Directed Markovnikov Hydroarylation and Hydroalkenylation of Alkenes Under Nickel Catalysis

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General Information

Unless otherwise stated, all materials were used as received from commercial sources without further purification. All glassware and magnetic stir bars were dried in an oven at 100 °C overnight unless otherwise stated. All solvents were purchased from MilliporeSigma (sure-seal) and used as received. 2-Dram (8-mL) reaction tubes were purchased from Fisher (Cat#: 1495925A). Caps with TFE septa were purchased from Chemglass (Cat#: CG-4910-15). Ambient (room) temperature refers to 21–24 °C. Elevated temperatures were maintained by an IKA heating block for 1-dram vials or a silicon oil bath for larger vessels. Thin-layer chromatography (TLC) was performed using EMD Millipore 250 mm silica gel F-254 plates (250 μm) with F-254 fluorescent indicator and visualized by UV fluorescence quenching, iodine, Seebach's stain, or potassium permanganate stain. SiliCycle SiliaFlash P60 silica gel (particle size 40–63 μm) was used for flash chromatography. Analtech thin layer chromatography products (20 cm × 20 cm, 1000 micron) were used for preparative TLC. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker DRX equipped with a 5 mm DCH cryoprobe (600 MHz and 150 MHz, respectively). ^{1}H NMR spectra were reported relative to Me_4Si (δ 0.0) unless otherwise stated. ^{13}C NMR spectra were calibrated to residual solvent signals ($CDCl_3$ at 77.16 ppm). Kinetic data were obtained using ^{1}H NMR spectra on a JEOL (400 MHz). High-resolution mass spectra (HRMS) were recorded on an Agilent LC/MSD TOF mass spectrometer by electrospray ionization time of flight experiments.

Chemical and Supplier:

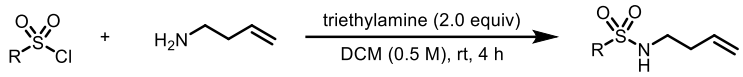
The following chemicals were purchased from the suppliers indicated:

$Ni(cod)_2$: Strem (1295-35-8)

All arylboronic acids and alkenylboronic acids were purchased from Combi-Blocks. All other commercial reagents were purchased from MilliporeSigma, Alfa Aesar, Oakwood, TCI or Strem and used as received.

Substrate Synthesis

General Procedure A for the Synthesis of Alkenyl Sulfonamides



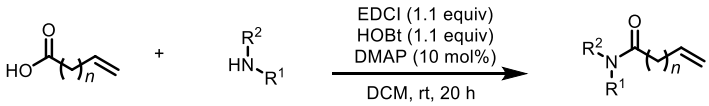
The reaction was carried out according to a literature procedure.[1] To a solution of homoallylamine (460 μL, 5.0 mmol), triethylamine (1.4 mL, 10 mmol) in DCM (10 mL) at 0 °C was added sulfonyl chloride (6.0 mmol, 1.2 equiv) in small batches. The reaction was warmed to ambient temperature and stirred for 4 h. After this time, the reaction was quenched with water. The aqueous solution was extracted with DCM (×3). The combined organic layers were washed with brine and dried over Na_2SO_4. The organic solvent was removed under reduced pressure, and the residue was subjected to flash column chromatography on silica gel with hexanes/ethyl acetate (5:1) as the eluent to afford the products. Analytical data were in agreement with literature values.

General Procedure B for the Synthesis of β,γ-Unsaturated Ketones

The reaction was carried out according to a modified literature procedure.[2] To a 100-mL Schlenk flask was added the corresponding aldehyde (10 mmol) and THF (20 mL) under an inert atmosphere. The solution was cooled to 0 °C. Allyl magnesium bromide (15 mmol, 1.7 M in THF) was added dropwise, and the solution was stirred for 3 h under ambient temperature or until the aldehyde was full consumed (as monitored by TLC). Then, the reaction was quenched with NH_4Cl (sat.). The organic layer was separated. The aqueous solution was extracted with ethyl acetate (3 × 20 mL). The combined organic layers were dried over Na_2SO_4. The organic solvent was removed under reduced pressure, and the residue was subjected to flash column chromatography on silica gel with hexanes/ethyl acetate as the eluent to afford the corresponding alcohol.

To the solution of the alcohol in DCM (20 mL) was added Dess–Martin periodinane (12 mmol, 1.2 equiv). The solution was stirred at room temperature for 2 h or until the aldehyde was fully consumed (as monitored by TLC). Then, the reaction was quenched with water. The organic layer was separated. The aqueous solution was extracted with DCM (3 × 20 mL). The combined organic layers were dried over Na_2SO_4. The organic solvent was removed under reduced pressure, and the residue was subjected to flash column chromatography on silica gel with hexanes/ethyl acetate as the eluent to afford the corresponding β,γ-unsaturated ketone.

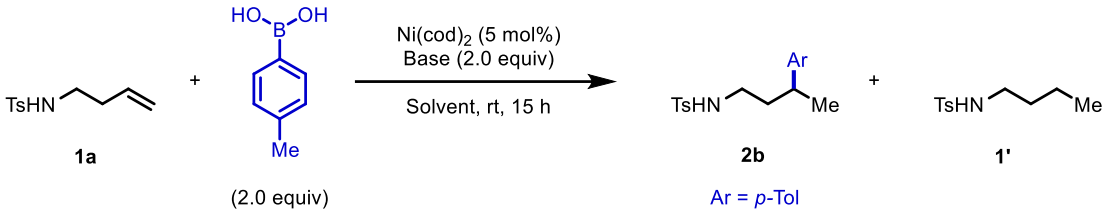
General Procedure C for the Synthesis of Alkenyl Amides



The reaction was carried out according to a modified literature procedure.[3] To a solution of EDCI (1.1 equiv), HOBt (1.1 equiv) and DMAP (10 mol%) in DCM (0.5 M) were added the corresponding alkenyl acid (1.0 equiv) and amine (0.9 equiv) successively. The solution was stirred under ambient temperature for 20 h. Then, the reaction was quenched with water. The organic layer was separated. The aqueous solution was extracted with DCM (3 × 20 mL). The combined organic layers were dried over Na_2SO_4. The organic solvent was removed under reduced pressure, and the residue was subjected to flash column chromatography on silica gel with hexanes/acetone as the eluent to afford the corresponding alkenyl amides.

Optimization of Reaction Conditions

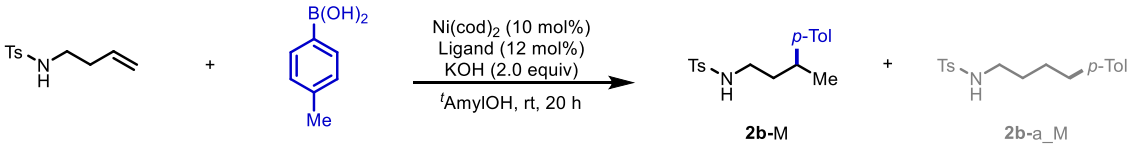
Table S1: Optimization of Reaction Conditions for Alkenyl Sulfonamides[a]



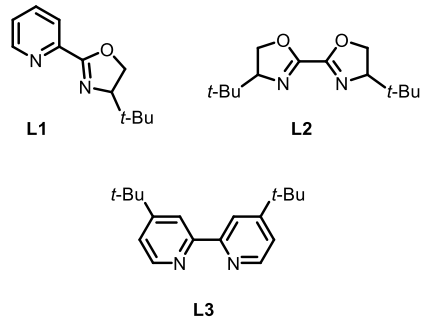
Entry	Base	Solvent	Yield (%)[b] **2b**/**1'**
1	KO*t*-Bu	*s*-BuOH	60/17
2	NaO*t*-Bu	*s*-BuOH	12/41
3	LiO*t*-Bu	*s*-BuOH	trace/31
4	NaOMe	*s*-BuOH	25/41
5	NaOEt	*s*-BuOH	29/30
6	KOH	*s*-BuOH	80/5
7	K_3PO_4	*s*-BuOH	49/4
8	Cs_2CO_3	*s*-BuOH	28/11
9	KOH	MeOH	trace/trace
10	KOH	EtOH	11/6
11	KOH	*n*-PrOH	30/7
12	KOH	*n*-BuOH	46/6
13	KOH	*i*-PrOH	64/4
14	KOH	*i*-BuOH	60/7
15	KOH	*t*-AmylOH	96/trace
16[c]	KOH	*t*-AmylOH	71/16

[a] The reactions were performed on 0.1 mmol scale. [b]Yields were determined by ^{1}H NMR analysis of the crude reaction mixture with CH_2Br_2 as internal standard. [c]40 °C instead of rt.

Table S2: Ligand Screening for Alkenyl Sulfonamides[a]

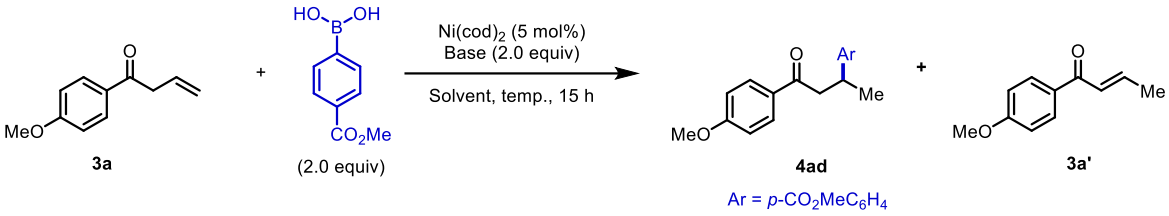


Entry	Ligand	Yield (%)[b] **2b**-M/**2b**-a_M
1	No Ligand	90/trace
2	PPh_3	18/trace
3	PCy_3	26/trace
4	dppe	64/trace
5	dppb	trace/trace
6	**L1**	21/trace
7	**L2**	94/trace
8	**L3**	trace/trace



[a] The reactions were performed on 0.1 mmol scale. [b]Yields were determined by ^{1}H NMR analysis of the crude reaction mixture with CH_2Br_2 as internal standard.

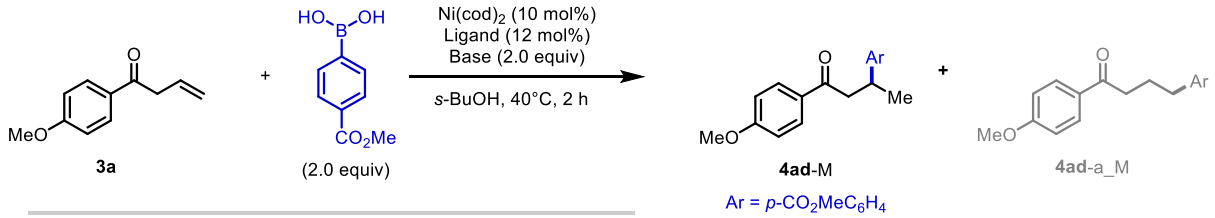
Table S3: Optimization of Reaction Conditions for Alkenyl Ketone[a]



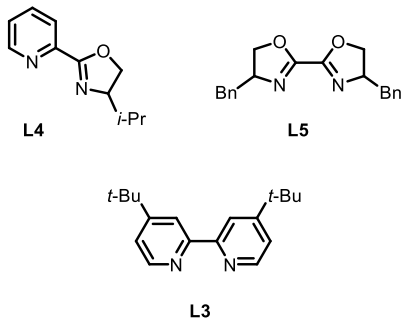
Entry	Base	Solvent	Temp. (°C)	**3a**/**3a'**[b]	Yield (%)[b] **4ad**
1	KO*t*-Bu (20 mol%)	*i*-PrOH	60	24/38	10
2	KO*t*-Bu	*i*-PrOH	60	trace/trace	22
3	NaO*t*-Bu	*i*-PrOH	60	trace/trace	16
4	LiO*t*-Bu	*i*-PrOH	60	trace/trace	27
5	K_2CO_3	*i*-PrOH	60	trace/63	7
6	Cs_2CO_3	*i*-PrOH	60	trace/trace	83
7	K_3PO_4	*i*-PrOH	60	trace/trace	82
8	NaOMe	*i*-PrOH	60	trace/trace	20
9	Cs_2CO_3	EtOH	60	trace/7	40
10	Cs_2CO_3	*n*-PrOH	60	trace/7	43
11	Cs_2CO_3	*s*-BuOH	60	-/-	99
12	Cs_2CO_3	*t*-AmylOH	60	trace/7	38
13	Cs_2CO_3	*s*-BuOH	40	-/-	99
14	Cs_2CO_3	*s*-BuOH	40 (2 h)	-/-	99

[a]The reactions were performeed on 0.1 mmol scale. [b]Yields were determined by ^{1}H NMR analysis of the crude reaction mixture with CH_2Br_2 as internal standard.

Table S4: Ligand Screening for Alkenyl Sulfonamides[a]



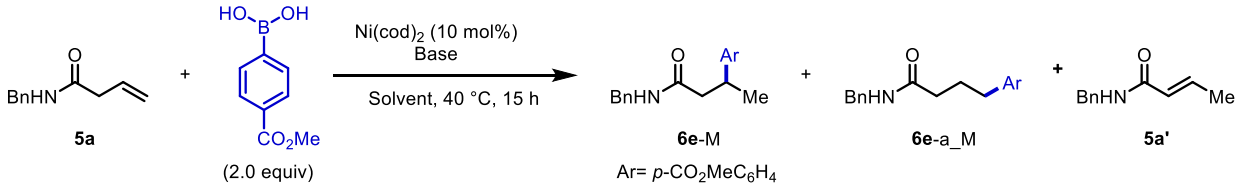
Entry	Ligand	Yield (%)[b] **4ad**-M/**4ad**-a_M
1	No Ligand	99/trace
2	PPh_3	36/trace
3	PCy_3	trace/trace
4	dppe	30/trace
5	dppb	10/trace
6	**L4**	trace/trace
7	**L5**	32/trace
8	**L3**	trace/trace



L4 **L5** **L3**

[a] The reactions were performed on 0.1 mmol scale. [b]Yields were determined by ^{1}H NMR analysis of the crude reaction mixture with CH_2Br_2 as internal standard.

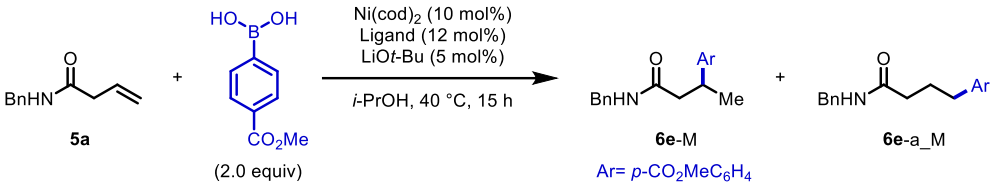
Table S5: Optimization of Reaction Conditions for Alkenyl Amide[a]



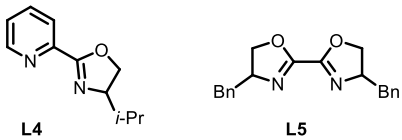
Entry	Base	Solvent	**5a**/ **5a'**[b]	Yield (%)[b] **6e**-M/**6e**-a_M
1	LiO*t*-Bu (5 mol%)	*i*-PrOH	trace/4	86/12
2	LiO*t*-Bu (5 mol%)	*i*-PrOH	trace/trace	82/11
3	LiO*t*-Bu (5 mol%)	*i*-PrOH	50/43	7/trace
4	LiO*t*-Bu (5 mol%)	*i*-PrOH	0/3	80/12
5	NaOMe (5 mol%)	*i*-PrOH	0/68	32/trace
6	Cs_2CO_3 (2.0 equiv)	*i*-PrOH	28/62	9/trace
7	K_3PO_4 (2.0 equiv)	*i*-PrOH	80/4	11/2
8	LiO*t*-Bu (5 mol%)	*t*-AmylOH	trace/2	82/15
9	LiO*t*-Bu (5 mol%)	*s*-BuOH	trace/2	86/12
10	LiO*t*-Bu (5 mol%)	*n*-PrOH	trace/6	76/11

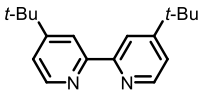
[a]The reactions were performeed on 0.1 mmol scale. [b]Yields were determined by ^{1}H NMR analysis of the crude reaction mixture with CH_2Br_2 as internal standard.

Table S6: Ligand Screening for Alkenyl Sulfonamides[a]



Entry	Ligand	Yield (%)[b] **6e**-M/**6e**-a_M
1	No Ligand	86/12
2	PPh_3	trace/trace
3	PCy_3	trace/trace
4	dppe	11/6
5	dppb	trace/trace
6	**L4**	trace/trace
7	**L5**	trace/trace
8	**L3**	trace/trace

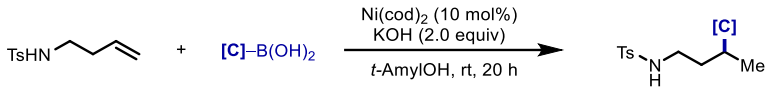




[a] The reactions were performed on 0.1 mmol scale. [b]Yields were determined by ^{1}H NMR analysis of the crude reaction mixture with CH_2Br_2 as internal standard.

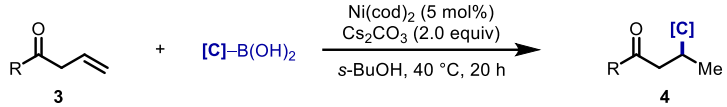
General Procedures for Markovnikov-Selective Hydroarylation/Hydroalkenylation

General Procedure D (Alkenyl Sulfonamides)



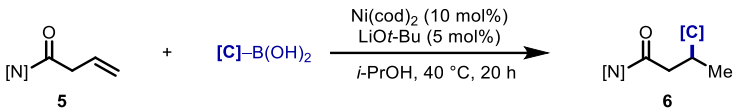
To an oven-dried 2-dram (8-mL) reaction tube equipped with a magnetic stir bar were added the appropriate alkenyl sulfonamide (0.1 mmol) and aryl- or alkenylboronic acid (0.2 mmol) outside of the glovebox. The vial was then introduced into an argon-filled glovebox antechamber. Once transferred inside the glovebox, $Ni(cod)_2$ (2.8 mg, 10 mol%) and KOH (11.2 mg, 0.2 mmol) were added to the vial, followed by *t*-AmylOH (0.5 mL). The vial was sealed with a screw-top septum cap, removed from the glovebox, and left to stir at rt for 20 h. After this time, the reaction was quenched with 2 M HCl (1 mL) and then diluted with brine (10 mL). The aqueous solution was then extracted with ethyl acetate (3 × 2 mL). The combined organic layers were dried by passage through a pad of silica gel with ethyl acetate as eluent. The filtrate was concentrated and purified by preparative thin-layer chromatography (PTLC) to furnish the desired product.

General Procedure E (Alkenyl Ketones)



To an oven-dried 2-dram (8-mL) reaction tube equipped with a magnetic stir bar were added the appropriate alkenyl ketone (0.1 mmol), aryl- or alkenylboronic acid (0.2 mmol) outside of the glovebox. The vial was then introduced into an argon-filled glovebox antechamber. Once transferred inside the glovebox, $Ni(cod)_2$ (1.4 mg, 5 mol%) and Cs_2CO_3 (65 mg, 0.2 mmol) were added to the vial, followed by *s*-BuOH (0.5 mL). The vial was sealed with a screw-top septum cap, removed from the glovebox, and left to stir at 40 °C for 20 h. After this time, the reaction was quenched with 2 M HCl (1 mL) and then diluted with brine (10 mL). The aqueous solution was then extracted with ethyl acetate (3 × 2 mL). The combined organic layers were dried by passage through a pad of silica gel with ethyl acetate as eluent. The filtrate was concentrated and purified by preparative thin-layer chromatography (PTLC) to furnish the desired product.

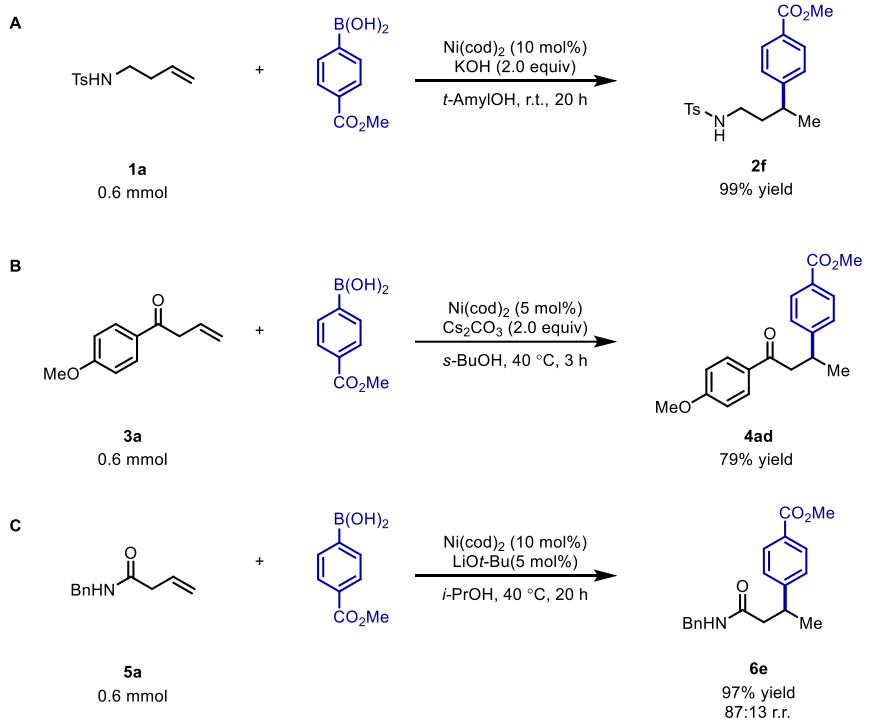
General Procedure F (Alkenyl Amides)



To an oven-dried 2-dram (8-mL) reaction tube equipped with a magnetic stir bar were added the appropriate alkenyl amide (0.1 mmol), aryl- or alkenylboronic acid (0.2 mmol) outside of the glovebox. The vial was then introduced into an argon-filled glovebox antechamber. Once transferred inside the glovebox, $Ni(cod)_2$ (2.8 mg, 10 mol%) and LiO*t*-Bu (0.4 mg, 0.005 mmol) were added to the vial, followed by *i*-PrOH (0.5 mL). The vial was sealed with a screw-top septum cap, removed from the glovebox, and left to stir at 40 °C for 20 h. After this time, the reaction was quenched with 2 M HCl (1 mL) and then diluted with brine (10 mL). The aqueous solution was then extracted with ethyl acetate (3 × 2 mL). The combined organic layers were dried by passage through a pad of silica gel with ethyl acetate as eluent. The filtrate was concentrated and purified by preparative thin-layer chromatography (PTLC) to furnish the desired product.

Large-Scale Experiments

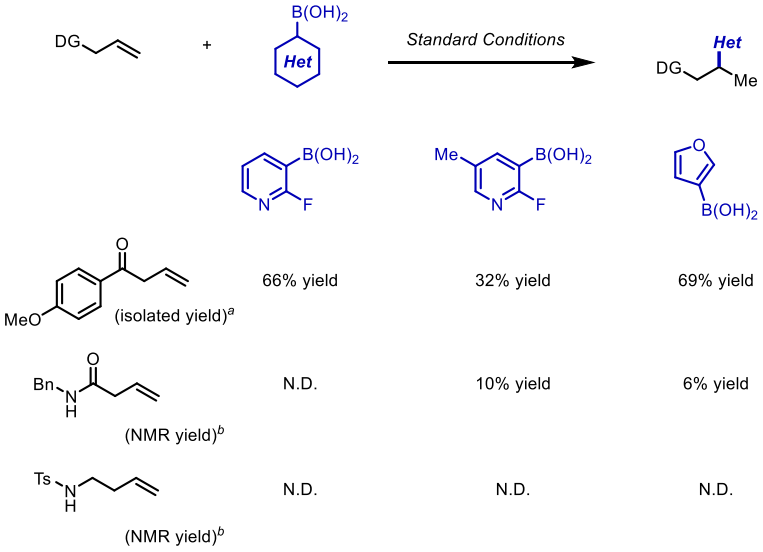
The experiments were performed on 0.6 mmol scale following General Procedure D, E, and F with purification being performed via silica gel column chromatography rather than PTLC. Percentages represent isolated yields.



Scheme S1. Large-Scale Experiments.

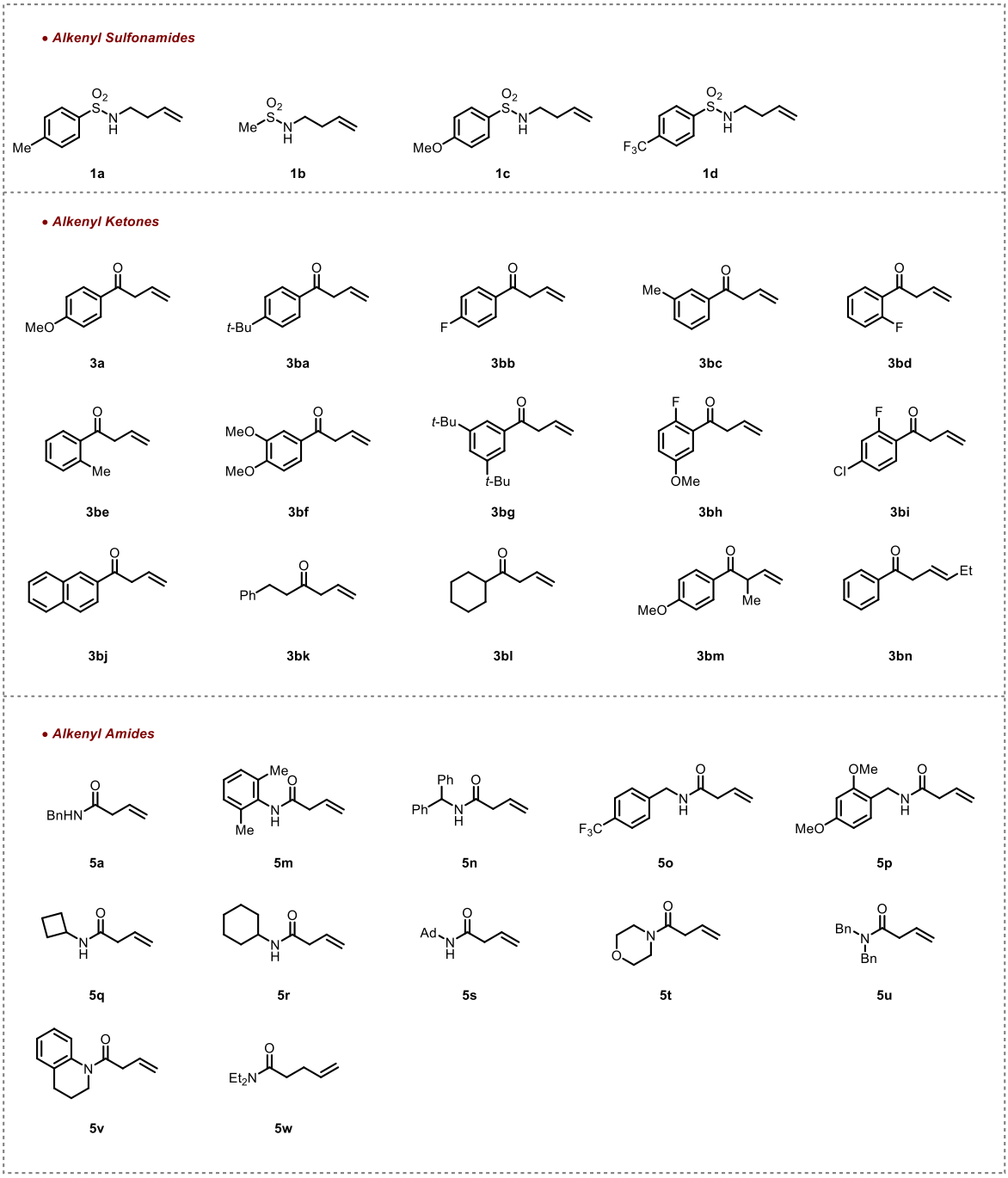
Reactions with Heteroaryl Boronic Acids

The experiments were performed on 0.1 mmol scale following General Procedure D, E, and F.



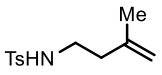
Scheme S2. Reactions with Heteroaryl Boronic Acids. [a]3.0 equivalent of heteroaryl boronic acids were used. [b]Yields were determined by ^{1}H NMR analysis of the crude reaction mixture with CH_2Br_2 as internal standard.

Table of Substrates



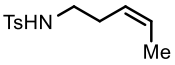
Scheme S3. List of alkenyl sulfonamides[1], ketones[2] and amides[3] used in this study.

Limitations



N.R.

N.R.



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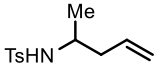

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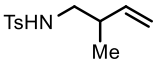

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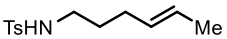

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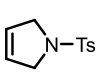

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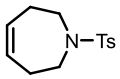

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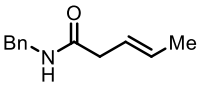

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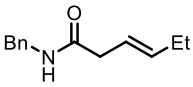

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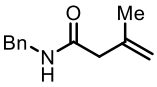

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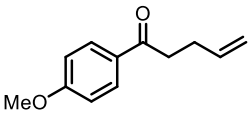
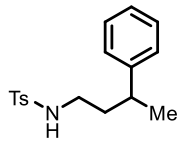
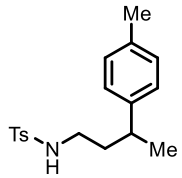


N.R.

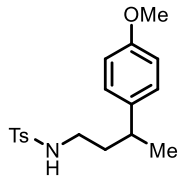
Representative Procedures and Analytical Data



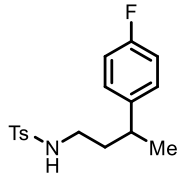
4-methyl-*N*-(3-phenylbutyl)benzenesulfonamide (2a): The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), phenylboronic acid (24.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 28.7 mg (95%) of **2a** as a colorless oil. Analytical data were in agreement with literature values.[4] **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.29–7.23 (m, 4H), 7.19–7.14 (m, 1H), 7.07 (m, 2H), 4.49 (t, *J* = 6.2 Hz, 1H), 2.83 (q, *J* = 6.8 Hz, 2H), 2.71 (dp, *J* = 8.7, 6.8 Hz, 1H), 2.42 (s, 3H), 1.81–1.67 (m, 2H), 1.19 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 145.98, 143.44, 136.99, 129.78, 128.70, 127.21, 126.96, 126.45, 41.69, 37.96, 37.35, 22.32, 21.63. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{22}NO_2S^+$ [M+H] 304.1371, found 304.1371.



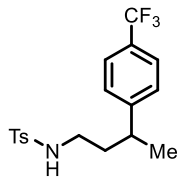
4-methyl-*N*-(3-(p-tolyl)butyl)benzenesulfonamide (2b): The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), *p*-tolylboronic acid (27.2 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 28.5 mg (90%) of **2b** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.2 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.06 (d, *J* = 7.9 Hz, 2H), 6.96 (d, *J* = 8.0 Hz, 2H), 4.42 (t, *J* = 6.2 Hz, 1H), 2.90–2.78 (m, 2H), 2.67 (dp, *J* = 9.0, 6.8 Hz, 1H), 2.42 (s, 3H), 2.30 (s, 3H), 1.81–1.64 (m, 2H), 1.17 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 143.41, 142.91, 137.03, 135.94, 129.76, 129.38, 127.22, 126.83, 41.74, 37.99, 36.96, 22.44, 21.64, 21.11. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{24}NO_2S^+$ [M+H] 318.1528, found 318.1531.



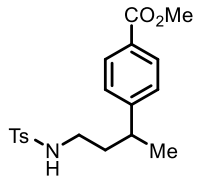
***N*-(3-(4-methoxyphenyl)butyl)-4-methylbenzenesulfonamide (2c):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (4-methoxyphenyl)boronic acid (30.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 18.6 mg (56%) of **2c** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 8.1 Hz, 2H), 6.99 (d, *J* = 8.7 Hz, 2H), 6.79 (d, *J* = 8.6 Hz, 2H), 4.43 (t, *J* = 6.2 Hz, 1H), 3.78 (s, 3H), 2.89–2.79 (m, 2H), 2.67 (dp, *J* = 9.2, 6.9 Hz, 1H), 2.42 (s, 3H), 1.85–1.63 (m, 2H), 1.16 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 158.15, 143.43, 138.00, 137.01, 129.78, 127.84, 127.21, 114.07, 55.37, 41.72, 38.12, 36.52, 22.55, 21.64. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{24}NO_3S^+$ [M+H] 334.1477, found 334.1472.



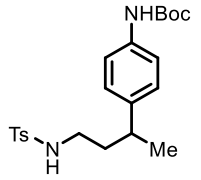
***N*-(3-(4-fluorophenyl)butyl)-4-methylbenzenesulfonamide (2d):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (4-fluorophenyl)boronic acid (28.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 29.8 mg (93%) of **2d** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.06–7.01 (m, 2H), 6.95–6.90 (m, 2H), 4.59 (t, *J* = 6.1 Hz, 1H), 2.88–2.76 (m, 2H), 2.72 (dq, *J* = 9.1, 6.7 Hz, 1H), 2.42 (s, 3H), 1.83–1.64 (m, 2H), 1.17 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.47 (d, J_{C-F} = 243.8 Hz), 143.54, 141.61 (d, J_{C-F} = 3.2 Hz), 136.90, 129.80, 128.32 (d, J_{C-F} = 7.8 Hz), 127.20, 115.39 (d, J_{C-F} = 21.0 Hz), 41.52, 38.06, 36.50, 22.43, 21.63. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –119.62. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{21}FNO_2S^+$ [M+H] 322.1277, found 322.1285.



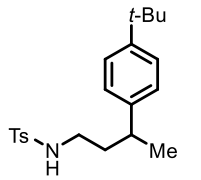
4-methyl-*N*-(3-(4-(trifluoromethyl)phenyl)butyl)benzenesulfonamide (2e): The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (4-(trifluoromethyl)phenyl)boronic acid (38.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 34.8 mg (94%) of **2e** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.49 (d, *J* = 8.1 Hz, 2H), 7.27 (d, *J* = 10.6 Hz, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 4.67 (t, *J* = 6.1 Hz, 1H), 2.88–2.73 (m, 3H), 2.42 (s, 3H), 1.91–1.70 (m, 2H), 1.21 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 150.15, 143.65, 136.80, 129.83, 128.74 (q, $J_{C–F}$ = 32.3 Hz), 127.37, 127.21, 125.61 (q, $J_{C–F}$ = 3.8 Hz), 124.35 (d, $J_{C–F}$ = 271.8 Hz), 41.38, 37.74, 37.01, 22.04, 21.60. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –65.01. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{21}F_3NO_2S^+$ [M+H] 372.1245, found 372.1240.



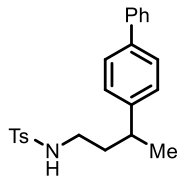
methyl 4-(4-((4-methylphenyl)sulfonamido)butan-2-yl)benzoate (2f): The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 29.6 mg (82%) of **2f** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.3 Hz, 2H), 7.68 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 7.9 Hz, 2H), 7.14 (d, *J* = 8.3 Hz, 2H), 4.72 (t, *J* = 6.2 Hz, 1H), 3.90 (s, 3H), 2.86–2.74 (m, 3H), 2.42 (s, 3H), 1.83–1.71 (m, 2H), 1.20 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 167.12, 151.51, 143.55, 136.86, 130.03, 129.81, 128.38, 127.18, 127.04, 52.15, 41.43, 37.69, 37.21, 21.98, 21.61. **HRMS** (ESI-TOF) Calcd for $C_{19}H_{24}NO_4S^+$ [M+H] 362.1426, found 362.1428.



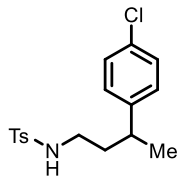
***tert*-butyl (4-(4-((4-methylphenyl)sulfonamido)butan-2-yl)phenyl)carbamate (2g):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (4-((*tert*-butoxycarbonyl)amino)phenyl)boronic acid (47.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 33.8 mg (81%) of **2g** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.67 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 9.1 Hz, 1H), 7.23 (d, *J* = 8.1 Hz, 2H), 6.98 (d, *J* = 8.5 Hz, 2H), 4.57 (t, *J* = 6.1 Hz, 1H), 2.81 (qd, *J* = 6.8, 1.6 Hz, 2H), 2.66 (dp, *J* = 9.2, 6.8 Hz, 1H), 2.41 (s, 3H), 1.79–1.63 (m, 2H), 1.51 (s, 9H), 1.15 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 153.02, 143.43, 140.64, 136.96, 136.64, 129.78, 127.41, 127.18, 119.01, 41.63, 37.96, 36.67, 28.46, 22.40, 21.61. **HRMS** (ESI-TOF) Calcd for $C_{22}H_{30}N_2O_4SNa^+$ [M+Na] 441.1824, found 441.1819.



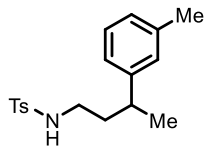
***N*-(3-(4-(*tert*-butyl)phenyl)butyl)-4-methylbenzenesulfonamide (2h):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (4-(*tert*-butyl)phenyl)boronic acid (35.6 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 31.6 mg (88%) of **2h** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.27 (dd, *J* = 8.4, 6.6 Hz, 4H), 7.00 (d, *J* = 8.3 Hz, 2H), 4.49 (t, *J* = 6.2 Hz, 1H), 2.84 (q, *J* = 7.0 Hz, 2H), 2.74–2.62 (m, 1H), 2.42 (s, 3H), 1.77–1.66 (m, 2H), 1.30 (s, 9H), 1.17 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 149.19, 143.39, 142.83, 137.02, 129.75, 127.23, 126.56, 125.51, 41.75, 37.99, 36.79, 34.47, 31.50, 22.23, 21.64. **HRMS** (ESI-TOF) Calcd for $C_{21}H_{30}NO_2S^+$ [M+H] 360.1997, found 360.1994.



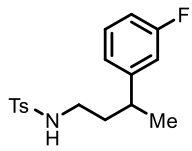
***N*-(3-([1,1'-biphenyl]-4-yl)butyl)-4-methylbenzenesulfonamide (2i):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), [1,1'-biphenyl]-4-ylboronic acid (39.6 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 31.1 mg (82%) of **2i** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.56 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.47 (d, *J* = 8.3 Hz, 2H), 7.45–7.39 (m, 2H), 7.36–7.30 (m, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.2 Hz, 2H), 4.57 (t, *J* = 6.2 Hz, 1H), 2.92–2.81 (m, 2H), 2.81–2.72 (m, 1H), 2.38 (s, 3H), 1.83–1.70 (m, 2H), 1.22 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 145.07, 143.46, 141.00, 139.35, 136.96, 129.78, 128.86, 127.40, 127.38, 127.24, 127.22, 127.08, 41.66, 37.94, 36.92, 22.31, 21.61. **HRMS** (ESI-TOF) Calcd for $C_{23}H_{26}NO_2S^+$ [M+H] 380.1684, found 380.1684.



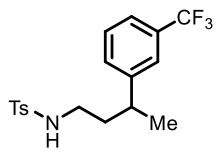
***N*-(3-(4-chlorophenyl)butyl)-4-methylbenzenesulfonamide (2j):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (4-chlorophenyl)boronic acid (31.2 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 30.3 mg (90%) of **2j** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.1 Hz, 2H), 7.20 (d, *J* = 8.5 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 2H), 4.65 (t, *J* = 6.2 Hz, 1H), 2.85–2.75 (m, 2H), 2.75–2.66 (m, 1H), 2.42 (s, 3H), 1.78–1.64 (m, 2H), 1.16 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 144.45, 143.56, 136.85, 131.98, 129.81, 128.75, 128.35, 127.19, 41.45, 37.85, 36.60, 22.24, 21.64. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{21}ClNO_2S^+$ [M+H] 338.0982, found 338.0981.



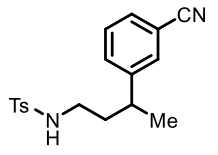
4-methyl-*N*-(3-(m-tolyl)butyl)benzenesulfonamide (2k): The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), *m*-tolylboronic acid (27.2 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 28.5 mg (90%) of **2k** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.32–7.25 (m, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 7.01–6.97 (m, 1H), 6.92–6.84 (m, 2H), 4.48 (t, *J* = 6.2 Hz, 1H), 2.84 (q, *J* = 6.8 Hz, 2H), 2.67 (dp, *J* = 8.6, 6.8 Hz, 1H), 2.42 (s, 3H), 2.30 (s, 3H), 1.79–1.65 (m, 2H), 1.17 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 145.95, 143.41, 138.23, 137.04, 129.76, 128.59, 127.74, 127.22, 127.20, 123.95, 41.75, 37.93, 37.32, 22.34, 21.63, 21.58. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{24}NO_2S^+$ [M+H] 318.1528, found 318.1540.



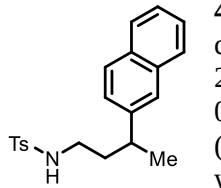
***N*-(3-(3-fluorophenyl)butyl)-4-methylbenzenesulfonamide (2l):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (3-fluorophenyl)boronic acid (28.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 28.5 mg (89%) of **2l** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.20 (td, *J* = 7.9, 6.0 Hz, 1H), 6.88–6.84 (m, 2H), 6.75 (dt, *J* = 10.1, 2.1 Hz, 1H), 4.63 (t, *J* = 6.2 Hz, 1H), 2.89–2.78 (m, 2H), 2.77–2.69 (m, 1H), 2.42 (s, 3H), 1.83–1.66 (m, 2H), 1.18 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 163.11 (d, $J_{C–F}$ = 245.7 Hz), 148.74 (d, $J_{C–F}$ = 6.7 Hz), 143.58, 136.89, 130.11 (d, $J_{C–F}$ = 8.3 Hz), 129.83, 127.20, 122.74 (d, $J_{C–F}$ = 2.7 Hz), 113.71 (d, $J_{C–F}$ = 21.0 Hz), 113.28 (d, $J_{C–F}$ = 21.0 Hz), 41.49, 37.80, 37.05, 22.12, 21.62. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –115.74. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{21}FNO_2S^+$ [M+H] 322.1277, found 322.1281.



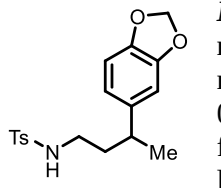
4-methyl-*N*-(3-(3-(trifluoromethyl)phenyl)butyl)benzenesulfonamide (2m): The reaction was carried out according to General Procedure D using **2a** (22.5 mg, 0.1 mmol), (3-(trifluoromethyl)phenyl)boronic acid (38.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 36.7 mg (99%) of **2m** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 7.7 Hz, 1H), 7.37 (t, *J* = 7.7 Hz, 1H), 7.33 (s, 1H), 7.31–7.26 (m, 3H), 4.79 (t, *J* = 6.2 Hz, 1H), 2.93–2.73 (m, 3H), 2.41 (s, 3H), 1.82–1.70 (m, 2H), 1.21 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 147.10, 143.63, 136.85, 130.91 (m), 130.60–130.55 (m), 129.84, 129.13, 127.17, 125.20, 123.59 (q, $J_{C–F}$ = 3.7 Hz), 123.33 (q, $J_{C–F}$ = 3.9 Hz), 41.42, 37.80, 37.01, 21.99, 21.59. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –65.14. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{21}F_3NO_2S^+$ [M+H] 372.1245, found 372.1247.



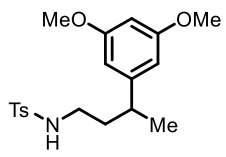
***N*-(3-(3-cyanophenyl)butyl)-4-methylbenzenesulfonamide (2n):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (3-cyanophenyl)boronic acid (29.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 14.1 mg (43%) of **2n** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.3 Hz, 2H), 7.50–7.47 (m, 1H), 7.39–7.34 (m, 3H), 7.30 (d, *J* = 8.1 Hz, 2H), 4.63 (t, *J* = 6.2 Hz, 1H), 2.90–2.76 (m, 3H), 2.43 (s, 3H), 1.82–1.68 (m, 2H), 1.21 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 147.57, 143.76, 136.81, 131.83, 130.58, 130.27, 129.91, 129.53, 127.18, 119.04, 112.69, 41.30, 37.73, 36.81, 21.93, 21.67. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{21}N_2O_2S^+$ [M+H] 329.1324, found 329.1326.



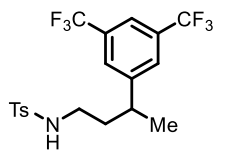
4-methyl-*N*-(3-(naphthalen-2-yl)butyl)benzenesulfonamide (2o): The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), naphthalen-2-ylboronic acid (34.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 33.3 mg (94%) of **2o** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.81–7.76 (m, 1H), 7.75–7.71 (m, 2H), 7.63 (d, *J* = 8.3 Hz, 2H), 7.50 (s, 1H), 7.43 (dddd, *J* = 16.4, 8.2, 6.8, 1.4 Hz, 2H), 7.23 (dd, *J* = 8.5, 1.8 Hz, 1H), 7.18 (d, *J* = 8.0 Hz, 2H), 4.58 (t, *J* = 5.7 Hz, 1H), 2.96–2.73 (m, 3H), 2.36 (s, 3H), 1.87–1.79 (m, 2H), 1.27 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 143.40, 143.35, 136.87, 133.66, 132.42, 129.73, 128.41, 127.71, 127.67, 127.15, 126.13, 125.49, 125.43, 125.33, 41.66, 37.76, 37.40, 22.37, 21.59. **HRMS** (ESI-TOF) Calcd for $C_{21}H_{24}NO_2S^+$ [M+H] 354.1528, found 354.1530.



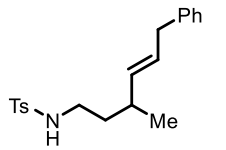
***N*-(3-(benzo[d][1,3]dioxol-5-yl)butyl)-4-methylbenzenesulfonamide (2p):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), benzo[d][1,3]dioxol-5-ylboronic acid (33.2 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 22.5 mg (65%) of **2p** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.3 Hz, 2H), 7.36–7.20 (m, 2H), 6.68 (d, *J* = 7.9 Hz, 1H), 6.56 (d, *J* = 1.8 Hz, 1H), 6.52 (dd, *J* = 7.9, 1.8 Hz, 1H), 5.91 (s, 2H), 4.49 (t, *J* = 6.2 Hz, 1H), 2.91–2.74 (m, 2H), 2.68–2.58 (m, 1H), 2.42 (s, 3H), 1.77–1.54 (m, 2H), 1.14 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 147.89, 146.01, 143.49, 139.91, 136.99, 129.79, 127.22, 119.98, 108.34, 107.08, 100.96, 41.66, 38.06, 37.15, 22.61, 21.64. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{22}NO_4S^+$ [M+H] 348.1270, found 348.1274.



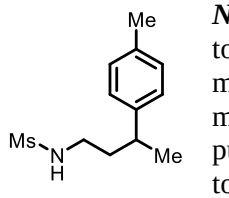
***N*-(3-(3,5-dimethoxyphenyl)butyl)-4-methylbenzenesulfonamide (2q):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (3,5-dimethoxyphenyl)boronic acid (36.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 31.9 mg (88%) of **2q** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.3 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 6.29 (t, *J* = 2.3 Hz, 1H), 6.26 (d, *J* = 2.3 Hz, 2H), 4.59 (t, *J* = 6.2 Hz, 1H), 3.76 (s, 6H), 2.84 (q, *J* = 6.8 Hz, 2H), 2.71–2.60 (m, 1H), 2.41 (s, 3H), 1.78–1.62 (m, 2H), 1.17 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 161.00, 148.58, 143.43, 136.98, 129.78, 127.16, 105.14, 98.10, 55.36, 41.68, 37.82, 37.67, 22.23, 21.61. **HRMS** (ESI-TOF) Calcd for $C_{19}H_{26}NO_4S^+$ [M+H] 364.1583, found 364.1588.



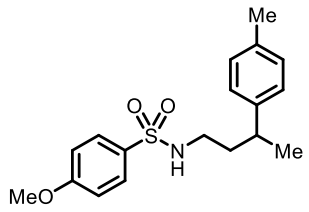
***N*-(3-(3,5-bis(trifluoromethyl)phenyl)butyl)-4-methylbenzenesulfonamide (2r):** The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (3,5-bis(trifluoromethyl)phenyl)boronic acid (51.6 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 43.7 mg (99%) of **2r** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.74–7.65 (m, 3H), 7.56 (d, *J* = 1.9 Hz, 2H), 7.29 (d, *J* = 8.1 Hz, 2H), 4.98 (t, *J* = 6.2 Hz, 1H), 3.03–2.91 (m, 1H), 2.86 (qd, *J* = 6.7, 4.3 Hz, 2H), 2.41 (s, 3H), 1.82–1.72 (m, 2H), 1.24 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 148.87, 143.80, 136.75, 131.88 (q, $J_{C–F}$ = 33.0 Hz), 129.89, 127.35–127.24 (m), 127.16, 123.47 (q, $J_{C–F}$ = 272.6 Hz), 120.55 (p, $J_{C–F}$ = 3.8 Hz), 41.17, 37.67, 36.81, 21.65, 21.57. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –65.45. **HRMS** (ESI-TOF) Calcd for $C_{19}H_{20}F_6NO_2S^+$ [M+H] 440.1119, found 440.1119.



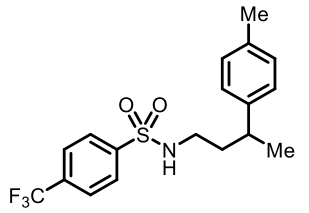
(*E*)-4-methyl-*N*-(3-methyl-6-phenylhex-4-en-1-yl)benzenesulfonamide (2s): The reaction was carried out according to General Procedure D using **1a** (22.5 mg, 0.1 mmol), (*E*)-(3-phenylprop-1-en-1-yl)boronic acid (32.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 30.2 mg (88%) of **2s** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 7.8 Hz, 4H), 7.22–7.17 (m, 1H), 7.14–7.11 (m, 2H), 5.53–5.43 (m, 1H), 5.33–5.16 (m, 1H), 4.58 (t, *J* = 6.2 Hz, 1H), 3.27 (dd, *J* = 6.8, 1.4 Hz, 2H), 3.04–2.81 (m, 2H), 2.41 (s, 3H), 2.13 (ddd, *J* = 14.3, 7.8, 5.9 Hz, 1H), 1.51–1.34 (m, 2H), 0.93 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 143.40, 140.75, 137.10, 136.39, 129.78, 128.62, 128.55, 128.53, 127.22, 126.08, 41.63, 39.00, 36.60, 34.54, 21.63, 20.90. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{26}NO_2S^+$ [M+H] 344.1684, found 344.1679.



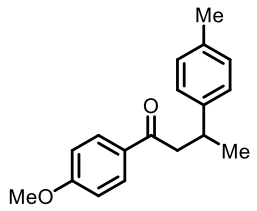
***N*-(3-(p-tolyl)butyl)methanesulfonamide (2t):** The reaction was carried out according to General Procedure D using **1b** (14.9 mg, 0.1 mmol), *p*-tolylboronic acid (27.2 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 24.0 mg (99%) of **2t** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.12 (d, *J* = 7.9 Hz, 2H), 7.07 (d, *J* = 8.1 Hz, 2H), 4.35 (t, *J* = 6.3 Hz, 1H), 3.13–2.96 (m, 2H), 2.86 (s, 3H), 2.80–2.71 (m, 1H), 2.32 (s, 3H), 1.95–1.74 (m, 2H), 1.26 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 142.83, 136.11, 129.48, 126.85, 41.88, 40.20, 38.44, 37.11, 22.66, 21.10. **HRMS** (ESI-TOF) Calcd for $C_{12}H_{20}NO_2S^+$ [M+H] 242.1215, found 242.1218.



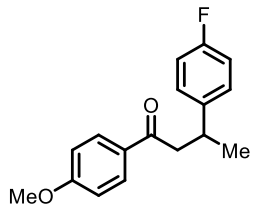
4-methoxy-*N*-(3-(p-tolyl)butyl)benzenesulfonamide (2u): The reaction was carried out according to General Procedure D using **1c** (24.1 mg, 0.1 mmol), *p*-tolylboronic acid (27.2 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 32.3 mg (97%) of **2u** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.9 Hz, 2H), 7.11–7.04 (m, 2H), 6.99–6.89 (m, 4H), 4.53 (t, *J* = 6.2 Hz, 1H), 3.86 (s, 3H), 2.89–2.78 (m, 2H), 2.67 (dp, *J* = 9.0, 6.8 Hz, 1H), 2.30 (s, 3H), 1.76–1.61 (m, 2H), 1.17 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 162.90, 142.93, 135.88, 131.59, 129.35, 129.30, 126.81, 114.28, 55.71, 41.67, 37.93, 36.92, 22.43, 21.08. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{24}NO_3S^+$ [M+H] 334.1477, found 334.1474.



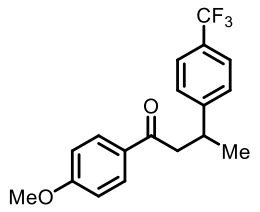
***N*-(3-(p-tolyl)butyl)-4-(trifluoromethyl)benzenesulfonamide (2v):** The reaction was carried out according to General Procedure D using **1d** (27.9 mg, 0.1 mmol), *p*-tolylboronic acid (27.2 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), KOH (11.2 mg, 0.2 mmol), and *t*-AmylOH (0.5 mL). The reaction was run for 20 h at room temperature (20 °C), and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 33.3 mg (90%) of **2v** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.2 Hz, 2H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.06 (d, *J* = 7.8 Hz, 2H), 6.95 (d, *J* = 8.1 Hz, 2H), 4.68 (t, *J* = 6.0 Hz, 1H), 2.94–2.82 (m, 2H), 2.67 (dp, *J* = 9.2, 6.8 Hz, 1H), 2.30 (s, 3H), 1.88–1.66 (m, 2H), 1.18 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 143.62, 142.58, 136.13, 134.40 (q, $J_{C–F}$ = 33.0 Hz), 129.45, 127.67, 126.76, 126.34 (q, $J_{C–F}$ = 3.7 Hz), 126.13–120.48 (m), 41.84, 37.91, 36.98, 22.53, 21.06. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –65.75. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{21}F_3NO_2S^+$ [M+H] 372.1245, found 372.1254.



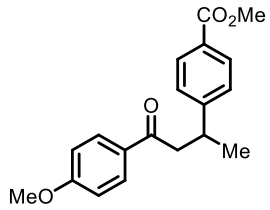
1-(4-methoxyphenyl)-3-(p-tolyl)butan-1-one (4aa): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), *p*-tolylboronic acid (40.8 mg, 0.3 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 21.4 mg (80%) of **4aa** as a white solid. Analytical data were in agreement with literature values.[5] **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.9 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 7.9 Hz, 2H), 6.91 (d, *J* = 8.9 Hz, 2H), 3.86 (s, 3H), 3.50–3.40 (m, 1H), 3.29–3.04 (m, 2H), 2.31 (s, 3H), 1.31 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.90, 163.51, 143.89, 135.83, 130.51, 130.49, 129.33, 126.85, 113.81, 55.60, 46.95, 35.50, 22.08, 21.13. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{21}O_2^+$ [M+H] 269.1542, found 269.1546.



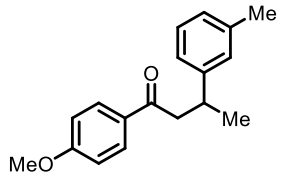
3-(4-fluorophenyl)-1-(4-methoxyphenyl)butan-1-one (4ab): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (4-fluorophenyl)boronic acid (28.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 12.8 mg (47%) of **4ab** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.90 (d, *J* = 8.9 Hz, 2H), 7.22 (dd, *J* = 8.5, 5.5 Hz, 2H), 6.97 (t, *J* = 8.7 Hz, 2H), 6.92–6.89 (m, 2H), 3.86 (s, 1H), 3.52–3.44 (m, 1H), 3.27–3.05 (m, 2H), 1.31 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.58, 163.59, 161.46 (d, $J_{C–F}$ = 243.7 Hz), 142.46, 130.47, 130.38, 128.38 (d, $J_{C–F}$ = 7.8 Hz), 115.33 (d, $J_{C–F}$ = 21.2 Hz), 113.85, 55.61, 46.87, 35.19, 22.25. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –119.84. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{18}FO_2^+$ [M+H] 273.1291, found 273.1284.



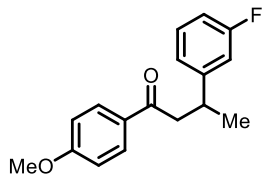
1-(4-methoxyphenyl)-3-(4-(trifluoromethyl)phenyl)butan-1-one (4ac): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), 4-(trifluoromethyl)phenyl)boronic acid (38.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 23.2 mg (72%) of **4ac** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.90 (d, *J* = 9.0 Hz, 2H), 7.59–7.52 (m, 2H), 7.38 (d, *J* = 8.1 Hz, 2H), 6.91 (d, *J* = 9.0 Hz, 2H), 3.86 (s, 3H), 3.57 (h, *J* = 7.0 Hz, 1H), 3.31–3.11 (m, 2H), 1.35 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.08, 163.68, 150.91 (q, $J_{C–F}$ = 1.4 Hz), 130.45, 130.22, 128.64 (q, $J_{C–F}$ = 32.3 Hz), 127.41, 125.58 (q, $J_{C–F}$ = 3.8 Hz), 127.21–121.37 (m), 113.89, 55.61, 46.30, 35.61, 21.99. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –64.98. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{18}F_3O_2^+$ [M+H] 323.1259, found 323.1262.



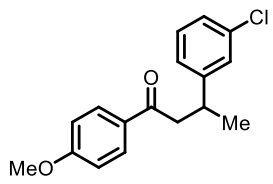
methyl 4-(4-(4-methoxyphenyl)-4-oxobutan-2-yl)benzoate (4ad): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 31.2 mg (99%) of **4ad** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.4 Hz, 2H), 7.90 (d, *J* = 9.0 Hz, 2H), 7.34 (d, *J* = 8.3 Hz, 2H), 6.91 (d, *J* = 8.9 Hz, 2H), 3.89 (s, 3H), 3.85 (s, 3H), 3.56 (h, *J* = 7.0 Hz, 1H), 3.32–3.08 (m, 2H), 1.34 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.18, 167.15, 163.62, 152.25, 130.44, 130.26, 130.01, 128.30, 127.07, 113.86, 55.58, 52.10, 46.27, 35.82, 21.89. **HRMS** (ESI-TOF) Calcd for $C_{19}H_{21}O_4^+$ [M+H] 313.1440, found 313.1439.



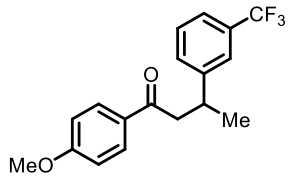
1-(4-methoxyphenyl)-3-(m-tolyl)butan-1-one (4ae): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), *m*-tolylboronic acid (27.2 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 16.1 mg (60%) of **4ae** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.9 Hz, 2H), 7.19 (t, *J* = 7.5 Hz, 1H), 7.07 (dt, *J* = 9.2, 1.9 Hz, 2H), 7.01 (ddd, *J* = 7.4, 1.8, 1.0 Hz, 1H), 6.91 (d, *J* = 8.9 Hz, 2H), 3.86 (s, 3H), 3.48–3.39 (m, 1H), 3.26–2.99 (m, 2H), 2.33 (s, 3H), 1.31 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.87, 163.51, 146.88, 138.17, 130.50, 130.49, 128.54, 127.82, 127.12, 123.94, 113.81, 55.59, 46.85, 35.81, 21.98, 21.63. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{21}O_2^+$ [M+H] 269.1542, found 269.1536.



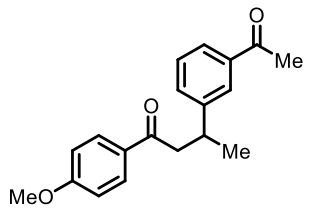
3-(3-fluorophenyl)-1-(4-methoxyphenyl)butan-1-one (4af): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (3-fluorophenyl)boronic acid (28.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 19.6 mg (72%) of **4af** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.91 (d, *J* = 8.9 Hz, 2H), 7.27–7.22 (m, 1H), 7.08–7.02 (m, 1H), 6.97 (ddd, *J* = 10.3, 2.6, 1.7 Hz, 1H), 6.91 (d, *J* = 9.0 Hz, 2H), 6.87 (tdd, *J* = 8.3, 2.6, 1.0 Hz, 1H), 3.86 (s, 3H), 3.50 (dq, *J* = 13.9, 6.7 Hz, 1H), 3.34–3.02 (m, 2H), 1.32 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.31, 163.62, 163.11 (d, $J_{C–F}$ = 224.6 Hz), 149.53 (d, $J_{C–F}$ = 6.6 Hz), 130.47, 130.32, 130.04 (d, $J_{C–F}$ = 8.4 Hz), 122.76 (d, $J_{C–F}$ = 2.7 Hz), 113.86, 113.83 (d, $J_{C–F}$ = 21.0 Hz) 113.18 (d, $J_{C–F}$ = 21.0 Hz), 55.60, 46.49, 35.57 (d, $J_{C–F}$ = 2.0 Hz), 21.94. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –115.95. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{18}FO_2^+$ [M+H] 273.1291, found 273.1289.



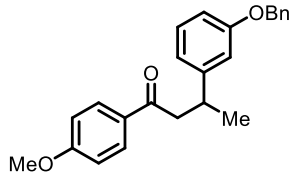
3-(3-chlorophenyl)-1-(4-methoxyphenyl)butan-1-one (4ag): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (3-chlorophenyl)boronic acid (31.2 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 21.3 mg (74%) of **4ag** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.93–7.87 (m, 2H), 7.26 (d, *J* = 2.3 Hz, 1H), 7.23–7.20 (m, 1H), 7.18–7.13 (m, 2H), 6.95–6.88 (m, 2H), 3.86 (s, 3H), 3.53–3.43 (m, 1H), 3.25–3.03 (m, 2H), 1.31 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.22, 163.62, 148.97, 134.36, 130.47, 130.29, 129.90, 127.15, 126.52, 125.40, 113.87, 55.60, 46.44, 35.54, 21.94. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{18}ClO_2^+$ [M+H] 289.0995, found 289.0995.



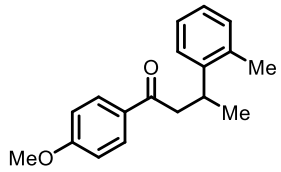
1-(4-methoxyphenyl)-3-(3-(trifluoromethyl)phenyl)butan-1-one (4ah): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (3-(trifluoromethyl)phenyl)boronic acid acid (38.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 24.5 mg (76%) of **4ah** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.93–7.88 (m, 2H), 7.51 (d, *J* = 1.9 Hz, 1H), 7.46 (ddd, *J* = 10.5, 5.9, 1.7 Hz, 2H), 7.42–7.38 (m, 1H), 7.00–6.87 (m, 2H), 3.86 (s, 3H), 3.58 (h, *J* = 7.0 Hz, 1H), 3.30–3.05 (m, 2H), 1.35 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.13, 163.67, 147.75, δ 130.88 (q, $J_{C–F}$ = 32.0 Hz), 130.69 (q, $J_{C–F}$ = 1.4 Hz), 130.47, 130.26, 129.05, 124.37 (q, $J_{C–F}$ = 272.3 Hz), 123.67 (q, $J_{C–F}$ = 3.8 Hz), 123.26 (q, $J_{C–F}$ = 3.9 Hz), 113.88, 55.61, 46.43, 35.64, 21.96. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –65.13. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{18}F_3O_2^+$ [M+H] 323.1259, found 323.1252.



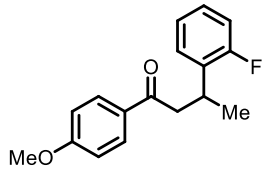
3-(3-acetylphenyl)-1-(4-methoxyphenyl)butan-1-one (4ai): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (3-acetylphenyl)boronic acid (32.8 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 22.2 mg (75%) of **4ai** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.95–7.90 (m, 2H), 7.88 (d, *J* = 1.9 Hz, 1H), 7.77 (dt, *J* = 7.8, 1.4 Hz, 1H), 7.49 (dt, *J* = 7.7, 1.5 Hz, 1H), 7.39 (t, *J* = 7.7 Hz, 1H), 6.91 (d, *J* = 9.0 Hz, 2H), 3.86 (s, 3H), 3.57 (h, *J* = 7.0 Hz, 1H), 3.31–3.10 (m, 2H), 2.59 (s, 3H), 1.36 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 198.44, 197.32, 163.62, 147.44, 137.50, 132.17, 130.46, 130.28, 128.84, 126.66, 126.55, 113.85, 55.59, 46.43, 35.72, 26.83, 22.11. **HRMS** (ESI-TOF) Calcd for $C_{19}H_{21}O_3^+$ [M+H] 297.1491, found 297.1482.



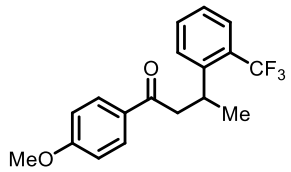
3-(3-(benzyloxy)phenyl)-1-(4-methoxyphenyl)butan-1-one (4aj): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (3-(benzyloxy)phenyl)boronic acid (45.6 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 23.7 mg (76%) of **4aj** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.98–7.87 (m, 2H), 7.46–7.42 (m, 2H), 7.40–7.35 (m, 2H), 7.35–7.29 (m, 1H), 7.21 (t, *J* = 7.9 Hz, 1H), 6.97–6.87 (m, 4H), 6.81 (ddd, *J* = 8.2, 2.6, 1.0 Hz, 1H), 5.04 (s, 2H), 3.85 (s, 3H), 3.52–3.38 (m, 1H), 3.33–2.94 (m, 2H), 1.31 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.72, 163.52, 159.08, 148.65, 137.20, 130.49, 130.43, 129.63, 128.69, 128.06, 127.70, 119.72, 113.97, 113.81, 112.25, 70.09, 55.58, 46.70, 35.88, 21.91. **HRMS** (ESI-TOF) Calcd for $C_{24}H_{25}O_3^+$ [M+H] 361.1804, found 361.1800.



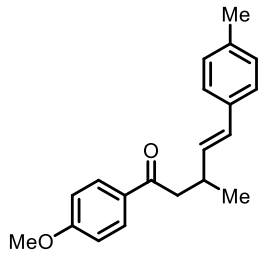
1-(4-methoxyphenyl)-3-(o-tolyl)butan-1-one (4ak): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), *o*-tolylboronic acid (27.2 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 9.6 mg (36%) of **4ak** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.00–7.89 (m, 2H), 7.25 (d, *J* = 9.2 Hz, 1H), 7.20–7.16 (m, 1H), 7.14 (d, *J* = 7.2 Hz, 1H), 7.09 (td, *J* = 7.3, 1.4 Hz, 1H), 6.94–6.87 (m, 2H), 3.86 (s, 3H), 3.74 (dqd, *J* = 8.7, 6.9, 5.1 Hz, 1H), 3.26–3.11 (m, 2H), 2.38 (s, 3H), 1.28 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.86, 163.54, 145.08, 135.45, 130.60, 130.49, 130.47, 126.38, 126.05, 125.36, 113.83, 55.60, 46.09, 30.79, 21.50, 19.68. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{21}O_2^+$ [M+H] 269.1542, found 269.1546.



3-(2-fluorophenyl)-1-(4-methoxyphenyl)butan-1-one (4al): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (2-fluorophenyl)boronic acid (28.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 23.4 mg (86%) of **4al** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.98–7.84 (m, 2H), 7.27 (td, *J* = 7.7, 1.9 Hz, 1H), 7.17 (dddd, *J* = 8.1, 7.1, 5.2, 1.8 Hz, 1H), 7.07 (td, *J* = 7.5, 1.3 Hz, 1H), 7.01 (ddd, *J* = 10.9, 8.1, 1.3 Hz, 1H), 6.96–6.89 (m, 2H), 3.86 (s, 3H), 3.77–3.68 (m, 1H), 3.40–2.87 (m, 2H), 1.34 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.50, 163.56, 160.92 (d, $J_{C–F}$ = 245.0 Hz), 133.25 (d, $J_{C–F}$ = 14.1 Hz), 130.50, 130.29, 128.52 (d, $J_{C–F}$ = 5.5 Hz), 127.80 (d, $J_{C–F}$ = 8.2 Hz), 124.28 (d, $J_{C–F}$ = 3.4 Hz), 115.71 (d, $J_{C–F}$ = 22.6 Hz), 113.83, 55.58, 45.17 (d, $J_{C–F}$ = 1.6 Hz), 30.21 (d, $J_{C–F}$ = 1.6 Hz), 20.44 (d, $J_{C–F}$ = 1.3 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ –120.42. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{18}FO_2^+$ [M+H] 273.1291, found 273.1294.

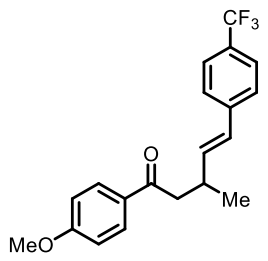


1-(4-methoxyphenyl)-3-(2-(trifluoromethyl)phenyl)butan-1-one (4am): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (2-(trifluoromethyl)phenyl)boronic acid (38.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 25.7 mg (80%) of **4am** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.8 Hz, 2H), 7.74–7.60 (m, 1H), 7.58–7.42 (m, 2H), 7.30 (t, *J* = 7.5 Hz, 1H), 6.92 (d, *J* = 8.9 Hz, 2H), 3.94–3.88 (m, 1H), 3.86 (s, 3H), 3.36–2.89 (m, 2H), 1.33 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 196.95, 163.63, 146.00, 132.21, 130.55, 130.09, 127.87 (q, $J_{C–F}$ = 30.2 Hz), 127.77, 126.25, 126.01 (q, $J_{C–F}$ = 5.9 Hz), 124.66 (q, $J_{C–F}$ = 274.0 Hz), 113.86, 55.60, 46.50, 31.18 (d, $J_{C–F}$ = 1.7 Hz), 22.19. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –61.59. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{18}F_3O_2^+$ [M+H] 323.1259, found 323.1259.

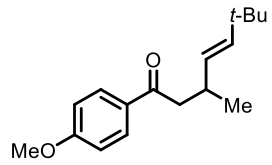


(*E*)-1-(4-methoxyphenyl)-3-methyl-5-(p-tolyl)pent-4-en-1-one (4an): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (*E*)-(4-methylstyryl)boronic acid (32.4 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 25.0 mg (85%) of **4an** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.10–7.81 (m, 2H), 7.23–7.20 (m, 2H), 7.08 (d, *J* = 7.9 Hz, 2H), 7.00–6.85 (m, 2H), 6.37 (d, *J* = 15.9 Hz, 1H), 6.17 (dd, *J* = 15.9, 6.8 Hz, 1H), 3.86 (s, 3H), 3.13–2.85 (m, 3H), 2.31 (s, 3H), 1.17 (d, *J* = 6.4 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 198.00, 163.52, 136.85, 134.87, 134.22, 130.57, 130.54, 129.28, 128.35,

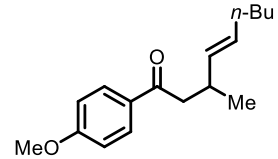
126.10, 113.83, 55.58, 45.42, 33.45, 21.26, 20.39. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{23}O_2^+$ [M+H] 295.1698, found 295.1704.



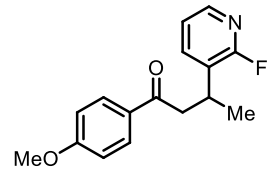
(*E*)-1-(4-methoxyphenyl)-3-methyl-5-(4-(trifluoromethyl)phenyl)pent-4-en-1-one (4ao): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (*E*)-(4-(trifluoromethyl)styryl)boronic acid (43.2 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 31.7 mg (91%) of **4ao** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.08–7.83 (m, 2H), 7.52 (d, *J* = 8.1 Hz, 2H), 7.40 (d, *J* = 8.1 Hz, 2H), 7.00–6.90 (m, 2H), 6.43 (d, *J* = 15.9 Hz, 1H), 6.33 (dd, *J* = 15.9, 7.0 Hz, 1H), 4.06–3.58 (m, 3H), 3.16–2.83 (m, 3H), 1.20 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.60, 163.64, 141.18, 138.02, 130.52, 130.43, 128.95 (q, $J_{C–F}$ = 32.2 Hz), 127.47, 126.35, 125.53 (q, $J_{C–F}$ = 3.8 Hz), 124.40 (q, $J_{C–F}$ = 271.7 Hz), 113.89, 55.61, 45.10, 33.39, 20.25. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –65.05. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{20}F_3O_2^+$ [M+H] 349.1415, found 349.1405.



(*E*)-1-(4-methoxyphenyl)-3,6,6-trimethylhept-4-en-1-one (4ap): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (*E*)-(3,3-dimethylbut-1-en-1-yl)boronic acid (25.6 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 18.5 mg (71%) of **4ap** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.9 Hz, 2H), 6.93 (d, *J* = 8.9 Hz, 2H), 5.41 (dd, *J* = 15.6, 0.9 Hz, 1H), 5.27 (dd, *J* = 15.6, 6.8 Hz, 1H), 3.87 (s, 3H), 3.17–2.65 (m, 3H), 1.05 (d, *J* = 6.3 Hz, 3H), 0.93 (s, 9H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 198.73, 163.42, 140.32, 130.83, 130.63, 129.26, 113.76, 55.59, 45.86, 33.71, 32.74, 29.81, 20.84. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{25}O_2^+$ [M+H] 261.1855, found 261.1860.

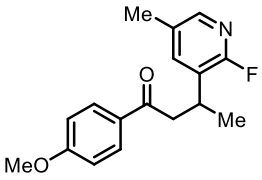


(*E*)-1-(4-methoxyphenyl)-3-methylnon-4-en-1-one (4aq): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (*E*)-hex-1-en-1-ylboronic acid (25.6 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 16.4 mg (63%) of **4aq** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.39–7.31 (m, 2H), 7.07–6.65 (m, 2H), 5.57–5.26 (m, 2H), 3.87 (s, 3H), 3.09–2.72 (m, 3H), 1.94 (dt, *J* = 8.8, 3.4 Hz, 2H), 1.35–1.06 (m, 4H), 1.05 (d, *J* = 6.4 Hz, 3H), 0.96–0.74 (m, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 198.55, 163.44, 134.79, 130.72, 130.58, 129.30, 113.78, 55.58, 45.69, 33.42, 32.31, 31.80, 22.27, 20.72, 14.08. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{25}O_2^+$ [M+H] 261.1855, found 261.1860.

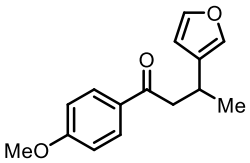


3-(2-fluoropyridin-3-yl)-1-(4-methoxyphenyl)butan-1-one (4ar): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (2-fluoropyridin-3-yl)boronic acid (28.2 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 18.1 mg (66%) of **4ar** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.05 (ddd, *J* = 4.9, 1.9, 1.2 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 1H), 7.75–7.67 (m, 1H), 7.13 (ddd, *J* = 7.4, 4.8, 1.8 Hz, 1H), 6.92 (d, *J* = 8.9 Hz, 1H), 3.86 (s, 3H), 3.67 (h, *J* = 7.0 Hz, 1H), 3.46–3.04 (m, 1H), 1.37 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 196.87, 163.71, 161.72 (d, $J_{C–F}$ = 238.8 Hz), 145.30 (d, $J_{C–F}$ = 15.1 Hz), 139.53 (d, $J_{C–F}$ = 6.3 Hz),

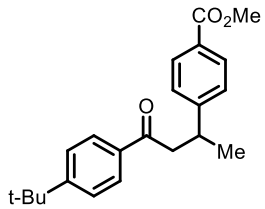
130.45, 130.04, 128.03 (d, $J_{C–F}$ = 28.5 Hz), 121.67 (d, $J_{C–F}$ = 4.2 Hz), 113.91, 55.61, 44.29 (d, $J_{C–F}$ = 2.1 Hz), 30.60 (d, $J_{C–F}$ = 3.0 Hz), 20.01 (d, $J_{C–F}$ = 1.6 Hz). **^{19}F NMR** (376 MHz, $CDCl_3$) δ -73.38. **HRMS** (ESI-TOF) Calcd for $C_{16}H_{17}FNO_2^+$ [M+H] 274.1243, found 274.1030.



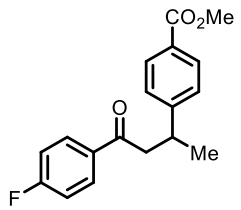
3-(2-fluoro-5-methylpyridin-3-yl)-1-(4-methoxyphenyl)butan-1-one (4as): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), (2-fluoro-5-methylpyridin-3-yl)boronic acid (31.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 9.8 mg (32%) of **4as** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 9.0 Hz, 1H), 7.83 (dd, *J* = 1.6, 0.8 Hz, 1H), 7.53–7.48 (m, 1H), 6.92 (d, *J* = 8.9 Hz, 2H), 3.87 (s, 3H), 3.69–3.55 (m, 1H), 3.43–3.00 (m, 2H), 2.29 (s, 3H), 1.35 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.01, 163.70, 160.19 (d, $J_{C–F}$ = 236.5 Hz), 144.78 (d, $J_{C–F}$ = 14.9 Hz), 140.32 (d, $J_{C–F}$ = 6.1 Hz), 131.06 (d, $J_{C–F}$ = 4.6 Hz), 130.47, 130.10, 127.11 (d, $J_{C–F}$ = 29.1 Hz), 113.91. **^{19}F NMR** (376 MHz, $CDCl_3$) δ -78.88. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{19}FNO_2^+$ [M+H] 288.1400, found 288.1090.



3-(furan-3-yl)-1-(4-methoxyphenyl)butan-1-one (4at): The reaction was carried out according to General Procedure E using **3a** (17.6 mg, 0.1 mmol), furan-3-ylboronic acid (22.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 16.9 mg (69%) of **4at** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 9.0 Hz, 1H), 7.38–7.31 (m, 1H), 7.25–7.23 (m, 1H), 6.92 (d, *J* = 8.9 Hz, 1H), 6.33 (dd, *J* = 1.9, 0.9 Hz, 1H), 3.86 (s, 3H), 3.50–3.36 (m, 1H), 3.27–2.89 (m, 2H), 1.28 (d, *J* = 6.9 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.76, 163.58, 142.98, 138.20, 130.49, 130.46, 130.36, 113.85, 109.70, 55.60, 46.21, 26.60, 21.20. **HRMS** (ESI-TOF) Calcd for $C_{15}H_{17}O_3^+$ [M+H] 245.1178, found 245.0794.

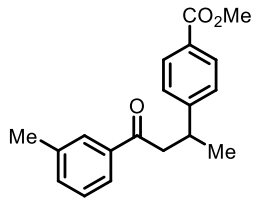


methyl 4-(4-(4-(*tert*-butyl)phenyl)-4-oxobutan-2-yl)benzoate (4ba): The reaction was carried out according to General Procedure E using **3ba** (20.2 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 26.4 mg (78%) of **4ba** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.6 Hz, 2H), 7.45 (d, *J* = 8.6 Hz, 2H), 7.34 (d, *J* = 8.4 Hz, 2H), 3.89 (s, 3H), 3.58 (h, *J* = 7.0 Hz, 1H), 3.37–3.05 (m, 2H), 1.34 (d, *J* = 6.8 Hz, 3H), 1.33 (s, 9H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 198.29, 167.15, 157.00, 152.21, 136.31–131.62 (m), 130.03, 128.32, 128.14, 127.09, 125.68, 52.11, 46.55, 35.69, 35.22, 31.19, 21.88. **HRMS** (ESI-TOF) Calcd for $C_{22}H_{27}O_3^+$ [M+H] 339.1960, found 339.1969.

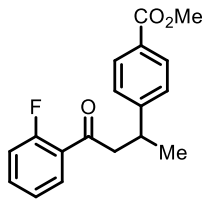


methyl 4-(4-(4-fluorophenyl)-4-oxobutan-2-yl)benzoate (4bb): The reaction was carried out according to General Procedure E using **3bb** (17.4 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 20.1 mg (67%) of **4bb** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.09–7.81 (m, 4H), 7.33 (d, *J* = 8.3 Hz, 2H), 7.19–7.04 (m, 2H), 3.90 (s, 3H), 3.56 (h, *J* = 7.0 Hz, 1H), 3.36–3.06 (m, 2H), 1.35 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.01, 167.11, 165.88 (d, $J_{C–F}$ = 254.8 Hz), 151.91, 133.58

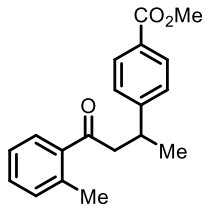
(d, $J_{C–F}$ = 3.2 Hz), 130.79 (d, $J_{C–F}$ = 9.3 Hz), 130.07, 128.45, 127.07, 115.84 (d, $J_{C–F}$ = 21.8 Hz), 52.14, 46.54, 35.67, 21.91. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –107.77. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{18}FO_3^+$ [M+H] 301.1240, found 301.1241.



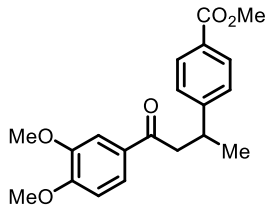
methyl 4-(4-oxo-4-(m-tolyl)butan-2-yl)benzoate (4bc): The reaction was carried out according to General Procedure E using **3bc** (16.0 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 26.9 mg (91%) of **4bc** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.02–7.87 (m, 2H), 7.80–7.62 (m, 2H), 7.42–7.30 (m, 4H), 3.89 (s, 3H), 3.57 (h, *J* = 7.0 Hz, 1H), 3.38–3.01 (m, 2H), 2.39 (d, *J* = 1.1 Hz, 3H), 1.35 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 198.84, 167.14, 152.15, 138.54, 137.19, 133.99, 130.03, 128.67, 128.60, 128.34, 127.09, 125.37, 52.11, 46.68, 35.64, 21.88, 21.46. **HRMS** (ESI-TOF) Calcd for $C_{19}H_{21}O_3^+$ [M+H] 297.1491, found 297.1490.



methyl 4-(4-(2-fluorophenyl)-4-oxobutan-2-yl)benzoate (4bd): The reaction was carried out according to General Procedure E using **3bd** (16.4 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 17.4 mg (58%) of **4bd** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.09–7.93 (m, 2H), 7.76 (td, *J* = 7.6, 1.9 Hz, 1H), 7.50 (dddd, *J* = 8.3, 7.1, 5.0, 1.9 Hz, 1H), 7.37–7.30 (m, 2H), 7.20 (td, *J* = 7.5, 1.1 Hz, 1H), 7.12 (ddd, *J* = 11.3, 8.3, 1.1 Hz, 1H), 3.89 (s, 3H), 3.63–3.48 (m, 1H), 3.43–3.01 (m, 2H), 1.34 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.11, 167.17, 161.90 (d, $J_{C–F}$ = 254.2 Hz), 151.97, 134.67 (d, $J_{C–F}$ = 9.1 Hz), 130.75 (d, $J_{C–F}$ = 2.7 Hz), 130.01, 128.33, 127.12, 125.93 (d, $J_{C–F}$ = 13.1 Hz), 124.67, 116.77 (d, $J_{C–F}$ = 24.2 Hz), 52.12, 51.55 (d, $J_{C–F}$ = 7.1 Hz), 35.51 (d, $J_{C–F}$ = 1.7 Hz), 21.99. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –112.14. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{18}FO_3^+$ [M+H] 301.1240, found 301.1250.

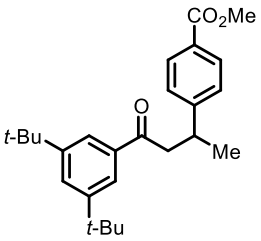


methyl 4-(4-oxo-4-(*o*-tolyl)butan-2-yl)benzoate (4be): The reaction was carried out according to General Procedure E using **3be** (16.0 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 16.9 mg (57%) of **4be** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.00–7.89 (m, 2H), 7.53 (dd, *J* = 7.8, 1.4 Hz, 1H), 7.34 (td, *J* = 7.5, 1.4 Hz, 1H), 7.32–7.29 (m, 2H), 7.25–7.14 (m, 2H), 3.90 (s, 3H), 3.53 (h, *J* = 7.0 Hz, 1H), 3.37–2.84 (m, 2H), 2.35 (s, 3H), 1.34 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 203.03, 167.15, 151.86, 138.33, 138.04, 132.06, 131.35, 130.02, 128.38, 128.25, 127.12, 125.76, 52.13, 49.68, 35.99, 22.03, 21.08. **HRMS** (ESI-TOF) Calcd for $C_{19}H_{21}O_3^+$ [M+H] 297.1491, found 297.1494.

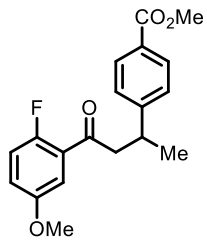


methyl 4-(4-(3,4-dimethoxyphenyl)-4-oxobutan-2-yl)benzoate (4bf): The reaction was carried out according to General Procedure E using **3bf** (20.6 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 29.1 mg (85%) of **4bf** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.55 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.48 (d, *J* = 2.1 Hz, 1H), 7.34 (d, *J* = 8.3 Hz, 2H), 6.86 (d, *J* = 8.4 Hz, 1H), 3.93 (s, 3H), 3.91 (s, 3H), 3.89 (s, 3H), 3.56 (p, *J* = 7.0 Hz, 1H), 3.36–3.02 (m,

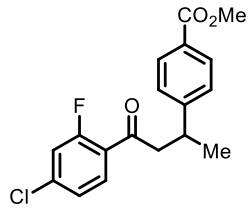
2H), 1.35 (d, J = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 197.36, 167.20, 153.45, 152.19, 149.16, 130.38, 130.02, 128.29, 127.07, 122.84, 110.23, 110.07, 56.19, 56.07, 52.13, 46.13, 35.96, 21.88. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{23}O_5^+$ [M+H] 343.1545, found 343.1555.



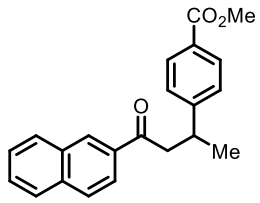
methyl 4-(4-(3,5-di-*tert*-butylphenyl)-4-oxobutan-2-yl)benzoate (4bg): The reaction was carried out according to General Procedure E using **3bg** (25.8 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 26.8 mg (68%) of **4bg** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.98 (d, J = 8.4 Hz, 2H), 7.75 (d, J = 1.9 Hz, 2H), 7.63 (t, J = 1.9 Hz, 1H), 7.36 (d, J = 8.3 Hz, 2H), 3.89 (s, 3H), 3.59 (h, J = 7.0 Hz, 1H), 3.43–3.06 (m, 2H), 1.37 (d, J = 7.0 Hz, 3H), 1.34 (s, 18H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 199.32, 167.16, 152.31, 151.37, 136.84, 130.06, 128.34, 127.52, 127.14, 122.35, 52.11, 46.91, 35.82, 35.11, 31.50, 21.85. **HRMS** (ESI-TOF) Calcd for $C_{26}H_{35}O_3^+$ [M+H] 395.2586, found 395.2582.



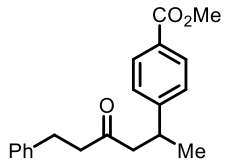
methyl 4-(4-(2-fluoro-5-methoxyphenyl)-4-oxobutan-2-yl)benzoate (4bh): The reaction was carried out according to General Procedure E using **3bh** (19.4 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 22.1 mg (67%) of **4bh** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, J = 8.4 Hz, 2H), 7.32 (d, J = 8.3 Hz, 2H), 7.23 (ddd, J = 5.5, 2.7, 0.9 Hz, 1H), 7.10–6.97 (m, 2H), 3.89 (s, 3H), 3.78 (s, 3H), 3.64–3.49 (m, 1H), 3.29 (dddd, J = 65.2, 17.3, 7.0, 3.1 Hz, 2H), 1.34 (d, J = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 196.82 (d, $J_{C–F}$ = 4.4 Hz), 167.17, 157.38, 155.83 (d, $J_{C–F}$ = 28.5 Hz), 152.00, 130.00, 128.33, 127.12, 125.82 (d, $J_{C–F}$ = 14.8 Hz), 121.62 (d, $J_{C–F}$ = 8.8 Hz), 117.76 (d, $J_{C–F}$ = 26.4 Hz), 112.96 (d, $J_{C–F}$ = 3.0 Hz), 56.00, 52.11, 51.49 (d, $J_{C–F}$ = 7.7 Hz), 35.54, 22.03. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –122.09. **HRMS** (ESI-TOF) Calcd for $C_{19}H_{20}FO_4^+$ [M+H] 331.1346, found 331.1349.



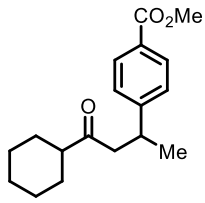
methyl 4-(4-(4-chloro-2-fluorophenyl)-4-oxobutan-2-yl)benzoate (4bi): The reaction was carried out according to General Procedure E using **3bi** (19.8 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 13.4 mg (43%) of **4bi** as a colorless oil. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, J = 8.4 Hz, 2H), 7.73 (t, J = 8.2 Hz, 1H), 7.31 (d, J = 8.2 Hz, 2H), 7.23–7.10 (m, 2H), 3.90 (s, 3H), 3.61–3.48 (m, 1H), 3.38–2.97 (m, 2H), 1.33 (d, J = 6.9 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 195.74 (d, $J_{C–F}$ = 4.4 Hz), 167.14, 161.72 (d, $J_{C–F}$ = 257.5 Hz), 151.75, 140.20 (d, $J_{C–F}$ = 10.7 Hz), 131.83 (d, $J_{C–F}$ = 3.4 Hz), 130.04, 128.42, 127.10, 125.36 (d, $J_{C–F}$ = 3.3 Hz), 124.32 (d, $J_{C–F}$ = 13.4 Hz), 117.47 (d, $J_{C–F}$ = 27.5 Hz), 52.14, 51.48 (d, $J_{C–F}$ = 7.1 Hz), 35.47 (d, $J_{C–F}$ = 1.7 Hz), 22.00. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –109.67. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{17}ClFO_3^+$ [M+H] 335.0850, found 335.0860.



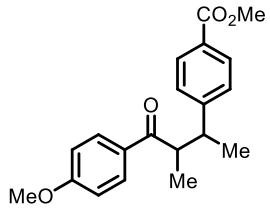
methyl 4-(4-(naphthalen-2-yl)-4-oxobutan-2-yl)benzoate (4bj): The reaction was carried out according to General Procedure E using **3bj** (19.6 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 22.2 mg (67%) of **4bj** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 8.42 (d, *J* = 1.8 Hz, 1H), 7.98 (dd, *J* = 8.5, 2.4 Hz, 3H), 7.94 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.91–7.82 (m, 2H), 7.59 (ddd, *J* = 8.2, 6.9, 1.3 Hz, 1H), 7.54 (ddd, *J* = 8.1, 6.9, 1.3 Hz, 1H), 7.42–7.35 (m, 2H), 3.89 (s, 3H), 3.64 (h, *J* = 7.0 Hz, 1H), 3.54–3.14 (m, 2H), 1.39 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 198.58, 167.14, 152.12, 135.71, 134.49, 132.61, 130.07, 129.82, 129.67, 128.63, 128.40, 127.90, 127.13, 126.95, 123.92, 52.12, 46.71, 35.80, 21.95. **HRMS** (ESI-TOF) Calcd for $C_{22}H_{21}O_3^+$ [M+H] 333.1491, found 333.1482.



methyl 4-(4-oxo-7-phenylheptan-2-yl)benzoate (4bk): The reaction was carried out according to General Procedure E using **3bk** (17.4 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 24.3 mg (75%) of **4bk** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96–7.91 (m, 2H), 7.30–7.21 (m, 4H), 7.20–7.14 (m, 1H), 7.14–7.02 (m, 2H), 3.90 (s, 3H), 3.37 (h, *J* = 7.0 Hz, 1H), 2.89–2.77 (m, 2H), 2.75–2.44 (m, 4H), 1.24 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 208.45, 167.11, 151.70, 141.00, 130.04, 128.60, 128.39, 126.99, 126.23, 52.14, 51.02, 45.07, 35.43, 29.67, 21.85. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{23}O_3^+$ [M+H] 311.1647, found 311.1651.

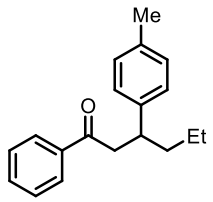


methyl 4-(4-cyclohexyl-4-oxobutan-2-yl)benzoate (4bl): The reaction was carried out according to General Procedure E using **3bl** (15.2 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 10.9 mg (38%) of **4bl** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.2 Hz, 2H), 3.90 (s, 3H), 3.40 (h, *J* = 7.0 Hz, 1H), 2.89–2.54 (m, 2H), 2.32–2.15 (m, 1H), 1.83–1.67 (m, 4H), 1.66–1.62 (m, 1H), 1.25 (d, *J* = 7.0 Hz, 3H), 1.34–1.09 (m, 5H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 212.44, 167.19, 152.19, 129.98, 128.28, 127.05, 52.13, 51.37, 48.81, 35.15, 28.38, 28.25, 25.93, 25.76, 25.70, 21.80. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{25}O_3^+$ [M+H] 289.1804, found 289.1804.

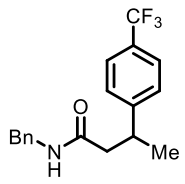


3:1 dr

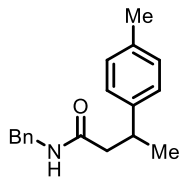
methyl 4-(4-(4-methoxyphenyl)-3-methyl-4-oxobutan-2-yl)benzoate (4bm): The reaction was carried out according to General Procedure E using **3bm** (19.0 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (1.4 mg, 0.005 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 27.7 mg (85%, 3:1 dr) of **4bm** as a white solid with diastereoselectivity dertermined by ^{1}H NMR analysis. **^{1}H NMR** (600 MHz, $CDCl_3$) (major) δ 8.01 (dd, *J* = 8.7, 7.4 Hz, 4H), 7.33 (d, *J* = 8.3 Hz, 2H), 6.98 (d, *J* = 8.9 Hz, 2H), 3.92 (s, 3H), 3.89 (s, 3H), 3.63 (dq, *J* = 10.0, 6.9 Hz, 1H), 3.23 (dq, *J* = 10.0, 6.9 Hz, 1H), 1.20 (d, *J* = 6.9 Hz, 3H), 0.91 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) (major) δ 202.68, 167.18, 163.76, 150.85, 130.72, 129.96, 129.77, 127.93, 127.51, 114.02, 55.63, 52.14, 46.59, 43.38, 20.89, 17.54. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{23}O_4^+$ [M+H] 327.1596, found 327.1590.



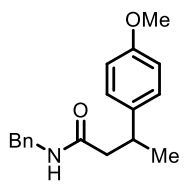
1-phenyl-3-(*p*-tolyl)hexan-1-one (4bn): The reaction was carried out according to General Procedure E using **3bn** (17.4 mg, 0.1 mmol), *p*-tolylboronic acid (40.8 mg, 0.3 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), Cs_2CO_3 (65.0 mg, 0.2 mmol), and *s*-BuOH (0.5 mL). The reaction was run for 16 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/ethyl acetate (5:1) to afford 14.8 mg (56%) of **4bn** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.93–7.81 (m, 2H), 7.57–7.49 (m, 1H), 7.42 (dd, *J* = 8.2, 7.3 Hz, 2H), 7.18–7.06 (m, 4H), 3.34–3.27 (m, 1H), 3.28–3.17 (m, 2H), 2.30 (s, 3H), 1.72–1.63 (m, 1H), 1.64–1.52 (m, 1H), 1.24–1.13 (m, 2H), 0.84 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 199.43, 142.04, 137.43, 135.79, 132.99, 129.24, 128.64, 128.20, 127.55, 46.21, 40.80, 38.75, 21.15, 20.78, 14.14. **HRMS** (ESI-TOF) Calcd for $C_{19}H_{23}O^+$ [M+H] 267.1749, found 267.1337.



***N*-benzyl-3-(4-(trifluoromethyl)phenyl)butanamide (6a):** The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), (4-(trifluoromethyl)phenyl)boronic acid (38.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the reaction mixture was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 27.7 mg (85%) of an inseparable mixture of **6a** (major) and **6a'** (minor) (90:10 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. Analytical data for the major isomer agree with literature values.[6] The ensuing data corresponds to the major isomer. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.1 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 1.1 Hz, 2H), 7.08–6.93 (m, 2H), 5.57 (s, 1H), 4.33 (ddd, *J* = 81.2, 14.7, 5.7 Hz, 2H), 3.43 (h, *J* = 7.1 Hz, 1H), 2.61–2.28 (m, 2H), 1.34 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.95, 149.94, 138.05, 128.92, 128.84 (d, J_{C-F} = 18.5 Hz), 127.73, 127.67, 127.41, 125.66 (q, J_{C-F} = 3.7 Hz), 124.37 (q, J_{C-F} = 271.9 Hz), 45.62, 43.67, 37.01, 21.68. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –64.98. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{23}O_4^+$ [M+H] 322.1419, found 322.1425.

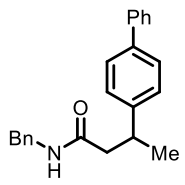


***N*-benzyl-3-(*p*-tolyl)butanamide (6b):** The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), *p*-tolylboronic acid (27.2 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 20.6 mg (77%) of an inseparable mixture of **6b** (major) and **6b'** (minor) (93:7 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. Analytical data for the major isomer agree with literature values.[7] **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.27–7.22 (m, 2H), 7.13–7.06 (m, 4H), 7.04–6.98 (m, 2H), 5.56 (t, *J* = 5.9 Hz, 1H), 4.32 (ddd, *J* = 62.8, 14.8, 5.7 Hz, 2H), 3.28 (h, *J* = 7.1 Hz, 1H), 2.44 (dd, *J* = 7.6, 1.7 Hz, 2H), 2.32 (s, 3H), 1.30 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.68, 142.83, 138.25, 136.06, 129.42, 128.66, 127.72, 127.44, 126.82, 46.09, 43.56, 36.85, 22.09, 21.14. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{23}O_4^+$ [M+H] 268.1701, found 268.1704.

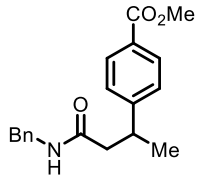


***N*-benzyl-3-(4-methoxyphenyl)butanamide (6c):** The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), (4-methoxyphenyl)boronic acid (30.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 24.0 mg (85%) of an inseparable mixture of **6c** (major) and **6c'** (minor) (94:6 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. Analytical data for the major isomer agree with literature values.[7] **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.27–7.21 (m, 2H), 7.16–7.12 (m, 2H), 7.04–6.97 (m, 2H), 6.84–6.80 (m, 2H), 5.58 (s, 1H), 4.32 (ddd, *J* = 73.6, 14.8, 5.7 Hz, 2H), 3.78 (s, 3H), 3.28 (dt, *J* = 8.1, 6.8 Hz, 1H), 2.42 (qd, *J* = 13.9, 7.6 Hz, 2H), 1.29 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.68, 158.27, 138.25, 137.90,

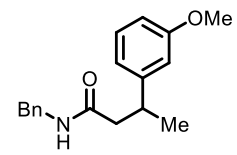
128.67, 127.88, 127.70, 127.46, 114.10, 55.35, 46.25, 43.52, 36.46, 22.17. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{23}O_4^+$ [M+H] 284.1651, found 284.1657.



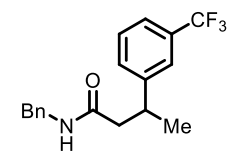
3-([1,1'-biphenyl]-4-yl)-*N*-benzylbutanamide (6d): The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), [1,1'-biphenyl]-4-ylboronic acid (39.6 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 22.0 mg (67%) of an inseparable mixture of **6d** (major) and **6d'** (minor) (90:10 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.60–7.55 (m, 2H), 7.52 (d, *J* = 8.3 Hz, 2H), 7.45–7.41 (m, 2H), 7.36–7.31 (m, 1H), 7.31–7.27 (m, 2H), 7.21–7.15 (m, 2H), 7.07–6.96 (m, 2H), 5.60 (s, 1H), 4.33 (ddd, *J* = 69.8, 14.8, 5.7 Hz, 2H), 3.38 (h, *J* = 7.2 Hz, 1H), 2.54–2.42 (m, 2H), 1.36 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.52, 144.95, 140.97, 139.52, 138.18, 128.88, 128.72, 127.72, 127.49, 127.43, 127.42, 127.11, 124.95, 45.99, 43.63, 36.92, 21.97. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{23}O_4^+$ [M+H] 330.1858, found 330.1858.



methyl 4-(4-(benzylamino)-4-oxobutan-2-yl)benzoate (6e): The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (3:1) to afford 25.2 mg (81%) of an inseparable mixture of **6e** (major) and **6e'** (minor) (91:9 r.r.), obtained as a colorless oil. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.3 Hz, 2H), 7.24–7.20 (m, 2H), 7.14–6.81 (m, 2H), 5.71 (s, 1H), 4.32 (ddd, *J* = 58.0, 14.8, 5.7 Hz, 2H), 3.90 (s, 3H), 3.41 (h, *J* = 7.1 Hz, 1H), 2.58–2.39 (m, 2H), 1.33 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.08, 167.12, 151.31, 138.12, 130.07, 128.71, 128.51, 127.71, 127.54, 127.06, 52.15, 45.51, 43.58, 37.15, 21.61. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{23}O_4^+$ [M+H] 312.1600, found 312.1602.

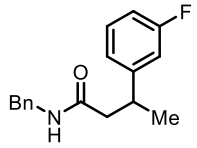


***N*-benzyl-3-(3-methoxyphenyl)butanamide (6f):** The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), 3-methoxyphenylboronic acid (30.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 26.6 mg (94%) of an inseparable mixture of **6f** (major) and **6f'** (minor) (92:8 r.r.), obtained as a colorless oil. The r.r. values of the crude reaction mixture and purified sample were consistent. Analytical data for the major isomer agree with literature values.[7] **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.28–7.19 (m, 4H), 7.06–7.02 (m, 3H), 6.84–6.73 (m, 3H), 5.67 (s, 1H), 4.33 (ddd, *J* = 57.6, 14.8, 5.7 Hz, 2H), 3.76 (s, 3H), 3.30 (h, *J* = 7.1 Hz, 1H), 2.52–2.41 (m, 2H), 1.30 (d, *J* = 7.0 Hz, 3H).**^{13}C NMR** (151 MHz, $CDCl_3$) δ 171.57, 159.90, 147.63, 138.23, 129.73, 128.69, 127.67, 127.44, 119.26, 112.91, 111.69, 55.26, 45.86, 43.55, 37.26, 21.92. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{22}NO_2^+$ [M+H] 284.1651, found 284.1654.

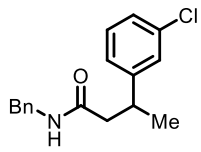


***N*-benzyl-3-(3-(trifluoromethyl)phenyl)butanamide (6g):** The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), (3-(trifluoromethyl)phenyl)boronic acid (38.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 30.2 mg (94% of an inseparable mixture of **6g** (major) and **6g'** (minor) (90:10 r.r.), obtained as a white solid. The r.r. values of the crude reaction

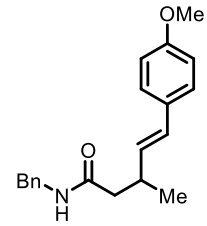
mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.49–7.44 (m, 2H), 7.40–7.36 (m, 2H), 7.27–7.19 (m, 3H), 7.08–6.98 (m, 2H), 4.32 (ddd, *J* = 53.4, 14.7, 5.7 Hz, 2H), 3.41 (h, *J* = 7.2 Hz, 1H), 2.47 (h, *J* = 7.9, 7.4 Hz, 2H), 1.33 (d, *J* = 7.1 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 171.56, 146.63, 137.70, 131.03 (d, $J_{C–F}$ = 31.71 Hz), 130.81 (d, $J_{C–F}$ = 31.9 Hz), 129.22, 128.83, 127.71, 127.67, 123.55 (q, $J_{C–F}$ = 3.8 Hz), 123.43 (q, $J_{C–F}$ = 4.0 Hz), 45.56, 43.78, 36.98, 21.67. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –65.13. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{19}F_3NO^+$ [M+H] 322.1419, found 322.1426.



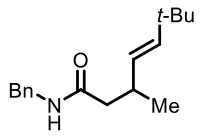
***N*-benzyl-3-(3-fluorophenyl)butanamide (6h):** The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), (3-fluorophenyl)boronic acid (28.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 23.3 mg (86%) of an inseparable mixture of **6h** (major) and **6h'** (minor) (91:9 r.r.), obtained as a colorless oil. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.29–7.21 (m, 4H), 7.09–7.04 (m, 2H), 7.00–6.97 (m, 1H), 6.94–6.86 (m, 2H), 5.68 (s, 1H), 4.33 (ddd, *J* = 59.4, 14.8, 5.7 Hz, 2H), 3.35 (h, *J* = 7.1 Hz, 1H), 2.51–2.34 (m, 2H), 1.30 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.20, 163.95, 162.32, 148.56, 138.17, 130.16 (d, $J_{C–F}$ = 8.3 Hz), 128.75, 127.63 (d, $J_{C–F}$ = 24.2 Hz), 122.79 (d, $J_{C–F}$ = 3.2 Hz), 113.74 (d, $J_{C–F}$ = 20.9 Hz), 113.41 (d, $J_{C–F}$ = 21.0 Hz), 45.67, 43.60, 36.90 (d, $J_{C–F}$ = 1.7 Hz), 21.75. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –115.66. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{19}FNO^+$ [M+H] 272.1451, found 272.1453.



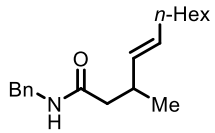
***N*-benzyl-3-(3-chlorophenyl)butanamide (6i):** The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), (3-chlorophenyl)boronic acid (31.2 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 10.0 mg (35%) of an inseparable mixture of **6i** (major) and **6i'** (minor) (87:13 r.r.), obtained as a colorless oil. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.31–7.18 (m, 6H), 7.13–7.09 (m, 1H), 7.07–7.04 (m, 2H), 5.56 (s, 1H), 4.35 (ddd, *J* = 65.9, 14.8, 5.7 Hz, 2H), 3.34 (h, *J* = 7.1 Hz, 1H), 2.49–2.36 (m, 2H), 1.31 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.07, 148.01, 138.14, 134.51, 130.02, 128.81, 127.74, 127.60, 127.06, 126.79, 125.43, 45.72, 43.65, 36.92, 21.76. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{19}ClNO^+$ [M+H] 288.1155, found 288.1152.



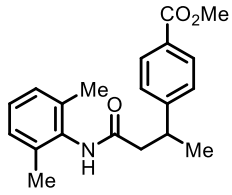
(*E*)-*N*-benzyl-5-(4-methoxyphenyl)-3-methylpent-4-enamide (6j): The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), (*E*)-(4-methoxystyryl)boronic acid (35.4 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 17.6 mg (68% yield, >95:5 r.r.) of **6j** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.32–7.16 (m, 7H), 6.83 (d, *J* = 8.7 Hz, 2H), 6.35 (dd, *J* = 15.9, 1.1 Hz, 1H), 6.35 (d, *J* = 15.9 Hz, 1H), 5.97 (dd, *J* = 15.9, 7.7 Hz, 1H), 5.89 (t, *J* = 5.8 Hz, 1H), 4.60–4.23 (m, 2H), 3.80 (s, 3H), 2.96–2.79 (m, 1H), 2.36–2.19 (m, 2H), 1.15 (d, *J* = 6.8 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.93, 159.04, 138.26, 132.18, 130.20, 128.78, 127.88, 127.55, 127.39, 114.05, 55.43, 44.61, 43.70, 34.70, 20.61. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{26}NO^+$ [M+H] 260.2014, found 260.2013.



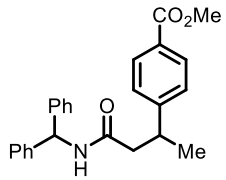
(*E*)-*N*-benzyl-3,6,6-trimethylhept-4-enamide (6k): The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), (*E*)-(3,3-dimethylbut-1-en-1-yl)boronic acid (25.6 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 17.6 mg (68% yield, >95:5 r.r.) of **6k** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.34–7.30 (m, 2H), 7.29–7.23 (m, 3H), 5.80 (s, 1H), 5.48 (dd, *J* = 15.7, 1.1 Hz, 1H), 5.22 (dd, *J* = 15.7, 7.5 Hz, 1H), 4.60–4.19 (m, 2H), 2.69–2.53 (m, 1H), 2.30–2.12 (m, 2H), 1.03 (d, *J* = 6.8 Hz, 3H), 0.94 (s, 9H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.01, 141.22, 138.48, 129.04, 128.82, 128.00, 127.62, 44.74, 43.69, 34.20, 32.80, 29.80, 20.97. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{26}NO^+$ [M+H] 260.2014, found 260.2013.



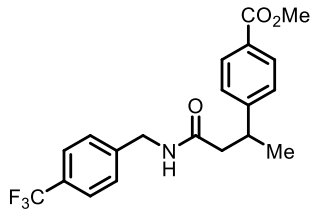
(*E*)-*N*-benzyl-3-methyl-6-oxoundec-4-enamide (6l): The reaction was carried out according to General Procedure F using **5a** (17.5 mg, 0.1 mmol), (*E*)-(3-oxooct-1-en-1-yl)boronic acid (34.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 17.6 mg (68% yield, >95:5 r.r.) of **6l** as a white solid. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.32 (dd, *J* = 8.4, 6.3 Hz, 2H), 7.28–7.24 (m, 3H), 5.81 (t, *J* = 5.6 Hz, 1H), 5.54–5.10 (m, 2H), 4.57–4.11 (m, 2H), 2.64 (h, *J* = 7.0 Hz, 1H), 2.18 (h, *J* = 7.4 Hz, 2H), 2.04–1.85 (m, 2H), 1.33–1.18 (m, 8H), 1.03 (d, *J* = 6.8 Hz, 3H), 0.88 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 172.03, 138.49, 134.35, 130.25, 128.80, 127.95, 127.60, 44.62, 43.68, 34.25, 32.62, 31.84, 29.55, 28.97, 22.76, 20.82, 14.23. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{26}NO^+$ [M+H] 260.2014, found 260.2013.



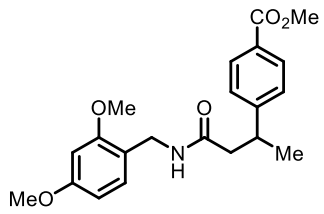
methyl 4-(4-((2,6-dimethylphenyl)amino)-4-oxobutan-2-yl)benzoate (6m): The reaction was carried out according to General Procedure F using **5m** (18.9 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 26.7 mg (82%) of an inseparable mixture of **6m** (major) and **6m'** (minor) (90:10 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.3 Hz, 2H), 7.12–7.02 (m, 1H), 6.99 (d, *J* = 7.5 Hz, 2H), 6.80 (s, 1H), 3.90 (s, 3H), 3.53–3.42 (m, 1H), 2.71–2.61 (m, 2H), 1.98 (s, 6H), 1.37 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 169.71, 167.13, 151.36, 135.48, 133.78, 130.13, 128.59, 128.23, 127.48, 127.21, 52.18, 45.08, 37.13, 22.05, 18.34. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{24}NO_3^+$ [M+H] 326.1756, found 326.1751.



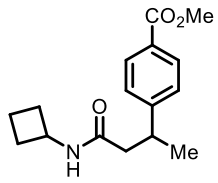
methyl 4-(4-(benzhydrylamino)-4-oxobutan-2-yl)benzoate (6n): The reaction was carried out according to General Procedure F using **5n** (25.1 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 31.0 mg (80%) of an inseparable mixture of **6n** (major) and **6n'** (minor) (89:11 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.3 Hz, 2H), 7.32–7.23 (m, 5H), 7.19–7.15 (m, 3H), 7.12–7.06 (m, 2H), 6.85 (d, *J* = 7.5 Hz, 2H), 6.12 (d, *J* = 8.0 Hz, 1H), 5.98 (d, *J* = 8.0 Hz, 1H), 3.91 (s, 3H), 3.49–3.31 (m, 1H), 2.63–2.36 (m, 2H), 1.31 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.25, 167.12, 151.18, 141.52, 141.21, 130.15, 128.79, 128.74, 128.58, 127.58, 127.51, 127.39, 127.24, 127.12, 56.92, 52.17, 45.59, 37.29, 21.80. **HRMS** (ESI-TOF) Calcd for $C_{25}H_{26}NO_3^+$ [M+H] 388.1913, found 388.1912.



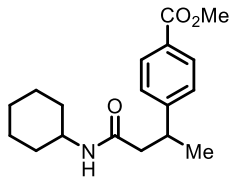
methyl 4-(4-oxo-4-((4-(trifluoromethyl)benzyl)amino)butan-2-yl)benzoate (6o): The reaction was carried out according to General Procedure F using **5o** (24.3 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 26.1 mg (69%) of an inseparable mixture of **6o** (major) and **6o'** (minor) (93:7 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.92 (d, *J* = 8.3 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.04 (d, *J* = 8.0 Hz, 2H), 5.84 (s, 1H), 4.36 (ddd, *J* = 149.1, 15.4, 6.0 Hz, 2H), 3.91 (s, 3H), 3.46–3.33 (m, 1H), 2.65–2.32 (m, 2H), 1.34 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (151 MHz, $CDCl_3$) δ 171.28, 167.10, 151.09, 142.32, 130.11, 128.65, 127.71, 127.14, 125.56 (q, J_{C-F} = 3.8 Hz), δ 124.17 (q, J_{C-F} = 271.9 Hz), 52.20, 45.54, 42.90, 37.29, 21.73. **^{19}F NMR** (376 MHz, $CDCl_3$) δ –65.24. **HRMS** (ESI-TOF) Calcd for $C_{20}H_{21}F_3NO_3^+$ [M+H] 380.1474, found 380.1461.



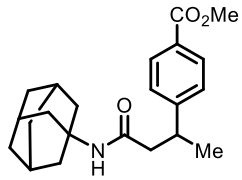
methyl 4-(4-((2,4-dimethoxybenzyl)amino)-4-oxobutan-2-yl)benzoate (6p): The reaction was carried out according to General Procedure F using **5p** (24.3 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 17.6 mg (69%) of an inseparable mixture of **6p** (major) and **6p'** (minor) (86:14 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.87 (d, *J* = 8.3 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 6.97 (d, *J* = 8.0 Hz, 1H), 6.46–6.32 (m, 2H), 5.81–5.67 (m, 1H), 4.30–4.12 (m, 2H), 3.90 (s, 3H), 3.78 (s, 3H), 3.73 (s, 3H), 3.34 (h, *J* = 7.1 Hz, 1H), 2.40 (qd, *J* = 13.9, 7.5 Hz, 2H), 1.29 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.97, 167.12, 160.57, 158.45, 151.29, 130.47, 129.91, 128.36, 126.94, 118.67, 103.85, 98.62, 55.46, 55.32, 52.10, 45.67, 38.94, 37.18, 21.45. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{26}NO^+$ [M+H] 260.2014, found 260.2013.



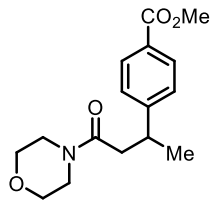
methyl 4-(4-(cyclobutylamino)-4-oxobutan-2-yl)benzoate (6q): The reaction was carried out according to General Procedure F using **5q** (13.9 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 23.7 mg (86%) of an inseparable mixture of **6q** (major) and **6q'** (minor) (92:8 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.4 Hz, 2H), 7.29 (d, *J* = 8.3 Hz, 2H), 5.50 (d, *J* = 8.0 Hz, 1H), 4.30 (q, *J* = 7.9 Hz, 1H), 3.90 (d, *J* = 1.0 Hz, 3H), 3.36 (h, *J* = 7.2 Hz, 1H), 2.37 (d, *J* = 7.5 Hz, 2H), 2.32–2.24 (m, 1H), 2.24–2.18 (m, 1H), 1.85–1.77 (m, 1H), 1.75–1.67 (m, 1H), 1.67–1.57 (m, 3H), 1.31 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.28, 167.14, 151.51, 130.01, 128.45, 127.02, 52.15, 45.50, 44.67, 37.07, 37.07, 31.26, 31.21, 21.38, 15.14. **HRMS** (ESI-TOF) Calcd for $C_{16}H_{22}NO_3^+$ [M+H] 276.1600, found 276.1602.



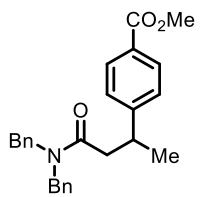
methyl 4-(4-(cyclohexylamino)-4-oxobutan-2-yl)benzoate (6r): The reaction was carried out according to General Procedure F using **5r** (16.7 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), Li*O*t-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 26.4 mg (87% of an inseparable mixture of **6r**(major) and **6r'** (minor) (89:11 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 5.18 (d, *J* = 8.3 Hz, 1H), 3.90 (d, *J* = 1.0 Hz, 4H), 3.71–3.62 (m, 1H), 3.37 (h, *J* = 7.2 Hz, 1H), 2.44–2.30 (m, 2H), 1.87–1.81 (m, 1H), 1.71–1.61 (m, 2H), 1.61–1.51 (m, 2H), 1.32 (d, *J* = 7.1 Hz, 3H), 1.30–1.23 (m, 2H), 1.16–0.98 (m, 2H), 0.94–0.82 (m, 1H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.21, 167.15, 151.50, 130.00, 128.44, 127.04, 52.15, 48.12, 45.81, 37.21, 33.21, 33.09, 25.56, 24.89, 24.83, 21.44. **HRMS** (ESI-TOF) Calcd for $C_{18}H_{26}NO_3^+$ [M+H] 304.1913, found 304.1909.



methyl 4-(4-(adamantan-1-ylamino)-4-oxobutan-2-yl)benzoate (6s): The reaction was carried out according to General Procedure F using **5s** (21.9 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), Li*O*t-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 33.4 mg (94%) of an inseparable mixture of **6s** (major) and **6s'** (minor) (93:7 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.3 Hz, 2H), 7.29 (d, *J* = 8.4 Hz, 2H), 4.96 (s, 1H), 3.91 (s, 3H), 3.34 (h, *J* = 7.2 Hz, 1H), 2.45–2.26 (m, 2H), 2.09–1.96 (m, 3H), 1.91–1.81 (m, 6H), 1.69–1.60 (m, 6H), 1.31 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.33, 167.18, 151.67, 129.96, 128.36, 127.10, 52.14, 52.00, 46.56, 41.64, 37.17, 36.40, 29.47, 21.35. **HRMS** (ESI-TOF) Calcd for $C_{22}H_{30}NO_3^+$ [M+H] 356.2226, found 356.2234.

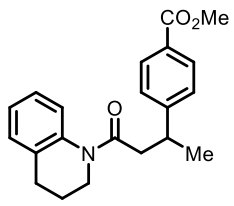


methyl 4-(4-(morpholinoamino)-4-oxobutan-2-yl)benzoate (6t): The reaction was carried out according to General Procedure F using **5t** (15.5 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), Li*O*t-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (3:1) to afford 25.7 mg (88%) of an inseparable mixture of **6t** (major) and **6t'** (minor) (97:3 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.4 Hz, 2H), 3.90 (s, 3H), 3.64–3.50 (m, 5H), 3.43 (h, *J* = 7.0 Hz, 1H), 3.39–3.21 (m, 3H), 2.73–2.44 (m, 2H), 1.36 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.04, 167.04, 151.67, 130.00, 128.50, 127.09, 66.95, 66.57, 52.14, 46.22, 42.03, 41.02, 36.84, 21.69. **HRMS** (ESI-TOF) Calcd for $C_{16}H_{22}NO_4^+$ [M+H] 292.1549, found 292.1548.

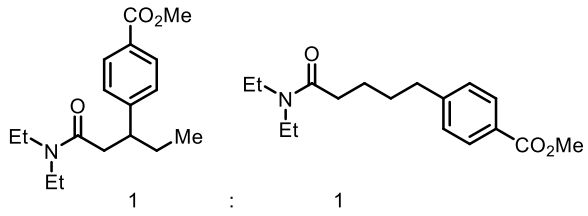


methyl 4-(4-(dibenzylamino)-4-oxobutan-2-yl)benzoate (6u): The reaction was carried out according to General Procedure F using **5u** (26.5 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), Li*O*t-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 35.3 mg (88%) of an inseparable mixture of **6u** (major) and **6u'** (minor) (86:14 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.95 (d, *J* = 8.4 Hz, 2H), 7.39–7.21 (m, 8H), 7.11–6.99 (m, 4H), 4.69–4.43 (m, 2H), 4.41–4.27 (m, 2H), 3.91 (s, 3H), 3.58 (h, *J* = 7.1 Hz, 1H), 2.95–2.57 (m, 2H), 1.33 (d, *J* = 7.0 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.91, 167.16, 151.78,

137.30, 136.49, 129.98, 129.08, 128.65, 128.39, 128.26, 127.76, 127.48, 127.24, 126.35, 52.13, 49.98, 48.45, 41.29, 36.83, 21.79. **HRMS** (ESI-TOF) Calcd for $C_{26}H_{28}NO_3^+$ [M+H] 402.2069, found 402.2079.



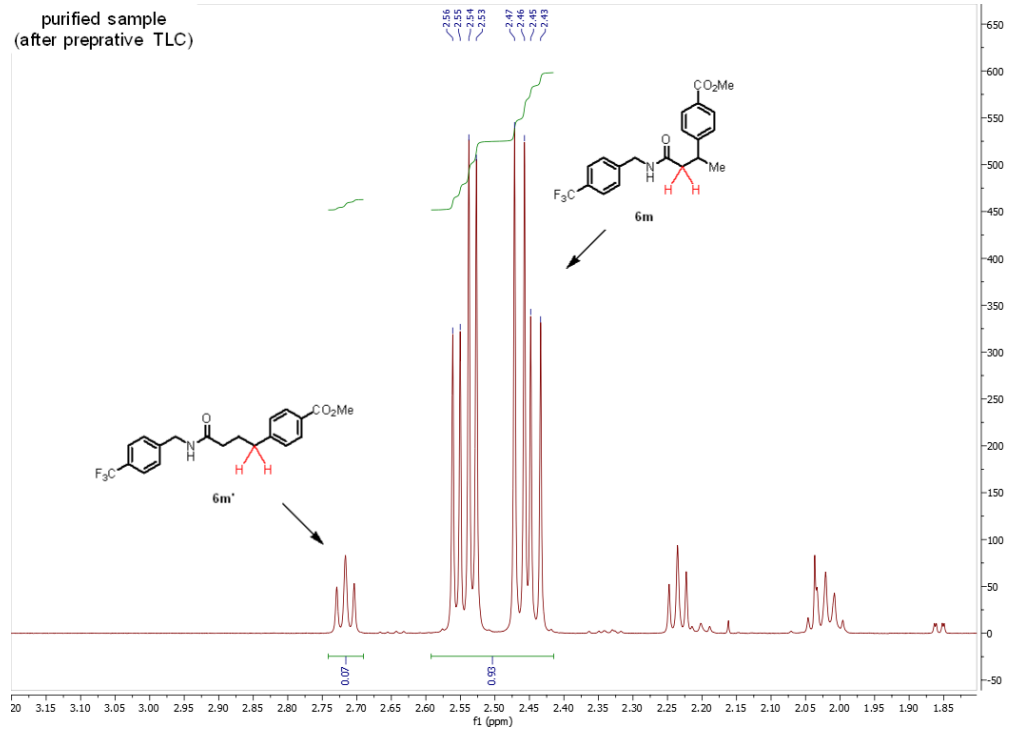
methyl 4-(4-(3,4-dihydroquinolin-1(2H)-yl)-4-oxobutan-2-yl)benzoate (6v): The reaction was carried out according to General Procedure F using **5v** (20.1 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 29.0 mg (86%) of an inseparable mixture of **6v** (major) and **6v'** (minor) (95:5 r.r.), obtained as a colorless oil. The r.r. values of the crude reaction mixture and purified sample were consistent. **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 7.9 Hz, 2H), 7.19–6.95 (m, 6H), 3.89 (s, 3H), 3.82–3.73 (m, 1H), 3.59–3.35 (m, 2H), 2.95 (dd, *J* = 14.6, 8.3 Hz, 1H), 2.69 (dd, *J* = 14.6, 6.6 Hz, 1H), 2.61–2.48 (m, 1H), 2.31 (br, 1H), 1.79–1.58 (m, 2H), 1.34–1.20 (m, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.34, 167.15, 151.53, 147.37, 139.13, 129.81, 128.62, 128.28, 127.05, 126.16, 125.55, 124.91, 52.11, 26.60, 24.07, 21.96. **HRMS** (ESI-TOF) Calcd for $C_{21}H_{23}NO_3Na^+$ [M+Na] 360.1576, found 360.1583.

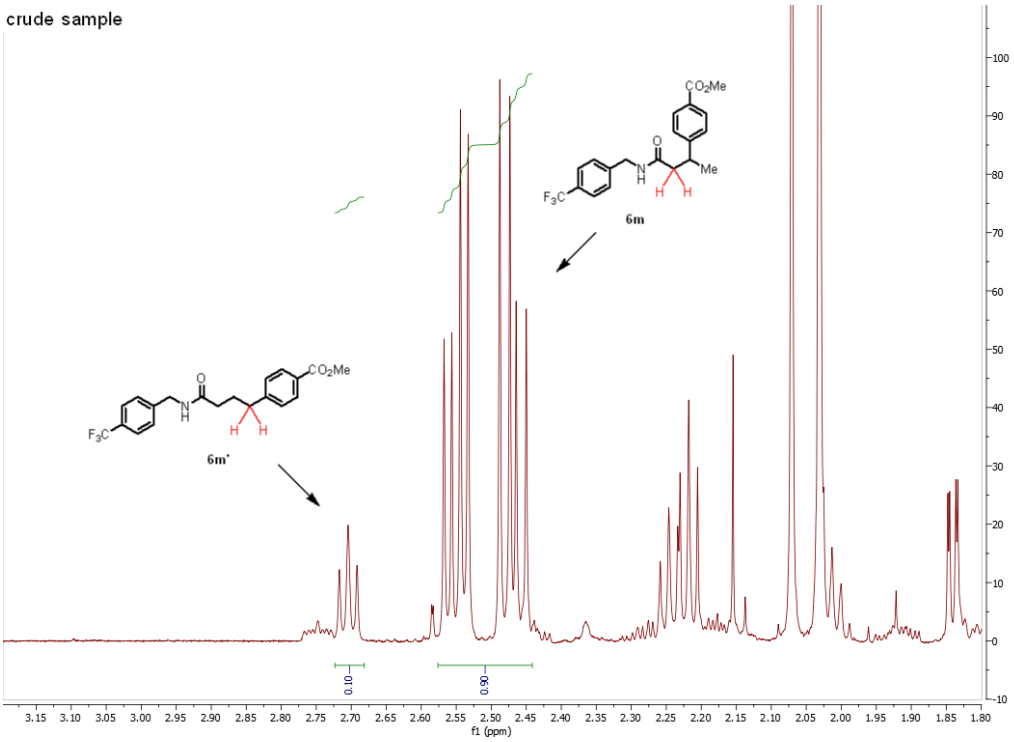


methyl 4-(1-(diethylamino)-1-oxopentan-3-yl)benzoate (6w) and methyl 4-(5-(diethylamino)-5-oxopentyl)benzoate (6w'): The reaction was carried out according to General Procedure F using **5w** (15.5 mg, 0.1 mmol), (4-(methoxycarbonyl)phenyl)boronic acid (36.0 mg, 0.2 mmol), $Ni(cod)_2$ (2.8 mg, 0.01 mmol), LiO*t*-Bu (0.4 mg, 0.005 mmol), and *i*-PrOH (0.5 mL). The reaction was run for 20 h at 40 °C, and the product was purified by preparative thin-layer chromatography (PTLC) with hexanes/acetone (5:1) to afford 18.0 mg (62%) of a mixture of **6w** and **6w'** (50:50 r.r.), obtained as a white solid. The r.r. values of the crude reaction mixture and purified sample were consistent. **6w**: **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.3 Hz, 2H), 7.28 (d, *J* = 8.3 Hz, 2H), 3.90 (s, 3H), 3.39–3.29 (m, 1H), 3.29–3.19 (m, 2H), 3.19–3.09 (m, 2H), 2.68–2.48 (m, 1H), 1.84–1.75 (m, 1H), 1.71–1.59 (m, 1H), 1.06 (t, *J* = 7.1 Hz, 3H), 1.00 (t, *J* = 7.1 Hz, 3H), 0.79 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 170.53, 167.28, 150.53, 129.82, 128.32, 127.93, 52.12, 44.32, 42.09, 40.41, 39.94, 28.82, 14.51, 13.13, 12.22. **6w'**: **^{1}H NMR** (600 MHz, $CDCl_3$) δ 7.94 (d, *J* = 8.3 Hz, 2H), 7.25 (d, *J* = 8.2 Hz, 2H), 3.90 (s, 3H), 3.36 (q, *J* = 7.1 Hz, 2H), 3.27 (q, *J* = 7.1 Hz, 2H), 2.70 (t, *J* = 7.0 Hz, 2H), 2.31 (t, *J* = 7.0 Hz, 2H), 1.78–1.61 (m, 4H), 1.15 (t, *J* = 7.2 Hz, 3H), 1.10 (t, *J* = 7.1 Hz, 3H). **^{13}C NMR** (150 MHz, $CDCl_3$) δ 171.97, 167.32, 148.11, 129.81, 128.57, 127.87, 52.10, 42.08, 40.23, 36.04, 33.00, 31.07, 25.21, 14.52, 13.25. **HRMS** (ESI-TOF) Calcd for $C_{17}H_{26}NO_3^+$ [M+H] 292.1913, found 292.1907.

Determination of Regioisomeric Ratios of the Hydroarylated Amide Products

^{1}H NMR was deemed to be a robust method for the analysis of the r.r. of the hydroarylated or hydroalkenylated amide products. In all cases, the regioisomers were found to be inseparable by PTLC. The r.r. values of the crude reaction mixture and isolated sample are generally consistent with one another (±5%). Below is a representative example (**6m**) of r.r. determination from a purified sample and crude reaction mixture:

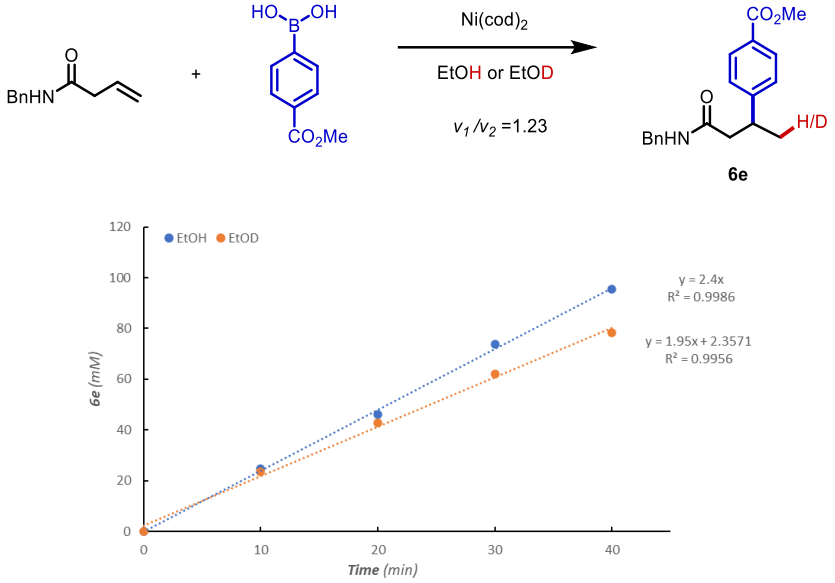




Mechanistic Investigation

Kinetic Isotope Effect Determination

All reactions were performed following a slightly modified version of General Procedure F. To a 2-dram (8-mL) scintillation vial equipped with a magnetic stir bar were added alkene **5** (87.5 mg, 0.5 mmol) and 4-methoxycarbonylphenyl boronic acid (180 mg, 1.0 mmol) outside of the glovebox. The vial was then introduced into an argon-filled glovebox antechamber. Once transferred inside the glovebox, $Ni(cod)_2$ (14.0 mg, 10 mol%) was added, followed by a solution of LiO*t*-Bu (2.0 mg) and 1,3,5-trimethoxybenzene (5.0 mg) in ethanol or ethanol-d_1 (2.5 mL) The vial was sealed with a screw-top septum cap and left to stir at 40 °C on a preheated heating block in the glovebox. Subsequently, aliquots of 200 µL were taken and quenched with acetonitrile (0.5 mL) at 10 min, 20 min, 30 min, 40 min and 50 min. The aliquots were removed from the glovebox, and then diluted with brine (10 mL). A solution of 1M HCl (0.5 mL) were added, and the aqueous solution was extracted with ethyl acetate (2 × 2 mL). The combined organic layers were dried by passage through a pad of silica gel with ethyl acetate as eluent. The filtrate was concentrated, and a ^1H NMR spectrum was collected to determine reaction progress using 1,3,5-trimethoxybenzene as internal standard.

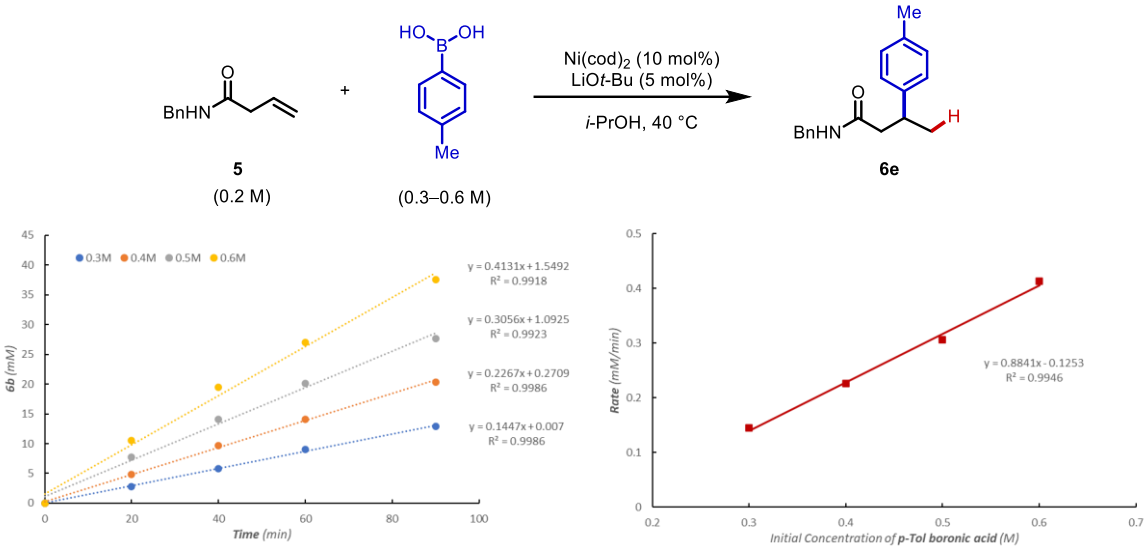


Scheme S4. Kinetic Isotope Effect Determination.

Reaction Order of Arylboronic Acid Determination

All reactions were performed following slightly modified version of General Procedure F. To a 2-dram (8-mL) scintillation vial equipped with a magnetic stir bar were added alkene **5** (87.5 mg, 0.5 mmol) and the appropriate amount of *p*-tolylboronic acid (102 mg, 136 mg, 170 mg or 204 mg) outside of the glovebox. The vial was then introduced into an argon-filled glovebox antechamber. Once transferred inside the glovebox, $Ni(cod)_2$ (14.0 mg, 10 mol%) was added, followed by a solution of LiO*t*-Bu (2.0 mg) and 1,3,5-trimethoxybenzene (5.0 mg) in *i*-PrOH (2.5 mL) (an aliquot of premade stock solution that was used for all four data sets). The vial was sealed with a screw-top septum cap and left to stir at 40 °C on a preheated heating block in the glovebox. Subsequently, aliquots of 200 µL were taken and quenched with acetonitrile (0.5 mL) at 20 min, 40 min, 60 min, 90 min and 120 min. The aliquots were removed from the glovebox, and then diluted with brine (10 mL). A solution of 1M HCl (0.5 mL) were added, and the aqueous solution was extracted with ethyl acetate (2 × 2 mL). The combined organic layers were dried by passage through a

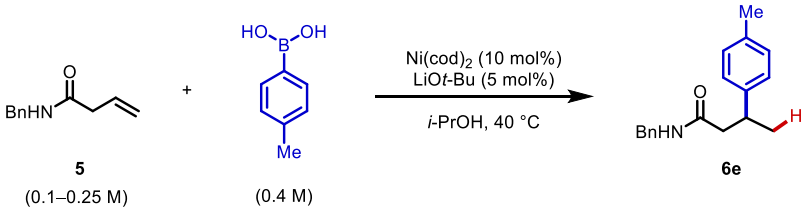
pad of silica gel with ethyl acetate as eluent. The filtrate was concentrated, and an ^{1}H NMR spectrum was collected to determine reaction progress with 1,3,5-trimethoxybenzene as internal standard.

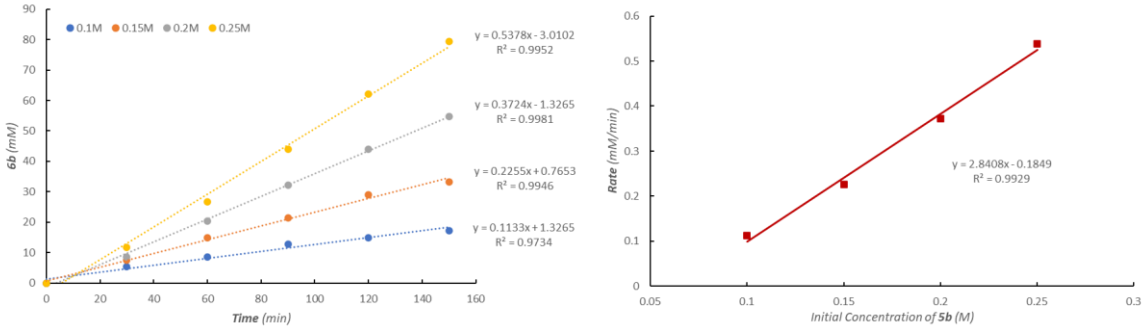


Scheme S5. Reaction Order of Arylboronic Acid Determination.

Reaction Order of Alkene Substrate Determination

All reactions were performed following slightly modified version of General Procedure F. To a 2-dram (8-mL) scintillation vial equipped with a magnetic stir bar were added appropriate amount of alkene **5** (43.8 mg, 65.6 mg, 87.5 mg and 109.4mg, respectively) and the *p*-tolboronic acid (136 mg, 1.0 mmol) outside of the glovebox. The vial was then introduced into an argon-filled glovebox antechamber. Once transferred inside the glovebox, $Ni(cod)_2$ (14.0 mg, 10 mol%) was added, followed by a solution of LiO*t*-Bu (2.0 mg) and 1,3,5-trimethoxybenzene (5.0 mg) in *i*-PrOH (2.5 mL) (an aliquot of premade stock solution that was used for all four data sets). The vial was sealed with a screw-top septum cap and left to stir at 40 °C on a preheated heating block in the glovebox. Subsequently, aliquots of 200 μL were taken and quenched with acetonitrile (0.5 mL) at 30 min, 60 min, 90 min, 120 min and 150 min. The aliquots were removed from the glovebox, and then diluted with brine (10 mL). A solution of 1M HCl (0.5 mL) were added, and the aqueous solution was extracted with ethyl acetate (2 × 2 mL). A solution of 1M HCl (0.5 mL) were added, and the aqueous solution was extracted with ethyl acetate (2 × 2 mL). The combined organic layers were dried by passage through a pad of silica gel with ethyl acetate as eluent. The filtrate was concentrated, and an ^{1}H NMR spectrum was collected to determine reaction progress with 1,3,5-trimethoxybenzene as internal standard.

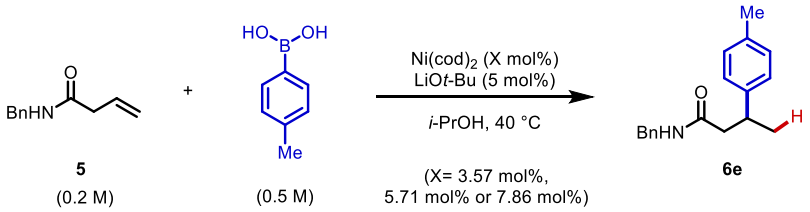


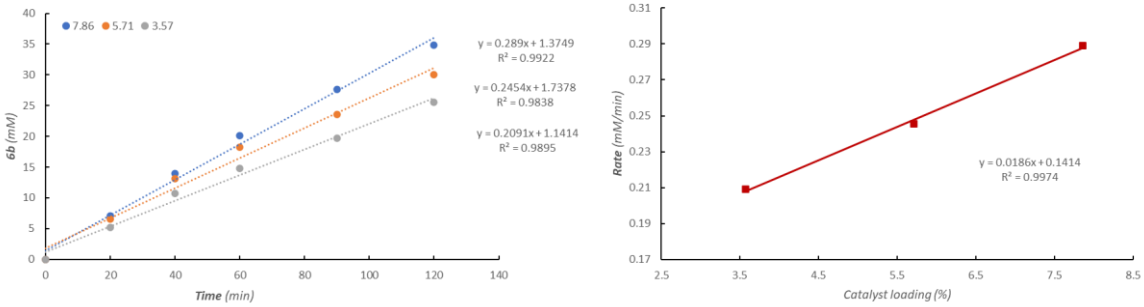


Scheme S6. Reaction Order of Alkene Substrate Determination.

Reaction Order of Ni(cod)$_2$ Determination

All reactions were performed following slightly modified version of General Procedure F. To a 2-dram (8-mL) scintillation vial equipped with a magnetic stir bar were added appropriate amount of alkene **5** (87.5 mg, 0.5 mmol) and the *p*-tolboronic acid (170 mg, 1.25 mmol) outside of the glovebox. The vial was then introduced into an argon-filled glovebox antechamber. Once transferred inside the glovebox, Ni(cod)$_2$ (11.0 mg, 8.0 mg and 5.0 mg, respctively) was added, followed by a solution of LiO*t*-Bu (2.0 mg) and 1,3,5-trimethoxybenzene (5.0 mg) in *i*-PrOH (2.5 mL) (an aliquot of premade stock solution that was used for all four data sets). The vial was sealed with a screw-top septum cap and left to stir at 40 °C on a preheated heating block in the glovebox. Subsequently, aliquots of 200 μL were taken and quenched with acetonitrile (0.5 mL) at 20 min, 40 min, 60 min, 90 min and 120 min. The aliquots were removed from the glovebox, and then diluted with brine (10 mL). A solution of 1M HCl (0.5 mL) were added, and the aqueous solution was extracted with ethyl acetate (2 × 2 mL). A solution of 1M HCl (0.5 mL) were added, and the aqueous solution was extracted with ethyl acetate (2 × 2 mL). The combined organic layers were dried by passage through a pad of silica gel with ethyl acetate as eluent. The filtrate was concentrated, and an ^{1}H NMR spectrum was collected to determine reaction progress with 1,3,5-trimethoxybenzene as internal standard.



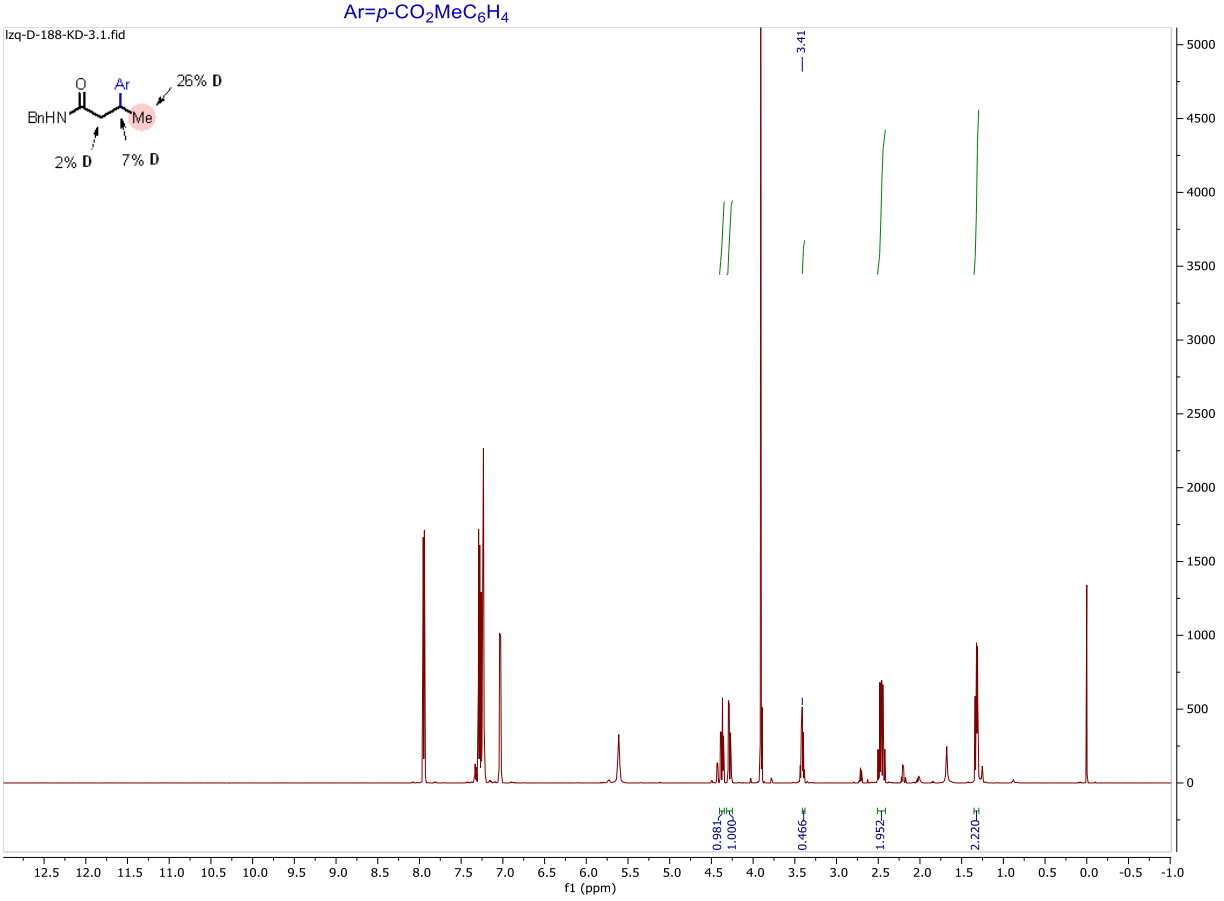


Scheme S7. Reaction Order of Ni(cod)$_2$ Determination.

Deuterium Labeling Experiments

Following slightly modified General Procedure A and B, the reactions were performed with ethanol-d_1. Deuterium incorporation was determined by ^{1}H NMR (600 MHz, $CDCl_3$, relaxation delay *d1*=10 s) with the integration of the methyl group (s, 3H) as internal standard.

Ar=*p*-$CO_2MeC_6H_4$



Computational Details

All calculations were performed with Gaussian 09.6 The B3LYP density functional and a mixed basis set of 6-31G* (for C, H, O, N) and SDD (for Ni) were used in geometry optimizations. Single-point energies were calculated with B3LYP and a mixed basis set of 6-311+G** (for C, H, O, N) and SDD (for Ni). All structures have been optimized considering solvent effects using the SMD model for 2-propanol. To confirm the nature of the stationary points, vibrational frequency calculations were performed for all optimized structures. All optimized transition state structures have only one imaginary (negative) frequency, and all minima (reactants, products, and intermediates) have no imaginary frequencies.

Complete Citation for Gaussian 09

Gaussian 09, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 09, Revision D.01; Gaussian, Inc.: Wallingford, CT, 2013.

Potential Energy Profile for Transmetalation and Reductive Elimination

We computed the energy profile for the transmetalation and reductive elimination steps. Considering the overall pH of the reaction solution, deprotonation of the directing group was not considered. Two possible coordination modes of the amide directing group were evaluated. For both Markovnikov and anti-Markovnikov selectivity, oxygen-coordination is preferred over nitrogen-coordination. For the oxygen-coordinated transition states, the $\Delta\Delta G_{sol}$ is 1.0 kcal/mol. The small energy difference explains the moderate selectivity of Markovnikov over anti-Markovnikov hydroarylation. Analysis of the energy-minimized 3D structures reveals a late transition state for the Markovnikov selectivity, with a Ni−C(Ph) bond length of 2.02 Å. On the other hand, a Ni−C(Ph) bond length of 2.08 Å is observed in the anti-Markovnikov pathway. The energy barrier of reductive elimination is 16.7 (17.3) kcal/mol, in agreement with transmetalation being rate-limiting step. Ethylene was used as model olefin ligand, representing a second molecule of alkene starting material, which could be carried on to an additional turnover.

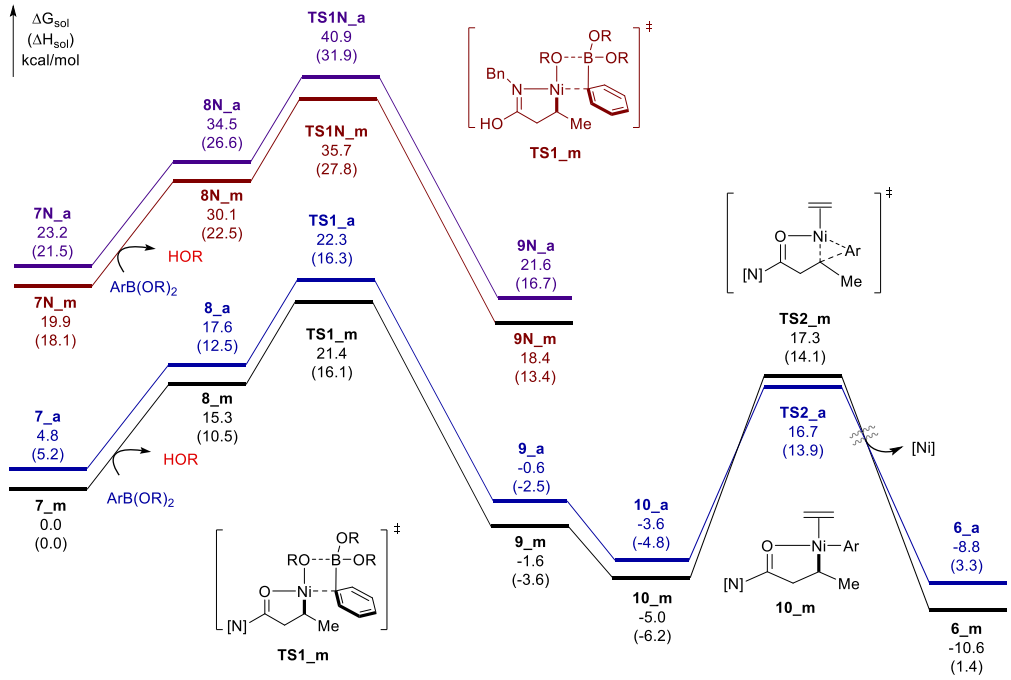


Figure S1. Potential Energy Profile

Other Coordination Modes for Transmetalation

We also considered other coordination modes for the transmetalation step. First, a three-coordinate transition state without the directing group bound was considered. However, due to the unsaturated coordination environment, a higher energy barrier was observed. Then, we tried to saturate the coordination environment with an ethylene molecule. However, the π-accepting nature of the ethylene ligand led to even higher energy barrier.

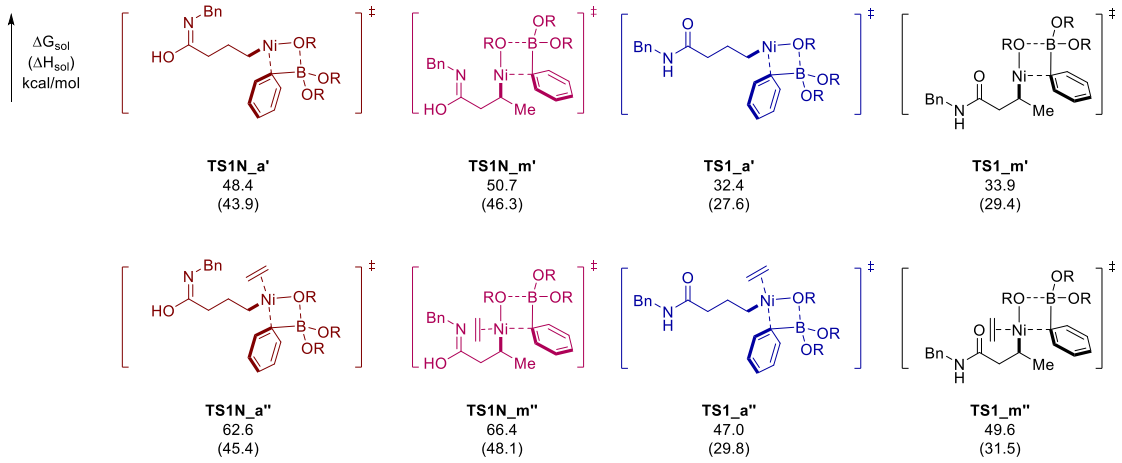
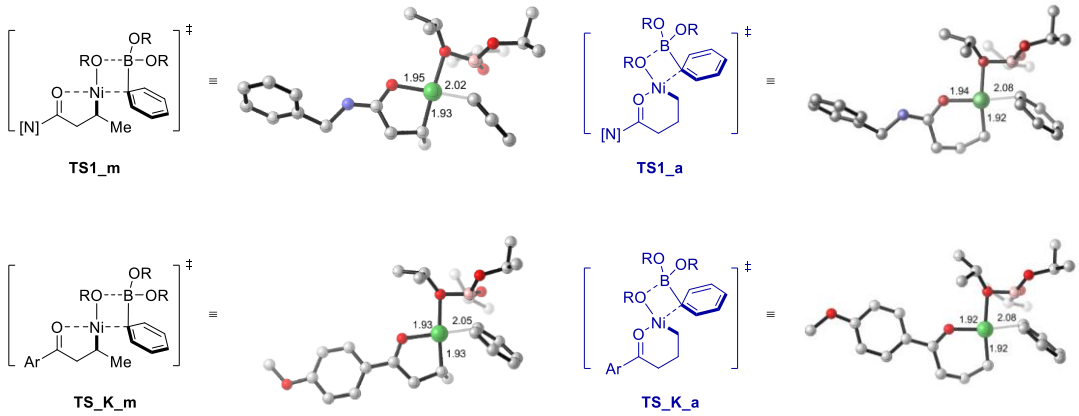


Figure S2. Other Coordination Modes for Transmetalation.

Comparison of Amide and Ketone Substrates in Transmetalation

Experimentally, moderate selectivity was observed with amide substrates, while ketone substrates gave excellent selectivity. We calculated the transition states of transmetalation for both substrates. The $\Delta\Delta G_{sol}$ for the amide substrate is 1.0 kcal/mol, while the ketone substrate has a 2.4 kcal/mol energy difference.



TS1	O(DG)–Ni (Å)	C(Ph)–Ni (Å)	C(Alkyl)–Ni (Å)	$\Delta\Delta G_{sol}$ (kcal/mol)	$\Delta\Delta H_{sol}$ (kcal/mol)
TS1_m	1.95	2.02	1.93	1.0	0.3
TS1_a	1.94	2.08	1.92		
TS1_K_m	1.93	2.05	1.93	2.4	1.9
TS1_K_a	1.92	2.08	1.92		

Figure S3. Comparison of Amide and Ketone Substrates in Transmetalation.

Mathematical Analysis

After obtaining the kinetic and computational data, we derived a rate expression that would represent the envisioned sequence of elementary reactions. A simplified catalytic system is considered herein, with a fast equilibrium (hydrometalation) followed by a slow rate-determining step (transmetalation) and a fast product-forming step (reductive elimination). A theoretical rate law could be written as equation (1). When K[A] ≪1, the rate law can be simplified as equation (2). This is in agreement with our experimental results.

For a catalytic system:
$A + \ * \ \rightleftharpoons A*,\ k_1\ and\ k_{-1}$ (A = **5a,** * = Cat.)
$A* + B \rightarrow AB*, k_{AB}$ (B = **ArB(OH)$_2$**, AB = **INT_O**)
$AB* \rightarrow P + \ *, k_p$ (P = **6**)

The rate law can be written as follows:

$$r = k_p[B]k_{AB}\frac{k_1}{k_{-1}+k_{AB}} \cdot \frac{[A][*]_{total}}{1+\frac{k_1}{k_{-1}+k_{AB}}[A]} = k'K\frac{[A][B][*]_{total}}{1+K[A]} \quad (1)$$

$$K = \frac{k_1}{k_{-1}+k_{AB}}$$

$$K[A] \ll 1$$

$$r_{theo} = k_{obs}[A][B][*]_{total} \quad (2)$$

Cartesian Coordinates (Å) and Energies of Optimized Structures

PhB(O*i*-Pr)$_2$
SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -644.33135551 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.245472 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -644.08588351 a.u.

0 1

B	0.00006900	-0.74185500	-0.00001200
C	-0.00003500	0.84279700	0.00005500
C	0.53884700	1.57466200	1.07457000
C	-0.53906900	1.57446500	-1.07454000
C	0.53507300	2.97057000	1.08136300
H	0.96574300	1.04516500	1.92433400
C	-0.53556200	2.97036900	-1.08146900
H	-0.96587200	1.04480200	-1.92424600
C	-0.00030900	3.67245200	-0.00008400
H	0.95180000	3.51005500	1.92830200
H	-0.95239400	3.50970000	-1.92845400
H	-0.00041200	4.75945900	-0.00013200
O	1.14096300	-1.49199800	0.02048600
O	-1.14074900	-1.49210400	-0.02061100
C	2.48068500	-1.01053400	-0.13749800
H	2.47563100	0.08590700	-0.16425600
C	-2.48052500	-1.01083600	0.13748100
H	-2.47564800	0.08561000	0.16413400
C	-3.29747700	-1.48321800	-1.06298700
H	-4.33813900	-1.15035700	-0.97822300
H	-2.88314200	-1.08517200	-1.99557300
H	-3.28518400	-2.57704500	-1.12497900
C	-3.02562500	-1.54109100	1.46254200
H	-3.00569200	-2.63649200	1.47151500
H	-2.41959500	-1.18100900	2.30073800
H	-4.05869400	-1.20897300	1.61683700
C	3.29758100	-1.48266300	1.06311000
H	3.28547000	-2.57648700	1.12520400
H	4.33819500	-1.14963100	0.97843900
H	2.88306500	-1.08460300	1.99561000
C	3.02600400	-1.54082700	-1.46245200
H	3.00627200	-2.63623200	-1.47130900
H	2.41998600	-1.18094500	-2.30074300
H	4.05902600	-1.20853600	-1.61668400

ethylene
SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -78.61663322 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.02842000 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -78.58821322 a.u.

0 1

C	0.00000000	0.66542900	0.00000000
H	0.92369100	1.23953300	0.00000000
H	-0.92365300	1.23957600	0.00000000
C	0.00000000	-0.66542900	0.00000000
H	-0.92369100	-1.23953300	0.00000000
H	0.92365300	-1.23957600	0.00000000

B(O*i*-Pr)$_3$
SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -606.48063395 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.25505200 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -606.22558195 a.u.

0 1

B	0.15398300	-0.38885400	-0.03824100
O	1.33301100	-1.08300000	-0.07168500
O	-0.93582500	-1.12177200	-0.43750800
C	2.60867500	-0.47093100	0.16035100
H	2.47625400	0.39289900	0.82218600
C	-2.30841500	-0.96251500	-0.07903700
H	-2.66054200	0.02999300	-0.39334800
C	-3.08951200	-2.01681900	-0.85924200
H	-4.16360500	-1.92993400	-0.66061400
H	-2.92250800	-1.89673700	-1.93430900
H	-2.75942500	-3.02129500	-0.57286500
C	-2.49060200	-1.10633700	1.43260700
H	-2.15012600	-2.09504600	1.76001900
H	-1.91215600	-0.34969300	1.97434100
H	-3.54507700	-0.99315300	1.70953200
C	3.48854300	-1.51072900	0.84887000
H	3.61234900	-2.39089600	0.20790900
H	4.47973700	-1.09719900	1.06745800
H	3.03317200	-1.83610900	1.78993500
C	3.19255600	0.00375900	-1.16998300
H	3.29152300	-0.83822800	-1.86445700
H	2.54140800	0.75513600	-1.62933600
H	4.18223900	0.45235200	-1.02396900
O	0.18933300	0.92455300	0.37544700
C	-0.78127100	1.95583400	0.17441600
H	-1.74878500	1.63102400	0.57938600
C	-0.30852800	3.16798100	0.97220600
H	0.66027700	3.51686800	0.59751100
H	-1.02935700	3.98913300	0.89168100
H	-0.19316900	2.90889800	2.02948300
C	-0.93507100	2.26207300	-1.31561700
H	-1.25391200	1.37279400	-1.86959600
H	-1.67912100	3.05094000	-1.47480400
H	0.02051700	2.60038900	-1.73239700

6_m
SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -789.49459132 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.26944100 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -789.22515032 a.u.

0 1

C	-3.01580000	-0.08844700	-0.07356600
C	-3.22806200	0.57118900	-1.29360300
C	-3.09688600	0.66311600	1.10678900
C	-3.51824700	1.93548400	-1.33247800
H	-3.17257600	0.01585100	-2.22702600
C	-3.38671200	2.02843900	1.07259400
H	-2.91801100	0.17134400	2.05949800
C	-3.60028500	2.67008200	-0.14783100
H	-3.68371100	2.42435100	-2.28942500
H	-3.44655200	2.58932600	2.00186300
H	-3.82964500	3.73207000	-0.17694600
C	-0.23310600	-1.19648100	0.59822600
O	-0.31547800	-1.44406200	1.79762300
C	-2.67072200	-1.57186500	-0.01349600
C	-1.19519700	-1.81733500	-0.41232500
H	-1.01023200	-1.45008100	-1.42994800
H	-1.00260700	-2.89807800	-0.41550800
C	1.68902000	0.33825900	0.90365000
H	1.65551300	-0.15428800	1.88057400
H	1.36958000	1.37815700	1.05756100
C	3.08639500	0.31319500	0.31705600
C	3.80023200	1.50146200	0.12938400
C	3.69441200	-0.90066700	-0.03373100
C	5.09622300	1.48262800	-0.39155700
H	3.33797000	2.45013700	0.39390900

C	4.98607100	-0.92292400	-0.55688000
C	5.69208200	0.26995000	-0.73691000
H	5.63592200	2.41571900	-0.53078400
H	5.44502100	-1.87193200	-0.82193000
N	0.72226100	-0.37147500	0.07539600
H	0.68412300	-0.14193200	-0.90776000
H	3.14662600	-1.82951400	0.10390900
H	6.69930300	0.25210400	-1.14458200
H	-2.75424200	-1.88705300	1.03255000
C	-3.61739100	-2.44616300	-0.85211800
H	-3.39289400	-3.50855400	-0.70141700
H	-4.66085400	-2.27448000	-0.56737800
H	-3.52689700	-2.23986200	-1.92515300

6_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -789.49166060 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.26947500 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -789.22218560 a.u.

0 1

C	-0.61702700	1.34405600	-0.13299200
C	2.32342300	0.27867400	-0.84569100
H	2.15887400	1.35800400	-0.76493300
O	0.08677300	2.06972700	0.56070200
C	1.20315800	-0.44252200	-0.06876500
H	1.33545900	-1.52715400	-0.16902200
C	-0.20547000	-0.06918800	-0.54297900
H	-0.94438700	-0.77031200	-0.13148400
H	-0.27836200	-0.16617200	-1.63579300
C	-2.86738200	1.03005200	-1.27468600
H	-2.40190300	0.41183000	-2.05020200
H	-3.49091600	1.75578100	-1.81199100
C	-3.75983200	0.15223900	-0.40012800
C	-4.56560600	-0.81753600	-1.01187000
C	-3.82623400	0.30513600	0.98769500
C	-5.42386300	-1.61306700	-0.25451400
H	-4.51934800	-0.95160100	-2.09130000
C	-4.68341100	-0.49343800	1.74941800
C	-5.48544200	-1.45272300	1.13203800
H	-6.03989000	-2.36218300	-0.74506100
H	-4.72059400	-0.36388800	2.82787000
N	-1.83711300	1.78908700	-0.58671700
H	-2.07280300	2.71227400	-0.24350000
H	-3.20025900	1.04579600	1.47696100
H	-6.15061600	-2.07440300	1.72511000
H	2.24880800	0.01551500	-1.91001800
H	1.29550500	-0.20507900	0.99613100
C	3.70398600	-0.06819200	-0.33191900
C	4.47045000	-1.07726500	-0.92909400
C	4.23391100	0.59754000	0.78294700
C	5.72976900	-1.41491100	-0.42972600
H	4.07759500	-1.60076400	-1.79869400
C	5.49117300	0.26345500	1.28645400
H	3.65151400	1.38634700	1.25439600
C	6.24432100	-0.74525900	0.68126400
H	6.30991400	-2.19829000	-0.91125400
H	5.88575000	0.79449000	2.14918500
H	7.22572500	-1.00391300	1.07028700

Ni-ethylene

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -249.5446226 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.025694 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -249.51892863 a.u.

0 1

Ni	-0.63303200	-0.00002100	-0.00001300
C	1.03020200	-0.73089100	0.00000400
H	1.34084200	-1.25995600	0.90619000
C	1.03010000	0.73098000	-0.00004900
H	1.34108100	1.26029800	-0.90590500
H	1.34024800	1.25991000	0.90637000
H	1.34091400	-1.26020400	-0.90601000

7_m_ethylene

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1001.18433032 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.32457100 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1000.85975932 a.u.

0 1

C	2.42309100	2.43528100	-1.34487200
H	3.41437100	2.19850300	-1.71609700
C	-0.64935500	-0.20309000	-0.29840500
C	1.74841600	-2.13233500	-1.33995800
H	1.19292300	-1.69327400	-2.18060400
H	2.80989700	-2.10862300	-1.60757000
C	2.22005200	2.73894200	-0.04000700
H	1.24558500	3.05879000	0.32050200
O	0.08574500	0.76130300	-0.63873800
C	1.49770600	-1.38005800	-0.02947700
H	2.07465400	-1.84052800	0.77607300
C	0.00375700	-1.39128500	0.35543100
H	-0.11443100	-1.25924900	1.44158400
H	-0.51205500	-2.32891600	0.09481200
C	-2.98791600	-1.13239700	-0.18863800
H	-2.64967600	-1.68567600	0.69297900
H	-3.07542300	-1.85323500	-1.01218500
C	-4.33409600	-0.48958600	0.07741000
C	-4.49202000	0.41729300	1.13553000
C	-5.43709000	-0.79254900	-0.72754500
C	-5.73083800	1.00702400	1.38210000
H	-3.64006500	0.66142300	1.76586200
C	-6.68051400	-0.20595000	-0.47925300
C	-6.82896700	0.69532200	0.57501200
H	-5.84122600	1.70673400	2.20595500
H	-7.52895400	-0.45129700	-1.11199800
Ni	1.98126100	0.48412100	-0.26705000
N	-1.97510900	-0.12009400	-0.50359000
H	-2.29014900	0.72485800	-0.96855600
H	1.61784400	2.50152200	-2.07210900
H	3.04381400	2.75495200	0.66496500
H	-7.79459800	1.15407100	0.76864500
H	-5.32404600	-1.49172900	-1.55293400
H	1.44563200	-3.19211700	-1.27216500
O	3.76157400	0.33867000	0.00830600
C	4.49214600	-0.67486500	0.63772400
H	4.15557600	-1.67660500	0.31276200
C	4.36048200	-0.60559400	2.16852500
H	4.93210000	-1.40215700	2.66394500
H	4.72986200	0.36170700	2.53202900
H	3.30980300	-0.69685100	2.46747400
C	5.96029600	-0.53340600	0.20728900
H	6.04079700	-0.60006500	-0.88306400
H	6.35171700	0.44326700	0.51731000
H	6.58704800	-1.31651900	0.65316100

7_a_ethylene

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1001.17745214 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.32117500 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1000.85627714 a.u.

0 1

N	1.99392300	0.43563900	-0.39594300

C	0.70006400	0.81355900	-0.34409800
C	0.35409400	2.19212300	0.16883300
O	-0.16518800	-0.00640000	-0.72977200
C	3.17814500	1.22146900	-0.02626100
C	-1.00993000	2.67350100	-0.34245700
C	-2.17054700	1.80741000	0.13713100
Ni	-2.09407700	-0.02815900	-0.43313800
H	2.15323500	-0.49563600	-0.76445200
H	1.15115000	2.89531700	-0.09898000
H	0.33824900	2.14121000	1.26906400
H	3.40438300	1.95970000	-0.80664900
H	2.95907300	1.77252600	0.89399500
H	-1.12855700	3.71499500	-0.00277800
H	-0.98171000	2.71458700	-1.44035300
H	-3.12508400	2.17351200	-0.24861500
H	-2.22604100	1.82122100	1.23541000
O	-3.90535100	-0.16609000	-0.24718700
C	-4.51244800	-0.77067400	0.85850400
H	-4.06910300	-1.76811000	1.07433700
C	-5.98910000	-1.00647300	0.50292700
H	-6.52130600	-1.52250600	1.31259400
H	-6.48457700	-0.04671900	0.31332300
H	-6.06579600	-1.61101300	-0.40732500
C	-4.39368400	0.05031600	2.15494000
H	-3.34398300	0.16673300	2.44690300
H	-4.81934500	1.05094100	2.01075600
H	-4.92490200	-0.43786700	2.98321600
C	-2.14964700	-1.78305600	-1.92965200
H	-3.17415400	-1.66214100	-2.26386700
H	-1.36247200	-1.48755000	-2.61871900
C	-1.86325400	-2.36748400	-0.74506700
H	-0.83805800	-2.54868000	-0.43567200
H	-2.64755000	-2.74509900	-0.09717500
C	4.36978100	0.31120600	0.18398200
C	4.43008700	-0.52613900	1.30723100
C	5.41586900	0.27958600	-0.74464100
C	5.51777700	-1.37734400	1.49717300
H	3.62213300	-0.50819100	2.03518200
C	6.50784100	-0.57065000	-0.55467800
H	5.37809700	0.92537800	-1.61899200
C	6.55969400	-1.40058900	0.56570100
H	5.55527400	-2.01893000	2.37314900
H	7.31503300	-0.58335000	-1.28171800
H	7.40854400	-2.06200300	0.71510600

7_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1117.009345230 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.37480200 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1116.634543230 a.u.

0 1

C	-1.01591500	-0.38008700	-0.44794400
C	1.28724500	-2.12149300	-2.03018500
H	0.86232200	-1.35474400	-2.69338400
H	2.36987100	-2.12661700	-2.19427300
O	-0.15268500	0.53263700	-0.35657800
C	0.96546900	-1.84882800	-0.55829600
H	1.41163700	-2.63228600	0.06314400
C	-0.55755700	-1.80875000	-0.29889500
H	-0.77892900	-2.10348500	0.73793200
H	-1.13457200	-2.48633000	-0.94751400
C	-3.45618500	-0.93342200	-0.75956000
H	-3.20251900	-1.87411800	-0.26217800
H	-3.65181900	-1.16737900	-1.81445400
C	-4.69438200	-0.32345000	-0.13151000
C	-4.68807200	0.07663500	1.21253300
C	-5.86330400	-0.16234500	-0.88244000
C	-5.83144200	0.62457600	1.79205500
H	-3.78272400	-0.03905000	1.80366600
C	-7.01148400	0.38236500	-0.30214200
C	-6.99704700	0.77750100	1.03562700
H	-5.81441400	0.93019300	2.83459000
H	-7.91262400	0.50128100	-0.89738000
Ni	1.62888500	-0.12196700	-0.05043300
N	-2.30245500	-0.04000000	-0.64305900
H	-2.47519000	0.95636200	-0.72770200
H	-7.88789900	1.20417000	1.48816700
H	-5.87681900	-0.46519500	-1.92703600
H	0.89172600	-3.09538100	-2.36877000
O	3.40763000	-0.51238900	0.17906800
C	3.97412900	-1.65744600	0.75755600
H	3.60743000	-2.56274600	0.24005500
C	3.61902400	-1.78989200	2.24660700
H	4.06140100	-2.69132700	2.69162000
H	3.98652700	-0.91613800	2.80030700
H	2.53168500	-1.83687900	2.37673400
C	5.49451500	-1.59806900	0.55451600
H	5.73022600	-1.51068800	-0.51149900
H	5.91081700	-0.72191700	1.06798200
H	5.98823600	-2.49517900	0.94911300
O	2.40099400	1.71607400	0.53954100
H	3.25349500	1.20505300	0.59132100
C	2.52778400	2.88416600	-0.29850900
H	1.49482500	3.21580800	-0.45050200
C	3.29839100	3.96506400	0.45890600
H	4.33403400	3.64904500	0.63675200
H	3.32396900	4.89959200	-0.11405800
H	2.82848100	4.16284000	1.42742700
C	3.15581900	2.54421100	-1.64983700
H	2.57495800	1.77262700	-2.16520000
H	3.19745900	3.43558900	-2.28723900
H	4.17739200	2.16698500	-1.52122000

7_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1117.001072880 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.37422500 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1116.626847880 a.u.

0 1

N	-2.34081500	-0.44120700	-0.47229200
C	-1.09052700	-0.95072300	-0.51297600
C	-0.91234900	-2.45192200	-0.50602300
O	-0.12918600	-0.14921800	-0.54484300
C	-3.60999000	-1.17705000	-0.44459900
C	0.45807900	-2.89601100	-1.03413500
C	1.62556100	-2.35467500	-0.20888000
Ni	1.77826300	-0.45795500	-0.30787000
H	-2.39442200	0.57071300	-0.49916700
H	-1.72725100	-2.91743600	-1.07322100
H	-1.02963200	-2.78750700	0.53699400
H	-3.85053600	-1.56492800	-1.44324600
H	-3.49878800	-2.03827200	0.22260300
H	0.45057000	-3.99818100	-1.03796500
H	0.54986900	-2.59022200	-2.08569900
H	2.57470800	-2.75269300	-0.57808100
H	1.51361000	-2.67289300	0.83963500
O	3.59083700	-0.43637600	-0.14380900
C	4.27820200	-0.40934200	1.07588700
H	3.89491100	0.39817500	1.73815500
C	5.75071000	-0.08189300	0.77386100
H	6.34295400	0.00473200	1.69424700
H	6.18596800	-0.87191800	0.14997200
H	5.83044200	0.86106600	0.22095200
C	4.18584200	-1.71780900	1.87978000
H	3.15091100	-1.93017600	2.16466400
H	4.55363400	-2.55920800	1.27960500

H	4.78644000	-1.65816600	2.79777600
C	-4.73025500	-0.28238400	0.04373500
C	-4.73838400	0.18337300	1.36668300
C	-5.76523300	0.09860200	-0.81691900
C	-5.76362300	1.01350400	1.81776200
H	-3.93884200	-0.10787900	2.04409700
C	-6.79555700	0.92707200	-0.36557700
H	-5.76721500	-0.25617200	-1.84499500
C	-6.79558500	1.38649800	0.95170100
H	-5.76081000	1.36539700	2.84569200
H	-7.59448200	1.21309500	-1.04400000
H	-7.59585700	2.03114300	1.30435700
O	1.77541600	1.62996500	-0.70667900
H	0.90569200	2.02092400	-0.52373000
C	2.83263000	2.58120900	-0.44796800
H	3.72266100	1.94919800	-0.46846800
C	2.88203600	3.60964100	-1.57548400
H	1.97221900	4.22538200	-1.59215300
H	3.73803500	4.28267000	-1.44764100
H	2.97756300	3.10875500	-2.54367700
C	2.66235100	3.20805100	0.93332500
H	2.62184100	2.43227200	1.70403000
H	3.50017100	3.87670400	1.16163700
H	1.74000500	3.80481900	0.98564900

7N_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1001.16110253 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.374802000 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1000.83506753 a.u.

0 1

C	-0.53636500	2.25297200	-0.54592700
C	1.08617900	1.48888300	2.22250600
H	0.00503000	1.35069400	2.36648500
H	1.59388000	0.62056800	2.65148100
C	1.46214400	1.63179500	0.74957800
H	2.54200700	1.76029200	0.65695000
C	0.72587100	2.78785400	0.05626300
H	1.33049200	3.20377700	-0.76363900
H	0.48878200	3.63301100	0.72892700
C	-1.85307200	0.45637500	-1.37528100
H	-1.56026700	-0.25199300	-2.15534000
H	-2.39916800	1.26475900	-1.87424100
C	-2.78300100	-0.24688700	-0.39615200
C	-2.81271400	0.06514500	0.96690600
C	-3.67780400	-1.20833900	-0.88720800
C	-3.71793600	-0.56933100	1.82084800
H	-2.11924400	0.79761300	1.36724800
C	-4.58681500	-1.83836200	-0.03730500
C	-4.60901600	-1.52049400	1.32265200
H	-3.72209800	-0.31983300	2.87857900
H	-5.27191700	-2.58176500	-0.43617800
N	-0.62455400	0.98633400	-0.76789400
Ni	1.00099800	-0.00143200	-0.20055800
C	0.91972800	-1.45024400	-1.95089400
H	0.35386900	-0.91636400	-2.70980100
C	0.31724100	-2.06752400	-0.90493600
H	0.89040800	-2.66828000	-0.20759200
O	-1.54434300	3.09300000	-0.86858900
H	-1.29153800	3.99547800	-0.61595000
H	-0.76029100	-2.05605000	-0.76878300
H	1.97783400	-1.57997700	-2.15253200
H	-5.31140600	-2.01446300	1.98836900
H	-3.66303700	-1.46503400	-1.94482700
H	1.37630100	2.37918000	2.80721400
O	2.41011100	-0.81323400	0.65373100
C	3.57917700	-1.28780300	0.05928200
H	3.36309700	-2.05771000	-0.71510000
C	4.41152000	-1.98697400	1.14556900
H	3.82245000	-2.78068400	1.61729100
H	5.32584000	-2.42966000	0.72965100
H	4.69213400	-1.26649300	1.92311900
C	4.39941500	-0.17966400	-0.62542700
H	3.80306900	0.31742900	-1.40078900
H	4.69563400	0.57919700	0.10952400
H	5.30862900	-0.58047000	-1.09318000

7N_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1001.15638625 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.32643700 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1000.82994925 a.u.

0 1

O	1.57991900	3.53934300	0.30800800
C	0.57270300	2.66670500	0.05508200
C	-0.65906400	3.20201500	-0.62439600
N	0.71517300	1.41680800	0.32400400
C	-1.00704800	2.29246900	-1.81974300
C	-1.53318400	0.93612500	-1.35813700
Ni	-0.83260400	0.19116600	0.28457000
C	2.02923100	0.95835600	0.81397800
O	-2.14897200	-1.06135400	0.40425100
C	-3.13894500	-1.49898200	-0.48007100
C	-3.11364500	-3.03548500	-0.53279300
C	-4.52020100	-0.98373400	-0.03993000
H	1.33032600	4.41770700	-0.01836700
H	-0.47714000	4.23749700	-0.94701700
H	-1.49889700	3.22523300	0.08074000
H	-1.74857100	2.81674000	-2.44041000
H	-0.10638900	2.18700700	-2.44002800
H	-1.38649700	0.17263600	-2.13164600
H	-2.60688800	1.01312300	-1.15842800
H	2.76753600	1.75611300	0.68688900
H	1.95494700	0.77678600	1.89201400
H	-2.95977500	-1.13777300	-1.50724600
H	-3.86820200	-3.42968700	-1.22635400
H	-2.12637700	-3.38275200	-0.85714600
H	-3.31005100	-3.45189800	0.46324500
H	-5.31680100	-1.31589300	-0.71920300
H	-4.52752600	0.11217000	-0.00930800
H	-4.75104800	-1.34893000	0.96873800
C	-0.78123900	0.04941800	2.64536000
H	-1.86445300	0.06629900	2.69678700
H	-0.25488200	0.93559300	2.99442300
C	-0.12222400	-1.07133500	2.27931400
H	0.96024600	-1.14200500	2.30500100
H	-0.66812200	-1.95825900	1.98285100
C	2.53040400	-0.29585100	0.11935400
C	3.42013800	-1.13832700	0.79958500
C	2.19270900	-0.60107700	-1.20421300
C	3.95934900	-2.26322300	0.17477300
H	3.69391400	-0.91183400	1.82858000
C	2.72744100	-1.72981000	-1.82937500
H	1.49757900	0.03549300	-1.74191100
C	3.61193400	-2.56389100	-1.14390600
H	4.64403300	-2.90720700	0.72034400
H	2.44756600	-1.95758400	-2.85452700
H	4.02444300	-3.44301300	-1.63138700

8_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.88765346 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.54758300 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.34007046 a.u.

0 1

O	3.29448700	-0.48410200	1.27863600
B	2.71385700	-0.41729900	-0.04599200
C	2.29005600	1.18230800	-0.27881900
C	1.64729400	1.58343800	-1.47863900
C	2.75269900	2.22357800	0.57000600
C	1.50429000	2.93806600	-1.83022500
H	1.35477900	0.82382900	-2.19985400
C	2.62440100	3.56235700	0.22492700
H	3.24906700	1.93682000	1.49254400
C	1.99918500	3.92234700	-0.98278500
H	1.03113100	3.21111900	-2.77064900
H	3.01319400	4.33764000	0.88130300
H	1.90986200	4.97175200	-1.25454800
O	1.34452100	-1.11464400	-0.12015000
C	1.09292500	-2.32827500	-0.84806800
H	2.06600900	-2.80337600	-0.99982100
O	3.50222200	-0.98328300	-1.12343500
C	-2.38909300	0.47739200	0.53790100
C	-0.42442800	2.16422300	2.36737700
H	-0.78344100	1.25104900	2.86227300
H	0.62468300	2.29422200	2.64972300
O	-1.42803100	-0.33781800	0.47876800
C	-0.58490500	2.10095400	0.84502900
H	-0.16857300	3.00085000	0.38528100
C	-2.06445700	1.94466000	0.44115800
H	-2.21238600	2.24013900	-0.60838500
H	-2.75331400	2.55712000	1.04306700
C	-4.88165000	0.77680600	0.74584700
H	-4.71869700	1.73070200	0.23534100
H	-5.11539100	1.00399600	1.79404800
C	-6.03755800	0.02947200	0.11107400
C	-5.98069600	-0.36028600	-1.23482200
C	-7.18072000	-0.27250700	0.85828900
C	-7.04936800	-1.03766500	-1.81995400
H	-5.09519400	-0.13374000	-1.82411200
C	-8.25469300	-0.94677000	0.27210900
C	-8.19023400	-1.33116400	-1.06729800
H	-6.99390600	-1.33416900	-2.86372100
H	-9.13680400	-1.17436200	0.86407300
Ni	0.29277200	0.51418300	0.20373000
N	-3.63848700	0.00429600	0.66138900
H	-3.71280000	-1.00550900	0.73297100
H	-7.23263700	0.02162500	1.90409700
H	-9.02314400	-1.85822800	-1.52422300
C	0.49206800	-2.02685300	-2.22191200
H	1.18744000	-1.42274100	-2.81215800
H	0.29682000	-2.95623300	-2.77161000
H	-0.45670600	-1.48505100	-2.11921800
C	0.20183400	-3.24758900	-0.01207400
H	0.66615200	-3.45712600	0.95666200
H	-0.77410900	-2.78577100	0.16794700
H	0.04714000	-4.20177700	-0.53139600
H	-0.98937300	3.00871100	2.79887200
C	4.86884300	-0.64613400	-1.28957400
H	5.24529000	-0.16979200	-0.37219000
C	5.65892600	-1.93607600	-1.53022000
H	5.28173100	-2.44497800	-2.42583000
H	6.72691000	-1.73063000	-1.67460500
H	5.54891200	-2.61970600	-0.68173900
C	5.03766100	0.33352400	-2.45823700
H	4.65863300	-0.11670100	-3.38413900
H	4.48096900	1.25800200	-2.27651800
H	6.09356900	0.59207900	-2.60845900
C	3.55570600	-1.72737000	1.90610000
H	3.46254200	-2.54609800	1.17512800
C	2.54064700	-1.95757000	3.03318900
H	2.70285500	-2.92377700	3.52867600
H	2.63273900	-1.16540600	3.78680800
H	1.52159900	-1.93191500	2.63612600
C	4.98934000	-1.72269500	2.44612700
H	5.71242100	-1.60140000	1.63314300
H	5.12149500	-0.88706300	3.14427400
H	5.21902300	-2.65505000	2.97702700

TS1_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.87760473 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.54712400 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.33048073 a.u.

0 1

O	3.01550900	-0.70172100	1.28340600
B	2.54064100	-0.63550900	-0.05486900
C	2.06371400	1.29319000	-0.20551000
C	1.94723600	1.84150000	-1.50667000
C	2.77372500	2.07015500	0.73596200
C	2.47499200	3.08851900	-1.84078100
H	1.43715200	1.27237300	-2.28065300
C	3.33101000	3.30809200	0.40938100
H	2.91151900	1.67215900	1.73647100
C	3.17161700	3.82742300	-0.87789300
H	2.35589200	3.48261400	-2.84790500
H	3.88421800	3.87185300	1.15758300
H	3.59569100	4.79575500	-1.13399800
O	1.24728100	-1.29583300	-0.26677000
C	0.99524700	-2.24911700	-1.32311900
H	1.95073600	-2.74325700	-1.52336500
O	3.42240600	-0.89727900	-1.12173300
C	-2.37469900	0.45405700	0.52961200
C	-0.35878300	2.00595800	2.46304300
H	-0.77573200	1.10208700	2.92913200
H	0.69124600	2.06892400	2.76564800
O	-1.46314200	-0.40845700	0.42011200
C	-0.49231900	1.98252200	0.93635100
H	-0.04913800	2.89044800	0.51692200
C	-1.97461800	1.90644000	0.51022200
H	-2.09341100	2.25449900	-0.52696900
H	-2.64570600	2.52244500	1.12946500
C	-4.84853200	0.87773300	0.76685900
H	-4.63866200	1.84399100	0.29865000
H	-5.06300600	1.06969800	1.82637900
C	-6.04868400	0.22438600	0.11035700
C	-6.02292500	-0.10744800	-1.25197000
C	-7.20216100	-0.04719500	0.85340800
C	-7.13166900	-0.69737000	-1.85697000
H	-5.12981100	0.09605100	-1.83810100
C	-8.31602400	-0.63400100	0.24783000
C	-8.28219600	-0.96081200	-1.10788300
H	-7.09995300	-0.94894200	-2.91351400
H	-9.20553100	-0.83861500	0.83719900
Ni	0.31389500	0.37524900	0.23051800
N	-3.65075600	0.04458000	0.63366700
H	-3.77988500	-0.96165800	0.65675100
H	-7.23063500	0.20243000	1.91162200
H	-9.14630400	-1.41973200	-1.58024900
C	0.52824800	-1.56221800	-2.60499800
H	1.29601900	-0.87500100	-2.97006000
H	0.33809400	-2.30879200	-3.38603900
H	-0.40011100	-1.00457300	-2.43148900
C	-0.01382500	-3.26844000	-0.79969300
H	0.36356400	-3.75143500	0.10751300
H	-0.96313300	-2.78014400	-0.55843100
H	-0.19650300	-4.04394500	-1.55335500
H	-0.88150700	2.87063700	2.90846600
C	4.82955500	-0.67686600	-1.02851500
H	5.06187200	-0.24611800	-0.04660900
C	5.54318100	-2.02485100	-1.16219400
H	5.29912200	-2.48829700	-2.12588000

H	6.63160400	-1.90082400	-1.10655700
H	5.23466900	-2.71170500	-0.36672100
C	5.26124200	0.30021700	-2.12363000
H	5.01181300	-0.10444300	-3.11220200
H	4.75566900	1.26272200	-2.00911100
H	6.34437300	0.46946700	-2.08516400
C	3.04364900	-1.95079100	1.97304700
H	2.99229600	-2.77719100	1.24694200
C	1.84556600	-2.05823200	2.92159000
H	1.86161700	-3.00902100	3.46981700
H	1.87217300	-1.23926300	3.65046100
H	0.90802800	-1.99091400	2.36281900
C	4.37004500	-2.04672000	2.72912300
H	5.21800500	-1.99070700	2.03892400
H	4.45651700	-1.21709700	3.44076300
H	4.43819100	-2.98842600	3.28713200

9_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.91121940 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.54415600 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.36706340 a.u.

0 1

O	2.66985600	-1.45448700	1.34989800
B	2.53229400	-1.34661100	-0.00251200
C	1.96416800	1.83430600	-0.26900500
C	2.10352800	2.60309700	-1.44474700
C	3.05443900	1.86697900	0.62442700
C	3.26296600	3.33159800	-1.72814600
H	1.28457400	2.64069700	-2.16241900
C	4.21938600	2.59641600	0.35348600
H	3.00821200	1.30672500	1.55610200
C	4.33219200	3.33027000	-0.82873200
H	3.32927000	3.90726800	-2.65003700
H	5.03736700	2.59379500	1.07237500
H	5.23368000	3.90035800	-1.04149300
O	1.28781200	-1.09367100	-0.59221200
C	1.01731600	-1.61231500	-1.93453700
H	1.91707700	-2.14519500	-2.25238300
O	3.60411500	-1.53053700	-0.82187700
C	-2.28108600	0.60363800	0.47260900
C	-0.28491600	2.46182400	2.24697400
H	-0.56070300	1.54662800	2.79039100
H	0.76911000	2.66486800	2.46242200
O	-1.31716400	-0.18699800	0.32241100
C	-0.51614800	2.33157400	0.73700900
H	-0.20742600	3.26093600	0.24927900
C	-2.00913100	2.08767400	0.41898300
H	-2.23848400	2.41306200	-0.60709500
H	-2.68856600	2.64520200	1.08315500
C	-4.77391200	0.83686000	0.82469500
H	-4.63725900	1.83944600	0.41005600
H	-4.99493900	0.95630500	1.89379100
C	-5.93184700	0.13943300	0.13704700
C	-5.89635800	-0.10672600	-1.24309200
C	-7.05638800	-0.25749300	0.86784400
C	-6.96702200	-0.73461000	-1.87747100
H	-5.02494400	0.19422500	-1.81985400
C	-8.13232500	-0.88371700	0.23350500
C	-8.08915400	-1.12376500	-1.13991500
H	-6.92829600	-0.91778800	-2.94781400
H	-8.99971700	-1.18584100	0.81394600
Ni	0.41178300	0.80226700	0.03687600
N	-3.52101500	0.10192600	0.64366400
H	-3.57081600	-0.91110500	0.66977500
H	-7.09239000	-0.07447800	1.93943600
H	-8.92386500	-1.61213500	-1.63513200
C	0.75648100	-0.47209400	-2.90998100
H	1.60750000	0.21199300	-2.94666900
H	0.59118200	-0.88237500	-3.91396700
H	-0.13316900	0.09914400	-2.62009800
C	-0.15172500	-2.58782300	-1.82933000
H	0.09200200	-3.41956100	-1.15916700
H	-1.03805600	-2.07974500	-1.43810900
H	-0.38541500	-3.00403800	-2.81658900
H	-0.87688700	3.28536200	2.68406700
C	4.93190700	-1.78505700	-0.32589100
H	4.97600200	-1.47821600	0.72440800
C	5.21660500	-3.28216000	-0.42732200
H	5.13463500	-3.61771100	-1.46781800
H	6.22785100	-3.50908600	-0.07026600
H	4.50379500	-3.85226600	0.17833100
C	5.89552200	-0.93458900	-1.14758800
H	5.84493800	-1.21249500	-2.20683000
H	5.64009600	0.12549300	-1.05539300
H	6.92541400	-1.07941700	-0.80081700
C	1.58679500	-1.50290200	2.29581500
H	0.80942800	-0.79644600	1.97986800
C	2.15011000	-1.06722000	3.64471700
H	1.36437800	-1.07743800	4.40852400
H	2.95148200	-1.74443400	3.96268500
H	2.55920600	-0.05395600	3.58505700
C	1.00325200	-2.91456000	2.33468700
H	0.59245900	-3.19077200	1.35856200
H	1.77715300	-3.64133900	2.60930800
H	0.19497300	-2.97584900	3.07278400

8_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.88467350 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.54812700 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.33654650 a.u.

0 1

O	2.93769100	-1.09900600	1.42168200
B	2.60257000	-0.80291600	0.04215200
C	2.73779900	0.82140800	-0.35991000
C	2.32138000	1.23305200	-1.65416800
C	3.48615200	1.77354500	0.38654300
C	2.63431400	2.50891000	-2.17352000
H	1.88603100	0.49793000	-2.32805100
C	3.80501400	3.02201300	-0.12246600
H	3.85286500	1.49155700	1.36883500
C	3.36960200	3.39911200	-1.40976200
H	2.31785700	2.77732400	-3.17882300
H	4.40428400	3.71479700	0.46449300
H	3.62835500	4.37886900	-1.80412400
O	1.12460600	-1.03141000	-0.30143400
C	0.64864900	-2.22915400	-0.93818500
H	1.53092000	-2.84834200	-1.11969000
O	3.38670800	-1.61506900	-0.85586200
C	0.00274100	-1.89644800	-2.28482800
H	0.72281900	-1.40875300	-2.95025300
H	-0.34420100	-2.81200300	-2.78013500
H	-0.85908700	-1.23102800	-2.15319700
C	-0.31042900	-2.98130100	-0.01349200
H	0.19172600	-3.26134500	0.91653100
H	-1.17680400	-2.35806600	0.23585200
H	-0.66892000	-3.89840200	-0.49829900
C	4.77228900	-1.81596100	-0.63047800
H	5.16667100	-1.01343200	0.01215700
C	5.00673800	-3.15300500	0.08085000
H	4.61902300	-3.97816800	-0.53016400
H	6.07646500	-3.32832900	0.25606800
H	4.48505200	-3.15410800	1.04102300
C	5.48710000	-1.75467800	-1.98318200
H	5.09313700	-2.52982800	-2.65203300

H	5.32508000	-0.78163600	-2.45988600
H	6.56716300	-1.91206300	-1.87163300
C	2.33193400	-0.51104600	2.55171300
H	1.91500900	0.47970400	2.29480500
C	3.40914900	-0.32182100	3.62650700
H	2.99775800	0.14645300	4.52917300
H	3.83167200	-1.29516200	3.90298000
H	4.22988400	0.30179600	3.25537500
C	1.18133600	-1.37629100	3.08405800
H	0.38542300	-1.45758200	2.34040800
H	1.54692100	-2.38530600	3.31098100
H	0.75942500	-0.94793800	4.00329200
N	-3.49135300	0.37728600	0.40626600
C	-2.30631000	1.01750300	0.39326700
C	-2.26195700	2.48554100	0.75511300
O	-1.29155900	0.35989400	0.06528700
C	-4.80285600	0.92386500	0.77481400
C	-0.84697200	2.98082000	1.07187700
C	0.14606700	2.72558900	-0.05968400
Ni	0.53359200	0.86871400	-0.28407800
H	-3.44847900	-0.60824400	0.16929000
H	-2.94671300	2.67503900	1.59037700
H	-2.66457600	3.04251000	-0.10581200
H	-4.89808700	0.98296000	1.86694900
H	-4.87479100	1.94459500	0.38456400
H	-0.92740200	4.05730600	1.29001800
H	-0.49991500	2.51033500	2.00251900
H	1.09145500	3.23823000	0.13942300
H	-0.25376800	3.11046800	-1.01206800
C	-5.91628200	0.06906100	0.20623900
C	-6.09263900	-0.03399500	-1.18131300
C	-6.78022000	-0.63010500	1.05560700
C	-7.11538700	-0.82221500	-1.70688000
H	-5.42633800	0.50569900	-1.85051300
C	-7.80850900	-1.41649200	0.53063200
H	-6.64971200	-0.55869000	2.13290200
C	-7.97670900	-1.51443200	-0.85077000
H	-7.24331700	-0.89350300	-2.78338900
H	-8.47352200	-1.95320500	1.20137900
H	-8.77486100	-2.12698200	-1.26064100

TS1_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.87731414 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.54835200 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.32896214 a.u.

0 1

O	3.21976800	-0.73339000	1.38830500
B	2.48760500	-0.82060200	0.16436100
C	2.40267200	0.86351800	-0.62830000
C	2.04602000	0.89539700	-2.00061300
C	3.35685800	1.82285900	-0.21734500
C	2.57853600	1.82788400	-2.89301900
H	1.35349400	0.14963100	-2.38350100
C	3.91858100	2.74319400	-1.09961000
H	3.67427900	1.83472900	0.82064500
C	3.52055300	2.75508000	-2.44086700
H	2.27376900	1.82471400	-3.93723300
H	4.66329900	3.45391500	-0.74828500
H	3.95180200	3.47646100	-3.13128400
O	1.04260800	-1.15704000	0.29170700
C	0.50218100	-2.41707400	-0.15682900
H	1.33967700	-3.12026600	-0.17446300
O	3.10605400	-1.67104700	-0.79083500
C	-0.05631600	-2.29892300	-1.57480900
H	0.73860400	-2.01688200	-2.27029300
H	-0.47295300	-3.25925800	-1.90363300
H	-0.85328800	-1.54628600	-1.61646200
C	-0.54615700	-2.90194500	0.84347700
H	-0.10771400	-3.02657800	1.83808800
H	-1.36931700	-2.18497100	0.91937700
H	-0.95047700	-3.87094400	0.52567100
C	4.52280800	-1.72253600	-0.92268000
H	4.95959800	-0.78933500	-0.53960400
C	5.08195400	-2.89199500	-0.10744600
H	4.64920200	-3.83753200	-0.45784800
H	6.17319800	-2.95573600	-0.20669300
H	4.83144000	-2.76289600	0.94848100
C	4.85280400	-1.84723300	-2.41123000
H	4.40358600	-2.75898000	-2.82398700
H	4.45705500	-0.98922000	-2.96427400
H	5.93681700	-1.89516800	-2.57138700
C	2.74789600	-0.14628900	2.58633100
H	2.04698700	0.67494700	2.34927300
C	3.95145000	0.42875200	3.33983800
H	3.63781600	0.91132700	4.27319200
H	4.65578000	-0.37478100	3.58612700
H	4.48647100	1.16573600	2.73214200
C	2.00645100	-1.17319400	3.45028700
H	1.12648100	-1.55003800	2.92555700
H	2.66726400	-2.01915000	3.67509900
H	1.68263300	-0.72570600	4.39881300
N	-3.57007900	0.53934600	0.47189800
C	-2.35388400	1.12002700	0.49857100
C	-2.24482100	2.62320500	0.39932900
O	-1.35059900	0.37805300	0.61520300
C	-4.87901200	1.19636700	0.36354900
C	-0.94833200	3.13817700	1.03773500
C	0.31161000	2.65687900	0.32103900
Ni	0.50473400	0.74991400	0.20617300
H	-3.56508300	-0.47064300	0.56461000
H	-3.12522800	3.09006200	0.85501700
H	-2.26402800	2.89077800	-0.66891900
H	-5.16245900	1.64262900	1.32565000
H	-4.80156700	2.00969800	-0.36556800
H	-1.00435000	4.23808100	1.03836900
H	-0.93243200	2.83409600	2.09389800
H	1.19551600	3.04526100	0.84005400
H	0.33933700	3.05778900	-0.70400700
C	-5.93511600	0.20355600	-0.07469700
C	-5.89948900	-0.34440900	-1.36517100
C	-6.95229900	-0.18798000	0.80235200
C	-6.86453600	-1.26615500	-1.76851800
H	-5.11338300	-0.04606100	-2.05514100
C	-7.92255800	-1.10821600	0.39846700
H	-6.98731700	0.23005300	1.80576400
C	-7.87924400	-1.64929900	-0.88673200
H	-6.82800100	-1.68229300	-2.77143600
H	-8.70837400	-1.40185800	1.08878200
H	-8.63247400	-2.36582100	-1.20223900

9_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.90959420 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.54405800 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.36553620 a.u.

0 1

O	-2.43569800	1.39601000	1.51287600
B	-2.24244700	1.43966200	0.16374300
C	-2.33320800	-1.80275000	-0.49097300
C	-2.47731300	-2.43916500	-1.74221900
C	-3.51839400	-1.61526400	0.24954100
C	-3.72350900	-2.83351700	-2.24036900
H	-1.59381300	-2.64491000	-2.34599200
C	-4.77087200	-2.01018800	-0.23716000
H	-3.47436600	-1.14903100	1.23181600

C	-4.88126200	-2.61730400	-1.48981700
H	-3.78909100	-3.31779400	-3.21349600
H	-5.66111300	-1.84899200	0.36915400
H	-5.85199000	-2.92730600	-1.87002400
O	-1.08934900	0.92851200	-0.44095400
C	-0.67292700	1.49040400	-1.72487400
H	-1.56150700	1.92530200	-2.18792600
O	-3.17253000	2.03842800	-0.63371600
C	-0.13082500	0.39459800	-2.63245500
H	-0.88737000	-0.37377200	-2.80832800
H	0.14818000	0.83322400	-3.59873900
H	0.75691700	-0.07821000	-2.19952300
C	0.35121500	2.58956400	-1.44914600
H	-0.07880200	3.37904400	-0.82273600
H	1.22291400	2.17347900	-0.93262100
H	0.68430600	3.04688900	-2.38842000
C	-4.41516700	2.56362200	-0.13336000
H	-4.57838600	2.17326200	0.87655600
C	-4.31527600	4.08658800	-0.07541500
H	-4.10348600	4.49478500	-1.07061900
H	-5.25437000	4.52319600	0.28394700
H	-3.51245900	4.39482500	0.60322600
C	-5.52416500	2.07056000	-1.05820500
H	-5.36425500	2.43773600	-2.07870500
H	-5.53791500	0.97651800	-1.08414500
H	-6.50109800	2.42699000	-0.71117900
C	-1.48230300	0.96452700	2.49830300
H	-0.97387700	0.06616100	2.12365600
C	-2.27160300	0.61039000	3.75481200
H	-1.59776400	0.25838200	4.54404600
H	-2.81417900	1.48723000	4.12759200
H	-2.99865700	-0.18017600	3.54436000
C	-0.45399900	2.06759500	2.74246000
H	0.10990100	2.27826100	1.82896100
H	-0.95106400	2.98799700	3.07192000
H	0.25672000	1.76290100	3.51980400
N	3.41797700	-0.43043800	0.50804600
C	2.24415000	-1.08908100	0.64756500
C	2.26899700	-2.55884100	1.00515200
O	1.18242400	-0.45492300	0.47392000
C	4.77357800	-0.96104600	0.68569900
C	0.95408800	-3.03384800	1.63667700
C	-0.25562000	-2.96139300	0.69839100
Ni	-0.64248700	-1.19219700	0.08496400
H	3.33026100	0.55649000	0.29332300
H	3.11759800	-2.75922500	1.67008800
H	2.46044300	-3.12411600	0.07908900
H	5.01260200	-1.05893900	1.75320200
H	4.81528600	-1.96493000	0.24969700
H	1.12092600	-4.07005700	1.97233400
H	0.77130600	-2.44752900	2.54853600
H	-1.12996200	-3.37871800	1.20970000
H	-0.07765900	-3.59332000	-0.18742600
C	5.79059700	-0.06226200	0.01312500
C	5.78753000	0.09240700	-1.38088800
C	6.74286200	0.62801800	0.77041300
C	6.72041600	0.92118500	-2.00264900
H	5.05164900	-0.44019200	-1.97900000
C	7.68129800	1.45552800	0.14890400
H	6.75235600	0.51646500	1.85221700
C	7.67068800	1.60424900	-1.23816600
H	6.70957800	1.03075700	-3.08357900
H	8.41666700	1.98376800	0.74941600
H	8.39898200	2.24816700	-1.72330700

8N_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.86852488 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.55188900 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.31663588 a.u.

0 1

O	-1.28944500	-1.39793500	-1.10217400
C	-1.24150800	-2.81778300	-1.10028300
B	-1.80351700	-0.65967400	0.03158200
C	-1.98445500	0.91912000	-0.48119000
C	-2.21248700	1.95888800	0.45458200
C	-2.15569500	1.25264600	-1.84998100
C	-2.60742000	3.24765700	0.05633600
H	-2.17252200	1.73627800	1.51821500
C	-2.55592300	2.52026500	-2.25264000
H	-1.98505600	0.47024900	-2.58406500
C	-2.78278300	3.52423600	-1.29516800
H	-2.79396700	4.01684400	0.80208100
H	-2.69970800	2.74056500	-3.30796600
H	-3.10231500	4.51407300	-1.61275800
O	-0.70190200	-0.54574800	1.13133900
C	-1.05639300	-0.66779200	2.52656600
H	-2.10994200	-0.38957200	2.62986800
O	-2.97808600	-1.20187800	0.68067800
C	-4.22918100	-1.27405700	0.01302400
C	2.55813400	1.99224900	0.69523200
C	1.28007100	2.16121900	-2.18787000
H	2.08707600	1.42171400	-2.11042900
H	0.49294900	1.72381500	-2.80893500
C	0.74067300	2.57055400	-0.81569800
H	-0.06975900	3.29548800	-0.93262300
C	1.85510700	3.16001900	0.07048500
H	1.43773700	3.78781000	0.87092800
H	2.57824000	3.78896500	-0.48071400
C	2.57164900	-0.34048900	1.25660300
H	1.77619900	-1.07871300	1.37219900
H	3.00276200	-0.14570300	2.24559500
C	3.65065700	-0.86216100	0.32218500
C	3.34037300	-1.20412300	-1.00200300
C	4.96394500	-1.03001600	0.77368600
C	4.32664000	-1.70131000	-1.85405100
H	2.32203600	-1.08577200	-1.36035600
C	5.95098400	-1.53588500	-0.07549200
C	5.63488000	-1.87061000	-1.39274900
H	4.07114200	-1.96504100	-2.87700600
H	6.96598900	-1.66315100	0.29202900
Ni	0.07759900	1.05562800	0.18832100
N	1.91329200	0.87987700	0.75092800
O	3.80903400	2.09193100	1.18142400
H	4.15091400	2.98304200	1.00389200
H	1.68601500	3.03008300	-2.73386100
H	6.40135300	-2.26276100	-2.05598500
H	5.21666200	-0.75903800	1.79613900
C	-0.21220400	0.26377800	3.39749500
H	-0.56024700	0.21137500	4.43621900
H	0.84574600	-0.01799400	3.38717500
H	-0.29208000	1.30556800	3.06673900
C	-0.91264300	-2.12900900	2.95550000
H	-1.55750500	-2.76196200	2.34162100
H	0.12491000	-2.46794800	2.84493700
H	-1.20358700	-2.25350600	4.00629500
H	-1.82771000	-3.20168200	-0.25426200
H	-4.08876000	-1.09845000	-1.06475500
C	-4.81161600	-2.67782900	0.20615600
H	-4.92499500	-2.89109400	1.27596500
H	-5.79667300	-2.76557800	-0.26833800
H	-4.15398100	-3.43948600	-0.22394300
C	-5.18520000	-0.20784500	0.56345000
H	-6.16662600	-0.26914200	0.07669700
H	-5.32642100	-0.35478700	1.64136600
H	-4.78731800	0.79867900	0.40513200
C	0.20156400	-3.30773500	-0.94952200

H	0.24656200	-4.40422400	-0.93171300
H	0.81398200	-2.95548600	-1.78820800
H	0.63940000	-2.92918800	-0.02138900
C	-1.86680200	-3.32739800	-2.40241300
H	-2.90928000	-3.00232400	-2.48650200
H	-1.31762700	-2.92784600	-3.26408400
H	-1.84081700	-4.42293200	-2.45619300

TS1N_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.85867789 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.55099900 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.30767889 a.u.

0 1

O	1.08807600	1.35831500	-1.02537800
C	0.87798400	2.76640400	-1.17922700
B	1.58704300	0.83817400	0.19336000
C	1.93152400	-1.12224900	-0.33178700
C	2.55338500	-1.97345300	0.61333400
C	2.43989100	-1.17942800	-1.64737300
C	3.57886800	-2.85449800	0.26496000
H	2.22349400	-1.95584800	1.65081400
C	3.48515800	-2.03381300	-2.00539000
H	2.00881000	-0.52411700	-2.39924100
C	4.04772200	-2.88753100	-1.05234000
H	4.01880200	-3.50776900	1.01571900
H	3.85608100	-2.04327300	-3.02825000
H	4.85198900	-3.56494300	-1.32997500
O	0.55637100	0.65736200	1.22554400
C	0.95588100	0.62857200	2.62398400
H	1.99277500	0.28414900	2.66814700
O	2.79662400	1.29681800	0.73560000
C	3.96517000	1.59054500	-0.03309400
C	-2.43869300	-2.17173700	0.44410100
C	-0.93256100	-2.07469500	-2.38101800
H	-1.80670600	-1.41178000	-2.34124800
H	-0.14153900	-1.53949500	-2.91566100
C	-0.46961300	-2.49638500	-0.98404600
H	0.39028300	-3.16611900	-1.07283300
C	-1.59499900	-3.21975600	-0.21736400
H	-1.17974400	-3.86925600	0.56719900
H	-2.22837600	-3.86418300	-0.85599300
C	-2.71740400	0.06880000	1.22514800
H	-2.01880400	0.88705300	1.41750200
H	-3.11732500	-0.26098100	2.19189300
C	-3.86237700	0.55458000	0.34946800
C	-3.65989700	0.85464400	-1.00467400
C	-5.13427700	0.74833700	0.89921600
C	-4.70820100	1.33806300	-1.78838000
H	-2.67741500	0.70800200	-1.44299600
C	-6.18322700	1.23943100	0.11884200
C	-5.97322400	1.53458800	-1.22878200
H	-4.53512200	1.56615800	-2.83698600
H	-7.16483000	1.38329000	0.56306100
Ni	-0.02813000	-0.96241700	0.12287100
N	-1.91693000	-1.00997700	0.62219700
O	-3.69373600	-2.43870300	0.85703700
H	-3.92818700	-3.34369000	0.59481500
H	-1.21427500	-2.94611600	-2.99740600
H	-6.78852800	1.91329000	-1.83950400
H	-5.30722500	0.50773700	1.94586900
C	0.07284200	-0.33444100	3.41171200
H	0.42174500	-0.38221600	4.45004200
H	-0.97069200	-0.00403300	3.42322100
H	0.11064000	-1.34517500	2.99210400
C	0.88822600	2.05289600	3.17211000
H	1.54423700	2.70987600	2.59616900
H	-0.13665700	2.43970900	3.11957900
H	1.21036600	2.07487500	4.22030300
H	1.40953700	3.30229400	-0.38095600
H	3.75435400	1.40994100	-1.09492000
C	4.33651500	3.06229200	0.16889000
H	4.50526100	3.26412000	1.23333900
H	5.25662300	3.30594200	-0.37547900
H	3.54544100	3.73082800	-0.18378700
C	5.10385500	0.67237900	0.41428400
H	6.01749000	0.89023200	-0.15200400
H	5.31515900	0.82733500	1.47937100
H	4.84387400	-0.37690700	0.26201700
C	-0.61157000	3.09601700	-1.06947600
H	-0.77901200	4.17548700	-1.17169600
H	-1.17406200	2.58607000	-1.85940100
H	-1.00925100	2.77573200	-0.10222700
C	1.45136100	3.19246300	-2.53115700
H	2.52466100	2.98356800	-2.58561200
H	0.95632300	2.63978600	-3.33846600
H	1.29802900	4.26460500	-2.70316800

9N_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.88358575 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.54833000 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.33525575 a.u.

0 1

O	0.53866400	1.67629700	-0.47451700
C	0.67865400	2.92232700	-1.17421000
B	1.29805100	1.21494400	0.56371000
C	1.72902600	-1.65131300	-0.66185900
C	2.64565000	-2.50318200	-0.00720800
C	2.20792100	-1.02287100	-1.83259700
C	3.94762500	-2.71041400	-0.47716700
H	2.33805200	-3.03584200	0.89287400
C	3.50735900	-1.22116700	-2.31523300
H	1.54580800	-0.36533600	-2.39384500
C	4.38716900	-2.06906200	-1.63820600
H	4.61757600	-3.38032600	0.05976300
H	3.82993300	-0.71952000	-3.22668000
H	5.39523800	-2.23312000	-2.01227500
O	0.64567600	0.25641500	1.35609300
C	1.25945800	-0.16682800	2.61234200
H	2.30927100	-0.39236000	2.40346300
O	2.54396300	1.60530100	0.95569800
C	3.64389000	2.11434500	0.18144000
C	-2.58614200	-2.25066400	0.41834700
C	-1.12969200	-2.31073800	-2.47721900
H	-1.87219800	-1.50376600	-2.41537300
H	-0.27070400	-1.92625700	-3.03639800
C	-0.70332100	-2.80716500	-1.09230200
H	0.04517500	-3.59667700	-1.20851600
C	-1.90462100	-3.37387300	-0.30838000
H	-1.57017100	-4.10436700	0.44347200
H	-2.63746800	-3.90044500	-0.94947600
C	-2.57235500	-0.05540400	1.34131900
H	-1.76539900	0.60826000	1.65983700
H	-3.08485600	-0.42201300	2.23917600
C	-3.56004300	0.70432600	0.47149400
C	-3.14322700	1.27162800	-0.74180000
C	-4.89069900	0.86605900	0.87011900
C	-4.04192500	1.98571400	-1.53507100
H	-2.11028500	1.14813900	-1.05432400
C	-5.79012300	1.58783200	0.08101300
C	-5.36839400	2.14867700	-1.12477000
H	-3.70703300	2.41815600	-2.47482800
H	-6.82055500	1.70529400	0.40686400
Ni	-0.03357700	-1.35589100	-0.00680500
N	-1.92328300	-1.17360300	0.63561900

O	-3.85681300	-2.39197800	0.86131500
H	-4.19438900	-3.25574900	0.57449900
H	-1.57851400	-3.11955400	-3.08057300
H	-6.06696000	2.70726200	-1.74226100
H	-5.22696400	0.41927900	1.80284600
C	0.55630600	-1.42496300	3.10770900
H	1.04354900	-1.77436900	4.02559400
H	-0.49707500	-1.22584100	3.33283700
H	0.60427500	-2.22392300	2.36197900
C	1.16346700	0.96695000	3.63312800
H	1.68735400	1.85972700	3.28391200
H	0.11433600	1.22111400	3.82575400
H	1.61746400	0.65499500	4.58090500
H	1.71985500	3.25566300	-1.13153300
H	3.39280800	2.05035500	-0.88377900
C	3.90507800	3.56560300	0.58228900
H	4.14272900	3.62142300	1.65059000
H	4.75343800	3.97158500	0.01999700
H	3.03401500	4.20242800	0.39524700
C	4.85029700	1.21845900	0.45195000
H	5.71998800	1.57384800	-0.11291800
H	5.10098300	1.23621800	1.51903900
H	4.64178100	0.18775400	0.15392400
C	-0.20335600	3.97145400	-0.49615800
H	-0.13015500	4.93222200	-1.01899900
H	-1.25058900	3.65110100	-0.49935400
H	0.10519300	4.12485400	0.54416800
C	0.30265000	2.68950100	-2.63463200
H	0.94772000	1.92775100	-3.08300600
H	-0.73551800	2.35031300	-2.71715600
H	0.40935300	3.61751200	-3.20754200

8N_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.86260456 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.55310300 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.30950156 a.u.

0 1

O	1.26453900	1.63979400	-0.50806600
C	1.61969400	2.94171600	-0.06257500
B	1.76805200	0.43353600	0.12784000
C	1.56385600	-0.80673900	-0.95898500
C	1.68208700	-2.15210800	-0.52754600
C	1.47165700	-0.59576900	-2.36014800
C	1.74580700	-3.22450400	-1.44053100
H	1.86325900	-2.36057100	0.52524500
C	1.54008100	-1.64611000	-3.26375500
H	1.37733400	0.42749500	-2.71264500
C	1.68025200	-2.96962700	-2.80309100
H	1.87048300	-4.24212000	-1.07766100
H	1.49253100	-1.45256000	-4.33303900
H	1.74301000	-3.78794700	-3.51641500
O	0.81691900	0.00892200	1.28836000
C	1.33575200	-0.38004500	2.57459600
H	2.31086200	-0.85532900	2.41935100
O	3.10006900	0.50780000	0.69200500
C	4.25422700	0.67783100	-0.11759800
O	-4.02393100	-1.29228600	1.81824000
C	-2.85723500	-1.60123000	1.20476500
C	-2.57243800	-3.03353700	0.83790000
N	-2.00714900	-0.67915300	0.93897600
C	-2.21664800	-3.19294600	-0.66772500
C	-1.41270200	-2.02246600	-1.25430500
Ni	-0.35374300	-1.08644000	0.04751800
C	-2.31356300	0.73755400	1.24916700
H	-4.53771500	-2.10236800	1.95901900
H	-3.42333300	-3.67433300	1.10684900
H	-1.72353100	-3.36238700	1.44887400
H	-1.65097400	-4.12708700	-0.76291500
H	-3.15303700	-3.34045100	-1.22515000
H	-2.08566600	-1.26129400	-1.66828900
H	-0.75973700	-2.37391500	-2.05588900
H	-2.90816800	0.79179500	2.16663300
H	-1.35017600	1.21597700	1.42653900
C	-3.04773900	1.41432300	0.10504000
C	-4.43194500	1.61686100	0.16396100
C	-2.34364000	1.83715800	-1.03304000
C	-5.10676000	2.22845200	-0.89511200
H	-4.98259600	1.29448800	1.04402400
C	-3.02022700	2.44415200	-2.09239000
H	-1.26536200	1.70081600	-1.07901100
C	-4.40217400	2.64079500	-2.02727500
H	-2.46447700	2.77134600	-2.96738500
H	-4.92532700	3.11837600	-2.85172500
H	-6.18072000	2.38526500	-0.83321700
C	1.54865300	0.86095700	3.44353900
H	1.97376000	0.58134300	4.41589900
H	2.23983600	1.54759700	2.95027800
H	0.59773400	1.37826600	3.62137800
C	0.39519800	-1.37882000	3.24819900
H	-0.59443600	-0.93949900	3.41681500
H	0.27158400	-2.28239600	2.63939300
H	0.80363500	-1.68076100	4.22006400
C	0.49267500	3.58049500	0.75813900
H	0.78528300	4.57872800	1.10836500
H	-0.41821100	3.68471200	0.15751900
H	0.26039700	2.96790800	1.63429500
C	1.96256700	3.79059500	-1.29031800
H	1.09682000	3.85096200	-1.96144700
H	2.24691800	4.81077500	-1.00446700
H	2.79247500	3.34368600	-1.84843700
C	5.18508400	1.68369600	0.56751100
H	5.45443200	1.32092500	1.56681400
H	6.10790200	1.82336600	-0.00834400
H	4.70007000	2.65837500	0.68069600
C	4.97194800	-0.66235800	-0.32823500
H	5.88622900	-0.52807900	-0.91984300
H	5.25064000	-1.09203100	0.64188800
H	4.33128000	-1.37956200	-0.84823400
H	2.50813000	2.87383300	0.57792800
H	3.96589800	1.07956200	-1.10174400

TS1N_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.85255661 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.55317300 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.29938361 a.u.

0 1

O	0.85872700	1.45101000	-0.79010900
C	0.79577800	2.87618700	-0.88317100
B	1.51139400	0.76432100	0.26366300
C	1.87611900	-1.04219100	-0.62185000
C	2.61322600	-2.00159700	0.11260300
C	2.26765200	-0.85644400	-1.96555900
C	3.64231300	-2.75278600	-0.45847100
H	2.37088700	-2.17934000	1.15904500
C	3.31122500	-1.57966400	-2.54518400
H	1.73797400	-0.11712000	-2.56071700
C	3.99343200	-2.54313900	-1.79562600
H	4.17385200	-3.49459400	0.13405400
H	3.58863700	-1.40310900	-3.58243500
H	4.79843300	-3.11895200	-2.24654800
O	0.58907800	0.32727200	1.32258000
C	1.09663300	0.03159700	2.65037300
H	2.13514800	-0.29766800	2.55012800
O	2.73250400	1.20294600	0.79461500

C	3.83274100	1.72491400	0.04975200
O	-3.83272800	-2.06739900	1.37250700
C	-2.63990700	-2.12690400	0.73270800
C	-2.26083000	-3.41571400	0.05461900
N	-1.90984500	-1.07405200	0.65622800
C	-1.77756300	-3.10905600	-1.37587400
C	-0.42116800	-2.40402300	-1.38580800
Ni	-0.07490900	-1.07704000	-0.02012000
C	-2.47585400	0.19780600	1.16953900
H	-4.27494600	-2.92788700	1.30658300
H	-3.12869800	-4.09096300	0.04603800
H	-1.46535300	-3.91997300	0.61844000
H	-1.73177500	-4.05990100	-1.92805600
H	-2.54580800	-2.49943100	-1.87027000
H	-0.25384800	-1.92175000	-2.35705000
H	0.37171300	-3.15311400	-1.25973100
H	-2.96253900	0.03212000	2.13658000
H	-1.62914200	0.86607300	1.32580600
C	-3.46619700	0.80752200	0.19211600
C	-4.78474100	1.07092500	0.57821900
C	-3.06639500	1.12788000	-1.11473100
C	-5.68873500	1.64950300	-0.31633200
H	-5.10720200	0.81771700	1.58541300
C	-3.97076000	1.69770400	-2.01144300
H	-2.04253900	0.93037700	-1.42165400
C	-5.28470300	1.96212200	-1.61473800
H	-3.64725400	1.94081600	-3.02040300
H	-5.98705300	2.40924400	-2.31335100
H	-6.70886300	1.85012500	0.00126700
C	1.06805800	1.31082800	3.48630200
H	1.46396000	1.11734700	4.49077500
H	1.68191900	2.08336500	3.01779200
H	0.04172400	1.68326900	3.58844900
C	0.27105600	-1.08343800	3.28631200
H	-0.77475100	-0.78193000	3.41088300
H	0.29668200	-1.99352200	2.67783200
H	0.67575600	-1.32172000	4.27710600
C	-0.16024600	3.47542200	0.15271500
H	-0.18915900	4.56822200	0.05894100
H	-1.17584900	3.09214100	0.00493300
H	0.15734300	3.22958200	1.17043600
C	0.37367200	3.21723800	-2.31163400
H	-0.62834800	2.82421200	-2.51813700
H	0.35559200	4.30267300	-2.46404700
H	1.06973300	2.77631100	-3.03293500
C	4.21960600	3.07789900	0.65463500
H	4.52043500	2.94561900	1.70058600
H	5.06037600	3.52227000	0.10918800
H	3.38301700	3.78342500	0.63135300
C	5.00931400	0.74858600	0.10712900
H	5.87401700	1.16280700	-0.42574800
H	5.30039700	0.57409300	1.14997900
H	4.75196100	-0.21033200	-0.34524600
H	1.79520500	3.29517400	-0.71138300
H	3.53476900	1.86052200	-0.99878000

9N_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.87876240 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.54872700 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.33003540 a.u.

0 1

O	0.65603600	1.74921400	-0.08163300
C	0.87171800	3.05012300	-0.64657000
B	1.46159400	1.03166500	0.75716400
C	1.52801300	-1.57610900	-1.03949400
C	2.53147300	-2.43229200	-0.53947600
C	1.86173200	-0.85408300	-2.20597900
C	3.78508600	-2.55638300	-1.14952300
H	2.33328700	-3.03774800	0.34500700
C	3.11258400	-0.96382200	-2.82460400
H	1.11899100	-0.19752300	-2.65620100
C	4.08414000	-1.81950800	-2.29844700
H	4.52677000	-3.23537000	-0.73139300
H	3.32382300	-0.39240300	-3.72753500
H	5.05366500	-1.91877700	-2.78152900
O	0.78996900	-0.01815500	1.39774900
C	1.43591400	-0.71534100	2.49983700
H	2.44729600	-0.97852100	2.17498100
O	2.76446600	1.24049600	1.09880100
C	3.81673800	1.94478000	0.42093600
O	-3.94454900	-1.65463000	1.55287500
C	-2.83765800	-1.92178600	0.81311400
C	-2.72160300	-3.29051000	0.19347500
N	-1.96605900	-1.00196100	0.61677700
C	-2.25189700	-3.17904600	-1.26809500
C	-0.78058000	-2.77758100	-1.38930100
Ni	-0.17948500	-1.36942200	-0.22168200
C	-2.28945000	0.35757100	1.11057000
H	-4.51979300	-2.43533700	1.56226000
H	-3.69837700	-3.79291200	0.25224200
H	-2.01372900	-3.90237100	0.76879300
H	-2.42893600	-4.15276400	-1.75134000
H	-2.90062800	-2.45577100	-1.78036300
H	-0.55435100	-2.50883600	-2.42799900
H	-0.15144800	-3.64647500	-1.14596800
H	-2.65969300	0.31110200	2.14072900
H	-1.35527100	0.91664500	1.11138500
C	-3.31030100	1.05692400	0.22871100
C	-4.49616000	1.56770600	0.76687800
C	-3.06599500	1.22297300	-1.14359200
C	-5.41858700	2.23747000	-0.04117700
H	-4.70077100	1.43589800	1.82675400
C	-3.98930700	1.88478500	-1.95395300
H	-2.14882700	0.82498700	-1.57061500
C	-5.16855800	2.39640800	-1.40456800
H	-3.78712200	2.00385300	-3.01551200
H	-5.88632200	2.91359300	-2.03597300
H	-6.33433800	2.62871800	0.39497400
C	1.50331900	0.20368900	3.72028900
H	1.97601700	-0.32071800	4.55894600
H	2.08854700	1.10144800	3.50801100
H	0.49410800	0.50130600	4.02898100
C	0.64931300	-1.98463900	2.80392600
H	-0.36769900	-1.74375300	3.13294400
H	0.58188000	-2.62618700	1.91984900
H	1.14923000	-2.54213400	3.60468800
C	-0.31148400	3.93302900	-0.25245100
H	-0.18923200	4.94177200	-0.66343000
H	-1.24770100	3.51164200	-0.63296600
H	-0.38837300	4.01244300	0.83731500
C	1.02611800	2.92093800	-2.16007700
H	0.11731400	2.49309700	-2.59735600
H	1.19912300	3.90392100	-2.61312600
H	1.86430600	2.26460000	-2.41348100
C	4.17796100	3.19100000	1.22847000
H	4.50954000	2.90421000	2.23287200
H	4.99097000	3.74119800	0.74168900
H	3.32153900	3.86583700	1.33416700
C	4.99774600	0.98761400	0.27995500
H	5.82967000	1.48532800	-0.23199300
H	5.34372900	0.66661700	1.26931800
H	4.71279800	0.10289000	-0.29540600
H	1.78423400	3.48454300	-0.22503500
H	3.47679600	2.23229600	-0.58027800

10_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1039.05131219 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.31626000 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1038.73505219 a.u.

0 1

C	3.00347100	0.44437700	-0.09920000
C	3.06845000	1.67437000	-0.78143500
C	4.13311200	0.07386900	0.65421000
C	4.20673400	2.48567900	-0.72800500
H	2.21363000	2.01406200	-1.36562900
C	5.27337700	0.88331900	0.71775000
H	4.13163700	-0.86443800	1.20851900
C	5.31659600	2.09407200	0.02435000
H	4.22344800	3.42907500	-1.27108900
H	6.12857900	0.56514800	1.31150500
H	6.20103900	2.72492600	0.07133900
C	-1.14153800	-1.17957800	0.34067600
C	1.03829200	-0.30620200	2.55336800
H	0.82514700	-1.38410300	2.59868200
H	2.10834200	-0.17716000	2.74498000
O	-0.21785600	-1.75201300	-0.28843500
C	0.64583600	0.30750600	1.20401600
H	0.90565400	1.36974200	1.20522300
C	-0.87079100	0.17134800	0.94853100
H	-1.20869600	0.91295000	0.21017800
H	-1.48562400	0.33790700	1.84782200
C	-3.55461200	-1.25507800	1.05863100
H	-3.32843300	-0.94162300	2.08316700
H	-4.24496700	-2.10248000	1.14277300
C	-4.22237200	-0.11261600	0.30760700
C	-4.79870900	0.94300000	1.02276300
C	-4.31326400	-0.11347000	-1.09004100
C	-5.45999900	1.97708600	0.35727000
H	-4.72692200	0.95962400	2.10827100
C	-4.96850000	0.92165700	-1.75756500
C	-5.54573900	1.96910900	-1.03556500
H	-5.89829300	2.79183300	0.92709800
H	-5.02748000	0.91044000	-2.84254700
N	-2.34348200	-1.78621000	0.43384400
H	-2.39728800	-2.67933900	-0.04118800
Ni	1.49893300	-0.68285900	-0.24836200
C	2.51210300	-2.29552300	-1.26810700
H	3.54253900	-2.22210400	-0.93431700
C	2.01326500	-1.44447200	-2.21130100
H	1.04000500	-1.61582600	-2.66421800
H	2.63026100	-0.66855700	-2.65366300
H	1.95113000	-3.16891000	-0.94519300
H	-3.86116300	-0.92113100	-1.66020100
H	-6.05383000	2.77593200	-1.55635000
H	0.49410200	0.16293100	3.39180300

TS2_m
SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1039.05131219 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.31626000 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1038.73505219 a.u.

0 1

C	1.82446700	0.93481400	0.27881300
C	0.95951500	1.62629700	-0.60111300
C	2.79537900	1.70703600	0.96499300
C	1.11178100	2.99620400	-0.83947800
H	0.18768400	1.08544700	-1.14270200
C	2.93724000	3.06920700	0.72748400
H	3.45277400	1.21975300	1.68174200
C	2.09824800	3.72912700	-0.18109400
H	0.44953200	3.48825100	-1.54905400
H	3.70958500	3.62517200	1.25517800
H	2.21023900	4.79455300	-0.36241500
C	-0.58130000	-1.55830500	-0.20694100
C	1.67080800	-1.55914600	2.14149000
H	1.71758300	-2.48380700	1.55555200
H	2.69069400	-1.30389600	2.44358100
O	0.39249100	-1.72844400	-0.96371800
C	0.99712900	-0.37951600	1.40261400
H	0.93927000	0.41610100	2.14515900
C	-0.45966500	-0.67087800	1.01172800
H	-0.98776300	0.26461800	0.78734600
H	-0.99042300	-1.11847400	1.86396900
C	-3.03057200	-2.00618900	0.21870700
H	-2.87978900	-2.20445900	1.28594600
H	-3.68095800	-2.80821200	-0.14946000
C	-3.71745700	-0.65897400	0.04202400
C	-4.40666300	-0.08592200	1.11686600
C	-3.71326700	0.00489600	-1.19127500
C	-5.08527700	1.12461000	0.96385400
H	-4.41102500	-0.58797100	2.08228100
C	-4.38606100	1.21753500	-1.34491400
C	-5.07579500	1.77998400	-0.26824000
H	-5.61194900	1.55858300	1.80942200
H	-4.37016000	1.72378000	-2.30621100
N	-1.76244700	-2.16060800	-0.49041300
H	-1.74944500	-2.70223900	-1.34631600
Ni	2.16063300	-0.84690900	-0.32897100
C	4.12850200	-0.91653100	-0.42936700
H	4.56507300	0.06772300	-0.58463500
C	3.53671500	-1.61254700	-1.50384800
H	3.46589200	-2.70122100	-1.48506700
H	3.49297100	-1.17248100	-2.50011700
H	4.54548000	-1.46768900	0.41624100
H	-3.17308400	-0.42200000	-2.03242200
H	-5.59721500	2.72552300	-0.38795600
H	1.10213900	-1.78198900	3.05993400

Post-TS2_m
SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1039.06899010 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.31907000 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1038.74992010 a.u.

0 1

C	1.63381800	0.74744200	0.93319700
C	1.29002200	1.29315200	-0.33905100
C	2.83335600	1.23252000	1.53603100
C	2.11706900	2.27276800	-0.94754000
H	0.30497200	1.13232000	-0.76833700
C	3.62360300	2.19361900	0.93174700
H	3.11023000	0.86700800	2.52182700
C	3.26695200	2.72300900	-0.32458400
H	1.81597200	2.68505500	-1.90761300
H	4.52099400	2.54571300	1.43423400
H	3.88811000	3.47985300	-0.79584900
C	-0.70543000	-1.30721800	0.07036500
C	1.21445300	-1.24458400	2.51664400
H	1.45292000	-2.01486500	1.77732800
H	2.13335400	-1.01771100	3.06464900
O	0.30905100	-1.54111000	-0.60483700
C	0.63257700	0.01624500	1.84436400
H	0.39506400	0.72323700	2.65481700
C	-0.73436500	-0.29565800	1.20232500
H	-1.20058700	0.62073600	0.81719800
H	-1.40691500	-0.65561700	1.98924500
C	-3.17945800	-1.79742900	0.35706600
H	-3.12606200	-1.88591500	1.44838300
H	-3.77700600	-2.65110000	0.01624000
C	-3.87882700	-0.49652000	-0.01593800

C	-4.70702700	0.13816800	0.91689900
C	-3.74567500	0.06172200	-1.29345400
C	-5.39600200	1.30500900	0.58059100
H	-4.81277900	-0.28157400	1.91535400
C	-4.42897800	1.23096400	-1.63007700
C	-5.25774600	1.85503700	-0.69475700
H	-6.03220700	1.78759300	1.31756900
H	-4.31309800	1.65475600	-2.62394000
N	-1.85181700	-1.98302500	-0.22062900
H	-1.75524500	-2.60896300	-1.01129900
Ni	2.15609400	-0.61725900	-0.64455500
C	4.02782100	-0.69672800	-1.16265300
H	4.26383200	0.02620300	-1.94463900
C	3.35859100	-1.90505300	-1.48681400
H	3.50015700	-2.79829300	-0.87539800
H	3.06062700	-2.11389500	-2.51617000
H	4.69830500	-0.65420600	-0.30363600
H	-3.09818700	-0.41451000	-2.02510100
H	-5.78761900	2.76650200	-0.95708900
H	0.49632400	-1.65780900	3.23670200

10_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1039.049481910 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.316622 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1038.732859910 a.u.

0 1

C	-3.61853500	-0.18701800	0.09248900
C	-4.05521200	-0.64611700	1.34907100
C	-4.61263600	0.13322700	-0.85062200
C	-5.41481400	-0.79499900	1.64502600
H	-3.32503600	-0.89243000	2.11957100
C	-5.97375300	-0.01408700	-0.56235100
H	-4.32577600	0.51248500	-1.83096700
C	-6.38253800	-0.48101500	0.68868300
H	-5.71709600	-1.15426500	2.62732800
H	-6.71589600	0.24148800	-1.31679900
H	-7.43980700	-0.59433300	0.91636800
Ni	-1.77839500	-0.08541300	-0.31546300
C	-1.82470400	-1.73759800	-1.72233200
H	-2.83549200	-1.71947400	-2.11720700
C	-1.55743700	-2.25746800	-0.48981300
H	-0.53608300	-2.42637800	-0.16060700
H	-2.34829900	-2.66053200	0.13474000
H	-1.02397900	-1.47935000	-2.41015200
N	2.37173500	0.42234300	-0.26583600
C	1.06662800	0.76163900	-0.18065800
C	0.68883000	2.06368100	0.48747200
O	0.21833500	-0.01834800	-0.66419100
C	3.53433600	1.19022900	0.19885200
C	-0.65692100	2.60583700	-0.01357400
C	-1.86234800	1.73731500	0.35990700
H	2.55485700	-0.45235600	-0.74491700
H	1.48783500	2.79919300	0.33920700
H	0.63262700	1.87911000	1.57191200
H	3.70292400	2.05757500	-0.45276200
H	3.32715600	1.57100200	1.20471500
H	-0.76486600	3.61861000	0.40678200
H	-0.59743200	2.73729500	-1.10336100
H	-2.77690300	2.22852500	0.01252100
H	-1.94601400	1.66908000	1.45693500
C	4.76881300	0.31401800	0.21833600
C	4.92377400	-0.66998500	1.20530300
C	5.76014400	0.45808600	-0.75866600
C	6.04974400	-1.49244800	1.21388300
H	4.15970800	-0.78913700	1.97024100
C	6.89007200	-0.36294800	-0.75035600
H	5.64930400	1.21849000	-1.52826600
C	7.03584300	-1.33983900	0.23521700
H	6.16041400	-2.24872600	1.98605000
H	7.65384200	-0.23822100	-1.51290200
H	7.91452900	-1.97876500	0.24371400

TS2_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1039.01796 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.317405 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1038.70055511 a.u.

0 1

C	2.61932500	0.77003600	0.30613900
C	1.63756800	1.73872200	-0.01427800
C	3.93877200	1.23498000	0.51153400
C	1.98005600	3.07809000	-0.20428800
H	0.60331800	1.43773200	-0.14822000
C	4.27261000	2.57525600	0.32823400
H	4.71304400	0.52827700	0.79812200
C	3.29816100	3.50929900	-0.03670900
H	1.20610600	3.79132400	-0.48128700
H	5.30433600	2.89163600	0.46738000
H	3.55996200	4.55442200	-0.17800700
Ni	2.28055600	-0.93838700	-0.48031100
C	3.99010600	-1.64643700	-1.14182800
H	4.67822300	-0.84785500	-1.41351400
C	2.92913200	-1.99474300	-2.00841700
H	2.50896000	-3.00159100	-1.99181000
H	2.77488100	-1.45738800	-2.94425300
H	4.41295300	-2.39297900	-0.46572700
N	-1.97052900	-0.85206400	-0.12536900
C	-0.66102700	-1.04813600	0.16997400
C	-0.28132200	-1.33351600	1.61364700
O	0.18632600	-0.97627900	-0.73412100
C	-3.12320100	-0.98802000	0.76682300
C	1.19047800	-1.72650800	1.78747500
C	2.21844100	-0.58330600	1.57997100
H	-2.15967500	-0.70460500	-1.11087200
H	-0.92797100	-2.13275600	1.99849400
H	-0.51074300	-0.44166900	2.21608300
H	-3.41228100	-2.04327900	0.87164100
H	-2.83188500	-0.63409400	1.76155300
H	1.30994900	-2.07079500	2.82671700
H	1.41008000	-2.59726600	1.15734000
H	3.20909400	-0.92841200	1.88625500
H	1.93337200	0.21065600	2.27565000
C	-4.30354500	-0.18507000	0.25785900
C	-4.19829300	1.20287000	0.08648300
C	-5.51533500	-0.81594800	-0.04179700
C	-5.28650300	1.94280700	-0.37361400
H	-3.25911900	1.70235900	0.31214600
C	-6.60830300	-0.07554200	-0.49897000
H	-5.60580200	-1.89259900	0.08312700
C	-6.49538500	1.30474900	-0.66630500
H	-5.19280400	3.01772000	-0.50143400
H	-7.54357100	-0.57902500	-0.72760000
H	-7.34330600	1.88218900	-1.02411100

TS1_m'

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.85512976 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.544581 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.31054876 a.u.

0 1

O	3.53028500	-0.29036500	1.26494100
B	2.90793500	-0.15940800	-0.01219800
C	1.64616300	1.21333300	0.06521500

C	1.22468900	1.76350300	-1.17402100
C	1.67693500	2.10576600	1.16403800
C	0.85608700	3.10421900	-1.30780200
H	1.21771700	1.13251200	-2.05922000
C	1.33620000	3.45078200	1.03954600
H	1.99927200	1.73366500	2.13154100
C	0.91555400	3.95086000	-0.19863800
H	0.53732900	3.49053200	-2.27298700
H	1.39559600	4.11300200	1.90030000
H	0.64480600	4.99946700	-0.29811600
O	2.03521400	-1.31184200	-0.41512000
C	2.32364400	-2.20123600	-1.52205900
H	3.40755600	-2.35476100	-1.50434700
O	3.80877100	0.16649500	-1.05355800
C	-2.41739800	-1.28460700	-0.87005300
C	-1.36069200	0.64710300	2.25060700
H	-0.88946800	-0.08479800	2.91866900
H	-0.89063500	1.61772900	2.43600800
O	-1.86727200	-1.38243200	-1.96406600
C	-1.20921700	0.25807100	0.78934200
H	-1.61134800	1.01363000	0.10802300
C	-1.59541900	-1.16183600	0.40859200
H	-1.98928200	-1.73375800	1.25608700
H	-0.65070300	-1.77119700	0.13950500
C	-4.59308900	-1.12594800	0.44933200
H	-3.98556400	-0.65278300	1.22688900
H	-4.87933700	-2.11948700	0.82385000
C	-5.84338700	-0.30093700	0.20519100
C	-5.75567800	0.97841700	-0.36193800
C	-7.10096000	-0.80011300	0.55989800
C	-6.90451100	1.74183000	-0.56536300
H	-4.78352900	1.37187900	-0.64840900
C	-8.25275600	-0.03500400	0.36112800
C	-8.15671000	1.23736500	-0.20281800
H	-6.82299000	2.73197900	-1.00563700
H	-9.22276100	-0.43692200	0.64091400
Ni	0.42778400	-0.40962700	0.13979900
N	-3.77645400	-1.23875500	-0.75594900
H	-4.26314000	-1.33322100	-1.64016300
H	-7.18089200	-1.79450400	0.99360400
H	-9.05137400	1.83294700	-0.36238500
C	1.92171100	-1.58445000	-2.86067300
H	2.47376600	-0.65755600	-3.02953800
H	2.15385300	-2.27923000	-3.67752800
H	0.84391800	-1.38278700	-2.88199000
C	1.60744200	-3.52472200	-1.26825400
H	1.87278400	-3.93910300	-0.29040000
H	0.51960300	-3.39022300	-1.31380000
H	1.88306500	-4.25530900	-2.03739800
H	-2.41728700	0.73395800	2.55289100
C	4.89759700	1.06074500	-0.83236500
H	4.66068000	1.72078600	0.01444400
C	6.16524200	0.27114100	-0.49616200
H	6.41302500	-0.41222800	-1.31774000
H	7.01742800	0.94476100	-0.33995800
H	6.00984200	-0.31583800	0.41243300
C	5.06498100	1.91259400	-2.09139700
H	5.27252100	1.27167600	-2.95692600
H	4.15070400	2.47913800	-2.29644600
H	5.89516700	2.62046800	-1.98041100
C	2.96050400	-0.94425100	2.38272000
H	1.85883500	-0.84252100	2.35403700
C	3.48533100	-0.26829500	3.65283900
H	3.06384600	-0.73635100	4.55028200
H	4.57708400	-0.35716000	3.69755200
H	3.23653000	0.79770300	3.66940900
C	3.30714400	-2.43795400	2.37867000
H	2.92253300	-2.92047800	1.47748400
H	4.39555300	-2.56814400	2.40188300
H	2.88042500	-2.94269600	3.25483600

TS1_a'

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.85794759 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.545124 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.31282359 a.u.

0 1

O	-4.01965000	-0.81828400	0.05813300
B	-2.91850100	-0.06935000	0.56332000
C	-2.24761900	1.02968700	-0.79772700
C	-1.48690300	2.14741200	-0.36481100
C	-2.98903400	1.20677700	-1.99022700
C	-1.46728200	3.35418700	-1.06656900
H	-0.93172900	2.07643200	0.56752800
C	-2.99390700	2.41125900	-2.69106500
H	-3.58911600	0.38251000	-2.36250700
C	-2.22552300	3.48682900	-2.23275300
H	-0.87676400	4.19167800	-0.70211100
H	-3.59059800	2.51652800	-3.59414800
H	-2.22527300	4.42737200	-2.77875200
O	-1.69179800	-0.86457100	0.89930000
C	-1.22681100	-1.08961400	2.25144600
H	-2.12716500	-1.14566200	2.87149700
O	-3.25841700	0.78160800	1.64258600
C	-0.36645900	0.07497700	2.73945200
H	-0.93957700	1.00442800	2.71259000
H	-0.03831900	-0.10269500	3.77095400
H	0.53007700	0.18066900	2.11470600
C	-0.48008800	-2.41940400	2.29557100
H	-1.12017100	-3.24114000	1.95942100
H	0.41557300	-2.39711500	1.66394600
H	-0.16273000	-2.63522700	3.32282800
C	-4.52804600	1.42940800	1.69803300
H	-4.94171000	1.50904500	0.68295700
C	-5.49593200	0.60873700	2.55427000
H	-5.09739200	0.49291000	3.56983400
H	-6.47433500	1.10102600	2.62284000
H	-5.63240700	-0.38349300	2.11665500
C	-4.31247700	2.83622300	2.25768800
H	-3.87523900	2.78183800	3.26223400
H	-3.62996400	3.40407600	1.61686900
H	-5.26116300	3.38220500	2.32498000
C	-3.92104200	-1.94057500	-0.79958400
H	-3.02150100	-1.84704600	-1.43647000
C	-5.16240400	-1.96599400	-1.69611500
H	-5.12779200	-2.81234700	-2.39222700
H	-6.06417900	-2.06188800	-1.08011600
H	-5.25267200	-1.04250700	-2.27723000
C	-3.80393600	-3.23718800	0.00905900
H	-2.90914600	-3.21906200	0.63466300
H	-4.67916400	-3.35273800	0.65948000
H	-3.74833200	-4.10948600	-0.65427900
N	4.40269000	-1.27213100	-0.32308100
C	3.07863800	-1.55052300	-0.51884100
C	2.32978000	-0.70771600	-1.55233100
O	2.51564100	-2.43058000	0.12778700
C	5.25232600	-0.33516700	-1.05156300
C	0.90572900	-1.21157200	-1.80005700
C	-0.03402600	-0.25089300	-2.46027200
Ni	-0.84068900	-0.42143200	-0.77280100
H	4.85658000	-1.89106100	0.33932800
H	2.87503400	-0.70062700	-2.50432400
H	2.29773700	0.33601000	-1.21056900
H	5.69268600	-0.80883400	-1.94153800
H	4.62476100	0.48777000	-1.41031300
H	0.90823900	-2.20891300	-2.25145800
H	0.50916100	-1.48780500	-0.73415200
H	-0.63036700	-0.65096900	-3.28292100

H	0.36499600	0.73937400	-2.69007500
C	6.36212300	0.21491500	-0.17431500
C	6.07783300	0.74801800	1.09080600
C	7.68542600	0.21669400	-0.62794100
C	7.09812500	1.27440400	1.88230200
H	5.05404900	0.74297200	1.45626900
C	8.70818500	0.74796800	0.16125100
H	7.91853300	-0.20115200	-1.60483900
C	8.41660700	1.27742400	1.41867400
H	6.86413700	1.68369800	2.86138600
H	9.73130200	0.74081100	-0.20470300
H	9.21100300	1.68714900	2.03643000

TS1N_m'

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.82765335 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.543904 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.28374935 a.u.

0 1

O	2.82916100	-0.58538100	1.36539000
C	3.18321800	-1.78945600	2.05093800
B	2.43294000	-0.62703200	-0.00276500
C	1.97230700	1.22656900	-0.33578900
C	1.63944800	1.60171300	-1.66141500
C	2.75271000	2.14150700	0.40565400
C	2.04583600	2.81925200	-2.20909800
H	1.06436500	0.91880000	-2.28378400
C	3.19190000	3.34673300	-0.14261600
H	3.03442300	1.87556600	1.42002900
C	2.82729300	3.69392400	-1.44764400
H	1.76598300	3.08321100	-3.22617600
H	3.81029700	4.02135100	0.44516400
H	3.15802200	4.63859600	-1.87275600
O	1.12807300	-1.32250900	-0.19311900
C	0.80483500	-2.08590900	-1.38571900
H	1.21894500	-1.55445900	-2.25037100
O	3.35079300	-1.00949200	-1.00139700
C	4.72079300	-0.60532500	-0.98442600
C	-2.87144400	1.08904400	0.48814200
C	-0.00282700	2.38316900	2.52811200
H	0.28775600	1.58195600	3.21857800
H	0.87767100	3.00963600	2.35804800
C	-0.52825600	1.83296400	1.21132100
H	-0.73709800	2.62209800	0.48149300
C	-1.62583700	0.78377500	1.28568600
H	-1.87883900	0.52409700	2.32311500
H	-1.26640300	-0.22370100	0.86310400
C	-4.43253200	0.77718000	-1.25557000
H	-4.25182800	0.53732700	-2.30938600
H	-4.64067900	1.85192800	-1.18559200
C	-5.63404600	-0.00858100	-0.75897200
C	-5.82185900	-1.34092800	-1.14999400
C	-6.56069600	0.57435900	0.11421200
C	-6.91207800	-2.07441500	-0.68132500
H	-5.10670100	-1.80324500	-1.82641800
C	-7.65494100	-0.15601600	0.58277800
C	-7.83334300	-1.48260600	0.18651800
H	-7.04561300	-3.10618200	-0.99649400
H	-8.36903700	0.31261500	1.25532500
Ni	0.32939900	0.36592400	0.40325500
N	-3.21421400	0.40635800	-0.52296600
O	-3.58982600	2.16252200	0.94739600
H	-3.07724700	2.62361000	1.63108400
H	-0.74849700	3.00798800	3.04909900
H	-8.68581000	-2.05133000	0.54873900
H	-6.41986300	1.60530400	0.42851100
C	-0.71187200	-2.18325500	-1.50481500
H	-0.97965300	-2.73629900	-2.41281500
H	-1.12926900	-2.72345000	-0.64621600
H	-1.19362500	-1.20091400	-1.55044200
C	1.45568900	-3.46479200	-1.28863500
H	2.54017000	-3.37260700	-1.20601000
H	1.07317300	-4.00588200	-0.41508600
H	1.22345500	-4.05301700	-2.18458300
H	3.42316100	-2.57284400	1.31733200
H	4.90468900	0.01209000	-0.09516700
C	5.60234400	-1.85508300	-0.91504700
H	5.41142400	-2.49948900	-1.78146600
H	6.66479900	-1.58356100	-0.91723000
H	5.39829800	-2.43332400	-0.00837400
C	5.02067100	0.21761200	-2.23902000
H	6.07372900	0.52359200	-2.25729900
H	4.82075400	-0.37885600	-3.13736200
H	4.39940000	1.11587400	-2.27737000
C	2.01091900	-2.27102400	2.91166300
H	2.27196100	-3.19057500	3.45037100
H	1.74669700	-1.50423400	3.65023400
H	1.13447600	-2.47015100	2.28841100
C	4.42542600	-1.50766700	2.89683100
H	5.26163100	-1.18576400	2.26766100
H	4.21478700	-0.70813700	3.61714600
H	4.73417100	-2.40042300	3.45361500

TS1N_a'

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1566.83130226 a.u.
Thermal correction to Gibbs free energy at 313 K: 0.543908 a.u.
Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1566.28739426 a.u.

0 1

O	2.22613200	1.36149400	-1.14077400
C	1.92290300	2.75841500	-1.19014800
B	2.37978900	0.70475700	0.11303100
C	2.58478200	-1.15729600	-0.43879300
C	2.90717400	-2.10342300	0.56495600
C	3.22180200	-1.31849800	-1.68992100
C	3.80063800	-3.15026700	0.33571700
H	2.46401900	-2.00534500	1.55418700
C	4.13707800	-2.34537500	-1.92282100
H	3.00281100	-0.60264800	-2.47665300
C	4.41967400	-3.27032800	-0.91277800
H	4.02419700	-3.86428400	1.12512500
H	4.62435700	-2.43391800	-2.89119100
H	5.12523700	-4.07762300	-1.09483800
O	1.11154000	0.66584200	0.89124300
C	1.09137800	0.64358600	2.34031400
H	2.01906800	0.17544500	2.68561900
O	3.46714300	1.01380600	0.95359000
C	4.78070500	1.26192500	0.45066800
O	-4.32994900	-2.71184800	0.87062700
C	-3.37680500	-1.83481700	0.41466900
C	-2.25424000	-2.46024900	-0.38653600
N	-3.42042600	-0.59163800	0.65351100
C	-1.32175800	-1.45501000	-1.06676700
C	-0.03059600	-1.99946100	-1.60781700
Ni	0.62654600	-0.79501700	-0.33437800
C	-4.53984000	-0.03911900	1.42739800
H	-4.10336400	-3.61336400	0.59224800
H	-2.68909500	-3.11124400	-1.15932300
H	-1.67142800	-3.11713800	0.27627000
H	-1.87032600	-0.83659900	-1.78333000
H	-1.10864500	-0.66610200	-0.24002300
H	0.20238200	-1.73535200	-2.64111300
H	0.16961300	-3.05446900	-1.40409600
H	-4.97359500	-0.77781700	2.11200000
H	-4.13341800	0.78025700	2.03087800
C	-5.62086400	0.50141000	0.50731500

C	-6.76614900	-0.25462000	0.22830700
C	-5.47656300	1.75596400	-0.09926400
C	-7.74965100	0.23450000	-0.63399800
H	-6.88282400	-1.23247000	0.68866000
C	-6.45589800	2.24650200	-0.96353700
H	-4.58975100	2.34999100	0.10924200
C	-7.59696000	1.48663900	-1.23236900
H	-6.33082900	3.22333100	-1.42375500
H	-8.36299500	1.86962300	-1.90157000
H	-8.63617700	-0.36148200	-0.83586400
C	1.04628900	2.08365300	2.84632000
H	1.04602800	2.10433100	3.94281900
H	1.92077300	2.63468500	2.49153300
H	0.13985100	2.58694300	2.49017400
C	-0.10946700	-0.17478200	2.80425600
H	-1.04300400	0.23860600	2.40633300
H	-0.02840500	-1.21712100	2.47262500
H	-0.16878900	-0.17375100	3.89895000
C	0.42805500	2.96317500	-1.45491300
H	0.18247100	4.03135700	-1.50854200
H	0.14801100	2.49749400	-2.40765600
H	-0.16888100	2.50823800	-0.65935400
C	2.78271700	3.39263800	-2.28395600
H	2.57056000	2.91771500	-3.24920500
H	2.57658700	4.46583800	-2.37481700
H	3.84820300	3.26171100	-2.06865000
C	5.19326400	2.68477400	0.83580200
H	5.17413900	2.80069700	1.92606700
H	6.20854500	2.90505800	0.48474800
H	4.51261200	3.42443200	0.40238700
C	5.74664100	0.22486000	1.02723600
H	6.76888300	0.41230500	0.67678500
H	5.74429400	0.27575300	2.12282300
H	5.45910500	-0.78657400	0.72912800
H	2.17544800	3.22286900	-0.22548900
H	4.77029000	1.17568100	-0.64381300

TS1_m''

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1645.472545 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.598838 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1644.87370653 a.u.

0 1

O	3.47987900	-0.47213000	1.42614500
B	3.20223100	-0.31040500	0.05062200
C	1.84099100	1.14538700	-0.11535800
C	1.67746300	1.67824500	-1.41756800
C	1.93759400	2.08417200	0.93548200
C	1.57927800	3.05125500	-1.65479100
H	1.65093500	1.00556700	-2.27366400
C	1.87808900	3.45828600	0.71048500
H	2.08403600	1.72539400	1.95029500
C	1.68008100	3.94557600	-0.58619300
H	1.43982200	3.42448600	-2.66698500
H	1.97594900	4.15291500	1.54148500
H	1.61595700	5.01652600	-0.76240700
O	2.46610900	-1.38280300	-0.63340900
C	3.15306000	-2.17256800	-1.64160800
H	4.21233100	-2.14604000	-1.36967600
O	4.27207300	0.17711900	-0.71681400
C	-3.22598900	1.45333600	0.45413100
C	-0.88512900	0.16629600	2.07939100
H	-1.22155900	-0.86216200	2.26832100
H	0.09753400	0.28413400	2.54682100
O	-2.88654400	2.42277000	1.12126600
C	-0.85016500	0.51836800	0.58845100
H	-0.54419600	1.55831200	0.48905100
C	-2.22966200	0.40362900	-0.06693200
H	-2.66412000	-0.59605100	0.06918500
H	-2.15588500	0.56645700	-1.15189100
C	-5.15029700	0.36280100	-0.83257400
H	-4.51850800	-0.52884100	-0.90127500
H	-5.16684700	0.81053700	-1.83854800
C	-6.56144600	-0.04234600	-0.44309400
C	-6.85660800	-0.44348400	0.86712200
C	-7.58487500	-0.04351200	-1.39702300
C	-8.14801300	-0.84145300	1.21195500
H	-6.07025300	-0.43153100	1.61713300
C	-8.87802700	-0.44579200	-1.05513000
C	-9.16278300	-0.84545000	0.25104700
H	-8.36320900	-1.14820900	2.23216300
H	-9.66238000	-0.43837300	-1.80731200
Ni	0.62094500	-0.50699600	-0.22991800
N	-4.55583300	1.26796600	0.14187200
H	-5.13383500	2.04501300	0.44447100
H	-7.36972900	0.27556200	-2.41464600
H	-10.16923400	-1.15352100	0.52114300
C	3.01141100	-1.55589300	-3.03263100
H	3.41576600	-0.54187000	-3.03291000
H	3.56825200	-2.15263100	-3.76539900
H	1.96400000	-1.52276500	-3.35634200
C	2.67217400	-3.62188700	-1.58631000
H	2.76977200	-4.03166400	-0.57626400
H	1.62843600	-3.72560000	-1.90123100
H	3.28161700	-4.23561500	-2.25989900
H	-1.57492800	0.84224700	2.60243800
C	5.27331300	1.02946700	-0.15665200
H	4.85422800	1.55601700	0.71062800
C	6.46828200	0.19259300	0.30534600
H	6.89534300	-0.35957800	-0.54099600
H	7.25312800	0.83173300	0.72861200
H	6.15393100	-0.52405600	1.06887700
C	5.66054200	2.05423500	-1.22236200
H	6.05567400	1.54725100	-2.11120100
H	4.78926200	2.64478000	-1.52195400
H	6.43136100	2.73706200	-0.84550300
C	2.80256900	-1.35458000	2.30751600
H	1.76283600	-1.49473500	1.96997800
C	2.78633600	-0.72235100	3.70057400
H	2.29790200	-1.38461400	4.42483000
H	3.81213100	-0.53549800	4.03854500
H	2.25218800	0.23303600	3.69653200
C	3.50007900	-2.71862300	2.32971000
H	3.52492800	-3.15804100	1.32888900
H	4.53344800	-2.60720700	2.67891900
H	2.98279900	-3.41461900	3.00172100
C	-0.37775600	-2.34822900	-0.13402400
H	0.41976100	-3.03937600	0.11965800
H	-1.18916700	-2.27154700	0.58142300
C	-0.49178000	-1.82358600	-1.39966600
H	-1.39728500	-1.32871300	-1.73056700
H	0.20650200	-2.09500900	-2.18423000

TS1_a''

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1645.475732 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.597866 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1644.87786628 a.u.

0 1

O	4.01174600	0.18096800	1.11654200
B	3.30521500	0.34537300	-0.10107600
C	1.51367800	1.01994500	0.33341300
C	0.75067500	1.50226100	-0.75724600
C	1.49329900	1.81115300	1.50429000
C	-0.00362400	2.67667200	-0.68118000
H	0.76770400	0.96371700	-1.70295200

C	0.77430100	3.00201400	1.58465300
H	2.07616500	1.49220700	2.36335200
C	0.00969400	3.43169800	0.49341700
H	-0.58424100	3.01060000	-1.53827000
H	0.80444500	3.59822300	2.49397800
H	-0.55970200	4.35605000	0.55580300
O	2.92670500	-0.87259500	-0.84162400
C	3.53977300	-1.14635500	-2.13015600
H	4.51336100	-0.64876000	-2.10648900
O	3.83663700	1.33252900	-0.95021300
C	2.72909300	-0.54096500	-3.27521600
H	2.65090300	0.54064100	-3.14649400
H	3.22523400	-0.74050900	-4.23280800
H	1.72047400	-0.96844400	-3.32584700
C	3.76157800	-2.64910300	-2.29368500
H	4.34808600	-3.05402100	-1.46316700
H	2.81884000	-3.20271800	-2.35439500
H	4.31572900	-2.83859200	-3.22040900
C	4.48507800	2.49587300	-0.43535000
H	4.11326000	2.69707700	0.57823900
C	5.99606400	2.26272600	-0.36786500
H	6.39105900	2.04299900	-1.36750100
H	6.51225500	3.15094300	0.01731300
H	6.21640700	1.41770400	0.28960800
C	4.11795800	3.67102500	-1.34119000
H	4.45592500	3.48010500	-2.36698200
H	3.03324700	3.81663200	-1.35842800
H	4.58894800	4.59717200	-0.99072200
C	3.88357100	-0.92334500	1.99610700
H	2.86448400	-1.34262400	1.91726100
C	4.09848700	-0.42915400	3.42865300
H	4.03570000	-1.25948400	4.14169800
H	5.08902400	0.03128400	3.52040700
H	3.34989800	0.31870700	3.70831500
C	4.89288300	-2.01766900	1.63439800
H	4.73372000	-2.36557500	0.61087400
H	5.91409300	-1.62546800	1.70788200
H	4.80330700	-2.87553700	2.31240300
N	-4.81042100	-1.20383200	-0.14569200
C	-3.49067400	-1.50630100	-0.35791300
C	-2.39843400	-0.67396700	0.29557000
O	-3.18677900	-2.45130300	-1.08743300
C	-5.41717900	-0.28763700	0.81440100
C	-1.59653600	-1.50750700	1.32125600
C	-0.19801400	-0.94766800	1.57814800
Ni	1.14239900	-1.00887300	0.16681900
H	-5.43666000	-1.86572600	-0.59200700
H	-2.75893300	0.24735400	0.76166300
H	-1.72735000	-0.37301700	-0.51609500
H	-5.57738700	-0.77971600	1.78518600
H	-4.71977100	0.53654100	0.99151200
H	-2.15741700	-1.52901400	2.27003600
H	-1.56090200	-2.54725200	0.97987200
H	0.29810200	-1.51969800	2.37848400
H	-0.28080700	0.08638200	1.91812300
C	-6.73852500	0.26124800	0.30711400
C	-6.83425800	0.83032700	-0.97055100
C	-7.87798000	0.22419900	1.11773800
C	-8.04454400	1.35424500	-1.42336800
H	-5.95666000	0.85334000	-1.61143900
C	-9.09069200	0.75198000	0.66790600
H	-7.81701400	-0.22195500	2.10803300
C	-9.17663800	1.31801300	-0.60429000
H	-8.10486800	1.79202600	-2.41626500
H	-9.96706900	0.71394800	1.30937900
H	-10.11964800	1.72552500	-0.95844700
C	1.05388200	-3.11757300	0.09096400
H	2.10016700	-3.38735300	-0.01459800
H	0.55549300	-3.47044500	0.98880900
C	0.33721600	-2.60314000	-0.96073400
H	-0.74823900	-2.55030200	-0.96000600
H	0.81307000	-2.44932100	-1.92449800

TS1N_m''

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1645.445537 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.598573 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1644.84696442 a.u.

0 1

O	-2.78604100	-0.55508600	-1.22653700
C	-3.93729100	-1.17513400	-1.81892100
B	-2.91702300	0.26116200	-0.07350100
C	-0.96831700	0.99538000	0.06266500
C	-0.68373300	1.78853000	1.19685600
C	-0.55229100	1.51274400	-1.18384500
C	0.00428000	3.00243000	1.10436900
H	-1.00467800	1.45509200	2.18244500
C	0.10448700	2.73744000	-1.29594000
H	-0.75311000	0.93765900	-2.08463100
C	0.40106900	3.47920800	-0.14647400
H	0.22607100	3.57527300	2.00191300
H	0.39842100	3.11236400	-2.27379900
H	0.93186800	4.42441900	-0.22839200
O	-2.94811300	-0.47178700	1.18819400
C	-3.66750500	0.10721500	2.31284100
H	-3.58066200	1.19482800	2.23977300
O	-3.74819100	1.38120300	-0.06825700
C	-3.88367300	2.31528000	-1.14292100
C	3.23783700	-1.88954100	-0.30548300
C	0.39295500	-1.85761600	-1.64350000
H	0.18747300	-2.93411500	-1.54067600
H	-0.51112300	-1.40636600	-2.06228400
C	0.77661000	-1.21156200	-0.30505000
H	1.13717100	-0.19991200	-0.49104300
C	1.91527200	-1.94496600	0.43514900
H	1.66248500	-3.00183100	0.61473400
H	2.10010400	-1.47304300	1.40276500
C	5.38522100	-1.06194800	-0.74913200
H	5.16556600	-0.88736700	-1.81442300
H	5.86857700	-2.05120100	-0.71621800
C	6.36889200	-0.00993600	-0.26302100
C	6.06076700	0.87210700	0.77660500
C	7.62510300	0.08760000	-0.87817800
C	6.98832800	1.83169200	1.19185100
H	5.08932100	0.79224700	1.25200900
C	8.55216100	1.04407800	-0.46604200
C	8.23591600	1.92262000	0.57406300
H	6.73271500	2.51031000	2.00235900
H	9.52141400	1.10382400	-0.95523600
Ni	-0.90927500	-0.95227200	0.67757000
N	4.15343700	-1.07813300	0.02636400
O	3.39508200	-2.75120300	-1.36517700
H	2.57927700	-3.26024100	-1.48944800
H	1.19234300	-1.74279600	-2.39113200
H	8.95661600	2.66920200	0.89806100
H	7.87908200	-0.59403000	-1.68862700
C	-3.07076500	-0.35368200	3.63695700
H	-3.61746800	0.11663700	4.46214400
H	-3.15783800	-1.43983800	3.75869400
H	-2.01826700	-0.06724200	3.73082200
C	-5.14181800	-0.28168300	2.19889900
H	-5.56002300	0.07728000	1.25600200
H	-5.25746800	-1.37107100	2.24902000
H	-5.71627200	0.16247200	3.02071900
H	-4.83772500	-0.62708300	-1.51125600
H	-3.20646700	2.02925900	-1.95764300
C	-5.32742600	2.29380500	-1.65141600
H	-6.01840500	2.53172700	-0.83416900

H	-5.46571600	3.03862700	-2.44381600
H	-5.60004100	1.31448800	-2.05590800
C	-3.50220000	3.70569100	-0.63277200
H	-3.59079600	4.44690200	-1.43596600
H	-4.17173600	4.00286100	0.18335500
H	-2.47544400	3.72016400	-0.26108600
C	-4.07213300	-2.62421000	-1.34538100
H	-4.93772200	-3.10539700	-1.81685600
H	-3.17545500	-3.19785700	-1.60748500
H	-4.20754800	-2.66562300	-0.26055000
C	-3.79391200	-1.08176200	-3.33701100
H	-3.71240400	-0.03761600	-3.65608700
H	-2.89049700	-1.60944200	-3.66508700
H	-4.65687100	-1.53210800	-3.84125800
C	-0.60771600	-2.36365800	2.19964700
H	0.45266300	-2.45836200	2.39890200
H	-1.20501400	-1.97073300	3.01300200
C	-1.20259600	-2.98228400	1.12780100
H	-2.28191100	-3.07102000	1.05832000
H	-0.62678900	-3.57864500	0.42754400

TS1N_a''

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1645.449791 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.596763 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1644.85302759 a.u.

0 1

O	2.93481900	-0.20889500	1.53044100
C	4.07309300	-0.62161400	2.30163000
B	3.07469900	0.16940300	0.16548900
C	1.17728700	0.78695500	-0.21954600
C	0.92523800	1.14166300	-1.56480000
C	0.71372700	1.69374200	0.75888000
C	0.23345700	2.30518200	-1.91677000
H	1.28466900	0.49824000	-2.36566700
C	0.04852100	2.87457500	0.42576900
H	0.89786400	1.46894500	1.80685800
C	-0.20720600	3.17766500	-0.91705900
H	0.05356300	2.53923900	-2.96396300
H	-0.27644600	3.55806900	1.20711700
H	-0.72623200	4.09641900	-1.18100100
O	3.14966800	-0.96741200	-0.75309200
C	3.84368500	-0.84201700	-2.02016200
H	3.73491200	0.19080500	-2.36581000
O	3.91867300	1.21510500	-0.22173700
C	4.06897700	2.45102800	0.47920600
O	-3.87613800	1.08291000	-1.56041400
C	-3.57912300	-0.05681700	-0.84575800
C	-2.17439400	-0.08973300	-0.29637800
N	-4.41415000	-0.99585900	-0.67970200
C	-1.81877100	-1.32640100	0.52519200
C	-0.39290300	-1.32700200	1.08532700
Ni	1.17109200	-1.28696200	-0.06591000
C	-5.75680200	-0.86884200	-1.25826200
H	-3.08698400	1.64923200	-1.58413500
H	-2.02154300	0.81589600	0.30746900
H	-1.48025500	0.00636400	-1.14187100
H	-2.52547600	-1.39706800	1.36534600
H	-2.01915900	-2.21749900	-0.08031600
H	-0.24383800	-2.24099300	1.67606000
H	-0.24287900	-0.47525900	1.75573900
H	-5.76311300	-0.25087100	-2.16501100
H	-6.07763600	-1.87868200	-1.54133100
C	-6.73974800	-0.29757700	-0.25053200
C	-7.13235100	1.04507900	-0.31192600
C	-7.25224900	-1.10163300	0.77632200
C	-8.02276300	1.57198500	0.62635600
H	-6.73131400	1.67914100	-1.09843500
C	-8.13953500	-0.57843300	1.71719900
H	-6.94864100	-2.14416700	0.83638500
C	-8.52922100	0.76137500	1.64374800
H	-8.53045700	-1.21666400	2.50584600
H	-9.22426300	1.16911900	2.37337200
H	-8.32179800	2.61532100	0.56107700
C	5.32781400	-1.13369500	-1.79811300
H	5.88110000	-1.02866200	-2.73913000
H	5.74799700	-0.43334600	-1.07282900
H	5.46858700	-2.15656600	-1.42879800
C	3.22775500	-1.78819500	-3.04478900
H	3.29618800	-2.83068900	-2.71218000
H	2.17618700	-1.54823100	-3.23372500
H	3.76504300	-1.70378500	-3.99604900
C	4.07666000	-2.14245300	2.46481700
H	4.92567800	-2.46452400	3.08000300
H	3.15218200	-2.47384000	2.95208800
H	4.15166200	-2.63527300	1.49141600
C	4.01750900	0.09384300	3.65094100
H	3.09344200	-0.17031600	4.17854000
H	4.86807300	-0.19008400	4.28187800
H	4.03378100	1.18042300	3.51807900
C	5.51436200	2.57747100	0.96737200
H	6.20480100	2.52952000	0.11708500
H	5.66630200	3.53563500	1.47806500
H	5.77439400	1.77525800	1.66438900
C	3.70288700	3.59954400	-0.46234300
H	3.81389500	4.56441400	0.04679000
H	4.36536600	3.59484400	-1.33624200
H	2.67141500	3.50927000	-0.81033400
H	4.99109500	-0.32587000	1.77539600
H	3.39267300	2.46203300	1.34387300
C	0.63168100	-3.07682200	-0.98163500
H	-0.43247200	-3.22900200	-0.84435900
H	0.96392900	-2.95223200	-2.00793800
C	1.52939500	-3.35444000	0.02287800
H	2.59348400	-3.42051500	-0.17731000
H	1.20112200	-3.71538300	0.99255200

TS1_K_m

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1586.723228 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.535743 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1586.18748541 a.u.

0 1

O	2.94854800	-1.00498800	1.32969100
B	2.49145600	-0.75640700	0.00111300
C	2.23751400	1.10503300	-0.18412100
C	2.18154300	1.62739700	-1.50199400
C	2.87407300	1.92031700	0.77856500
C	2.69164000	2.88450300	-1.83012100
H	1.74736900	1.02150200	-2.29407800
C	3.40871500	3.16894400	0.46287500
H	2.97393900	1.54652700	1.79270700
C	3.30641400	3.66002600	-0.84253900
H	2.62404200	3.25545800	-2.85047700
H	3.90529500	3.76124500	1.22823600
H	3.71703700	4.63573300	-1.09222500
O	1.13589900	-1.27235300	-0.31765900
C	0.90800000	-2.31990600	-1.28484300
H	1.79400800	-2.96197000	-1.25152100
O	3.41613300	-1.11237800	-1.01231400
C	-2.38872800	0.85765700	0.01247000
C	-0.43165900	2.21036300	2.18682100
H	-1.00615600	1.37627300	2.61337000
H	0.57614500	2.16243600	2.61139200
O	-1.55150400	-0.07922600	0.00130100
C	-0.39267500	2.16469000	0.65489900

H	0.20603900	3.00026300	0.28026300
C	-1.81590100	2.24769400	0.05960800
H	-1.77297500	2.60134600	-0.98307500
H	-2.47751800	2.94630500	0.59425300
Ni	0.29790300	0.47082500	0.05053000
C	0.77148300	-1.75358700	-2.69779300
H	1.68756100	-1.23192100	-2.98413700
H	0.59549800	-2.56340100	-3.41675100
H	-0.07495700	-1.05750300	-2.75589100
C	-0.32230200	-3.11900100	-0.86036800
H	-0.20111700	-3.51630900	0.15217300
H	-1.21601300	-2.48730500	-0.87532900
H	-0.47777200	-3.96148300	-1.54496000
H	-0.89721900	3.14146900	2.55325600
C	4.81906200	-0.94136900	-0.82688400
H	4.99564500	-0.15110300	-0.08334500
C	5.44574400	-2.24116300	-0.31501600
H	5.27183000	-3.05335700	-1.03185000
H	6.52905800	-2.12789500	-0.18053600
H	5.00016800	-2.51844900	0.64346000
C	5.41745900	-0.50225200	-2.16441300
H	5.23200000	-1.26475300	-2.93095400
H	4.96416900	0.43678100	-2.49791300
H	6.50109800	-0.35531400	-2.08097500
C	2.10311900	-1.29767300	2.42953200
H	1.11380400	-0.83492100	2.27804800
C	2.73142900	-0.71022300	3.69619200
H	2.13165000	-0.95617100	4.58060900
H	3.73953400	-1.11716200	3.83750900
H	2.81244800	0.37986200	3.63281600
C	1.91569300	-2.81311000	2.56646500
H	1.48427500	-3.23222800	1.65388600
H	2.88414200	-3.29721400	2.74129300
H	1.25230100	-3.05437600	3.40674700
C	-3.81975200	0.55104700	-0.05036500
C	-4.79811200	1.56490200	-0.13569200
C	-4.24730900	-0.78944400	-0.03721700
C	-6.14328200	1.24923800	-0.20820400
H	-4.50108300	2.60812900	-0.15328600
C	-5.59462800	-1.11909000	-0.10313900
H	-3.50132600	-1.57403300	0.03102700
C	-6.55490200	-0.09606900	-0.19074200
H	-6.90270000	2.02104900	-0.27755300
H	-5.89085800	-2.16133500	-0.08643300
O	-7.89019900	-0.29996000	-0.26184900
C	-8.38468400	-1.63535700	-0.25326500
H	-8.11712100	-2.15393100	0.67546500
H	-9.46987200	-1.54856500	-0.32092200
H	-8.00966700	-2.20492300	-1.11231600

TS1_K_a

SCF energy [B3LYP]/6-311+G**-SDD/SMD (2-propanol): -1586.720545 a.u.

Thermal correction to Gibbs free energy at 313 K: 0.536918 a.u.

Gibbs free energy at 313 K [B3LYP]/6-311+G**-SDD/SMD (2-propanol)]: -1586.18362735 a.u.

0 1

O	2.76430300	-1.11357700	1.38264100
B	2.36485000	-0.85069600	0.03657900
C	2.48704600	0.96907300	-0.31605100
C	2.41523300	1.34372800	-1.68141400
C	3.36502900	1.73174000	0.48908600
C	3.13858300	2.41812700	-2.20324600
H	1.79935900	0.75571500	-2.35849600
C	4.11653600	2.78757900	-0.02104300
H	3.46780900	1.47616200	1.53962200
C	3.99356900	3.14248200	-1.36933900
H	3.04988000	2.68119600	-3.25488500
H	4.79577200	3.33888900	0.62526800
H	4.57209300	3.97208600	-1.76930100
O	0.92872600	-1.09786000	-0.28194900
C	0.49876700	-2.13529100	-1.18941300
H	1.40635200	-2.55513600	-1.62925400
O	3.19970600	-1.48747600	-0.91865000
C	-0.36870400	-1.55262400	-2.30417800
H	0.17931700	-0.79120100	-2.86917600
H	-0.66071000	-2.34449600	-3.00478300
H	-1.27970300	-1.09730200	-1.90193300
C	-0.22469600	-3.22766400	-0.40211100
H	0.43164800	-3.64696500	0.36601100
H	-1.11790900	-2.82746800	0.09213500
H	-0.53583500	-4.04019900	-1.07044100
C	4.60483100	-1.59644800	-0.71983300
H	4.93883000	-0.80788100	-0.03039200
C	4.94276300	-2.95668200	-0.10275200
H	4.60710600	-3.76553300	-0.76381000
H	6.02477000	-3.06285800	0.04804100
H	4.44083800	-3.06280000	0.86224900
C	5.28689900	-1.39026000	-2.07331100
H	4.94867500	-2.15101700	-2.78757100
H	5.03871200	-0.40458700	-2.48011800
H	6.37716200	-1.46560800	-1.98064400
C	2.05630200	-0.73836000	2.54838500
H	1.51684500	0.20967300	2.36822400
C	3.07734200	-0.52136400	3.66930100
H	2.58490100	-0.20426200	4.59626900
H	3.61808300	-1.45458200	3.86674300
H	3.81436700	0.23886600	3.39007500
C	1.02534600	-1.80235700	2.94467700
H	0.26719400	-1.91423600	2.16675900
H	1.52209600	-2.76986400	3.08744900
H	0.52596000	-1.52945300	3.88334200
C	-2.42556300	1.18021800	0.20268000
C	-2.25166900	2.67391800	0.33685000
O	-1.42405600	0.43281700	0.20202400
C	-1.05137700	3.02545500	1.23035400
C	0.29368400	2.63337600	0.62801300
Ni	0.45688000	0.79826400	0.09280200
H	-3.16857100	3.13137200	0.71871300
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H	-1.19202200	2.54738300	2.21045000
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H	-9.41220100	-1.44287000	-0.57871600
H	-8.84760000	-0.01928900	0.33993100

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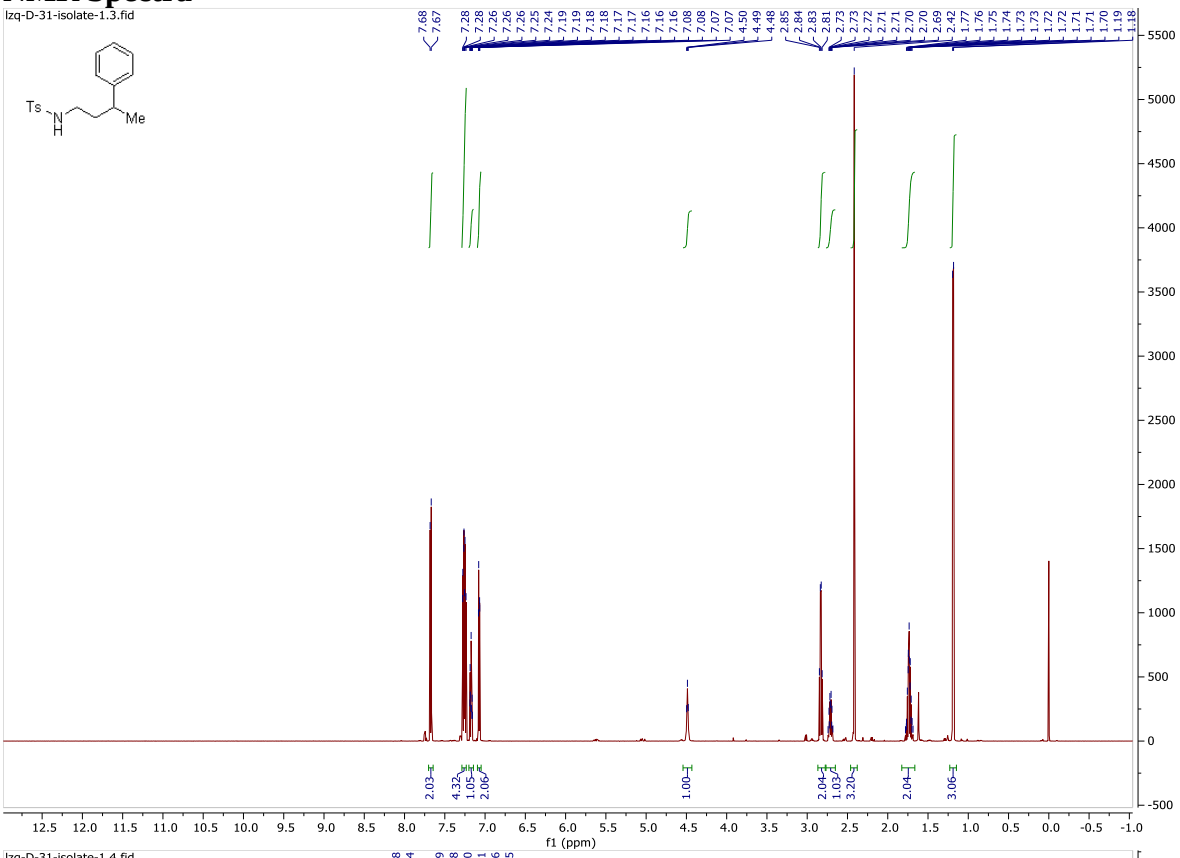
NMR Spectra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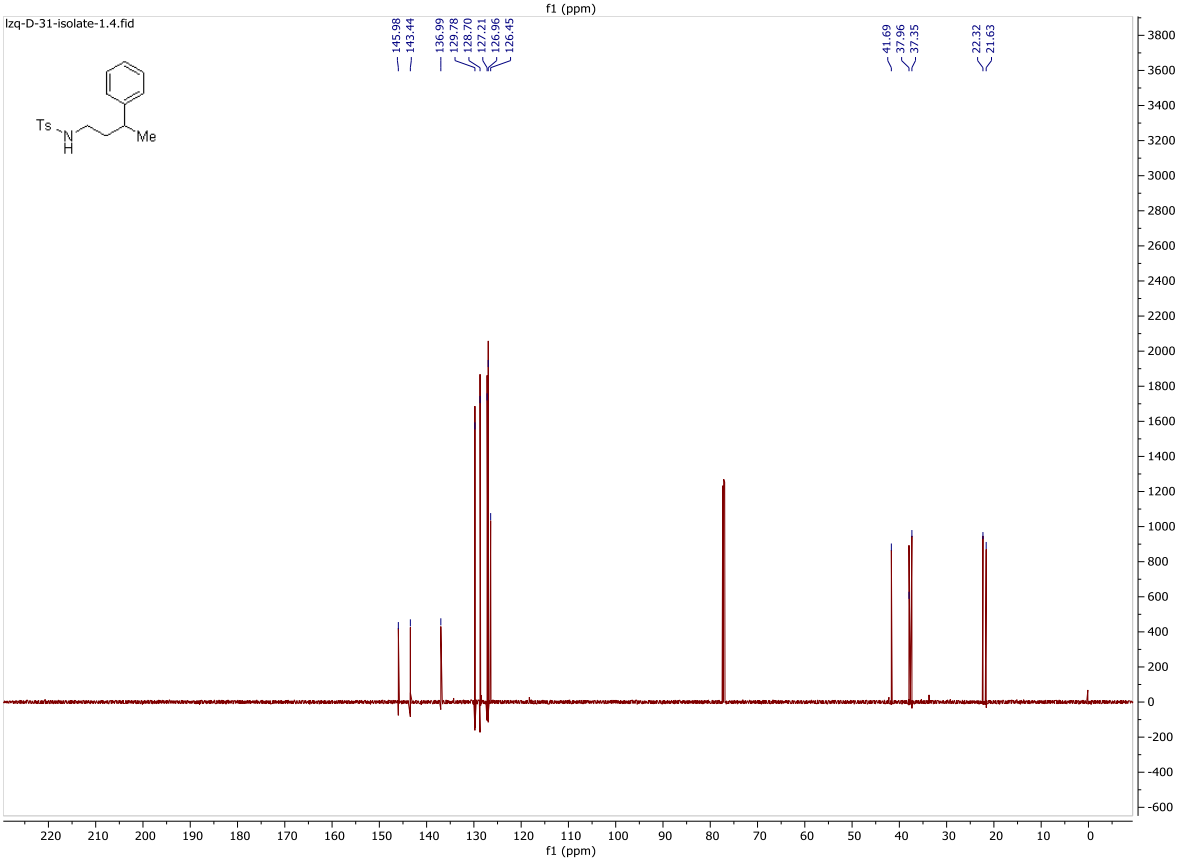
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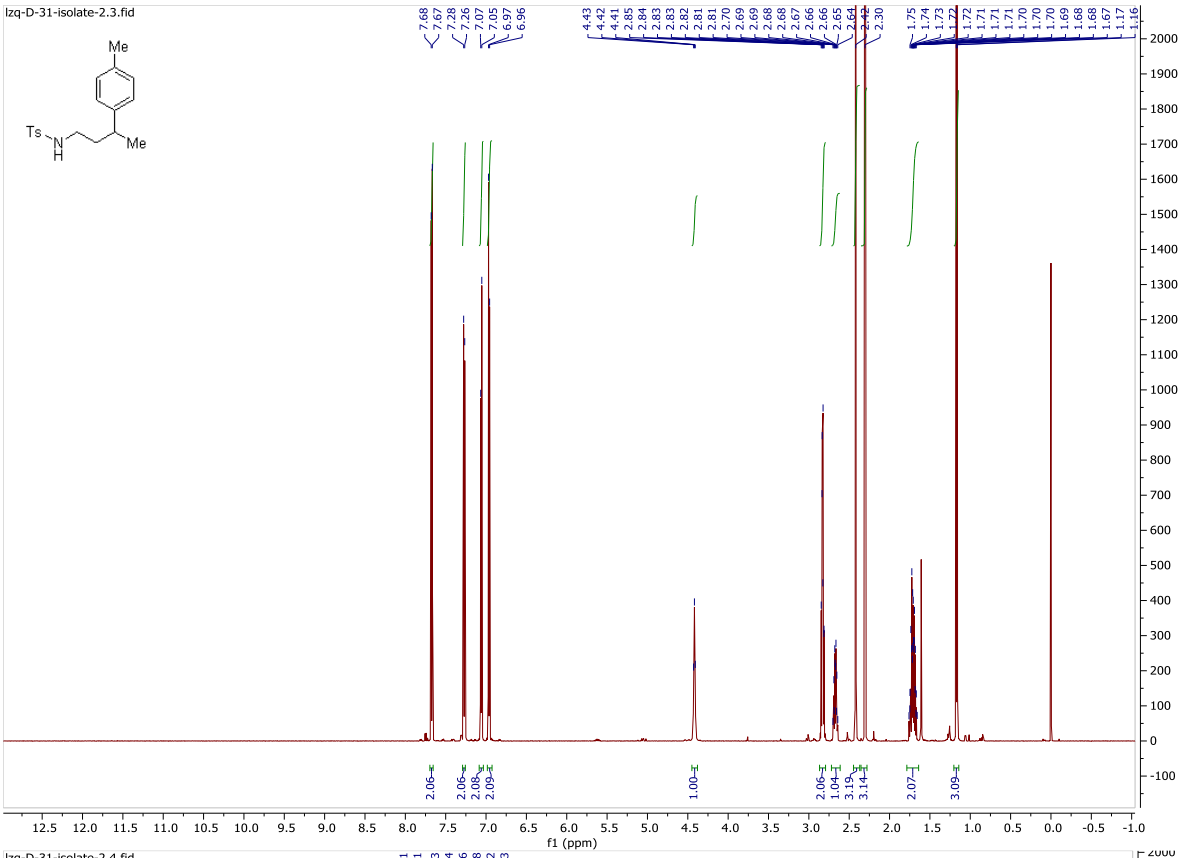
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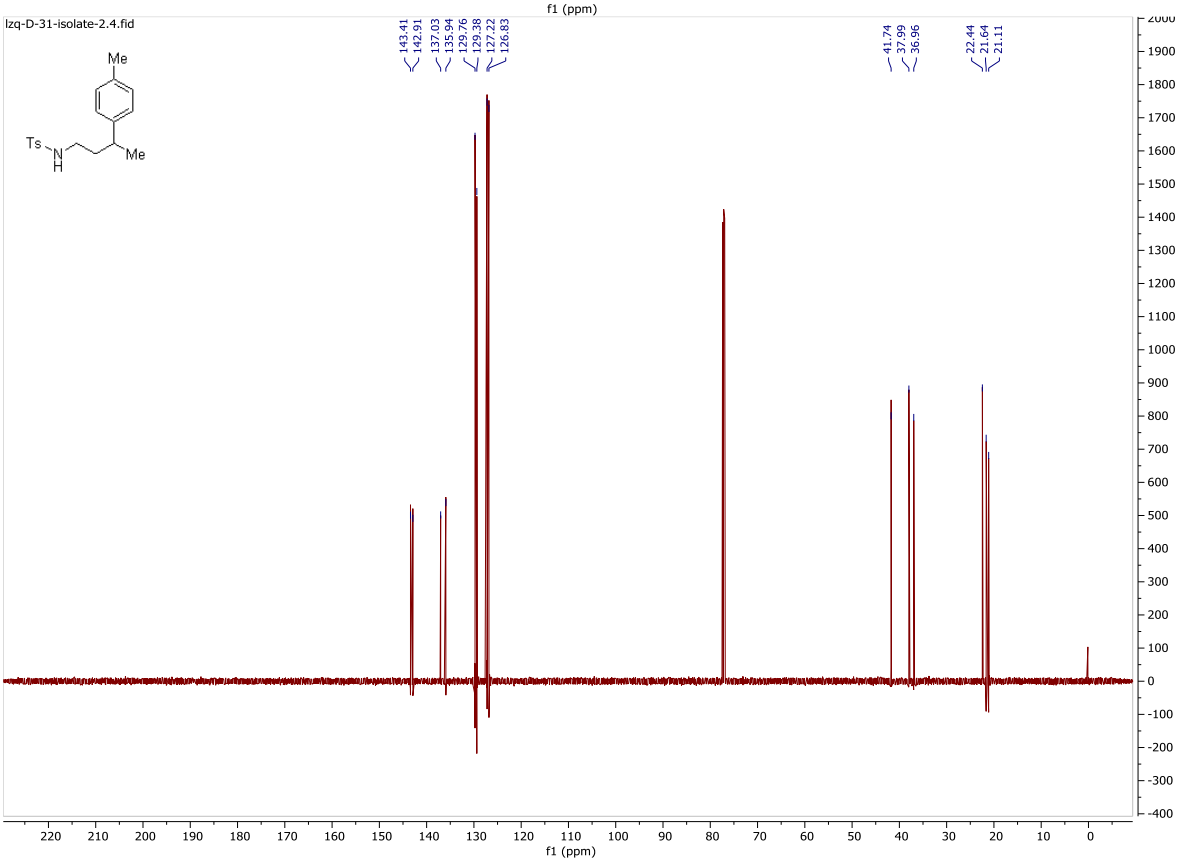
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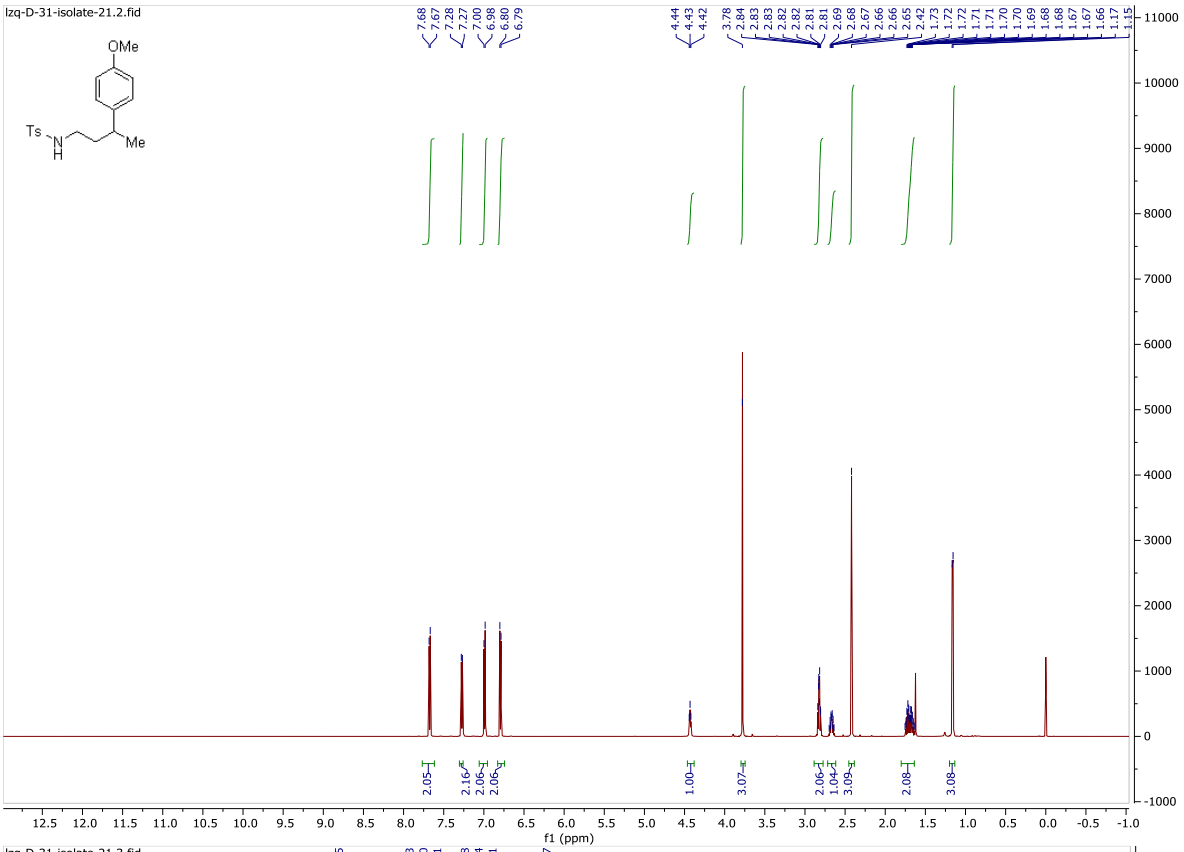
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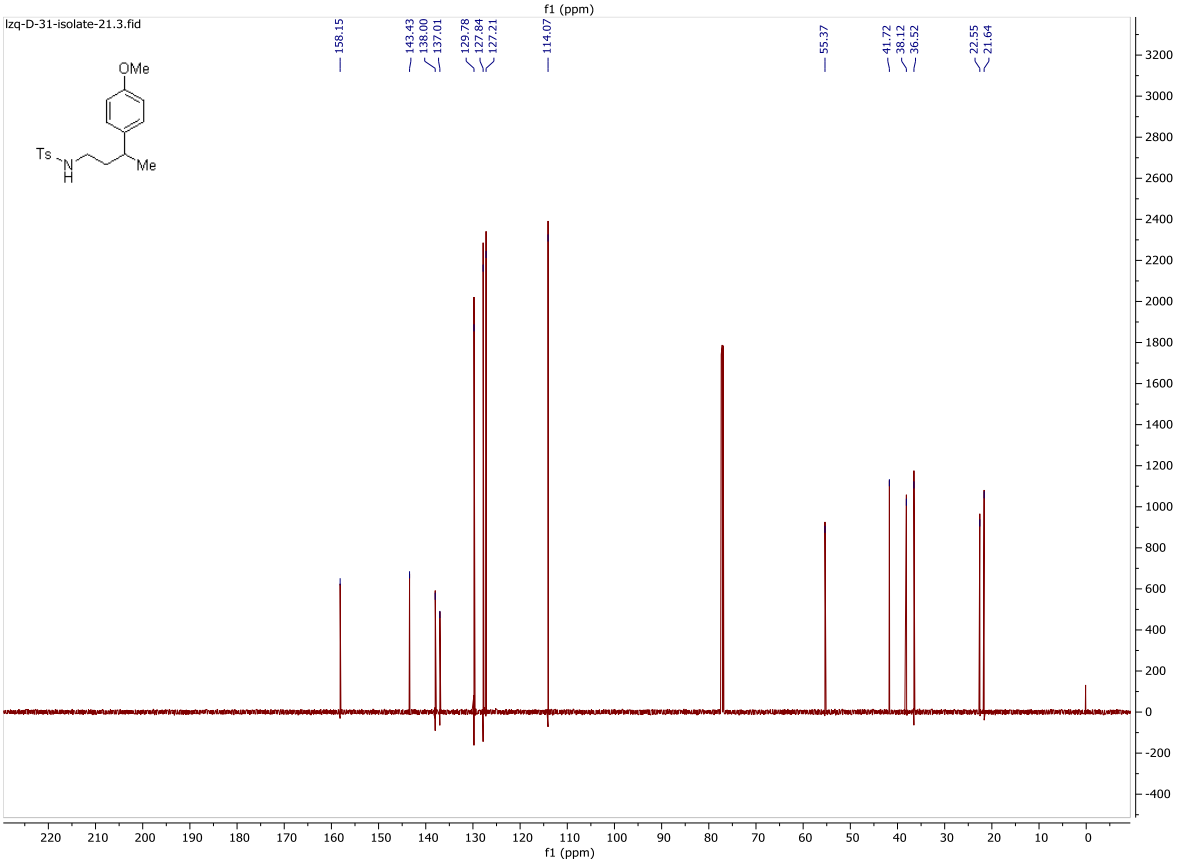
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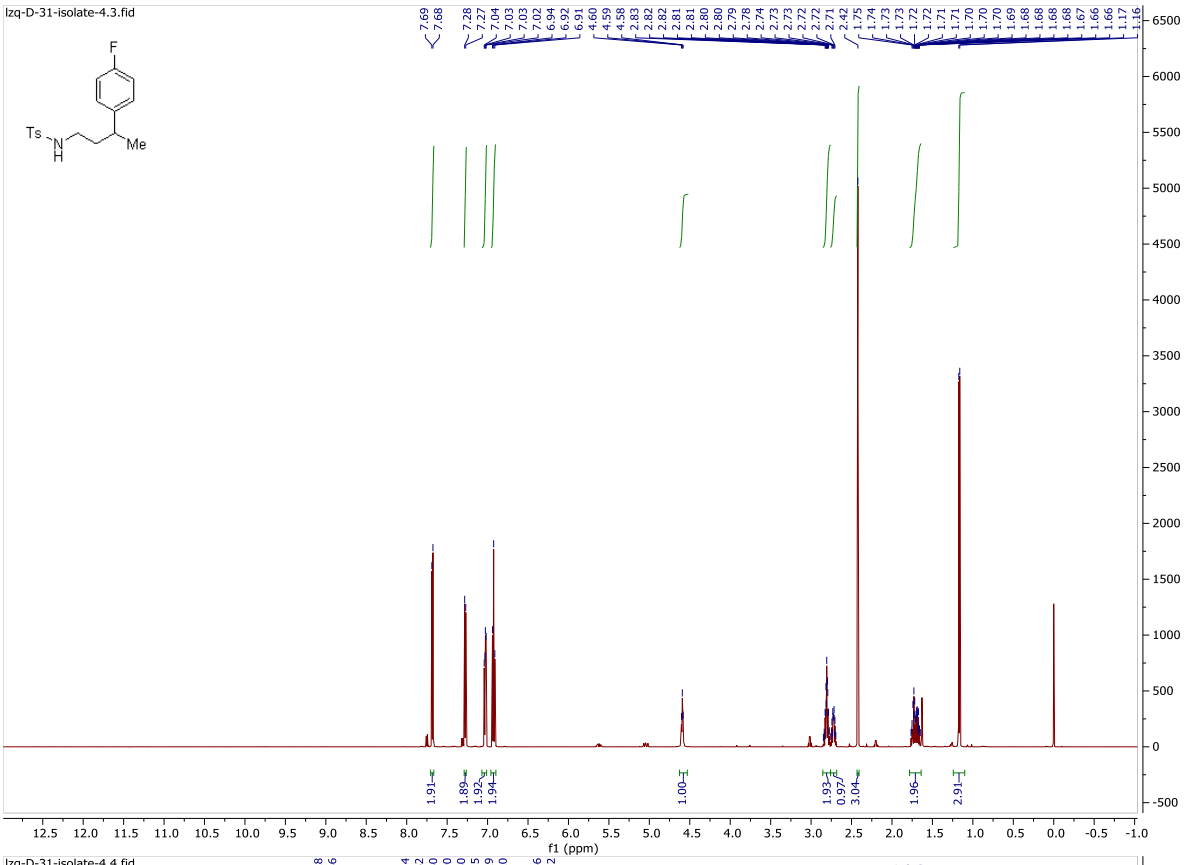
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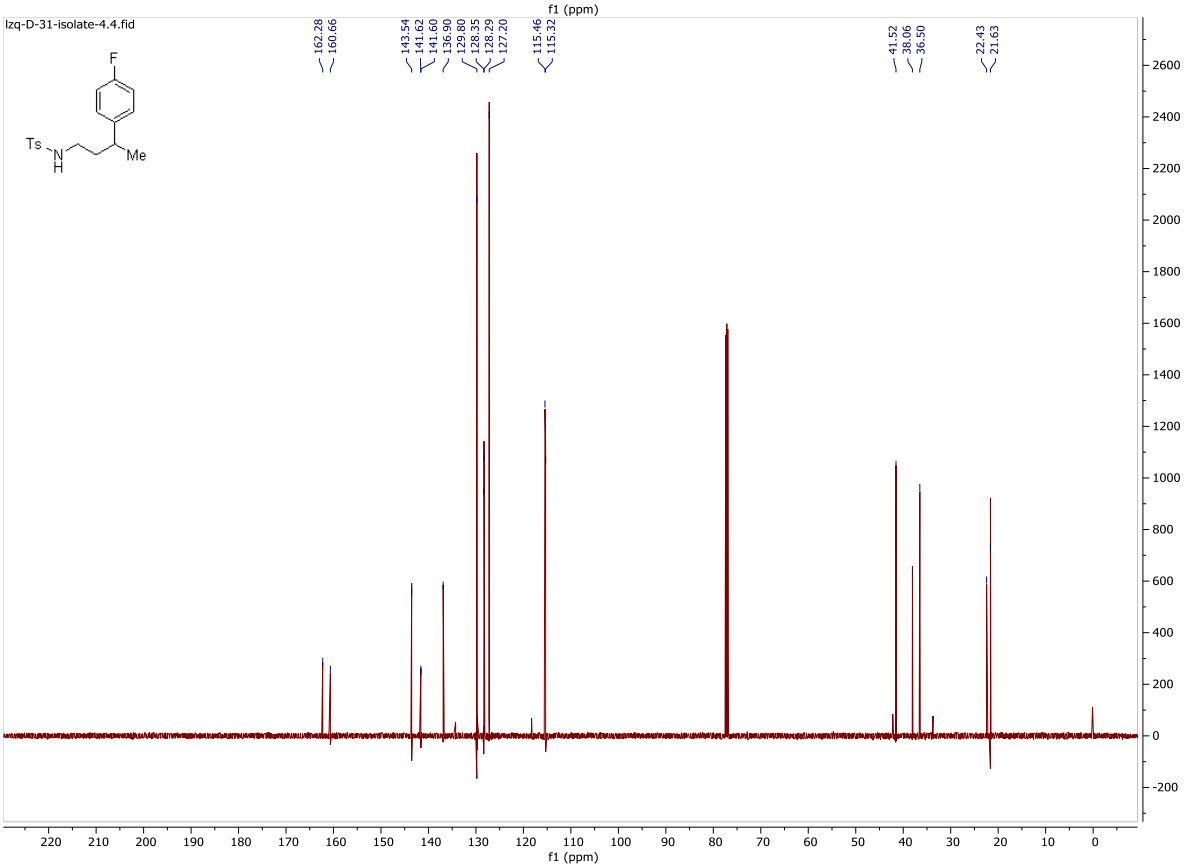
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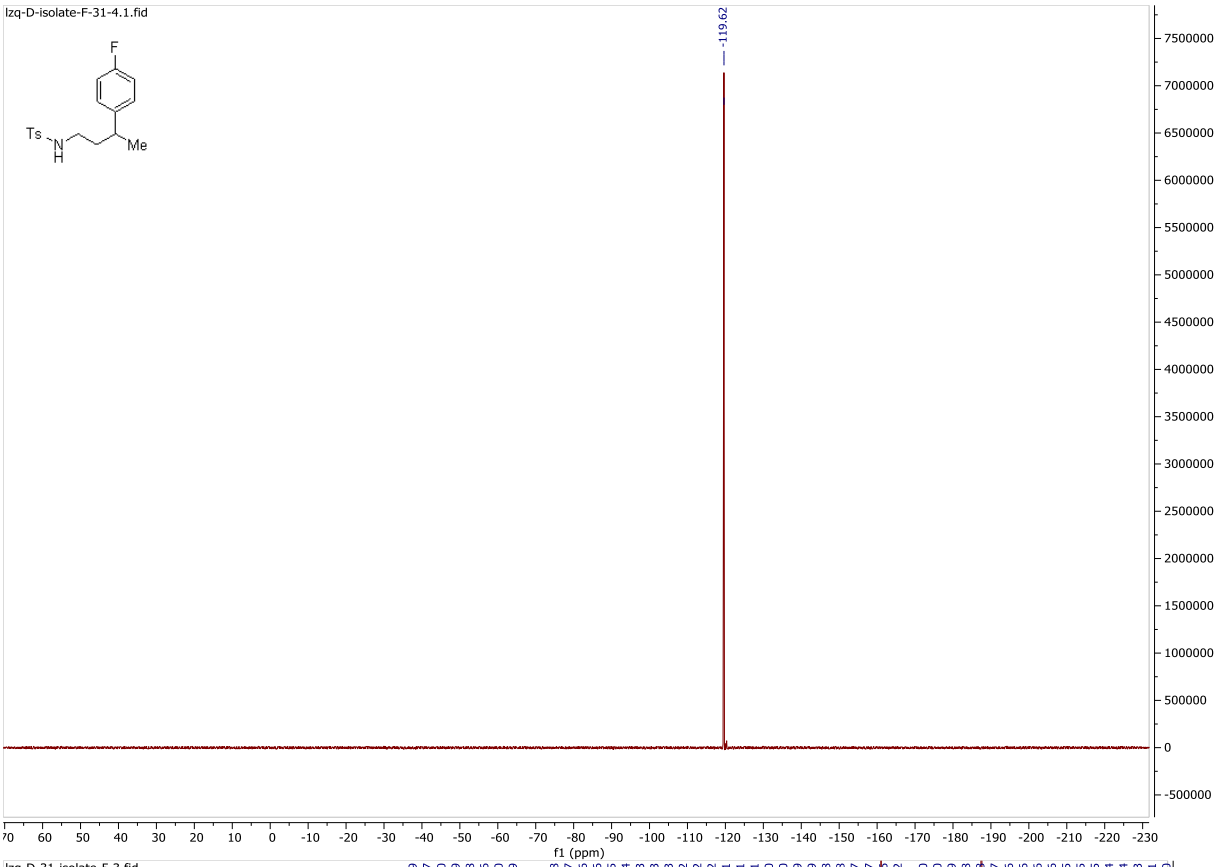
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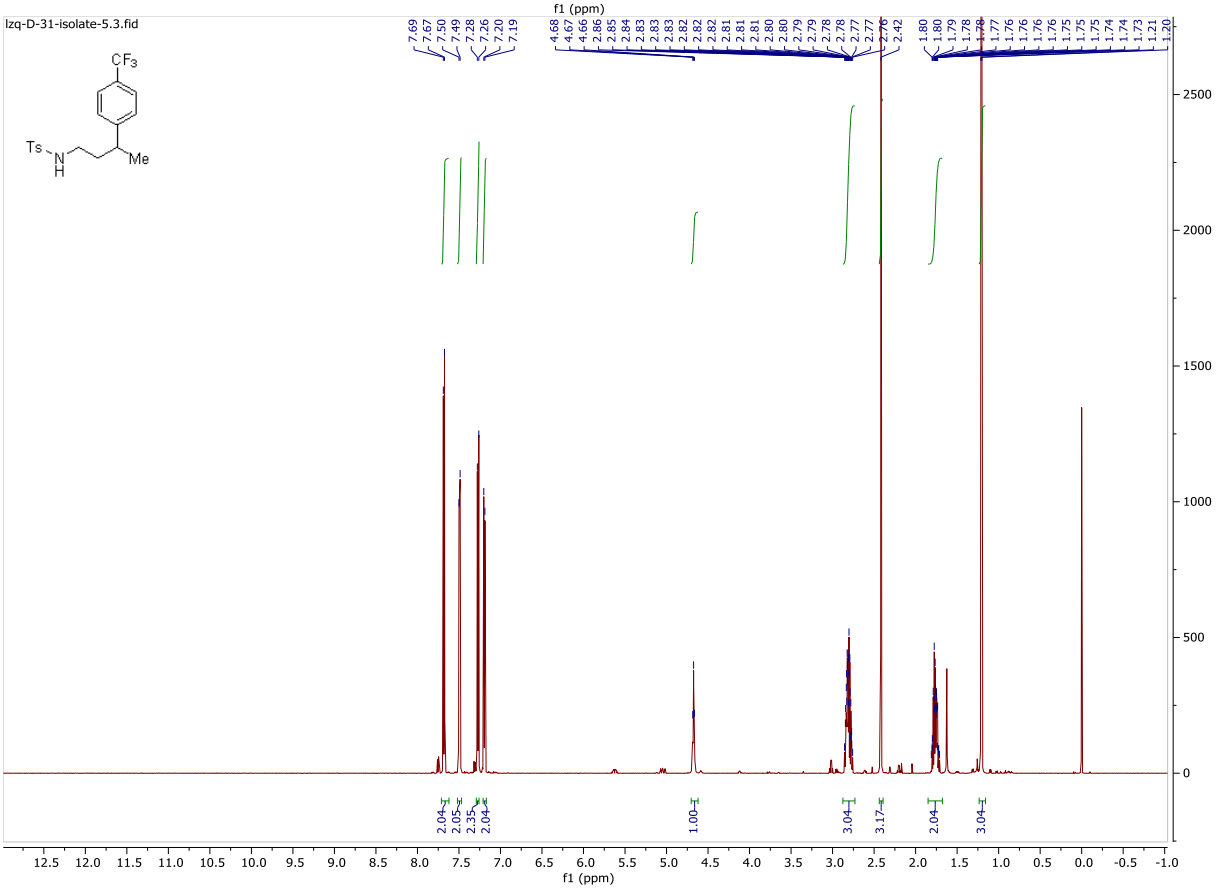
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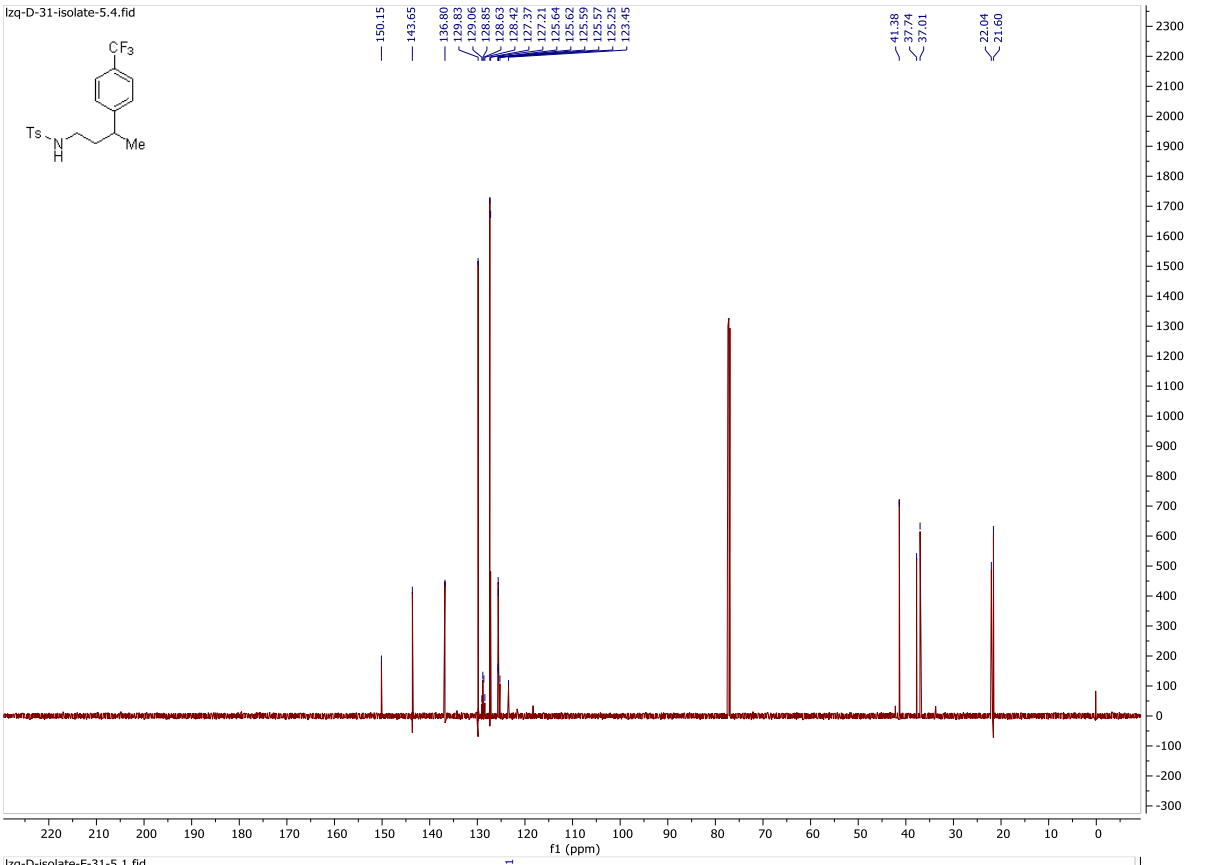
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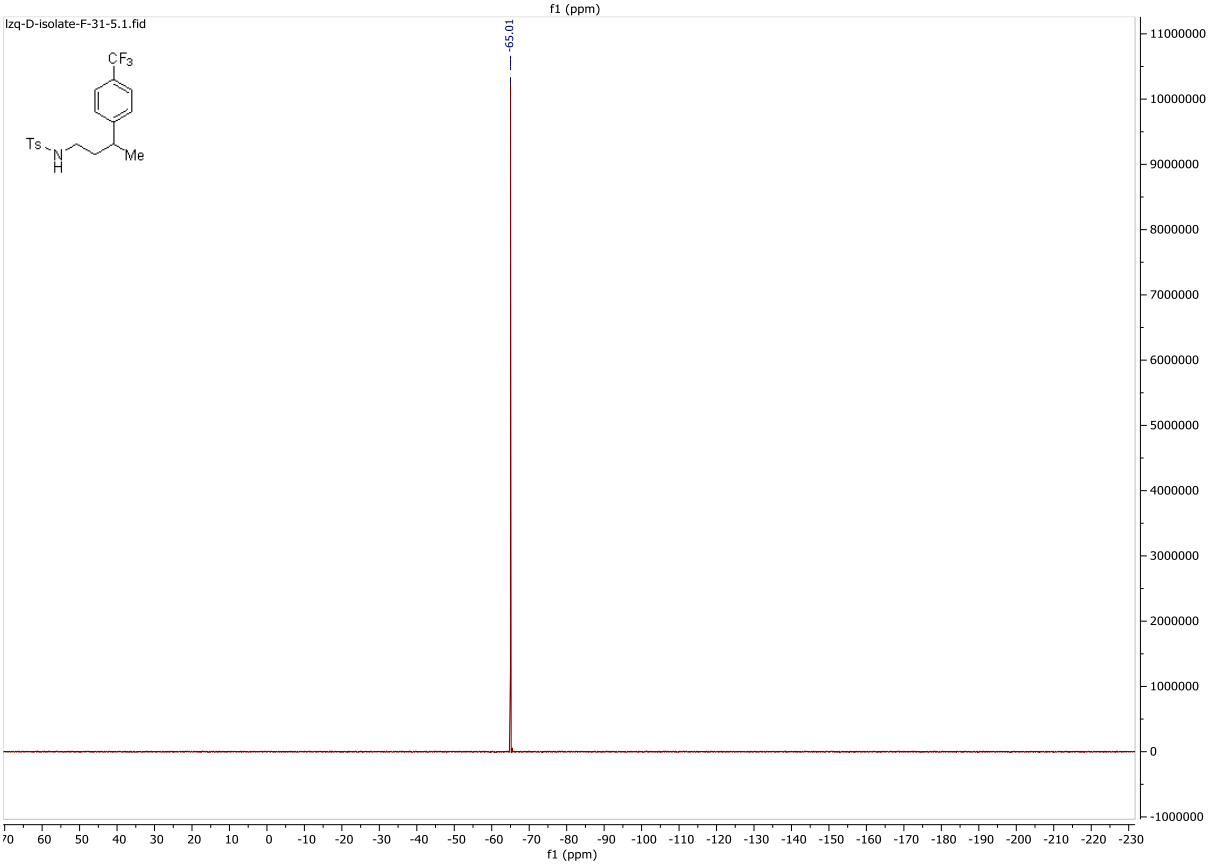
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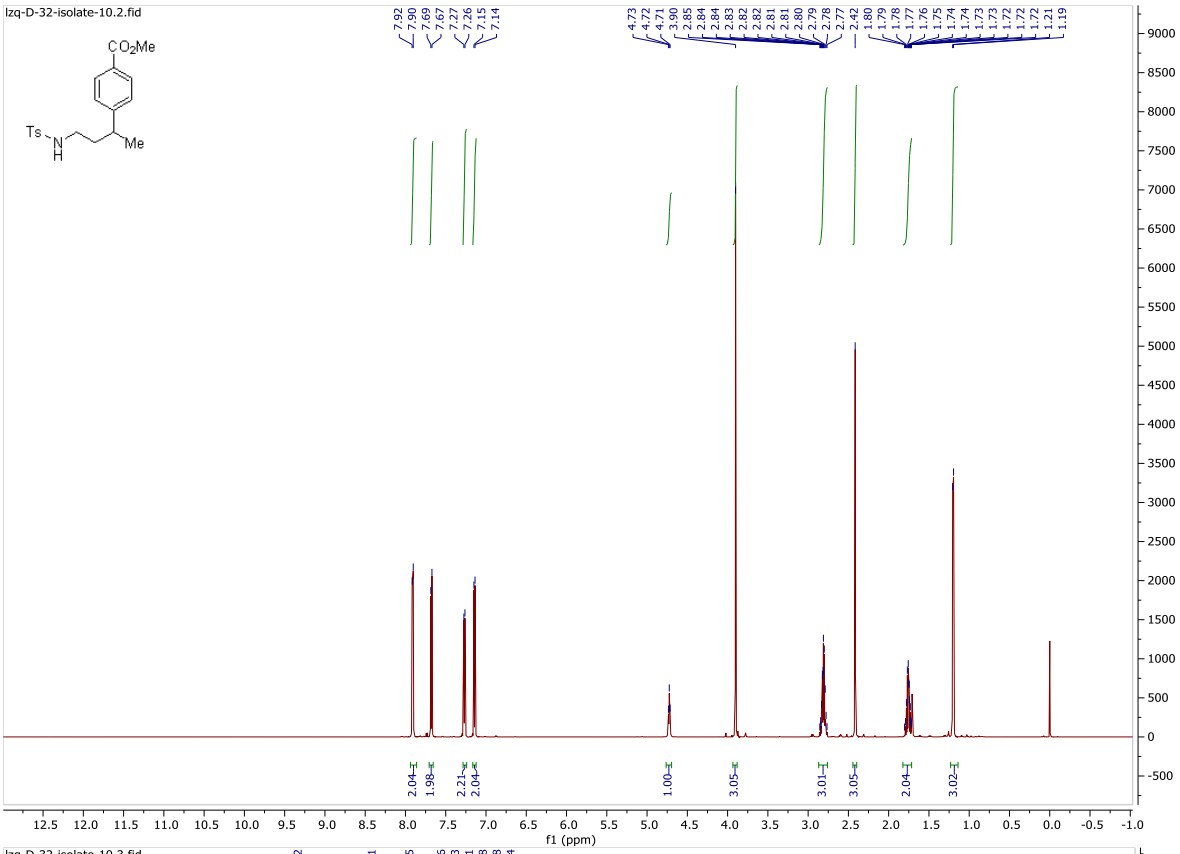
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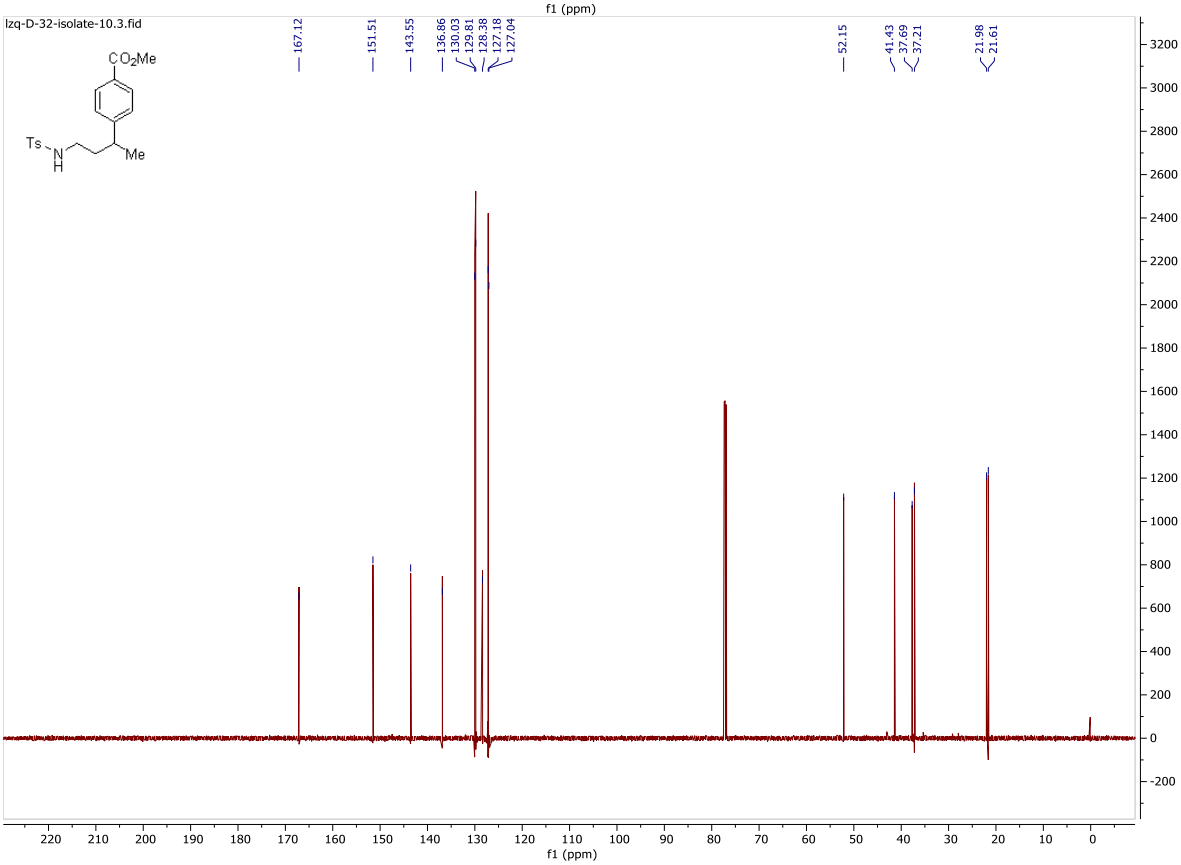
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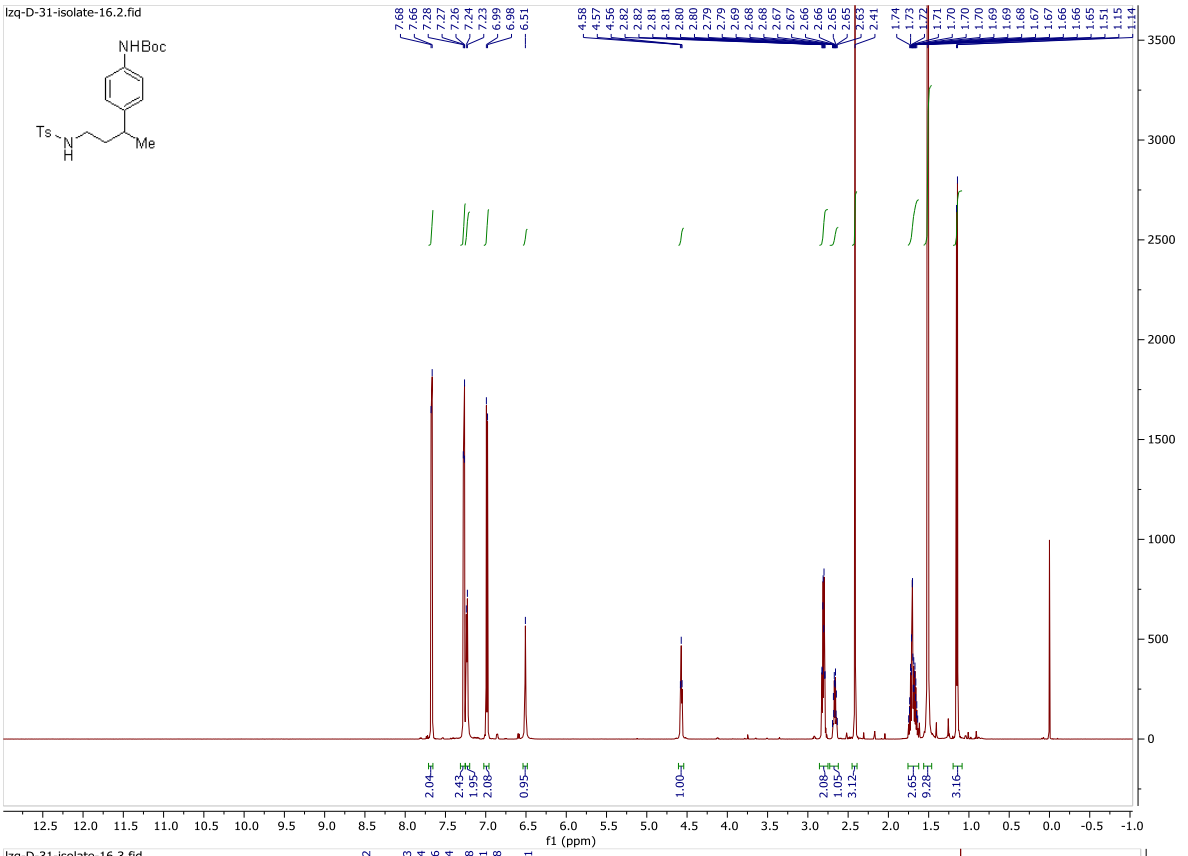
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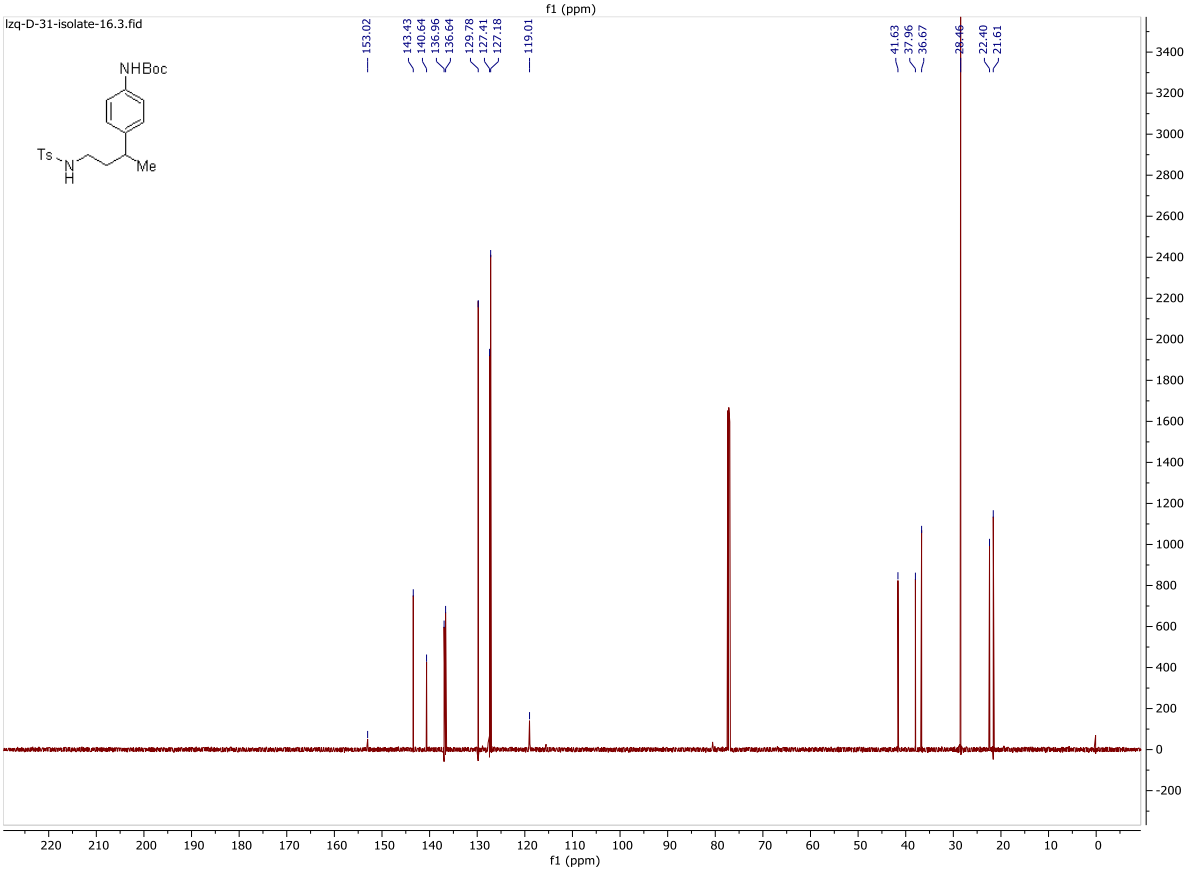
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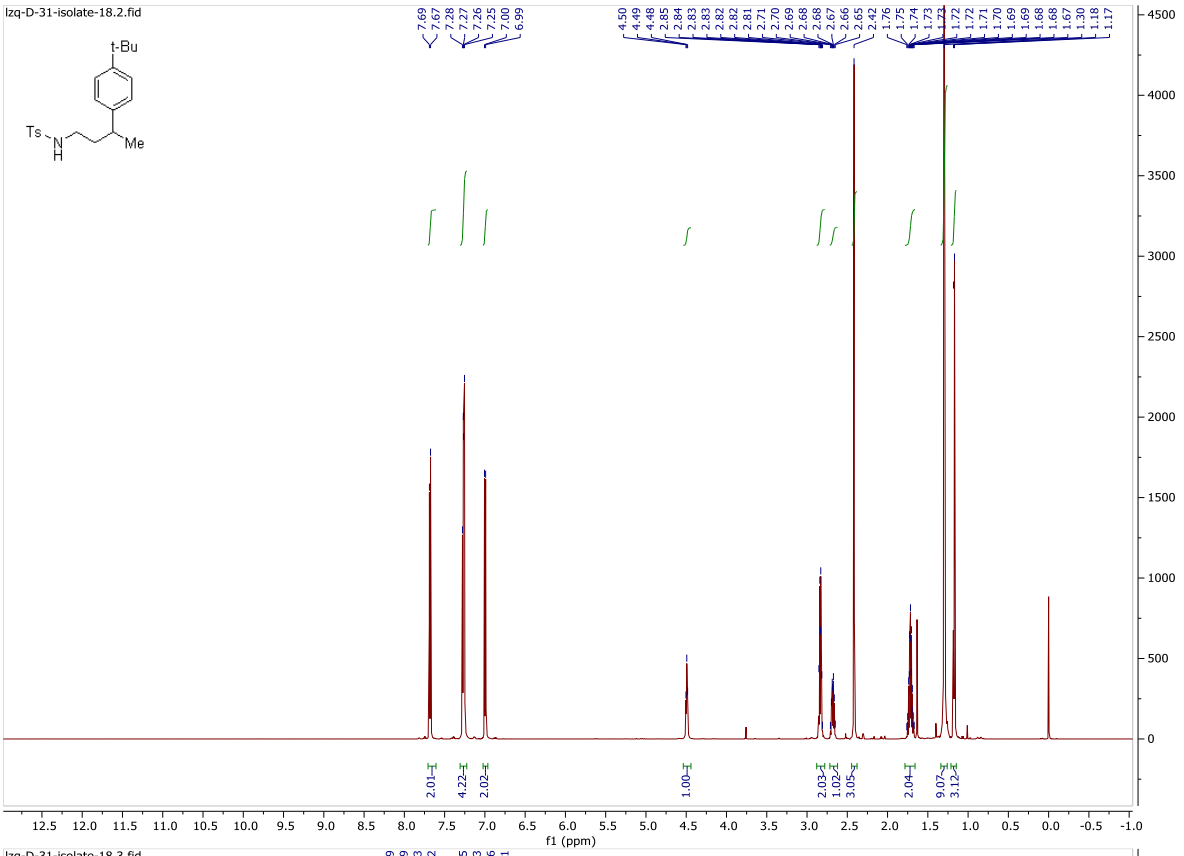
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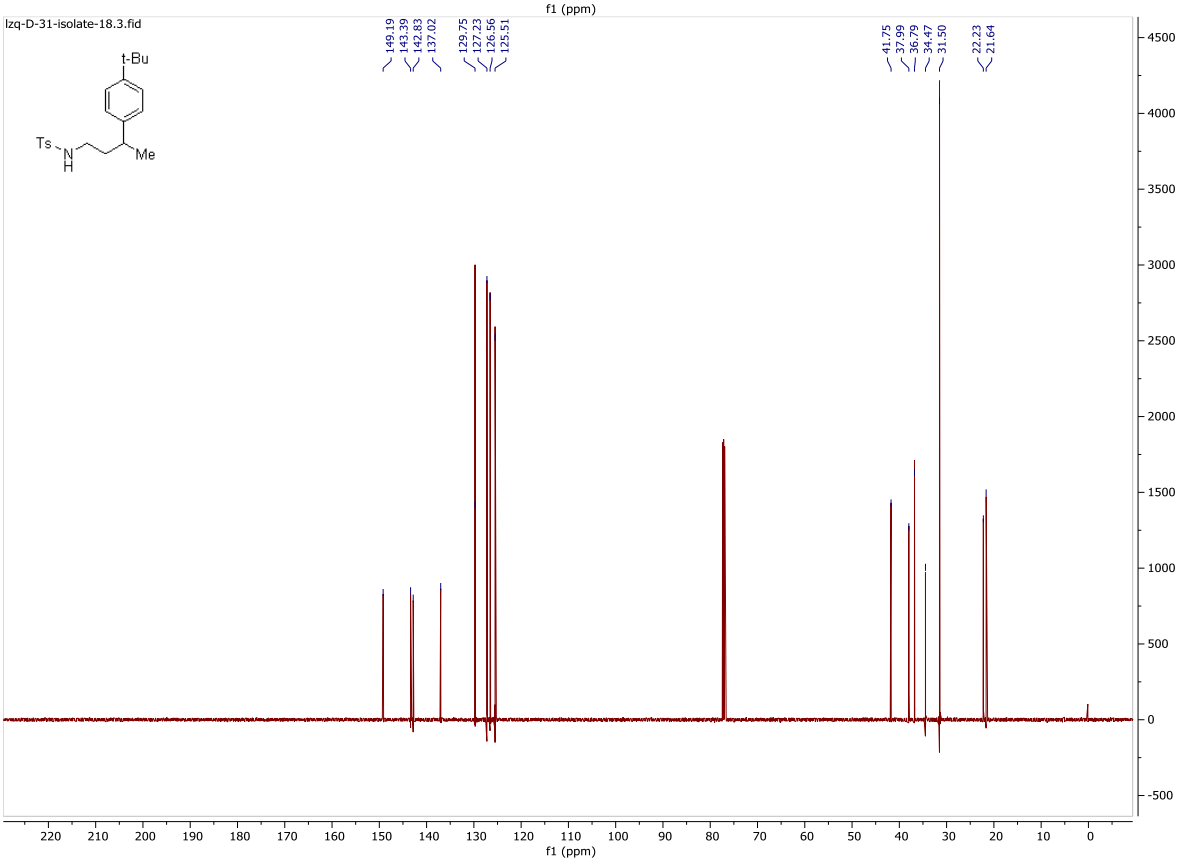
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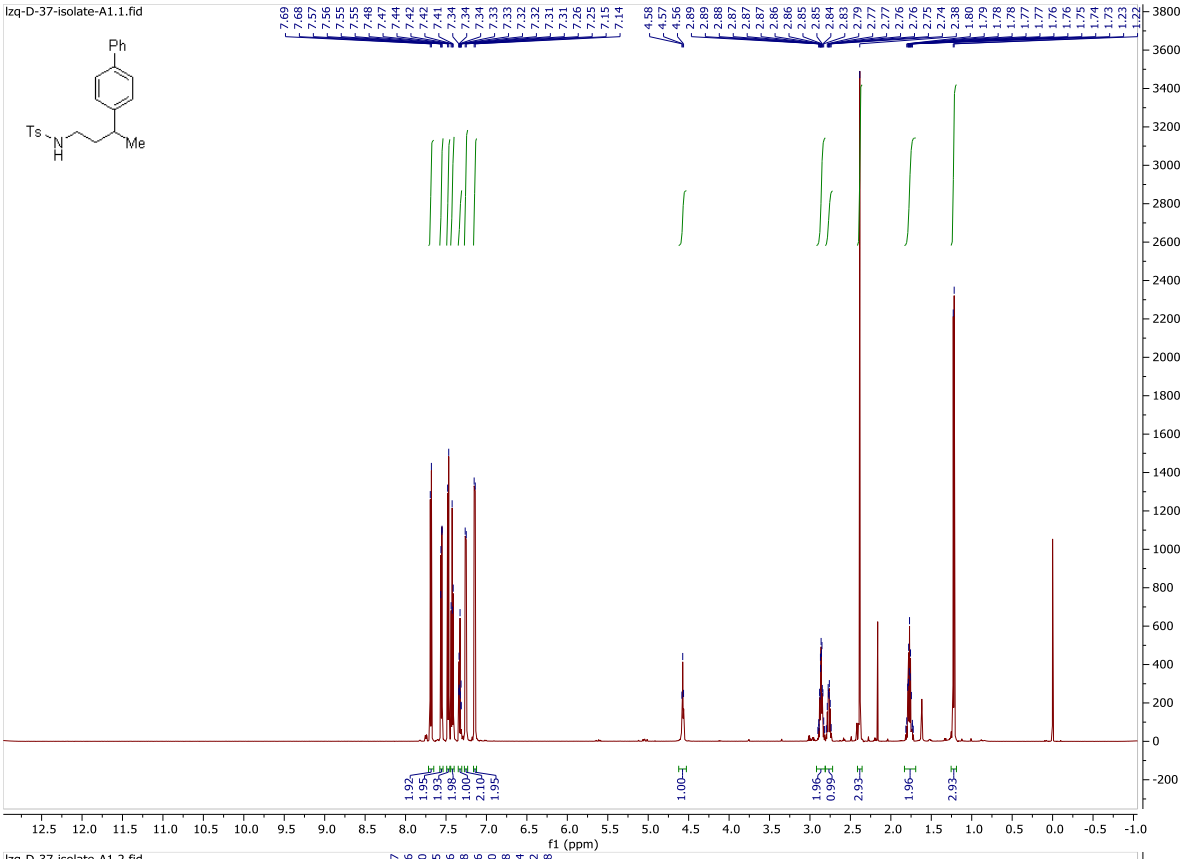
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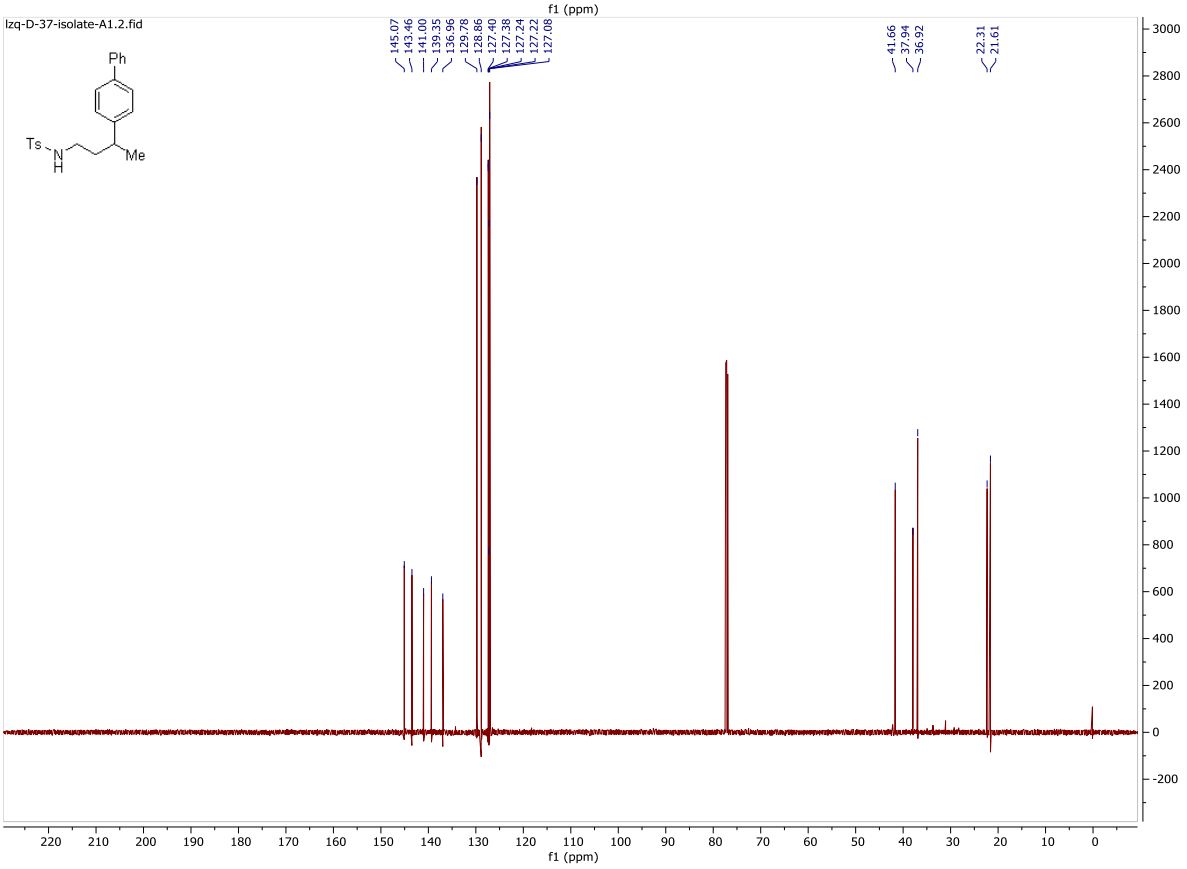
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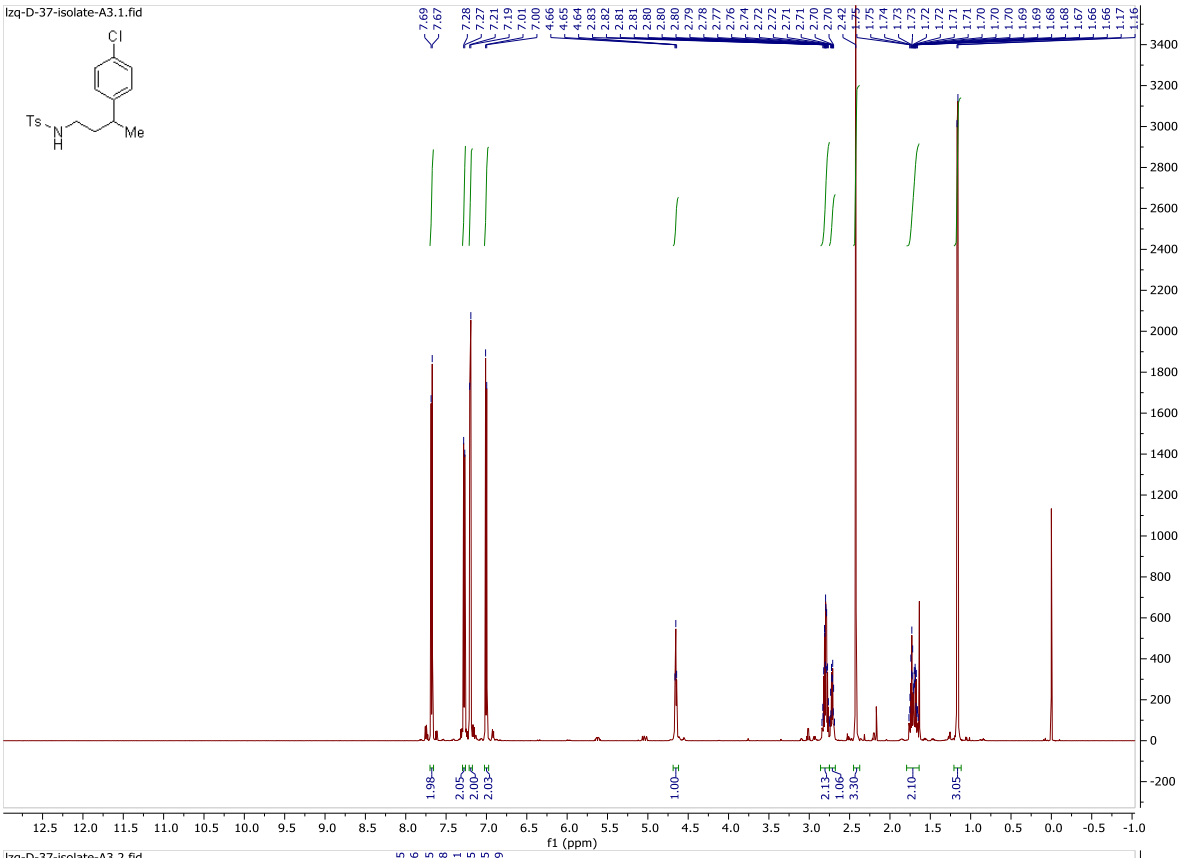
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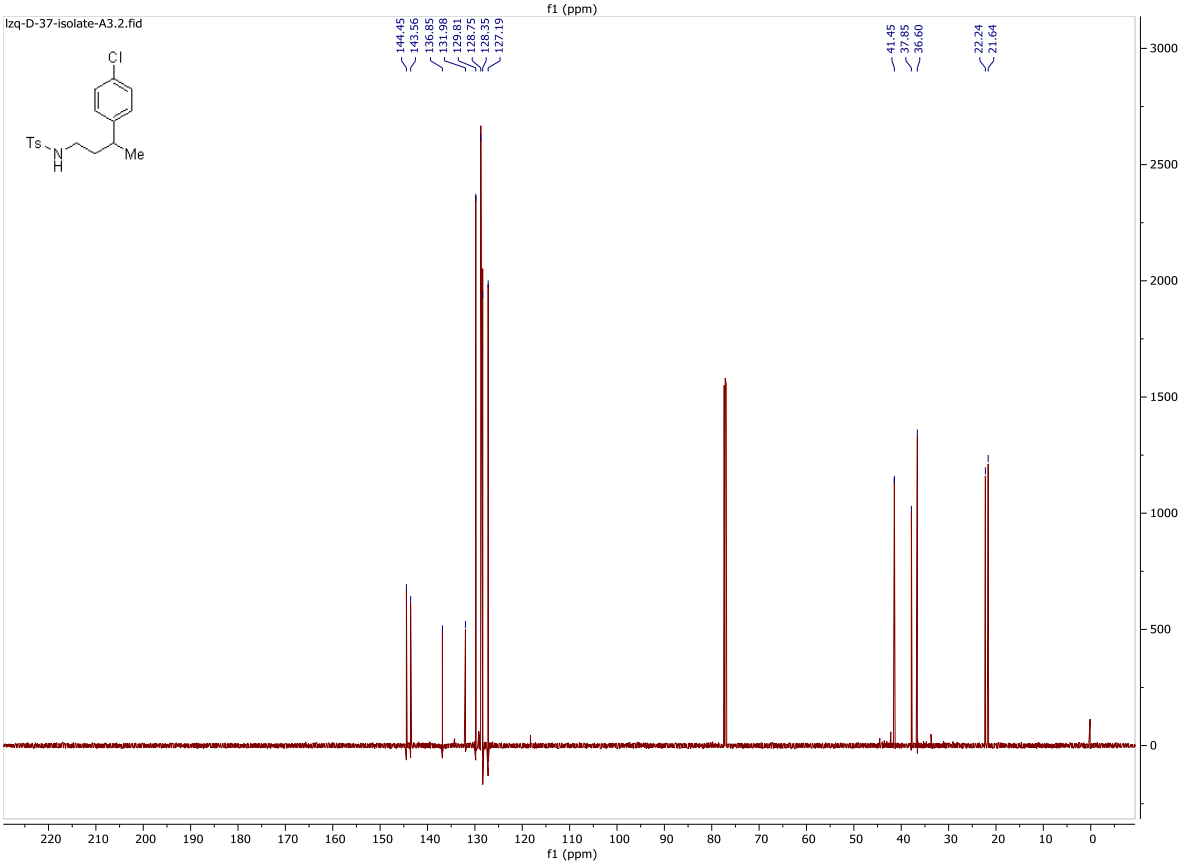
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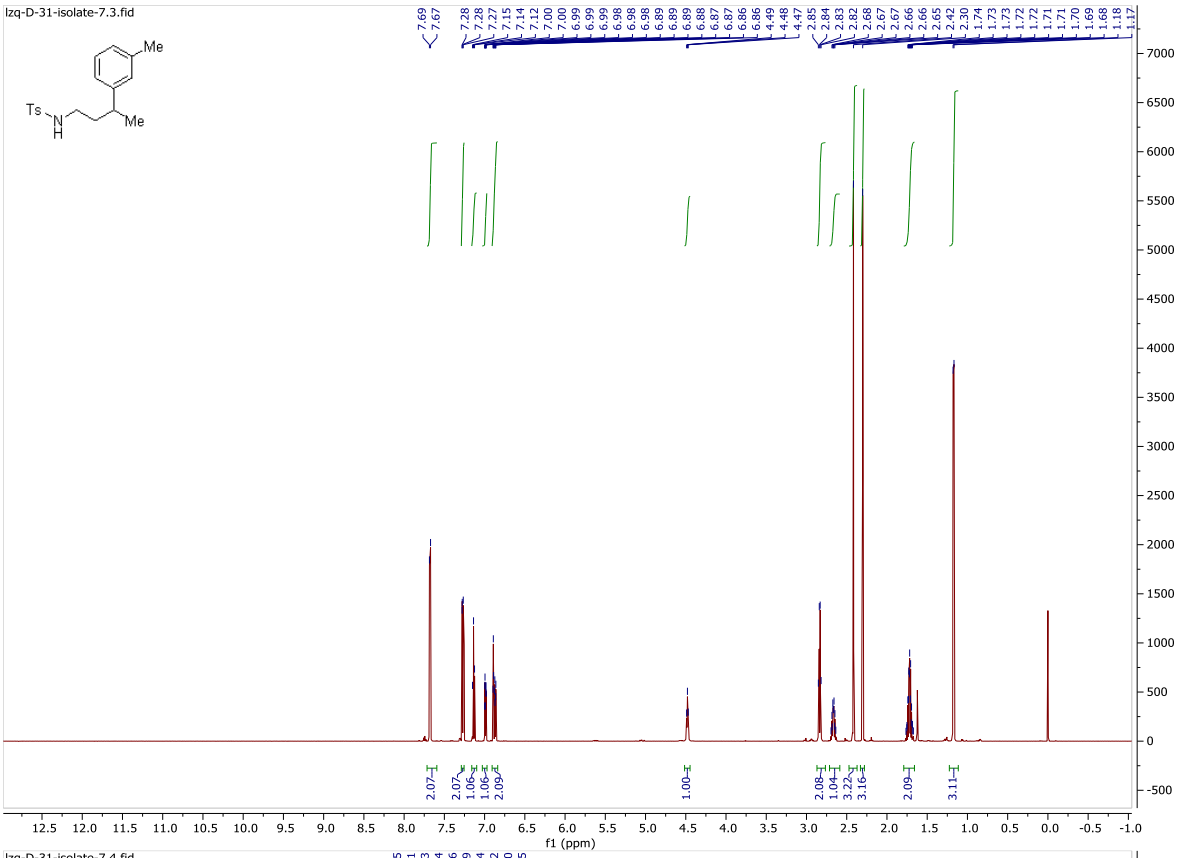
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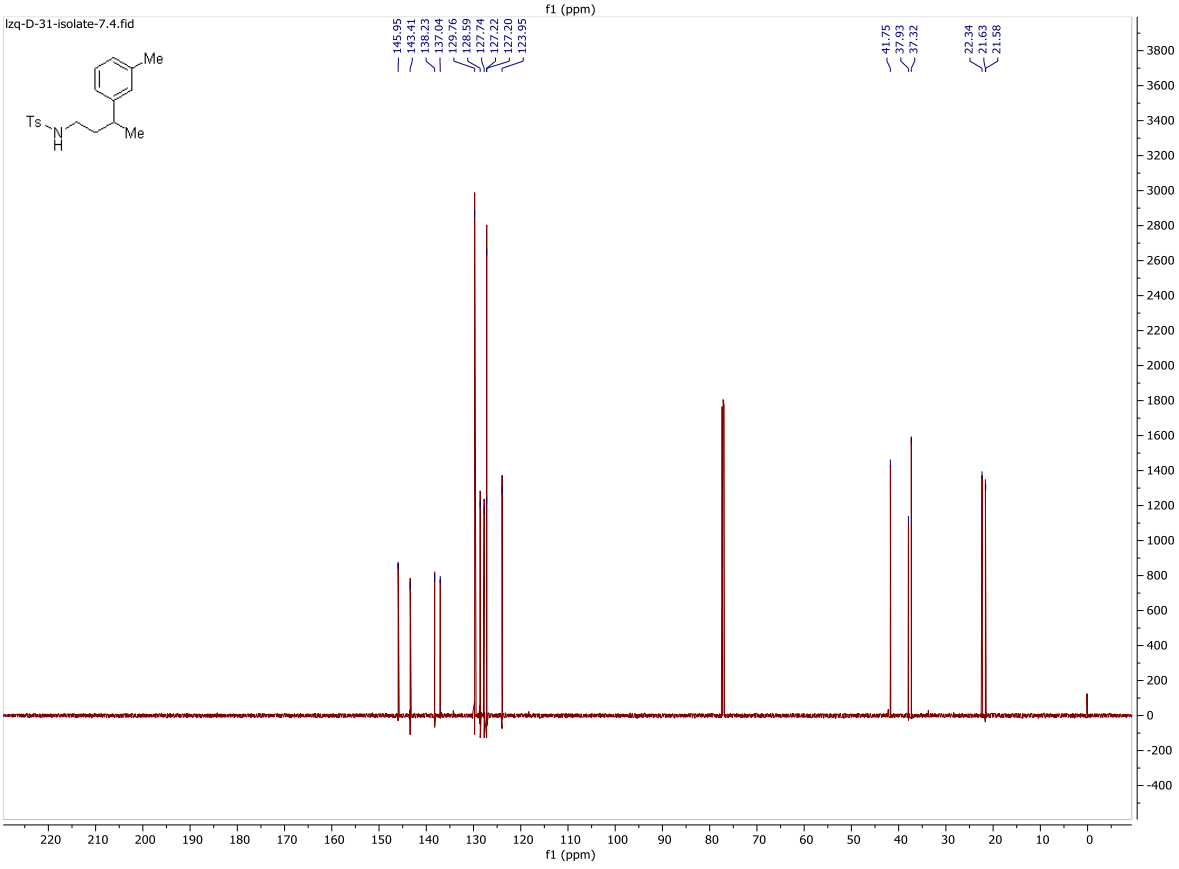
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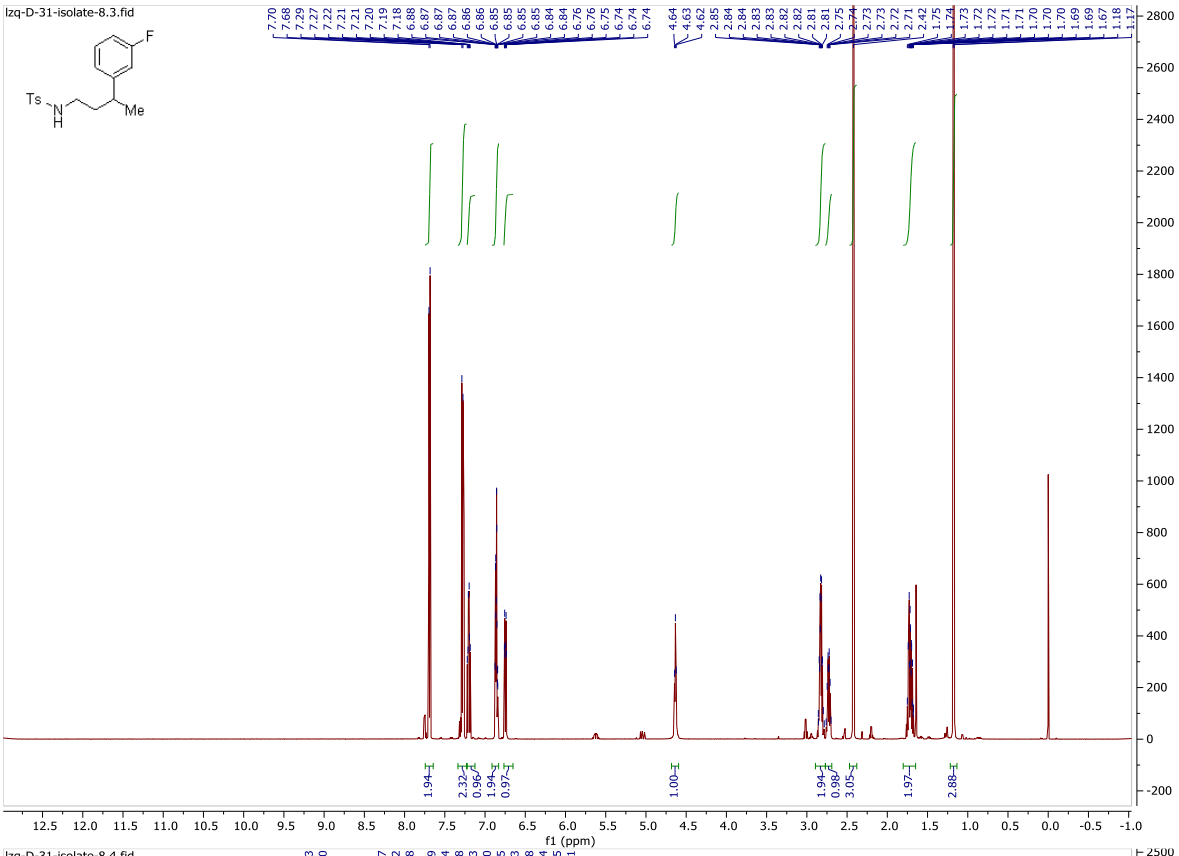
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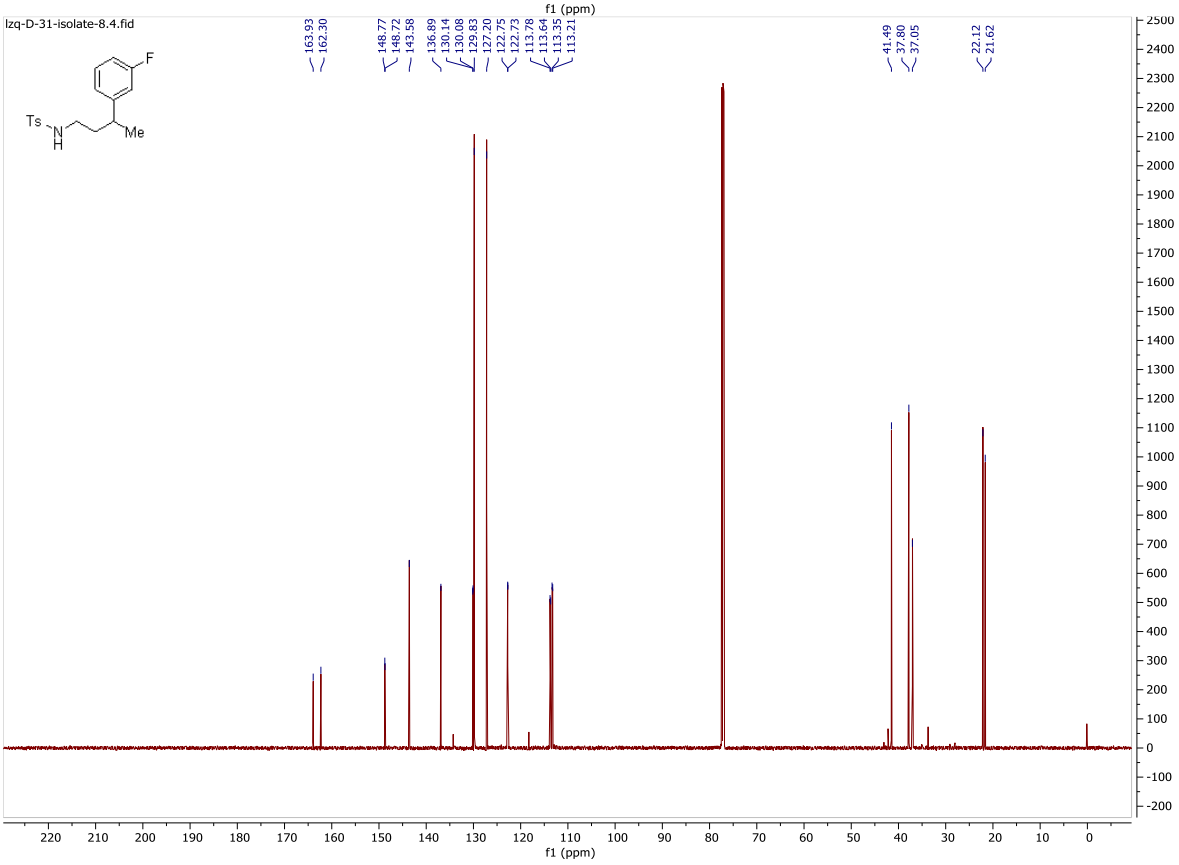
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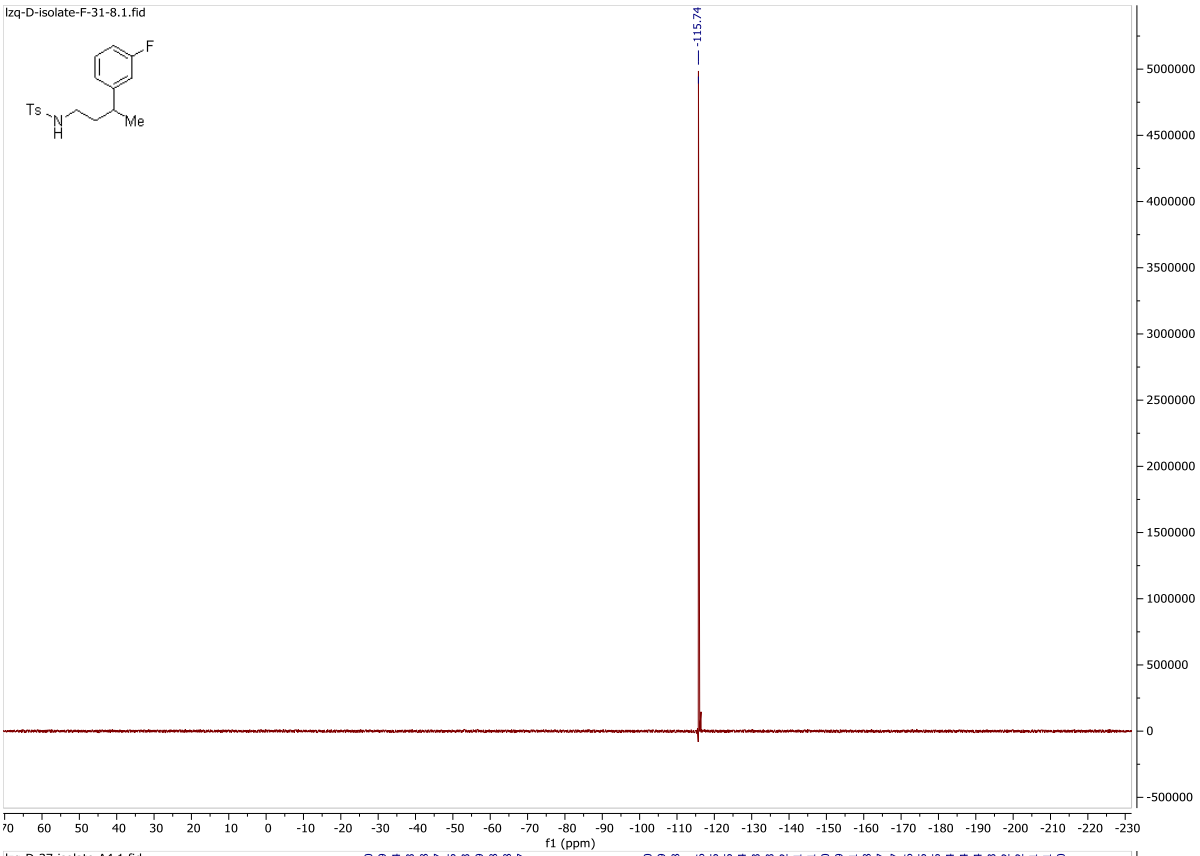
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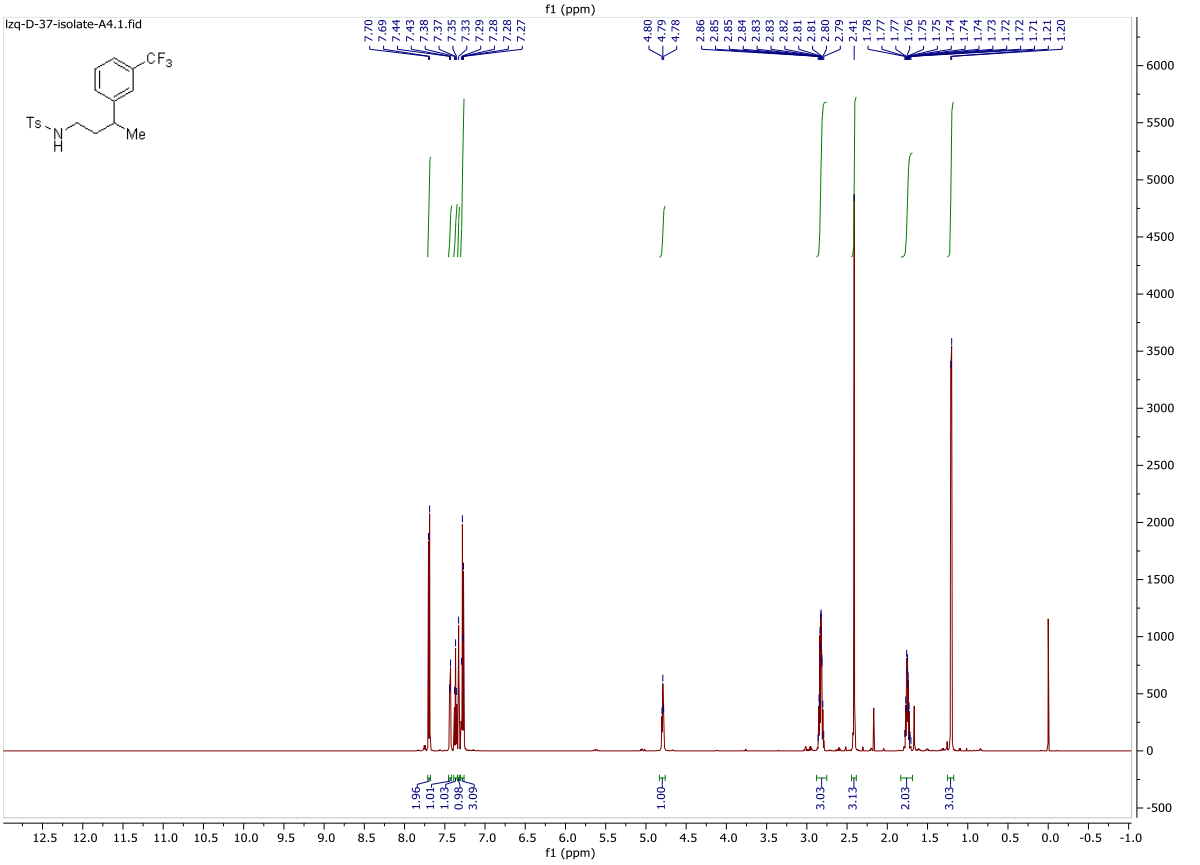
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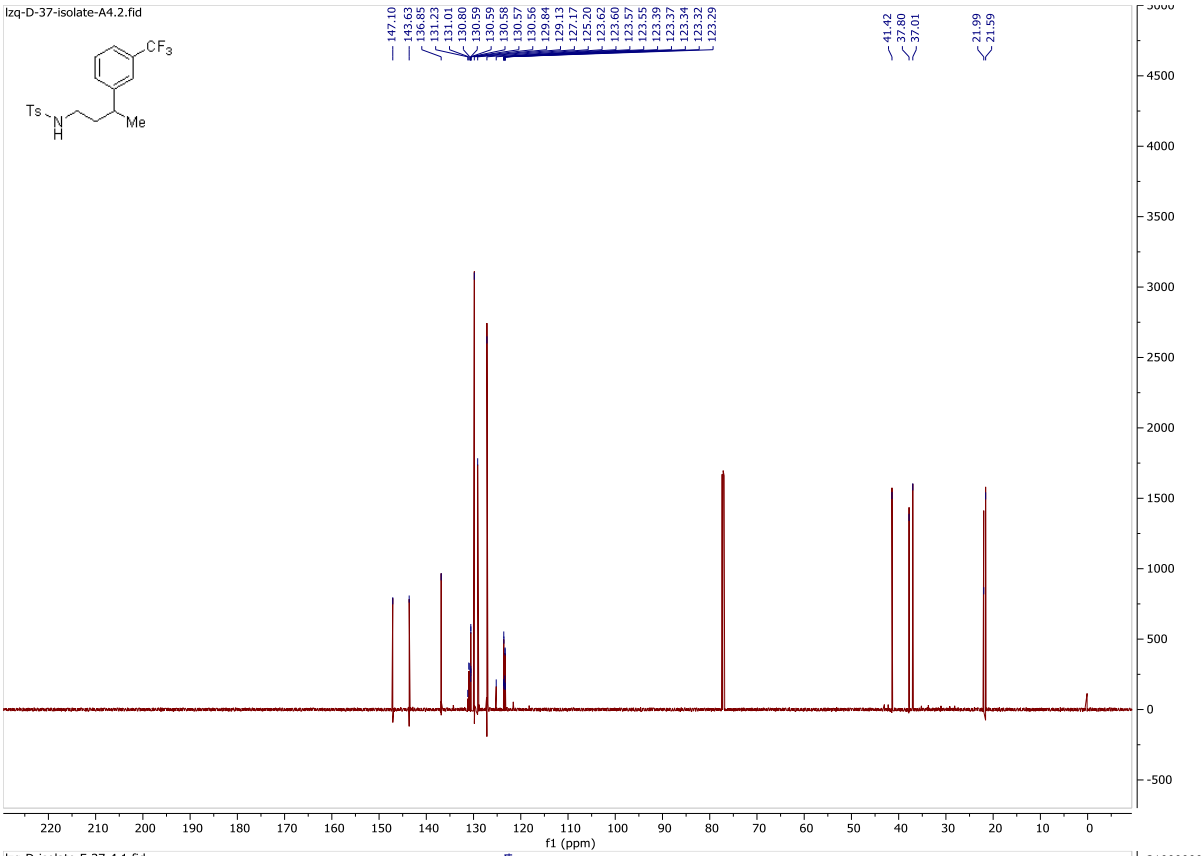
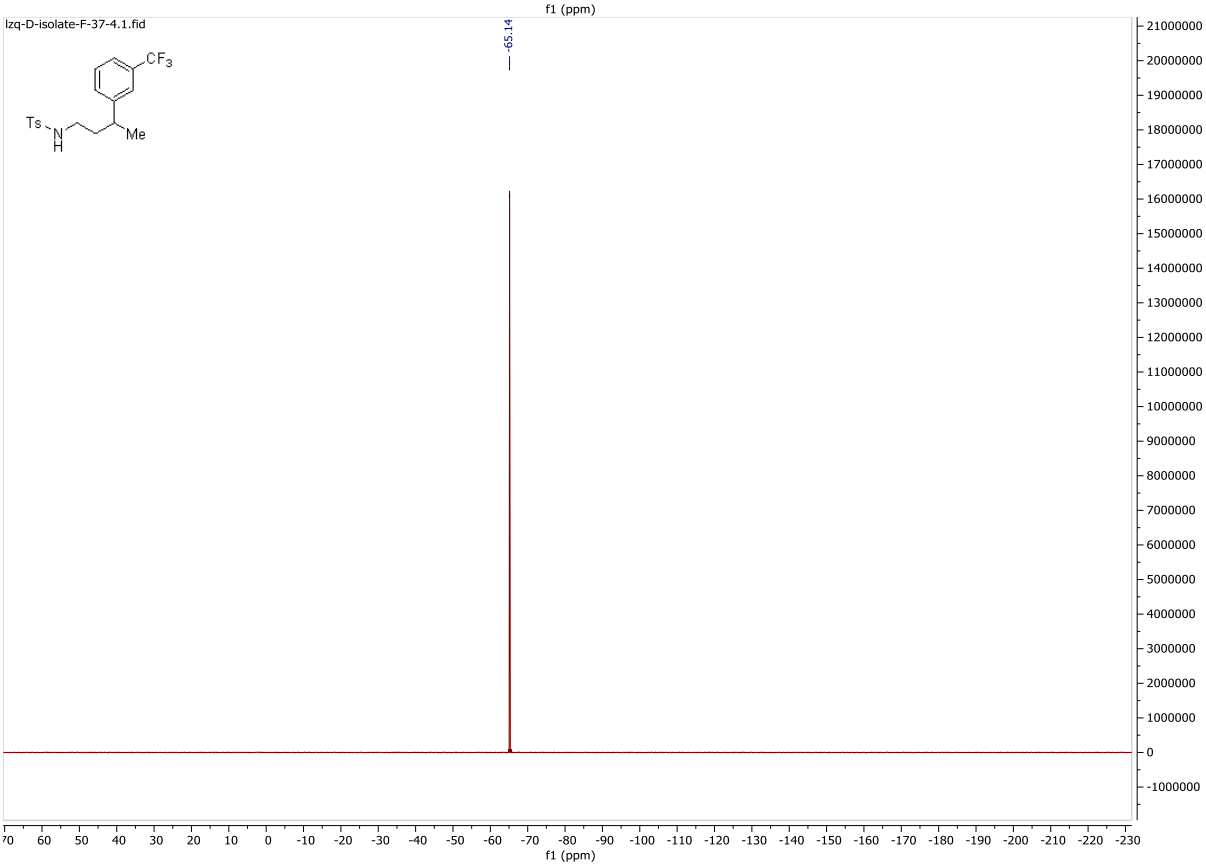
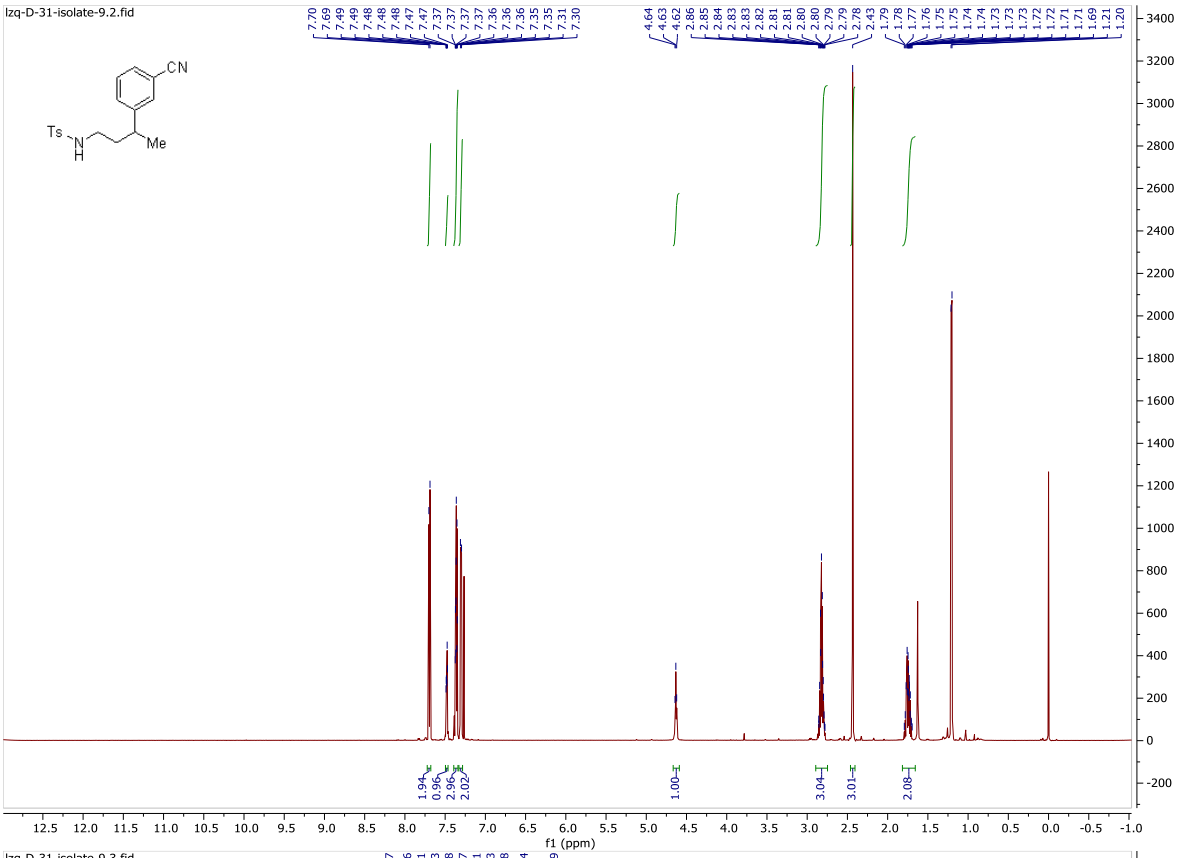
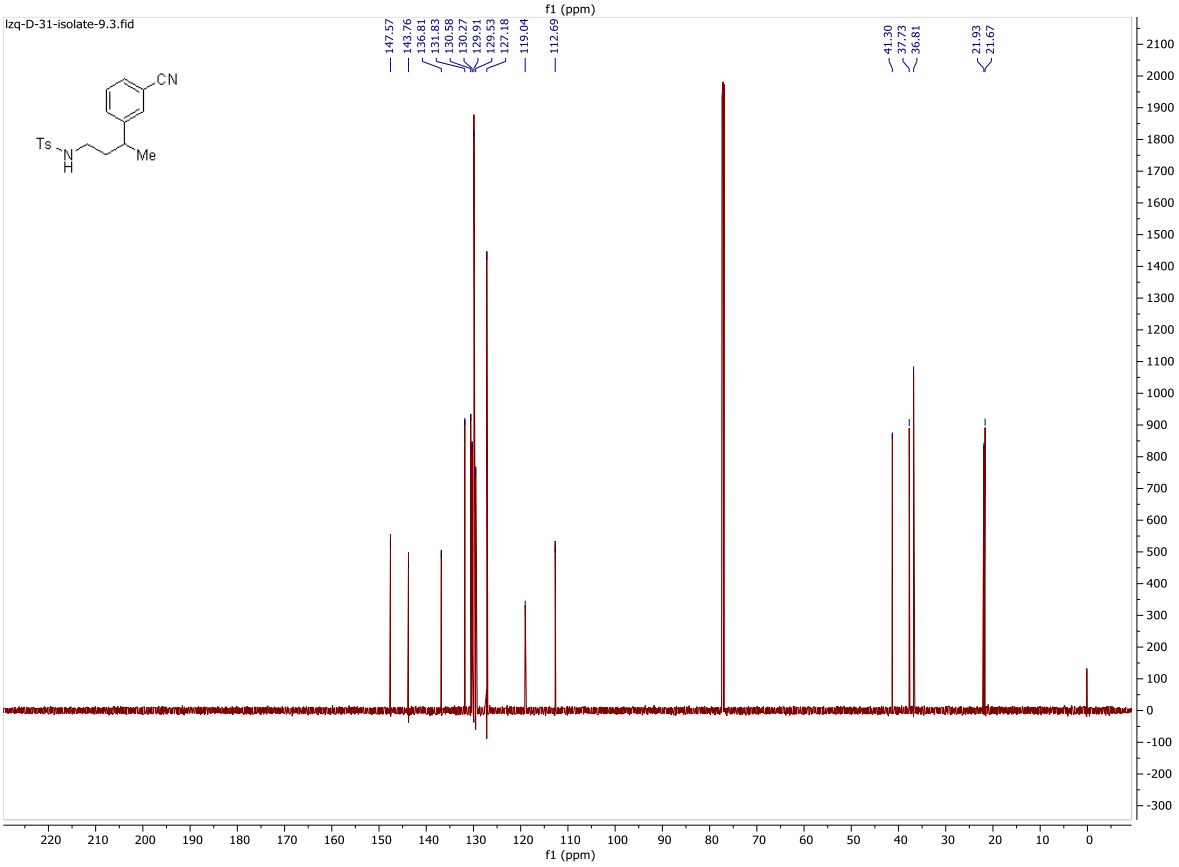
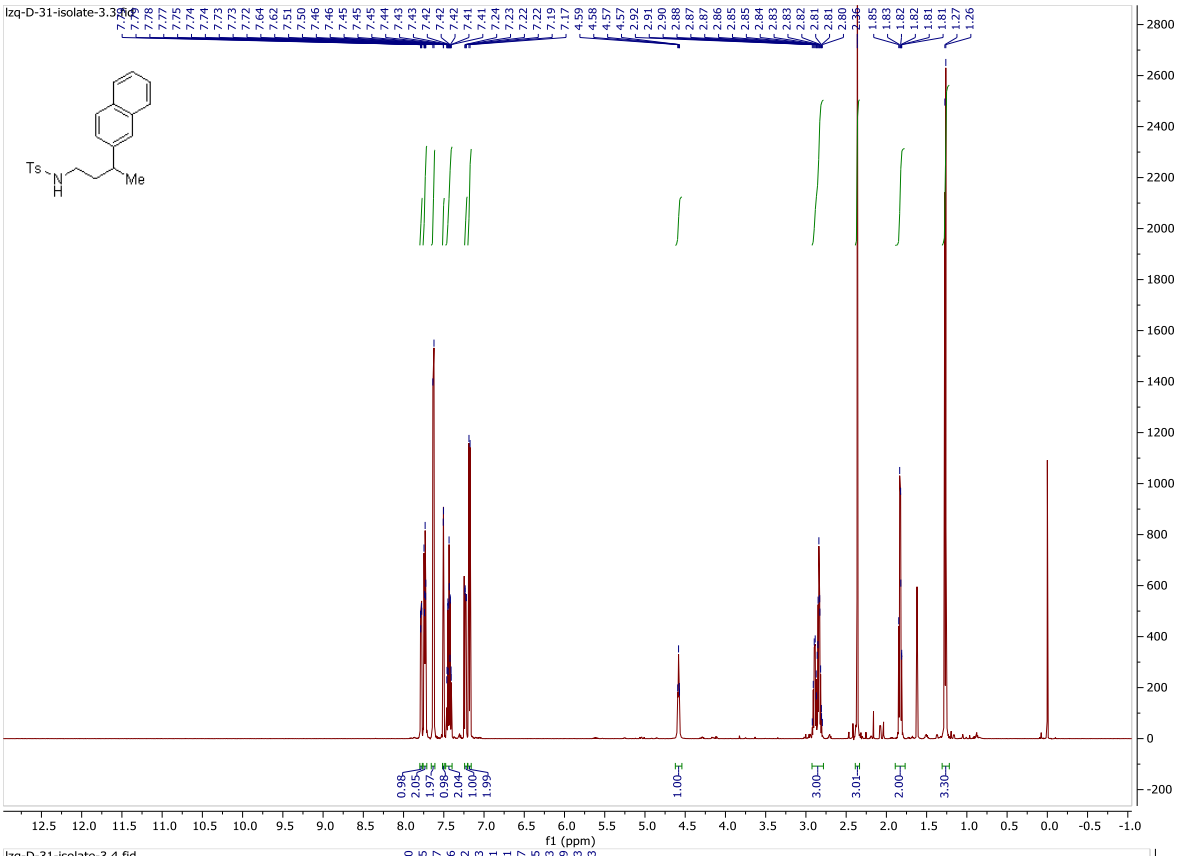
3.03
f1 (ppm)

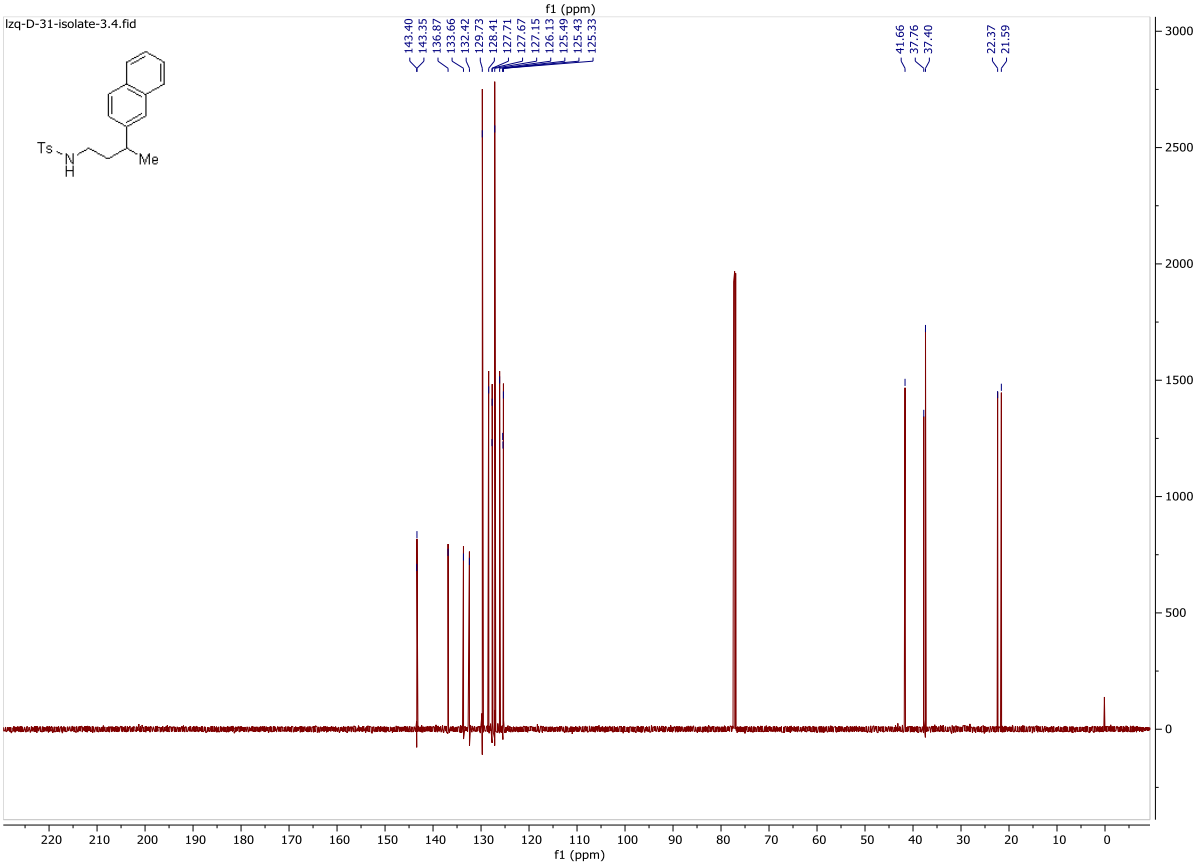

lzq-D-37-isolate-A4.2.fid
147.10
143.63
136.85
131.23
131.01
130.80
130.59
130.59
130.58
130.57
130.56
129.84
129.13
127.17
125.20
123.62
123.60
123.57
123.55
123.39
123.37
123.34
123.32
123.29
41.42
37.80
37.01
21.99
21.59
Ts
N
H
CF3
Me
f1 (ppm)

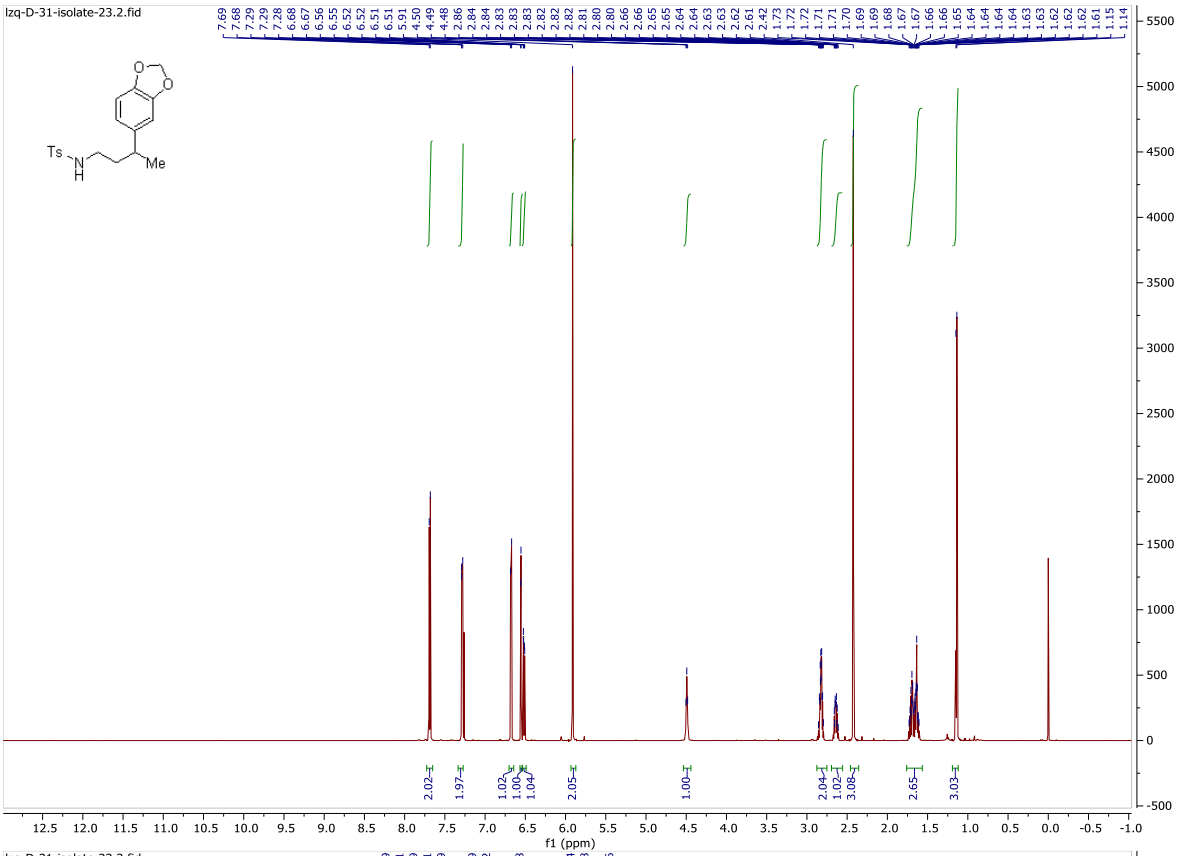

lzq-D-isolate-F-37-4.1.fid
-65.14
Ts
N
H
CF3
Me
f1 (ppm)

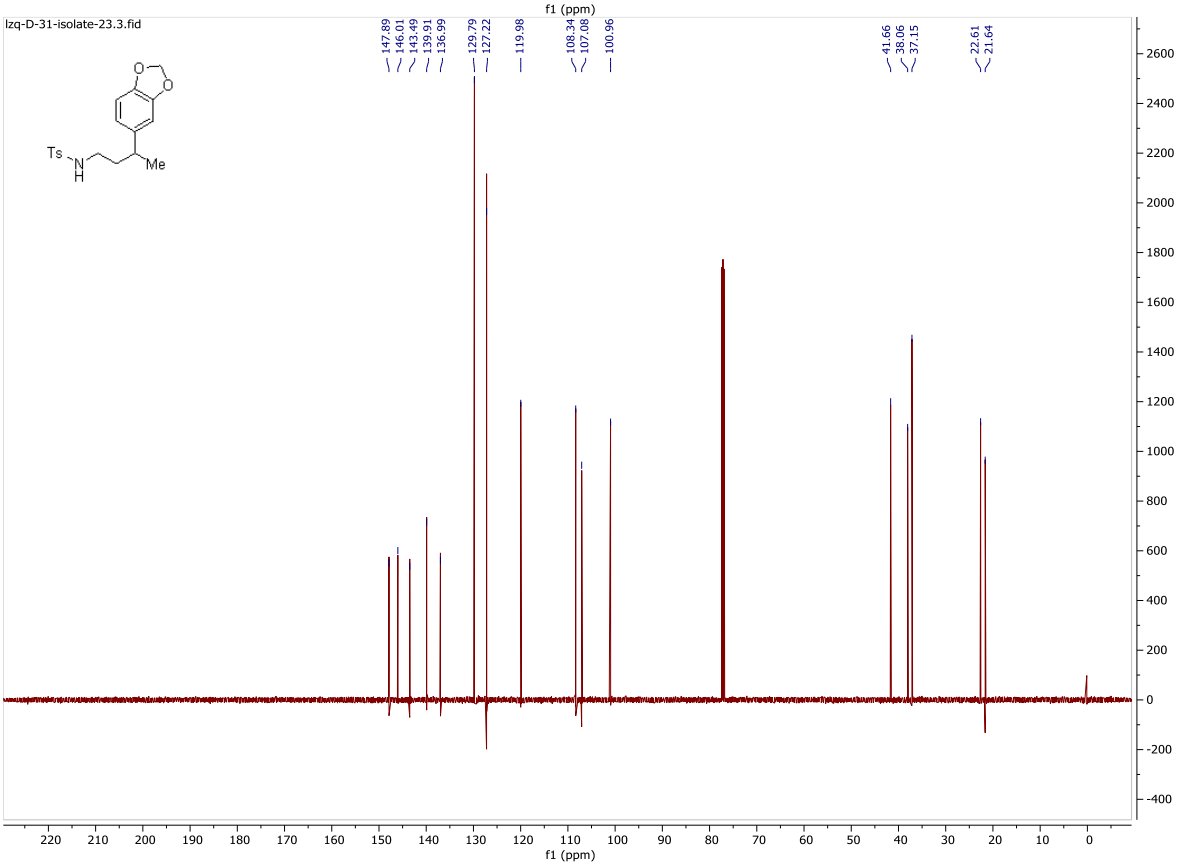

lzq-D-31-isolate-9.2.fid
CN
Ts
N
H
Me
7.70 7.69 7.49 7.49 7.48 7.48 7.48 7.47 7.47 7.37 7.37 7.37 7.36 7.36 7.35 7.35 7.31 7.30
4.64 4.63 4.62 2.86 2.85 2.84 2.83 2.82 2.81 2.81 2.80 2.80 2.79 2.79 2.78 2.43 1.79 1.78 1.77 1.76 1.75 1.75 1.74 1.74 1.73 1.73 1.72 1.72 1.71 1.71 1.69 1.21 1.20
1.94 0.96 2.96 2.02 1.00 3.04 3.01 2.08
f1 (ppm)

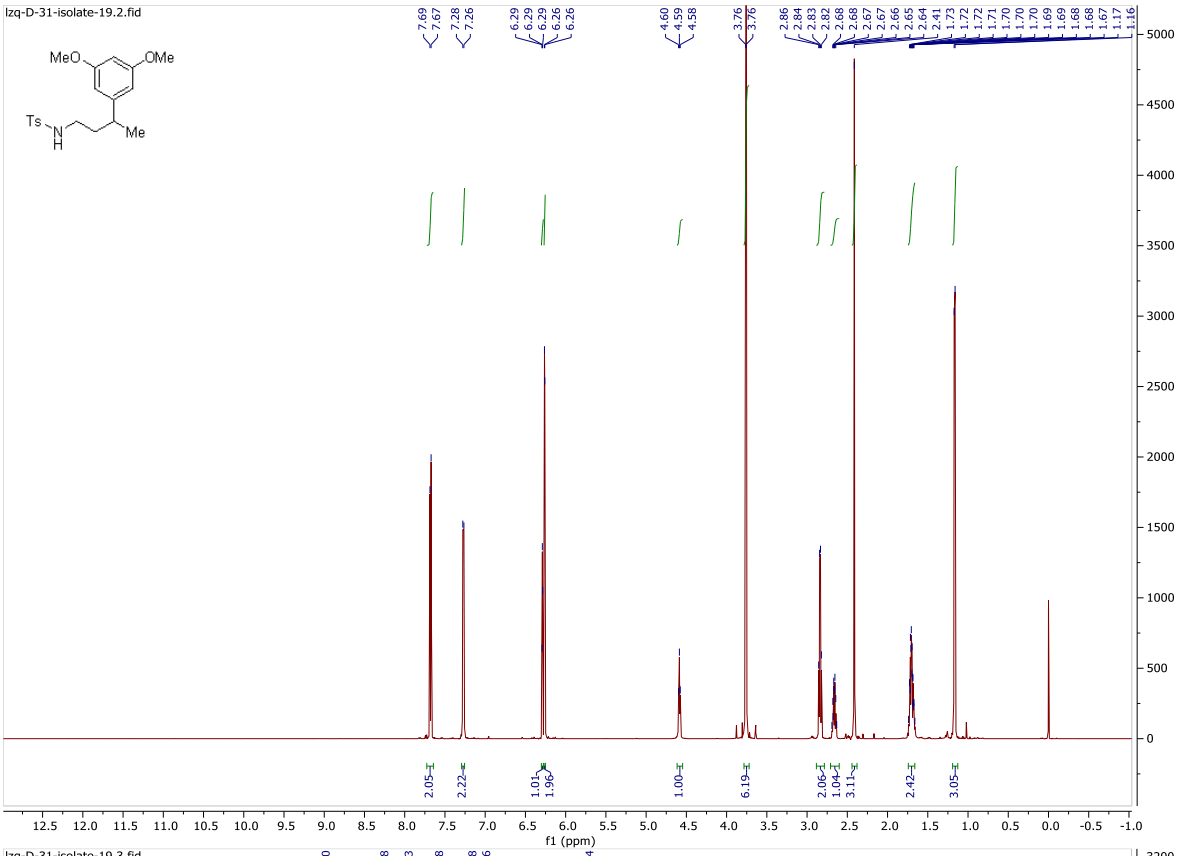

lzq-D-31-isolate-9.3.fid
CN
Ts
N
H
Me
147.57 143.76 136.81 131.83 130.58 130.27 129.91 129.53 127.18 119.04 112.69
41.30 37.73 36.81 21.93 21.67
f1 (ppm)

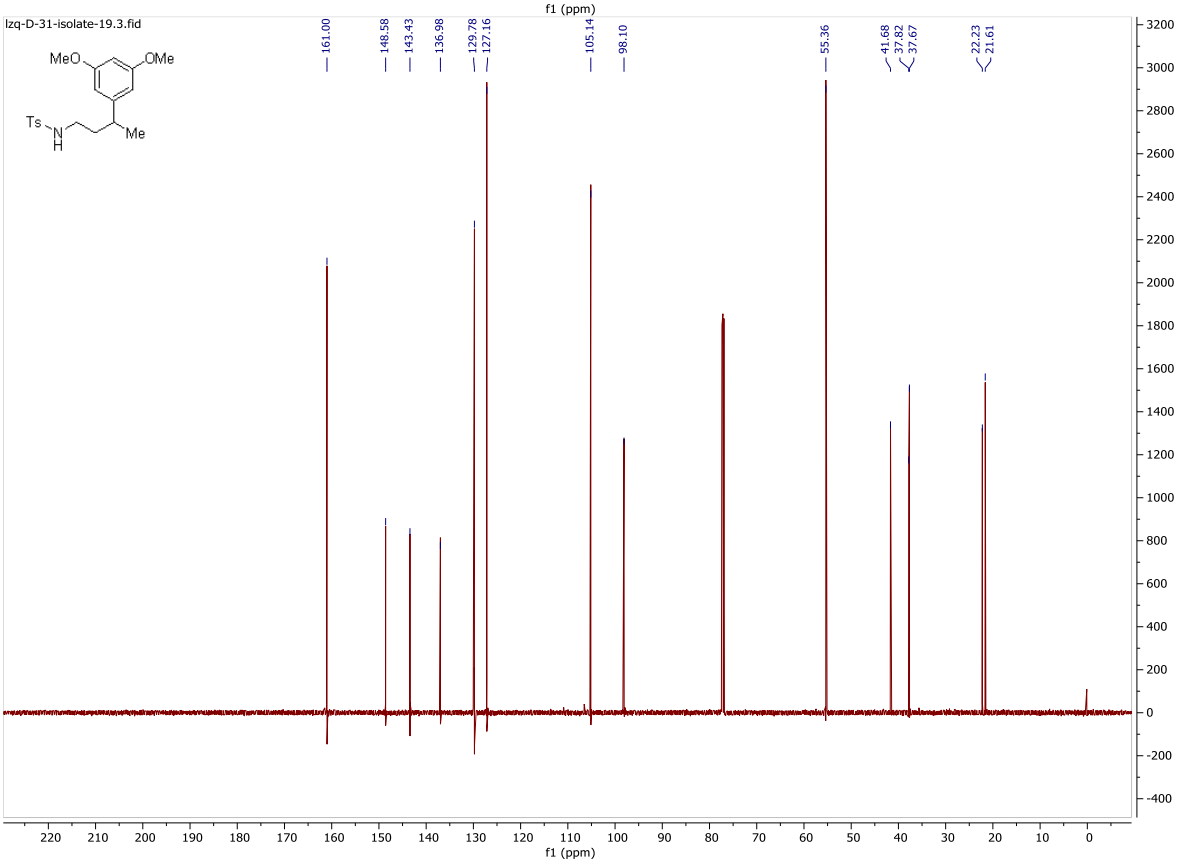

lzq-D-31-isolate-3.3.fid
Ts
N
H
Me
f1 (ppm)

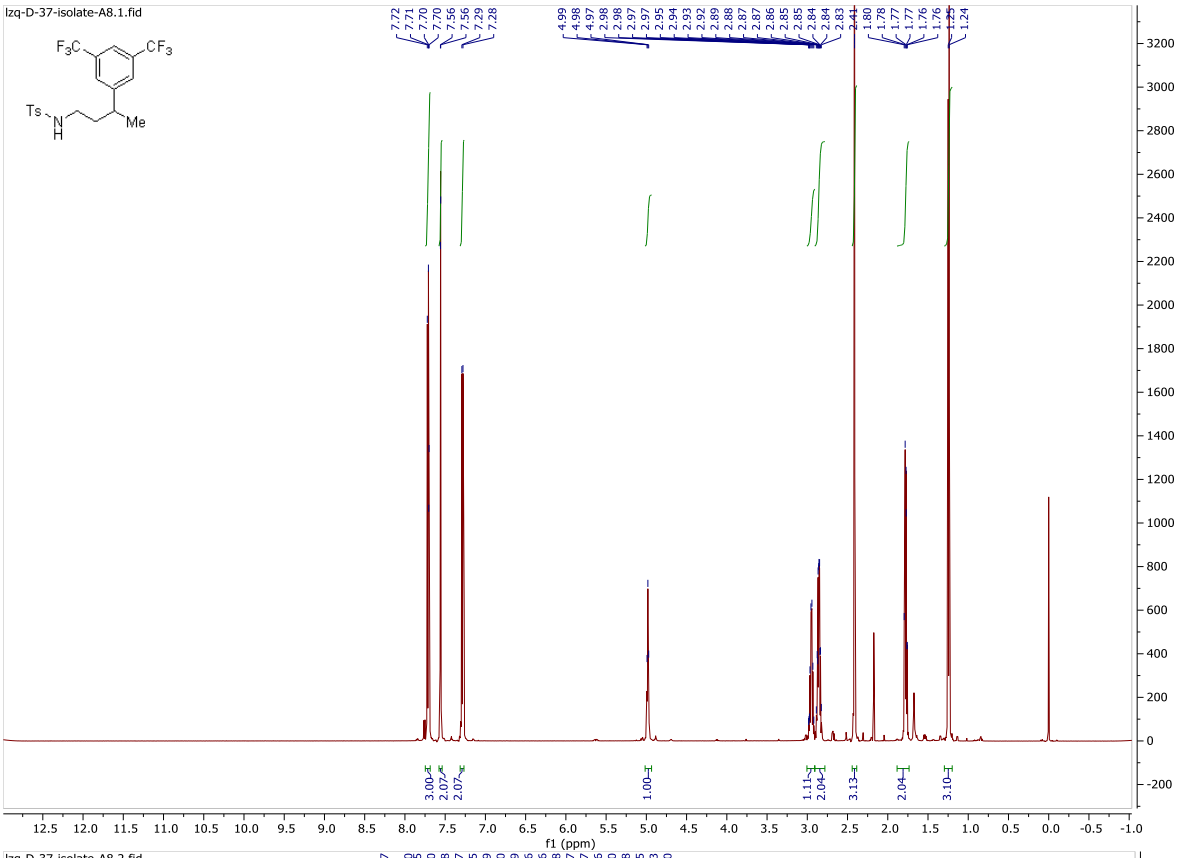

lzq-D-31-isolate-3.4.fid
Ts
N
H
Me
f1 (ppm)

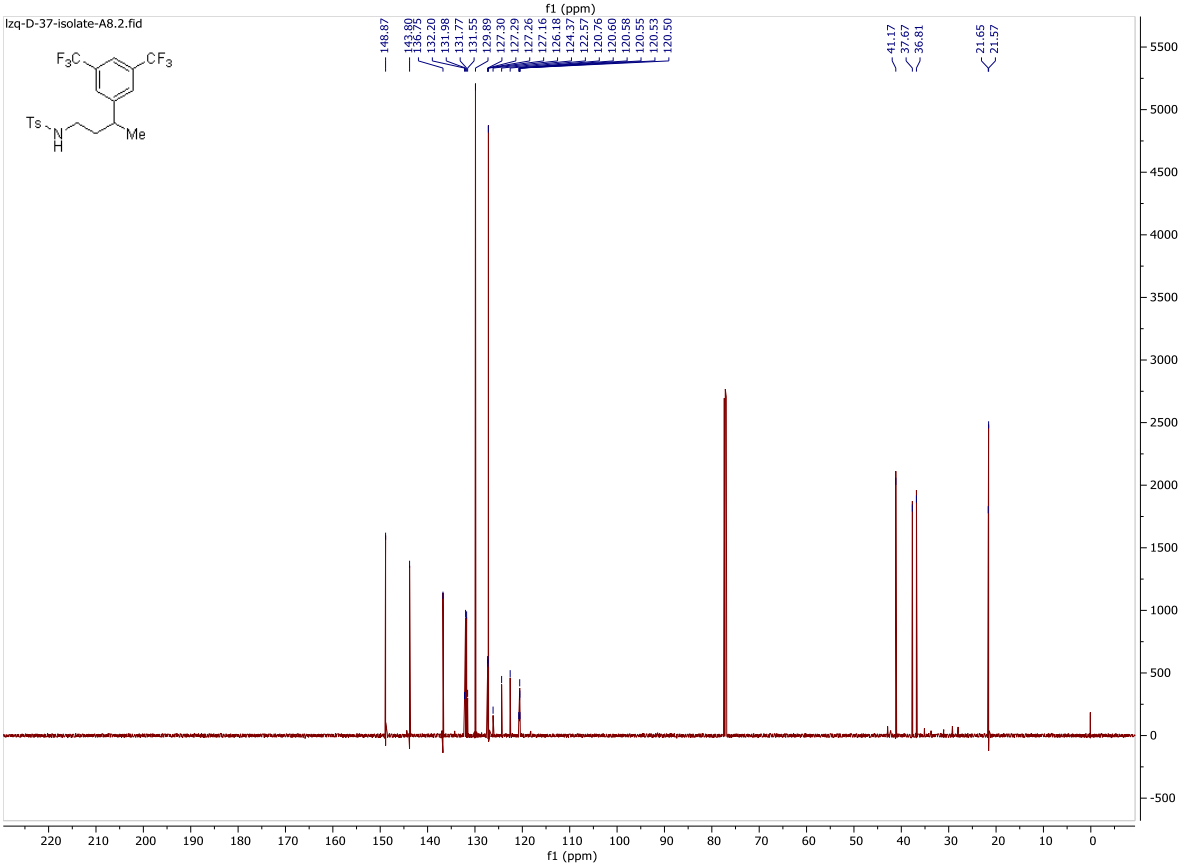

lzq-D-31-isolate-23.2.fid
Ts
N
H
Me
f1 (ppm)

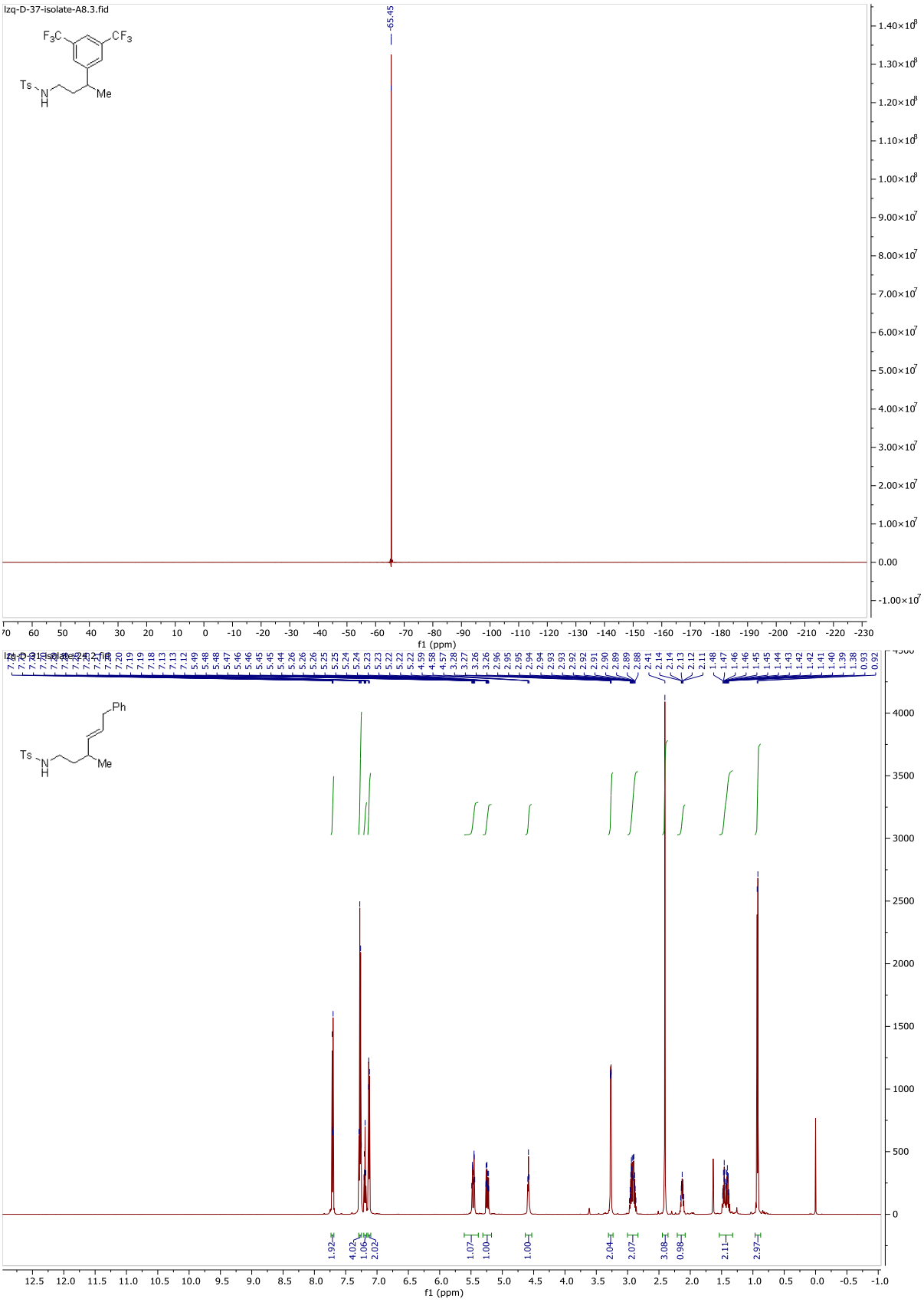

lzq-D-31-isolate-23.3.fid
147.89
146.01
143.49
139.91
136.99
129.79
127.22
119.98
108.34
107.08
100.96
41.66
38.06
37.15
22.61
21.64
Ts
N
H
Me
f1 (ppm)

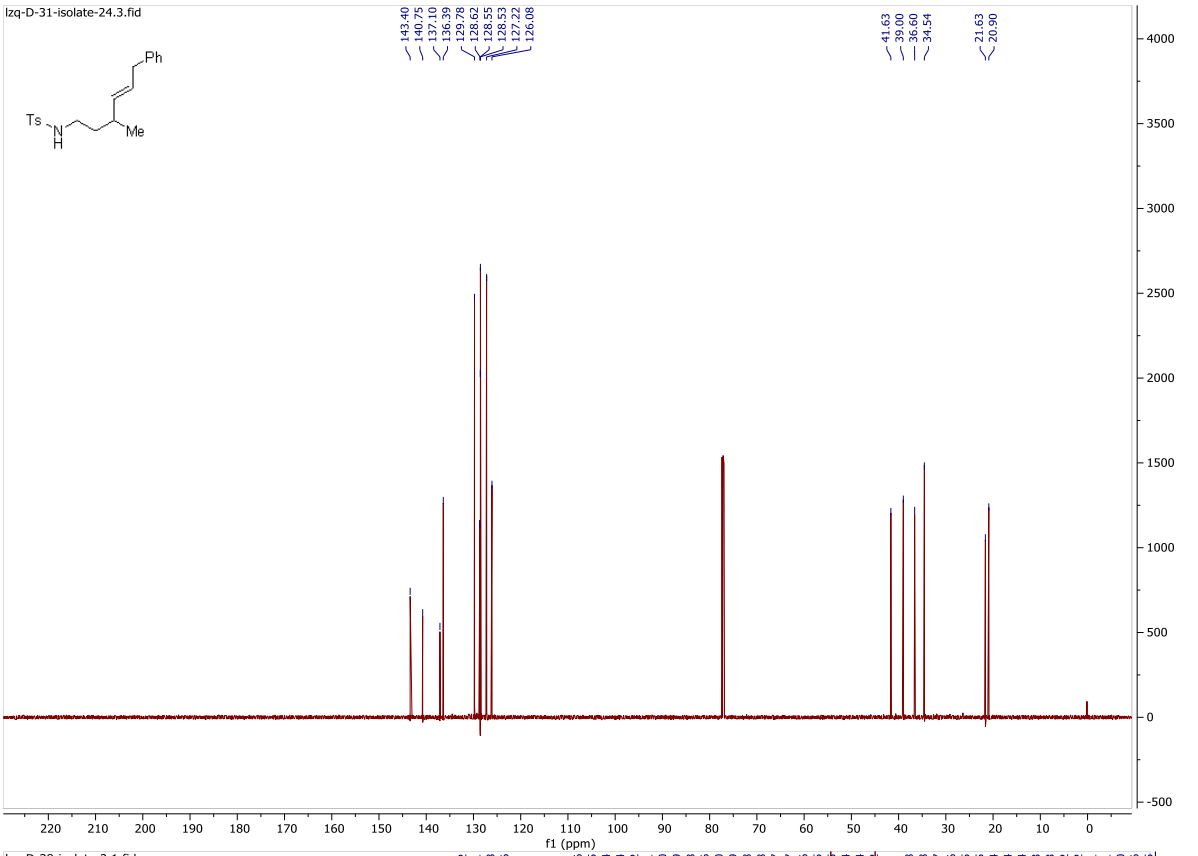

lzq-D-31-isolate-19.2.fid
MeO
OMe
Ts
N
H
Me
f1 (ppm)

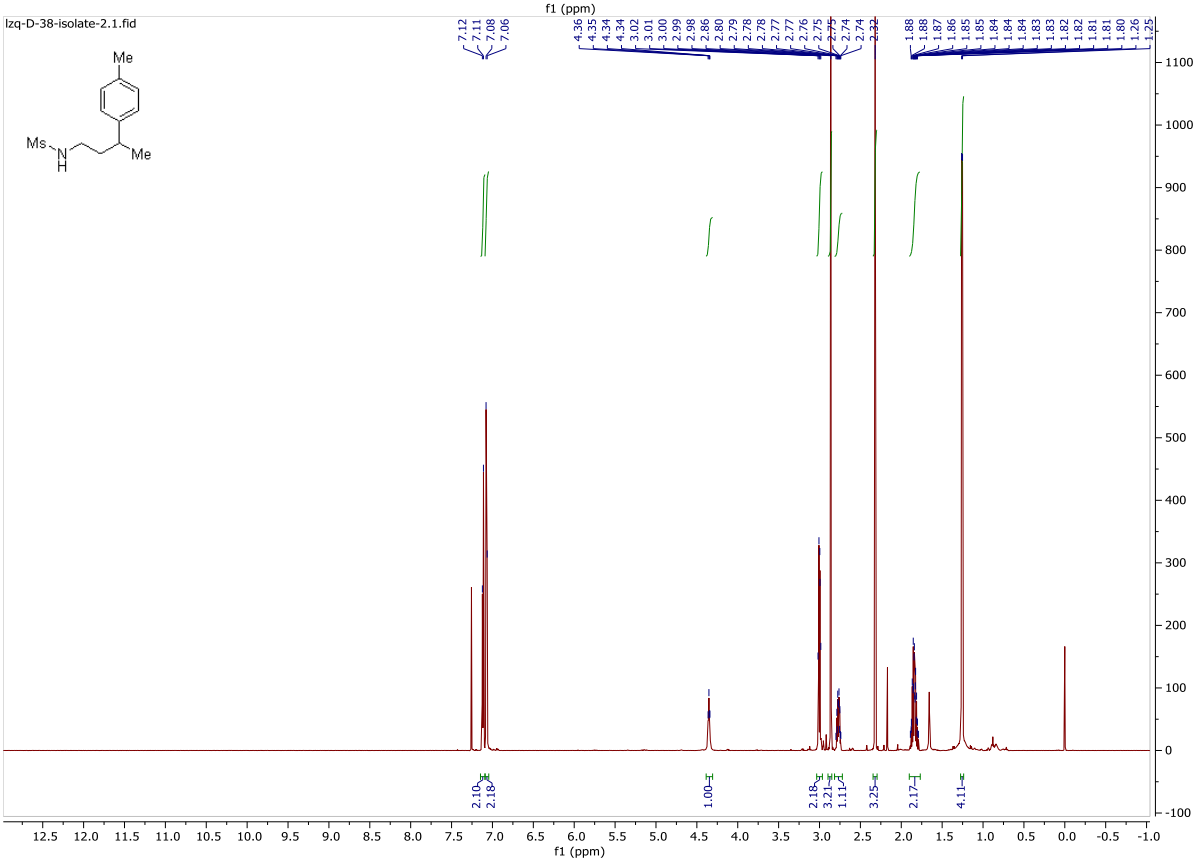

lzq-D-31-isolate-19.3.fid
MeO
OMe
Ts
N
H
Me
f1 (ppm)

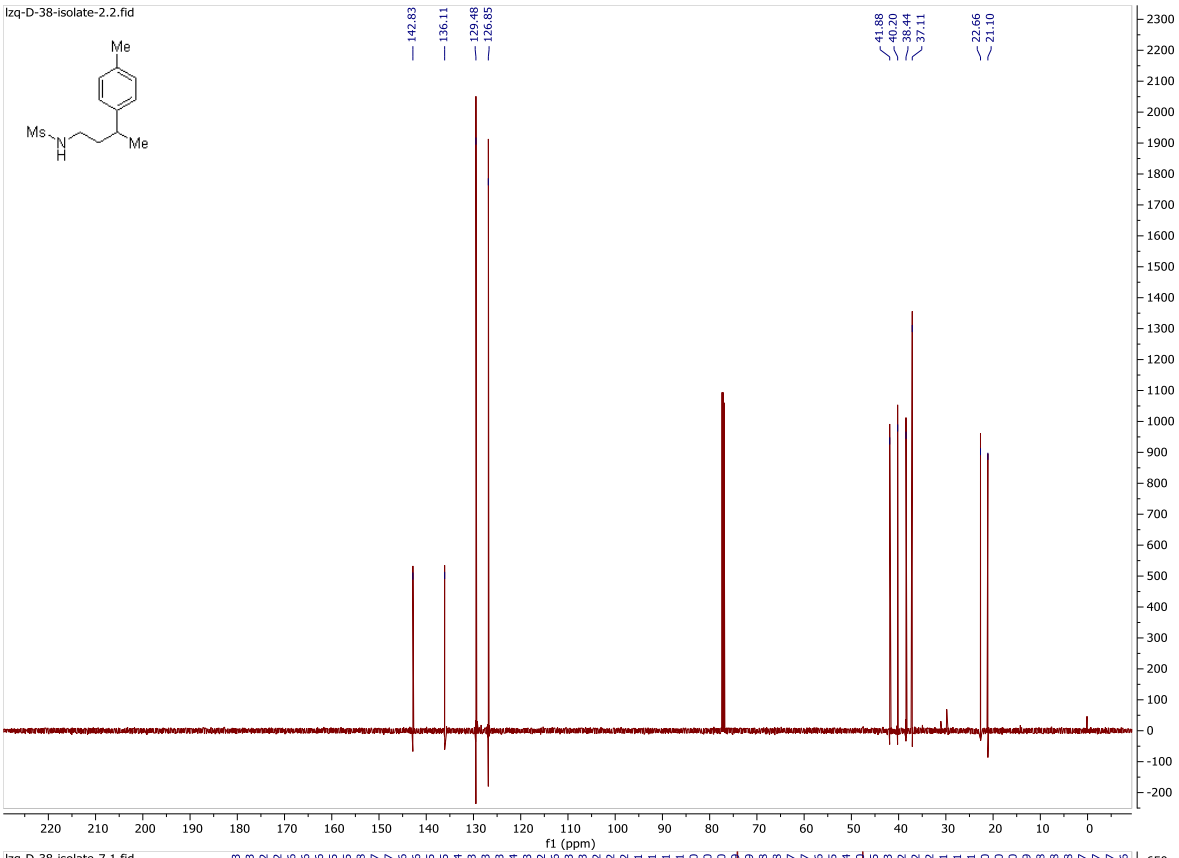

lzq-D-37-isolate-A8.1.fid
f1 (ppm)

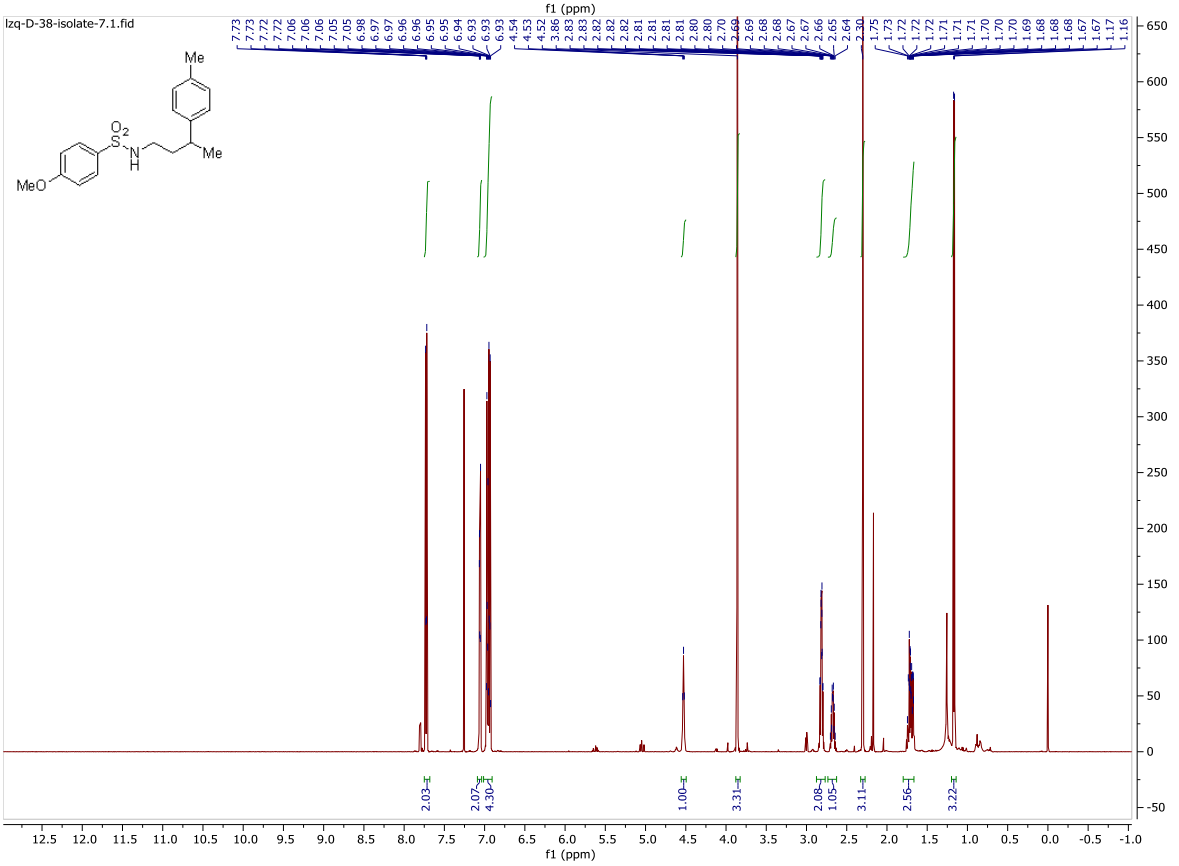

lzq-D-37-isolate-A8.2.fid
f1 (ppm)

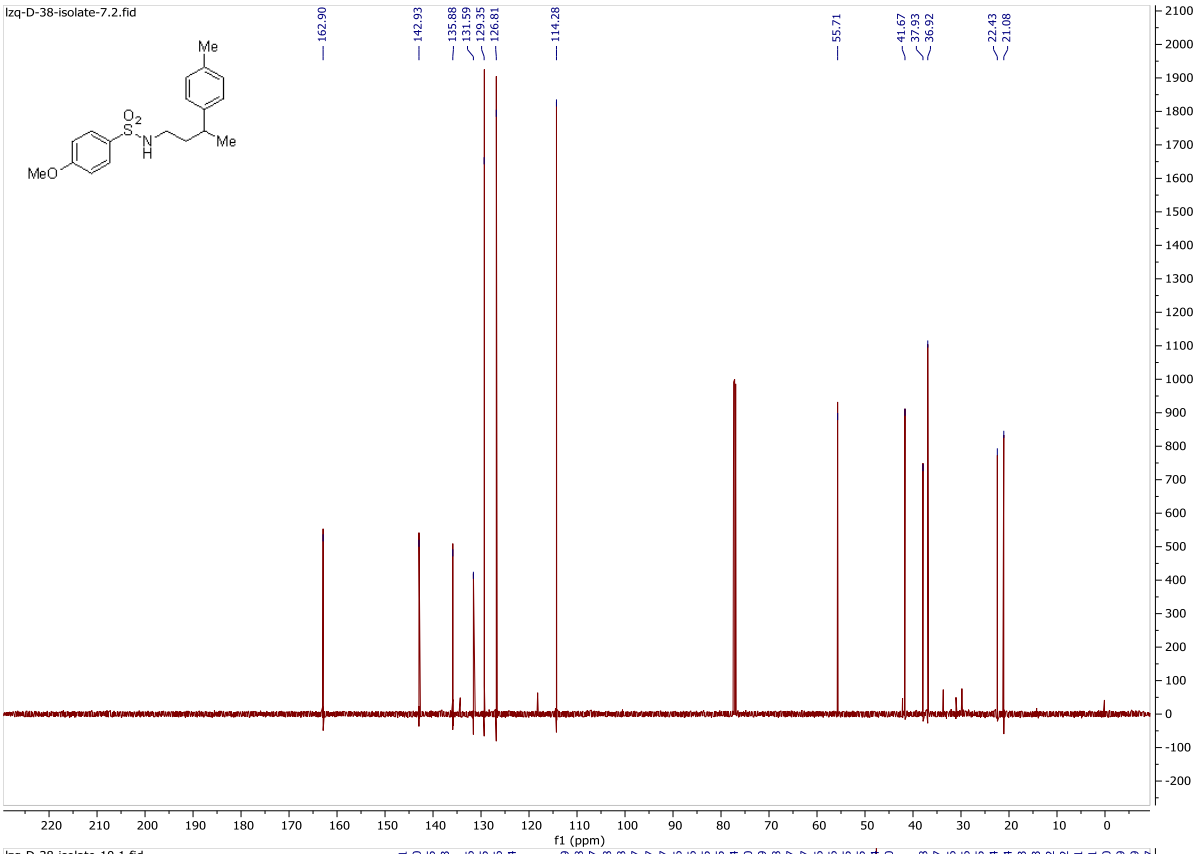

lzq-D-37-isolate-A8.3.fid
-65.45
f1 (ppm)
lzq-D-21-isolate-24-2.fid
1.92
4.02
1.06
2.02
1.07
1.00
1.00
2.04
2.07
3.08
0.98
2.11
2.97
f1 (ppm)

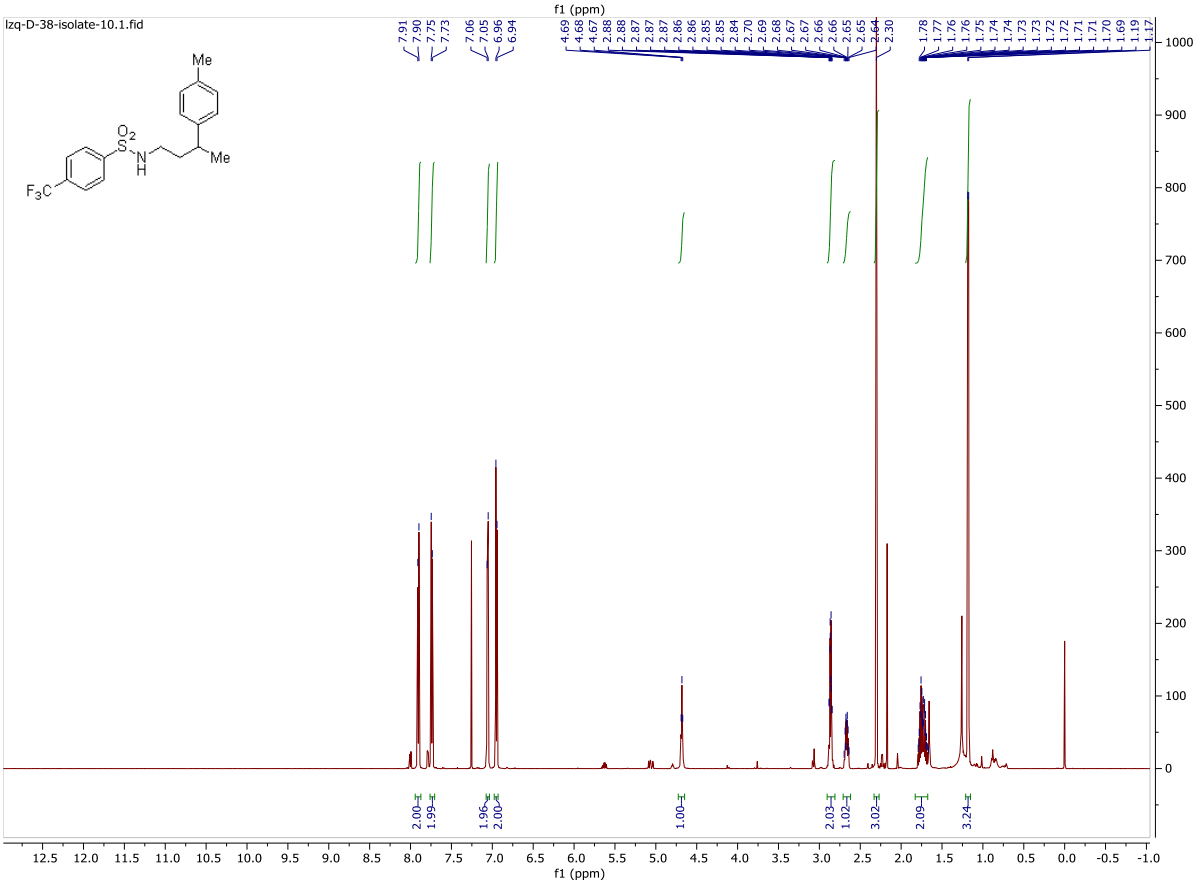

lzq-D-31-isolate-24.3.fid
143.40
140.75
137.10
136.39
129.78
128.62
128.55
128.53
127.22
126.08
41.63
39.00
36.60
34.54
21.63
20.90
Ph
Ts
N
H
Me
f1 (ppm)

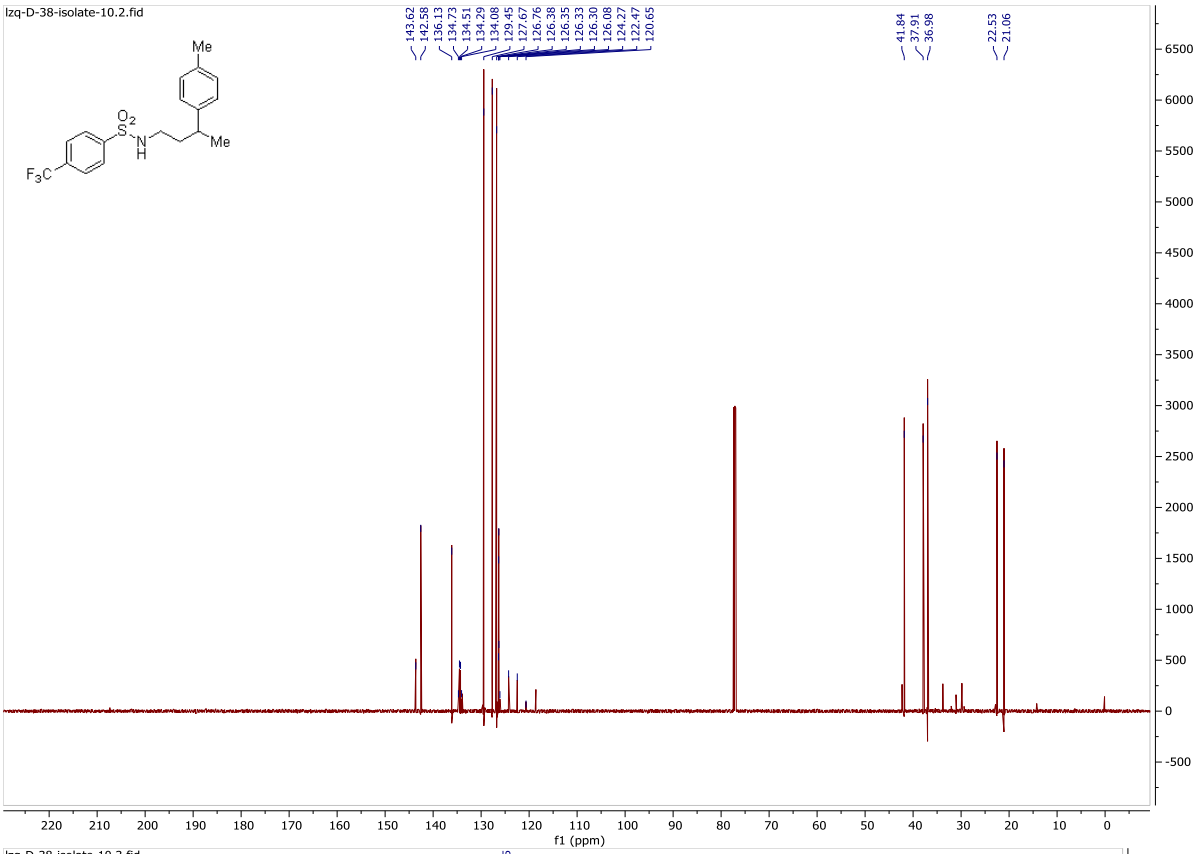

lzq-D-38-isolate-2.1.fid
Me
Ms
N
H
Me
f1 (ppm)

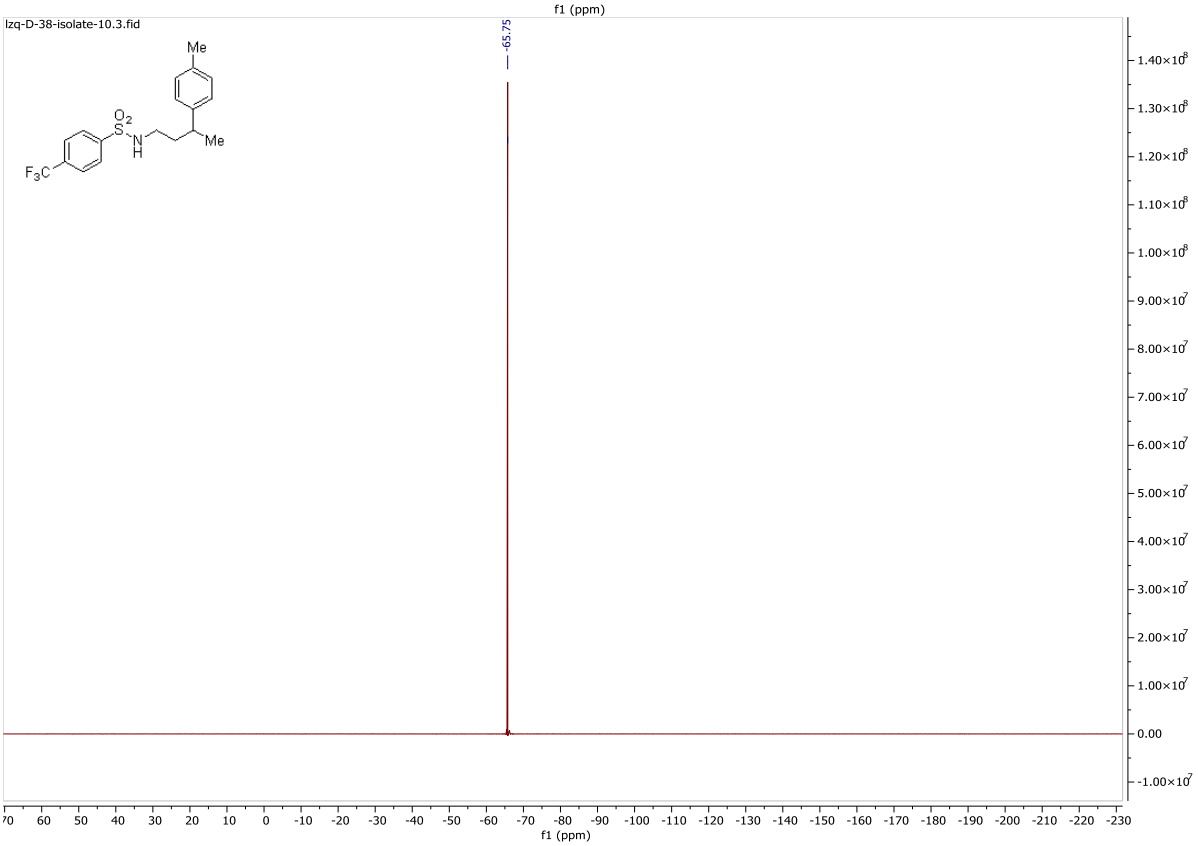

lzq-D-38-isolate-2.2.fid
Me
Ms
N
H
Me
142.83
136.11
129.48
126.85
41.88
40.20
38.44
37.11
22.66
21.10
f1 (ppm)

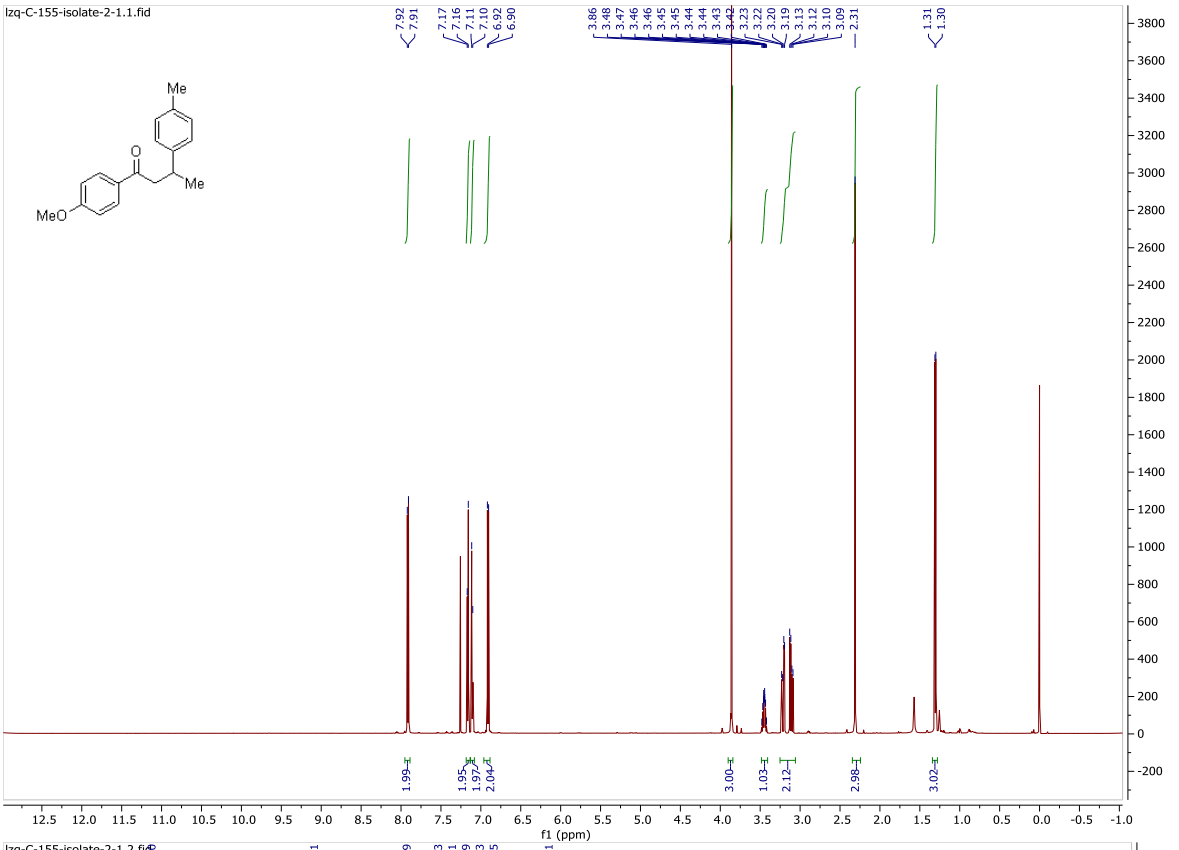

lzq-D-38-isolate-7.1.fid
Me
O2
S
N
H
Me
MeO
2.03
2.07
4.30
1.00
3.31
2.08
1.05
3.11
2.56
3.22
f1 (ppm)

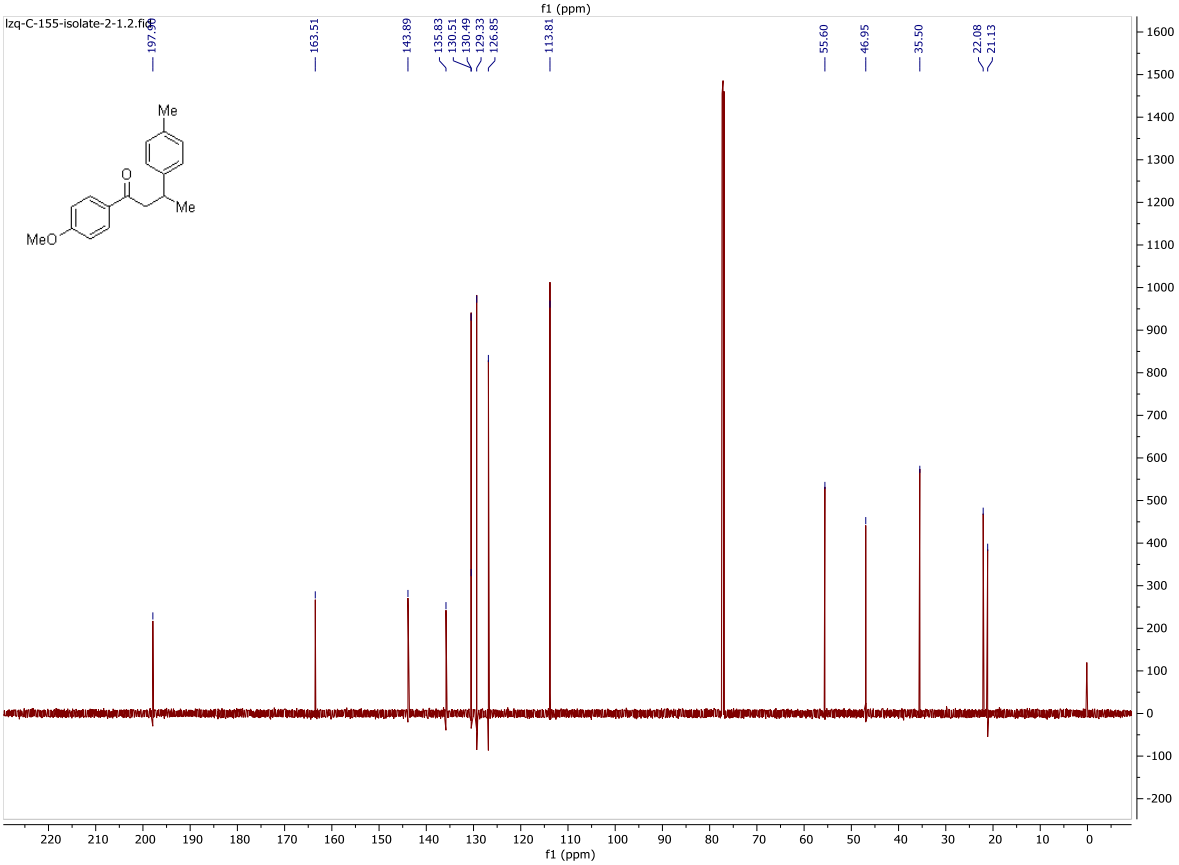

lzq-D-38-isolate-7.2.fid
162.90
142.93
135.88
131.59
129.35
126.81
114.28
55.71
41.67
37.93
36.92
22.43
21.08
Me
MeO
Me
f1 (ppm)

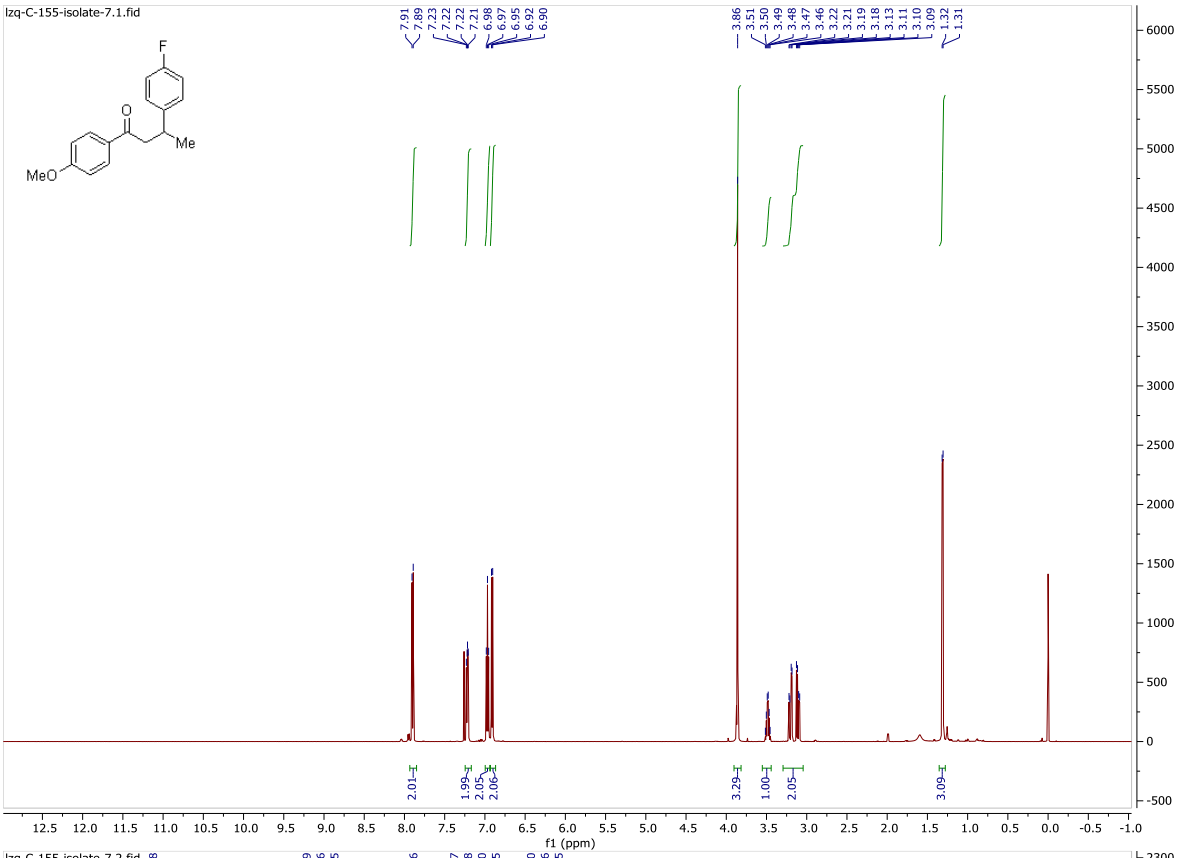

lzq-D-38-isolate-10.1.fid
7.91
7.90
7.75
7.73
7.06
7.05
6.96
6.94
4.69
4.68
4.67
2.88
2.87
2.86
2.85
2.84
2.70
2.69
2.68
2.67
2.66
2.65
2.64
2.30
1.78
1.77
1.76
1.75
1.74
1.73
1.72
1.71
1.70
1.69
1.19
1.17
2.00
1.99
1.96
2.00
1.00
2.03
1.02
3.02
2.09
3.24
Me
F3C
Me
f1 (ppm)

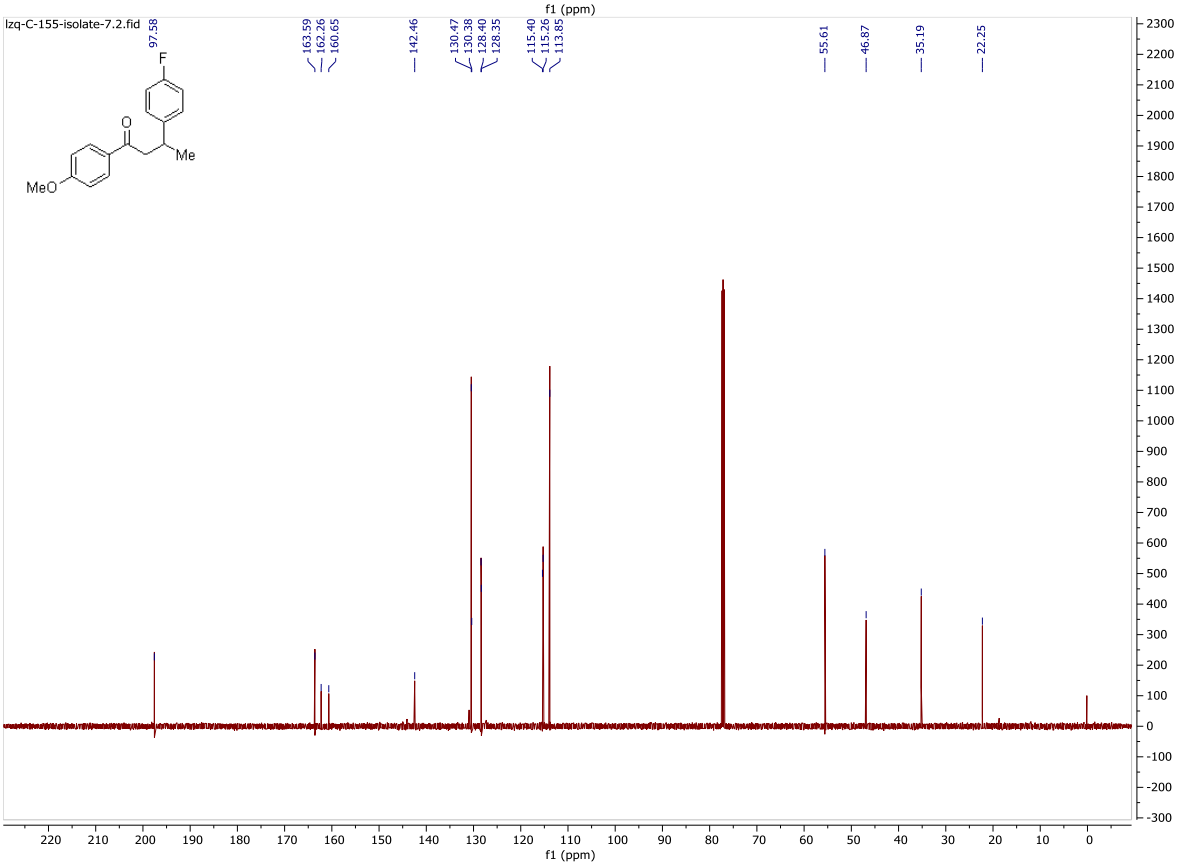

lzq-D-38-isolate-10.2.fid
143.62
142.58
136.13
134.73
134.51
134.29
134.08
129.45
127.67
126.76
126.38
126.35
126.33
126.30
126.08
124.27
122.47
120.65
41.84
37.91
36.98
22.53
21.06
Me
O2
S
N
H
Me
F3C
f1 (ppm)

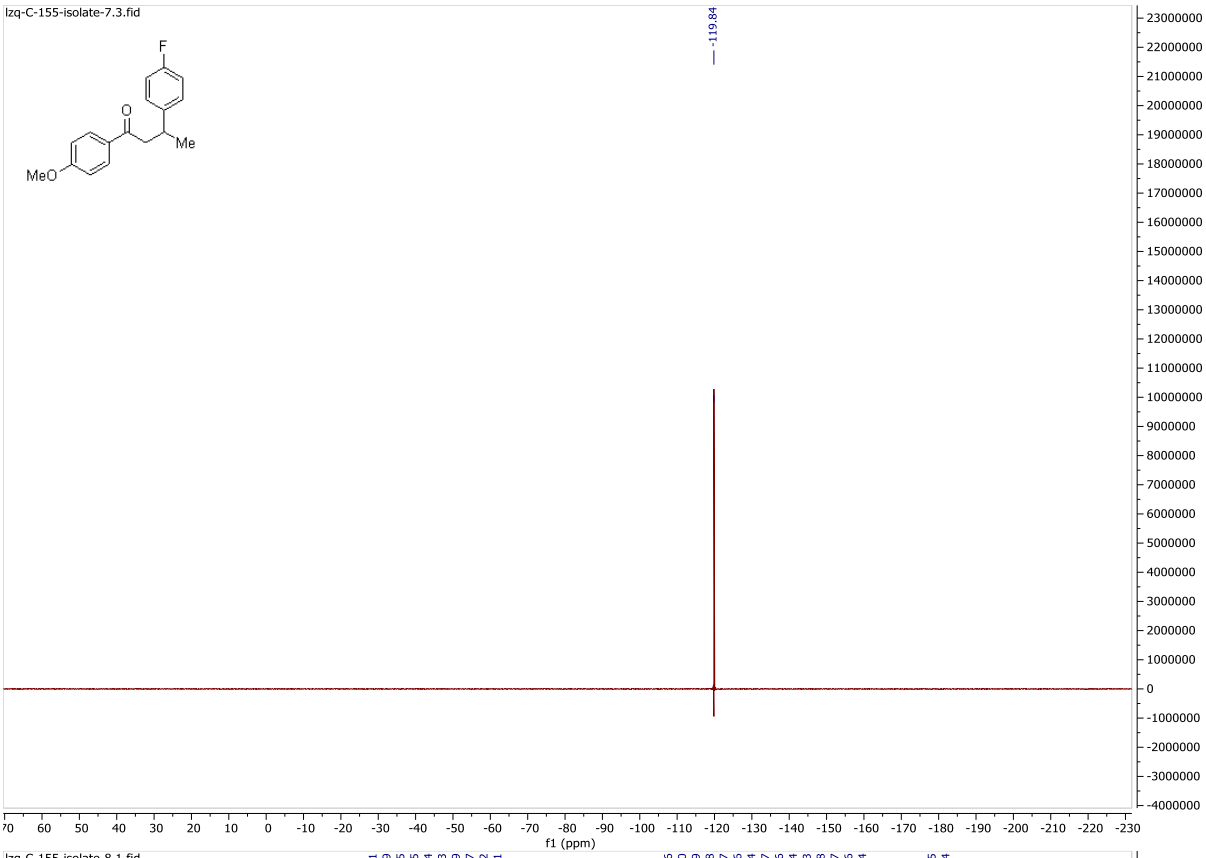

lzq-D-38-isolate-10.3.fid
-65.75
Me
O2
S
N
H
Me
F3C
f1 (ppm)

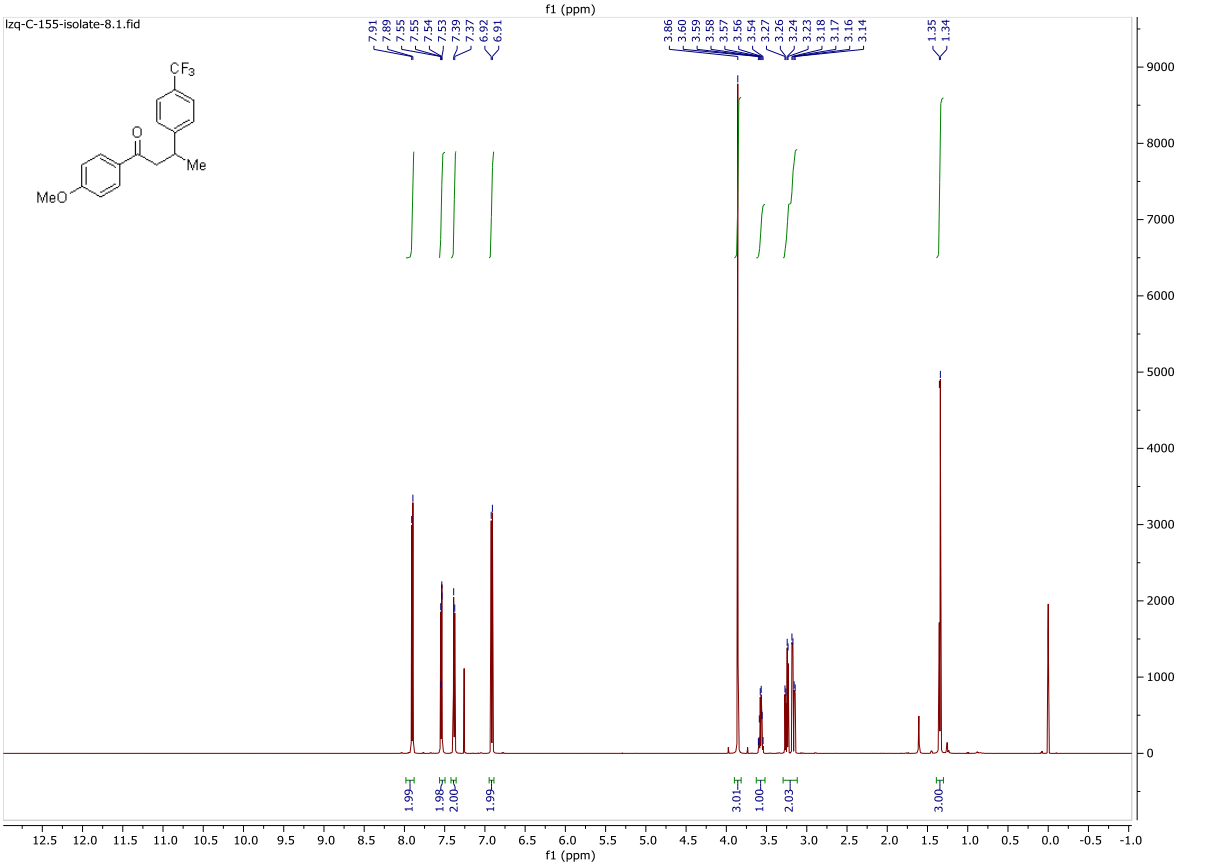

lzq-C-155-isolate-2-1.1.fid
Me
O
Me
MeO
f1 (ppm)

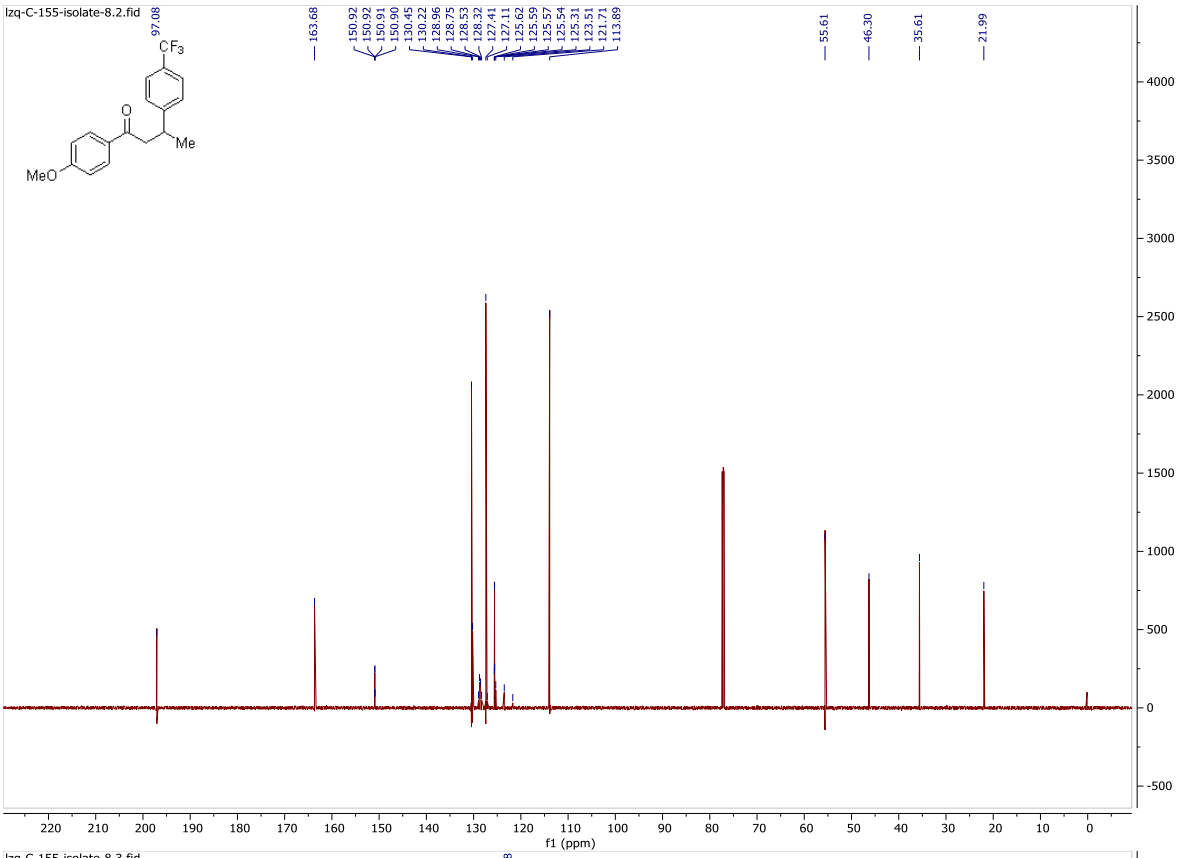

lzq-C-155-isolate-2-1.2.fid
Me
O
Me
MeO
f1 (ppm)

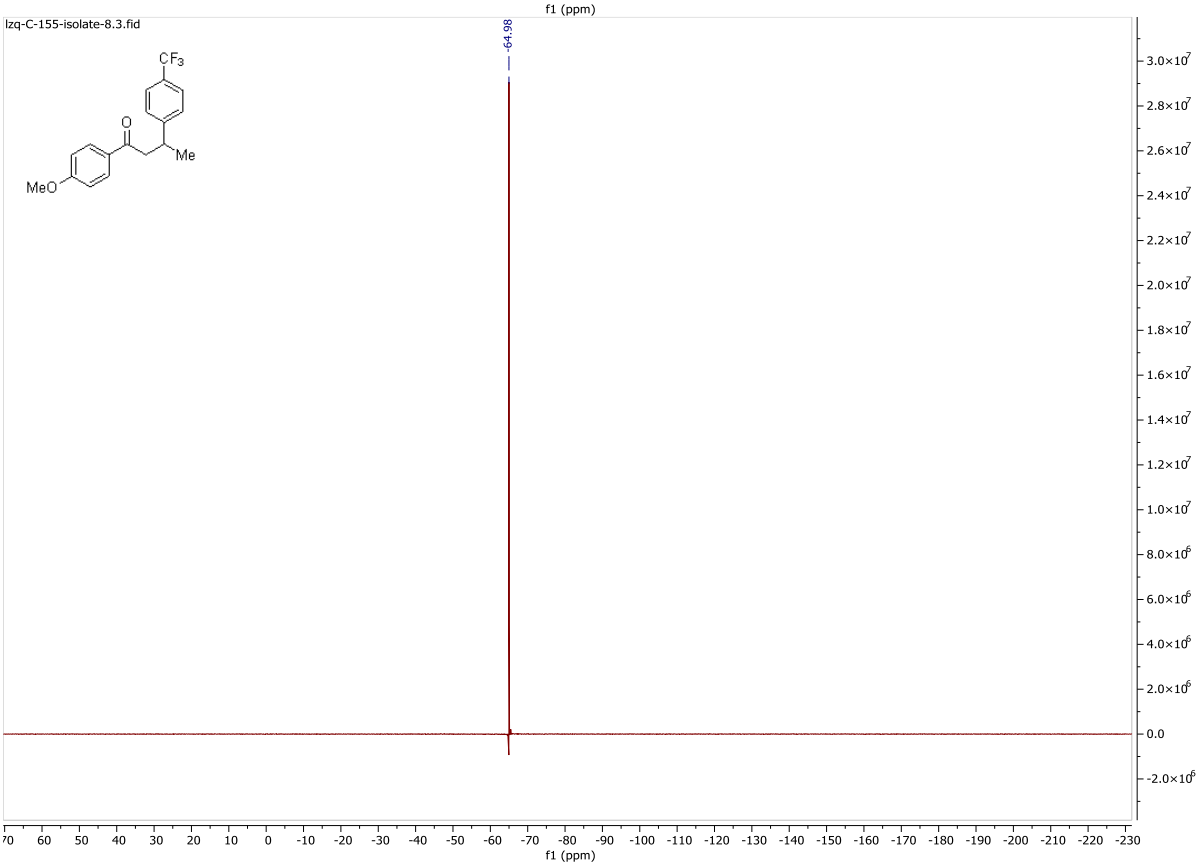

lzq-C-155-isolate-7.1.fid
F
O
Me
MeO
7.91
7.89
7.23
7.22
7.22
7.21
6.98
6.97
6.95
6.92
6.90
3.86
3.51
3.50
3.49
3.48
3.47
3.46
3.22
3.21
3.19
3.18
3.13
3.11
3.10
3.09
1.32
1.31
2.01
1.99
2.05
2.06
3.29
1.00
2.05
3.09
f1 (ppm)

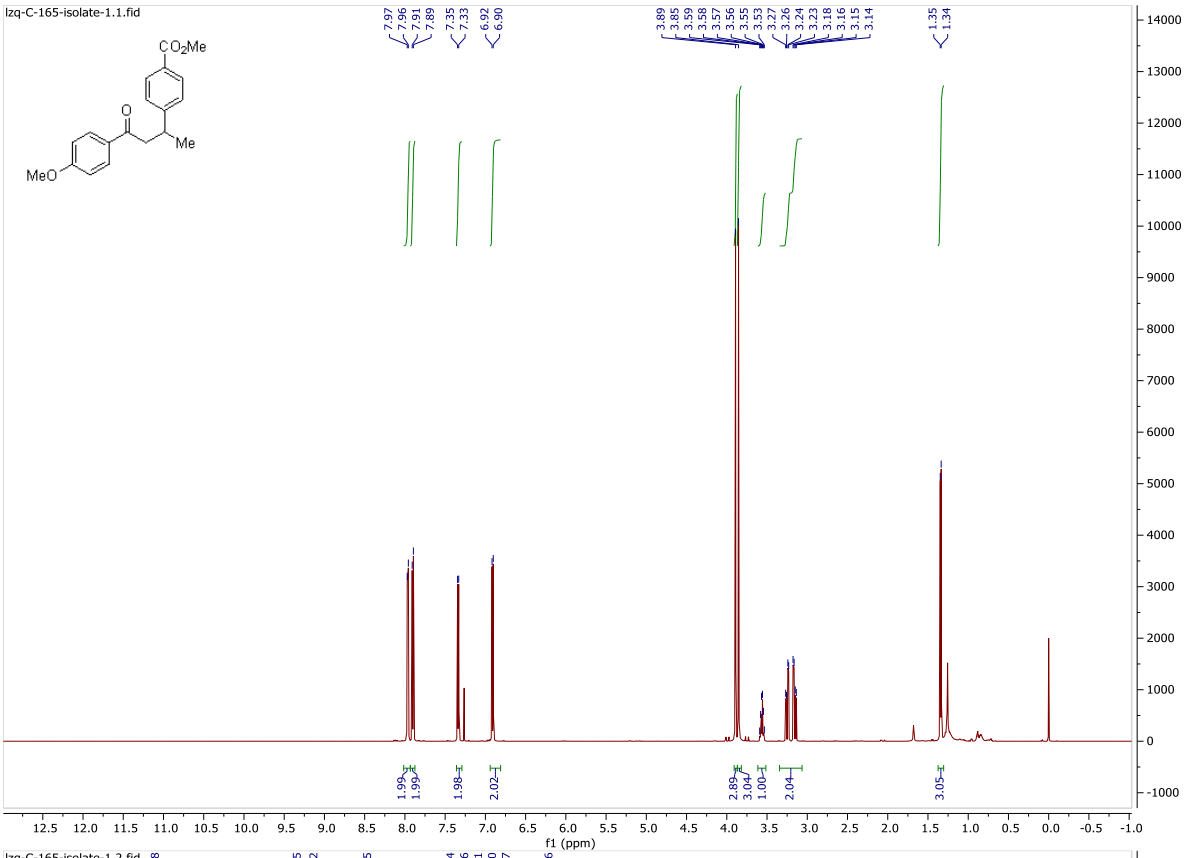

lzq-C-155-isolate-7.2.fid
F
O
Me
MeO
97.58
163.59
162.26
160.65
142.46
130.47
130.38
128.40
128.35
115.40
115.26
113.85
55.61
46.87
35.19
22.25
f1 (ppm)

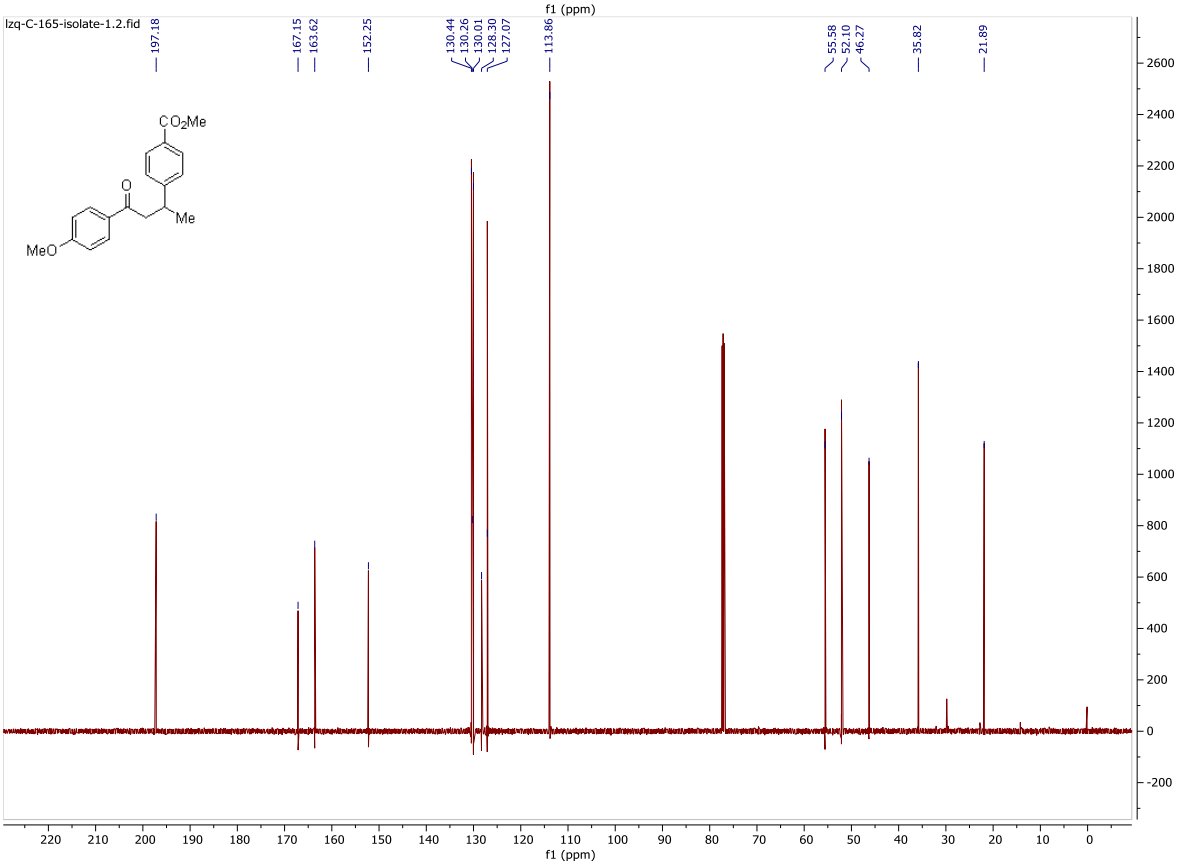

lzq-C-155-isolate-7.3.fid
F
O
Me
MeO
-119.84
f1 (ppm)

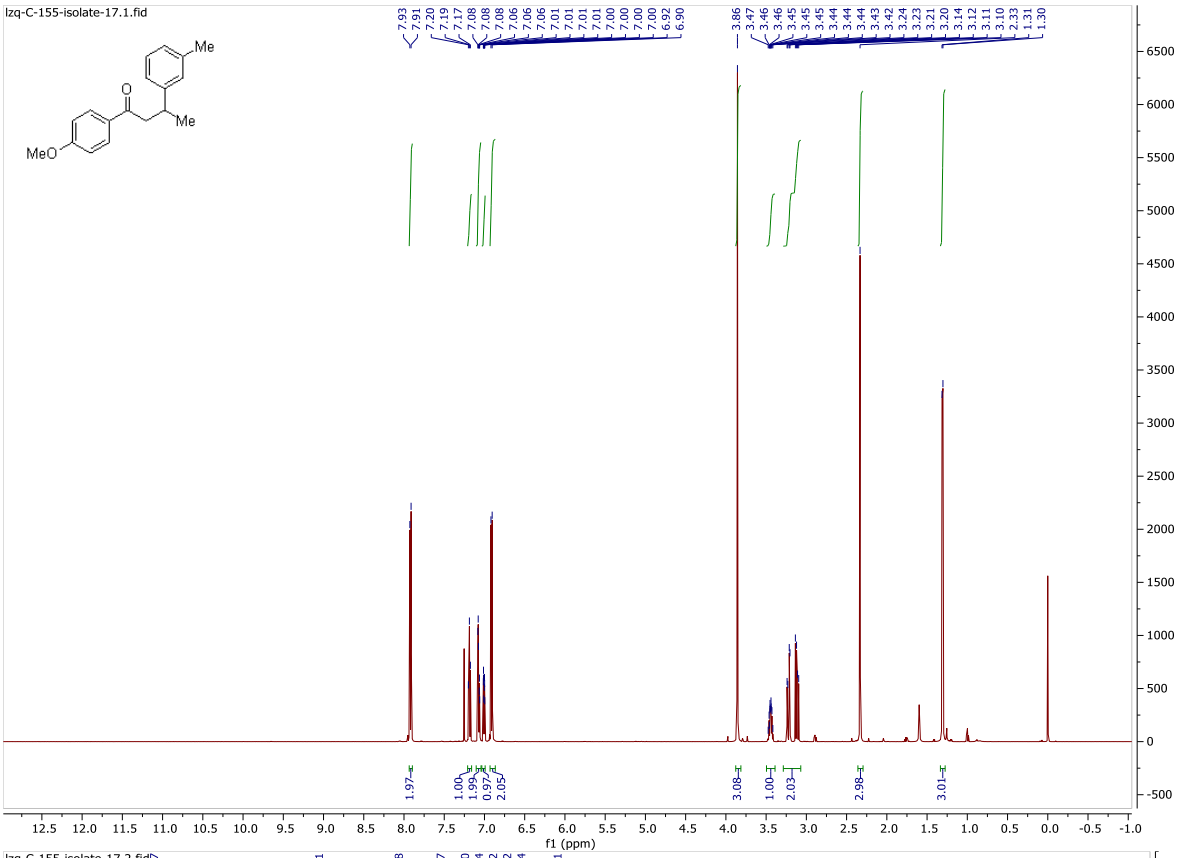

lzq-C-155-isolate-8.1.fid
CF3
O
Me
MeO
7.91
7.89
7.55
7.55
7.54
7.53
7.39
7.37
6.92
6.91
3.86
3.60
3.59
3.58
3.57
3.56
3.54
3.27
3.26
3.24
3.23
3.18
3.17
3.16
3.14
1.35
1.34
1.99
1.98
2.00
1.99
3.01
1.00
2.03
3.00
f1 (ppm)

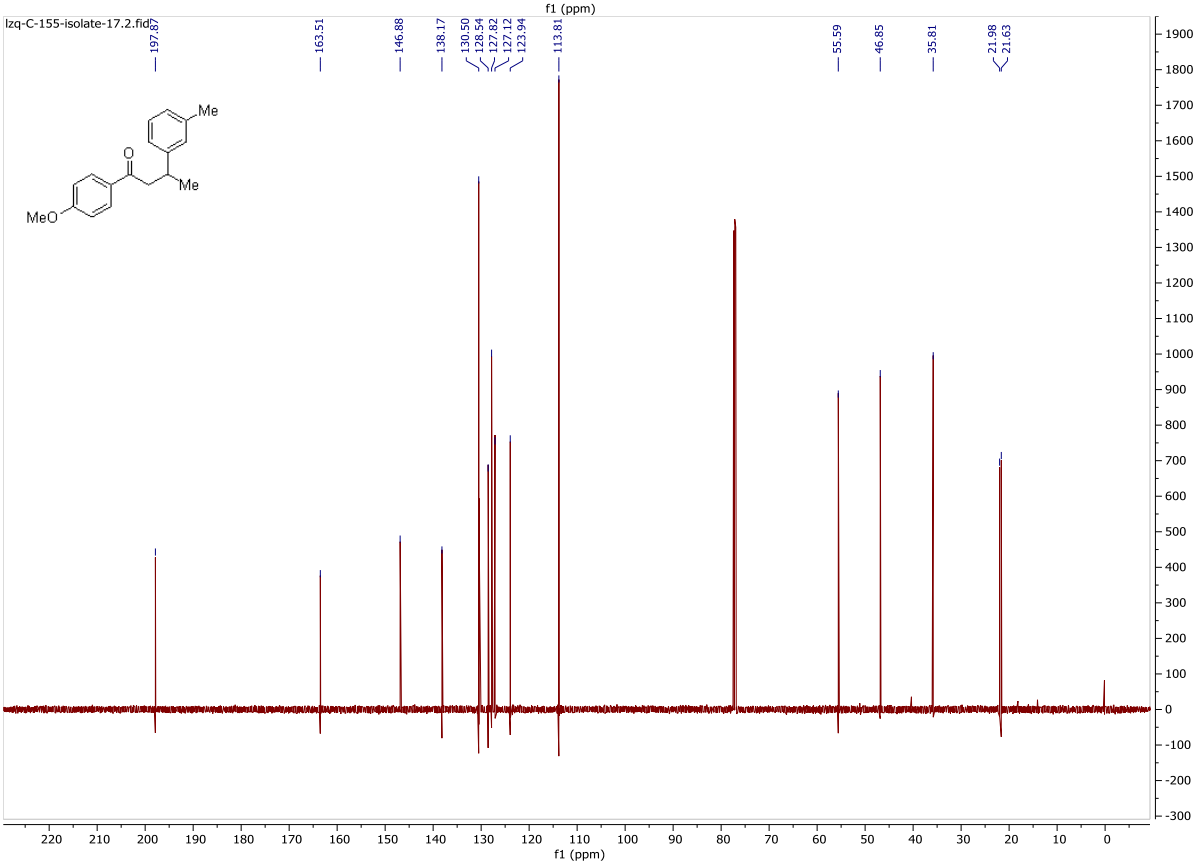

lzq-C-155-isolate-8.2.fid
97.08
163.68
150.92
150.92
150.91
150.90
130.45
130.22
128.96
128.75
128.53
128.32
127.41
127.11
125.62
125.59
125.57
125.54
125.31
123.51
121.71
113.89
55.61
46.30
35.61
21.99
CF3
O
Me
MeO
f1 (ppm)

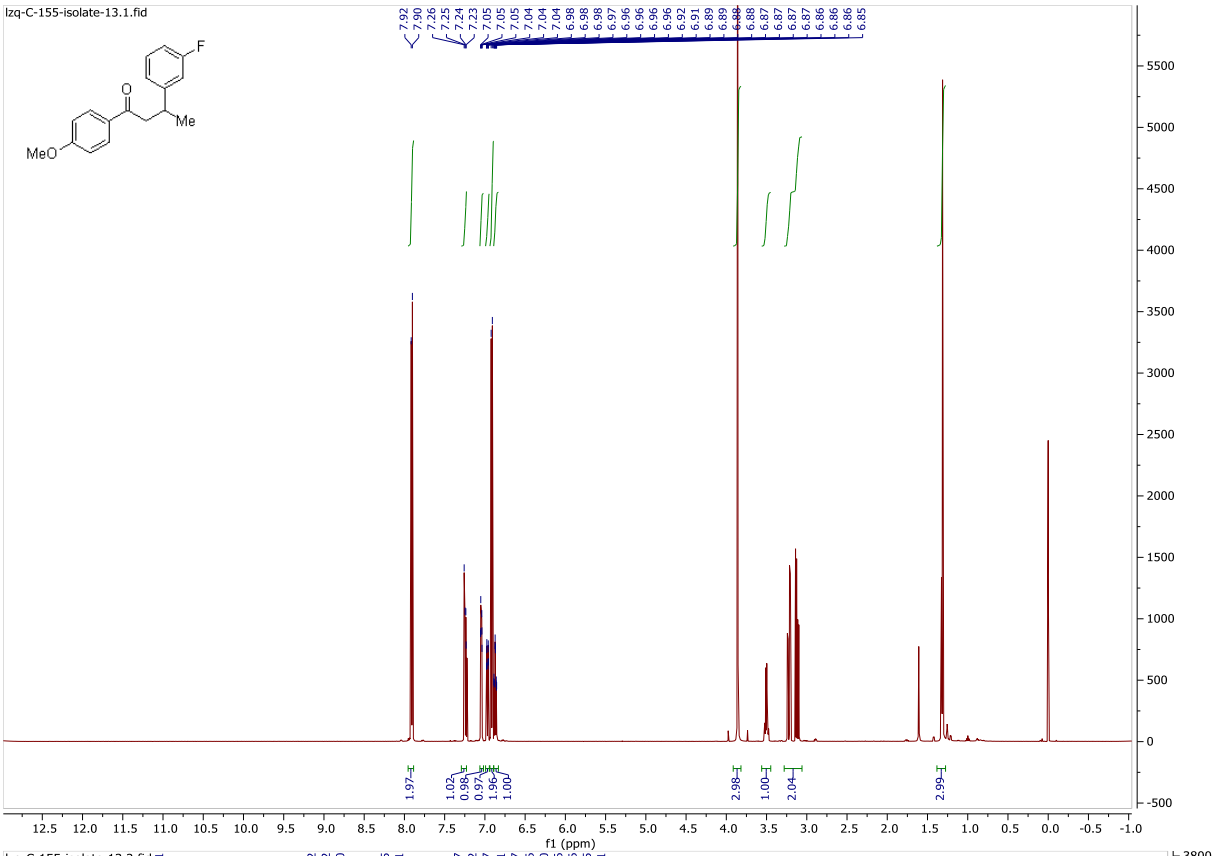

lzq-C-155-isolate-8.3.fid
-64.98
CF3
O
Me
MeO
f1 (ppm)

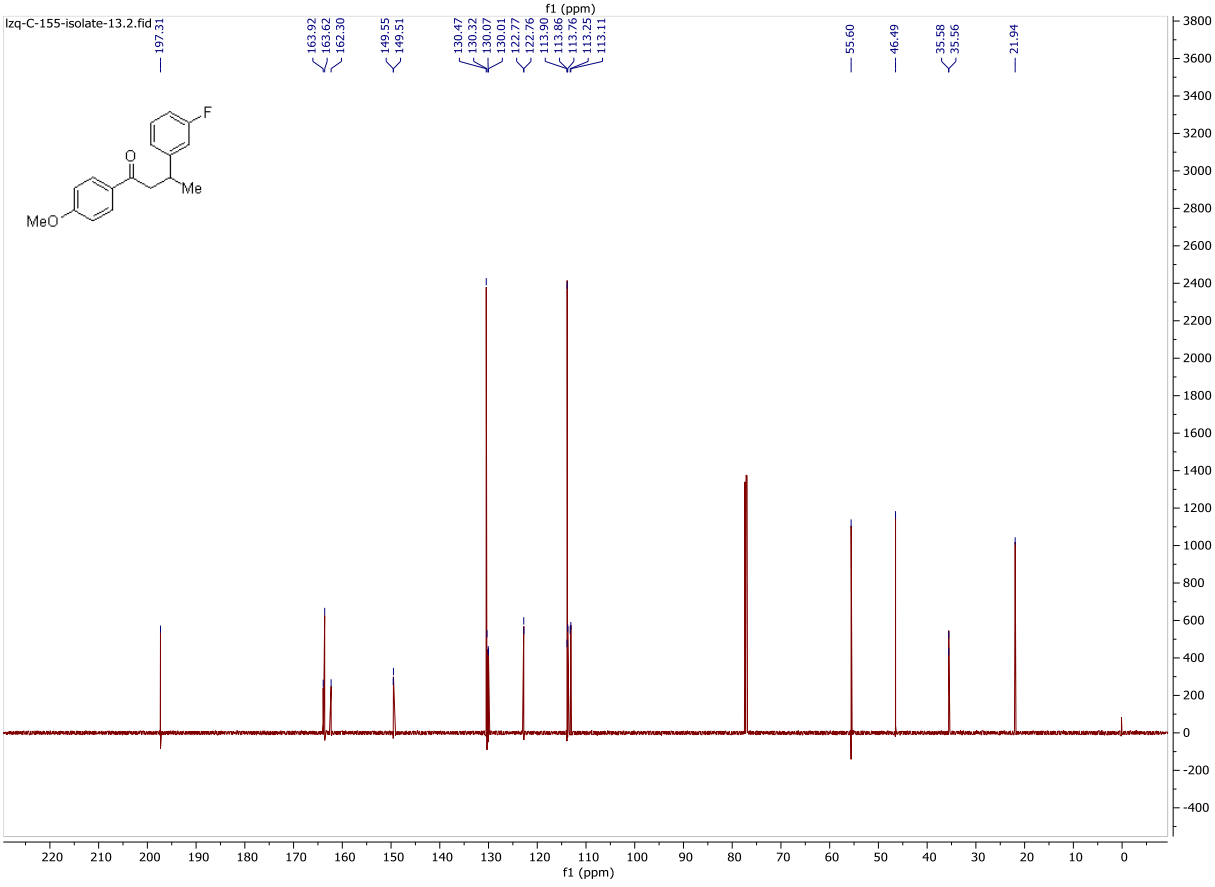

lzq-C-165-isolate-1.1.fid
CO2Me
O
Me
MeO
7.97
7.96
7.91
7.89
7.35
7.33
6.92
6.90
3.89
3.85
3.59
3.58
3.57
3.56
3.55
3.53
3.27
3.26
3.24
3.23
3.18
3.16
3.15
3.14
1.35
1.34
1.99
1.99
1.98
2.02
2.89
3.04
1.00
2.04
3.05
f1 (ppm)

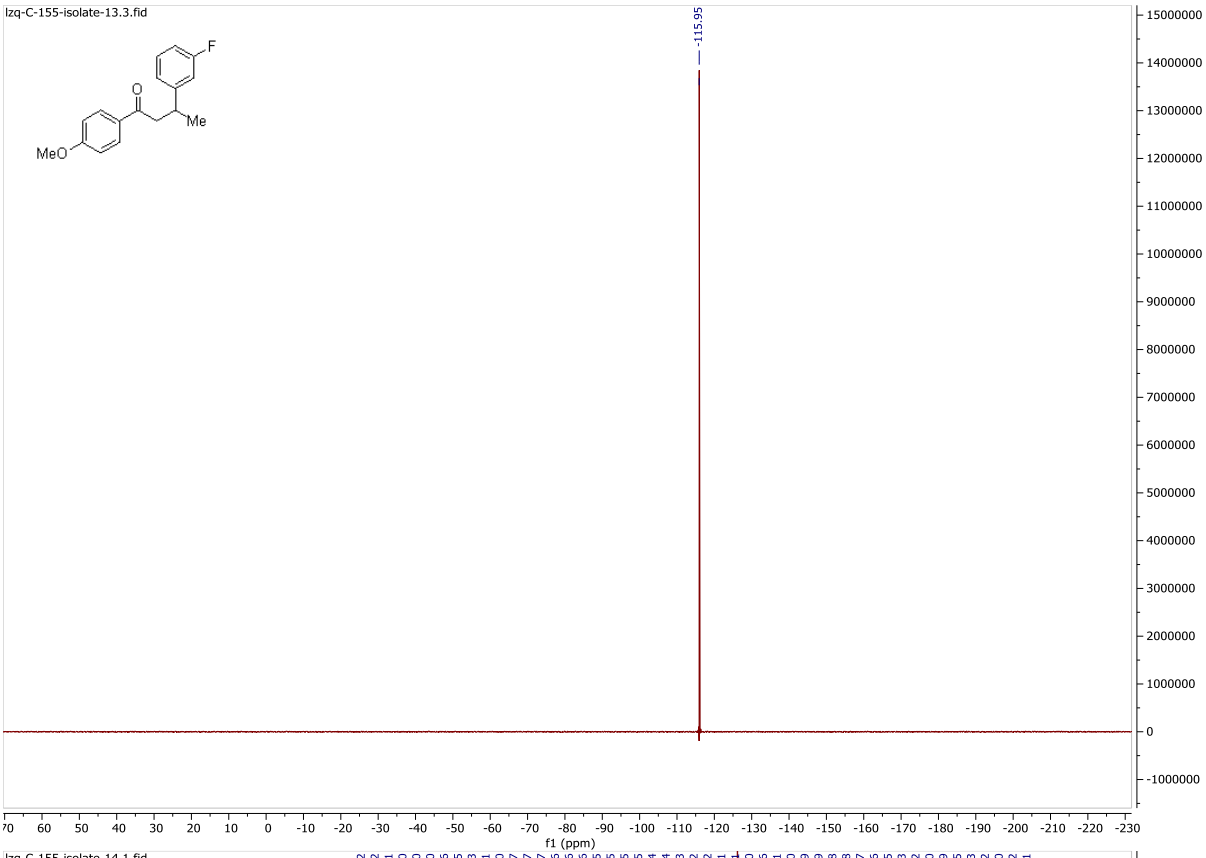

lzq-C-165-isolate-1.2.fid
CO2Me
O
Me
MeO
197.18
167.15
163.62
152.25
130.44
130.26
130.01
128.30
127.07
113.86
55.58
52.10
46.27
35.82
21.89
f1 (ppm)

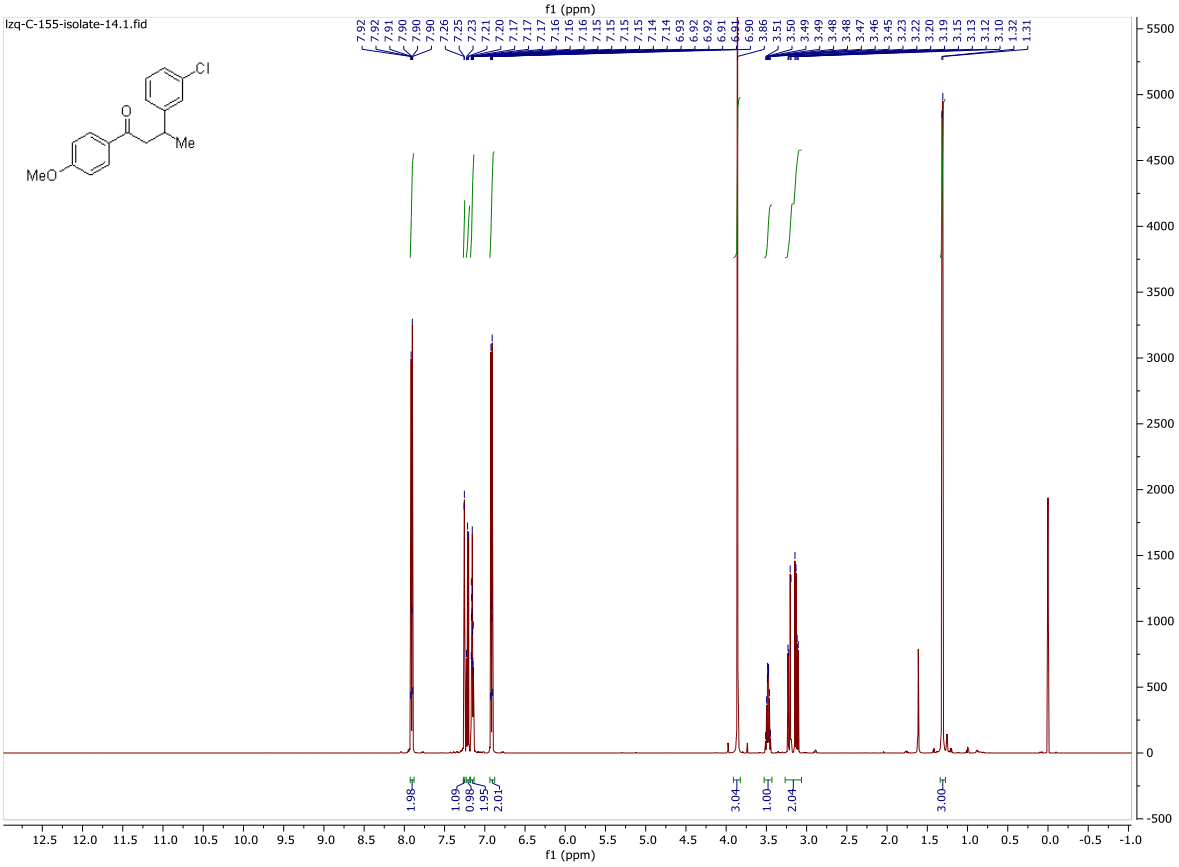

lzq-C-155-isolate-17.1.fid
Me
O
Me
MeO
7.93
7.91
7.20
7.19
7.17
7.08
7.08
7.08
7.06
7.06
7.06
7.01
7.01
7.01
7.00
7.00
7.00
7.00
6.92
6.90
3.86
3.47
3.46
3.46
3.45
3.45
3.44
3.44
3.44
3.43
3.42
3.24
3.23
3.21
3.20
3.14
3.12
3.11
3.10
2.33
1.31
1.30
1.97
1.00
1.99
0.97
2.05
3.08
1.00
2.03
2.98
3.01
f1 (ppm)

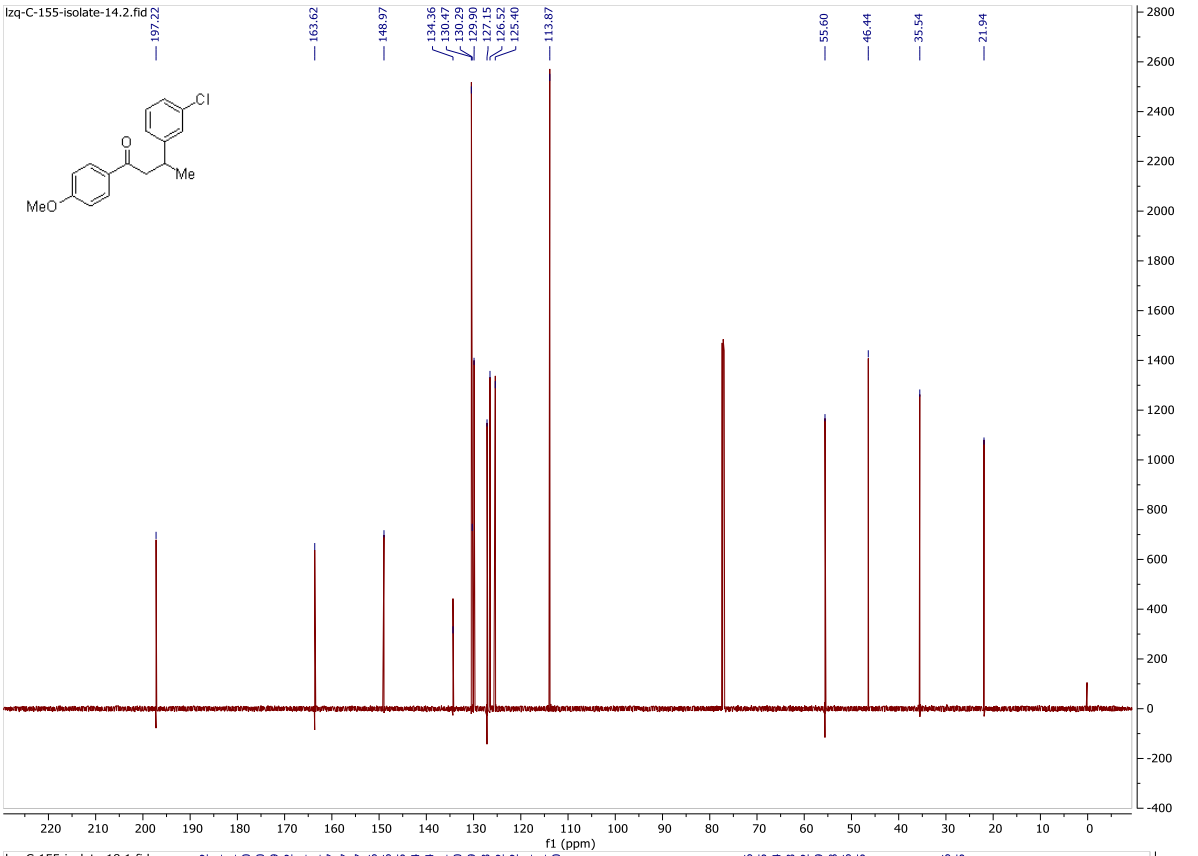

lzq-C-155-isolate-17.2.fid
Me
O
Me
MeO
197.87
163.51
146.88
138.17
130.50
128.54
127.82
127.12
123.94
113.81
55.59
46.85
35.81
21.98
21.63
f1 (ppm)

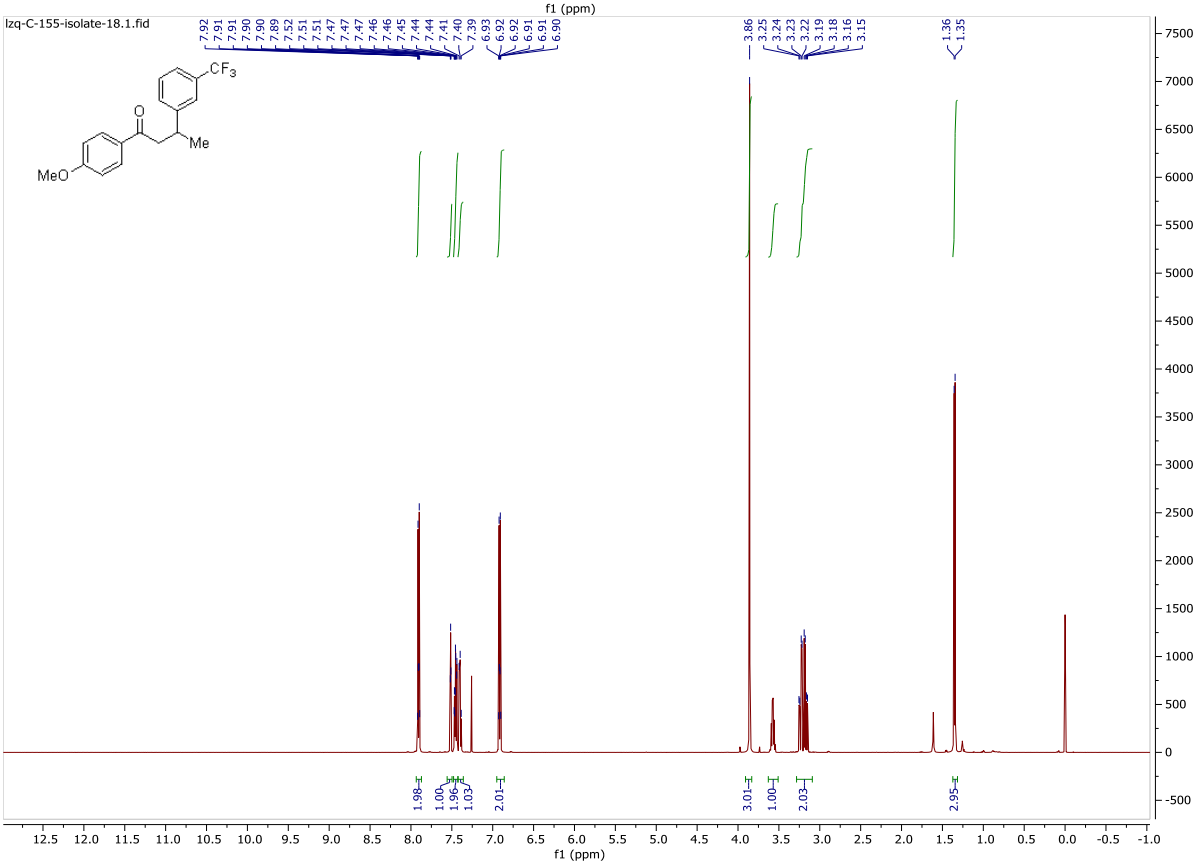

lzq-C-155-isolate-13.1.fid
F
O
Me
MeO
f1 (ppm)

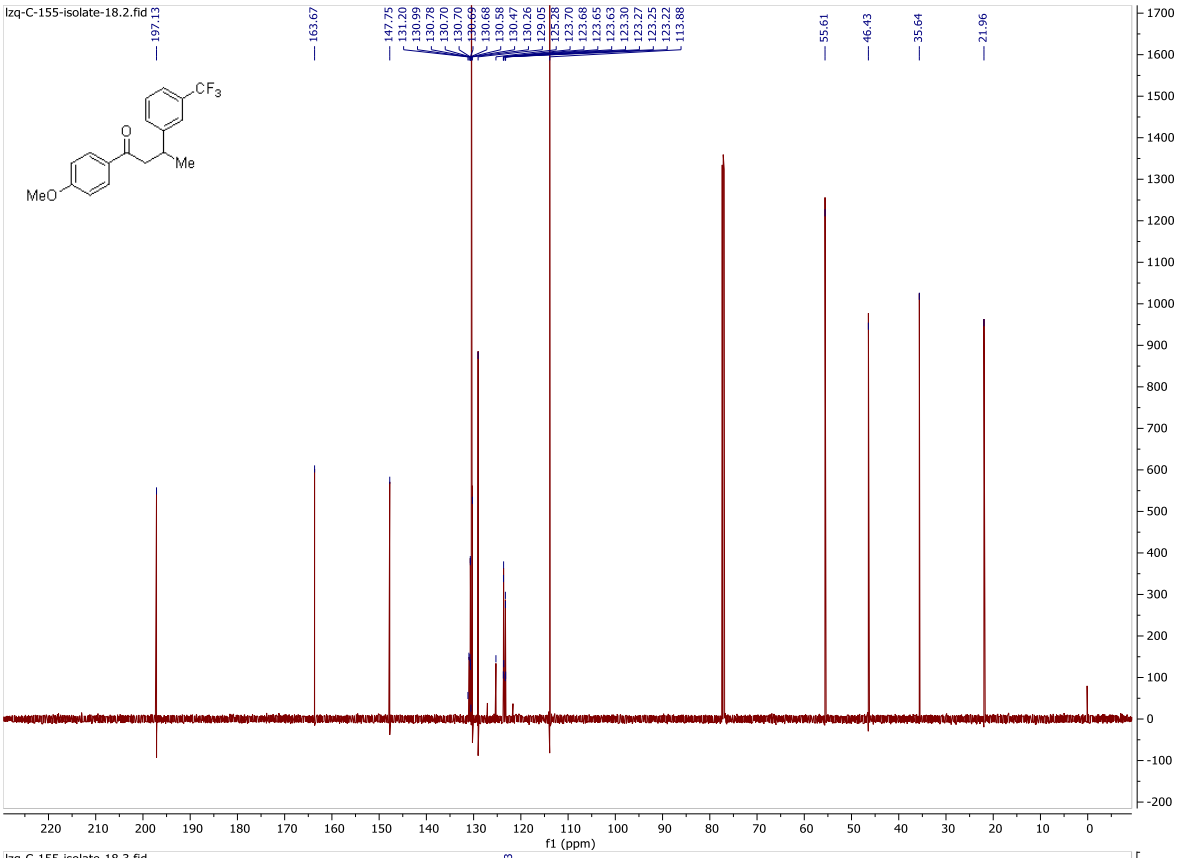

lzq-C-155-isolate-13.2.fid
F
O
Me
MeO
f1 (ppm)

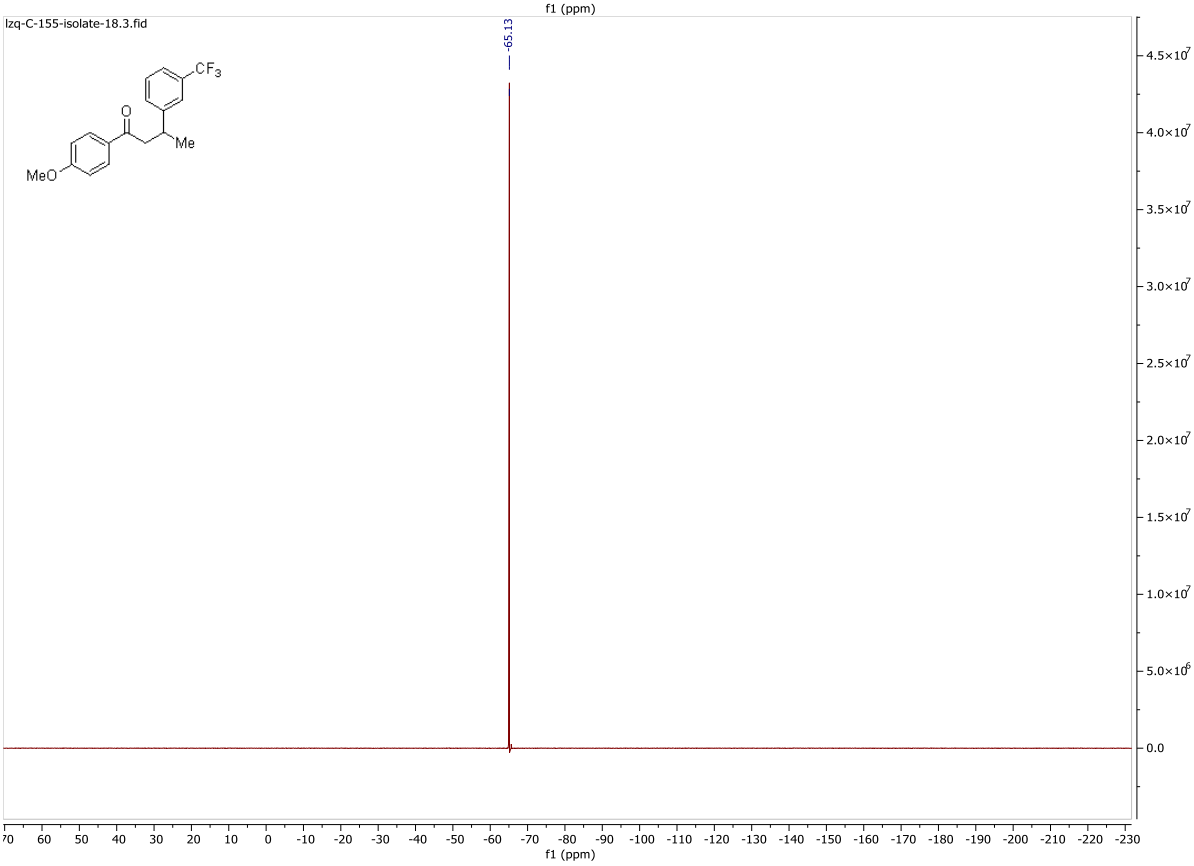

lzq-C-155-isolate-13.3.fid
F
O
Me
MeO
-115.95
f1 (ppm)

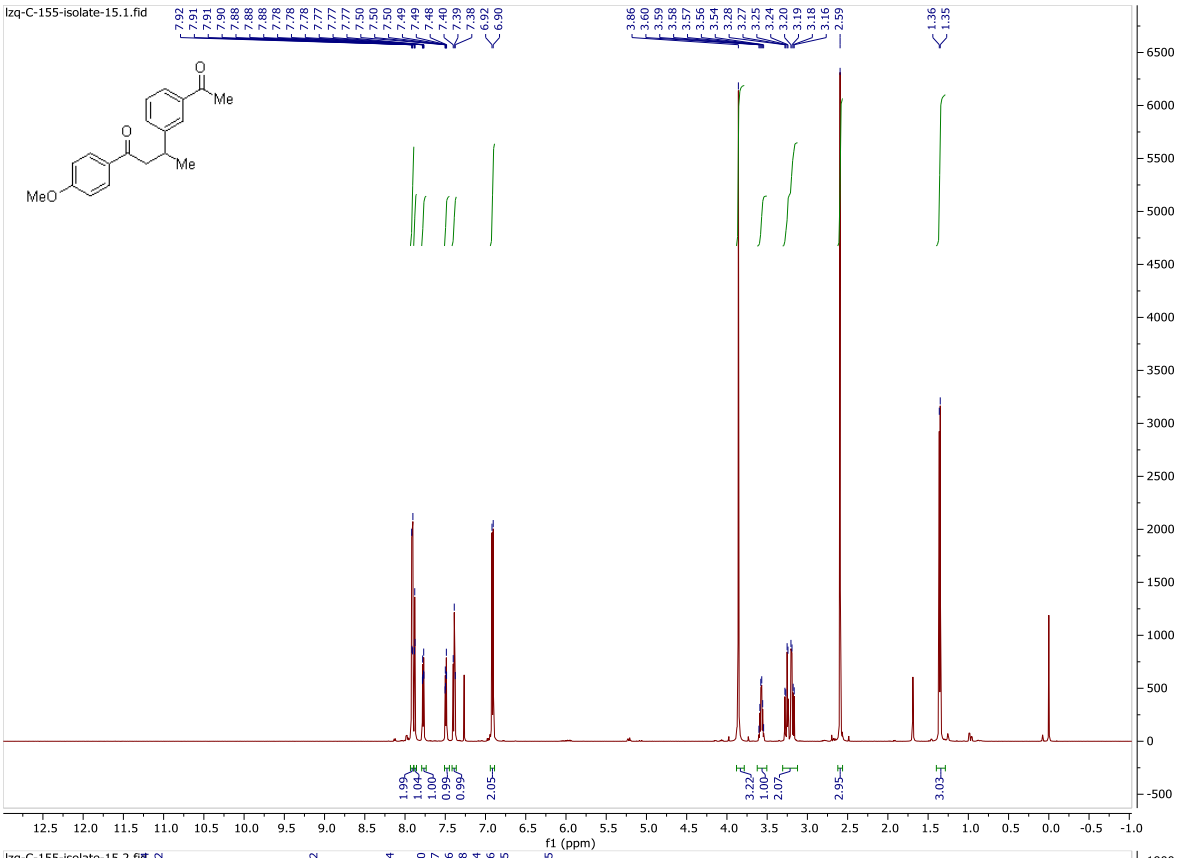

lzq-C-155-isolate-14.1.fid
Cl
O
Me
MeO
7.92
7.91
7.90
7.26
7.25
7.23
7.21
7.20
7.17
7.16
7.15
6.93
6.92
6.91
6.90
3.86
3.51
3.50
3.49
3.48
3.47
3.46
3.45
3.23
3.22
3.20
3.19
3.15
3.13
3.12
3.10
1.32
1.31
1.98
1.09
0.98
1.95
2.01
3.04
1.00
2.04
3.00
f1 (ppm)

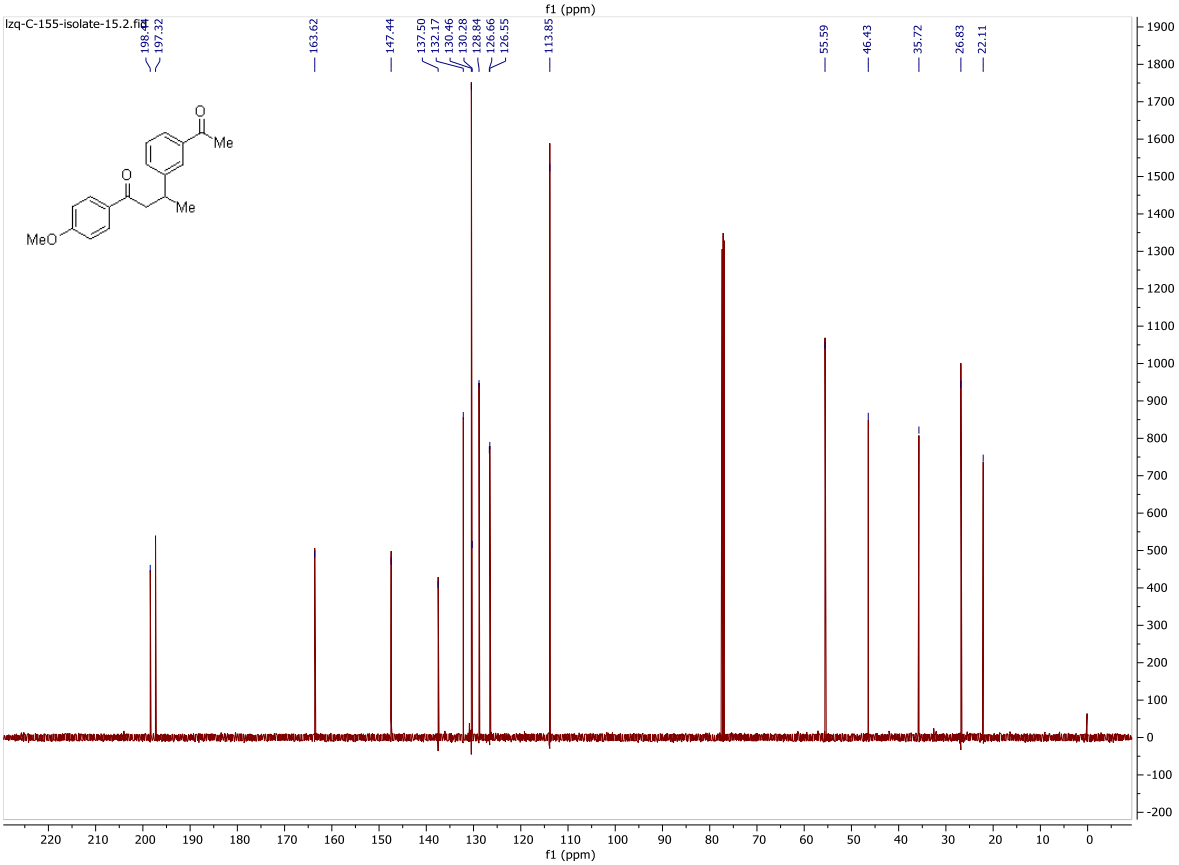

lzq-C-155-isolate-14.2.fid
197.22
163.62
148.97
134.36
130.47
130.29
129.90
127.15
126.52
125.40
113.87
55.60
46.44
35.54
21.94
Cl
O
Me
MeO
f1 (ppm)

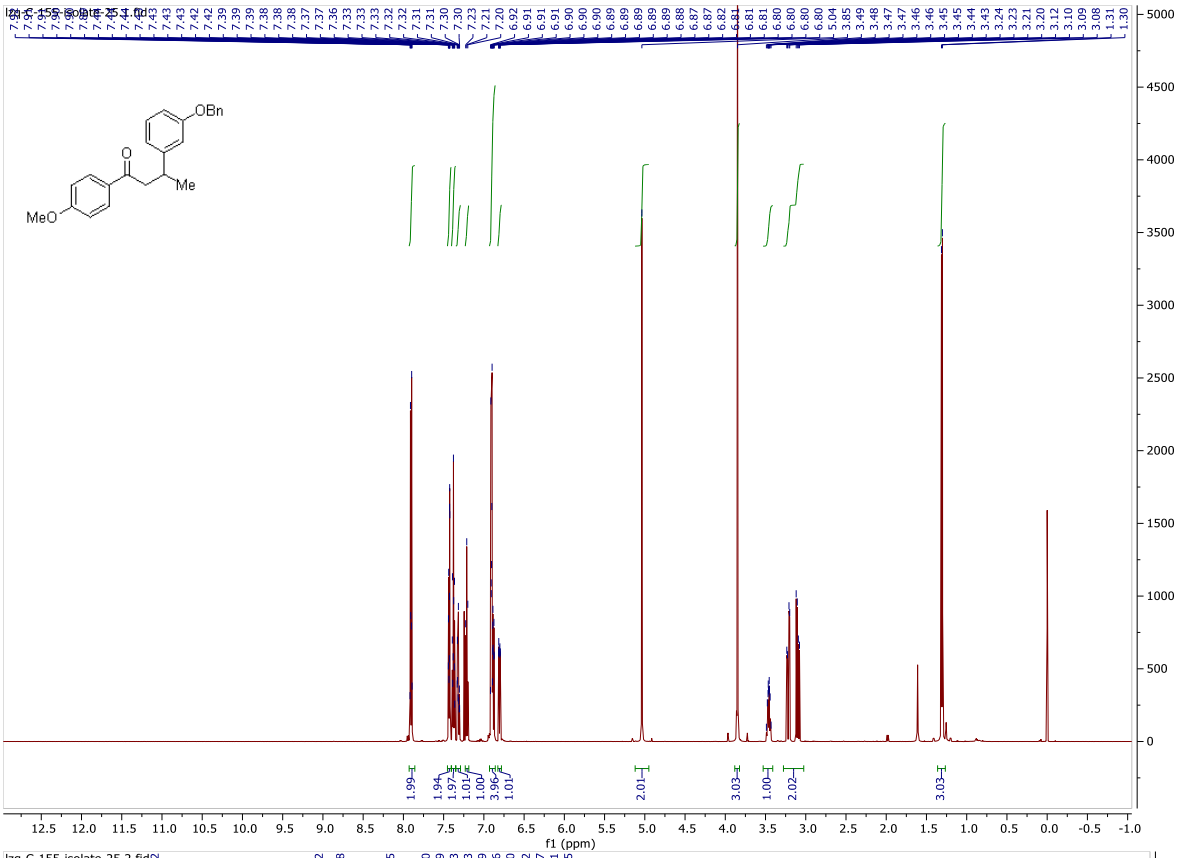

lzq-C-155-isolate-18.1.fid
7.92
7.91
7.91
7.90
7.90
7.89
7.52
7.51
7.51
7.47
7.47
7.47
7.46
7.46
7.46
7.45
7.44
7.44
7.41
7.40
7.39
6.93
6.92
6.92
6.91
6.91
6.90
3.86
3.25
3.24
3.23
3.22
3.19
3.18
3.16
3.15
1.36
1.35
CF3
O
Me
MeO
1.98
1.00
1.96
1.03
2.01
3.01
1.00
2.03
2.95
f1 (ppm)

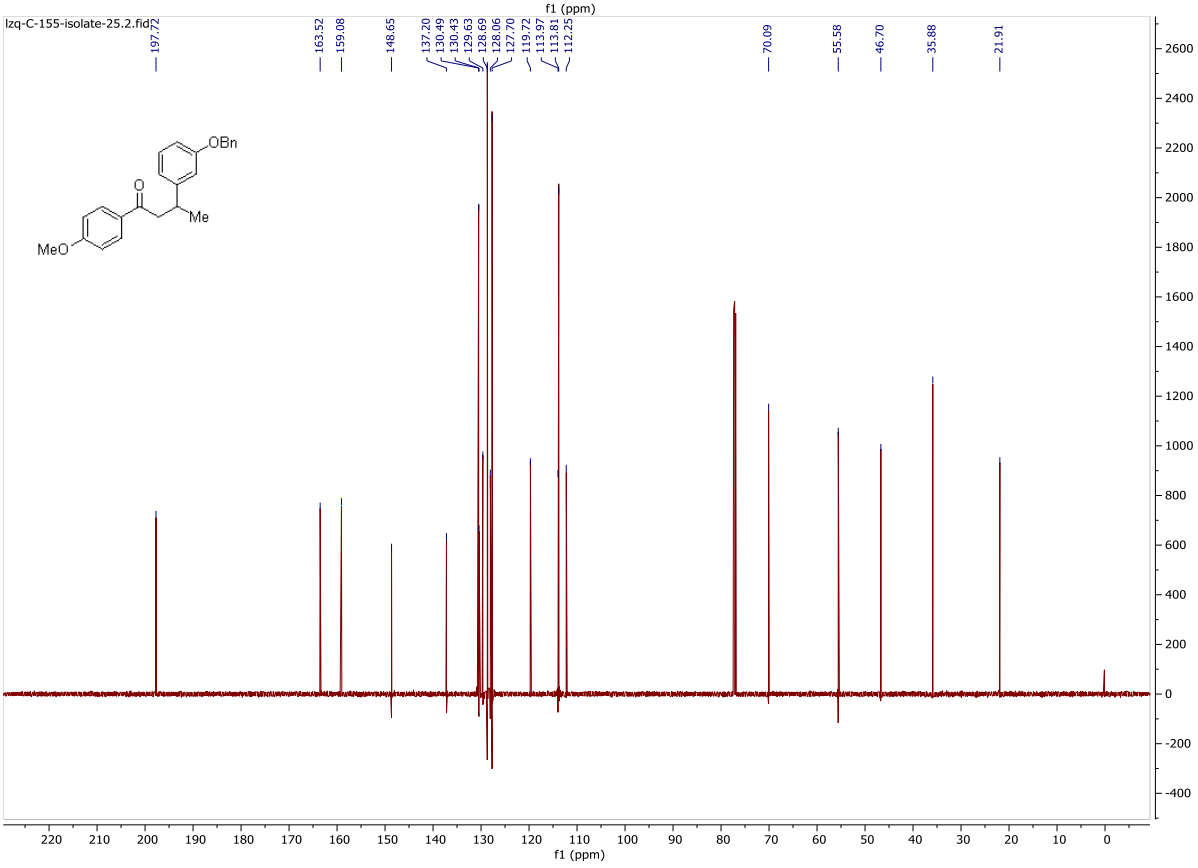

lzq-C-155-isolate-18.2.fid
197.13
163.67
147.75
131.20
130.99
130.78
130.70
130.70
130.69
130.68
130.58
130.47
130.26
129.05
125.28
123.70
123.68
123.65
123.63
123.30
123.27
123.25
123.22
113.88
55.61
46.43
35.64
21.96
CF3
O
Me
MeO
f1 (ppm)

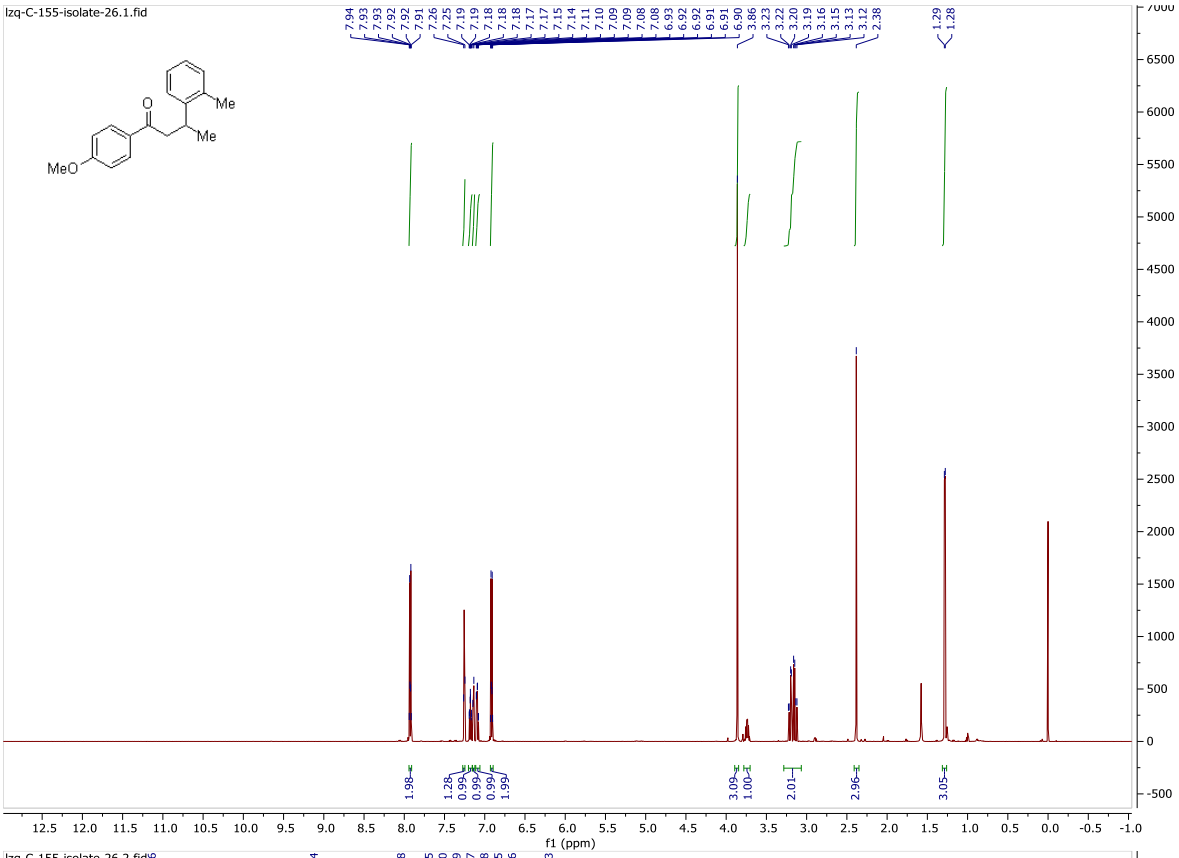

lzq-C-155-isolate-18.3.fid
-65.13
CF3
O
Me
MeO
f1 (ppm)

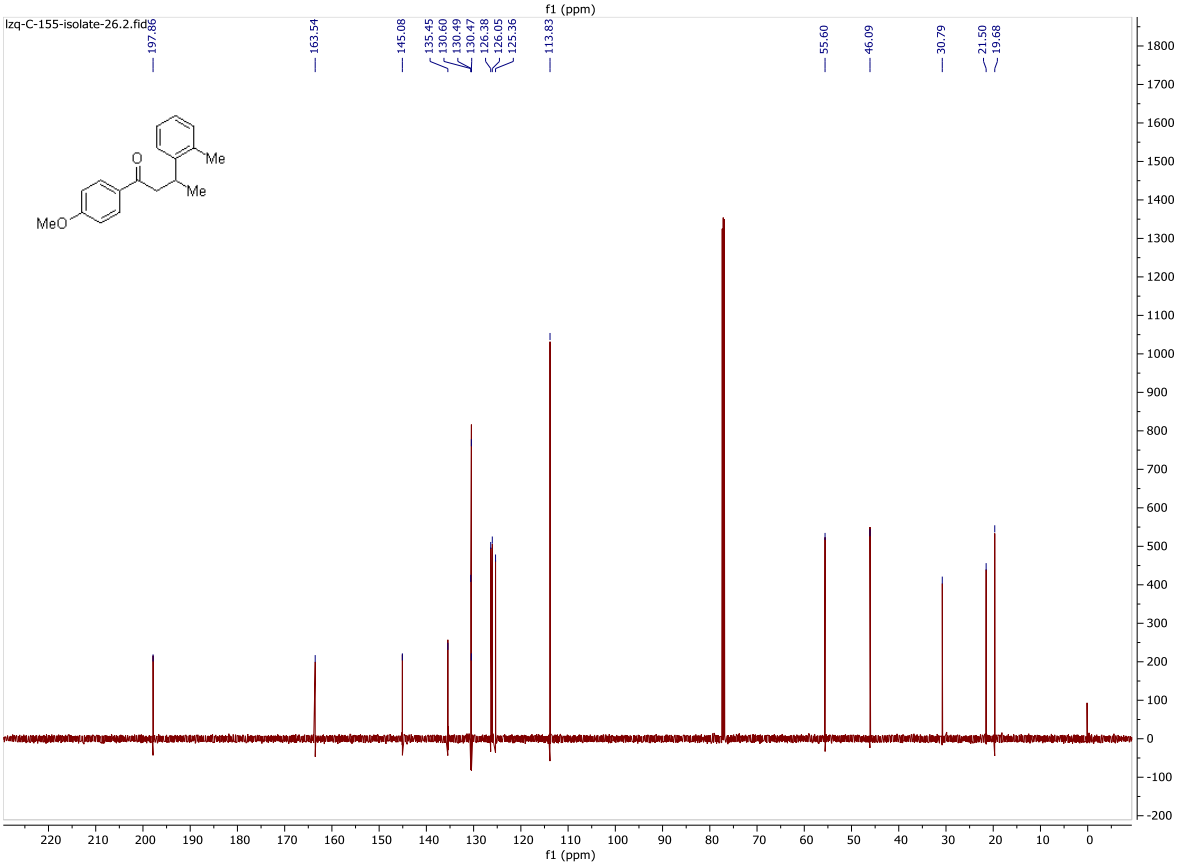

lzq-C-155-isolate-15.1.fid
7.92 7.91 7.91 7.90 7.88 7.88 7.88 7.78 7.78 7.78 7.77 7.77 7.77 7.50 7.50 7.50 7.49 7.49 7.48 7.40 7.39 7.38 6.92 6.90
3.86 3.60 3.59 3.58 3.57 3.56 3.54 3.28 3.27 3.25 3.24 3.20 3.19 3.18 3.16 2.59
1.36 1.35
O
Me
O
Me
MeO
1.99 1.04 1.00 0.99 0.99 2.05 3.22 1.00 2.07 2.95 3.03
f1 (ppm)

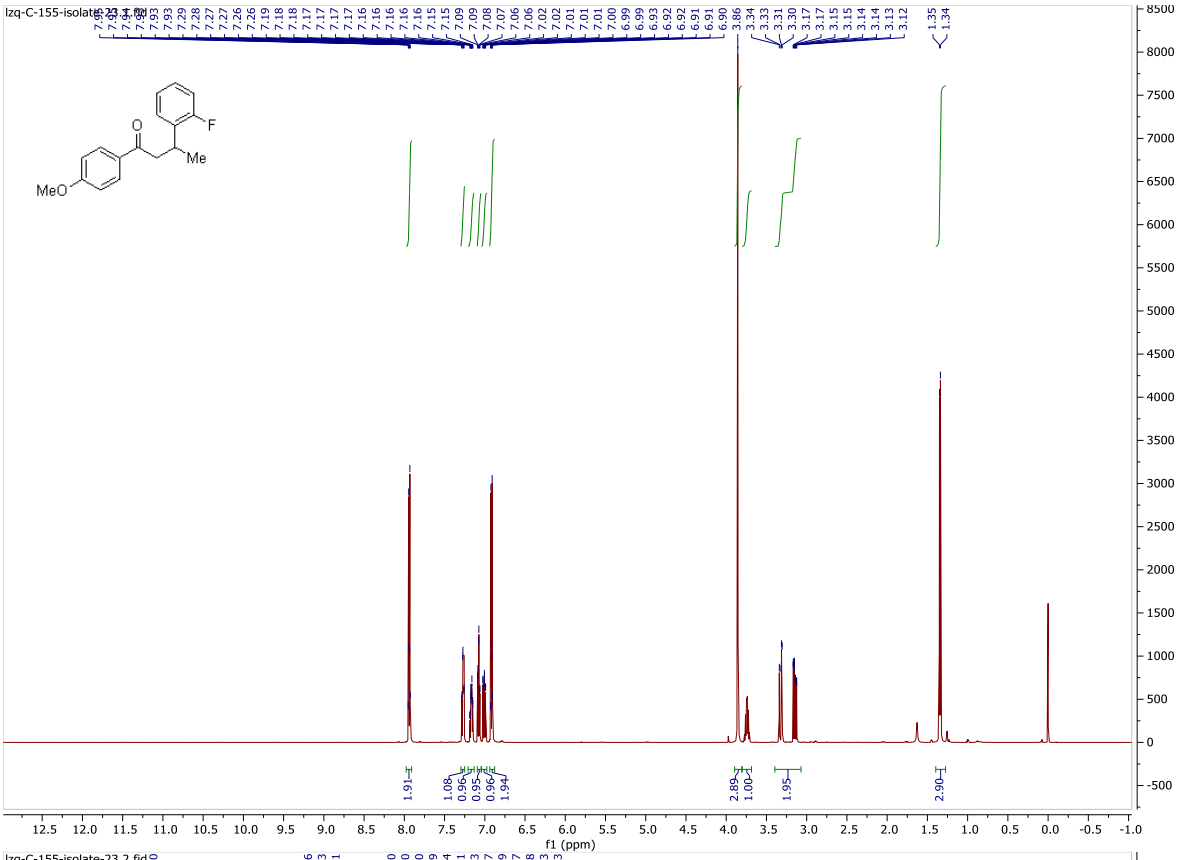

lzq-C-155-isolate-15.2.fid
198.45 197.32 163.62 147.44 137.50 132.17 130.46 130.28 128.84 126.66 126.55 113.85 55.59 46.43 35.72 26.83 22.11
O
Me
O
Me
MeO
f1 (ppm)

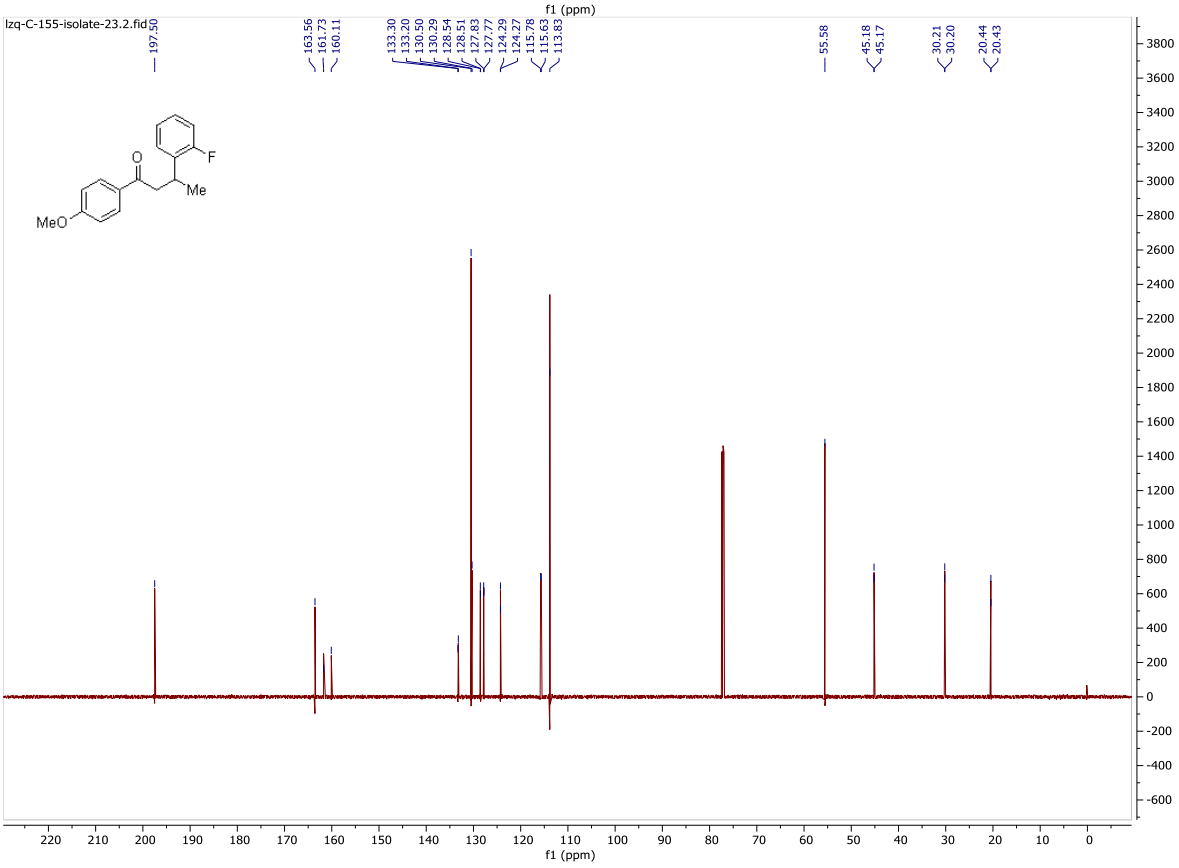

OBn
O
Me
MeO
f1 (ppm)

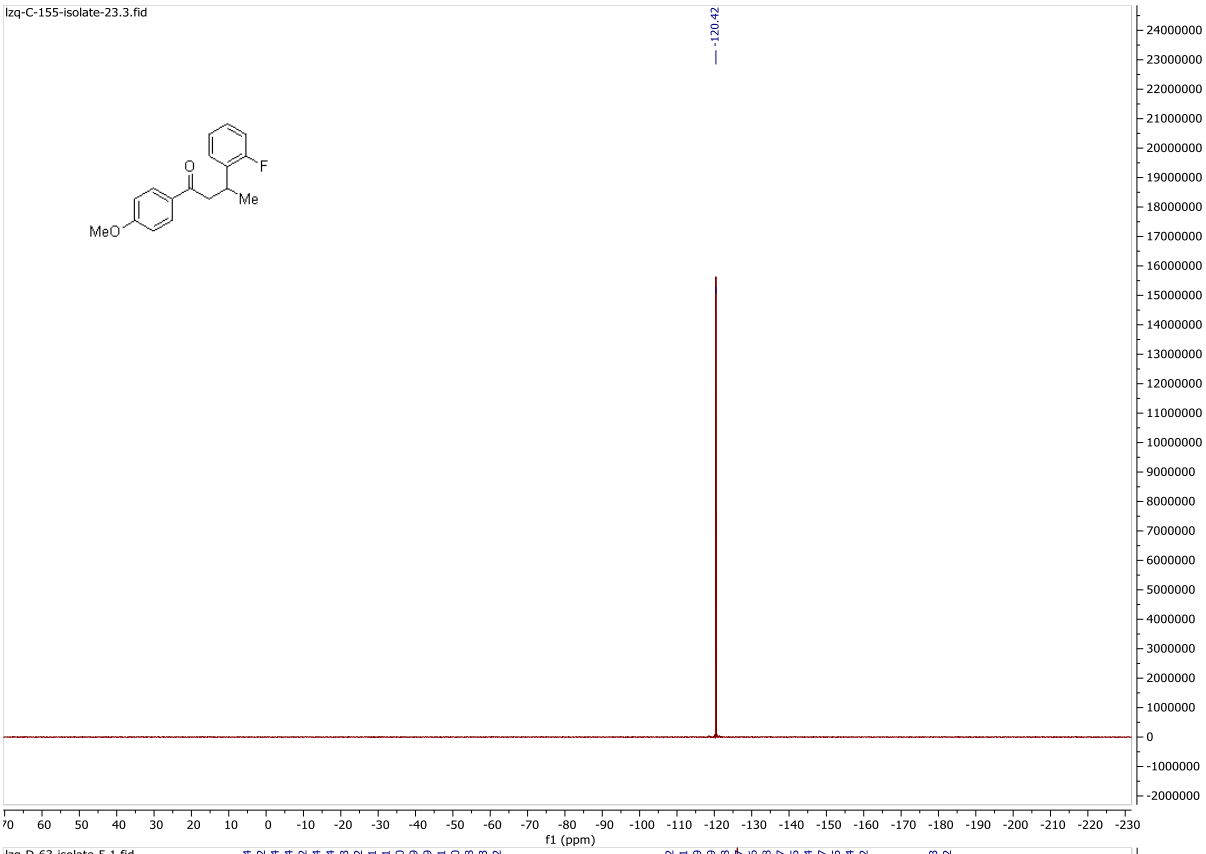

lzq-C-155-isolate-25.2.fid
197.72
163.52
159.08
148.65
137.20
130.49
130.43
129.63
128.69
128.06
127.70
119.72
113.97
113.81
112.25
70.09
55.58
46.70
35.88
21.91
OBn
O
Me
MeO
f1 (ppm)

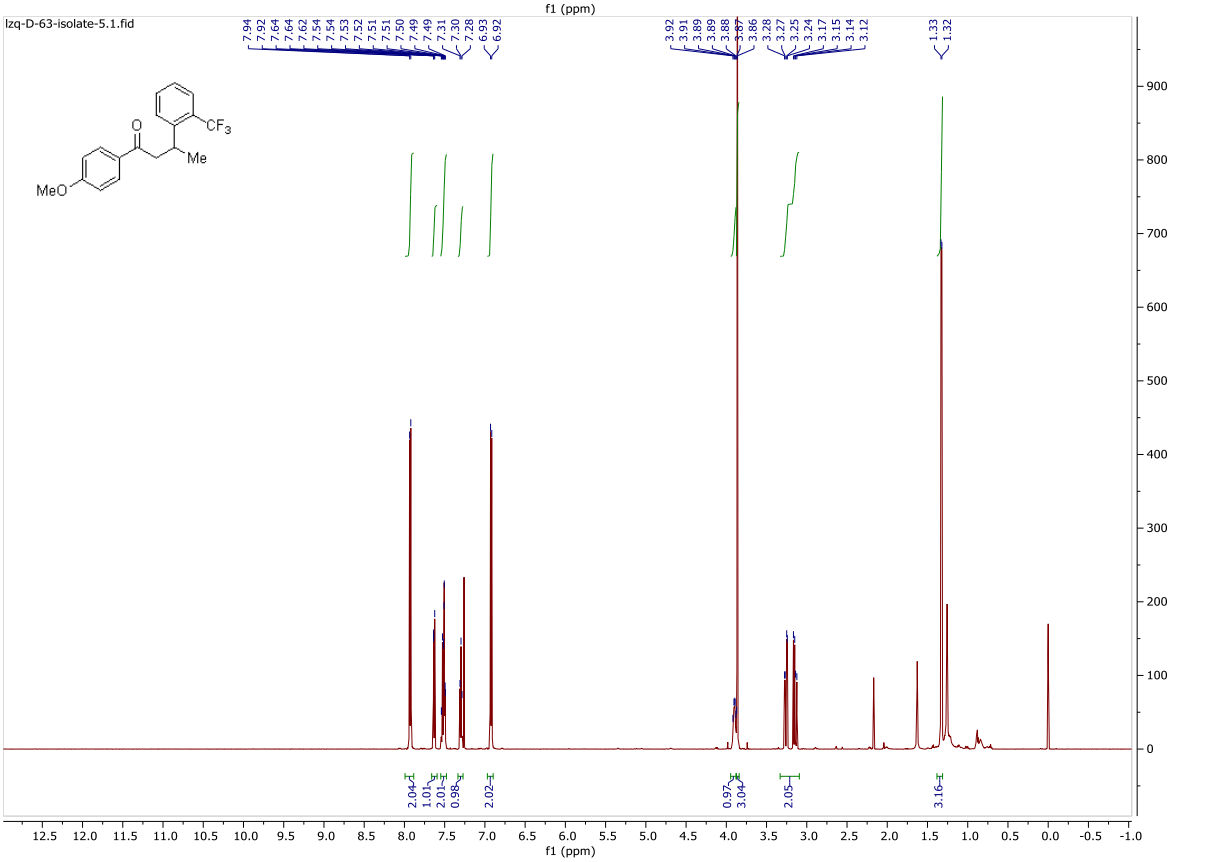

lzq-C-155-isolate-26.1.fid
Me
Me
O
MeO
f1 (ppm)

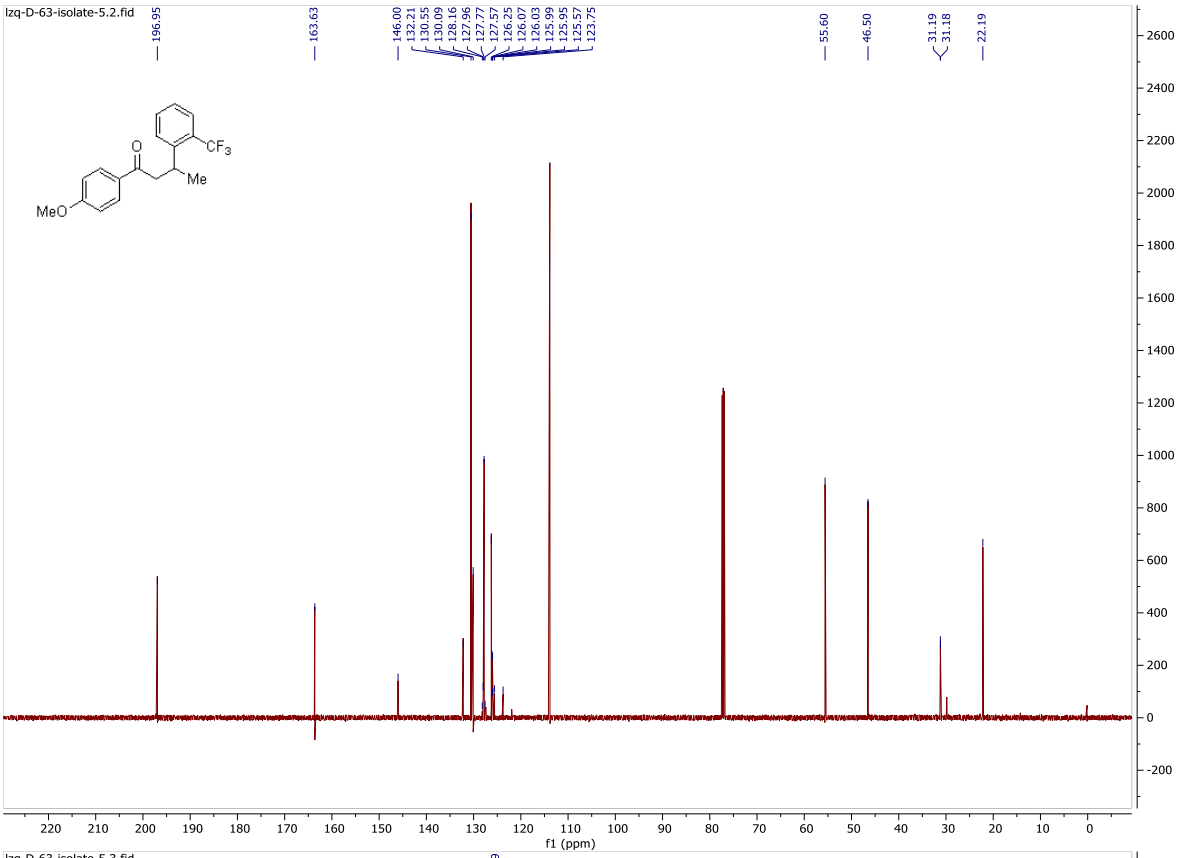

lzq-C-155-isolate-26.2.fid
197.86
163.54
145.08
135.45
130.60
130.49
130.47
126.38
126.05
125.36
113.83
55.60
46.09
30.79
21.50
19.68
Me
Me
O
MeO
f1 (ppm)

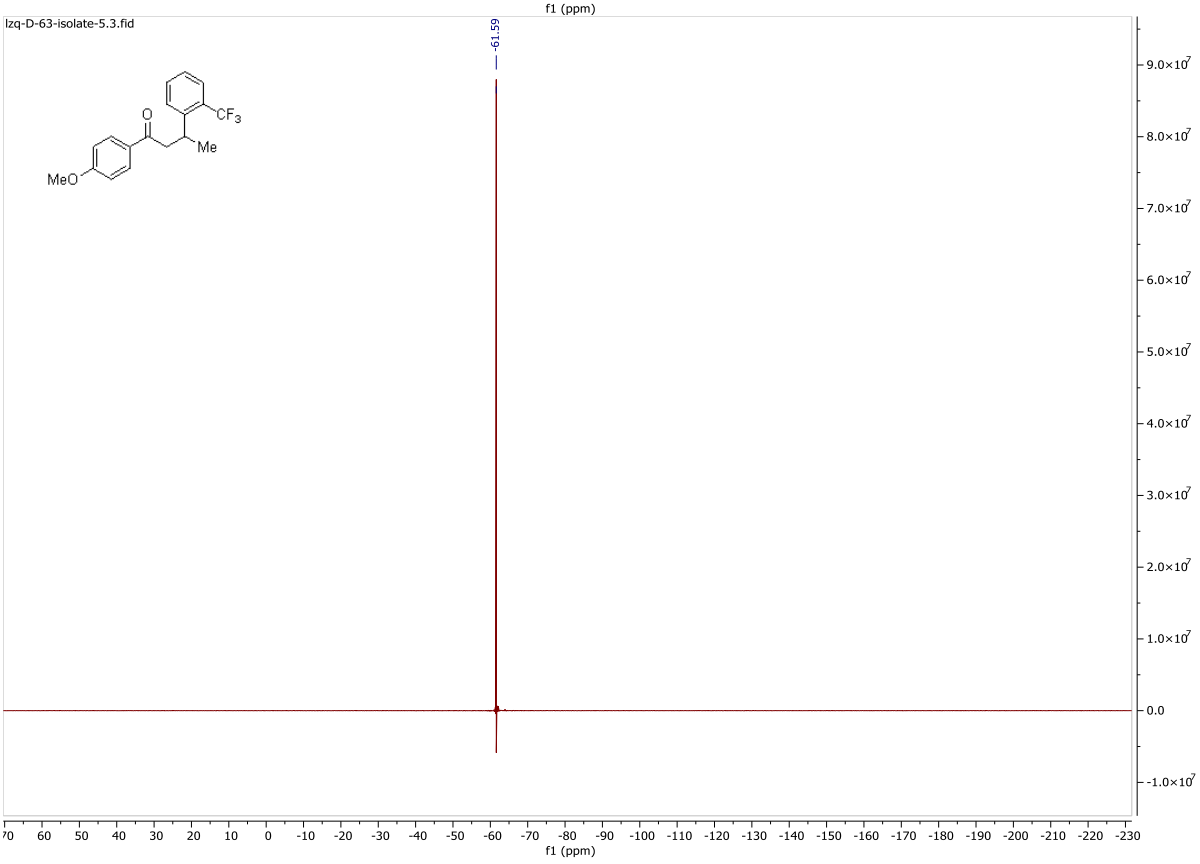

lzq-C-155-isolate-23.1.fid
O
F
Me
MeO
f1 (ppm)

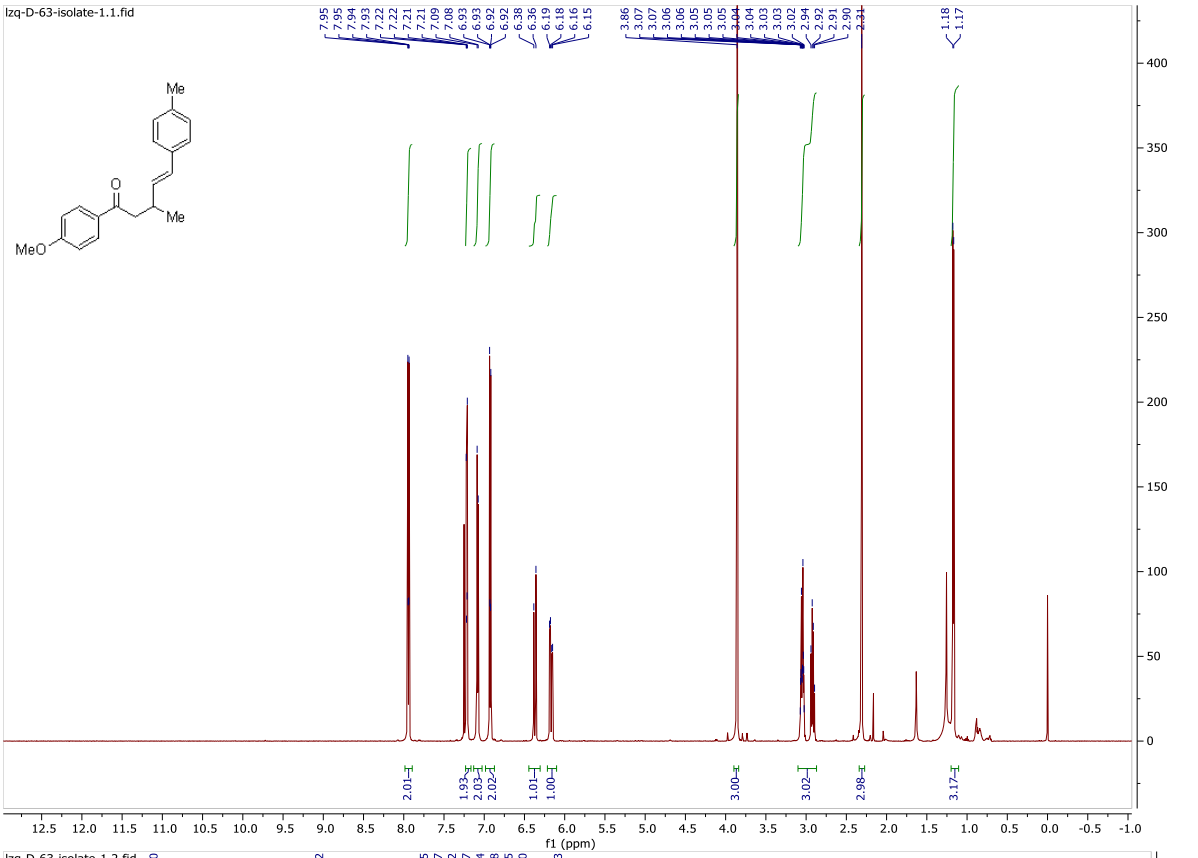

lzq-C-155-isolate-23.2.fid
197.50
163.56
161.73
160.11
133.30
133.20
130.50
130.29
128.54
128.51
127.83
127.77
124.29
124.27
115.78
115.63
113.83
55.58
45.18
45.17
30.21
30.20
20.44
20.43
O
F
Me
MeO
f1 (ppm)

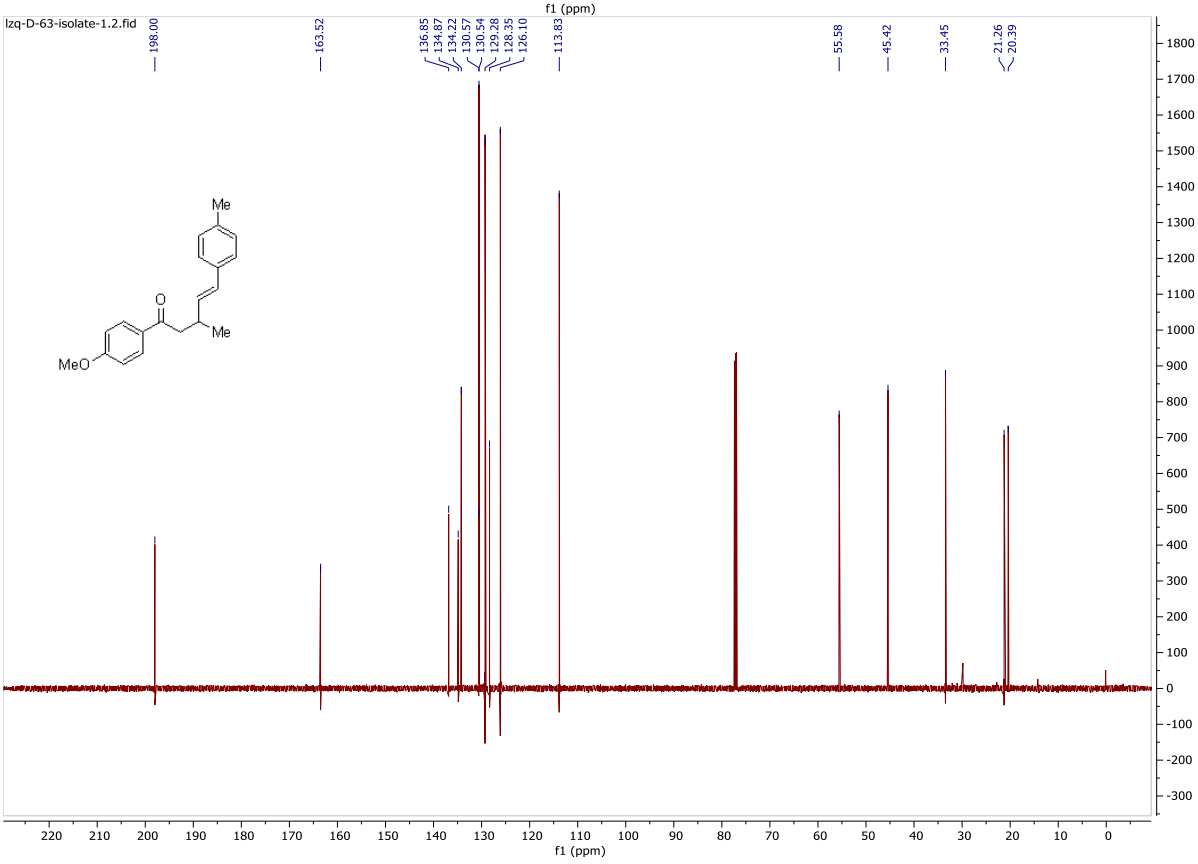

lzq-C-155-isolate-23.3.fid
-120.42
O
F
Me
MeO
f1 (ppm)

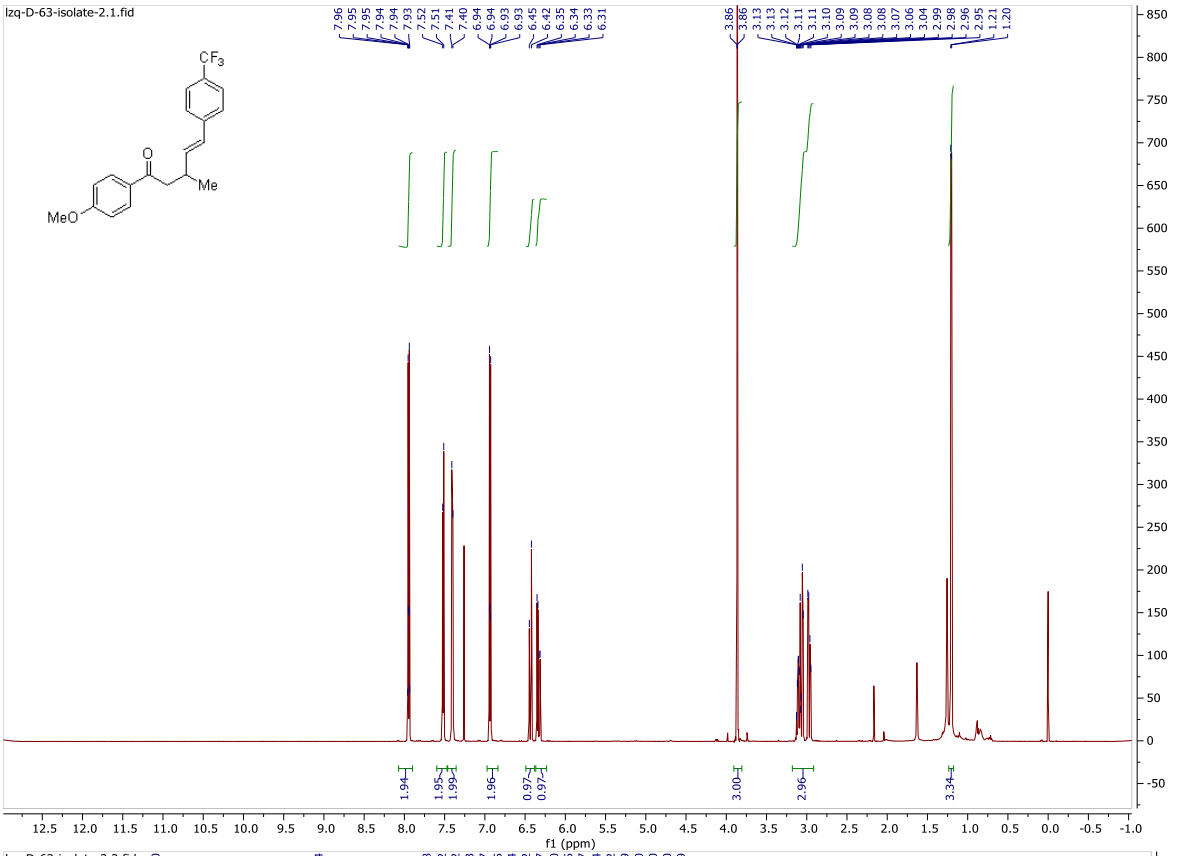

lzq-D-63-isolate-5.1.fid
7.94
7.92
7.64
7.64
7.62
7.54
7.54
7.53
7.52
7.51
7.51
7.50
7.49
7.49
7.31
7.30
7.28
6.93
6.92
3.92
3.91
3.89
3.89
3.88
3.87
3.86
3.28
3.27
3.25
3.24
3.17
3.15
3.14
3.12
1.33
1.32
O
CF3
Me
MeO
2.04
1.01
2.01
0.98
2.02
0.97
3.04
2.05
3.16
f1 (ppm)

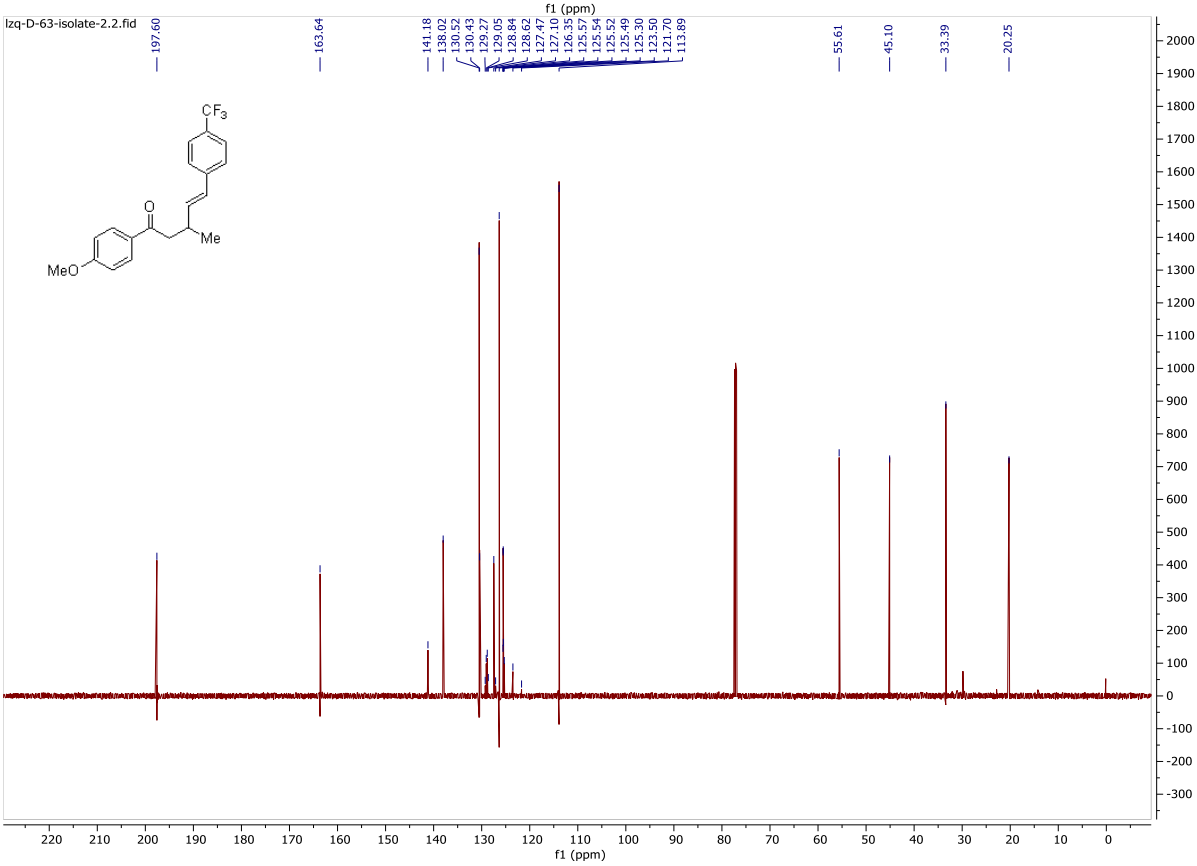

lzq-D-63-isolate-5.2.fid
196.95
163.63
146.00
132.21
130.55
130.09
128.16
127.96
127.77
127.57
126.25
126.07
126.03
125.99
125.95
125.57
123.75
55.60
46.50
31.19
31.18
22.19
O
CF3
Me
MeO
f1 (ppm)

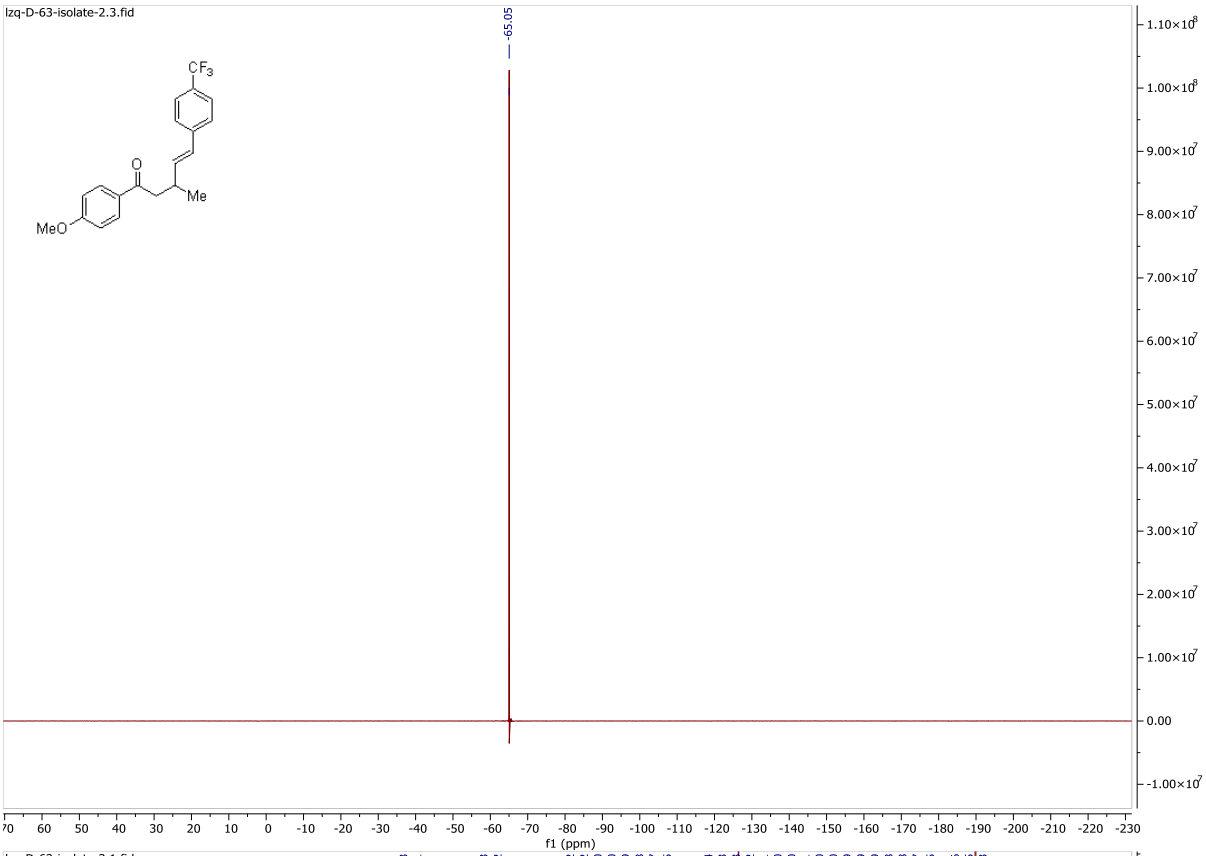

lzq-D-63-isolate-5.3.fid
-61.59
O
CF3
Me
MeO
f1 (ppm)

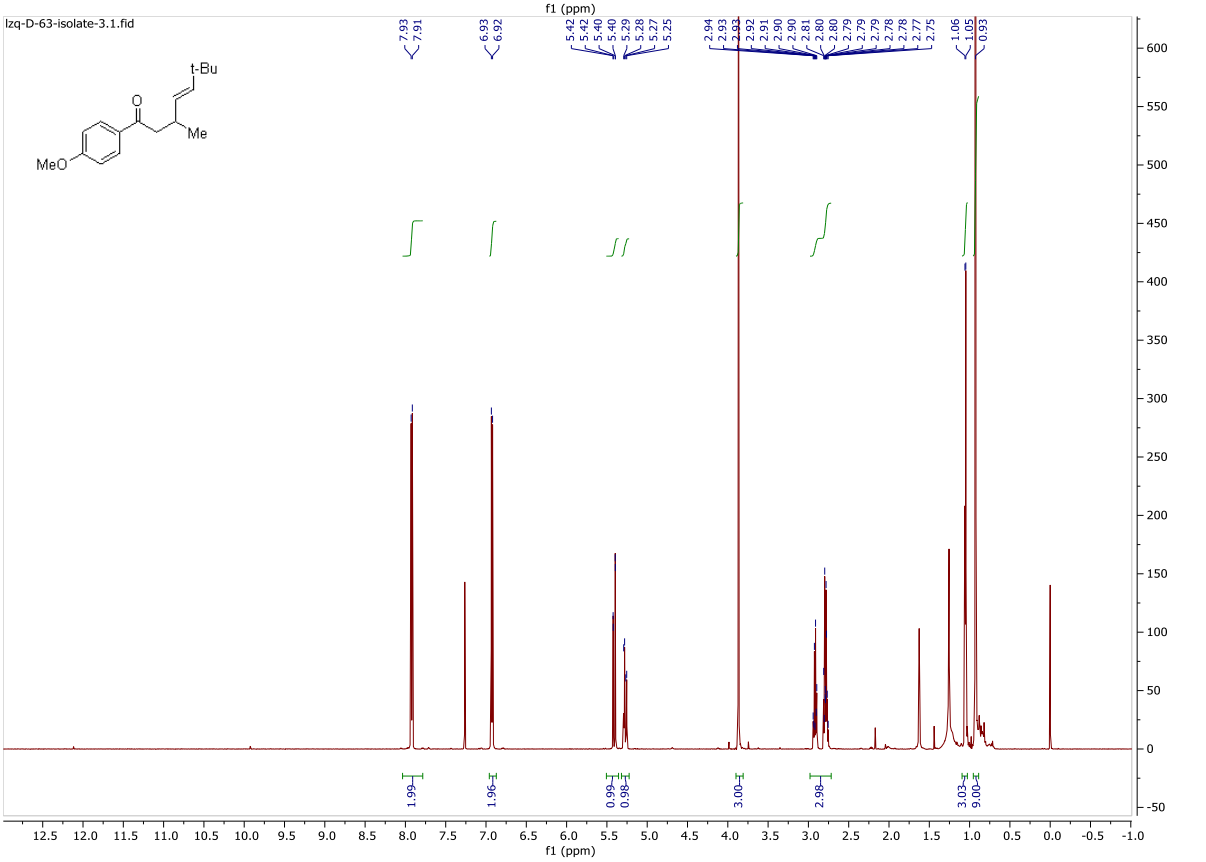

lzq-D-63-isolate-1.1.fid
Me
O
Me
MeO
f1 (ppm)

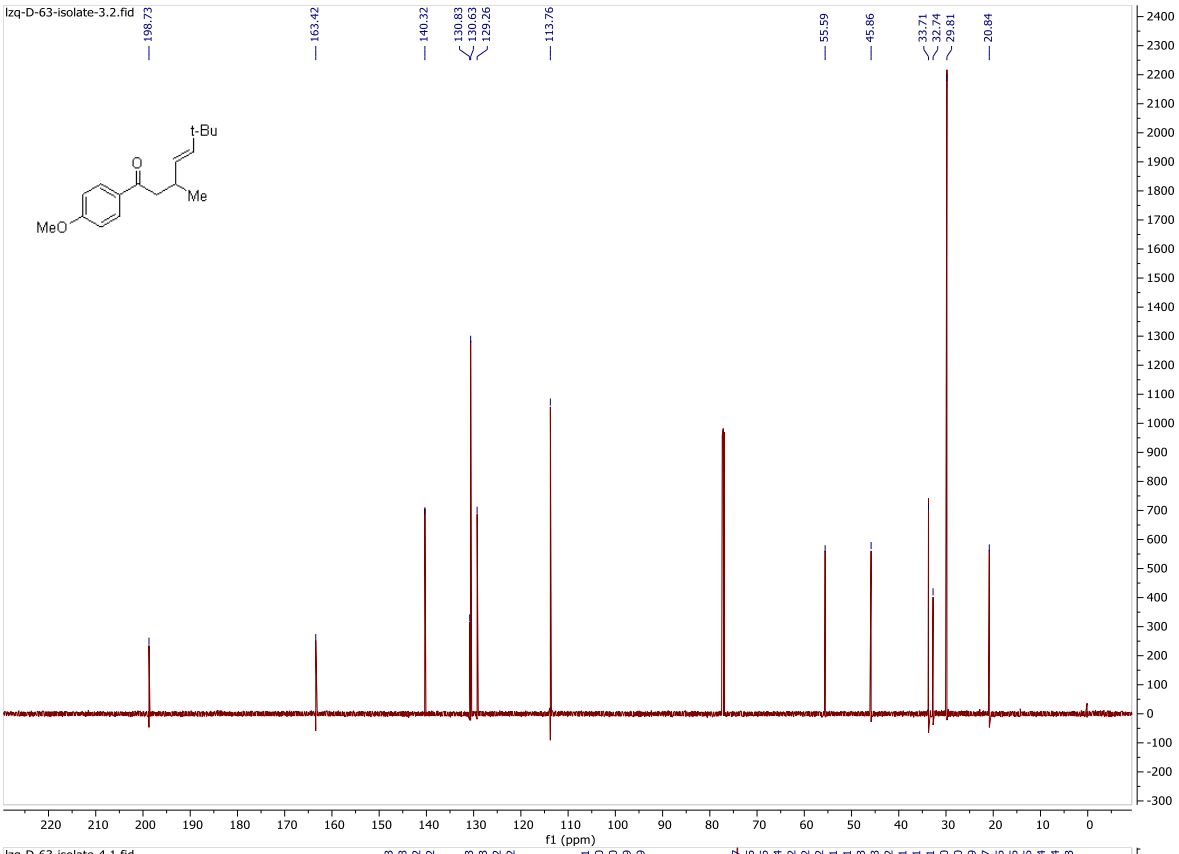

lzq-D-63-isolate-1.2.fid
198.00
163.52
136.85
134.87
134.22
130.57
130.54
129.28
128.35
126.10
113.83
55.58
45.42
33.45
21.26
20.39
Me
O
Me
MeO
f1 (ppm)

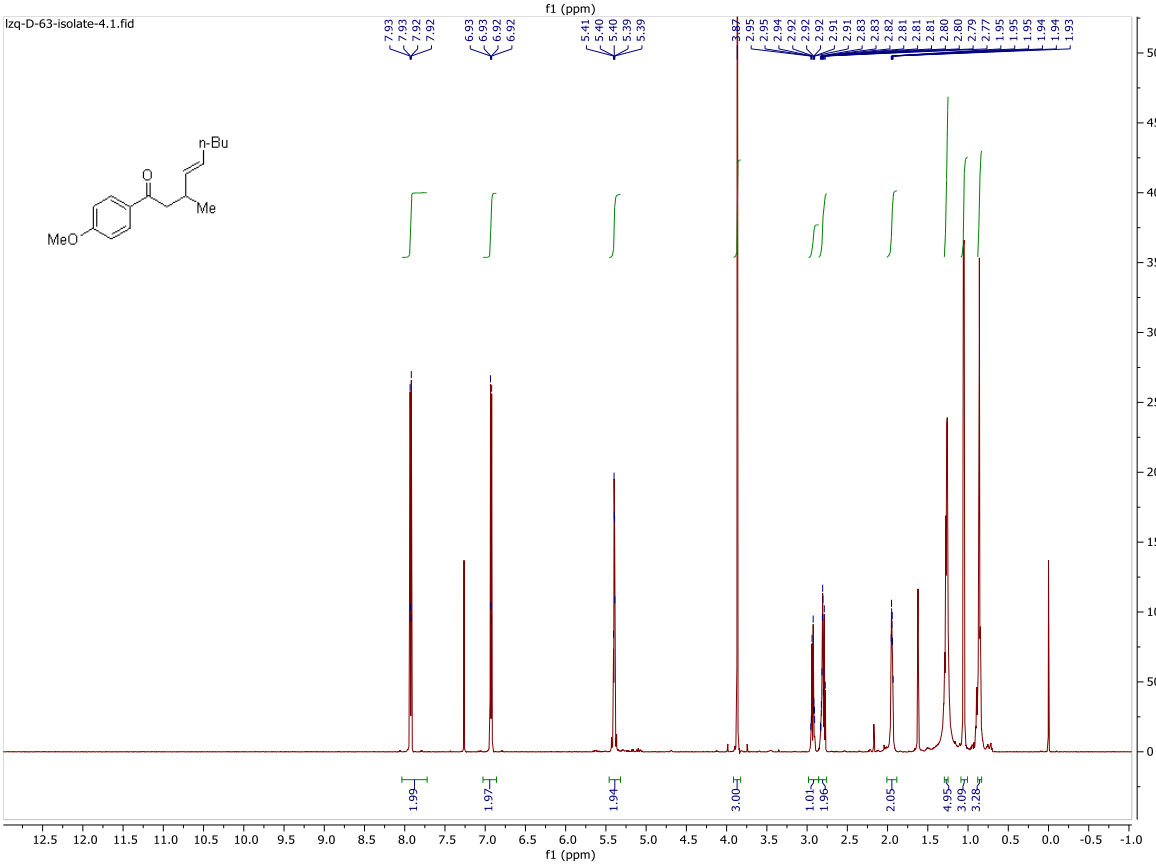

lzq-D-63-isolate-2.1.fid
CF3
O
Me
MeO
f1 (ppm)

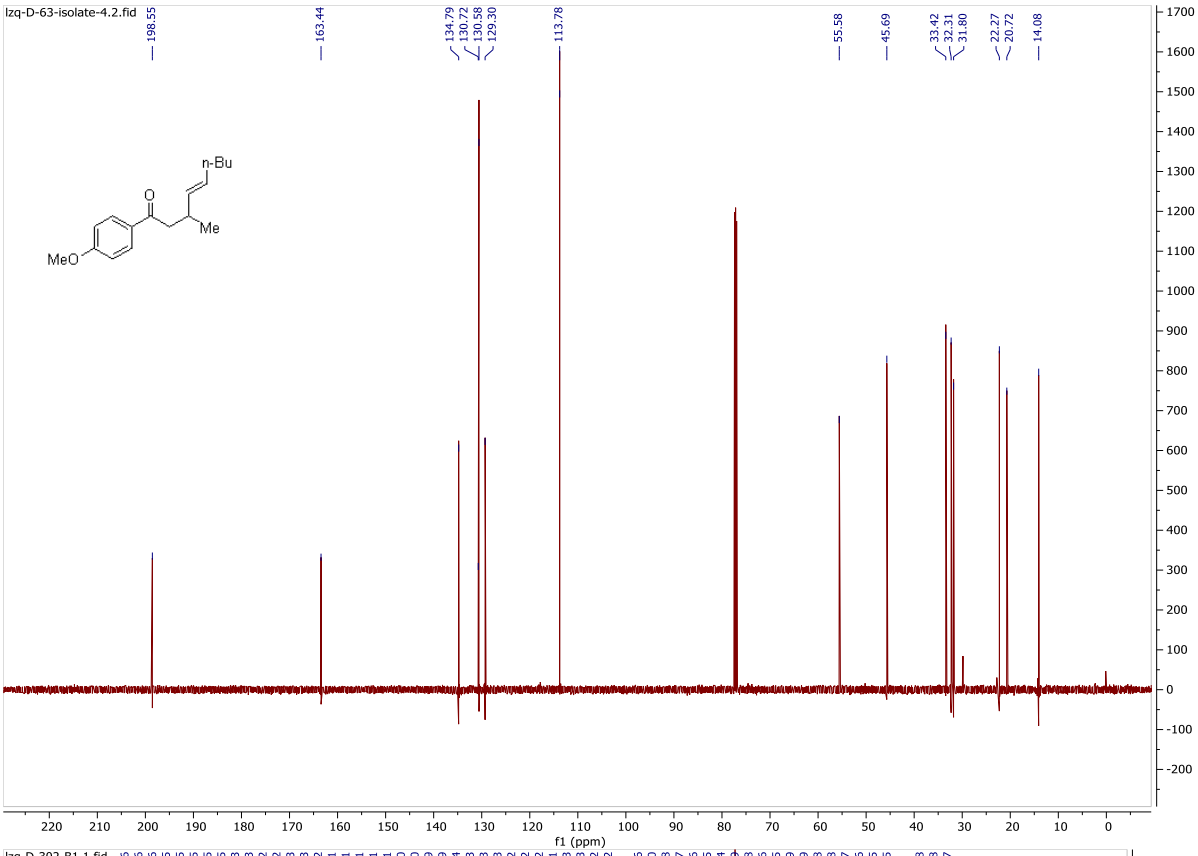

lzq-D-63-isolate-2.2.fid
CF3
O
Me
MeO
f1 (ppm)

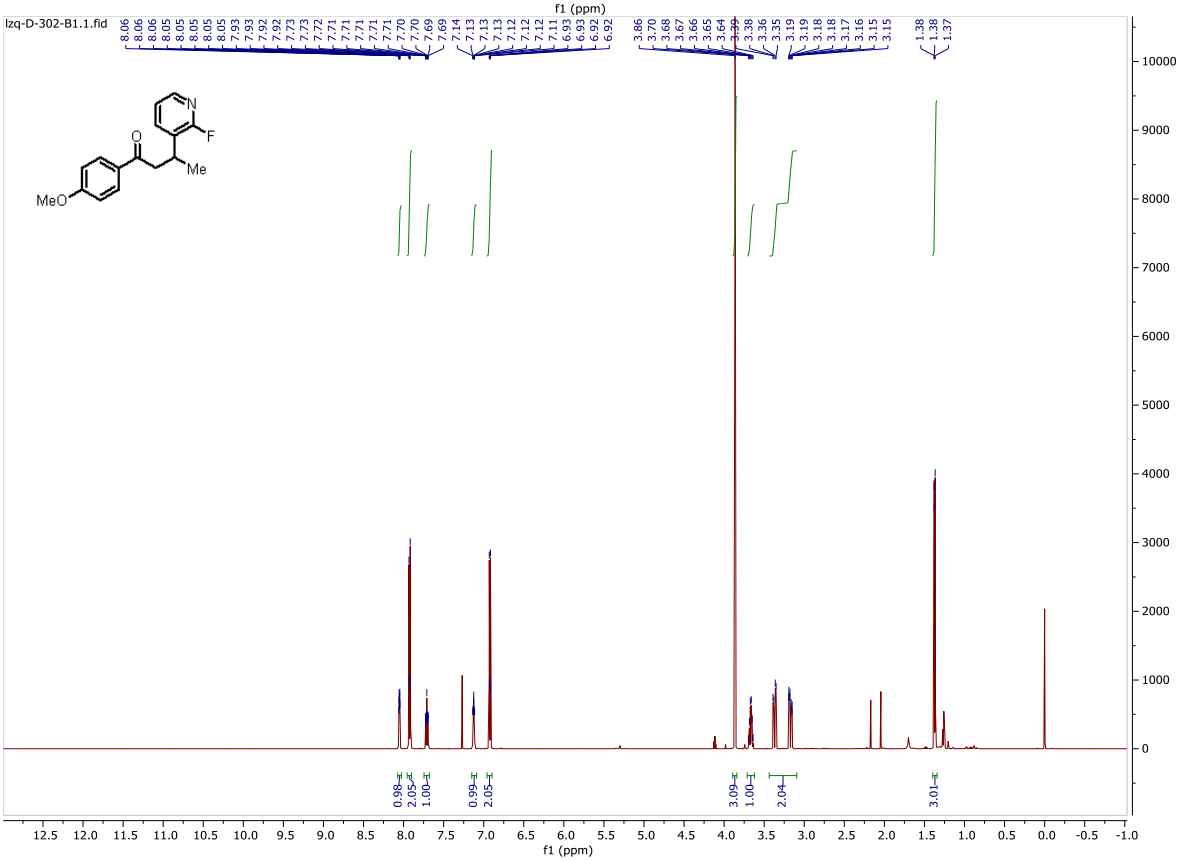

lzq-D-63-isolate-2.3.fid
-65.05
CF3
O
Me
MeO
f1 (ppm)

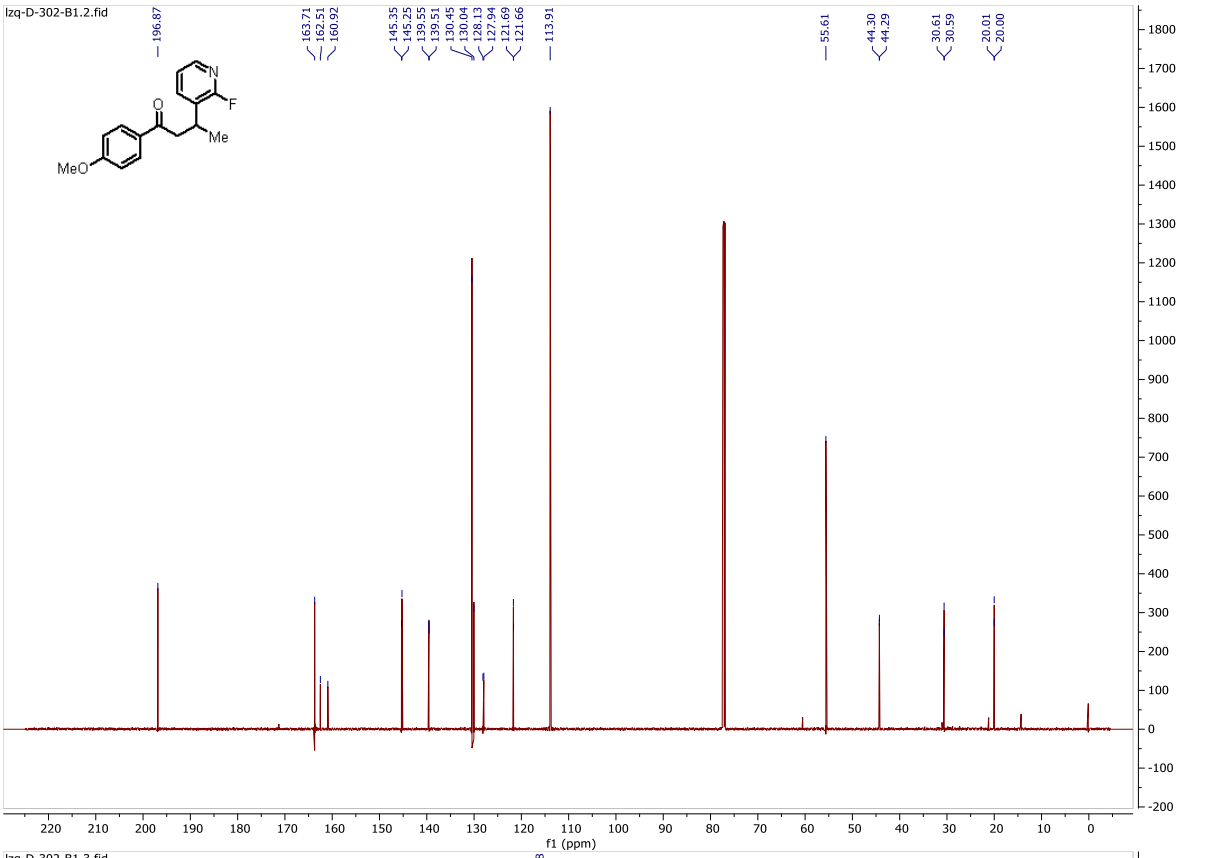

lzq-D-63-isolate-3.1.fid
t-Bu
O
Me
MeO
7.93
7.91
6.93
6.92
5.42
5.42
5.40
5.40
5.29
5.28
5.27
5.25
2.94
2.93
2.93
2.92
2.91
2.90
2.90
2.81
2.80
2.80
2.79
2.79
2.79
2.78
2.78
2.77
2.75
1.06
1.05
0.93
1.99
1.96
0.99
0.98
3.00
2.98
3.03
9.00
f1 (ppm)

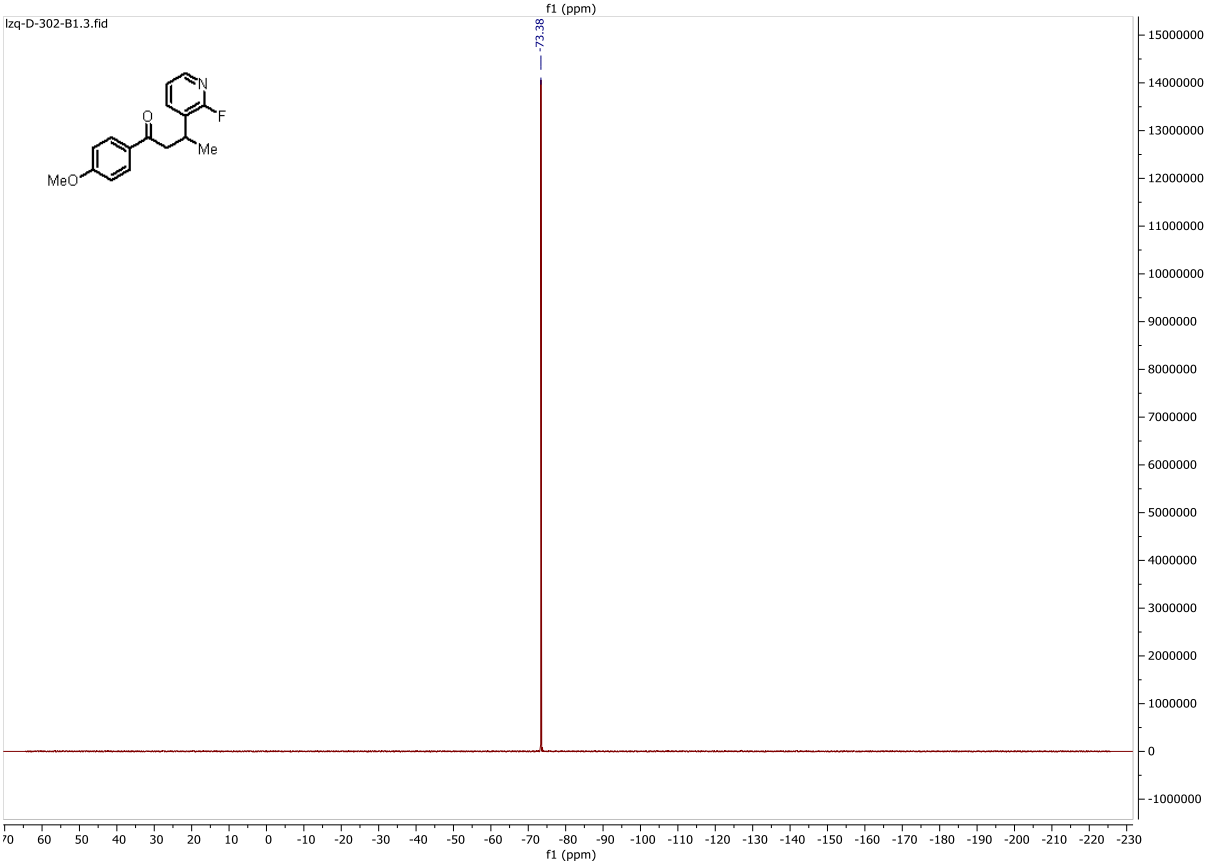

lzq-D-63-isolate-3.2.fid
198.73
163.42
140.32
130.83
130.63
129.26
113.76
55.59
45.86
33.71
32.74
29.81
20.84
t-Bu
O
Me
MeO
f1 (ppm)

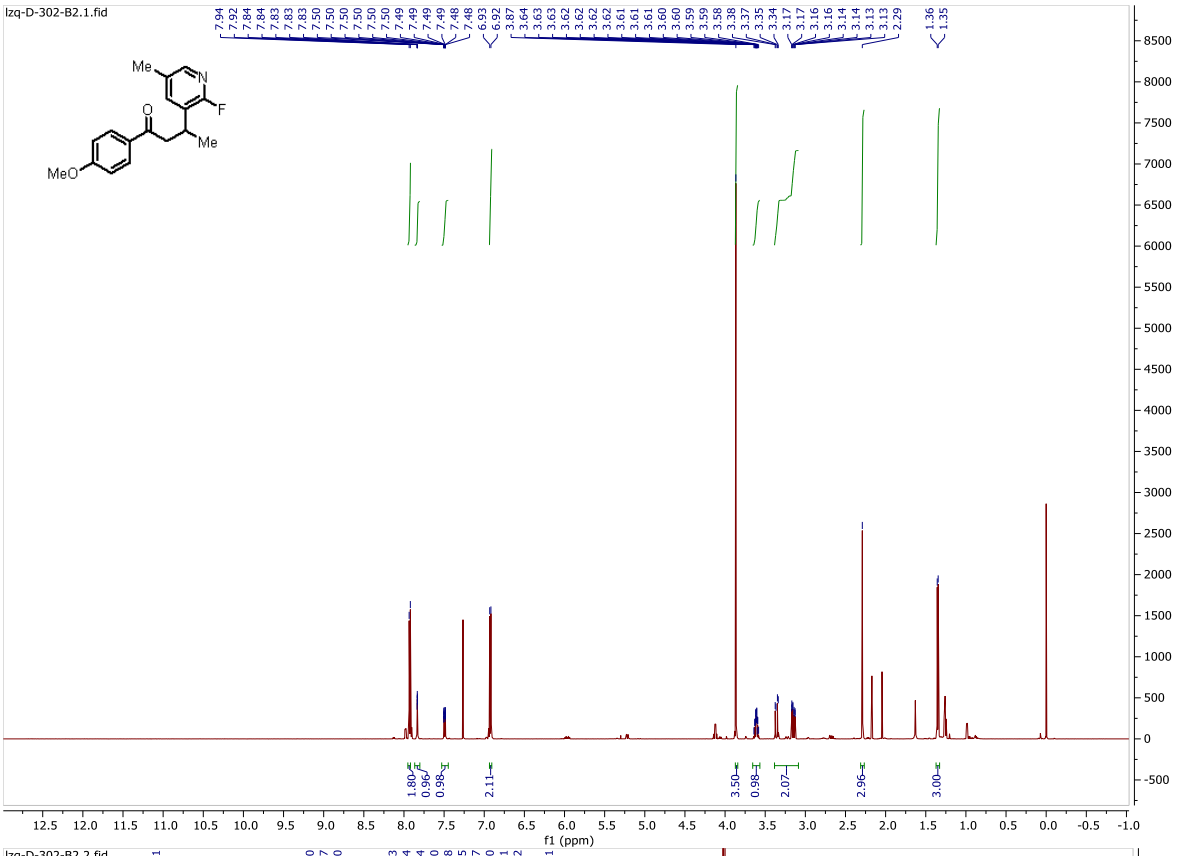

lzq-D-63-isolate-4.1.fid
n-Bu
O
Me
MeO
1.99
1.97
1.94
3.00
1.01
1.96
2.05
4.95
3.09
3.28
f1 (ppm)

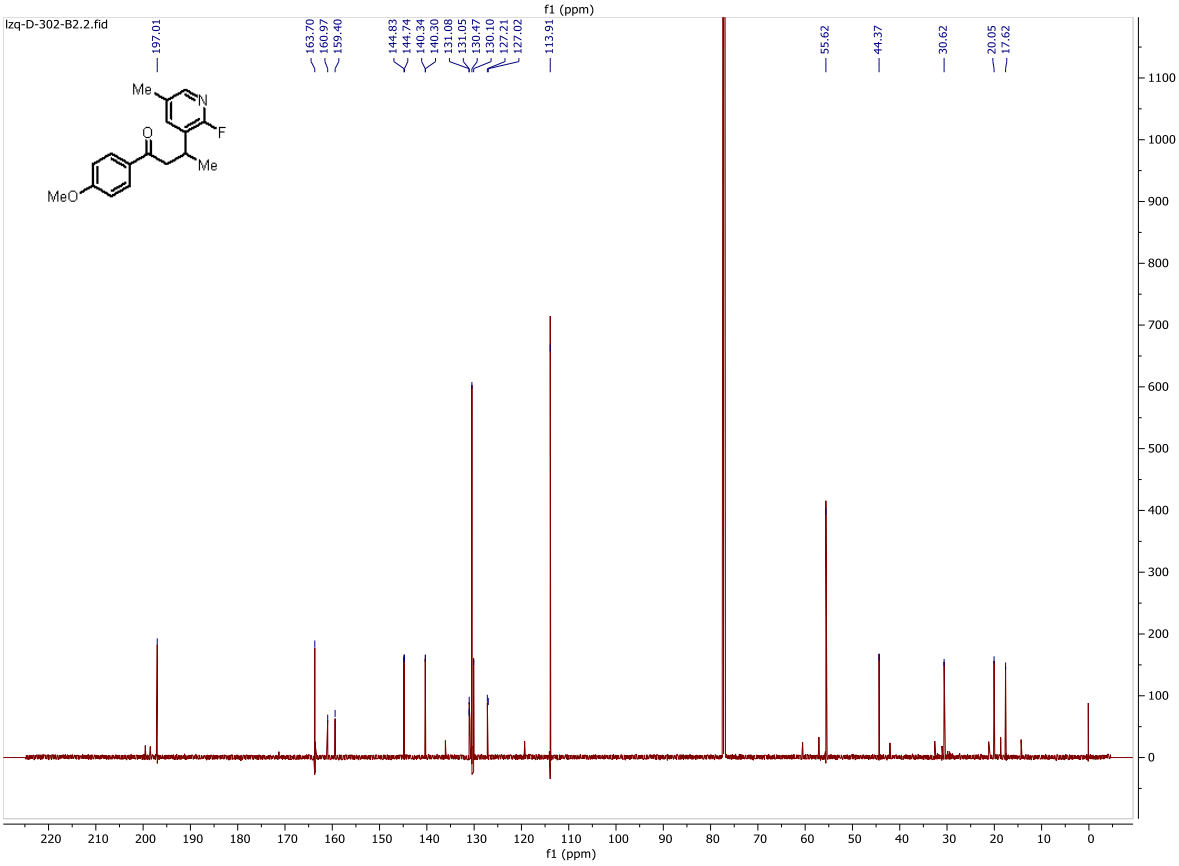

lzq-D-63-isolate-4.2.fid
198.55
163.44
134.79
130.72
130.58
129.30
113.78
55.58
45.69
33.42
32.31
31.80
22.27
20.72
14.08
n-Bu
O
Me
MeO
f1 (ppm)

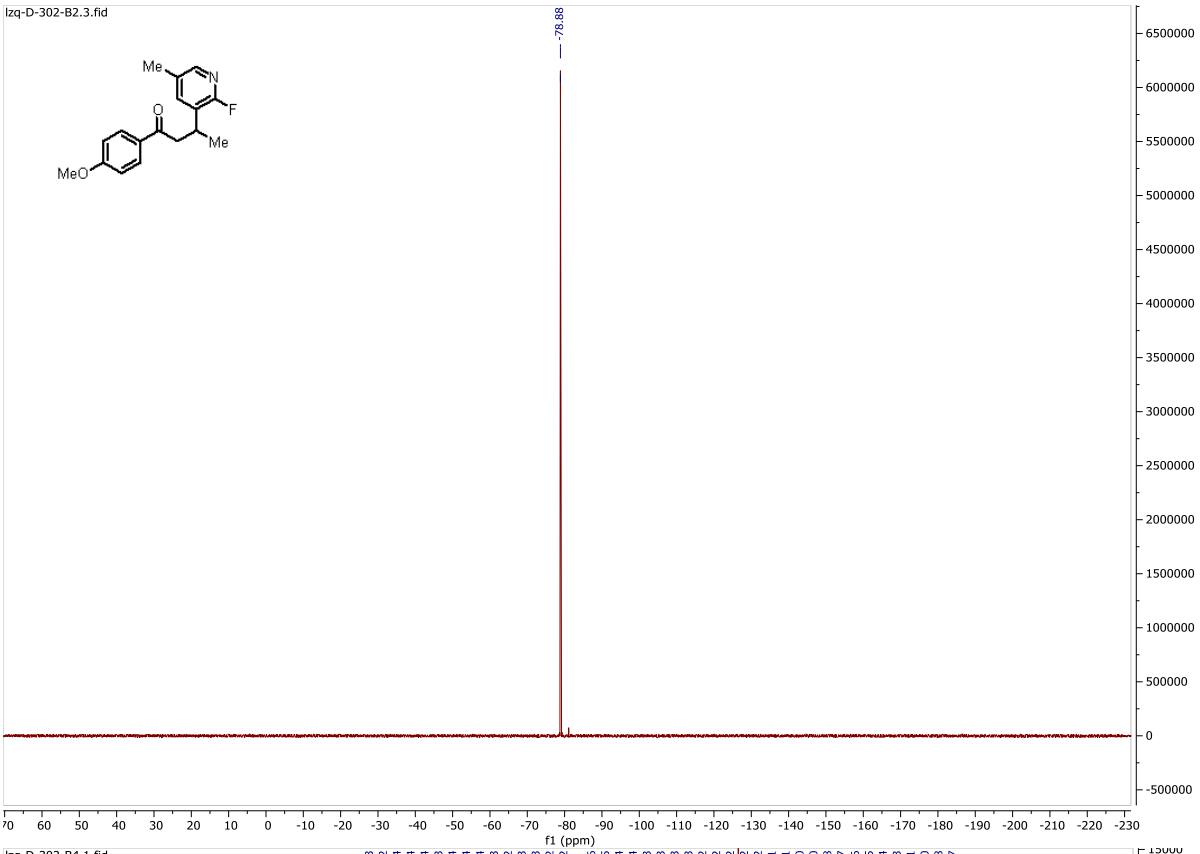

lzq-D-302-B1.1.fid
N
F
O
Me
MeO
0.98
2.05
1.00
0.99
2.05
3.09
1.00
2.04
3.01
f1 (ppm)

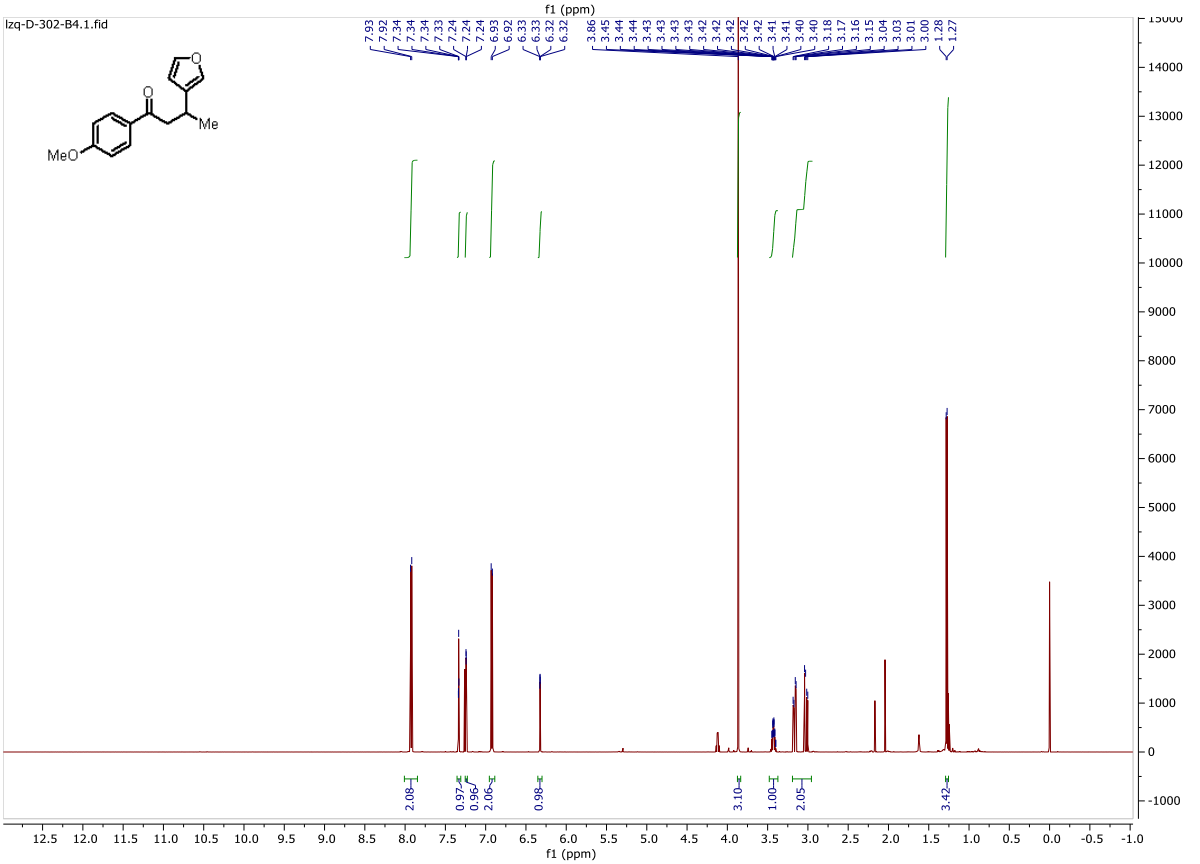

lzq-D-302-B1.2.fid
196.87
163.71
162.51
160.92
145.35
145.25
139.55
139.51
130.45
130.04
128.13
127.94
121.69
121.66
113.91
55.61
44.30
44.29
30.61
30.59
20.01
20.00
MeO
O
N
F
Me
f1 (ppm)

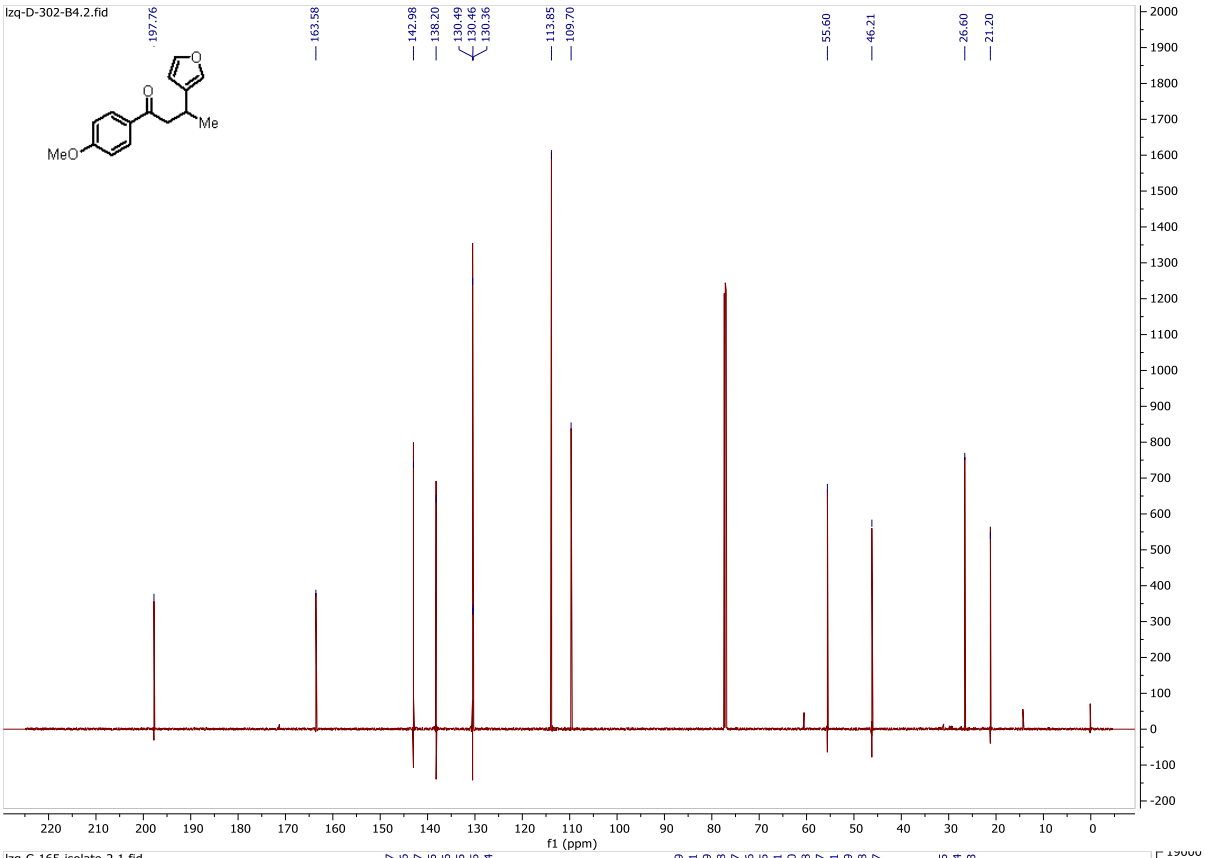

lzq-D-302-B1.3.fid
-73.38
MeO
O
N
F
Me
f1 (ppm)

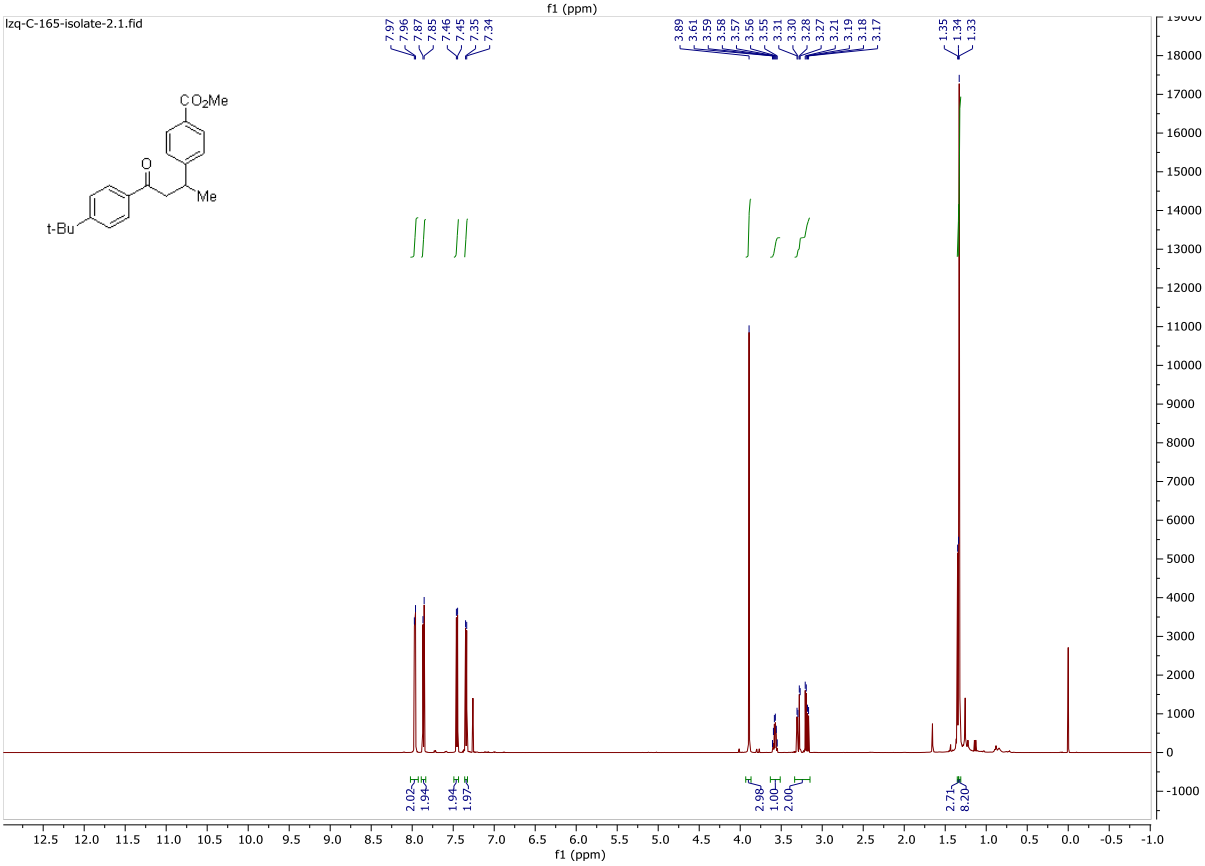

lzq-D-302-B2.1.fid
Me
N
F
O
Me
MeO
f1 (ppm)

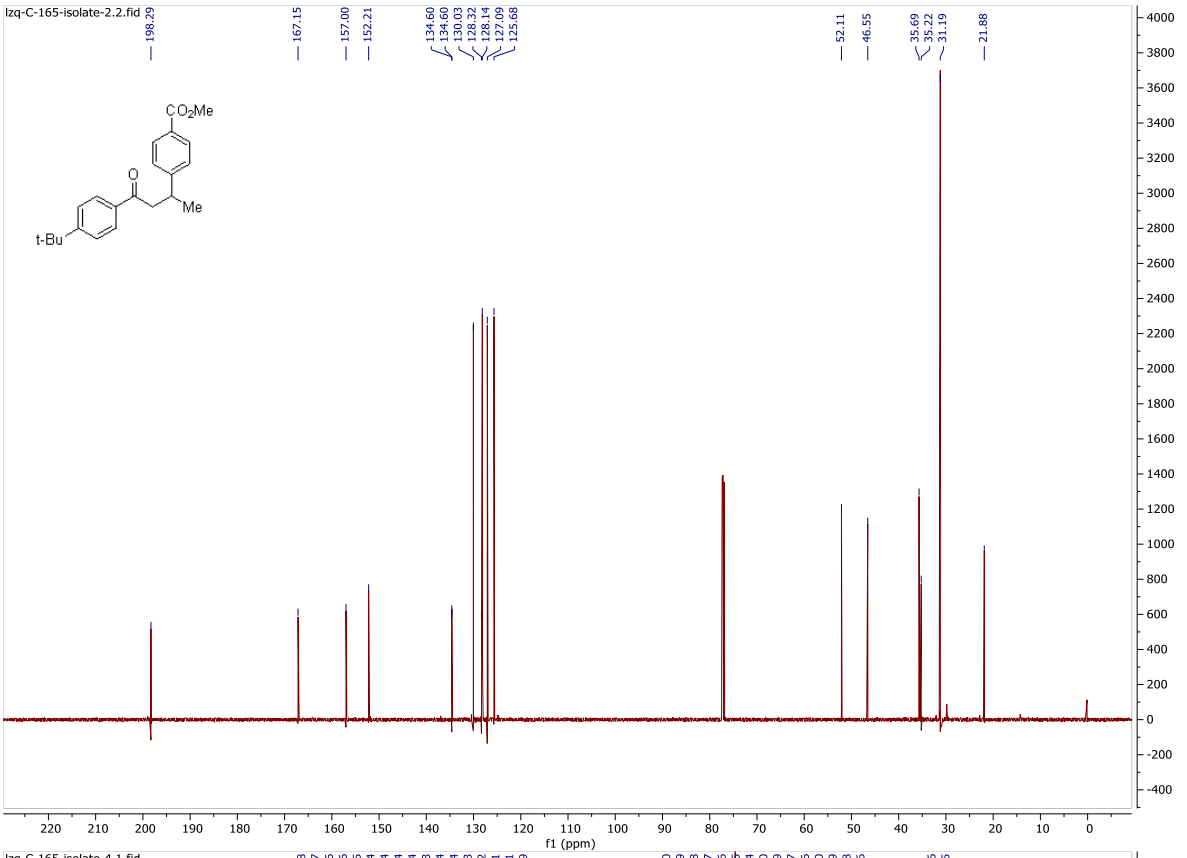

lzq-D-302-B2.2.fid
Me
N
F
O
Me
MeO
f1 (ppm)

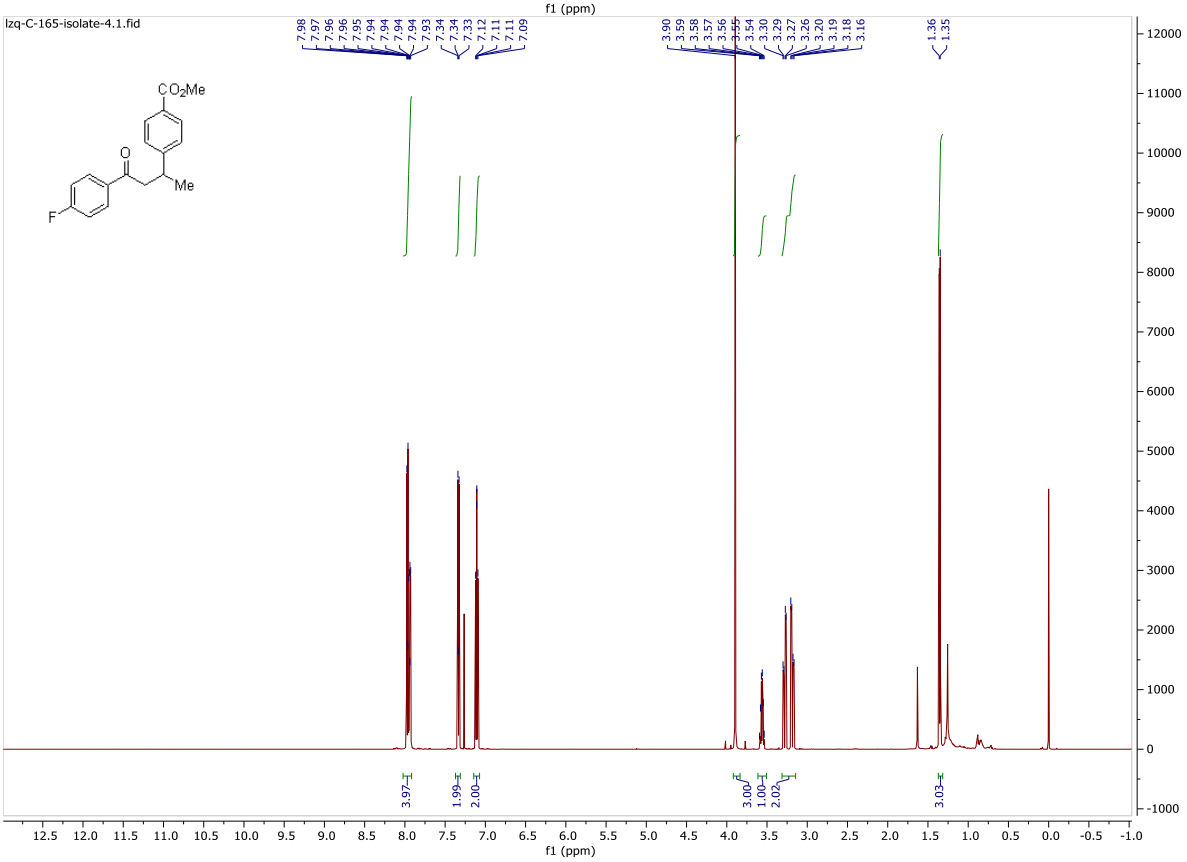

lzq-D-302-B2.3.fid
-78.88
Me
N
F
O
Me
MeO
f1 (ppm)

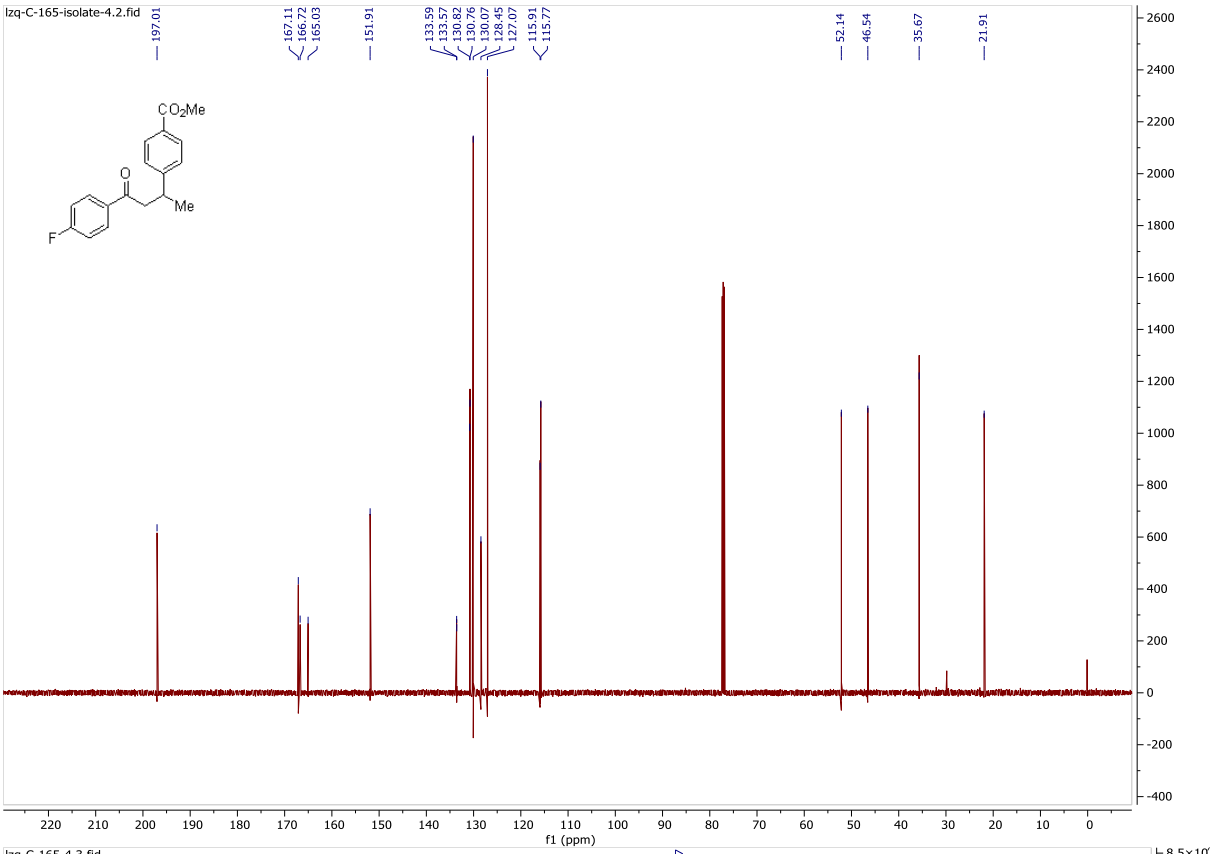

lzq-D-302-B4.1.fid
O
O
Me
MeO
2.08
0.97
0.96
2.06
0.98
3.10
1.00
2.05
3.42
f1 (ppm)

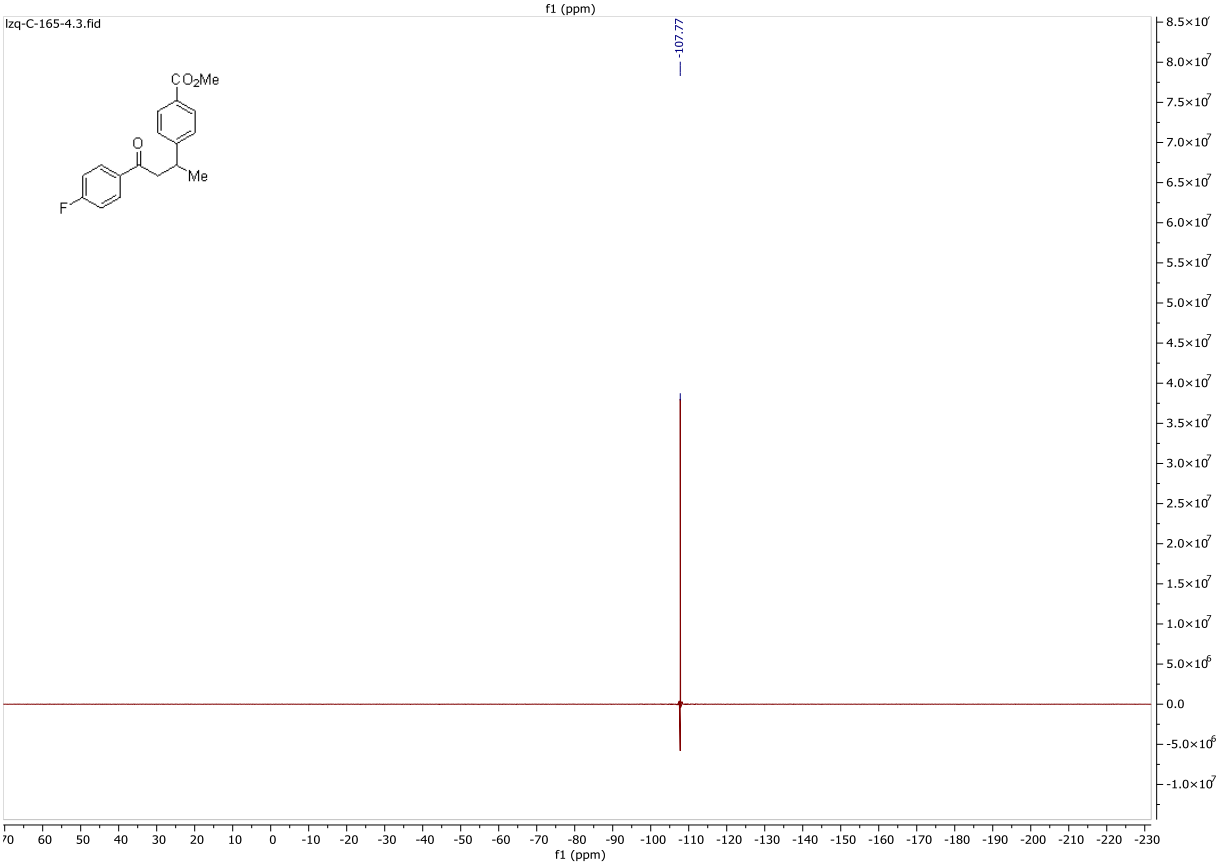

lzq-D-302-B4.2.fid
197.76
163.58
142.98
138.20
130.49
130.46
130.36
113.85
109.70
55.60
46.21
26.60
21.20
MeO
Me
f1 (ppm)

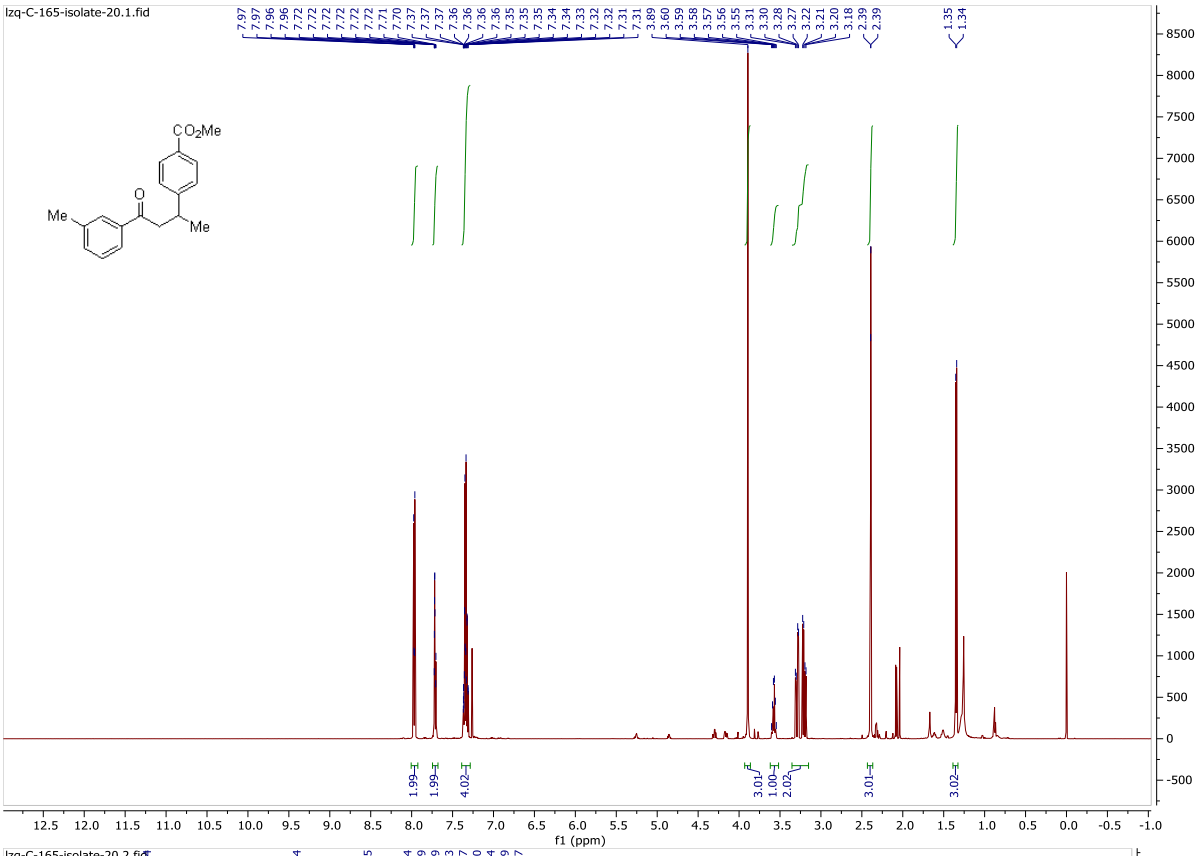

lzq-C-165-isolate-2.1.fid
7.97
7.96
7.87
7.85
7.46
7.45
7.35
7.34
3.89
3.61
3.59
3.58
3.57
3.56
3.55
3.31
3.30
3.28
3.27
3.21
3.19
3.18
3.17
1.35
1.34
1.33
CO2Me
Me
t-Bu
2.02
1.94
1.94
1.97
2.98
1.00
2.00
2.71
8.20
f1 (ppm)

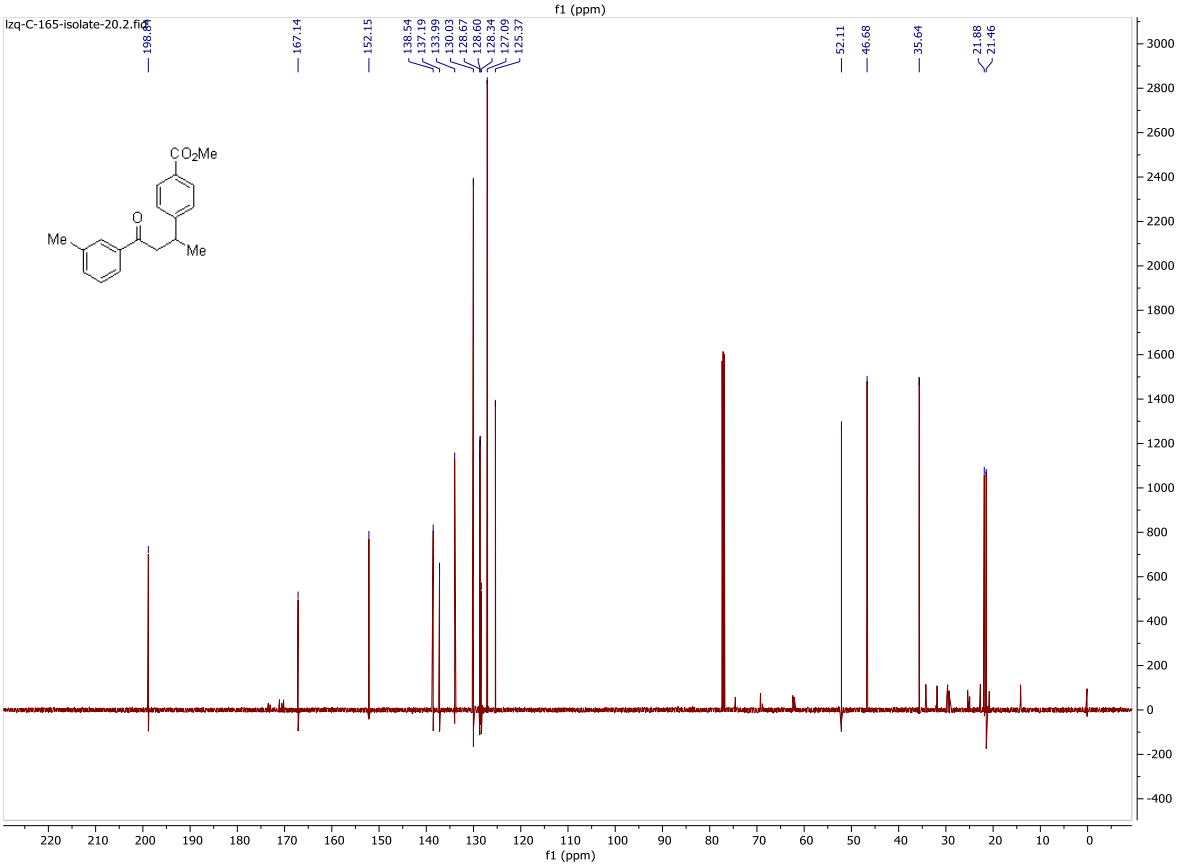

lzq-C-165-isolate-2.2.fid
198.29
167.15
157.00
152.21
134.60
134.60
130.03
128.32
128.14
127.09
125.68
52.11
46.55
35.69
35.22
31.19
21.88
CO2Me
O
Me
t-Bu
f1 (ppm)

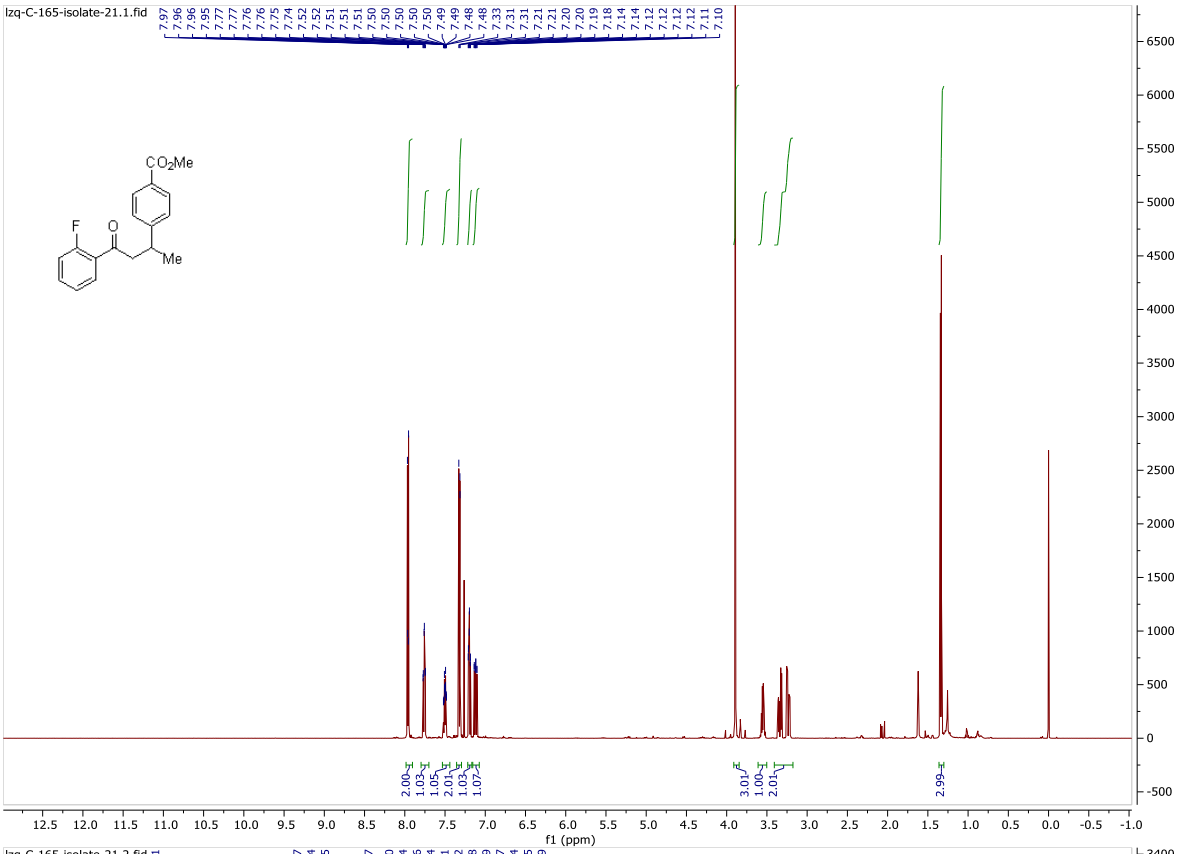

lzq-C-165-isolate-4.1.fid
7.98
7.97
7.96
7.96
7.95
7.94
7.94
7.94
7.93
7.34
7.34
7.33
7.12
7.11
7.11
7.09
3.90
3.59
3.58
3.57
3.56
3.55
3.54
3.30
3.29
3.27
3.26
3.20
3.19
3.18
3.16
1.36
1.35
CO2Me
O
Me
F
3.97
1.99
2.00
3.00
1.00
2.02
3.03
f1 (ppm)

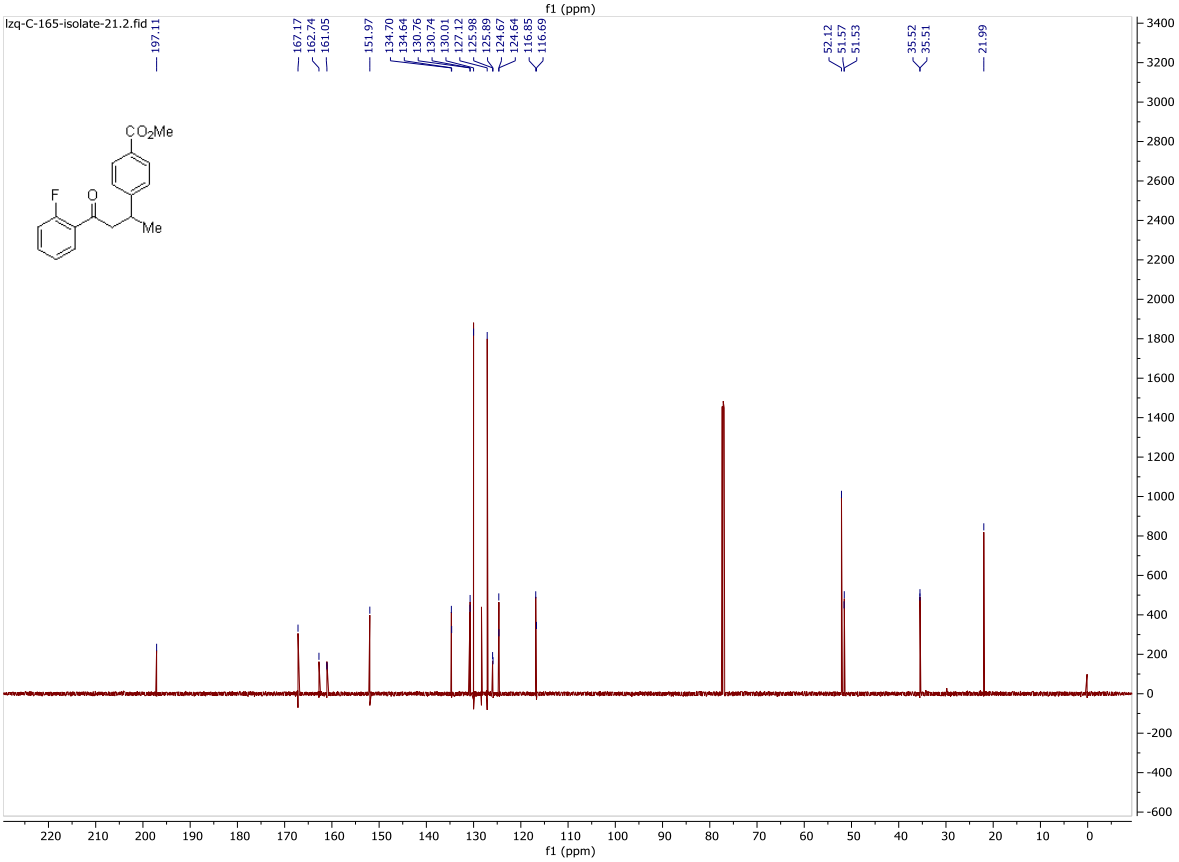

lzq-C-165-isolate-4.2.fid
197.01
167.11
166.72
165.03
151.91
133.59
133.57
130.82
130.76
130.07
128.45
127.07
115.91
115.77
52.14
46.54
35.67
21.91
CO2Me
O
Me
F
f1 (ppm)

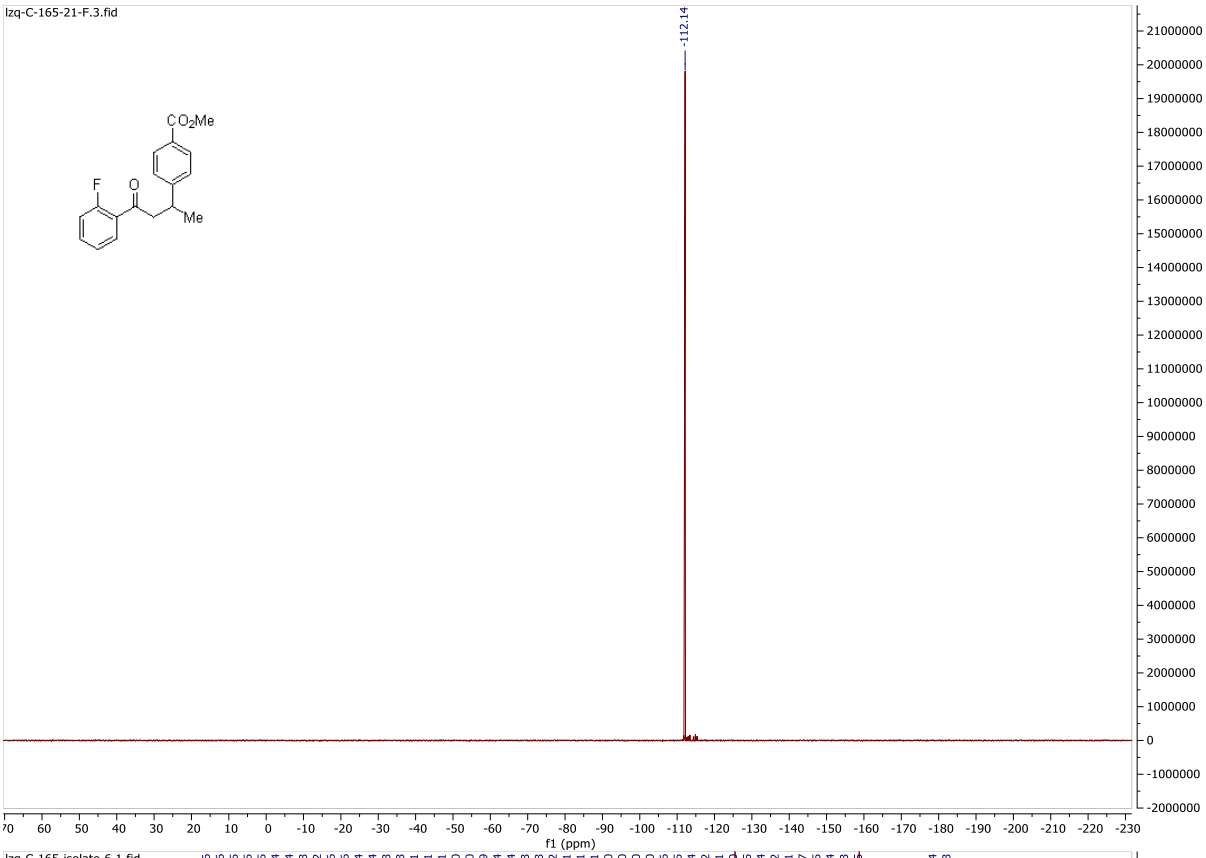

lzq-C-165-4.3.fid
-107.77
CO2Me
O
Me
F
f1 (ppm)

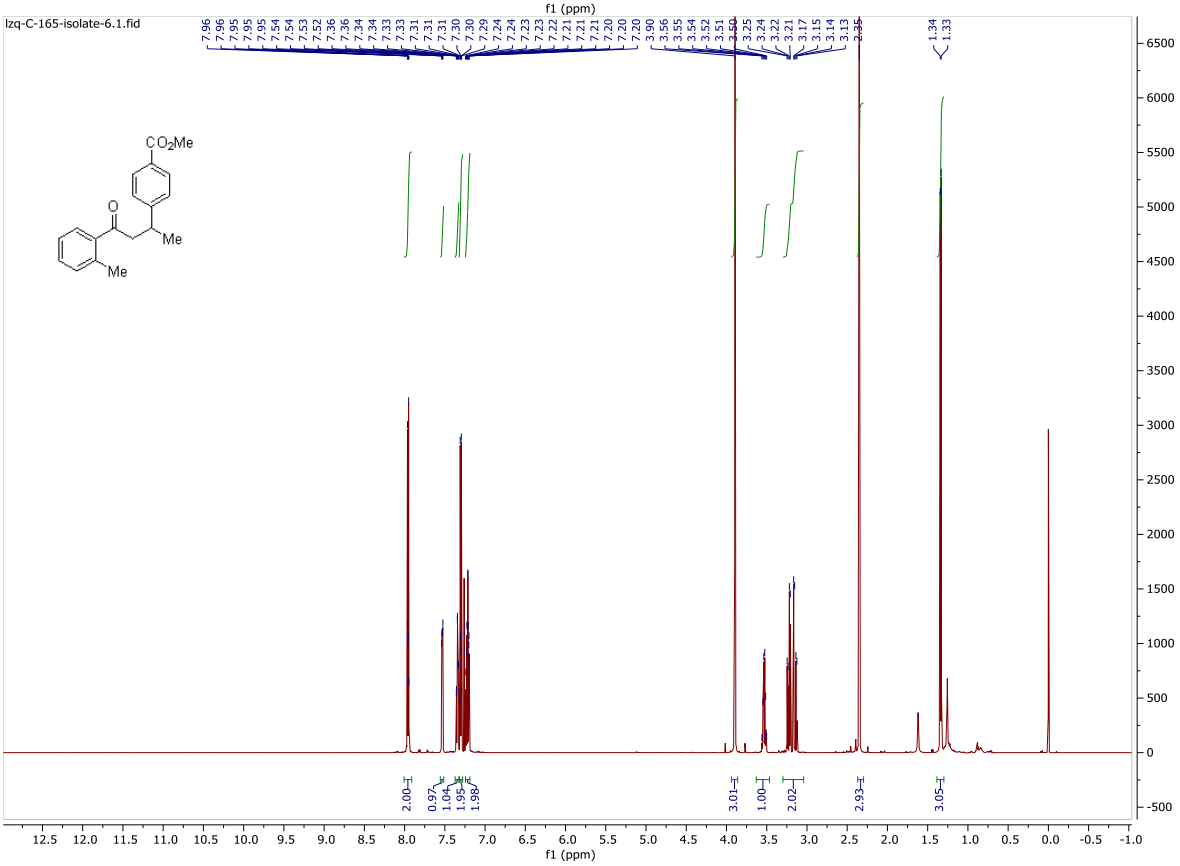

lzq-C-165-isolate-20.1.fid
CO2Me
O
Me
Me
f1 (ppm)

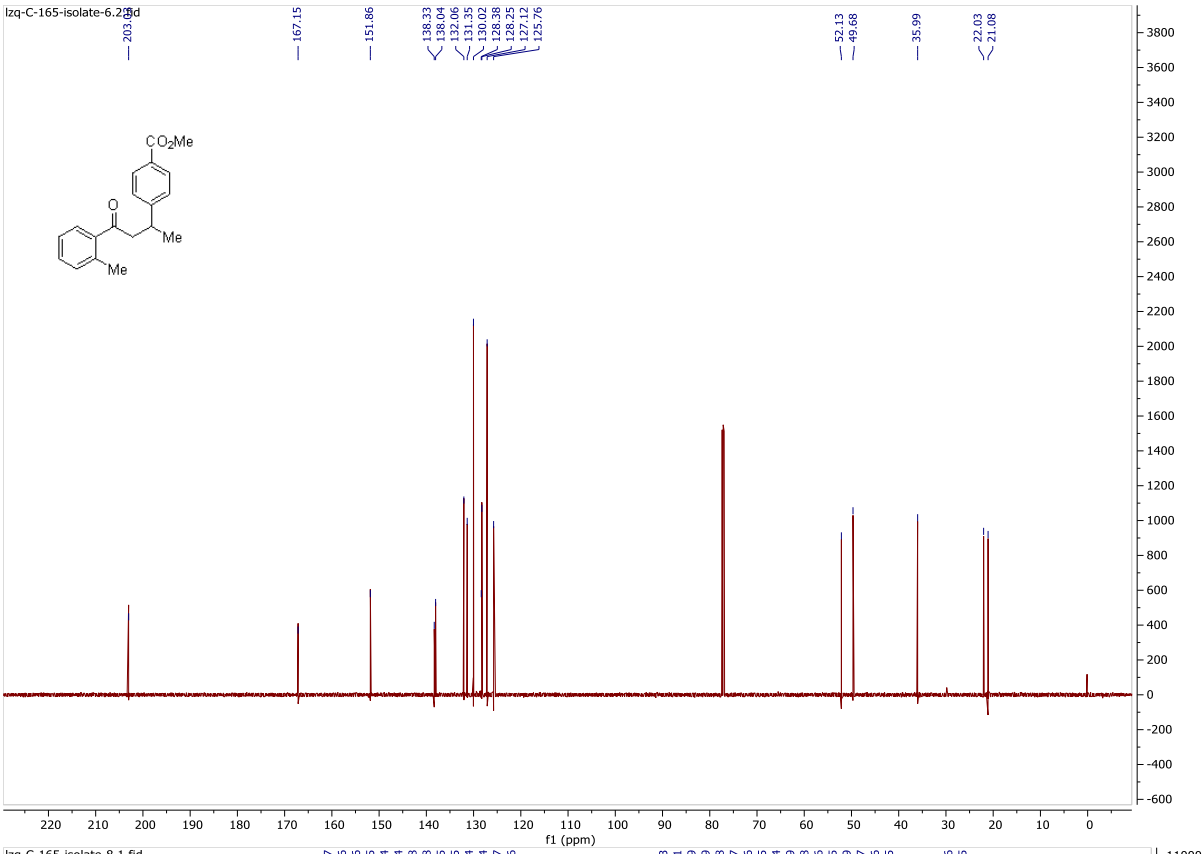

lzq-C-165-isolate-20.2.fid
CO2Me
O
Me
Me
f1 (ppm)

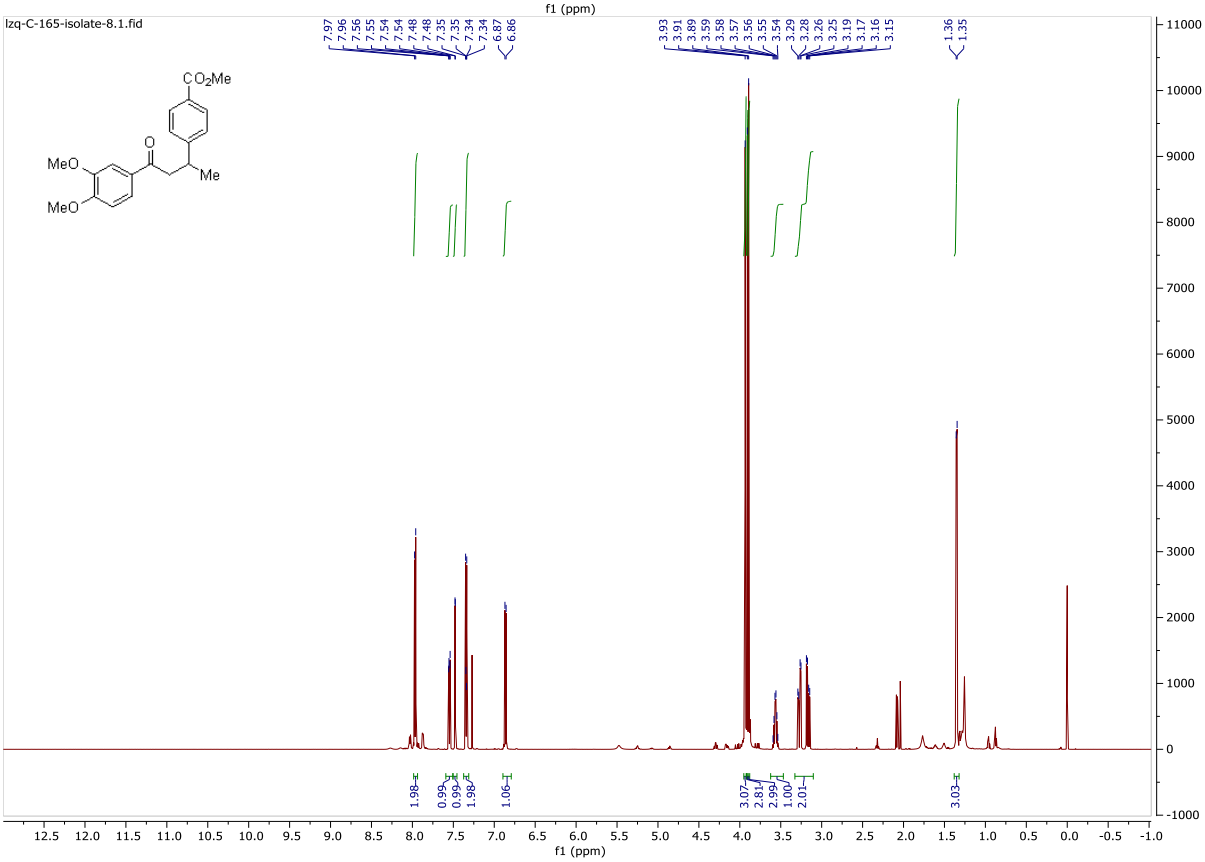

lzq-C-165-isolate-21.1.fid
CO2Me
F
O
Me
f1 (ppm)

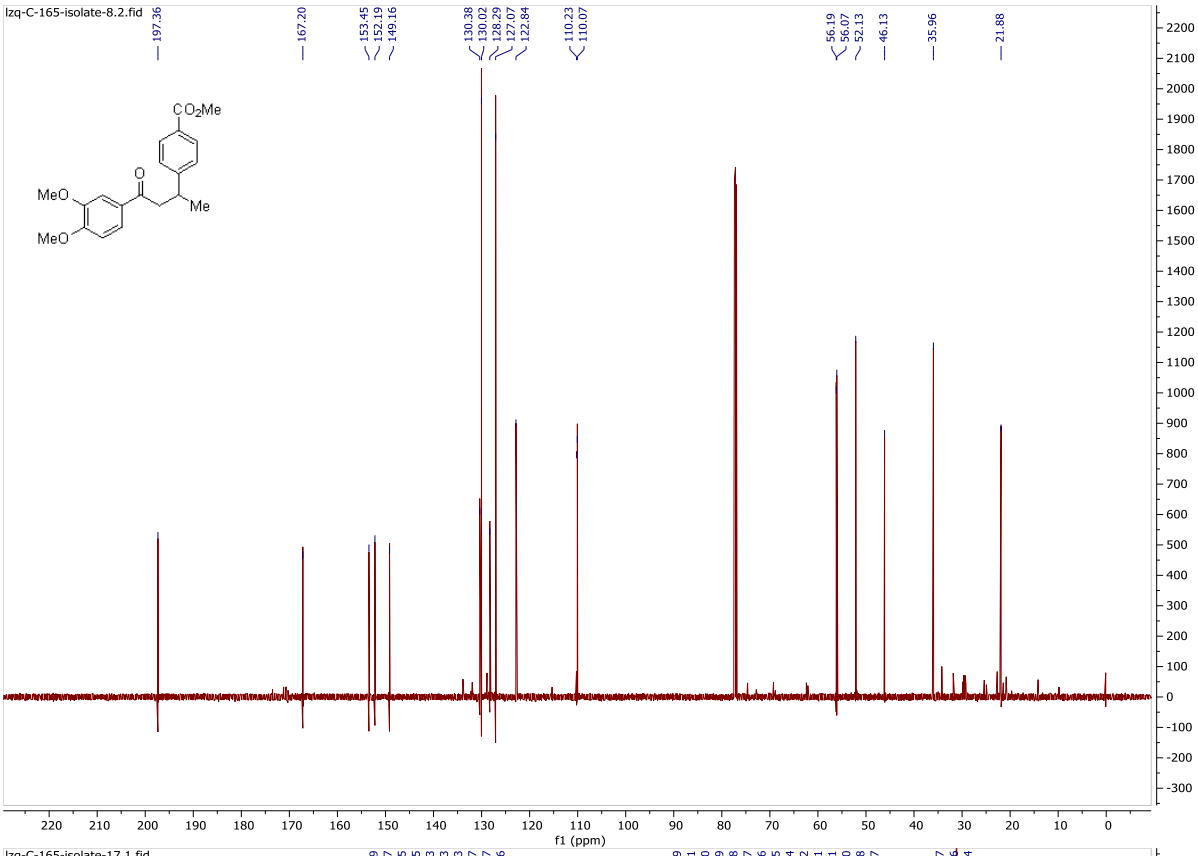

lzq-C-165-isolate-21.2.fid
CO2Me
F
O
Me
f1 (ppm)

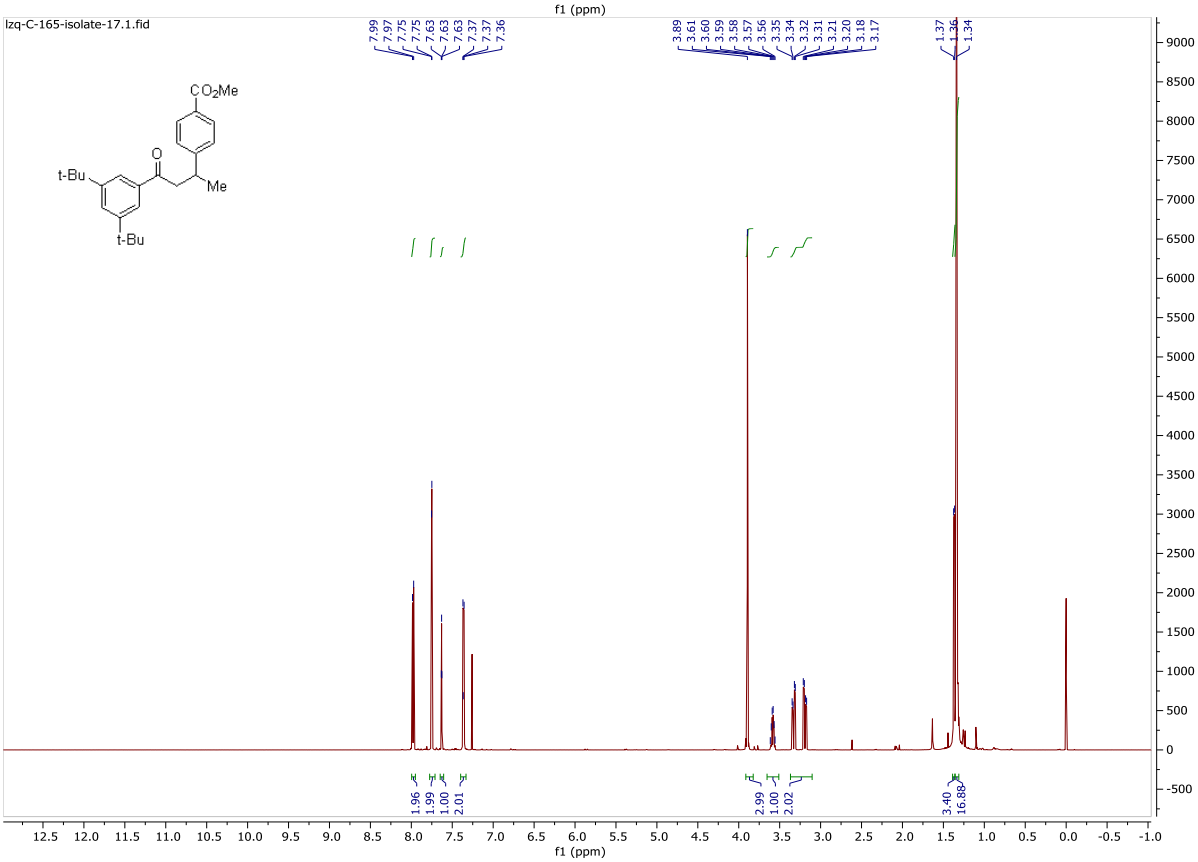

lzq-C-165-21-F.3.fid
-112.14
CO2Me
F
O
Me
f1 (ppm)

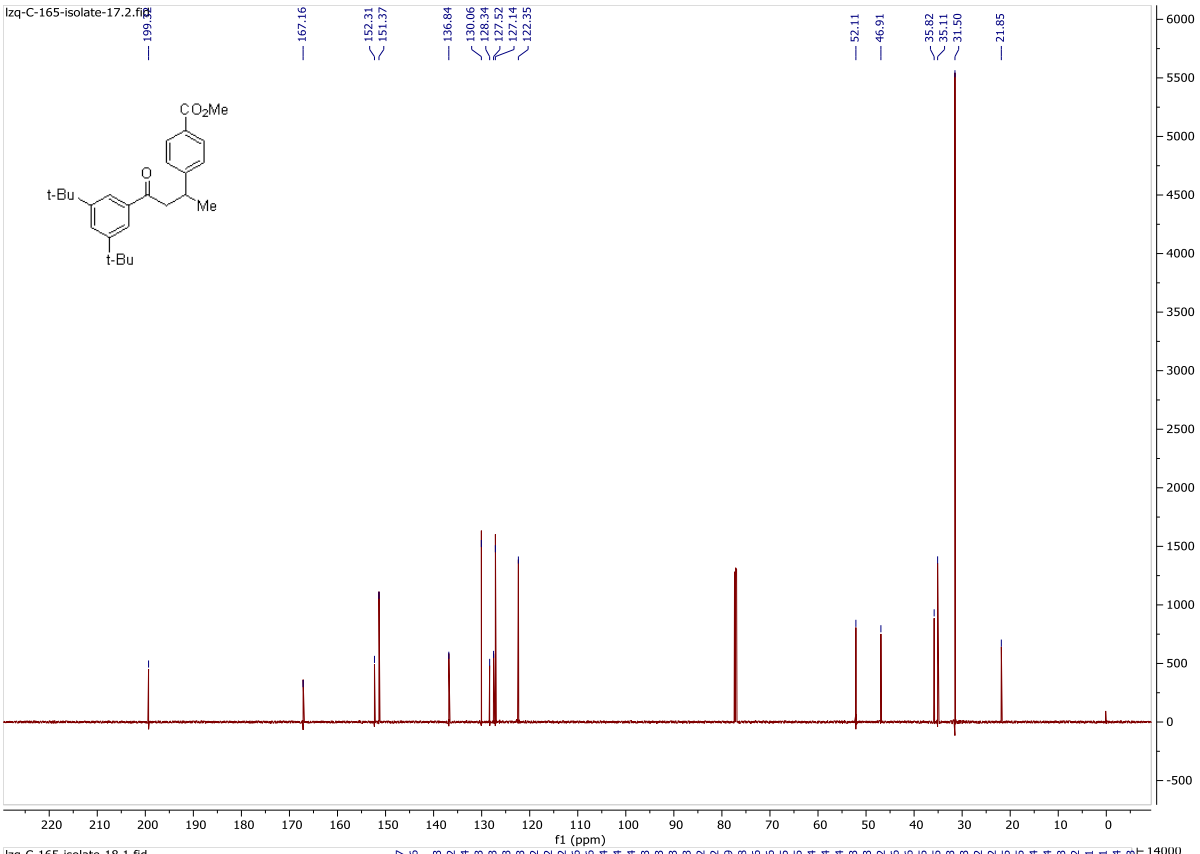

lzq-C-165-isolate-6.1.fid
CO2Me
O
Me
Me
2.00
0.97
1.04
1.95
1.98
3.01
1.00
2.02
2.93
3.05
f1 (ppm)

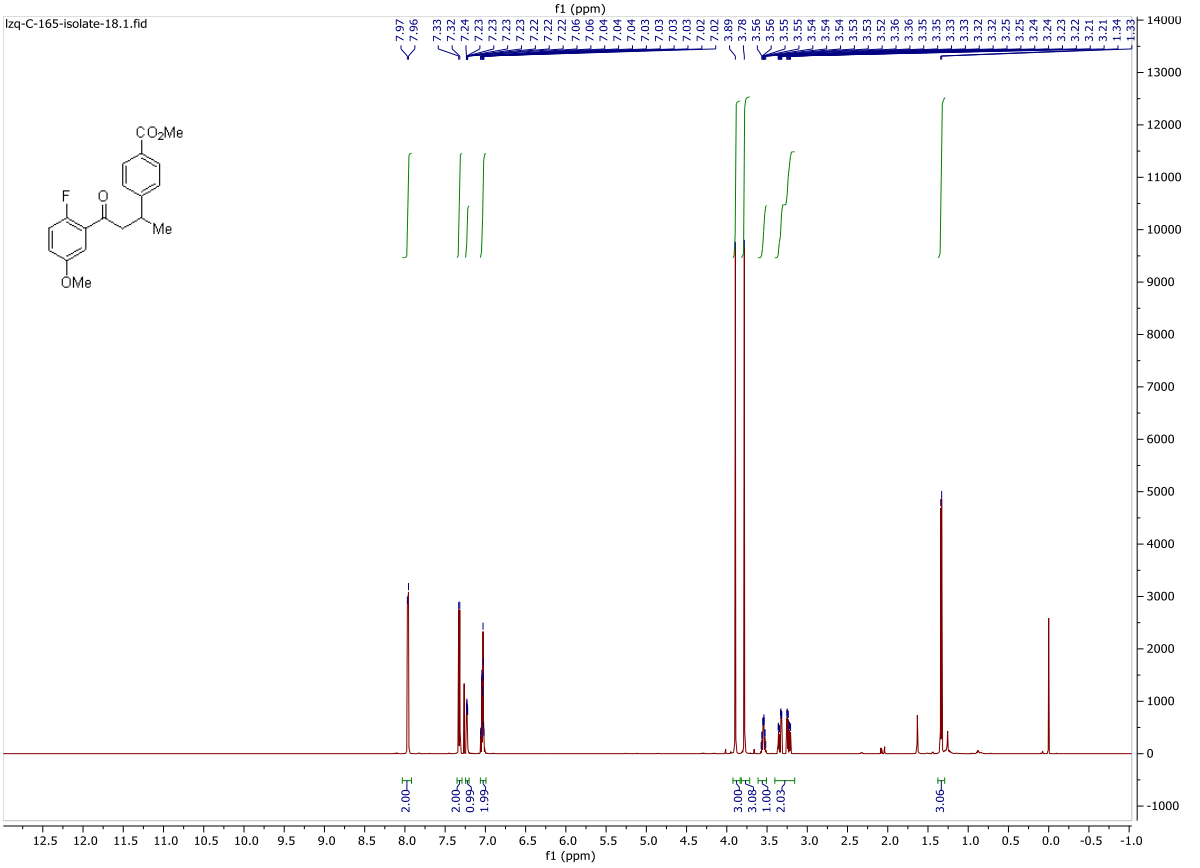

lzq-C-165-isolate-6.2.fid
203.05
167.15
151.86
138.33
138.04
132.06
131.35
130.02
128.38
128.25
127.12
125.76
52.13
49.68
35.99
22.03
21.08
CO2Me
O
Me
Me
f1 (ppm)

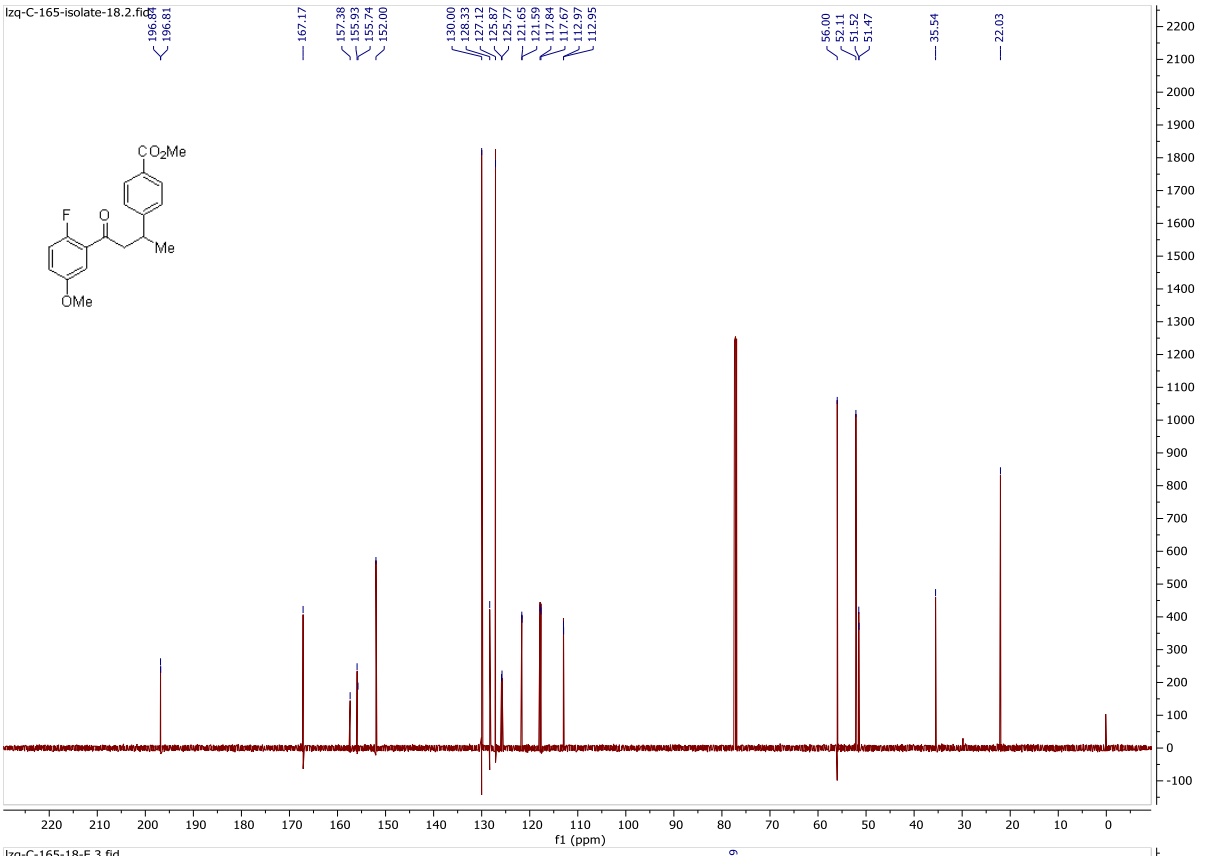

lzq-C-165-isolate-8.1.fid
7.97
7.96
7.56
7.55
7.54
7.54
7.48
7.48
7.35
7.35
7.34
7.34
6.87
6.86
3.93
3.91
3.89
3.59
3.58
3.57
3.56
3.55
3.54
3.29
3.28
3.26
3.25
3.19
3.17
3.16
3.15
1.36
1.35
CO2Me
O
MeO
MeO
Me
1.96
0.99
0.99
1.98
1.06
3.07
2.81
2.99
1.00
2.01
3.03
f1 (ppm)

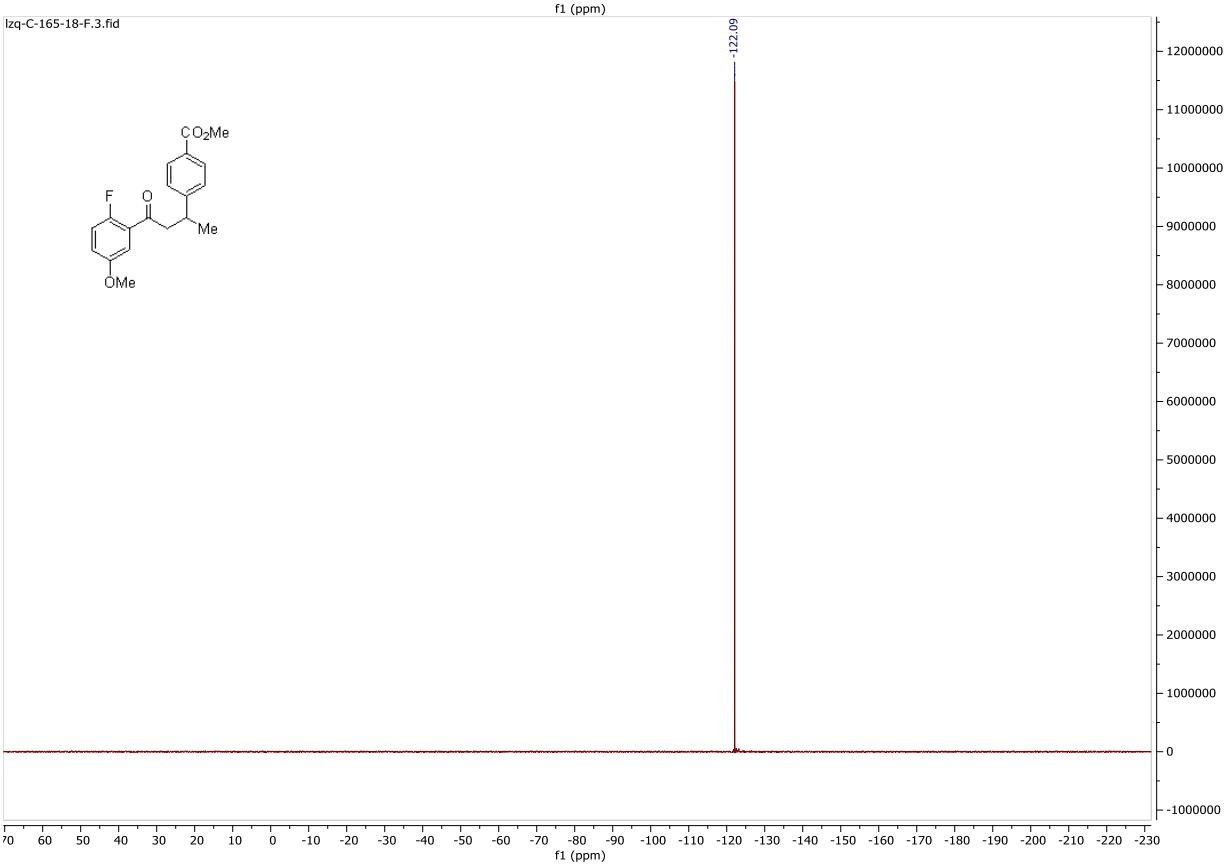

lzq-C-165-isolate-8.2.fid
197.36
167.20
153.45
152.19
149.16
130.38
130.02
128.29
127.07
122.84
110.23
110.07
56.19
56.07
52.13
46.13
35.96
21.88
CO2Me
O
MeO
MeO
Me
f1 (ppm)

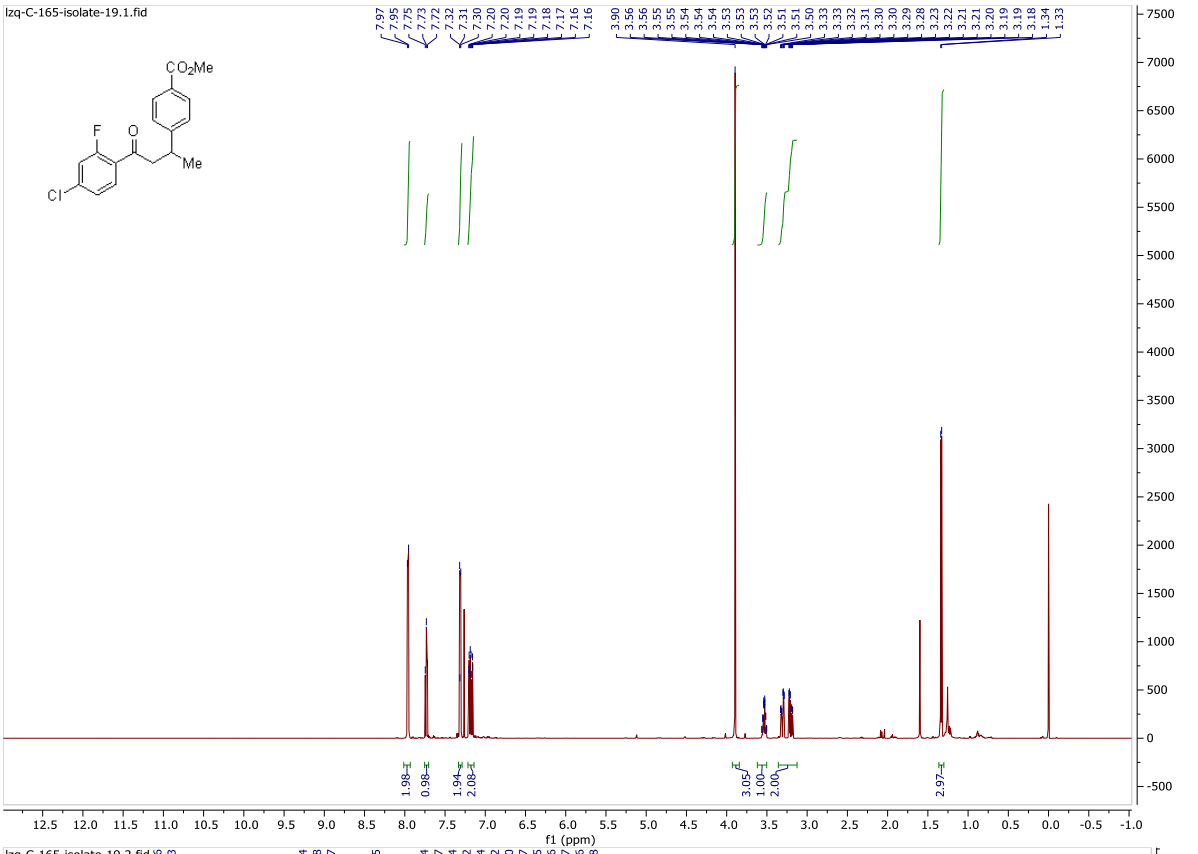

lzq-C-165-isolate-17.1.fid
7.99
7.97
7.75
7.75
7.63
7.63
7.63
7.37
7.37
7.36
3.89
3.61
3.60
3.59
3.58
3.57
3.56
3.35
3.34
3.32
3.31
3.21
3.20
3.18
3.17
1.37
1.36
1.34
CO2Me
O
t-Bu
t-Bu
Me
1.96
1.99
1.00
2.01
2.99
1.00
2.02
3.40
16.88
f1 (ppm)

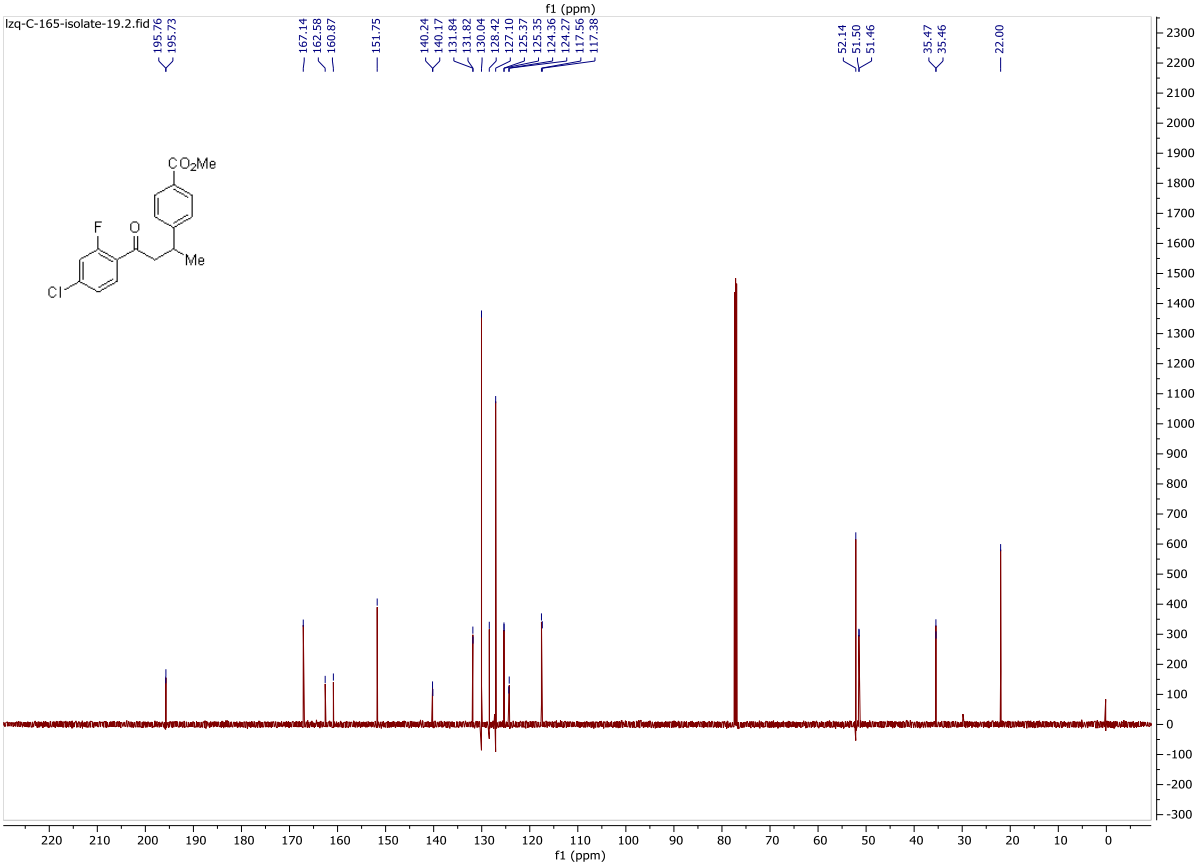

lzq-C-165-isolate-17.2.fid
199.32
167.16
152.31
151.37
136.84
130.06
128.34
127.52
127.14
122.35
52.11
46.91
35.82
35.11
31.50
21.85
CO2Me
O
t-Bu
Me
t-Bu
f1 (ppm)

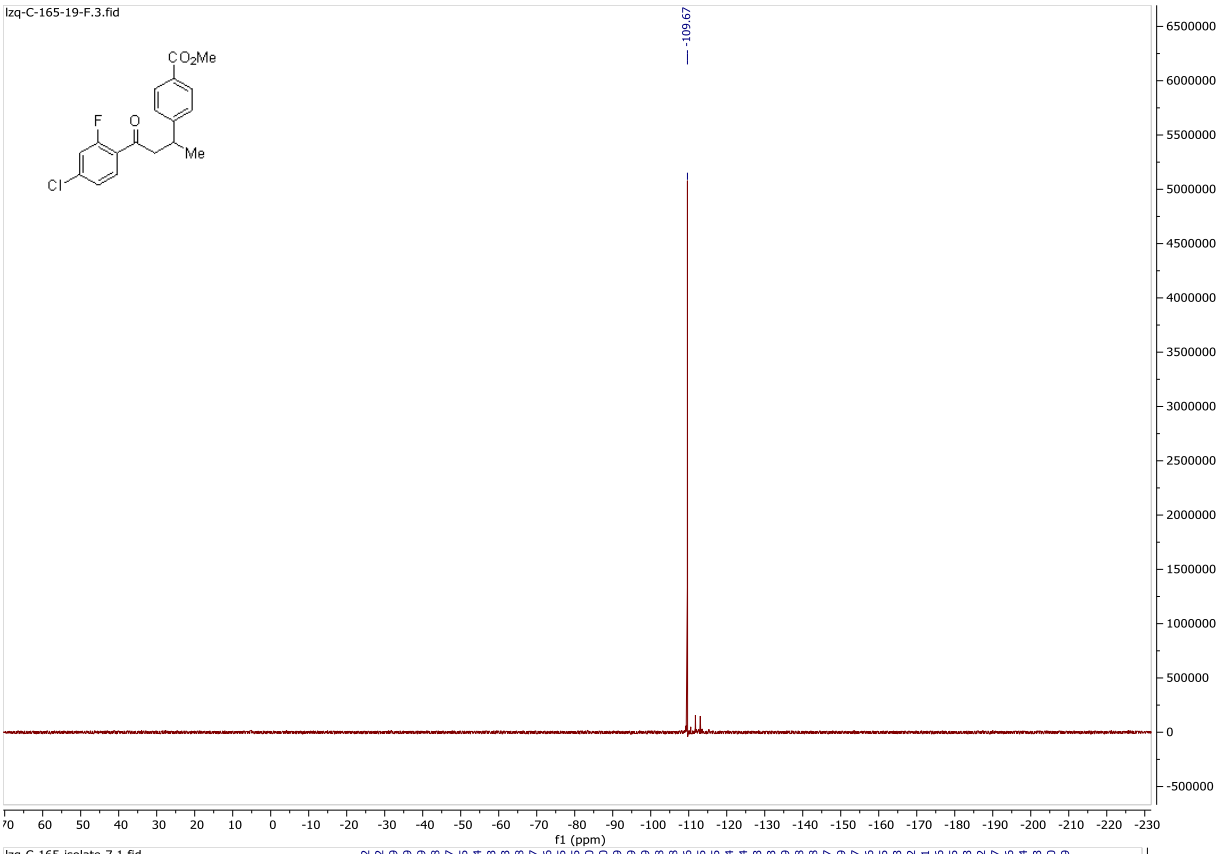

lzq-C-165-isolate-18.1.fid
7.97
7.96
7.33
7.32
7.24
7.23
3.89
3.78
3.56
3.55
3.54
3.53
3.52
3.36
3.35
3.33
3.32
3.25
1.34
1.33
CO2Me
F
O
Me
OMe
2.00
2.00
0.99
1.99
3.00
3.08
1.00
2.03
3.06
f1 (ppm)

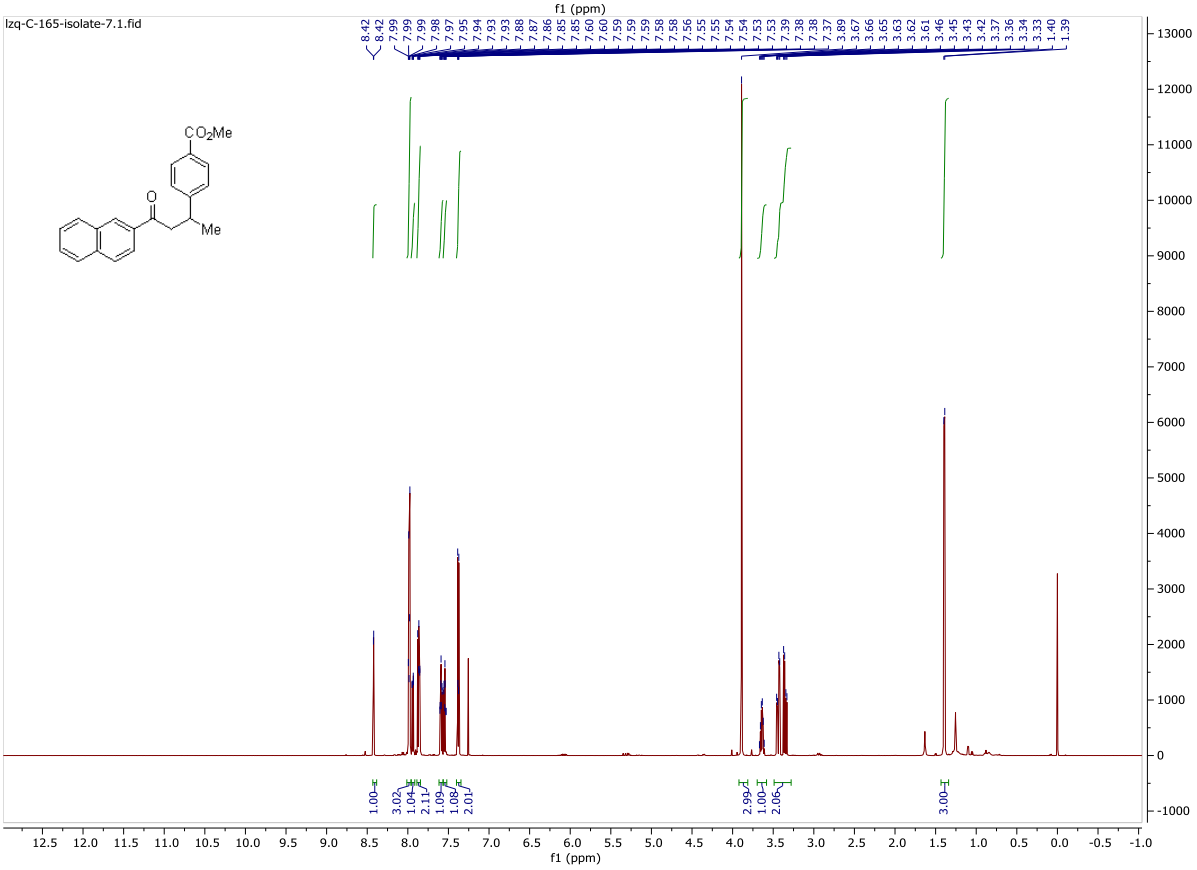

lzq-C-165-isolate-18.2.fid
196.84
196.81
167.17
157.38
155.93
155.74
152.00
130.00
128.33
127.12
125.87
125.77
121.65
121.59
117.84
117.67
112.97
112.95
56.00
52.11
51.52
51.47
35.54
22.03
CO2Me
F
O
Me
OMe
f1 (ppm)

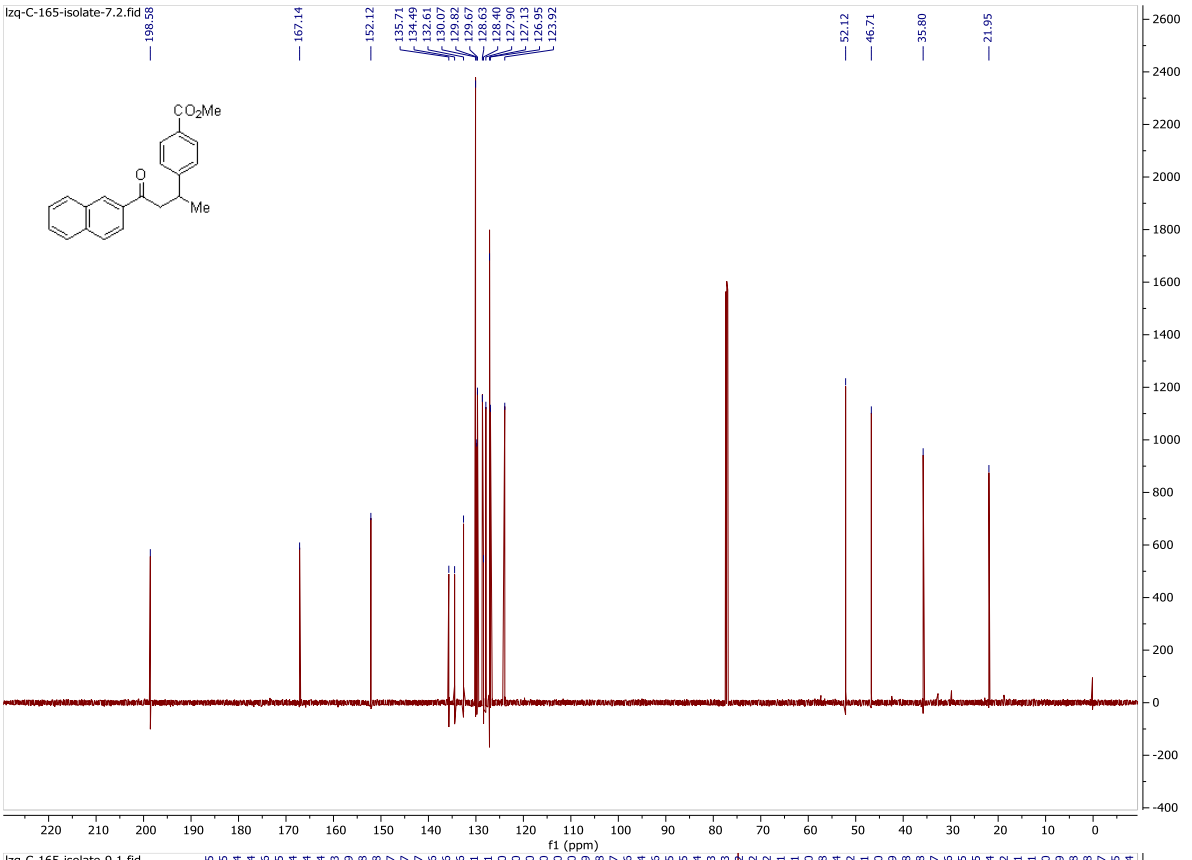

lzq-C-165-18-F.3.fid
-122.09
CO2Me
F
O
Me
OMe
f1 (ppm)

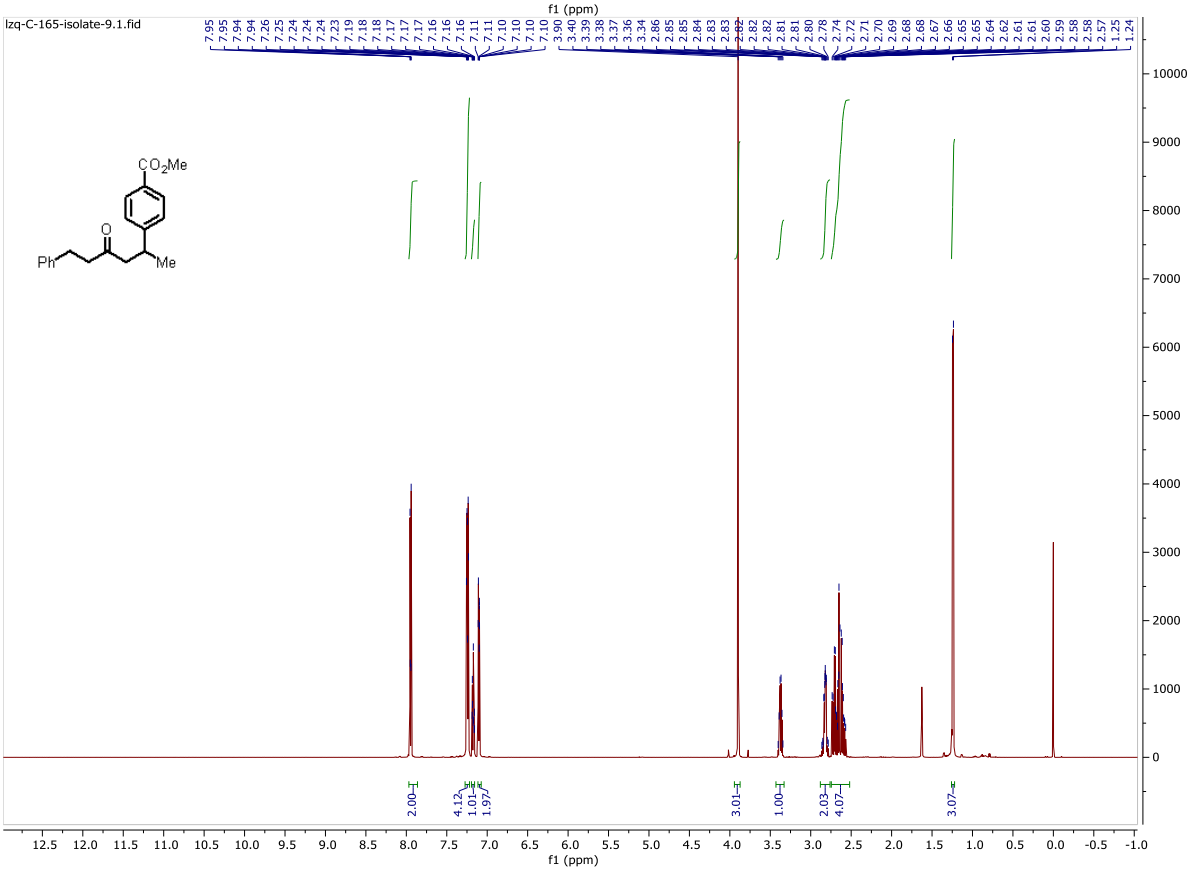

lzq-C-165-isolate-19.1.fid
CO2Me
F
O
Me
Cl
f1 (ppm)

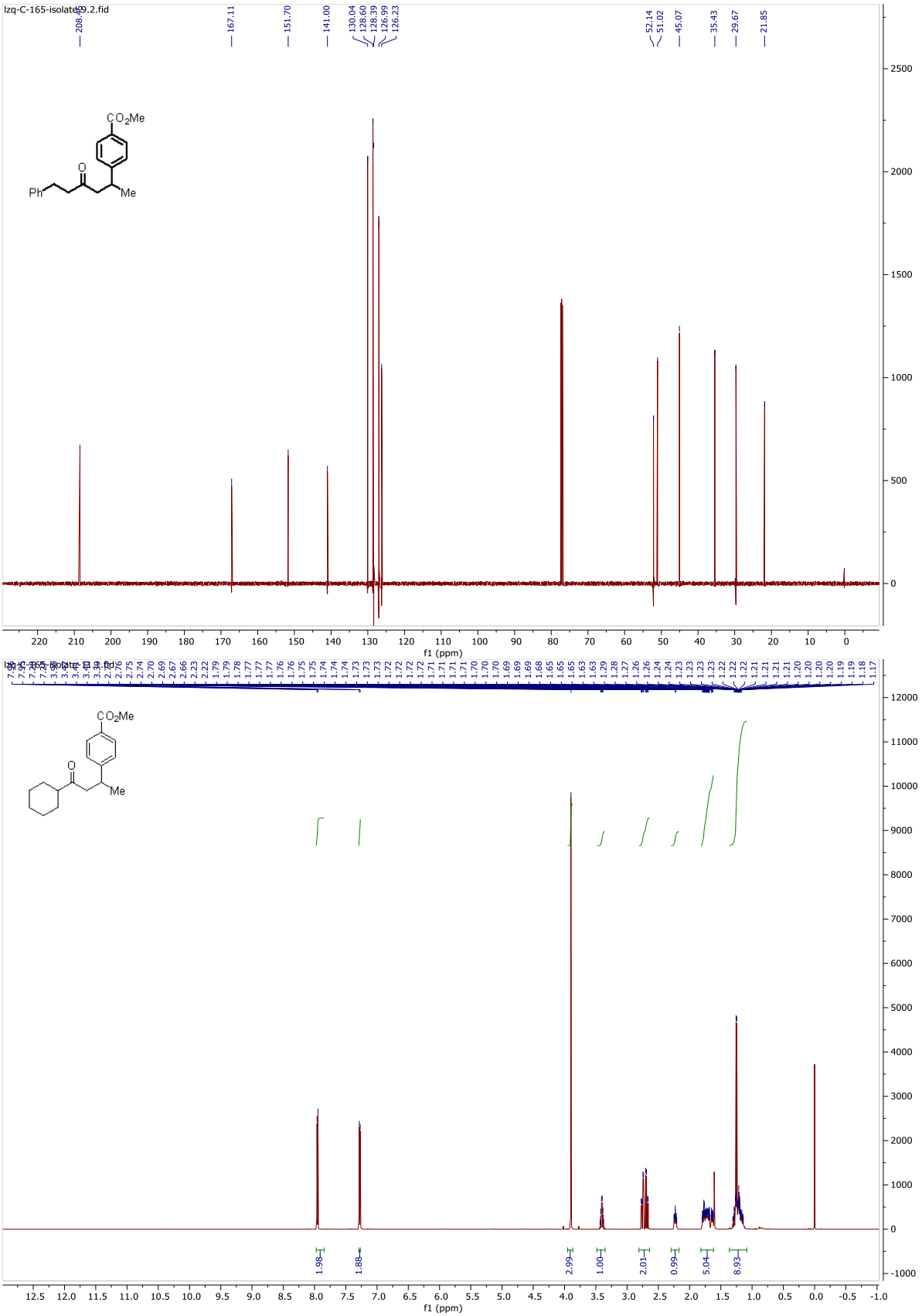

lzq-C-165-isolate-19.2.fid
CO2Me
F
O
Me
Cl
f1 (ppm)

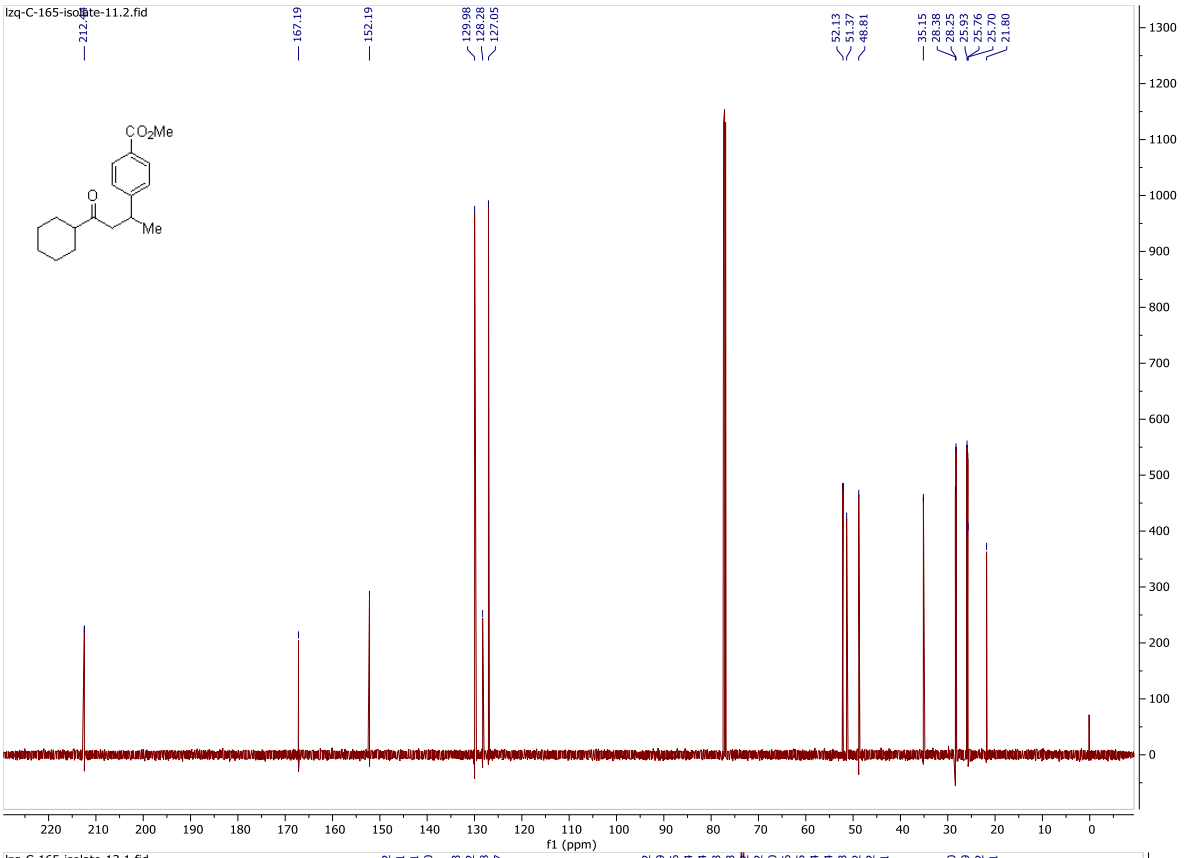

lzq-C-165-19-F.3.fid
-109.67
CO2Me
F
O
Me
Cl
f1 (ppm)

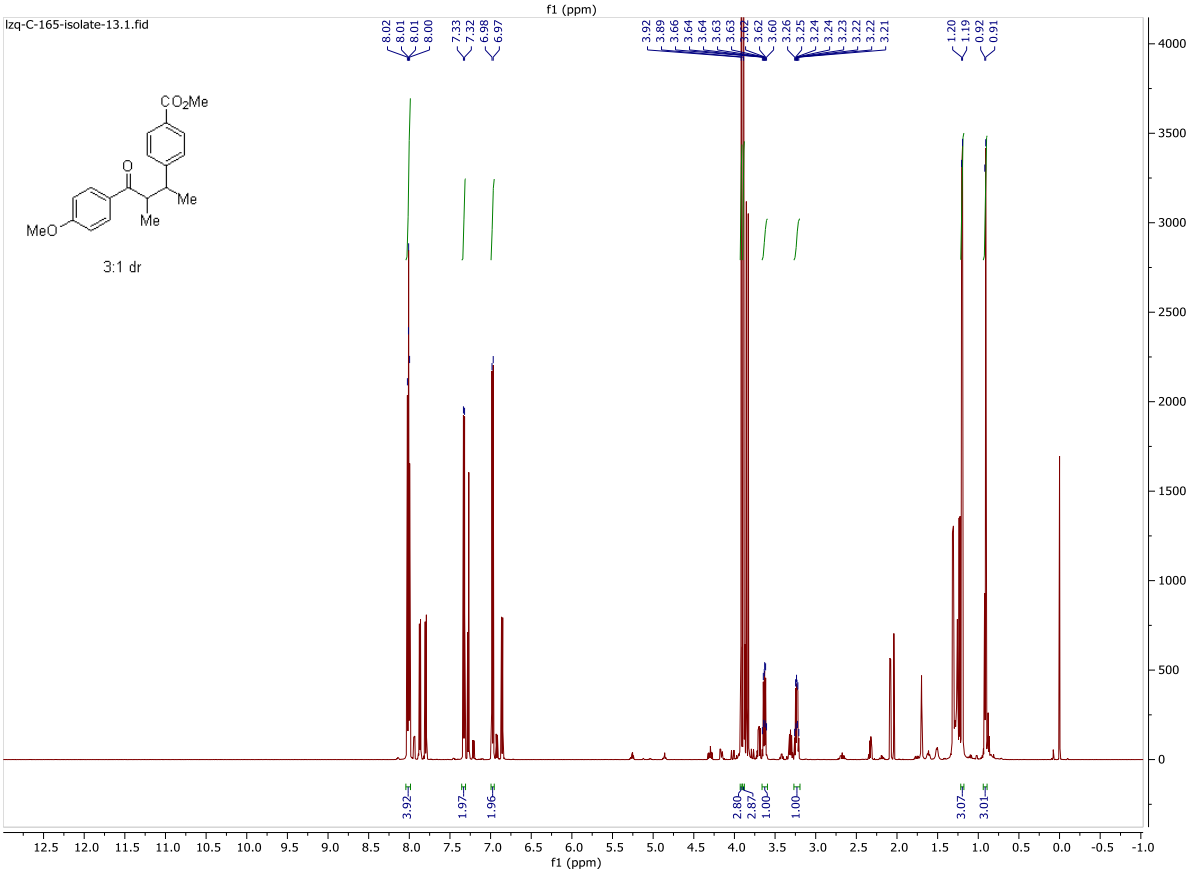

lzq-C-165-isolate-7.1.fid
CO2Me
O
Me
f1 (ppm)

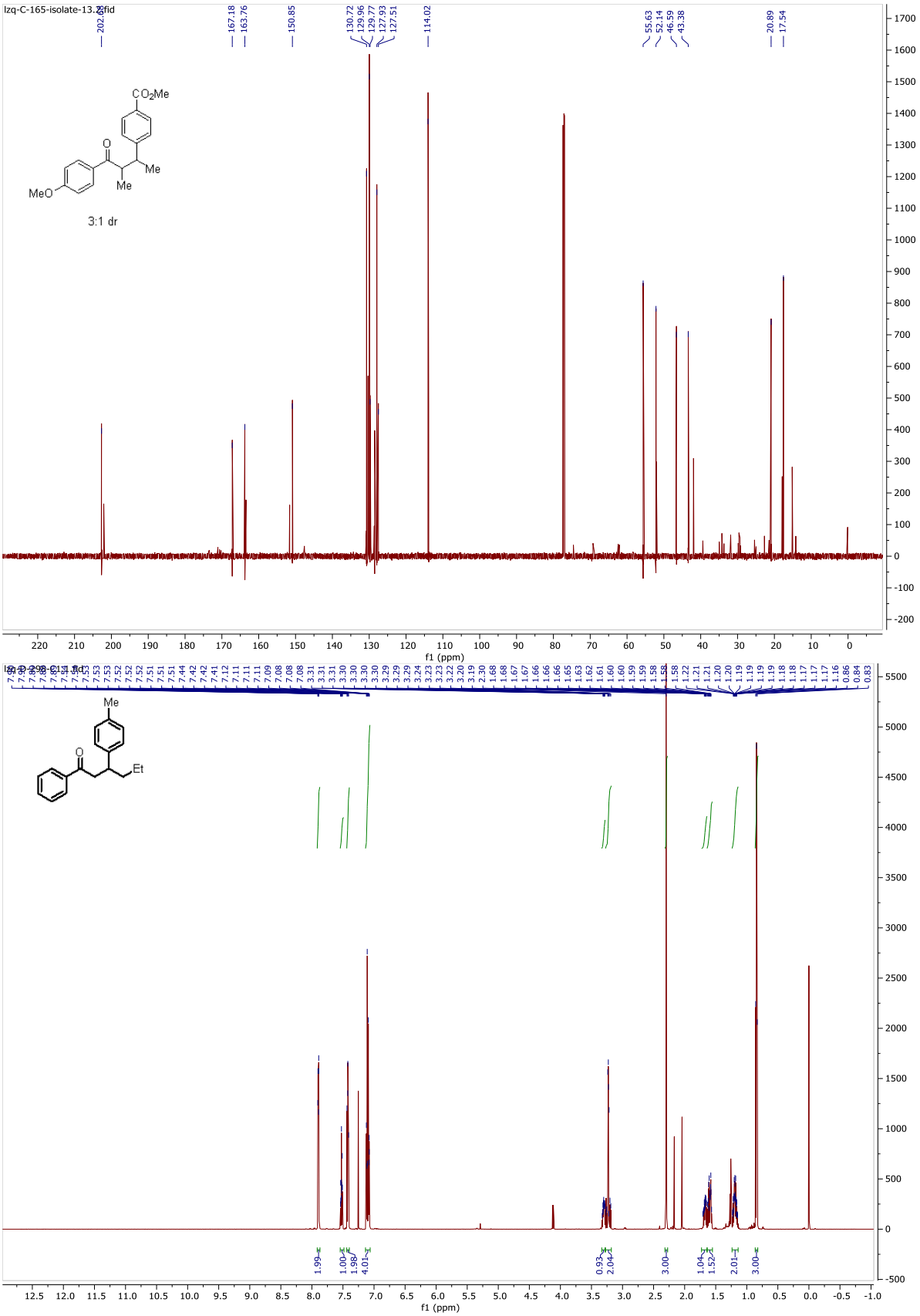

lzq-C-165-isolate-7.2.fid
198.58
167.14
152.12
135.71
134.49
132.61
130.07
129.82
129.67
128.63
128.40
127.90
127.13
126.95
123.92
52.12
46.71
35.80
21.95
CO2Me
O
Me
f1 (ppm)

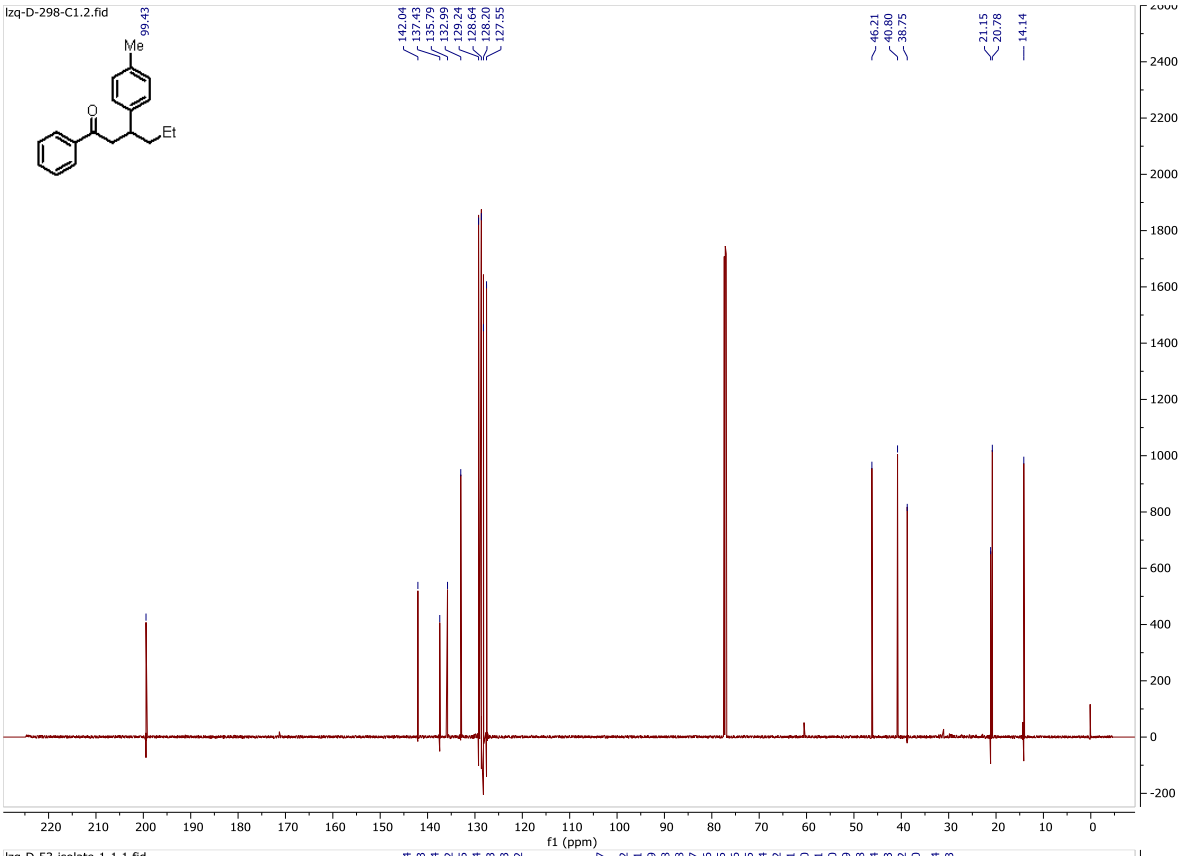

lzq-C-165-isolate-9.1.fid
CO2Me
O
Ph
Me
2.00
4.12
1.01
1.97
3.01
1.00
2.03
4.07
3.07
f1 (ppm)

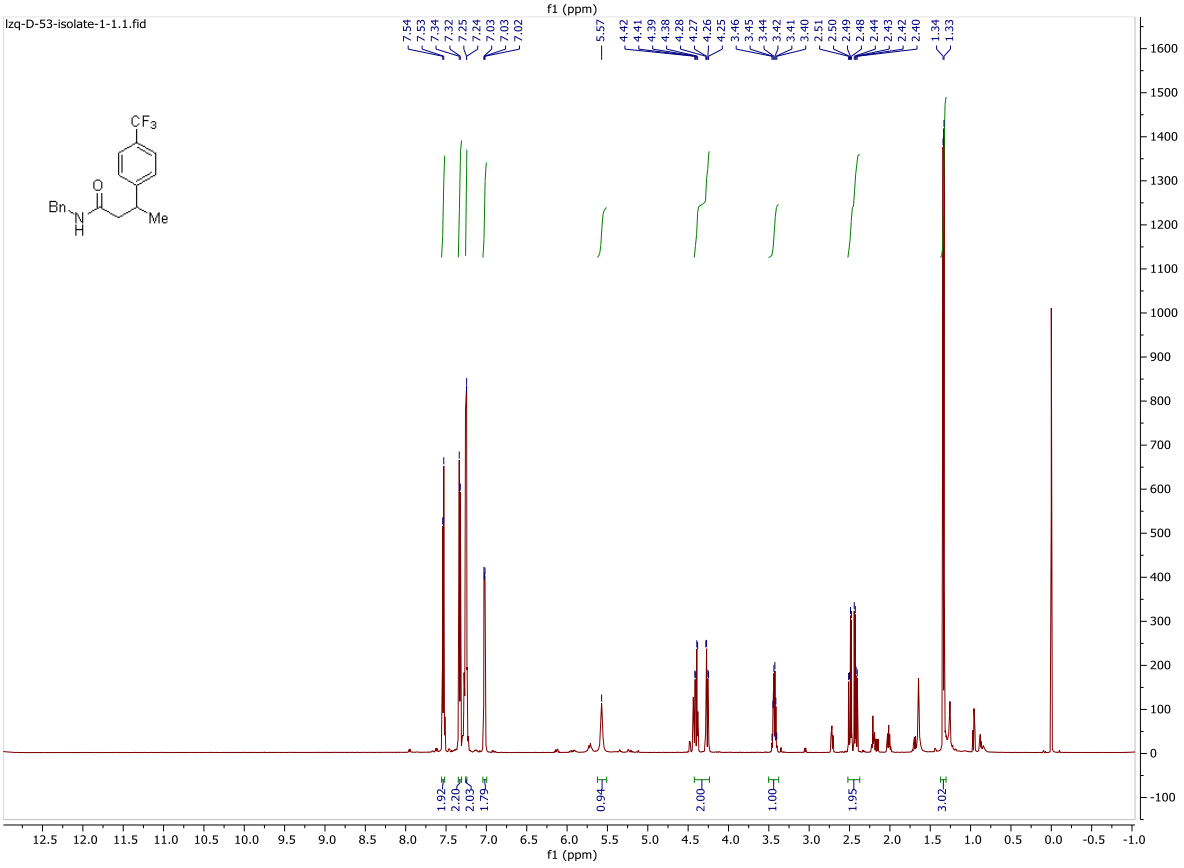

lzq-C-165-isolate-59.2.fid
208.45
167.11
151.70
141.00
130.04
128.60
128.39
126.99
126.23
52.14
51.02
45.07
35.43
29.67
21.85
CO2Me
O
Ph
Me
f1 (ppm)
CO2Me
O
Me
1.98
1.88
2.99
1.00
2.01
0.99
5.04
8.93
f1 (ppm)

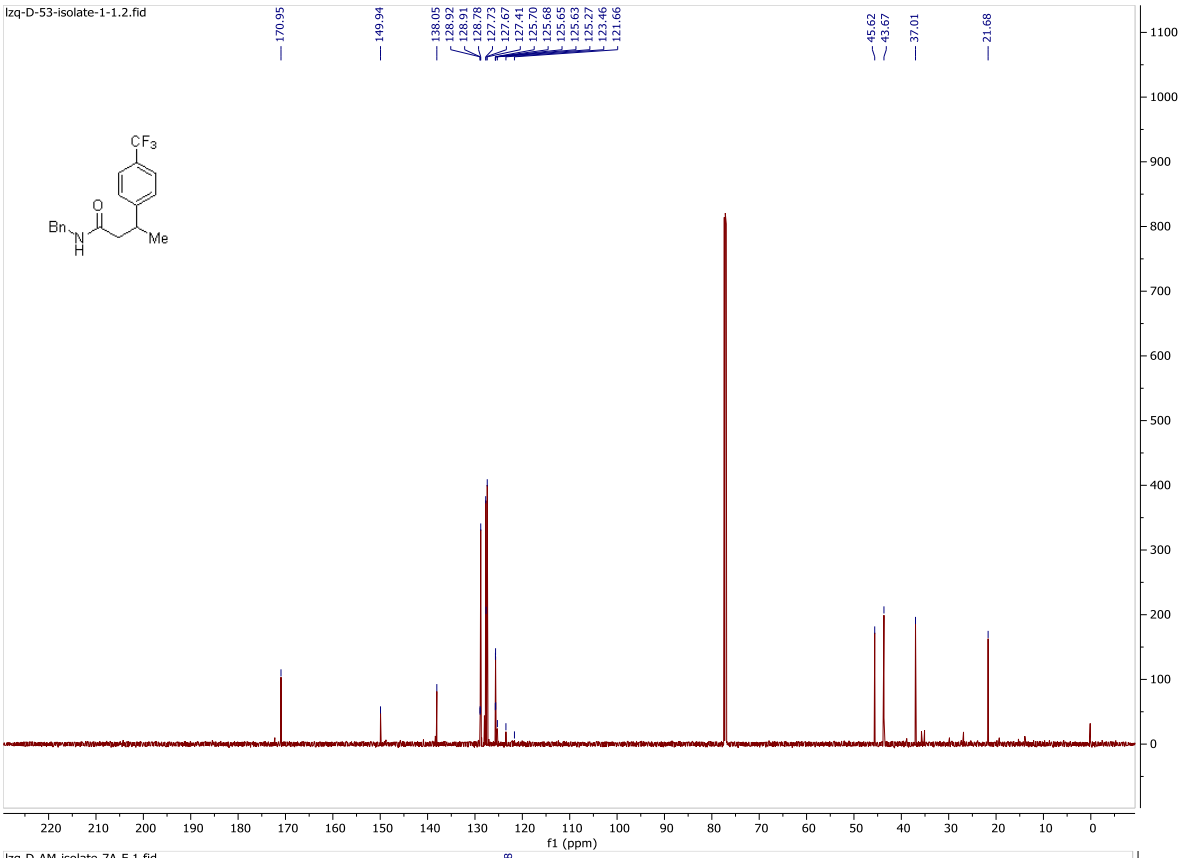

lzq-C-165-isolate-11.2.fid
212.73
167.19
152.19
129.98
128.28
127.05
52.13
51.37
48.81
35.15
28.38
28.25
25.93
25.76
25.70
21.80
CO2Me
O
Me
f1 (ppm)

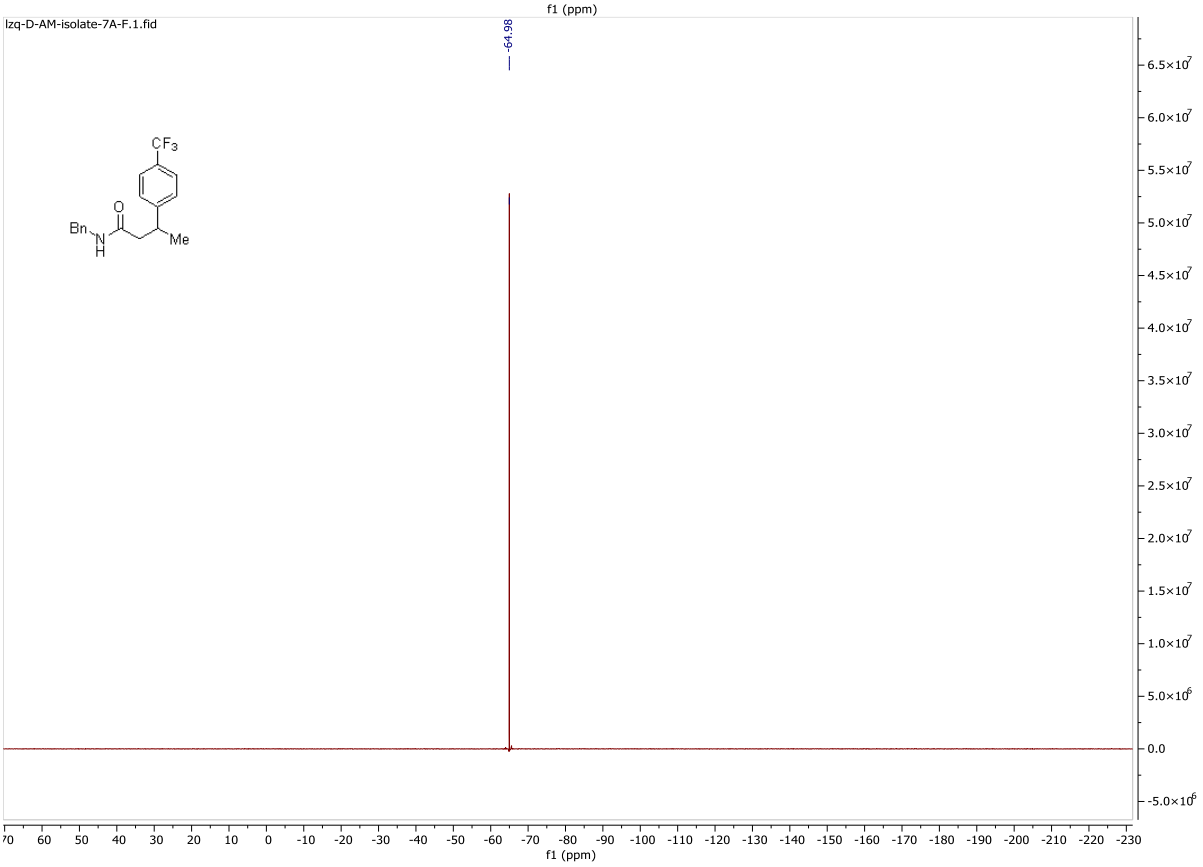

lzq-C-165-isolate-13.1.fid
8.02
8.01
8.01
8.00
7.33
7.32
6.98
6.97
3.92
3.89
3.66
3.64
3.64
3.63
3.63
3.62
3.60
3.26
3.25
3.24
3.24
3.23
3.22
3.22
3.21
1.20
1.19
0.92
0.91
CO2Me
O
Me
Me
MeO
3:1 dr
3.92
1.97
1.96
2.80
2.87
1.00
1.00
3.07
3.01
f1 (ppm)

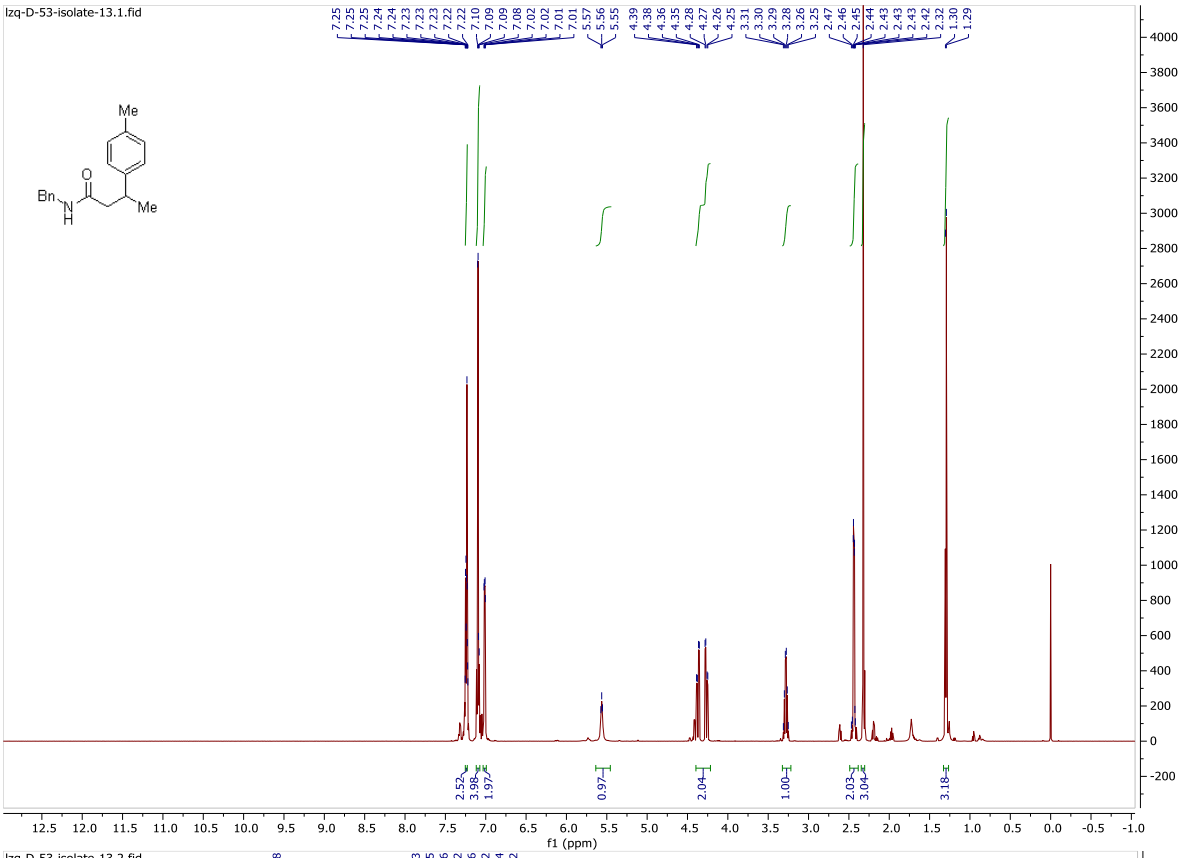

lzq-C-165-isolate-13.2.fid
202.48
167.18
163.76
150.85
130.72
129.96
129.77
127.93
127.51
114.02
55.63
52.14
46.59
43.38
20.89
17.54
CO2Me
O
Me
Me
MeO
3:1 dr
f1 (ppm)
Me
O
Et
1.99
1.00
1.98
4.01
0.93
2.04
3.00
1.04
1.52
2.01
3.00
f1 (ppm)

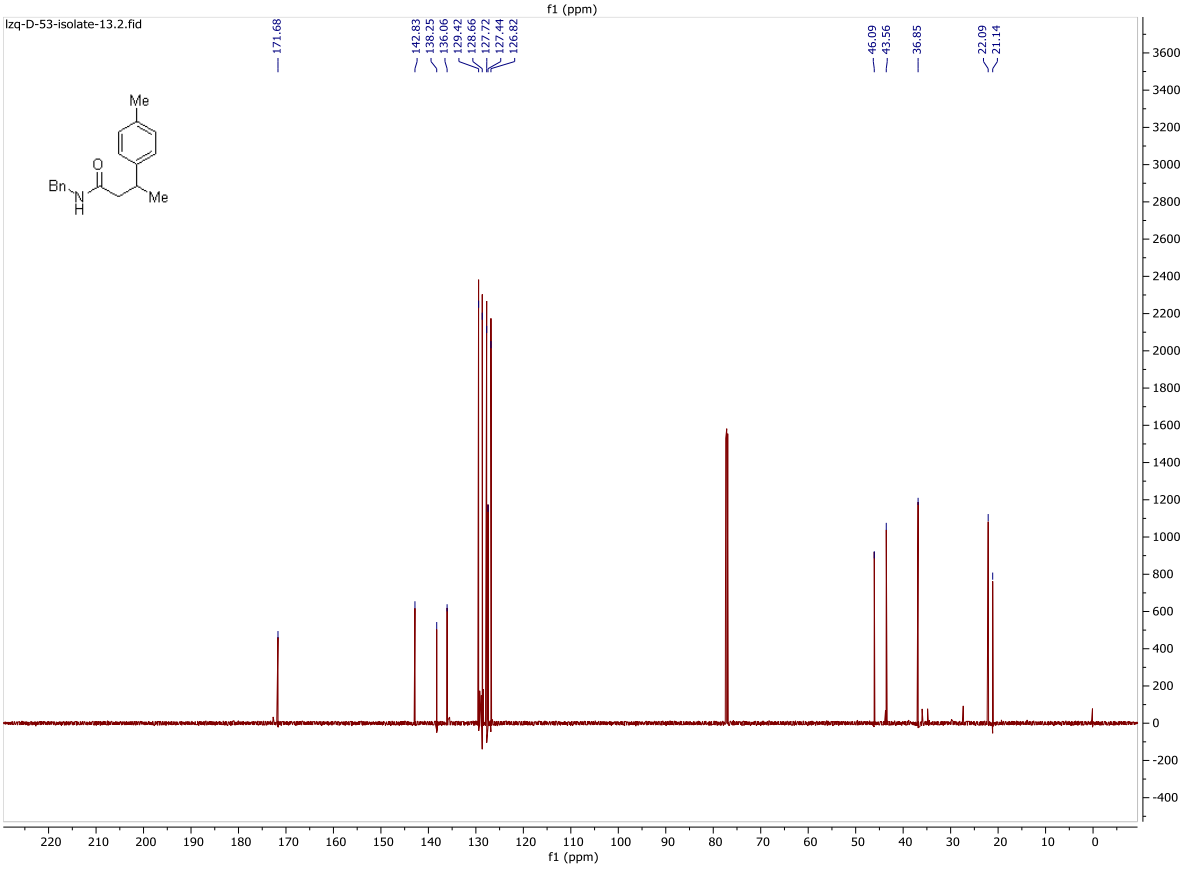

lzq-D-298-C1.2.fid
99.43
142.04
137.43
135.79
132.99
129.24
128.64
128.20
127.55
46.21
40.80
38.75
21.15
20.78
14.14
Me
O
Et
f1 (ppm)

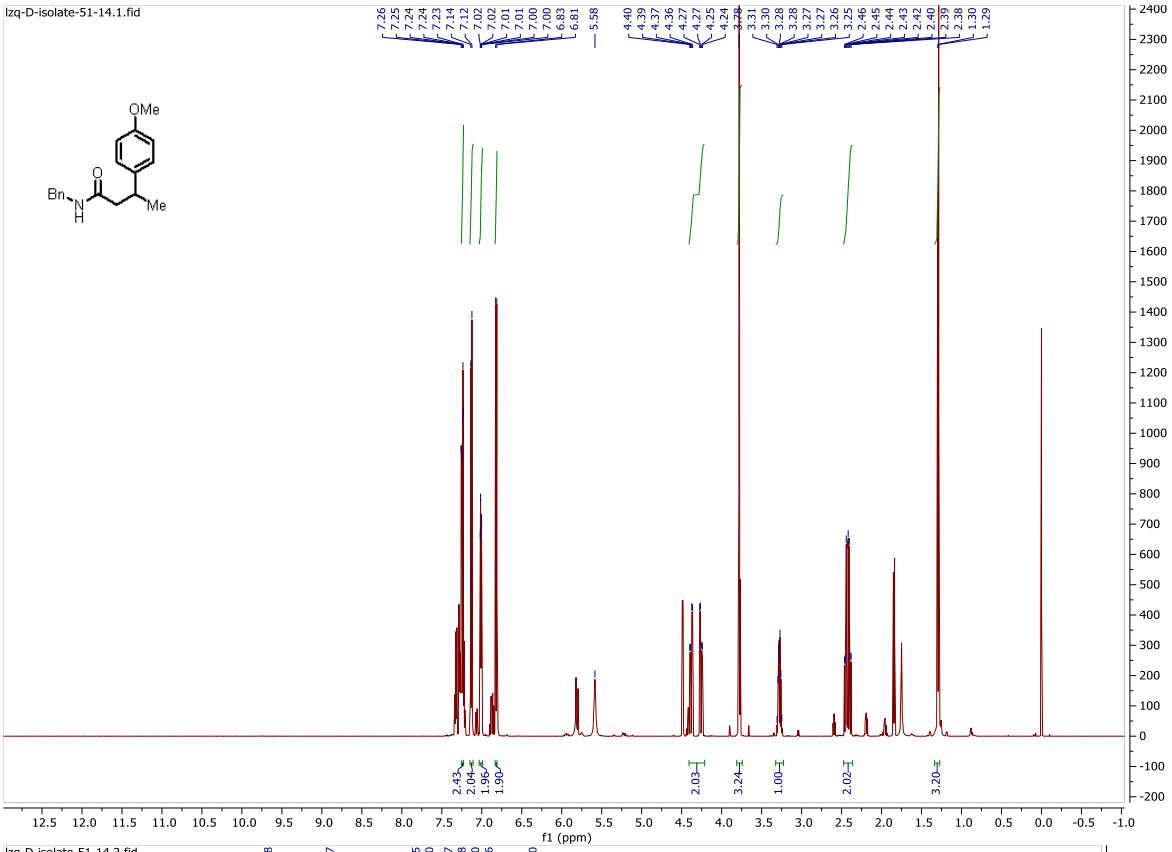

lzq-D-53-isolate-1-1.1.fid
7.54
7.53
7.34
7.32
7.25
7.24
7.03
7.03
7.02
5.57
4.42
4.41
4.39
4.38
4.28
4.27
4.26
4.25
3.46
3.45
3.44
3.42
3.41
3.40
2.51
2.50
2.49
2.48
2.44
2.43
2.42
2.40
1.34
1.33
CF3
Bn
N
H
O
Me
1.92
2.20
2.03
1.79
0.94
2.00
1.00
1.95
3.02
f1 (ppm)

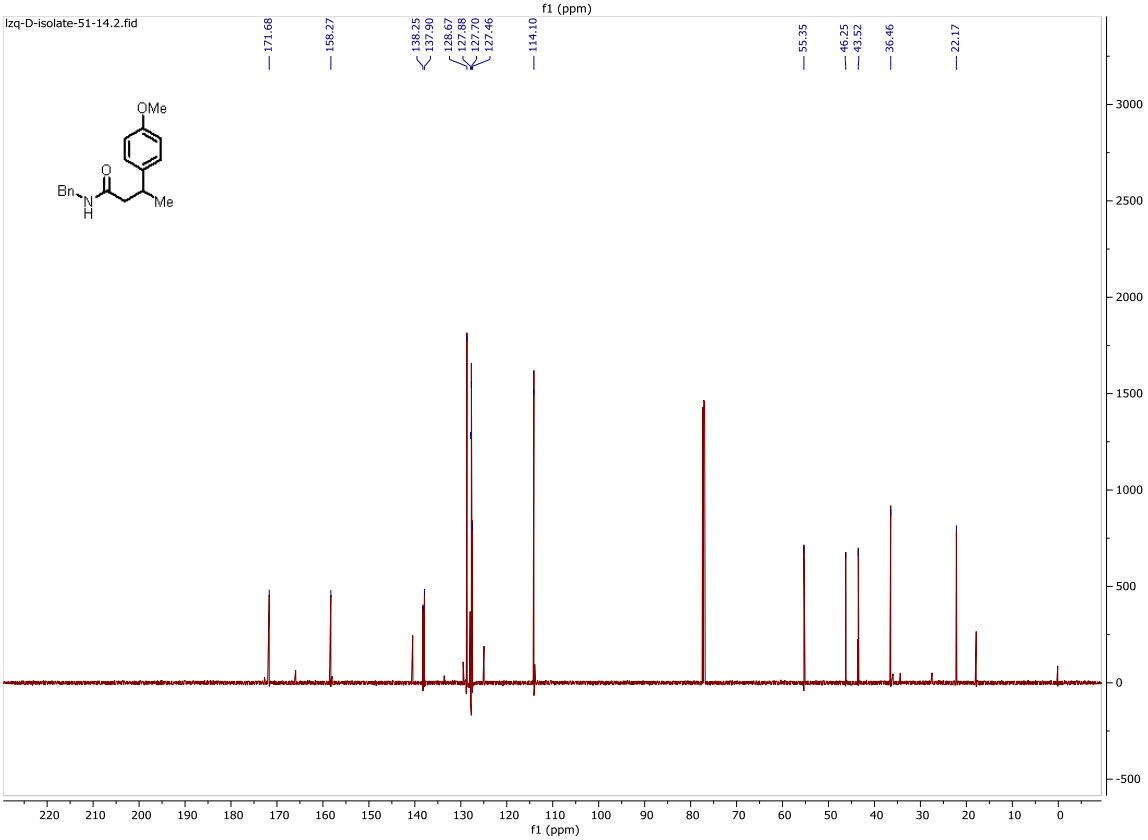

lzq-D-53-isolate-1-1.2.fid
170.95
149.94
138.05
128.92
128.91
128.78
127.73
127.67
127.41
125.70
125.68
125.65
125.63
125.27
123.46
121.66
45.62
43.67
37.01
21.68
CF3
Bn
N
H
O
Me
f1 (ppm)

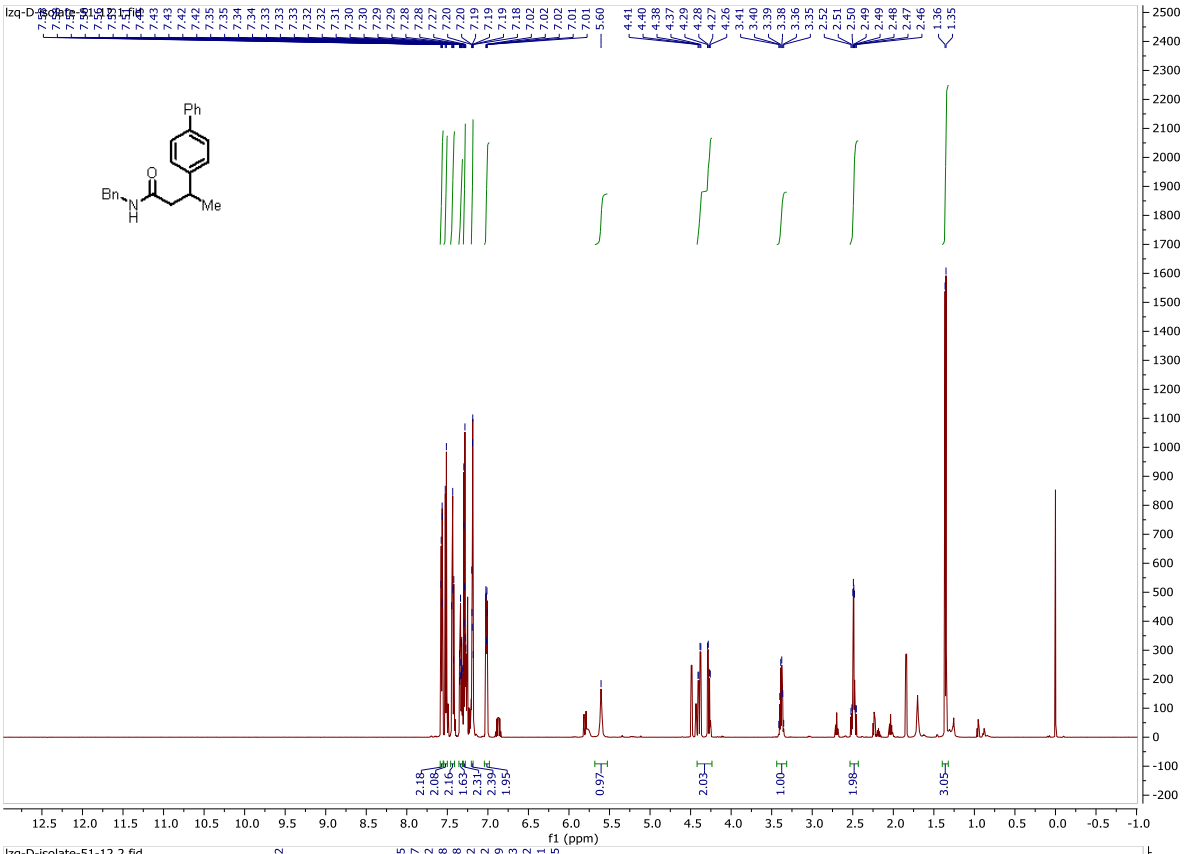

lzq-D-AM-isolate-7A-F.1.fid
-64.98
CF3
Bn
N
H
O
Me
f1 (ppm)

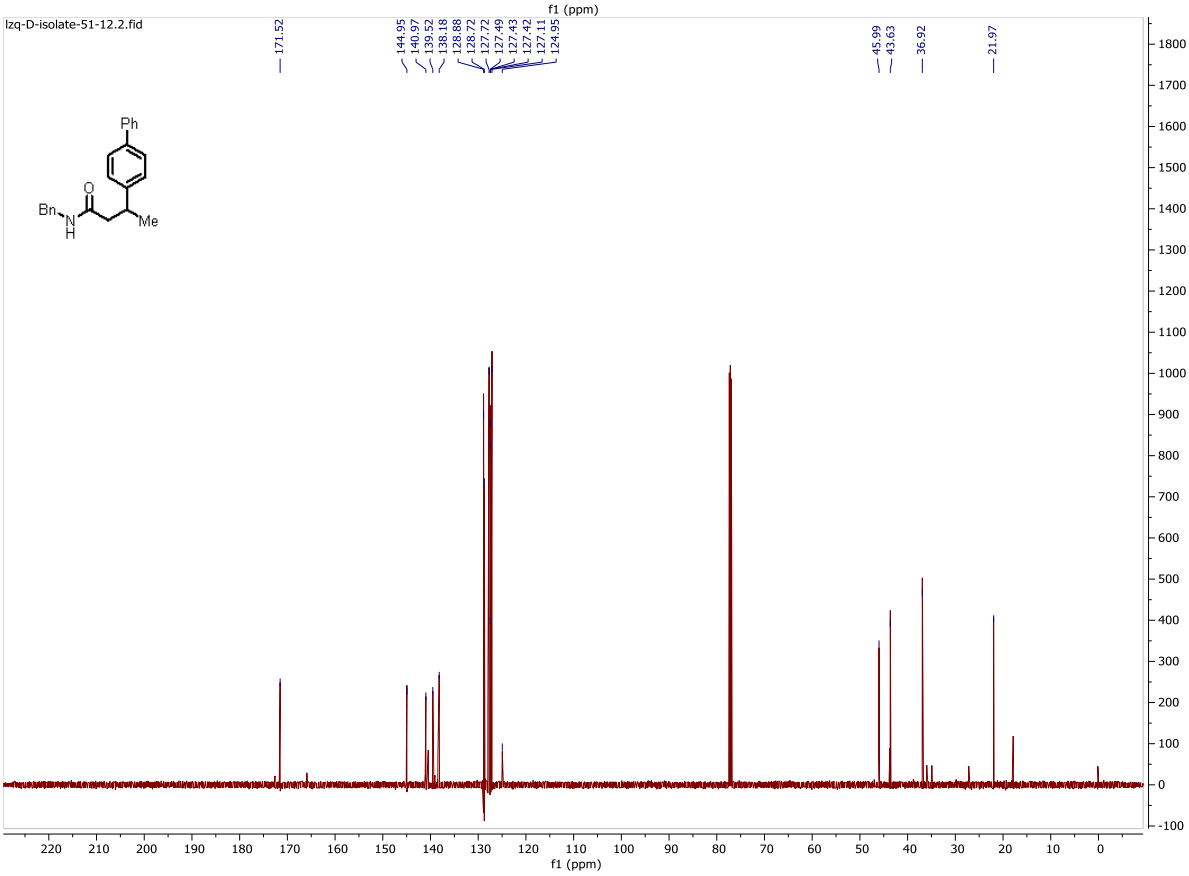

lzq-D-53-isolate-13.1.fid
Me
Bn
N
H
O
Me
f1 (ppm)

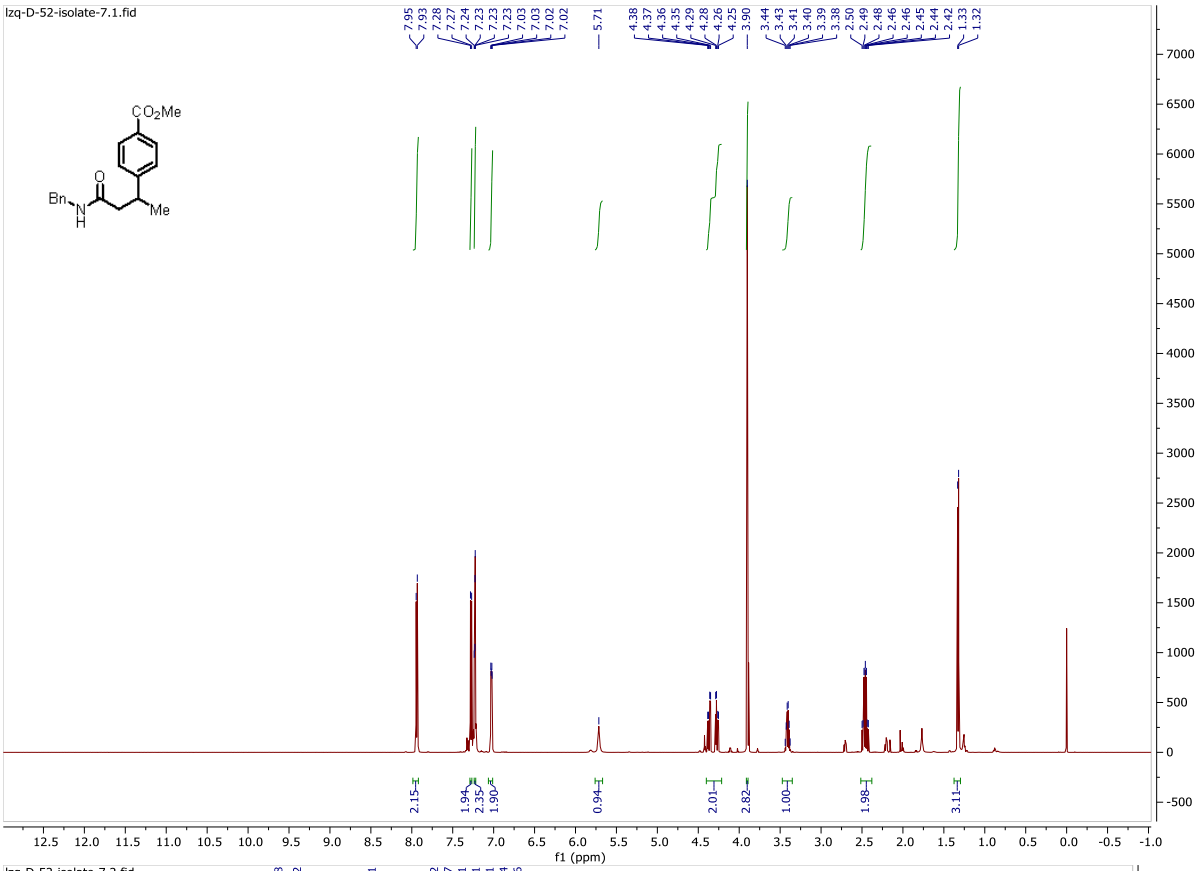

lzq-D-53-isolate-13.2.fid
171.68
142.83
138.25
136.06
129.42
128.66
127.72
127.44
126.82
46.09
43.56
36.85
22.09
21.14
Me
Bn
N
H
O
Me
f1 (ppm)

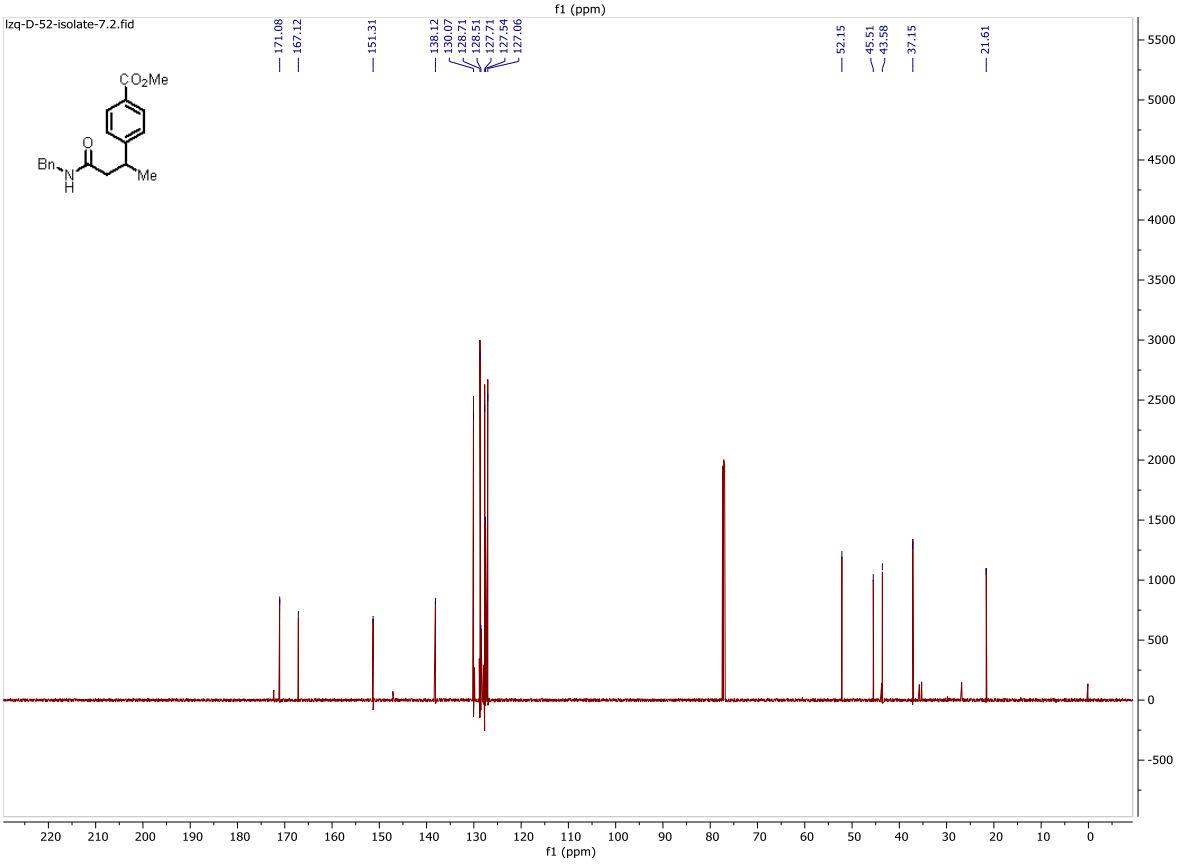

lzq-D-isolate-51-14.1.fid
OMe
Bn
N
H
O
Me
f1 (ppm)

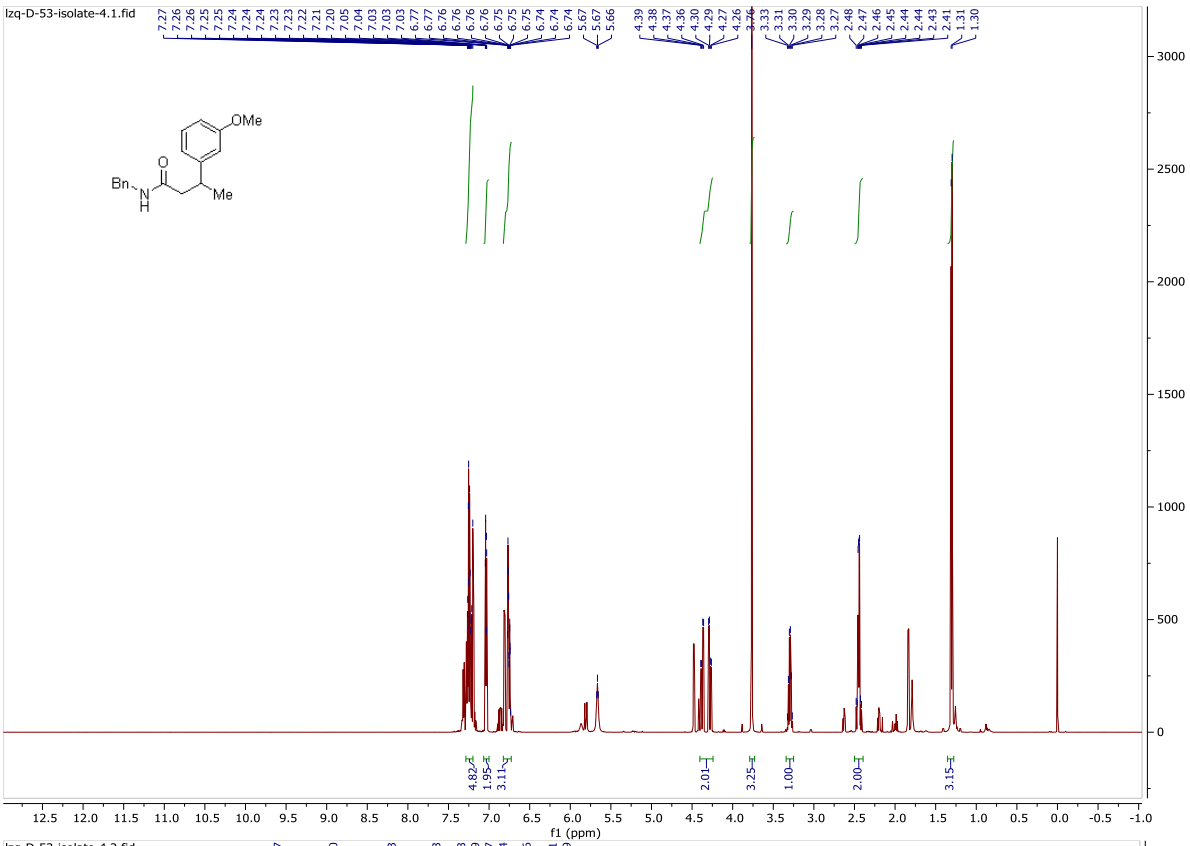

lzq-D-isolate-51-14.2.fid
OMe
Bn
N
H
O
Me
f1 (ppm)

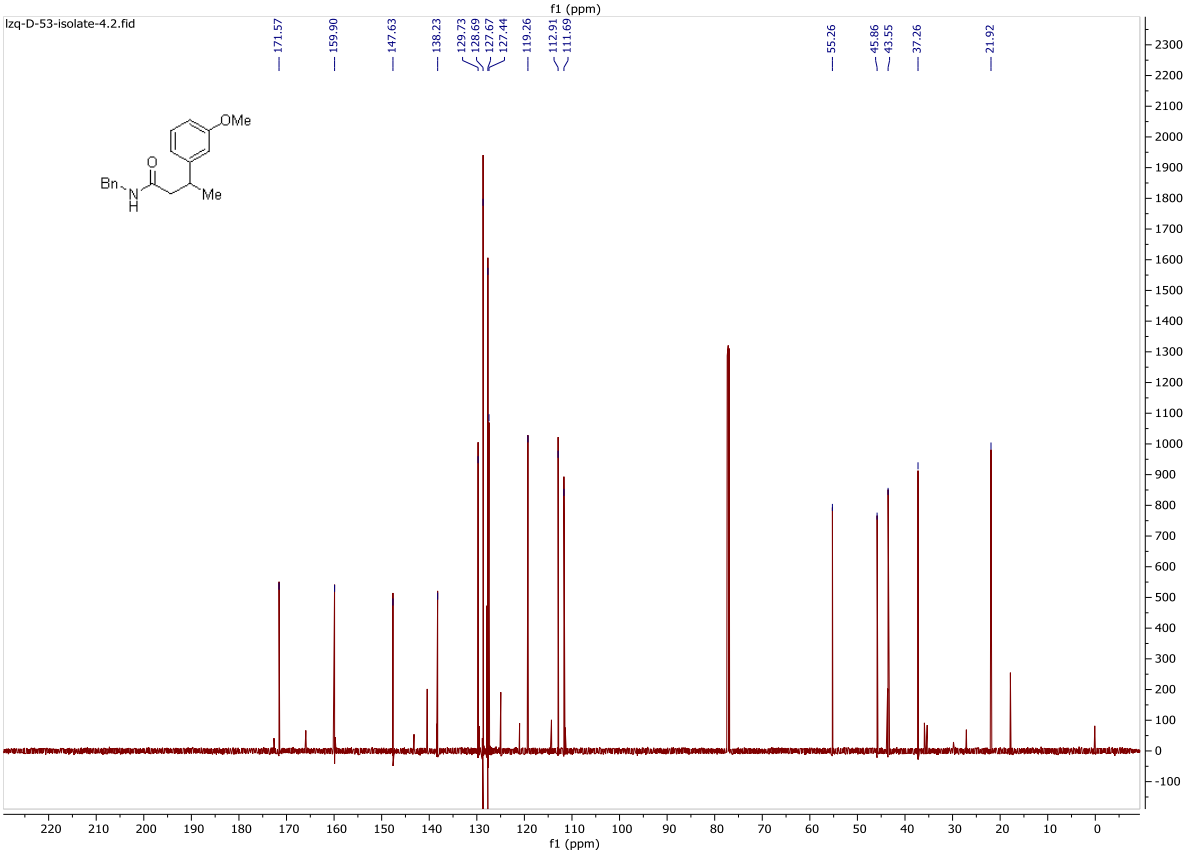

Ph
O
Bn
N
H
Me
f1 (ppm)

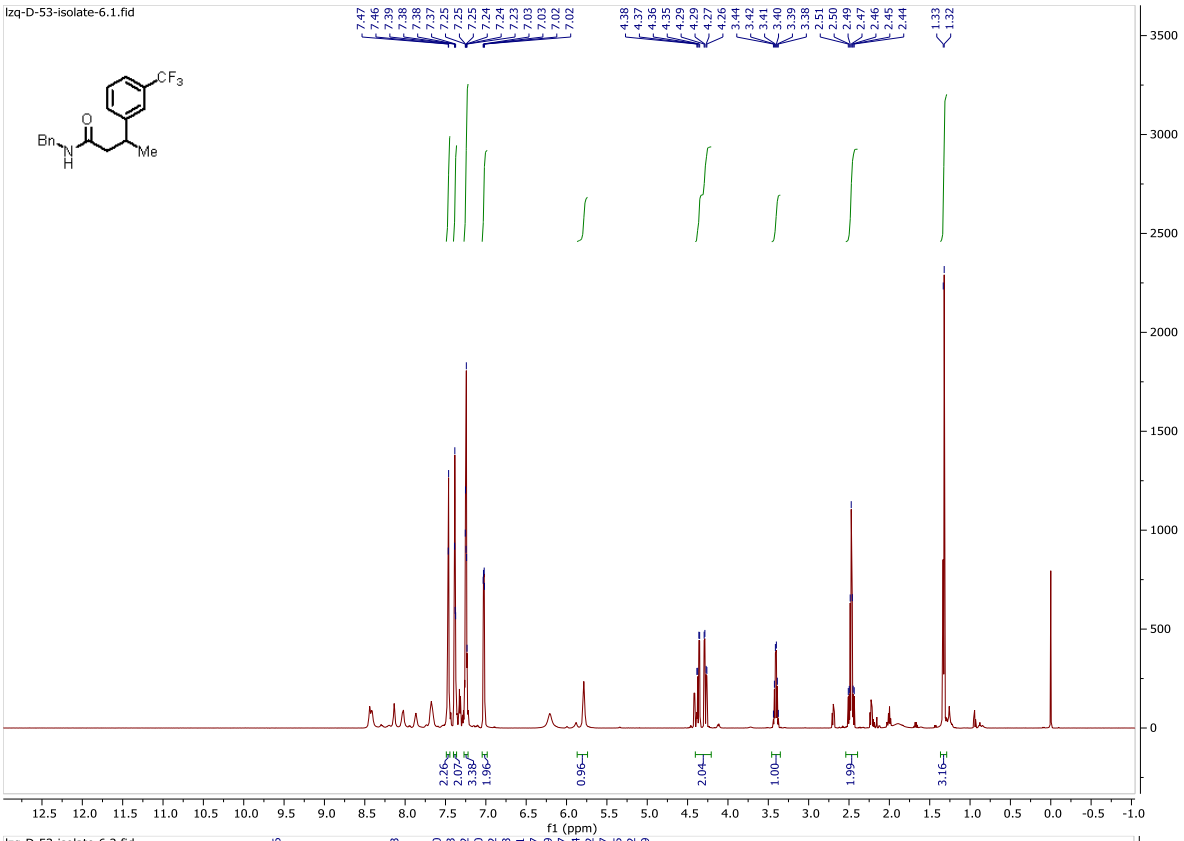

lzq-D-isolate-51-12.2.fid
171.52
144.95
140.97
139.52
138.18
128.88
128.72
127.72
127.49
127.43
127.42
127.11
124.95
45.99
43.63
36.92
21.97
Ph
O
Bn
N
H
Me
f1 (ppm)

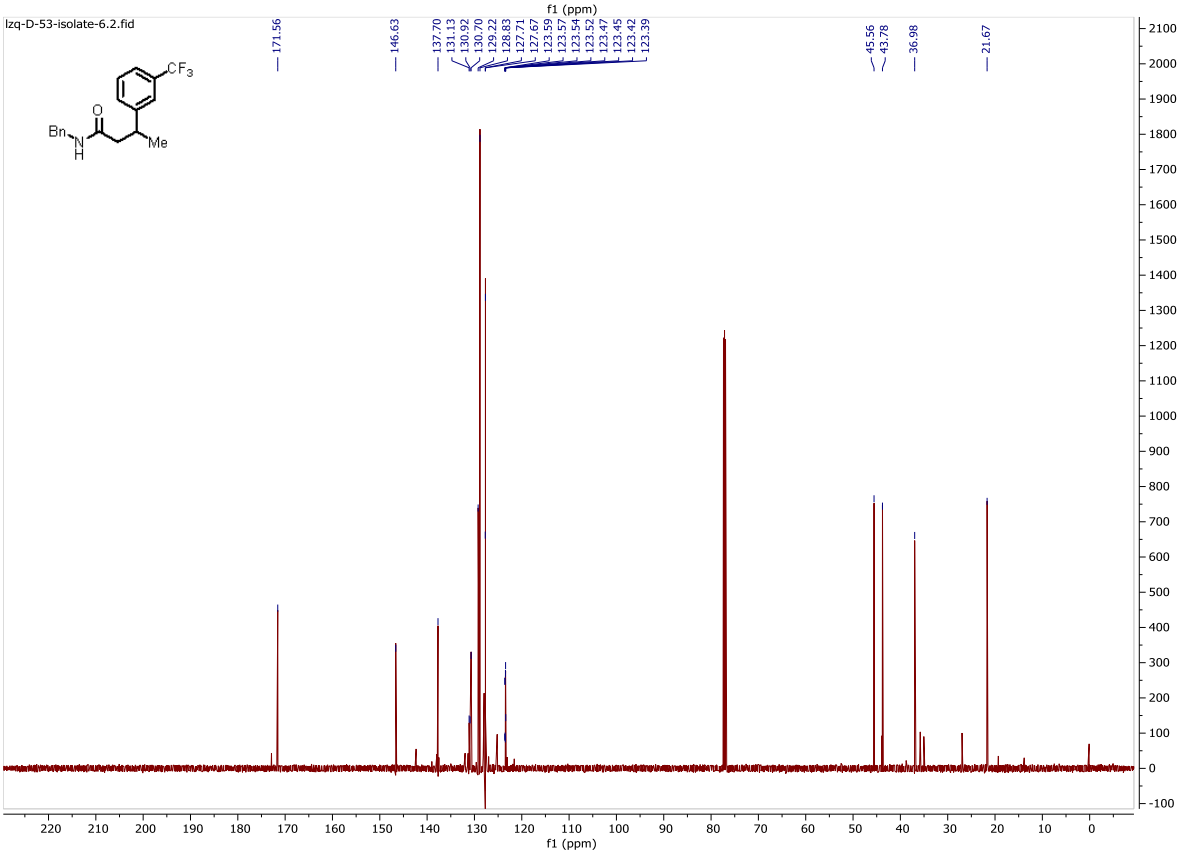

lzq-D-52-isolate-7.1.fid
CO2Me
Bn
N
H
O
Me
f1 (ppm)

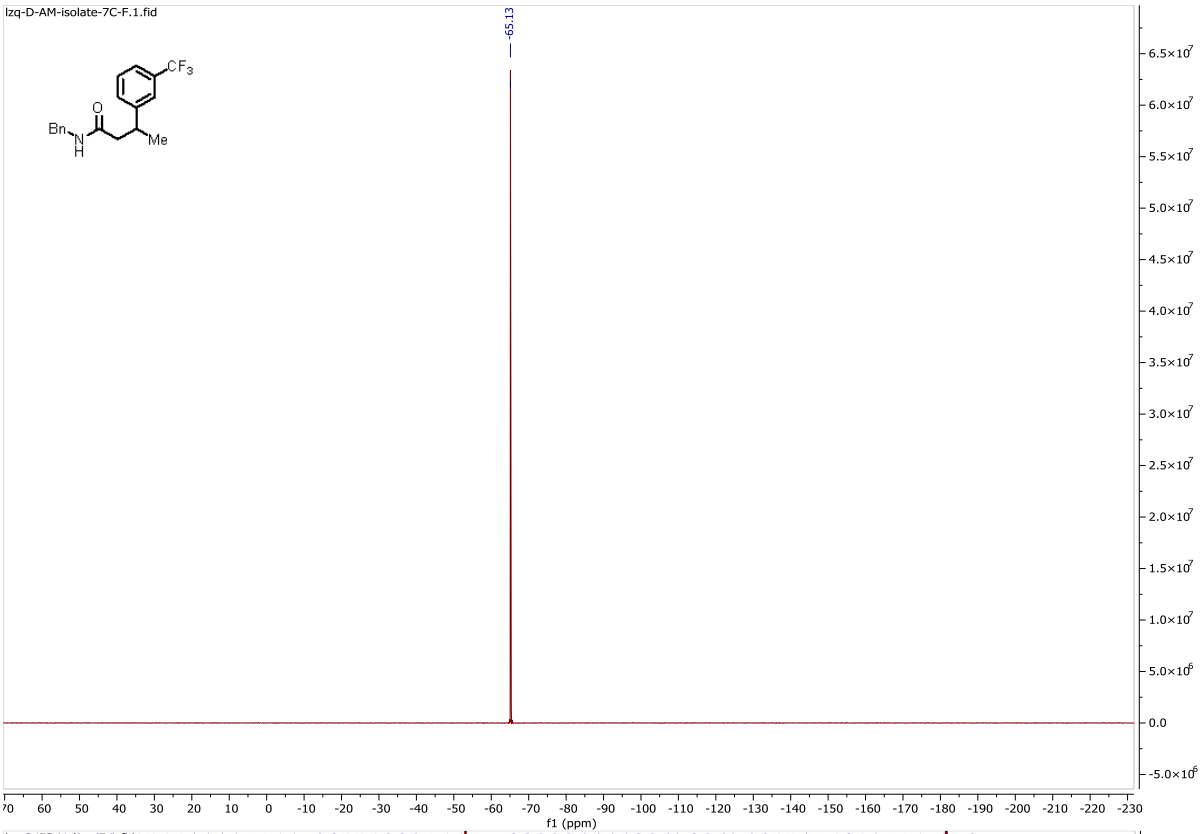

lzq-D-52-isolate-7.2.fid
CO2Me
Bn
N
H
O
Me
f1 (ppm)

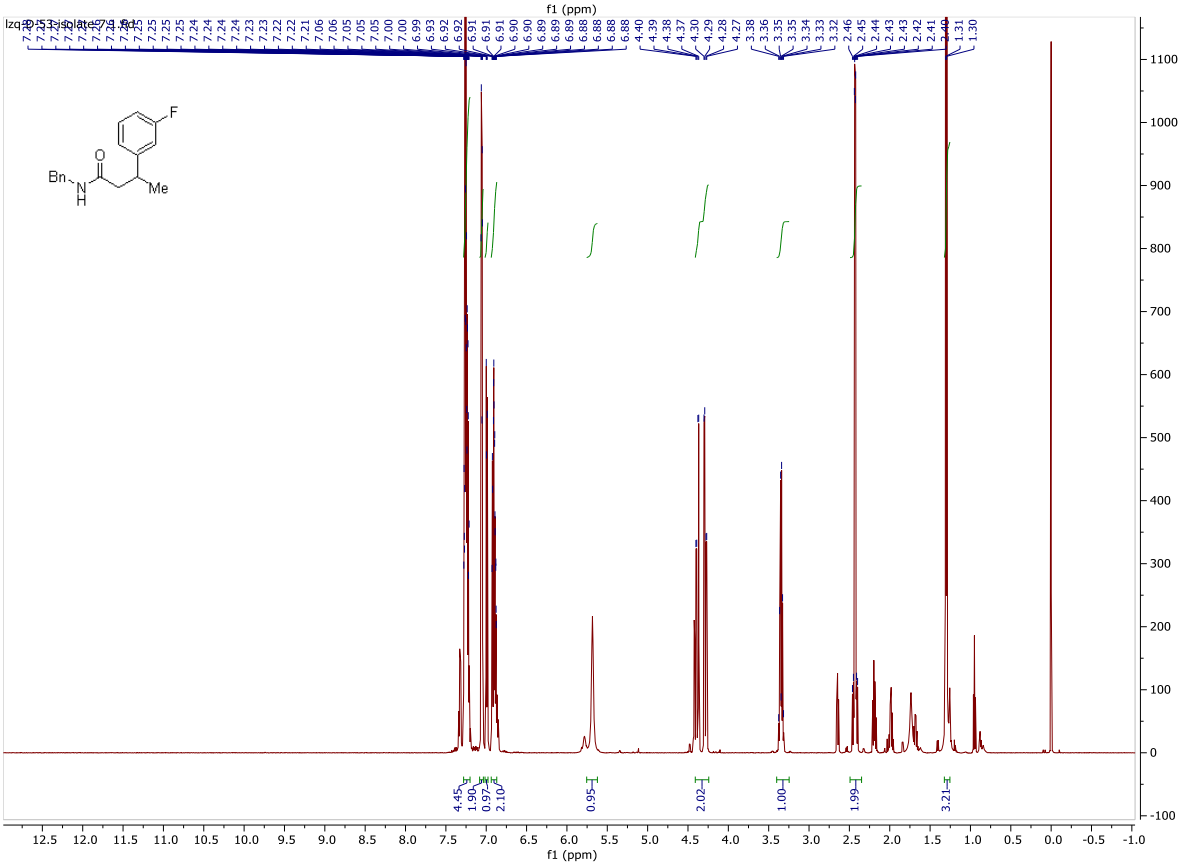

lzq-D-53-isolate-4.1.fid
OMe
Bn
N
H
O
Me
f1 (ppm)

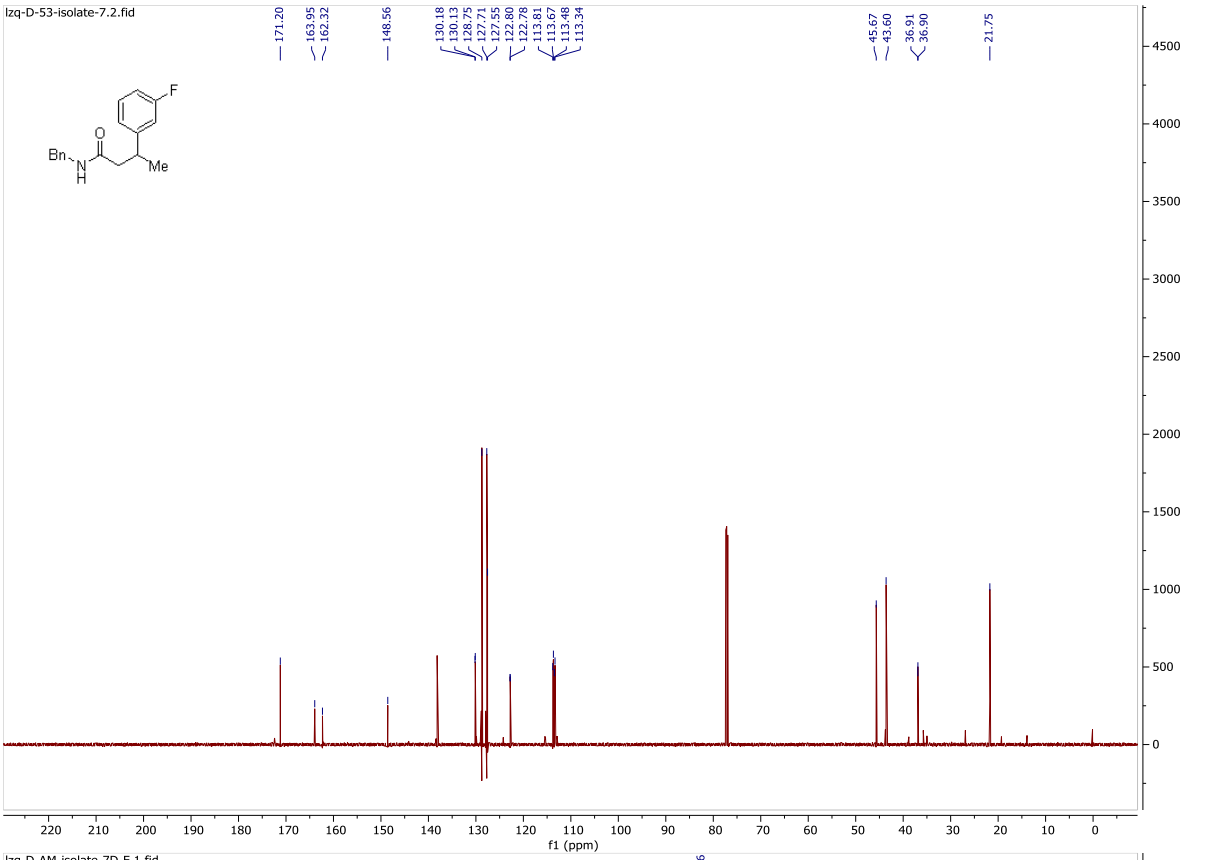

lzq-D-53-isolate-4.2.fid
171.57
159.90
147.63
138.23
129.73
128.69
127.67
127.44
119.26
112.91
111.69
55.26
45.86
43.55
37.26
21.92
OMe
Bn
N
H
O
Me
f1 (ppm)

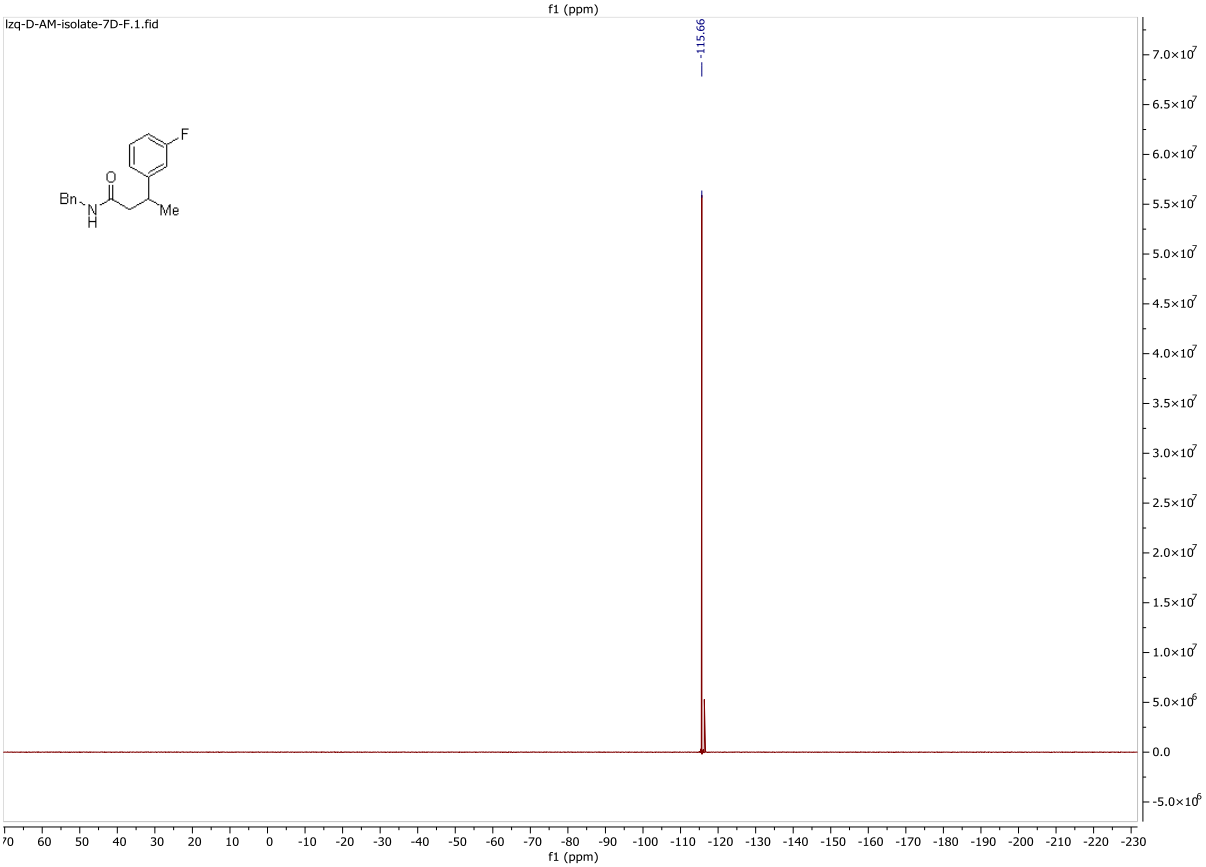

lzq-D-53-isolate-6.1.fid
7.47 7.46 7.39 7.38 7.38 7.37 7.25 7.25 7.25 7.24 7.24 7.23 7.03 7.02 7.02
4.38 4.37 4.36 4.35 4.29 4.29 4.27 4.26 3.44 3.42 3.41 3.40 3.39 3.38 2.51 2.50 2.49 2.47 2.46 2.45 2.44
1.33 1.32
CF3
O
Bn
N
H
Me
2.26 2.07 3.38 1.96 0.96 2.04 1.00 1.99 3.16
f1 (ppm)

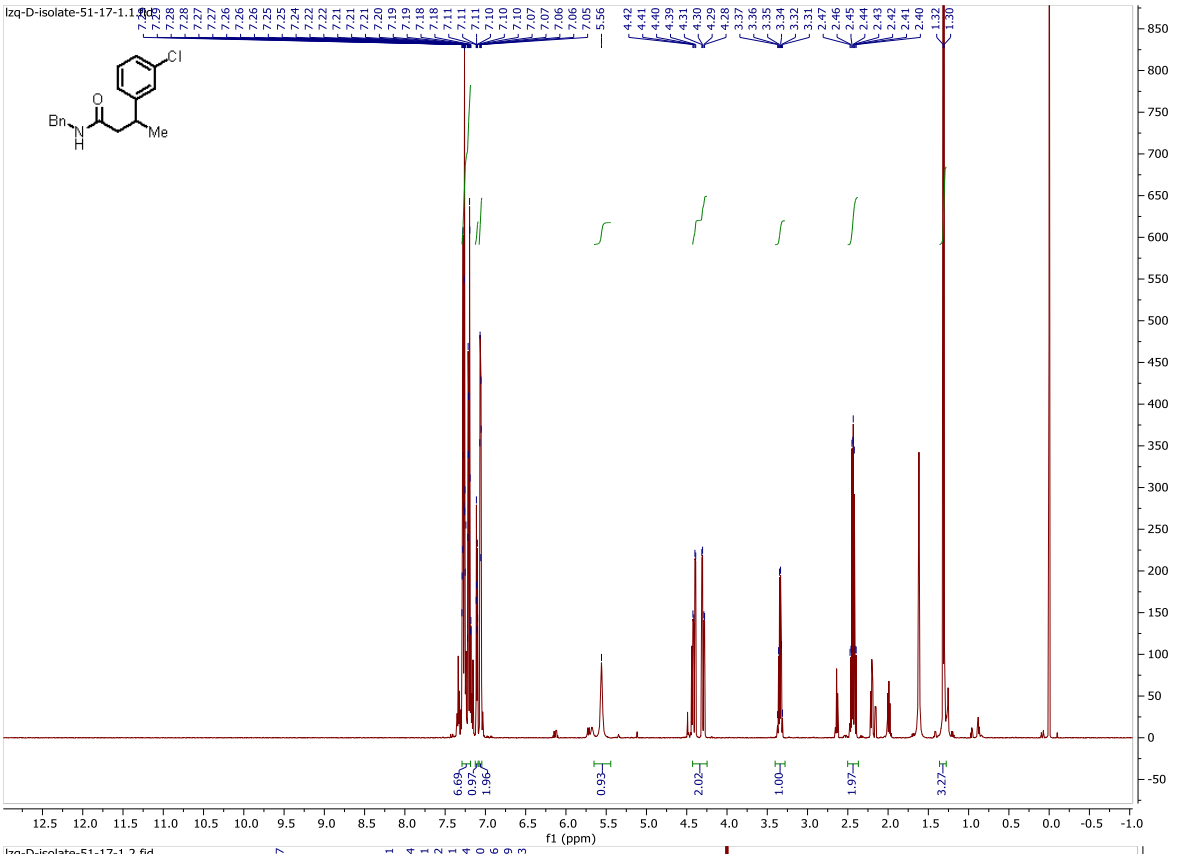

lzq-D-53-isolate-6.2.fid
171.56 146.63 137.70 131.13 130.92 130.70 129.22 128.83 127.71 127.67 123.59 123.57 123.54 123.52 123.47 123.45 123.42 123.39
45.56 43.78 36.98 21.67
CF3
O
Bn
N
H
Me
f1 (ppm)

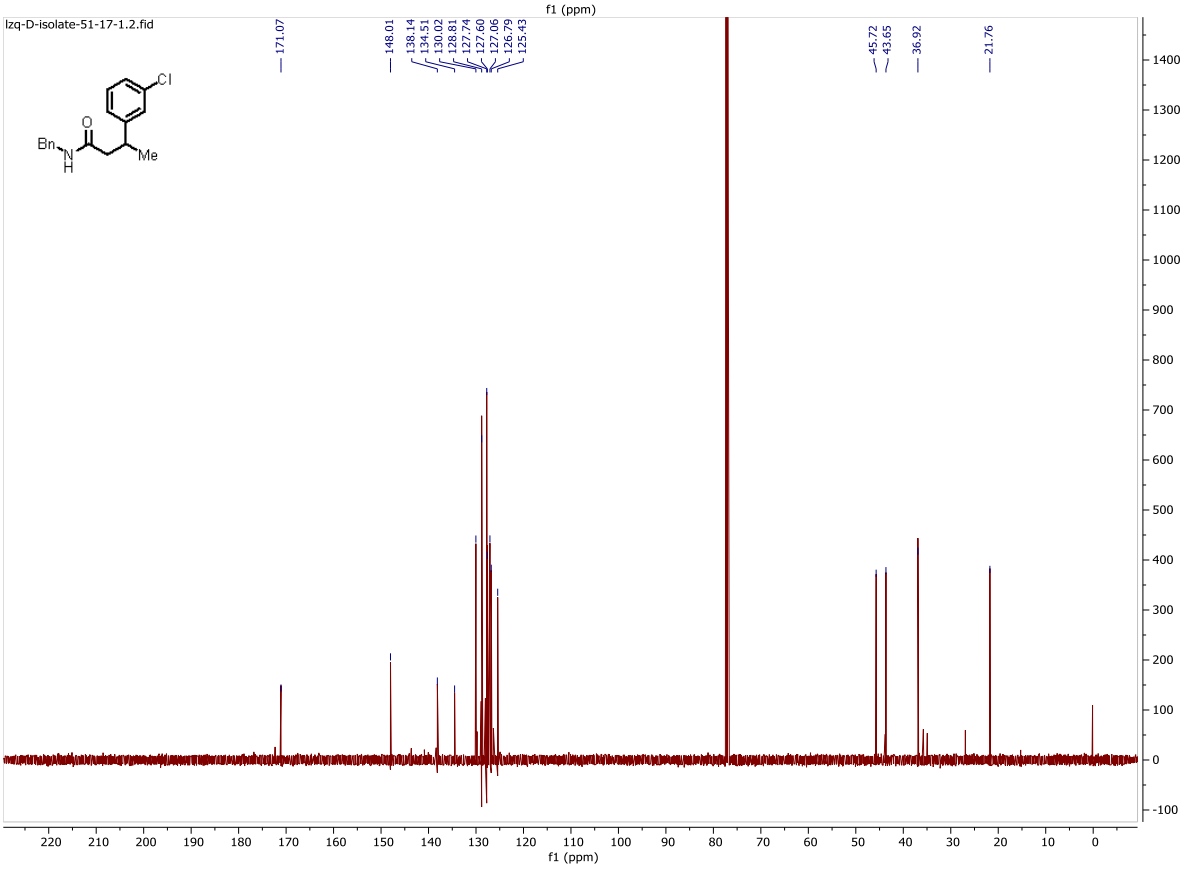

lzq-D-AM-isolate-7C-F.1.fid
-65.13
CF3
Bn
N
H
O
Me
f1 (ppm)

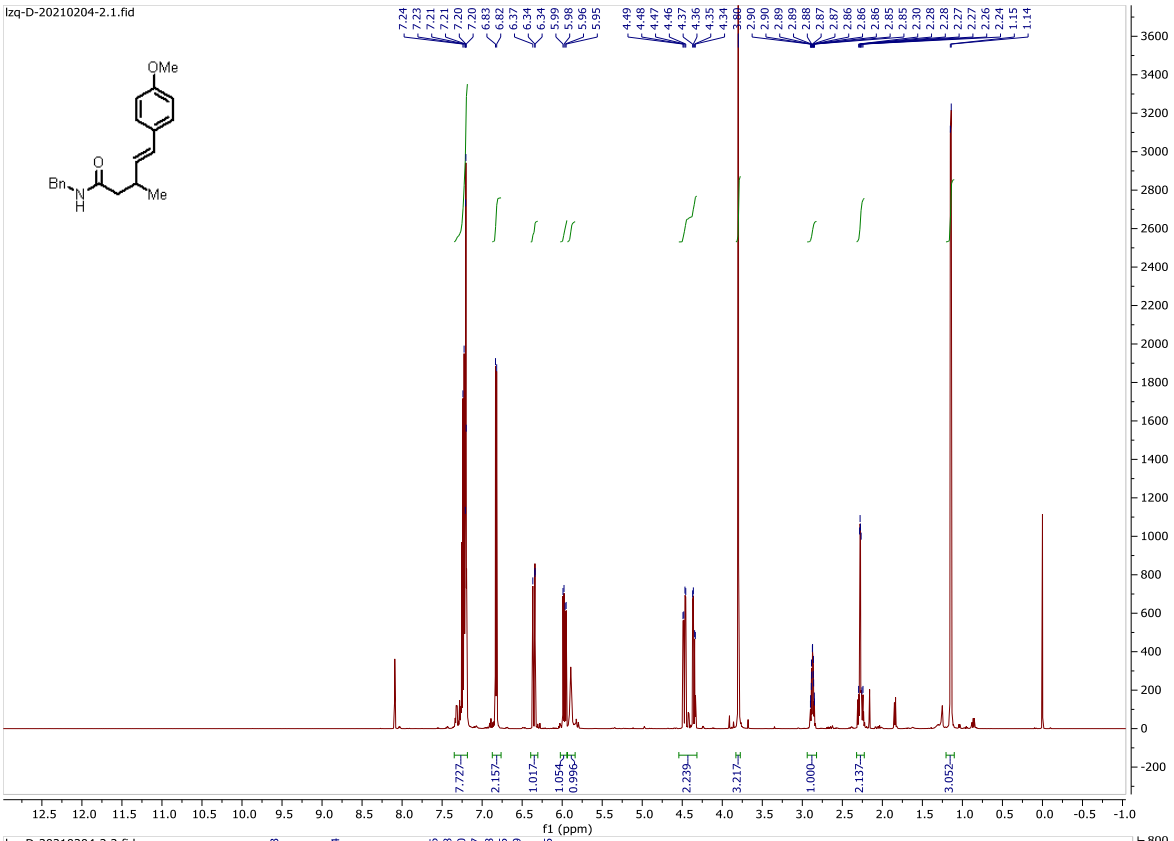

F
Bn
N
H
O
Me
4.45
1.90
0.97
2.10
0.95
2.02
1.00
1.99
3.21
f1 (ppm)

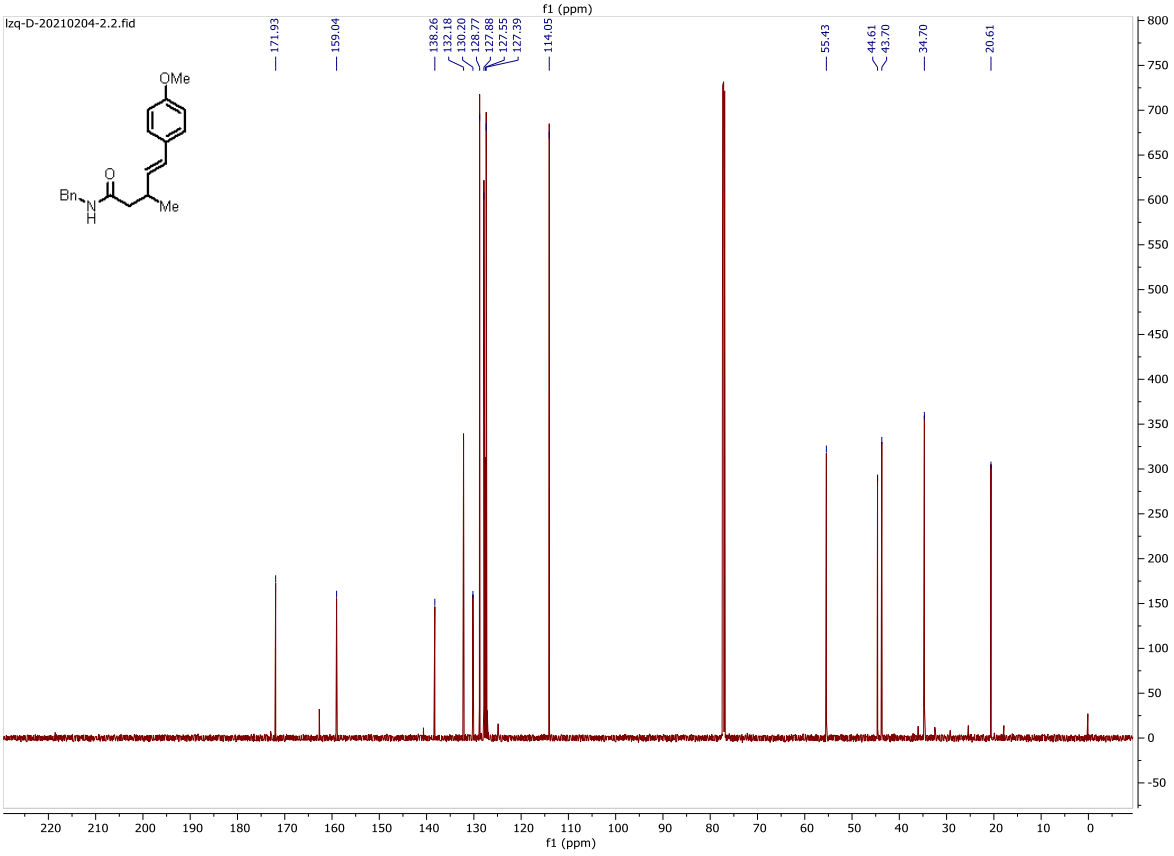

lzq-D-53-isolate-7.2.fid
171.20
163.95
162.32
148.56
130.18
130.13
128.75
127.71
127.55
122.80
122.78
113.81
113.67
113.48
113.34
45.67
43.60
36.91
36.90
21.75
F
O
Bn
N
H
Me
f1 (ppm)

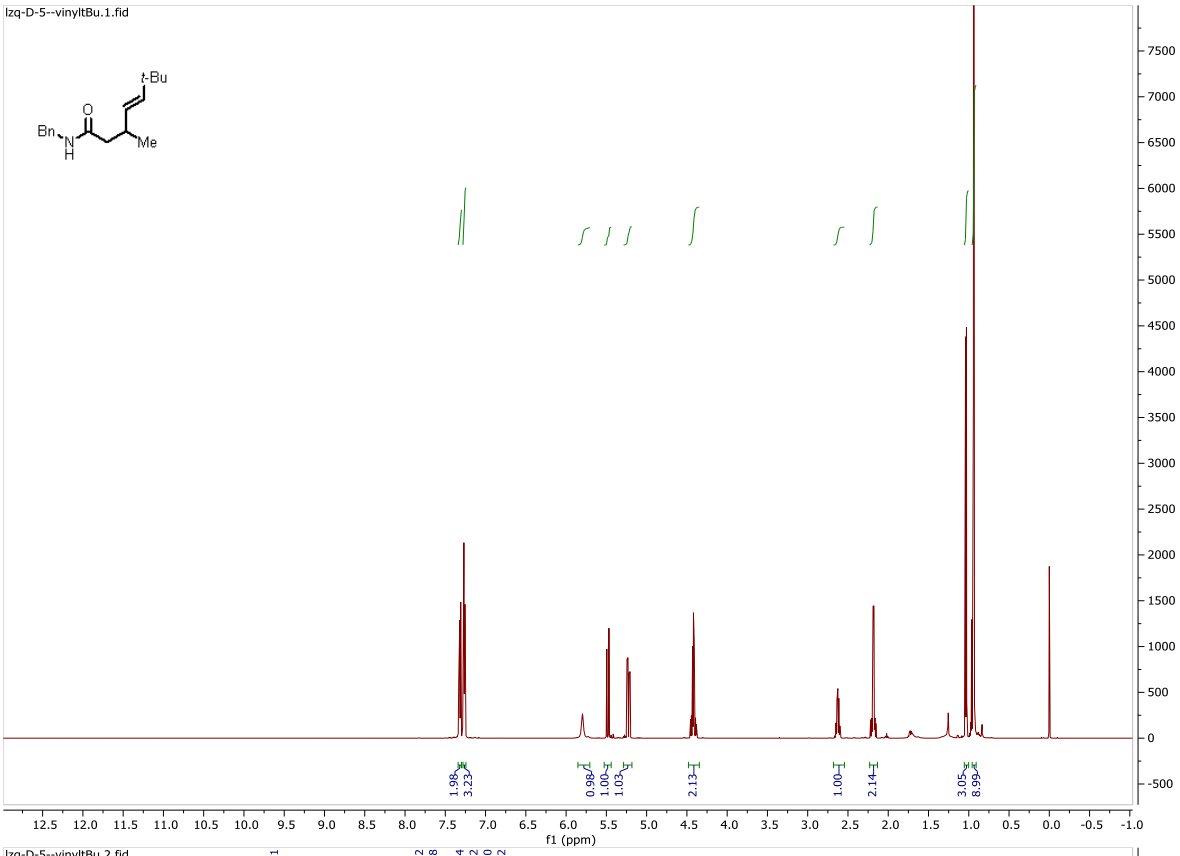

lzq-D-AM-isolate-7D-F.1.fid
-115.66
F
O
Bn
N
H
Me
f1 (ppm)

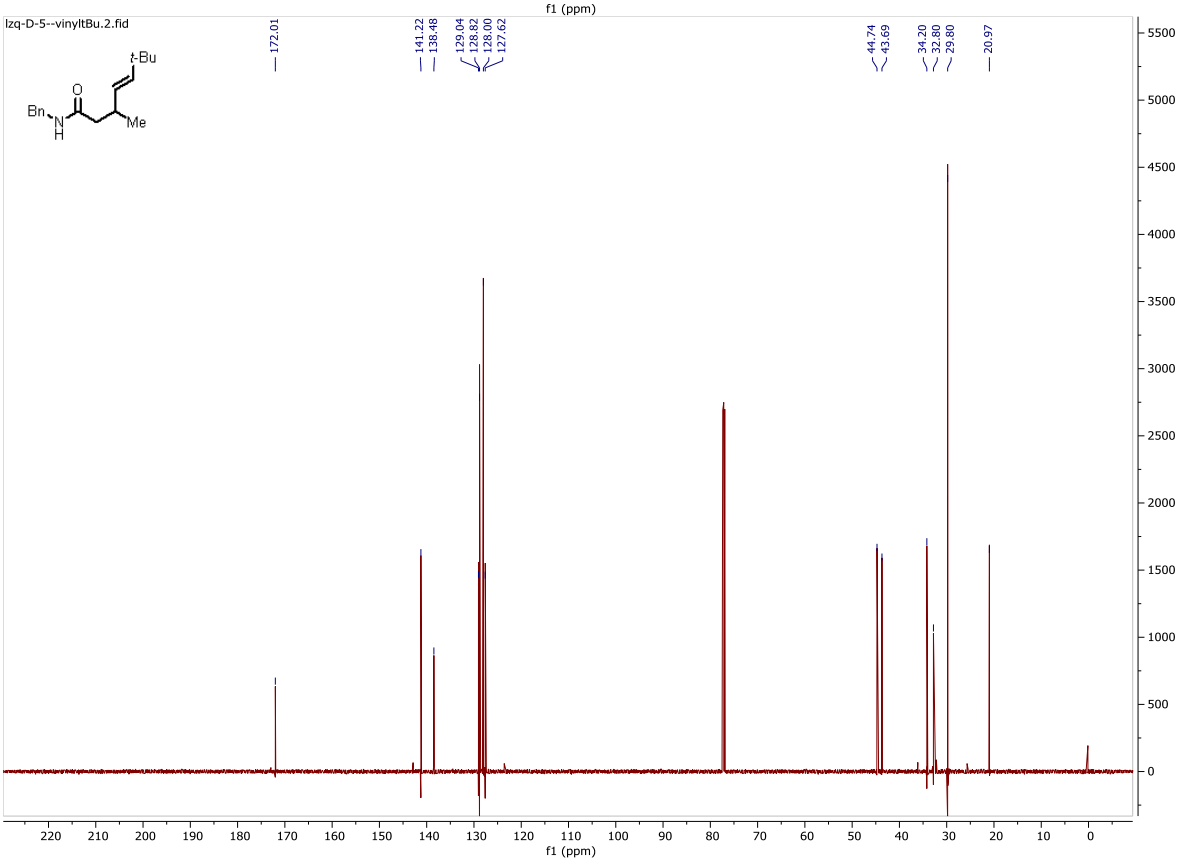

lzq-D-isolate-51-17-1.1.fid
Cl
Bn
N
H
O
Me
f1 (ppm)

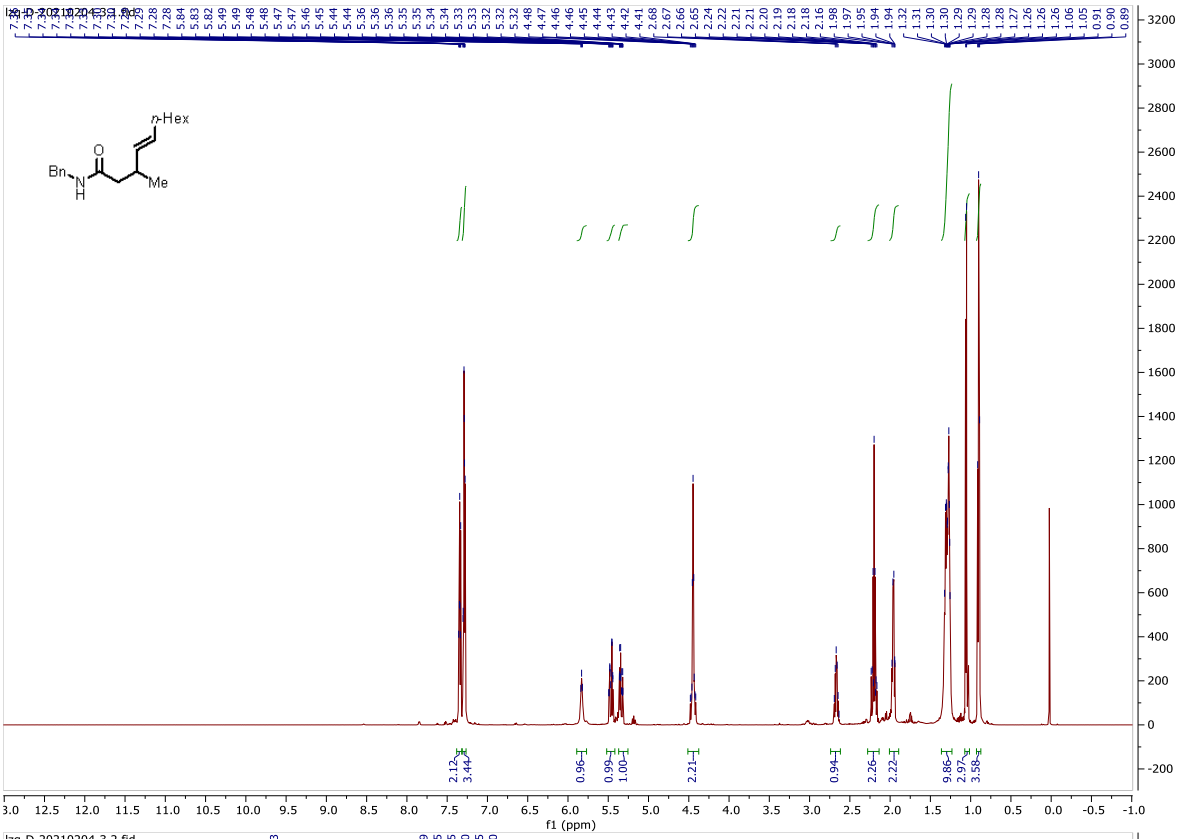

lzq-D-isolate-51-17-1.2.fid
171.07
148.01
138.14
134.51
130.02
128.81
127.74
127.60
127.06
126.79
125.43
45.72
43.65
36.92
21.76
Cl
Bn
N
H
O
Me
f1 (ppm)

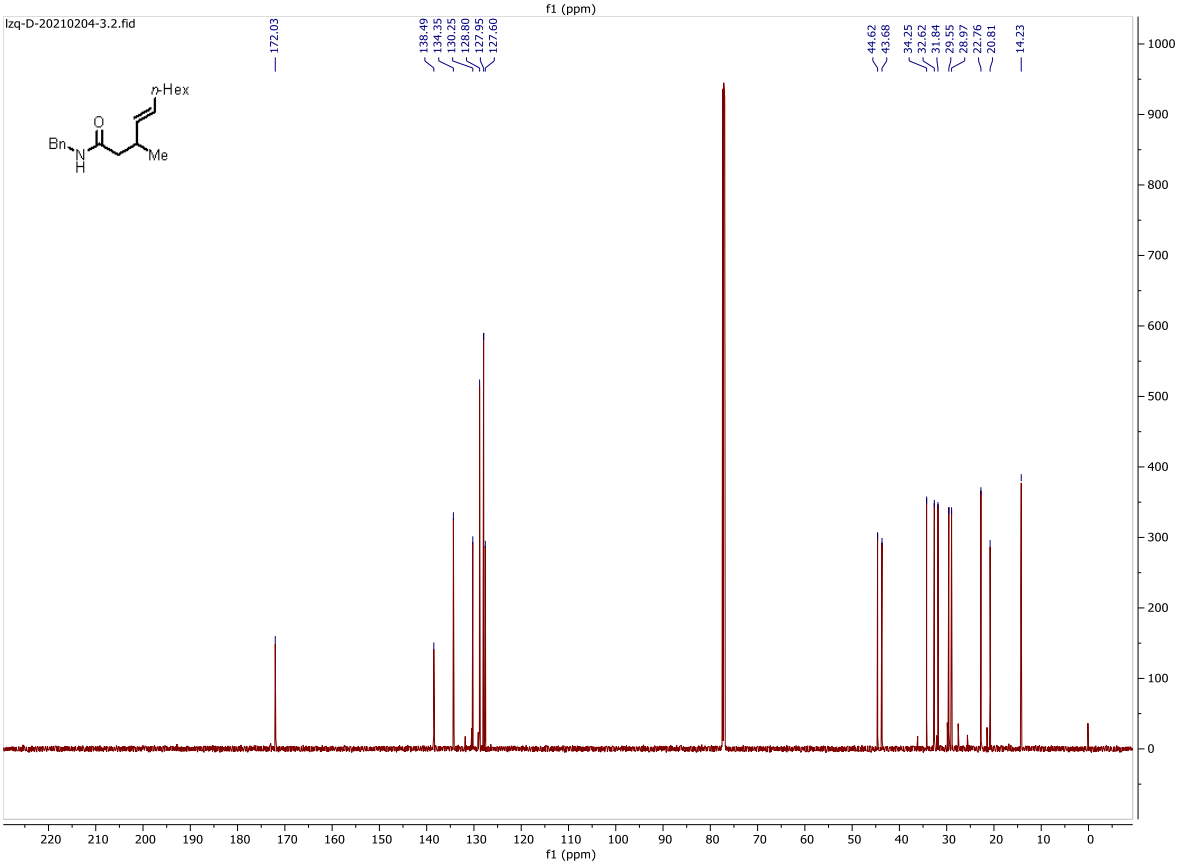

lzq-D-20210204-2.1.fid
OMe
Bn
N
H
O
Me
f1 (ppm)

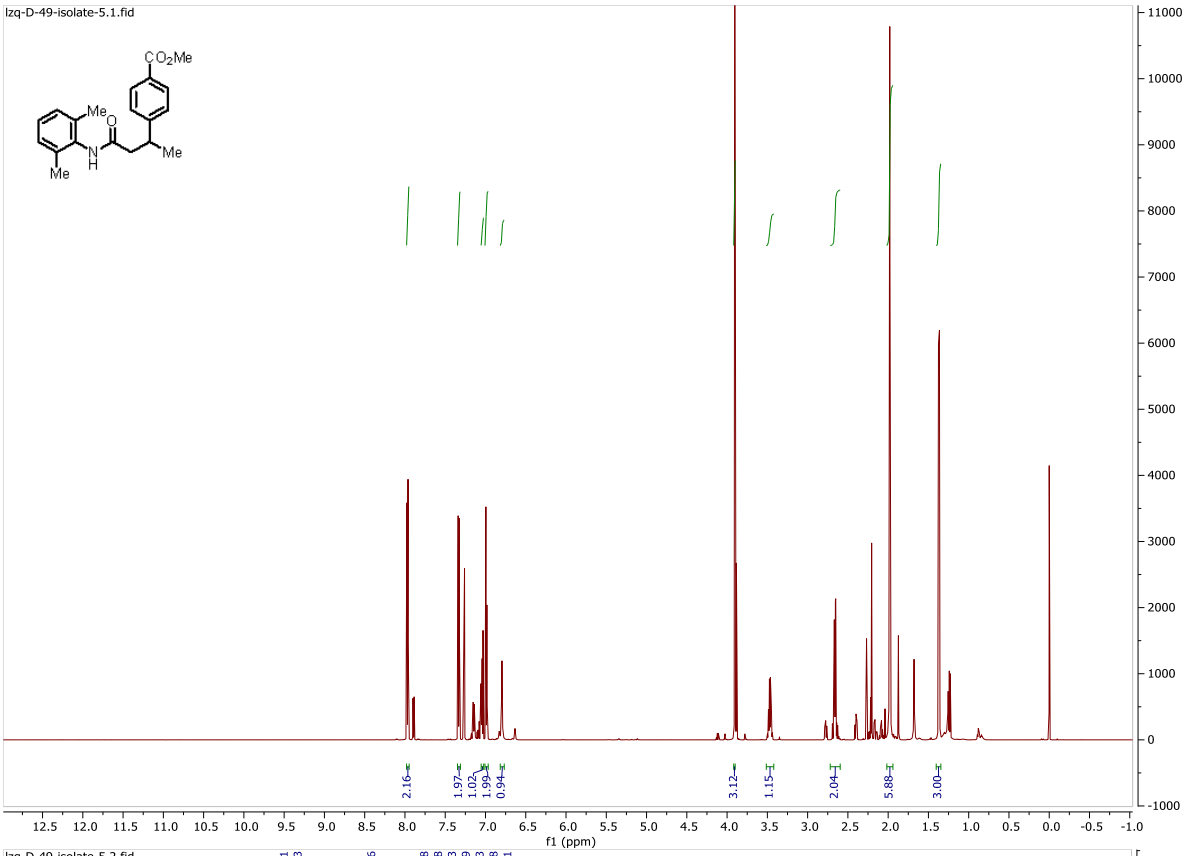

lzq-D-20210204-2.2.fid
OMe
Bn
N
H
O
Me
f1 (ppm)

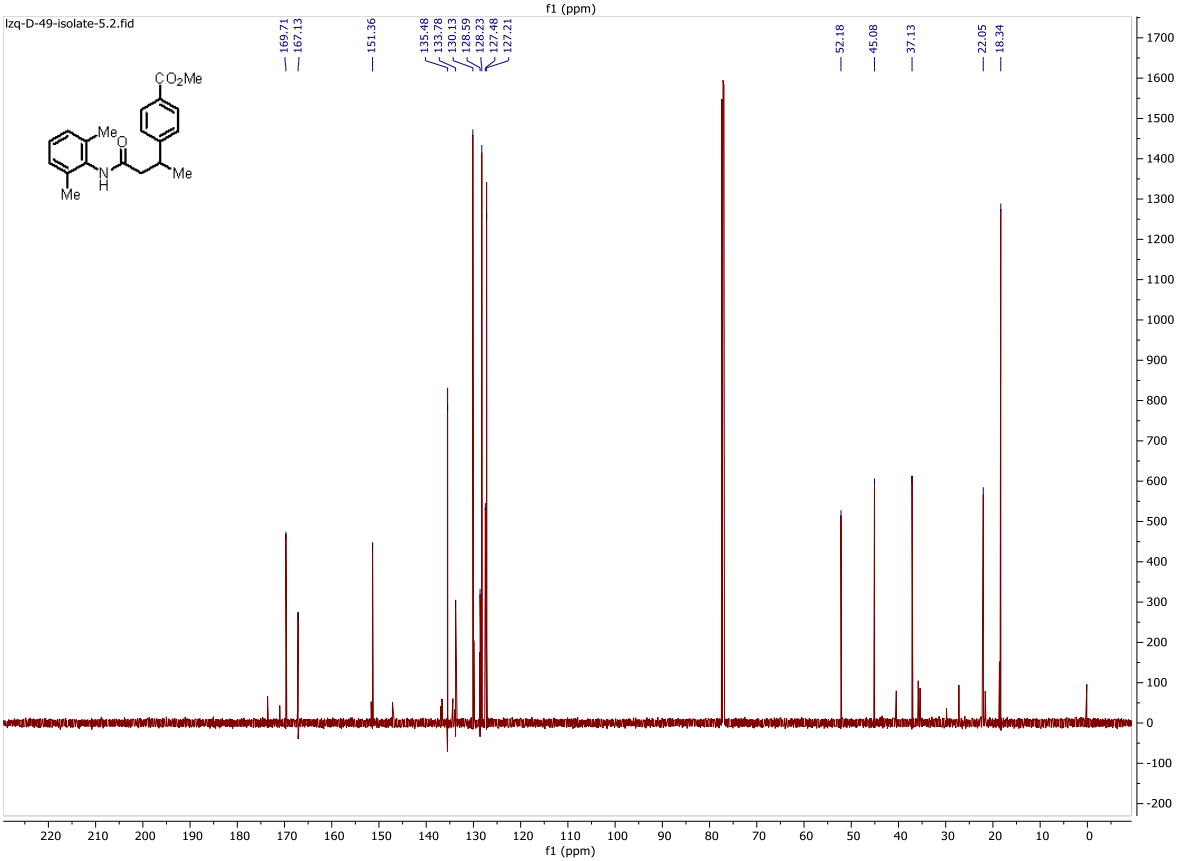

lzq-D-5--vinyltBu.1.fid
t-Bu
Bn
N
H
O
Me
1.98
3.23
0.98
1.00
1.03
2.13
1.00
2.14
3.05
8.99
f1 (ppm)

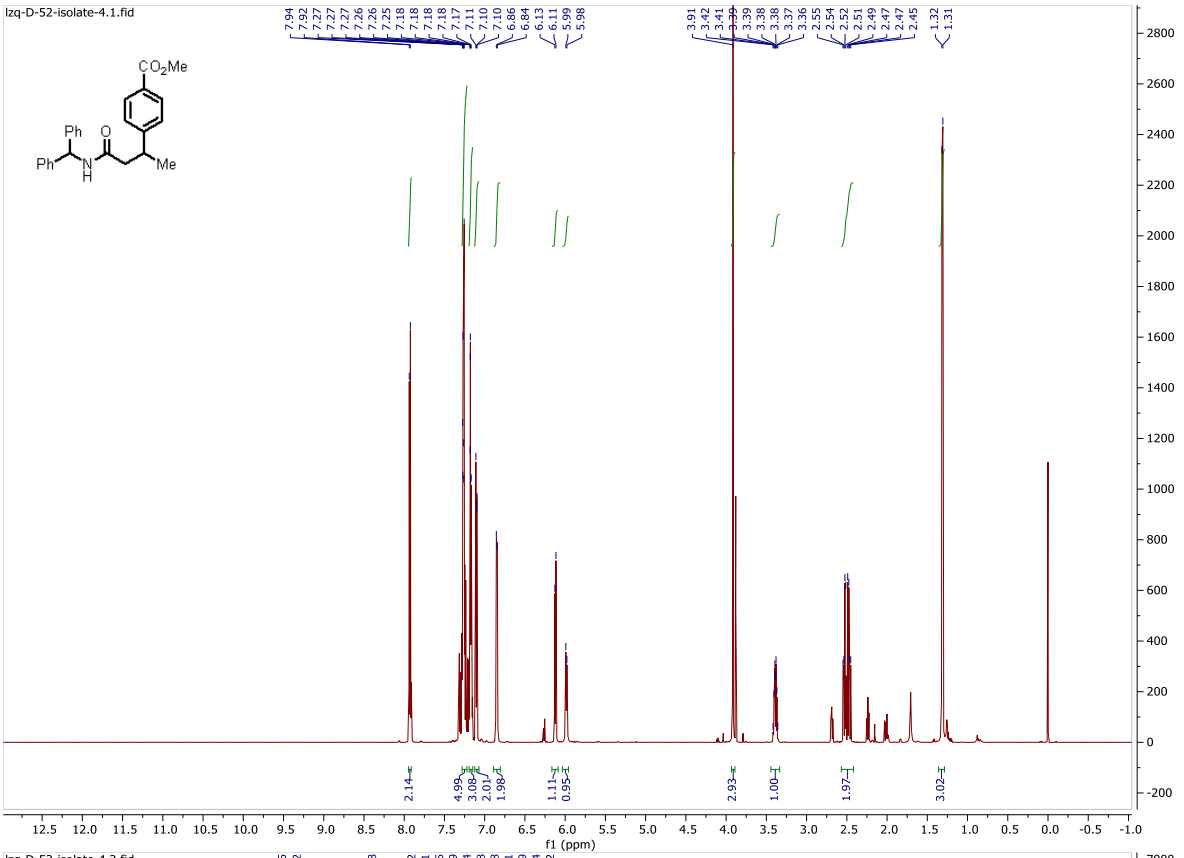

lzq-D-5--vinyltBu.2.fid
t-Bu
Bn
N
H
O
Me
172.01
141.22
138.48
129.04
128.82
128.00
127.62
44.74
43.69
34.20
32.80
29.80
20.97
f1 (ppm)

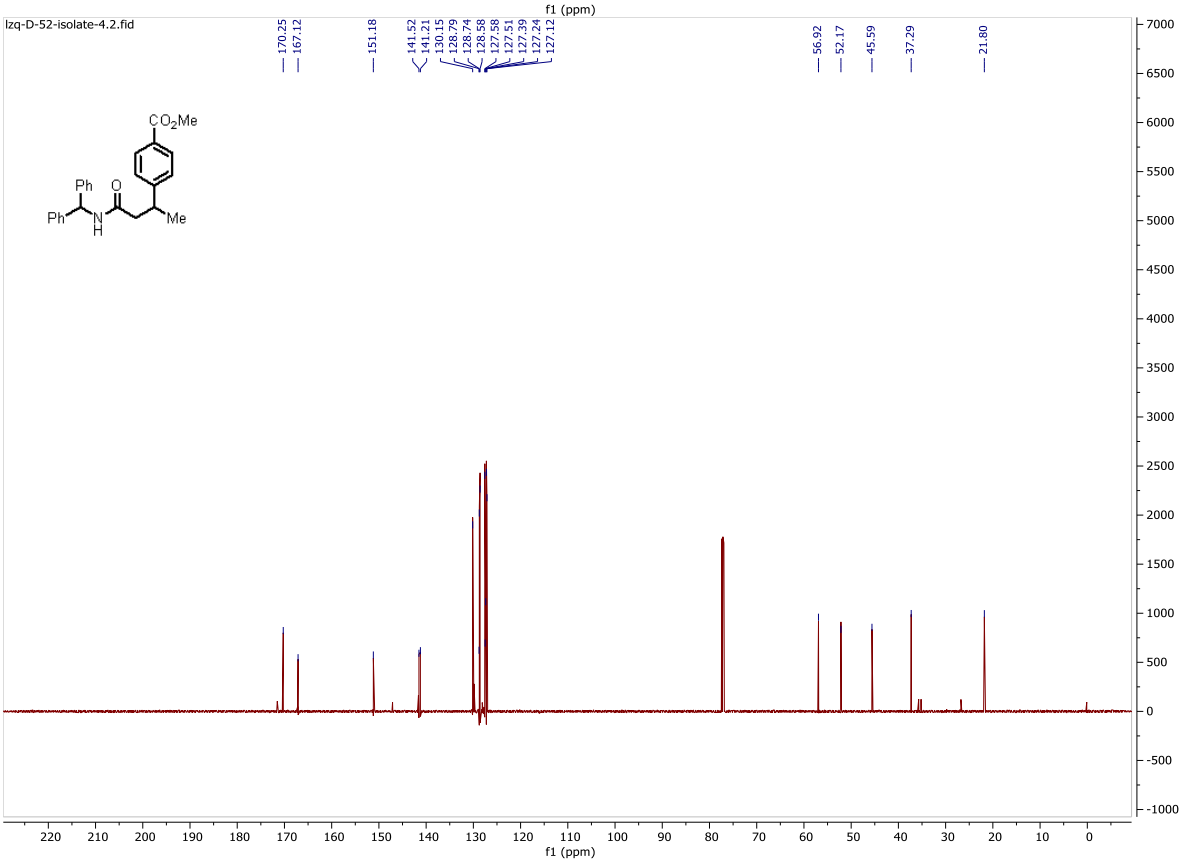

n-Hex
Bn
N
H
O
Me
f1 (ppm)

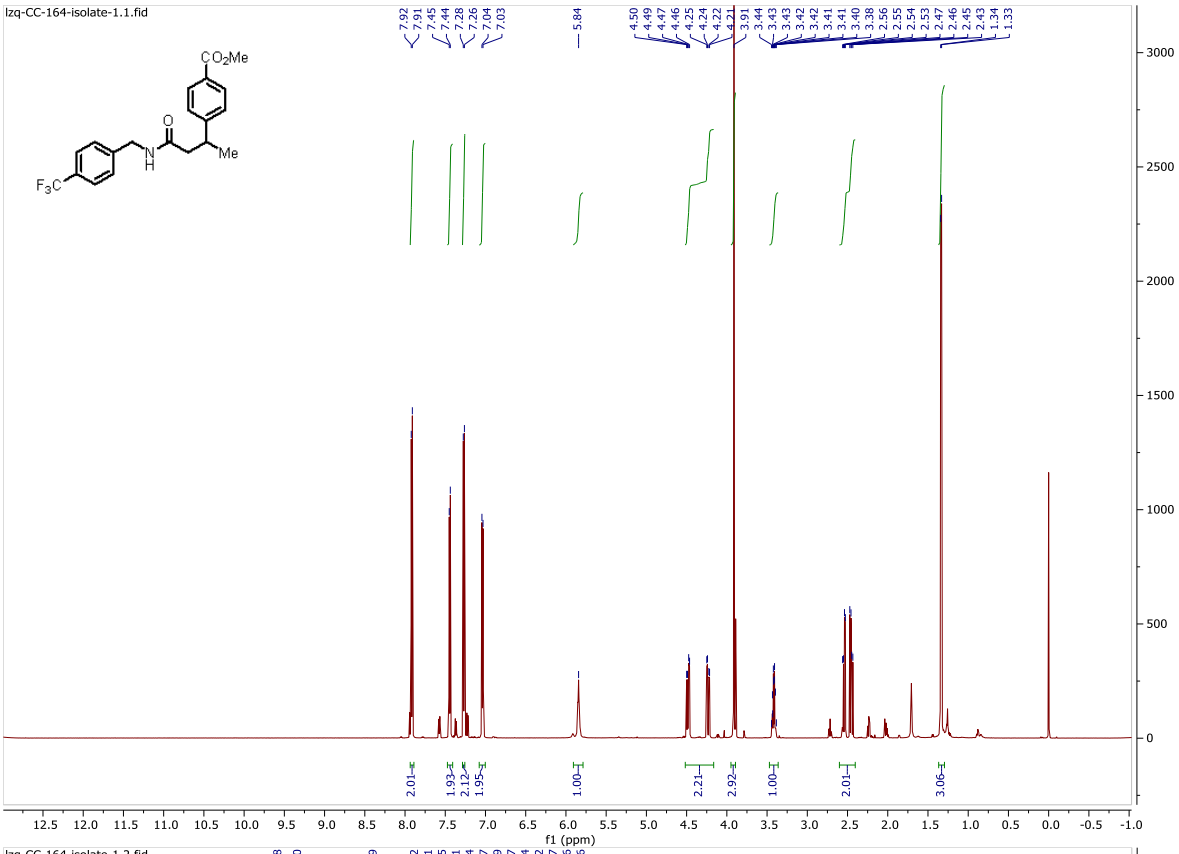

lzq-D-20210204-3.2.fid
n-Hex
Bn
N
H
O
Me
172.03
138.49
134.35
130.25
128.80
127.95
127.60
44.62
43.68
34.25
32.62
31.84
29.55
28.97
22.76
20.81
14.23
f1 (ppm)

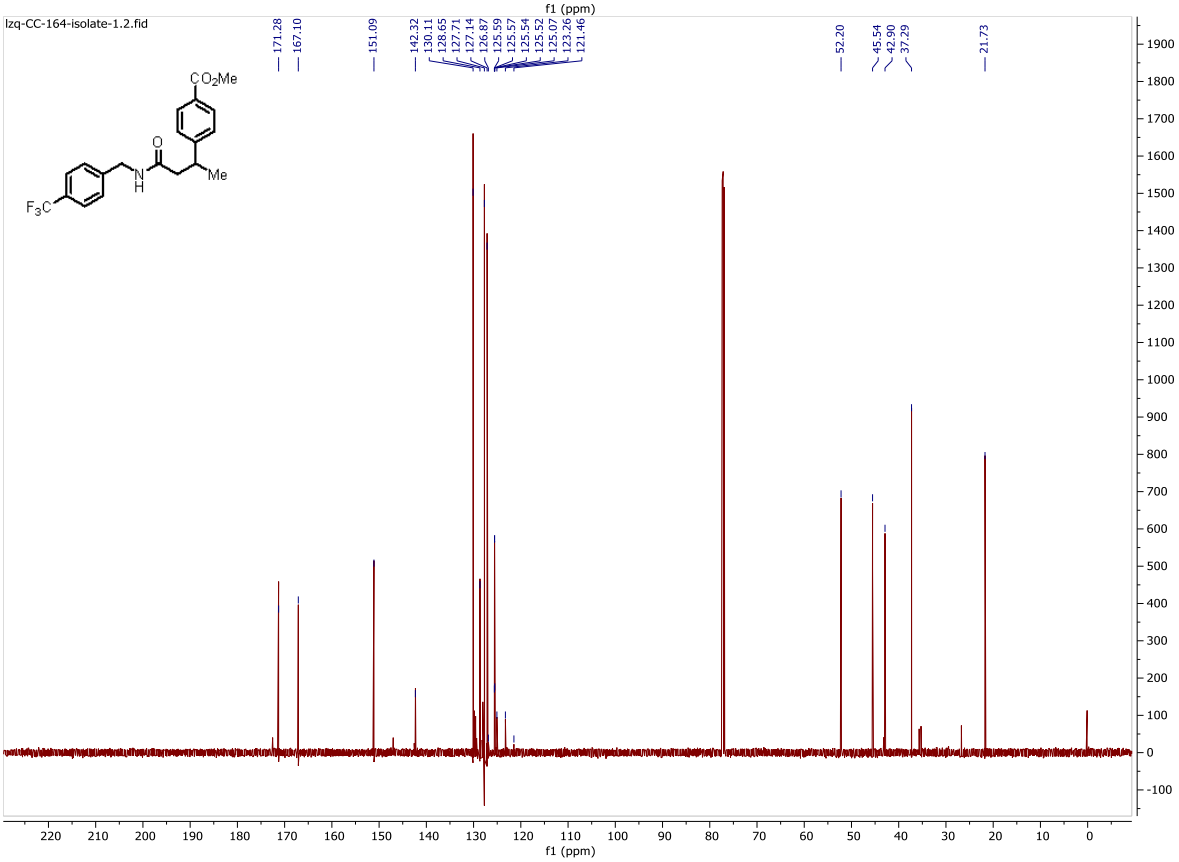

lzq-D-49-isolate-5.1.fid
CO2Me
Me
O
N
H
Me
Me
2.16
1.97
1.02
1.99
0.94
3.12
1.15
2.04
5.88
3.00
f1 (ppm)

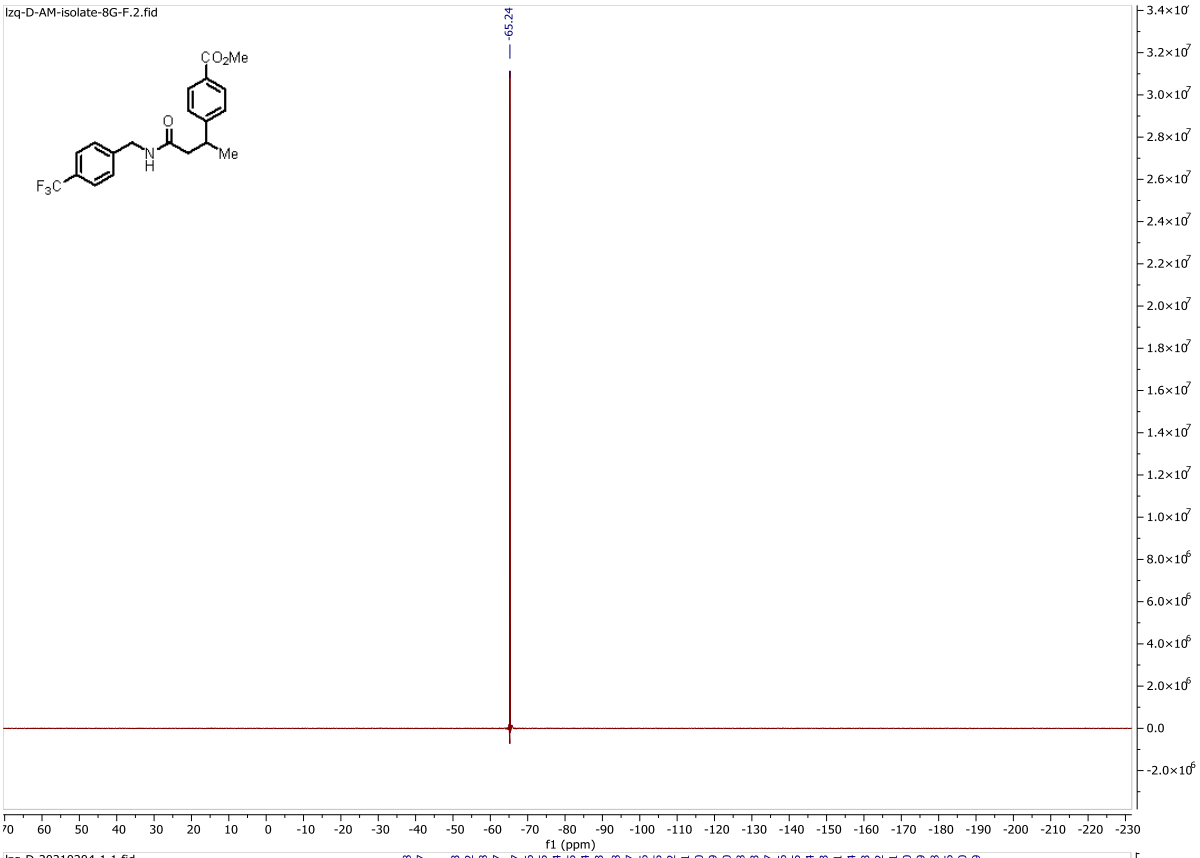

lzq-D-49-isolate-5.2.fid
CO2Me
Me
O
N
H
Me
Me
169.71
167.13
151.36
135.48
133.78
130.13
128.59
128.23
127.48
127.21
52.18
45.08
37.13
22.05
18.34
f1 (ppm)

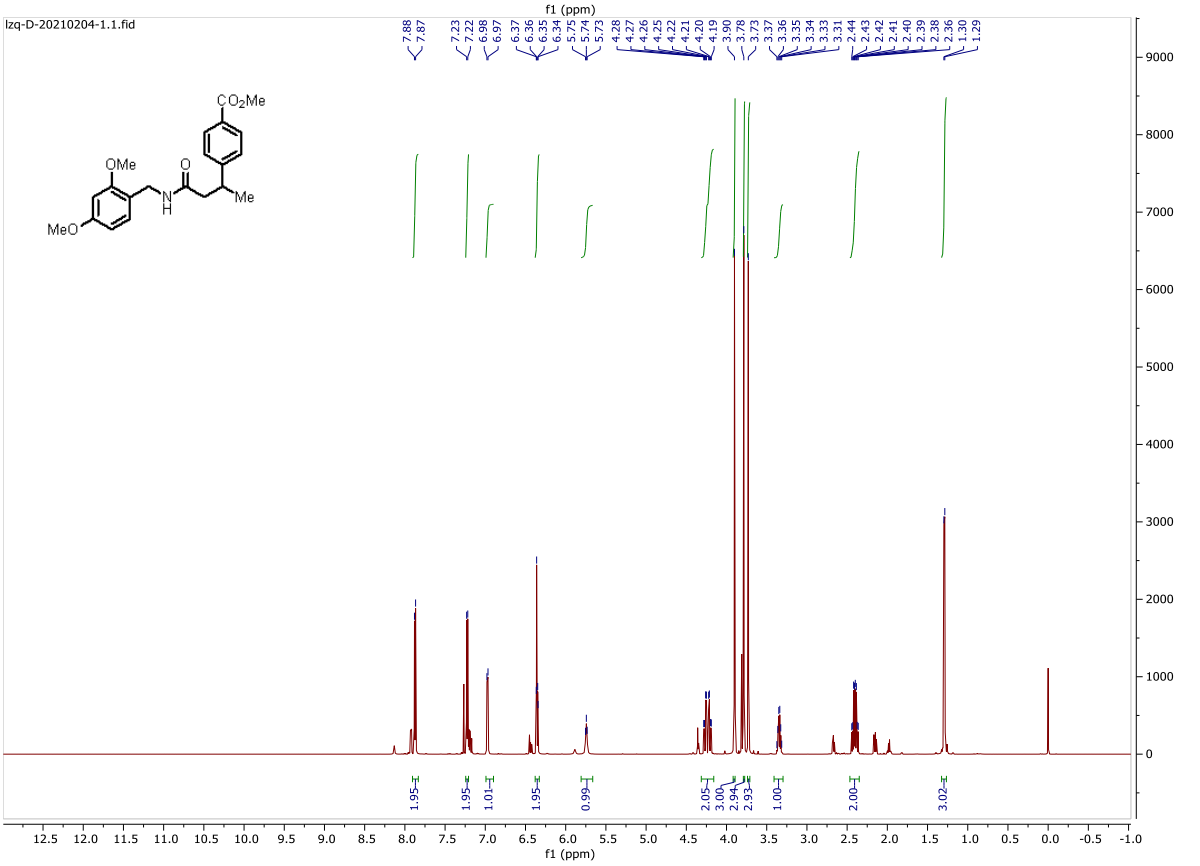

lzq-D-52-isolate-4.1.fid
CO2Me
Ph
O
Ph
N
H
Me
7.94 7.92 7.27 7.27 7.27 7.26 7.26 7.25 7.18 7.18 7.18 7.18 7.17 7.11 7.10 7.10 6.86 6.84 6.13 6.11 5.99 5.98
3.91 3.42 3.41 3.39 3.39 3.38 3.38 3.37 3.36 2.55 2.54 2.52 2.51 2.49 2.47 2.47 2.45 1.32 1.31
2.14 4.99 3.08 2.01 1.98 1.11 0.95 2.93 1.00 1.97 3.02
f1 (ppm)

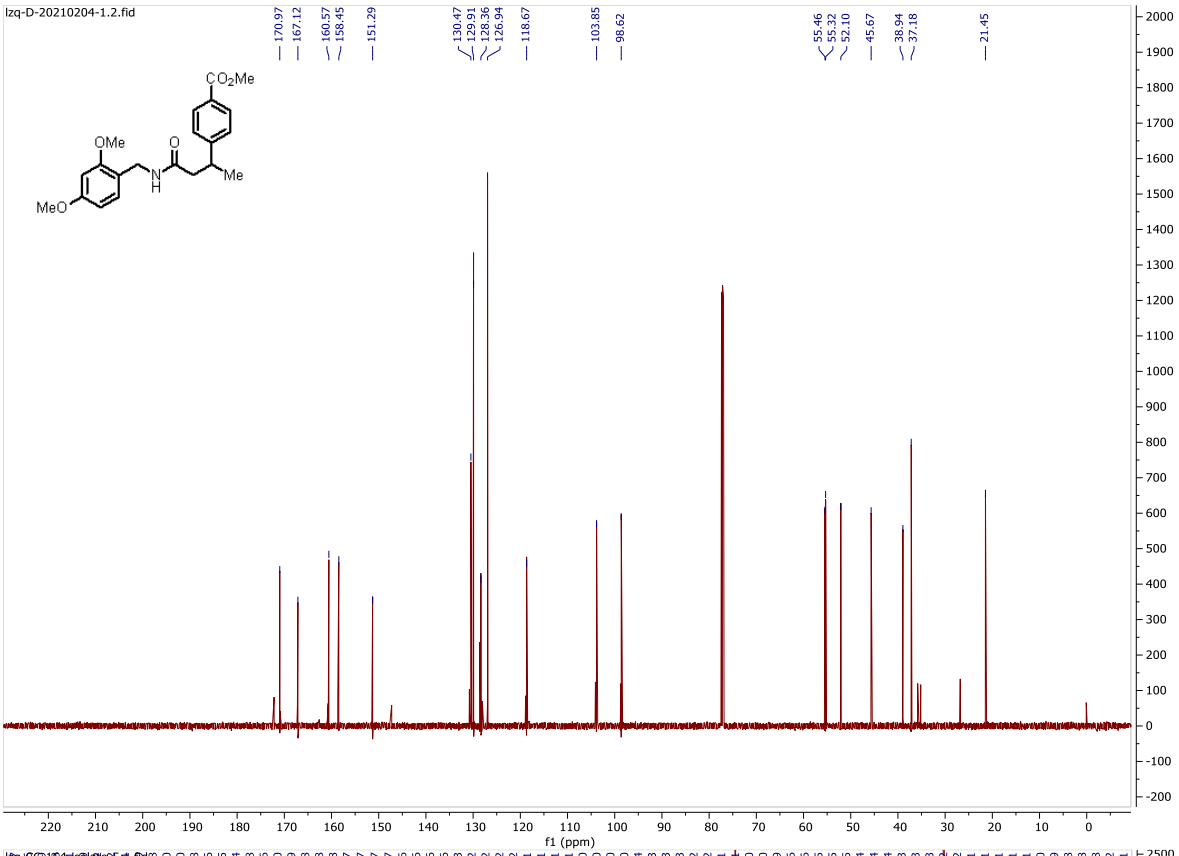

lzq-D-52-isolate-4.2.fid
CO2Me
Ph
O
Ph
N
H
Me
170.25 167.12 151.18 141.52 141.21 130.15 128.79 128.74 128.58 127.58 127.51 127.39 127.24 127.12 56.92 52.17 45.59 37.29 21.80
f1 (ppm)

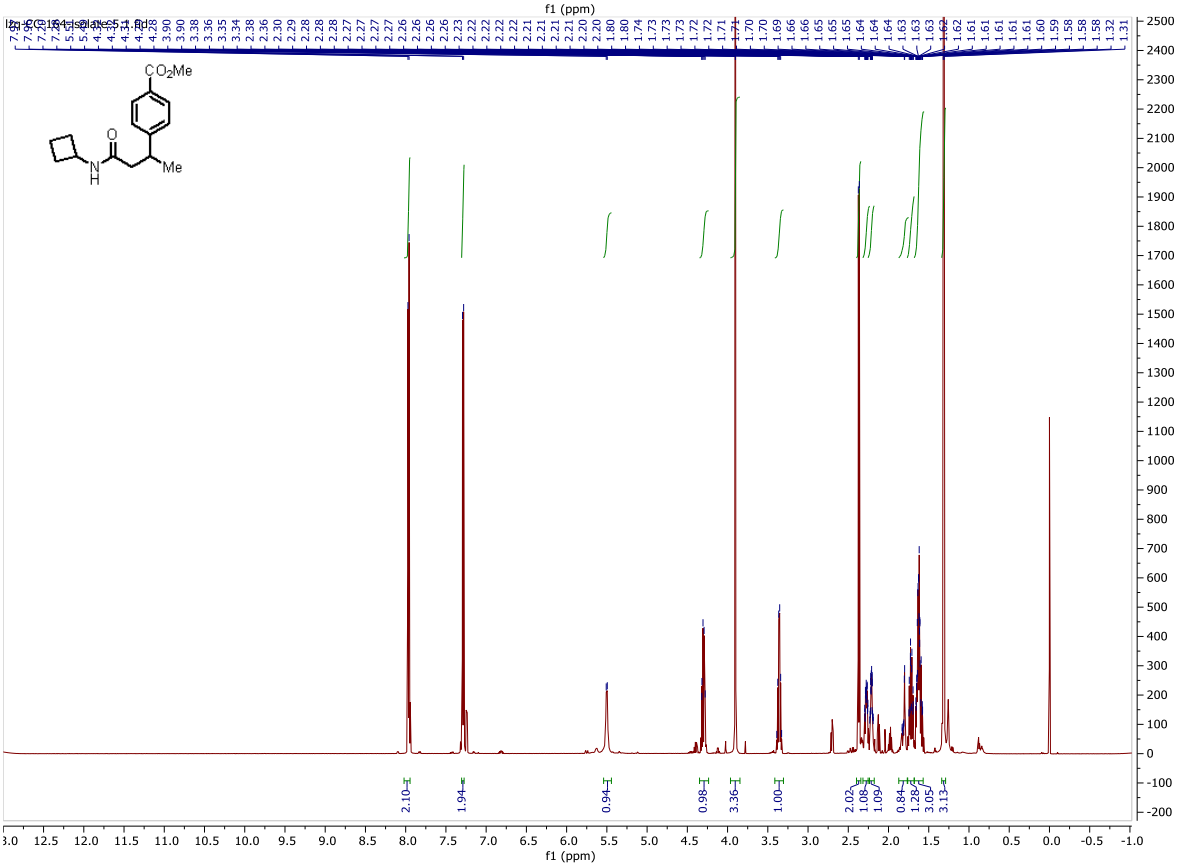

lzq-CC-164-isolate-1.1.fid
CO2Me
O
N
H
Me
F3C
7.92
7.91
7.45
7.44
7.28
7.26
7.04
7.03
5.84
4.50
4.49
4.47
4.46
4.25
4.24
4.22
4.21
3.91
3.44
3.43
3.43
3.42
3.42
3.41
3.41
3.40
3.38
2.56
2.55
2.54
2.53
2.47
2.46
2.45
2.43
1.34
1.33
2.01
1.93
2.12
1.95
1.00
2.21
2.92
1.00
2.01
3.06
f1 (ppm)

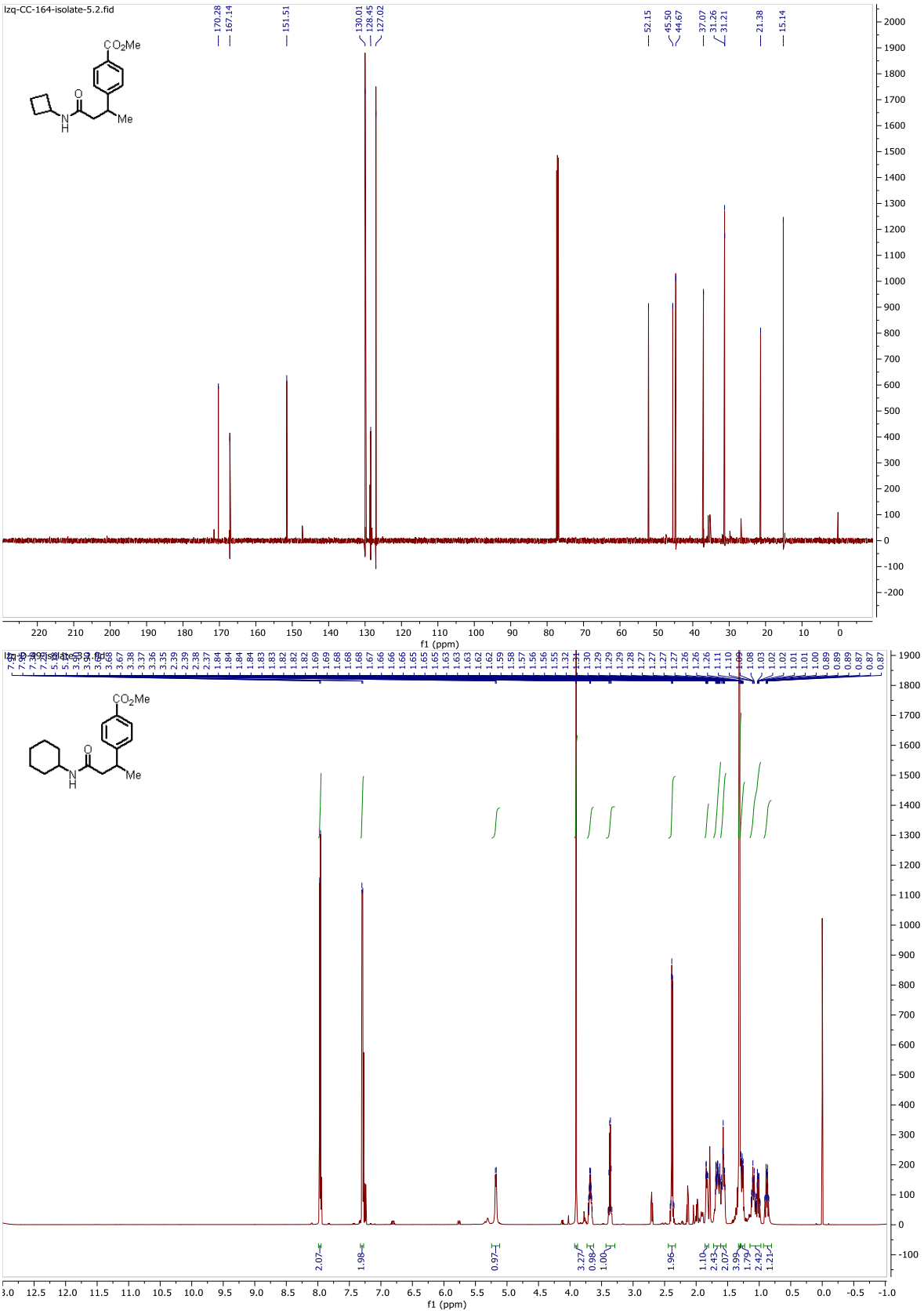

lzq-CC-164-isolate-1.2.fid
CO2Me
O
N
H
Me
F3C
171.28
167.10
151.09
142.32
130.11
128.65
127.71
127.14
126.87
125.99
125.57
125.54
125.52
125.07
123.26
121.46
52.20
45.54
42.90
37.29
21.73
f1 (ppm)

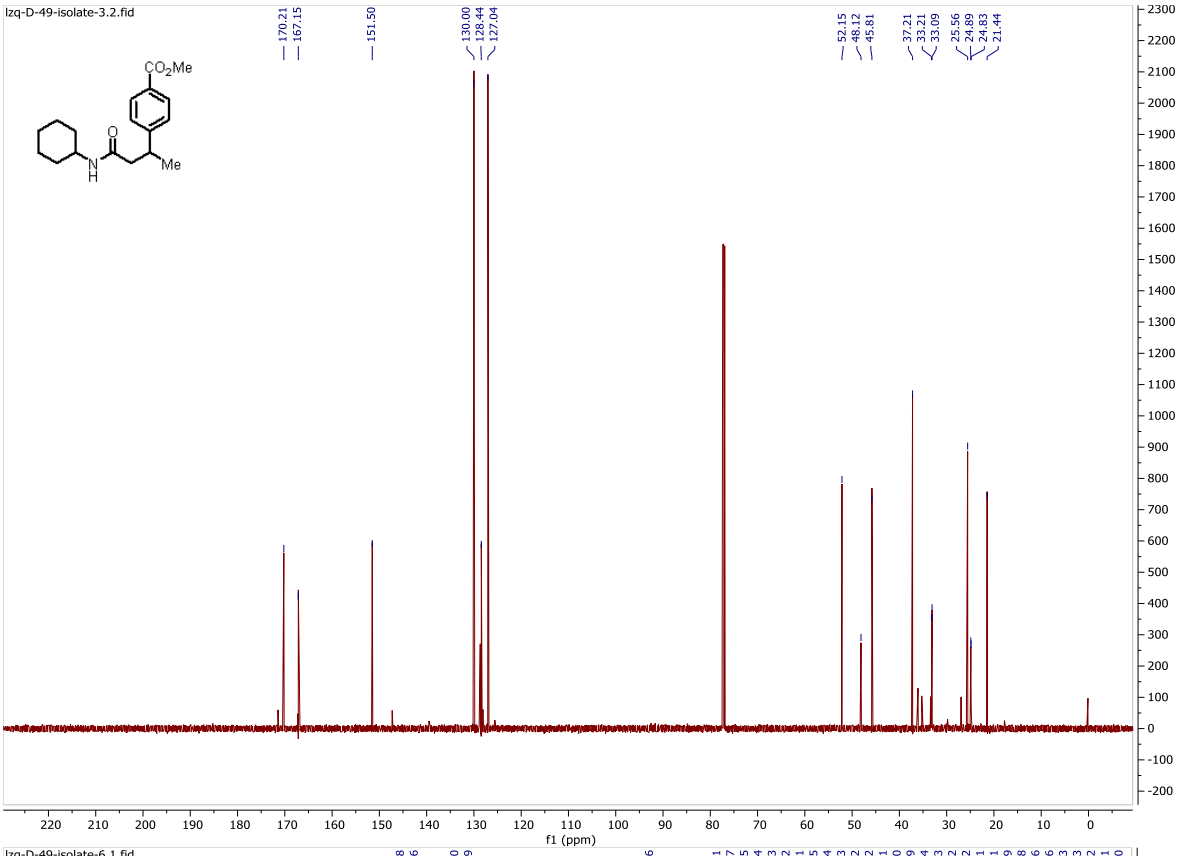

lzq-D-AM-isolate-8G-F.2.fid
-65.24
f1 (ppm)

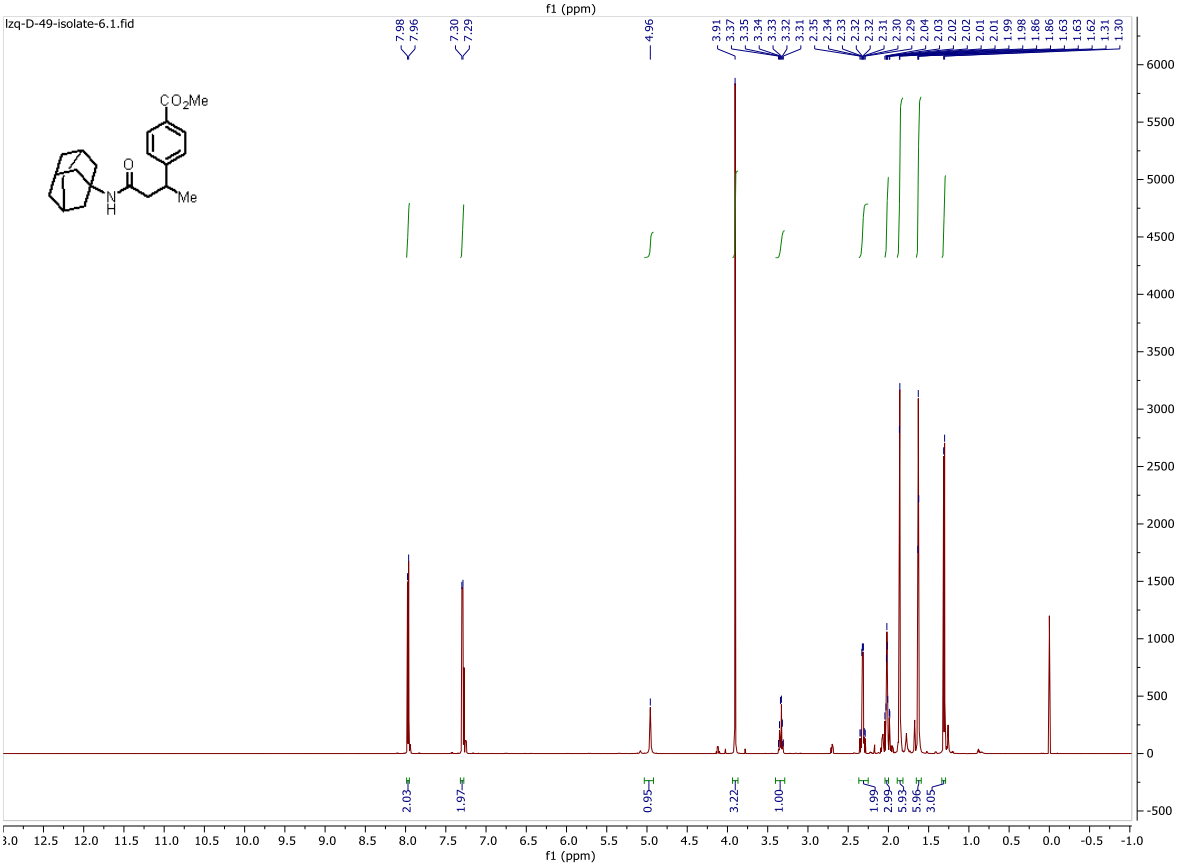

lzq-D-20210204-1.1.fid
f1 (ppm)

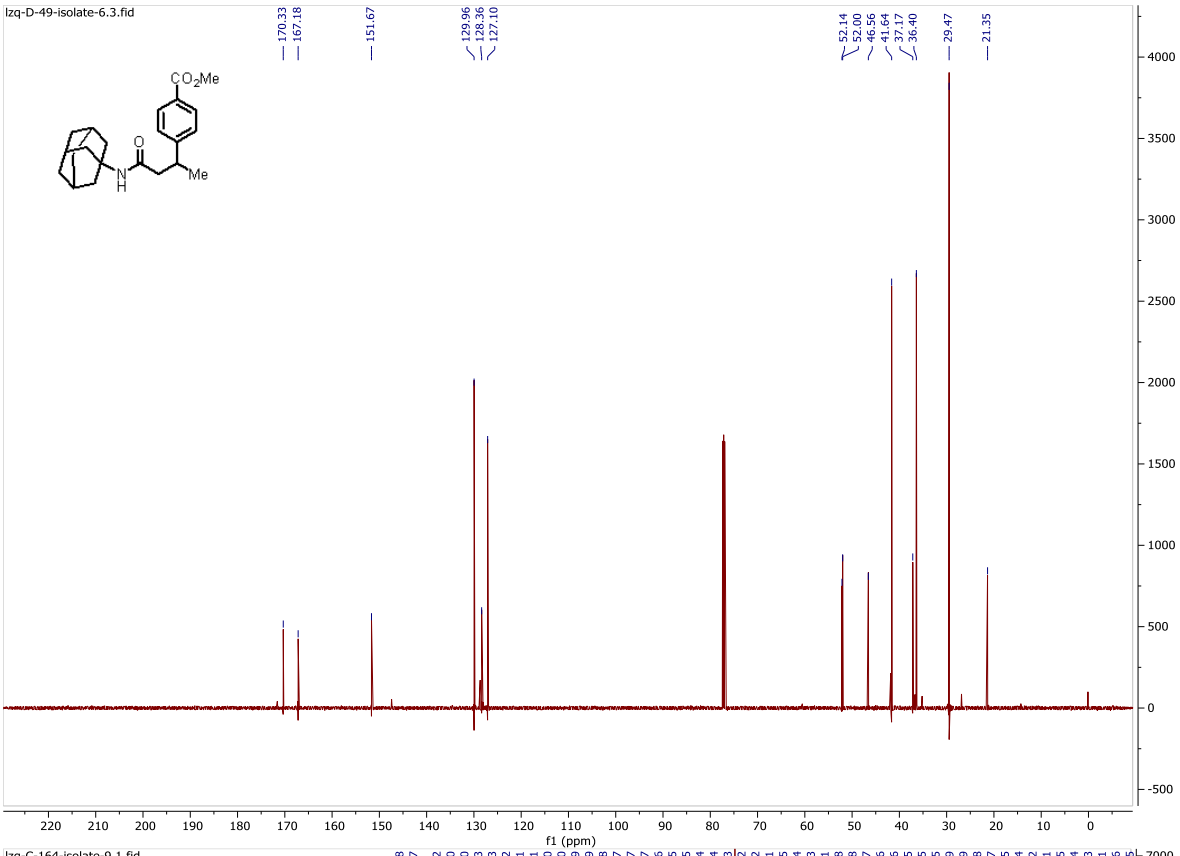

lzq-D-20210204-1.2.fid
170.97
167.12
160.57
158.45
151.29
130.47
129.91
128.36
126.94
118.67
103.85
98.62
55.46
55.32
52.10
45.67
38.94
37.18
21.45
CO2Me
OMe
O
N
H
Me
MeO
f1 (ppm)

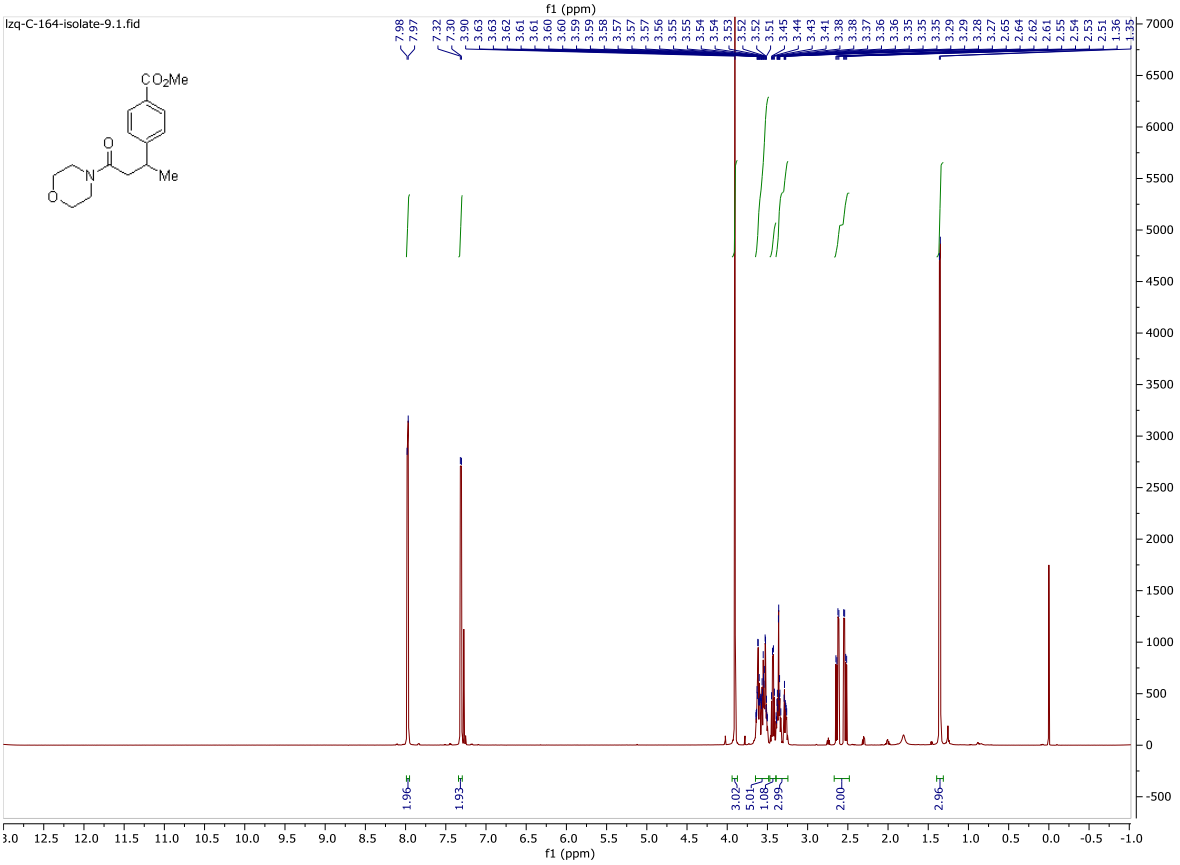

CO2Me
O
N
H
Me
2.10
1.94
0.94
0.98
3.36
1.00
2.02
1.08
1.09
0.84
1.28
3.05
3.13
f1 (ppm)

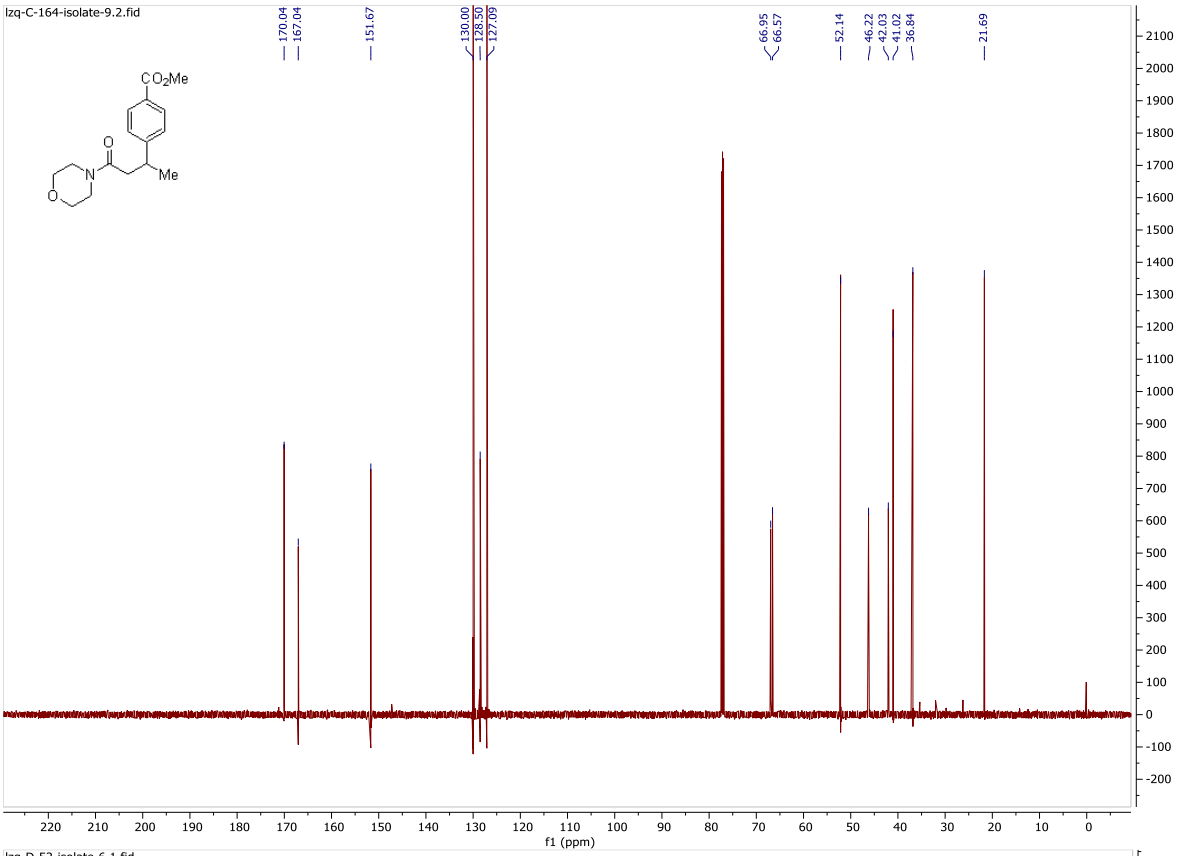

lzq-CC-164-isolate-5.2.fid
170.28
167.14
151.51
130.01
128.45
127.02
52.15
45.50
44.67
37.07
31.26
31.21
21.38
15.14
CO2Me
O
N
H
Me
f1 (ppm)
2.07
1.98
0.97
3.27
0.98
1.00
1.96
1.10
2.43
2.07
3.99
1.79
2.42
1.21

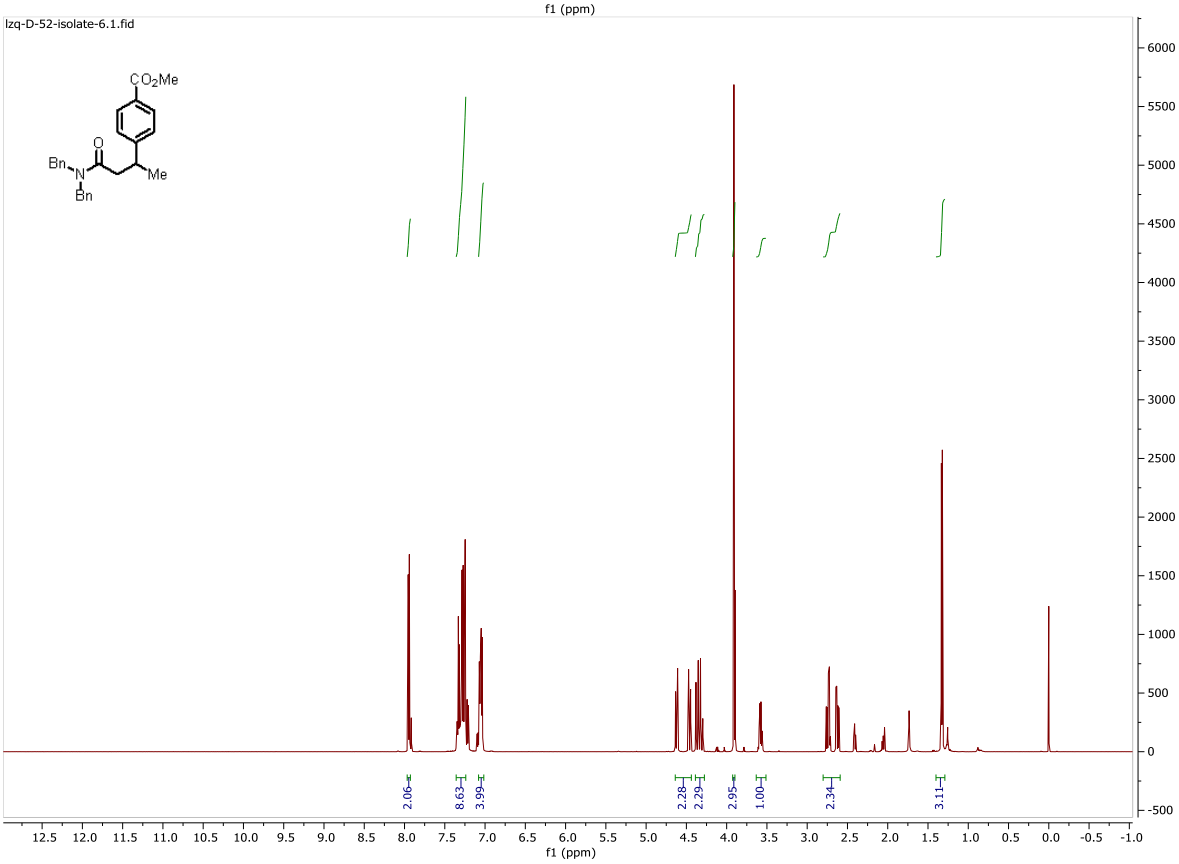

lzq-D-49-isolate-3.2.fid
170.21
167.15
151.50
130.00
128.44
127.04
52.15
48.12
45.81
37.21
33.21
33.09
25.56
24.89
24.83
21.44
CO2Me
O
N
H
Me
f1 (ppm)

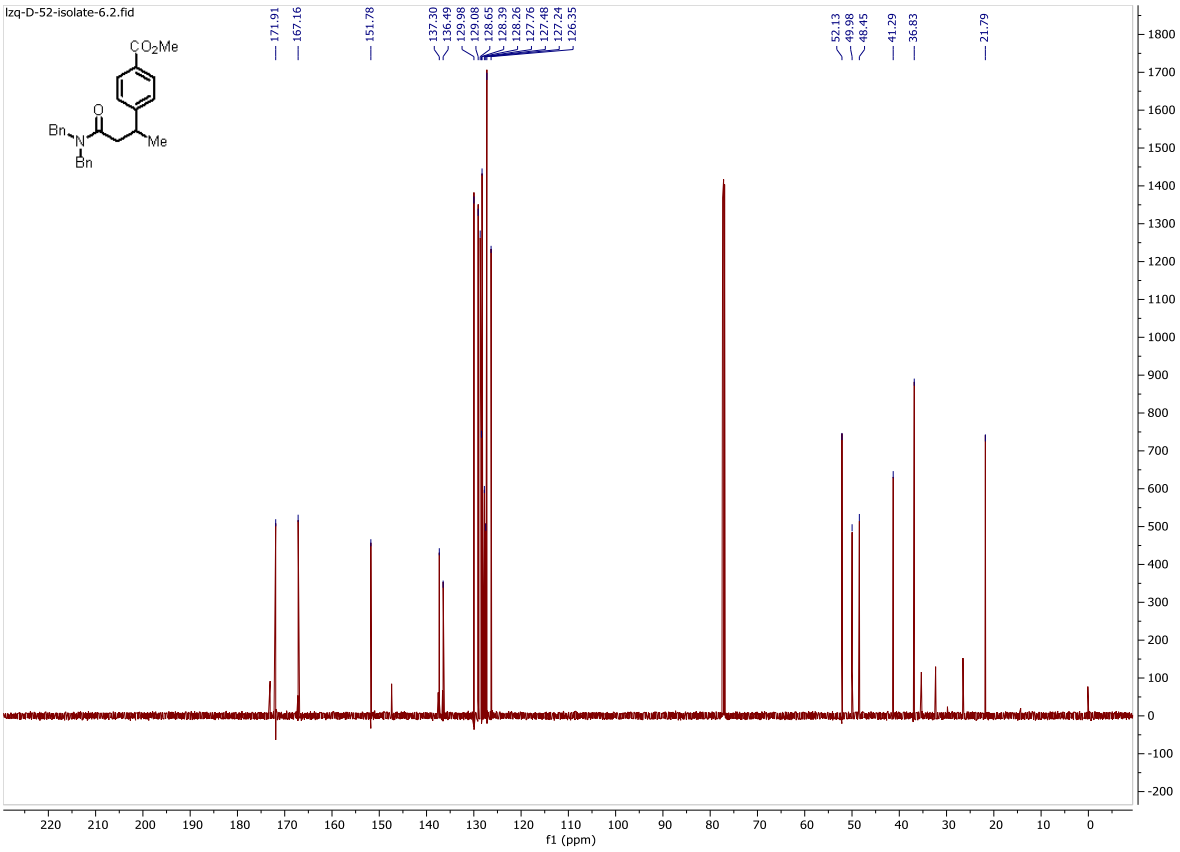

lzq-D-49-isolate-6.1.fid
7.98
7.96
7.30
7.29
4.96
3.91
3.37
3.35
3.34
3.33
3.32
3.31
2.35
2.34
2.33
2.32
2.32
2.31
2.30
2.29
2.04
2.03
2.02
2.02
2.01
2.01
1.99
1.98
1.86
1.86
1.63
1.63
1.62
1.31
1.30
CO2Me
O
N
H
Me
2.03
1.97
0.95
3.22
1.00
1.99
2.99
5.93
5.96
3.05
f1 (ppm)

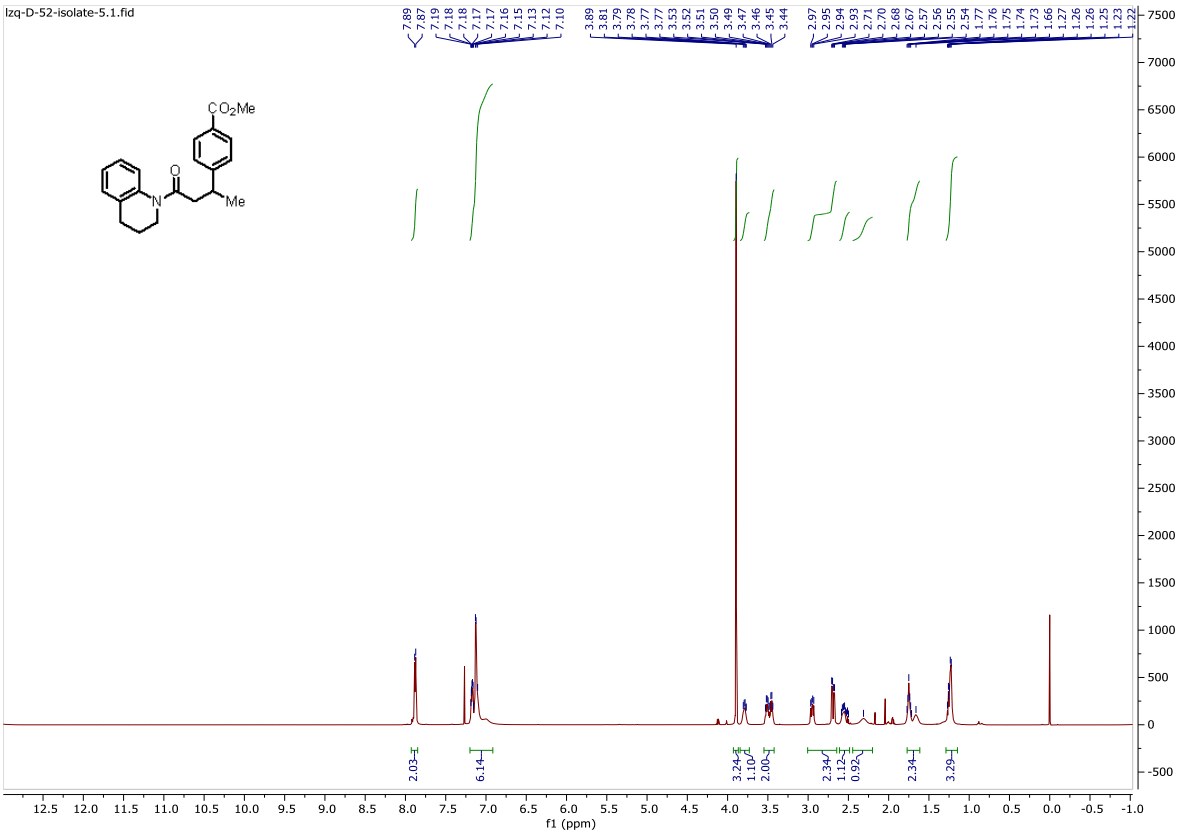

lzq-D-49-isolate-6.3.fid
170.33
167.18
151.67
129.96
128.36
127.10
52.14
52.00
46.56
41.64
37.17
36.40
29.47
21.35
CO2Me
O
N
H
Me
f1 (ppm)

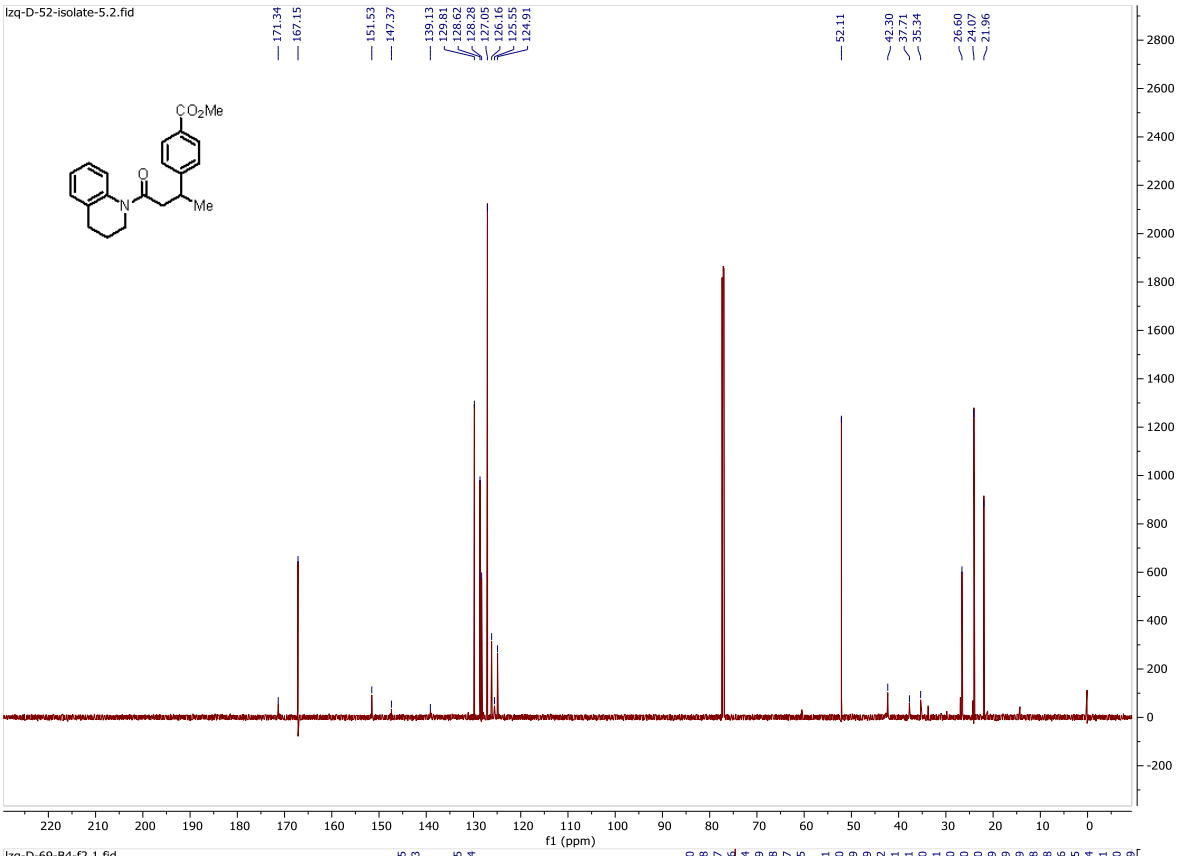

lzq-C-164-isolate-9.1.fid
CO2Me
O
N
O
Me
1.96
1.93
3.02
5.01
1.08
2.99
2.00
2.96
f1 (ppm)

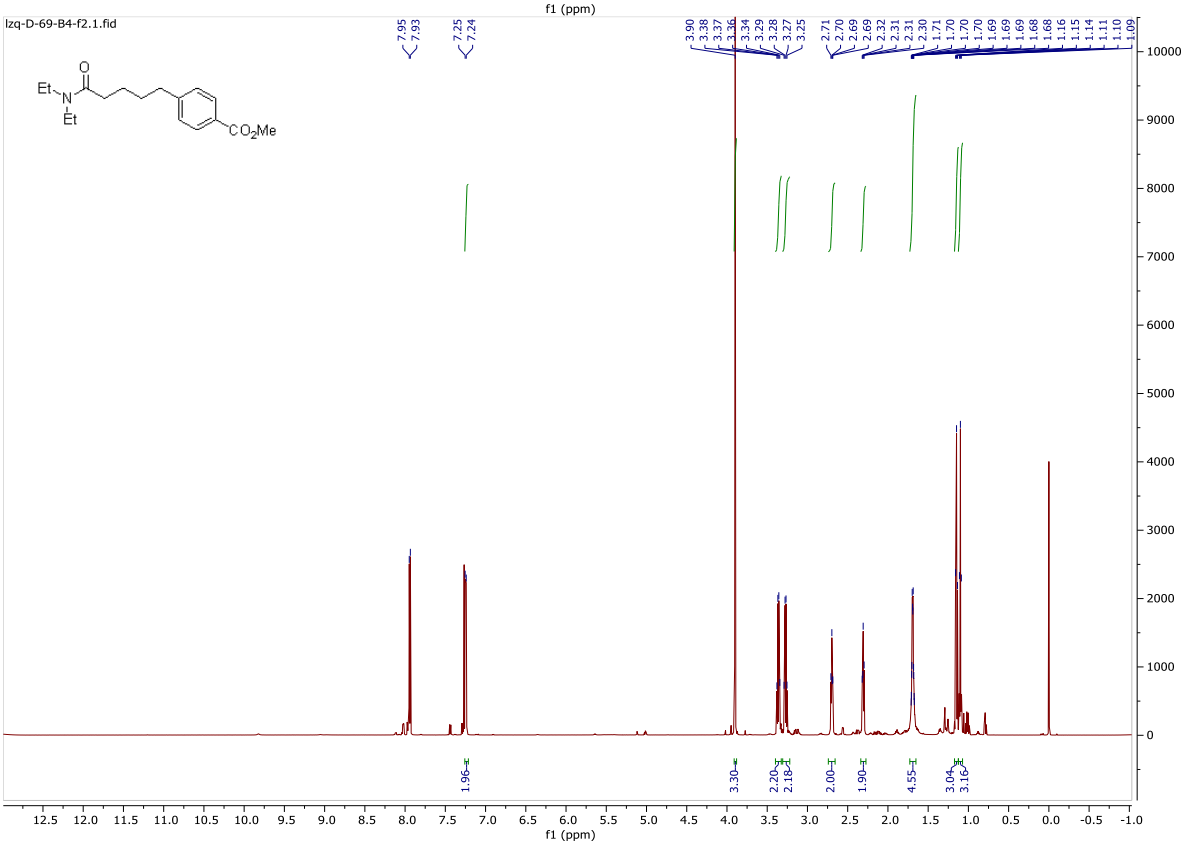

lzq-C-164-isolate-9.2.fid
170.04
167.04
151.67
130.00
128.50
127.09
66.95
66.57
52.14
46.22
42.03
41.02
36.84
21.69
CO2Me
O
N
O
Me
f1 (ppm)

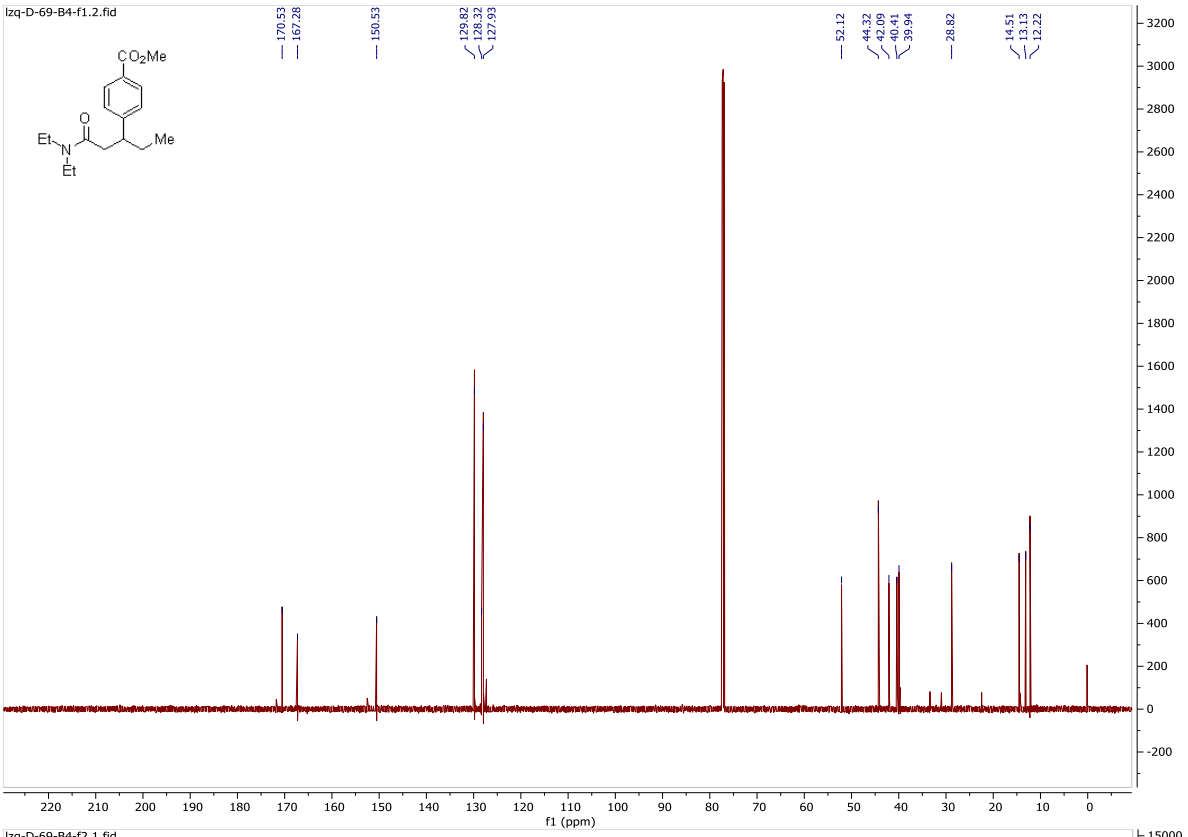

lzq-D-52-isolate-6.1.fid
CO2Me
O
Bn
N
Bn
Me
2.06
8.63
3.99
2.28
2.29
2.95
1.00
2.34
3.11
f1 (ppm)

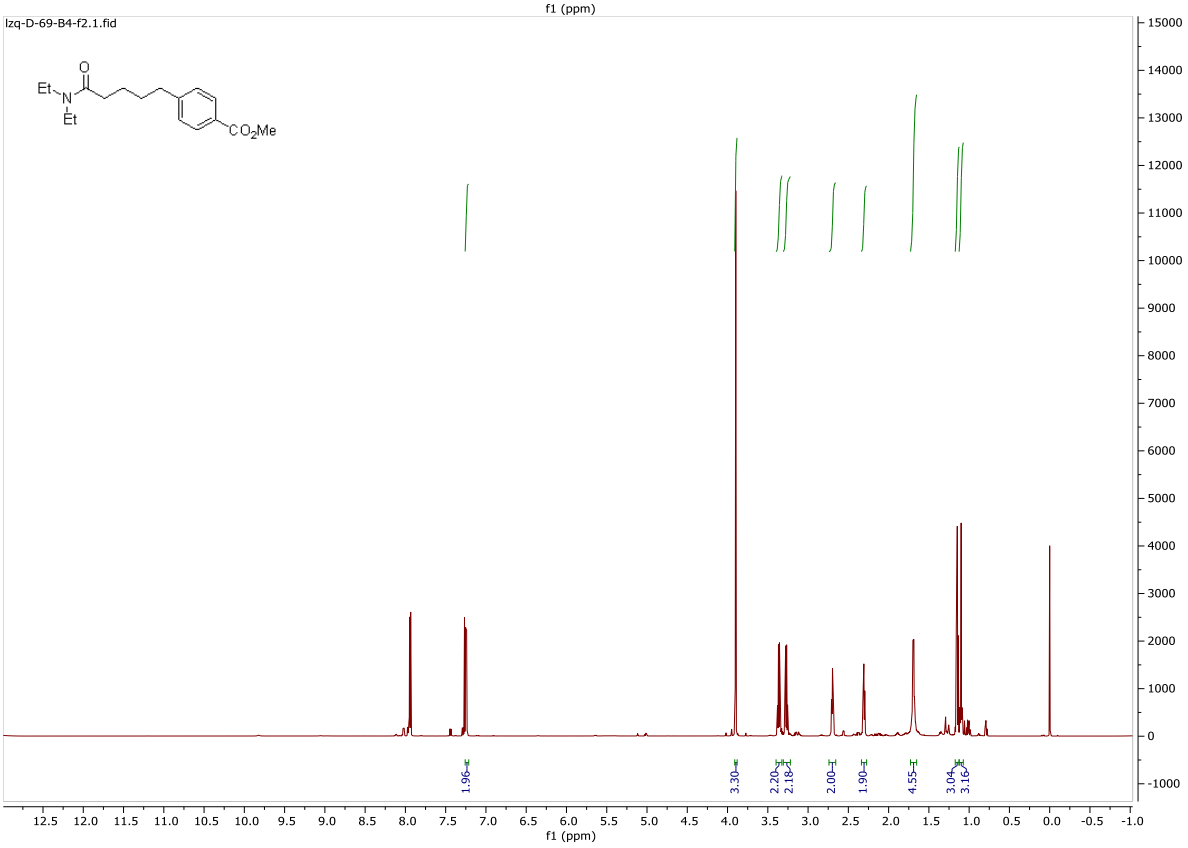

lzq-D-52-isolate-6.2.fid
171.91
167.16
151.78
137.30
136.49
129.98
129.08
128.65
128.39
128.26
127.76
127.48
127.24
126.35
52.13
49.98
48.45
41.29
36.83
21.79
CO2Me
Bn
N
Bn
O
Me
f1 (ppm)

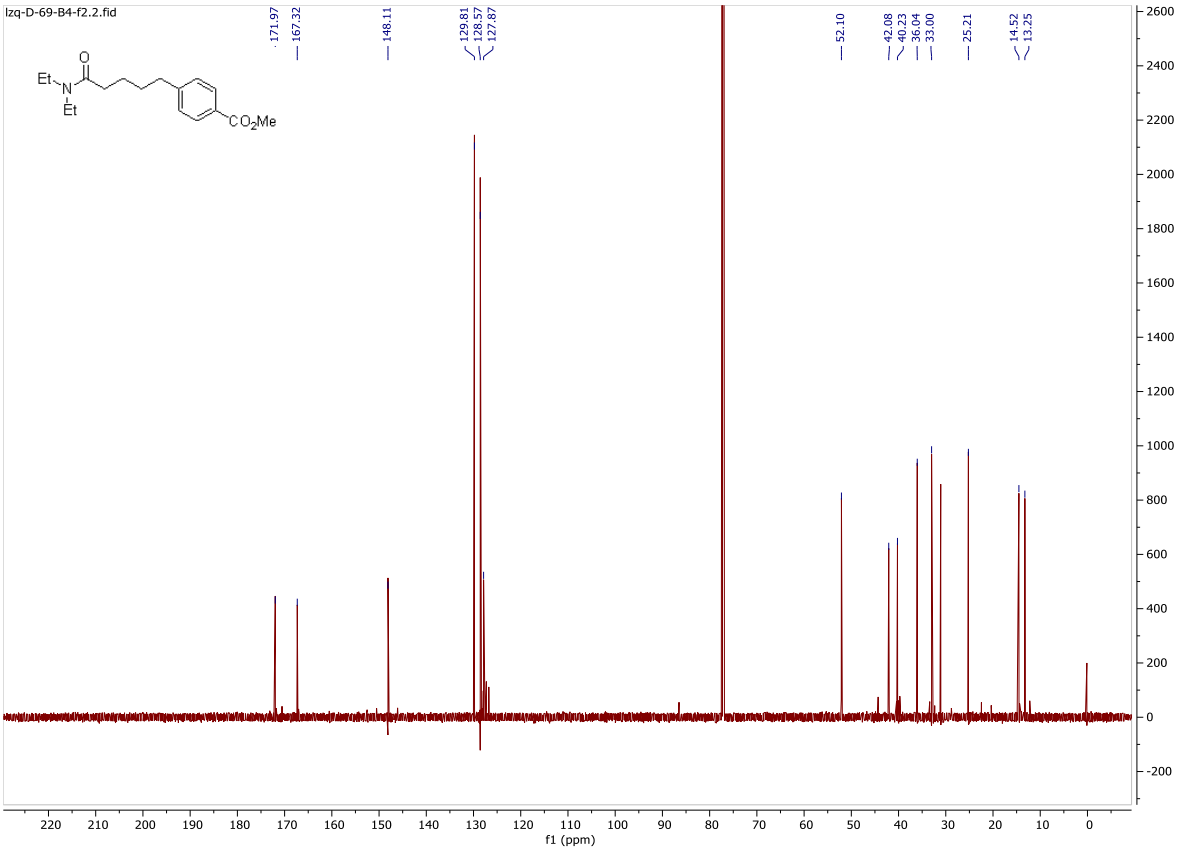

lzq-D-52-isolate-5.1.fid
7.89
7.87
7.19
7.18
7.18
7.17
7.17
7.16
7.15
7.13
7.12
7.10
3.89
3.81
3.79
3.78
3.77
3.77
3.53
3.52
3.51
3.50
3.49
3.47
3.46
3.45
3.44
2.97
2.95
2.94
2.93
2.71
2.70
2.68
2.67
2.57
2.56
2.55
2.54
1.77
1.76
1.75
1.74
1.73
1.66
1.27
1.26
1.26
1.25
1.23
1.22
CO2Me
N
O
Me
2.03
6.14
3.24
1.10
2.00
2.34
1.12
0.92
2.34
3.29
f1 (ppm)


lzq-D-52-isolate-5.2.fid
171.34
167.15
151.53
147.37
139.13
129.81
128.62
128.28
127.05
126.16
125.55
124.91
52.11
42.30
37.71
35.34
26.60
24.07
21.96
CO2Me
O
N
Me
f1 (ppm)


lzq-D-69-B4-f2.1.fid
7.95
7.93
7.25
7.24
3.90
3.38
3.37
3.36
3.34
3.29
3.28
3.27
3.25
2.71
2.70
2.69
2.69
2.32
2.31
2.31
2.30
1.71
1.70
1.70
1.70
1.69
1.69
1.69
1.68
1.68
1.16
1.15
1.14
1.11
1.10
1.09
Et
N
Et
O
CO2Me
1.96
3.30
2.20
2.18
2.00
1.90
4.55
3.04
3.16
f1 (ppm)


lzq-D-69-B4-f1.2.fid
170.53
167.28
150.53
129.82
128.32
127.93
52.12
44.32
42.09
40.41
39.94
28.82
14.51
13.13
12.22
CO2Me
Et
N
Et
O
Me
f1 (ppm)


lzq-D-69-B4-f2.1.fid
Et
N
Et
O
CO2Me
1.96
3.30
2.20
2.18
2.00
1.90
4.55
3.04
3.16
f1 (ppm)


lzq-D-69-B4-f2.2.fid
171.97
167.32
148.11
129.81
128.57
127.87
52.10
42.08
40.23
36.04
33.00
25.21
14.52
13.25
Et
N
Et
O
CO2Me
f1 (ppm)