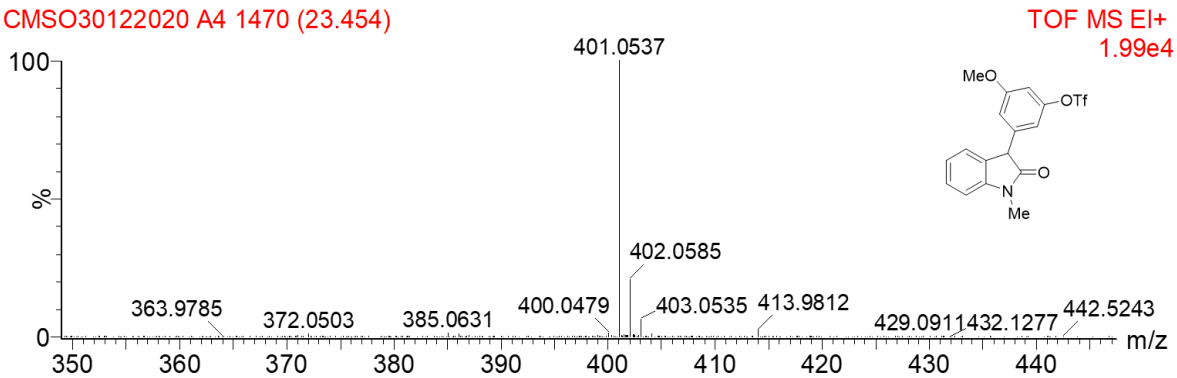

174.82
149.59
144.37
141.28
138.86
129.15
128.87
127.34
124.95
122.94
120.91
120.24
118.39
117.05
108.44
77.31
77.00
76.68
51.23
26.47
21.25
Current Data Parameters
NAME A816Z-20200917-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200917
Time 15.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 41
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 300.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127762 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
OTf
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

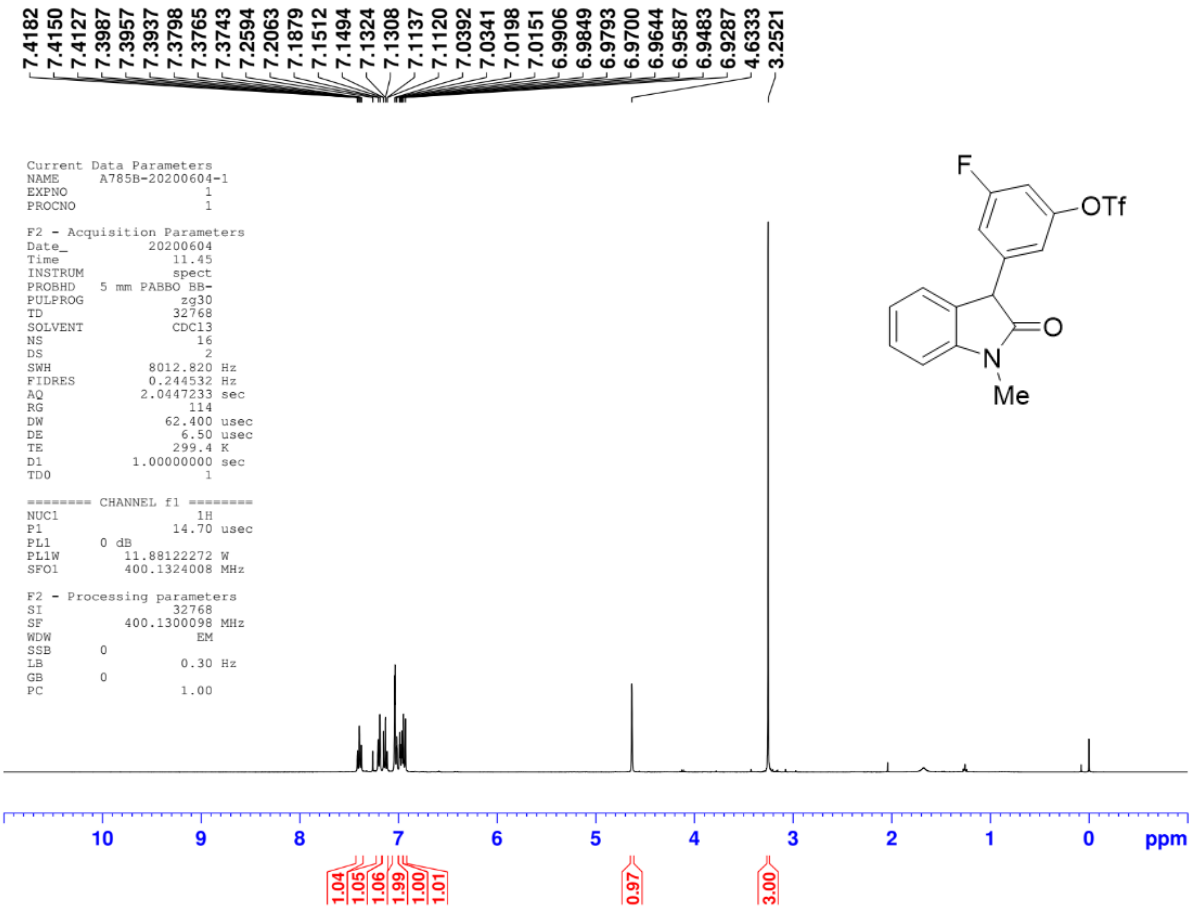

CMSO30122020 A9 1473 (22.594)
TOF MS EI+
1.65e4
100
%
0
385.0592
386.0641
384.0531
387.0602
356.0603
369.0695
401.0529
413.9796
429.0959
439.0186
m/z
350
360
370
380
390
400
410
420
430
440
Me
OTf
O
N
Me

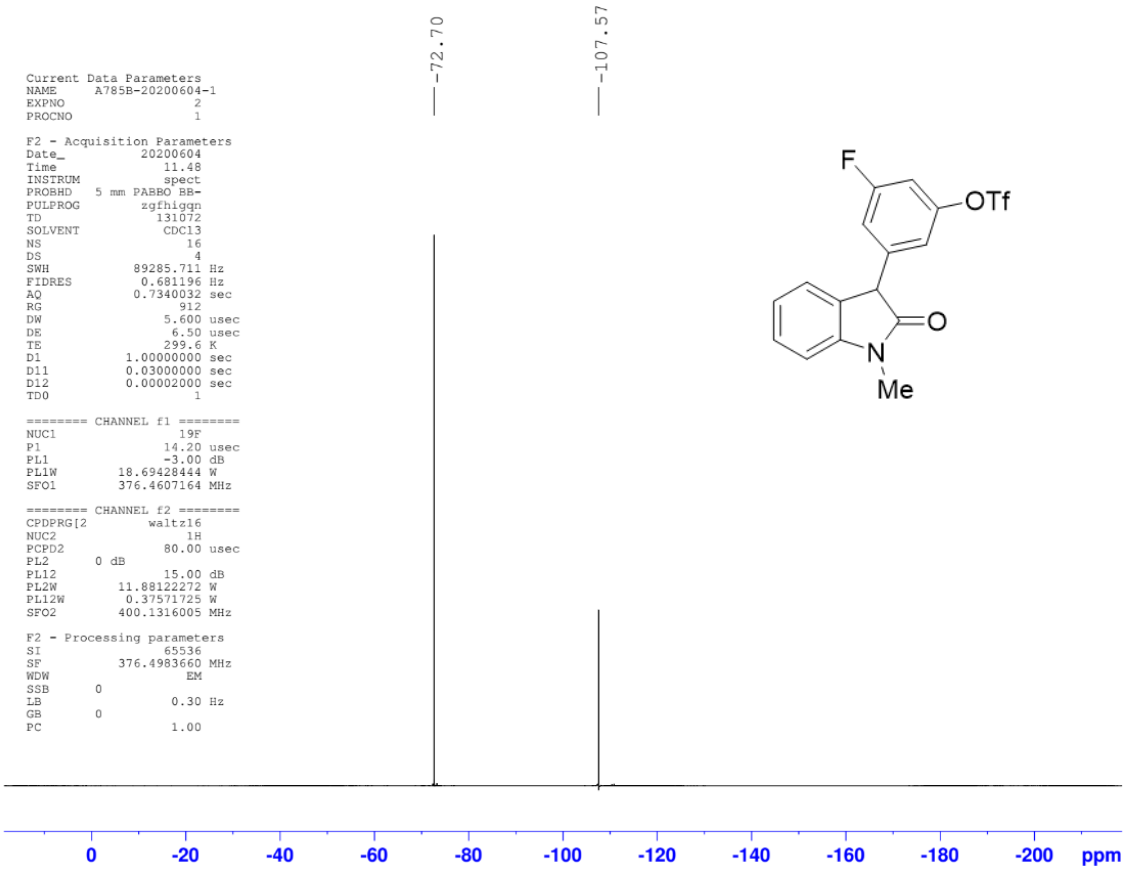

7.3863
7.3671
7.3478
7.2598
7.1923
7.1739
7.1219
7.1031
7.0844
6.9293
6.9098
6.8335
6.8287
6.8245
6.7362
6.7319
4.5923
3.7912
3.2450
Current Data Parameters
NAME A785A-reorg
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200919
Time 20.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
OTf
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.03
0.99
1.00
1.01
0.98
1.92
0.97
3.00
3.01

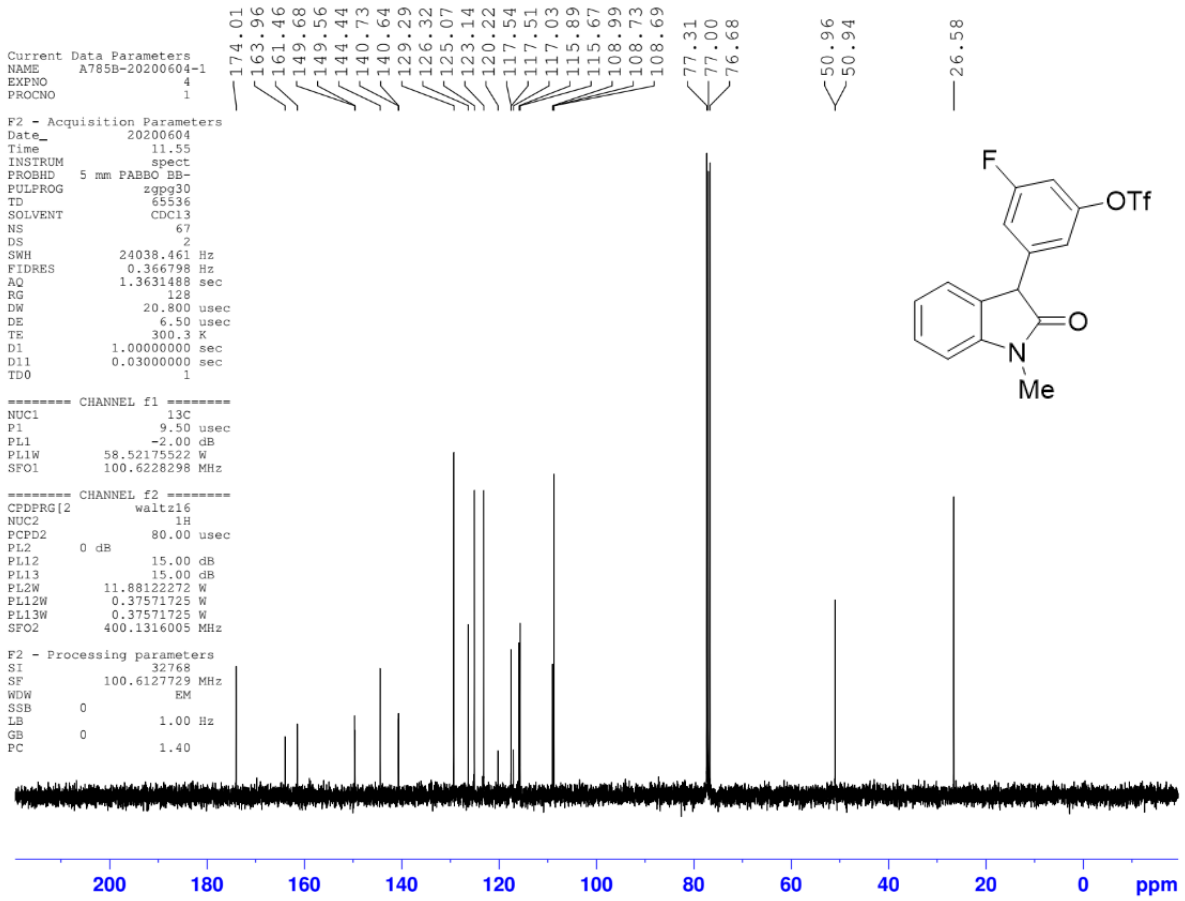

-72.85
Current Data Parameters
NAME A785A-reorg
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200919
Time 20.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDC13
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
MeO
OTf
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

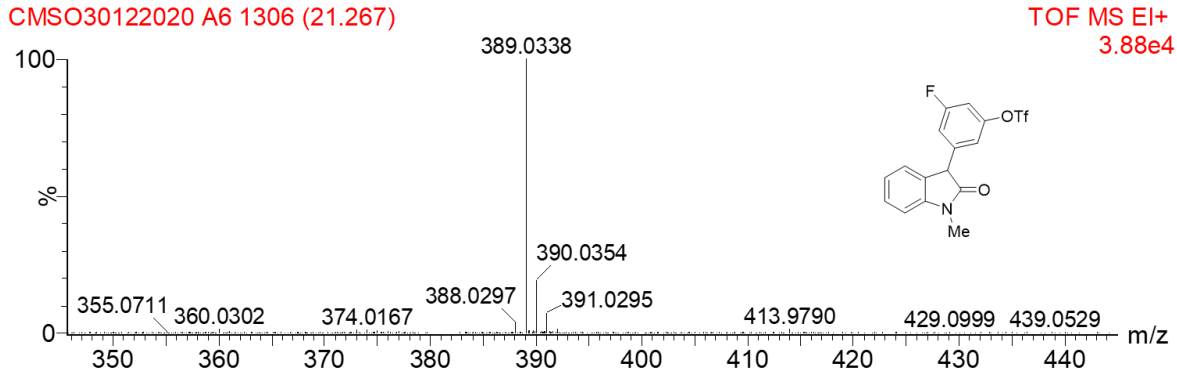

174.57
160.90
150.19
144.38
139.72
128.95
127.04
125.02
122.96
120.23
117.04
114.51
113.36
108.47
106.46
77.32
77.00
76.68
55.72
51.30
26.49
Current Data Parameters
NAME A785A-reorg
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200604
Time 11.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 51
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 256
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
MeO
OTf
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

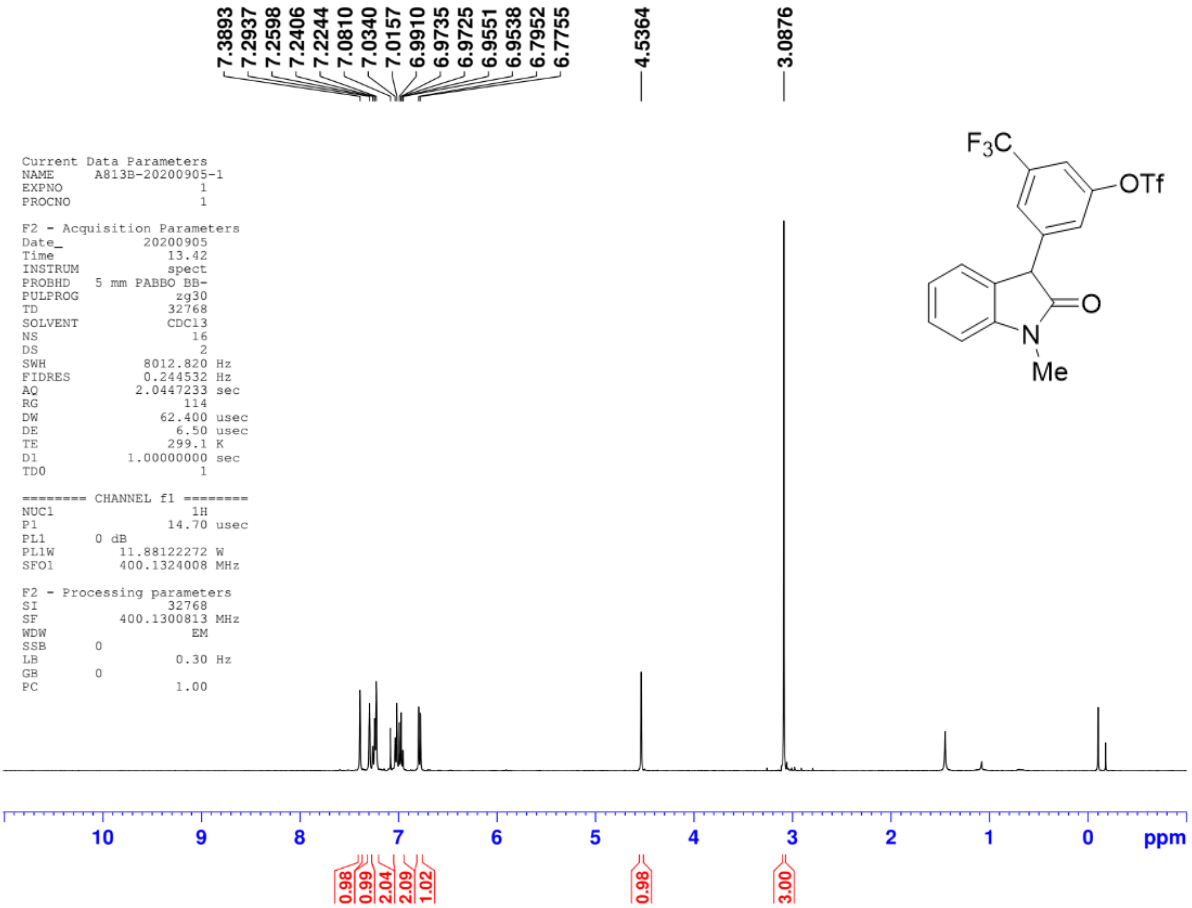

CMSO30122020 A4 1470 (23.454)
TOF MS EI+
1.99e4
100
%
0
401.0537
402.0585
363.9785
372.0503
385.0631
400.0479
403.0535
413.9812
429.0911
432.1277
442.5243
MeO
OTf
O
N
Me
350
360
370
380
390
400
410
420
430
440
m/z

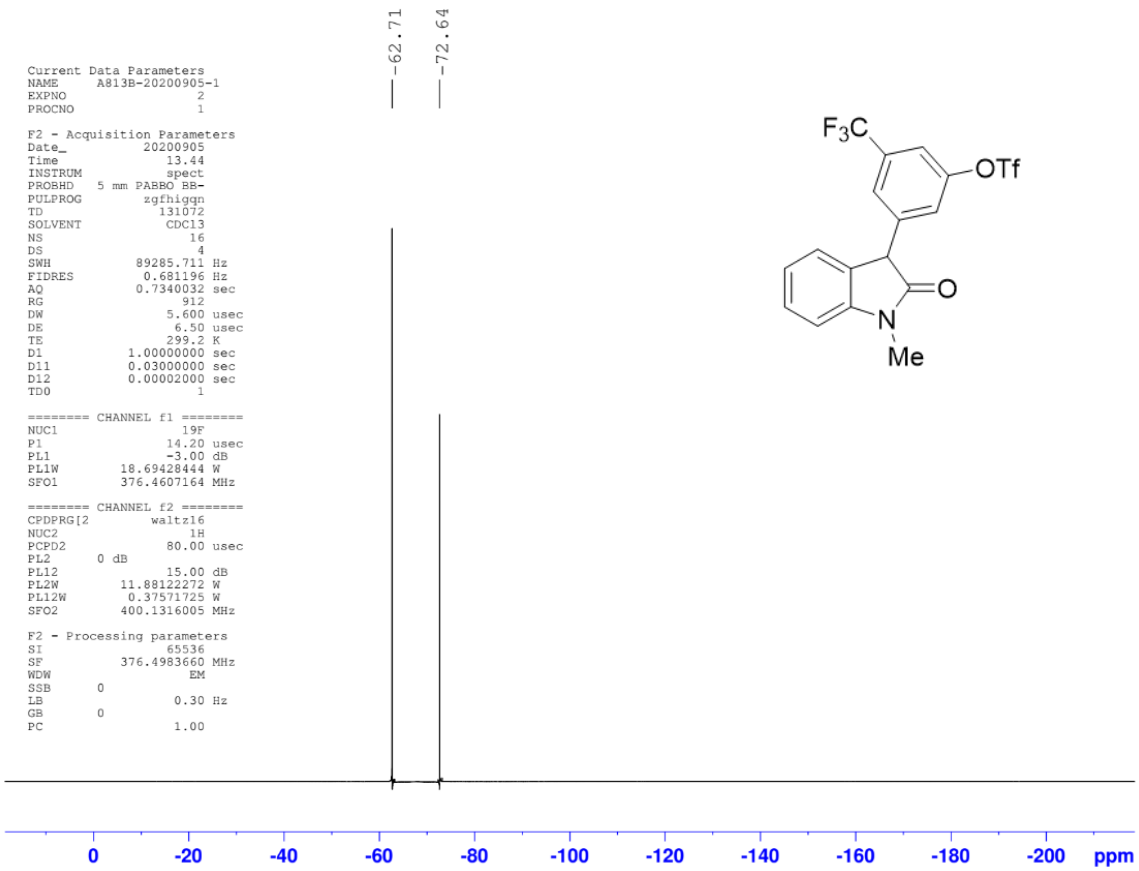

7.4182
7.4150
7.4127
7.3987
7.3957
7.3937
7.3798
7.3765
7.3743
7.2594
7.2063
7.1879
7.1512
7.1494
7.1324
7.1308
7.1137
7.1120
7.0392
7.0341
7.0198
7.0151
6.9906
6.9849
6.9793
6.9700
6.9644
6.9587
6.9483
6.9287
4.6333
3.2521
Current Data Parameters
NAME A785B-20200604-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200604
Time 11.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 299.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300098 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
F
OTf
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.04
1.05
1.06
1.99
1.00
1.01
0.97
3.00

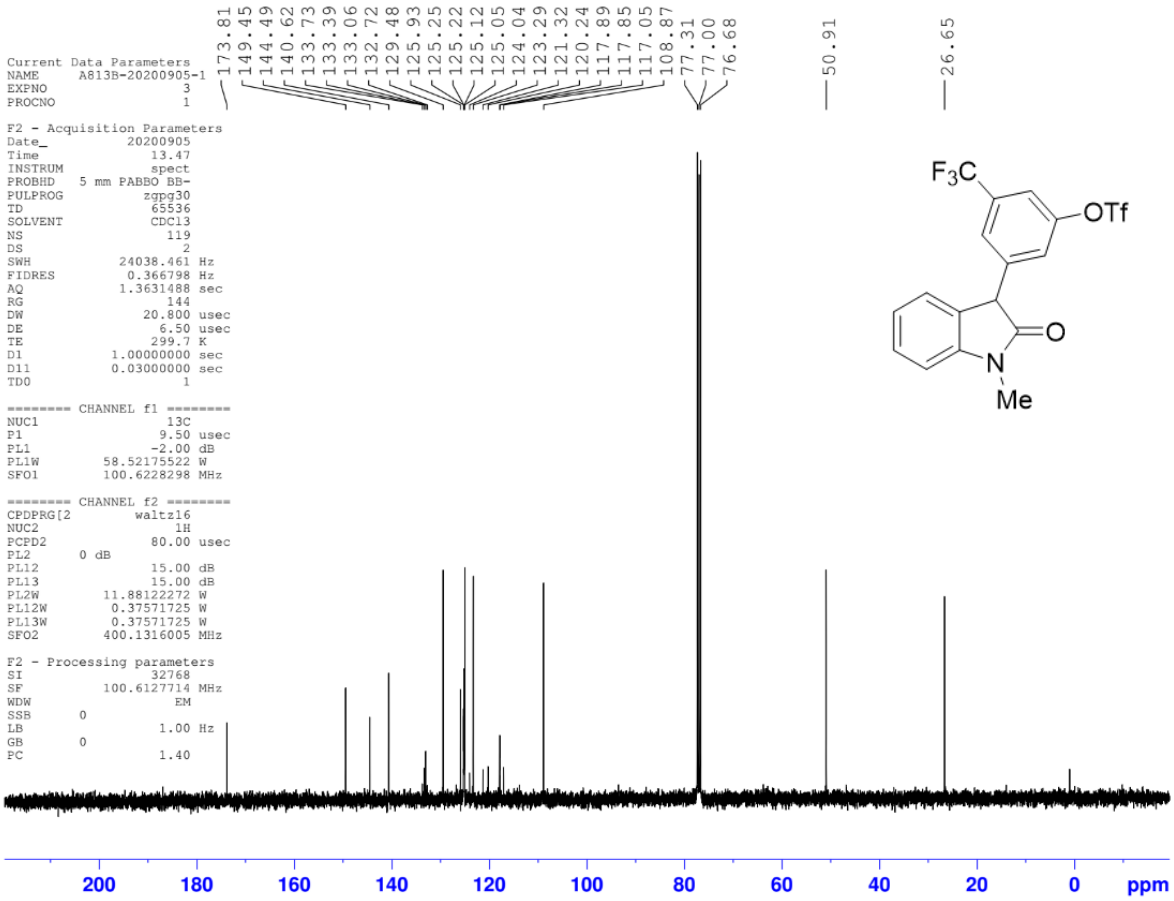

-72.70
-107.57
Current Data Parameters
NAME A785B-20200604-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200604
Time 11.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 299.6 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
F
OTf
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

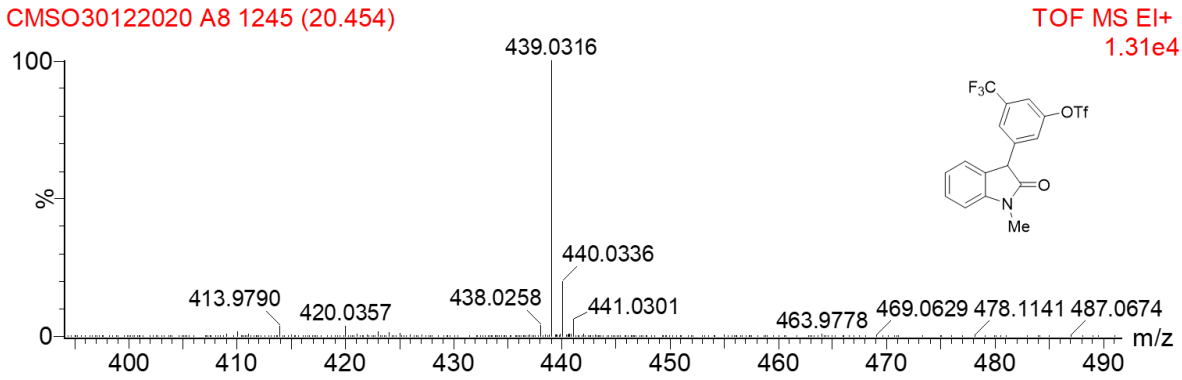

174.01
163.96
161.46
149.68
149.56
144.44
140.73
140.64
129.29
126.32
125.07
123.14
120.22
117.54
117.51
117.03
115.89
115.67
108.99
108.73
108.69
77.31
77.00
76.68
50.96
50.94
26.58
Current Data Parameters
NAME A785B-20200604-1
EXPNO 4
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200604
Time 11.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 67
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 128
DW 20.800 usec
DE 6.50 usec
TE 300.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
F
OTf
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

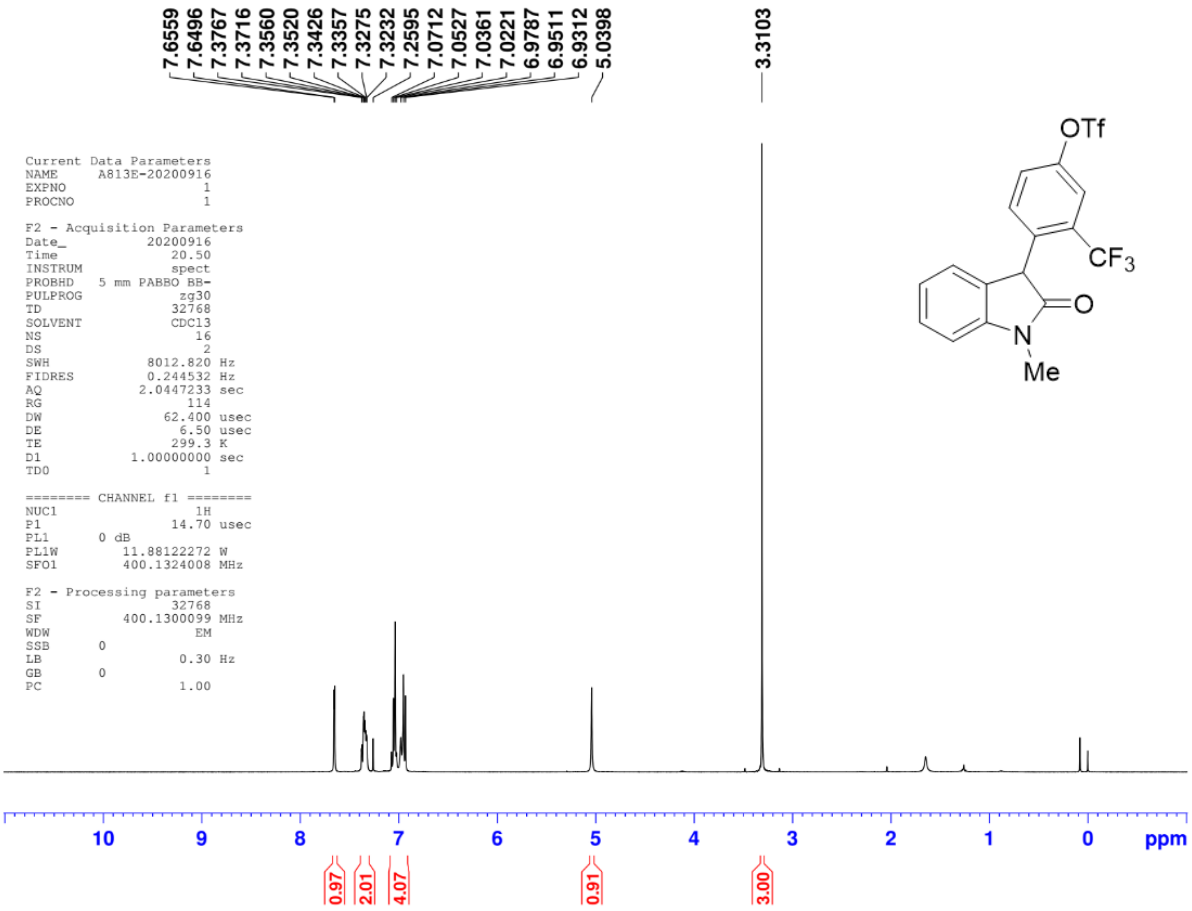

CMSO30122020 A6 1306 (21.267)
TOF MS EI+
3.88e4
100
%
0
389.0338
390.0354
388.0297
391.0295
355.0711
360.0302
374.0167
413.9790
429.0999
439.0529
m/z
350
360
370
380
390
400
410
420
430
440
F
OTf
O
N
Me

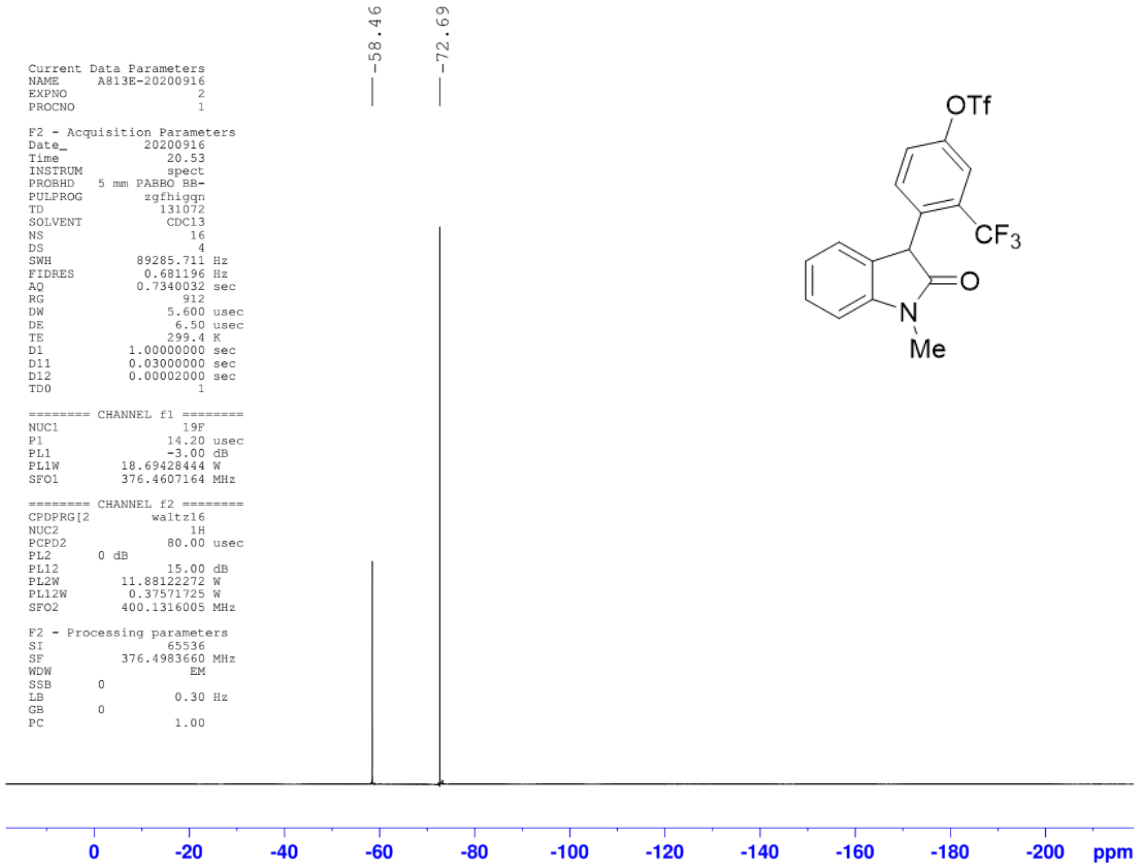

7.3893
7.2937
7.2598
7.2406
7.2244
7.0810
7.0340
7.0157
6.9910
6.9735
6.9725
6.9551
6.9538
6.7952
6.7755
4.5364
3.0876
Current Data Parameters
NAME A813B-20200905-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200905
Time 13.42
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300813 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
F3C
OTf
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
0.99
2.04
2.09
1.02
0.98
3.00

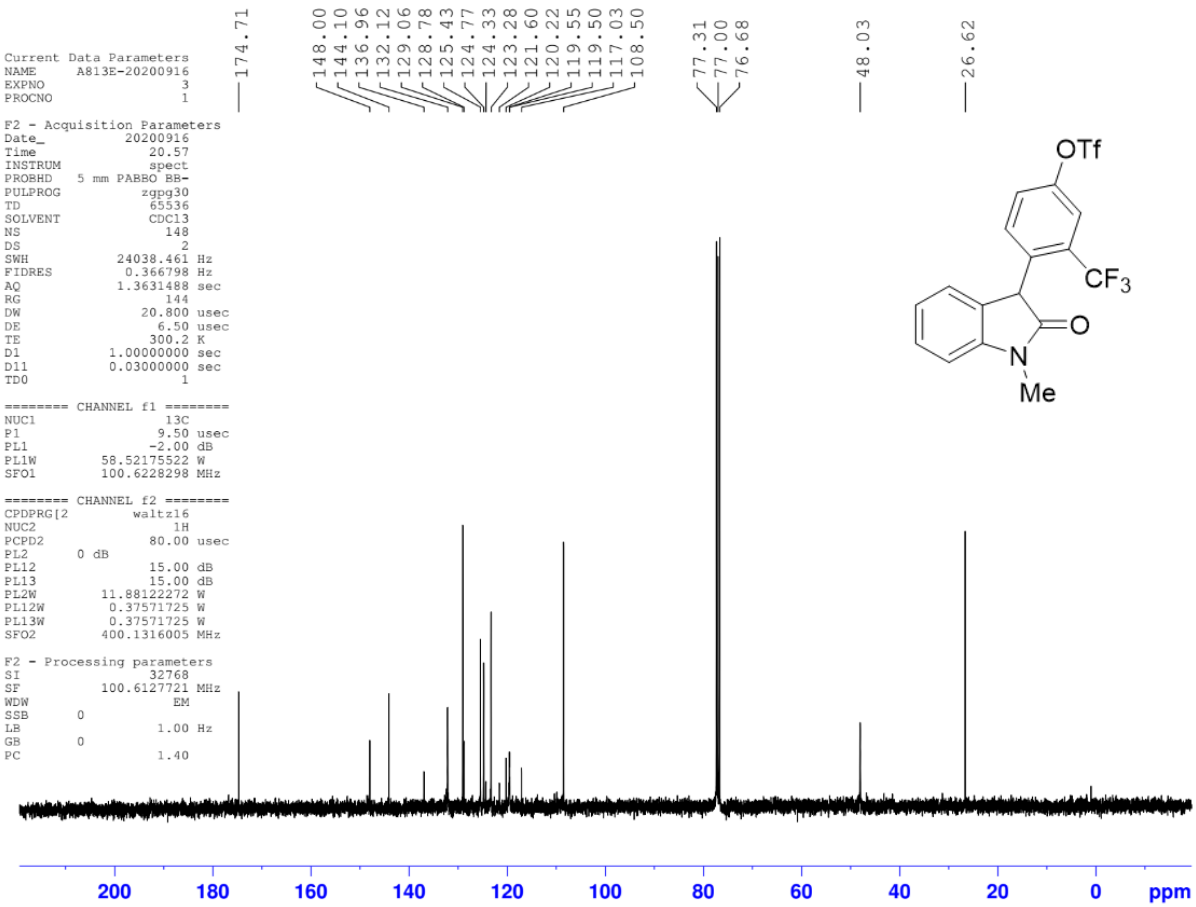

-62.71
-72.64
Current Data Parameters
NAME A813B-20200905-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200905
Time 13.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
F3C
OTf
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

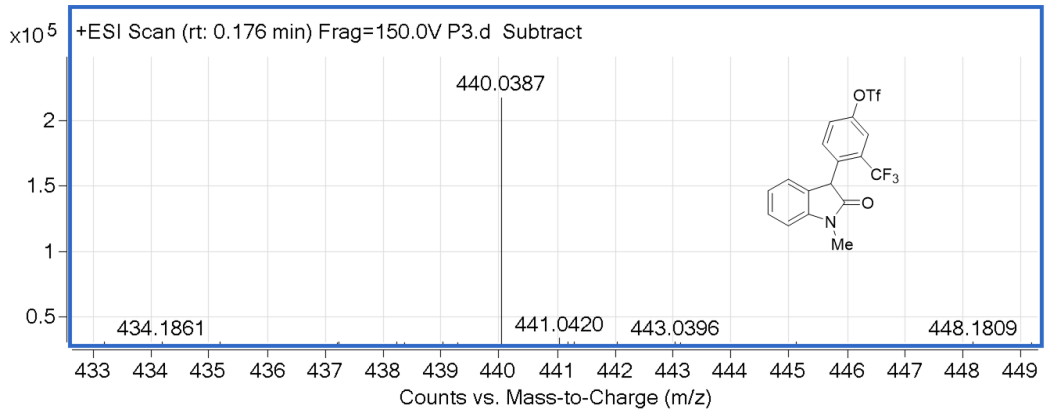

173.81
149.45
144.49
140.62
133.73
133.39
133.06
132.72
129.48
125.93
125.25
125.22
125.12
125.05
124.04
123.29
121.32
120.24
117.89
117.85
117.05
108.87
77.31
77.00
76.68
50.91
26.65
Current Data Parameters
NAME A813B-20200905-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200905
Time 13.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 119
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 299.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127714 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
F3C
OTf
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm


CMSO30122020 A8 1245 (20.454)
TOF MS EI+
1.31e4
100
%
0
439.0316
440.0336
413.9790
420.0357
438.0258
441.0301
463.9778
469.0629
478.1141
487.0674
F3C
OTf
O
N
Me
400
410
420
430
440
450
460
470
480
490
m/z

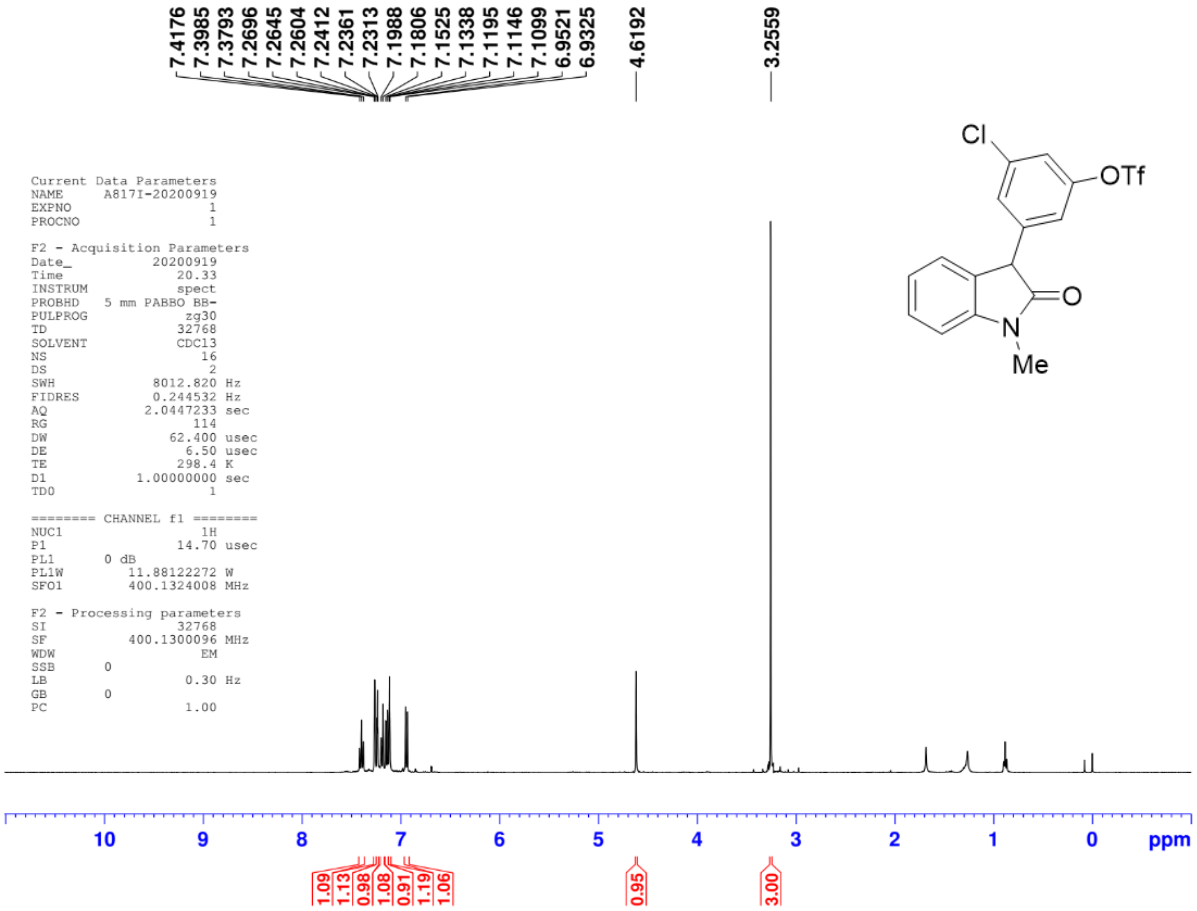

7.6559
7.6496
7.3767
7.3716
7.3560
7.3520
7.3426
7.3357
7.3275
7.3232
7.2595
7.0712
7.0527
7.0361
7.0221
6.9787
6.9511
6.9312
5.0398
3.3103
Current Data Parameters
NAME A813E-20200916
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200916
Time 20.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
CF3
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
2.01
4.07
0.91
3.00

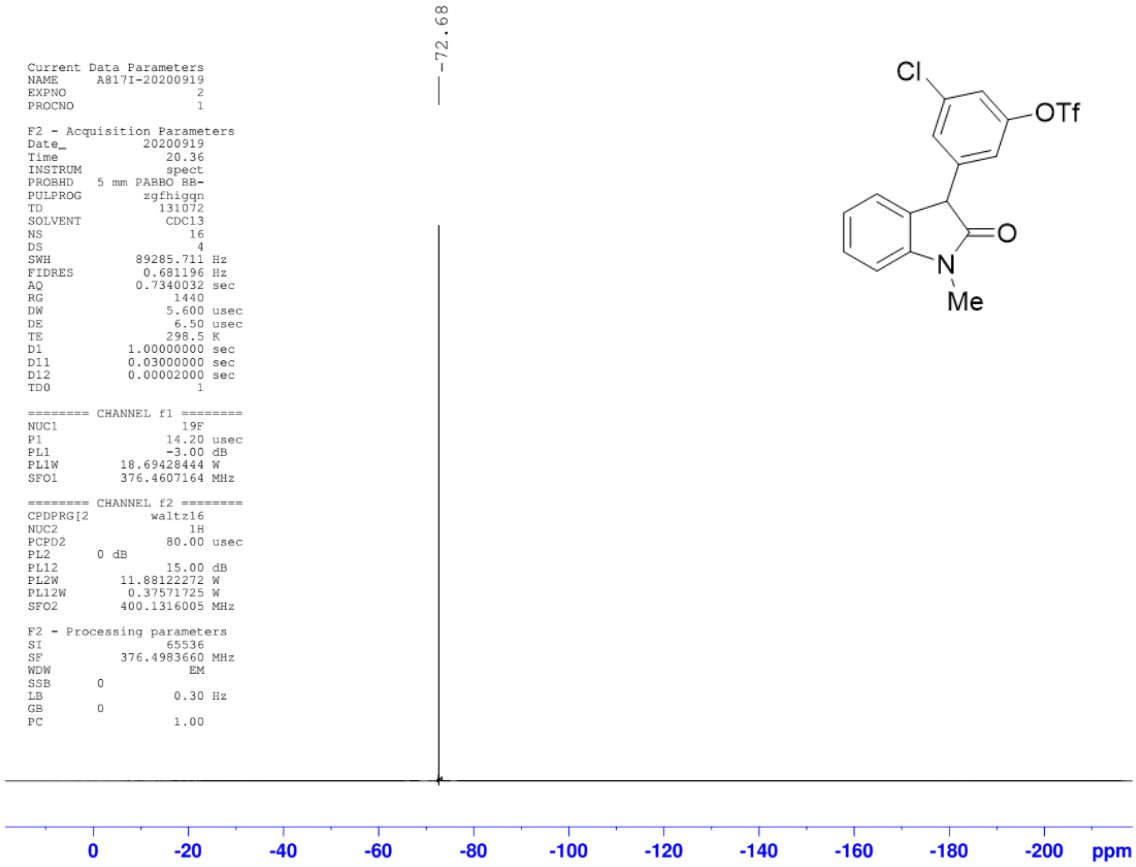

-58.46
-72.69
Current Data Parameters
NAME A813E-20200916
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200916
Time 20.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 299.4 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
CF3
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

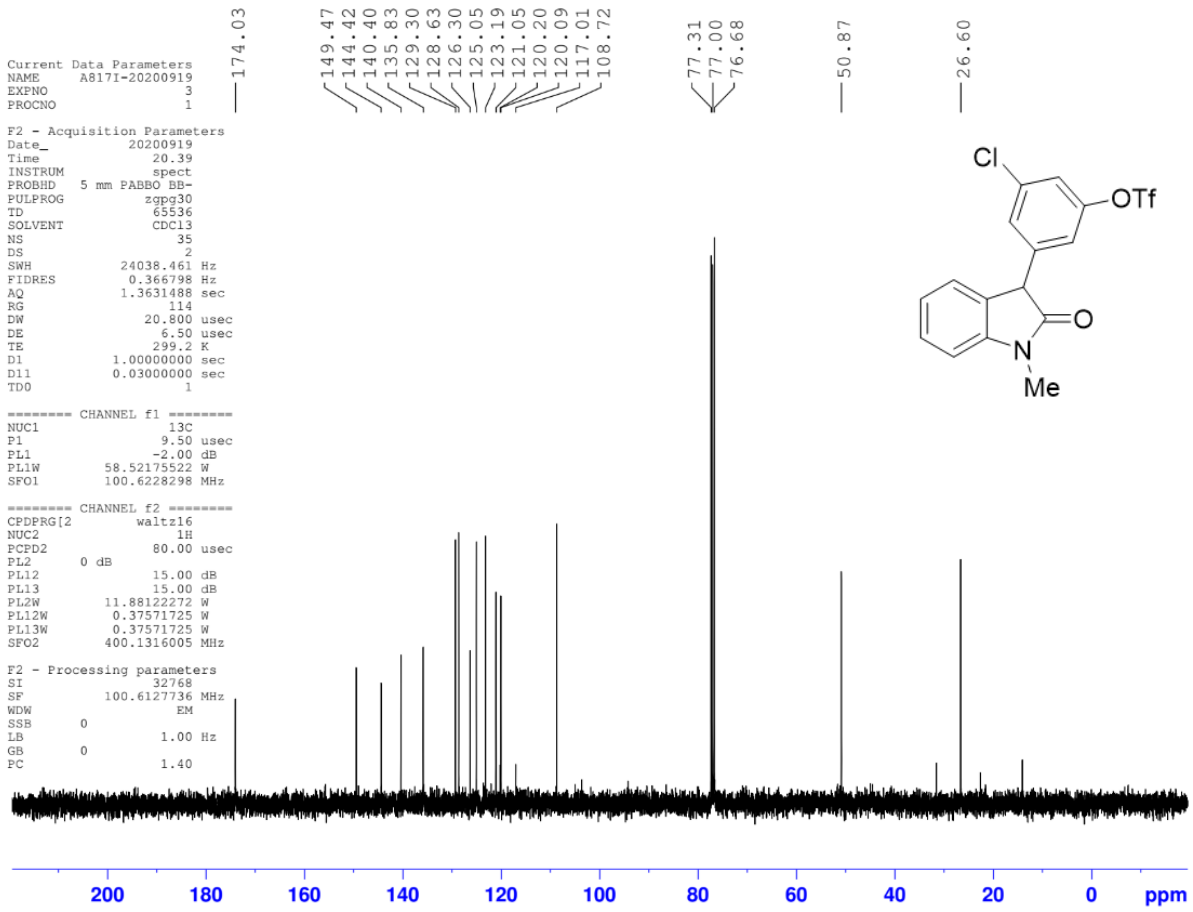


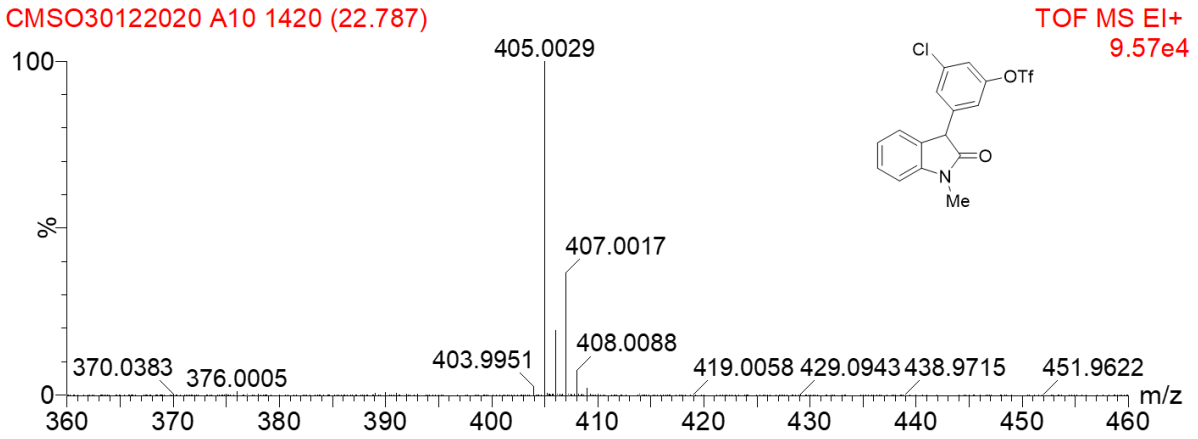


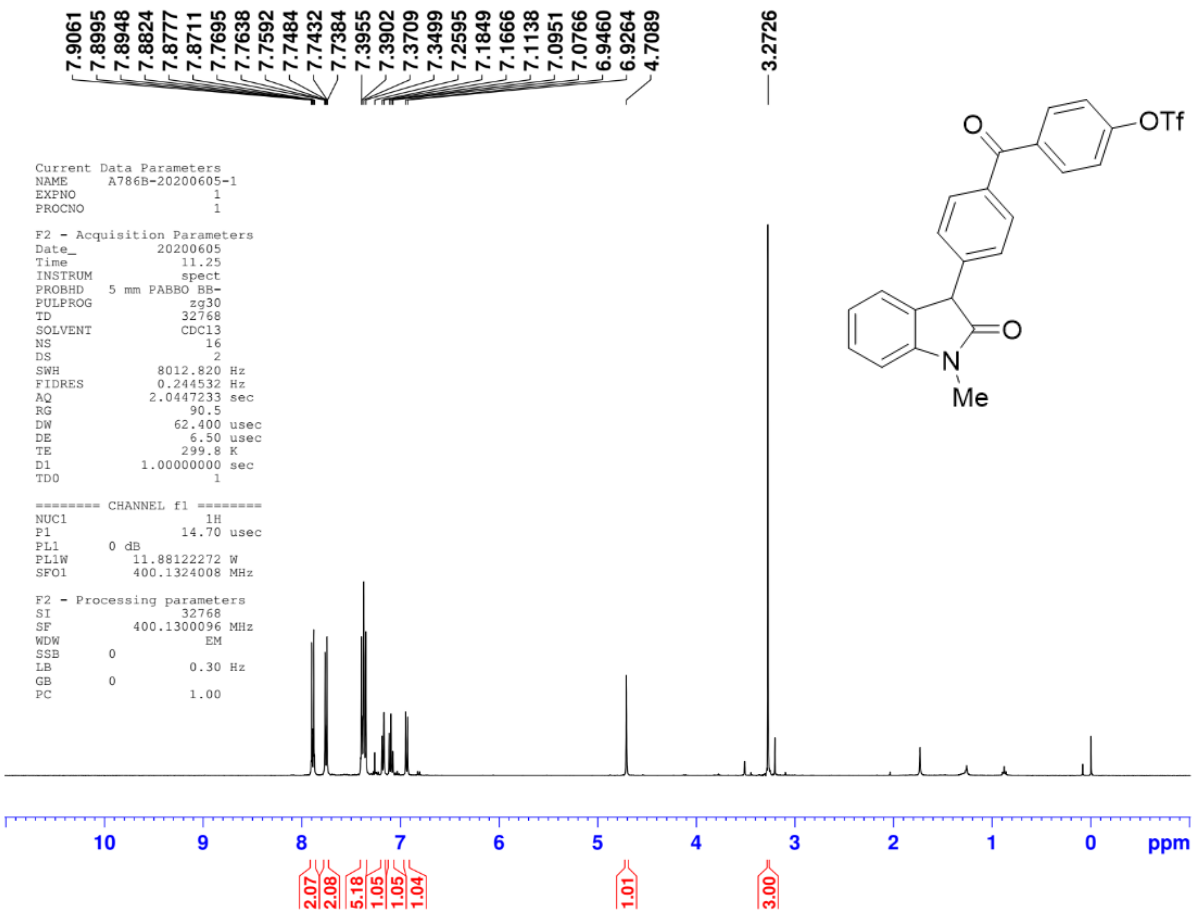
Mass	Calc. Mass	mDa	PPM	Formula
440.0387	440.0386	-0.13	-0.29	$C_{17}H_{12}F_6NO_4S$

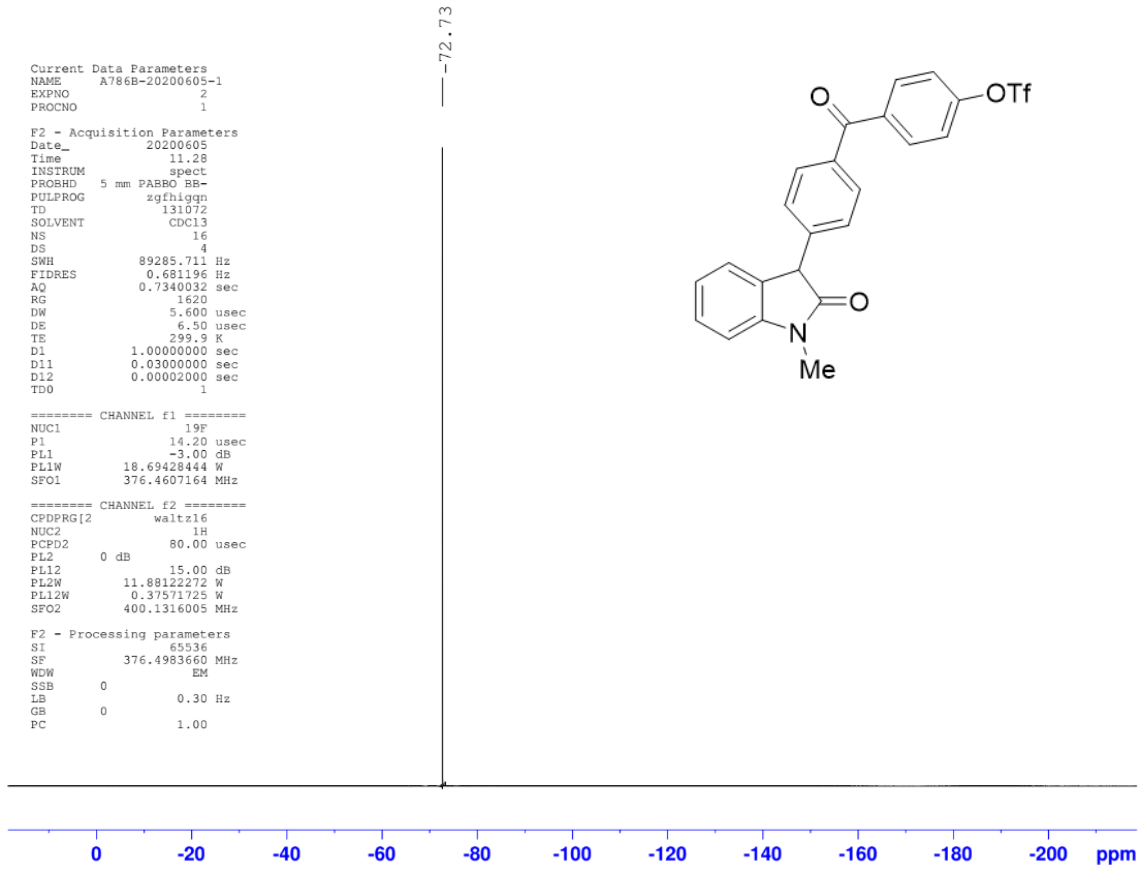

7.4176
7.3985
7.3793
7.2696
7.2645
7.2604
7.2412
7.2361
7.2313
7.1988
7.1806
7.1525
7.1338
7.1195
7.1146
7.1099
6.9521
6.9325
4.6192
3.2559
Current Data Parameters
NAME A817I-20200919
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200919
Time 20.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
OTf
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.09
1.13
0.98
1.08
0.91
1.19
1.06
0.95
3.00

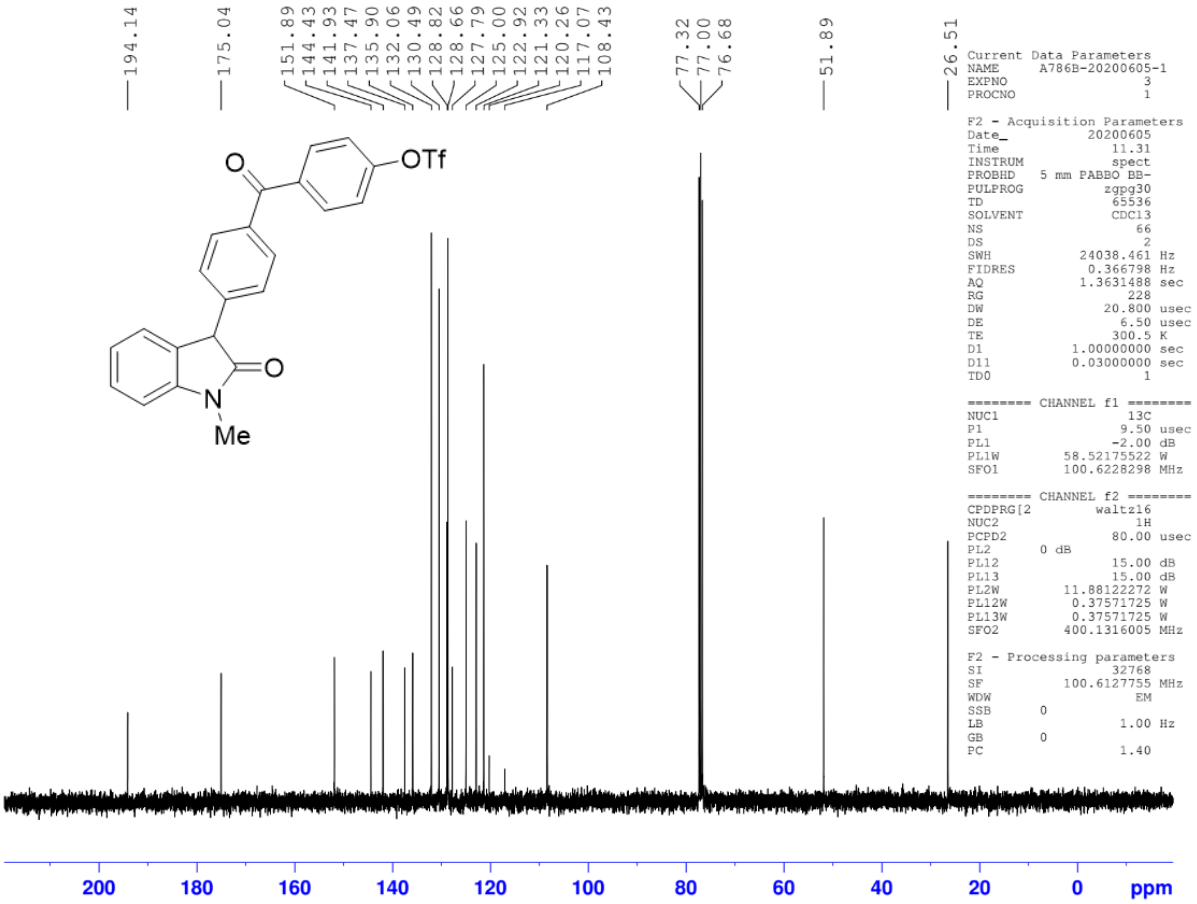

-72.68
Current Data Parameters
NAME A817I-20200919
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200919
Time 20.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 1440
DW 5.600 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Cl
OTf
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

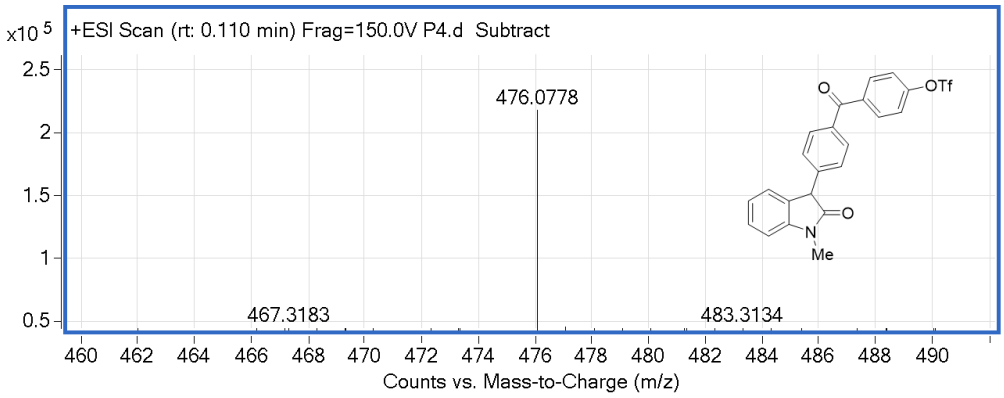

174.03
149.47
144.42
140.40
135.83
129.30
128.63
126.30
125.05
123.19
121.05
120.20
120.09
117.01
108.72
77.31
77.00
76.68
50.87
26.60
Current Data Parameters
NAME A817I-20200919
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200919
Time 20.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 35
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 114
DW 20.800 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127736 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Cl
OTf
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

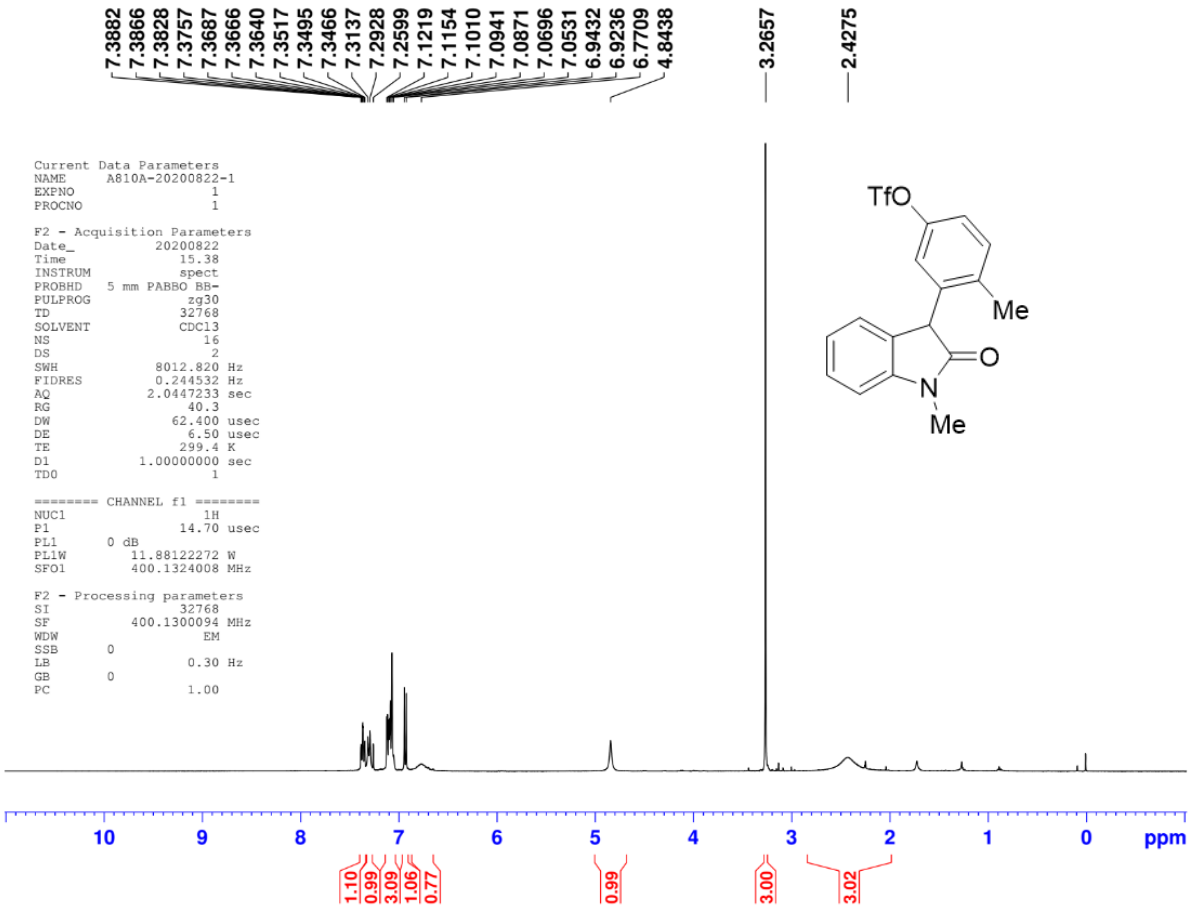

CMSO30122020 A10 1420 (22.787)
TOF MS EI+
9.57e4
100
%
0
405.0029
407.0017
408.0088
403.9951
370.0383
376.0005
419.0058
429.0943
438.9715
451.9622
m/z
360
370
380
390
400
410
420
430
440
450
460
Cl
OTf
O
N
Me

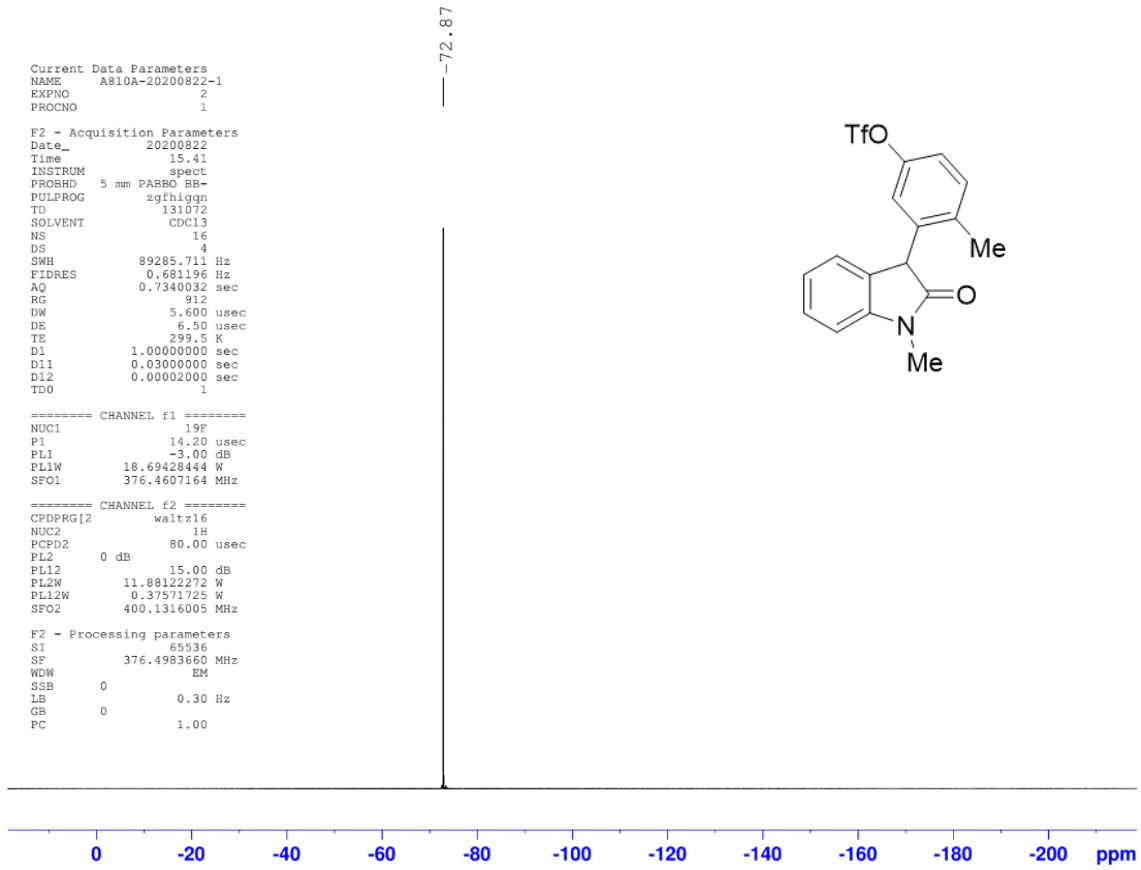

7.9061
7.8995
7.8948
7.8824
7.8777
7.8711
7.7695
7.7638
7.7592
7.7484
7.7432
7.7384
7.3955
7.3902
7.3709
7.3499
7.2595
7.1849
7.1666
7.1138
7.0951
7.0766
6.9460
6.9264
4.7089
3.2726
Current Data Parameters
NAME A786B-20200605-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200605
Time 11.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 90.5
DW 62.400 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
OTf
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
2.07
2.08
5.18
1.05
1.05
1.04
1.01
3.00

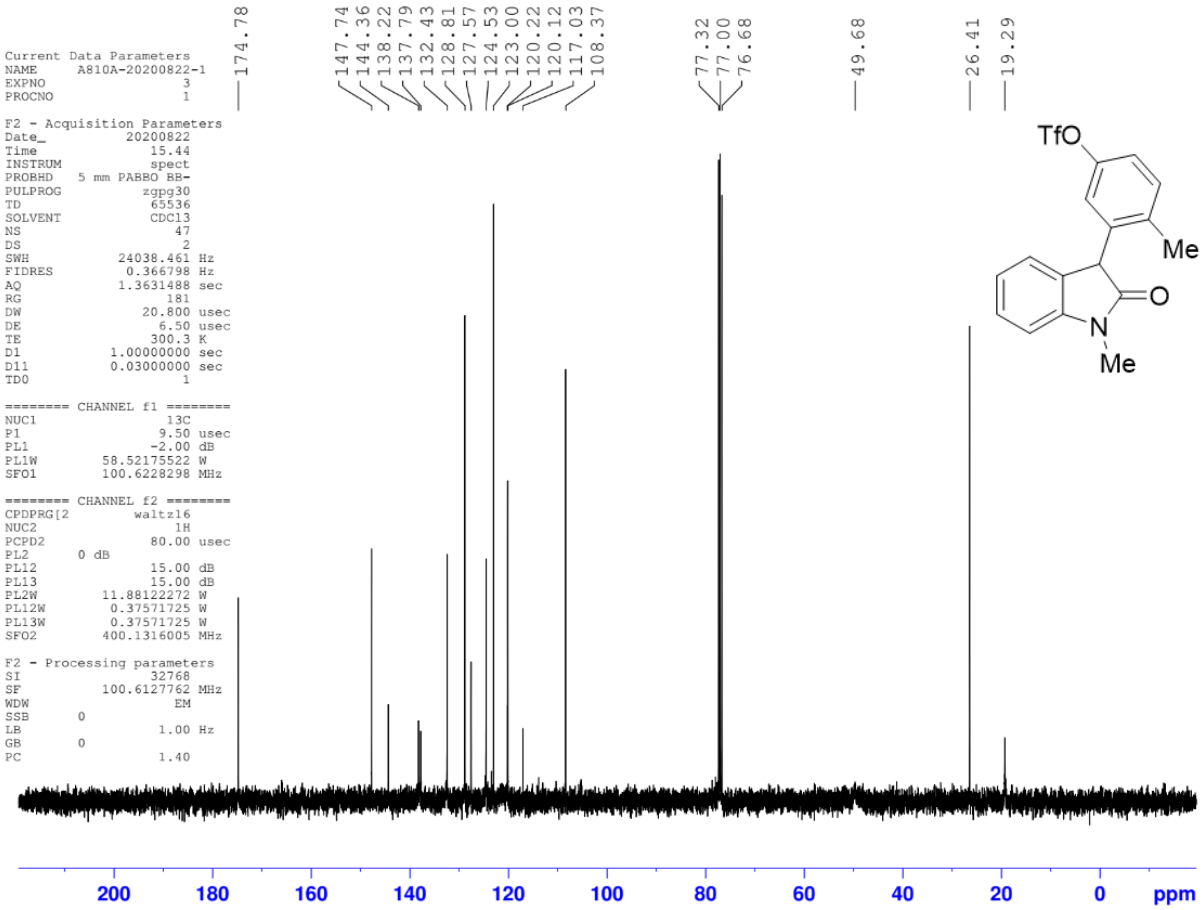

-72.73
Current Data Parameters
NAME A786B-20200605-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200605
Time 11.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 1620
DW 5.600 usec
DE 6.50 usec
TE 299.9 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
OTf
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

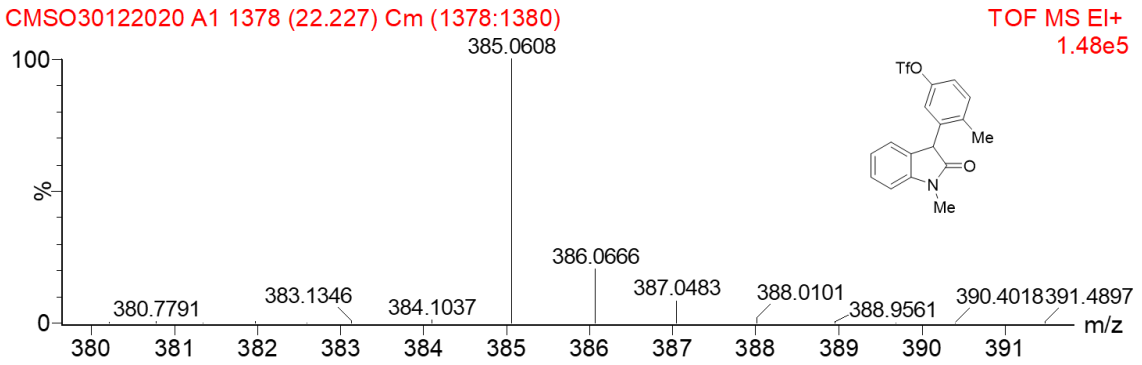

194.14
175.04
151.89
144.43
141.93
137.47
135.90
132.06
130.49
128.82
128.66
127.79
125.00
122.92
121.33
120.26
117.07
108.43
77.32
77.00
76.68
51.89
26.51
OTf
O
N
Me
Current Data Parameters
NAME A786B-20200605-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200605
Time 11.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 66
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 228
DW 20.800 usec
DE 6.50 usec
TE 300.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

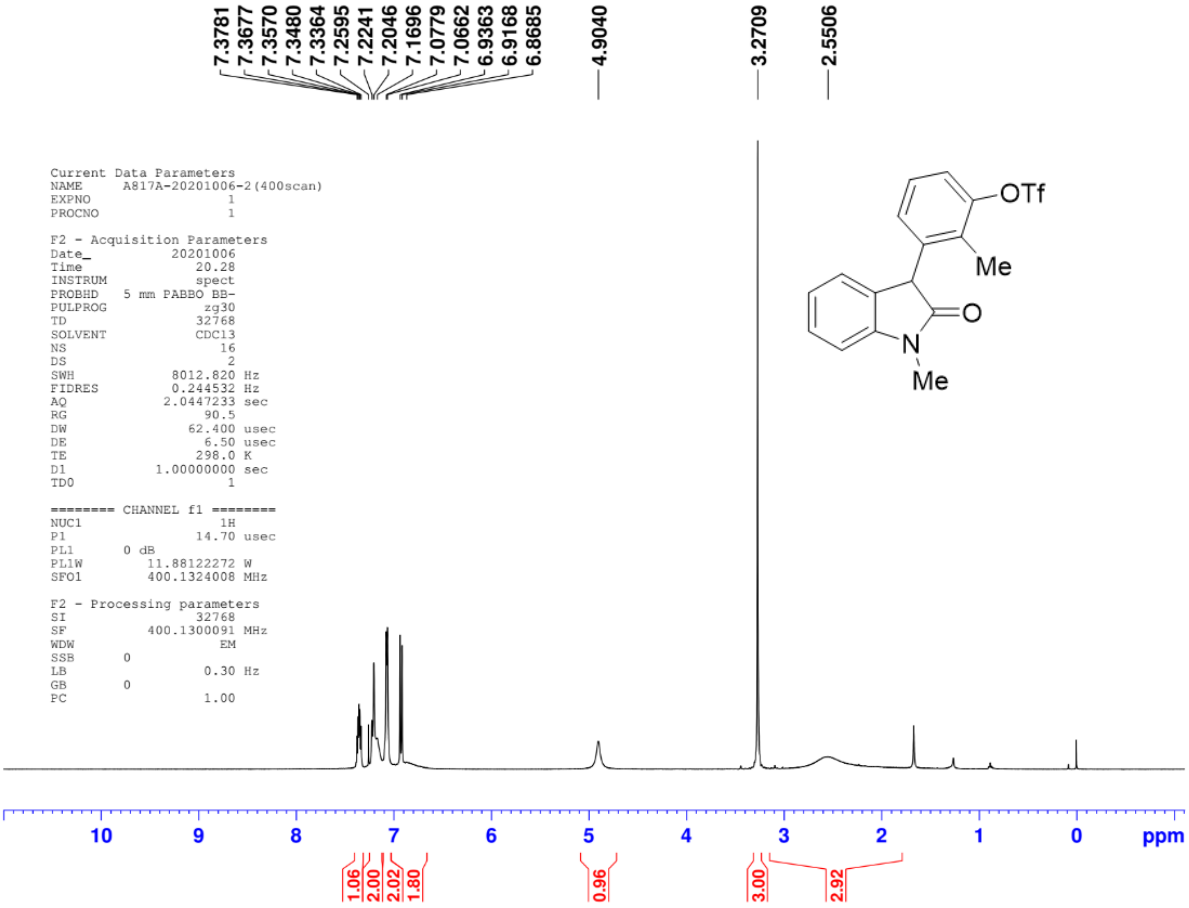

x10 5
+ESI Scan (rt: 0.110 min) Frag=150.0V P4.d Subtract
2.5
2
1.5
1
0.5
476.0778
467.3183
483.3134
OTf
O
N
Me
460
462
464
466
468
470
472
474
476
478
480
482
484
486
488
490
Counts vs. Mass-to-Charge (m/z)

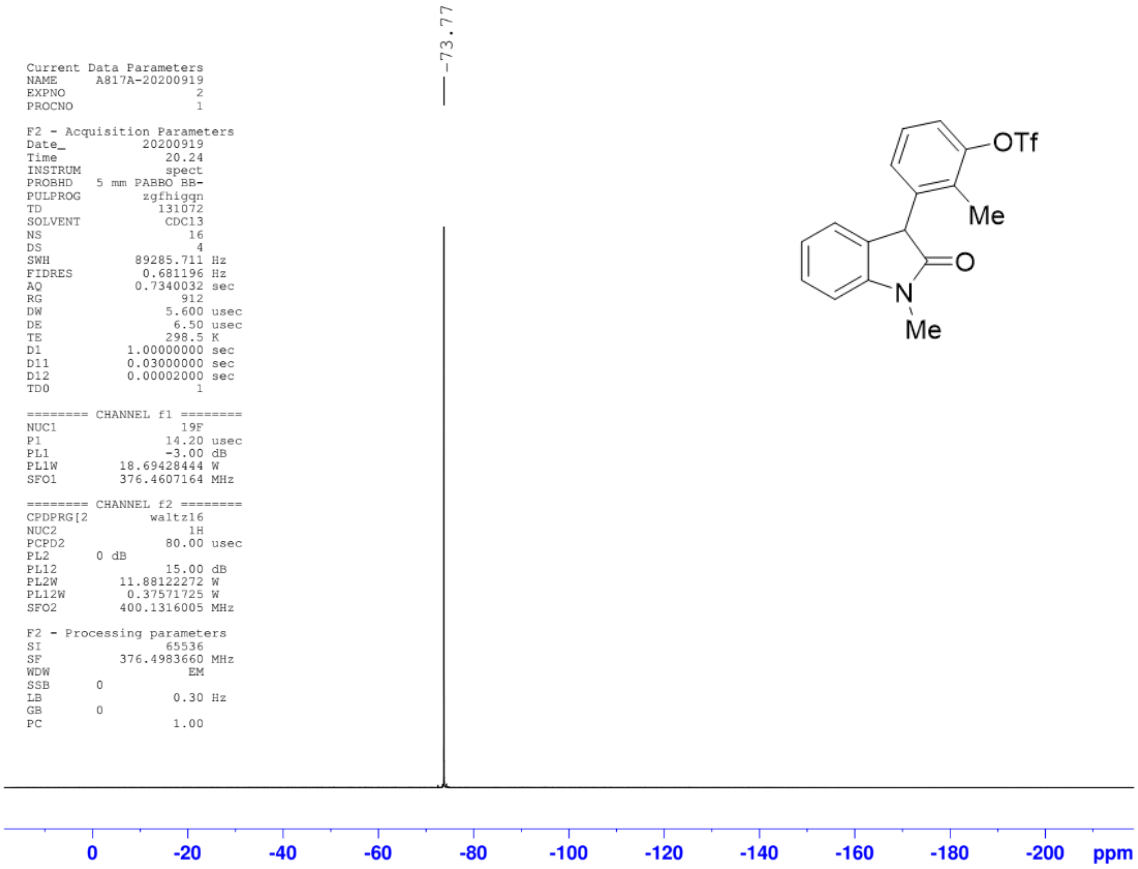

7.3882
7.3866
7.3828
7.3757
7.3687
7.3666
7.3640
7.3517
7.3495
7.3466
7.3137
7.2928
7.2599
7.1219
7.1154
7.1010
7.0941
7.0871
7.0696
7.0531
6.9432
6.9236
6.7709
4.8438
3.2657
2.4275
Current Data Parameters
NAME A810A-20200822-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200822
Time 15.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 40.3
DW 62.400 usec
DE 6.50 usec
TE 299.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
TfO
Me
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.10
0.99
3.09
1.06
0.77
0.99
3.00
3.02

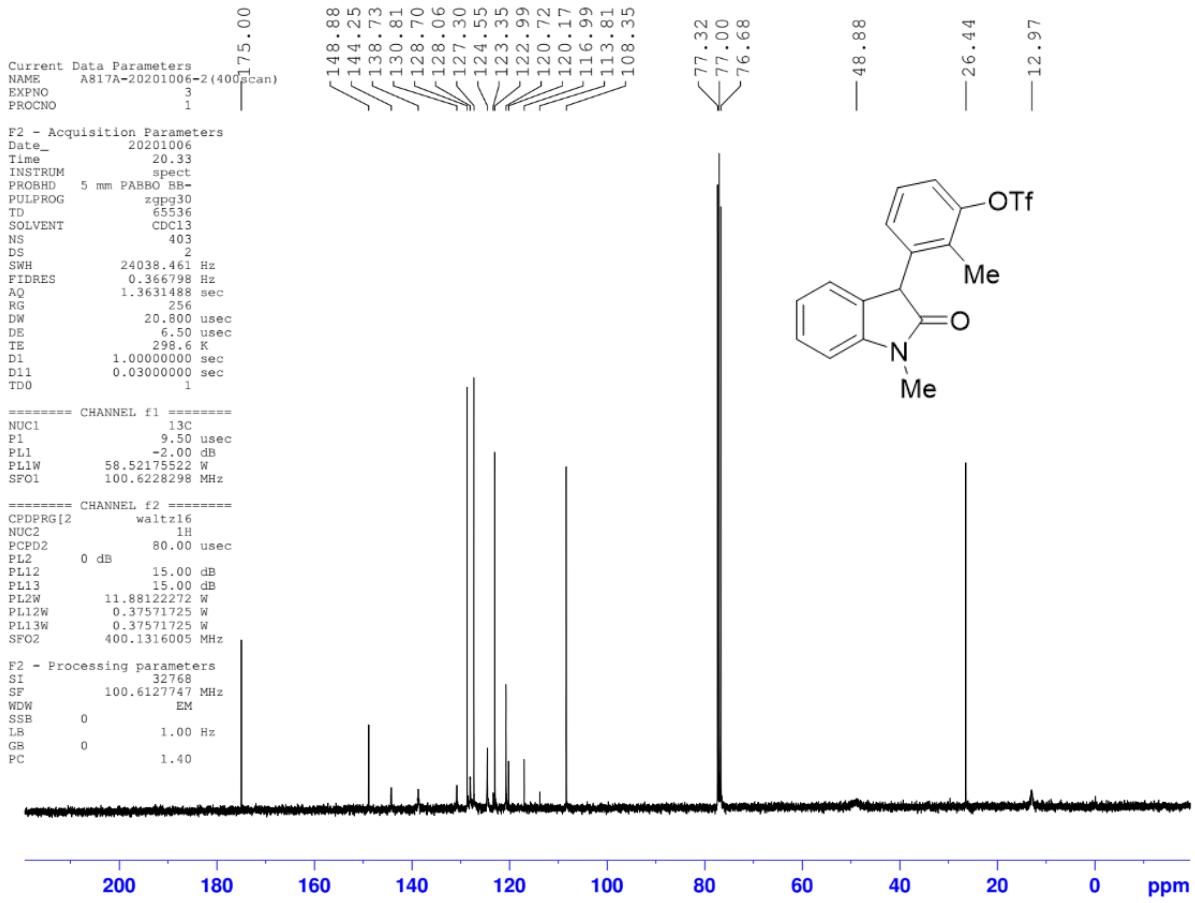

-72.87
Current Data Parameters
NAME A810A-20200822-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200822
Time 15.41
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
TfO
Me
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

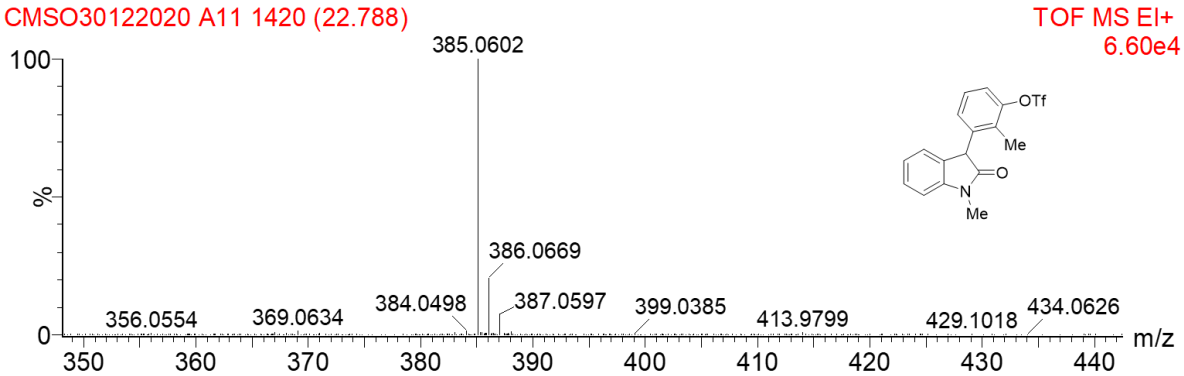

174.78
147.74
144.36
138.22
137.79
132.43
128.81
127.57
124.53
123.00
120.22
120.12
117.03
108.37
77.32
77.00
76.68
49.68
26.41
19.29
Current Data Parameters
NAME A810A-20200822-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200822
Time 15.44
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 47
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 181
DW 20.800 usec
DE 6.50 usec
TE 300.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127762 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
TfO
Me
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

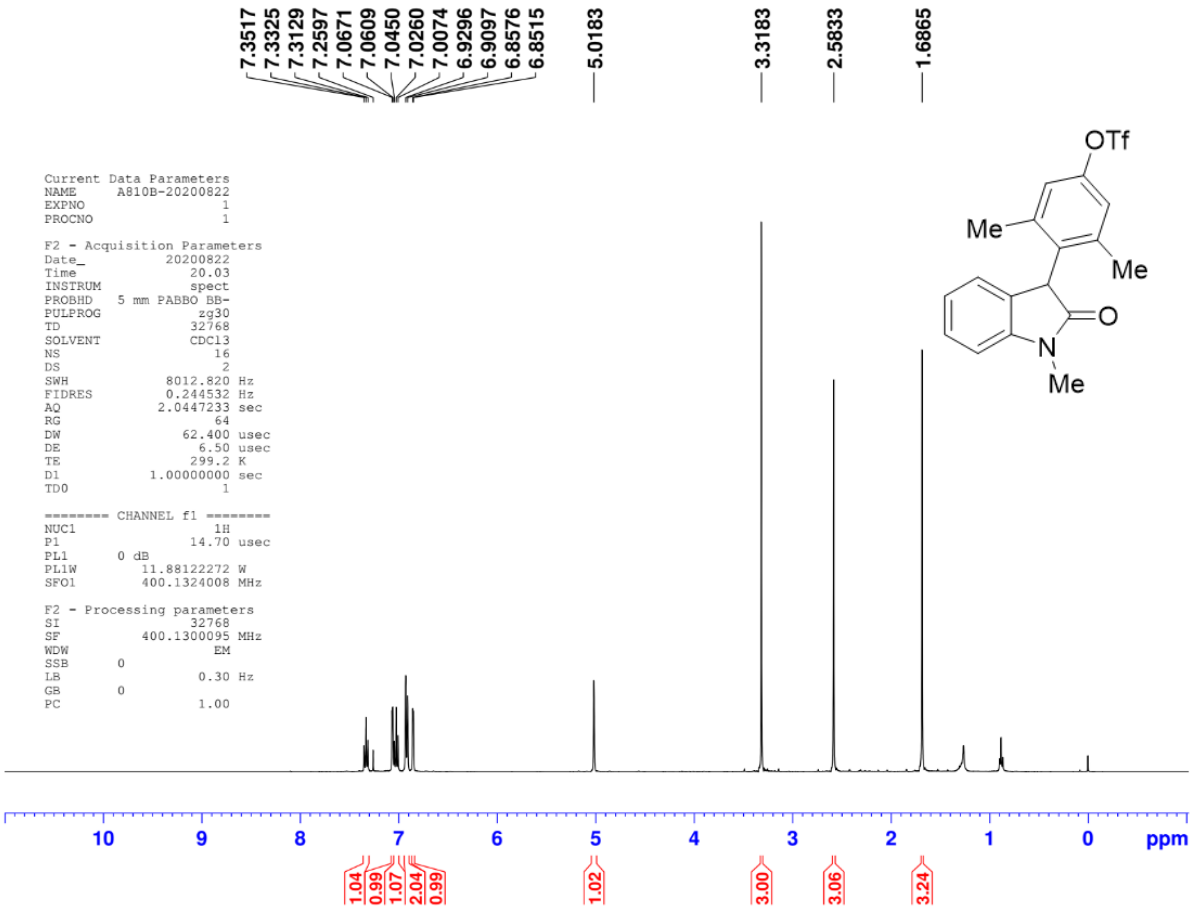

CMSO30122020 A1 1378 (22.227) Cm (1378:1380)
TOF MS EI+
1.48e5
100
%
0
385.0608
386.0666
387.0483
388.0101
388.9561
390.4018
391.4897
380.7791
383.1346
384.1037
TfO
Me
O
N
Me
380
381
382
383
384
385
386
387
388
389
390
391
m/z

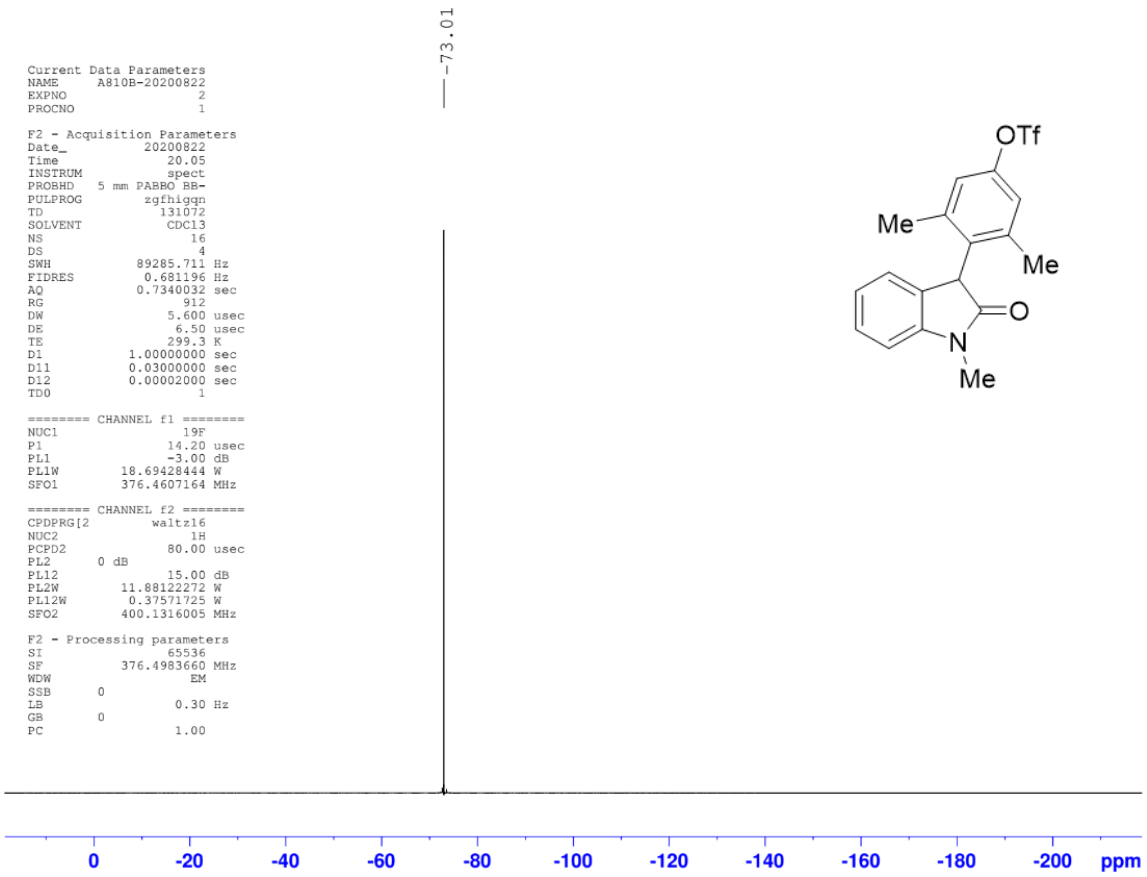

7.3781
7.3677
7.3570
7.3480
7.3364
7.2595
7.2241
7.2046
7.1696
7.0779
7.0662
6.9363
6.9168
6.8685
4.9040
3.2709
2.5506
Current Data Parameters
NAME A817A-20201006-2(400scan)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201006
Time 20.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 90.5
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
Me
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.06
2.00
2.02
1.80
0.96
3.00
2.92

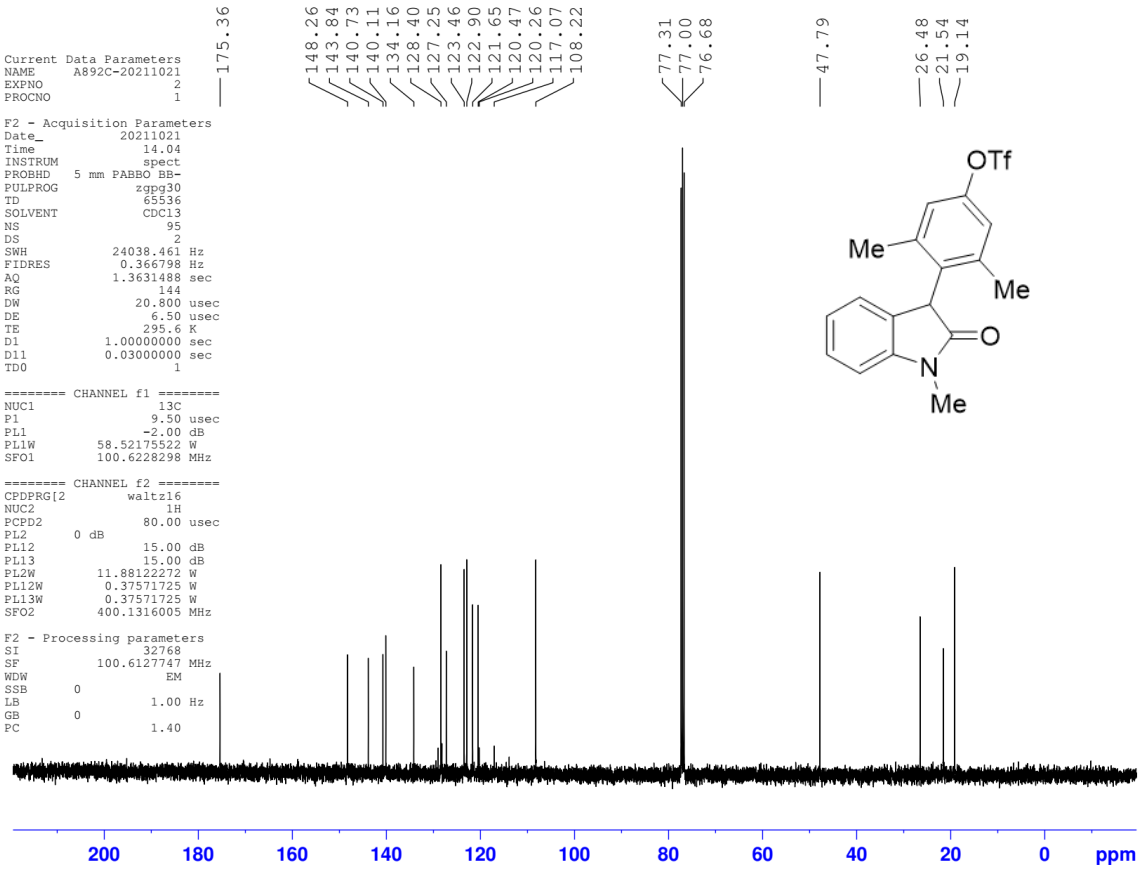

-73.77
Current Data Parameters
NAME A817A-20200919
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200919
Time 20.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
Me
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

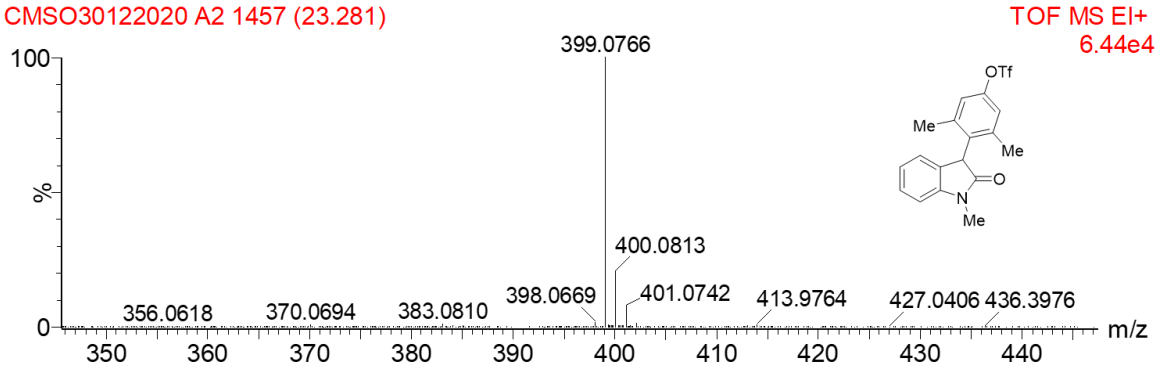

175.00
148.88
144.25
138.73
130.81
128.70
128.06
127.30
124.55
123.35
122.99
120.72
120.17
116.99
113.81
108.35
77.32
77.00
76.68
48.88
26.44
12.97
Current Data Parameters
NAME A817A-20201006-2(400scan)
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201006
Time 20.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 403
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 256
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127747 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OTf
Me
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm


CMSO30122020 A11 1420 (22.788)
TOF MS EI+
6.60e4
100
%
0
385.0602
386.0669
356.0554
369.0634
384.0498
387.0597
399.0385
413.9799
429.1018
434.0626
350
360
370
380
390
400
410
420
430
440
m/z
OTf
Me
O
N
Me

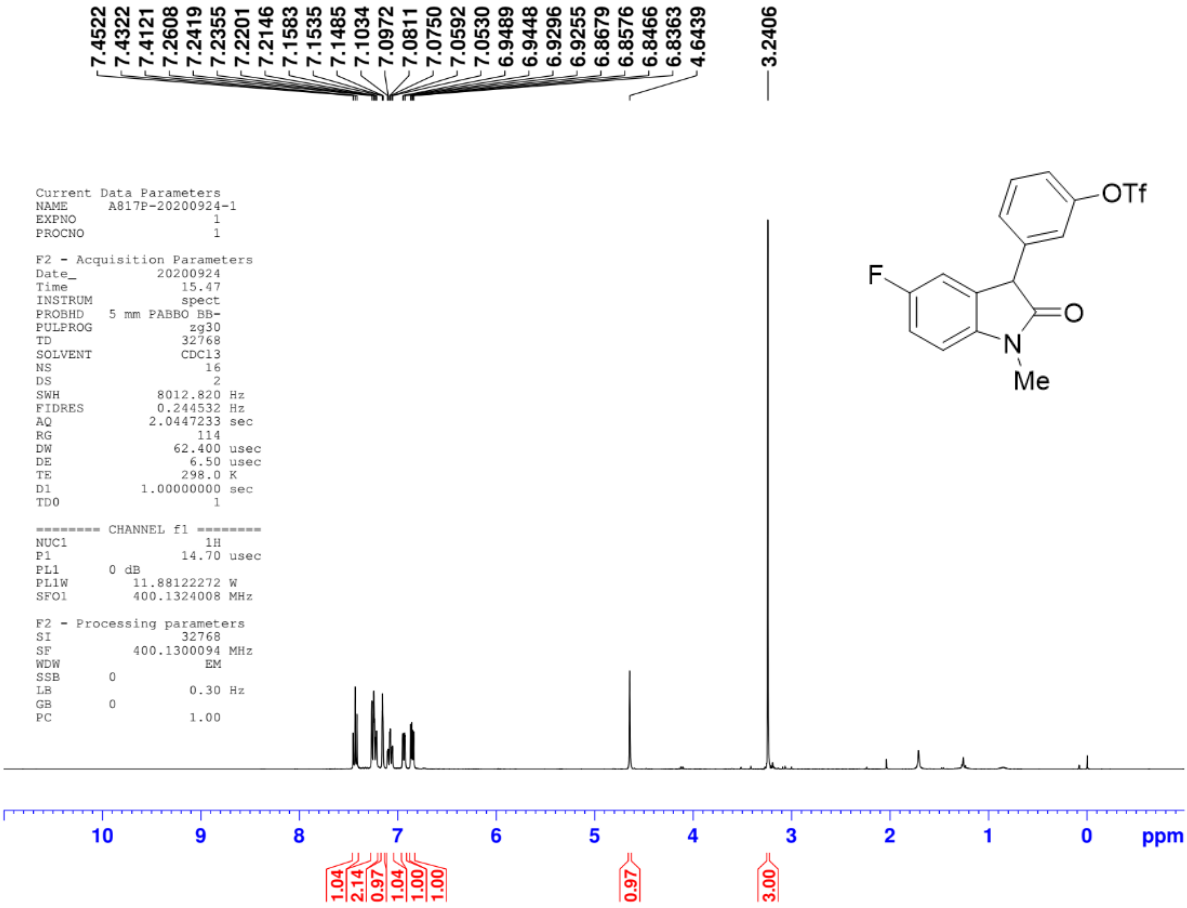

7.3517
7.3325
7.3129
7.2597
7.0671
7.0609
7.0450
7.0260
7.0074
6.9296
6.9097
6.8576
6.8515
5.0183
3.3183
2.5833
1.6865
Current Data Parameters
NAME A810B-20200822
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200822
Time 20.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 299.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
Me
Me
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.04
0.99
1.07
2.04
0.99
1.02
3.00
3.06
3.24

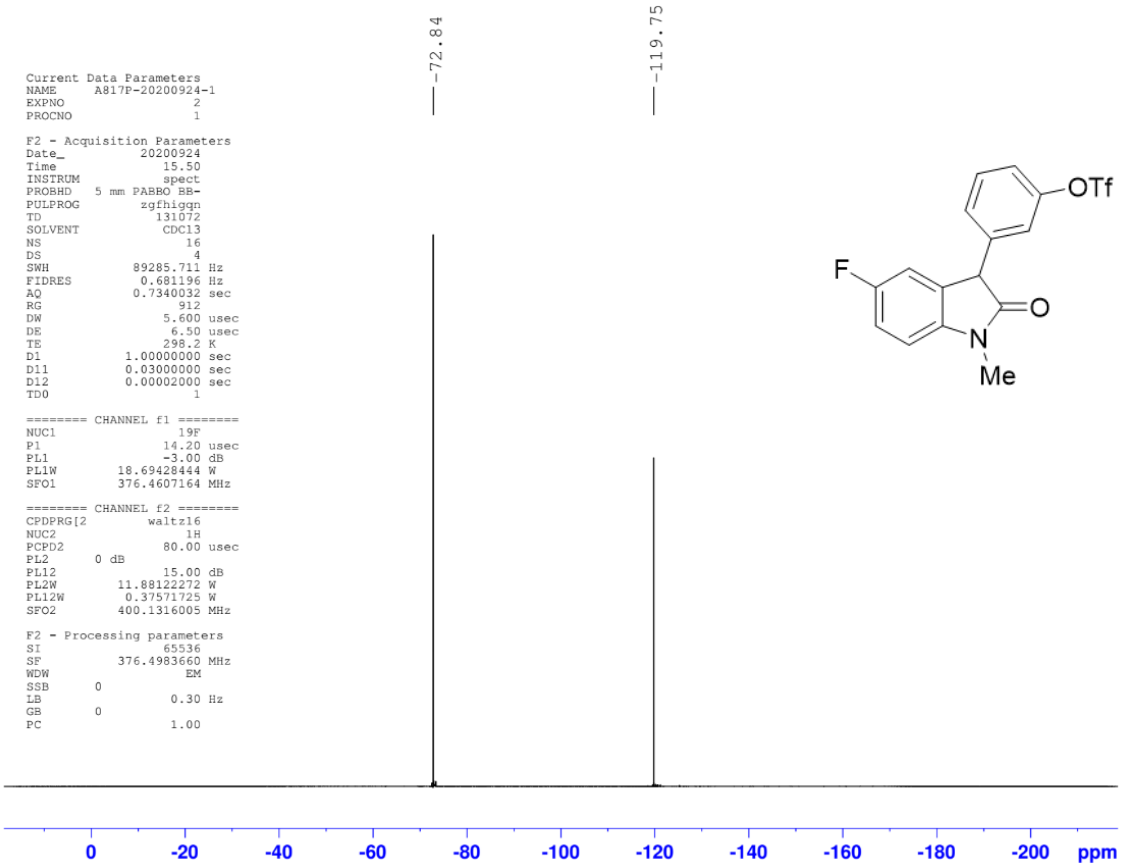

-73.01
Current Data Parameters
NAME A810B-20200822
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200822
Time 20.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
Me
Me
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

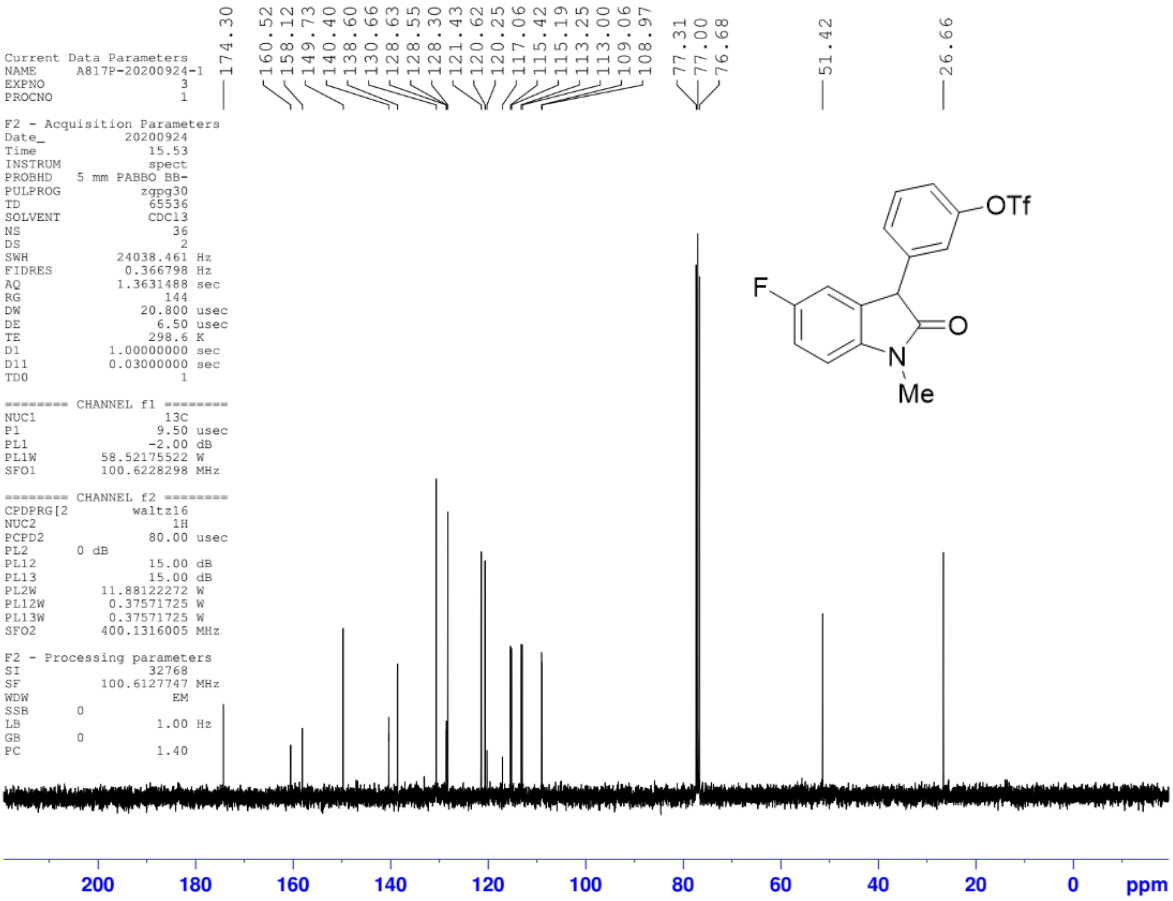


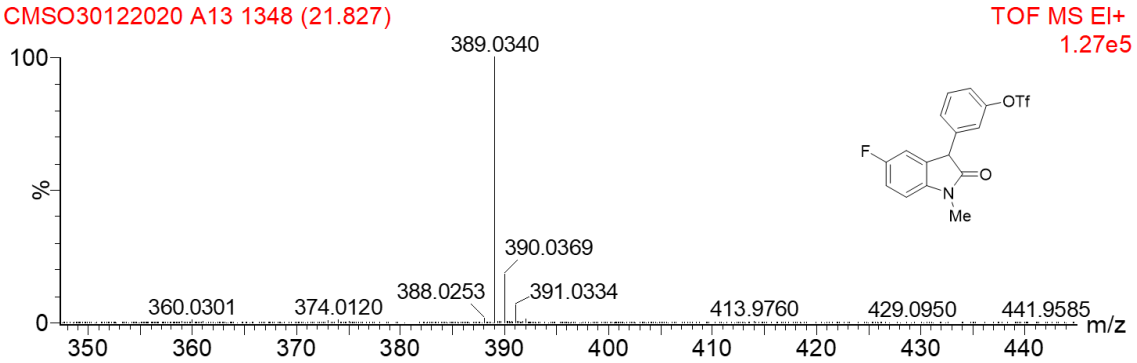


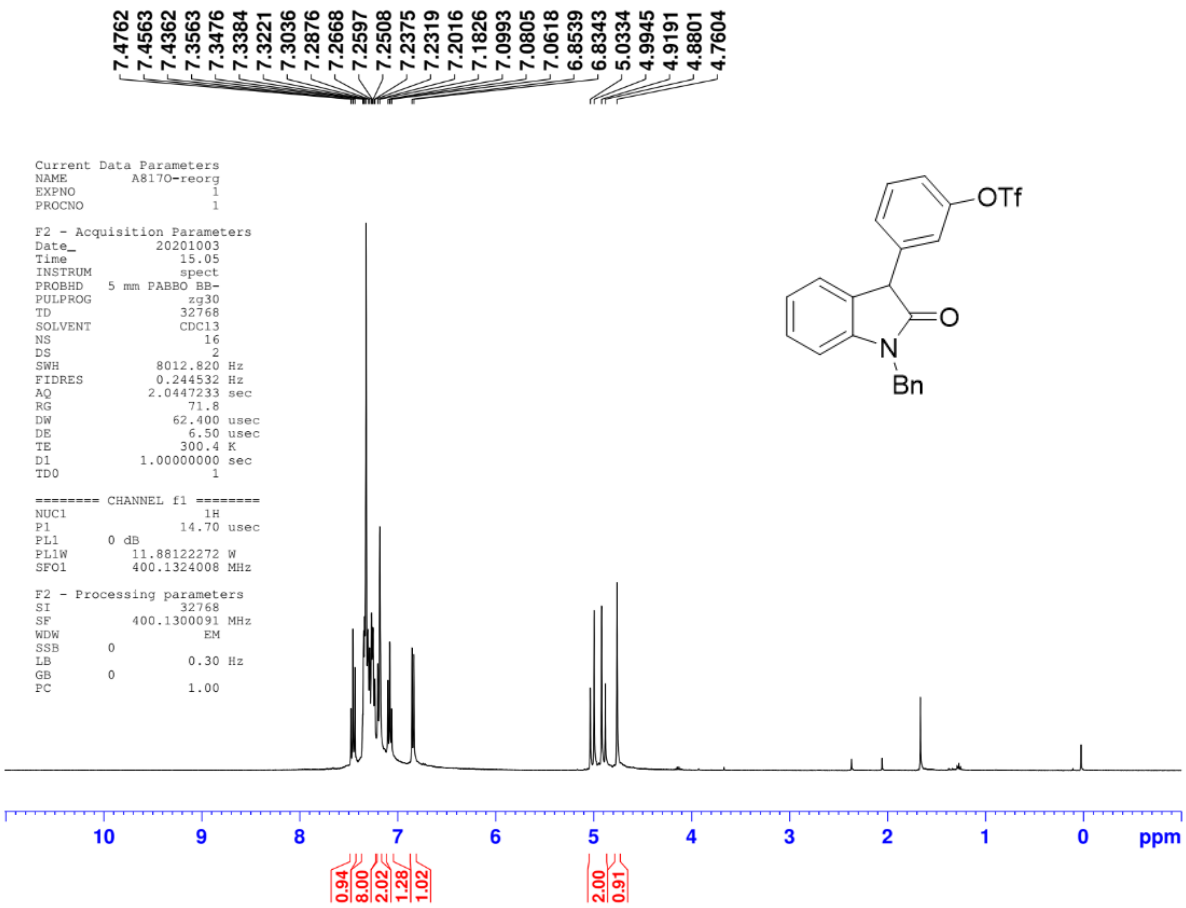
Mass	Calc. Mass	mDa	PPM	Formula
399.0766	399.0752	-1.39	-3.47	$C_{18}H_{16}F_3NO_4S$

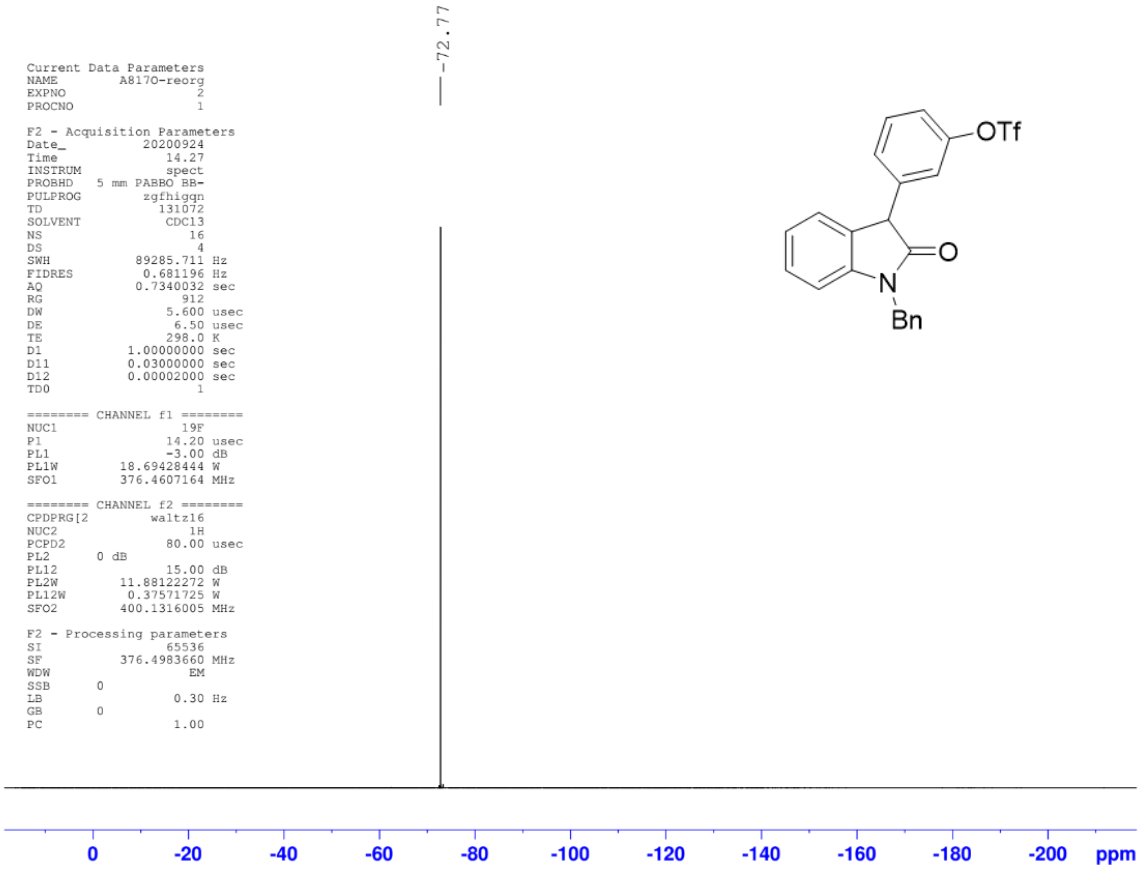

7.4522
7.4322
7.4121
7.2608
7.2419
7.2355
7.2201
7.2146
7.1583
7.1535
7.1485
7.1034
7.0972
7.0811
7.0750
7.0592
7.0530
6.9489
6.9448
6.9296
6.9255
6.8679
6.8576
6.8466
6.8363
4.6439
3.2406
Current Data Parameters
NAME A817P-20200924-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200924
Time 15.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
F
O
N
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.04
2.14
0.97
1.04
1.00
1.00
0.97
3.00

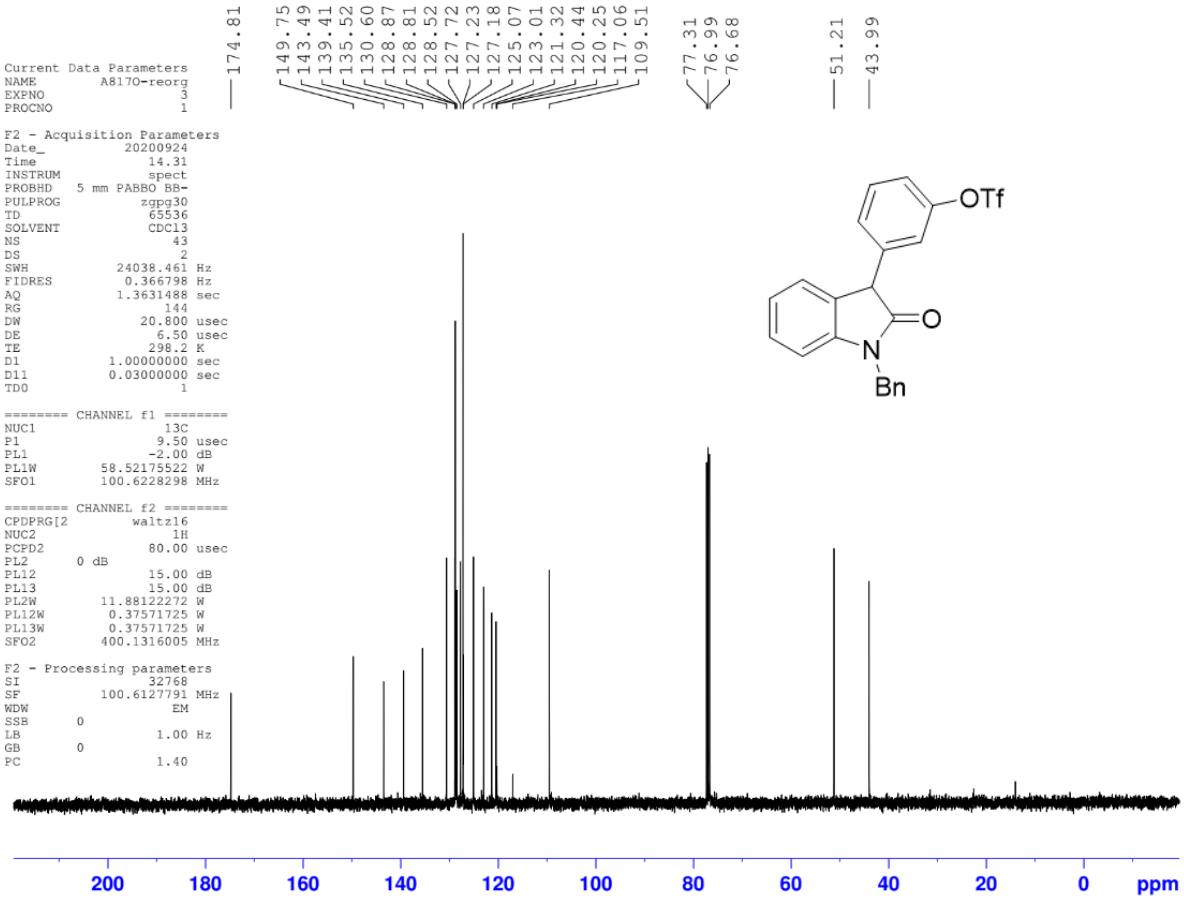

-72.84
-119.75
Current Data Parameters
NAME A817P-20200924-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200924
Time 15.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
F
O
N
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

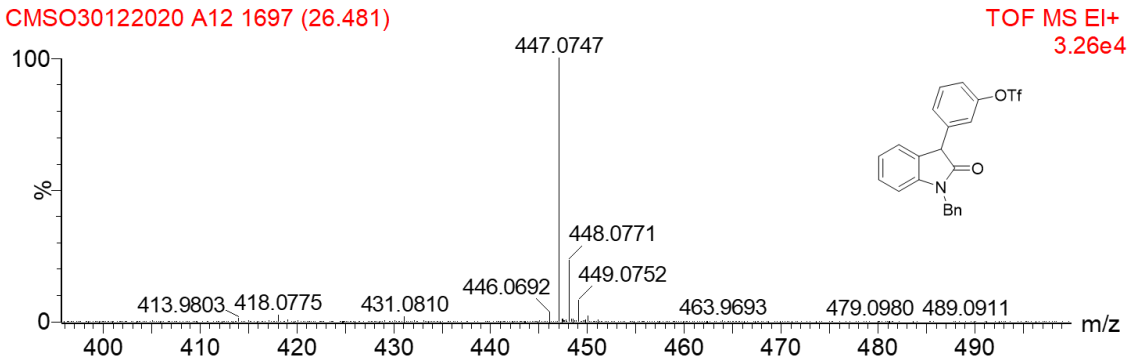

174.30
160.52
158.12
149.73
140.40
138.60
130.66
128.63
128.55
128.30
121.43
120.62
120.25
117.06
115.42
115.19
113.25
113.00
109.06
108.97
77.31
77.00
76.68
51.42
26.66
Current Data Parameters
NAME A817P-20200924-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200924
Time 15.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 36
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127747 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OTf
F
O
N
Me
200
180
160
140
120
100
80
60
40
20
0
ppm

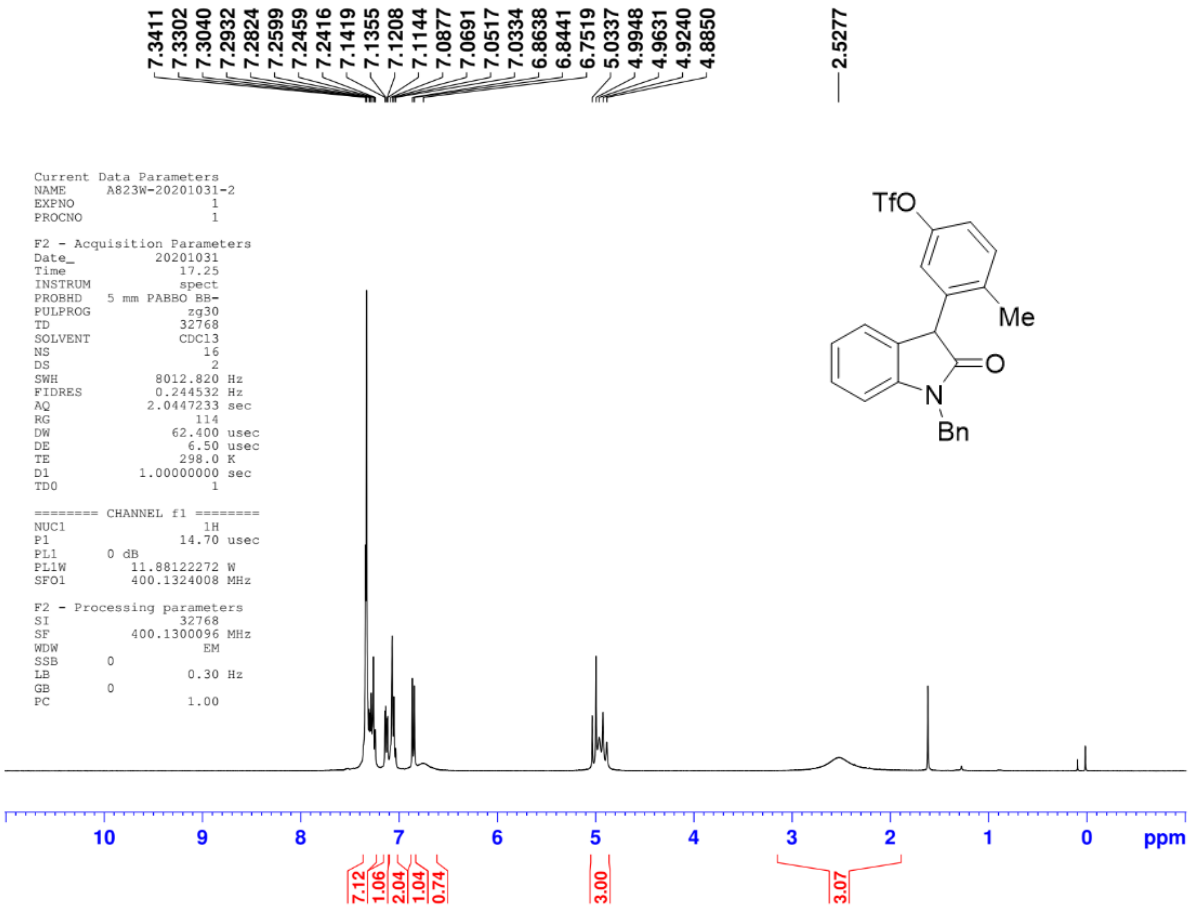

CMSO30122020 A13 1348 (21.827)
TOF MS EI+
1.27e5
100
%
0
389.0340
390.0369
388.0253
391.0334
360.0301
374.0120
413.9760
429.0950
441.9585
m/z
350
360
370
380
390
400
410
420
430
440
OTf
F
O
N
Me

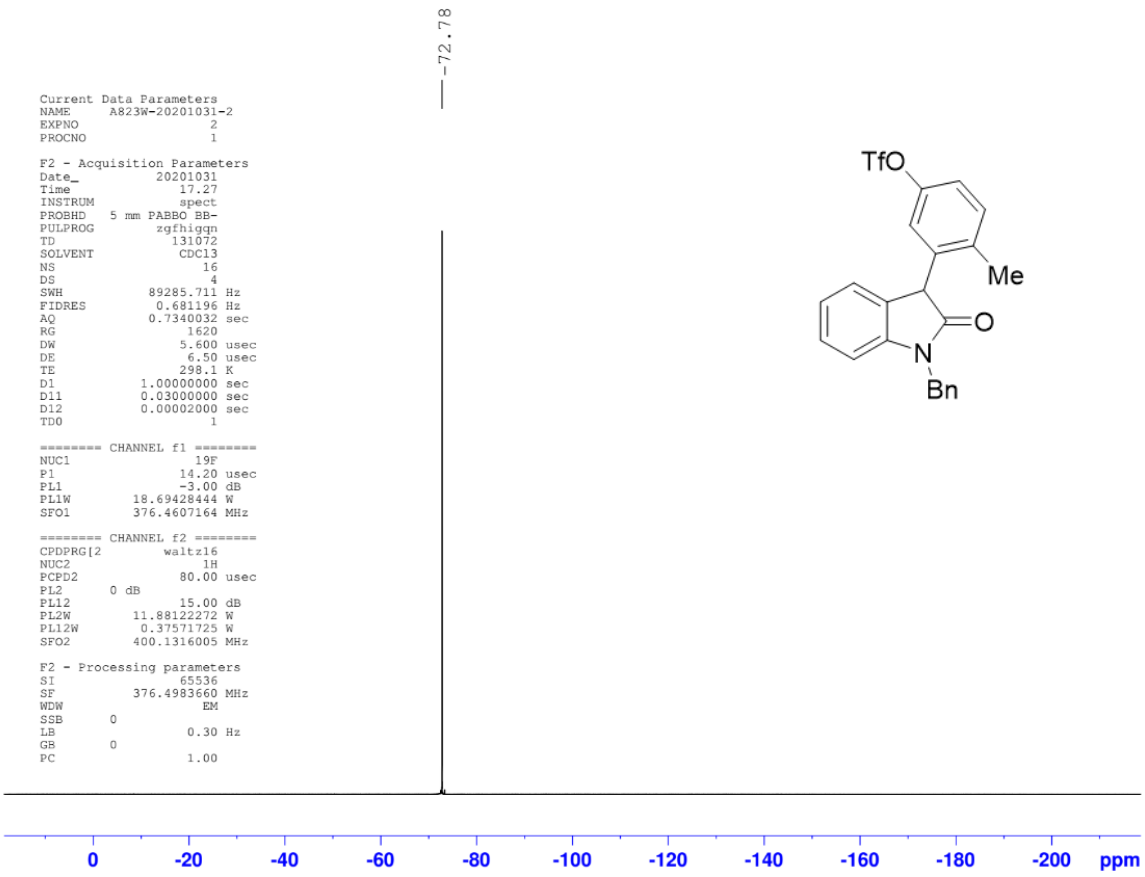

7.4762
7.4563
7.4362
7.3563
7.3476
7.3384
7.3221
7.3036
7.2876
7.2668
7.2597
7.2508
7.2375
7.2319
7.2016
7.1826
7.0993
7.0805
7.0618
6.8539
6.8343
5.0334
4.9945
4.9191
4.8801
4.7604
Current Data Parameters
NAME A817O-reorg
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201003
Time 15.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 300.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
N
Bn
10
9
8
7
6
5
4
3
2
1
0
ppm
0.94
8.00
2.02
1.28
1.02
2.00
0.91

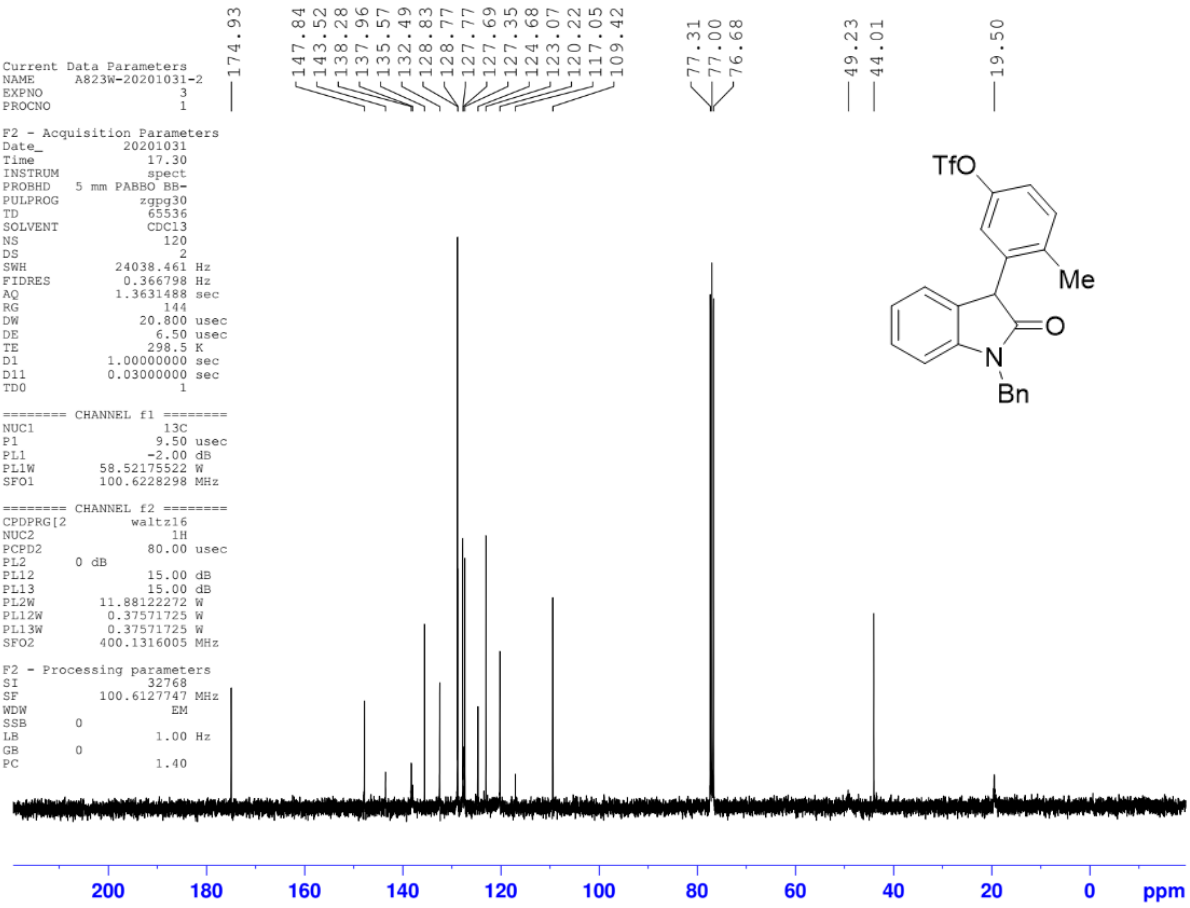

-72.77
Current Data Parameters
NAME A817O-reorg
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200924
Time 14.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
N
Bn
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

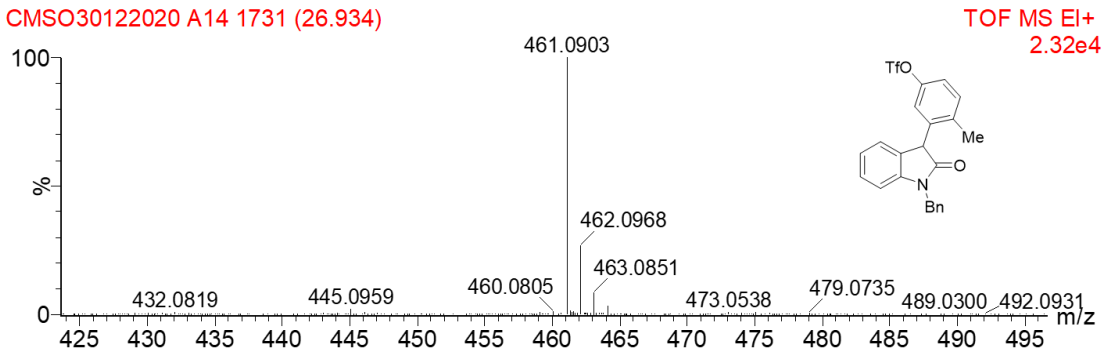

174.81
149.75
143.49
139.41
135.52
130.60
128.87
128.81
128.52
127.72
127.23
127.18
125.07
123.01
121.32
120.44
120.25
117.06
109.51
77.31
76.99
76.68
51.21
43.99
Current Data Parameters
NAME A817O-reorg
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200924
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 43
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127791 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OTf
O
N
Bn
200
180
160
140
120
100
80
60
40
20
0
ppm

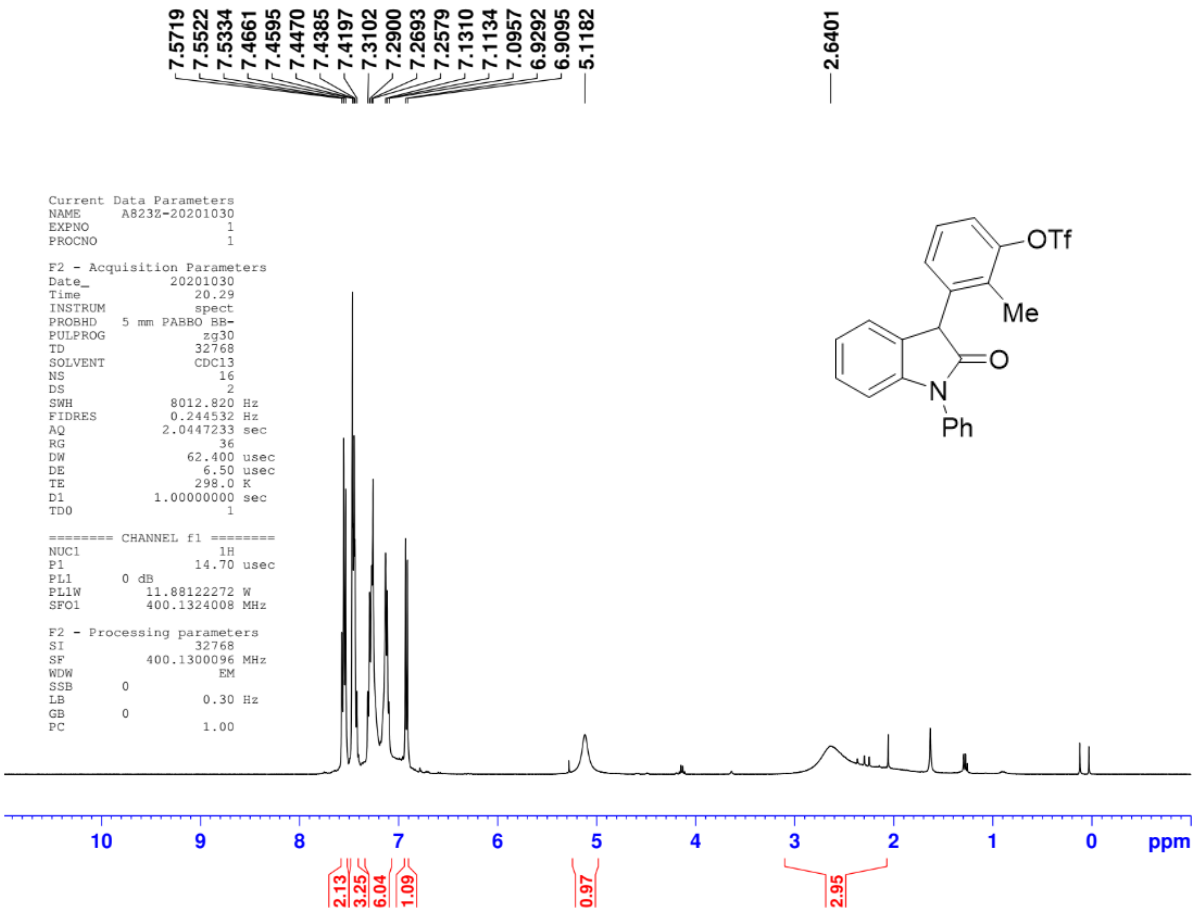

CMSO30122020 A12 1697 (26.481)
TOF MS EI+
3.26e4
100
%
0
447.0747
448.0771
449.0752
446.0692
413.9803
418.0775
431.0810
463.9693
479.0980
489.0911
OTf
O
N
Bn
400
410
420
430
440
450
460
470
480
490
m/z

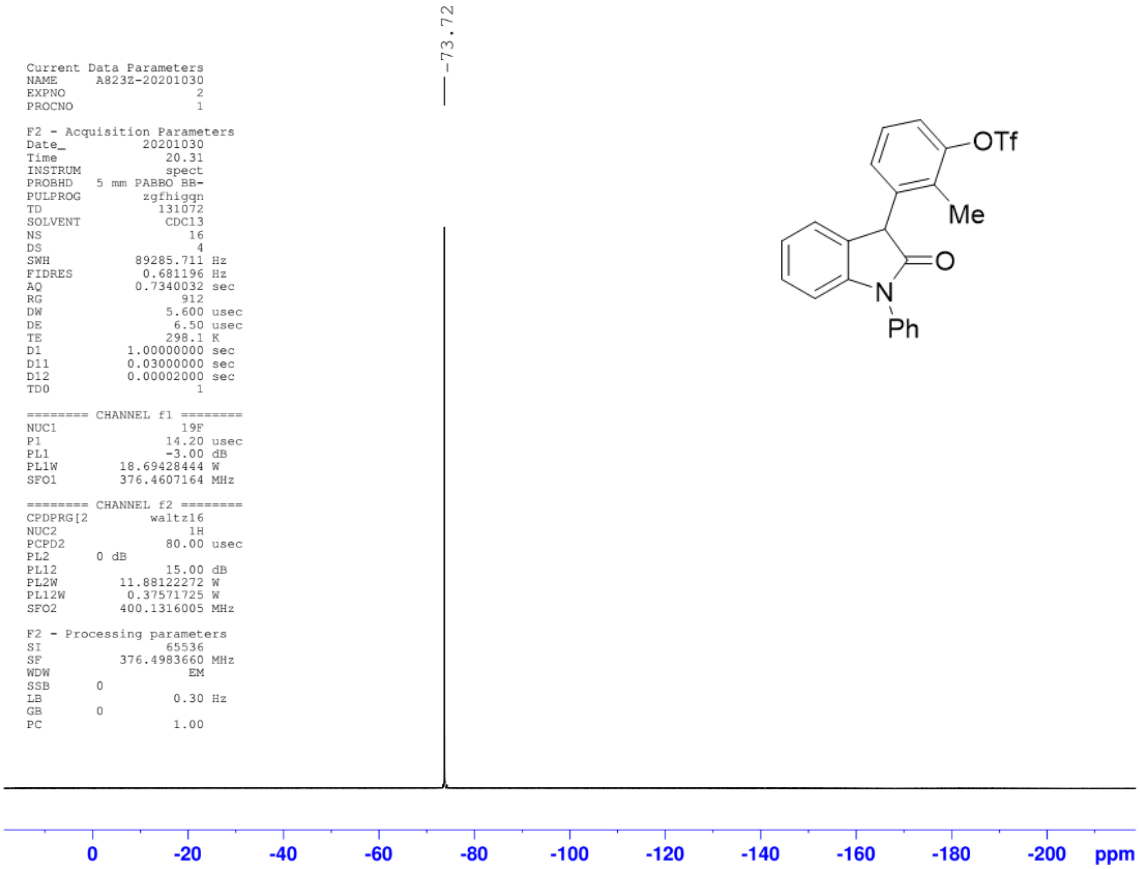

7.3411
7.3302
7.3040
7.2932
7.2824
7.2599
7.2459
7.2416
7.1419
7.1355
7.1208
7.1144
7.0877
7.0691
7.0517
7.0334
6.8638
6.8441
6.7519
5.0337
4.9948
4.9631
4.9240
4.8850
2.5277
Current Data Parameters
NAME A823W-20201031-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201031
Time 17.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
TfO
Me
O
N
Bn
10
9
8
7
6
5
4
3
2
1
0
ppm
7.12
1.06
2.04
1.04
0.74
3.00
3.07

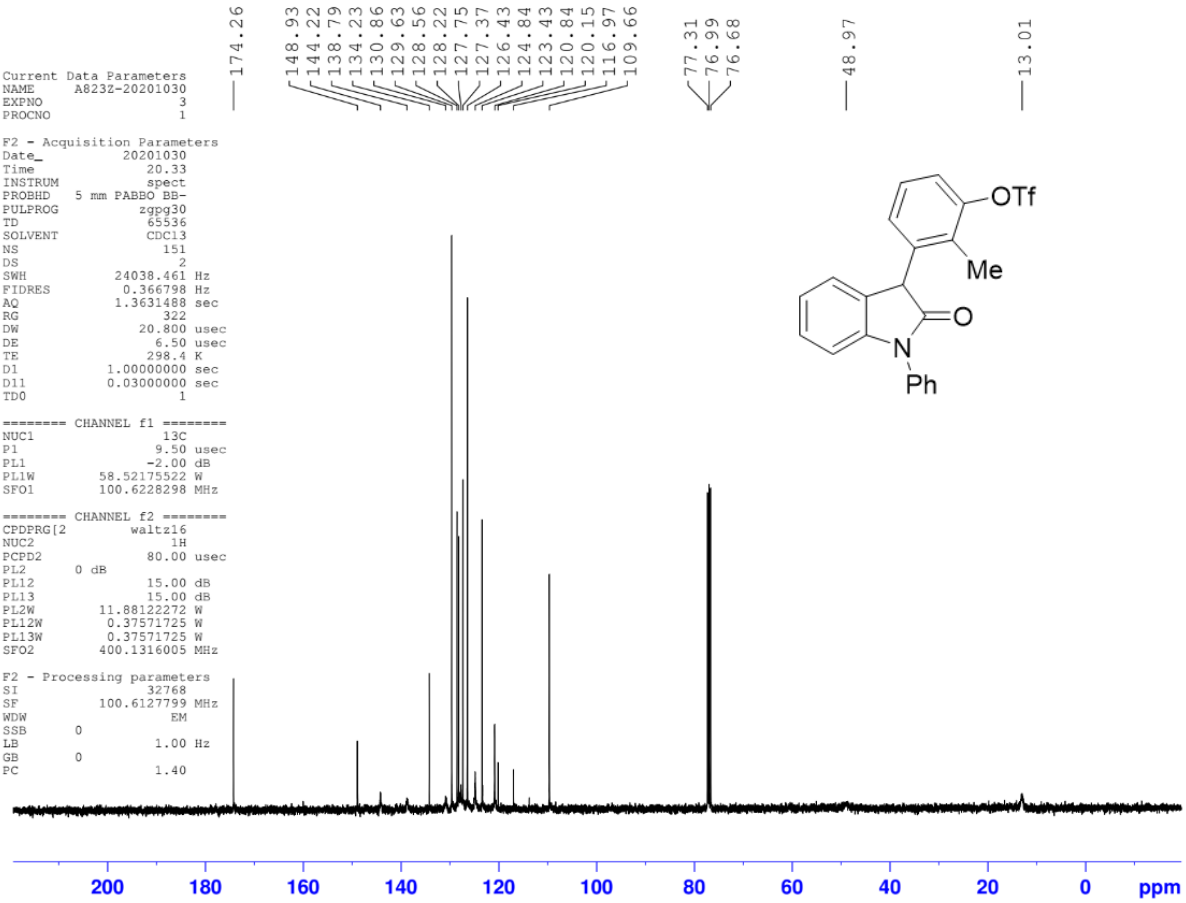

-72.78
Current Data Parameters
NAME A823W-20201031-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201031
Time 17.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 1620
DW 5.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
TfO
Me
O
N
Bn
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

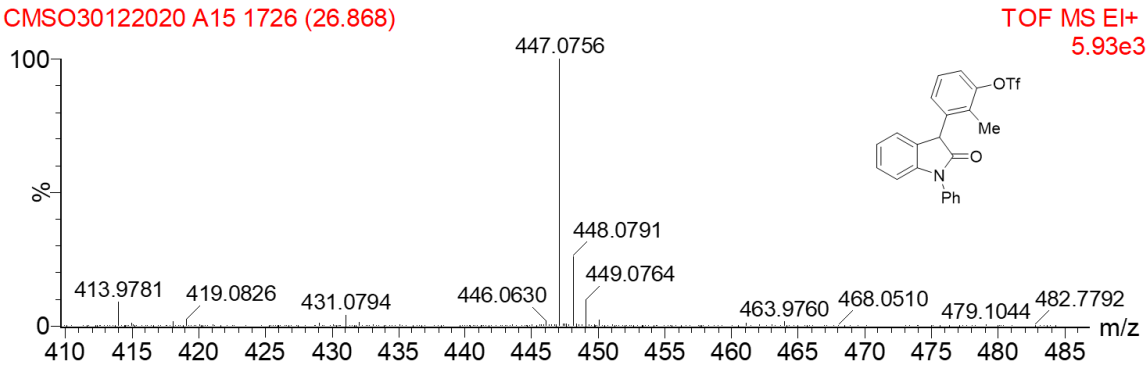

174.93
147.84
143.52
138.28
137.96
135.57
132.49
128.83
128.77
127.77
127.69
127.35
124.68
123.07
120.22
117.05
109.42
77.31
77.00
76.68
49.23
44.01
19.50
Current Data Parameters
NAME A823W-20201031-2
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201031
Time 17.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 120
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127747 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
TfO
Me
O
N
Bn
200
180
160
140
120
100
80
60
40
20
0
ppm

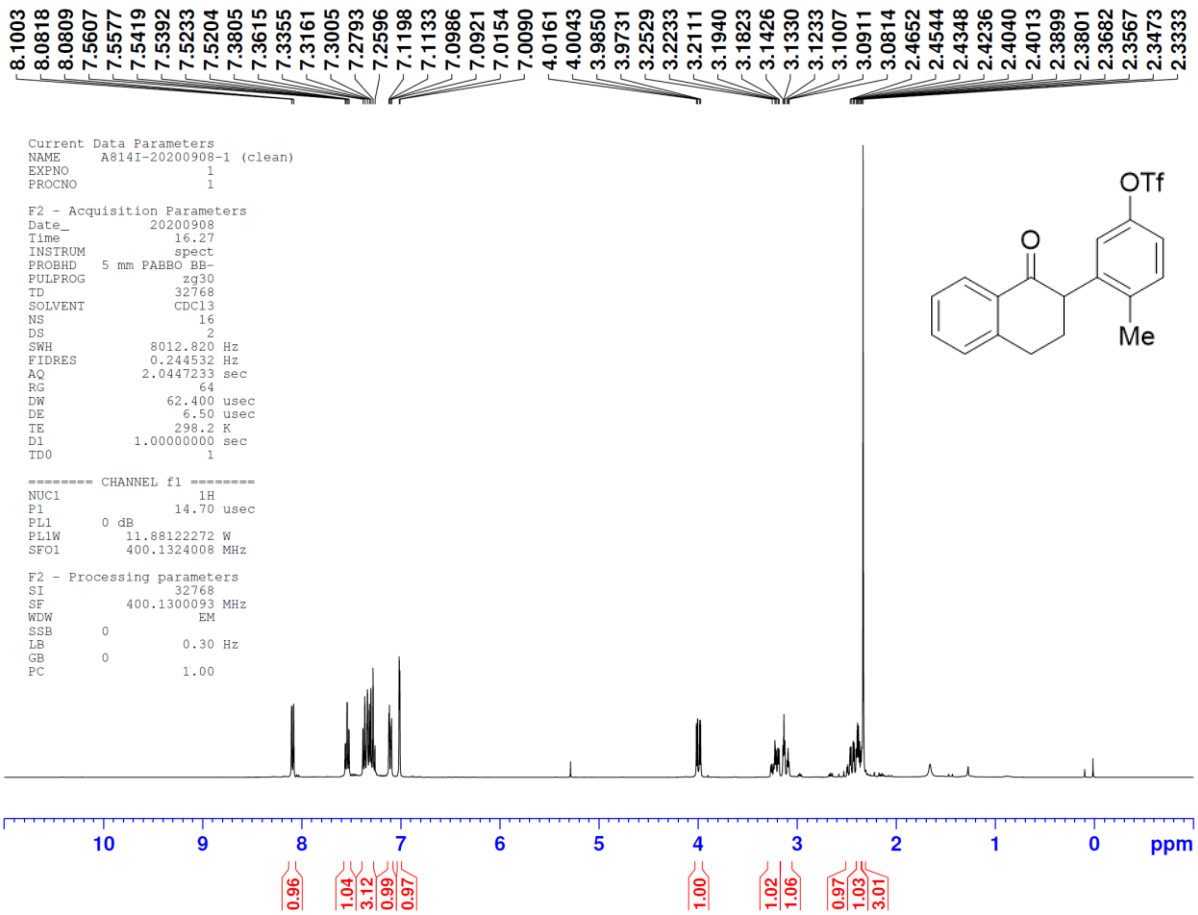

CMSO30122020 A14 1731 (26.934)
TOF MS EI+
2.32e4
100
%
0
461.0903
462.0968
463.0851
432.0819
445.0959
460.0805
473.0538
479.0735
489.0300
492.0931
m/z
425
430
435
440
445
450
455
460
465
470
475
480
485
490
495
TfO
Me
O
N
Bn

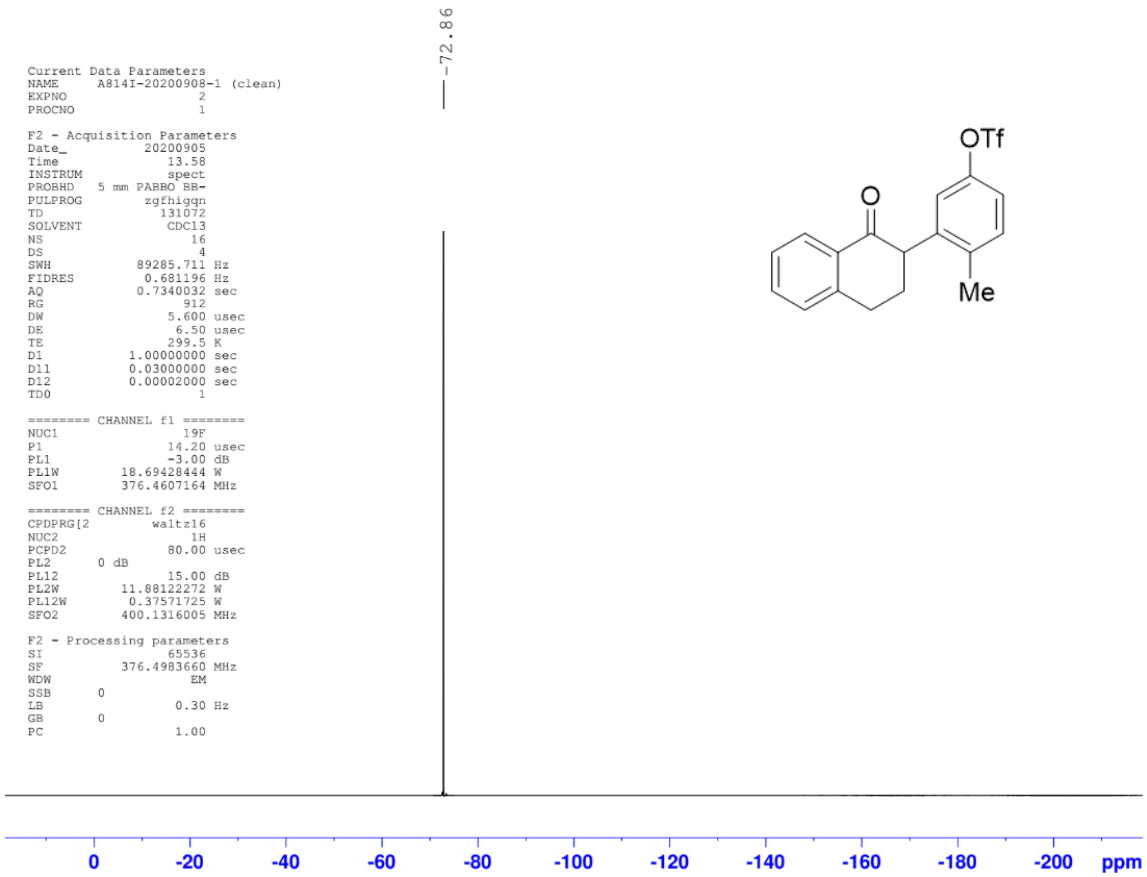

7.5719
7.5522
7.5334
7.4661
7.4595
7.4470
7.4385
7.4197
7.3102
7.2900
7.2693
7.2579
7.1310
7.1134
7.0957
6.9292
6.9095
5.1182
2.6401
Current Data Parameters
NAME A823Z-20201030
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201030
Time 20.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 36
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
Me
O
N
Ph
10
9
8
7
6
5
4
3
2
1
0
ppm
2.13
3.25
6.04
1.09
0.97
2.95

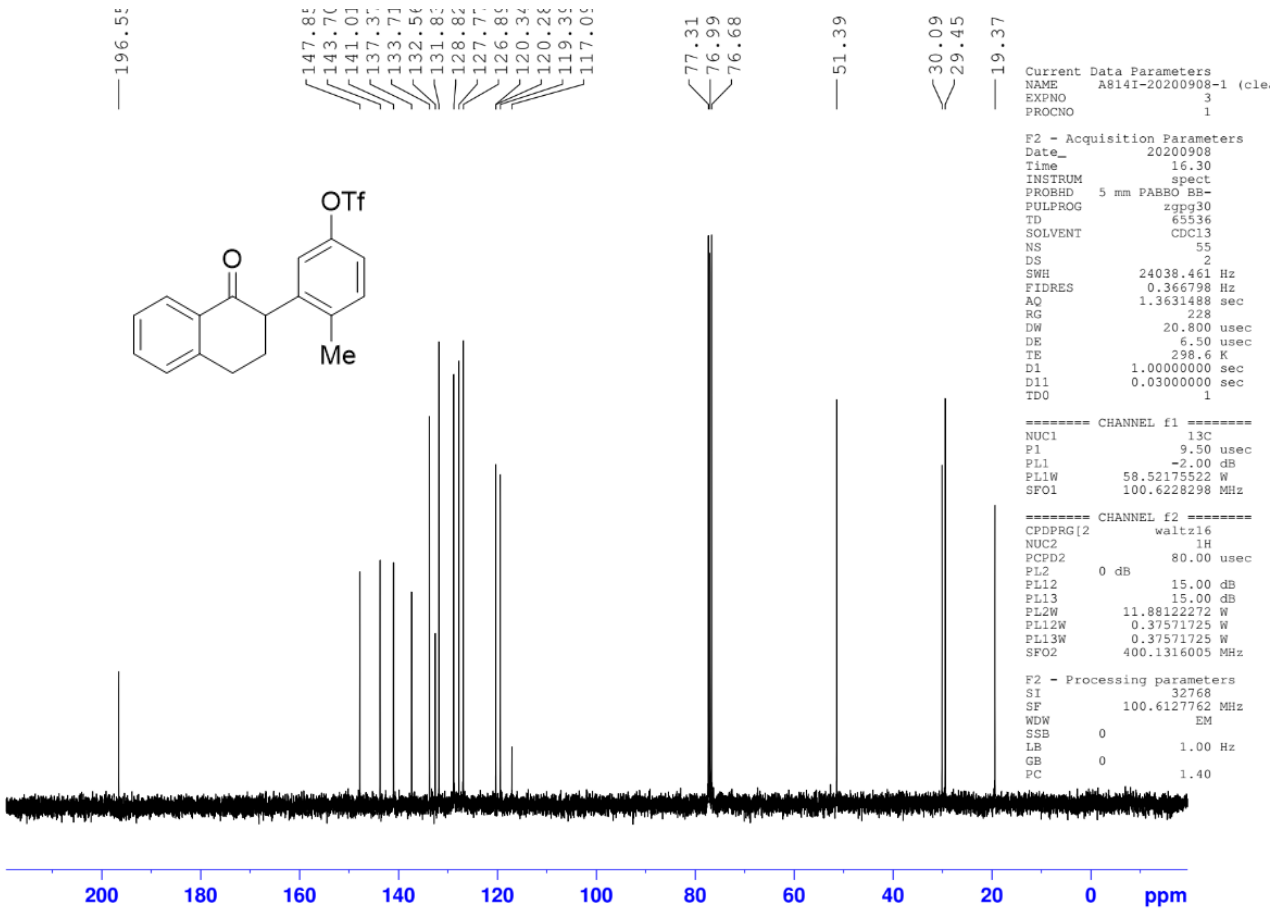

-73.72
Current Data Parameters
NAME A823Z-20201030
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201030
Time 20.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
Me
O
N
Ph
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

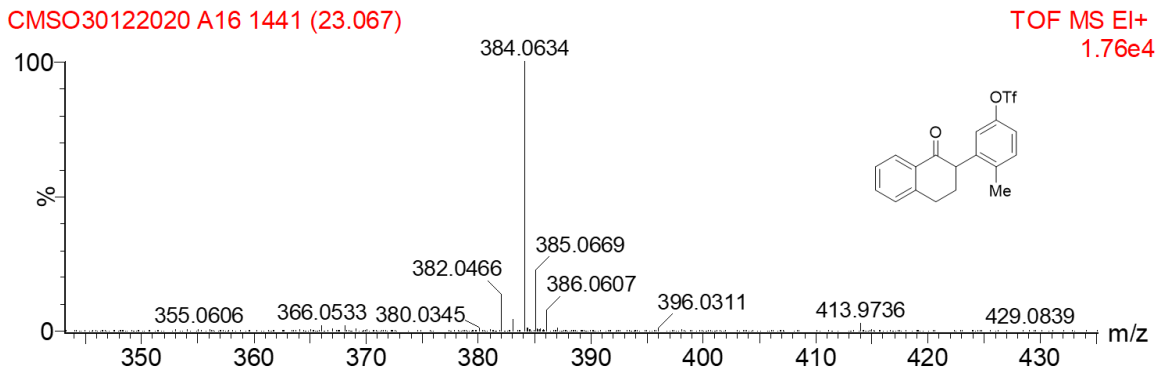

174.26
148.93
144.22
138.79
134.23
130.86
129.63
128.56
128.22
127.75
127.37
126.43
124.84
123.43
120.84
120.15
116.97
109.66
77.31
76.99
76.68
48.97
13.01
Current Data Parameters
NAME A823Z-20201030
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201030
Time 20.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 151
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 322
DW 20.800 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127799 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
OTf
Me
O
N
Ph
200
180
160
140
120
100
80
60
40
20
0
ppm

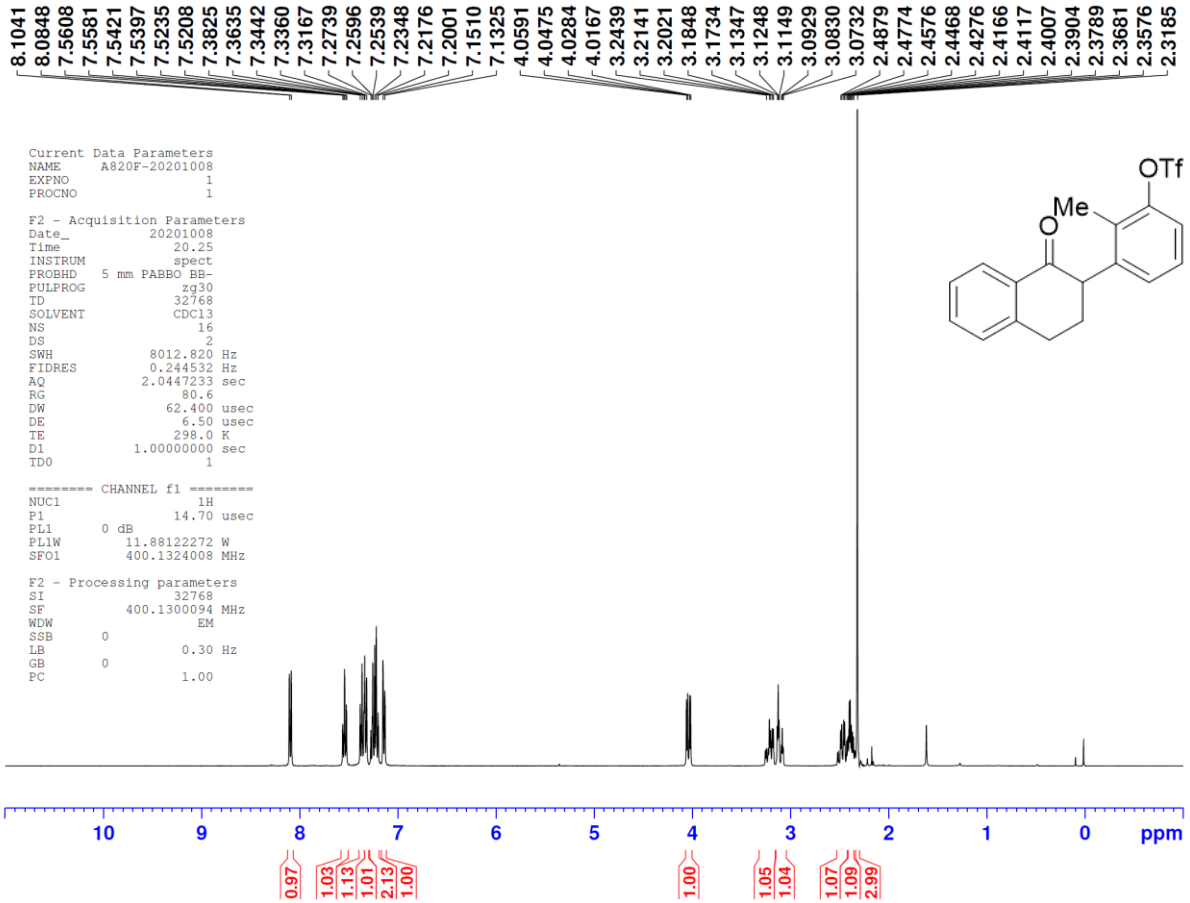

CMSO30122020 A15 1726 (26.868)
TOF MS EI+
5.93e3
100
%
0
447.0756
448.0791
449.0764
413.9781
419.0826
431.0794
446.0630
463.9760
468.0510
479.1044
482.7792
OTf
Me
O
N
Ph
410
415
420
425
430
435
440
445
450
455
460
465
470
475
480
485
m/z

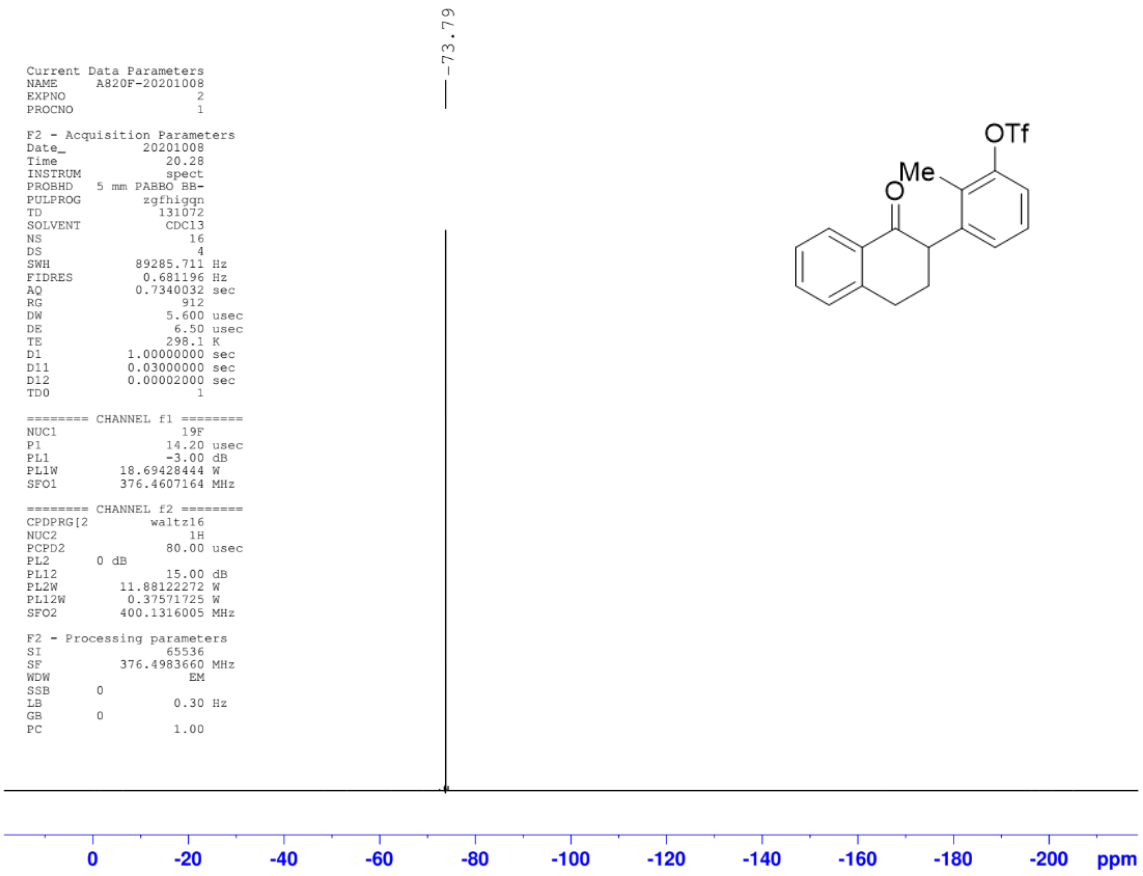

8.1003
8.0818
8.0809
7.5607
7.5577
7.5419
7.5392
7.5233
7.5204
7.3805
7.3615
7.3355
7.3161
7.3005
7.2793
7.2596
7.1198
7.1133
7.0986
7.0921
7.0154
7.0090
4.0161
4.0043
3.9850
3.9731
3.2529
3.2233
3.2111
3.1940
3.1823
3.1426
3.1330
3.1233
3.1007
3.0911
3.0814
2.4652
2.4544
2.4348
2.4236
2.4040
2.4013
2.3899
2.3801
2.3682
2.3567
2.3473
2.3333
Current Data Parameters
NAME A814I-20200908-1 (clean)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200908
Time 16.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 64
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
1.04
3.12
0.99
0.97
1.00
1.02
1.06
0.97
1.03
3.01

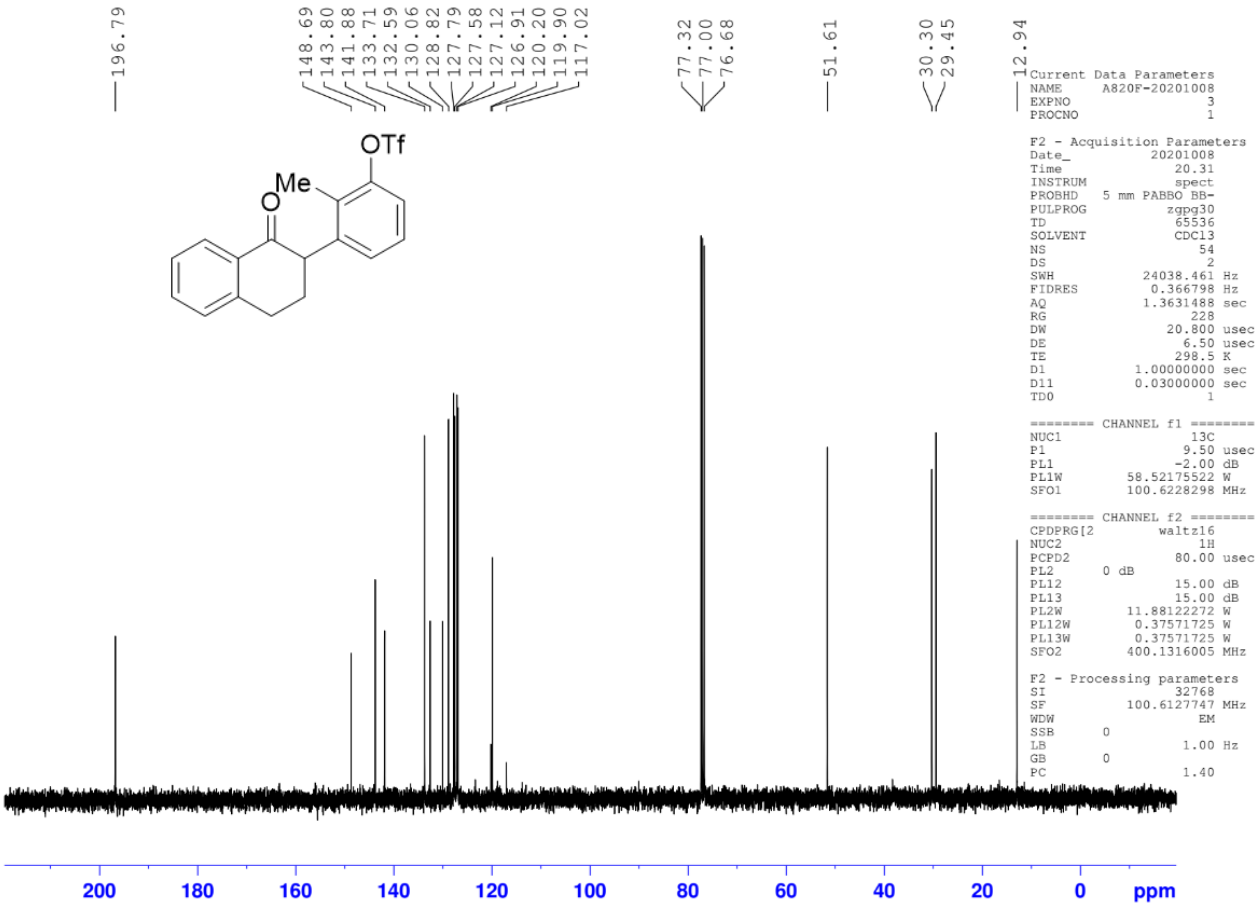

-72.86
Current Data Parameters
NAME A814I-20200908-1 (clean)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200905
Time 13.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 299.5 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
Me
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

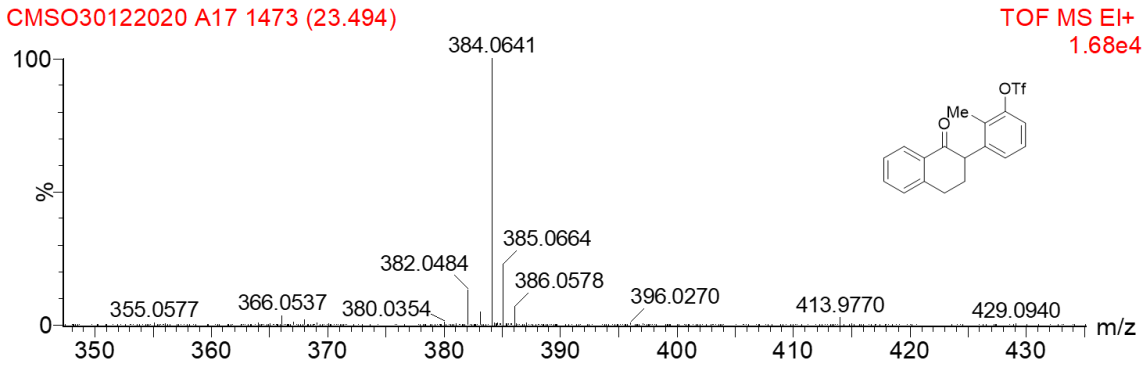

196.55
147.85
143.70
141.01
137.37
133.71
132.56
131.83
128.82
127.77
126.89
120.34
120.28
119.39
117.09
77.31
76.99
76.68
51.39
30.09
29.45
19.37
OTf
O
Me
Current Data Parameters
NAME A814I-20200908-1 (cle
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20200908
Time 16.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 55
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 228
DW 20.800 usec
DE 6.50 usec
TE 298.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127762 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

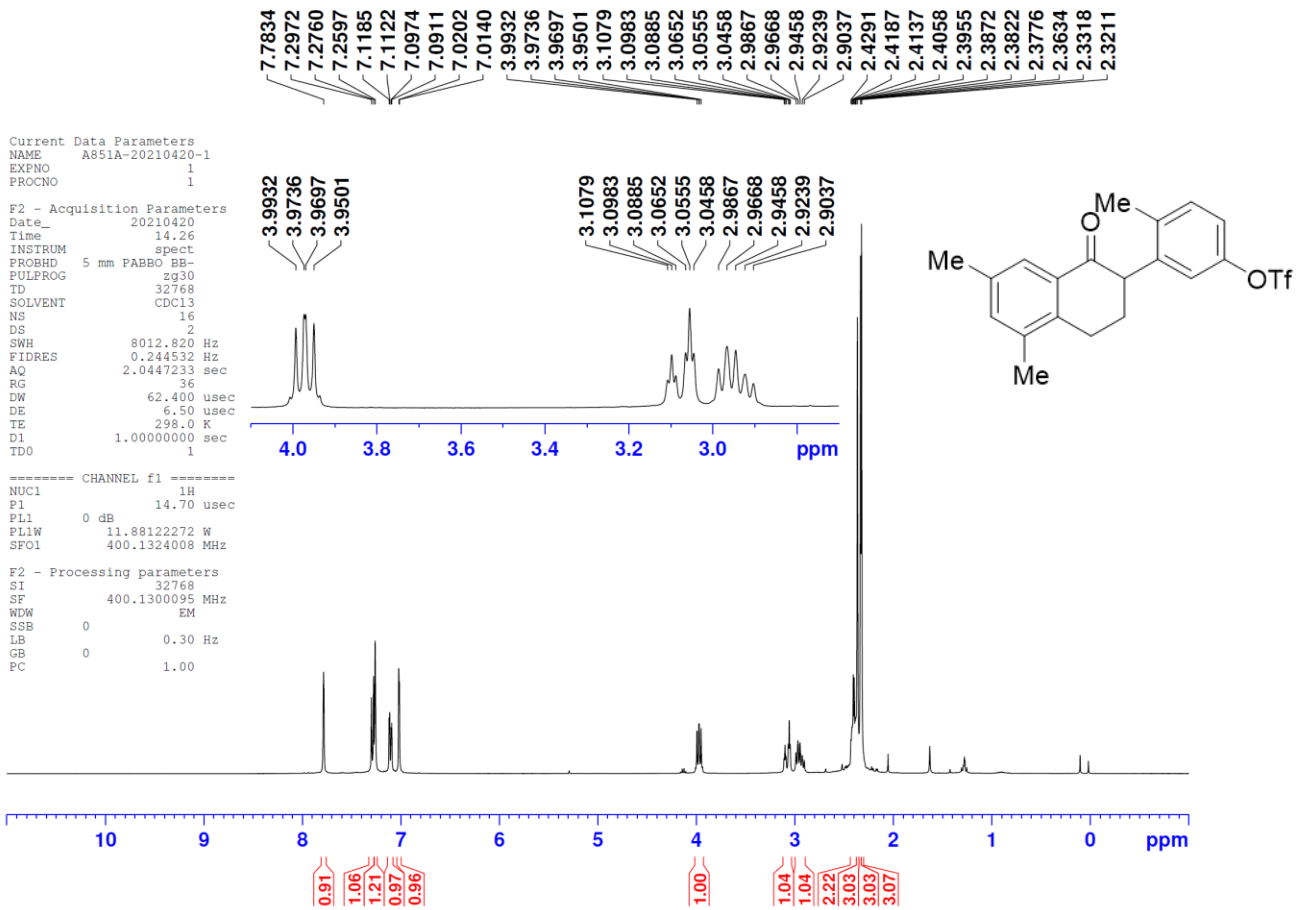

CMSO30122020 A16 1441 (23.067)
TOF MS EI+
1.76e4
100
%
0
384.0634
385.0669
382.0466
386.0607
355.0606
366.0533
380.0345
396.0311
413.9736
429.0839
OTf
O
Me
350
360
370
380
390
400
410
420
430
m/z

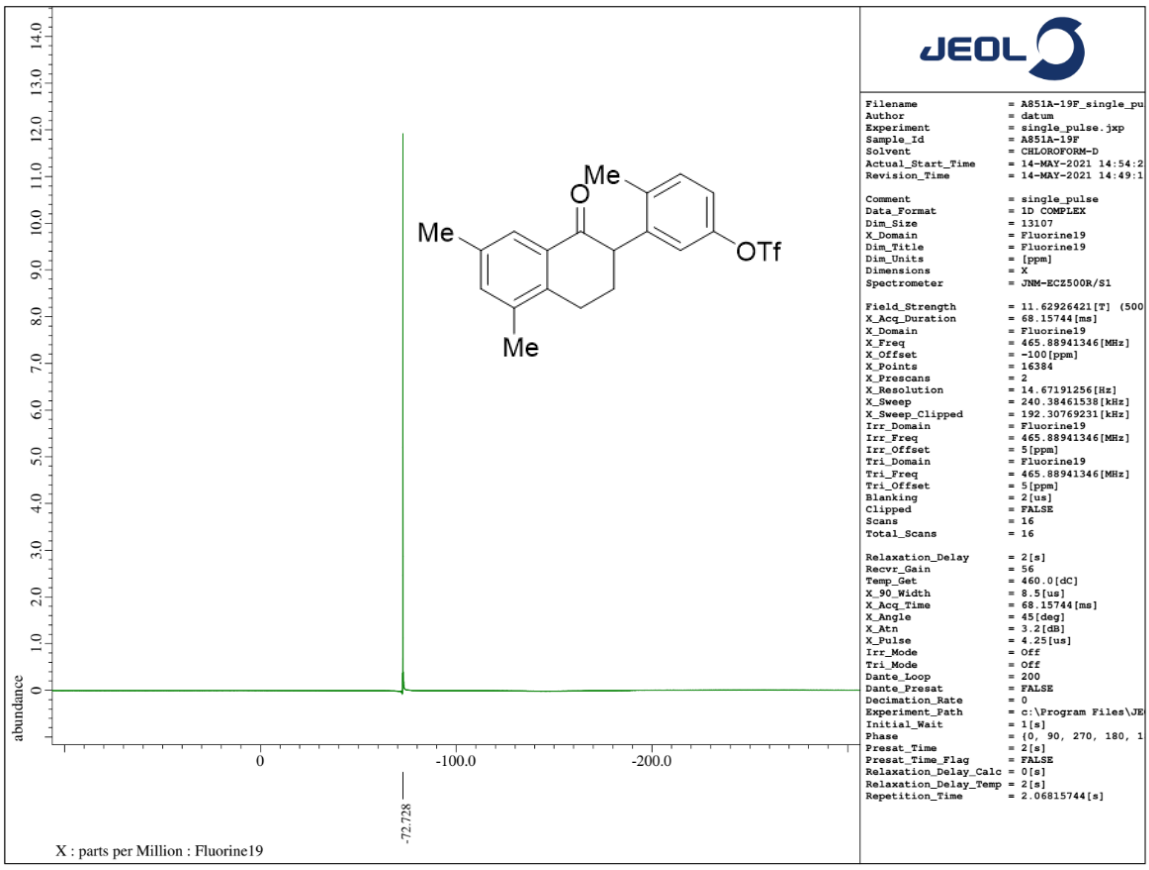

8.1041
8.0848
7.5608
7.5581
7.5421
7.5397
7.5235
7.5208
7.3825
7.3635
7.3442
7.3360
7.3167
7.2739
7.2596
7.2539
7.2348
7.2176
7.2001
7.1510
7.1325
4.0591
4.0475
4.0284
4.0167
3.2439
3.2141
3.2021
3.1848
3.1734
3.1347
3.1248
3.1149
3.0929
3.0830
3.0732
2.4879
2.4774
2.4576
2.4468
2.4276
2.4166
2.4117
2.4007
2.3904
2.3789
2.3681
2.3576
2.3185
Current Data Parameters
NAME A820F-20201008
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201008
Time 20.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 80.6
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
Me
O
10
9
8
7
6
5
4
3
2
1
0
ppm
0.97
1.03
1.13
1.01
2.13
1.00
1.00
1.05
1.04
1.07
1.09
2.99

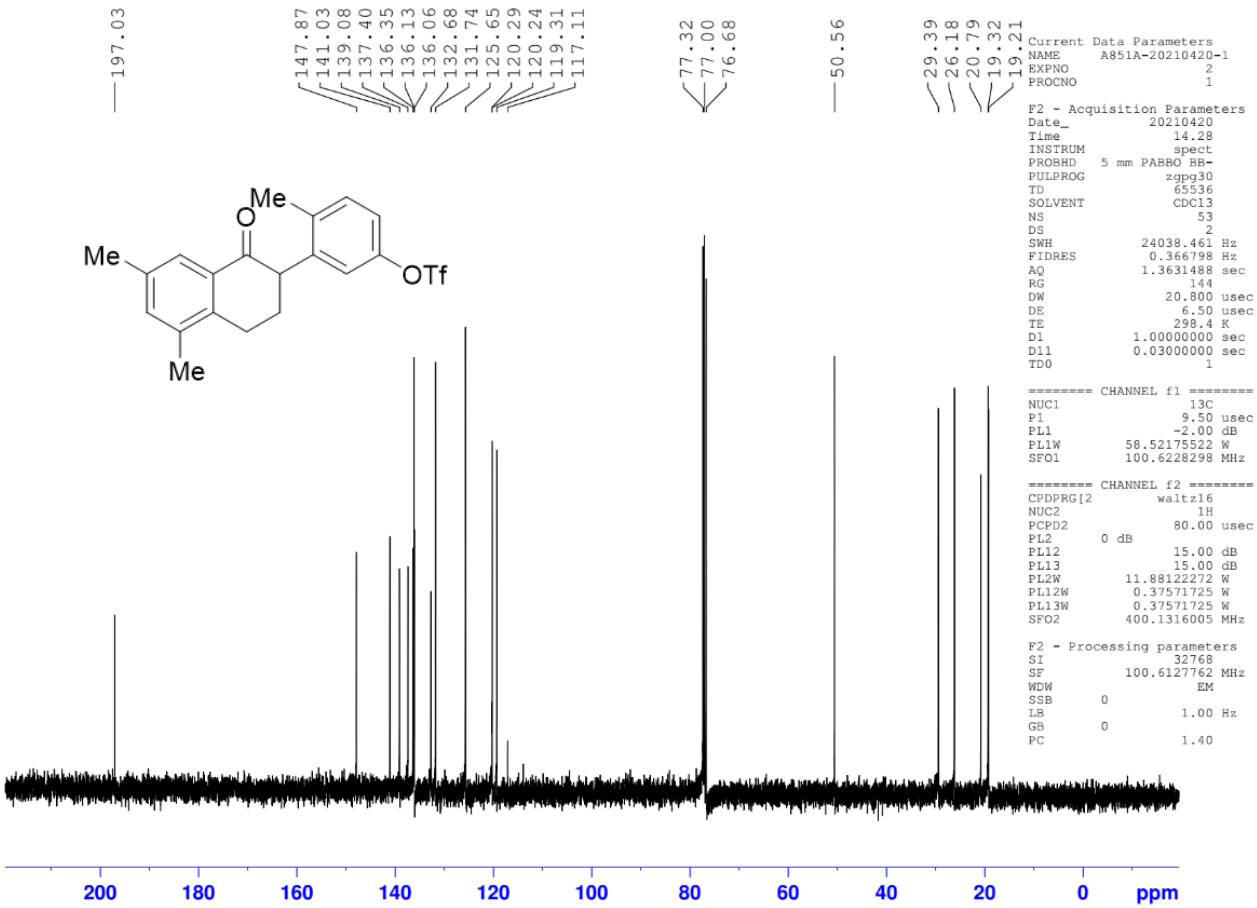

-73.79
Current Data Parameters
NAME A820F-20201008
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201008
Time 20.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
Me
O
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm


196.79
148.69
143.80
141.88
133.71
132.59
130.06
128.82
127.79
127.58
127.12
126.91
120.20
119.90
117.02
77.32
77.00
76.68
51.61
30.30
29.45
12.94
OTf
Me
O
Current Data Parameters
NAME A820F-20201008
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201008
Time 20.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 54
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 228
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127747 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

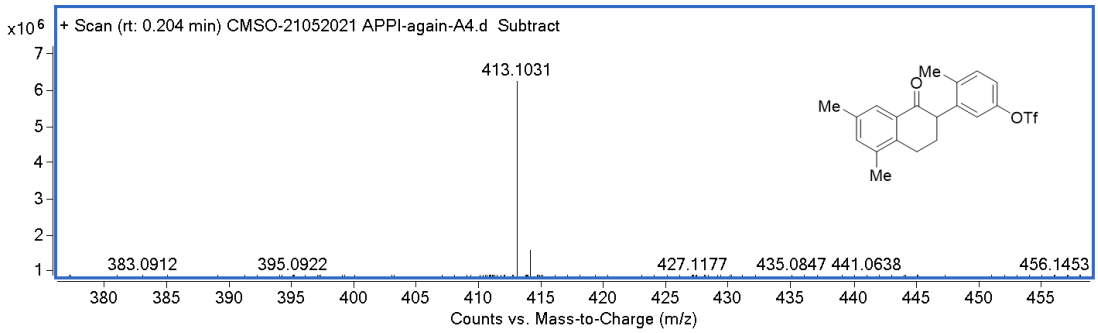

CMSO30122020 A17 1473 (23.494)
TOF MS EI+
1.68e4
100
%
0
384.0641
385.0664
382.0484
386.0578
355.0577
366.0537
380.0354
396.0270
413.9770
429.0940
m/z
350
360
370
380
390
400
410
420
430
OTf
Me
O

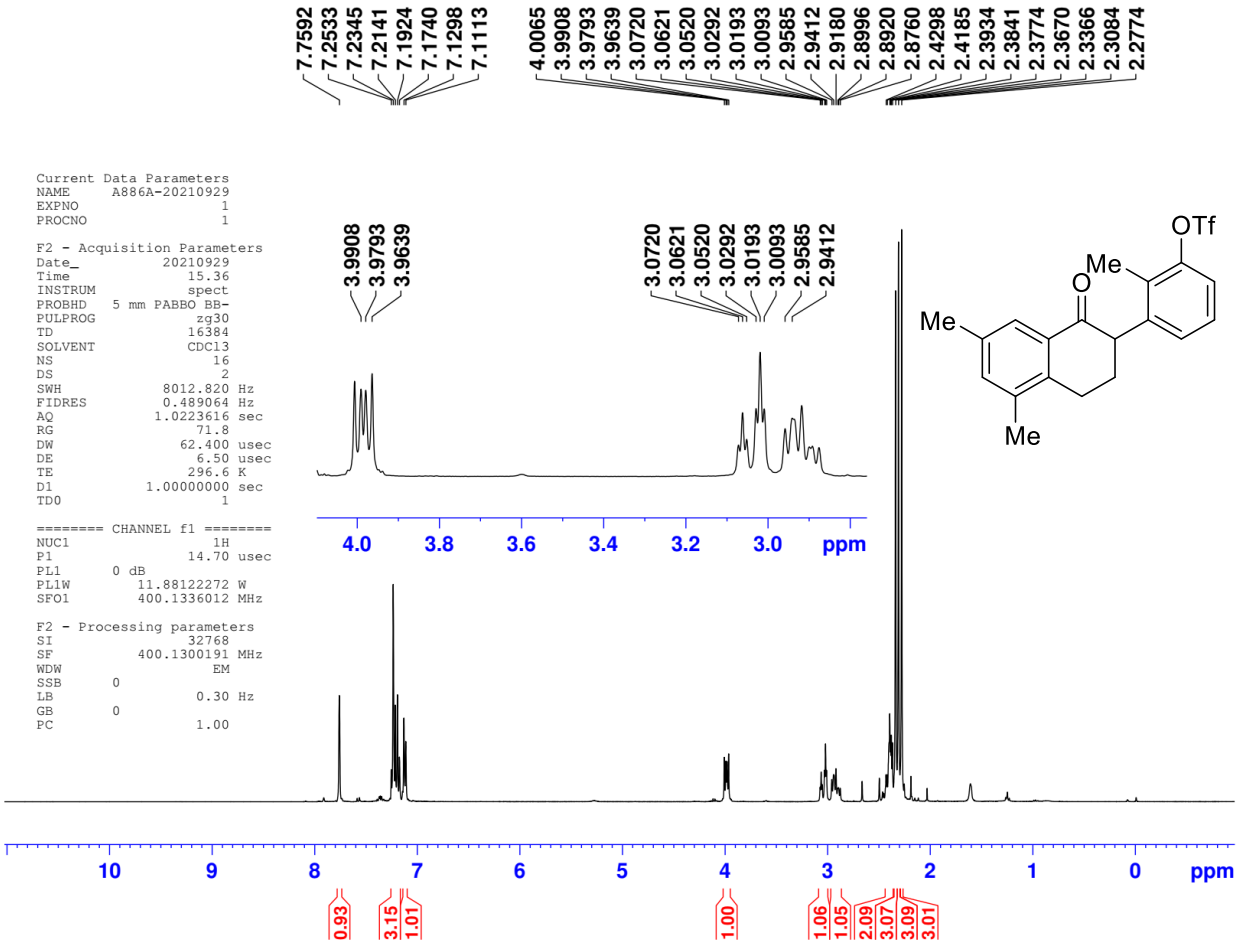

7.7834 7.2972 7.2760 7.2597 7.1185 7.1122 7.0974 7.0911 7.0202 7.0140 3.9932 3.9736 3.9697 3.9501 3.1079 3.0983 3.0885 3.0652 3.0555 3.0458 2.9867 2.9668 2.9458 2.9239 2.9037 2.4291 2.4187 2.4137 2.4058 2.3955 2.3872 2.3822 2.3776 2.3634 2.3318 2.3211
Current Data Parameters
NAME A851A-20210420-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210420
Time 14.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 36
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
O
Me
OTf
Me
4.0 3.8 3.6 3.4 3.2 3.0 ppm
10 9 8 7 6 5 4 3 2 1 0 ppm
0.91 1.06 1.21 0.97 0.96 1.00 1.04 1.04 2.22 3.03 3.03 3.07

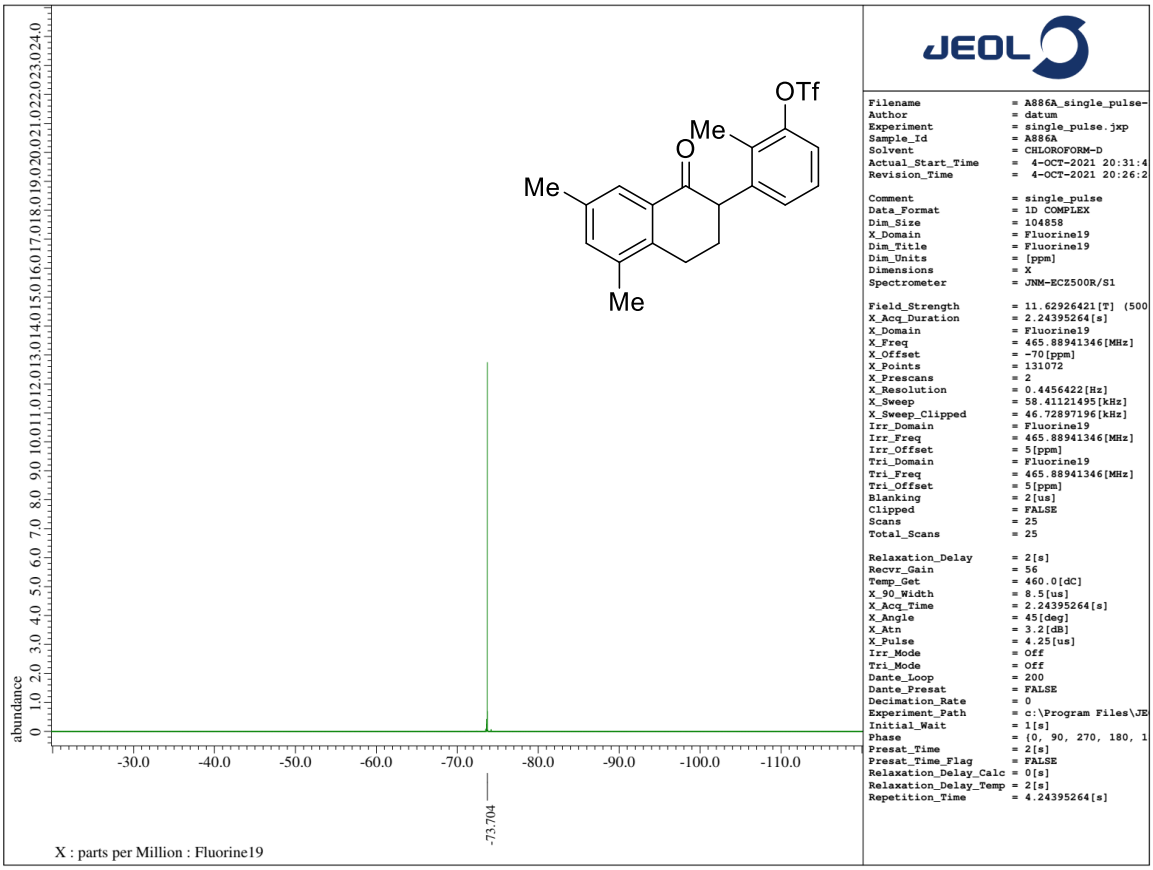

JEOL
Me
O
Me
OTf
Me
abundance
0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0 10.0 11.0 12.0 13.0 14.0
0 -100.0 -200.0
-72.728
X : parts per Million : Fluorine19
Filename = A851A-19F_single_pu
Author = datum
Experiment = single_pulse.jxp
Sample_Id = A851A-19F
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-MAY-2021 14:54:2
Revision_Time = 14-MAY-2021 14:49:1
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (500
X_Acq_Duration = 68.15744[ms]
X_Domain = Fluorine19
X_Freq = 465.88941346[MHz]
X_Offset = -100[ppm]
X_Points = 16384
X_Prescans = 2
X_Resolution = 14.67191256[Hz]
X_Sweep = 240.38461538[kHz]
X_Sweep_Clipped = 192.30769231[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 465.88941346[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 465.88941346[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 460.0[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 68.15744[ms]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 4.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 200
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 1
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 2.06815744[s]

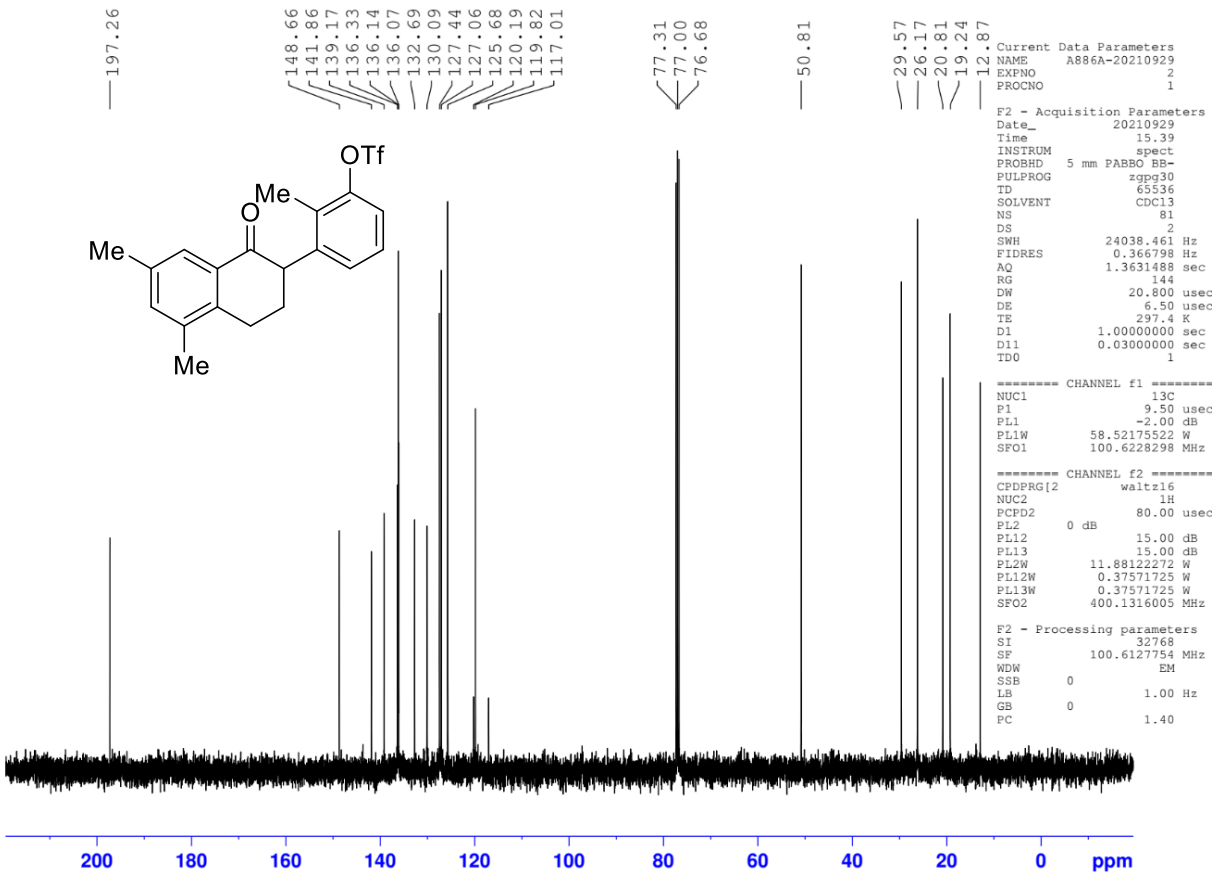


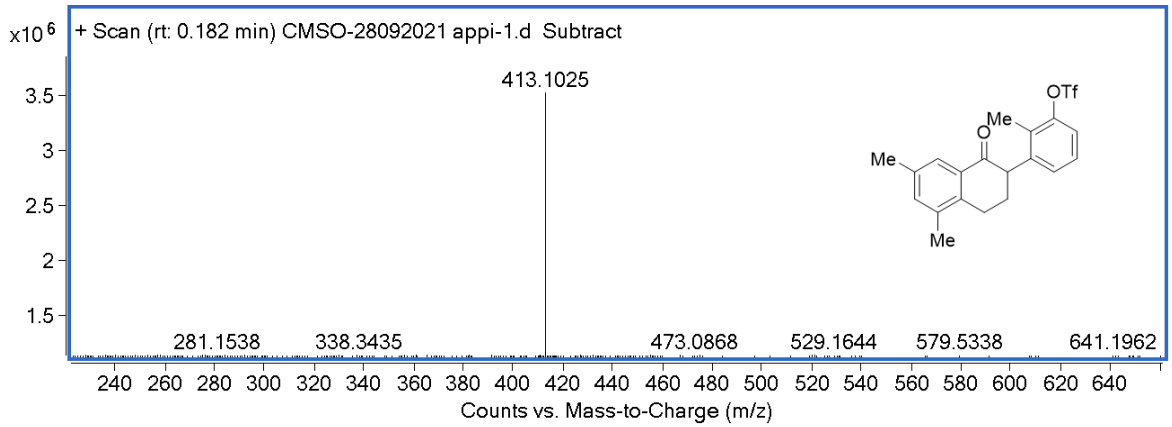

```
Current Data Parameters
NAME      A851A-20210420-1
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20210420
Time               14.28
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    53
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   144
DW                20.800 usec
DE                 6.50 usec
TE                298.4 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.50 usec
PL1               -2.00 dB
PL1W        58.52175522 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2       0 dB
PL12               15.00 dB
PL13               15.00 dB
PL2W        11.88122272 W
PL12W        0.37571725 W
PL13W        0.37571725 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF         100.6127762 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

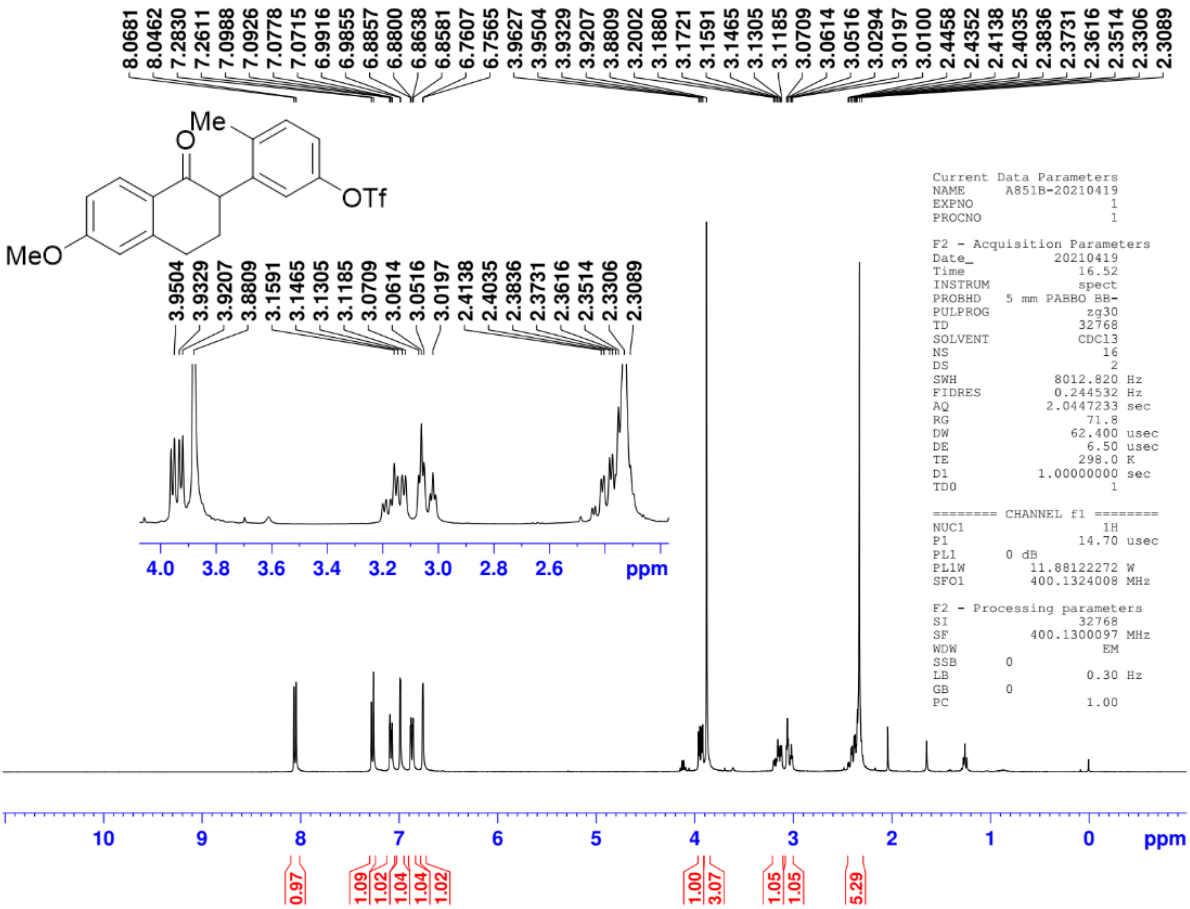


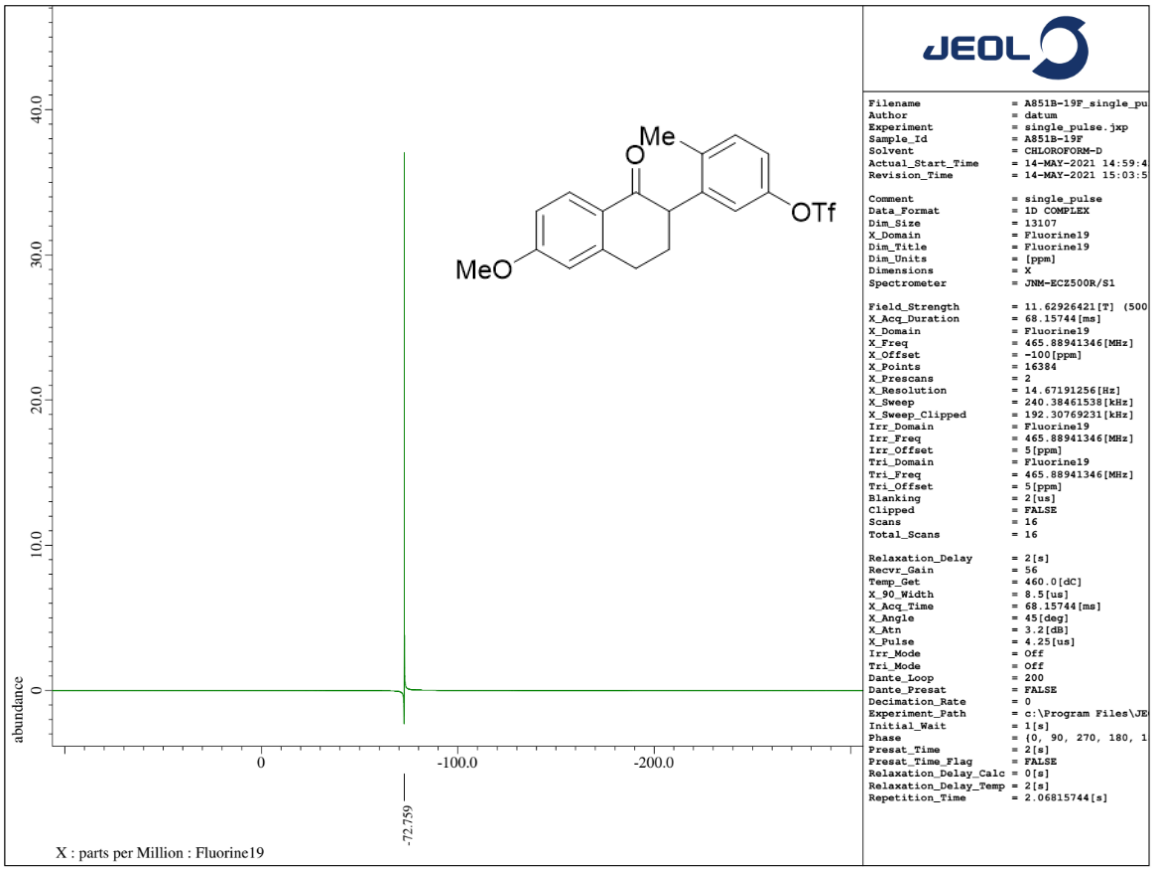

7.7592
7.2533
7.2345
7.2141
7.1924
7.1740
7.1298
7.1113
4.0065
3.9908
3.9793
3.9639
3.0720
3.0621
3.0520
3.0292
3.0193
3.0093
2.9585
2.9412
2.9180
2.8996
2.8920
2.8760
2.4298
2.4185
2.3934
2.3841
2.3774
2.3670
2.3366
2.3084
2.2774
Current Data Parameters
NAME A886A-20210929
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210929
Time 15.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 296.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300191 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
Me
O
Me
Me
4.0
3.8
3.6
3.4
3.2
3.0
ppm
10
9
8
7
6
5
4
3
2
1
0
ppm
0.93
3.15
1.01
1.00
1.06
1.05
2.09
3.07
3.09
3.01

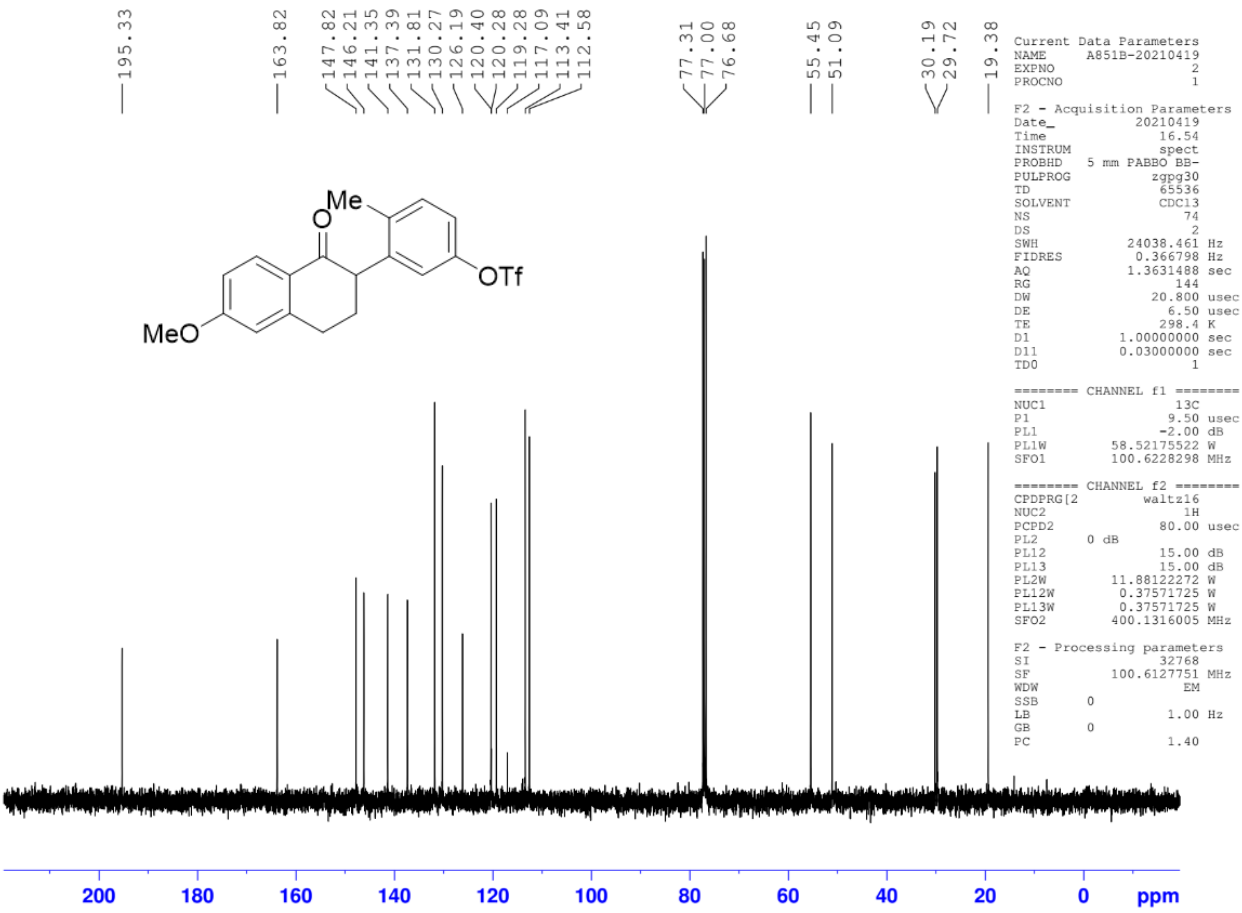

OTf
Me
O
Me
Me
abundance
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-73.704
X : parts per Million : Fluorine19
JEOL
Filename = A886A_single_pulse-
Author = datum
Experiment = single_pulse.jxp
Sample_Id = A886A
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-OCT-2021 20:31:4
Revision_Time = 4-OCT-2021 20:26:2
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (500
X_Acq_Duration = 2.24395264[s]
X_Domain = Fluorine19
X_Freq = 465.88941346[MHz]
X_Offset = -70[ppm]
X_Points = 131072
X_Prescans = 2
X_Resolution = 0.4456422[Hz]
X_Sweep = 58.41121495[kHz]
X_Sweep_Clipped = 46.72897196[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 465.88941346[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 465.88941346[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 25
Total_Scans = 25
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 460.0[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 2.24395264[s]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 4.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 200
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 1
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.24395264[s]


197.26
148.66
141.86
139.17
136.33
136.14
136.07
132.69
130.09
127.44
127.06
125.68
120.19
119.82
117.01
77.31
77.00
76.68
50.81
29.57
26.17
20.81
19.24
12.87
OTf
Me
O
Me
Me
Current Data Parameters
NAME A886A-20210929
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210929
Time 15.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 81
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127754 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

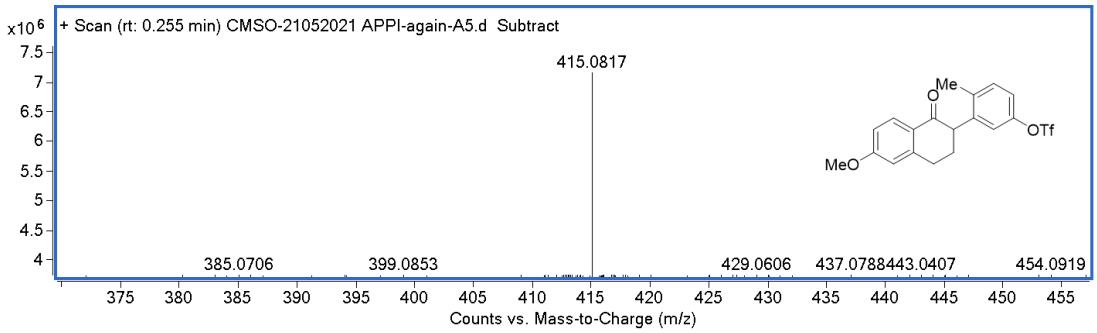

x10 6
+ Scan (rt: 0.182 min) CMSO-28092021 appi-1.d Subtract
413.1025
281.1538
338.3435
473.0868
529.1644
579.5338
641.1962
OTf
Me
O
Me
Me
3.5
3
2.5
2
1.5
240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640
Counts vs. Mass-to-Charge (m/z)

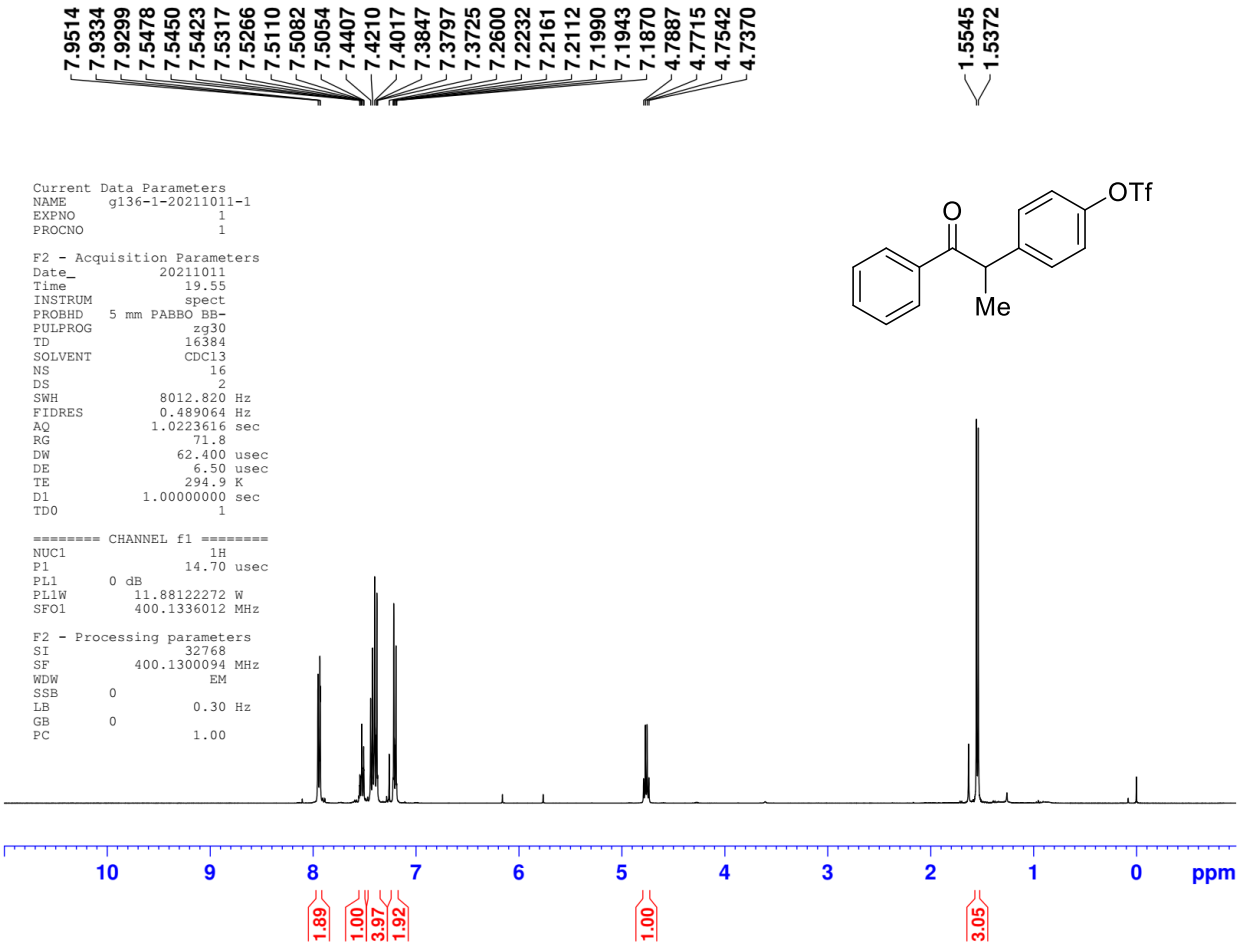

8.0681 8.0462 7.2830 7.2611 7.0988 7.0926 7.0778 7.0715 6.9916 6.9855 6.8857 6.8800 6.8638 6.8581 6.7607 6.7565 3.9627 3.9504 3.9329 3.9207 3.8809 3.2002 3.1880 3.1721 3.1591 3.1465 3.1305 3.1185 3.0709 3.0614 3.0516 3.0294 3.0197 3.0100 2.4458 2.4352 2.4138 2.4035 2.3836 2.3731 2.3616 2.3514 2.3306 2.3089
Me
O
OTf
MeO
3.9504 3.9329 3.9207 3.8809 3.1591 3.1465 3.1305 3.1185 3.0709 3.0614 3.0516 3.0197 2.4138 2.4035 2.3836 2.3731 2.3616 2.3514 2.3306 2.3089
4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 ppm
Current Data Parameters
NAME A851B-20210419
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210419
Time 16.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10 9 8 7 6 5 4 3 2 1 0 ppm
0.97 1.09 1.02 1.04 1.04 1.02 1.00 3.07 1.05 1.05 5.29

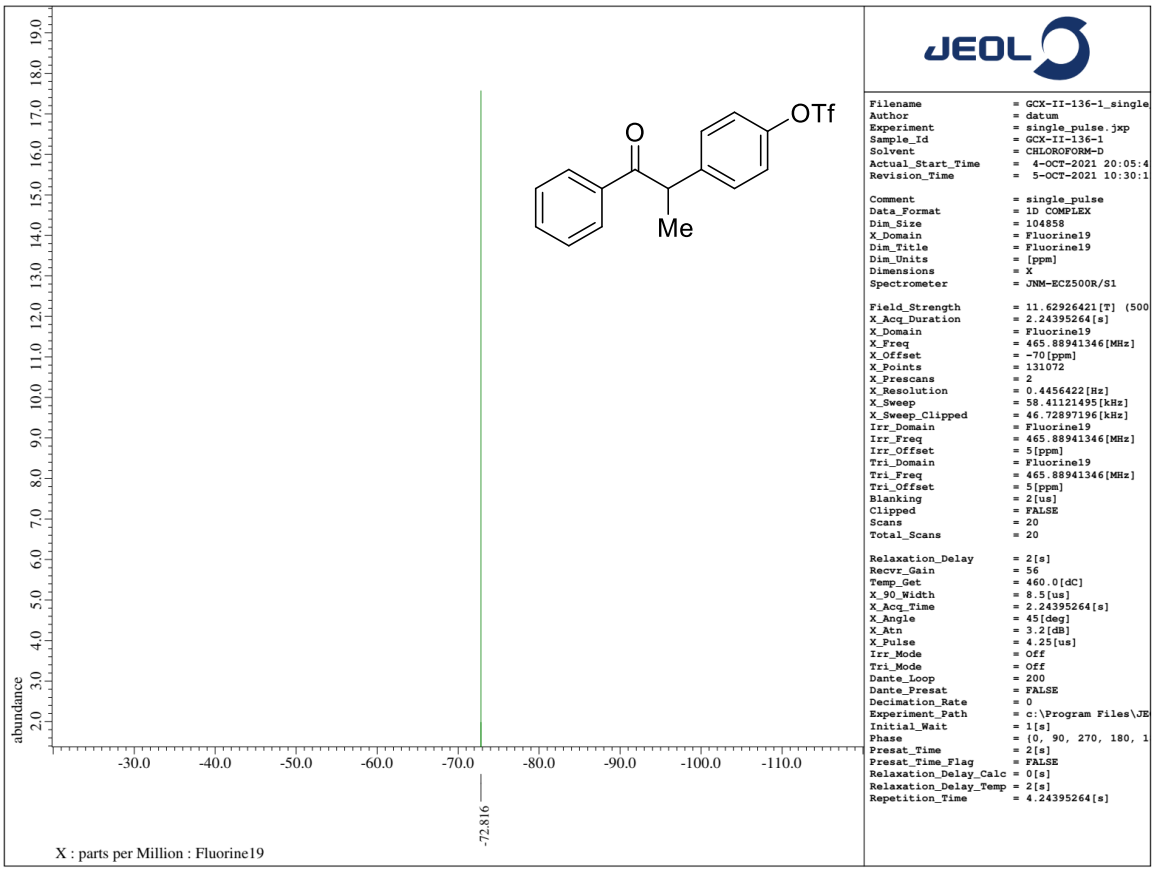

JEOL
Me
O
OTf
MeO
abundance
40.0
30.0
20.0
10.0
0
0
-100.0
-200.0
-72.759
X : parts per Million : Fluorine19
Filename = A851B-19F_single_pu
Author = datum
Experiment = single_pulse.jxp
Sample_Id = A851B-19F
Solvent = CHLOROFORM-D
Actual_Start_Time = 14-MAY-2021 14:59:4
Revision_Time = 14-MAY-2021 15:03:5
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (500
X_Acq_Duration = 68.15744[ms]
X_Domain = Fluorine19
X_Freq = 465.88941346[MHz]
X_Offset = -100[ppm]
X_Points = 16384
X_Prescans = 2
X_Resolution = 14.67191256[Hz]
X_Sweep = 240.38461538[kHz]
X_Sweep_Clipped = 192.30769231[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 465.88941346[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 465.88941346[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 460.0[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 68.15744[ms]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 4.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 200
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 1
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 2.06815744[s]

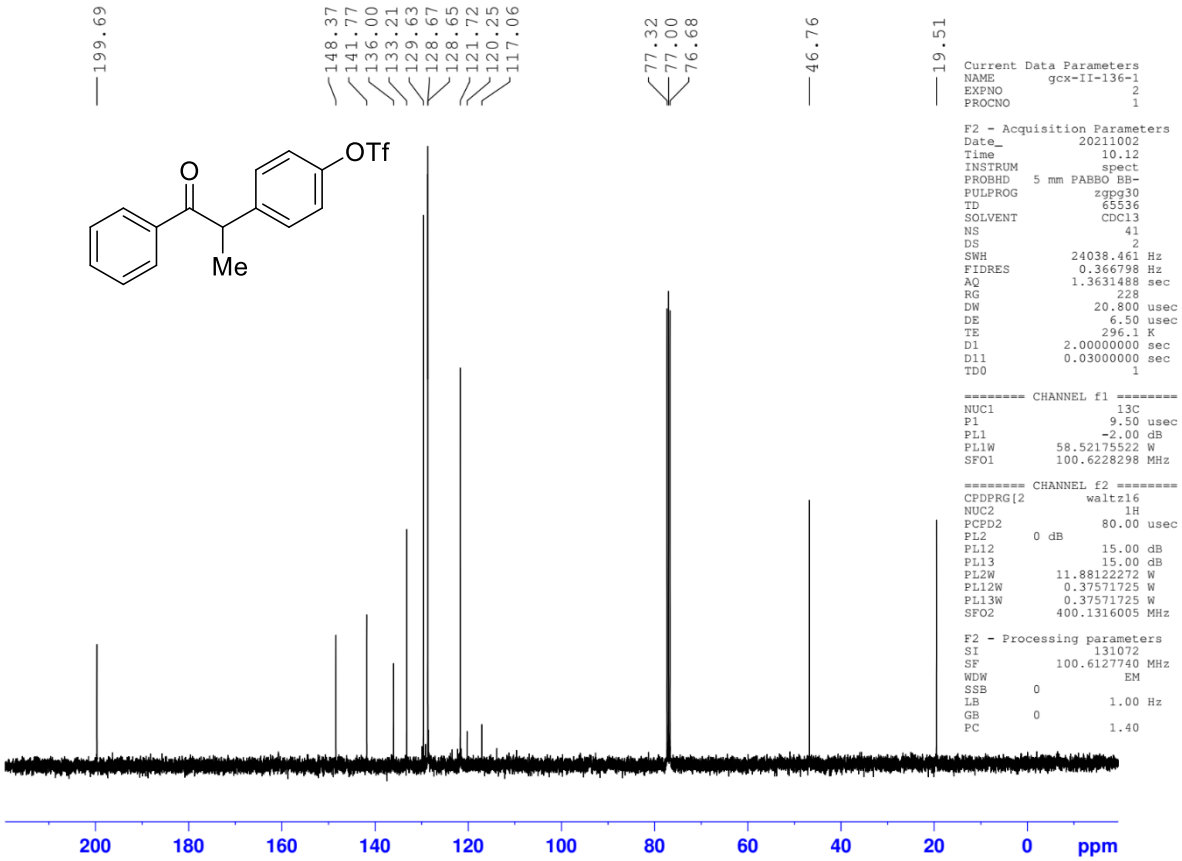


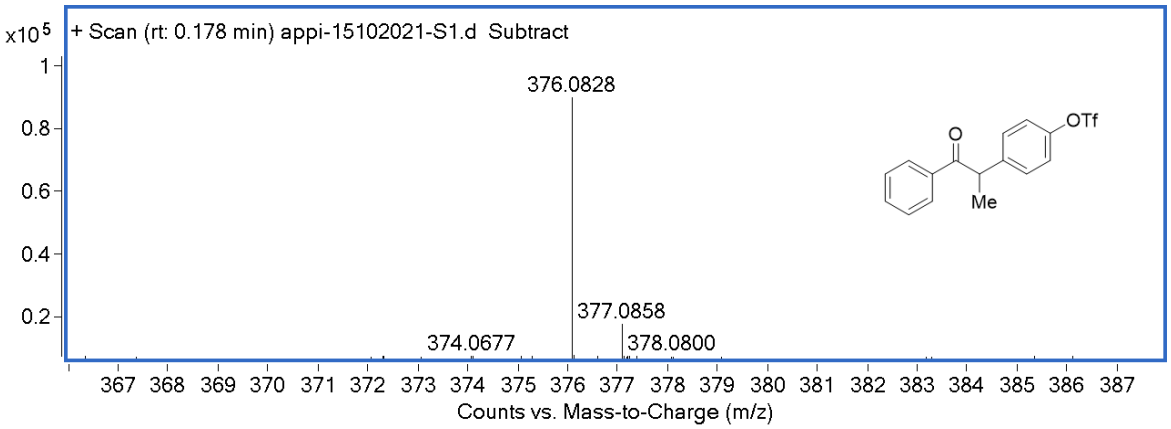

```
Current Data Parameters
NAME      A851B-20210419
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_            20210419
Time                16.54
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                    74
DS                     2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                   144
DW                20.800 usec
DE                 6.50 usec
TE                298.4 K
D1            1.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 9.50 usec
PL1               -2.00 dB
PL1W        58.52175522 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                   1H
PCPD2             80.00 usec
PL2       0 dB
PL12              15.00 dB
PL13              15.00 dB
PL2W        11.88122272 W
PL12W        0.37571725 W
PL13W        0.37571725 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                 32768
SF          100.6127751 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

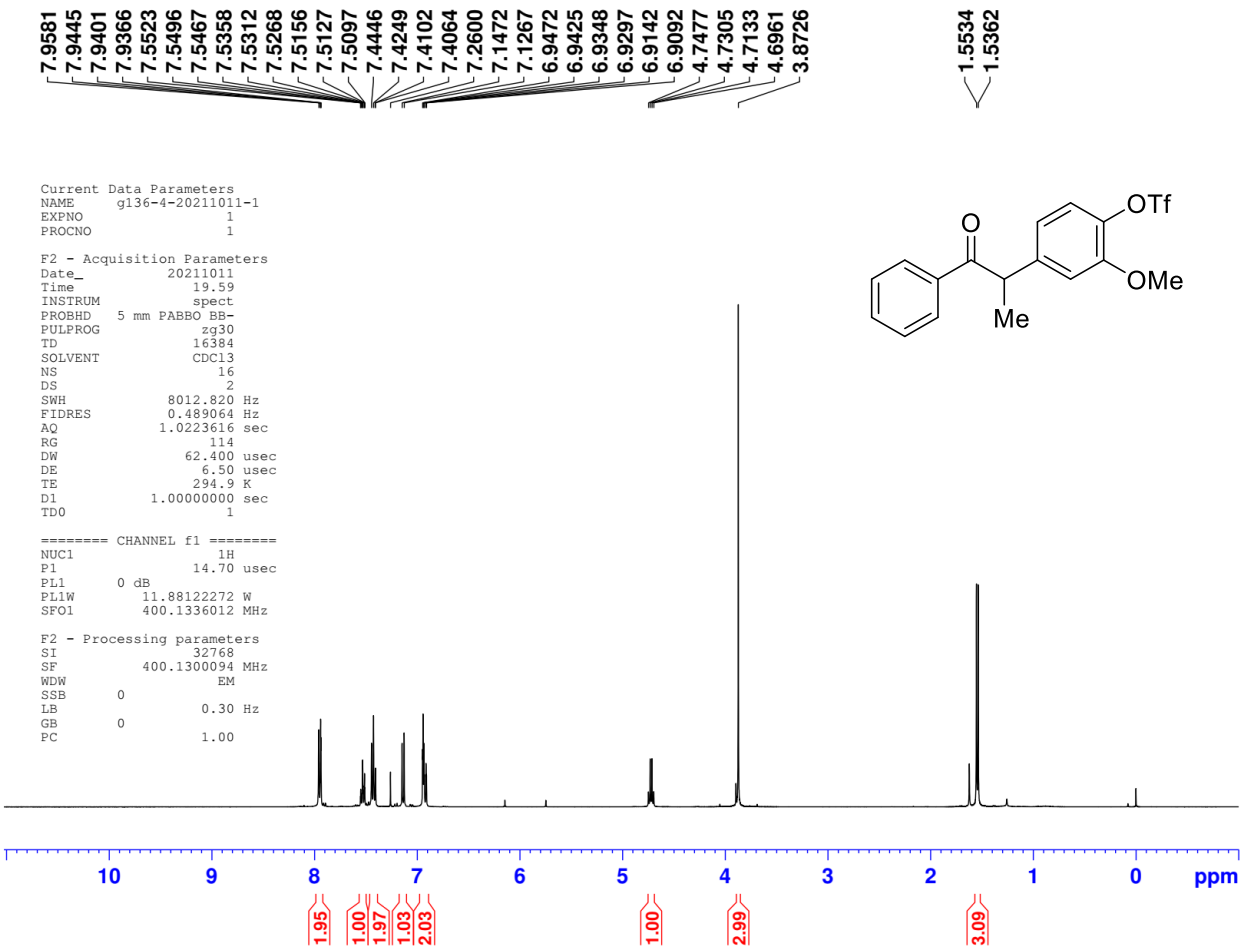


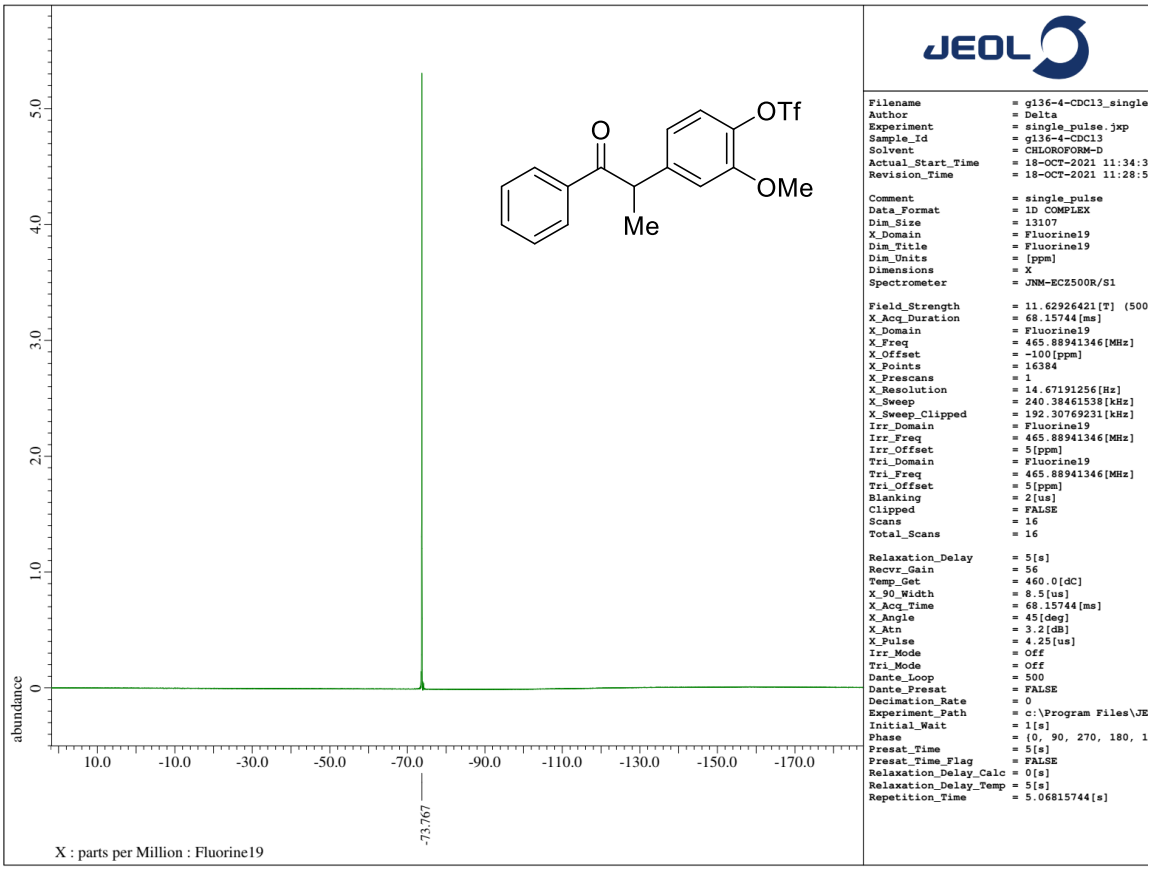

7.9514
7.9334
7.9299
7.5478
7.5450
7.5423
7.5317
7.5266
7.5110
7.5082
7.5054
7.4407
7.4210
7.4017
7.3847
7.3797
7.3725
7.2600
7.2232
7.2161
7.2112
7.1990
7.1943
7.1870
4.7887
4.7715
4.7542
4.7370
1.5545
1.5372
Current Data Parameters
NAME g136-1-20211011-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211011
Time 19.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.89
1.00
3.97
1.92
1.00
3.05

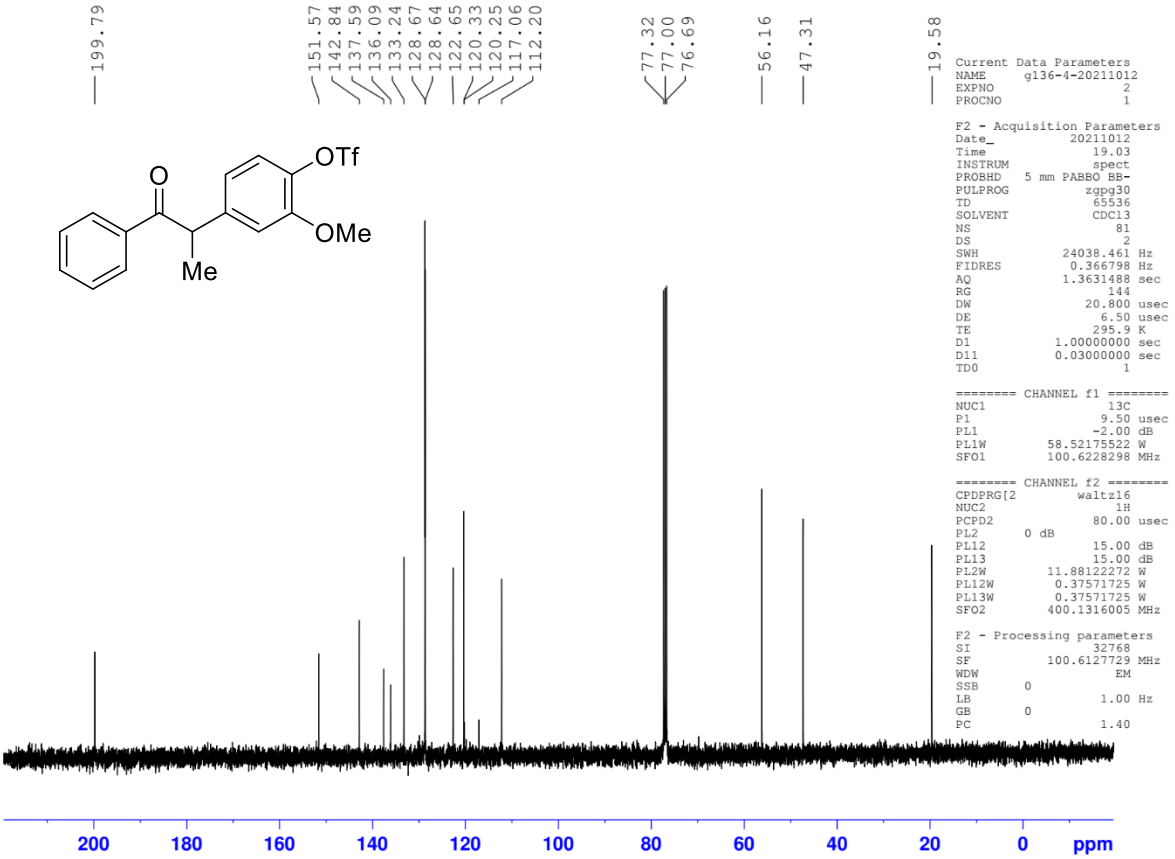

JEOL
OTf
O
Me
abundance
-30.0
-40.0
-50.0
-60.0
-70.0
-80.0
-90.0
-100.0
-110.0
-72.816
X : parts per Million : Fluorine19
Filename = GCX-II-136-1_single
Author = datum
Experiment = single_pulse.jxp
Sample_Id = GCX-II-136-1
Solvent = CHLOROFORM-D
Actual_Start_Time = 4-OCT-2021 20:05:4
Revision_Time = 5-OCT-2021 10:30:1
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (500
X_Acq_Duration = 2.24395264[s]
X_Domain = Fluorine19
X_Freq = 465.88941346[MHz]
X_Offset = -70[ppm]
X_Points = 131072
X_Prescans = 2
X_Resolution = 0.4456422[Hz]
X_Sweep = 58.41121495[kHz]
X_Sweep_Clipped = 46.72897196[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 465.88941346[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 465.88941346[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 20
Total_Scans = 20
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 460.0[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 2.24395264[s]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 4.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 200
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 1
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.24395264[s]

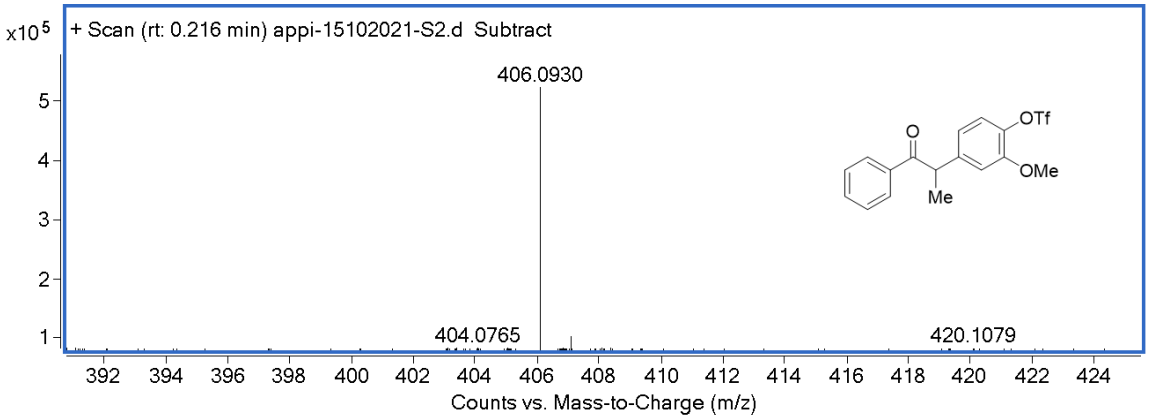

199.69
148.37
141.77
136.00
133.21
129.63
128.67
128.65
121.72
120.25
117.06
77.32
77.00
76.68
46.76
19.51
OTf
O
Me
Current Data Parameters
NAME gcx-II-136-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211002
Time 10.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 41
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 228
DW 20.800 usec
DE 6.50 usec
TE 296.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 131072
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

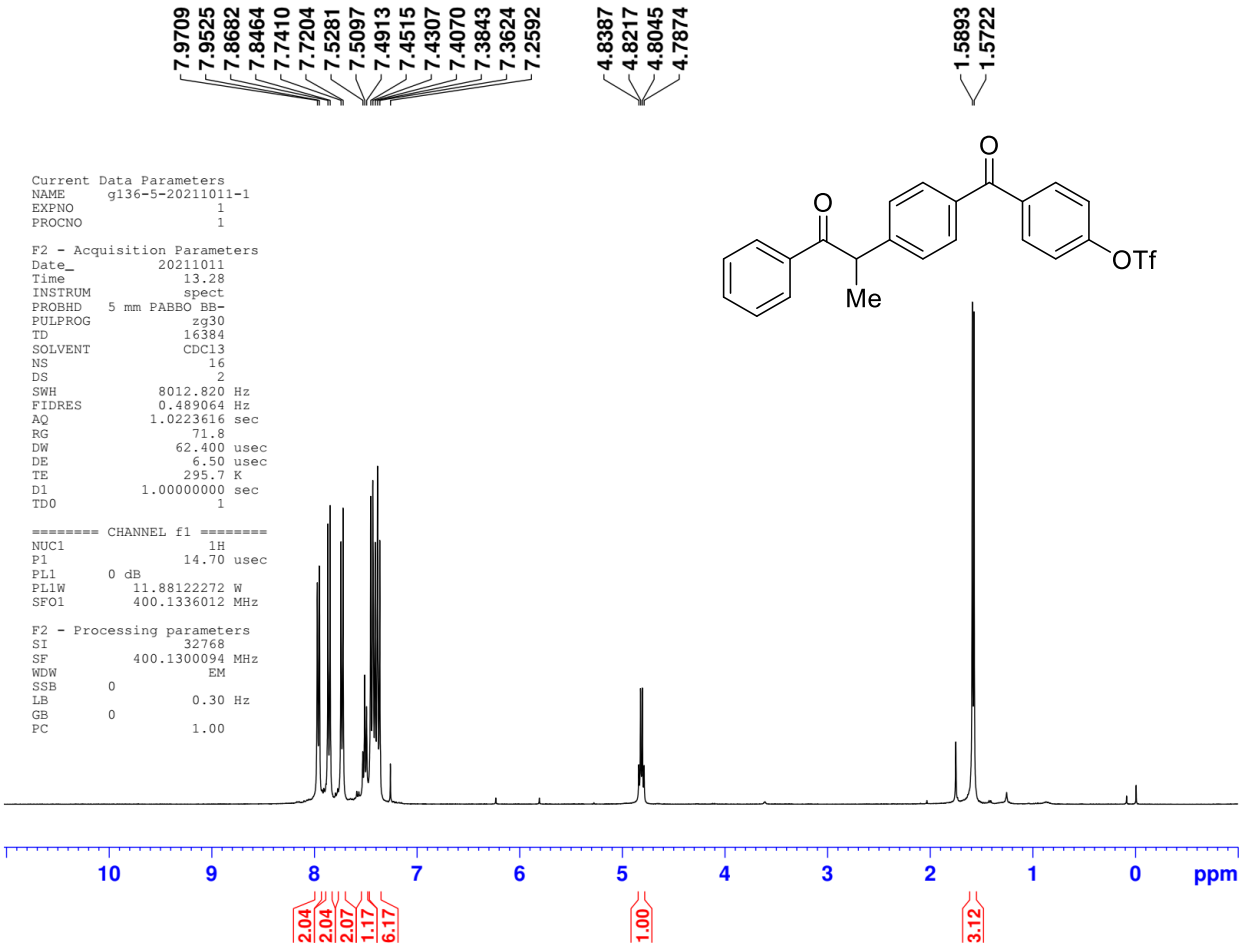

x10^5
+ Scan (rt: 0.178 min) appi-15102021-S1.d Subtract
1
0.8
0.6
0.4
0.2
376.0828
377.0858
374.0677
378.0800
OTf
O
Me
367 368 369 370 371 372 373 374 375 376 377 378 379 380 381 382 383 384 385 386 387
Counts vs. Mass-to-Charge (m/z)

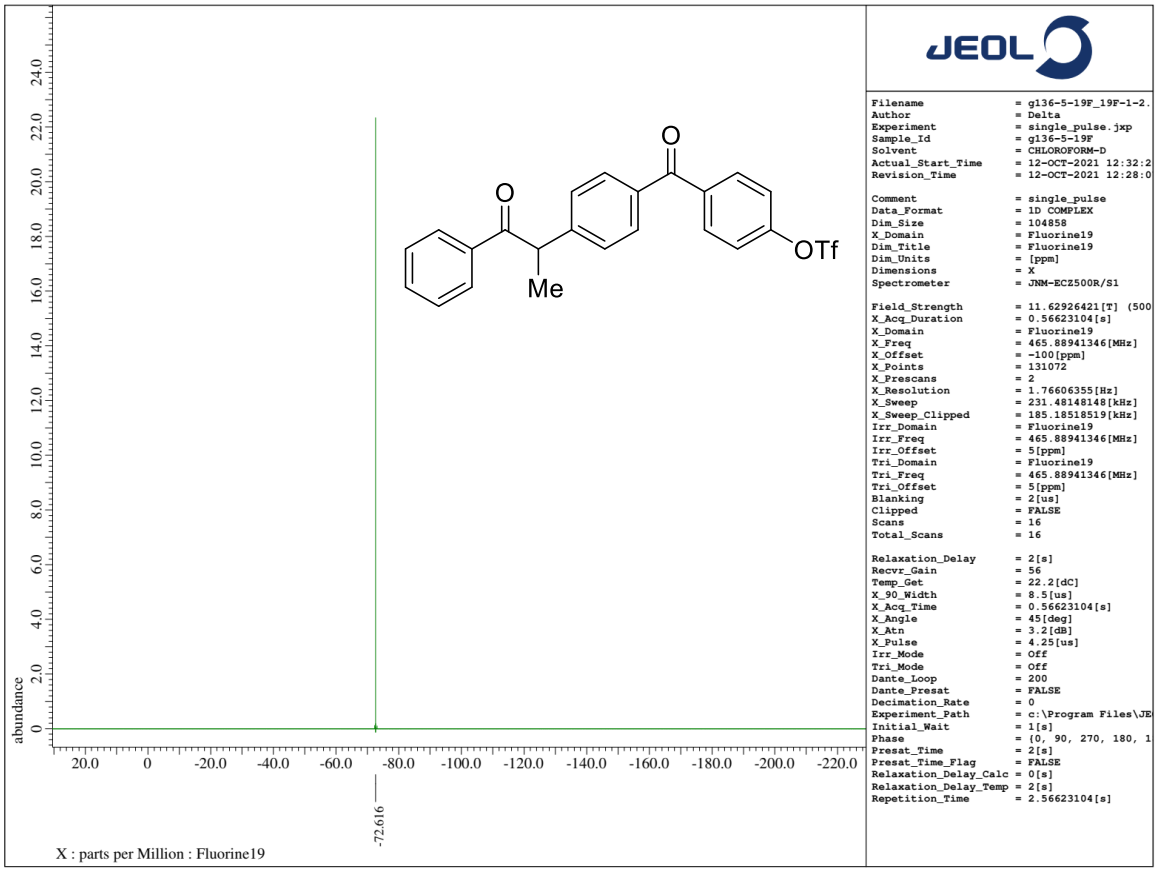

7.9581
7.9445
7.9401
7.9366
7.5523
7.5496
7.5467
7.5358
7.5312
7.5268
7.5156
7.5127
7.5097
7.4446
7.4249
7.4102
7.4064
7.2600
7.1472
7.1267
6.9472
6.9425
6.9348
6.9297
6.9142
6.9092
4.7477
4.7305
4.7133
4.6961
3.8726
1.5534
1.5362
Current Data Parameters
NAME g136-4-20211011-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211011
Time 19.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
OMe
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.95
1.00
1.97
1.03
2.03
1.00
2.99
3.09

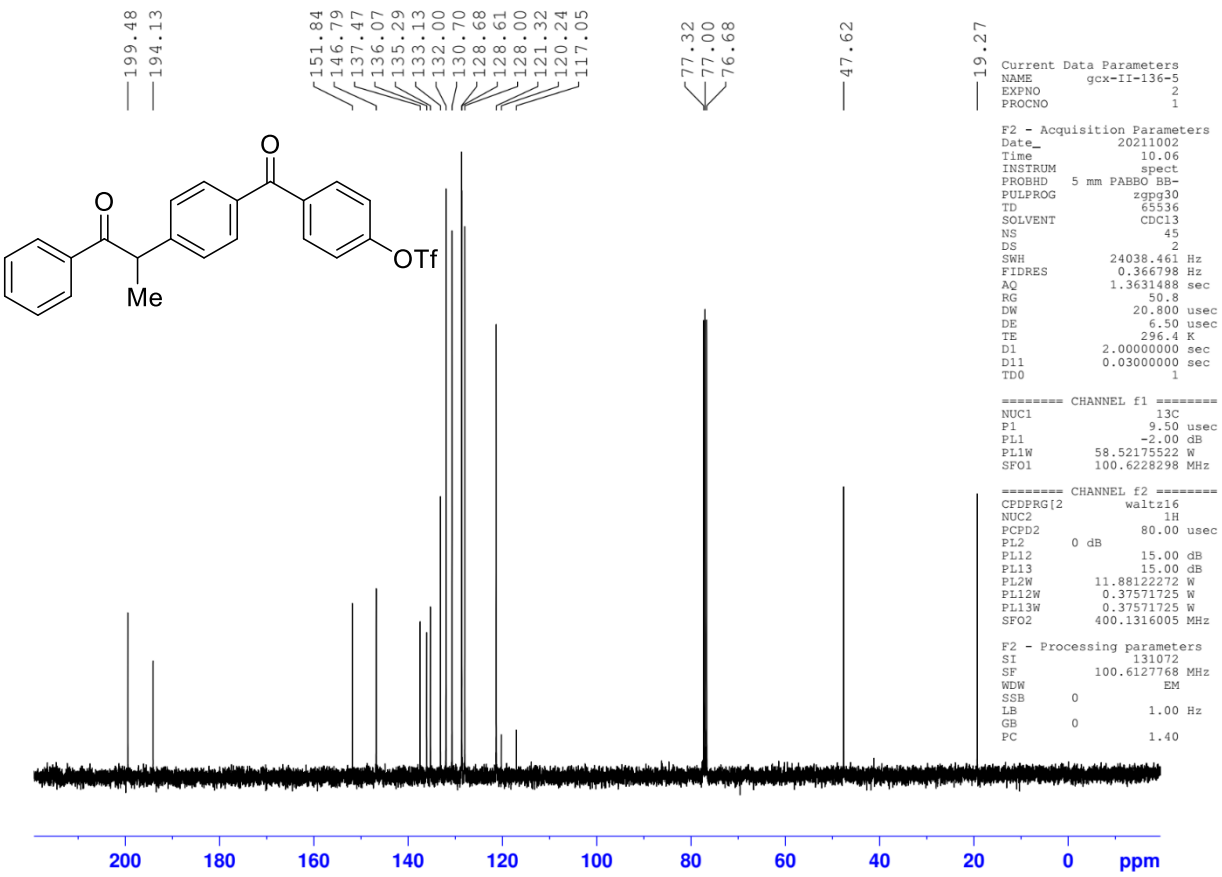

JEOL
OTf
O
OMe
Me
abundance
5.0
4.0
3.0
2.0
1.0
0
10.0
-10.0
-30.0
-50.0
-70.0
-90.0
-110.0
-130.0
-150.0
-170.0
-73.767
X : parts per Million : Fluorine19
Filename = g136-4-CDCl3_single
Author = Delta
Experiment = single_pulse.jxp
Sample_Id = g136-4-CDCl3
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-OCT-2021 11:34:3
Revision_Time = 18-OCT-2021 11:28:5
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (500
X_Acq_Duration = 68.15744[ms]
X_Domain = Fluorine19
X_Freq = 465.88941346[MHz]
X_Offset = -100[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 14.67191256[Hz]
X_Sweep = 240.38461538[kHz]
X_Sweep_Clipped = 192.30769231[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 465.88941346[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 465.88941346[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 460.0[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 68.15744[ms]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 4.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 1
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 5.06815744[s]

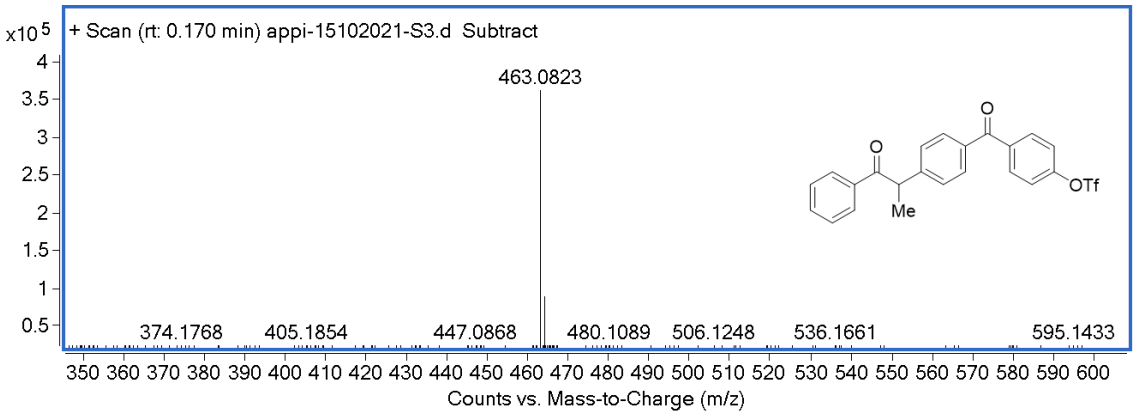

199.79
151.57
142.84
137.59
136.09
133.24
128.67
128.64
122.65
120.33
120.25
117.06
112.20
77.32
77.00
76.69
56.16
47.31
19.58
OTf
O
OMe
Me
Current Data Parameters
NAME g136-4-20211012
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211012
Time 19.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 81
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

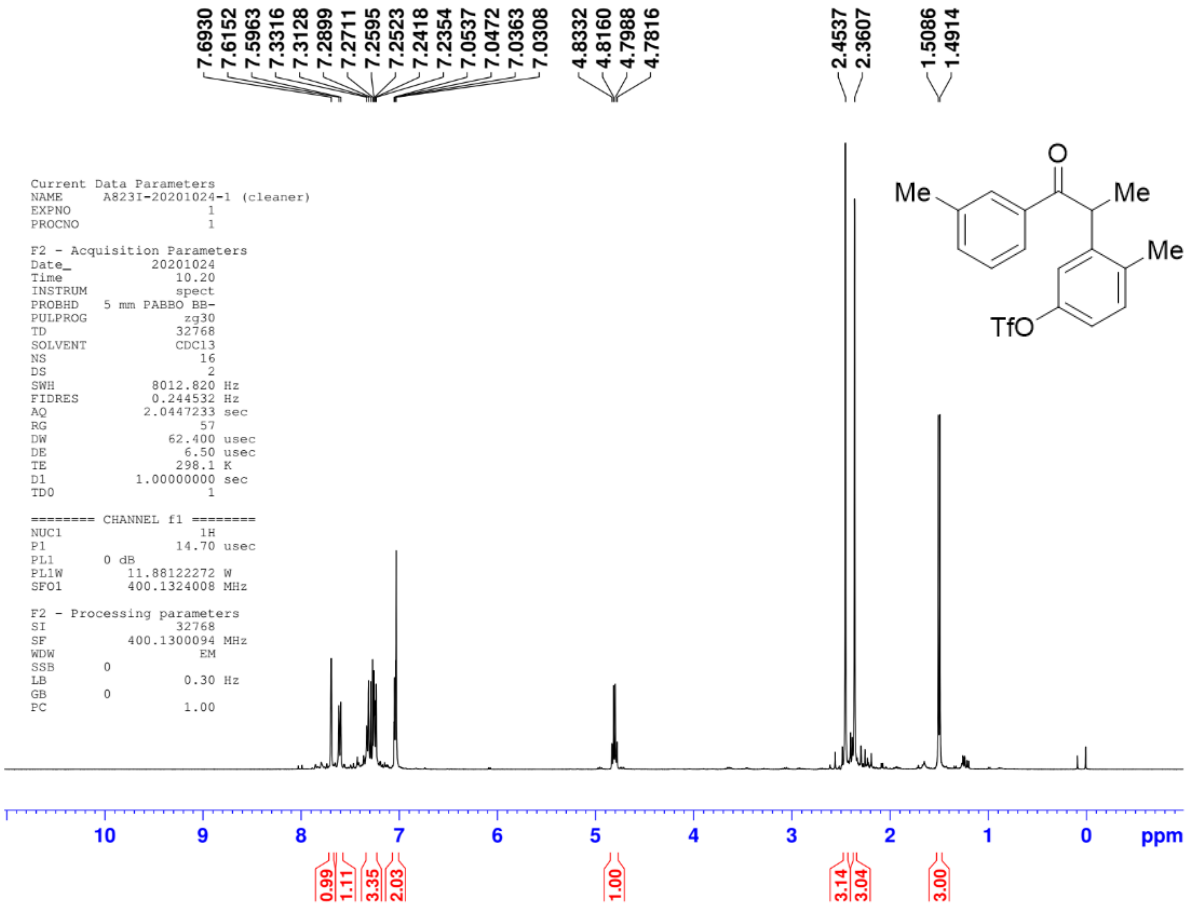

x10^5
+ Scan (rt: 0.216 min) appi-15102021-S2.d Subtract
406.0930
404.0765
420.1079
OTf
O
OMe
Me
5
4
3
2
1
392
394
396
398
400
402
404
406
408
410
412
414
416
418
420
422
424
Counts vs. Mass-to-Charge (m/z)

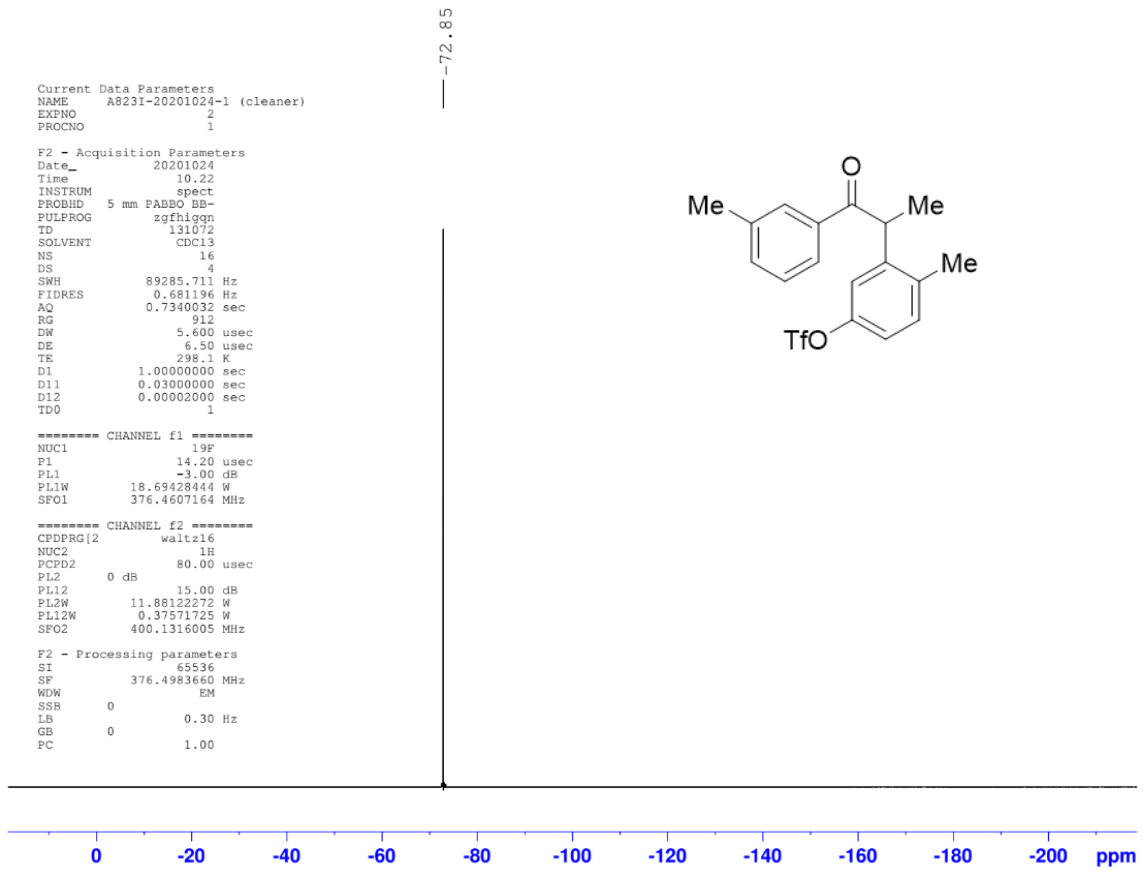

7.9709
7.9525
7.8682
7.8464
7.7410
7.7204
7.5281
7.5097
7.4913
7.4515
7.4307
7.4070
7.3843
7.3624
7.2592
4.8387
4.8217
4.8045
4.7874
1.5893
1.5722
Current Data Parameters
NAME g136-5-20211011-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211011
Time 13.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
O
OTf
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
2.04
2.04
2.07
1.17
6.17
1.00
3.12

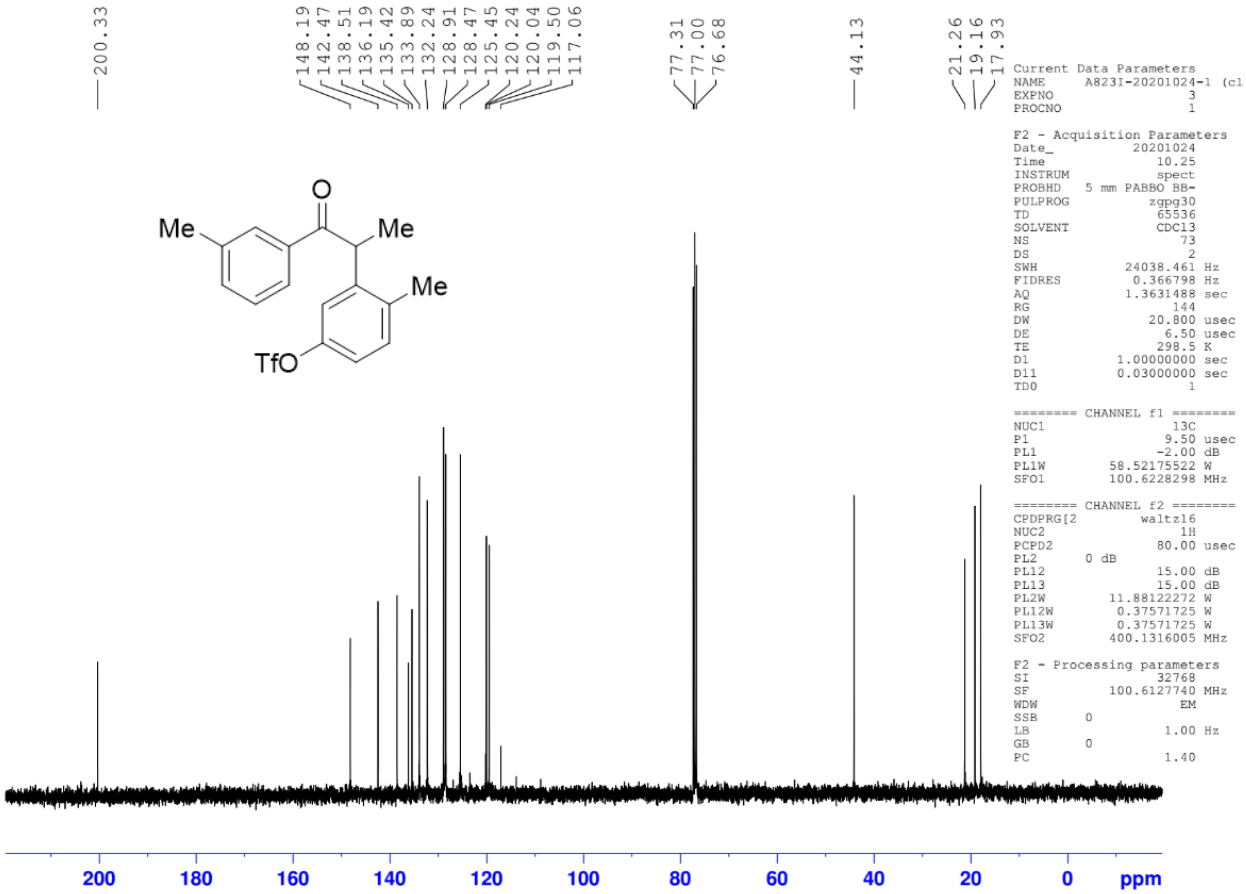

JEOL
Filename = g136-5-19F_19F-1-2.
Author = Delta
Experiment = single_pulse.jxp
Sample_Id = g136-5-19F
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-OCT-2021 12:32:2
Revision_Time = 12-OCT-2021 12:28:0
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (500
X_Acq_Duration = 0.56623104[s]
X_Domain = Fluorine19
X_Freq = 465.88941346[MHz]
X_Offset = -100[ppm]
X_Points = 131072
X_Prescans = 2
X_Resolution = 1.76606355[Hz]
X_Sweep = 231.48148148[kHz]
X_Sweep_Clipped = 185.18518519[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 465.88941346[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 465.88941346[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.2[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 0.56623104[s]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 4.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 200
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 1
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 2.56623104[s]
abundance
24.0
22.0
20.0
18.0
16.0
14.0
12.0
10.0
8.0
6.0
4.0
2.0
0
20.0
0
-20.0
-40.0
-60.0
-80.0
-100.0
-120.0
-140.0
-160.0
-180.0
-200.0
-220.0
-72.616
O
O
OTf
Me
X : parts per Million : Fluorine19

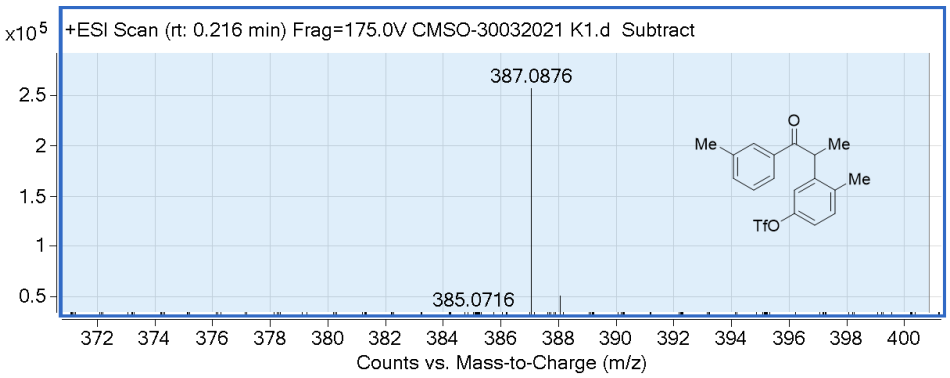

199.48
194.13
151.84
146.79
137.47
136.07
135.29
133.13
132.00
130.70
128.68
128.61
128.00
121.32
120.24
117.05
77.32
77.00
76.68
47.62
19.27
O
O
OTf
Me
Current Data Parameters
NAME gcx-II-136-5
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211002
Time 10.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 45
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 50.8
DW 20.800 usec
DE 6.50 usec
TE 296.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 131072
SF 100.6127768 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

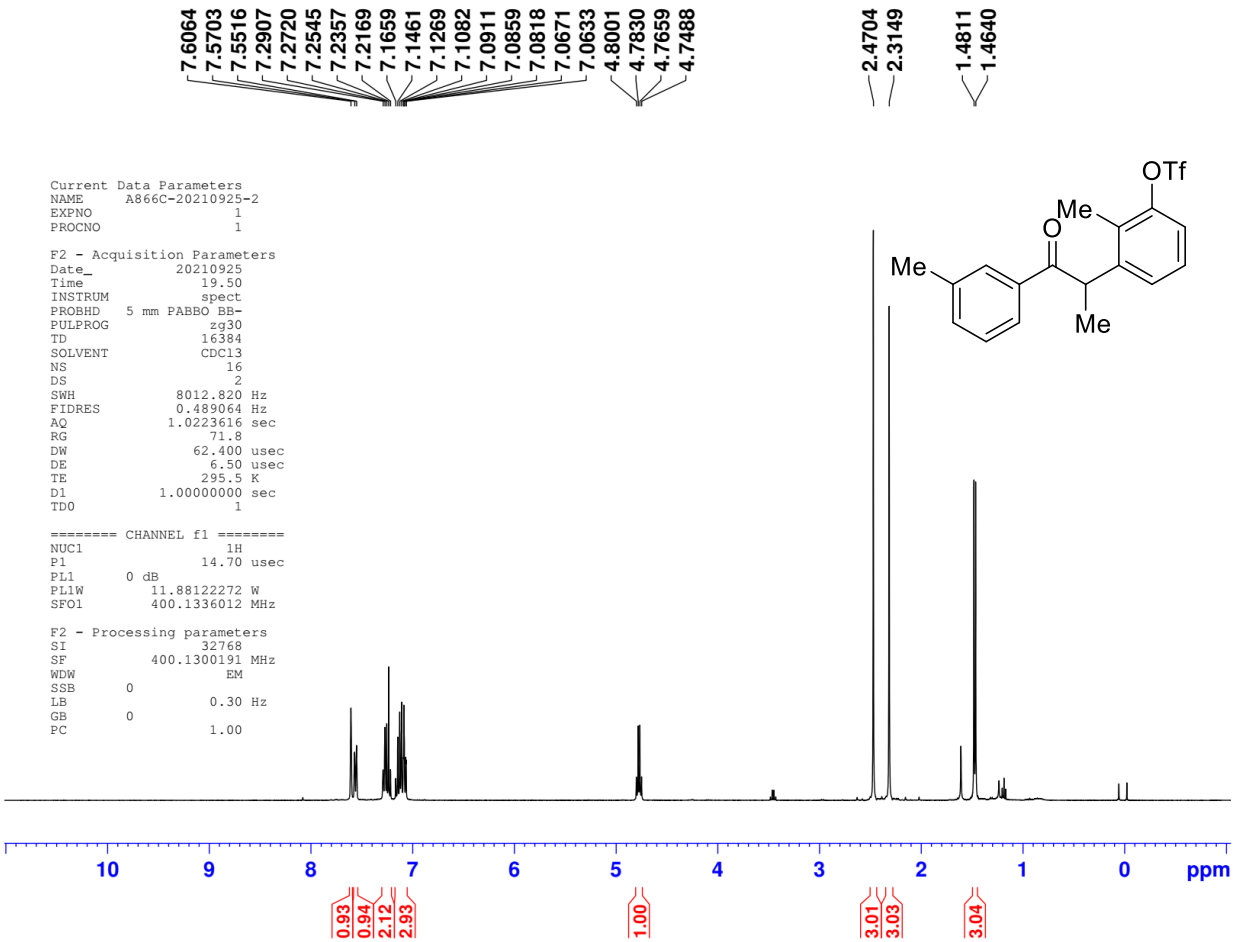

x10 5
+ Scan (rt: 0.170 min) appi-15102021-S3.d Subtract
463.0823
374.1768
405.1854
447.0868
480.1089
506.1248
536.1661
595.1433
O
O
OTf
Me
Counts vs. Mass-to-Charge (m/z)

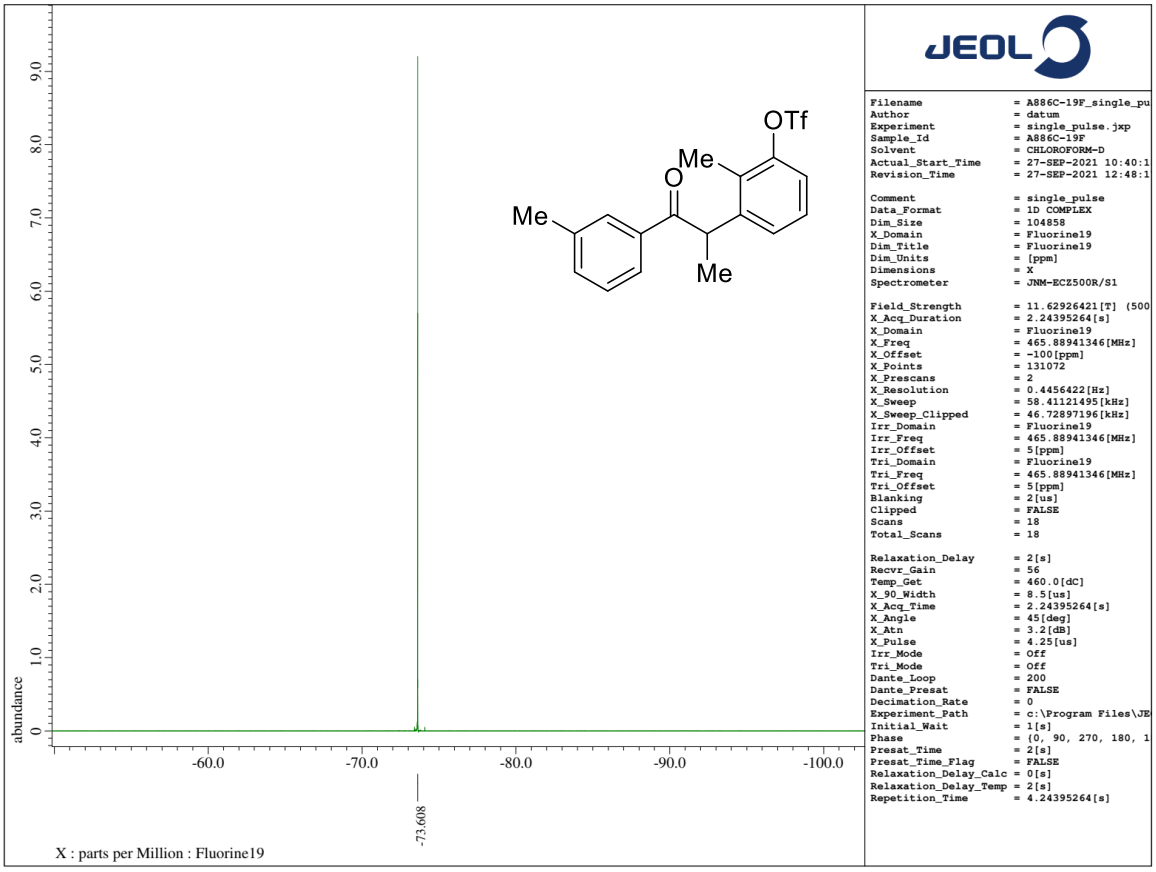

7.6930
7.6152
7.5963
7.3316
7.3128
7.2899
7.2711
7.2595
7.2523
7.2418
7.2354
7.0537
7.0472
7.0363
7.0308
4.8332
4.8160
4.7988
4.7816
2.4537
2.3607
1.5086
1.4914
Current Data Parameters
NAME A823I-20201024-1 (cleaner)
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201024
Time 10.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 57
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
Me
Me
O
TfO
10
9
8
7
6
5
4
3
2
1
0
ppm
0.99
1.11
3.35
2.03
1.00
3.14
3.04
3.00

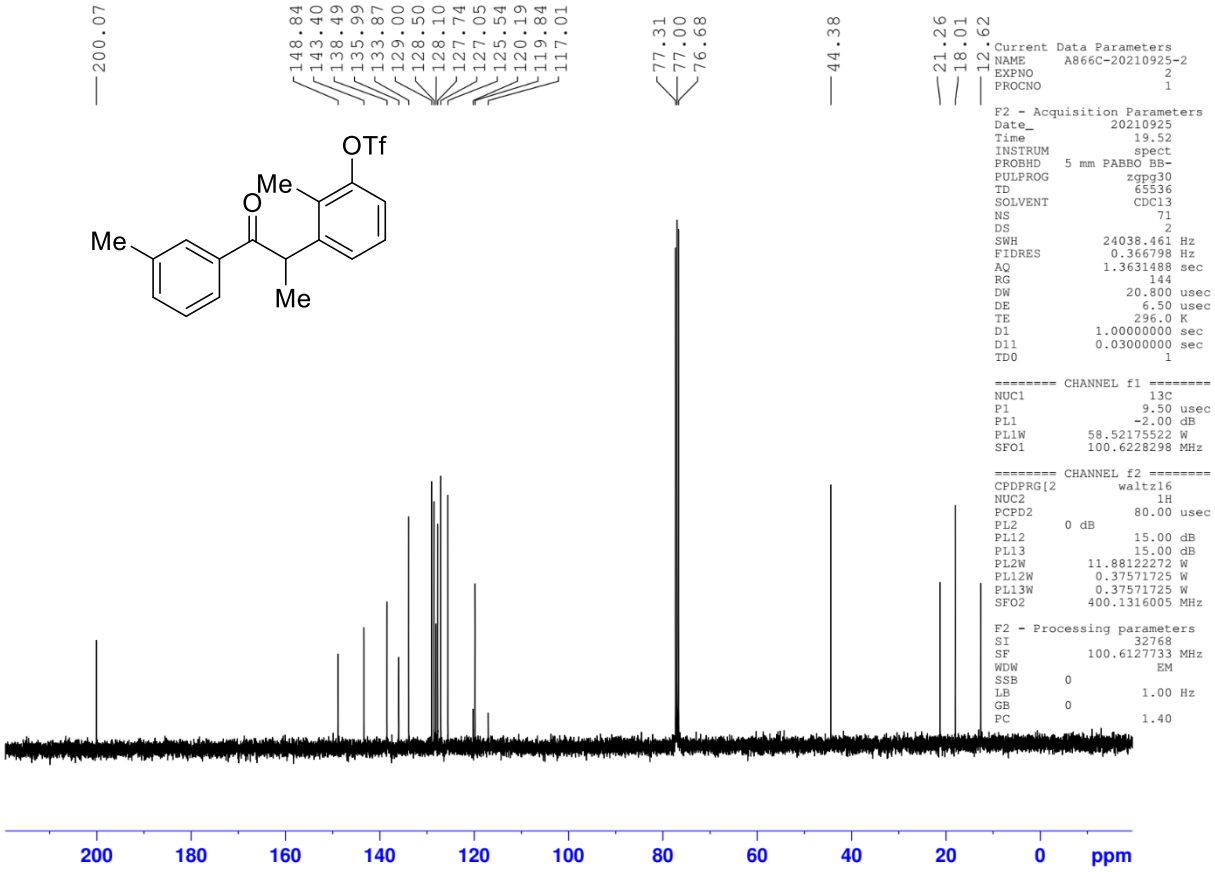

-72.85
Current Data Parameters
NAME A823I-20201024-1 (cleaner)
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201024
Time 10.22
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
Me
Me
O
TfO
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

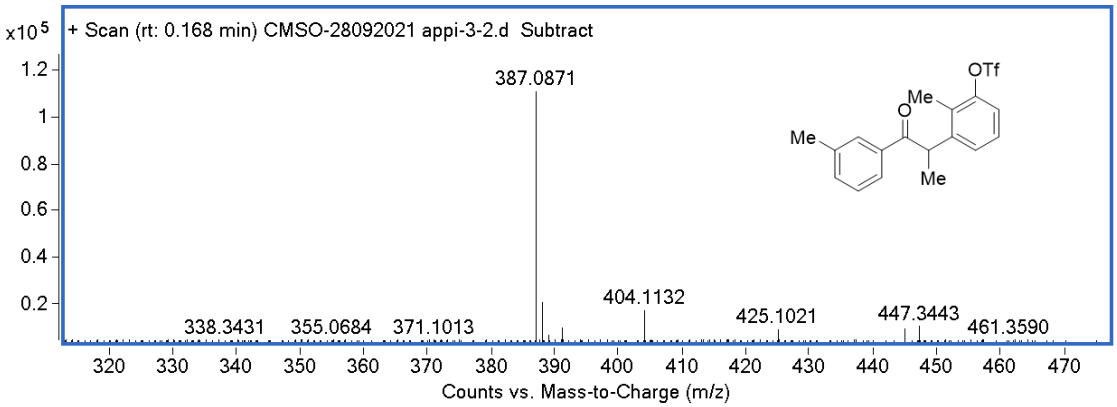

200.33
148.19
142.47
138.51
136.19
135.42
133.89
132.24
128.91
128.47
125.45
120.24
120.04
119.50
117.06
77.31
77.00
76.68
44.13
21.26
19.16
17.93
Me
Me
Me
TfO
O
Current Data Parameters
NAME A823I-20201024-1 (cl
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201024
Time 10.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 73
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

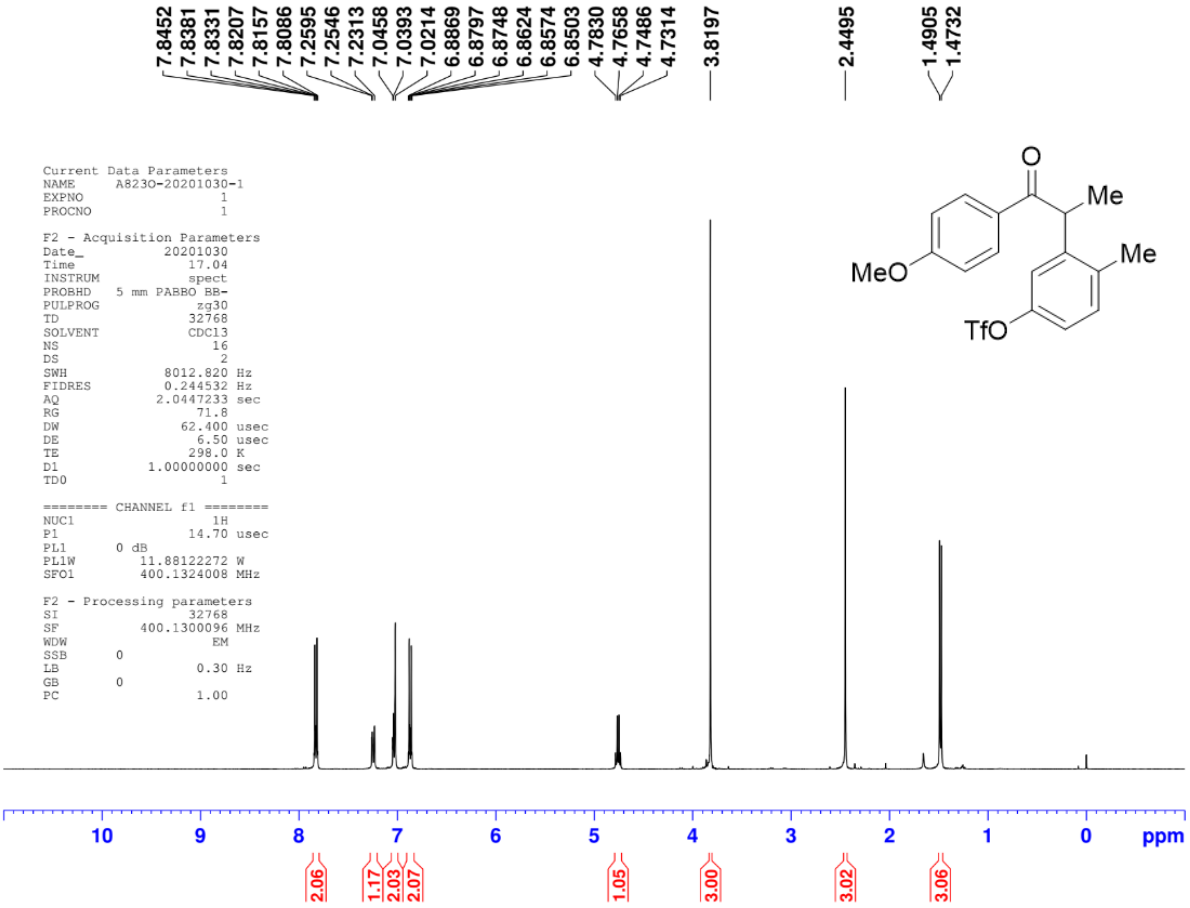

x10^5
+ESI Scan (rt: 0.216 min) Frag=175.0V CMSO-30032021 K1.d Subtract
387.0876
385.0716
2.5
2
1.5
1
0.5
Me
Me
Me
TfO
O
372
374
376
378
380
382
384
386
388
390
392
394
396
398
400
Counts vs. Mass-to-Charge (m/z)

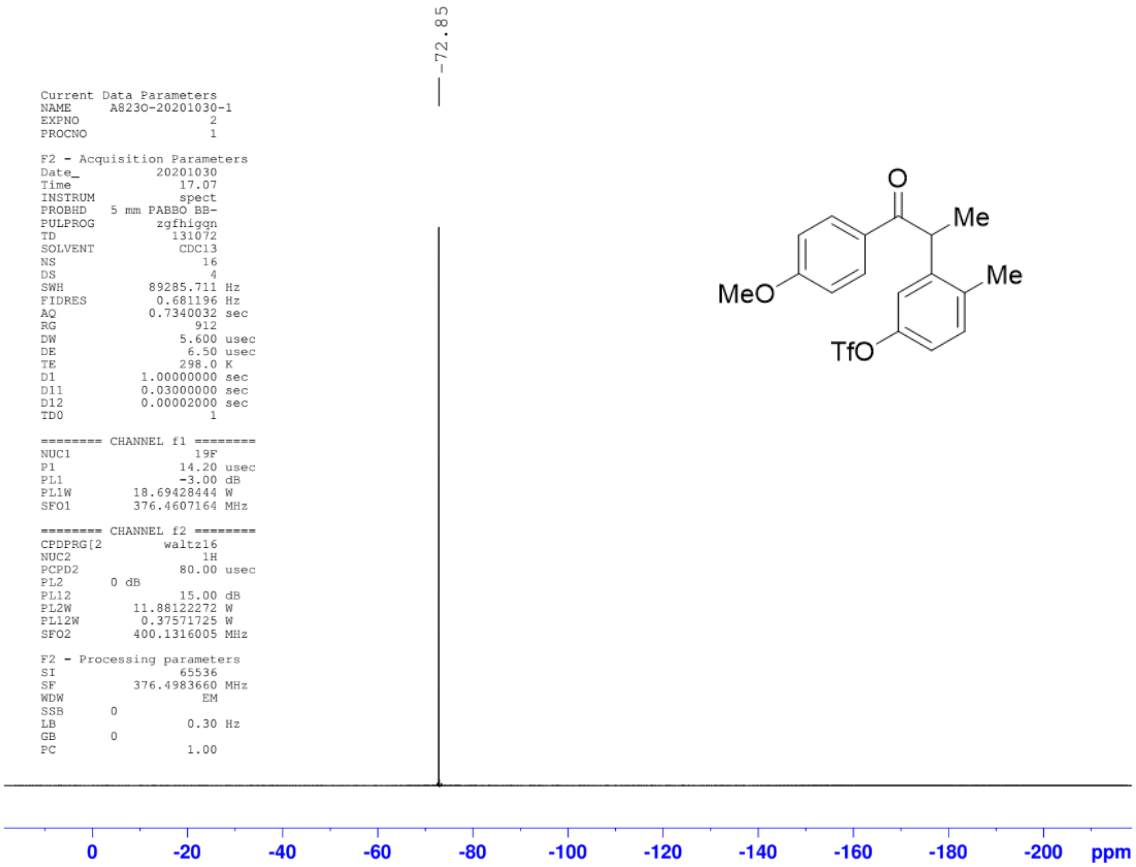

7.6064
7.5703
7.5516
7.2907
7.2720
7.2545
7.2357
7.2169
7.1659
7.1461
7.1269
7.1082
7.0911
7.0859
7.0818
7.0671
7.0633
4.8001
4.7830
4.7659
4.7488
2.4704
2.3149
1.4811
1.4640
Current Data Parameters
NAME A866C-20210925-2
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210925
Time 19.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300191 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
Me
O
Me
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
0.93
0.94
2.12
2.93
1.00
3.01
3.03
3.04

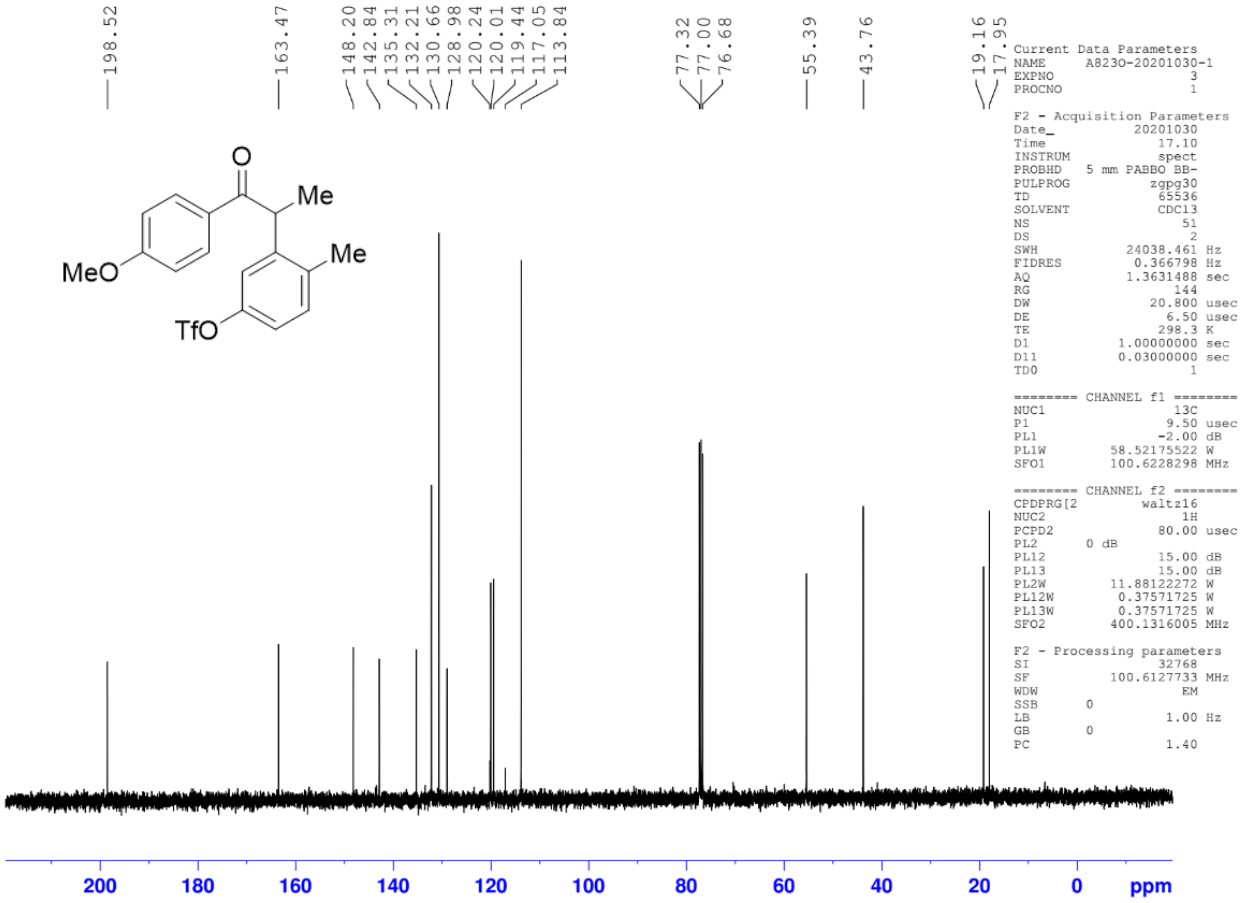

JEOL
Filename = A886C-19F_single_pu
Author = datum
Experiment = single_pulse.jxp
Sample_Id = A886C-19F
Solvent = CHLOROFORM-D
Actual_Start_Time = 27-SEP-2021 10:40:1
Revision_Time = 27-SEP-2021 12:48:1
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (500
X_Acq_Duration = 2.24395264[s]
X_Domain = Fluorine19
X_Freq = 465.88941346[MHz]
X_Offset = -100[ppm]
X_Points = 131072
X_Prescans = 2
X_Resolution = 0.4456422[Hz]
X_Sweep = 58.41121495[kHz]
X_Sweep_Clipped = 46.72897196[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 465.88941346[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 465.88941346[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 18
Total_Scans = 18
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 460.0[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 2.24395264[s]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 4.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 200
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 1
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 4.24395264[s]
OTf
Me
O
Me
Me
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-60.0
-70.0
-80.0
-90.0
-100.0
-73.608
X : parts per Million : Fluorine19

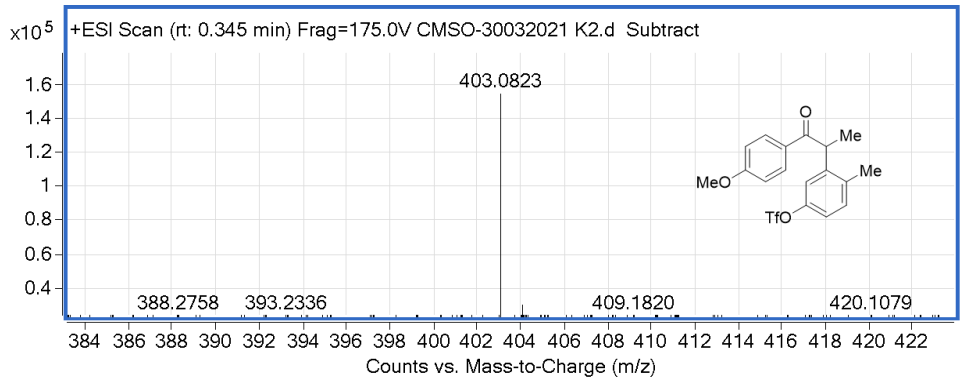

200.07
148.84
143.40
138.49
135.99
133.87
129.00
128.50
128.10
127.74
127.05
125.54
120.19
119.84
117.01
77.31
77.00
76.68
44.38
21.26
18.01
12.62
OTf
Me
O
Me
Me
Current Data Parameters
NAME A866C-20210925-2
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210925
Time 19.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 71
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127733 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

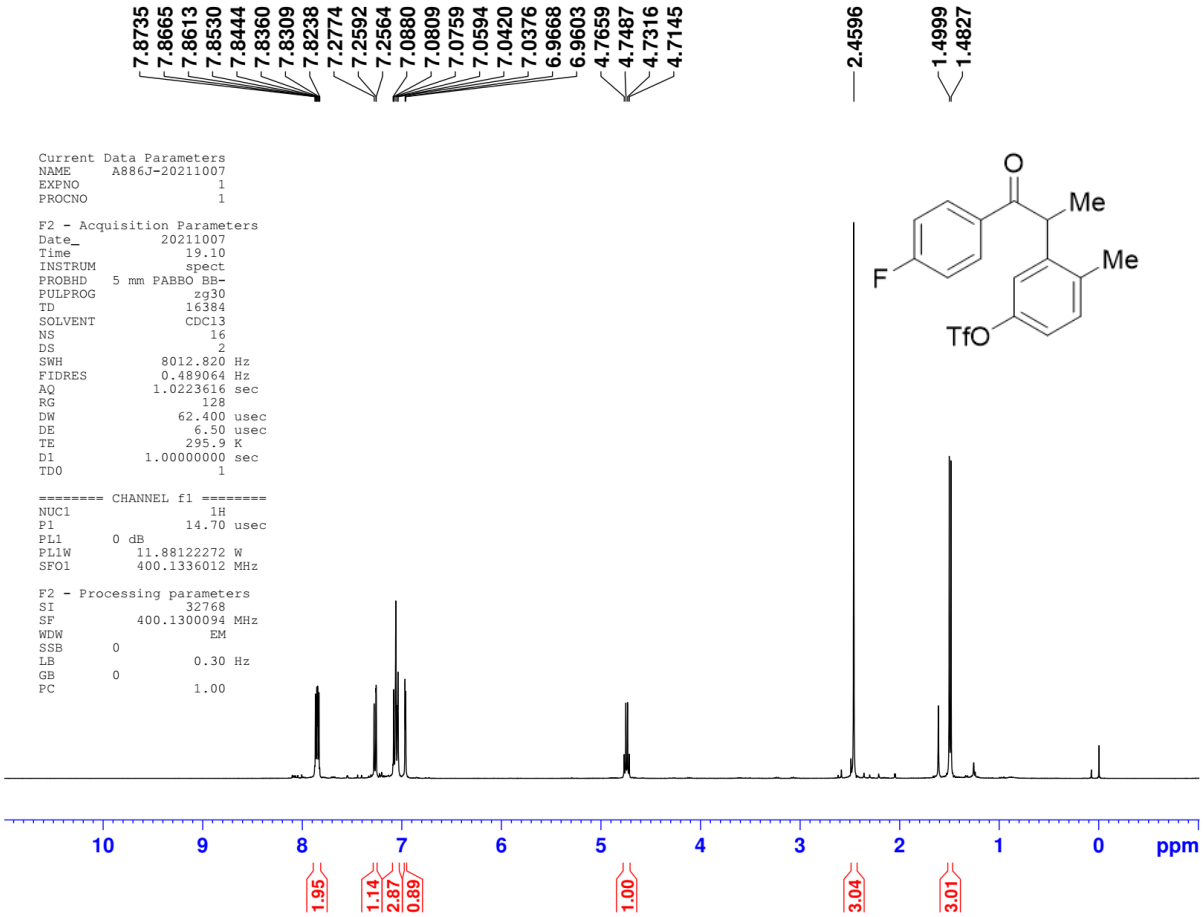

x10 5
+ Scan (rt: 0.168 min) CMSO-28092021 appi-3-2.d Subtract
1.2
1
0.8
0.6
0.4
0.2
387.0871
404.1132
338.3431
355.0684
371.1013
425.1021
447.3443
461.3590
OTf
Me
O
Me
Me
320
330
340
350
360
370
380
390
400
410
420
430
440
450
460
470
Counts vs. Mass-to-Charge (m/z)

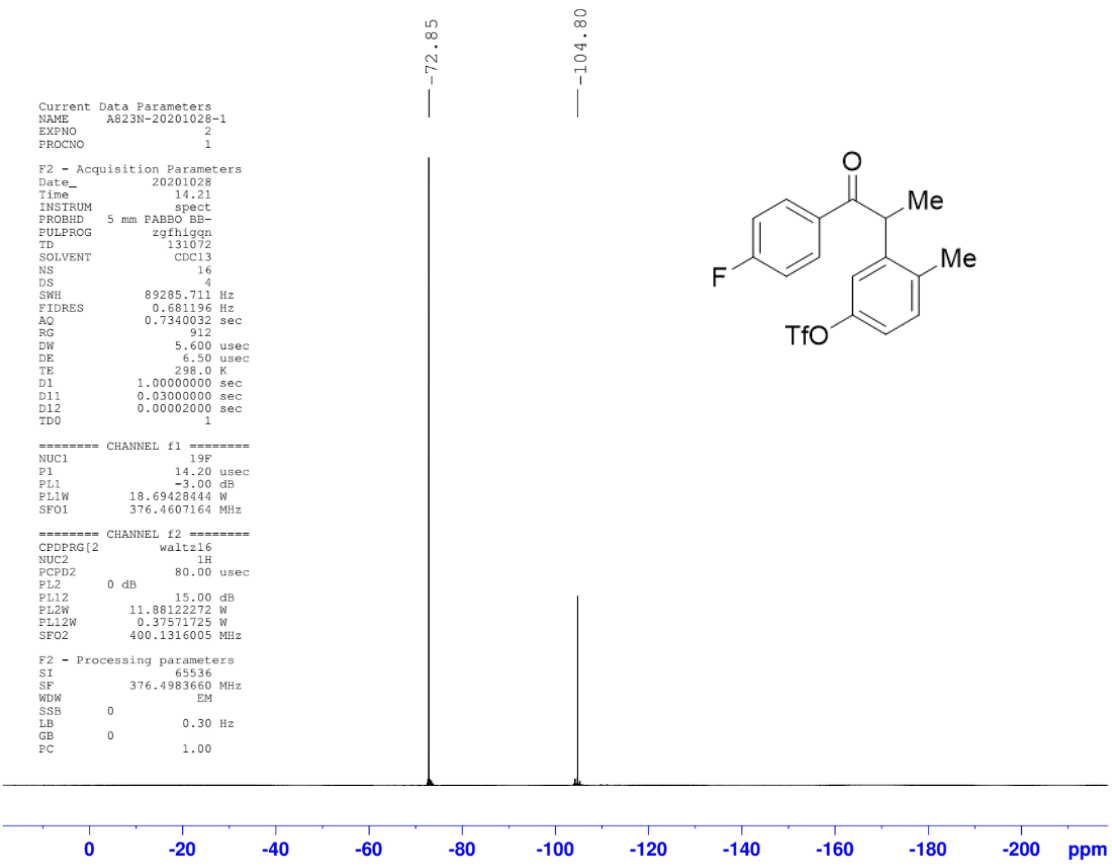

7.8452
7.8381
7.8331
7.8207
7.8157
7.8086
7.2595
7.2546
7.2313
7.0458
7.0393
7.0214
6.8869
6.8797
6.8748
6.8624
6.8574
6.8503
4.7830
4.7658
4.7486
4.7314
3.8197
2.4495
1.4905
1.4732
Current Data Parameters
NAME A8230-20201030-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201030
Time 17.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Me
Me
MeO
TfO
10
9
8
7
6
5
4
3
2
1
0
ppm
2.06
1.17
2.03
2.07
1.05
3.00
3.02
3.06

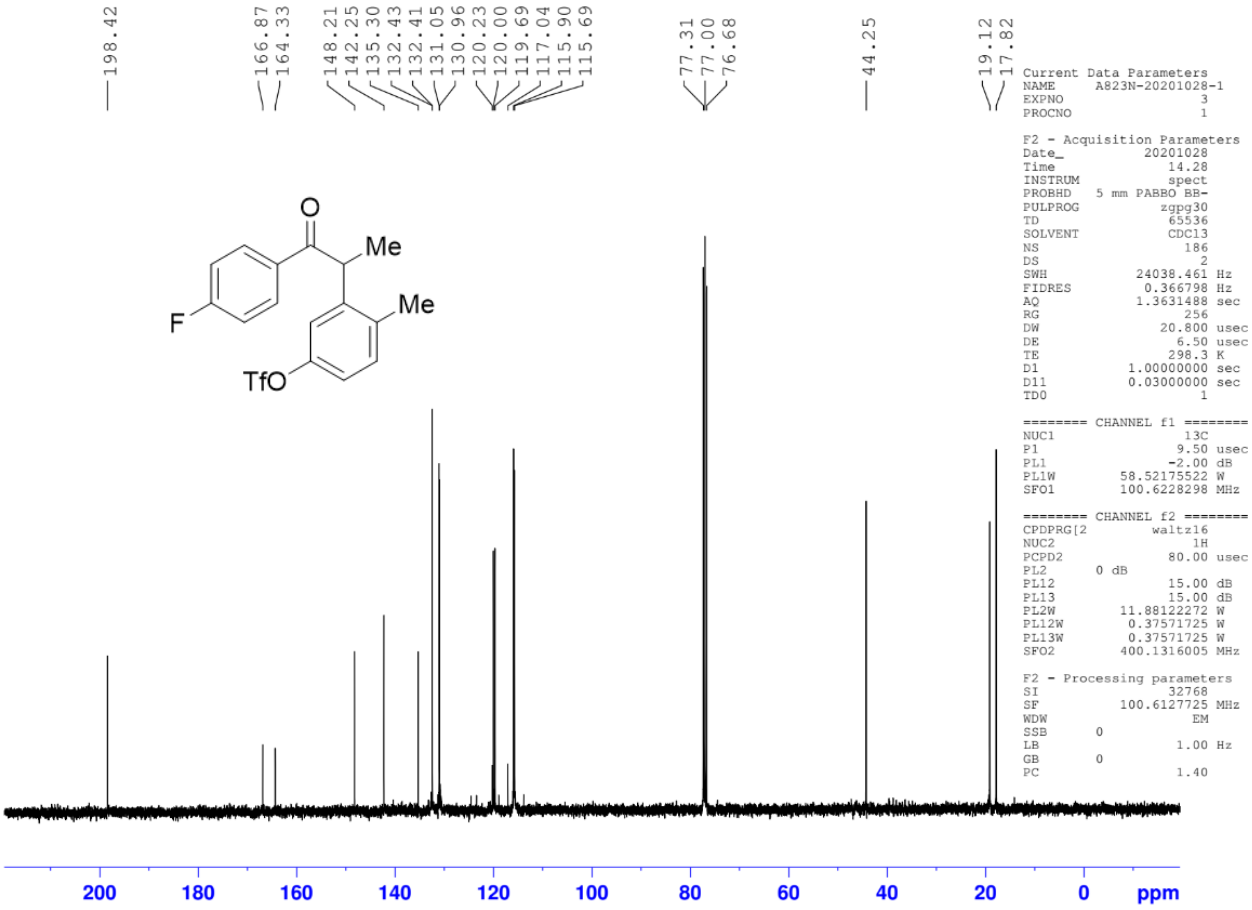

-72.85
Current Data Parameters
NAME A8230-20201030-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201030
Time 17.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Me
Me
MeO
TfO
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

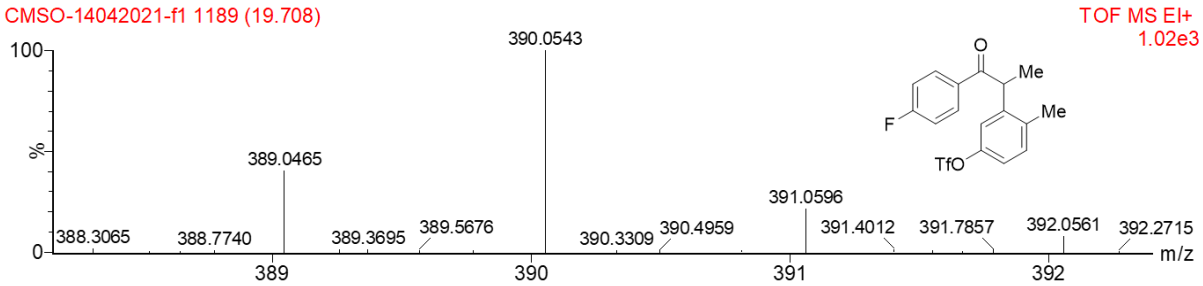

198.52
163.47
148.20
142.84
135.31
132.21
130.66
128.98
120.24
120.01
119.44
117.05
113.84
77.32
77.00
76.68
55.39
43.76
19.16
17.95
O
Me
Me
MeO
TfO
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME A8230-20201030-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201030
Time 17.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 51
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127733 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

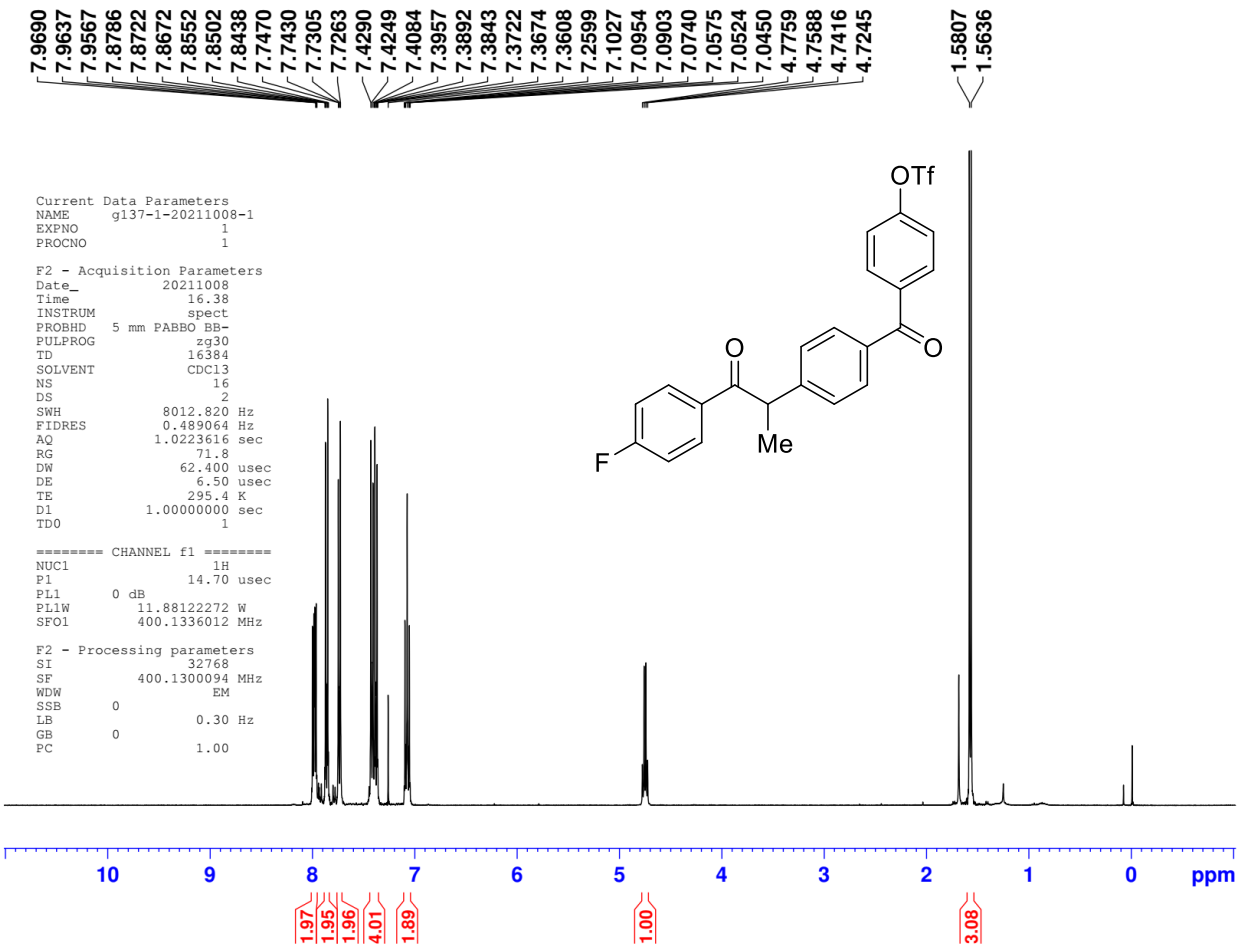

x10^5
+ESI Scan (rt: 0.345 min) Frag=175.0V CMSO-30032021 K2.d Subtract
1.6
1.4
1.2
1
0.8
0.6
0.4
403.0823
388.2758
393.2336
409.1820
420.1079
O
Me
Me
MeO
TfO
384 386 388 390 392 394 396 398 400 402 404 406 408 410 412 414 416 418 420 422
Counts vs. Mass-to-Charge (m/z)

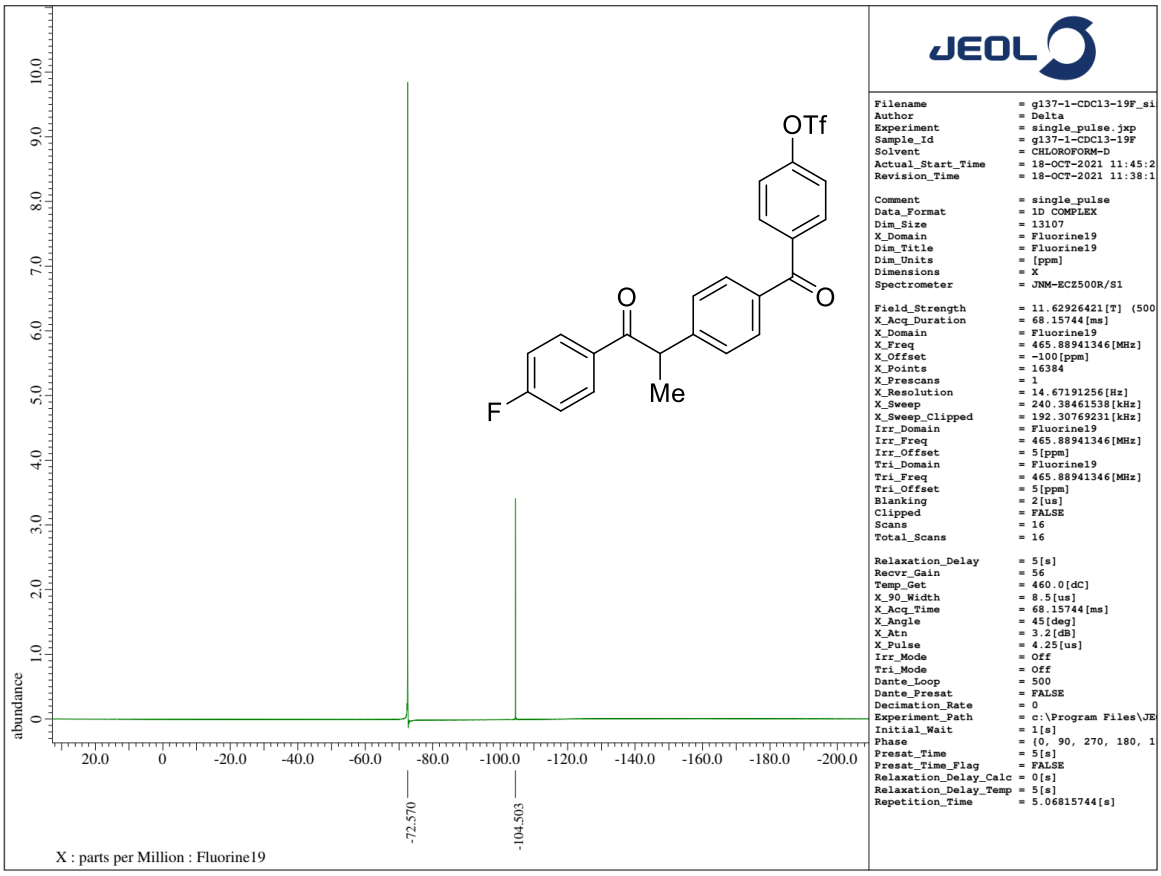

7.8735
7.8665
7.8613
7.8530
7.8444
7.8360
7.8309
7.8238
7.2774
7.2592
7.2564
7.0880
7.0809
7.0759
7.0594
7.0420
7.0376
6.9668
6.9603
4.7659
4.7487
4.7316
4.7145
2.4596
1.4999
1.4827
Current Data Parameters
NAME A886J-20211007
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211007
Time 19.10
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 128
DW 62.400 usec
DE 6.50 usec
TE 295.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Me
Me
F
TfO
10
9
8
7
6
5
4
3
2
1
0
ppm
1.95
1.14
2.87
0.89
1.00
3.04
3.01

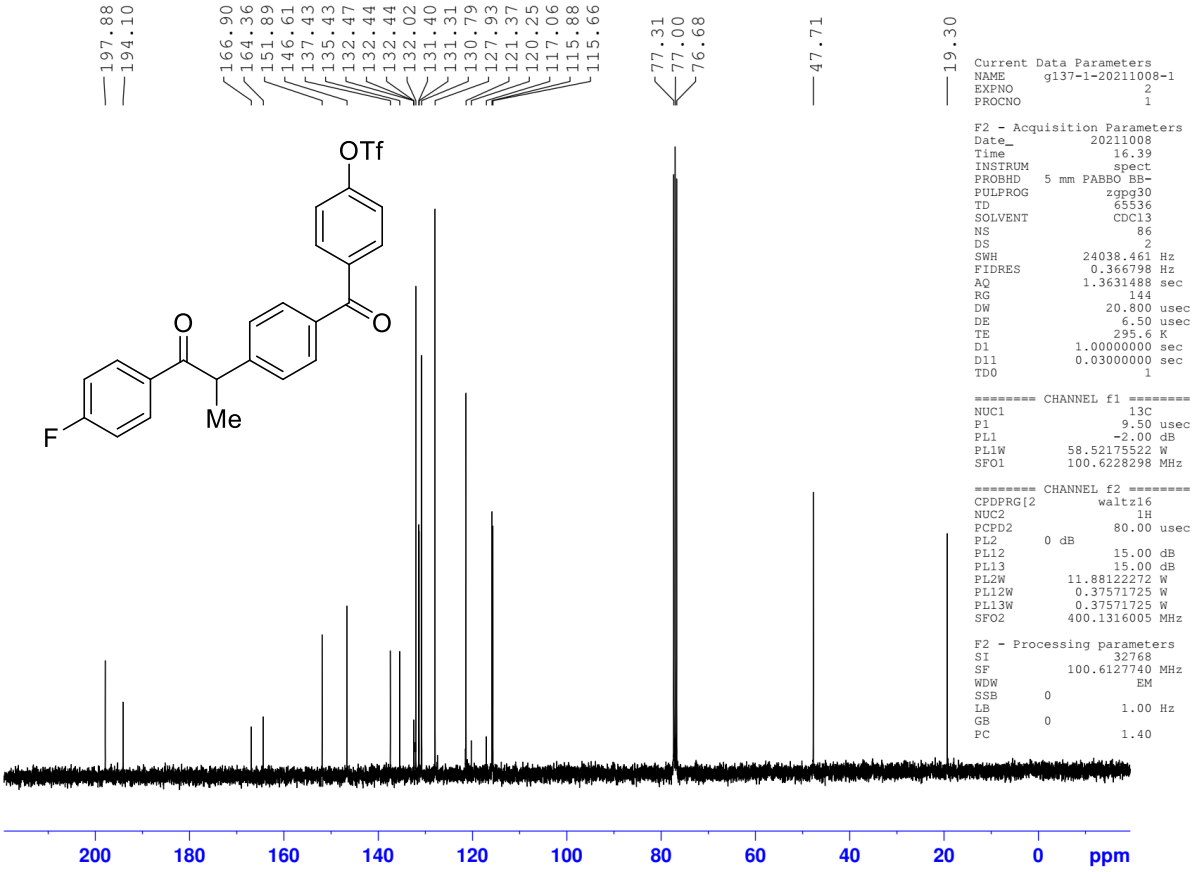

-72.85
-104.80
Current Data Parameters
NAME A823N-20201028-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201028
Time 14.21
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Me
Me
F
TfO
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

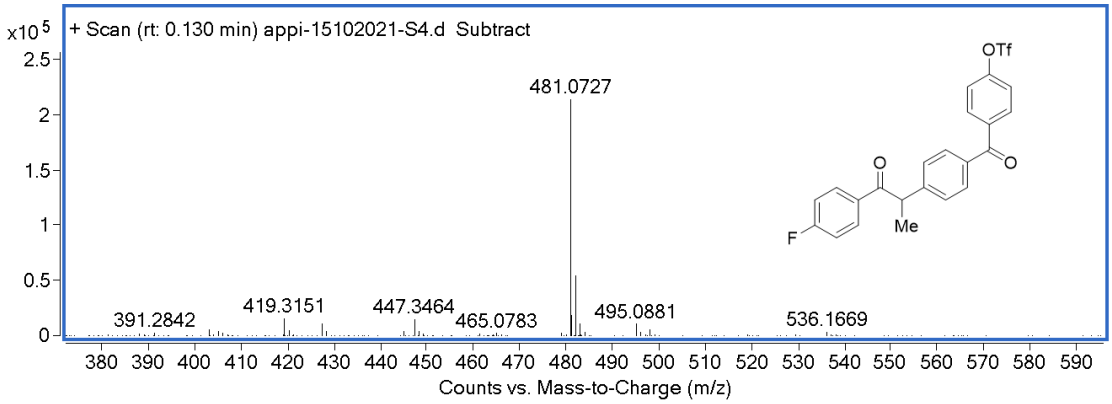

198.42
166.87
164.33
148.21
142.25
135.30
132.43
132.41
131.05
130.96
120.23
120.00
119.69
117.04
115.90
115.69
77.31
77.00
76.68
44.25
19.12
17.82
O
Me
Me
F
TfO
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME A823N-20201028-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201028
Time 14.28
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 186
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 256
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127725 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

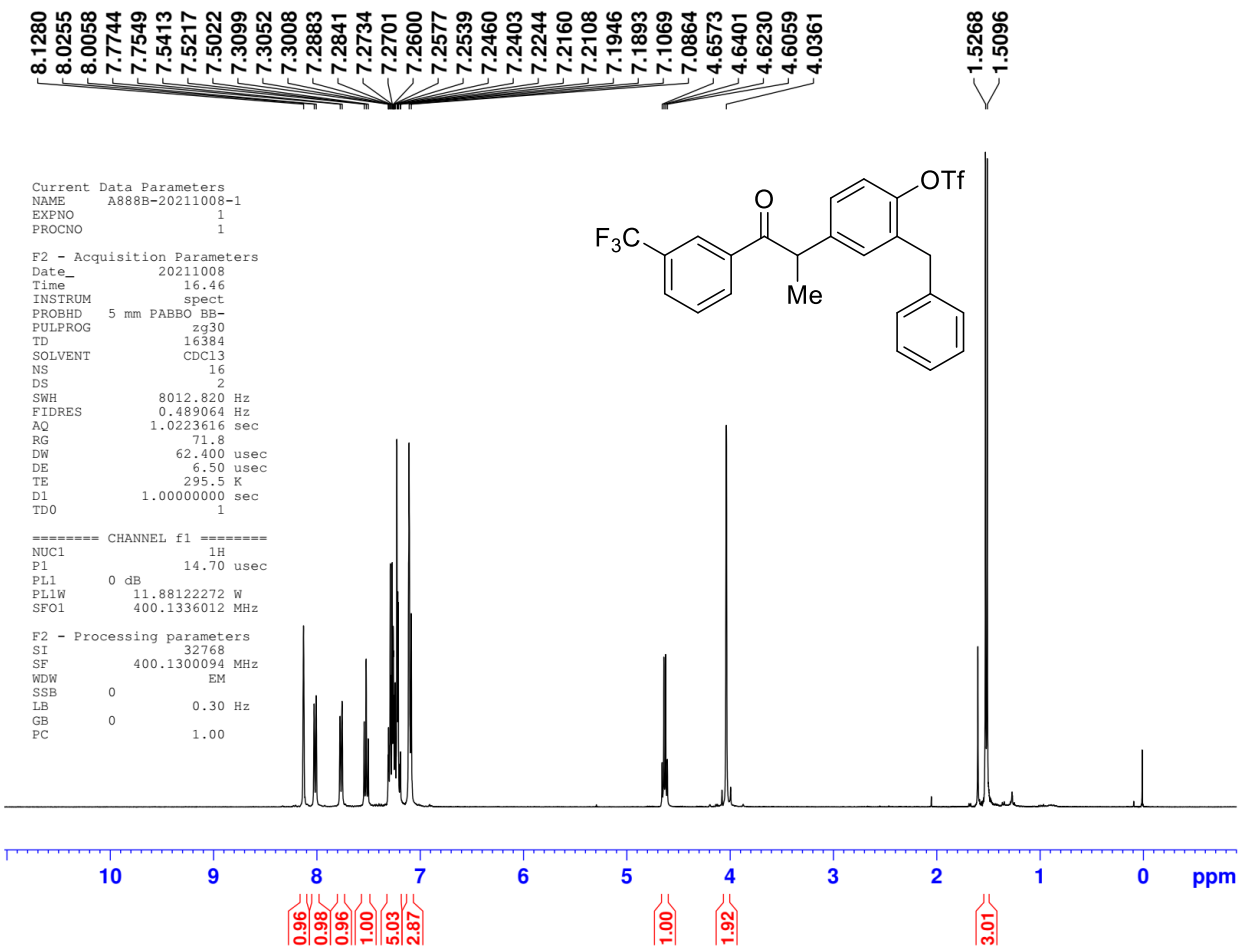

CMSO-14042021-f1 1189 (19.708)
TOF MS EI+
1.02e3
100
%
0
390.0543
389.0465
388.3065
388.7740
389.3695
389.5676
390.3309
390.4959
391.0596
391.4012
391.7857
392.0561
392.2715
389
390
391
392
m/z
O
Me
Me
F
TfO

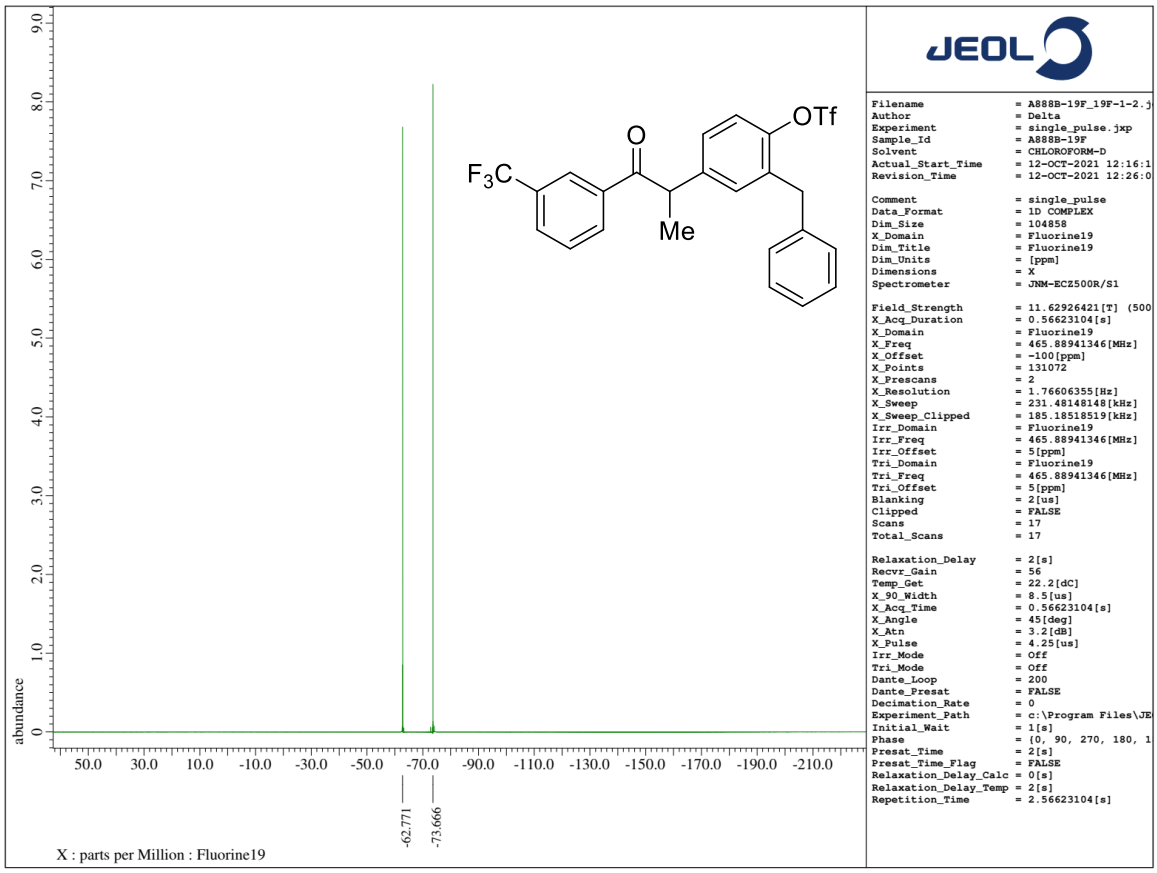

7.9690
7.9637
7.9567
7.8786
7.8722
7.8672
7.8552
7.8502
7.8438
7.7470
7.7430
7.7305
7.7263
7.4290
7.4249
7.4084
7.3957
7.3892
7.3843
7.3722
7.3674
7.3608
7.2599
7.1027
7.0954
7.0903
7.0740
7.0575
7.0524
7.0450
4.7759
4.7588
4.7416
4.7245
1.5807
1.5636
Current Data Parameters
NAME g137-1-20211008-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211008
Time 16.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 295.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
O
F
Me
10
9
8
7
6
5
4
3
2
1
0
ppm
1.97
1.95
1.96
4.01
1.89
1.00
3.08

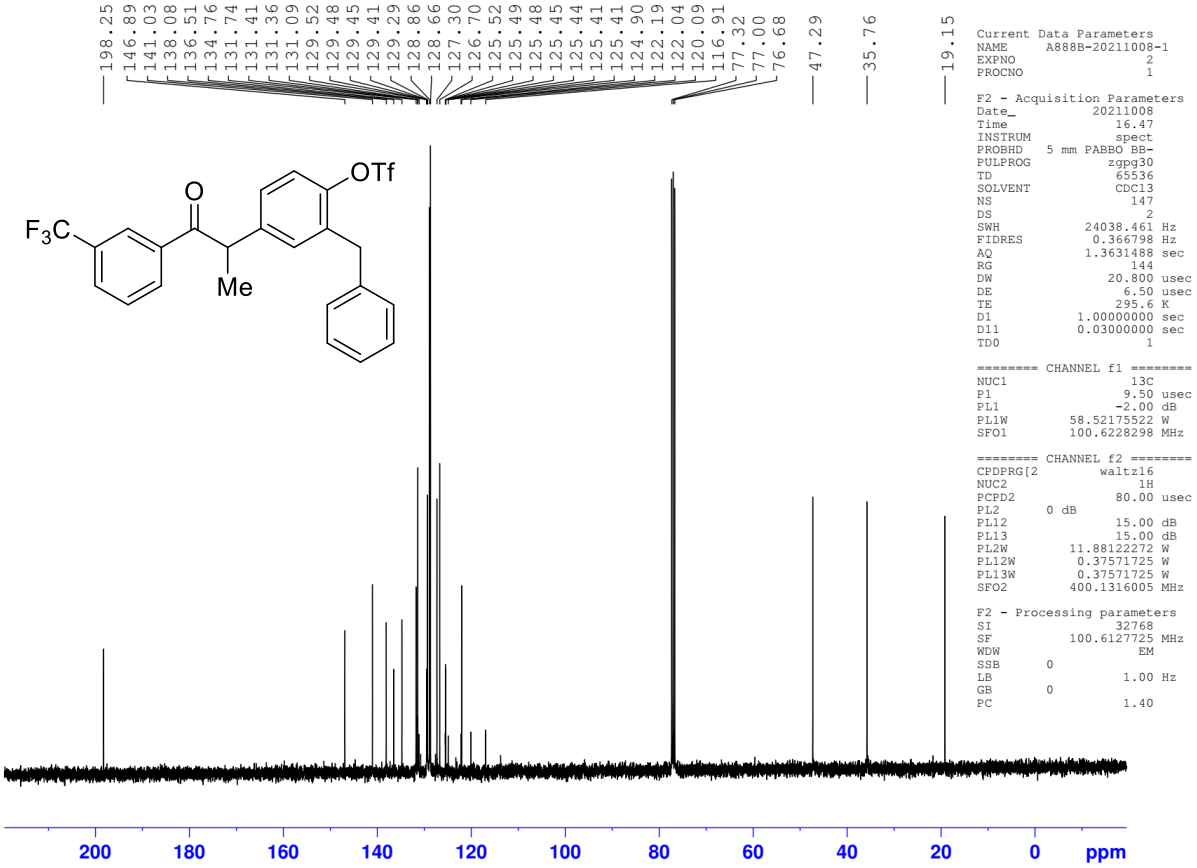

JEOL
Filename = g137-1-CDCl3-19F_si
Author = Delta
Experiment = single_pulse.jxp
Sample_Id = g137-1-CDCl3-19F
Solvent = CHLOROFORM-D
Actual_Start_Time = 18-OCT-2021 11:45:2
Revision_Time = 18-OCT-2021 11:38:1
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 13107
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (500
X_Acq_Duration = 68.15744[ms]
X_Domain = Fluorine19
X_Freq = 465.88941346[MHz]
X_Offset = -100[ppm]
X_Points = 16384
X_Prescans = 1
X_Resolution = 14.67191256[Hz]
X_Sweep = 240.38461538[kHz]
X_Sweep_Clipped = 192.30769231[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 465.88941346[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 465.88941346[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 5[s]
Recvr_Gain = 56
Temp_Get = 460.0[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 68.15744[ms]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 4.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 500
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 1
Presat_Time = 5[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 5[s]
Repetition_Time = 5.06815744[s]
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
20.0
0
-20.0
-40.0
-60.0
-80.0
-100.0
-120.0
-140.0
-160.0
-180.0
-200.0
-72.570
-104.503
OTf
O
O
F
Me
X : parts per Million : Fluorine19


197.88
194.10
166.90
164.36
151.89
146.61
137.43
135.43
132.47
132.44
132.44
132.02
131.40
131.31
130.79
127.93
121.37
120.25
117.06
115.88
115.66
77.31
77.00
76.68
47.71
19.30
OTf
O
O
Me
F
200
180
160
140
120
100
80
60
40
20
0
ppm
Current Data Parameters
NAME g137-1-20211008-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211008
Time 16.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 86
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

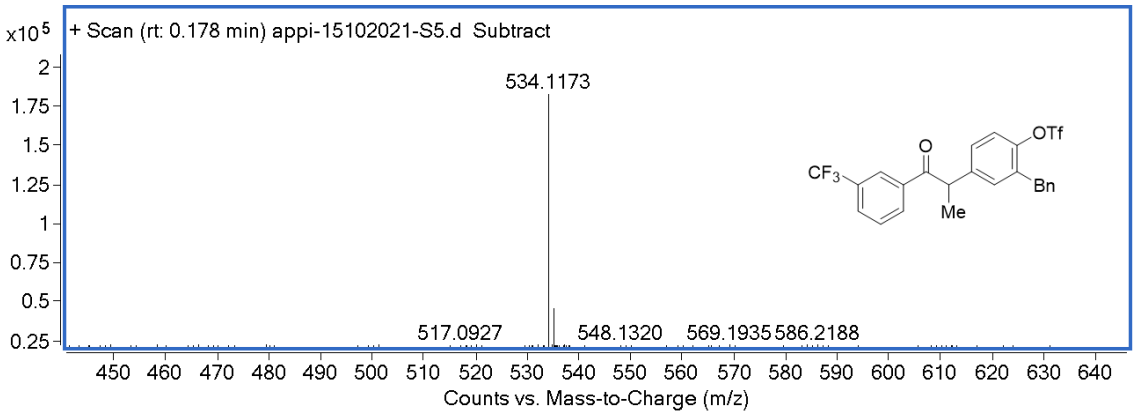

x10^5
+ Scan (rt: 0.130 min) appi-15102021-S4.d Subtract
2.5
2
1.5
1
0.5
0
481.0727
391.2842
419.3151
447.3464
465.0783
495.0881
536.1669
OTf
O
O
Me
F
380
390
400
410
420
430
440
450
460
470
480
490
500
510
520
530
540
550
560
570
580
590
Counts vs. Mass-to-Charge (m/z)

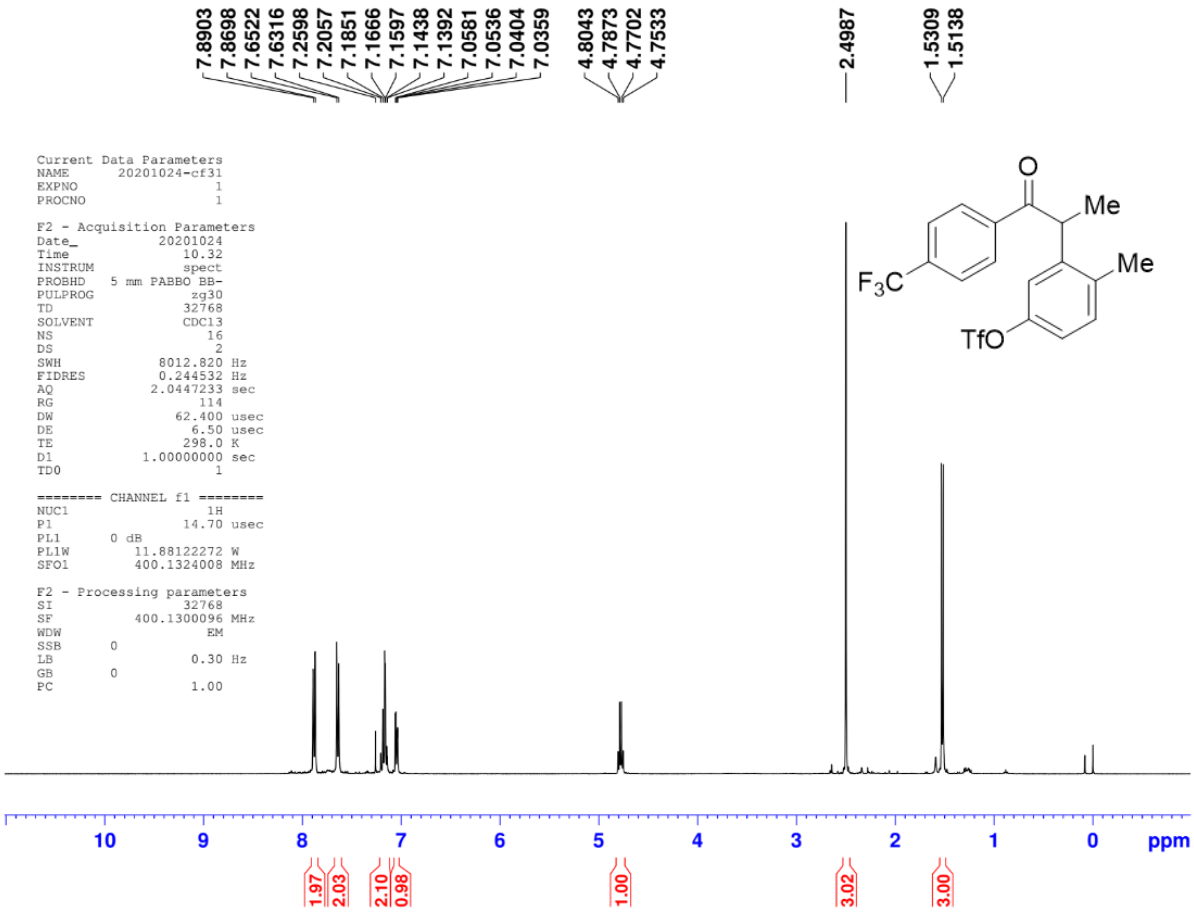

8.1280 8.0255 8.0058 7.7744 7.7549 7.5413 7.5217 7.5022 7.3099 7.3052 7.3008 7.2883 7.2841 7.2734 7.2701 7.2600 7.2577 7.2539 7.2460 7.2403 7.2244 7.2160 7.2108 7.1946 7.1893 7.1069 7.0864 4.6573 4.6401 4.6230 4.6059 4.0361
1.5268 1.5096
Current Data Parameters
NAME A888B-20211008-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211008
Time 16.46
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
F3C
Me
10 9 8 7 6 5 4 3 2 1 0 ppm
0.96 0.98 0.96 1.00 5.03 2.87 1.00 1.92 3.01

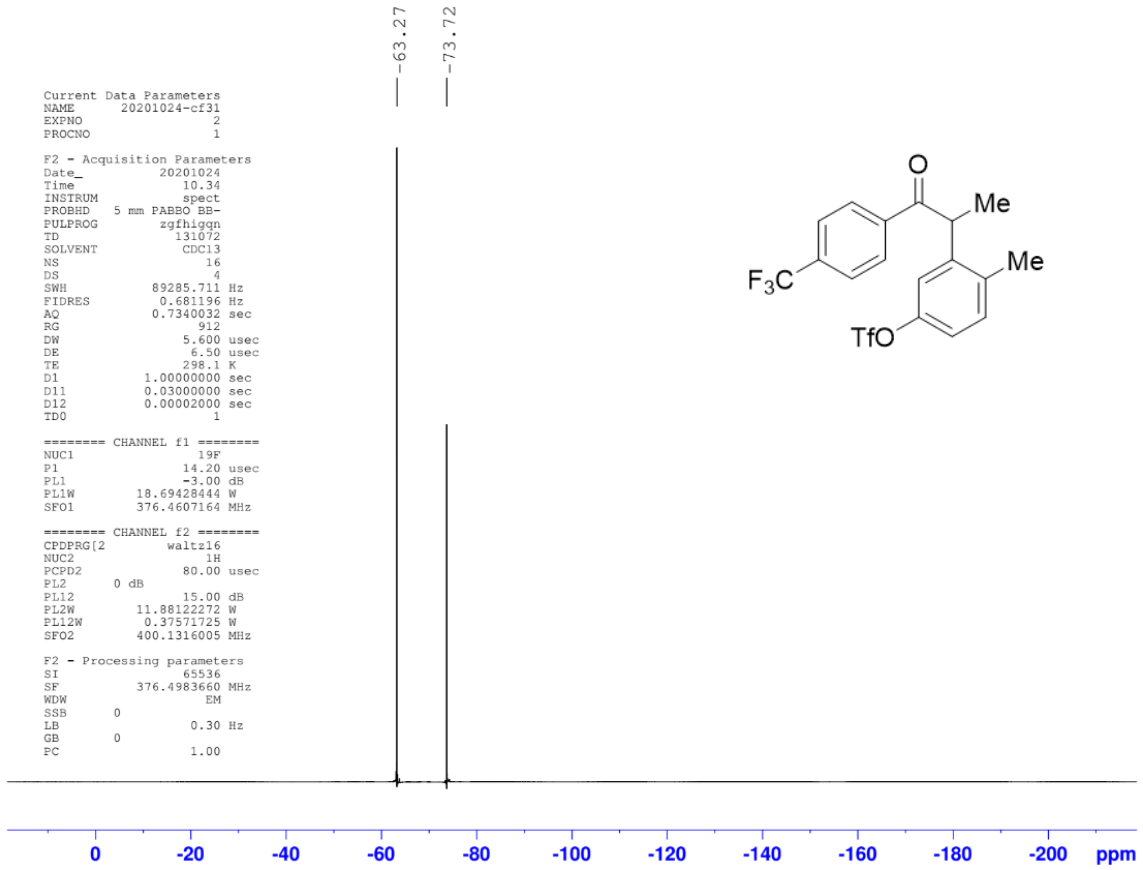

JEOL
Filename = A888B-19F_19F-1-2.j
Author = Delta
Experiment = single_pulse.jxp
Sample_Id = A888B-19F
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-OCT-2021 12:16:1
Revision_Time = 12-OCT-2021 12:26:0
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (500
X_Acq_Duration = 0.56623104[s]
X_Domain = Fluorine19
X_Freq = 465.88941346[MHz]
X_Offset = -100[ppm]
X_Points = 131072
X_Prescans = 2
X_Resolution = 1.76606355[Hz]
X_Sweep = 231.48148148[kHz]
X_Sweep_Clipped = 185.18518519[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 465.88941346[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 465.88941346[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 17
Total_Scans = 17
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.2[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 0.56623104[s]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 4.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 200
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = (0, 90, 270, 180, 1
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 2.56623104[s]
OTf
O
F3C
Me
abundance
9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0
50.0 30.0 10.0 -10.0 -30.0 -50.0 -70.0 -90.0 -110.0 -130.0 -150.0 -170.0 -190.0 -210.0
-62.771
-73.666
X : parts per Million : Fluorine19

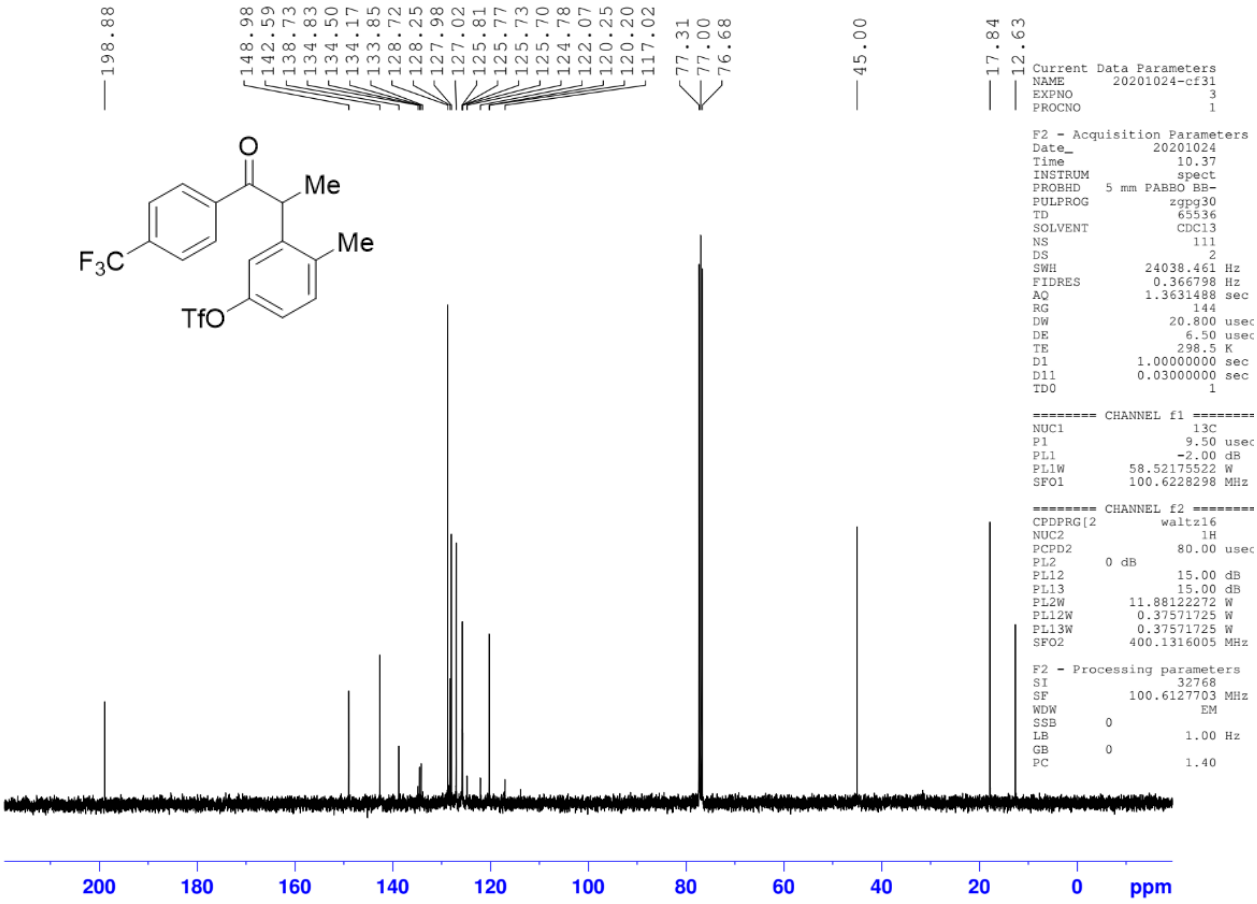


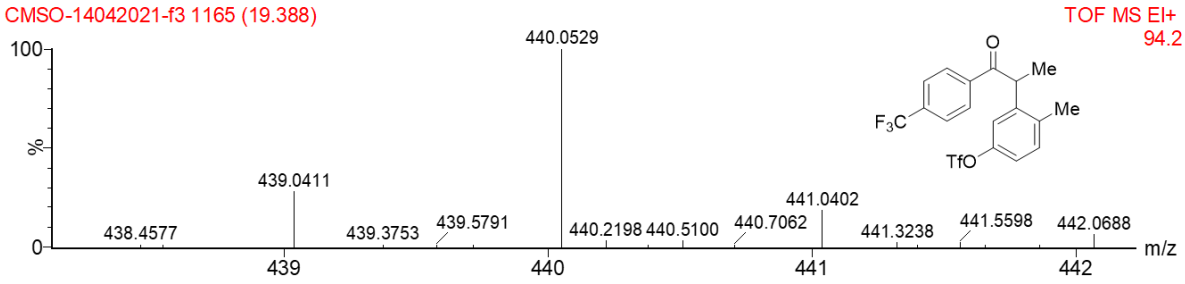

```
Current Data Parameters
NAME      A888B-20211008-1
EXPNO                    2
PROCNO                   1

F2 - Acquisition Parameters
Date_            20211008
Time               16.47
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  147
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ            1.3631488 sec
RG                  144
DW               20.800 usec
DE                6.50 usec
TE               295.6 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.50 usec
PL1               -2.00 dB
PL1W        58.52175522 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2       0 dB
PL12              15.00 dB
PL13              15.00 dB
PL2W        11.88122272 W
PL12W        0.37571725 W
PL13W        0.37571725 W
SFO2       400.1316005 MHz

F2 - Processing parameters
SI                  32768
SF         100.6127725 MHz
WDW                    EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

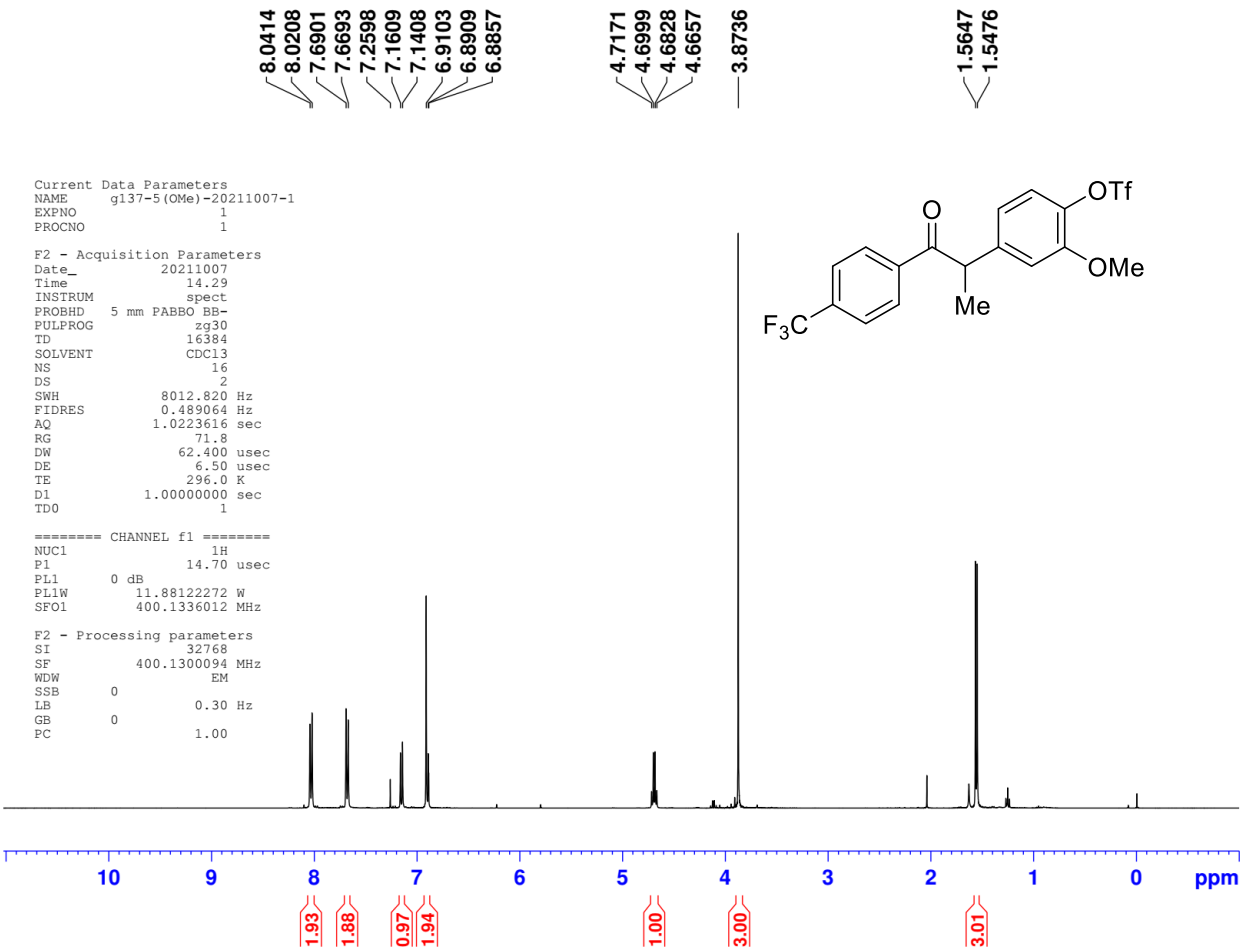


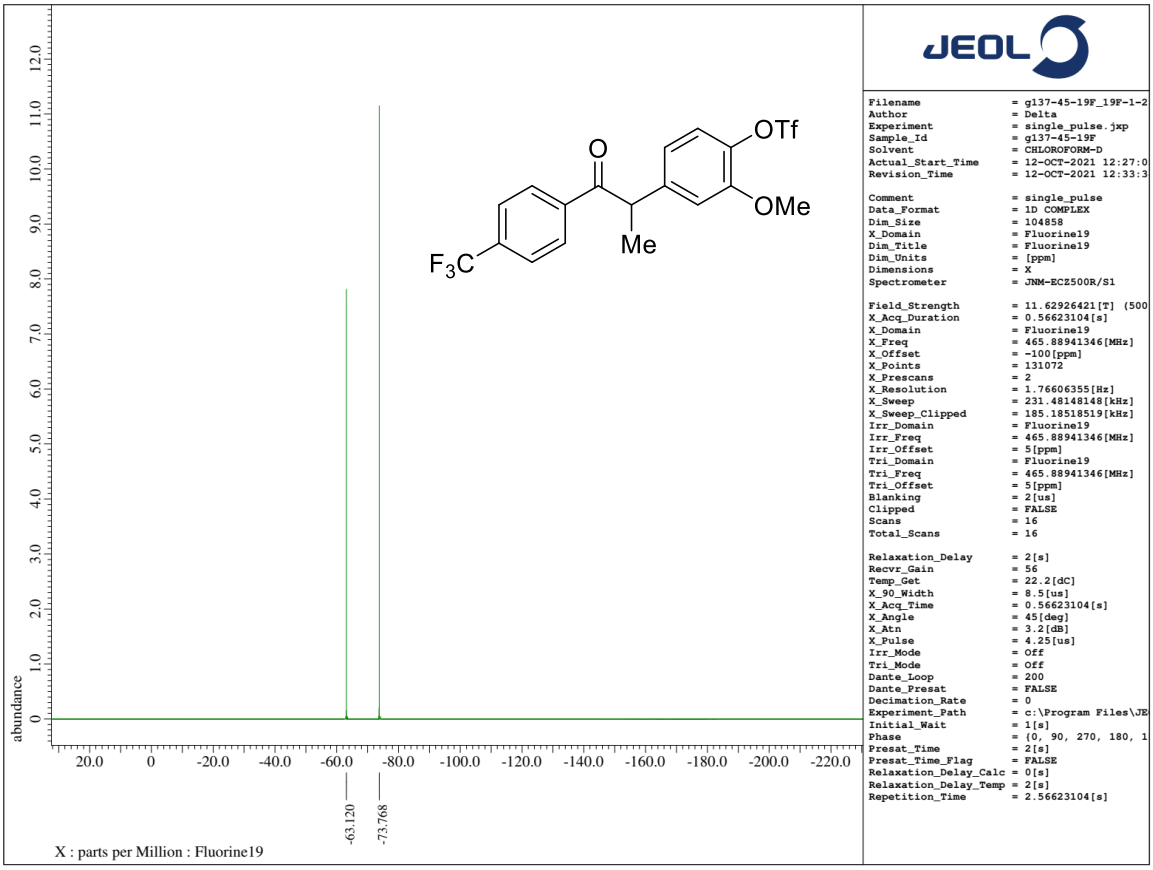

7.8903
7.8698
7.6522
7.6316
7.2598
7.2057
7.1851
7.1666
7.1597
7.1438
7.1392
7.0581
7.0536
7.0404
7.0359
4.8043
4.7873
4.7702
4.7533
2.4987
1.5309
1.5138
Current Data Parameters
NAME 20201024-cf31
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201024
Time 10.32
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Me
Me
F3C
TfO
10
9
8
7
6
5
4
3
2
1
0
ppm
1.97
2.03
2.10
0.98
1.00
3.02
3.00

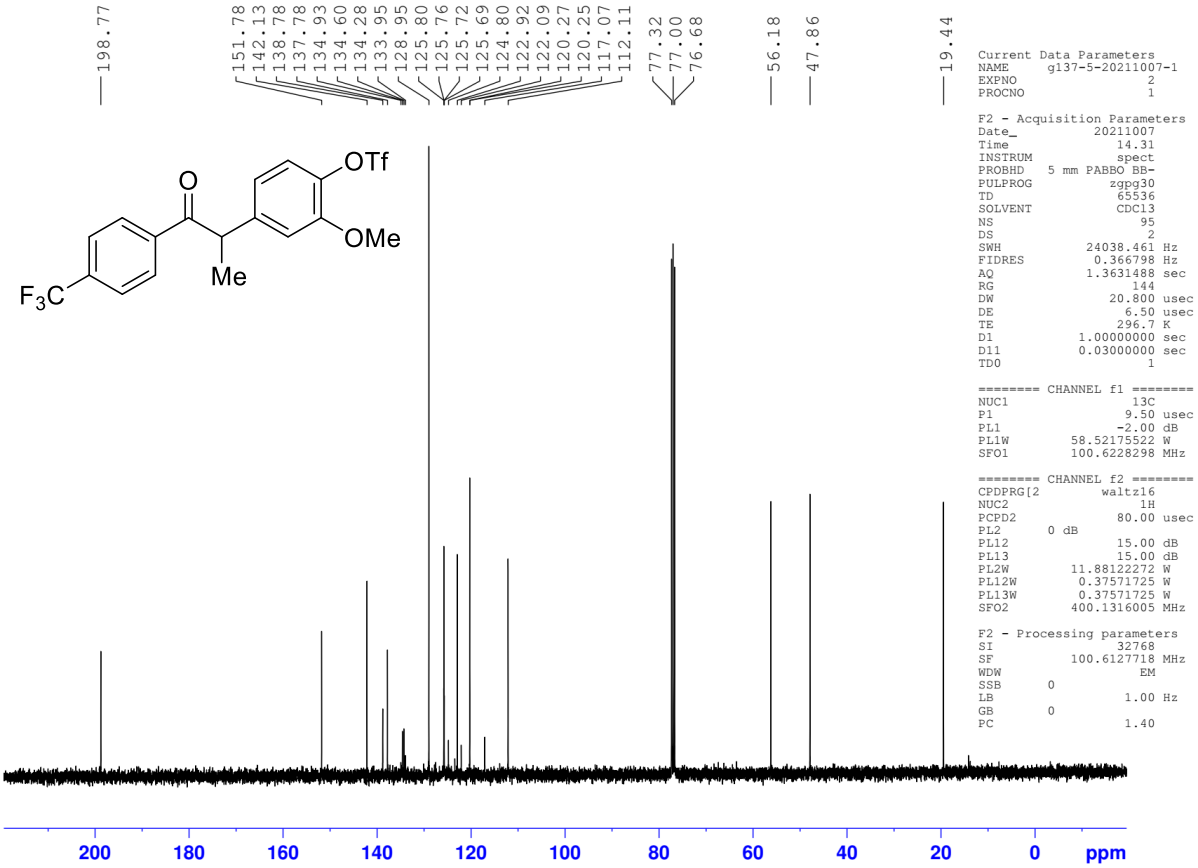

-63.27
-73.72
Current Data Parameters
NAME 20201024-cf31
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201024
Time 10.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
O
Me
Me
F3C
TfO
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

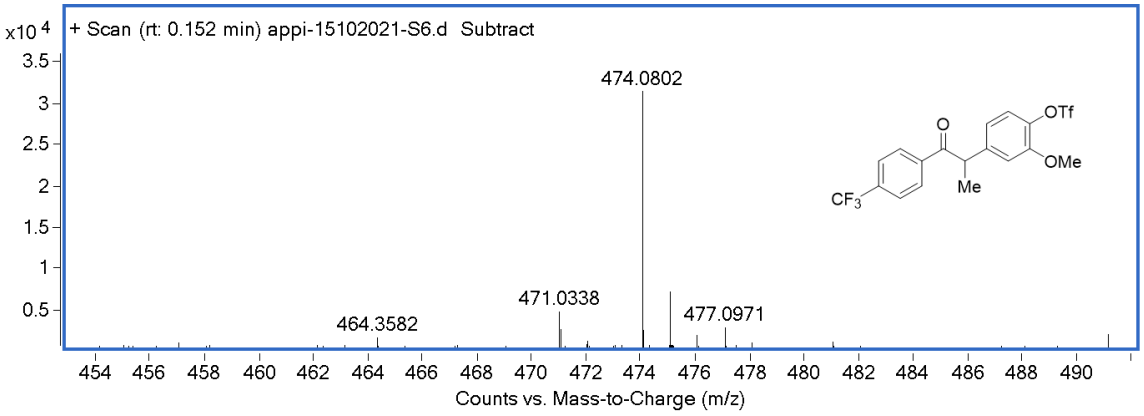

198.88
148.98
142.59
138.73
134.83
134.50
134.17
133.85
128.72
128.25
127.98
127.02
125.81
125.77
125.73
125.70
124.78
122.07
120.25
120.20
117.02
77.31
77.00
76.68
45.00
17.84
12.63
O
Me
Me
F3C
TfO
Current Data Parameters
NAME 20201024-cf31
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201024
Time 10.37
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 111
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.5 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127703 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

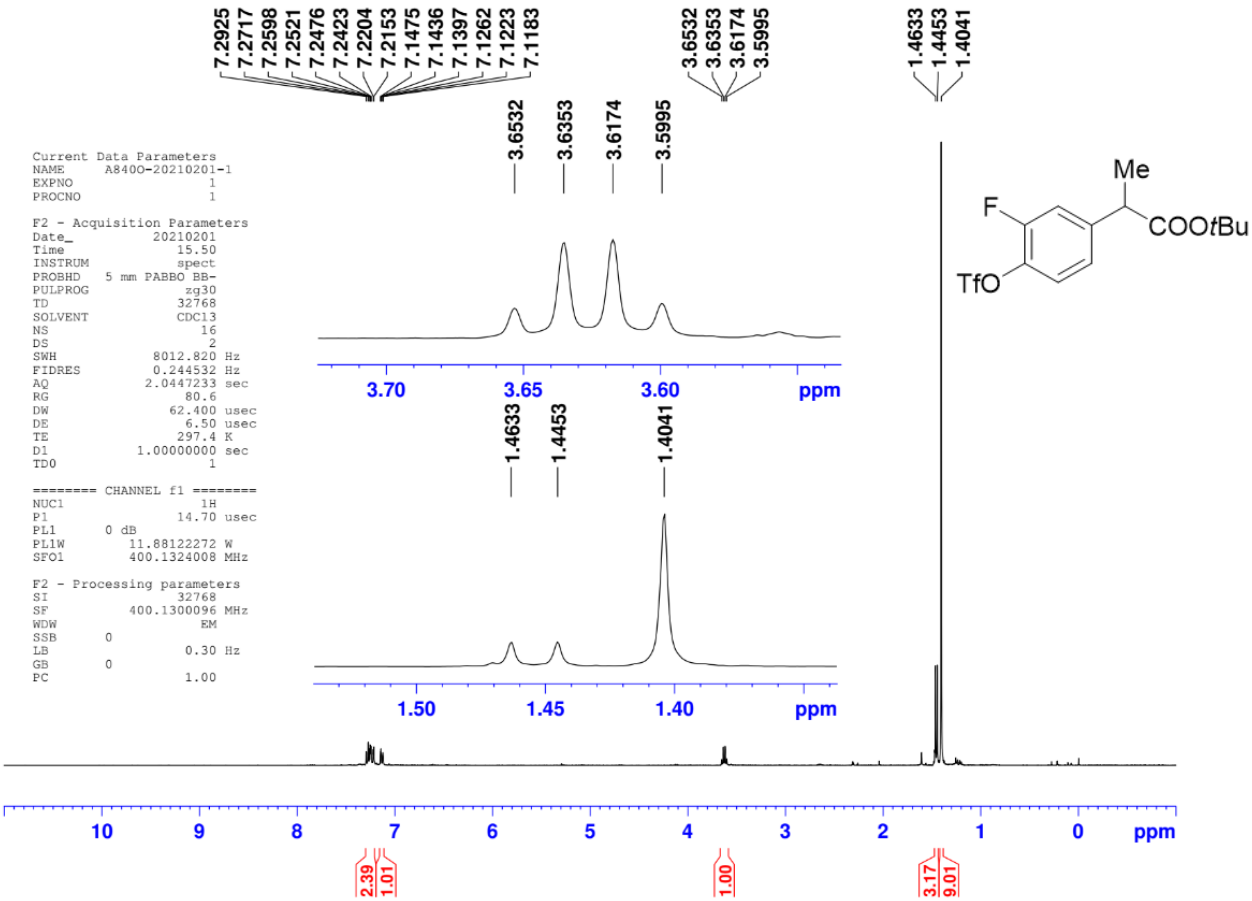

CMSO-14042021-f3 1165 (19.388)
TOF MS EI+
94.2
100
%
0
440.0529
439.0411
438.4577
439.3753
439.5791
440.2198
440.5100
440.7062
441.0402
441.3238
441.5598
442.0688
439
440
441
442
m/z
O
Me
Me
F3C
TfO

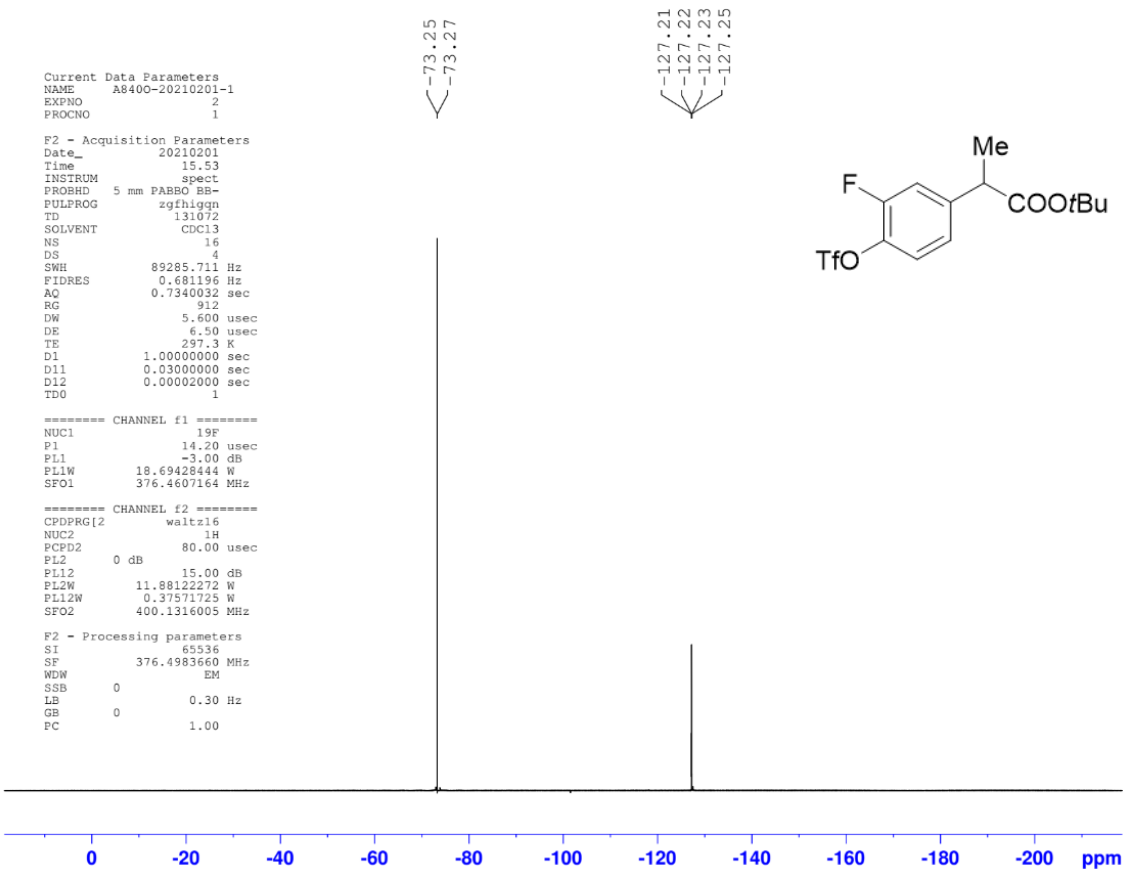

8.0414
8.0208
7.6901
7.6693
7.2598
7.1609
7.1408
6.9103
6.8909
6.8857
4.7171
4.6999
4.6828
4.6657
3.8736
1.5647
1.5476
Current Data Parameters
NAME g137-5(OMe)-20211007-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211007
Time 14.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 296.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OTf
O
OMe
Me
F3C
10
9
8
7
6
5
4
3
2
1
0
ppm
1.93
1.88
0.97
1.94
1.00
3.00
3.01

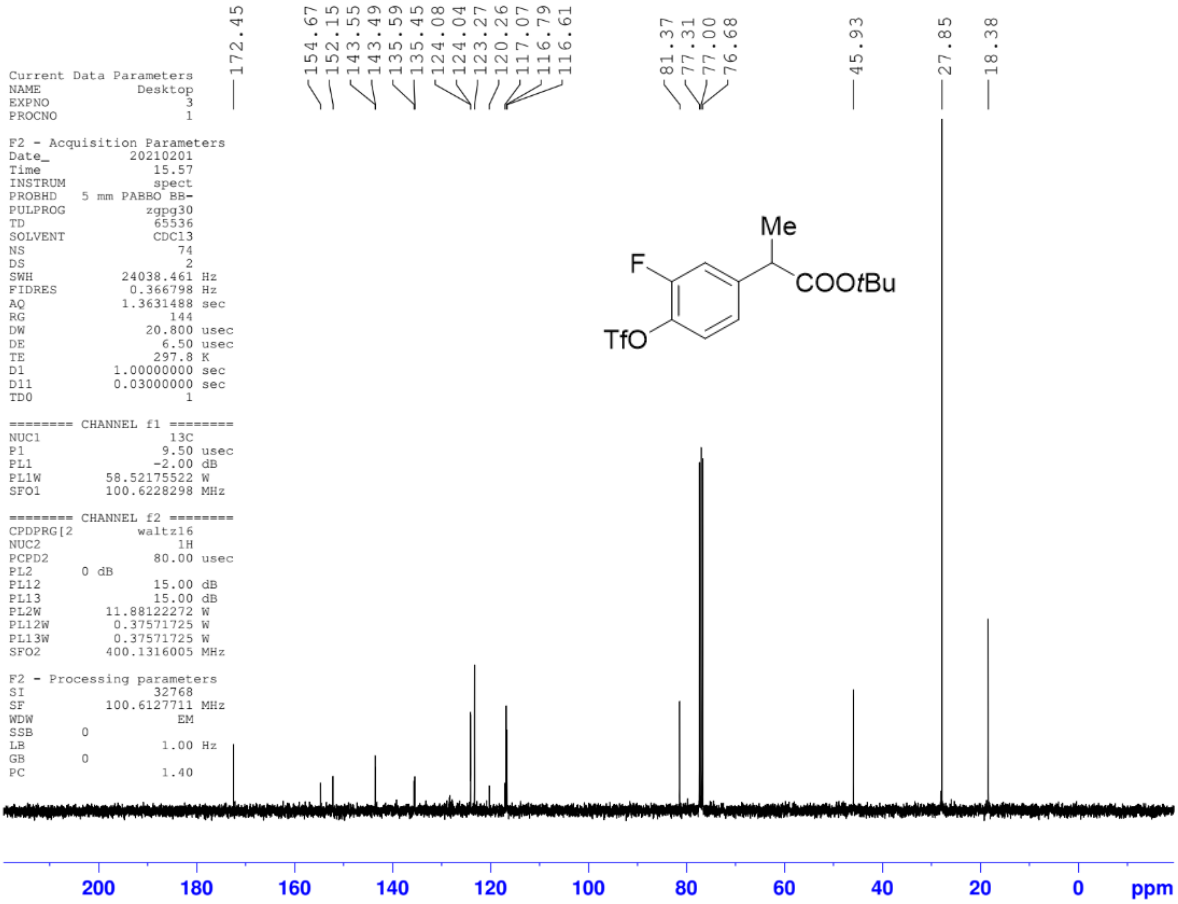

JEOL
Filename = g137-45-19F_19F-1-2
Author = Delta
Experiment = single_pulse.jxp
Sample_Id = g137-45-19F
Solvent = CHLOROFORM-D
Actual_Start_Time = 12-OCT-2021 12:27:0
Revision_Time = 12-OCT-2021 12:33:3
Comment = single_pulse
Data_Format = 1D COMPLEX
Dim_Size = 104858
X_Domain = Fluorine19
Dim_Title = Fluorine19
Dim_Units = [ppm]
Dimensions = X
Spectrometer = JNM-ECZ500R/S1
Field_Strength = 11.62926421[T] (500
X_Acq_Duration = 0.56623104[s]
X_Domain = Fluorine19
X_Freq = 465.88941346[MHz]
X_Offset = -100[ppm]
X_Points = 131072
X_Prescans = 2
X_Resolution = 1.76606355[Hz]
X_Sweep = 231.48148148[kHz]
X_Sweep_Clipped = 185.18518519[kHz]
Irr_Domain = Fluorine19
Irr_Freq = 465.88941346[MHz]
Irr_Offset = 5[ppm]
Tri_Domain = Fluorine19
Tri_Freq = 465.88941346[MHz]
Tri_Offset = 5[ppm]
Blanking = 2[us]
Clipped = FALSE
Scans = 16
Total_Scans = 16
Relaxation_Delay = 2[s]
Recvr_Gain = 56
Temp_Get = 22.2[dC]
X_90_Width = 8.5[us]
X_Acq_Time = 0.56623104[s]
X_Angle = 45[deg]
X_Atn = 3.2[dB]
X_Pulse = 4.25[us]
Irr_Mode = Off
Tri_Mode = Off
Dante_Loop = 200
Dante_Presat = FALSE
Decimation_Rate = 0
Experiment_Path = c:\Program Files\JE
Initial_Wait = 1[s]
Phase = {0, 90, 270, 180, 1
Presat_Time = 2[s]
Presat_Time_Flag = FALSE
Relaxation_Delay_Calc = 0[s]
Relaxation_Delay_Temp = 2[s]
Repetition_Time = 2.56623104[s]
OTf
O
OMe
Me
F3C
abundance
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
20.0
0
-20.0
-40.0
-60.0
-80.0
-100.0
-120.0
-140.0
-160.0
-180.0
-200.0
-220.0
-63.120
-73.768
X : parts per Million : Fluorine19


198.77
151.78
142.13
138.78
137.78
134.93
134.60
134.28
133.95
128.95
125.80
125.76
125.72
125.69
124.80
122.92
122.09
120.27
120.25
117.07
112.11
77.32
77.00
76.68
56.18
47.86
19.44
OTf
OMe
Me
F3C
O
Current Data Parameters
NAME g137-5-20211007-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20211007
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 95
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127718 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

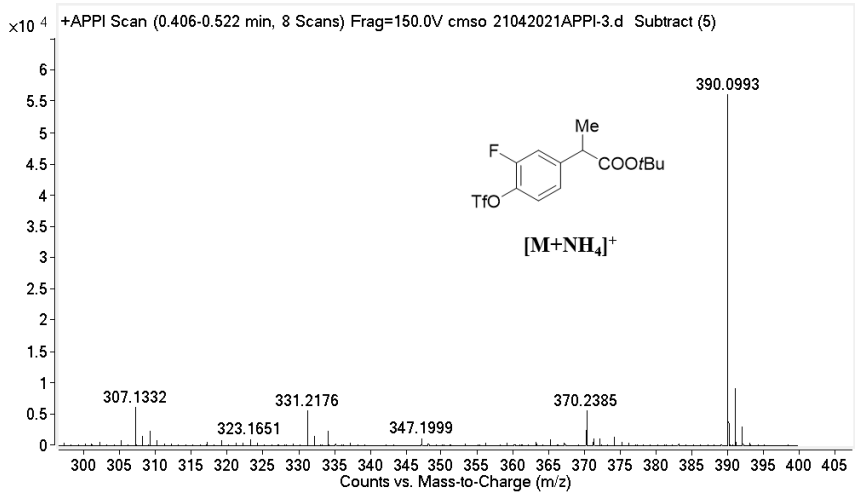

x10 4
+ Scan (rt: 0.152 min) appi-15102021-S6.d Subtract
474.0802
471.0338
477.0971
464.3582
OTf
OMe
Me
CF3
O
Counts vs. Mass-to-Charge (m/z)

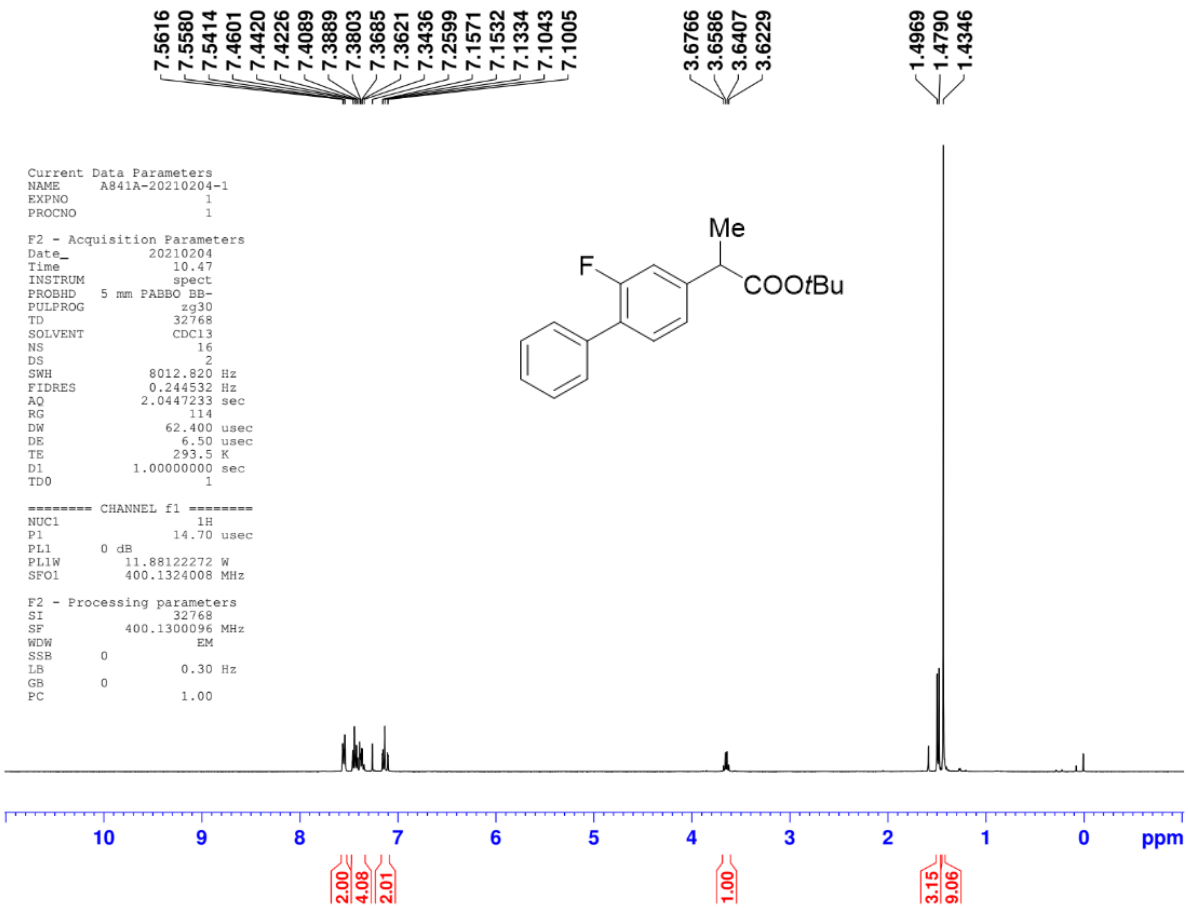

7.2925
7.2717
7.2598
7.2521
7.2476
7.2423
7.2204
7.2153
7.1475
7.1436
7.1397
7.1262
7.1223
7.1183
3.6532
3.6353
3.6174
3.5995
1.4633
1.4453
1.4041
Current Data Parameters
NAME A840O-20210201-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210201
Time 15.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 80.6
DW 62.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
3.70
3.65
3.60
ppm
1.50
1.45
1.40
ppm
Me
F
COOtBu
TfO
10
9
8
7
6
5
4
3
2
1
0
ppm
2.39
1.01
1.00
3.17
9.01

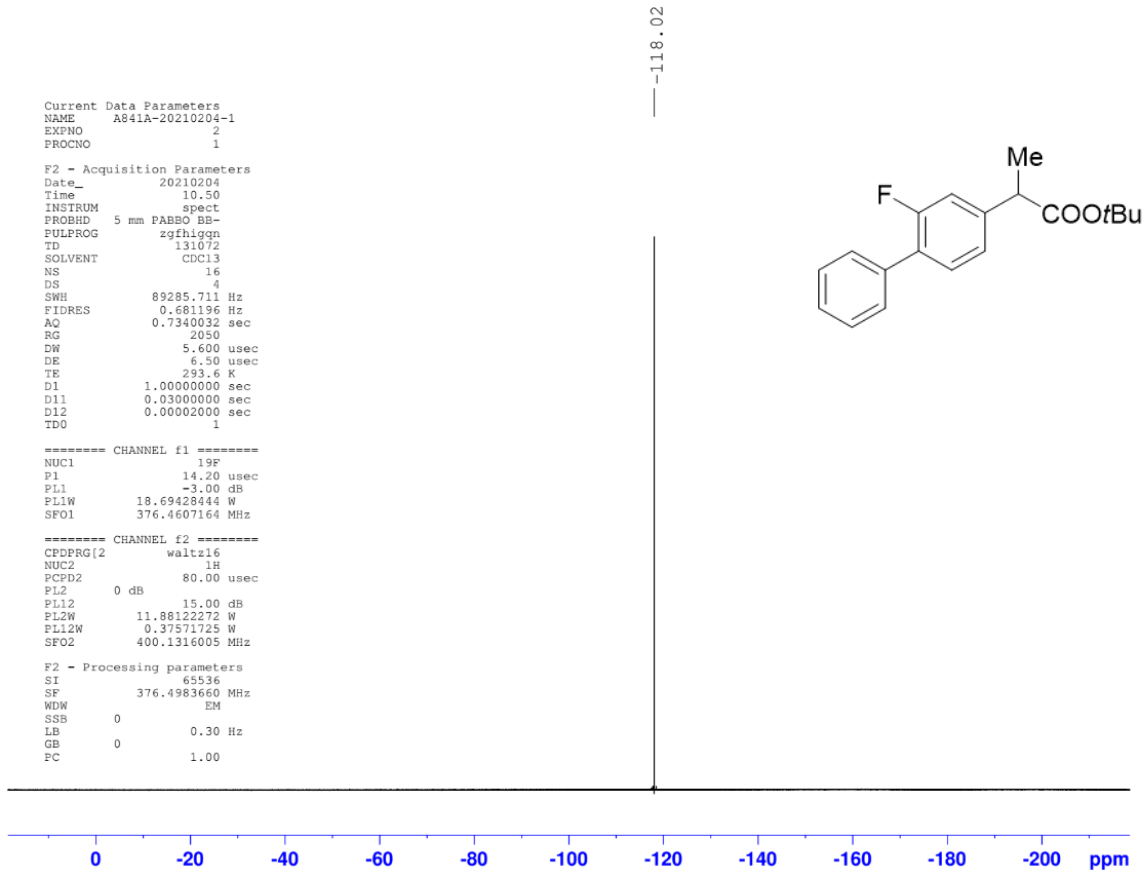

-73.25
-73.27
-127.21
-127.22
-127.23
-127.25
Current Data Parameters
NAME A840O-20210201-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210201
Time 15.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
F
COOtBu
TfO
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

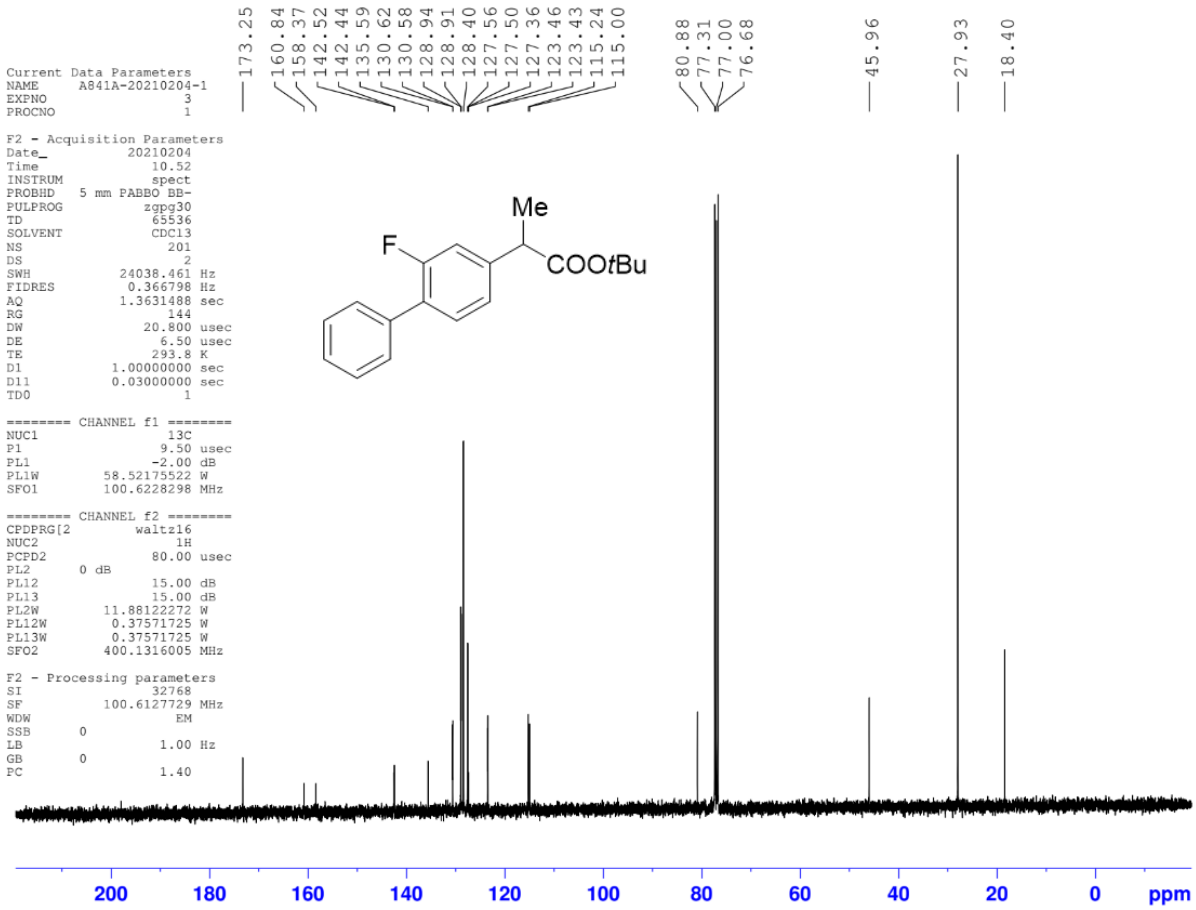


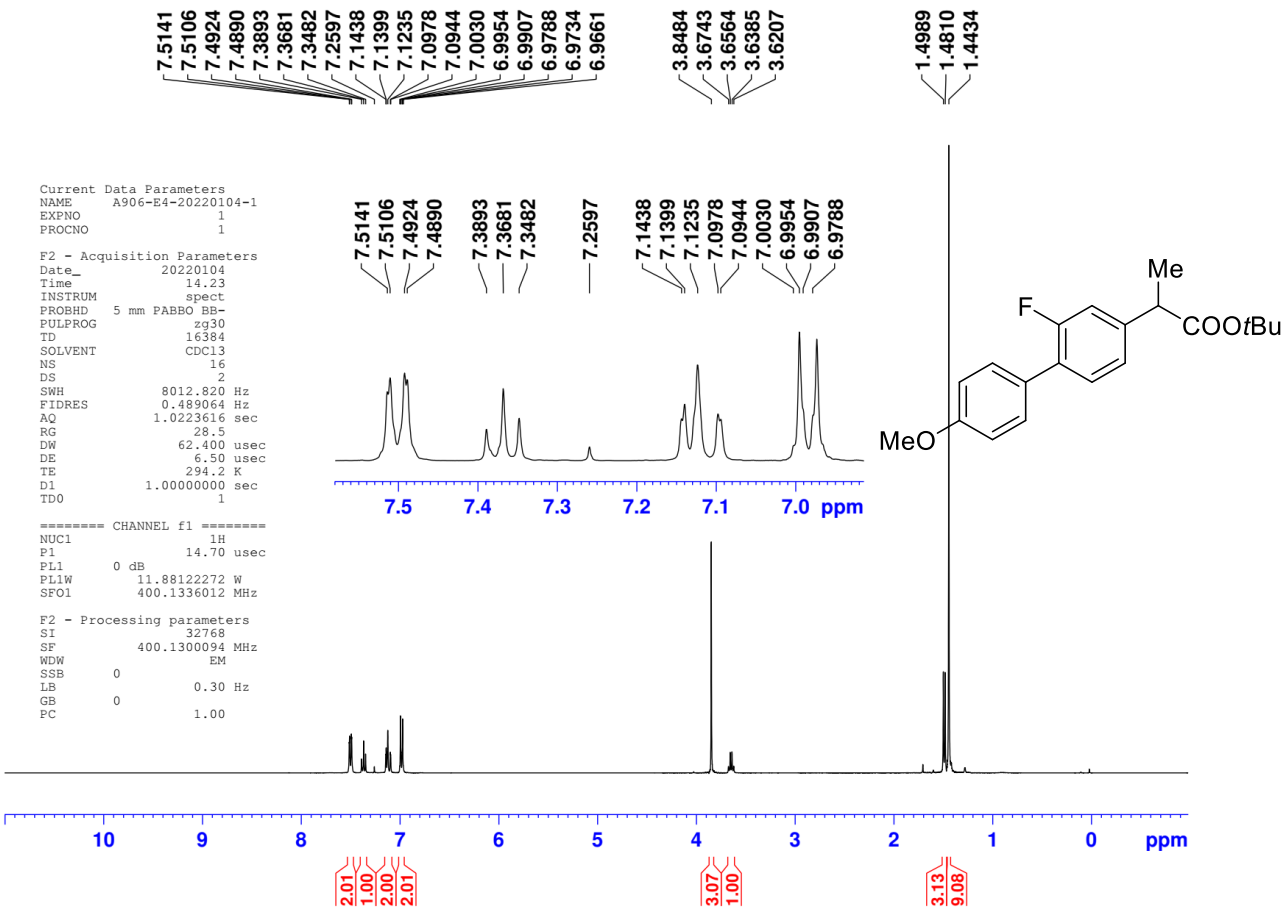

```
Current Data Parameters
NAME            Desktop
EXPNO                 3
PROCNO                1

F2 - Acquisition Parameters
Date_            20210201
Time               15.57
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   74
DS                    2
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ             1.3631488 sec
RG                  144
DW               20.800 usec
DE                6.50 usec
TE               297.8 K
D1           1.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 9.50 usec
PL1               -2.00 dB
PL1W        58.52175522 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2       0 dB
PL12              15.00 dB
PL13              15.00 dB
PL2W        11.88122272 W
PL12W        0.37571725 W
PL13W        0.37571725 W
SFO2        400.1316005 MHz

F2 - Processing parameters
SI                32768
SF          100.6127711 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

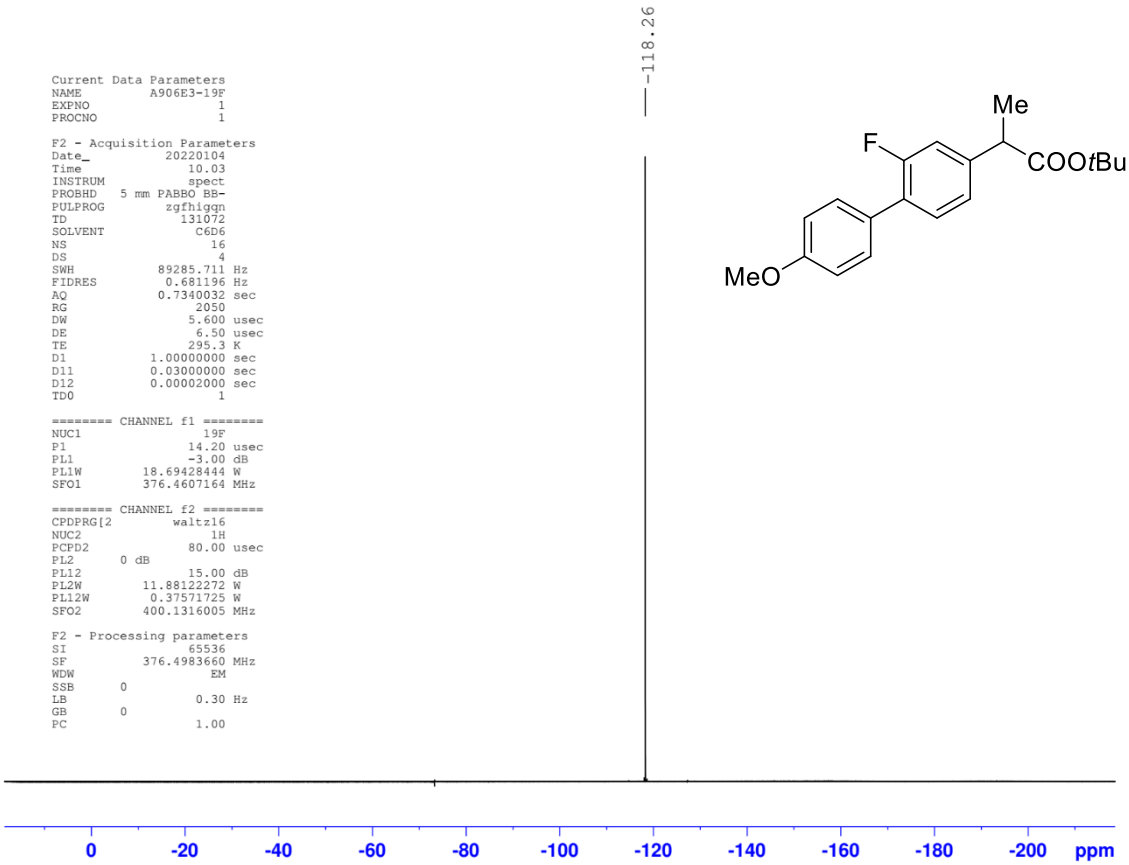


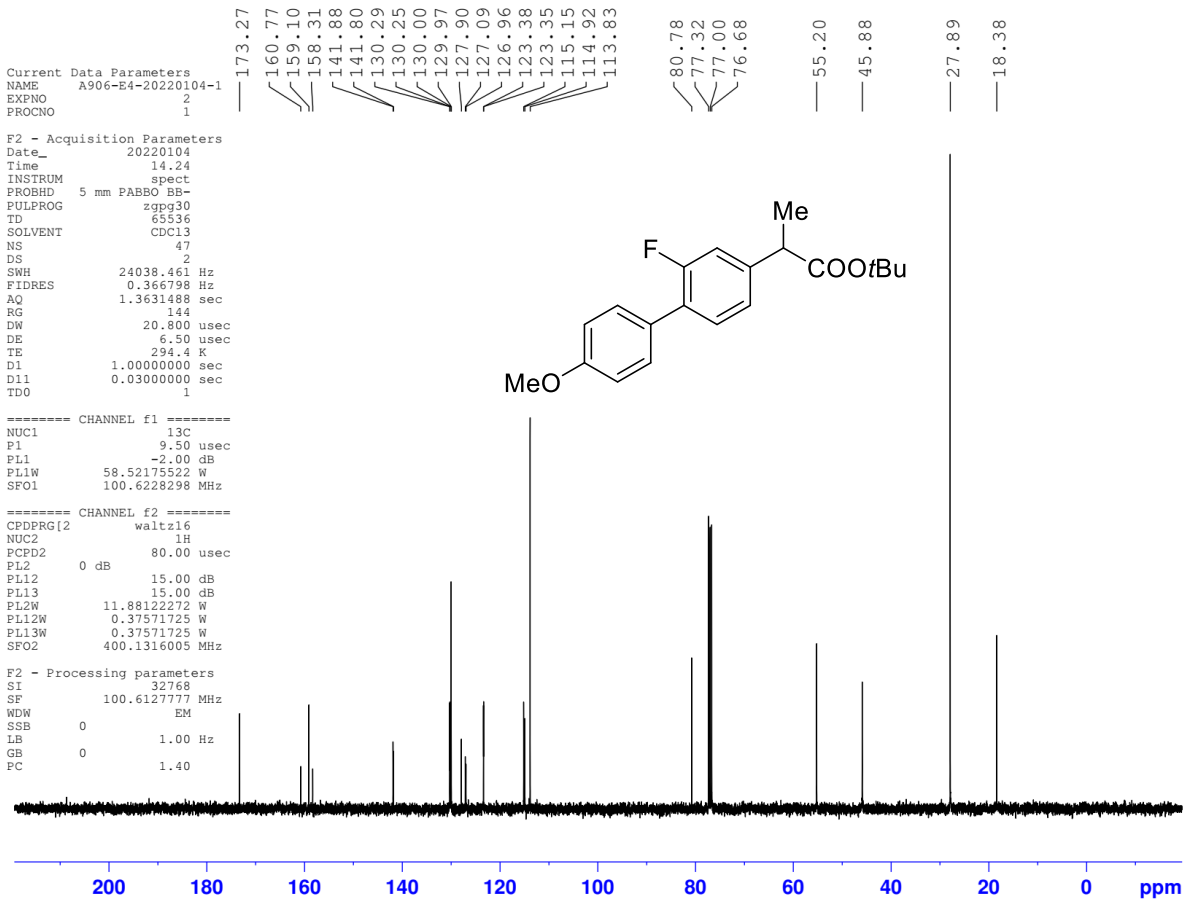

7.5616
7.5580
7.5414
7.4601
7.4420
7.4226
7.4089
7.3889
7.3803
7.3685
7.3621
7.3436
7.2599
7.1571
7.1532
7.1334
7.1043
7.1005
3.6766
3.6586
3.6407
3.6229
1.4969
1.4790
1.4346
Current Data Parameters
NAME A841A-20210204-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210204
Time 10.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 114
DW 62.400 usec
DE 6.50 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
F
COOtBu
10
9
8
7
6
5
4
3
2
1
0
ppm
2.00
4.08
2.01
1.00
3.15
9.06

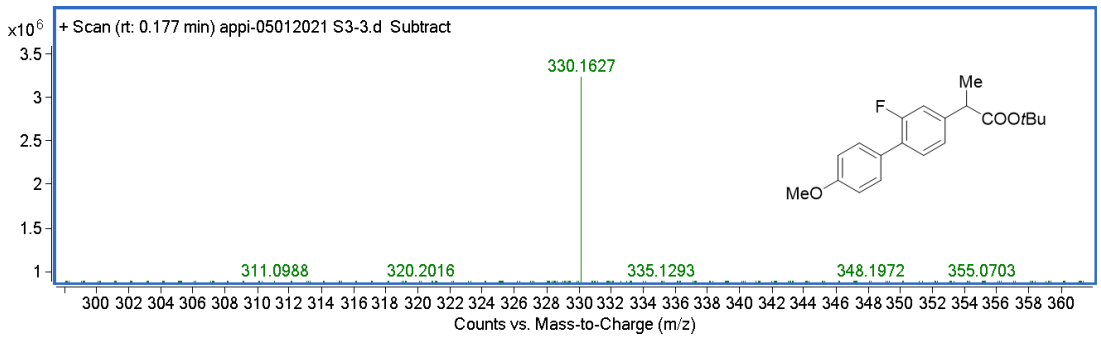

-118.02
Current Data Parameters
NAME A841A-20210204-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210204
Time 10.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 2050
DW 5.600 usec
DE 6.50 usec
TE 293.6 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
F
COOtBu
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

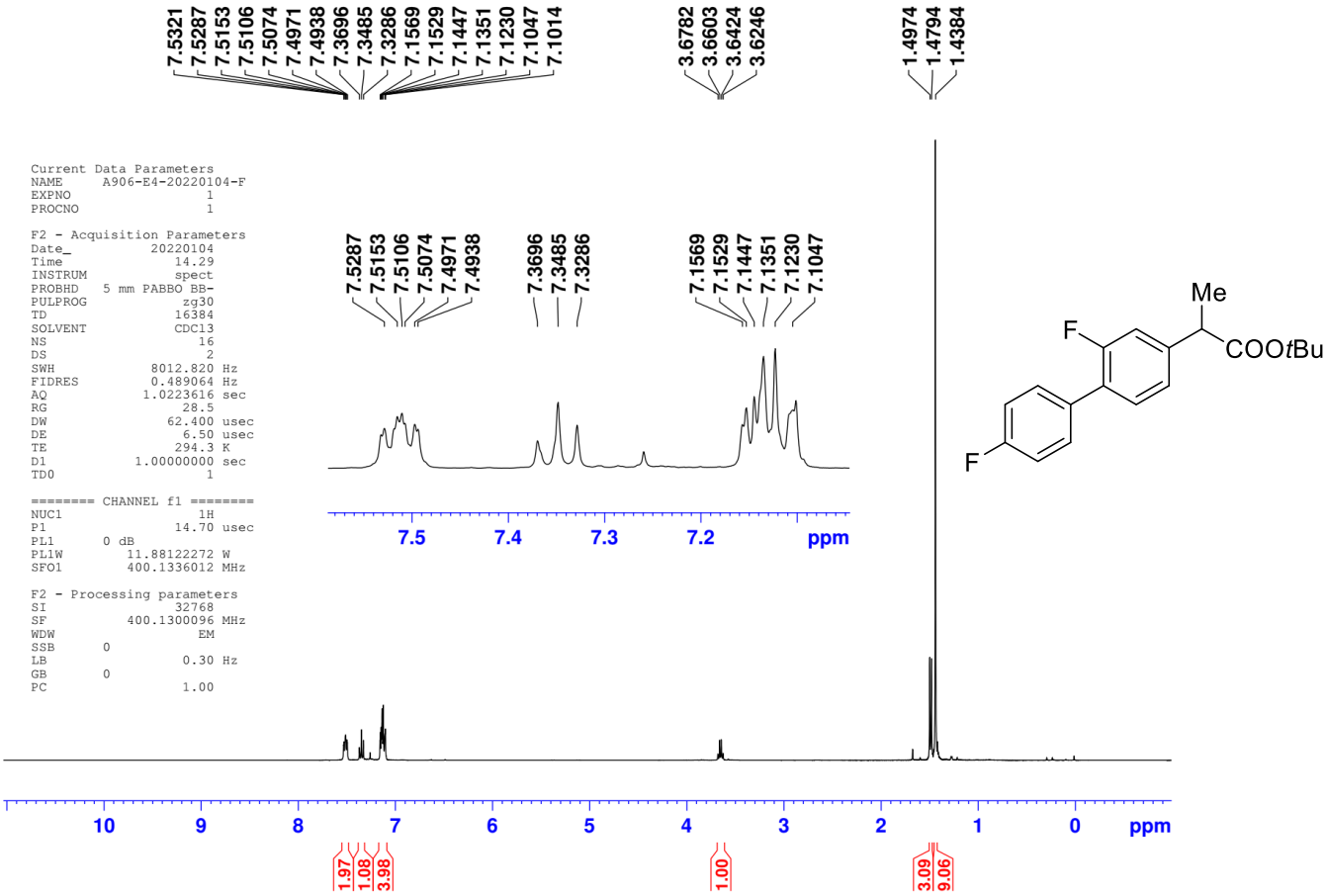

173.25
160.84
158.37
142.52
142.44
135.59
130.62
130.58
128.94
128.91
128.40
127.56
127.50
127.36
123.46
123.43
115.24
115.00
80.88
77.31
77.00
76.68
45.96
27.93
18.40
Current Data Parameters
NAME A841A-20210204-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210204
Time 10.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 201
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 293.8 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127729 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
F
COOtBu
200
180
160
140
120
100
80
60
40
20
0
ppm

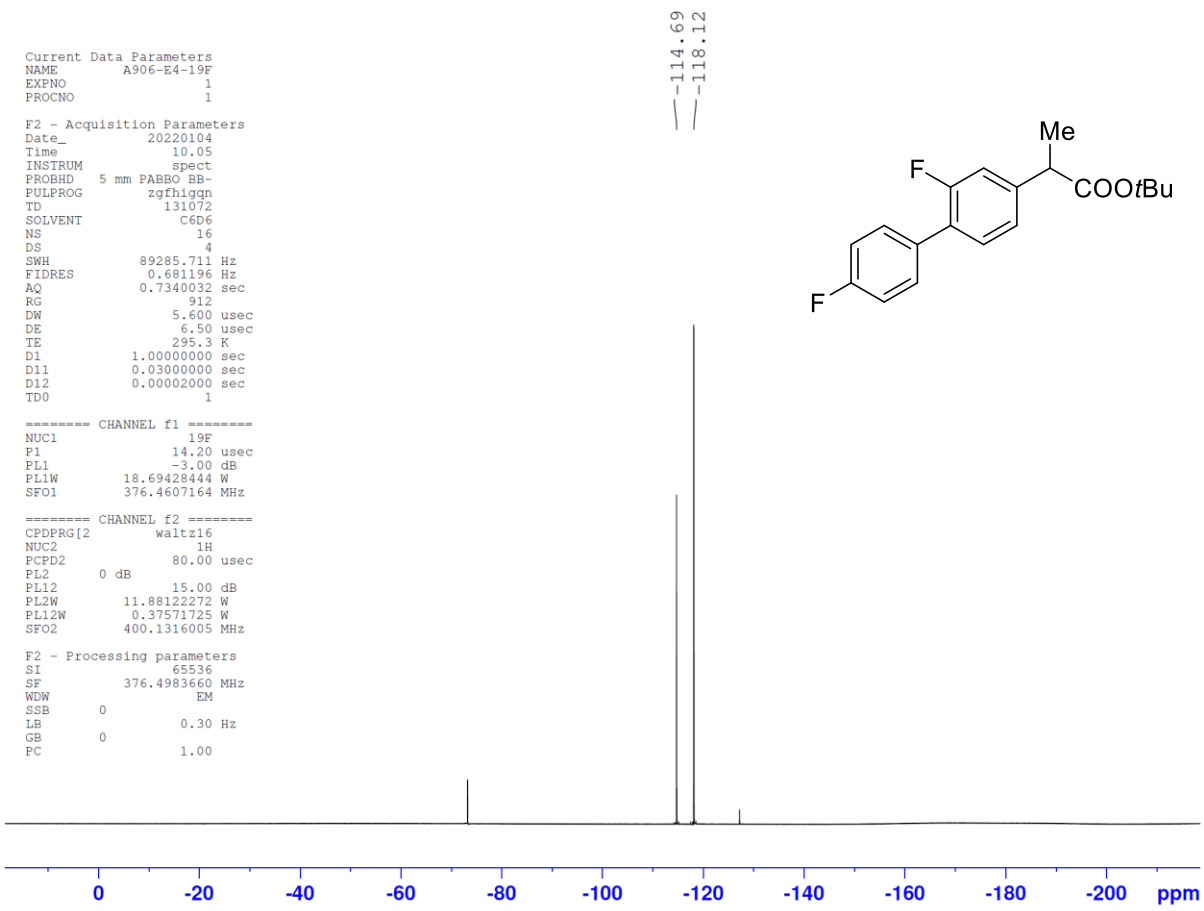

7.5141
7.5106
7.4924
7.4890
7.3893
7.3681
7.3482
7.2597
7.1438
7.1399
7.1235
7.0978
7.0944
7.0030
6.9954
6.9907
6.9788
6.9734
6.9661
3.8484
3.6743
3.6564
3.6385
3.6207
1.4989
1.4810
1.4434
Current Data Parameters
NAME A906-E4-20220104-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220104
Time 14.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 28.5
DW 62.400 usec
DE 6.50 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
F
COOtBu
MeO
7.5
7.4
7.3
7.2
7.1
7.0 ppm
10
9
8
7
6
5
4
3
2
1
0
ppm
2.01
1.00
2.00
2.01
3.07
1.00
3.13
9.08

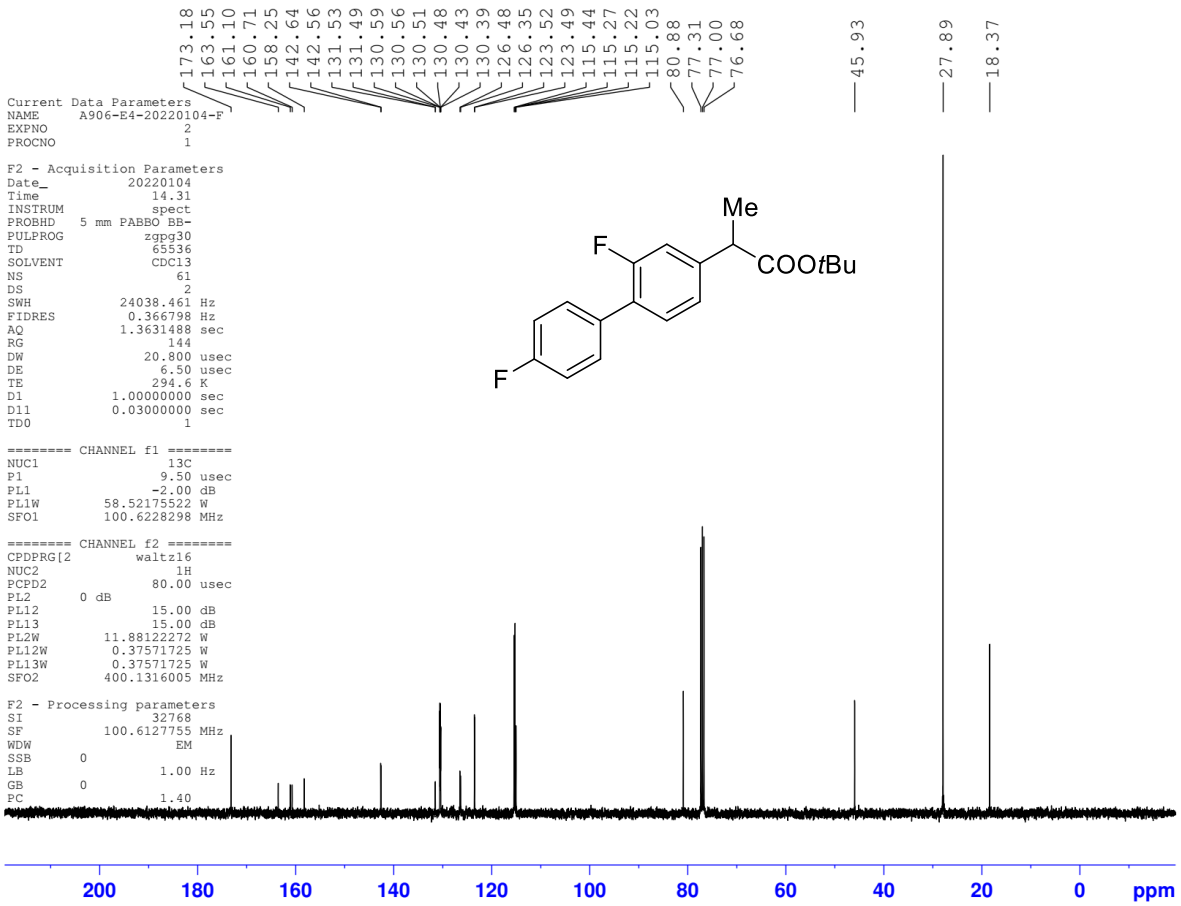

-118.26
Current Data Parameters
NAME A906E3-19F
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220104
Time 10.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT C6D6
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 2050
DW 5.600 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
F
COOtBu
MeO
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

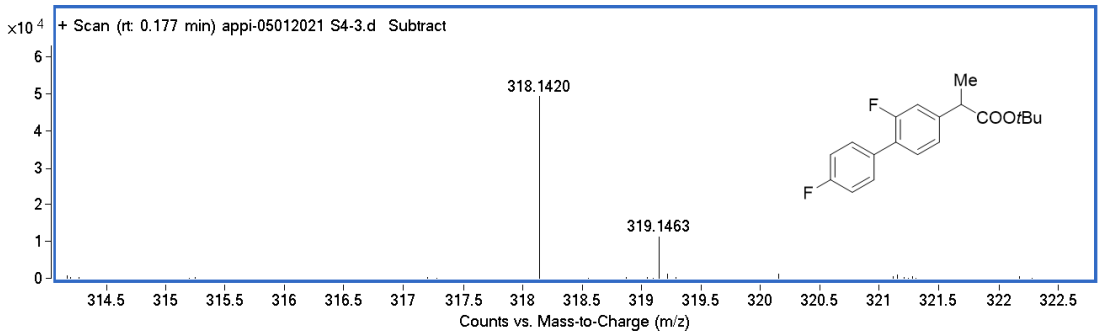

173.27
160.77
159.10
158.31
141.88
141.80
130.29
130.25
130.00
129.97
127.90
127.09
126.96
123.38
123.35
115.15
114.92
113.83
80.78
77.32
77.00
76.68
55.20
45.88
27.89
18.38
Current Data Parameters
NAME A906-E4-20220104-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220104
Time 14.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 47
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 294.4 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127777 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
F
COOtBu
MeO
200
180
160
140
120
100
80
60
40
20
0
ppm

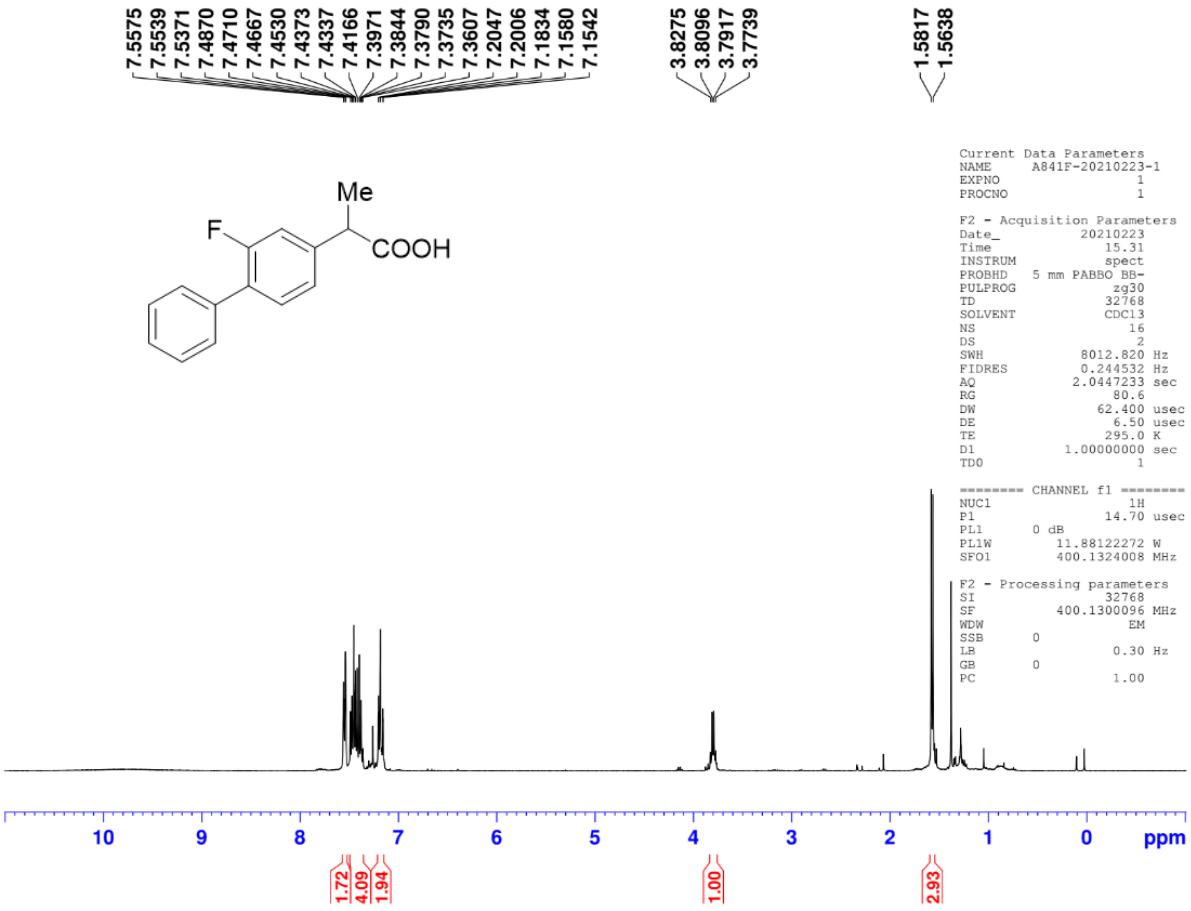

x10^6
+ Scan (rt: 0.177 min) appi-05012021 S3-3.d Subtract
3.5
3
2.5
2
1.5
1
330.1627
311.0988
320.2016
335.1293
348.1972
355.0703
Me
F
COOtBu
MeO
300 302 304 306 308 310 312 314 316 318 320 322 324 326 328 330 332 334 336 338 340 342 344 346 348 350 352 354 356 358 360
Counts vs. Mass-to-Charge (m/z)

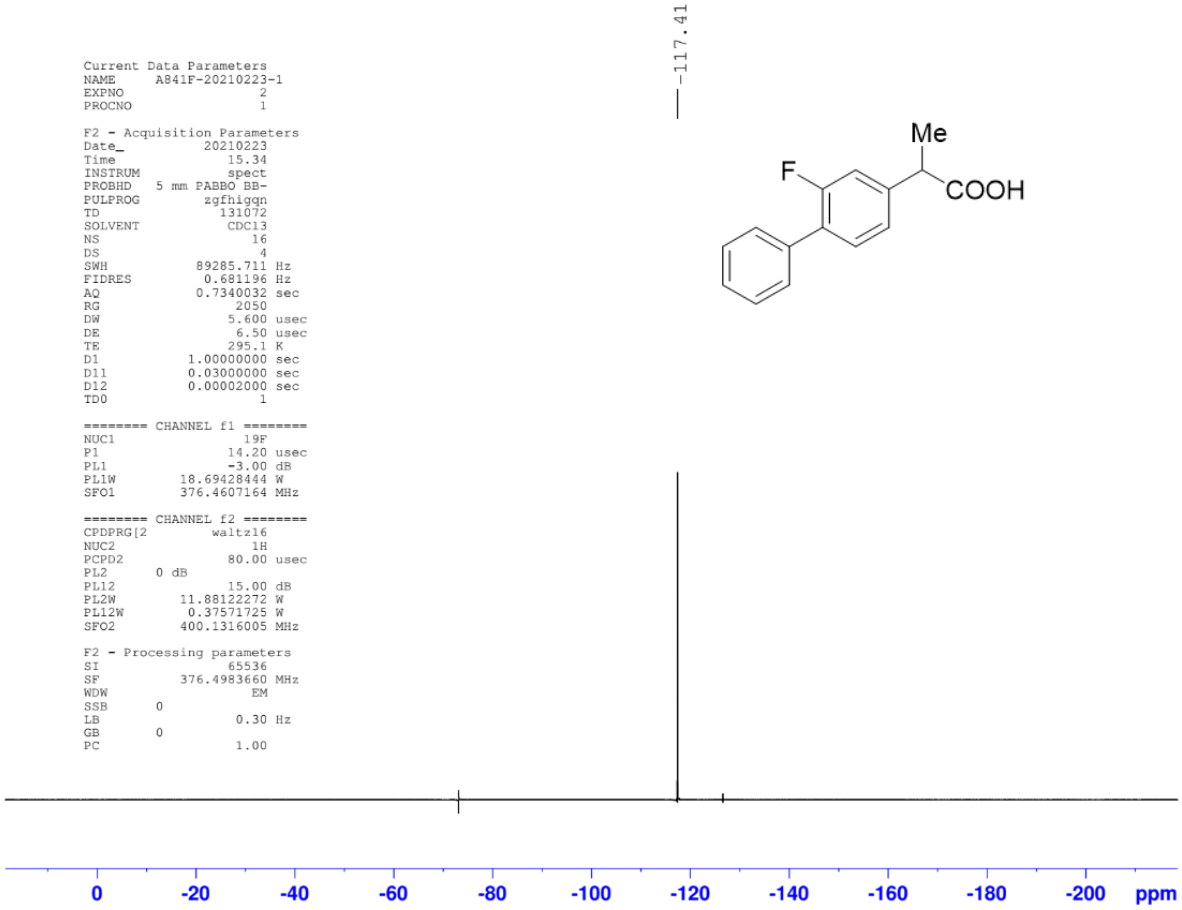

7.5321
7.5287
7.5153
7.5106
7.5074
7.4971
7.4938
7.3696
7.3485
7.3286
7.1569
7.1529
7.1447
7.1351
7.1230
7.1047
7.1014
3.6782
3.6603
3.6424
3.6246
1.4974
1.4794
1.4384
Current Data Parameters
NAME A906-E4-20220104-F
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220104
Time 14.29
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 28.5
DW 62.400 usec
DE 6.50 usec
TE 294.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.5287
7.5153
7.5106
7.5074
7.4971
7.4938
7.3696
7.3485
7.3286
7.1569
7.1529
7.1447
7.1351
7.1230
7.1047
7.5
7.4
7.3
7.2
ppm
Me
F
COOtBu
F
10
9
8
7
6
5
4
3
2
1
0
ppm
1.97
1.08
3.98
1.00
3.09
9.06

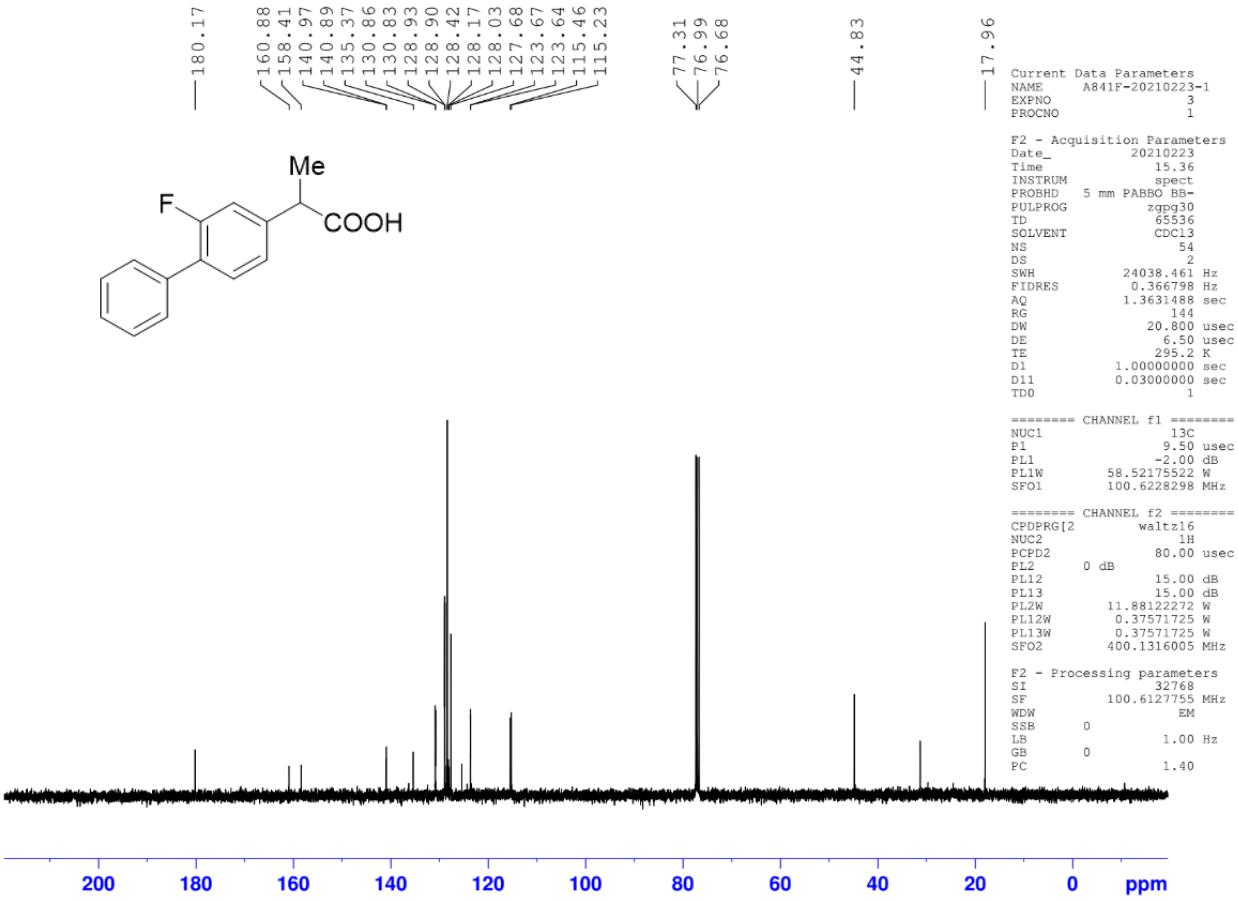

-114.69
-118.12
Current Data Parameters
NAME A906-E4-19F
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220104
Time 10.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT C6D6
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 912
DW 5.600 usec
DE 6.50 usec
TE 295.3 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
F
COOtBu
F
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

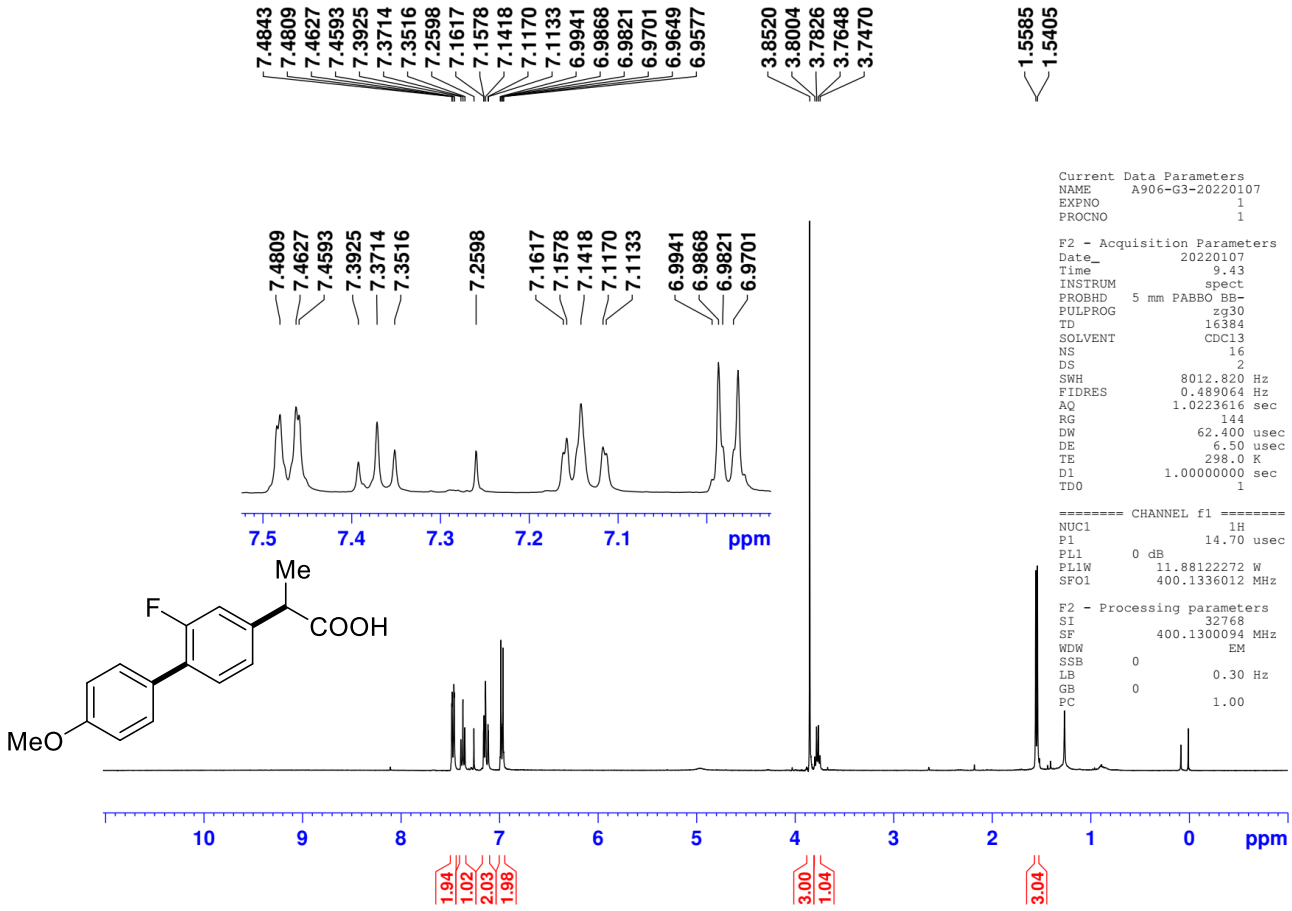

173.18
163.55
161.10
160.71
158.25
142.64
142.56
131.53
131.49
130.59
130.56
130.51
130.48
130.43
130.39
126.48
126.35
123.52
123.49
115.44
115.27
115.22
115.03
80.88
77.31
77.00
76.68
45.93
27.89
18.37
Current Data Parameters
NAME A906-E4-20220104-F
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220104
Time 14.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 61
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 294.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
F
COOtBu
F
200
180
160
140
120
100
80
60
40
20
0
ppm

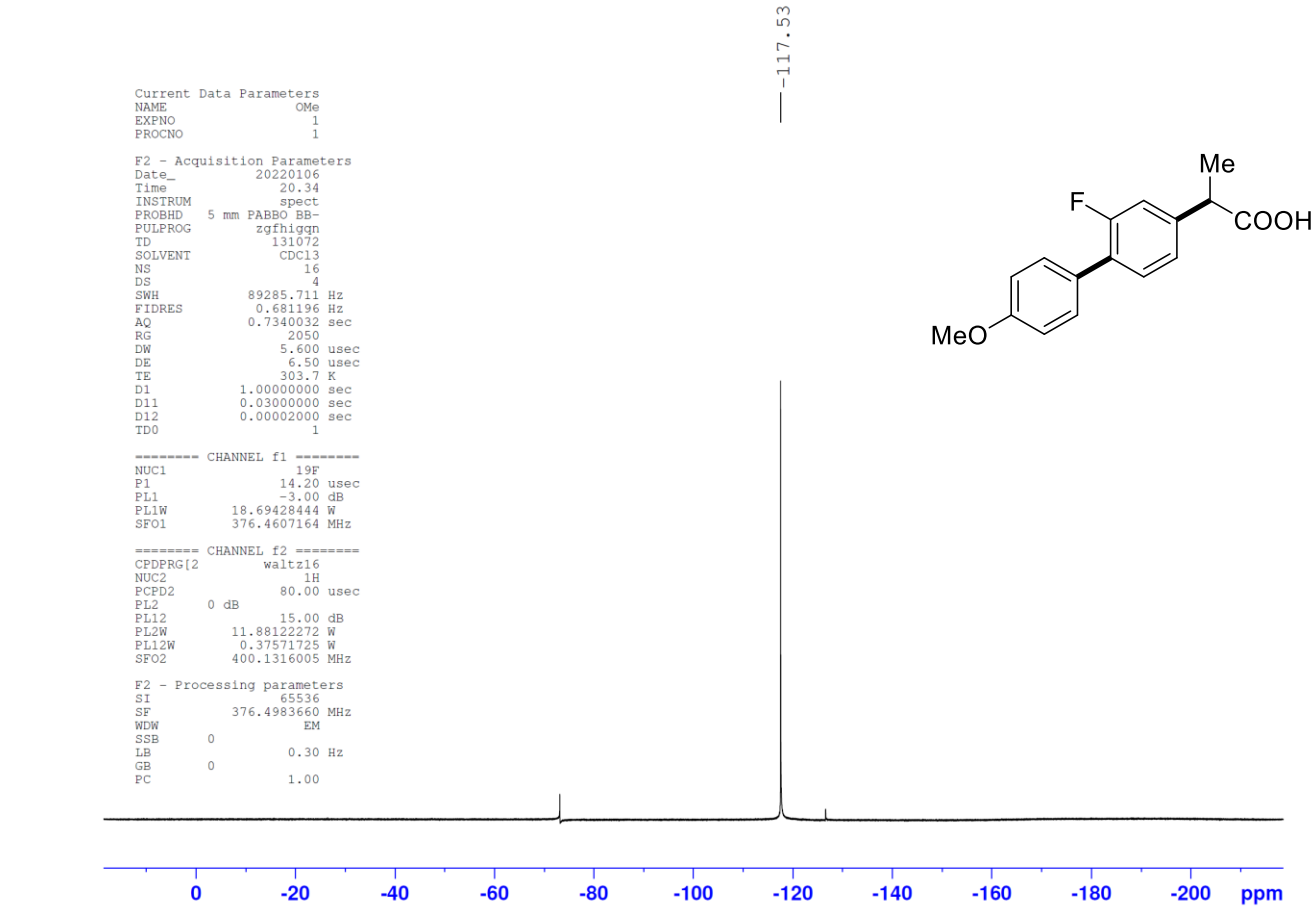

x10 4
+ Scan (rt: 0.177 min) appi-05012021 S4-3.d Subtract
318.1420
319.1463
Me
F
COOtBu
F
Counts vs. Mass-to-Charge (m/z)

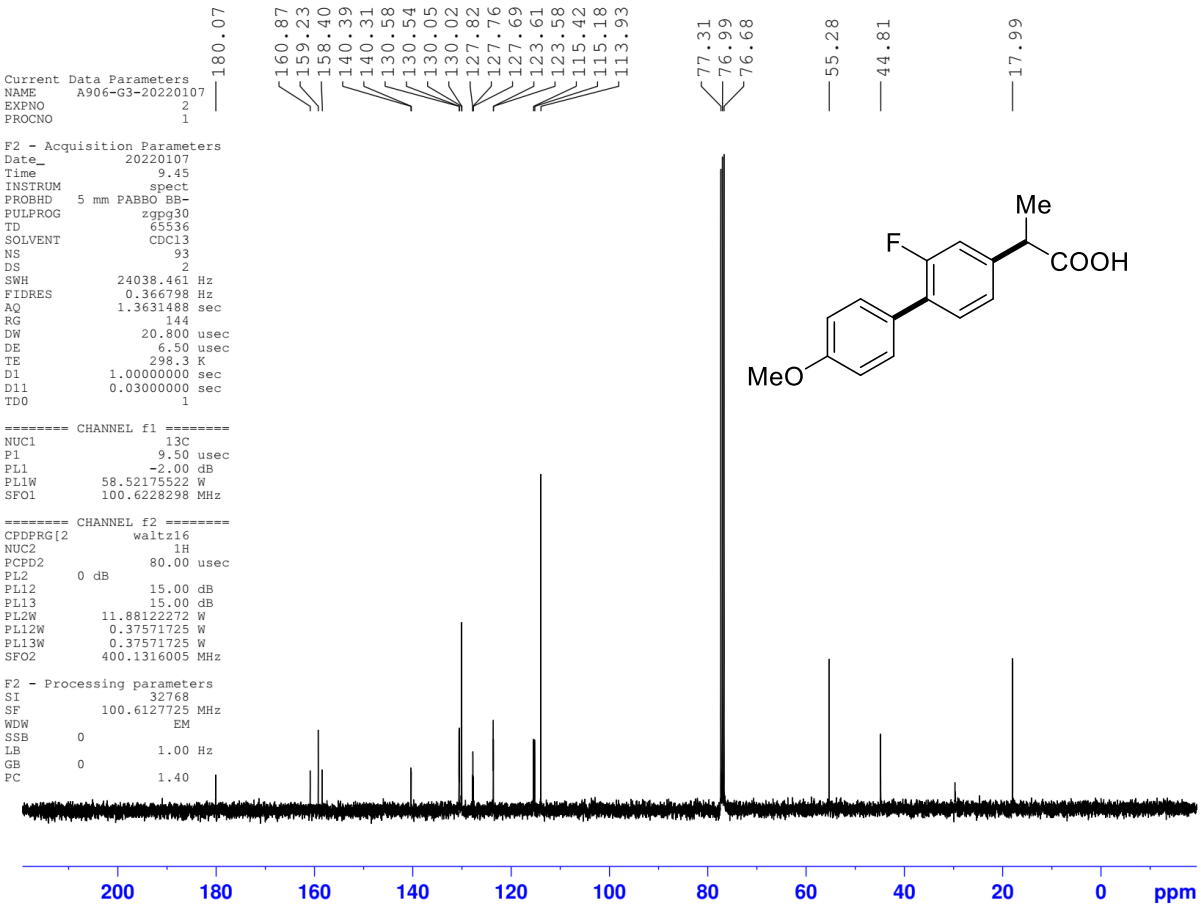

7.5575
7.5539
7.5371
7.4870
7.4710
7.4667
7.4530
7.4373
7.4337
7.4166
7.3971
7.3844
7.3790
7.3735
7.3607
7.2047
7.2006
7.1834
7.1580
7.1542
3.8275
3.8096
3.7917
3.7739
1.5817
1.5638
Me
F
COOH
Current Data Parameters
NAME A841F-20210223-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210223
Time 15.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 2.0447233 sec
RG 80.6
DW 62.400 usec
DE 6.50 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1324008 MHz
F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.72
4.09
1.94
1.00
2.93

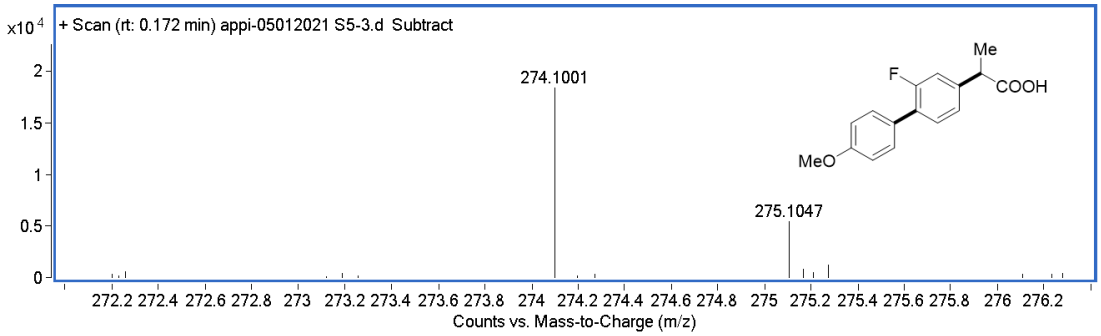

-117.41
Me
F
COOH
Current Data Parameters
NAME A841F-20210223-1
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210223
Time 15.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 2050
DW 5.600 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm

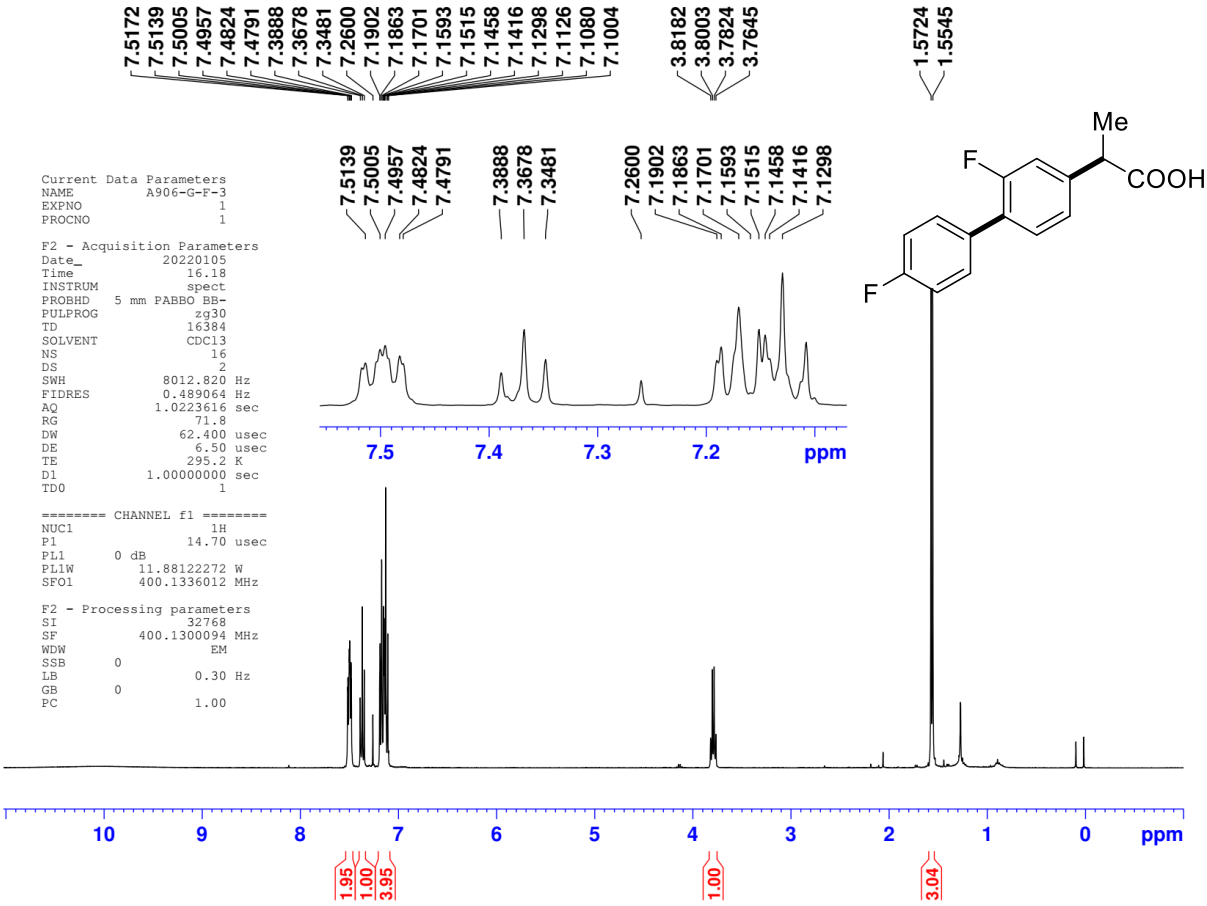

180.17
160.88
158.41
140.97
140.89
135.37
130.86
130.83
128.93
128.90
128.42
128.17
128.03
127.68
123.67
123.64
115.46
115.23
77.31
76.99
76.68
44.83
17.96
Me
F
COOH
Current Data Parameters
NAME A841F-20210223-1
EXPNO 3
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210223
Time 15.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 54
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

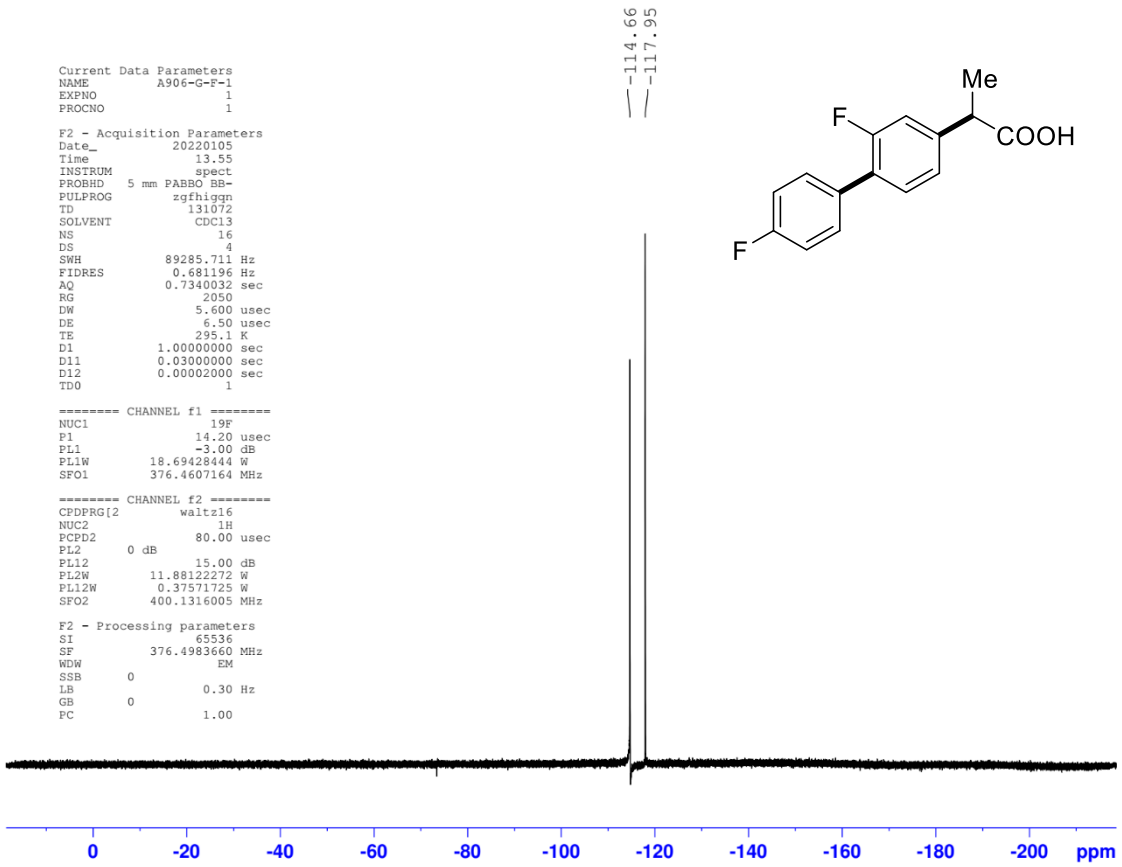

7.4843
7.4809
7.4627
7.4593
7.3925
7.3714
7.3516
7.2598
7.1617
7.1578
7.1418
7.1170
7.1133
6.9941
6.9868
6.9821
6.9701
6.9649
6.9577
3.8520
3.8004
3.7826
3.7648
3.7470
1.5585
1.5405
Current Data Parameters
NAME A906-G3-20220107
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220107
Time 9.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 144
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
F
COOH
MeO
ppm
1.94
1.02
2.03
1.98
3.00
1.04
3.04

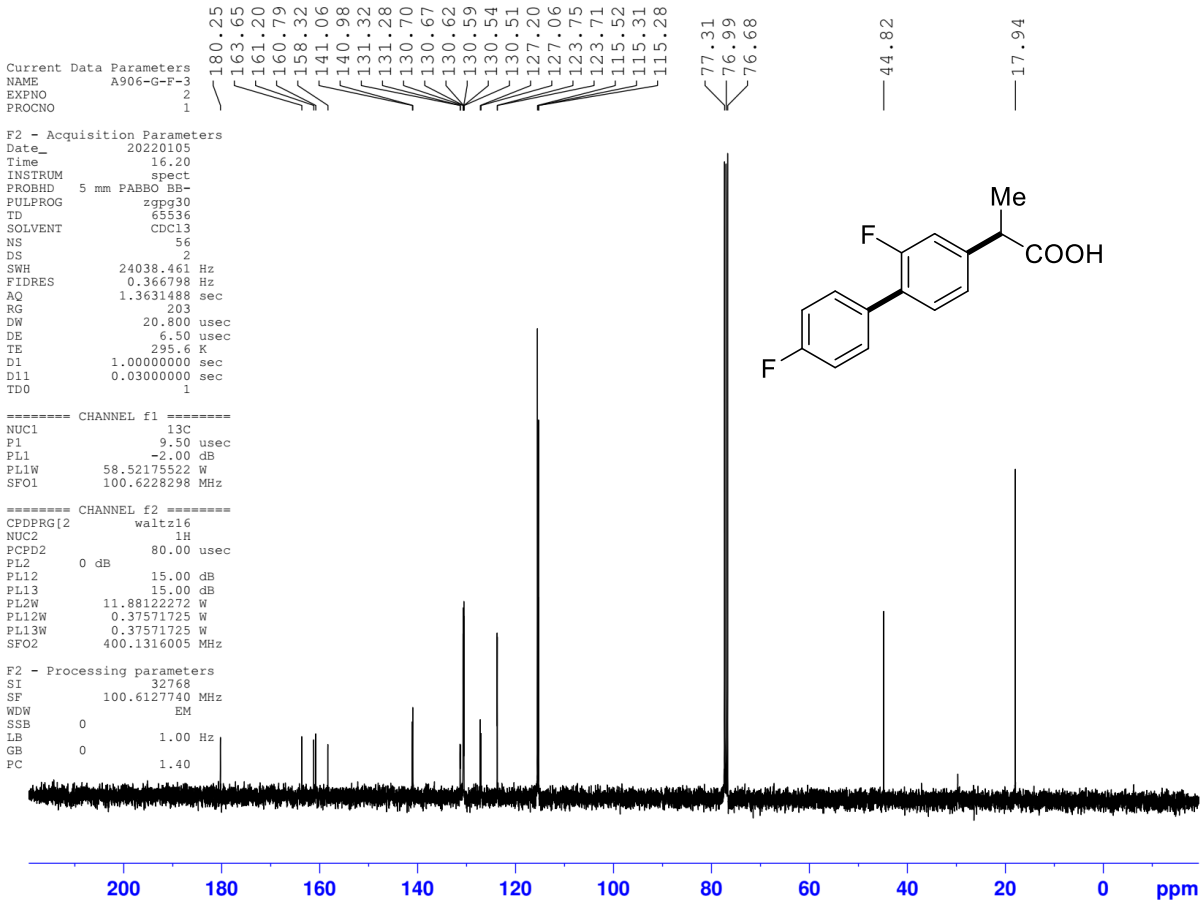

-117.53
Current Data Parameters
NAME OMe
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220106
Time 20.34
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 2050
DW 5.600 usec
DE 6.50 usec
TE 303.7 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
F
COOH
MeO
ppm

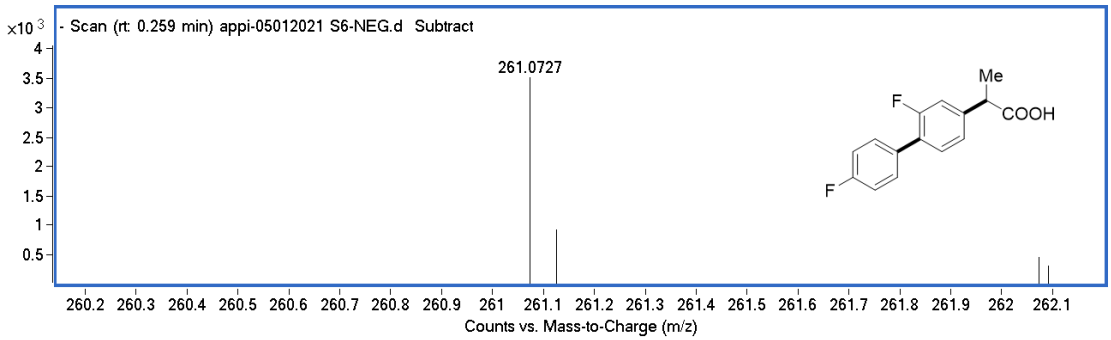

180.07
160.87
159.23
158.40
140.39
140.31
130.58
130.54
130.05
130.02
127.82
127.76
127.69
123.61
123.58
115.42
115.18
113.93
77.31
76.99
76.68
55.28
44.81
17.99
Current Data Parameters
NAME A906-G3-20220107
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220107
Time 9.45
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 93
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 144
DW 20.800 usec
DE 6.50 usec
TE 298.3 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127725 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
F
COOH
MeO
200
180
160
140
120
100
80
60
40
20
0
ppm


x10 4
+ Scan (rt: 0.172 min) appi-05012021 S5-3.d Subtract
274.1001
275.1047
Me
F
COOH
MeO
2
1.5
1
0.5
0
272.2 272.4 272.6 272.8 273 273.2 273.4 273.6 273.8 274 274.2 274.4 274.6 274.8 275 275.2 275.4 275.6 275.8 276 276.2
Counts vs. Mass-to-Charge (m/z)


7.5172
7.5139
7.5005
7.4957
7.4824
7.4791
7.3888
7.3678
7.3481
7.2600
7.1902
7.1863
7.1701
7.1593
7.1515
7.1458
7.1416
7.1298
7.1126
7.1080
7.1004
3.8182
3.8003
3.7824
3.7645
1.5724
1.5545
Current Data Parameters
NAME A906-G-F-3
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220105
Time 16.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 16384
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.489064 Hz
AQ 1.0223616 sec
RG 71.8
DW 62.400 usec
DE 6.50 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.70 usec
PL1 0 dB
PL1W 11.88122272 W
SFO1 400.1336012 MHz
F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
7.5
7.4
7.3
7.2
ppm
Me
F
COOH
F
10
9
8
7
6
5
4
3
2
1
0
ppm
1.95
1.00
3.95
1.00
3.04


-114.66
-117.95
Current Data Parameters
NAME A906-G-F-1
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220105
Time 13.55
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgfhigqn
TD 131072
SOLVENT CDCl3
NS 16
DS 4
SWH 89285.711 Hz
FIDRES 0.681196 Hz
AQ 0.7340032 sec
RG 2050
DW 5.600 usec
DE 6.50 usec
TE 295.1 K
D1 1.00000000 sec
D11 0.03000000 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 19F
P1 14.20 usec
PL1 -3.00 dB
PL1W 18.69428444 W
SFO1 376.4607164 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 65536
SF 376.4983660 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
Me
F
COOH
F
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
ppm


180.25
163.65
161.20
160.79
158.32
141.06
140.98
131.32
131.28
130.70
130.67
130.62
130.59
130.54
130.51
127.20
127.06
123.75
123.71
115.52
115.31
115.28
77.31
76.99
76.68
44.82
17.94
Current Data Parameters
NAME A906-G-F-3
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20220105
Time 16.20
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 56
DS 2
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 203
DW 20.800 usec
DE 6.50 usec
TE 295.6 K
D1 1.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.50 usec
PL1 -2.00 dB
PL1W 58.52175522 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG[2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0 dB
PL12 15.00 dB
PL13 15.00 dB
PL2W 11.88122272 W
PL12W 0.37571725 W
PL13W 0.37571725 W
SFO2 400.1316005 MHz
F2 - Processing parameters
SI 32768
SF 100.6127740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
Me
F
COOH
F
200
180
160
140
120
100
80
60
40
20
0
ppm


×10 3
- Scan (rt: 0.259 min) appi-05012021 S6-NEG.d Subtract
261.0727
Me
F
COOH
F
4
3.5
3
2.5
2
1.5
1
0.5
260.2
260.3
260.4
260.5
260.6
260.7
260.8
260.9
261
261.1
261.2
261.3
261.4
261.5
261.6
261.7
261.8
261.9
262
262.1
Counts vs. Mass-to-Charge (m/z)

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