Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Rhodium(III)-catalyzed synthesis of 3-trifluoromethylindanones from *N*-Methoxybenzamides via C-H activation and Claisen/Retro-Claisen reaction

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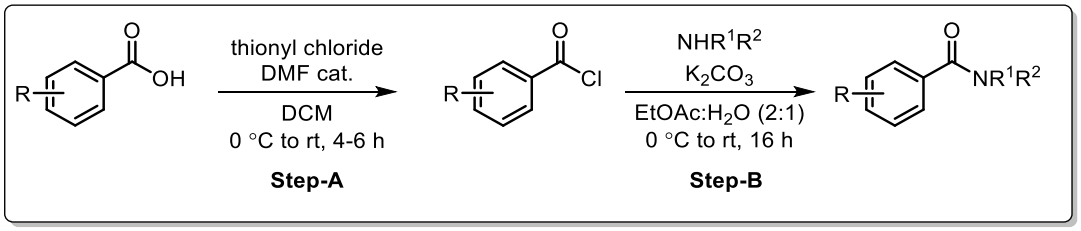
General Information: Commercially available chemicals were obtained from Sigma-Aldrich and used as received unless otherwise stated. Unless otherwise noted, all the reactions were carried out under air using the sealed pressure tubes. Reaction temperatures are reported as the temperature of the bath surrounding the vessel unless otherwise stated. NMR spectra were recorded on a Bruker AVANCE NEO 500 MHz (^{1}H = 500 MHz, ^{13}C = 125 MHz and ^{19}F = 470 MHz) spectrometer with $CDCl_3$ as reference solvent at ambient temperature. Chemical shifts are given in parts per million (ppm) relative to TMS. The residual solvent signals were used as references and the chemical shifts converted to the TMS scale ($CDCl_3$: δ_H = 7.26 ppm, δ_C = 77.16 ppm). Chromatographic separations were performed using 230-400 mesh silica gel. IR spectra were recorded as KBr pellet on Bruker Alpha FT-IR spectrometer. High Resolution Mass Spectra (HRMS) were recorded on Agilent Q-TOF LC/MS. Melting points were uncorrected and were taken on Buchi M-560. No attempts were made to optimize yields for starting materials synthesis.

Preparation of benzamide derivatives (1a-1y).[1]



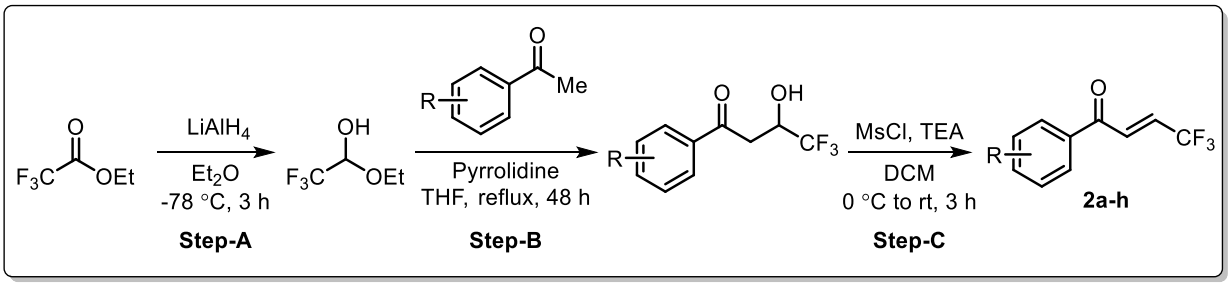
Following same procedure by Fagnou et. al.[1]

Step-A: To a solution of the carboxylic acid (3.0 mmol, 1.0 equiv) in DCM (10 mL, 0.3 M) at 0 °C was added thionyl chloride (3.6 mmol, 1.2 equiv) dropwise, followed by a catalytic amount of DMF (2 drops). The reaction was allowed to stir at rt until completion (typically 4–6 h). The solvent was then removed under reduced pressure to afford the corresponding crude acid chloride.

Step-B: Corresponding amine (3.6 mmol, 1.2 equiv.) was added to a biphasic mixture of K_2CO_3 (2.0 equiv.) in a 2:1 mixture of EtOAc:H_2O (36 mL, 0.08 M). The resulting solution was cooled to 0 °C followed by dropwise addition of the unpurified acid chloride dissolved in a minimum amount of EtOAc. The flask containing the acid chloride was then rinsed with additional EtOAc.

The reaction was allowed to stir for 16 h while reaching rt. Afterwards, the phases were separated and the aqueous phase was extracted twice with EtOAc (30 mL × 2). The combined organic layers were washed with aqueous K_2CO_3 solution (0.2 M, 20 mL), brine and dried over sodium sulfate, filtered, and evaporated under reduced pressure. The pure products were obtained without any further purification.

Preparation of β-trifluoromethyl-substituted enones (2a-h).[2, 3, 4]



Following same procedure by Xiao et. al.,[2] Yu et. al.,[3] and Konno et. al.[4]

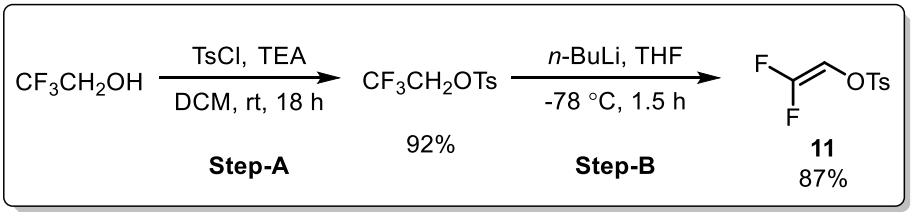
Step-A:[2] A solution of ethyl trifluoroacetate (14.2 g, 0.100 mol) in Et_2O (50 mL) was added slowly at -78 °C to a suspension of $LiAlH_4$ (1.33 g, 0.035 mol) in Et_2O (100 mL). The reaction mixture was stirred at this temperature for 3 h and then treated slowly with cooled H_2SO_4 (1.0 M, 100 mL). The upper layer was separated and the aqueous phase was extracted by Et_2O (100 mL × 2). The combined organic phases were dried over sodium sulfate, evaporated, and distilled under normal pressure. Ethyl trifluoroacetaldehyde hemiacetal was obtained at 95-100 °C (7.84 g, 54%).

Step-B:[3] To a solution of trifluoroacetaldehyde ethyl hemiacetal (1.44 g, 10.0 mmol) in THF (20 mL), pyrrolidine (0.49 g, 7.0 mmol) was added and the resulting mixture was stirred at room temperature for 30 min. Then corresponding acetophenone (10.0 mmol) was poured into the solution. The reaction mixture was stirred at reflux for 48 h. After cooling to ambient temperature, all the volatiles were removed under reduced pressure. The resulting residue was purified by silica gel column chromatography (eluent; hexane/EtOAc = 10:1) to afford β-trifluoromethyl-β-hydroxy ketones.

Step-C:[4] To a solution of β-hydroxy ketones (5 mmol), in dichloromethane (10 mL) was added methanesulfonyl chloride (0.86 g, 7.5 mmol) and triethylamine (1.52 g, 15 mmol) at 0 °C. After

being stirred at rt for 3 h, the reaction mixture was quenched with H_2O, followed by extraction with dichloromethane (30 mL × 2). The combined organic layers were dried over anhydrous sodium sulfate, concentrated under reduced pressure. The residue was purified by silica gel column chromatography (eluent; hexane/EtOAc = 40:1) to afford β-trifluoromethyl-substituted enones (**2a**-**2h**).

Preparation of 2,2-difluorovinyl tosylate (11).[5]

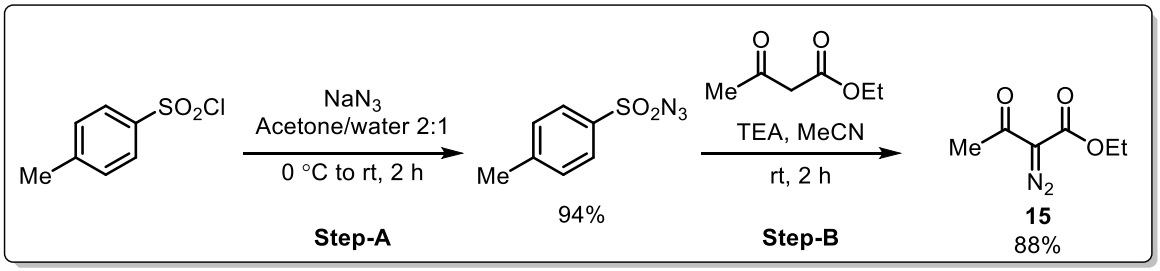


Following same procedure by Sandell et. al.[5]

Step-A: A solution of 2,2,2-trifluoroethanol (1.0 g, 10 mmol) and triethylamine (3.64 g, 36 mmol) in CH_2Cl_2 (10 mL) was cooled to 0 ℃. *p*-toluenesulfonyl chloride (2.3 g, 12 mmol) was added, and the solution was stirred at 0 ℃ for 1 h, then warmed to room temperature and stirred for a further 12 h. The CH_2Cl_2 layer was separated and washed with brine (2 mL), dried over sodium sulfate, filtered, and evaporated to afford 2,2,2-trifluoroethyltosylate as off white solid (2.34 g, 92%).

Step-B: To a solution of 2,2,2-trifluoroethyltosylate (2.34 g, 9.2 mmol) in THF (50 mL) at -78 ℃ was added dropwise 1.6 M n-butyllithium in hexanes (12.5 mL, 20 mmol). After stirring under a nitrogen atmosphere at -78 ℃ for 1 h, the solution was neutralized with a mixture of THF/H_2O (1:1, 30 mL). Water (~20 mL) was added, and the organic phase was extracted with ethyl acetate (30 mL × 2), dried over sodium sulfate, filtered, and evaporated. Purification by chromatography on silica gel to afford 2,2-difluorovinyl tosylate as a light yellowish oil (1.87 g, 87%).

Preparation ethyl-2-diazo-3-oxobutanoate (15).[6]

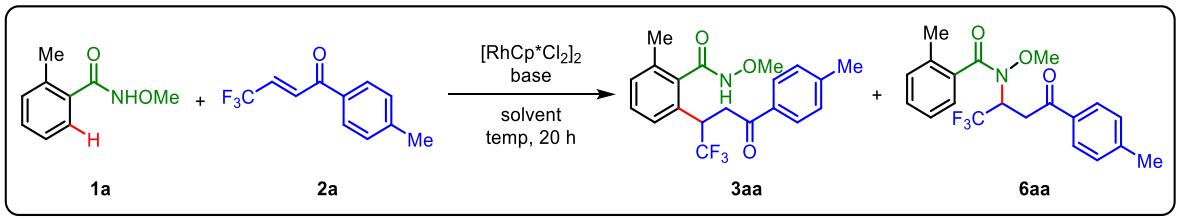


Following same procedure by Maguire et. al.[6]

Step-A: A solution of *p*-toluenesulfonyl chloride (1.90 g, 10 mmol) in acetone (10 mL) was added dropwise over 15 min to a stirring solution of sodium azide (0.65 g, 10 mmol) in water (5 mL) at 0 °C. The reaction mixture was allowed to reach room temperature and was stirred for 2 h after which time the acetone was removed under reduced pressure. The aqueous solution was extracted with dichloromethane (20 mL × 2) and the organic layer was then washed with water (15 mL × 2) and brine (10 mL). The organic layer was dried and concentrated under reduced pressure to give pure *p*-toluenesulfonyl azide as a colourless oil which crystallised to a white solid on refrigeration (1.85 g, 94%).

Step-B: Triethylamine (0.92 g, 9.9 mmol) was added to a stirring solution of ethyl 3-oxobutanoate (1.16 g, 8.93 mmol) in MeCN (80 mL). After 2 minutes *p*-toluenesulfonyl azide (1.85 g, 9.38 mmol) in acetonitrile (10 mL) was added dropwise, at room temperature, over 15 minutes. The reaction mixture was stirred in MeCN for 2 h. This was then concentrated under reduced pressure. The crude product was extracted with diethyl ether (30 mL × 2) and the organic layer was then washed with aqueous 9% KOH solution (12 mL × 2) and water (10 mL). The organic layer was dried and concentrated under reduced pressure to afford ethyl-2-diazo-3-oxobutanoate as a yellow oil (1.36 g, 88%).

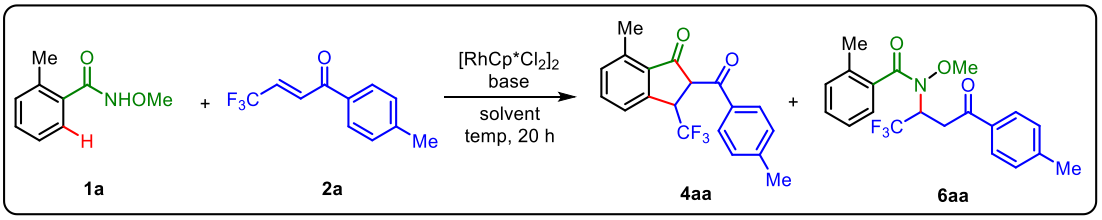
Optimization of C-H alkylated product (3):[a]



entry	base (mol %)	temp (°C)	solvent	yield (%)[b]	
				3aa	**6aa**
1	$AgSbF_6$ (6) AgOAc (20)	80	DCE	57	-
2	$AgSbF_6$ (6)	80	DCE	traces	-
3	AgOAc (20)	80	DCE	88	-
4	-	80	DCE	-	-
5[c]	AgOAc (20)	80	DCE	84	-
6[c]	**NaOAc (20)**	80	**DCE**	**84**	-
7[c]	KOAc (20)	80	DCE	86	-
8[c]	CsOAc (20)	80	DCE	62	-
9[c]	AcOH (20)	80	DCE	traces	
10[c]	Ag_2CO_3 (20)	80	DCE	54	
11[c]	K_2CO_3 (20)	80	DCE	23	47
12[c]	NaOAc (20)	80	TFE	77	-
13[c]	NaOAc (20)	50	DCE	69	-
14[c]	NaOAc (20)	rt	DCE	56	-
15[c]	K_2CO_3 (20)	rt	DCE	-	83
16[d]	K_2CO_3 (20)	rt	DCE	-	81

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.2 mmol), $[RhCp^*Cl_2]_2$ (1.5 mol %), base (quantity noted, mol %) in solvent (1.0 mL), temp (noted) for 20 h under air. [b]Isolated yield. [c]$[RhCp^*Cl_2]_2$ (1.0 mol %). [d]without $[RhCp^*Cl_2]_2$.

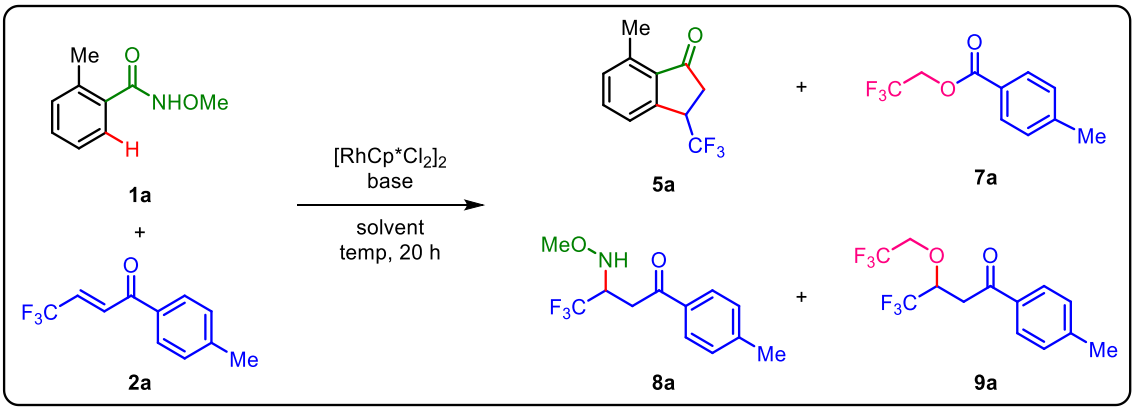
Optimization of 2-acyl-3-trifluoromethylindanone (4):[a]



entry	base (mol %)	temp (°C)	solvent	yield (%)[b]	
				4aa	**6aa**
1	CsOAc (20)	80	DCE	23	-
2	K_2CO_3 (20)	80	DCE	16	47
3	K_2CO_3 (20)	100	DCE	24	49
4	K_2CO_3 (20)	120	DCE	28	52
5	KOAc (100)	120	DCE	21	-
6[c]	KOAc (100)	120	DCE	29	-
7[d]	KOAc (100)	120	DCE	75	-
8[d]	**KOAc (150)**	120	**DCE**	**81**	-
9[d]	NaOAc (150)	120	DCE	76	-
10[d]	KOAc (150)	120	MeCN	24	35
11[d]	KOAc (150)	120	toluene	62	15
12[d]	KOAc (150)	120	THF	58	10
13[d]	KOAc (150)	120	1,4-dioxane	31	40
14[d,e]	KOAc (150)	120	DCE	68	-

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.2 mmol), $[RhCp^*Cl_2]_2$ (1.5 mol %), base (quantity noted, mol %) in solvent (1.0 mL), temp (noted) for 20 h under air. [b]Isolated yield. [c]Solvent (0.5 mL). [d] Solvent (0.2 mL). [e]$[RhCp^*Cl_2]_2$ (1.0 mol %).

Optimization of 3-trifluoromethylindanone (5):[a]

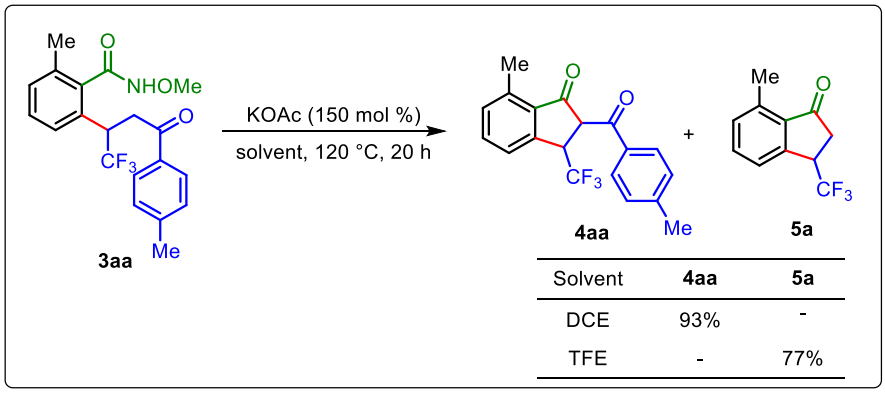


entry	base (mol %)	temp (°C)	solvent	yield (%)[b]			
				5a	**7a**	**8a**	**9a**
1	K_2CO_3 (20)	80	TFE	44	21	15	traces
2	K_2CO_3 (20)	100	TFE	42	ND	ND	ND
3	K_2CO_3 (20)	120	TFE	28	ND	ND	ND
4[c]	KOAc (150)	120	TFE	47	25	13	traces
5[c,d]	**KOAc (150)**	120	**TFE**	**70**	39	26	14
6[c,e]	KOAc (150)	120	TFE	72	41	44	49
7[c,d]	KOAc (150)	120	ethanol	30	-	-	-
8[c,d]	KOAc (150)	120	*t*-AmOH	15	-	-	-
9[c,d]	KOAc (150)	120	HFIP	23	-	-	-
10	K_2CO_3 (20)	50	TFE	-	-	-	74
11	K_2CO_3 (20)	rt	TFE	-	-	-	68

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.2 mmol), $[RhCp^*Cl_2]_2$ (1.5 mol %), base (quantity noted, mol %) in solvent (1.0 mL), temp. (noted) for 20 h under air. [b]Isolated yield. [c] Solvent (0.2 mL). [d]**2a** (0.3 mmol). [e]**2a** (0.4 mmol). ND = not determined.

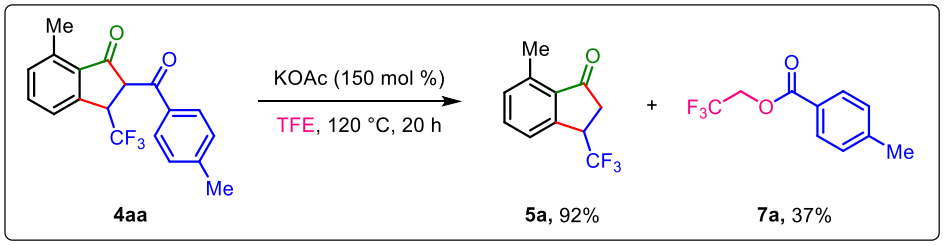
Claisen/retro-Claisen condensation investigation:

We performed few parallel reactions to understand the formation 3-trifluoromethylindanone products. It was found that only KOAc is required for the Claisen condensation in DCE to afford the 2-acylated-3-trifluoromethylindanone in 93% yield. Further, in TFE under basic condition, **3aa** initially undergoes Claisen condensation, which is subsequently followed by the retro-Claisen reaction to furnish **5a** in 77% yield. In addition, **4aa** under the similar condition in TFE produces **5a** in 92% yield along with 2,2,2-trifluoroethyl-4-methylbenzoate (**7a**) in 37% yield.



Solvent	4aa	5a
DCE	93%	-
TFE	-	77%

Procedure: To an oven-dried sealed tube charged with a stirring bar were added **3aa** (37.9 mg, 0.10 mmol, 100 mol) and KOAc (14.7 mg, 0.15 mmol, 150 mol %) in solvent (0.1 mL, 1.0 M). The reaction mixture was allowed to stir at 120 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide **4aa**.



Procedure: To an oven-dried sealed tube charged with a stirring bar were added **4aa** (33.2 mg, 0.10 mmol, 100 mol %) and KOAc (14.7 mg, 0.15 mmol, 150 mol %) in TFE (0.1 mL, 1.0 M). The reaction mixture was allowed to stir at 120 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide **5a** (92%) and **7a** (37%).

References:

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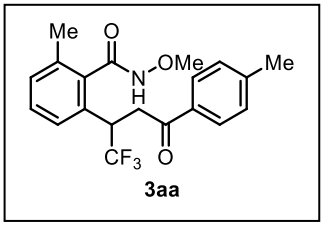
General procedure for synthesis of C-H alkylated products and spectral data (3aa-3ta):

To an oven-dried sealed charged tube with a stirring bar were added corresponding *N*-methoxybenzamides **1a-1t** (0.20 mmol, 100 mol %), (*E*)-4,4,4-trifluoro-1-(*p*-tolyl)but-2-en-1-one **2a** (42.8 mg, 0.20 mmol, 100 mol %), $[RhCp^*Cl_2]_2$ (1.2 mg, 2.0 μmol, 1.0 mol %) and NaOAc (3.3 mg, 0.04 mmol, 20 mol %) in 1,2-dichloroethane (1.0 mL, 0.2 M). The reaction mixture was allowed to stir at 80 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide corresponding C-H alkylated products (**3aa-3ta)**.

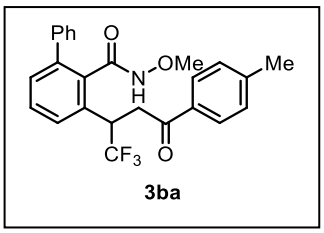
***N*-Methoxy-2-methyl-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3aa):**



3aa

64 mg (84%); White solid; **mp** = 145.0–146.2 °C; **R_F** (Hexane/EtOAc 60:40): 0.42; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.43 (s, 1H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.26 (d, *J* = 7.5 Hz, 2H), 7.23 (d, *J* = 7.5 Hz, 1H), 7.19–7.14 (m, 2H), 4.17–4.09 (m, 1H), 4.00 (s, 3H), 3.99–3.90 (m, 1H), 3.59 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.43 (s, 3H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.1, 167.2, 145.6, 137.4, 136.0, 133.4, 131.0, 130.6, 129.8, 129.7, 128.5, 126.3 (q, J_{C-F} = 278.4 Hz), 123.8, 64.5, 41.6 (q, J_{C-F} = 27.9 Hz), 38.3, 21.9, 19.5; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.5; **IR (KBr)** υ 3249, 3070, 2962, 2930, 2817, 1691, 1668, 1607, 1572, 1488, 1260, 1156, 1114, 1044, 882, 770, 658, 567 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{20}H_{21}F_3NO_3^+$ $[M+H]^+$ 380.1468, found 380.1496.

***N*-Methoxy-3-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-[1,1'-biphenyl]-2-carboxamide (3ba):**

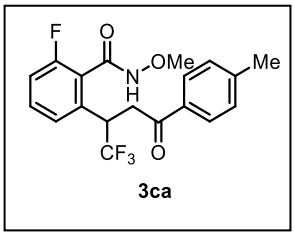


3ba

75 mg (85%); Light yellow solid; **mp** = 66.8–70.5 °C; **R_F** (Hexane/EtOAc 60:40): 0.58; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.62 (s, 1H), 7.84 (d, *J* = 8.5 Hz, 2H), 7.52–7.50 (m, 2H), 7.43–7.37 (m, 5H), 7.33 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.27 (d, *J* = 7.5 Hz, 2H), 4.34–4.26 (m, 1H), 3.92 (dd, *J* = 18.5, 11.0 Hz, 1H), 3.64 (dd, *J* = 18.5, 3.0 Hz, 1H), 3.58 (s, 3H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.3, 166.6, 145.3, 141.9, 139.9, 135.3, 133.5, 132.4, 130.2, 129.9, 129.6, 129.1, 128.4, 128.3, 127.9, 126.4 (q, J_{C-F} = 278.4 Hz),

125.7, 63.8, 41.6 (q, J_{C-F} = 27.7 Hz), 38.7, 21.9; **^{19}F NMR (470 MHz, CDCl$_3$)** δ -69.0; **IR (KBr)** υ 3248, 3062, 2976, 2936, 2817, 1674, 1607, 1461, 1439, 1307, 1256, 1160, 1112, 1034, 883, 812, 763, 702, 660, 571 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{25}H_{23}F_3NO_3^+$ $[M+H]^+$ 442.1625, found 442.1644.

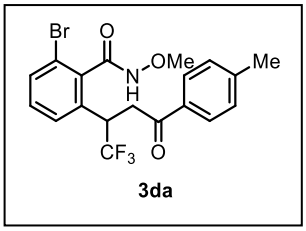
2-Fluoro-*N*-methoxy-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3ca):



3ca

51 mg (66%); Light yellow solid; **mp** = 112.1–113.7 °C; **R_F** (Hexane/EtOAc 60:40): 0.48; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 10.25 (s, 1H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.35 (td, *J* = 8.0, 5.5 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.08 (t, *J* = 8.5 Hz, 1H), 4.27–4.19 (m, 1H), 4.00 (s, 3H), 3.91 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.62 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 196.6, 162.3, 160.2 (d, J_{C-F} = 249.1 Hz), 145.7, 134.1, 133.2, 131.7 (d, J_{C-F} = 8.6 Hz), 129.7, 128.5, 126.1 (q, J_{C-F} = 278.1 Hz), 124.8 (d, J_{C-F} = 18.6 Hz), 122.5 (d, J_{C-F} = 3.1 Hz), 116.2 (d, J_{C-F} = 21.4 Hz), 64.7, 41.3 (q, J_{C-F} = 27.9 Hz), 38.4, 21.9; **^{19}F NMR (470 MHz, CDCl$_3$)** δ -69.3, -113.4; **IR (KBr)** υ 3255, 2970, 2938, 2822, 1700, 1669, 1609, 1580, 1461, 1310, 1264, 1159, 1115, 883, 819, 799, 660, 567 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{18}F_4NO_3^+$ $[M+H]^+$ 384.1217, found 384.1230.

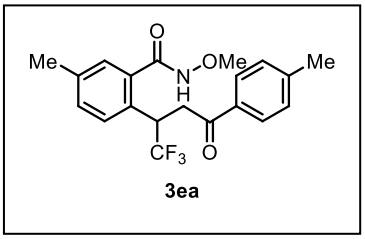
2-Bromo-*N*-methoxy-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3da):



3da

45 mg (51%); White solid; **mp** = 173.6–175.4 °C; **R_F** (Hexane/EtOAc 60:40): 0.52; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 10.25 (s, 1H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.56 (dd, *J* = 8.0, 1.0 Hz, 1H), 7.30 (d, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.22 (t, *J* = 8.0 Hz, 1H), 4.17–4.09 (m, 1H), 4.02 (s, 3H), 3.90 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.62 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.42 (s, 3H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 196.5, 165.0, 145.7, 137.5, 133.8, 133.2, 131.1, 129.7, 128.5, 126.0 (q, J_{C-F} = 278.4 Hz), 125.6, 122.4, 64.5, 42.2 (q, J_{C-F} = 28.2 Hz), 38.4, 21.9; **^{19}F NMR (470 MHz, CDCl$_3$)** δ -69.3; **IR (KBr)** υ 3248, 2969, 2933, 1698, 1667, 1606, 1492, 1439, 1278, 1259, 1156, 1110, 883, 812, 651, 595 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{18}BrF_3NO_3^+$ $[M+H]^+$ 444.0417, found 444.0433.

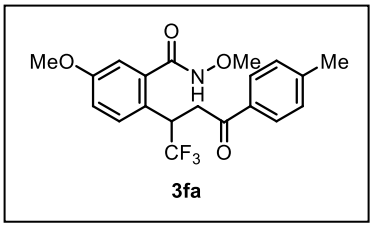
***N*-Methoxy-5-methyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3ea):**



3ea

65 mg (86%); White solid; **mp** = 164.4–165.7 °C; **R_F** (Hexane/EtOAc 60:40): 0.39; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.44 (s, 1H), 7.84 (d, *J* = 8.5 Hz, 2H), 7.38 (d, *J* = 2.0 Hz, 1H), 7.30–7.23 (m, 3H), 7.19 (dd, *J* = 8.0, 2.0 Hz, 1H), 4.52–4.44 (m, 1H), 3.98 (s, 3H), 3.95 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.60 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.41 (s, 3H), 2.32 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.1, 167.1, 145.5, 138.8, 136.0, 133.4, 131.5, 130.0, 129.7, 128.5, 128.2, 126.8, 126.4 (q, $J_{C\text{-}F}$ = 278.4 Hz), 64.6, 40.5 (q, $J_{C\text{-}F}$ = 27.7 Hz), 38.3, 21.9, 21.0; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.4; **IR (KBr)** υ 3178, 2987, 2963, 2936, 1690, 1650, 1608, 1573, 1493, 1383, 1358, 1299, 1261, 1222, 1164, 1155, 1118, 1067, 1038, 948, 873, 731, 688, 591 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{20}H_{21}F_3NO_3^+$ $[M+H]^+$ 380.1468, found 380.1484

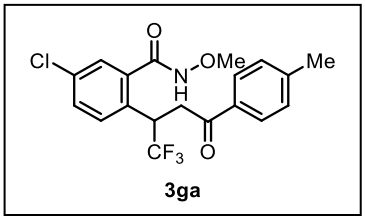
***N*,5-Dimethoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3fa):**



3fa

69 mg (87%); White solid; **mp** = 153.6–154.8 °C; **R_F** (Hexane/EtOAc 60:40): 0.27; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.57 (s, 1H), 7.85 (d, *J* = 8.5 Hz, 2H), 7.28–7.26 (m, 3H), 7.09 (d, *J* = 3.0 Hz, 1H), 6.92 (dd, *J* = 9.0, 3.0 Hz, 1H), 4.48–4.39 (m, 1H), 4.00 (s, 3H), 3.94 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.80 (s, 3H), 3.59 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.42 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.3, 166.7, 159.5, 145.6, 137.3, 133.4, 129.7, 128.5, 128.2, 126.5 (q, $J_{C\text{-}F}$ = 278.2 Hz), 122.9, 117.3, 113.9, 64.6, 55.6, 40.3 (q, $J_{C\text{-}F}$ = 27.9 Hz), 38.2, 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.7; **IR (KBr)** υ 3144, 2976, 2860, 2840, 1683, 1638,1606, 1541, 1466, 1413, 1334, 1303, 1260, 1246, 1166, 1116, 1102, 1062, 1036, 946, 865, 821,757, 692, 592 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{20}H_{21}F_3NO_4^+$ $[M+H]^+$ 396.1417, found 396.1436.

5-Chloro-*N*-methoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3ga):

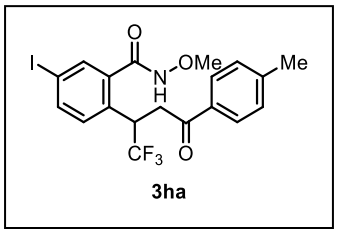


3ga

67 mg (84%); White solid; **mp** = 185.6–186.5 °C; **R_F** (Hexane/EtOAc 60:40): 0.55; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.42 (s, 1H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 2.5 Hz, 1H), 7.36 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.31 (d, *J* = 9.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 4.52–4.44 (m, 1H), 3.98 (s, 3H), 3.91 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.63 (dd, *J* =

18.5, 3.0 Hz, 1H), 2.42 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.8, 165.6, 145.8, 137.7, 134.9, 133.2, 130.9, 130.0, 129.7, 129.6, 128.5, 128.4, 126.2 (q, J_{C-F} = 280.4 Hz), 64.7, 40.6 (q, J_{C-F} = 28.3 Hz), 38.3, 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.3; **IR (KBr)** υ 3183, 2963, 2940, 2855, 1690, 1662, 1571, 1439, 1225, 1165, 1110, 1037, 888, 764, 685, 591 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{18}ClF_3NO_3^+$ $[M+H]^+$ 400.0922, found 400.0951.

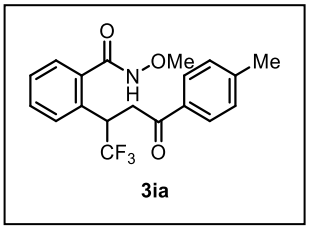
5-Iodo-*N*-methoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3ha):



3ha

60 mg (61%); Light yellow solid; **mp** = 151.0–152.7 °C; **R_F** (Hexane/EtOAc 60:40): 0.55; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.40 (s, 1H), 7.89 (d, *J* = 2.0 Hz, 1H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.71 (dd, *J* = 8.5, 2.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.5 Hz, 1H), 4.49–4.41 (m, 1H), 3.98 (s, 3H), 3.90 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.62 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.42 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.8, 165.3, 145.8, 139.7, 138.2, 138.0, 133.2, 131.1, 129.7, 128.6, 128.5, 126.1 (q, J_{C-F} = 278.6 Hz), 94.4, 64.7, 40.8 (q, J_{C-F} = 28.1 Hz), 38.2, 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.3; **IR (KBr)** υ 3201, 2985, 2941, 1691, 1650, 1438, 1271, 1159, 1098, 945, 894, 755, 680, 591 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{18}F_3INO_3^+$ $[M+H]^+$ 492.0278, found 492.0296.

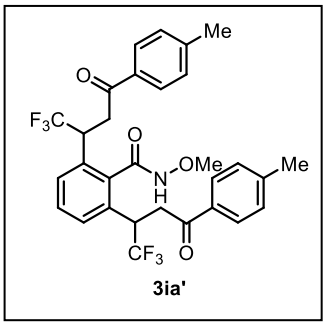
***N*-Methoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3ia):**



3ia

44 mg (60%); white solid; **mp** = 136.0–137.3 °C; **R_F** (Hexane/EtOAc 60:40): 0.33; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.35 (s, 1H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.55 (d, *J* = 7.5 Hz, 1H), 7.41–7.34 (m, 3H), 7.26 (d, *J* = 8.0 Hz, 2H), 4.59–4.50 (m, 1H), 3.98 (s, 3H), 3.95 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.62 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.9, 167.1, 145.5, 136.2, 133.4, 131.5, 130.7, 129.8, 129.4, 128.7, 128.5, 127.0, 126.3 (q, J_{C-F} = 278.2 Hz), 64.6, 40.8 (q, J_{C-F} = 27.9 Hz), 38.4, 21.8; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.3; **IR (KBr)** υ 3203, 2991, 2940, 1684, 1649, 1477, 1285, 1259, 1157, 1115, 938, 885, 971, 592 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{19}F_3NO_3^+$ $[M+H]^+$ 366.1312, found 366.1330.

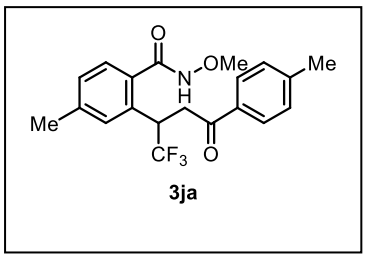
***N*-Methoxy-2,6-bis(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3ia'):**



3ia'

11 mg (9%); White solid; **mp** = 66.4–69.6 °C; **R_F** (Hexane/EtOAc 60:40): 0.58; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.42 (s, 1H), 7.81 (d, *J* = 8.5 Hz, 4H), 7.39–7.33 (m, 3H), 7.24 (d, *J* = 8.0 Hz, 4H), 4.39 (pd, *J* = 9.0, 3.5 Hz, 2H), 4.05 (s, 3H), 3.74 (dd, *J* = 18.0, 10.0 Hz, 2H), 3.64 (dd, *J* = 18.0, 4.0 Hz, 2H), 2.40 (s, 6H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 195.6, 165.2, 145.0, 138.1, 133.7, 133.3, 130.1, 129.6, 128.4, 127.2, 126.4 (q, $J_{C\text{-}F}$ = 278.6 Hz) 64.4, 41.8 (q, $J_{C\text{-}F}$ = 28.0 Hz), 38.8, 21.8; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.0; **IR (KBr)** υ 3277, 2930, 2864, 1682, 1607, 1455, 1419, 1368, 1304, 1260, 1163, 1109, 1037, 986, 885, 812, 762, 675, 587 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{30}H_{28}F_6NO_4^+$ $[M+H]^+$ 580.1917, found 580.1930.

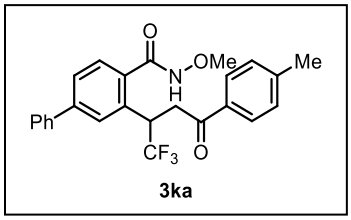
***N*-Methoxy-4-methyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3ja):**



3ja

48 mg (63%); White solid; **mp** = 117.9–119.4 °C; **R_F** (Hexane/EtOAc 60:40): 0.33; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.32 (s, 1H), 7.85 (d, *J* = 8.5 Hz, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.16 (d, *J* = 7.5 Hz, 1H), 7.15 (s, 1H), 4.58–4.51 (m, 1H), 3.97 (s, 3H), 3.93 (dd, *J* = 18.0, 11.0 Hz, 1H), 3.62 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.42 (s, 3H), 2.31 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.9, 167.3, 145.5, 140.9, 133.4, 133.3, 131.4, 129.7, 129.5, 129.4, 128.5, 127.5, 126.5 (q, $J_{C\text{-}F}$ = 278.0 Hz), 64.6, 40.8 (q, $J_{C\text{-}F}$ = 27.9 Hz), 38.4, 21.9, 21.6; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.2; **IR (KBr)** υ 3138, 2976, 2936, 2820, 1686, 1644, 1610, 1525, 1374, 1298, 1262, 1205, 1180, 1159, 1113, 1061, 1041, 942, 878, 821, 728, 639, 596 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{20}H_{21}F_3NO_3^+$ $[M+H]^+$ 380.1468, found 380.1485.

***N*-Methoxy-3-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-[1,1'-biphenyl]-4-carboxamide (3ka):**

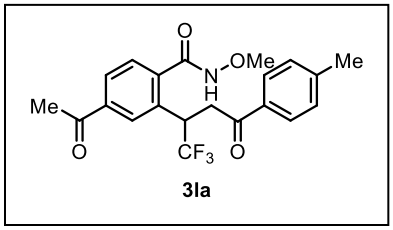


3ka

45 mg (51%); White solid; **mp** = 133.9–135.9 °C; **R_F** (Hexane/EtOAc 60:40): 0.33; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.41 (s, 1H), 7.85 (d, *J* = 8.0 Hz, 2H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.57 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.55 (s, 1H), 7.47 (d, *J* = 7.5 Hz, 2H), 7.42 (t, *J* = 7.5 Hz, 2H), 7.36 (t, *J* = 7.0 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 4.67–4.59 (m, 1H), 4.05–3.97

(m, 4H), 3.68 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 196.9, 167.0, 145.6, 143.8, 139.9, 134.9, 133.3, 132.1, 130.0, 129.7, 129.2, 128.5, 128.3, 127.6, 127.4, 126.4 (q, $J_{C\text{-}F}$ = 278.4), 125.8, 64.6, 40.9 (q, $J_{C\text{-}F}$ = 27.6 Hz), 38.5, 21.9; **^{19}F NMR (470 MHz, CDCl$_3$)** δ -69.1; **IR (KBr)** υ 3160, 3057, 3031, 2981, 2818, 1686, 1643, 1608, 1525, 1485, 1415, 1372, 1360, 1296, 1264, 1172, 1101, 1054, 1032, 969, 884, 809, 766, 699, 650, 585 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{25}H_{23}F_3NO_3^+$ $[M+H]^+$ 442.1625, found 442.1640.

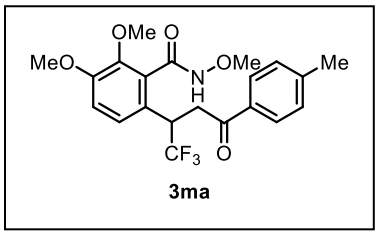
4-Acetyl-*N*-methoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3la):



3la

41 mg (50%); White solid; **mp** = 97.3–100.2 °C; **R_F** (Hexane/EtOAc 60:40): 0.18; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 10.50 (s, 1H), 7.99 (s, 1H), 7.90 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.83 (d, *J* = 8.5 Hz, 2H), 7.67 (d, *J* = 8.0 Hz, 1H), 7.27 (d, *J* = 8.0 Hz, 2H), 4.56–4.48 (m, 1H), 4.03 (dd, *J* = 18.5, 11.5 Hz, 1H), 4.00 (s, 3H), 3.69 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.56 (s, 3H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 197.0, 196.9, 166.1, 145.8, 140.3, 138.5, 133.1, 132.4, 130.0, 129.7, 128.8, 128.6, 126.4, 126.2 ($J_{C\text{-}F}$ = 278.2 Hz) 64.7, 41.0 ($J_{C\text{-}F}$ = 28.1 Hz), 38.4, 26.8, 21.9; **^{19}F NMR (470 MHz, CDCl$_3$)** δ -69.2; **IR (KBr)** υ 3190, 2994, 2943, 1692, 1656, 1508, 1412, 1267, 1158, 1103, 936, 895, 678, 588, 524 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{21}H_{21}F_3NO_4^+$ $[M+H]^+$ 408.1417, found 408.1433.

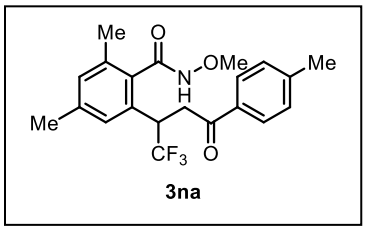
***N*,2,3-Trimethoxy-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3ma):**



3ma

76 mg (89%); White solid; **mp** = 151.4–152.0 °C; **R_F** (Hexane/EtOAc 60:40): 0.27; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 10.00 (s, 1H), 7.82 (d, *J* = 8.5 Hz, 2H), 7.26 (d, *J* = 8.5 Hz, 2H), 7.04 (d, *J* = 8.5 Hz, 1H), 6.88 (d, *J* = 8.5 Hz, 1H), 4.17–4.08 (m, 1H), 3.98 (s, 3H), 3.92 (s, 3H), 3.87–3.78 (m, 4H), 3.55 (dd, *J* = 18.0, 3.0 Hz, 1H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 196.5, 164.5, 152.7, 147.1, 145.3, 133.5, 131.7, 129.6, 128.4, 126.4 (q, $J_{C\text{-}F}$ = 278.1 Hz), 124.1, 122.7, 113.8, 64.5, 62.3, 55.9, 40.7 (q, $J_{C\text{-}F}$ = 28.0 Hz), 38.5, 21.8; **^{19}F NMR (470 MHz, CDCl$_3$)** δ -69.6; **IR (KBr)** υ 3247, 2982, 2946, 1680, 1660, 1498, 1311, 1259, 1157, 1111, 1033, 824, 744, 552, 514 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{21}H_{23}F_3NO_5^+$ $[M+H]^+$ 426.1523, found 426.1533.

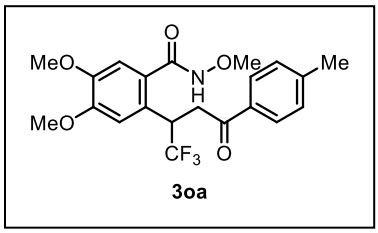
***N*-Methoxy-2,4-dimethyl-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3na):**



3na

68 mg (86%); White solid; **mp** = 157.5–160.0 °C; **R_F** (Hexane/EtOAc 60:40): 0.45; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.38 (s, 1H), 7.85 (d, *J* = 8.5 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 6.99 (s, 1H), 6.93 (s, 1H), 4.15–4.07 (m, 1H), 3.99 (s, 3H), 3.93 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.59 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.42 (s, 3H), 2.39 (s, 3H), 2.25 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.1, 167.5, 145.5, 139.7, 137.2, 133.4, 133.3, 131.5, 130.9, 129.7, 128.5, 126.4 ($J_{C\text{-}F}$ = 277.1 Hz), 124.4, 64.4, 41.5 ($J_{C\text{-}F}$ = 27.6 Hz), 38.3, 21.9, 21.5, 19.4; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.4; **IR (KBr)** υ 3273, 2970, 2926, 1683, 1665, 1494, 1316, 1266, 1159, 1106, 1034, 864, 751, 662, 565 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{21}H_{23}F_3NO_3^+$ $[M+H]^+$ 394.1625, found 394.1640.

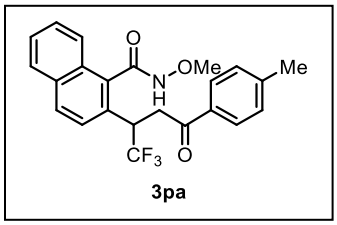
***N*,4,5-Trimethoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3oa):**



3oa

77 mg (91%); White solid; **mp** = 171.5–172.3 °C; **R_F** (Hexane/EtOAc 40:60): 0.15; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.65 (s, 1H), 7.86 (d, *J* = 8.5 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.08 (s, 1H), 6.75 (s, 1H), 4.56–4.48 (m, 1H), 3.98 (s, 3H), 3.91 (dd, *J* = 18.0, 11.5 Hz, 1H), 3.88 (s, 3H), 3.81 (s, 3H), 3.60 (dd, *J* = 18.4, 2.9 Hz, 1H), 2.42 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.2, 166.6, 150.7, 149.1, 145.7, 133.3, 129.7, 128.9, 128.5, 126.4 (q, $J_{C\text{-}F}$ = 279.9 Hz), 123.6, 112.1, 109.3, 64.6, 56.2, 56.1, 40.6 (q, $J_{C\text{-}F}$ = 27.7 Hz), 38.1, 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.4; **IR (KBr)** υ 3313, 2964, 2942, 1673, 1606, 1525, 1465, 1276, 1159, 1094, 938, 870, 736, 694, 568 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{21}H_{23}F_3NO_5^+$ $[M+H]^+$ 426.1523, found 426.1552.

***N*-Methoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-1-naphthamide (3pa):**

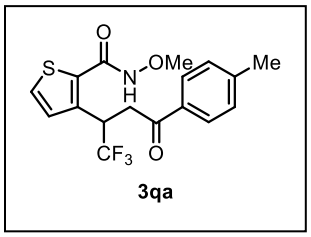


3pa

78 mg (94%); White solid; **mp** = 182.8–184.1 °C; **R_F** (Hexane/EtOAc 60:40): 0.45; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.79 (s, 1H), 8.08 (d, *J* = 8.5 Hz, 1H), 7.83 (t, *J* = 9.0 Hz, 3H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.59 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H), 7.53 (ddd, *J* = 8.0, 7.0, 1.0 Hz, 1H), 7.41 (d, *J* = 8.5 Hz, 1H), 7.26 (d, *J* = 8.0 Hz, 2H), 4.41–4.33 (m, 1H), 4.12 (dd, *J* = 18.5, 12.0 Hz, 1H), 4.10 (s, 3H), 3.67 (dd, *J* = 18.5, 2.5 Hz, 1H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.2, 166.5, 145.7, 134.0, 133.3, 133.0,

131.1, 130.7, 129.7, 128.5, 128.1, 128.0, 127.9, 127.2, 126.3 (q, $J_{C\text{-}F}$ = 278.4 Hz), 125.8, 122.7, 64.7, 42.1 (q, $J_{C\text{-}F}$ = 28.3 Hz), 37.7, 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.0; **IR (KBr)** υ 3247, 2965, 2936, 1693, 1668, 1488, 1260, 1164, 1106, 968, 890, 753, 699, 657, 569 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{23}H_{21}F_3NO_3^+$ $[M+H]^+$ 416.1468, found 416.1484.

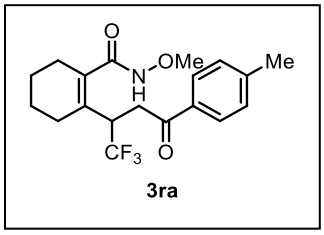
***N*-Methoxy-3-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)thiophene-2-carboxamide (3qa):**



3qa

21 mg (28%); Light yellow semi-solid; **R_F** (Hexane/EtOAc 60:40): 0.42; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.89 (s, 1H), 7.86 (d, *J* = 8.5 Hz, 2H), 7.42 (d, *J* = 5.0 Hz, 1H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.04 (d, *J* = 5.0 Hz, 1H), 4.79–4.71 (m, 1H), 3.98 (s, 3H), 3.80 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.61 (dd, *J* = 18.5, 2.5 Hz, 1H), 2.42 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.2, 161.2, 145.8, 136.0, 134.1, 133.2, 129.7, 129.4, 128.6, 126.8, 126.1 (q, $J_{C\text{-}F}$ = 278.2 Hz), 64.8, 39.2 (q, $J_{C\text{-}F}$ = 28.6 Hz), 38.6, 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.4; **IR (KBr)** υ 3219, 2973, 2926, 2854, 1667, 1607, 1426, 1306, 1264, 1159, 1108, 984, 881, 767, 682, 579, 511 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{17}H_{17}F_3NO_3S^+$ $[M+H]^+$ 372.0876, found 372.0885.

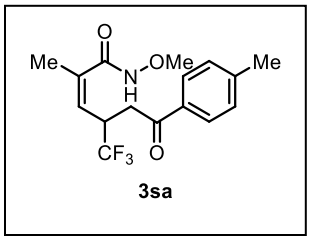
***N*-Methoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)cyclohex-1-ene-1-carboxamide (3ra):**



3ra

26 mg (35%); White solid; **mp** = 108.1–110.0 °C; **R_F** (Hexane/EtOAc 60:40): 0.33; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.47 (s, 1H), 7.89 (d, *J* = 8.5 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 4.00–3.92 (m, 1H), 3.88 (s, 3H), 3.72 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.19 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.61–2.55 (m, 1H), 2.44 (s, 3H), 2.17–2.05 (m, 2H), 1.78–1.71 (m, 1H), 1.65–1.59 (m, 2H), 1.55–1.45 (m, 2H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.6, 168.2, 145.7, 136.2, 133.4, 129.8, 128.6, 128.5, 126.4 (q, $J_{C\text{-}F}$ = 281.3 Hz), 64.3, 42.9 (q, $J_{C\text{-}F}$ = 27.4 Hz), 34.1, 28.0, 24.3, 22.0, 21.9, 21.6; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -67.9; **IR (KBr)** υ 3211, 2940, 2865, 1693, 1665, 1639, 1489, 1258, 1155, 1114, 1020, 887, 764, 977, 580 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{23}F_3NO_3^+$ $[M+H]^+$ 370.1625, found 370.1653.

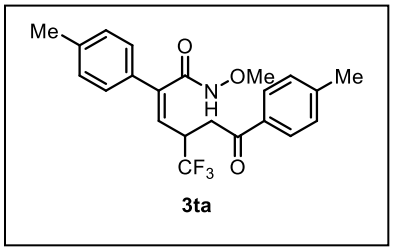
(*Z*)-*N*-Methoxy-2-methyl-6-oxo-6-(*p*-tolyl)-4-(trifluoromethyl)hex-2-enamide (3sa):



3sa

23 mg (35%); White solid; **mp** = 85.1–86.0 °C; **R_F** (Hexane/EtOAc 60:40): 0.33; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.92 (s, 1H), 7.88 (d, *J* = 8.5 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 2H), 5.22 (dd, *J* = 11.0, 2.0 Hz, 1H), 3.92 (s, 3H), 3.86–3.78 (m, 1H), 3.43–3.35 (m, 2H), 2.44 (s, 3H), 1.98 (d, *J* = 2.0 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.7, 165.8, 145.8, 138.6, 133.3, 129.8, 128.6, 126.1 (q, $J_{C\text{-}F}$ = 279.6 Hz), 123.1 (q, $J_{C\text{-}F}$ = 2.0 Hz), 64.5, 39.9 (q, $J_{C\text{-}F}$ = 28.1 Hz), 37.3, 21.9, 21.5; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.8; **IR (KBr)** υ 3172, 2951, 1693, 1669, 1644, 1357, 1262, 1150, 1115, 1035, 944, 882, 762, 639, 584, 555 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{16}H_{19}F_3NO_3^+$ $[M+H]^+$ 330.1312, found 330.1324.

(*Z*)-*N*-Methoxy-6-oxo-2,6-di-*p*-tolyl-4-(trifluoromethyl)hex-2-enamide (3ta):



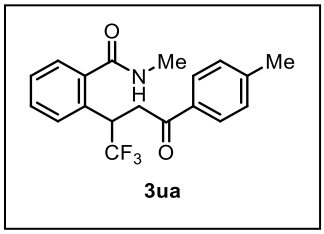
3ta

30 mg (37%); Light yellow solid; **mp** = 95.1–97.4 °C; **R_F** (Hexane/EtOAc 60:40): 0.58; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.65 (s, 1H), 7.88 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.5 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 5.69 (d, *J* = 11.0 Hz, 1H), 3.97 (s, 3H), 3.95–3.89 (m, 1H), 3.49–3.48 (m, 2H), 2.43 (s, 3H), 2.32 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.3, 165.3, 145.7, 142.0, 139.2, 133.4, 133.1, 129.7, 129.5, 128.6, 126.6, 126.1 (q, $J_{C\text{-}F}$ = 278.5 Hz), 122.6, 64.6, 40.5 (q, $J_{C\text{-}F}$ = 28.1 Hz), 37.6, 21.9, 21.3; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.3; **IR (KBr)** υ 3187, 2980, 2937, 1684, 1657, 1483, 1257, 1162, 1124, 977, 943, 819, 752, 638, 588 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{22}H_{23}F_3NO_3^+$ $[M+H]^+$ 406.1625, found 406.1639.

General procedure for synthesis of C-H alkylated products with different amides and spectral data (3ua-3ya):

To an oven-dried sealed charged tube with a stirring bar were added corresponding *N*-methoxybenzamides **1u-1y** (0.20 mmol, 100 mol %), (*E*)-4,4,4-trifluoro-1-(*p*-tolyl)but-2-en-1-one **2a** (42.8 mg, 0.20 mmol, 100 mol %), $[RhCp^*Cl_2]_2$ (1.9 mg, 3.0 μmol, 1.5 mol %), $AgSbF_6$ (4.1 mg, 12.0 μmol, 6.0 mol %) and KOAc (3.9 mg, 0.04 mmol, 20 mol %) in 1,2-dichloroethane (1.0 mL, 0.2 M). The reaction mixture was allowed to stir at 80 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide corresponding C-H alkylated products (**3ua-3ya)**.

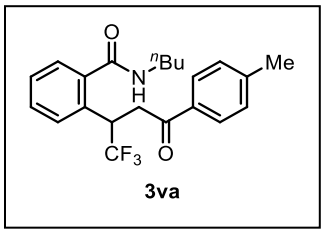
***N*-Methyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3ua):**



3ua

47 mg (67%); Light orange semi-solid; $\mathbf{R_F}$ (Hexane/EtOAc 60:40): 0.30; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.83 (d, *J* = 8.5 Hz, 2H), 7.59–7.52 (m, 2H), 7.38–7.31 (m, 3H), 7.83 (d, *J* = 7.5 Hz, 2H), 4.68–4.60 (m, 1H), 3.95 (dd, *J* = 18.0, 11.5 Hz, 1H), 3.61 (dd, *J* = 18.5, 3.0 Hz, 1H), 3.08 (d, *J* = 5.0 Hz, 3H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.7, 170.0, 145.3, 139.6, 133.5, 130.8, 130.0, 129.7, 128.9, 128.6, 128.4, 126.8, 126.6 (q, $J_{C\text{-}F}$ = 278.1 Hz), 40.6 (q, $J_{C\text{-}F}$ = 27.5 Hz), 38.4 (q, $J_{C\text{-}F}$ = 2.1 Hz), 26.9, 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.3; **IR (KBr)** υ 3322, 3067, 3034, 2924, 2854, 1680, 1605, 1547, 1446, 1412, 1305, 1259, 1182, 1157, 1113, 1061, 1000, 944, 894, 822, 759, 681, 666, 591 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{19}F_3NO_2^+$ $[M+H]^+$ 350.1362, found 350.1385.

***N*-Butyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3va):**

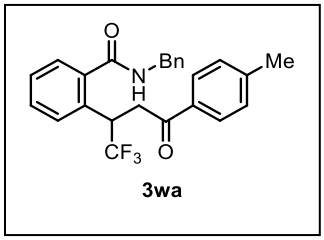


3va

49 mg (63%); Light yellow semi-solid; $\mathbf{R_F}$ (Hexane/EtOAc 60:40): 0.58; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.84 (d, *J* = 8.5 Hz, 2H), 7.54–7.51 (m, 1H), 7.50–7.46 (m, 1H), 7.37–7.31 (m, 3H), 7.26 (d, *J* = 8.0 Hz, 2H), 4.74–4.66 (m, 1H), 3.94 (dd, *J* = 18.0, 11.0 Hz, 1H), 3.60 (dd, *J* = 18.0, 3.0 Hz, 1H), 3.55–3.50 (m, 2H), 2.41 (s, 3H), 1.66 (p, *J* = 7.0 Hz, 2H), 1.46 (sextet, *J* = 7.5 Hz, 2H), 0.97 (t, *J* = 7.5 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.4, 169.2, 145.2, 139.8, 133.6, 130.8, 129.9, 129.6, 128.8, 128.6, 128.4, 126.8, 126.6 (q, $J_{C\text{-}F}$ = 278.2 Hz), 40.6 (q, $J_{C\text{-}F}$ = 27.6 Hz), 39.9, 38.3, 31.7, 21.8, 20.4, 13.9; **^{19}F NMR**

(470 MHz, $CDCl_3$) δ -69.3; **IR (KBr)** υ 3298, 2959, 2927, 2872, 1681,1659, 1605, 1537, 1469, 1305, 1261, 1182, 1158, 1114, 1059, 945, 803, 759, 665, 591 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{22}H_{25}F_3NO_2^+$ $[M+H]^+$ 392.1832, found 392.1795.

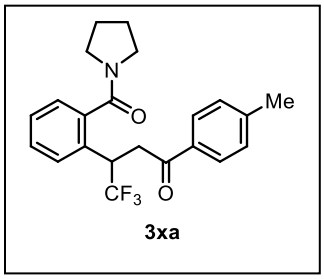
***N*-Benzyl-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3wa):**



3wa

52 mg (61%); White solid; **mp** = 127.7–130.1 °C; **R_F** (Hexane/EtOAc 60:40): 0.58; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.81–7.78 (m, 3H), 7.58–7.55 (m, 1H), 7.43 (d, *J* = 7.0 Hz, 2H), 7.38–7.32 (m, 5H), 7.28 (d, *J* = 8.5 Hz, 1H), 7.25 (d, *J* = 8.5 Hz, 2H), 4.76 (dd, *J* = 14.5, 6.0 Hz, 1H), 4.70 (dd, *J* = 14.5, 6.0 Hz, 1H), 4.69–4.63 (m, 1H), 3.89 (dd, *J* = 18.0, 11.0 Hz, 1H), 3.52 (dd, *J* = 18.0, 3.0 Hz, 1H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.2, 169.2, 145.2, 139.3, 138.5, 133.6, 131.2, 130.1, 129.6, 128.8, 128.8, 128.6, 128.4, 128.1, 127.5, 127.0, 126.6 (q, $J_{C\text{-}F}$ = 278.2 Hz), 44.2, 40.4, (q, $J_{C\text{-}F}$ = 27.6 Hz), 38.3, 21.8; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.3; **IR (KBr)** υ 3337, 3065, 3303, 2909, 1669, 1652, 1604, 1547, 1497, 1455, 1427, 1356, 1307, 1282, 1263, 1231, 1200, 1152, 1116, 1097, 984, 948, 820, 783, 747, 705, 663, 594 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{25}H_{23}F_3NO_2^+$ $[M+H]^+$ 426.1675, found 426.1692.

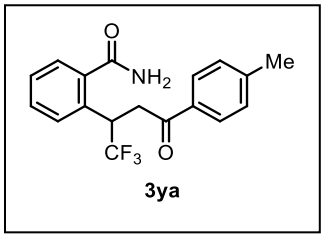
4,4,4-Trifluoro-3-(2-(pyrrolidine-1-carbonyl)phenyl)-1-(*p*-tolyl)butan-1-one (3xa):



3xa

45 mg (58%); Light yellow semi-solid; **R_F** (Hexane/EtOAc 60:40): 0.30; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.82 (d, *J* = 8.0 Hz, 2H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.38–7.35 (m, 1H), 7.32–7.28 (m, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 4.75–4.67 (m, 1H), 3.76–3.67 (m, 2H), 3.65–3.55 (m, 2H), 3.24–3.16 (m, 2H), 2.39 (s, 3H), 2.04–1.93 (m, 3H), 1.88–1.82 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 194.8, 168.8, 144.5, 139.2, 133.9, 132.6, 129.5, 129.4, 128.4, 128.3, 128.0, 127.1, 127.1 (q, $J_{C\text{-}F}$ = 278.6 Hz), 49.4, 45.9, 40.9 (q, $J_{C\text{-}F}$ = 27.6 Hz), 39.2, 26.2, 24.7, 21.8; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.5; **IR (KBr)** υ 3337, 2925, 2877, 1685, 1629, 1547, 1497, 1428, 1356, 1302, 1262, 1182, 1155, 1113, 1060, 946, 829, 784, 748, 683, 661, 591 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{22}H_{23}F_3NO_2^+$ $[M+H]^+$ 390.1675, found 390.1696.

2-(1,1,1-Trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3ya):



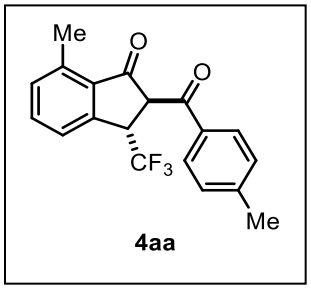
3ya

28 mg (42%); Yellowish orange semi-solid; $\mathbf{R_F}$ (Hexane/EtOAc 60:40): 0.24; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.83 (d, *J* = 8.5 Hz, 2H), 7.70 (bs, 1H), 7.62–7.59 (m, 1H), 7.43–7.33 (m, 3H), 7.26 (d, *J* = 8.0 Hz, 2H), 6.19 (bs, 1H), 4.87–4.79 (m, 1H), 3.97 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.63 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.6, 171.4, 145.3, 138.6, 133.5, 131.0, 130.4, 129.7, 129.0, 128.7, 128.4, 126.9, 126.6 (q, $J_{C\text{-}F}$ = 278.2 Hz), 40.9 (q, $J_{C\text{-}F}$ = 27.9 Hz), 38.3, 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.3; **IR (KBr)** υ 3345, 3188, 3035, 2924, 2855, 1674, 1606, 1494, 1451, 1380, 1316, 11260, 1182, 1159, 1112, 1058, 985, 944, 897, 806, 678, 629, 591 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{18}H_{17}F_3NO_2^+$ $[M+H]^+$ 336.1206, found 336.1224.

General procedure for synthesis of 2-acyl-3-trifluoromethylindanones and spectral data (4aa-4ca, 4ea-4ka, 4ma-4pa, 4ra, 4ab-4ah):

To an oven-dried sealed tube charged with a stirring bar were added corresponding *N*-methoxybenzamides **1a-1c, 1e-1k, 1m-1p, 1r** (0.20 mmol, 100 mol%), corresponding β-CF_3-substituted enones **2a-2h** (0.20 mmol, 100 mol %), $[RhCp^*Cl_2]_2$ (1.9 mg, 3.0 μmol, 1.5 mol %) and KOAc (29.4 mg, 0.30 mmol, 150 mol %) in 1,2-dichloroethane (0.2 mL, 1.0 M). The reaction mixture was allowed to stir at 120 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide corresponding 2-benzoyl-3-trifluoromethyl indanones (**4aa-4ca, 4ea-4ka, 4ma-4pa, 4ra, 4ab-4ah)**.

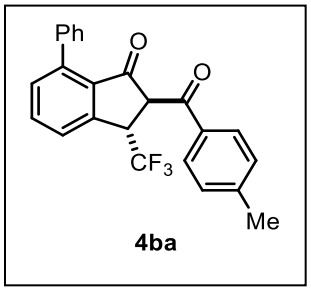
7-Methyl-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4aa)



4aa

54 mg (81%); Off white solid; **mp** = 132.3–133.0 °C; **R_F** (Hexane/EtOAc 85:15): 0.61; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.08 (d, *J* = 8.5 Hz, 2H), 7.62–7.55 (m, 2H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.28 (d, *J* = 6.0 Hz, 1H), 4.92 (d, *J* = 3.0 Hz, 1H), 4.89 (qd, *J* = 9.5, 3.5 Hz, 1H), 2.58 (s, 3H), 2.46 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.8, 191.0, 147.6 (q, J_{C-F} = 2.3 Hz), 145.4, 140.5, 135.2, 133.1, 133.1, 132.0, 130.6, 129.6, 126.4 (q, J_{C-F} = 278.2 Hz), 124.5, 57.9, 45.5 (q, J_{C-F} = 29.2 Hz), 21.9, 18.5; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9; **IR (KBr)** υ 2971, 1720, 1665, 1602, 1476, 1360, 1289, 1260, 1165, 1106, 991, 867, 784, 681, 590, 518 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{16}F_3O_2^+$ $[M+H]^+$ 333.1097, found 333.1112.

2-(4-Methylbenzoyl)-7-phenyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ba):

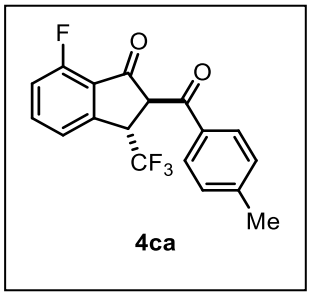


4ba

55 mg (70%) (exists as a 6.2:1 ratio of keto/enol tautomers); Off white solid; **mp** = 80.7–82.1 °C; **R_F** (Hexane/EtOAc 85:15): 0.55; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.03 (d, *J* = 8.5 Hz, 2H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.74 (t, *J* = 7.5 Hz, 1H), 7.43 (d, *J* = 7.5 Hz, 1H), 7.40–7.33 (m, 5H), 7.31 (d, *J* = 8.0 Hz, 2H), 4.99–4.88 (m, 2H), 2.43 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 194.9, 191.1, 148.1 (q, J_{C-F} = 2.1 Hz), 145.4, 143.1, 137.1, 135.2, 133.1, 132.3, 131.7, 130.6, 129.6, 129.3, 128.3, 128.0, 126.3 (q, J_{C-F} = 276.9

Hz), 126.0, 57.8, 45.5 (q, $J_{C\text{-}F}$ = 29.2 Hz), 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.8; **IR (KBr)** υ 2924, 1735, 1613, 1508, 1433, 1375, 1252, 1150, 1109, 902, 809, 734, 666, 577, 512 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{24}H_{18}F_3O_2^+$ $[M+H]^+$ 395.1253, found 395.1268.

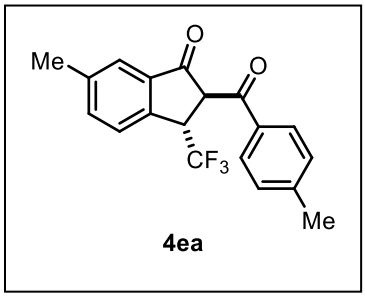
7-Fluoro-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ca):



4ca

31 mg (46%) (exists as a 5:1 ratio of keto/enol tautomers); White solid; **mp** = 102.9–104.0 °C; **R_F** (Hexane/EtOAc 85:15): 0.39; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.06 (d, *J* = 8.5 Hz, 2H), 7.72 (td, *J* = 8.0, 5.0 Hz, 1H), 7.56 (d, *J* = 7.5 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.17 (t, *J* = 8.5 Hz, 1H), 4.99–4.89 (m, 2H), 2.46 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 192.1 (d, $J_{C\text{-}F}$ = 1.9 Hz), 190.2, 159.5 (d, $J_{C\text{-}F}$ = 266.9 Hz), 148.6, 145.7, 138.0 (d, $J_{C\text{-}F}$ = 8.4 Hz), 132.8, 130.6, 129.6, 126.3 (q, $J_{C\text{-}F}$ = 276.7 Hz), 123.6 (d, $J_{C\text{-}F}$ = 13.2 Hz), 123.0 (d, $J_{C\text{-}F}$ = 4.3 Hz), 117.2 (d, $J_{C\text{-}F}$ = 18.7 Hz), 58.1, 46.0 (q, $J_{C\text{-}F}$ = 29.4 Hz), 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.8, -112.5; **IR (KBr)** υ 3031, 2972, 2951, 1714, 1665, 1609, 1452, 361, 1269, 1170, 1111, 1061, 998, 949, 861, 815, 776, 670, 597, 541, 527 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{18}H_{13}F_4O_2^+$ $[M+H]^+$ 337.0846, found 337.0843.

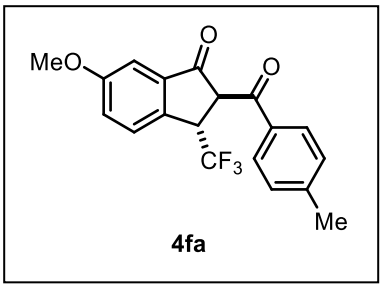
6-Methyl-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ea)



4ea

52 mg (78%) (exists as a 11.1:1 ratio of keto/enol tautomers); Yellowish orange semi-solid; **R_F** (Hexane/EtOAc 85:15): 0.55; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.07 (d, *J* = 8.5 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.56–7.54 (m, 2H), 7.36 (d, *J* = 8.0 Hz, 2H), 4.93 (d, *J* = 3.0 Hz, 1H), 4.89 (qd, *J* = 9.0, 3.5 Hz, 1H), 2.46 (s, 3H), 2.43 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.1, 190.9, 145.4, 144.4 (q, $J_{C\text{-}F}$ = 2.2 Hz), 140.5, 137.2, 136.0, 133.1, 130.5, 129.6, 129.4, 126.3 (q, $J_{C\text{-}F}$ = 276.7 Hz), 125.1, 58.1 (q, $J_{C\text{-}F}$ = 1.7 Hz), 45.8 (q, $J_{C\text{-}F}$ = 29.2 Hz), 21.9, 21.3; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.1; **IR (KBr)** υ 3035, 2951, 2927, 2865, 1726, 1677, 1608, 1494, 1375, 1285, 1263, 1157, 1112, 1032, 896, 865, 812, 688, 587 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{16}F_3O_2^+$ $[M+H]^+$ 333.1097, found 333.1114.

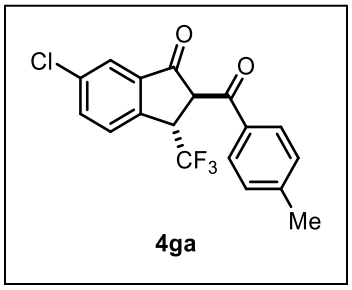
6-Methoxy-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4fa):



4fa

48 mg (69%); White solid; **mp** = 98.8–100.5 °C; **R_F** (Hexane/EtOAc 85:15): 0.42; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.06 (d, *J* = 8.5 Hz, 2H), 7.65 (d, *J* = 8.5 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.30 (dd, *J* = 8.5, 2.5 Hz, 1H), 7.17 (d, *J* = 2.5 Hz, 1H), 4.94 (d, *J* = 3.0 Hz, 1H), 4.83 (qd, *J* = 9.0, 3.0 Hz, 1H), 3.84 (s, 3H), 2.46 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.0, 190.8, 161.4, 145.4, 139.7 (q, $J_{C\text{-}F}$ = 2.2 Hz), 137.3, 133.1, 130.5, 129.6, 127.8, 126.4 (q, $J_{C\text{-}F}$ = 27.9 Hz), 125.0, 106.5, 58.4 (q, $J_{C\text{-}F}$ = 1.7 Hz), 55.9, 45.5 (q, $J_{C\text{-}F}$ = 29.4 Hz), 21.9. **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.3; **IR (KBr)** υ 2943, 1713, 1673, 1605, 1492, 1375, 1265, 1161, 1116, 1024, 880, 819, 759, 686, 590, 561, 516 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{16}F_3O_3^+$ $[M+H]^+$ 349.1046, found 349.1052.

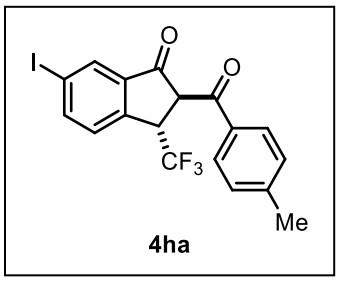
6-Chloro-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ga)



4ga

53 mg (75%) (exists as a 2.8:1 ratio of keto/enol tautomers); Light yellow solid; **mp** = 82.7–83.8 °C; **R_F** (Hexane/EtOAc 85:15): 0.61; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.05 (d, *J* = 8.5 Hz, 2H), 7.73–7.68 (m, 3H), 7.36 (d, *J* = 8.0 Hz, 2H), 4.96 (d, *J* = 3.0 Hz, 1H), 4.90 (qd, *J* = 9.0, 3.0 Hz, 1H), 2.47 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 194.7, 190.1, 145.1 (q, $J_{C\text{-}F}$ = 2.4 Hz), 136.1, 130.6, 129.7, 129.5, 129.3, 127.1, 124.9, 126.0 (q, $J_{C\text{-}F}$ = 276.7 Hz), 123.9, 122.7, 58.1, 45.7 (q, $J_{C\text{-}F}$ = 29.7 Hz), 22.0; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.0; **IR (KBr)** υ 3065, 2951, 2926, 2856, 1720, 1677, 1612, 1508, 1465, 1433, 1375, 1274, 1252, 1179, 1110, 1033, 905, 841, 809, 734, 701, 667, 578 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{18}H_{13}ClF_3O_2^+$ $[M+H]^+$ 353.0551, found 353.0569.

6-Iodo-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ha)

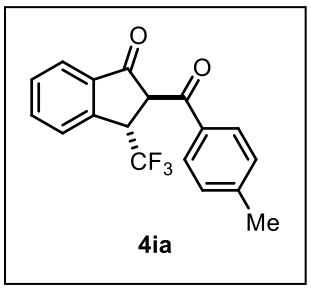


4ha

31 mg (35%); Yellowish orange solid; **mp** = 107.6–110.4 °C; **R_F** (Hexane/EtOAc 85:15): 0.52; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.10 (d, *J* = 1.5 Hz, 1H), 8.05–8.02 (m, 3H), 7.53 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 4.93 (d, *J* = 3.0 Hz, 1H), 4.87 (qd, *J* = 9.0, 3.0 Hz, 1H), 2.46 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 194.4, 190.1, 146.2 (q, $J_{C\text{-}F}$ = 2.3 Hz), 145.7, 144.6, 137.6, 134.2, 132.8, 130.5, 129.7, 128.7, 125.9 (q, $J_{C\text{-}F}$ =

278.5 Hz), 95.8, 57.7, 45.9 (q, J_{C-F} = 29.7 Hz), 22.0; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9; **IR (KBr)** υ 2926, 1721, 1679, 1605, 1457, 1377, 1297, 1266, 1232, 1168, 1109, 1030, 909, 863, 749, 622, 597, 526 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{18}H_{13}F_3IO_2^+$ $[M+H]^+$ 444.9907, found 444.9906.

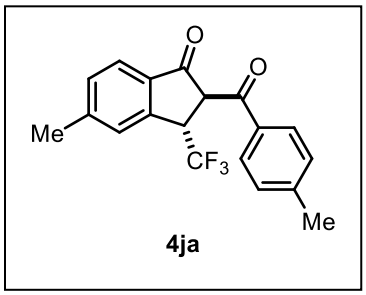
2-(4-Methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ia)



4ia

31 mg (49%) (exists as a 6.7:1 ratio of keto/enol tautomers); White solid; **mp** = 110.5–111.9 °C; **R_F** (Hexane/EtOAc 85:15): 0.48; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.07 (d, *J* = 8.5 Hz, 2H), 7.80–7.77 (m, 2H), 7.74 (td, *J* = 7.5, 1.0 Hz, 1H), 7.55 (t, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 4.99–4.91 (m, 2H), 2.46 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.0, 190.7, 147.0 (q, J_{C-F} = 2.6 Hz), 145.5, 136.0, 135.8, 133.0, 130.6, 130.1, 129.8, 126.3 (q, J_{C-F} = 276.6 Hz), 127.1, 125.2, 57.8, 46.1 (q, J_{C-F} = 29.5 Hz), 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9; **IR (KBr)** υ 2926, 1715, 1661, 1604, 1462, 1372, 1263, 1162, 1116, 1010, 908, 808, 760, 690, 572, 521 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{18}H_{14}F_3O_2^+$ $[M+H]^+$ 319.0940, found 319.0949.

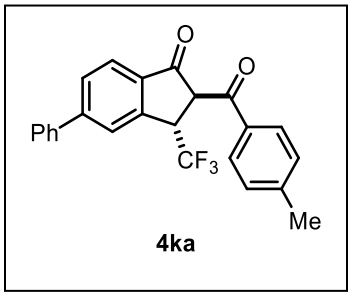
5-Methyl-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ja):



4ja

35 mg (53%) (exists as a 7.7:1 ratio of keto/enol tautomers); White solid; **mp** = 190.6–192.1 °C; **R_F** (Hexane/EtOAc 85:5): 0.52; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.06 (d, *J* = 8.5 Hz, 2H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.56 (s, 1H), 7.36–7.33 (m, 3H), 4.92 (d, *J* = 3.0 Hz, 1H), 4.88 (qd, *J* = 9.5, 3.5 Hz, 1H), 2.51 (s, 3H), 2.46 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 195.4, 191.0, 147.7, 147.4 (q, J_{C-F} = 2.3 Hz), 145.4, 133.5, 133.1, 131.3, 130.5, 129.6, 127.4, 126.3 (q, J_{C-F} = 276.7 Hz), 125.0, 58.0, 45.9 (q, J_{C-F} = 29.3 Hz), 22.4, 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.8; **IR (KBr)** υ 2925, 1712, 1665, 1606, 1456, 1410, 1371, 1263, 1161, 1115, 1016, 974, 868, 763, 665, 539, 519 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{16}F_3O_2^+$ $[M+H]^+$ 333.1037, found 333.1051.

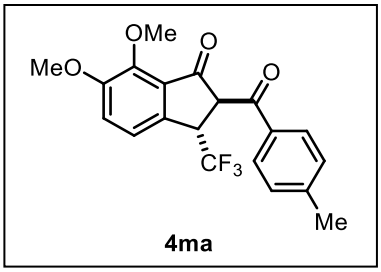
2-(4-Methylbenzoyl)-5-phenyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ka):



4ka

31 mg (39%); White solid; **mp** = 130.6–132.2 °C; **R_F** (Hexane/EtOAc 85:15): 0.48; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.09 (d, *J* = 8.5 Hz, 2H), 7.96 (s, 1H), 7.83 (d, *J* = 8.1 Hz, 1H), 7.76 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.70–7.63 (m, 2H), 7.52 (t, *J* = 8.1 Hz, 2H), 7.48–7.43 (m, 1H), 7.37 (d, *J* = 8.0 Hz, 2H), 5.04–4.95 (m, 2H), 2.47 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 195.5, 190.8, 149.3, 147.7 (q, J_{C-F} = 2.2 Hz), 145.5, 139.6, 134.5, 133.1, 130.6, 129.6, 129.4, 129.3, 129.0, 127.8, 126.3 (q, J_{C-F} = 276.7 Hz), 125.6, 125.5, 58.1, 46.1 (q, J_{C-F} = 29.4 Hz), 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.7; **IR (KBr)** υ 2958, 1721, 1679, 1662, 1605, 1414, 1371, 1251, 1154, 1111, 1012, 863, 760, 695, 579, 528 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{24}H_{18}F_3O_2^+$ $[M+H]^+$ 395.1253, found 395.1274.

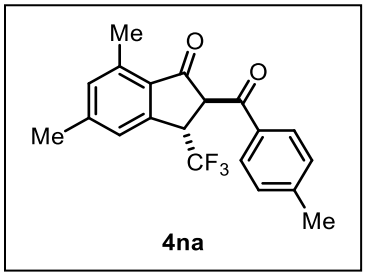
6,7-Dimethoxy-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ma):



4ma

29 mg (38%) (exists as a 7.1:1 ratio of keto/enol tautomers); Light yellow semi-solid; **R_F** (Hexane/EtOAc 85:15): 0.39; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.06 (d, *J* = 8.5 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.5 Hz, 1H), 4.90 (d, *J* = 3.0 Hz, 1H), 4.79 (qd, *J* = 9.0, 3.0 Hz, 1H), 3.94 (s, 3H), 3.91 (s, 3H), 2.45 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 193.6, 190.9, 153.5, 148.1, 145.4, 139.0 (d, J_{C-F} = 2.3 Hz), 133.0, 130.6, 129.6, 128.2, 126.3 (d, J_{C-F} = 278.1 Hz), 121.8, 120.5, 62.1, 58.7, 56.9, 44.9 (q, J_{C-F} = 29.4 Hz), 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.4; **IR (KBr)** υ 2933, 2850, 1724, 1676, 1607, 1495, 1423, 1277, 1167, 1115, 1012, 964, 820, 690, 590, 535 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{20}H_{18}F_3O_4^+$ $[M+H]^+$ 379.1152, found 379.1166.

5,7-Dimethyl-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4na):

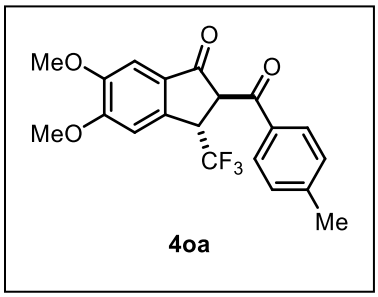


4na

45 mg (65%); White solid; **mp** = 103.0–104.3 °C; **R_F** (Hexane/EtOAc 85:15): 0.58; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.07 (d, *J* = 8.5 Hz, 2H), 7.38 (s, 1H), 7.36 (d, *J* = 8.0 Hz, 2H), 7.09 (s, 1H), 4.90 (d, *J* = 3.5 Hz, 1H), 4.83 (qd, *J* = 9.0, 3.0 Hz, 1H), 2.53 (s, 3H), 2.45 (s, 6H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.2, 191.3, 148.1 (q, J_{C-F} = 2.3 Hz), 146.8, 145.3, 140.2, 133.2, 133.1, 130.9, 130.6, 129.5, 126.4 (d, J_{C-F} =

278.4 Hz), 124.9, 58.1, 45.3 (q, $J_{C\text{-}F}$ = 29.2 Hz), 22.2, 21.9, 18.4; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.5; **IR (KBr)** υ 2951, 1714, 1665, 1609, 1448, 1360, 1269, 1170, 1111, 999, 861, 747, 670, 597 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{20}H_{18}F_3O_2^+$ $[M+H]^+$ 347.1253, found 347.1251.

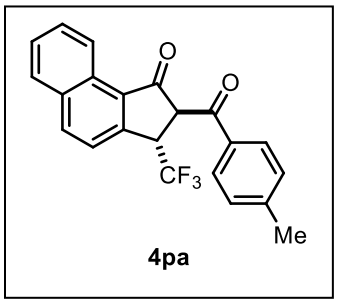
5,6-Dimethoxy-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4oa):



4oa

56 mg (74%); Off white solid; **mp** = 117.0–118.8 °C; **R_F** (Hexane/EtOAc 85:15): 0.21; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.07 (d, *J* = 8.5 Hz, 2H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.14 (d, *J* = 2.5 Hz, 2H), 4.90 (d, *J* = 3.0 Hz, 1H), 4.81 (qd, *J* = 9.0, 3.0 Hz, 1H), 4.03 (s, 3H), 3.90 (s, 3H), 2.45 (s, 3H). **^{13}C NMR (125 MHz, $CDCl_3$)** δ 194.5, 191.3, 156.3, 151.4, 145.3, 142.3 (q, $J_{C\text{-}F}$ = 2.5 Hz), 133.2, 130.5, 129.6, 128.8, 126.4 (q, $J_{C\text{-}F}$ = 278.5 Hz), 107.8, 105.2, 57.9, 56.6, 56.3, 45.8 (q, $J_{C\text{-}F}$ = 29.4 Hz), 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.0. **IR (KBr)** υ 2937, 2839, 1705, 1668, 1589, 1504, 1272, 1158, 1120, 1022, 589, 817, 749, 675, 589, 531 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{20}H_{18}F_3O_4^+$ $[M+H]^+$ 379.1152, found 379.1153.

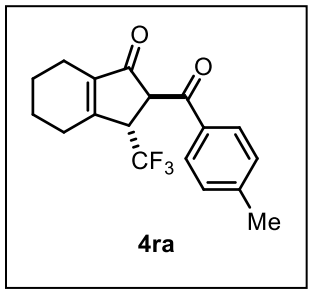
2-(4-Methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-cyclopenta[*a*]naphthalen-1-one (4pa):



4pa

31 mg (42%) (exists as a 11.1:1 ratio of keto/enol tautomers); Light yellow solid; **mp** = 136.3–139.2 °C; **R_F** (Hexane/EtOAc 85:15): 0.52; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.02 (d, *J* = 8.5 Hz, 1H), 8.20 (d, *J* = 8.5 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 2H), 7.95 (d, *J* = 9.0 Hz, 1H), 7.82 (d, *J* = 8.5 Hz, 1H), 7.68 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H), 7.62 (ddd, *J* = 8.0, 7.0, 1.5 Hz, 1H), 7.39 (d, *J* = 8.0 Hz, 2H), 5.07 (d, *J* = 3.0 Hz, 1H), 5.03 (dd, *J* = 9.0, 3.0 Hz, 1H), 2.48 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.5, 190.9, 150.1 (q, $J_{C\text{-}F}$ = 2.1 Hz), 145.5, 137.3, 133.9, 133.2, 130.6, 130.3, 129.9, 129.6, 129.4, 128.5, 127.9, 126.3 (q, $J_{C\text{-}F}$ = 278.7 Hz), 124.3, 123.3, 58.1, 46.1 (q, $J_{C\text{-}F}$ = 29.3 Hz), 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.3; **IR (KBr)** υ 2945, 1704, 1675, 1605, 1514, 1383, 1256, 1167, 1111, 1035, 928, 827, 751, 622, 532 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{22}H_{16}F_3O_2^+$ $[M+H]^+$ 369.1097, found 369.1118.

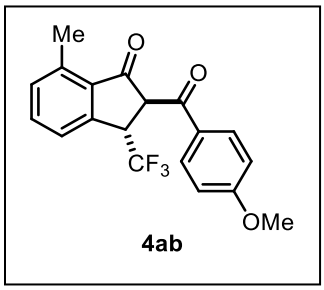
2-(4-Methylbenzoyl)-3-(trifluoromethyl)-2,3,4,5,6,7-hexahydro-1*H*-inden-1-one (4ra):



4ra

21 mg (33%); White solid; **mp** = 110.3–112.0 °C; **R_F** (Hexane/EtOAc 85:15): 0.55; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.01 (d, *J* = 8.5 Hz, 2H), 7.33 (d, *J* = 8.0 Hz, 2H), 4.59 (d, *J* = 2.5 Hz, 1H), 4.27 (qd, *J* = 9.0, 1.5 Hz, 1H), 2.59–2.50 (m, 2H), 2.44 (s, 3H), 2.24–2.18 (m, 1H), 2.12–2.05 (m, 1H), 1.90–1.83 (m, 1H), 1.78–1.68 (m, 2H), 1.66–1.60 (m, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 198.0, 191.5, 166.2, 145.2, 140.8, 133.3, 130.4, 129.5, 126.0 (q, *J* = 279.5 Hz), 55.8, 49.3 (q, *J* = 28.9 Hz), 27.4, 22.1, 21.9, 21.1, 20.6; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -67.5; **IR (KBr)** υ 2927, 1712, 1667, 1605, 1424, 1388, 1270, 1143, 1102, 1010, 946, 808, 689, 591, 525 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{18}H_{18}F_3O_2^+$ $[M+H]^+$ 323.1253, found 323.1264.

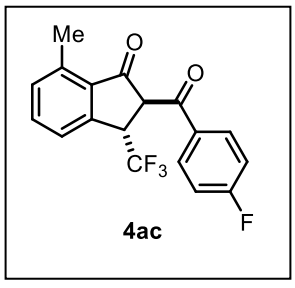
2-(4-Methoxybenzoyl)-7-methyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ab):



4ab

43 mg (62%); White solid; **mp** = 116.2–117.2 °C; **R_F** (Hexane/EtOAc 85:15): 0.45; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.16 (d, *J* = 9.0 Hz, 2H), 7.61–7.56 (m, 2H), 7.28 (d, *J* = 6.5 Hz, 1H), 7.03 (d, *J* = 9.0 Hz, 2H), 4.93–4.85 (m, 2H), 3.91 (s, 3H), 2.58 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 197.1, 189.6, 164.6, 147.7 (q, $J_{C\text{-}F}$ = 2.3 Hz), 140.5, 135.2, 133.1, 132.9, 132.0, 128.6, 126.4 (d, $J_{C\text{-}F}$ = 278.5 Hz), 124.5, 114.1, 57.7, 55.7, 45.5 (q, $J_{C\text{-}F}$ = 29.2 Hz), 18.5; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9; **IR (KBr)** υ 2975, 2924, 1714, 1658, 1600, 1479, 1266, 1168, 978, 837, 688, 595, 509 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{16}F_3O_3^+$ $[M+H]^+$ 349.1046, found 349.1051.

2-(4-Fluorobenzoyl)-7-methyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ac):

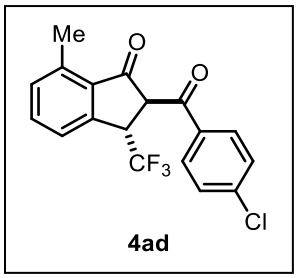


4ac

48 mg (71%); White solid; **mp** = 96.4–97.7 °C; **R_F** (Hexane/EtOAc 85:15): 0.61; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.24–8.20 (m, 2H), 7.63–7.56 (m, 2H), 7.31–7.29 (m, 1H), 7.24–7.21 (m, 2H), 4.92–4.86 (m, 2H), 2.58 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.5, 189.8, 166.6 (d, $J_{C\text{-}F}$ = 257.1 Hz), 147.5 (q, $J_{C\text{-}F}$ = 2.1 Hz), 140.6, 135.4, 133.3 (d, $J_{C\text{-}F}$ = 9.6 Hz), 132.9, 132.1, 132.0 (d, $J_{C\text{-}F}$ = 2.8 Hz), 126.3 (q, $J_{C\text{-}F}$ = 278.5 Hz), 124.5, 116.1 (d, $J_{C\text{-}F}$ = 22.1 Hz), 58.0, 45.4 (q, $J_{C\text{-}F}$ = 29.3 Hz), 18.5; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9, -103.2; **IR (KBr)** υ 2960, 2917, 1725, 1673, 1599, 1365, 1262, 1164,

1109, 993, 828, 786, 683, 593 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{18}H_{13}F_4O_2^+$ $[M+H]^+$ 337.0846, found 337.0853.

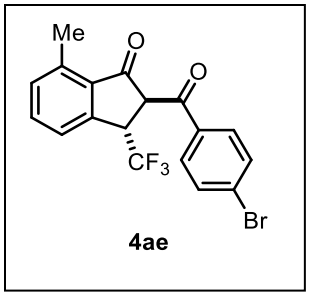
2-(4-Chlorobenzoyl)-7-methyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ad):



4ad

41 mg (58%); White solid; **mp** = 98.1–100.3 °C; **R_F** (Hexane/EtOAc 85:15): 0.61; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.12 (d, *J* = 8.5 Hz, 2H), 7.61–7.59 (m, 2H), 7.54 (d, *J* = 8.5 Hz, 2H), 7.31–7.29 (m, 1H), 4.89 (qd, *J* = 9.0, 3.5 Hz, 1H), 4.87 (d, *J* = 3.5 Hz, 1H), 2.58 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.4, 190.3, 147.5 (q, J_{C-F} = 2.1 Hz), 141.0, 140.7, 135.5, 133.9, 132.9, 132.1, 131.8, 129.2, 126.3 (q, J_{C-F} = 278.4 Hz), 124.5, 58.0 (q, J_{C-F} = 1.8 Hz), 45.4 (q, J_{C-F} = 29.4 Hz), 18.5; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9; **IR (KBr)** υ 2965, 2936, 1723, 1676, 1591, 1477, 1262, 1109, 982, 820, 787, 971, 528cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{18}H_{13}ClF_3O_2^+$ $[M+H]^+$ 353.0551, found 353.0564.

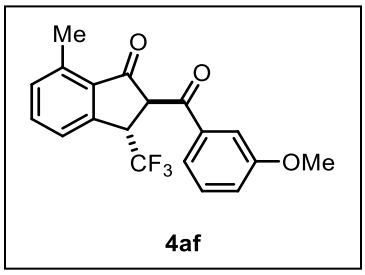
2-(4-Bromobenzoyl)-7-methyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ae):



4ae

56 mg (70%); White solid; **mp** = 104.6–106.9 °C; **R_F** (Hexane/EtOAc 85:15): 0.61; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.04 (d, *J* = 8.5 Hz, 2H), 7.71 (d, *J* = 8.5 Hz, 2H), 7.62–7.57 (m, 2H), 7.31–7.28 (m, 1H), 4.89 (qd, *J* = 9.0, 3.5 Hz, 1H), 4.86 (d, *J* = 3.5 Hz, 1H), 2.58 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.3, 190.5, 147.5 (q, J_{C-F} = 2.3 Hz), 140.7, 135.5, 134.3, 132.9, 132.2, 132.1, 131.9, 129.9, 126.3 (q, J_{C-F} = 278.5 Hz), 124.5, 58.0, 45.4 (q, J_{C-F} = 29.4 Hz), 18.5; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9; **IR (KBr)** υ 2967, 1723, 1676, 1588, 1364, 1260, 1164, 1107, 980, 819, 787, 664, 565 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{18}H_{13}BrF_3O_2^+$ $[M+H]^+$ 397.0046, found 397.0050.

2-(3-Methoxybenzoyl)-7-methyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4af):

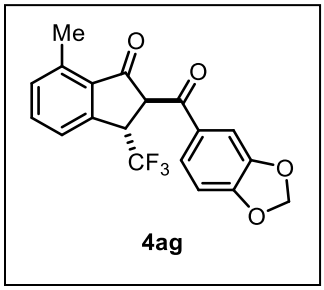


4af

37 mg (53%) (exists as a 10:1 ratio of keto/enol tautomers); Off white solid; **mp** = 76.0–76.9 °C; **R_F** (Hexane/EtOAc 85:15): 0.48; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.80 (d, *J* = 7.5 Hz, 1H), 7.66 (dd, *J* = 2.5, 1.5 Hz, 1H), 7.62–7.57 (m, 2H), 7.49 (t, *J* = 8.0 Hz, 1H), 7.30–7.28 (m, 1H), 7.21 (ddd, *J* = 8.5, 2.5, 1.0 Hz, 1H), 4.91 (d, *J* = 3.5 Hz, 1H), 4.87 (qd, *J* = 9.0, 3.5 Hz, 1H), 3.89 (s, 3H), 2.58 (s, 3H); **^{13}C NMR (125 MHz,**

$CDCl_3$) δ 196.6, 191.5, 160.0, 147.5 (q, J_{C-F} = 2.2 Hz), 140.6, 137.0, 135.3, 133.0, 132.1, 129.9, 126.3 (q, J_{C-F} = 278.4 Hz), 124.4, 123.3, 120.9, 114.1, 58.1, 55.6, 45.6 (q, J_{C-F} = 29.3 Hz), 18.5; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9; **IR (KBr)** υ 3082, 3030, 2945, 2842, 1714, 1671, 1596, 1471, 1430, 1368, 1339, 1264, 1199, 1164, 1090, 1041, 995, 948, 917, 807, 788, 760, 734, 691, 647, 626 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{16}F_3O_3^+$ $[M+H]^+$ 349.1046, found 349.1055.

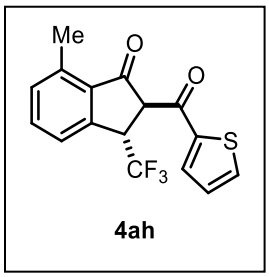
2-(Benzo[*d*][1,3]dioxole-5-carbonyl)-7-methyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ag):



4ag

53 mg (73%); Off white solid; **mp** = 126.6–128.0 °C; **R_F** (Hexane/EtOAc 85:15): 0.45; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.83 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.63–7.55 (m, 3H), 7.29–7.27 (m, 1H), 6.97 (d, *J* = 8.5 Hz, 1H), 6.09 (d, *J* = 1.5 Hz, 1H), 6.08 (d, *J* = 1.5 Hz, 1H), 4.86 (qd, *J* = 9.5, 3.0 Hz, 1H), 4.82 (d, *J* = 3.5 Hz, 1H), 2.58 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.9, 189.4, 153.0, 148.5, 147.6 (q, J_{C-F} = 2.0 Hz), 140.5, 135.3, 133.0, 132.0, 130.4, 127.8, 126.3 (q, J_{C-F} = 278.5 Hz), 124.5, 109.6, 108.2, 102.3, 57.8, 45.6 (q, J_{C-F} = 29.2 Hz), 18.5; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9; **IR (KBr)** υ 2888, 1714, 1659, 1598, 1444, 1369, 1258, 1158, 1115, 1038, 1006, 892, 793, 638, 579 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{19}H_{14}F_3O_4^+$ $[M+H]^+$ 363.0839, found 363.0847.

7-Methyl-2-(thiophene-2-carbonyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4ah):



4ah

47 mg (72%); White solid; **mp** = 102.2–103 °C; **R_F** (Hexane/EtOAc 85:15): 0.52; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.08 (dd, *J* = 4.0, 1.0 Hz, 1H), 7.80 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.60–7.56 (m, 2H), 7.32–7.26 (m, 2H), 4.87 (qd, *J* = 9.0, 3.5 Hz, 1H), 4.66 (d, *J* = 3.5 Hz, 1H), 2.60 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.3, 183.9, 147.5 (q, J_{C-F} = 2.1 Hz), 142.8, 140.6, 136.3, 136.1, 135.4, 133.0, 132.1, 128.8, 126.2 (q, J_{C-F} = 278.4 Hz), 124.5, 59.1 (q, J_{C-F} = 2.0 Hz), 45.2 (q, J_{C-F} = 29.4 Hz), 18.5; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9; **IR (KBr)** υ 2964, 2926, 1721, 1649, 1599, 1477, 1355, 1259, 1164, 1105, 991, 808, 731, 677, 573 516 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{16}H_{12}F_3O_2S^+$ $[M+H]^+$ 325.0505, found 325.0504.

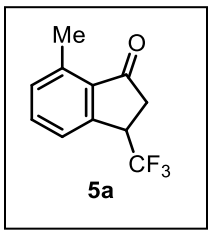
General procedure for synthesis of 3-trifluoromethylindanones and spectral data (5a-5p):

General procedure (reaction condition-A): To an oven-dried sealed tube charged with a stirring bar were added corresponding *N*-methoxybenzamides **1a-1p** (0.20 mmol, 100 mol %), (*E*)-4,4,4-trifluoro-1-(*p*-tolyl)but-2-en-1-one **2a** (64.3 mg, 0.30 mmol, 150 mol %), $[RhCp^*Cl_2]_2$ (1.9 mg, 3.0 μmol, 1.5 mol %) and KOAc (29.4 mg, 0.30 mmol, 150 mol %) in 2,2,2-trifluoroethanol (0.2 mL, 1.0 M). The reaction mixture was allowed to stir at 120 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide corresponding 3-trifluoromethyl indanones (**5a-5p)**.

General procedure (reaction condition-B): step-i): To an oven-dried sealed tube charged with a stirring bar were added corresponding *N*-methoxybenzamides **1a-1p** (0.20 mmol, 100 mol %), (*E*)-4,4,4-trifluoro-1-(*p*-tolyl)but-2-en-1-one **2a** (42.8 mg, 0.20 mmol, 100 mol %), $[RhCp^*Cl_2]_2$ (1.2 mg, 2.0 μmol, 1.0 mol %) and NaOAc (3.3 mg, 0.04 mmol, 20 mol %) in 1,2-dichloroethane (1.0 mL, 0.2 M). The reaction mixture was allowed to stir at 80 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide corresponding C-H alkylated products (**3aa-3ap)**.

step-ii): To an oven-dried sealed tube charged with a stirring bar were added corresponding C-H alkylated products **3aa-3ap** (100 mol %) and KOAc (150 mol %) in 2,2,2-trifluoroethanol (1.0 M). The reaction mixture was allowed to stir at 120 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide corresponding 3-trifluoromethyl indanones **(5a-5p)**.

7-Methyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5a):

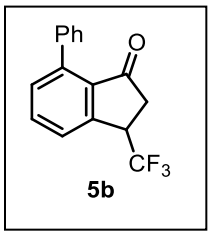


5a

Reaction condition-**A**: 30 mg (70%), reaction condition-**B**: 28 mg (65%); Light yellowish oil; $\mathbf{R_F}$ (Hexane/EtOAc 85:15): 0.55; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.57–7.48 (m, 2H), 7.27 (d, *J* = 7.5 Hz, 1H), 4.04 (pd, *J* = 9.0, 3.5 Hz, 1H), 2.90 (dd, *J* = 19.0, 8.5 Hz, 1H), 2.78 (dd, *J* = 19.0, 3.5 Hz, 1H), 2.66 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 203.2, 147.9, (q, $J_{C\text{-}F}$ = 2.4 Hz), 139.6, 134.9, 134.6, 131.7, 126.5 (q, $J_{C\text{-}F}$ = 276.6 Hz), 124.5, 42.1 (q, $J_{C\text{-}F}$ = 29.5 Hz), 37.5 (q, $J_{C\text{-}F}$ = 2.4 Hz), 18.4; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.3; **IR (KBr)** υ 3075, 2931, 2855, 1719, 1597, 1478,

1415, 1356, 1272, 1155, 1111, 1043, 944, 780, 756, 619 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{11}H_{10}F_3O^+$ $[M+H]^+$ 215.0678, found 215.0681.

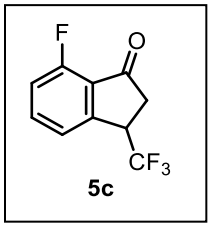
7-Phenyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5b):



5b

Reaction condition-**A**: 67%, reaction condition-**B**: 34 mg (62%); White solid; **mp** = 96.5–97.4 °C; $\mathbf{R_F}$ (Hexane/EtOAc 85:15): 0.48; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.74–7.65 (m, 2H), 7.48–7.39 (m, 6H), 4.10 (pd, *J* = 9.0, 3.5 Hz, 1H), 2.93 (dd, *J* = 19.0, 8.5 Hz, 1H), 2.82 (dd, *J* = 19.0, 3.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 200.8, 148.3 (q, $J_{C\text{-}F}$ = 2.3 Hz), 142.2, 137.4, 134.6, 133.6, 132.0, 129.4, 128.3, 128.0, 126.5 (q, $J_{C\text{-}F}$ = 278.2 Hz), 126.1, 42.0 (q, $J_{C\text{-}F}$ = 29.5 Hz), 37.6 (q, $J_{C\text{-}F}$ = 2.1 Hz); **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.2; **IR (KBr)** υ 2933, 1709, 1589, 1572, 1456, 1357, 1265, 1194, 1163, 1105, 1037, 943, 908, 765, 659, 561 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{16}H_{12}F_3O^+$ $[M+H]^+$ 277.0835, found 277.0843.

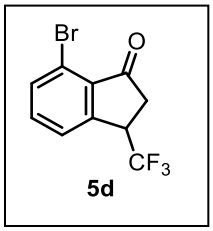
7-Fluoro-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5c):



5c

Reaction condition-**A**: 18 mg (41%), reaction condition-**B**: 16 mg (37%); Light yellowish oil; $\mathbf{R_F}$ (Hexane/EtOAc 85:15): 0.36; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.68 (td, *J* = 8.0, 5.0 Hz, 1H), 7.49 (d, *J* = 9.0 Hz, 1H), 7.17 (dd, *J* = 9.0, 8.0 Hz, 1H), 4.11 (pd, *J* = 8.5, 3.5 Hz, 1H), 2.97 (dd, *J* = 19.0, 8.5 Hz, 1H), 2.84 (dd, *J* = 19.0, 3.0 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 198.2 (d, $J_{C\text{-}F}$ = 1.8 Hz), 159.0 (d, $J_{C\text{-}F}$ = 265.3 Hz), 148.9 (p, $J_{C\text{-}F}$ = 5.0 Hz), 137.4 (d, $J_{C\text{-}F}$ = 8.4 Hz), 126.1 (d, $J_{C\text{-}F}$ = 278.2), 125.4 (d, $J_{C\text{-}F}$ = 13.6 Hz), 123.1 (d, $J_{C\text{-}F}$ = 4.1 Hz), 117.0 (d, $J_{C\text{-}F}$ = 19.2 Hz), 42.6 (q, $J_{C\text{-}F}$ = 29.8 Hz), 37.5 (q, $J_{C\text{-}F}$ = 2.2 Hz); **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.2, -113.5; **IR (KBr)** υ 2940, 1731, 1616, 1595, 1478, 1357, 1271, 1194, 1161, 1113, 987, 945, 783, 749, 664, 573, 509 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{10}H_7F_4O^+$ $[M+H]^+$ 219.0428, found 219.0439.

7-Bromo-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5d):

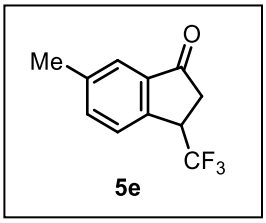


5d

Reaction condition-**A**: 23%, reaction condition-**B**: 21 mg (38%); Light yellowish oil; $\mathbf{R_F}$ (Hexane/EtOAc 85:15): 0.45; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.70 (d, *J* = 7.5 Hz, 1H), 7.66 (dd, *J* = 7.5, 1.5 Hz, 1H), 7.51 (t, *J* = 7.5 Hz, 1H), 4.05 (pd, *J* = 9.0, 3.5 Hz, 1H), 2.99 (dd, *J* = 19.0, 8.5 Hz, 1H), 2.87 (dd, *J* = 19.0, 3.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 199.1, 149.7 (q, $J_{C\text{-}F}$ = 2.5

Hz), 135.7, 135.1, 134.8, 126.3, 126.1 (q, $J_{C\text{-}F}$ = 276.5 Hz), 120.2, 41.6 (q, $J_{C\text{-}F}$ = 30.0 Hz), 37.8 (q, $J_{C\text{-}F}$ = 2.2 Hz); **^{19}F NMR (470 MHz, CDCl$_3$)** δ -70.2; **IR (KBr)** υ 2935, 1728, 1589, 1573, 1456, 1413, 1354, 1317, 1270, 1162, 1111, 1039, 944, 903, 750, 657, 588, 565 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{10}H_7BrF_3O^+$ $[M+H]^+$ 278.9627, found 278.9634.

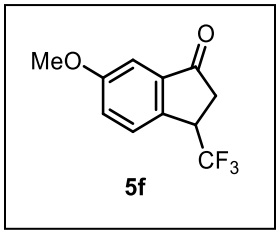
6-Methyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5e):



5e

Reaction condition-**A**: 61%, reaction condition-**B**: 28 mg (65%); Light yellowish oil; **R$_F$** (Hexane/EtOAc 85:15): 0.45; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.61 (s, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.50 (dd, *J* = 8.0, 1.5 Hz, 1H), 4.06 (pd, *J* = 9.0, 3.5 Hz, 1H), 2.92 (dd, *J* = 19.0, 8.5 Hz, 1H), 2.80 (dd, *J* = 19.0, 3.5 Hz, 1H), 2.44 (s, 3H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 202.4, 144.7 (q, $J_{C\text{-}F}$ = 2.4 Hz), 140.2, 137.8, 136.6, 126.8, 126.5 (q, $J_{C\text{-}F}$ = 276.5 Hz), 124.3, 42.3 (q, $J_{C\text{-}F}$ = 29.6 Hz), 37.4 (q, $J_{C\text{-}F}$ = 2.3 Hz), 21.3; **^{19}F NMR (470 MHz, CDCl$_3$)** δ -70.5; **IR (KBr)** υ 2927, 2855, 1725, 1677, 1617, 1585, 1494, 1412, 1359, 1268, 1160, 1109, 944, 830, 720, 656, 555 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{11}H_{10}F_3O^+$ $[M+H]^+$ 215.0678, found 215.0699.

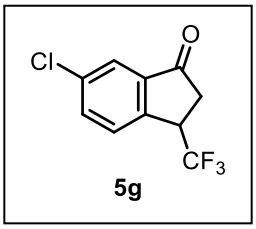
6-Methoxy-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5f):



5f

Reaction condition-**A**: 28 mg (61%), reaction condition-**B**: 29 mg (63%); White solid; **mp** = 63.4–64.6 °C; **R$_F$** (Hexane/EtOAc 85:15): 0.33; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.57 (d, *J* = 8.5 Hz, 1H), 7.28–7.22 (m, 2H), 4.03 (pd, *J* = 8.5, 3.5 Hz, 1H), 3.86 (s, 3H), 2.95 (dd, *J* = 19.2, 8.1 Hz, 1H), 2.81 (dd, *J* = 19.2, 3.3 Hz, 1H); **^{13}C NMR (125 MHz, CDCl$_3$)** δ 202.2, 161.2, 139.9 (q, $J_{C\text{-}F}$ = 2.4 Hz), 139.1, 127.9, 126.48 (q, $J_{C\text{-}F}$ = 278.1 Hz), 124.5, 105.6, 55.8, 42.06 (q, $J_{C\text{-}F}$ = 29.9 Hz), 37.72 (q, $J_{C\text{-}F}$ = 2.4 Hz); **^{19}F NMR (470 MHz, CDCl$_3$)** δ -70.7; **IR (KBr)** υ 2980, 2945, 1722, 1684, 1611, 1494, 1433, 1335, 1254, 1150, 1103, 940, 842, 663, 557, 511 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{11}H_{10}F_3O_2^+$ $[M+H]^+$ 231.0627, found 231.0633.

6-Chloro-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5g):

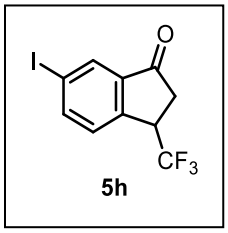


5g

Reaction condition-**A**: 62%, reaction condition-**B**: 26 mg (55%); White solid; **mp** = 101.2–102.5 °C; **R$_F$** (Hexane/EtOAc 85:15): 0.45; **^{1}H NMR (500 MHz, CDCl$_3$)** δ 7.78 (s, 1H), 7.67–7.63 (m, 2H), 4.08 (pd, *J* = 8.5, 3.5 Hz, 1H), 2.97 (dd, *J* = 19.5, 8.5 Hz, 1H), 2.84 (dd, *J* = 19.5, 3.5 Hz, 1H);

^{13}C NMR (125 MHz, $CDCl_3$) δ 200.7, 145.2 (q, J_{C-F} = 2.4 Hz), 139.2, 136.7, 135.5, 128.4, 126.1 (q, J_{C-F} = 276.6 Hz), 124.3, 42.4 (q, J_{C-F} = 30.1 Hz), 37.4 (q, J_{C-F} = 2.2 Hz); **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.4; **IR (KBr)** υ 2958, 2928, 1719, 1605, 1582, 1475, 1362, 1275, 1148, 1103, 1048, 945, 896, 833, 690, 655, 522 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{10}H_7ClF_3O^+$ $[M+H]^+$ 235.0132, found 235.0140.

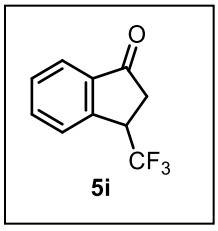
6-Iodo-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5h):



5h

Reaction condition-**A**: 49%, reaction condition-**B**: 20 mg (31%); White solid; **mp** = 97.5–100.9 °C; **R_F** (Hexane/EtOAc 85:15): 0.55; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.16 (d, J = 1.5 Hz, 1H), 7.99 (dd, J = 8.0, 1.5 Hz, 1H), 7.45 (d, J = 8.0 Hz, 1H), 4.05 (pd, J = 9.0, 3.5 Hz, 1H), 2.94 (dd, J = 19.5, 8.5 Hz, 1H), 2.82 (dd, J = 19.5, 3.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 200.4, 146.4 (q, J_{C-F} = 2.4 Hz), 144.0, 139.5, 133.6, 128.9, 126.1 (q, J_{C-F} = 278.3 Hz), 95.8, 42.5 (q, J_{C-F} = 30.1 Hz), 37.0 (q, J_{C-F} = 2.3 Hz); **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.3; **IR (KBr)** υ 2926, 1709, 1592, 1572, 1469, 1402, 1263, 1152, 1104, 945, 884, 804, 683, 654, 598 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{10}H_7F_3IO^+$ $[M+H]^+$ 326.9488, found 326.9499.

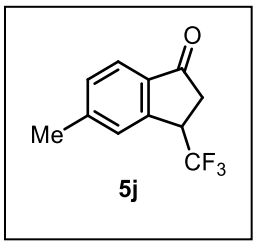
3-(Trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5i):



5i

Reaction condition-**A**: 18 mg (45%), reaction condition-**B**: 16 mg (40%); Light yellowish oil; **R_F** (Hexane/EtOAc 85:15): 0.42; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.83 (d, J = 7.5 Hz, 1H), 7.75–7.65 (m, 2H), 7.58–7.50 (m, 1H), 4.11 (pd, J = 9.0, 3.5 Hz, 1H), 2.94 (dd, J = 19.0, 8.5 Hz, 1H), 2.82 (dd, J = 19.0, 3.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 202.2, 147.2 (q, J_{C-F} = 2.4 Hz), 137.7, 135.4, 129.9, 127.2, 126.4 (q, J_{C-F} = 276.5 Hz), 124.3, 42.5 (q, J_{C-F} = 29.6 Hz), 37.3 (q, J_{C-F} = 2.3 Hz); **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.3; **IR (KBr)** υ 2957, 2928, 2871, 1725, 1607, 1466, 1413, 1358, 1266, 1158, 1112, 1045, 939, 763, 655, 581 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{10}H_8F_3O^+$ $[M+H]^+$ 201.0522, found 201.0529.

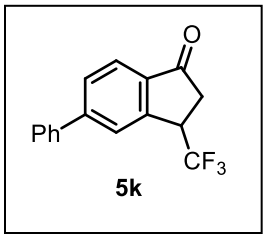
5-Methyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5j):



5j

Reaction condition-**A**: 22 mg (51%), reaction condition-**B**: 19 mg (44%); White solid; **mp** = 85.0-86.3 °C; $\mathbf{R_F}$ (Hexane/EtOAc 85:15): 0.39; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.71 (d, *J* = 8.0 Hz, 1H), 7.48 (s, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 4.05 (pd, *J* = 9.0, 3.5 Hz, 1H), 2.92 (dd, *J* = 19.0, 8.5 Hz, 1H), 2.79 (dd, *J* = 19.0, 3.5 Hz, 1H), 2.49 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 201.8, 147.7 (q, $J_{C\text{-}F}$ = 2.3 Hz), 146.9, 135.4, 131.0, 127.5, 126.5 (q, $J_{C\text{-}F}$ = 276.4 Hz), 124.1, 42.5 (q, $J_{C\text{-}F}$ = 29.6 Hz), 37.3 (q, $J_{C\text{-}F}$ = 2.3 Hz), 22.3; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.2; **IR (KBr)** υ 2950, 2925, 2853, 1716, 1608, 1417, 1368, 1268, 1162, 1102, 1042, 944, 831, 717, 662, 557, 521 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{11}H_{10}F_3O^+$ $[M+H]^+$ 215.0678, found 215.0684.

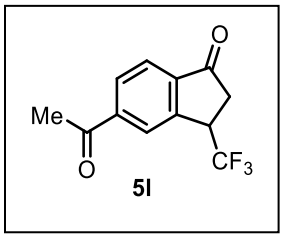
5-Phenyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5k):



5k

Reaction condition-**A**: 27 mg (49%), reaction condition-**B**: 20 mg (36%); White solid; **mp** = 74.0–75.5 °C; $\mathbf{R_F}$ (Hexane/EtOAc 85:15): 0.42; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.89 (d, *J* = 8.0 Hz, 2H), 7.76 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.65–7.63 (m, 2H), 7.52–7.48 (m, 2H), 7.46–7.43 (m, 1H), 4.16 (pd, *J* = 8.0, 3.5 Hz, 1H), 2.99 (dd, *J* = 19.0, 8.5 Hz, 1H), 2.87 (dd, *J* = 19.0, 3.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 201.7, 148.7, 147.9 (q, $J_{C\text{-}F}$ = 2.3 Hz), 139.7, 136.4, 129.2, 129.2, 128.9, 127.7, 126.5 (q, $J_{C\text{-}F}$ = 276.6 Hz), 125.3, 124.7, 42.7 (q, $J_{C\text{-}F}$ = 29.7 Hz) , 37.4 (q, $J_{C\text{-}F}$ = 2.3 Hz); **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.1; **IR (KBr)** υ 2943, 1713, 1606, 1578, 1509, 1455, 1414, 1364, 1269, 1168, 1105, 1055, 944, 847, 762, 691, 553 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{16}H_{12}F_3O^+$ $[M+H]^+$ 277.0835, found 277.0852.

5-Acetyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5l):

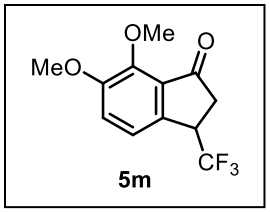


5l

Reaction condition-**A**: 23 mg (47%), reaction condition-**B**: 19 mg (39%); White solid; **mp** = 64.5–67.5 °C; $\mathbf{R_F}$ (Hexane/EtOAc 85:15): 0.18; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 8.24 (s, 1H), 8.10 (ddd, *J* = 8.0, 1.5, 1.0 Hz, 1H), 7.90 (d, *J* = 8.0 Hz, 1H), 4.17 (pd, *J* = 9.0, 3.5 Hz, 1H), 3.01 (dd, *J* = 19.5, 8.5 Hz, 1H), 2.89 (dd, *J* = 19.5, 3.5 Hz, 1H), 2.69 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 201.4, 197.1, 147.4 (q, $J_{C\text{-}F}$ = 2.3 Hz), 142.5, 140.5, 129.9, 126.2 (q, $J_{C\text{-}F}$ = 276.4 Hz), 127.0, 124.6, 42.7 (q, $J_{C\text{-}F}$ = 30.0 Hz), 37.5 (q, $J_{C\text{-}F}$ = 2.3 Hz), 27.3; **^{19}F NMR (470**

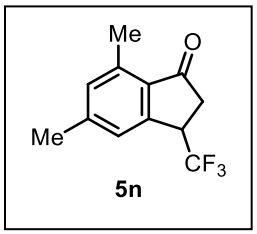
MHz, $CDCl_3$) δ -70.2; **IR (KBr)** υ 2938, 1722, 1687, 1610, 1585, 1482, 1416, 1364, 1293, 1270, 1145, 1108, 1037, 948, 859, 703, 654, 584, 518 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{12}H_{10}F_3O_2^+$ $[M+H]^+$ 243.0627, found 243.0635.

6,7-Dimethoxy-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5m):



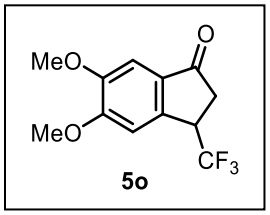
Reaction condition-**A**: 30 mg (58%), reaction condition-**B**: 32 mg (62%); Light yellow semi-solid; **R_F** (Hexane/EtOAc 85:15): 0.18; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.31 (d, *J* = 8.0 Hz, 1H), 7.22 (d, *J* = 8.0 Hz, 1H), 4.01 (s, 3H), 3.97 (pd, *J* = 9.0, 3.5 Hz, 1H), 3.90 (s, 3H), 2.92 (dd, *J* = 19.0, 8.5 Hz, 1H), 2.79 (dd, *J* = 19.0, 3.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 199.7, 153.3, 147.4, 139.4 (q, J_{C-F} = 2.3 Hz), 129.9, 126.5 (q, J_{C-F} = 278.2 Hz), 122.0, 119.8, 62.2, 56.8, 41.5 (q, J_{C-F} = 29.7 Hz), 38.3 (q, J_{C-F} = 2.2 Hz); **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.8; **IR (KBr)** υ 2939, 2843, 1722, 1690, 1589, 1494, 1413, 1358, 1273, 1157, 1113, 1025, 960, 826, 700, 682, 588, 535 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{12}H_{12}F_3O_3^+$ $[M+H]^+$ 261.0733, found 261.0739.

5,7-Dimethyl-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5n):



Reaction condition-**A**: 72%, reaction condition-**B**: 31 mg (68%); White solid; **mp** = 63.7–64.8 °C; **R_F** (Hexane/EtOAc 85:15): 0.55; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.29 (s, 1H), 7.08 (s, 1H), 3.98 (pd, *J* = 9.0, 3.5 Hz, 1H), 2.88 (dd, *J* = 19.0, 8.5 Hz, 1H), 2.76 (dd, *J* = 19.0 3.5 Hz, 1H), 2.61 (s, 3H), 2.43 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 202.6, 148.4 (q, J_{C-F} = 2.2 Hz), 145.9, 139.3, 132.8, 132.8, 126.6 (q, J_{C-F} = 278.1 Hz), 125.0, 41.9 (q, J_{C-F} = 29.5 Hz), 37.7 (q, J_{C-F} = 2.1 Hz), 22.1, 18.3; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.3; **IR (KBr)** υ 2928, 2853, 1708, 1613, 1594, 1412, 1357, 1245, 1178, 1162, 1107, 1054, 941, 864, 724, 657, 607, 574, 513 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{12}H_{12}F_3O^+$ $[M+H]^+$ 229.0835, found 229.0847.

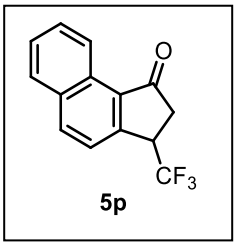
5,6-Dimethoxy-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (5o):



Reaction condition-**A**: 32 mg (62%), reaction condition-**B**: 34 mg (65%); White solid; **mp** = 105.2–107.9 °C; **R_F** (Hexane/EtOAc 85:15): 0.12; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.22 (s, 1H), 7.06 (s, 1H), 4.01 (pd, *J* = 8.5, 3.5 Hz, 1H), 3.99 (s, 3H), 3.93 (s, 3H), 2.91 (dd, *J* = 19.0, 8.0 Hz, 1H), 2.77 (dd, *J* = 19.0, 3.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 201.0, 155.8, 151.1, 142.2 (q,

$J_{C\text{-}F}$ = 2.4 Hz), 130.9, 126.5 (q, $J_{C\text{-}F}$ = 278.2 Hz), 107.8, 104.5, 56.6, 56.3, 42.3 (q, $J_{C\text{-}F}$ = 29.6 Hz), 37.3 (q, $J_{C\text{-}F}$ = 2.1 Hz); **^{19}F NMR (470 MHz, $CDCl_3$)** δ -70.4; **IR (KBr)** υ 2948, 2848, 1711, 1591, 1489, 1375, 1305, 1260, 1139, 1107, 1028, 974, 875, 698, 658, 535 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{12}H_{12}F_3O_3^+$ $[M+H]^+$ 261.0733, found 261.0741.

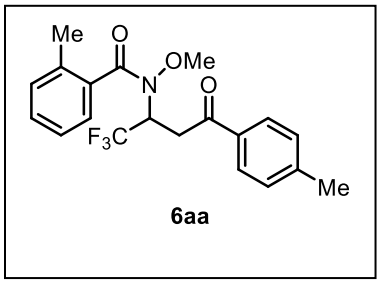
3-(Trifluoromethyl)-2,3-dihydro-1*H*-cyclopenta[*a*]naphthalen-1-one (5p):



5p

Reaction condition-**A**: 60%, reaction condition-**B**: 32 mg (64%); White solid; **mp** = 106.9–108.3 °C; **R_F** (Hexane/EtOAc 85:15): 0.48; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 9.18 (d, *J* = 8.5 Hz, 1H), 8.14 (d, *J* = 8.5 Hz, 1H), 7.94 (d, *J* = 8.0 Hz, 1H), 7.74–7.71 (m, 2H), 7.64 (ddd, *J* = 8.5, 7.0, 1.5 Hz, 1H), 4.18 (pd, *J* = 8.5, 3.5 Hz, 1H), 3.05 (dd, *J* = 19.0, 8.0 Hz, 1H), 2.93 (dd, *J* = 19.0, 3.5 Hz, 1H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 202.8, 149.9 (q, $J_{C\text{-}F}$ = 2.4 Hz), 136.6, 133.7, 132.4, 129.7, 129.2, 128.3, 127.9, 126.5 (q, $J_{C\text{-}F}$ = 278.7 Hz), 124.4, 123.4, 42.7 (q, $J_{C\text{-}F}$ = 29.7 Hz), 37.6 (q, $J_{C\text{-}F}$ = 2.2 Hz); **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.7; **IR (KBr)** υ 2973, 2933, 2854, 1711, 1572, 1512, 1351, 1266, 1160, 1106, 943, 835, 764, 685, 658, 578 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{14}H_{10}F_3O^+$ $[M+H]^+$ 251.0678, found 251.0689.

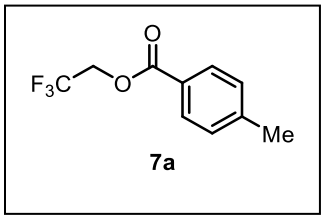
***N*-Methoxy-2-methyl-*N*-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (6aa):**



6aa

63 mg (83%); White solid; **mp** = 101.5–102.7 °C; **R_F** (Hexane/EtOAc 60:40): 0.76; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.90 (d, *J* = 8.0 Hz, 2H), 7.34–7.29 (m, 4H), 7.23–7.17 (m, 2H), 5.76 (bs, 1H), 3.92 (dd, *J* = 17.5, 10.5 Hz, 1H), 3.44 (bs, 3H), 3.24 (d, *J* = 17.5 Hz, 1H), 2.43 (s, 3H), 2.35 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 193.7, 172.4, 145.0, 135.9, 134.1, 133.6, 130.5, 129.8, 129.7, 128.4, 127.0, 125.3, 124.9, 63.8, 54.5, 33.2, 21.9, 19.3; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -72.8; **IR (KBr)** υ 3066, 2948, 2920, 1680, 1605, 1413, 1363, 1341, 1297, 1282, 1230, 1181, 1126, 1008, 816, 755, 645, 590 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{20}H_{21}F_3NO_3^+$ $[M+H]^+$ 380.1468, found 380.1479.

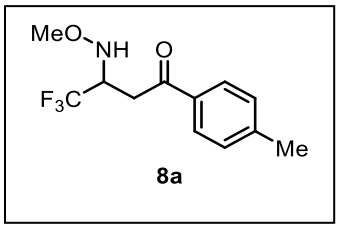
2,2,2-Trifluoroethyl-4-methylbenzoate (7a):



7a

16 mg (37%); Light yellowish oil; **R_F** (Hexane/EtOAc 85:15): 0.70; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.97 (d, *J* = 8.5 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 4.68 (q, *J* = 8.5 Hz, 2H), 2.43 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 165.1, 144.9, 130.2, 129.5, 125.8, 123.3 (q, $J_{C\text{-}F}$ = 275.4 Hz), 60.8 (q, $J_{C\text{-}F}$ = 36.2 Hz), 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -73.7; **IR (KBr)** υ 2970, 2929, 2860, 1738, 1681, 1614, 1444, 1413, 1297, 1258, 1172, 1109, 1025, 973, 839, 751, 690, 655, 569 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{10}H_{10}F_3O_2^+$ $[M+H]^+$ 219.0627, found 219.0643.

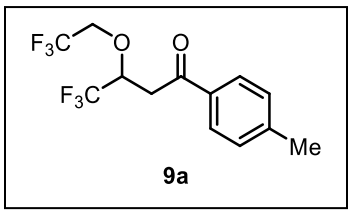
4,4,4-Trifluoro-3-(methoxyamino)-1-(*p*-tolyl)butan-1-one (8a):



8a

23 mg (44%); Yellowish brown oil; **R_F** (Hexane/EtOAc 85:15): 0.50; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.88 (d, *J* = 8.5 Hz, 2H), 7.28 (d, *J* = 8.0 Hz, 2H), 6.17 (s, 1H), 4.08–3.97 (m, 1H), 3.59 (dd, *J* = 18.0, 10.5 Hz, 1H), 3.50 (s, 3H), 3.13 (dd, *J* = 18.0, 3.0 Hz, 1H), 2.43 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.1, 145.0, 133.8, 129.6, 128.4, 125.8 (q, $J_{C\text{-}F}$ = 279.6 Hz), 62.5, 58.0 (q, $J_{C\text{-}F}$ = 28.6 Hz), 33.0, 21.8; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -73.5; **IR (KBr)** υ 3382, 3036, 2945, 2817, 1683, 1609, 1409, 1358, 1302, 1275, 1169, 1136, 1041, 986, 812, 759, 667,587 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{12}H_{15}F_3NO_2^+$ $[M+H]^+$ 262.1049, found 262.1063.

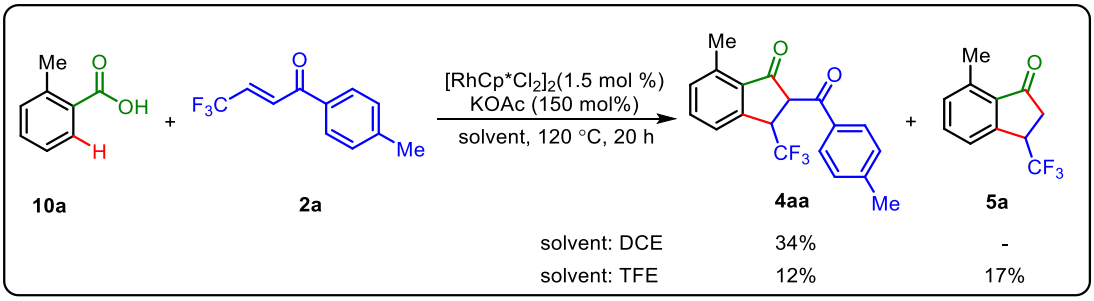
4,4,4-Trifluoro-1-(*p*-tolyl)-3-(2,2,2-trifluoroethoxy)butan-1-one (9a):



9a

31 mg (49%); Yellow oil; **R_F** (Hexane/EtOAc 85:15): 0.61; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.86 (d, *J* = 8.5 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 2H), 4.61–4.54 (m, 1H), 4.20 (dd, *J* = 8.5, 2.5 Hz, 1H), 4.17 (dd, *J* = 8.5, 3.0 Hz, 1H), 3.52 (dd, *J* = 18.0, 9.5 Hz, 1H), 3.17 (dd, *J* = 18.0, 2.0 Hz, 1H), 2.43 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 194.4, 145.2, 133.7, 129.7, 128.5, 124.9 (q, $J_{C\text{-}F}$ = 280.5 Hz), 123.1 (q, $J_{C\text{-}F}$ = 276.2 Hz), 75.3 (q, $J_{C\text{-}F}$ = 31.4 Hz), 70.2 (q, $J_{C\text{-}F}$ = 35.1 Hz), 38.5, 21.8; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -75.1, -77.3; **IR (KBr)** υ 3038, 2954, 2932, 2861, 1687, 1609, 1574, 1411, 1372, 1307, 1286, 1169, 1130, 1041, 967, 893, 810, 762, 682, 589 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{13}H_{13}F_6O_2^+$ $[M+H]^+$ 315.0814, found 315.0826.

Procedure for reaction of *o*-toluic acid (10a) with 2a:

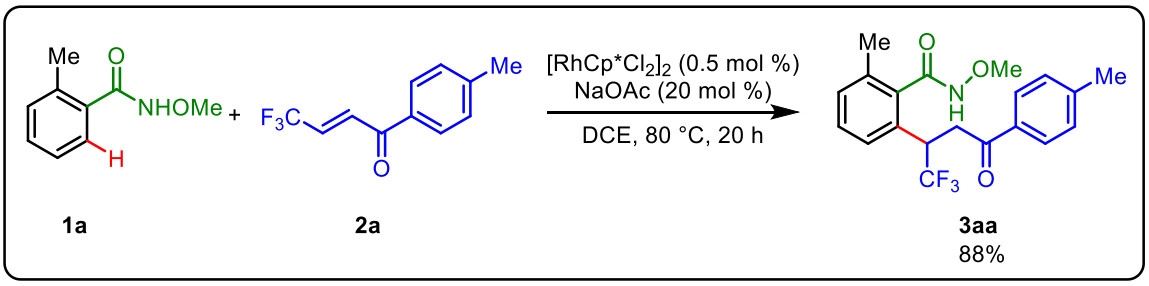


Procedure for reaction in DCE: To an oven-dried sealed tube charged with a stirring bar were added *o*-toluic acid **10a** (27.2 mg, 0.20 mmol, 100 mol %), (*E*)-4,4,4-trifluoro-1-(*p*-tolyl)but-2-en-1-one **2a** (42.8 mg, 0.20 mmol, 100 mol %), $[RhCp^*Cl_2]_2$ (1.9 mg, 3.0 μmol, 1.5 mol %) and KOAc (29.4 mg, 0.30 mmol, 150 mol %) in 1,2-dichloroethane (0.2 mL, 1.0 M). The reaction mixture was allowed to stir at 120 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide **4aa** (34%).

Procedure for reaction in TFE: To an oven-dried sealed tube charged with a stirring bar were added *o*-toluic acid **10a** (27.2 mg, 0.20 mmol, 100 mol %), (*E*)-4,4,4-trifluoro-1-(*p*-tolyl)but-2-en-1-one **2a** (64.3 mg, 0.30 mmol, 150 mol %), $[RhCp^*Cl_2]_2$ (1.9 mg, 3.0 μmol, 1.5 mol %) and KOAc (29.4 mg, 0.30 mmol, 150 mol %) in TFE (0.2 mL, 1.0 M). The reaction mixture was allowed to stir at 120 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide **4aa** (12%) and **5a** (17%).

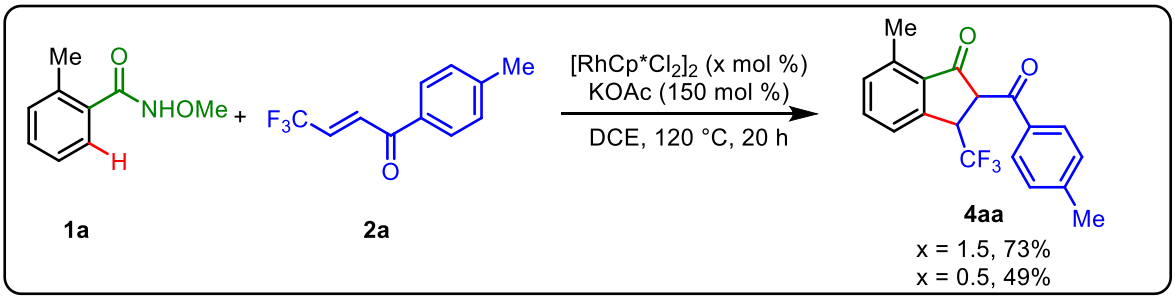
Procedure for scale up reactions:

***N*-Methoxy-2-methyl-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide (3aa):**



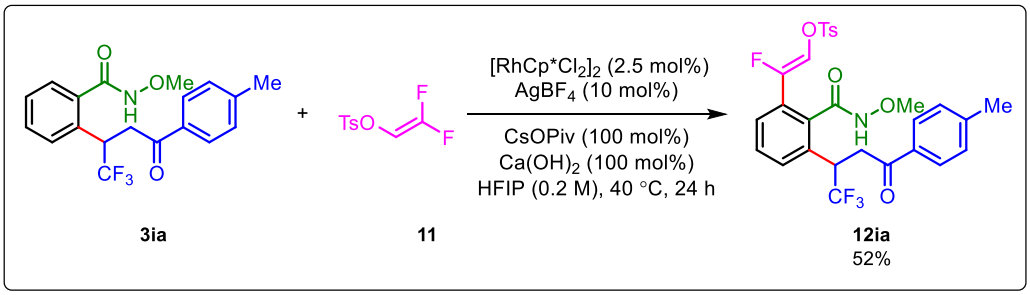
Procedure: To an oven-dried sealed tube charged with a stirring bar were added *N*-methoxy-2-methylbenzamide **1a** (495.6 mg, 3.0 mmol, 100 mol %), (*E*)-4,4,4-trifluoro-1-(*p*-tolyl)but-2-en-1-one **2a** (642.6 mg, 3.0 mmol, 100 mol %), $[RhCp^*Cl_2]_2$ (9.3 mg, 15.0 μmol, 0.5 mol %) and NaOAc (49.2 mg, 0.6 mmol, 20 mol %) in 1,2-dichloroethane (15.0 mL, 0.2 M). The reaction mixture was allowed to stir at 80 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide *N*-methoxy-2-methyl-6-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide **3aa** (1.00 g, 2.64 mmol, 88%).

7-Methyl-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one (4aa):



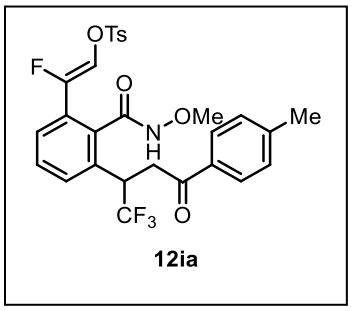
Procedure: To an oven-dried sealed tube charged with a stirring bar were added *N*-methoxy-2-methylbenzamide **1a** (495.6 mg, 3.0 mmol, 100 mol %), (*E*)-4,4,4-trifluoro-1-(*p*-tolyl)but-2-en-1-one **2a** (642.6 mg, 3.0 mmol, 100 mol %), $[RhCp^*Cl_2]_2$ (27.8 mg, 45.0 μmol, 1.5 mol %) and KOAc (441.6 mg, 4.5 mmol, 150 mol %) in 1,2-dichloroethane (3.0 mL, 1.0 M). The reaction mixture was allowed to stir at 120 °C for 20 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide 7-methyl-2-(4-methylbenzoyl)-3-(trifluoromethyl)-2,3-dihydro-1*H*-inden-1-one **4aa** (727.8 mg, 2.19 mmol, 73%).

Synthesis and characterization of 12ia:



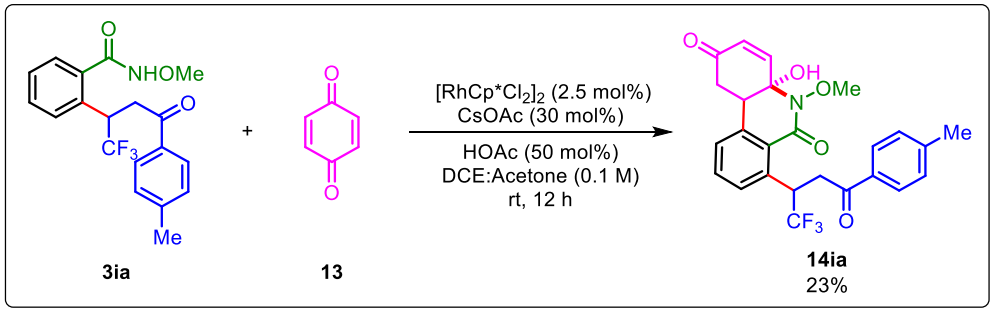
To an oven-dried sealed tube charged with a stirring bar were added *N*-methoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide **3ia** (36.5 mg, 0.10 mmol, 100 mol %), 2,2-difluorovinyl tosylate **11** (35.1 mg, 0.15 mmol, 150 mol %), $[Cp^*RhCl_2]_2$ (1.5 mg, 2.50 µmol, 2.5 mol %), $AgBF_4$ (1.9 mg, 10 µmol, 10 mol %), $Ca(OH)_2$ (7.4 mg, 0.10 mmol, 100 mol %) and CsOPiv (23.4 mg, 0.1 mmol, 100 mol %) in HFIP (0.5 mL, 0.2 M). The reaction was allowed to stir at 40 °C for 24 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide (*Z*)-2-fluoro-2-(2-(methoxycarbamoyl)-3-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)phenyl)vinyl 4-methylbenzenesulfonate **12ia** (30 mg, 52%).

(*Z*)-2-Fluoro-2-(2-(methoxycarbamoyl)-3-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)phenyl)-vinyl 4-methylbenzenesulfonate (12ia):



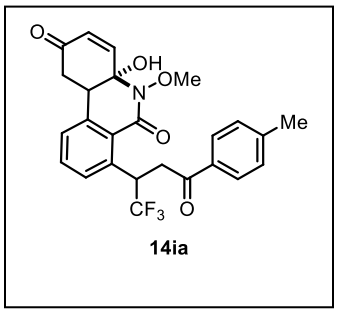
30 mg (52%); White solid; **mp** = 112.0–114.8 °C; **R_F** (Hexane/EtOAc 60:40): 0.55; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 10.30 (s, 1H), 7.89 (d, *J* = 8.5 Hz, 2H), 7.81 (d, *J* = 8.5 Hz, 2H), 7.40–7.36 (m, 5H), 7.27 (d, *J* = 7.5 Hz, 2H), 6.84 (d, *J* = 19.0 Hz, 1H), 4.17 (m, 1H), 3.92 (dd, *J* = 18.5, 11.5 Hz, 1H), 3.89 (s, 3H), 3.63 (dd, *J* = 18.5, 3.0 Hz, 1H), 2.46 (s, 3H), 2.41 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.7, 165.6, 149.1 (d, $J_{C\text{-}F}$ = 254.9 Hz), 145.9, 145.8, 134.4, 133.2, 132.7, 132.2, 130.2, 129.7, 128.9 (d, $J_{C\text{-}F}$ = 22.9 Hz), 128.5, 128.4, 128.4, 126.0 (q, $J_{C\text{-}F}$ = 278.6 Hz), 121.6 (d, $J_{C\text{-}F}$ = 13.4 Hz), 64.3, 41.4 (q, $J_{C\text{-}F}$ = 29.7 Hz), 38.4, 21.9; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -69.2, -118.5; **IR (KBr)** υ 3255, 2927, 2855, 1689, 1670, 1606, 1448, 1381, 1267, 1194, 1180, 1162, 1119, 1085, 1052, 885, 837, 815, 750, 687, 661, 552 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{28}H_{26}F_4NO_6S^+$ $[M+H]^+$ 580.1411, found 580.1423.

Synthesis and characterization of 14ia:



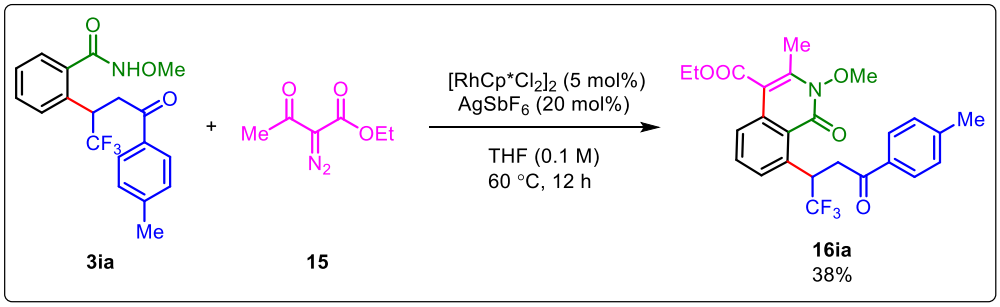
To an oven-dried sealed tube charged with a stirring bar were added *N*-methoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide **3ia** (36.5 mg, 0.10 mmol, 100 mol %), 1,4-benzoquinone **13** (21.6 mg, 0.20 mmol, 200 mol %), $[Cp^*RhCl_2]_2$ (1.5 mg, 2.5 μmol, 2.5 mol %) and CsOAc (5.8 mg, 30 μmol, 30 mol %) and HOAc (3.0 mg, 50 μmol, 50 mol %) in DCE/acetone (0.5 mL/0.5 mL 0.1 M). The reaction was allowed to stir at room temperature for 12 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide (4*aS*)-4*a*-hydroxy-5-methoxy-7-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-1,4*a*,5,10*b*-tetrahydrophenanthridine-2,6-dione **14ia** (11 mg, 23%).

(4*aS*)-4*a*-Hydroxy-5-methoxy-7-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-1,4*a*,5,10*b*-tetrahydrophenanthridine-2,6-dione (14ia):



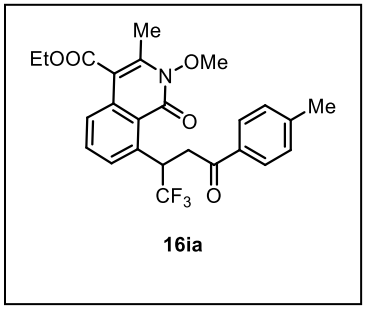
11 mg (23%); Light yellow solid; **mp** = 129.6–132.1 °C; **R_F** (Hexane/EtOAc 60:40): 0.21; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.81 (d, *J* = 8.5 Hz, 2H), 7.52–7.47 (m, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.20 (dd, *J* = 7.0, 2.0 Hz, 1H), 7.08 (d, *J* = 10.5 Hz, 1H), 6.89 (pd, *J* = 9.5, 5.0 Hz, 1H), 6.17 (d, *J* = 10.0 Hz, 1H), 5.25 (bs, 1H), 3.76 (dd, *J* = 17.5, 9.5 Hz, 1H), 3.71–3.62 (m, 5H), 2.73 (dd, *J* = 17.0, 13.0 Hz, 1H), 2.67 (ddd, *J* = 17.0, 5.0, 1.0 Hz, 1H), 2.39 (s, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 196.6, 195.1, 166.0, 147.2, 144.5, 140.3, 138.8, 134.0, 133.3, 129.5, 128.7, 128.6, 128.3, 128.2, 127.2 (q, $J_{C\text{-}F}$ = 278.6 Hz), 124.5, 85.7, 63.9, 46.5, 43.5, 38.6, 37.9 (q, $J_{C\text{-}F}$ = 26.1 Hz), 21.8; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.4; **IR (KBr)** υ 3317, 3023, 2935, 1684, 1658, 1608, 1596, 1475, 1360, 1334, 1305, 1279, 1267, 1174, 1152, 1109, 1083, 1048, 992, 885, 821, 777, 708 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{25}H_{23}F_3NO_5^+$ $[M+H]^+$ 474.1523, found 474.1536.

Synthesis and characterization of 16ia:



To an oven-dried sealed tube charged with a stirring bar were added *N*-methoxy-2-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)benzamide **3ia** (36.5 mg, 0.10 mmol, 100 mol %), ethyl 2-diazo-3-oxobutanoate **15** (18.7 mg, 0.12 mmol, 120 mol %), $[Cp^*RhCl_2]_2$ (3.1 mg, 5.0 μmol, 5.0 mol %) and $AgSbF_6$ (6.9 mg, 20 μmol, 20 mol %) in THF (1.0 mL, 0.1 M). The reaction was allowed to stir at 60 °C for 12 h. After cooling at room temperature, the reaction mixture was evaporated and the residue was purified by column chromatography to provide ethyl-2-methoxy-3-methyl-1-oxo-8-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-1,2-dihydroisoquinoline-4-carboxylate **16ia** (18 mg, 38%).

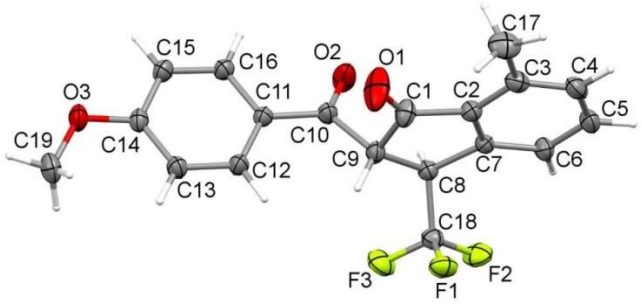
Ethyl-2-methoxy-3-methyl-1-oxo-8-(1,1,1-trifluoro-4-oxo-4-(*p*-tolyl)butan-2-yl)-1,2-dihydroisoquinoline-4-carboxylate (16ia):



18 mg (38%); Light yellow semi-solid; $\mathbf{R_F}$ (Hexane/EtOAc 60:40): 0.55; **^{1}H NMR (500 MHz, $CDCl_3$)** δ 7.80 (d, *J* = 8.5 Hz, 2H), 7.58–7.50 (m, 2H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 2H), 7.14 (pd, *J* = 10.0, 4.0 Hz, 1H), 4.44 (q, *J* = 7.0 Hz, 2H), 4.09 (s, 3H), 3.81 (dd, *J* = 17.5, 11.0 Hz, 1H), 3.68 (dd, *J* = 17.5, 4.0 Hz, 1H), 2.51 (s, 3H), 2.39 (s, 3H), 1.41 (t, *J* = 7.0 Hz, 3H); **^{13}C NMR (125 MHz, $CDCl_3$)** δ 195.1, 167.3, 158.8, 144.3, 140.3, 138.2, 135.1, 134.1, 131.9, 129.5, 128.3, 127.3 (q, $J_{C\text{-}F}$ = 278.6 Hz), 126.5, 124.2, 124.1, 109.9, 63.9, 61.9, 38.9, 38.1 (q, $J_{C\text{-}F}$ = 26.6 Hz), 21.8, 15.1, 14.4; **^{19}F NMR (470 MHz, $CDCl_3$)** δ -68.9; **IR (KBr)** υ 3015, 2947, 1687, 1663, 1582, 1473, 1371, 1322, 1305, 1294, 1256, 1177, 1113, 1083, 1048, 992, 885, 821, 777, 708 cm^{-1}; **HRMS (Q-TOF, ESI)** calcd for $C_{25}H_{25}F_3NO_5^+$ $[M+H]^+$ 476.1679, found 476.1693.

X-ray crystallographic data

Single Crystal data of 4ab (CCDC 1979536)



ORTEP diagram pf the organic compound with atom numbering scheme. (50% probability factor for the thermal ellipsoids)

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report
Datablock: SO4375F

Bond precision: C-C = 0.0014 A Wavelength=0.71073
Cell: a=7.8478(3) b=11.3684(5) c=17.6446(8)
alpha=90 beta=96.760(2) gamma=90
Temperature: 182 K

	Calculated	Reported
Volume	1563.25(12)	1563.25(12)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C19 H15 F3 O3	?
Sum formula	C19 H15 F3 O3	C38 H30 F6 O6
Mr	348.31	696.62
Dx,g cm-3	1.480	1.480
Z	4	2
Mu (mm-1)	0.123	0.123
F000	720.0	720.0
F000'	720.50	
h,k,lmax	13,18,29	13,18,29
Nref	7609	7579
Tmin,Tmax	0.962,0.973	0.941,0.973
Tmin'	0.941	

Correction method= # Reported T Limits: Tmin=0.941 Tmax=0.973 AbsCorr = MULTI SCAN
Data completeness= 0.996 Theta(max)= 36.410
R(reflections)= 0.0463(5570) wR2(reflections)= 0.1400(7579)
S = 1.054 Npar= 275

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C
PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -1.171 Report

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 17 Report
PLAT913_ALERT_3_C Missing # of Very Strong Reflections in FCF .... 14 Note

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Alert level G
PLAT045_ALERT_1_G Calculated and Reported Z Differ by a Factor ... 2.00 Check
PLAT066_ALERT_1_G Predicted and Reported Tmin&Tmax Range Identical ? Check
PLAT242_ALERT_2_G Low MainMol Ueq as Compared to Neighbors of C18 Check
PLAT434_ALERT_2_G Short Inter HL..HL Contact F1 ..F2 2.81 Ang.
1-x,1-y,2-z = 3_667 Check
PLAT793_ALERT_4_G Model has Chirality at C8 (Centro SPGR) S Verify
PLAT793_ALERT_4_G Model has Chirality at C9 (Centro SPGR) R Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 13 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 19 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 2 Check

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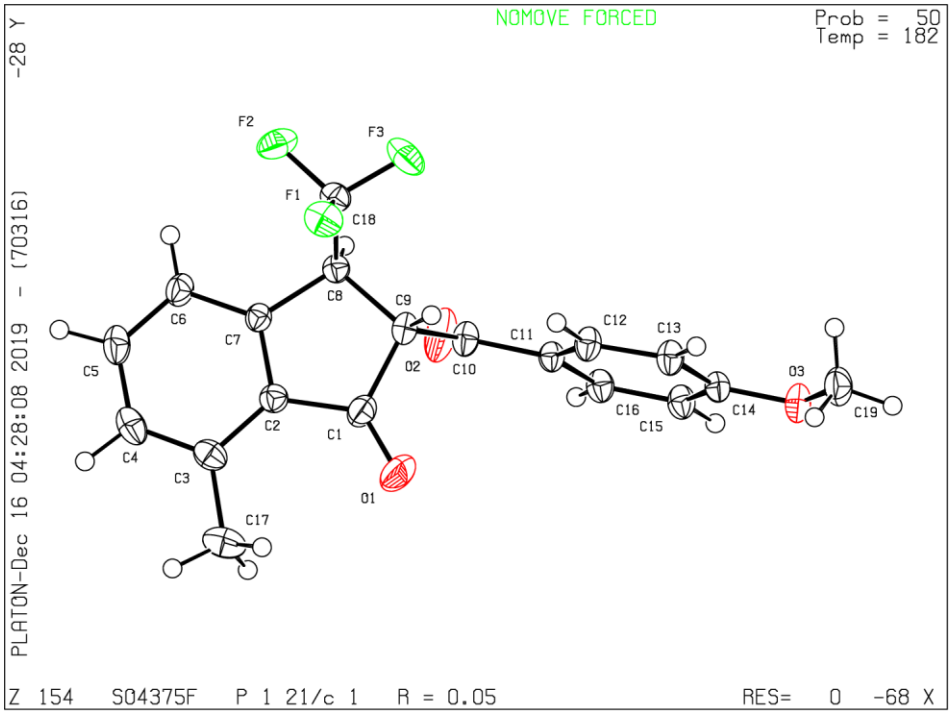
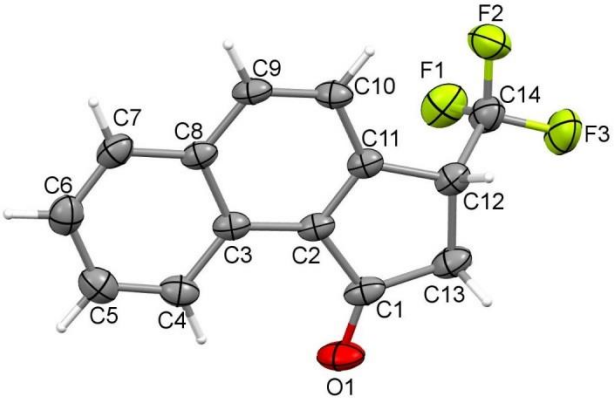
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
3 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
10 **ALERT level G** = General information/check it is not something unexpected

3 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
3 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
3 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

PLATON version of 11/12/2019; check.def file version of 11/12/2019



Single Crystal data of 5p (CCDC 1979537)



ORTEP digaram pf the organic compound with atom numbering scheme. (50% probability factor for the thermal ellipsoids)

No syntax errors found. CIF dictionary
Please wait while processing .... Interpreting this report

Datablock: SO4376

Bond precision: C-C = 0.0018 A Wavelength=0.71073

Cell: a=9.9108(4) b=11.6061(4) c=10.3846(4)
alpha=90 beta=113.481(1) gamma=90

Temperature: 182 K

	Calculated	Reported
Volume	1095.58(7)	1095.58(7)
Space group	P 21/c	P 1 21/c 1
Hall group	-P 2ybc	-P 2ybc
Moiety formula	C14 H9 F3 O	?
Sum formula	C14 H9 F3 O	C14 H9 F3 O
Mr	250.21	250.21
Dx,g cm-3	1.517	1.517
Z	4	4
Mu (mm-1)	0.129	0.129
F000	512.0	512.0
F000'	512.38	
h,k,lmax	14,16,14	14,16,14
Nref	3357	3342
Tmin,Tmax	0.963,0.983	0.831,0.972
Tmin'	0.956	

Correction method= # Reported T Limits: Tmin=0.831 Tmax=0.972 AbsCorr = MULTI SCAN

Data completeness= 0.996 Theta(max)= 30.570

R(reflections)= 0.0421(2673) wR2(reflections)= 0.1212(3342)

S = 1.038 Npar= 199

The following ALERTS were generated. Each ALERT has the format
test-name_ALERT_alert-type_alert-level.
Click on the hyperlinks for more details of the test.

Alert level C

PLAT905_ALERT_3_C Negative K value in the Analysis of Variance ... -0.033 Report

PLAT911_ALERT_3_C Missing FCF Refl Between Thmin & STh/L= 0.600 7 Report

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Alert level G

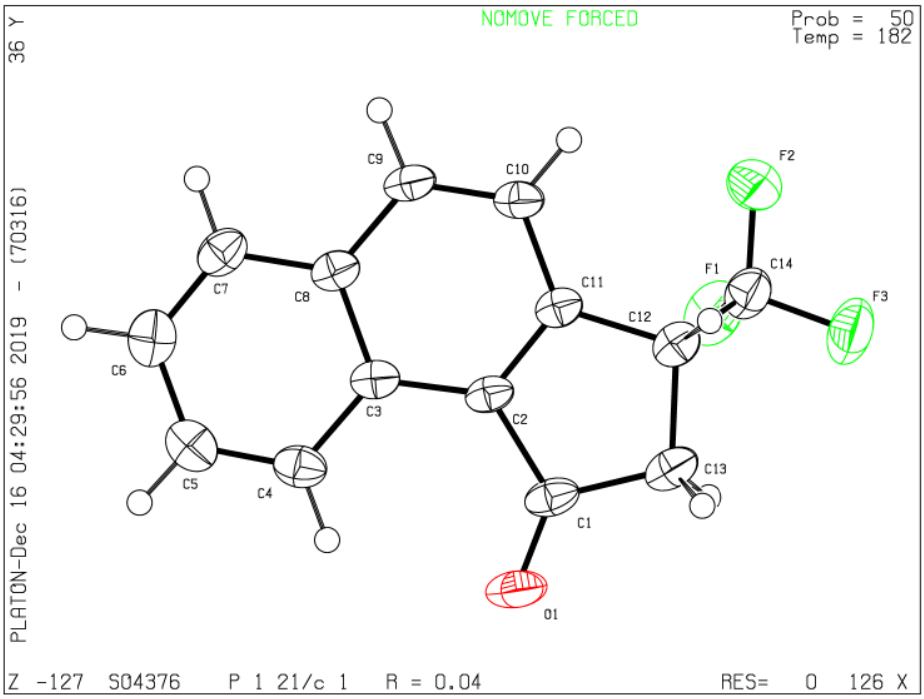
PLAT242_ALERT_2_G Low MainMol Ueq as Compared to Neighbors of C14 Check
PLAT793_ALERT_4_G Model has Chirality at C12 (Centro SPGR) R Verify
PLAT883_ALERT_1_G No Info/Value for _atom_sites_solution_primary . Please Do !
PLAT912_ALERT_4_G Missing # of FCF Reflections Above STh/L= 0.600 8 Note
PLAT913_ALERT_3_G Missing # of Very Strong Reflections in FCF .... 3 Note
PLAT978_ALERT_2_G Number C-C Bonds with Positive Residual Density. 17 Info
PLAT992_ALERT_5_G Repd & Actual _reflns_number_gt Values Differ by 1 Check

---

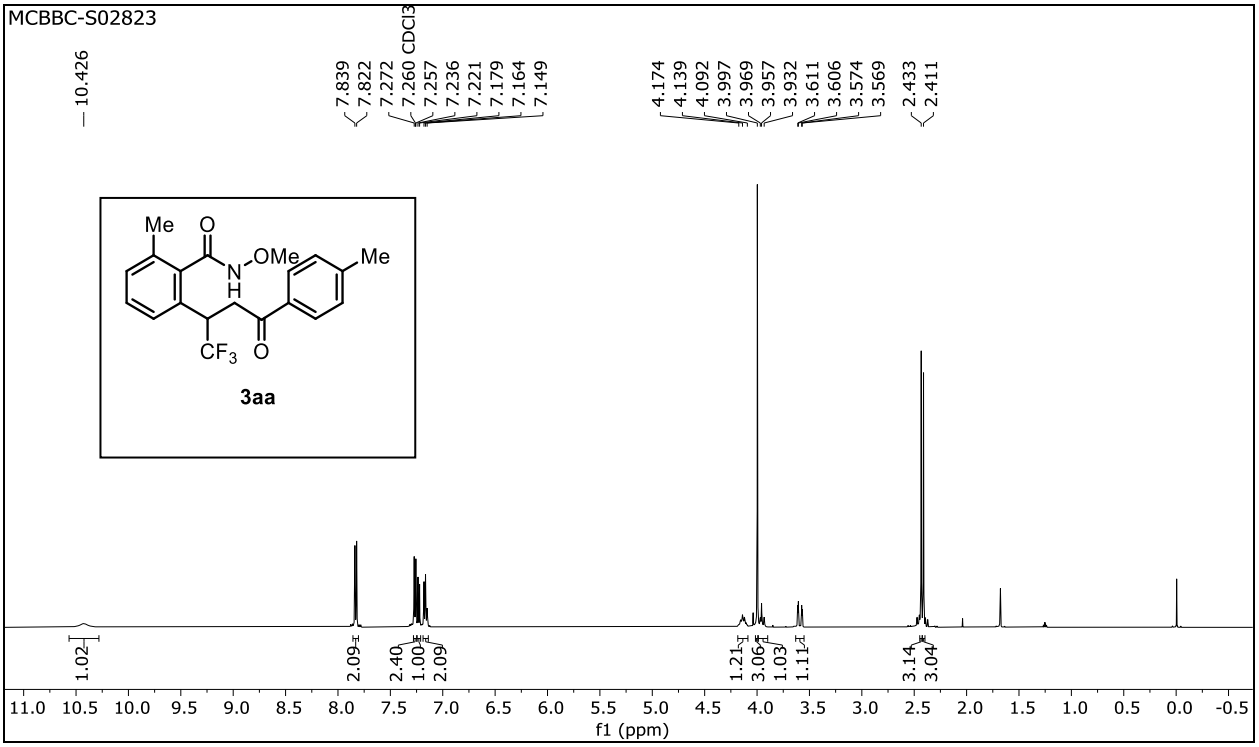
0 **ALERT level A** = Most likely a serious problem - resolve or explain
0 **ALERT level B** = A potentially serious problem, consider carefully
2 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight
7 **ALERT level G** = General information/check it is not something unexpected

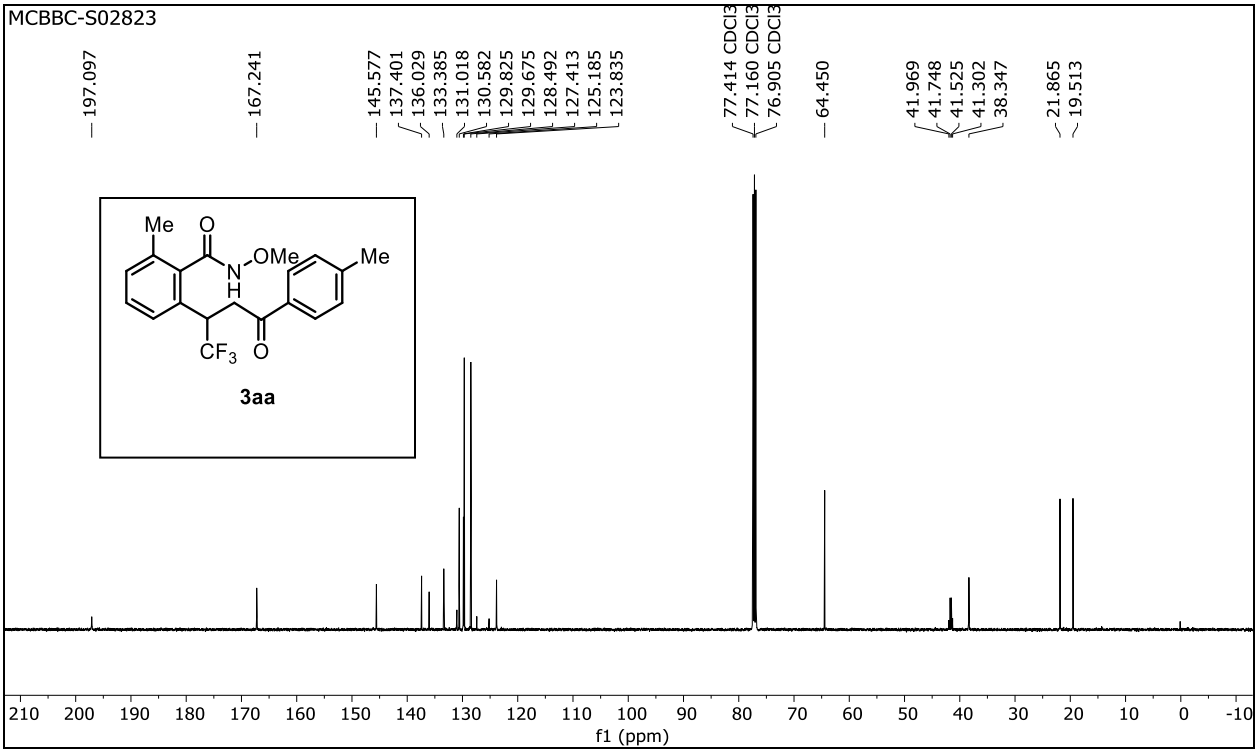
1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data
2 ALERT type 2 Indicator that the structure model may be wrong or deficient
3 ALERT type 3 Indicator that the structure quality may be low
2 ALERT type 4 Improvement, methodology, query or suggestion
1 ALERT type 5 Informative message, check

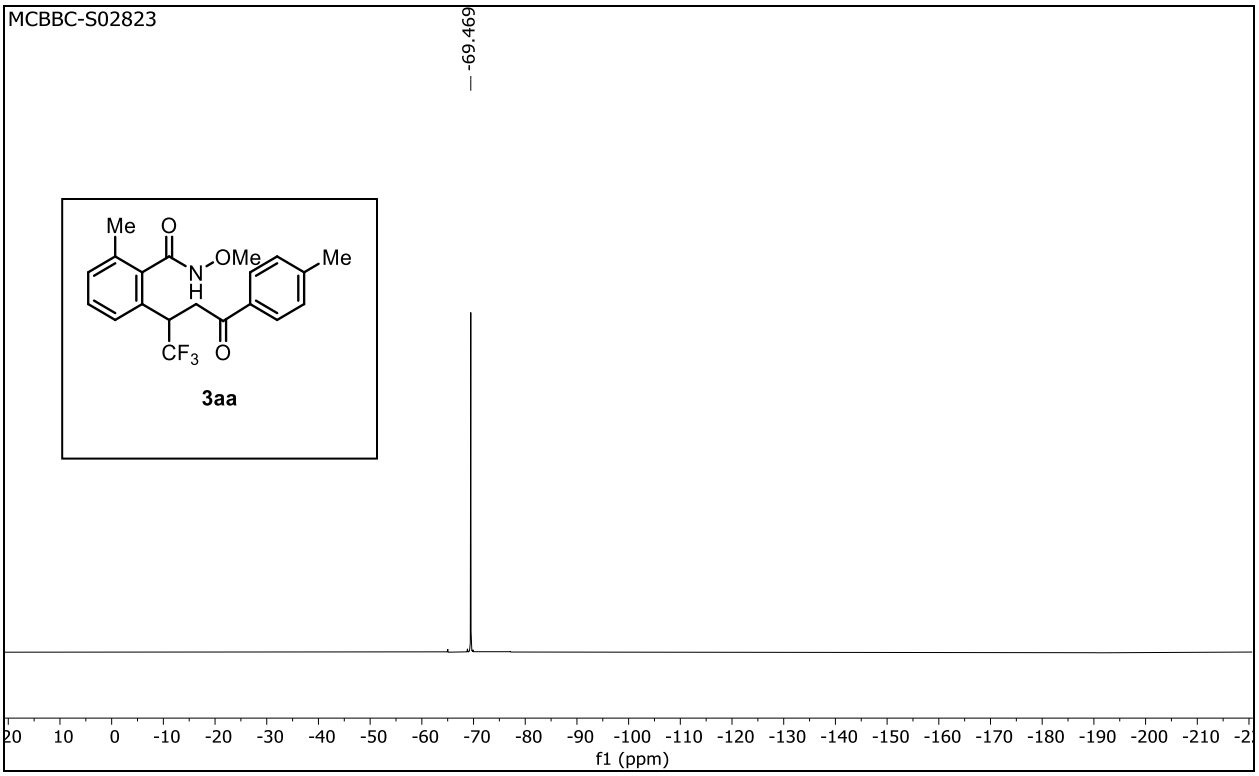
PLATON version of 11/12/2019; check.def file version of 11/12/2019



^{1}H NMR, ^{13}C NMR and ^{19}F NMR copies of all products



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N
H
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Me
CF3
O
3aa
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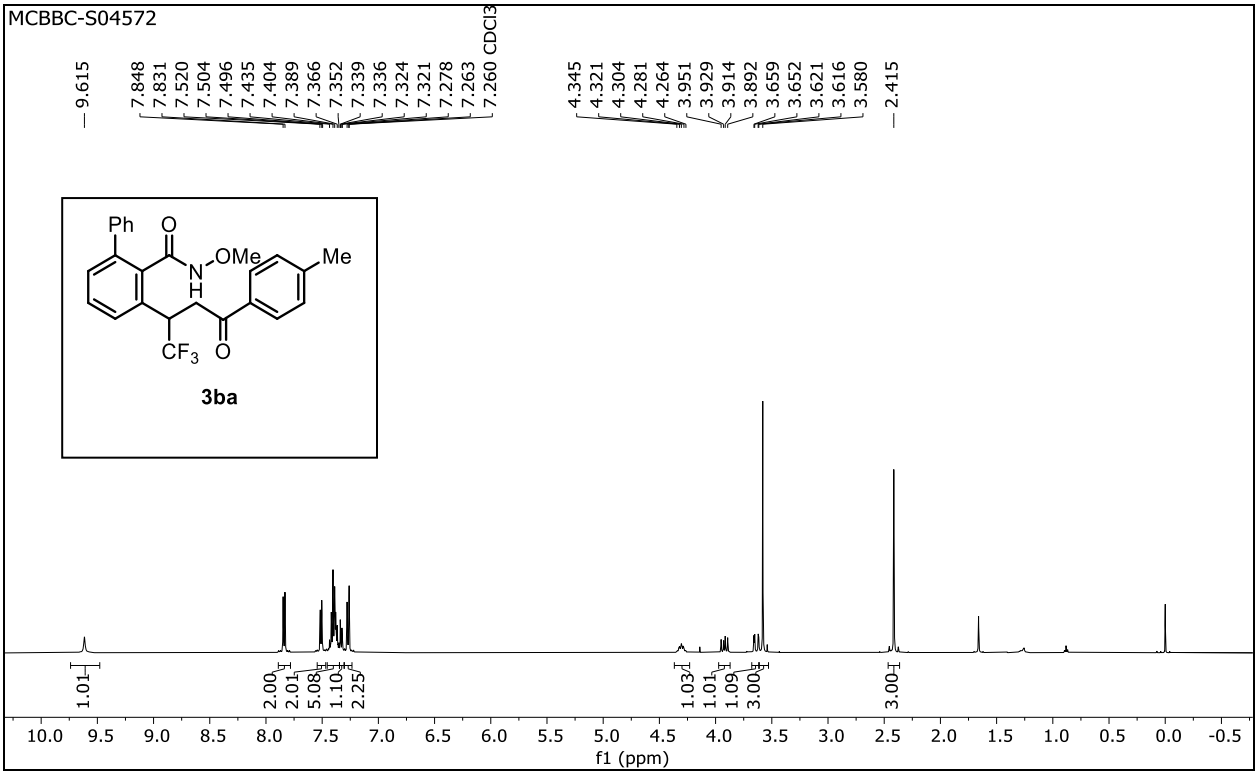
f1 (ppm)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7.352
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7.336
7.324
7.321
7.278
7.263
7.260 CDCl3
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4.321
4.304
4.281
4.264
3.951
3.929
3.914
3.892
3.659
3.652
3.621
3.616
3.580
2.415
Ph
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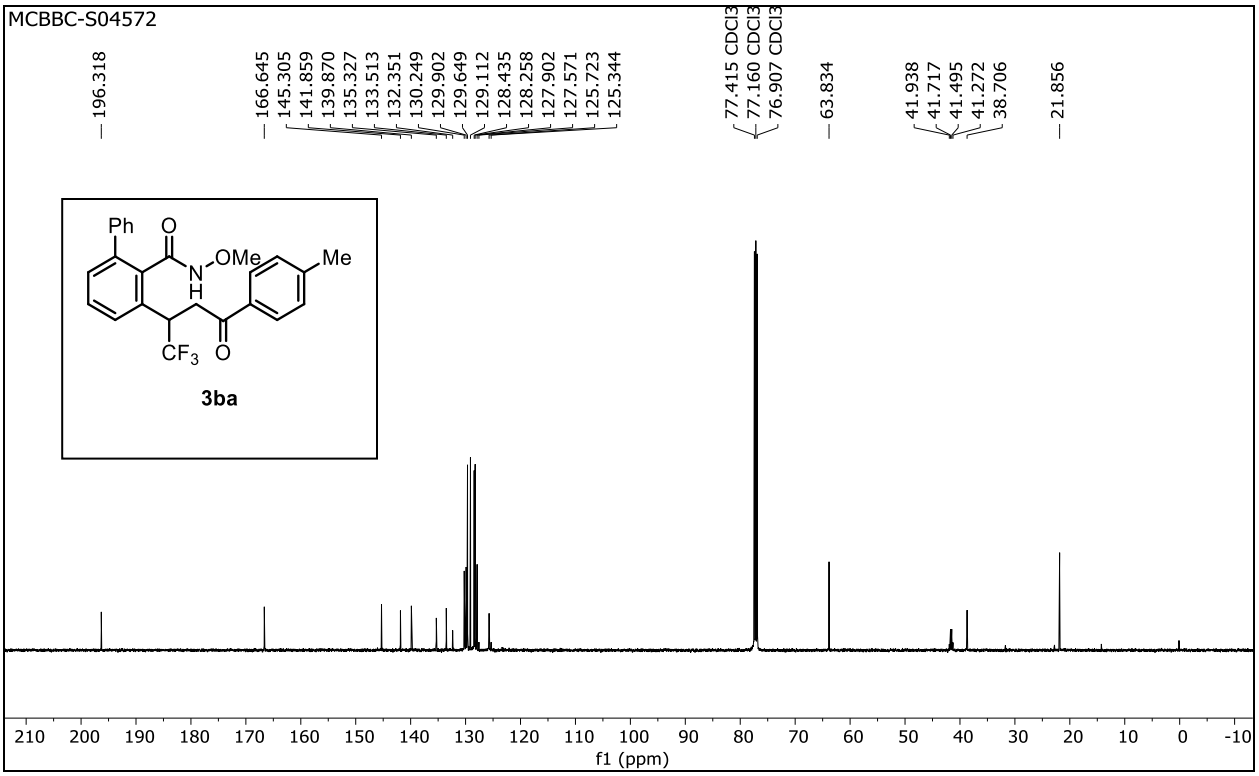
N
H
OMe
Me
CF3
O
3ba
1.01
2.00
2.01
5.08
1.10
2.25
1.03
1.01
1.09
3.00
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.649
129.112
128.435
128.258
127.902
127.571
125.723
125.344
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
63.834
41.938
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38.706
21.856
Ph
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OMe
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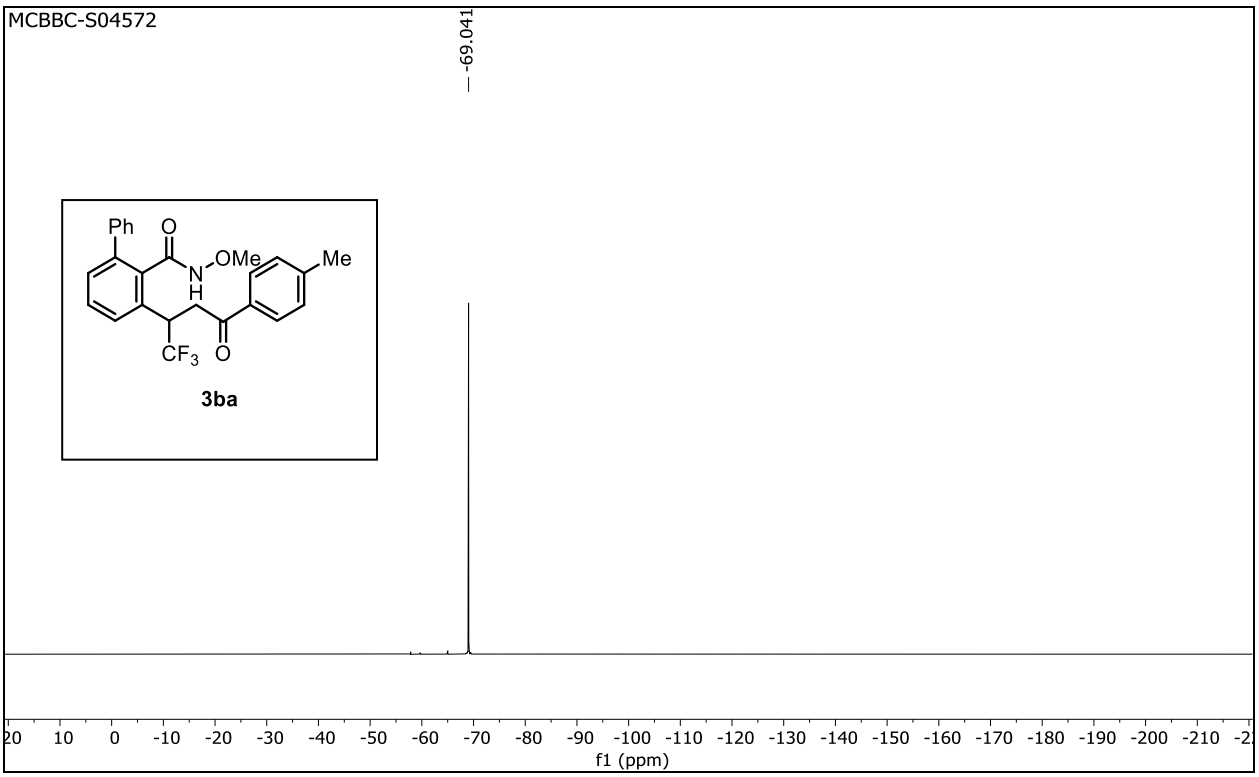
CF3
O
3ba
f1 (ppm)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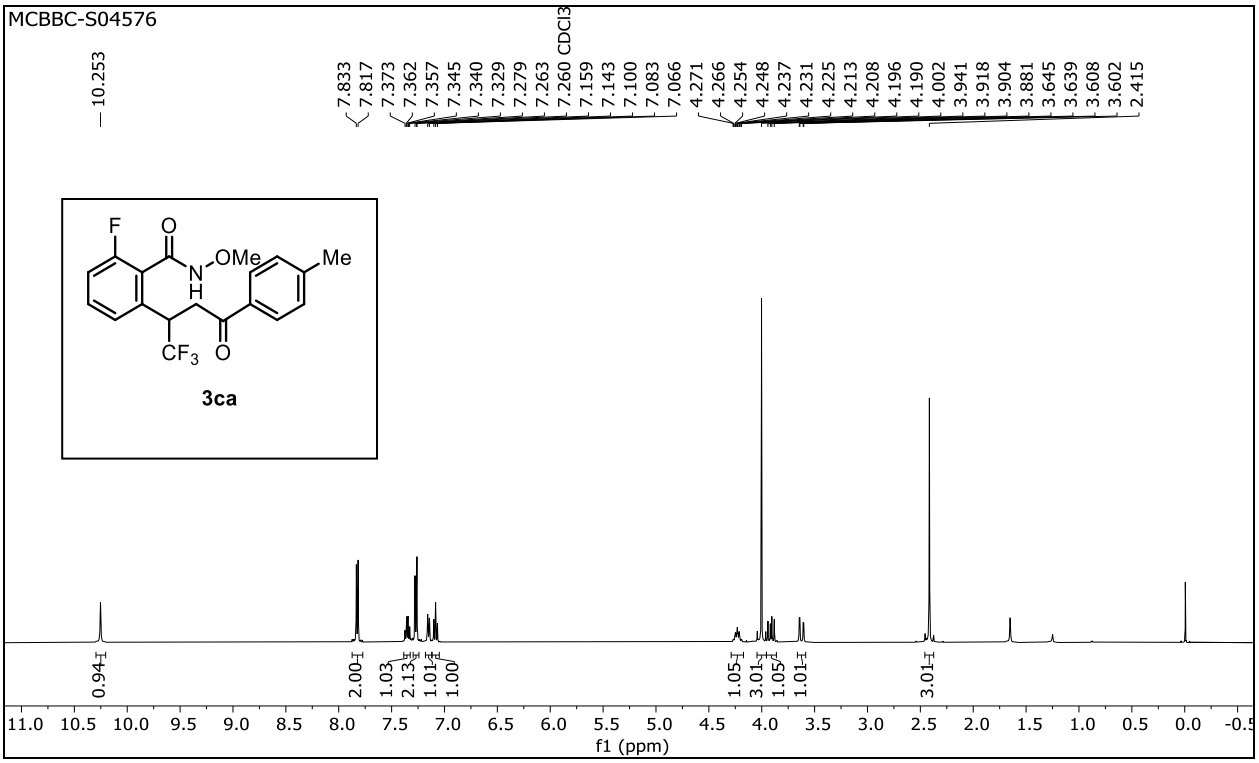
f1 (ppm)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7.143
7.100
7.083
7.066
4.271
4.266
4.254
4.248
4.237
4.231
4.225
4.213
4.208
4.196
4.190
4.002
3.941
3.918
3.904
3.881
3.645
3.639
3.608
3.602
2.415
F
O
N
H
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Me
CF3
O
3ca
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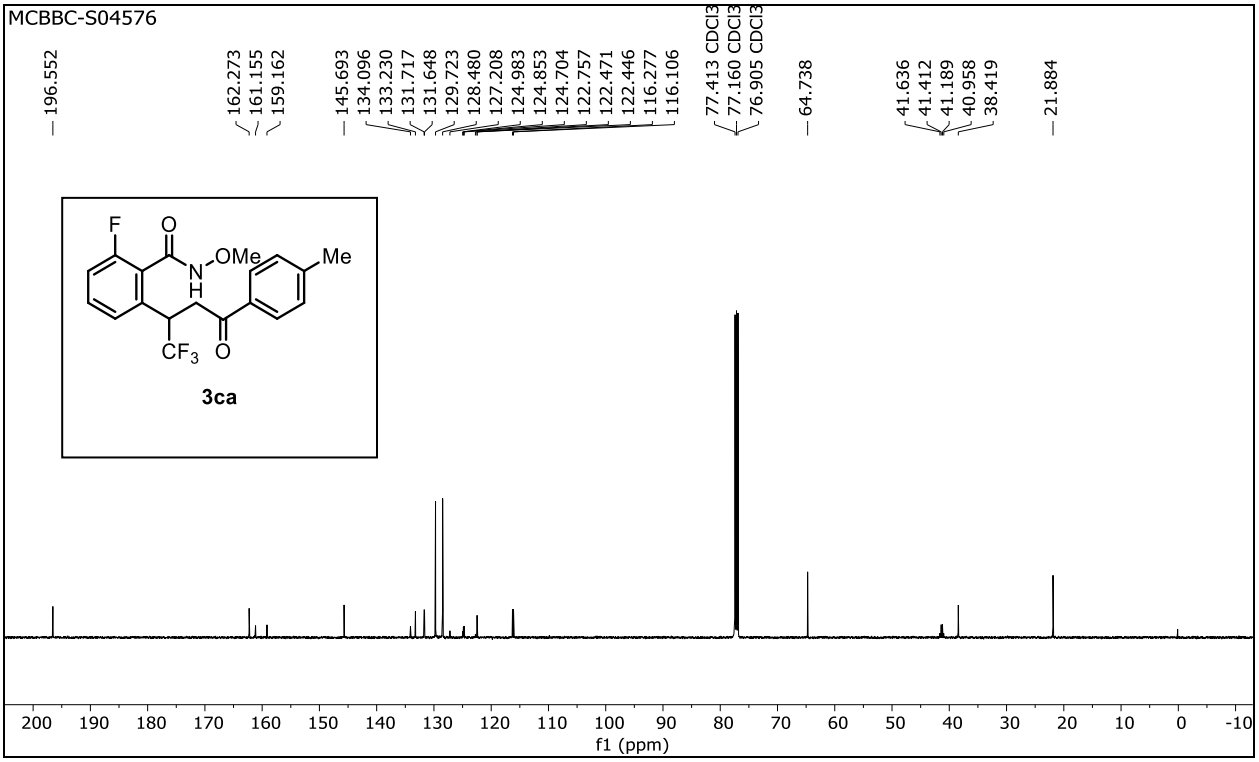
3.01
1.05
1.01
3.01
f1 (ppm)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124.983
124.853
124.704
122.757
122.471
122.446
116.277
116.106
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77.160 CDCl3
76.905 CDCl3
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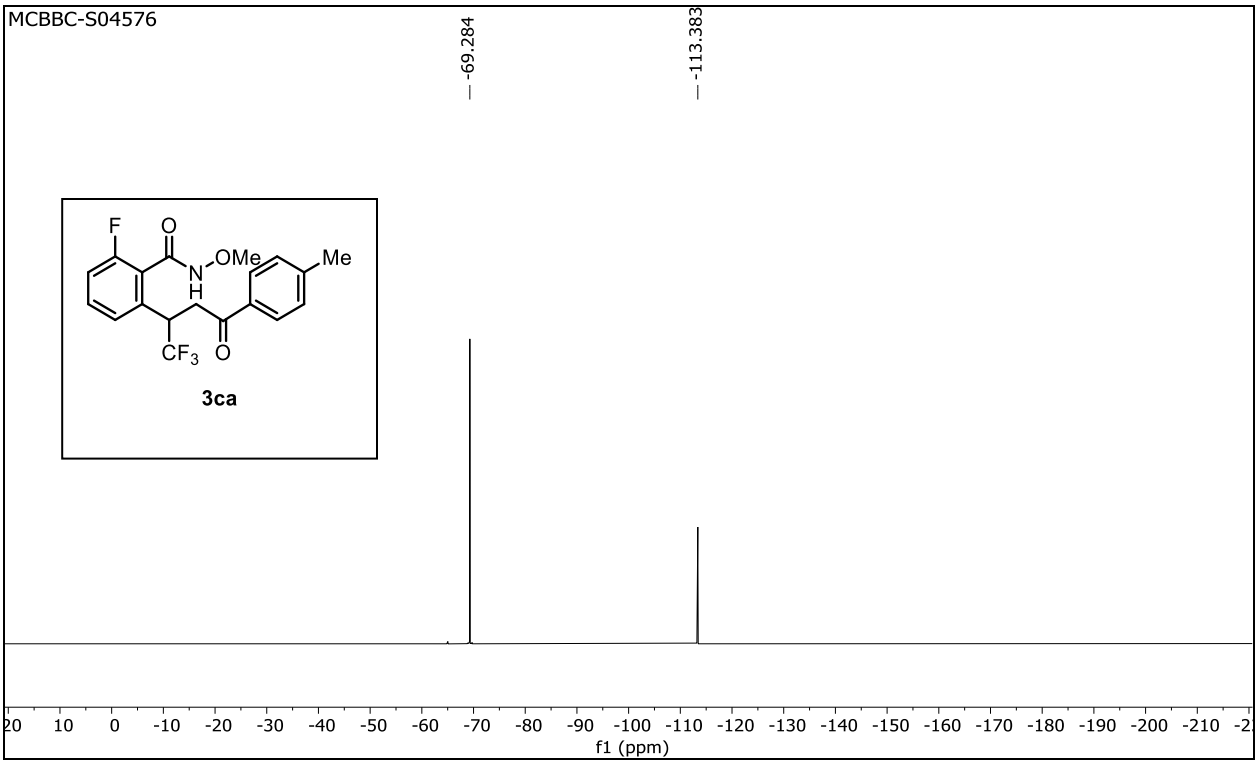
N
H
OMe
Me
CF3
O
3ca
f1 (ppm)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OMe
Me
CF3
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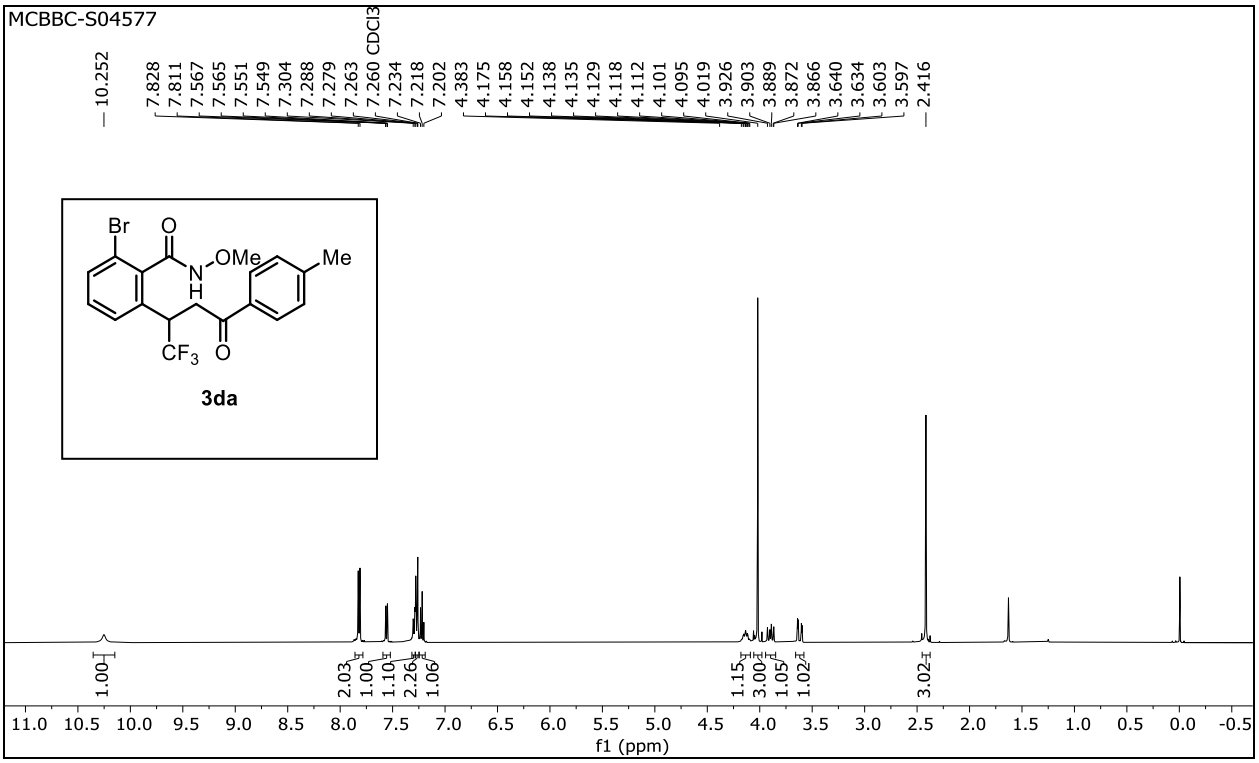
3ca
f1 (ppm)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7.260
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7.234
7.218
7.202
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4.158
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4.138
4.135
4.129
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3.903
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3.603
3.597
2.416
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N
H
OMe
Me
CF3
O
3da
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1.05
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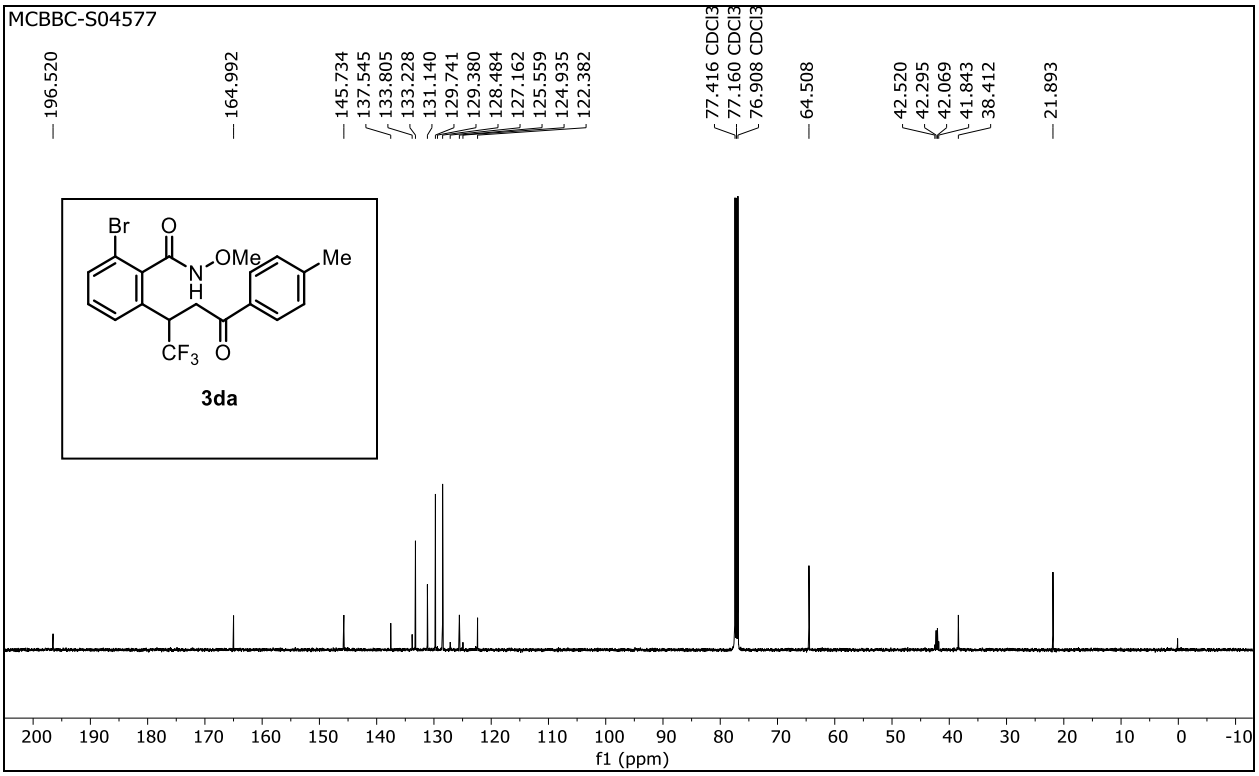
3.02
f1 (ppm)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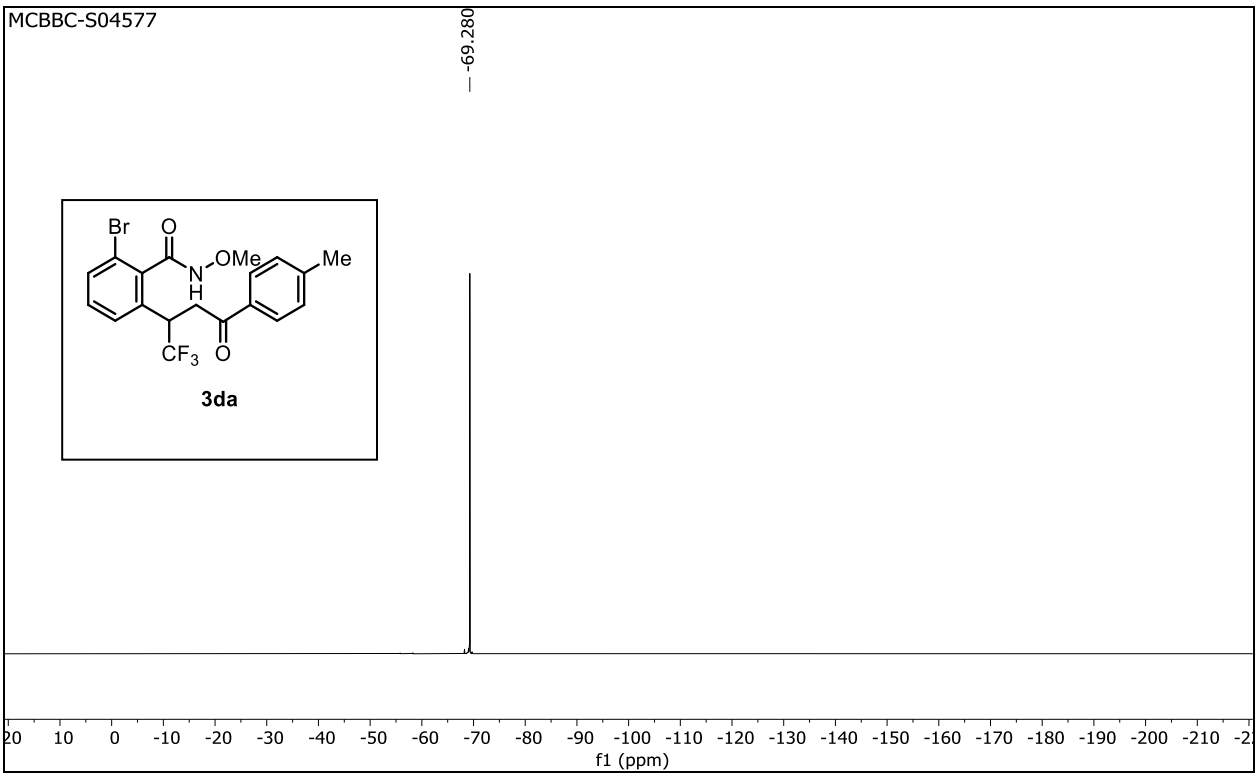
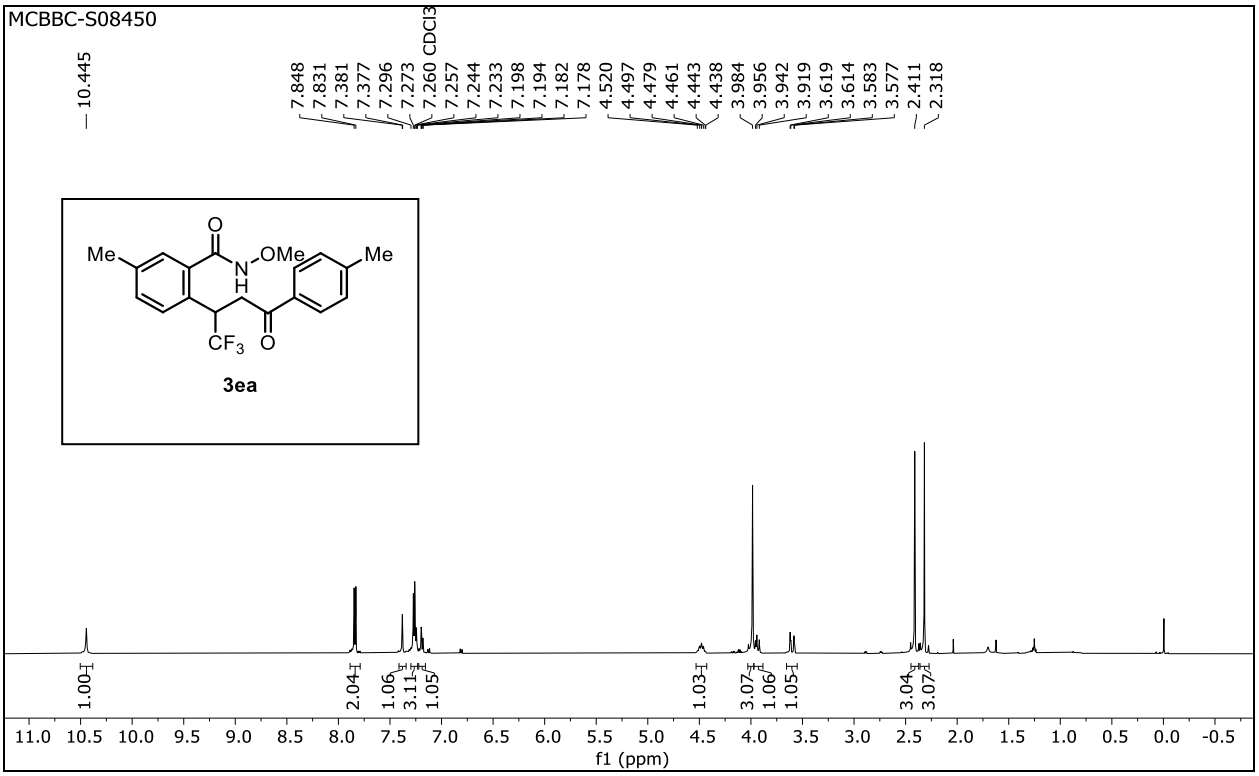
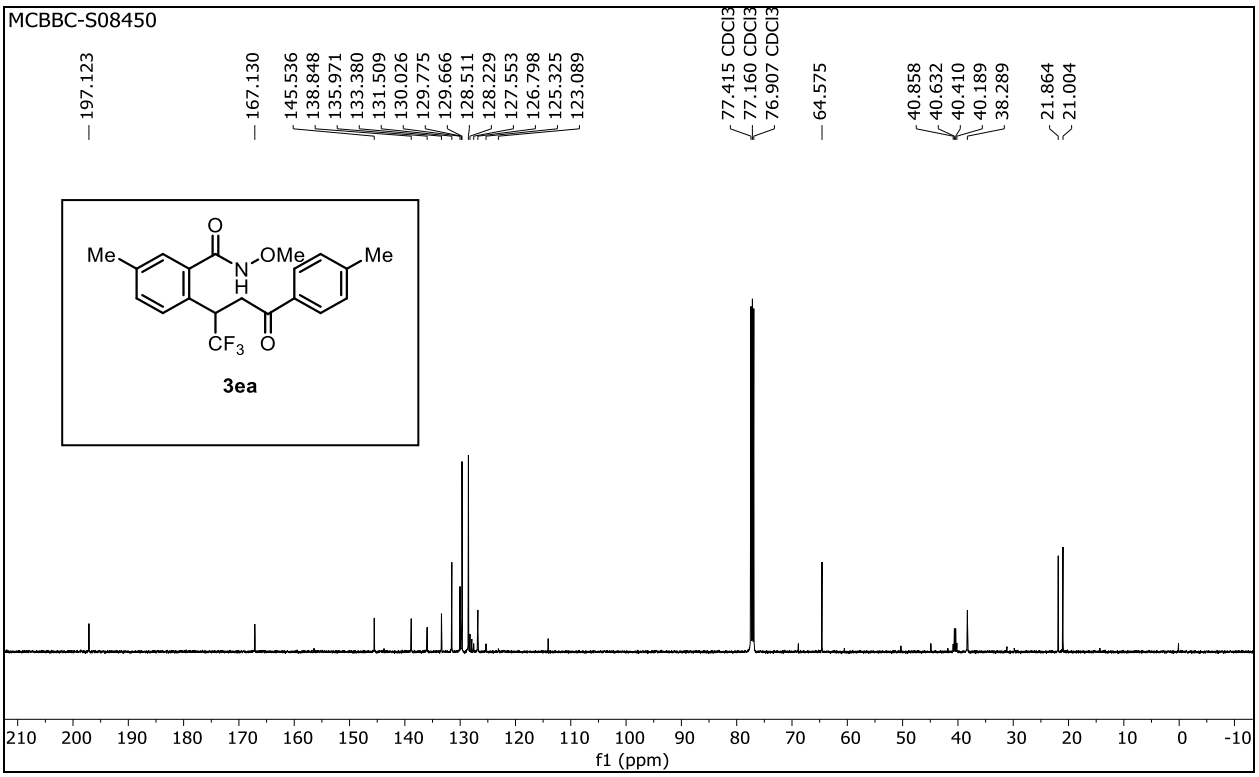
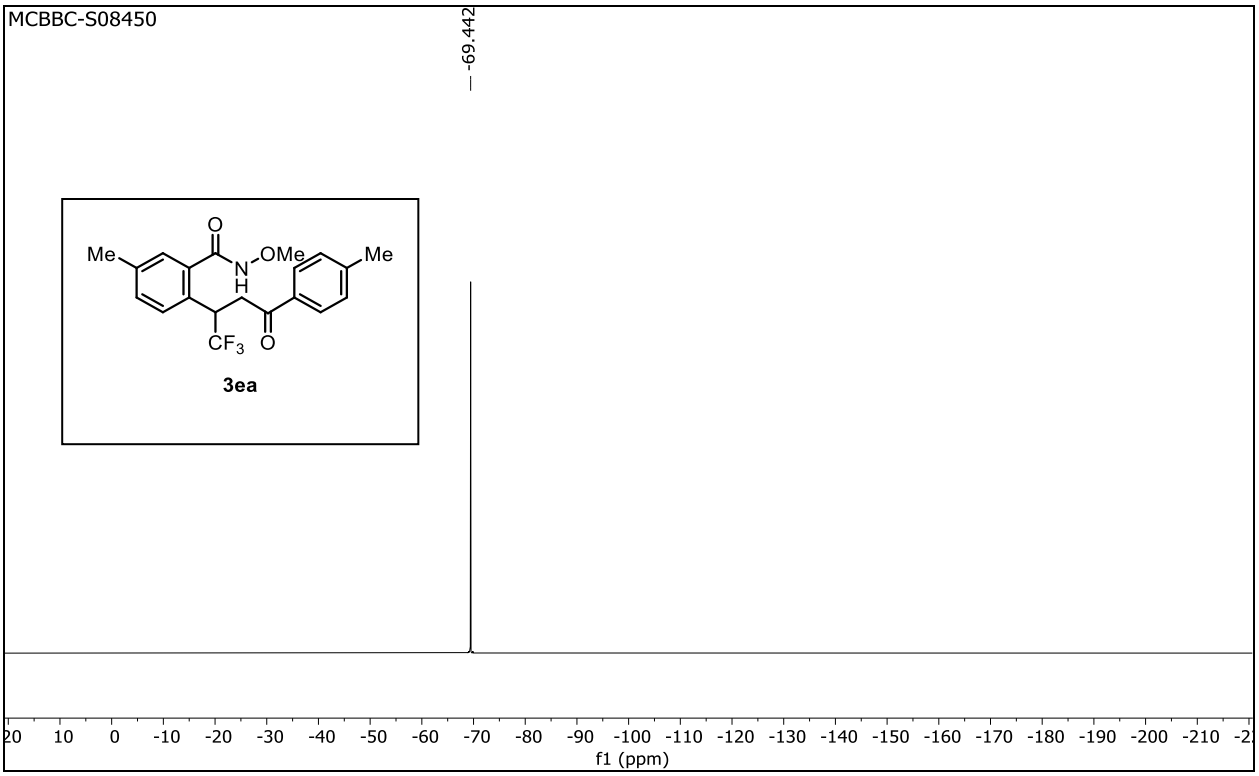
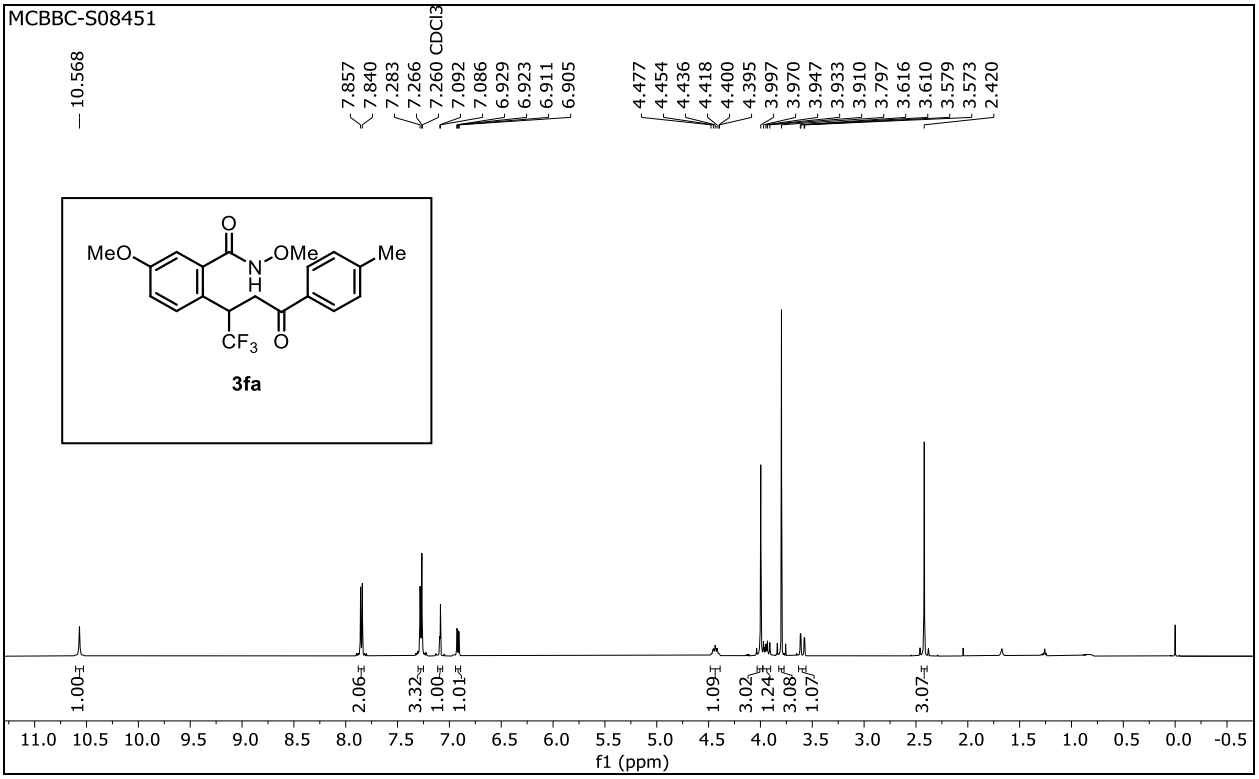
129.741
129.380
128.484
127.162
125.559
124.935
122.382
77.416 CDCl3
77.160 CDCl3
76.908 CDCl3
64.508
42.520
42.295
42.069
41.843
38.412
21.893
Br
O
N
H
OMe
Me
CF3
O
3da
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

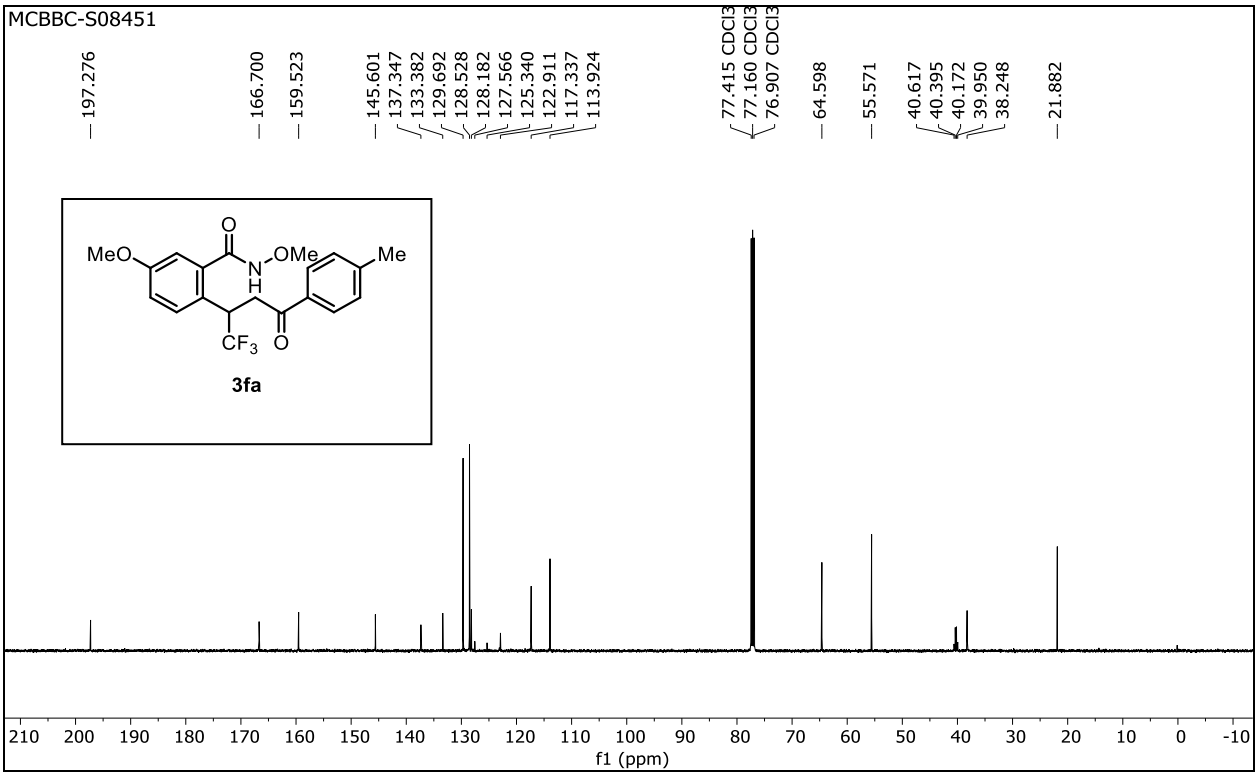

MCBBC-S04577
-69.280
Br
O
N
H
OMe
Me
CF3
O
3da
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

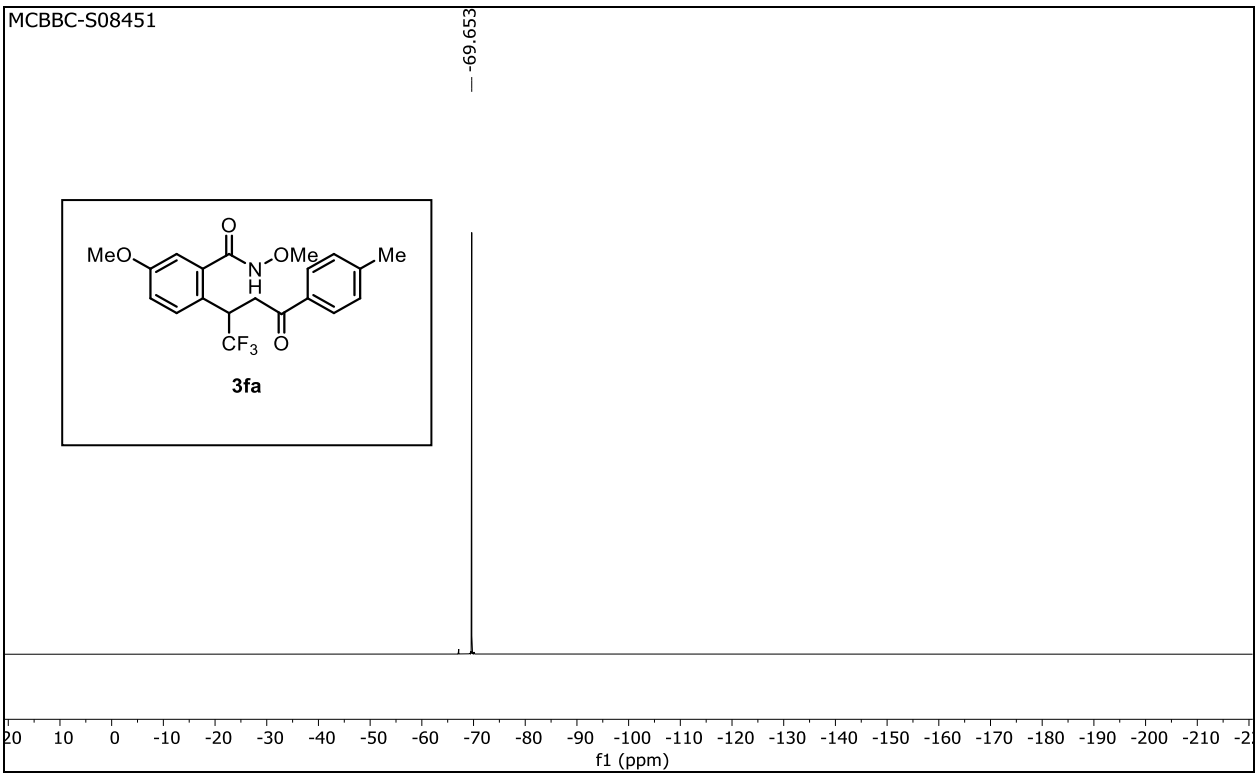

MCBBC-S08450
10.445
7.848
7.831
7.381
7.377
7.296
7.273
7.260 CDCl3
7.257
7.244
7.233
7.198
7.194
7.182
7.178
4.520
4.497
4.479
4.461
4.443
4.438
3.984
3.956
3.942
3.919
3.619
3.614
3.583
3.577
2.411
2.318
Me
OMe
Me
CF3
3ea
1.00
2.04
1.06
3.11
1.05
1.03
3.07
1.06
1.05
3.04
3.07
f1 (ppm)

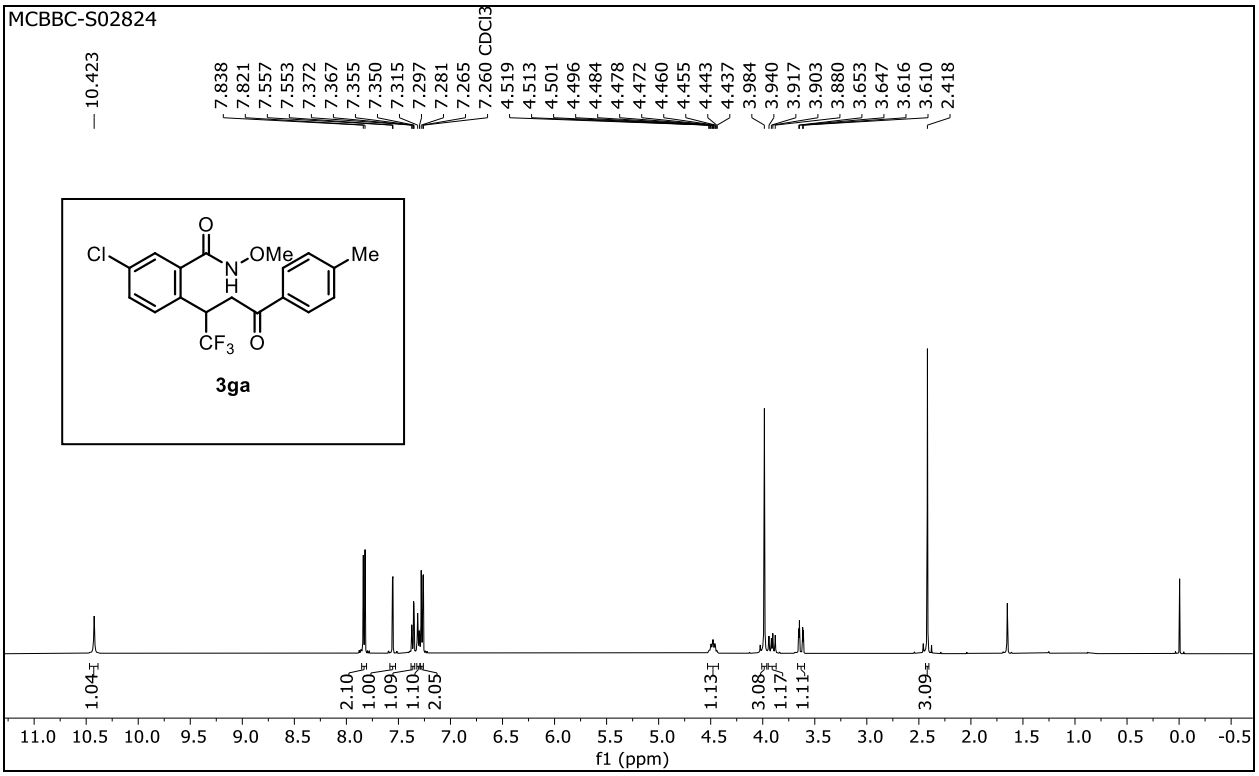

MCBBC-S08450
197.123
167.130
145.536
138.848
135.971
133.380
131.509
130.026
129.775
129.666
128.511
128.229
127.553
126.798
125.325
123.089
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
64.575
40.858
40.632
40.410
40.189
38.289
21.864
21.004
Me
OMe
Me
CF3
3ea
f1 (ppm)

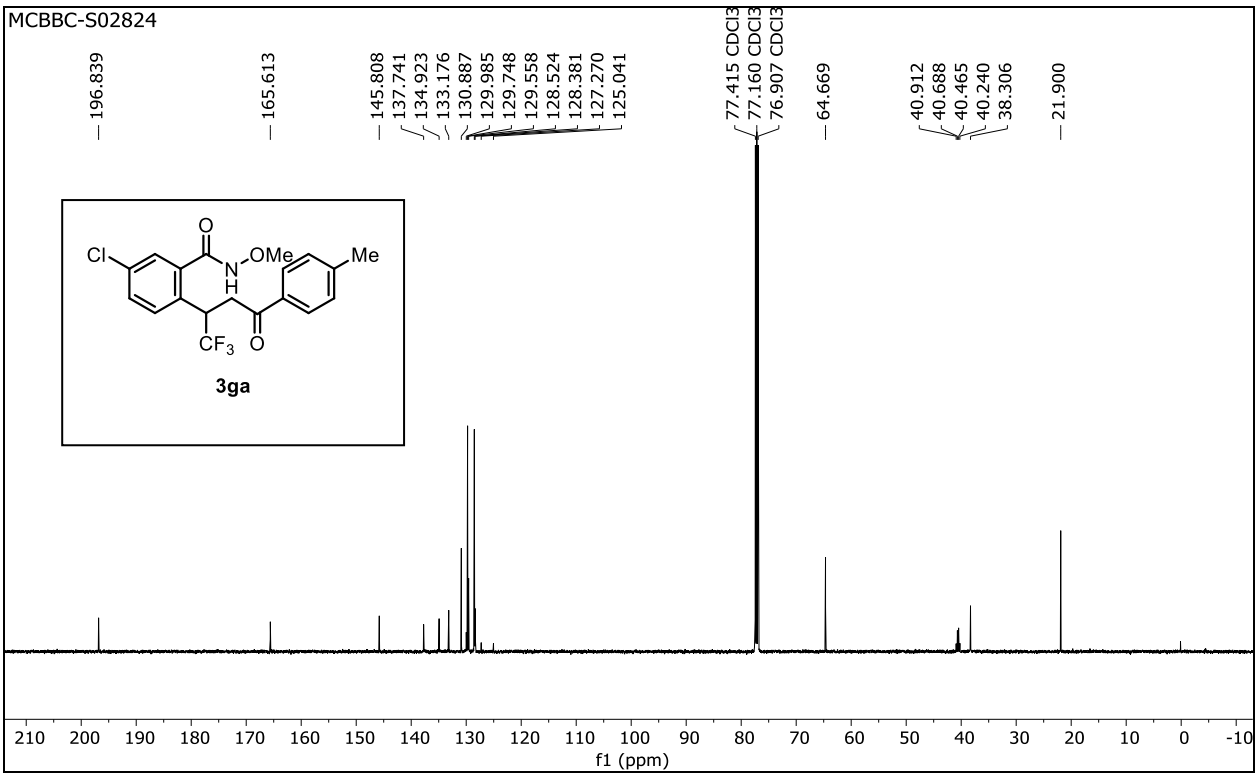

MCBBC-S08450
-69.442
Me
OMe
Me
N
H
O
O
CF3
3ea
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

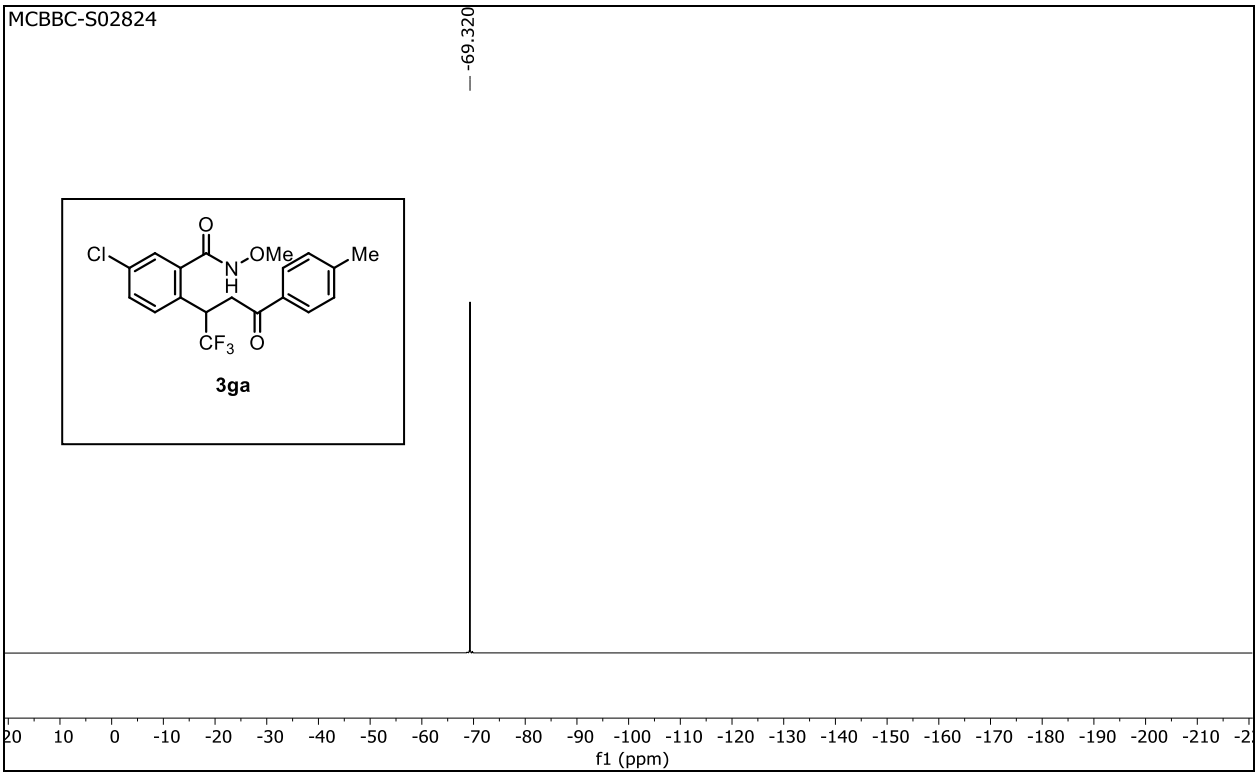

MCBBC-S08451
10.568
7.857
7.840
7.283
7.266
CDCl3
7.260
7.092
7.086
6.929
6.923
6.911
6.905
4.477
4.454
4.436
4.418
4.400
4.395
3.997
3.970
3.947
3.933
3.910
3.797
3.616
3.610
3.579
3.573
2.420
MeO
OMe
Me
N
H
O
O
CF3
3fa
1.00
2.06
3.32
1.00
1.01
1.09
3.02
1.24
3.08
1.07
3.07
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

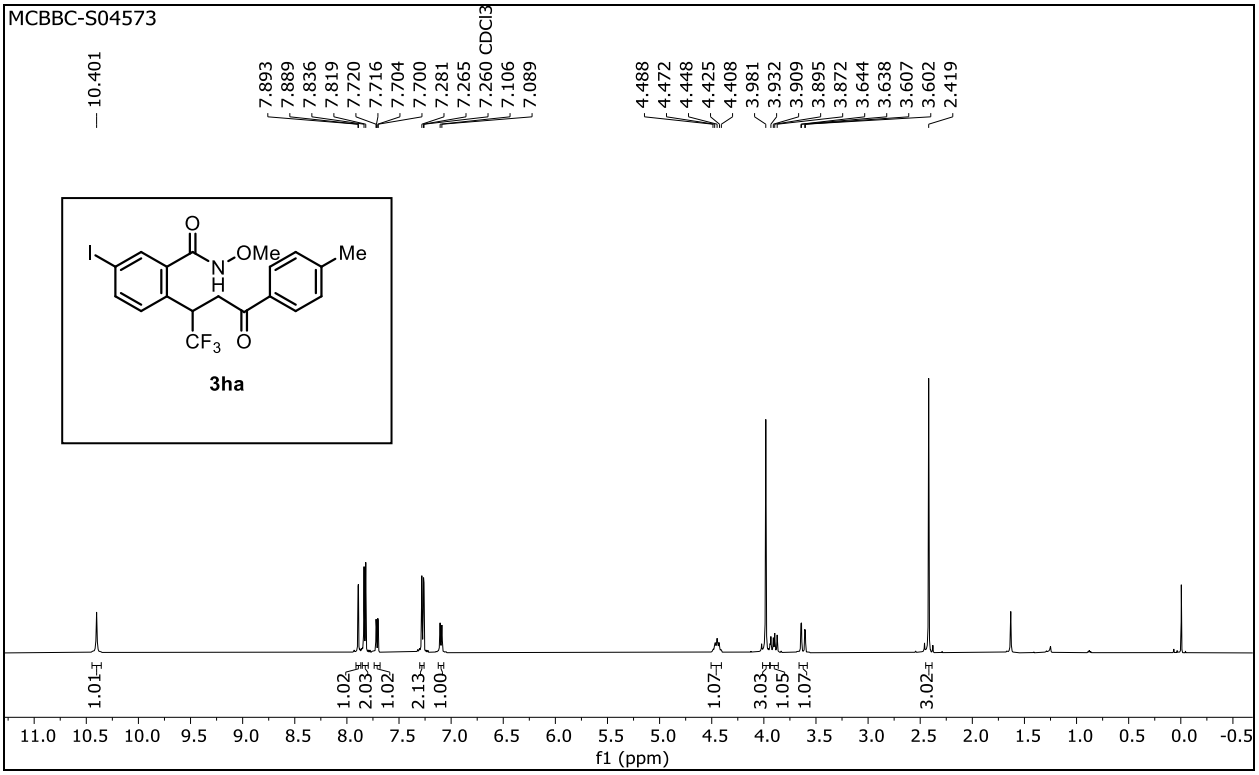

MCBBC-S08451
197.276
166.700
159.523
145.601
137.347
133.382
129.692
128.528
128.182
127.566
125.340
122.911
117.337
113.924
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
64.598
55.571
40.617
40.395
40.172
39.950
38.248
21.882
MeO
OMe
Me
N
H
O
CF3
3fa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

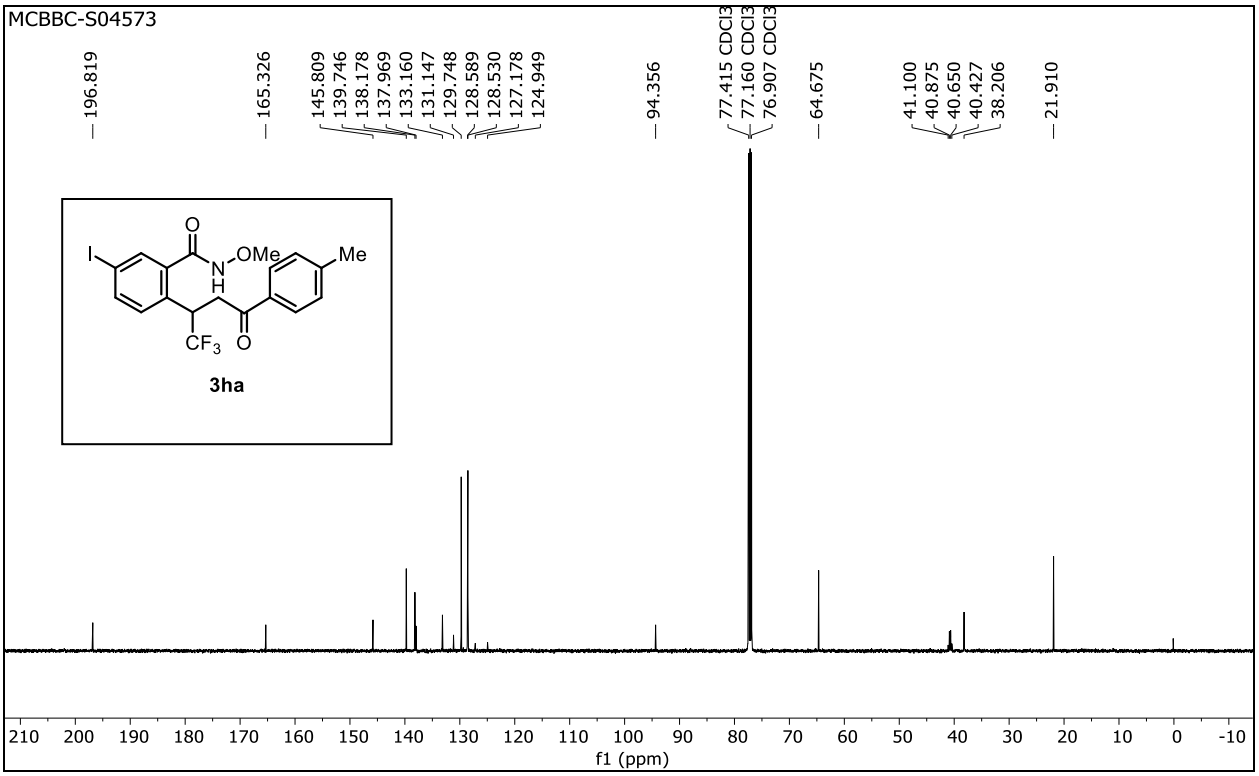

MCBBC-S08451
-69.653
MeO
OMe
Me
N
H
O
CF3
3fa
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

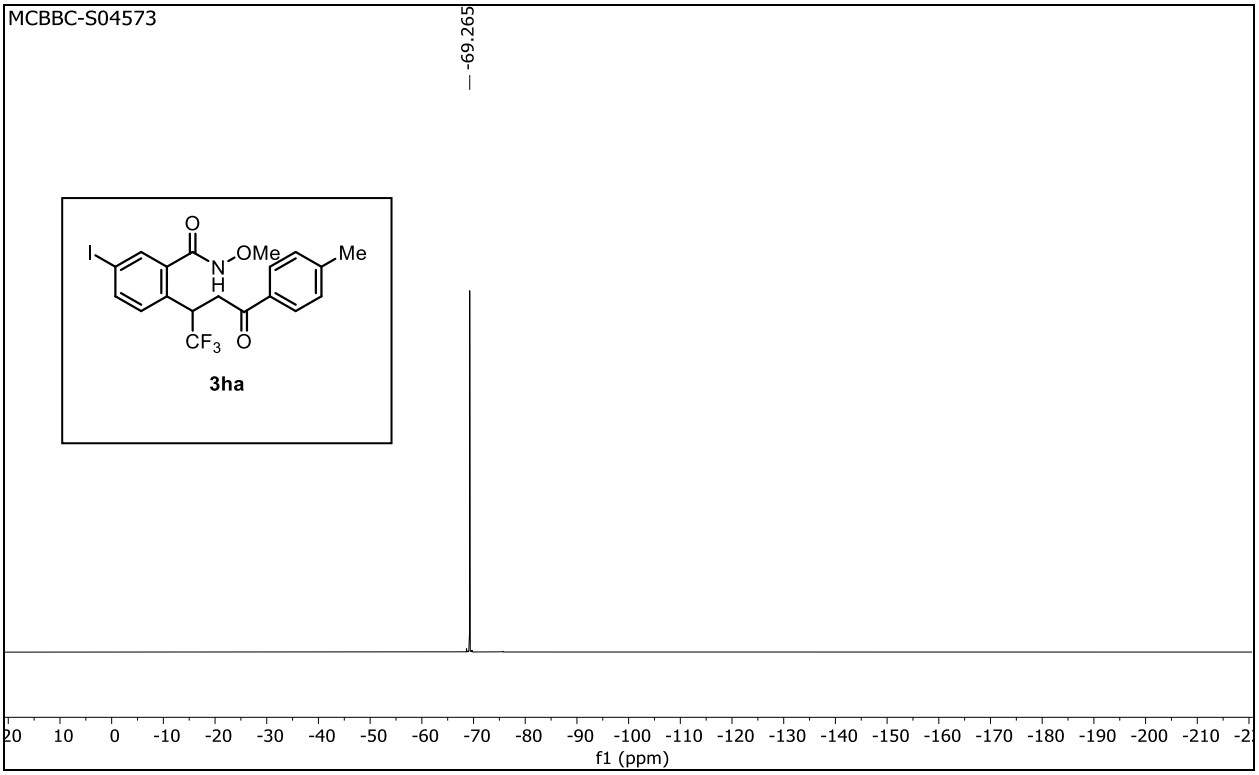

MCBBC-S02824
10.423
7.838
7.821
7.557
7.553
7.372
7.367
7.355
7.350
7.315
7.297
7.281
7.265
7.260 CDCl3
4.519
4.513
4.501
4.496
4.484
4.478
4.472
4.460
4.455
4.443
4.437
3.984
3.940
3.917
3.903
3.880
3.653
3.647
3.616
3.610
2.418
Cl
O
N
OMe
H
Me
CF3
O
3ga
1.04
2.10
1.00
1.09
1.10
2.05
1.13
3.08
1.17
1.11
3.09
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

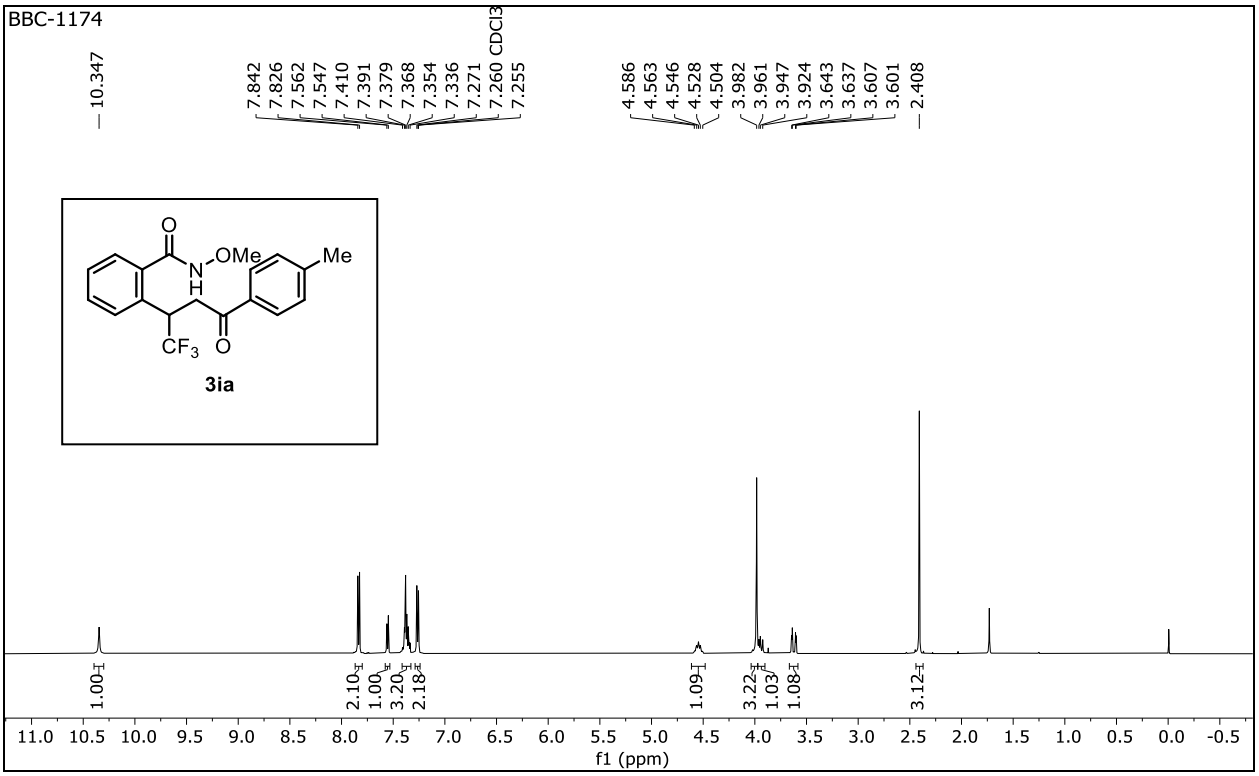

MCBBC-S02824
196.839
165.613
145.808
137.741
134.923
133.176
130.887
129.985
129.748
129.558
128.524
128.381
127.270
125.041
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
64.669
40.912
40.688
40.465
40.240
38.306
21.900
Cl
O
N
OMe
H
Me
CF3
O
3ga
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

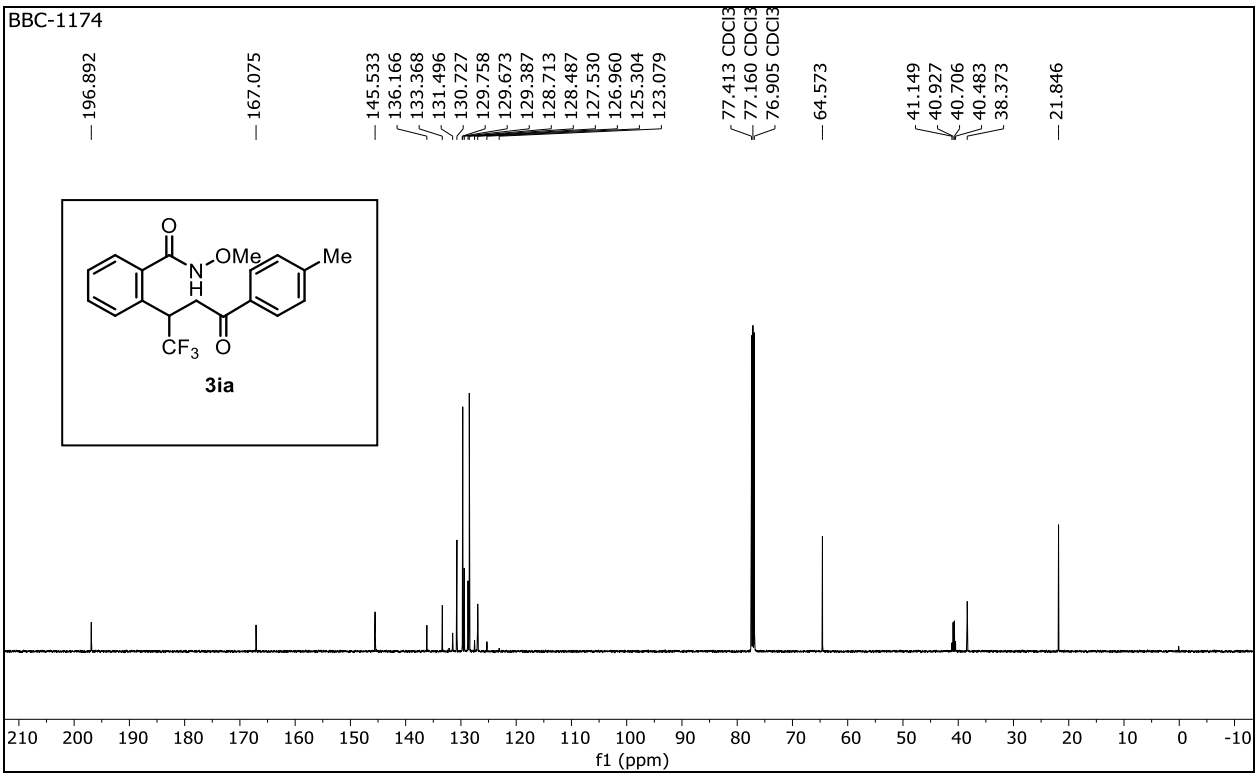

MCBBC-S02824
-69.320
Cl
O
N
H
OMe
Me
CF3
O
3ga
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

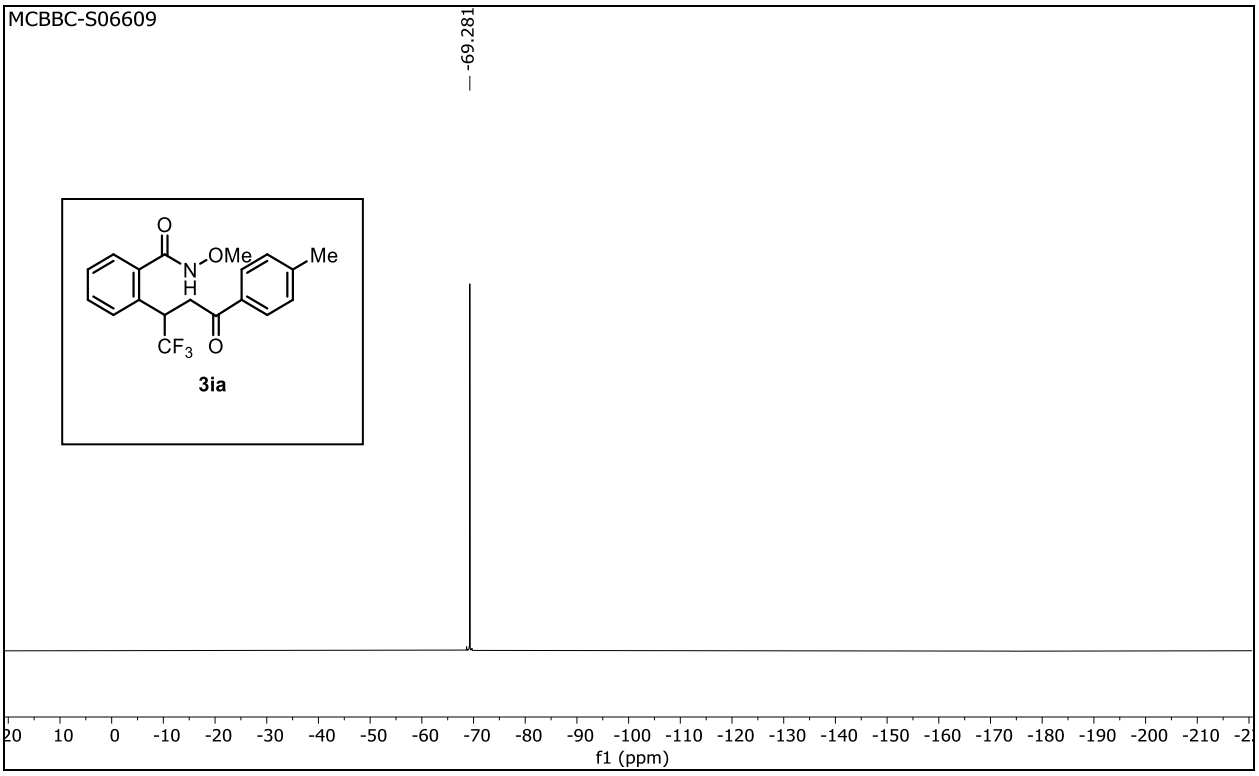

MCBBC-S04573
10.401
7.893
7.889
7.836
7.819
7.720
7.716
7.704
7.700
7.281
7.265
CDCl3
7.260
7.106
7.089
4.488
4.472
4.448
4.425
4.408
3.981
3.932
3.909
3.895
3.872
3.644
3.638
3.607
3.602
2.419
I
O
N
H
OMe
Me
CF3
O
3ha
1.01
1.02
2.03
1.02
2.13
1.00
1.07
3.03
1.05
1.07
3.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

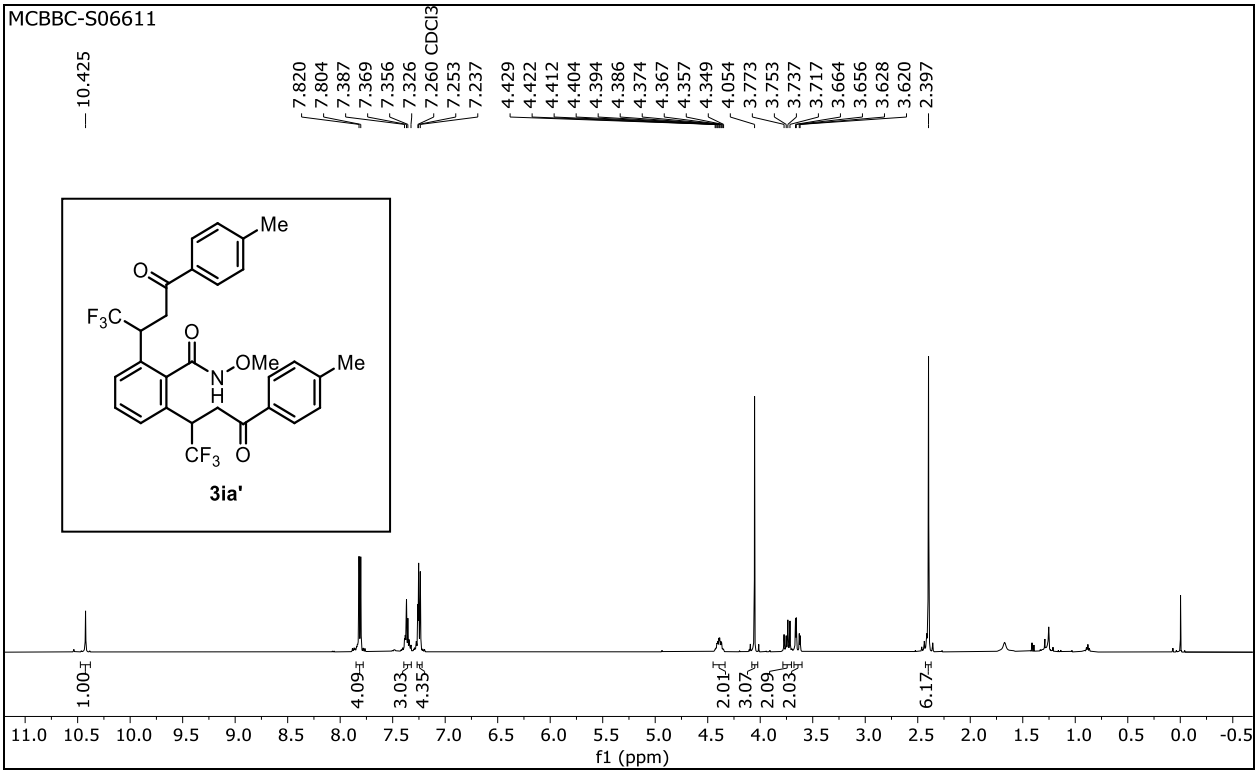

MCBBC-S04573
196.819
165.326
145.809
139.746
138.178
137.969
133.160
131.147
129.748
128.589
128.530
127.178
124.949
94.356
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
64.675
41.100
40.875
40.650
40.427
38.206
21.910
I
O
N
H
OMe
Me
CF3
O
3ha
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

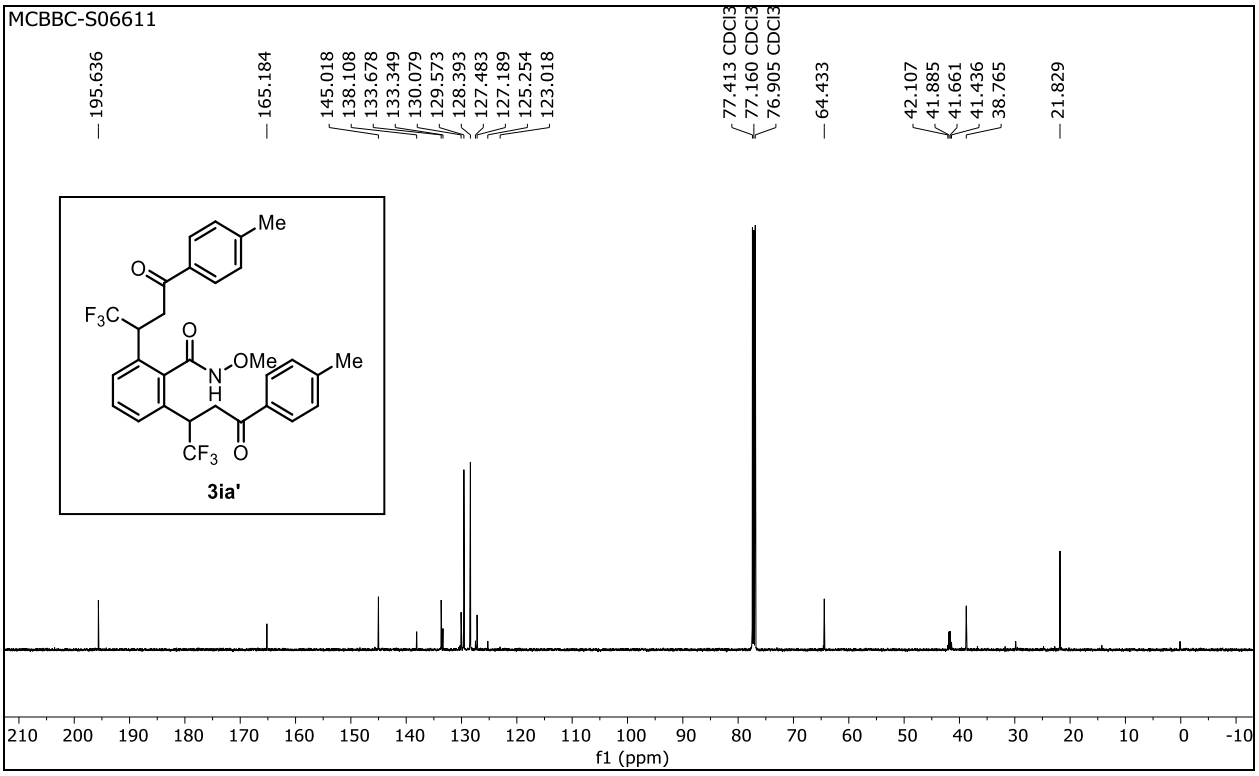

MCBBC-S04573
-69.265
I
O
N
H
OMe
Me
CF3
O
3ha
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

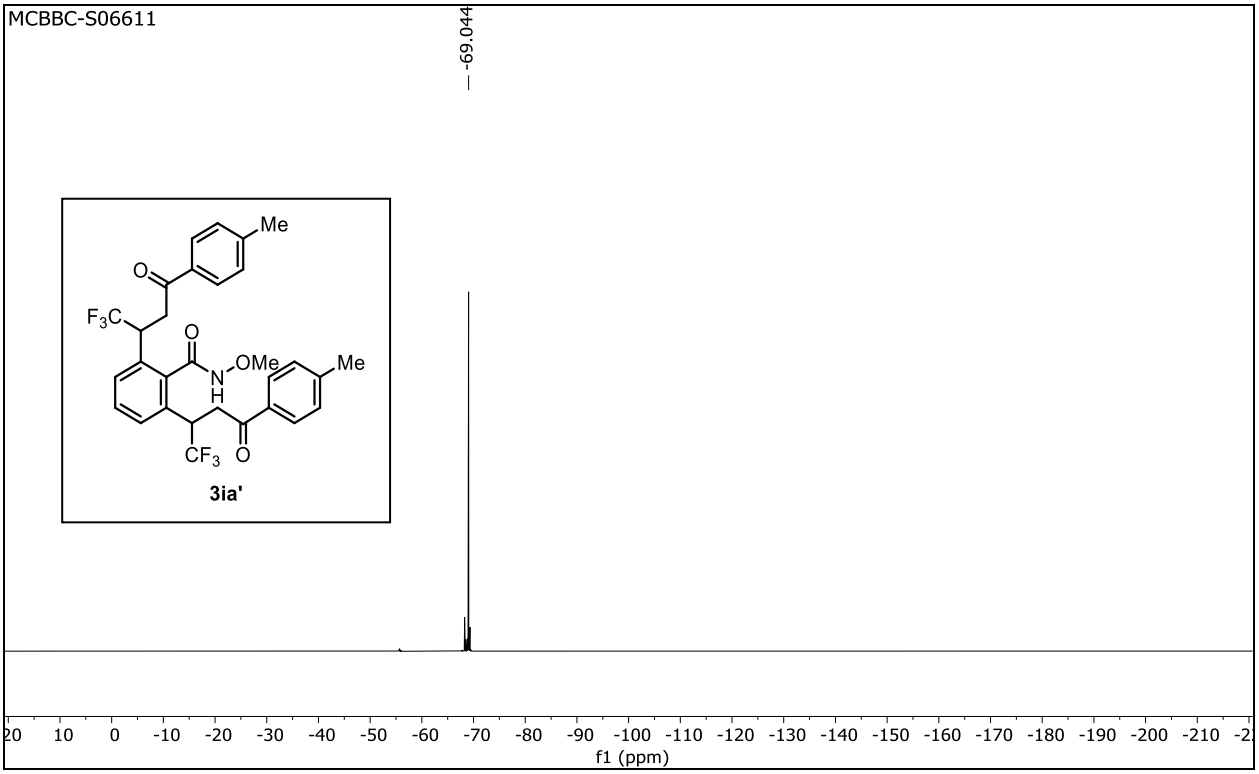

BBC-1174
10.347
7.842
7.826
7.562
7.547
7.410
7.391
7.379
7.368
7.354
7.336
7.271
7.260 CDCl3
7.255
4.586
4.563
4.546
4.528
4.504
3.982
3.961
3.947
3.924
3.643
3.637
3.607
3.601
2.408
1.00
2.10
1.00
3.20
2.18
1.09
3.22
1.03
1.08
3.12
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
O
N
H
OMe
Me
CF3
O
3ia

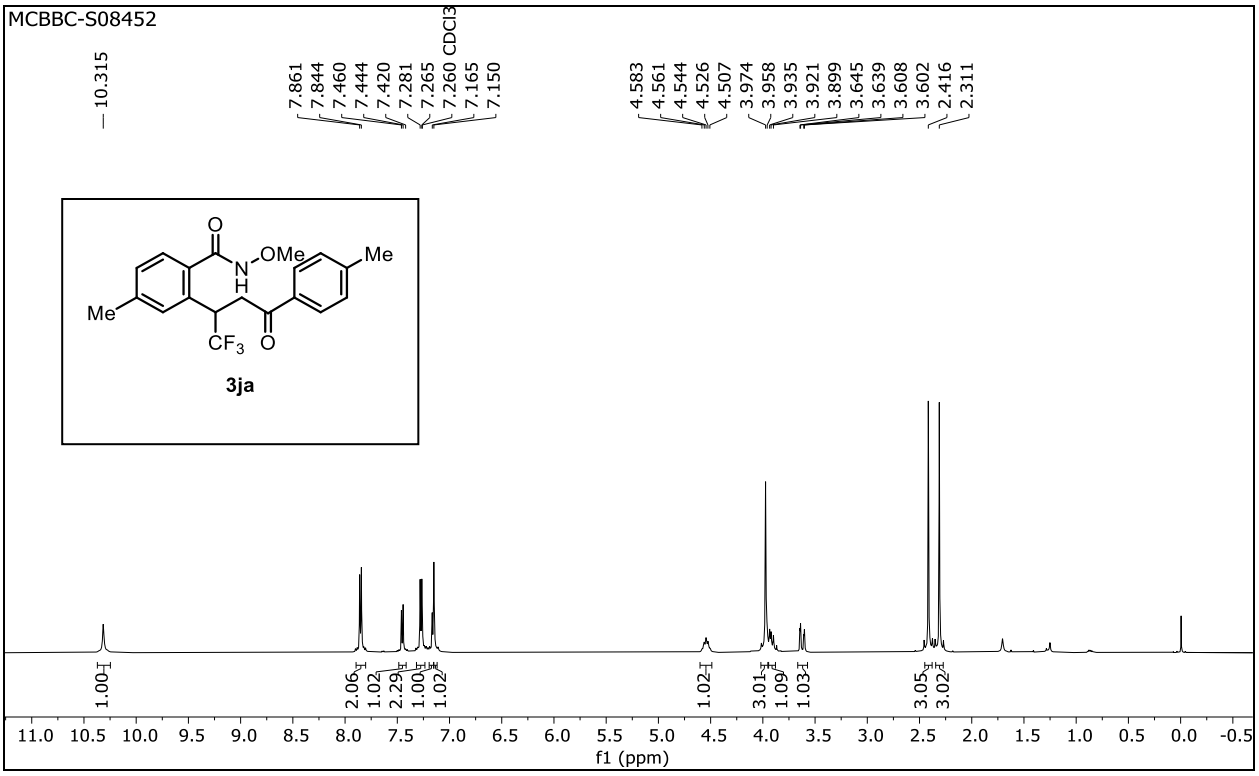

BBC-1174
196.892
167.075
145.533
136.166
133.368
131.496
130.727
129.758
129.673
129.387
128.713
128.487
127.530
126.960
125.304
123.079
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
64.573
41.149
40.927
40.706
40.483
38.373
21.846
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
O
N
H
OMe
Me
CF3
O
3ia

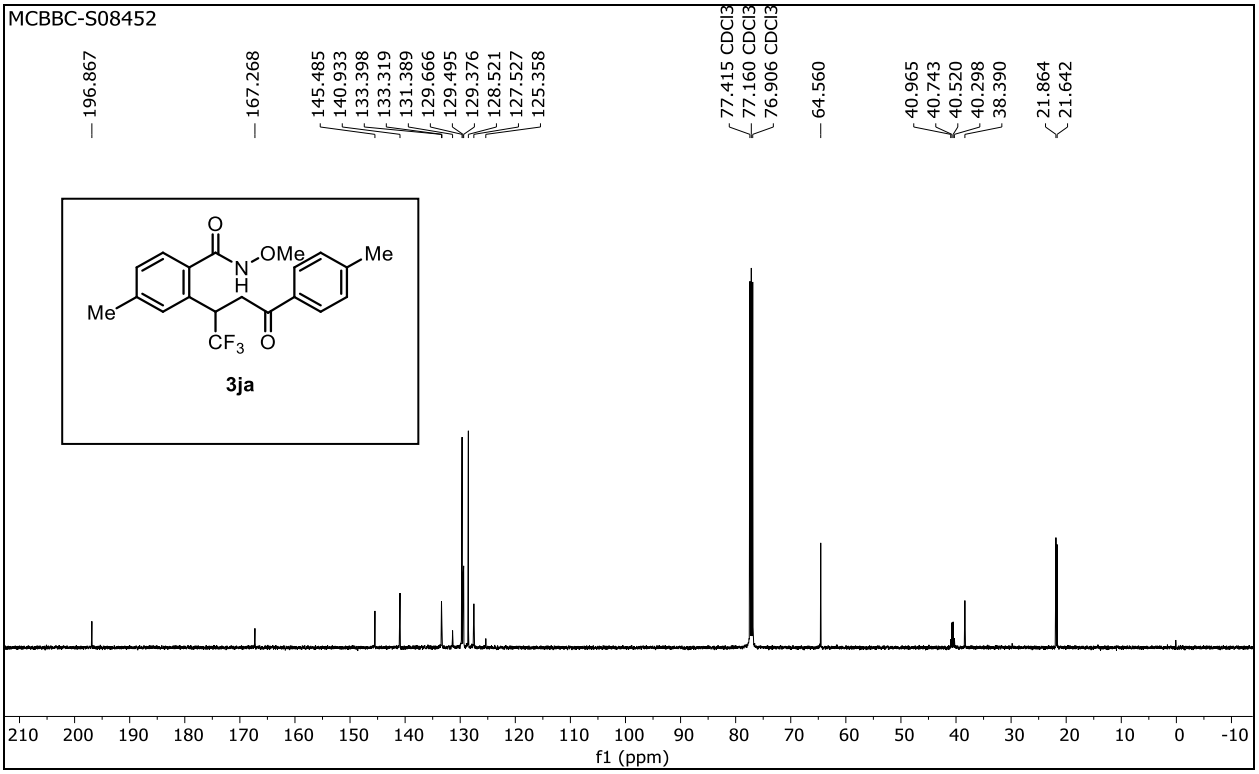

MCBBC-S06609
-69.281
O
N
H
OMe
Me
CF3
O
3ia
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

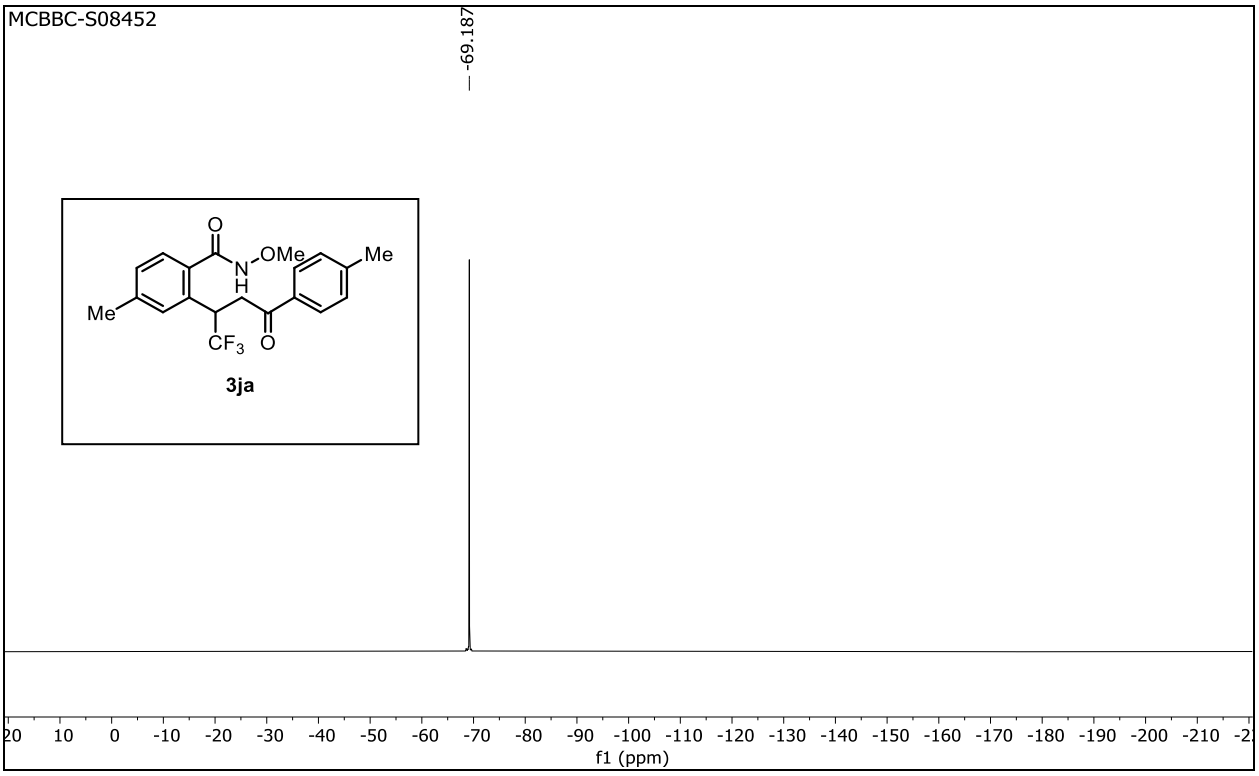

MCBBC-S06611
10.425
7.820
7.804
7.387
7.369
7.356
7.326
CDCl3
7.260
7.253
7.237
4.429
4.422
4.412
4.404
4.394
4.386
4.374
4.367
4.357
4.349
4.054
3.773
3.753
3.737
3.717
3.664
3.656
3.628
3.620
2.397
Me
O
F3C
O
N
H
OMe
Me
CF3
O
3ia'
1.00
4.09
3.03
4.35
2.01
3.07
2.09
2.03
6.17
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

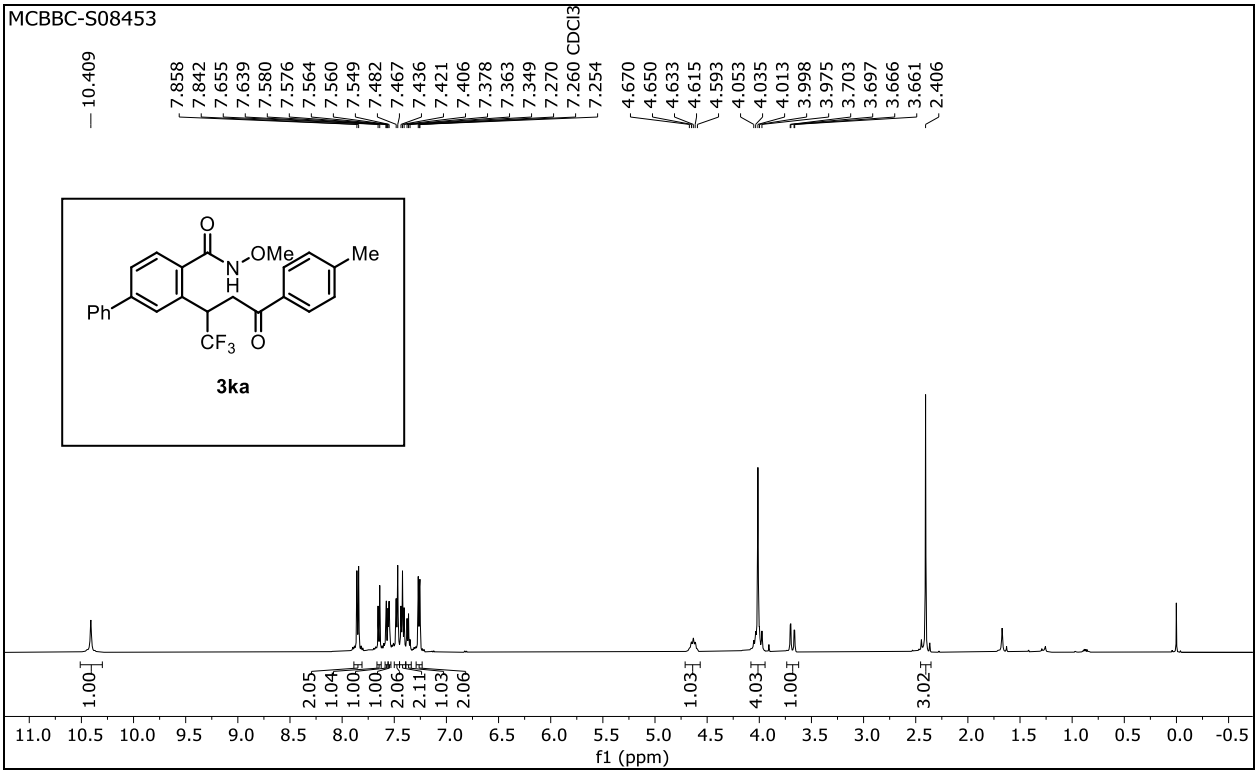

MCBBC-S06611
195.636
165.184
145.018
138.108
133.678
133.349
130.079
129.573
128.393
127.483
127.189
125.254
123.018
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
64.433
42.107
41.885
41.661
41.436
38.765
21.829
Me
O
F3C
O
N
H
OMe
Me
CF3
O
3ia'
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

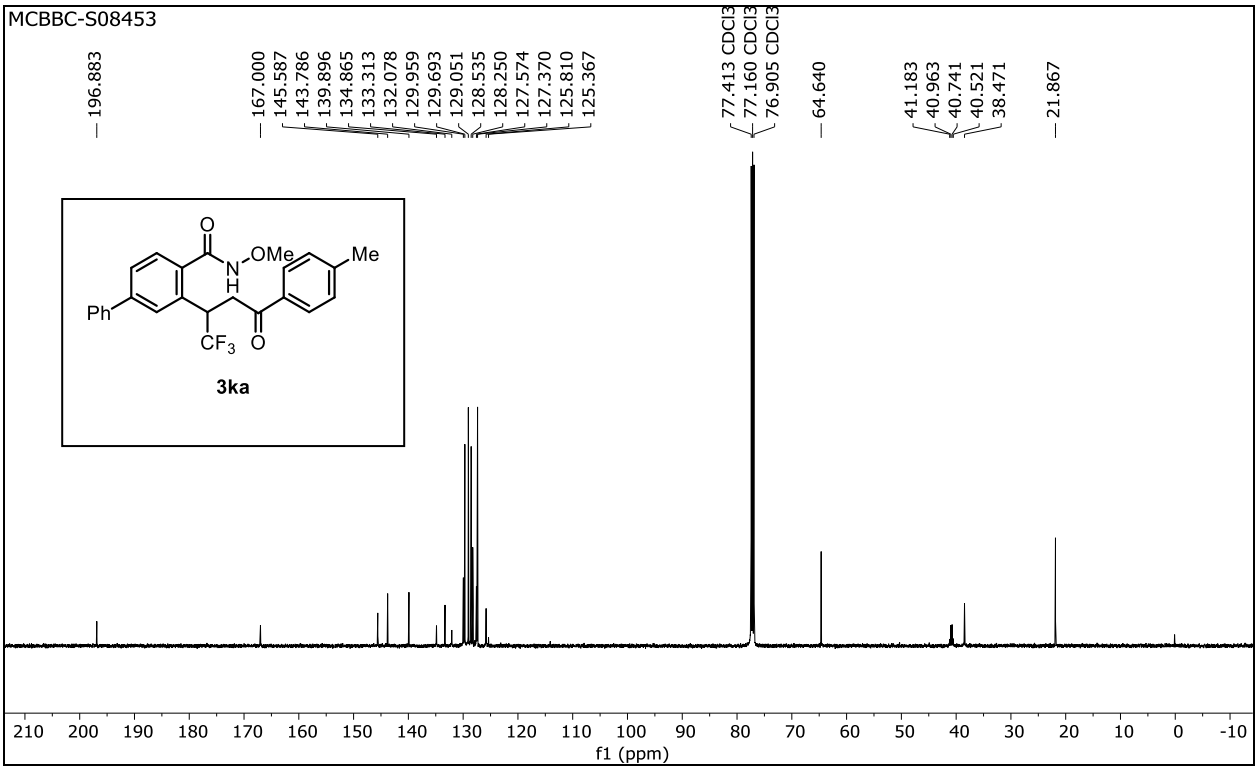

MCBBC-S06611
-69.044
Me
O
F3C
O
N
H
OMe
Me
CF3
O
3ia'
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

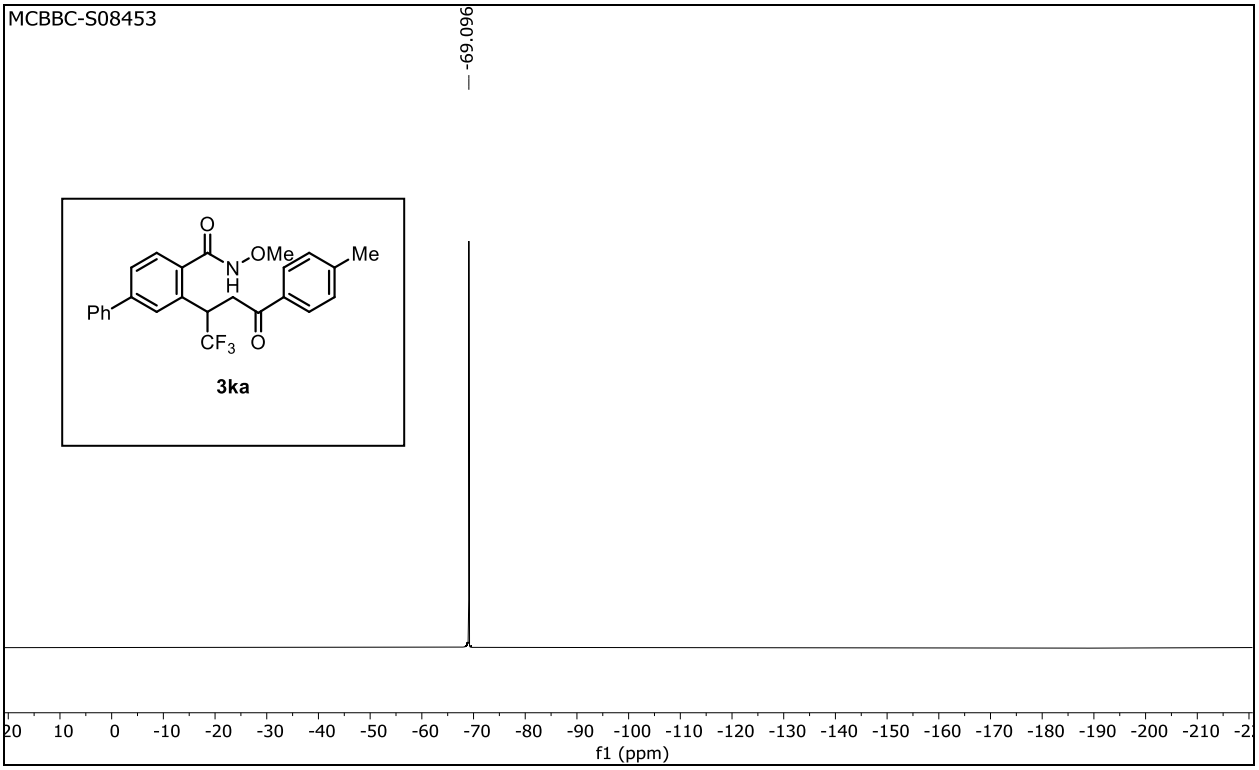

MCBBC-S08452
10.315
7.861
7.844
7.460
7.444
7.420
7.281
7.265
7.260 CDCl3
7.165
7.150
4.583
4.561
4.544
4.526
4.507
3.974
3.958
3.935
3.921
3.899
3.645
3.639
3.608
3.602
2.416
2.311
O
N
H
OMe
Me
Me
CF3
O
3ja
1.00
2.06
1.02
2.29
1.00
1.02
1.02
3.01
1.09
1.03
3.05
3.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

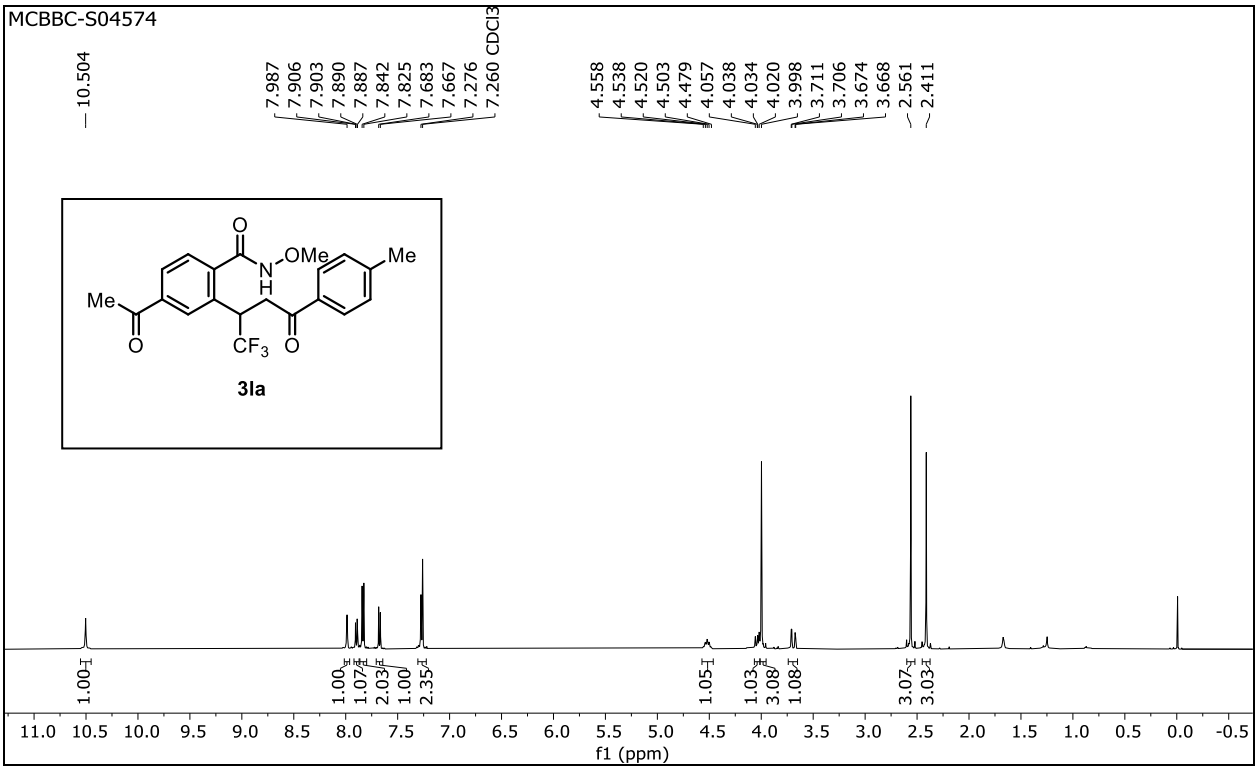

MCBBC-S08452
196.867
167.268
145.485
140.933
133.398
133.319
131.389
129.666
129.495
129.376
128.521
127.527
125.358
77.415 CDCl3
77.160 CDCl3
76.906 CDCl3
64.560
40.965
40.743
40.520
40.298
38.390
21.864
21.642
O
N
H
OMe
Me
Me
CF3
O
3ja
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

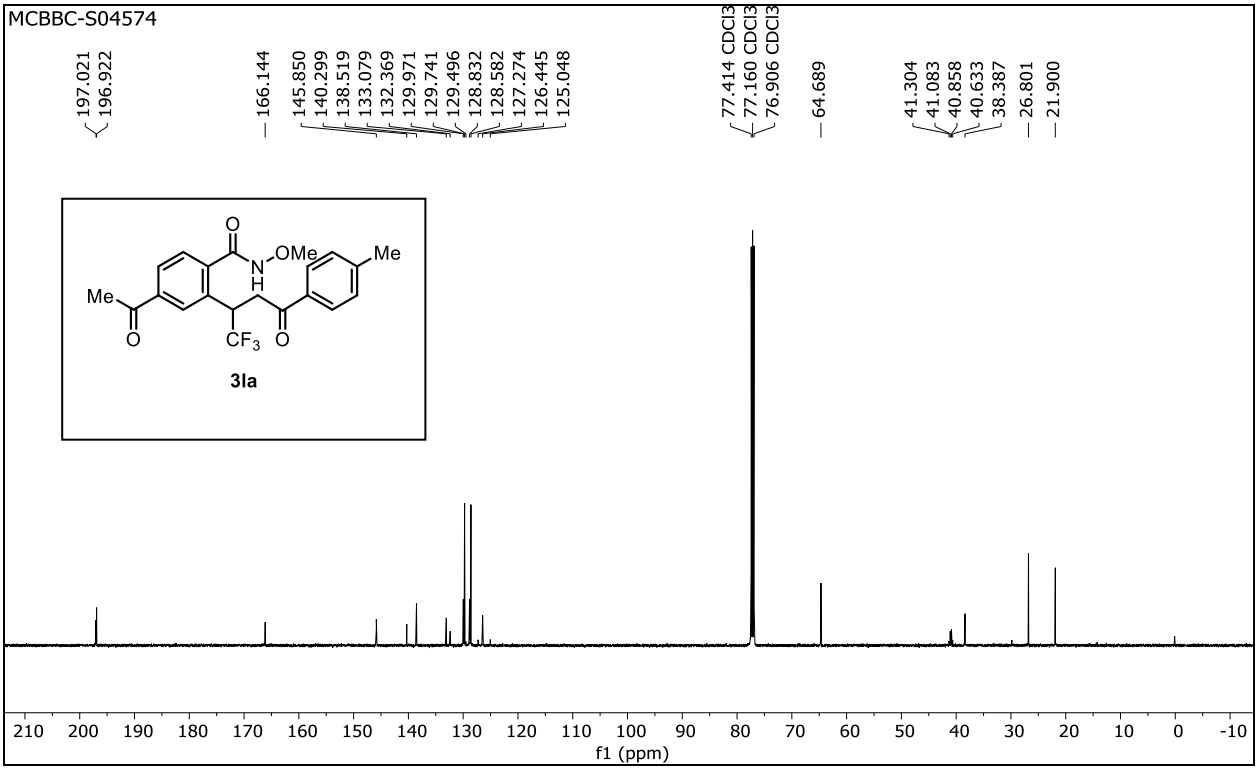

MCBBC-S08452
-69.187
O
N
H
OMe
Me
Me
CF3
O
3ja
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

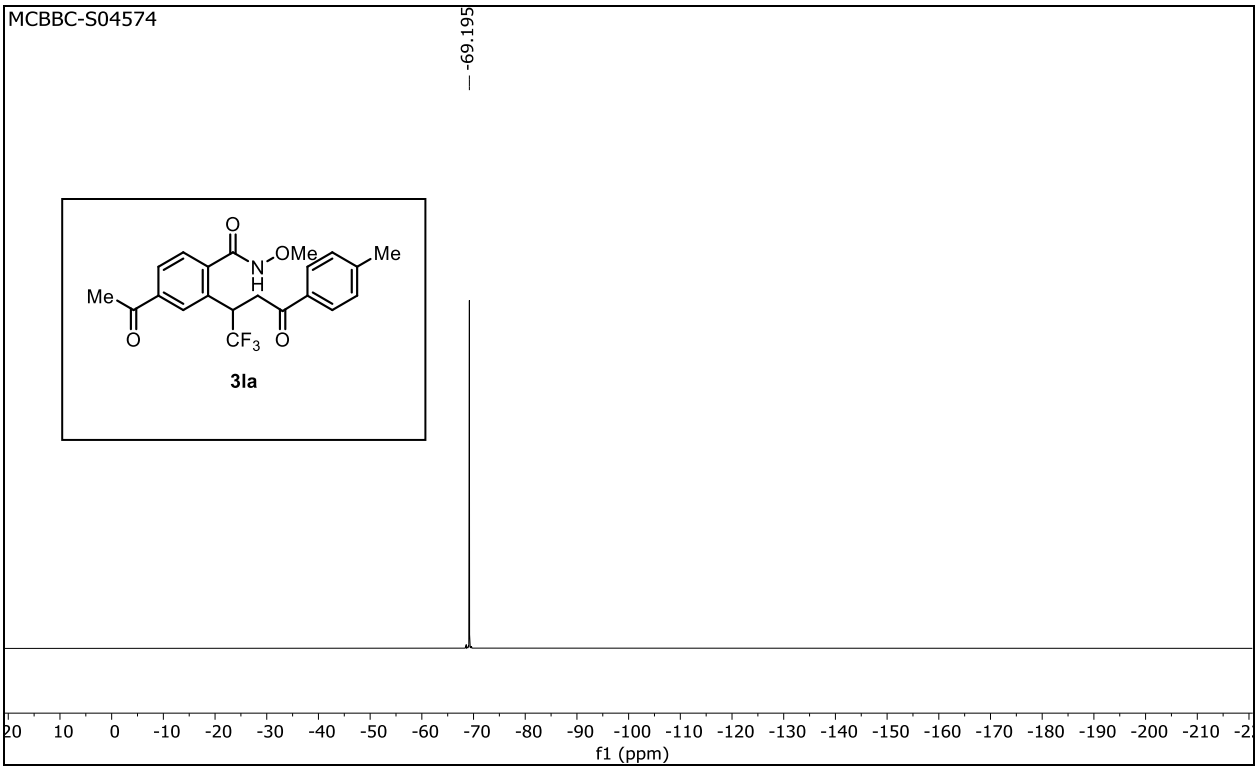

MCBBC-S08453
10.409
7.858
7.842
7.655
7.639
7.580
7.576
7.564
7.560
7.549
7.482
7.467
7.436
7.421
7.406
7.378
7.363
7.349
7.270
CDCl3
7.260
7.254
4.670
4.650
4.633
4.615
4.593
4.053
4.035
4.013
3.998
3.975
3.703
3.697
3.666
3.661
2.406
O
N
H
OMe
Me
Ph
CF3
O
3ka
1.00
2.05
1.04
1.00
1.00
2.06
2.11
1.03
2.06
1.03
4.03
1.00
3.02
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

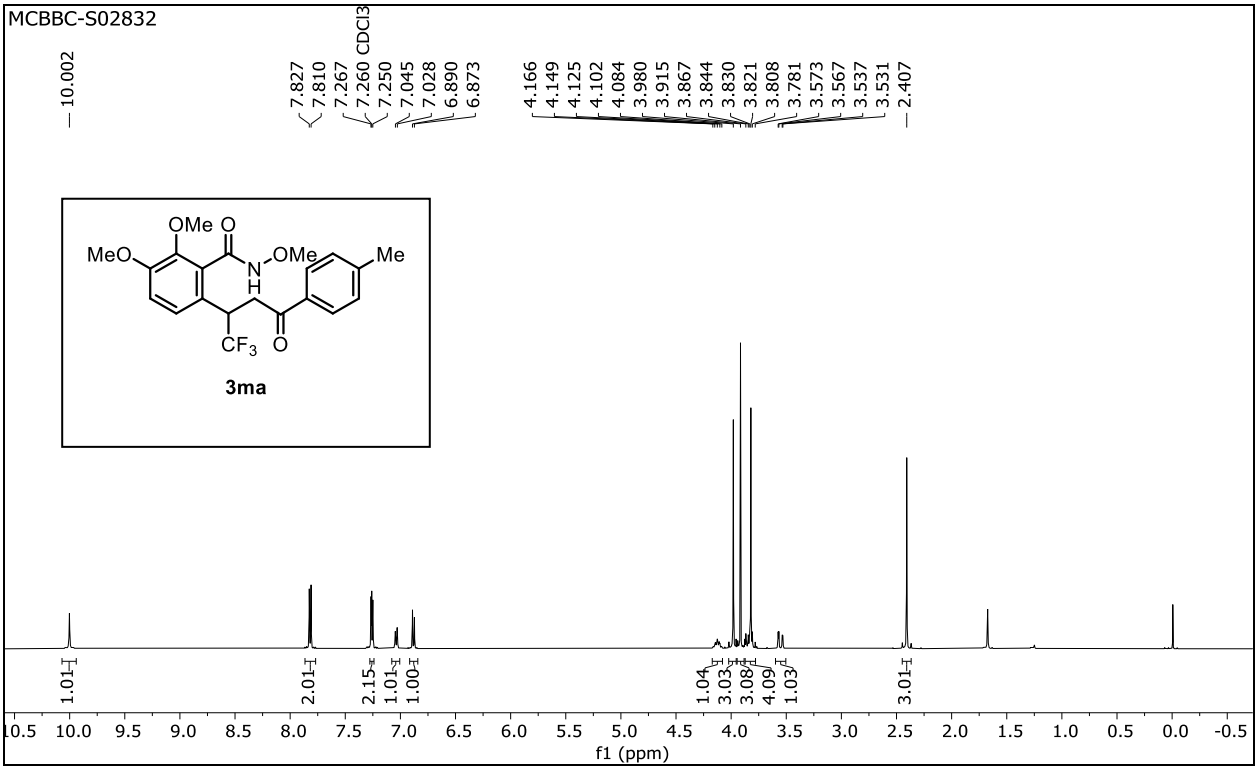

MCBBC-S08453
196.883
167.000
145.587
143.786
139.896
134.865
133.313
132.078
129.959
129.693
129.051
128.535
128.250
127.574
127.370
125.810
125.367
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
64.640
41.183
40.963
40.741
40.521
38.471
21.867
O
N
H
OMe
Me
Ph
CF3
O
3ka
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

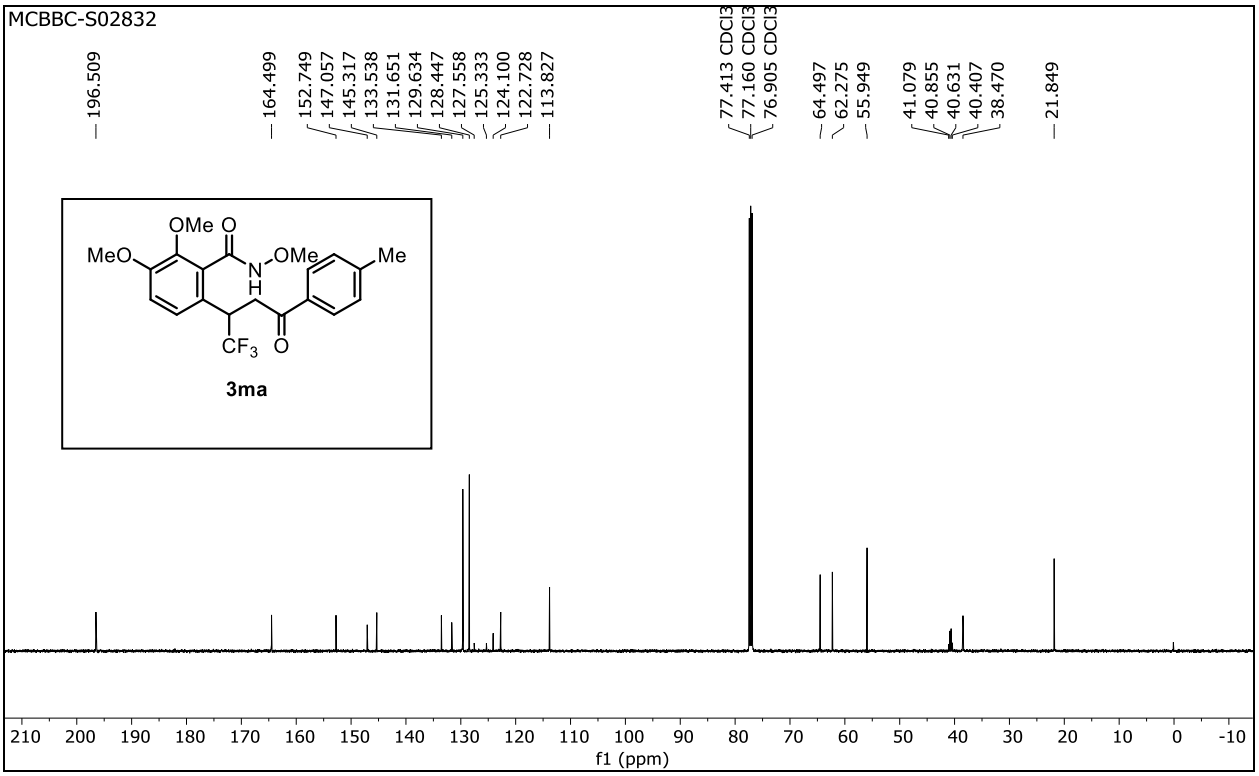

MCBBC-S08453
-69.096
O
N
H
OMe
Me
Ph
CF3
O
3ka
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

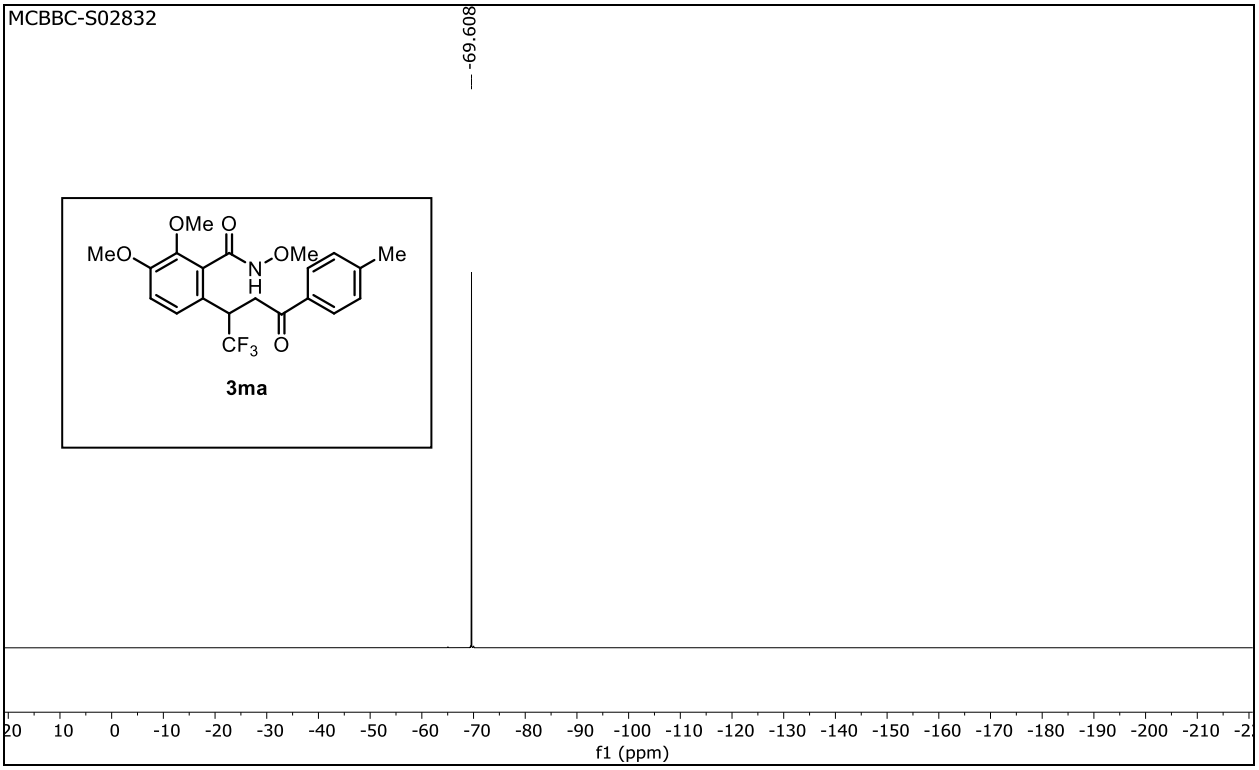

MCBBC-S04574
10.504
7.987
7.906
7.903
7.890
7.887
7.842
7.825
7.683
7.667
7.276
7.260 CDCl3
4.558
4.538
4.520
4.503
4.479
4.057
4.038
4.034
4.020
3.998
3.711
3.706
3.674
3.668
2.561
2.411
1.00
1.07
2.03
1.00
2.35
1.05
1.03
3.08
1.08
3.07
3.03
Me
OMe
Me
N
H
O
CF3
3la
f1 (ppm)

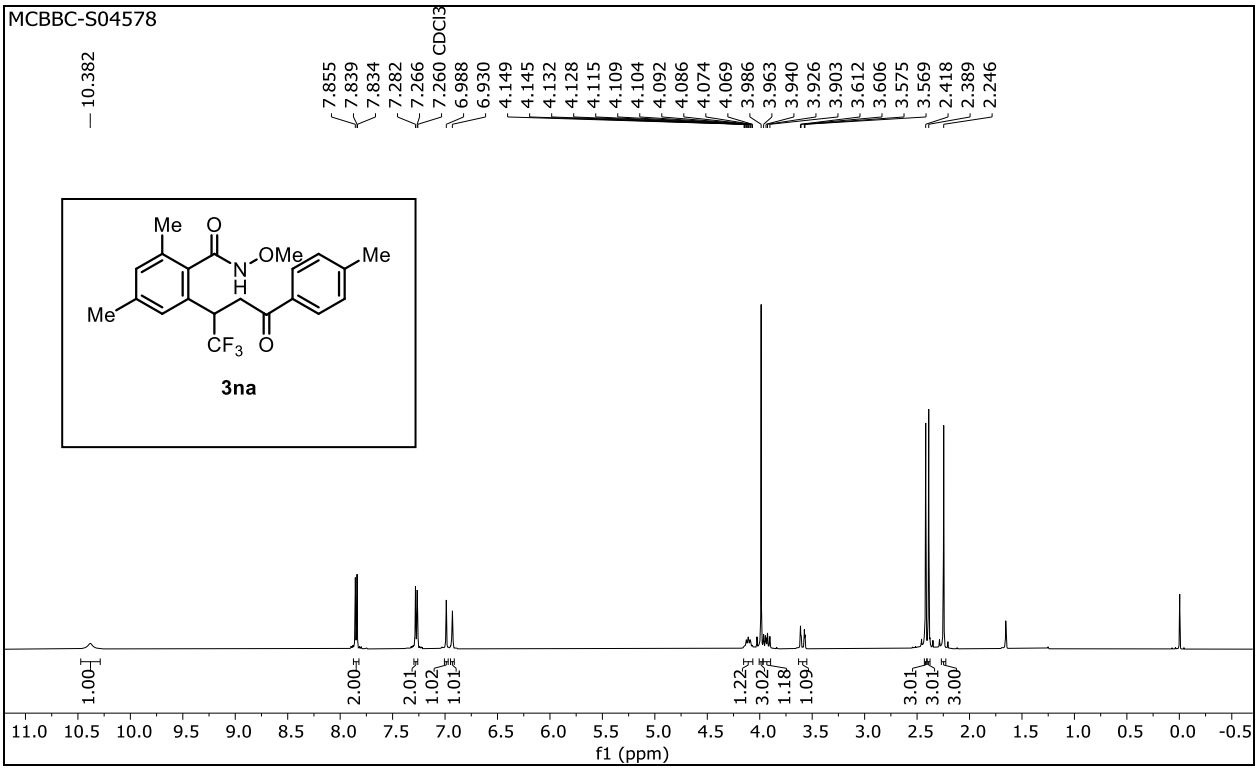

MCBBC-S04574
197.021
196.922
166.144
145.850
140.299
138.519
133.079
132.369
129.971
129.741
129.496
128.832
128.582
127.274
126.445
125.048
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
64.689
41.304
41.083
40.858
40.633
38.387
26.801
21.900
Me
OMe
Me
N
H
O
CF3
3la
f1 (ppm)

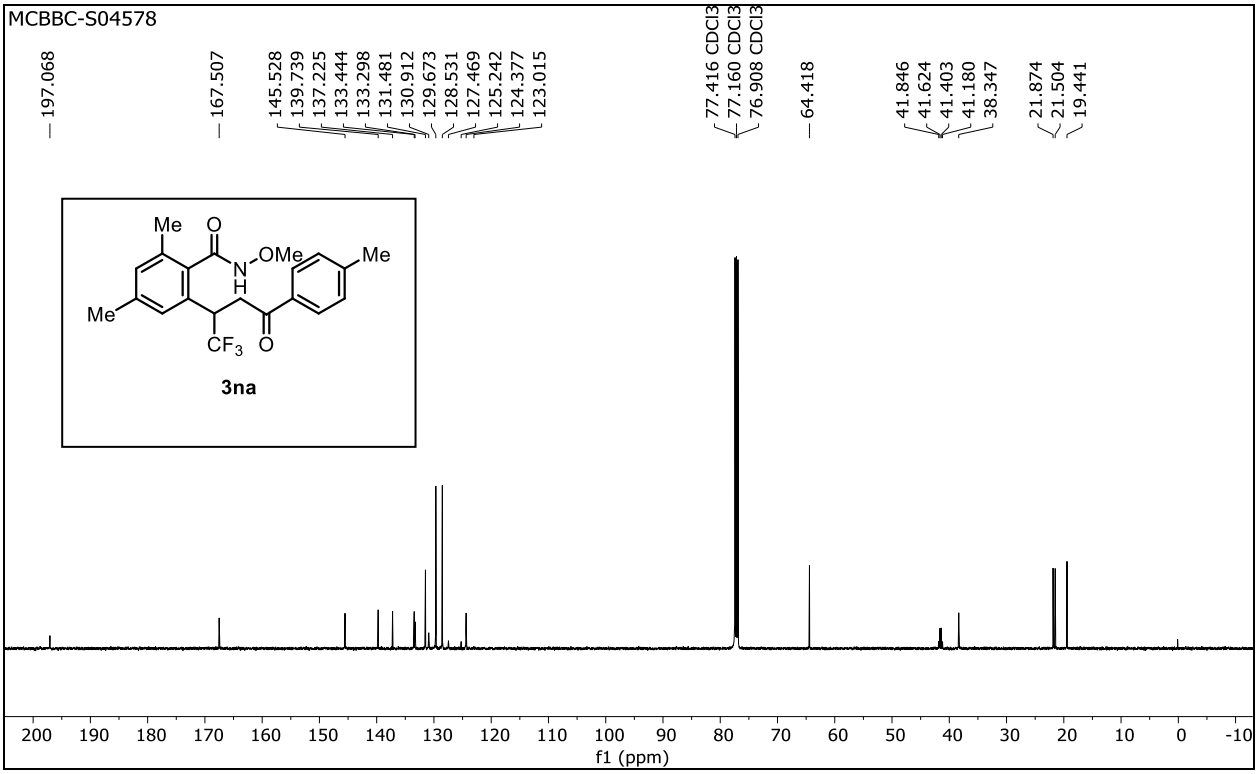

MCBBC-S04574
-69.195
3la
f1 (ppm)

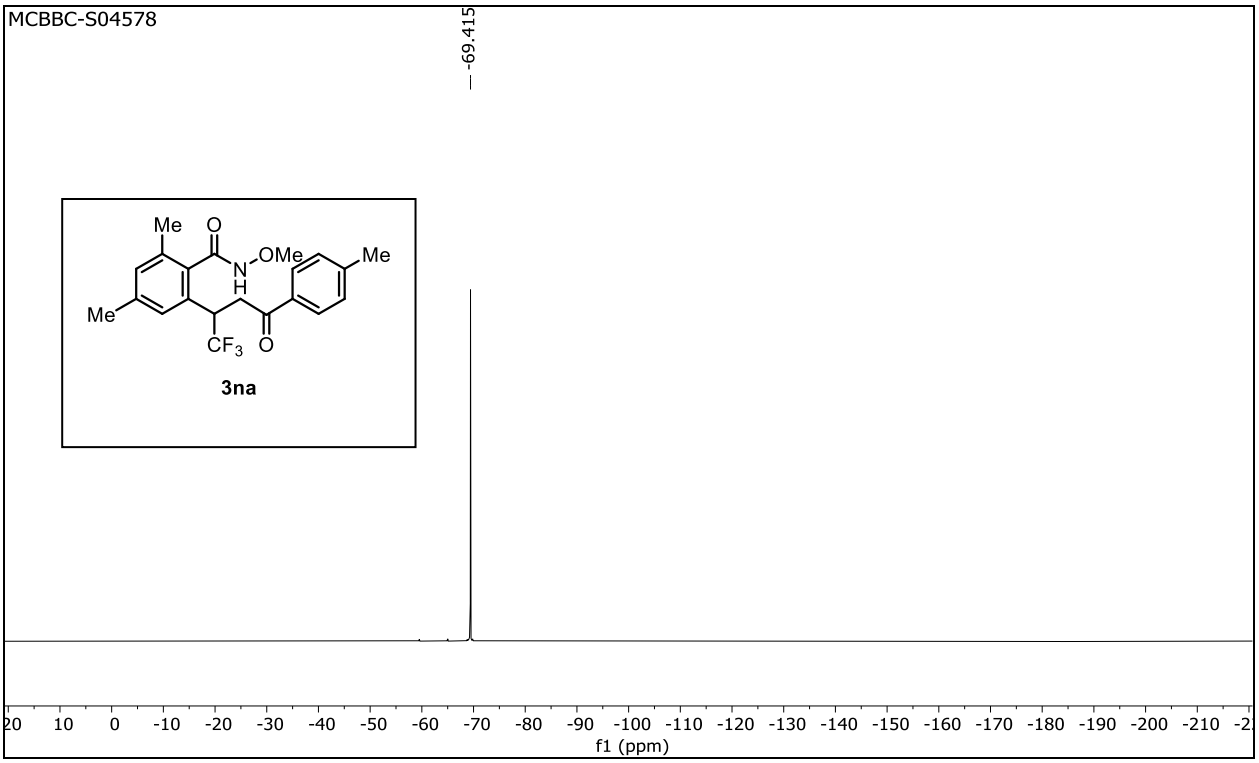

MCBBC-S02832
10.002
7.827
7.810
7.267
7.260 CDCl3
7.250
7.045
7.028
6.890
6.873
4.166
4.149
4.125
4.102
4.084
3.980
3.915
3.867
3.844
3.830
3.821
3.808
3.781
3.573
3.567
3.537
3.531
2.407
3ma
1.01
2.01
2.15
1.01
1.00
1.04
3.03
3.08
4.09
1.03
3.01
f1 (ppm)

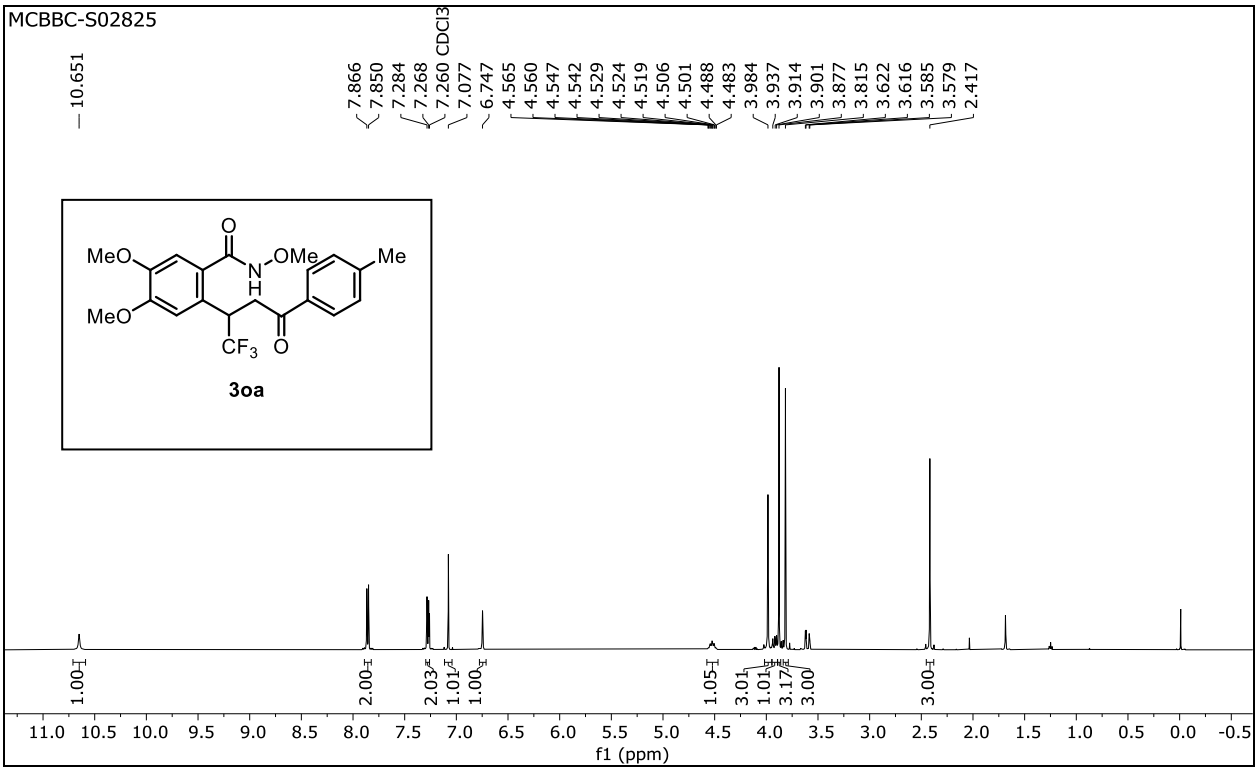

MCBBC-S02832
196.509
164.499
152.749
147.057
145.317
133.538
131.651
129.634
128.447
127.558
125.333
124.100
122.728
113.827
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
64.497
62.275
55.949
41.079
40.855
40.631
40.407
38.470
21.849
OMe O
MeO
N
OMe
Me
H
CF3 O
3ma
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

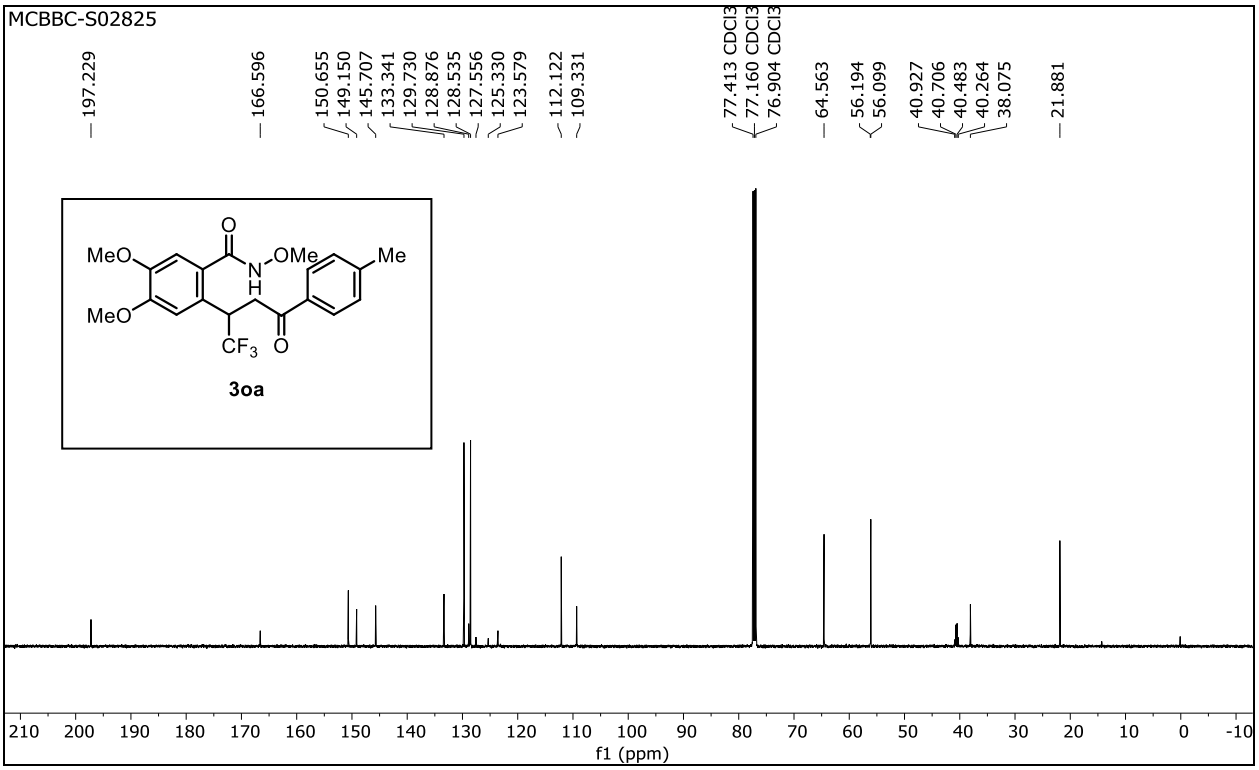

MCBBC-S02832
-69.608
OMe O
MeO
N
OMe
Me
H
CF3 O
3ma
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

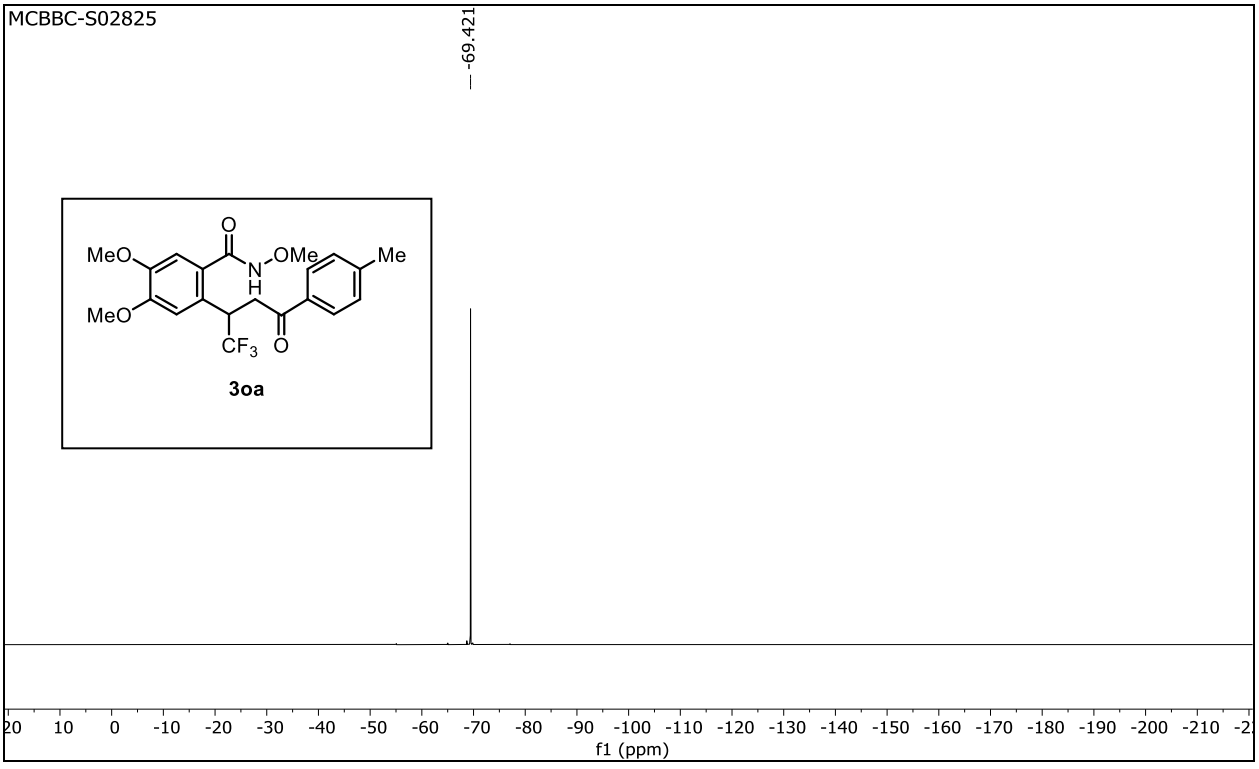

MCBBC-S04578
10.382
7.855
7.839
7.834
7.282
7.266
7.260 CDCl3
6.988
6.930
4.149
4.145
4.132
4.128
4.115
4.109
4.104
4.092
4.086
4.074
4.069
3.986
3.963
3.940
3.926
3.903
3.612
3.606
3.575
3.569
2.418
2.389
2.246
Me
O
N
OMe
H
Me
Me
CF3
O
3na
1.00
2.00
2.01
1.02
1.01
1.22
3.02
1.18
1.09
3.01
3.01
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

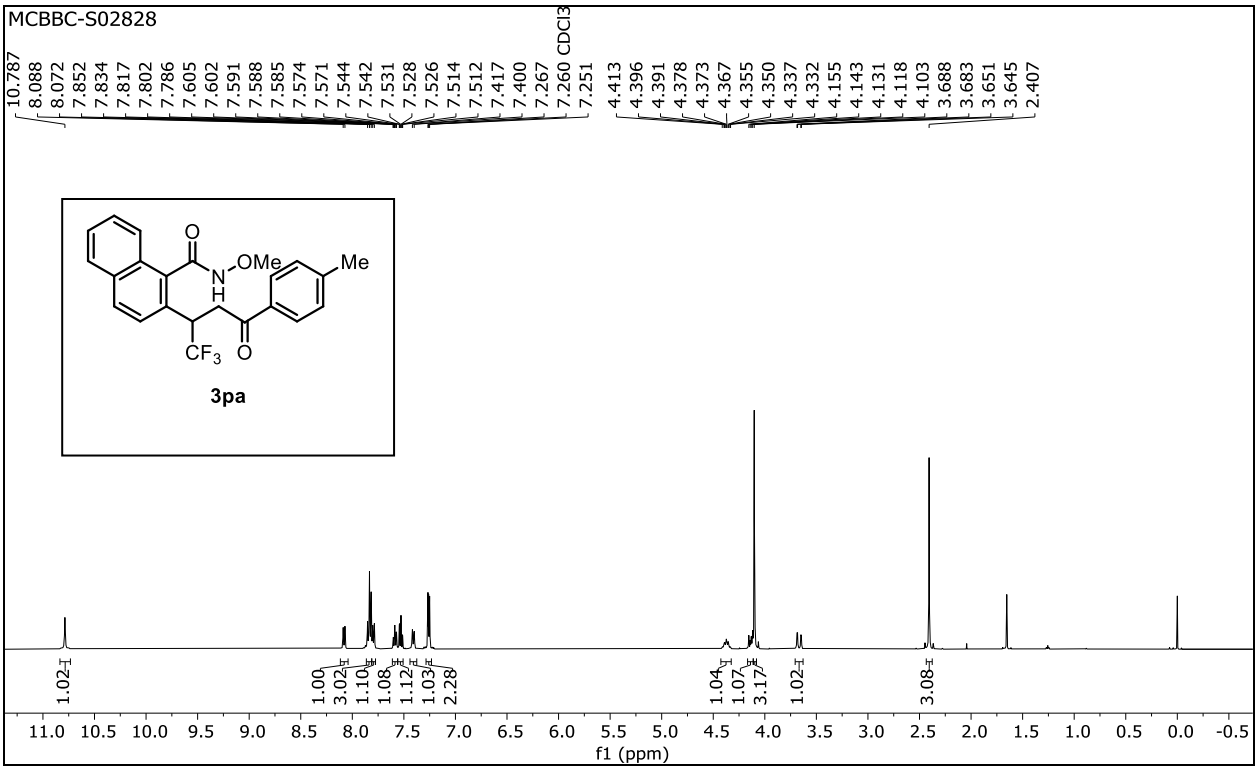

MCBBC-S04578
197.068
167.507
145.528
139.739
137.225
133.444
133.298
131.481
130.912
129.673
128.531
127.469
125.242
124.377
123.015
77.416 CDCl3
77.160 CDCl3
76.908 CDCl3
64.418
41.846
41.624
41.403
41.180
38.347
21.874
21.504
19.441
Me
O
N
OMe
H
Me
Me
CF3
O
3na
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

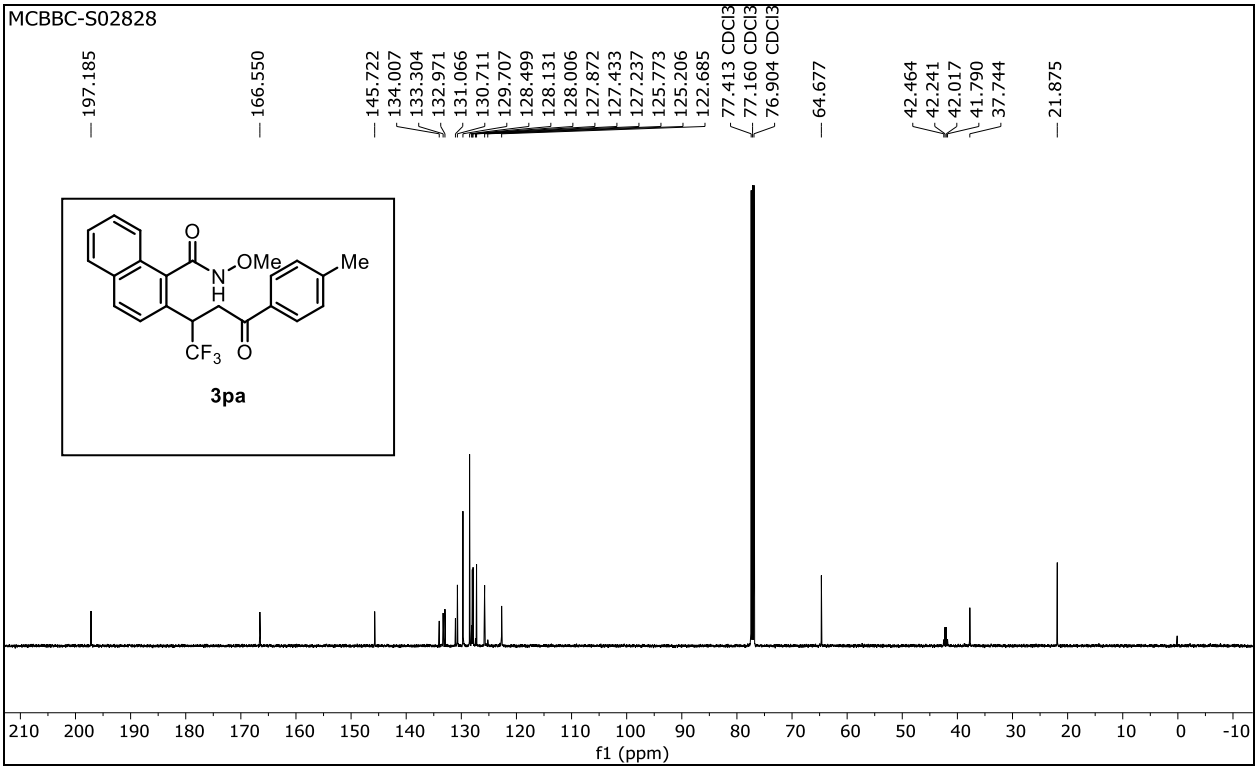

MCBBC-S04578
-69.415
Me
O
N
OMe
H
Me
Me
CF3
O
3na
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

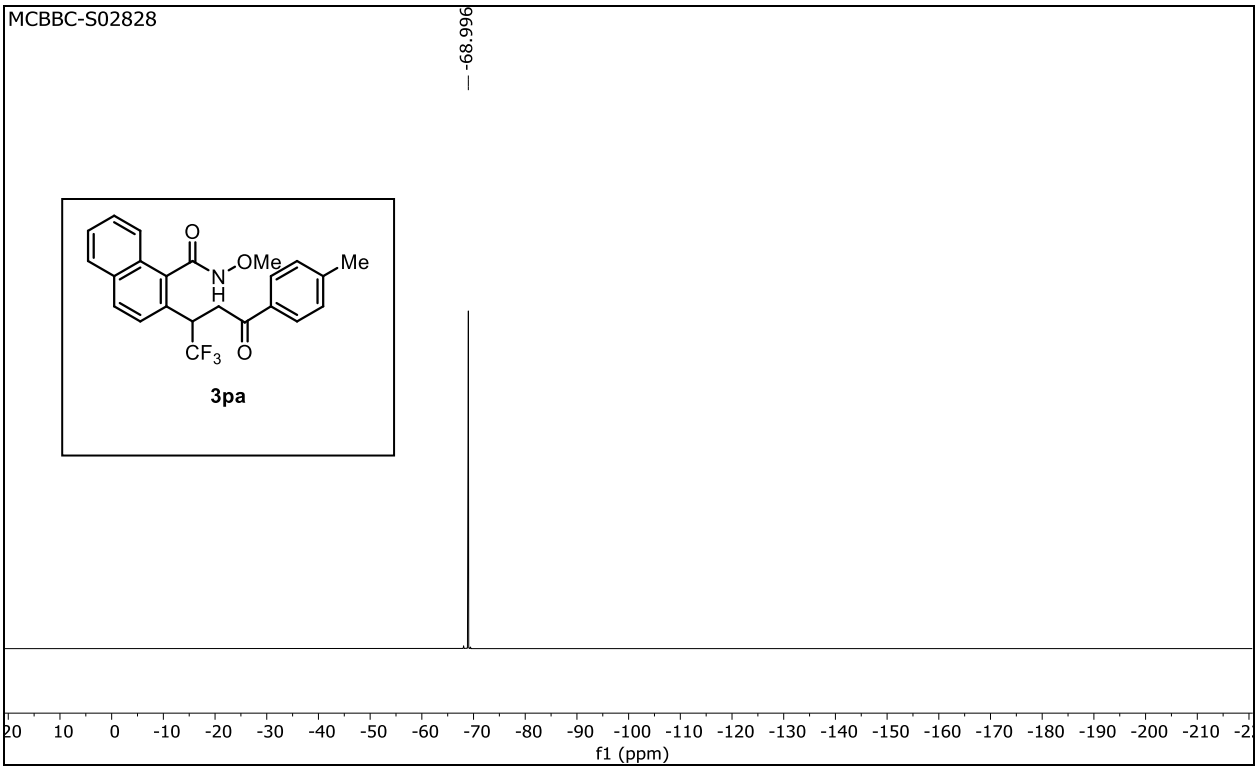

MCBBC-S02825
10.651
7.866
7.850
7.284
7.268
7.260 CDCl3
7.077
6.747
4.565
4.560
4.547
4.542
4.529
4.524
4.519
4.506
4.501
4.488
4.483
3.984
3.937
3.914
3.901
3.877
3.815
3.622
3.616
3.585
3.579
2.417
MeO
O
N
OMe
H
Me
MeO
CF3
O
3oa
1.00
2.00
2.03
1.01
1.00
1.05
3.01
1.01
3.17
3.00
3.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

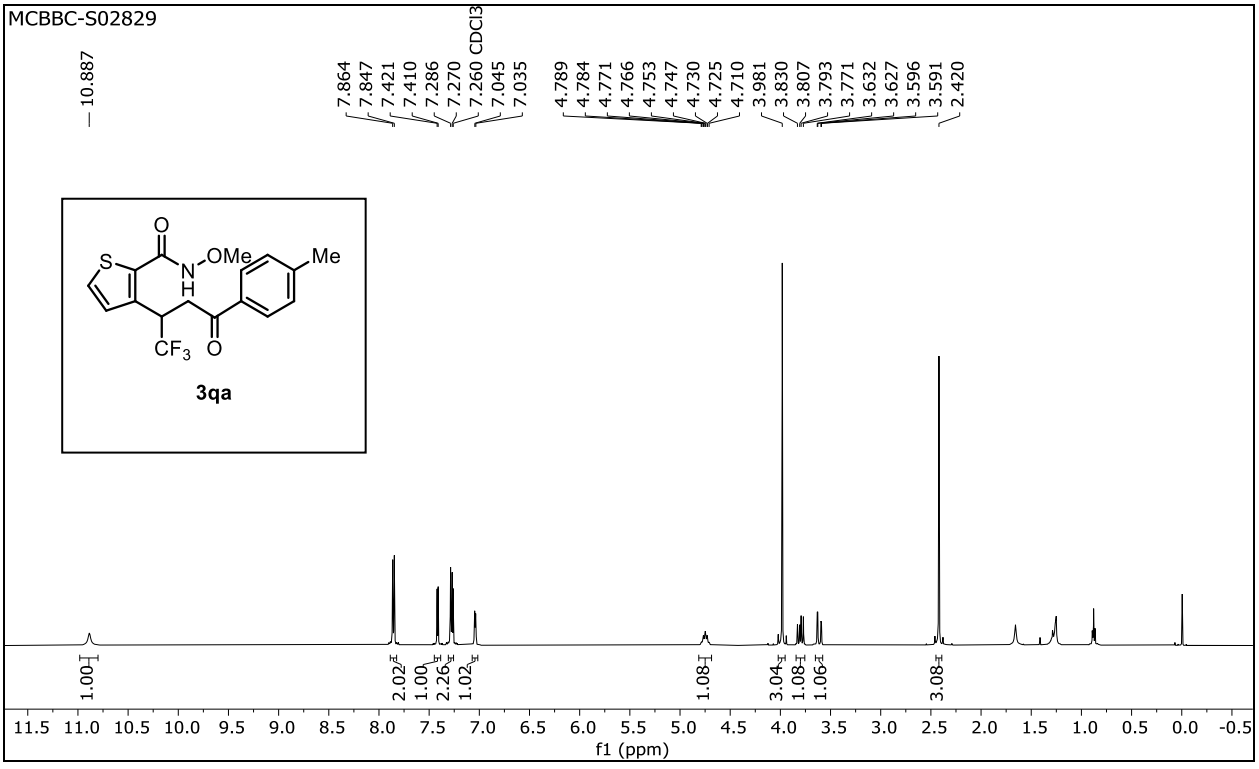

MCBBC-S02825
197.229
166.596
150.655
149.150
145.707
133.341
129.730
128.876
128.535
127.556
125.330
123.579
112.122
109.331
77.413 CDCl3
77.160 CDCl3
76.904 CDCl3
64.563
56.194
56.099
40.927
40.706
40.483
40.264
38.075
21.881
MeO
MeO
OMe
Me
N
H
O
CF3
3oa
f1 (ppm)

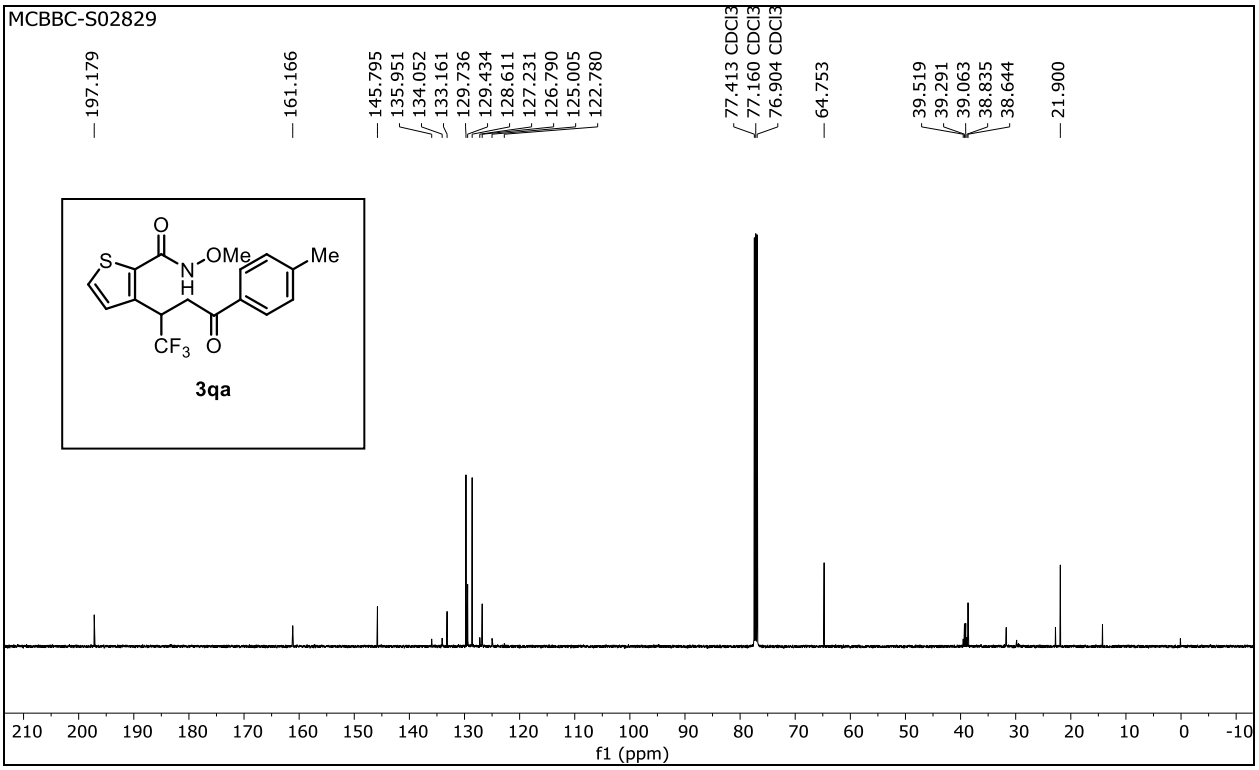

MCBBC-S02825
-69.421
MeO
MeO
OMe
Me
N
H
O
CF3
3oa
f1 (ppm)

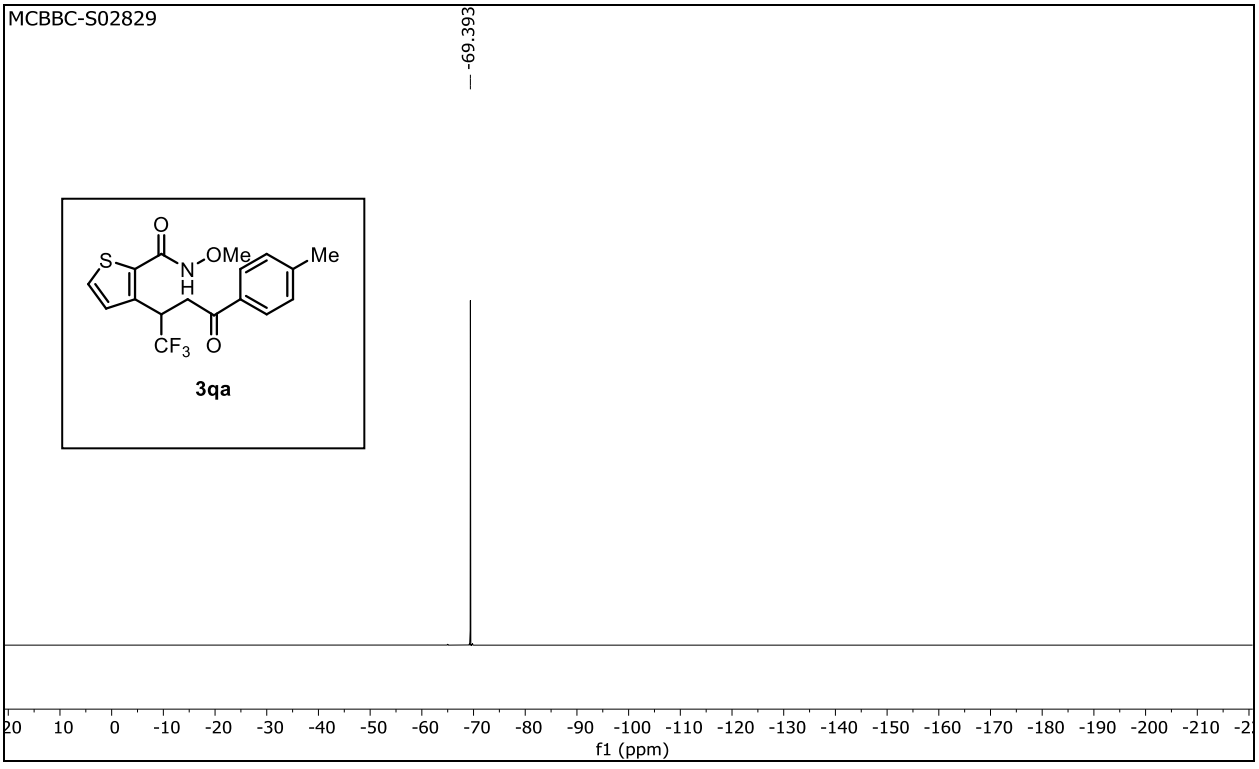

MCBBC-S02828
10.787
8.088
8.072
7.852
7.834
7.817
7.802
7.786
7.605
7.602
7.591
7.588
7.585
7.574
7.571
7.544
7.542
7.531
7.528
7.526
7.514
7.512
7.417
7.400
7.267
7.260 CDCl3
7.251
4.413
4.396
4.391
4.378
4.373
4.367
4.355
4.350
4.337
4.332
4.155
4.143
4.131
4.118
4.103
3.688
3.683
3.651
3.645
2.407
O
N
H
OMe
Me
CF3
O
3pa
1.02
1.00
3.02
1.10
1.08
1.12
1.03
2.28
1.04
1.07
3.17
1.02
3.08
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

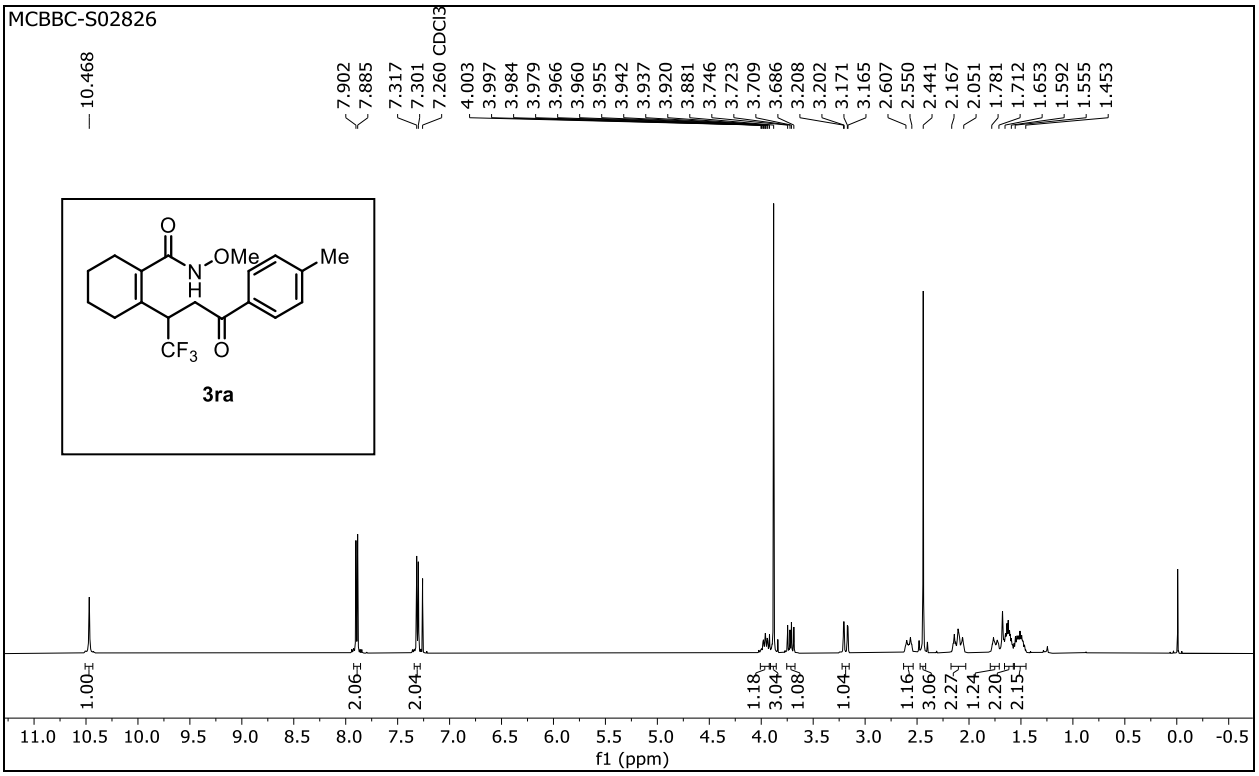

MCBBC-S02828
197.185
166.550
145.722
134.007
133.304
132.971
131.066
130.711
129.707
128.499
128.131
128.006
127.872
127.433
127.237
125.773
125.206
122.685
77.413 CDCl3
77.160 CDCl3
76.904 CDCl3
64.677
42.464
42.241
42.017
41.790
37.744
21.875
O
N
H
OMe
Me
CF3
O
3pa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

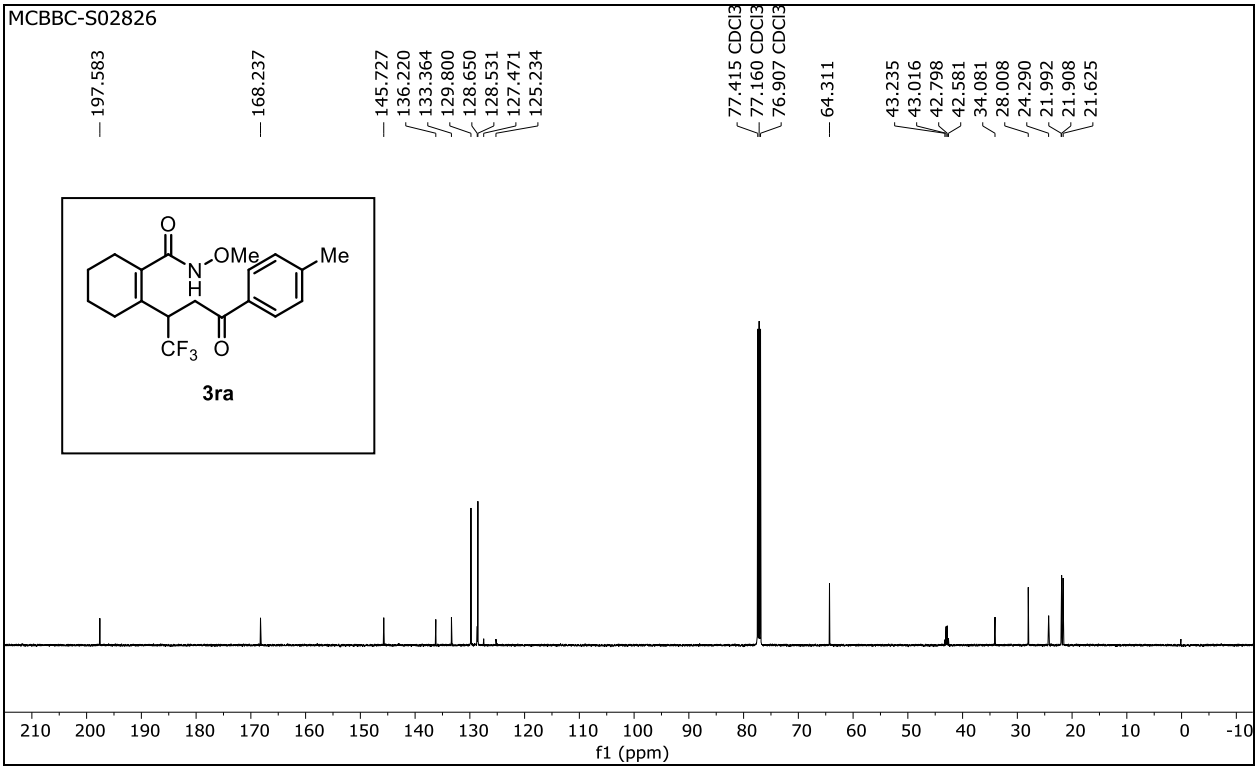

MCBBC-S02828
-68.996
O
N
H
OMe
Me
CF3
O
3pa
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

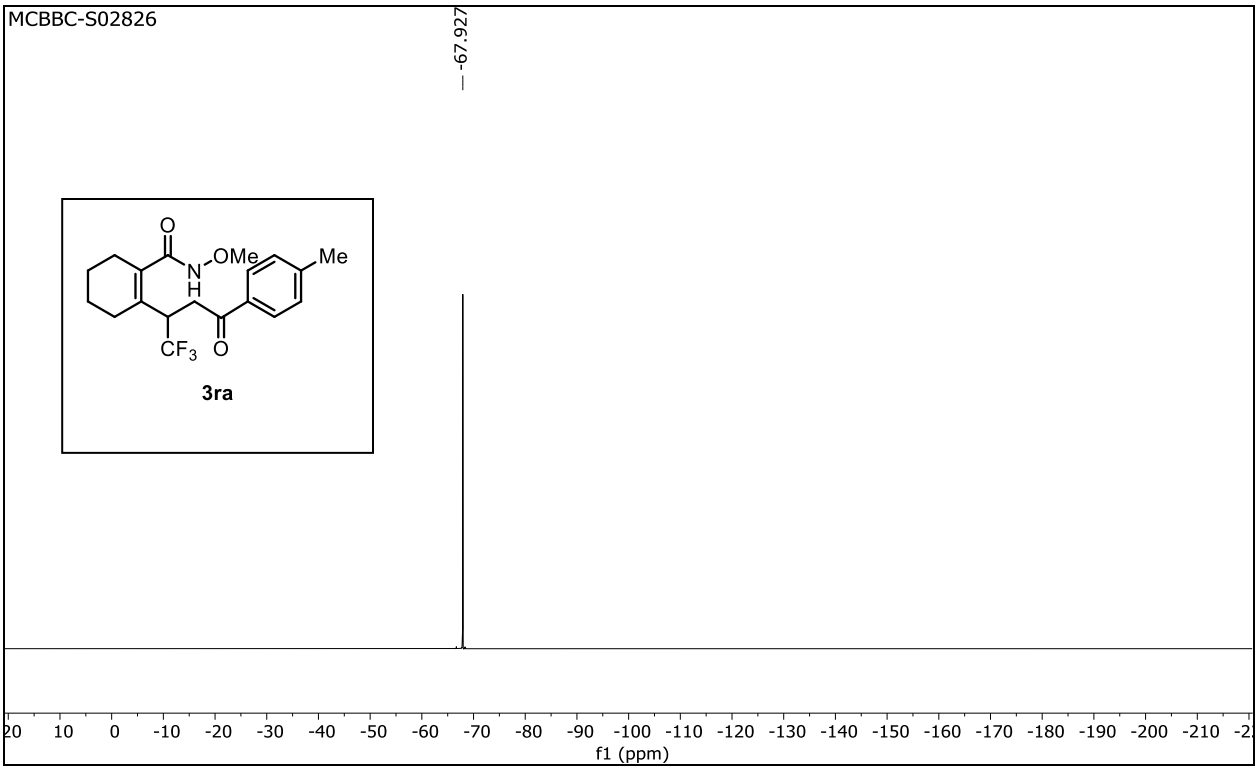

MCBBC-S02829
10.887
7.864
7.847
7.421
7.410
7.286
7.270
7.260 CDCl3
7.045
7.035
4.789
4.784
4.771
4.766
4.753
4.747
4.730
4.725
4.710
3.981
3.830
3.807
3.793
3.771
3.632
3.627
3.596
3.591
2.420
S
O
N
H
OMe
Me
CF3
O
3qa
1.00
2.02
1.00
2.26
1.02
1.08
3.04
1.08
1.06
3.08
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

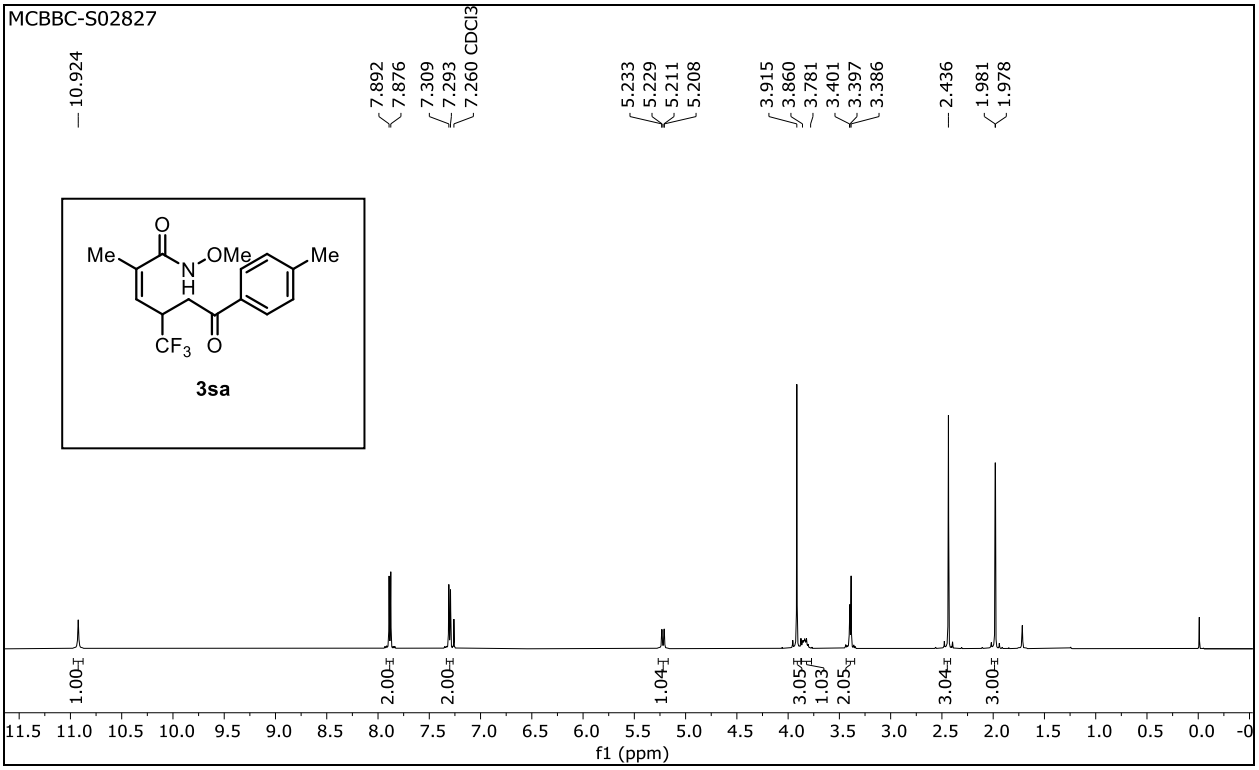

MCBBC-S02829
197.179
161.166
145.795
135.951
134.052
133.161
129.736
129.434
128.611
127.231
126.790
125.005
122.780
77.413 CDCl3
77.160 CDCl3
76.904 CDCl3
64.753
39.519
39.291
39.063
38.835
38.644
21.900
O
S
N
H
OMe
Me
CF3
O
3qa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

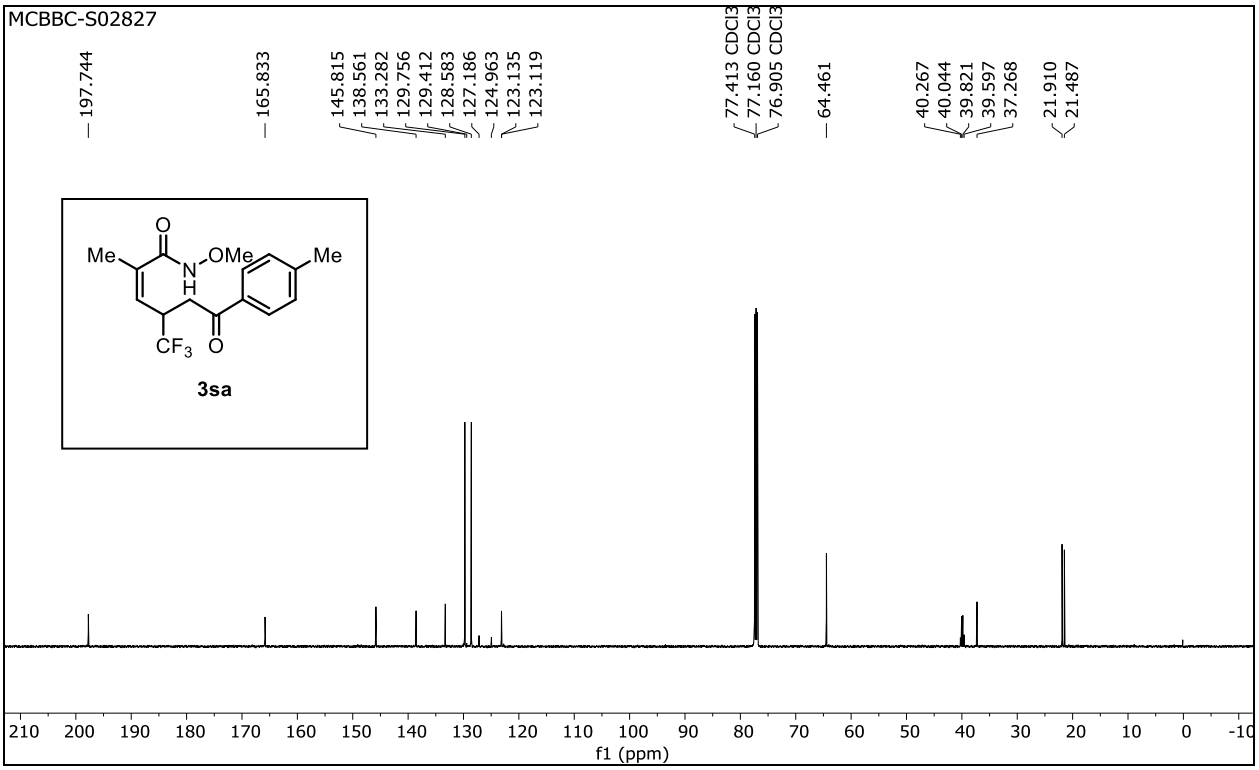

MCBBC-S02829
-69.393
O
S
N
H
OMe
Me
CF3
O
3qa
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

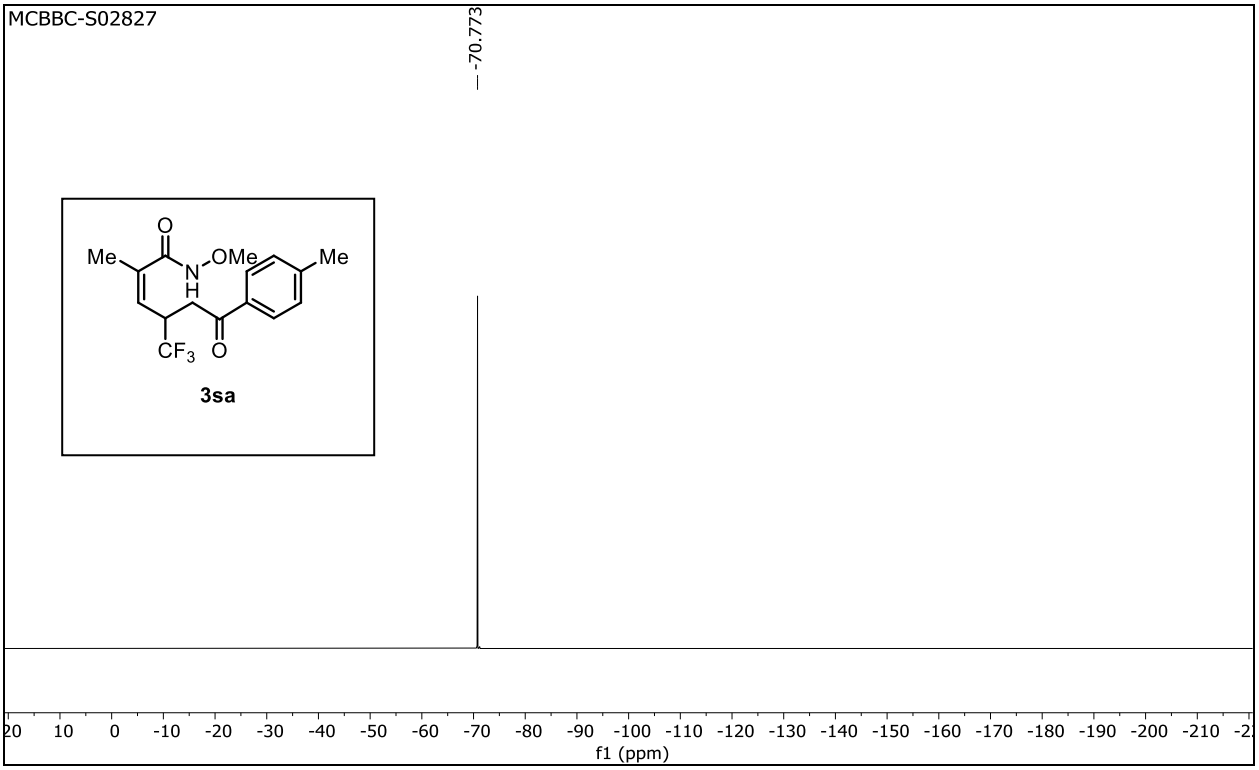

MCBBC-S02826
10.468
7.902
7.885
7.317
7.301
7.260 CDCl3
4.003
3.997
3.984
3.979
3.966
3.960
3.955
3.942
3.937
3.920
3.881
3.746
3.723
3.709
3.686
3.208
3.202
3.171
3.165
2.607
2.550
2.441
2.167
2.051
1.781
1.712
1.653
1.592
1.555
1.453
1.00
2.06
2.04
1.18
3.04
1.08
1.04
1.16
3.06
2.27
1.24
2.20
2.15
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)
O
N
H
OMe
Me
CF3
O
3ra

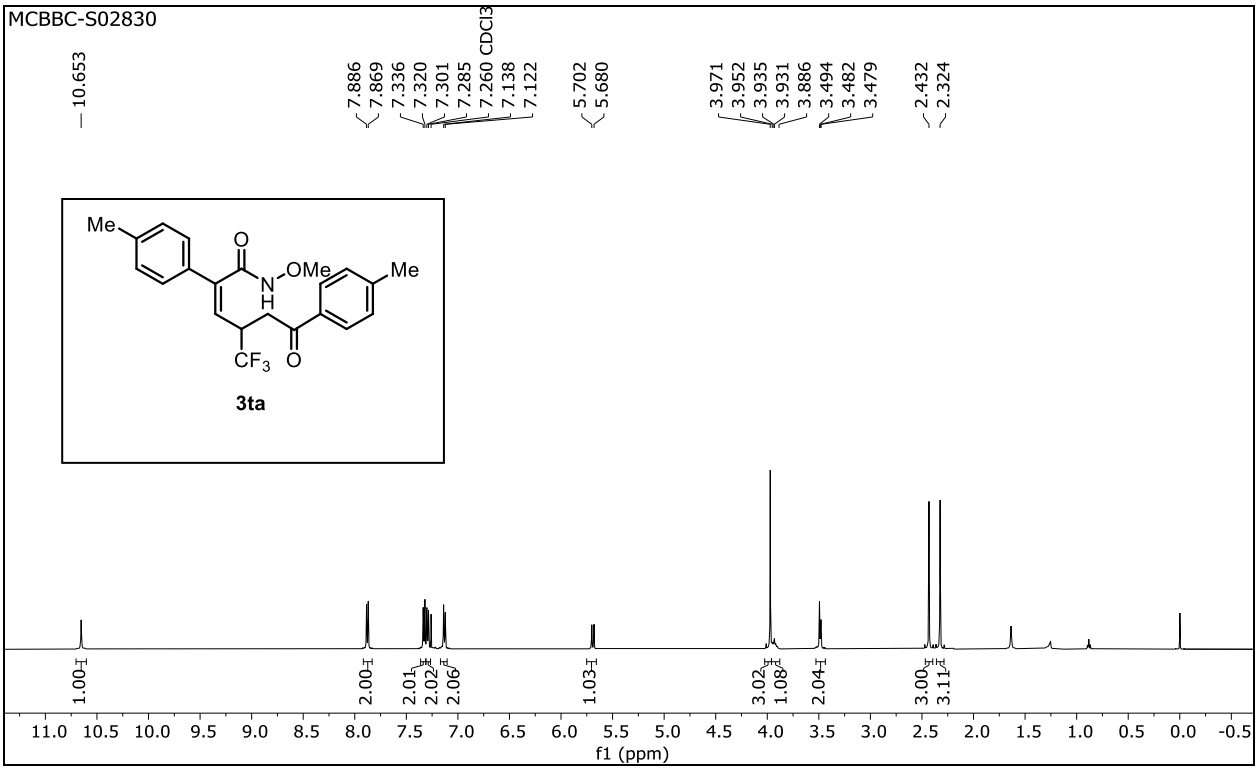

MCBBC-S02826
197.583
168.237
145.727
136.220
133.364
129.800
128.650
128.531
127.471
125.234
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
64.311
43.235
43.016
42.798
42.581
34.081
28.008
24.290
21.992
21.908
21.625
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
O
N
H
OMe
Me
CF3
O
3ra

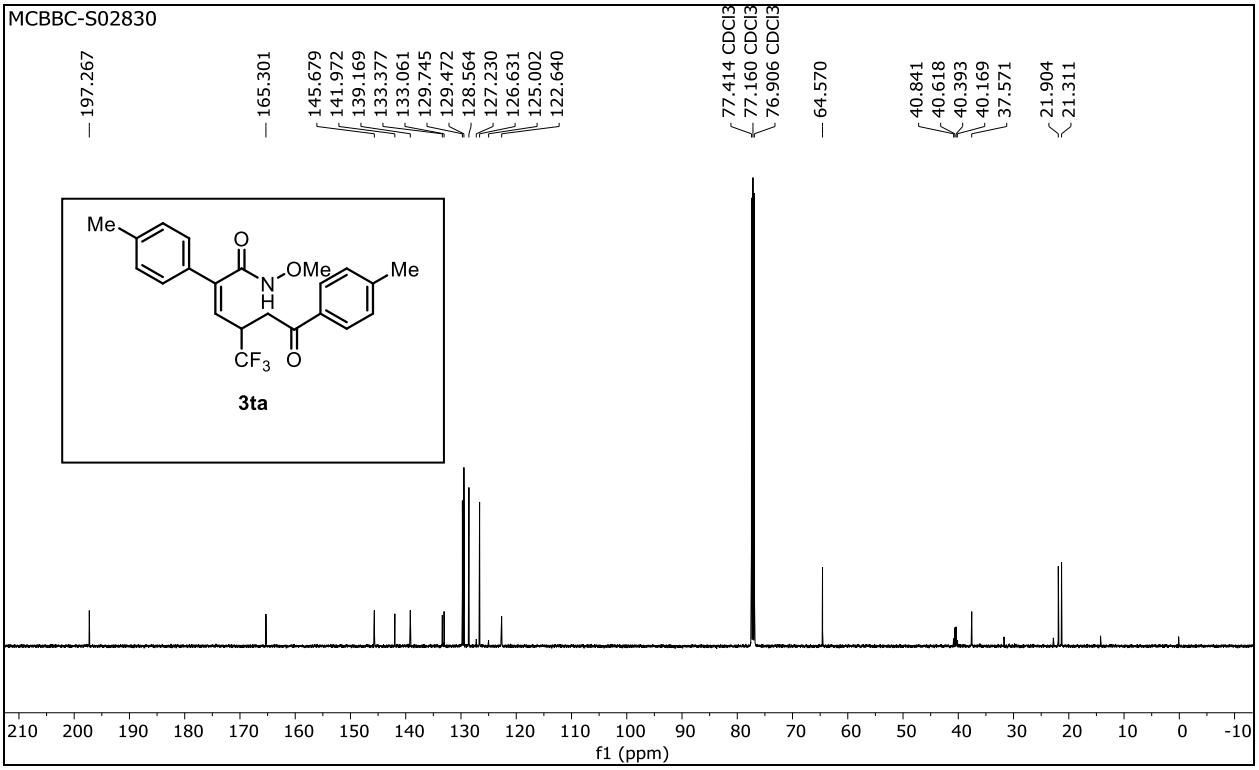

MCBBC-S02826
-67.927
3ra
f1 (ppm)

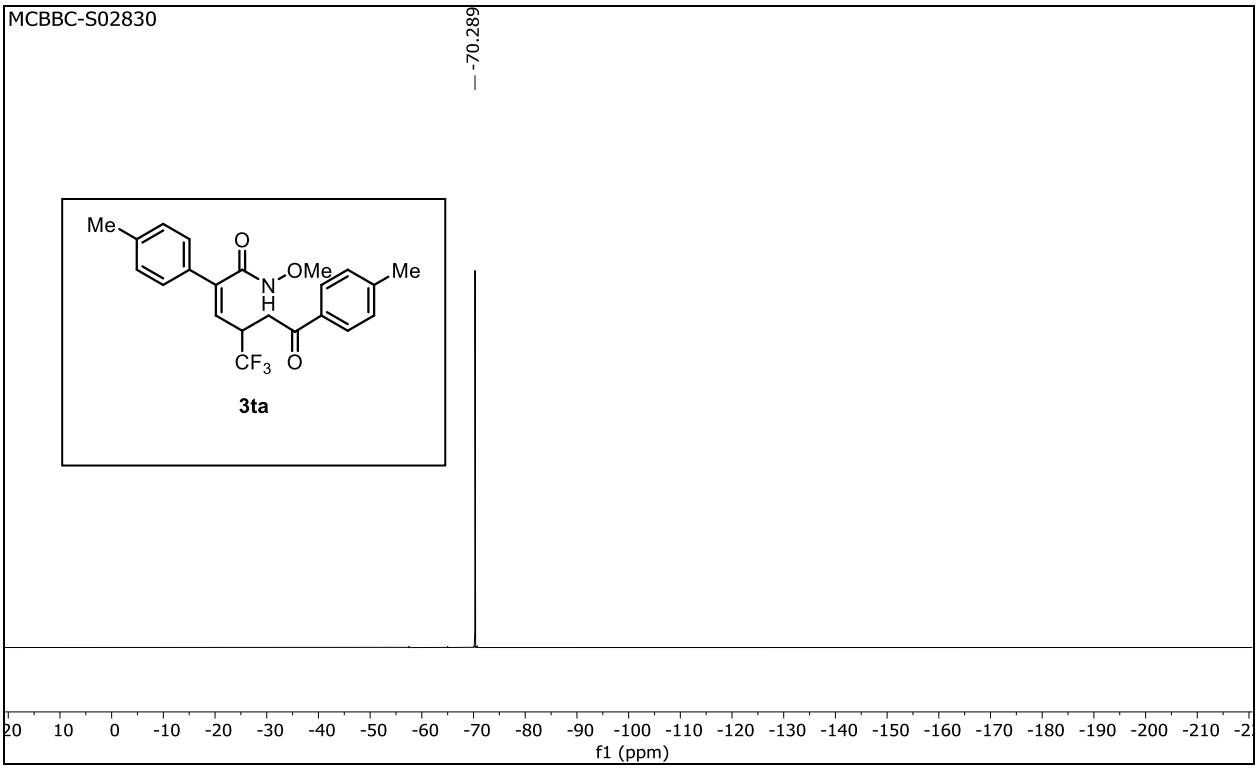

MCBBC-S02827
10.924
7.892
7.876
7.309
7.293
7.260 CDCl3
5.233
5.229
5.211
5.208
3.915
3.860
3.781
3.401
3.397
3.386
2.436
1.981
1.978
3sa
1.00
2.00
2.00
1.04
3.05
1.03
2.05
3.04
3.00
f1 (ppm)

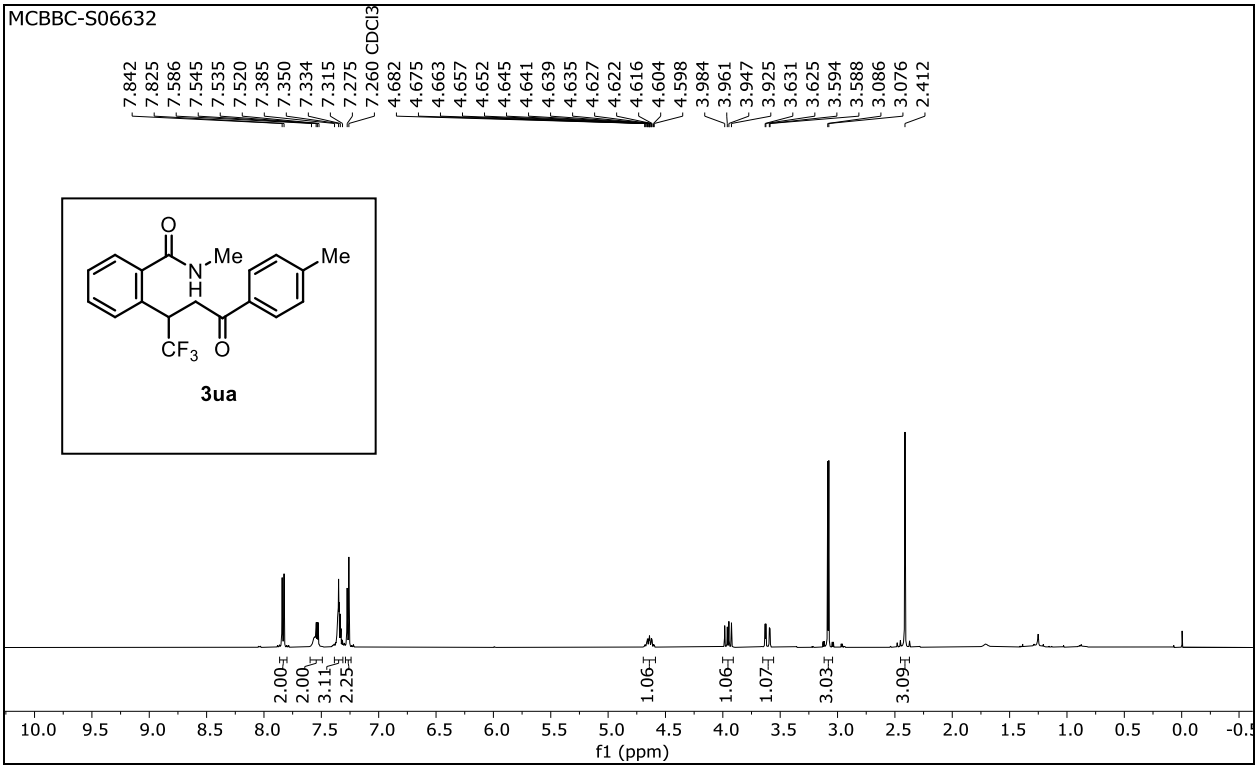

MCBBC-S02827
197.744
165.833
145.815
138.561
133.282
129.756
129.412
128.583
127.186
124.963
123.135
123.119
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
64.461
40.267
40.044
39.821
39.597
37.268
21.910
21.487
Me
N
H
OMe
Me
O
CF3
O
3sa
f1 (ppm)

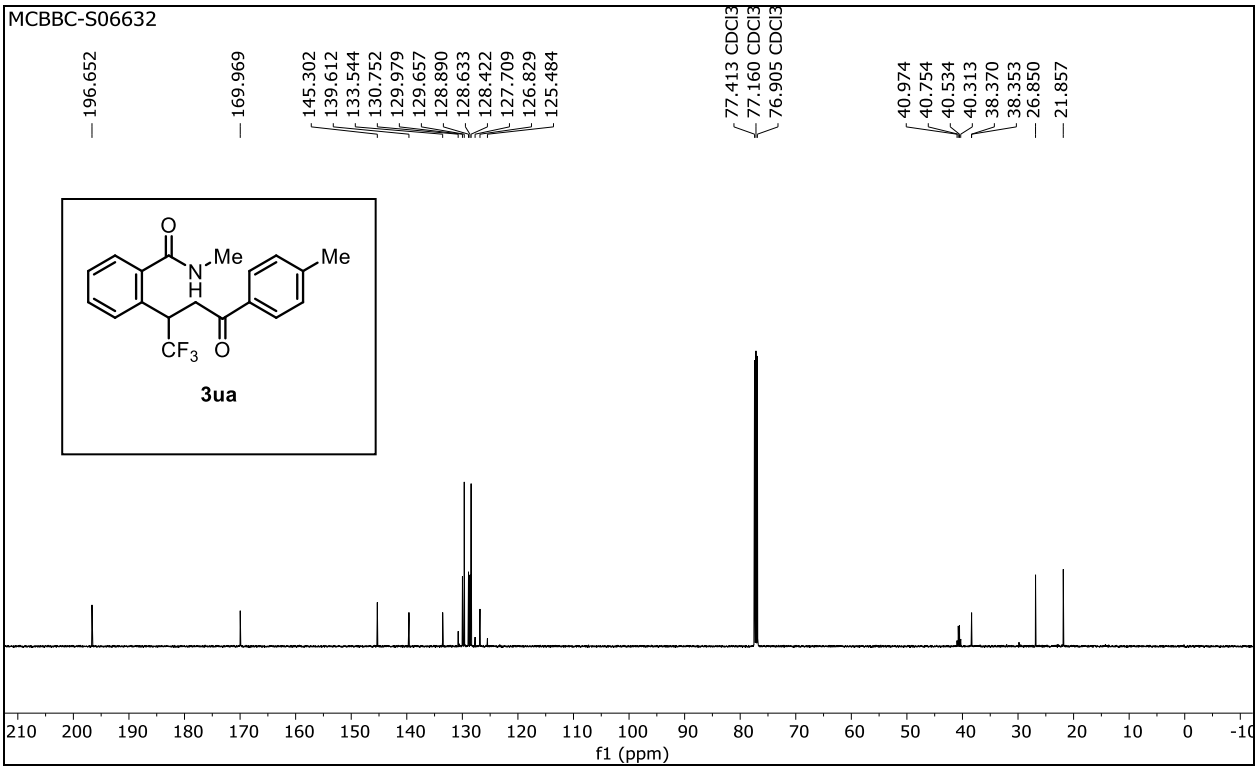

MCBBC-S02827
-70.773
Me
N
H
OMe
Me
O
CF3
O
3sa
f1 (ppm)

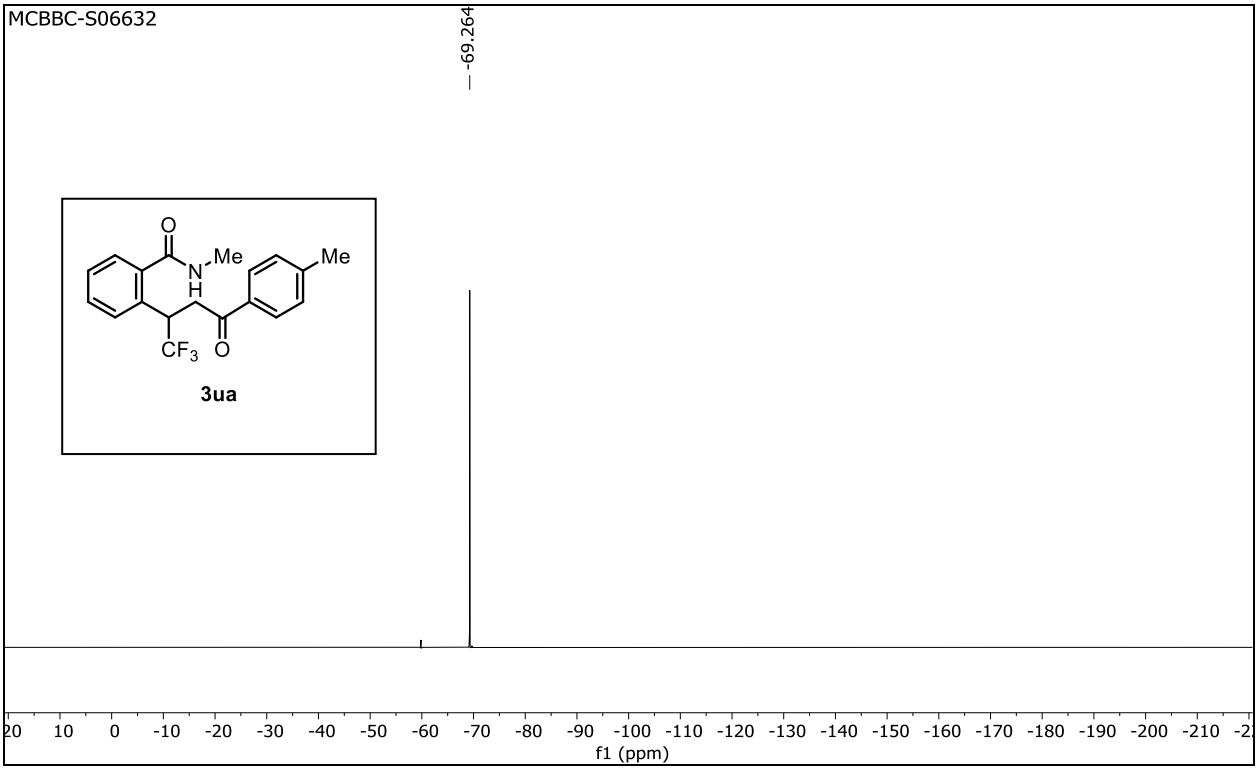

MCBBC-S02830
10.653
7.886
7.869
7.336
7.320
7.301
7.285
7.260 CDCl3
7.138
7.122
5.702
5.680
3.971
3.952
3.935
3.931
3.886
3.494
3.482
3.479
2.432
2.324
Me
O
N
OMe
H
Me
CF3
O
3ta
1.00
2.00
2.01
2.02
2.06
1.03
3.02
1.08
2.04
3.00
3.11
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

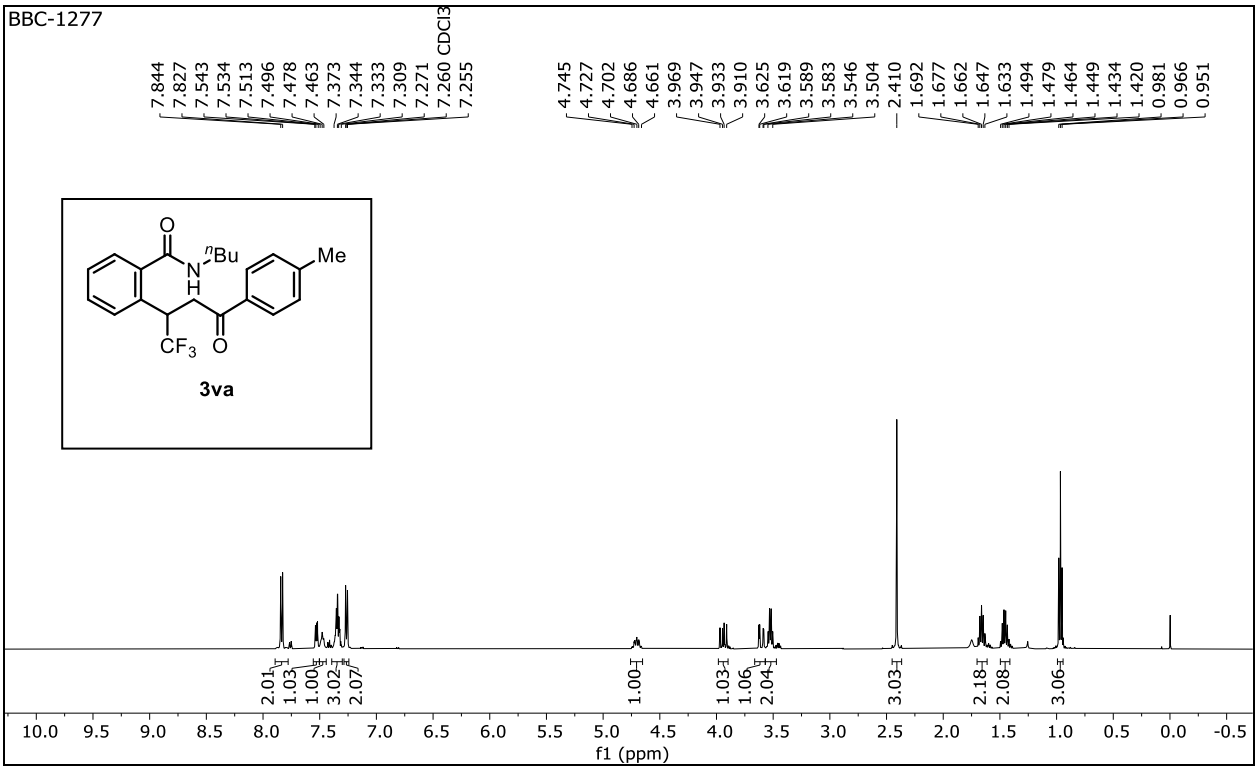

MCBBC-S02830
197.267
165.301
145.679
141.972
139.169
133.377
133.061
129.745
129.472
128.564
127.230
126.631
125.002
122.640
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
64.570
40.841
40.618
40.393
40.169
37.571
21.904
21.311
Me
O
N
OMe
H
Me
CF3
O
3ta
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

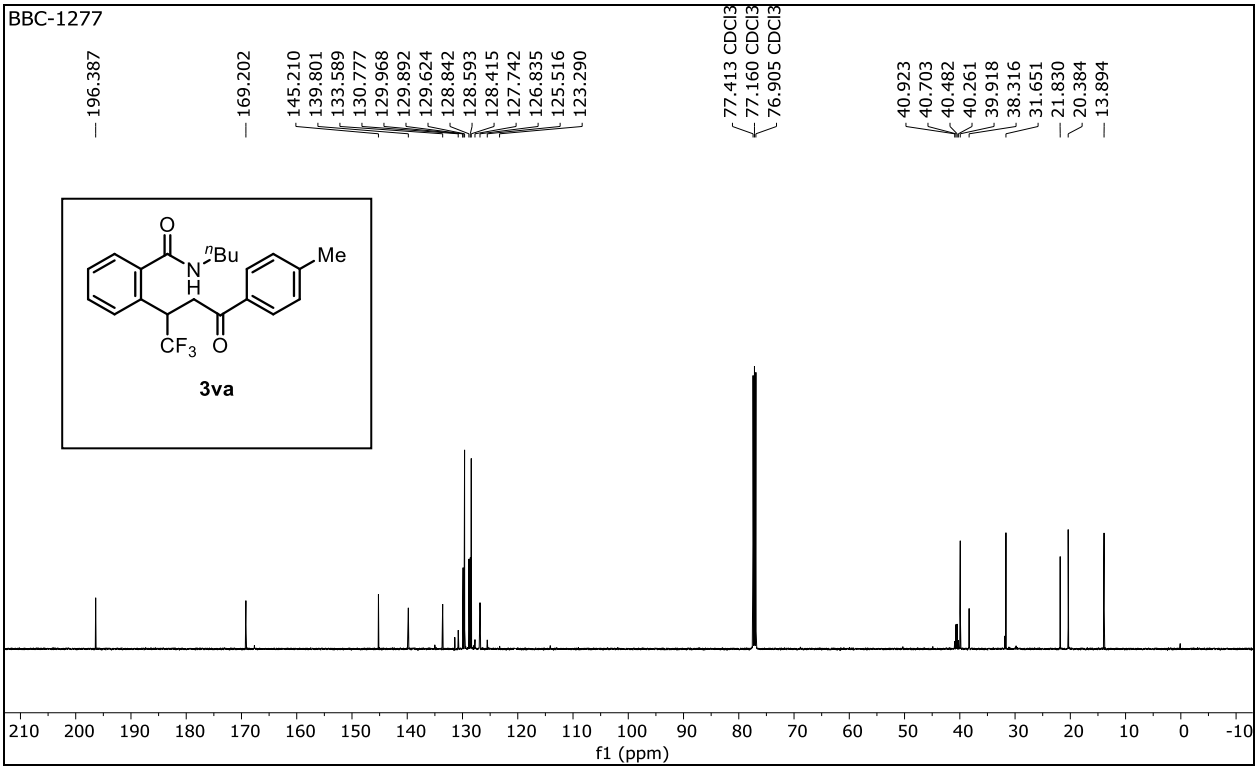

MCBBC-S02830
-70.289
Me
O
N
OMe
Me
H
CF3
O
3ta
f1 (ppm)

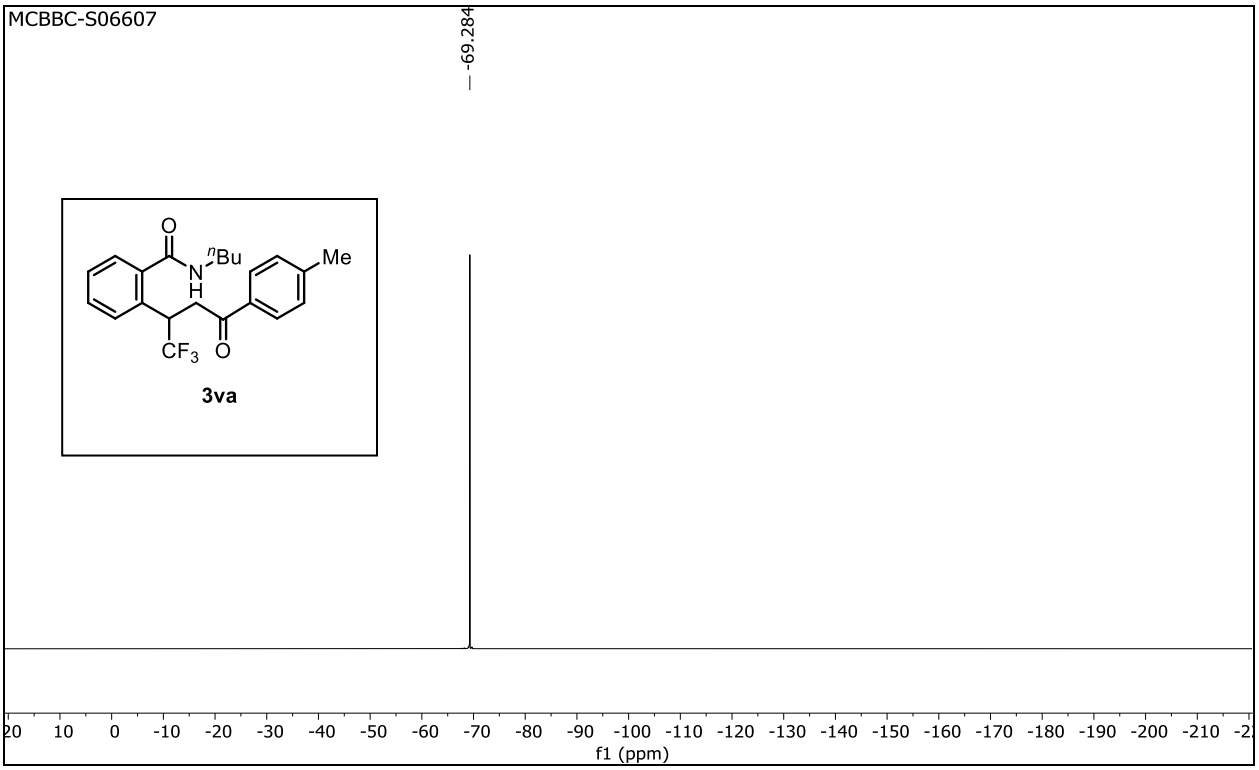

MCBBC-S06632
7.842
7.825
7.586
7.545
7.535
7.520
7.385
7.350
7.334
7.315
7.275
7.260 CDCl3
4.682
4.675
4.663
4.657
4.652
4.645
4.641
4.639
4.635
4.627
4.622
4.616
4.604
4.598
3.984
3.961
3.947
3.925
3.631
3.625
3.594
3.588
3.086
3.076
2.412
O
N
Me
Me
H
CF3
O
3ua
2.00
2.00
3.11
2.25
1.06
1.06
1.07
3.03
3.09
f1 (ppm)

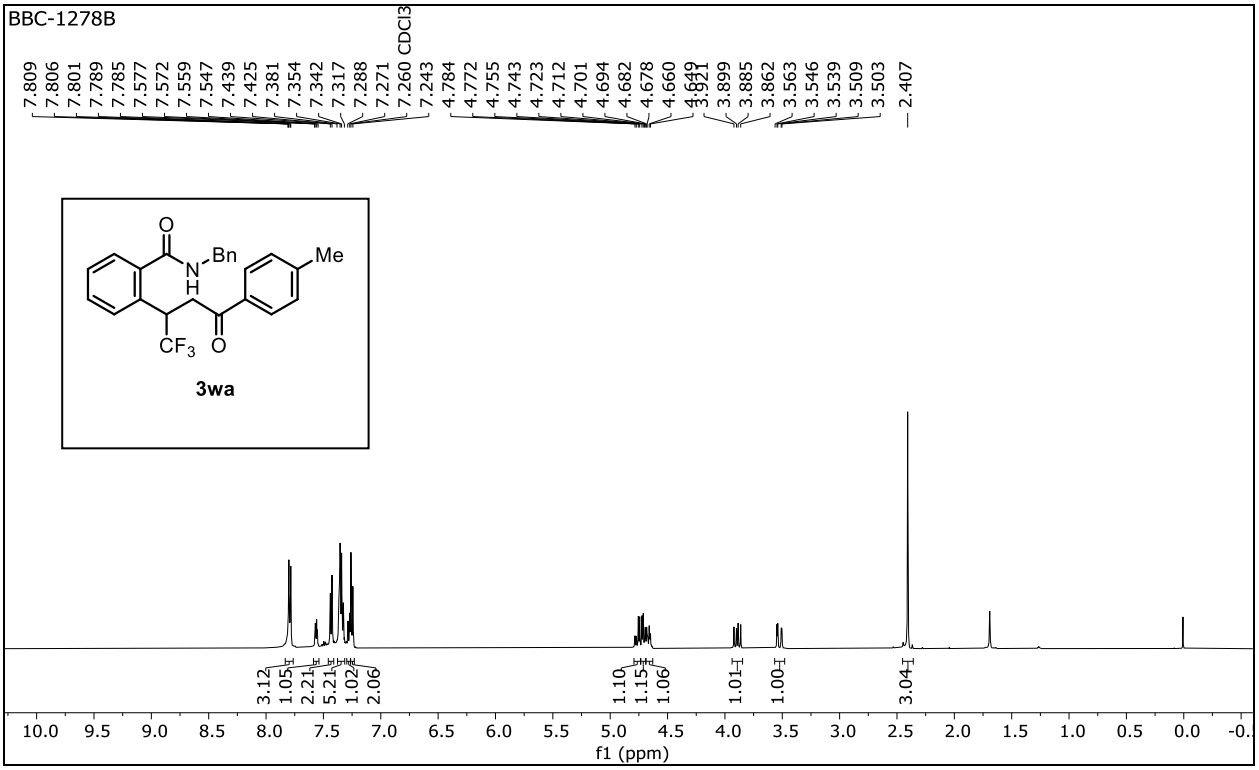

MCBBC-S06632
196.652
169.969
145.302
139.612
133.544
130.752
129.979
129.657
128.890
128.633
128.422
127.709
126.829
125.484
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
40.974
40.754
40.534
40.313
38.370
38.353
26.850
21.857
Me
Me
CF3
3ua
f1 (ppm)

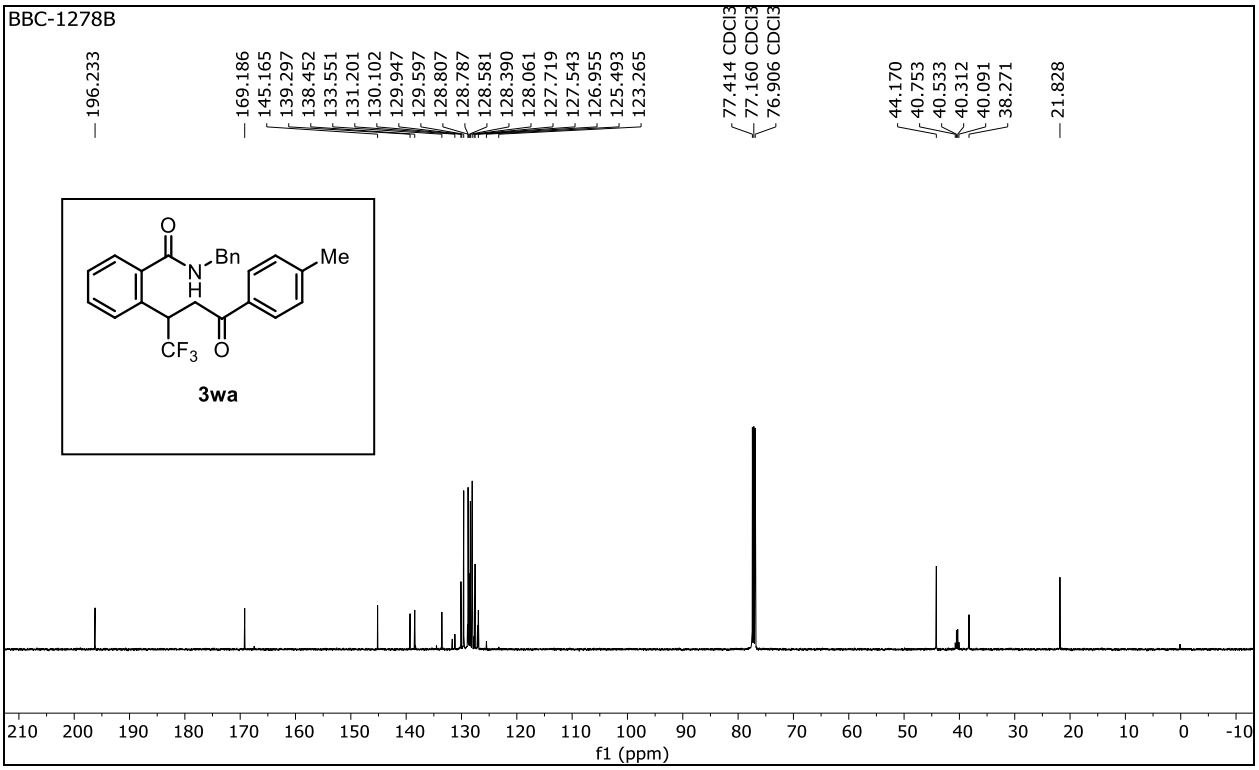

MCBBC-S06632
-69.264
Me
Me
CF3
3ua
f1 (ppm)

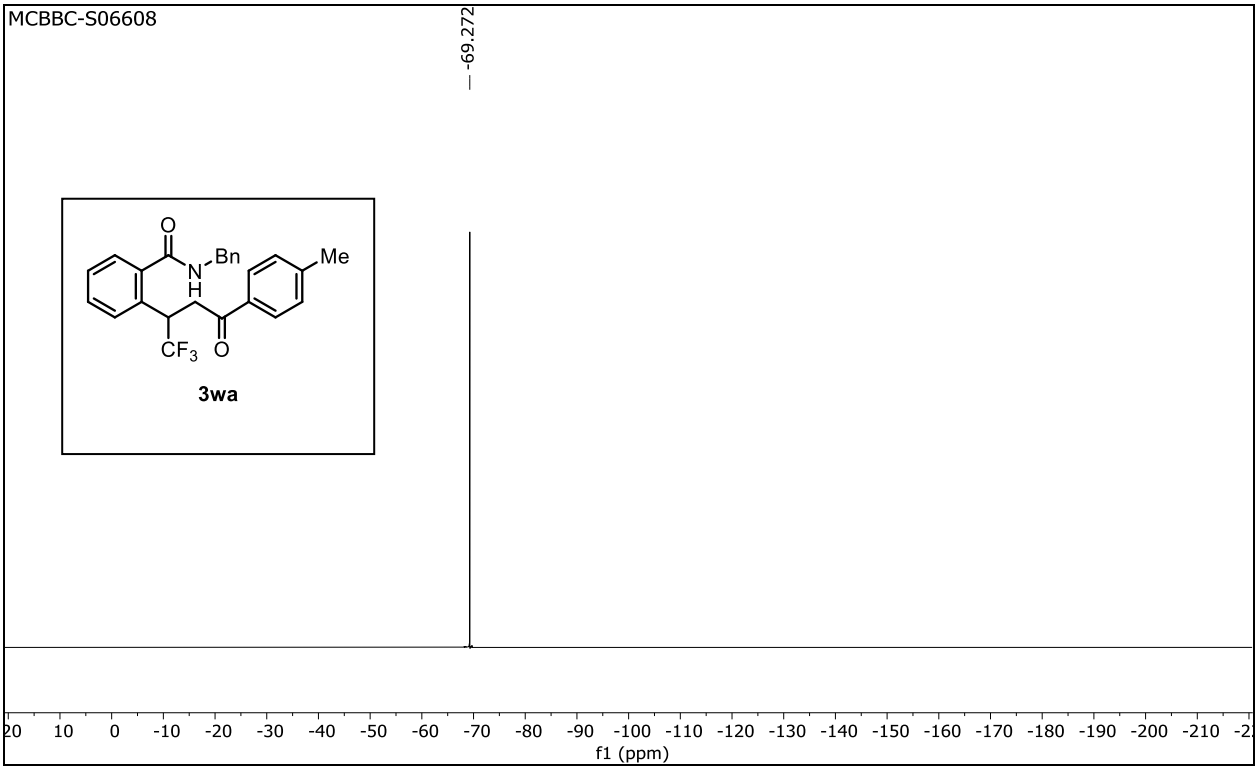

BBC-1277
7.844
7.827
7.543
7.534
7.513
7.496
7.478
7.463
7.373
7.344
7.333
7.309
7.271
7.260 CDCl3
7.255
4.745
4.727
4.702
4.686
4.661
3.969
3.947
3.933
3.910
3.625
3.619
3.589
3.583
3.546
3.504
2.410
1.692
1.677
1.662
1.647
1.633
1.494
1.479
1.464
1.449
1.434
1.420
0.981
0.966
0.951
O
nBu
N
H
Me
CF3
O
3va
2.01
1.03
1.00
3.02
2.07
1.00
1.03
1.06
2.04
3.03
2.18
2.08
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

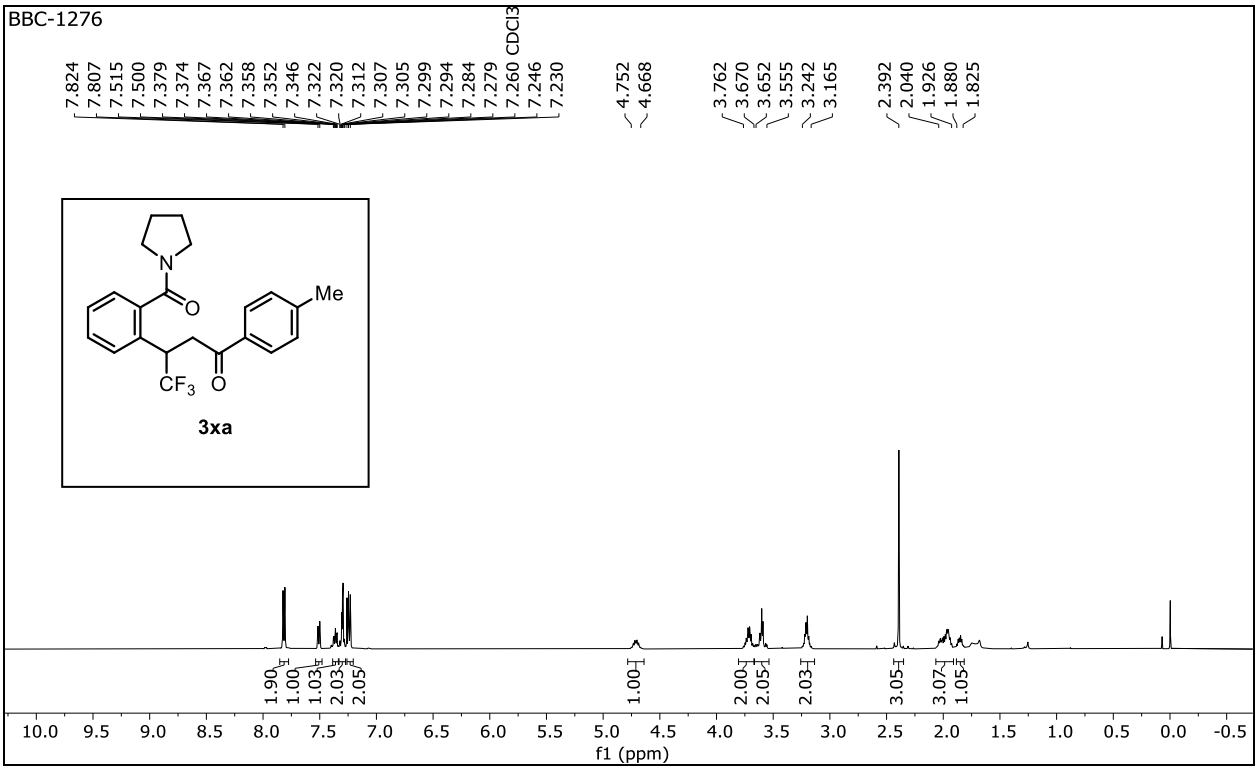

BBC-1277
196.387
169.202
145.210
139.801
133.589
130.777
129.968
129.892
129.624
128.842
128.593
128.415
127.742
126.835
125.516
123.290
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
40.923
40.703
40.482
40.261
39.918
38.316
31.651
21.830
20.384
13.894
O
nBu
N
H
Me
CF3
O
3va
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

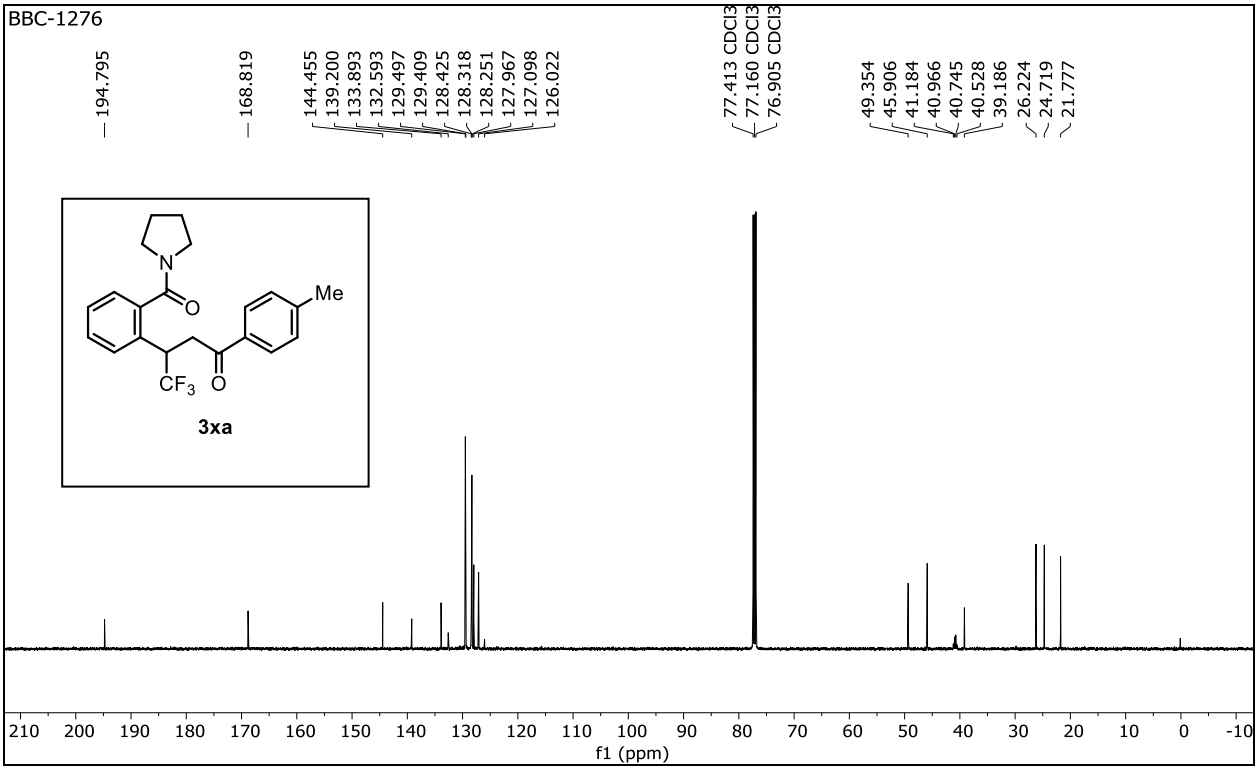

MCBBC-S06607
-69.284
3va
f1 (ppm)

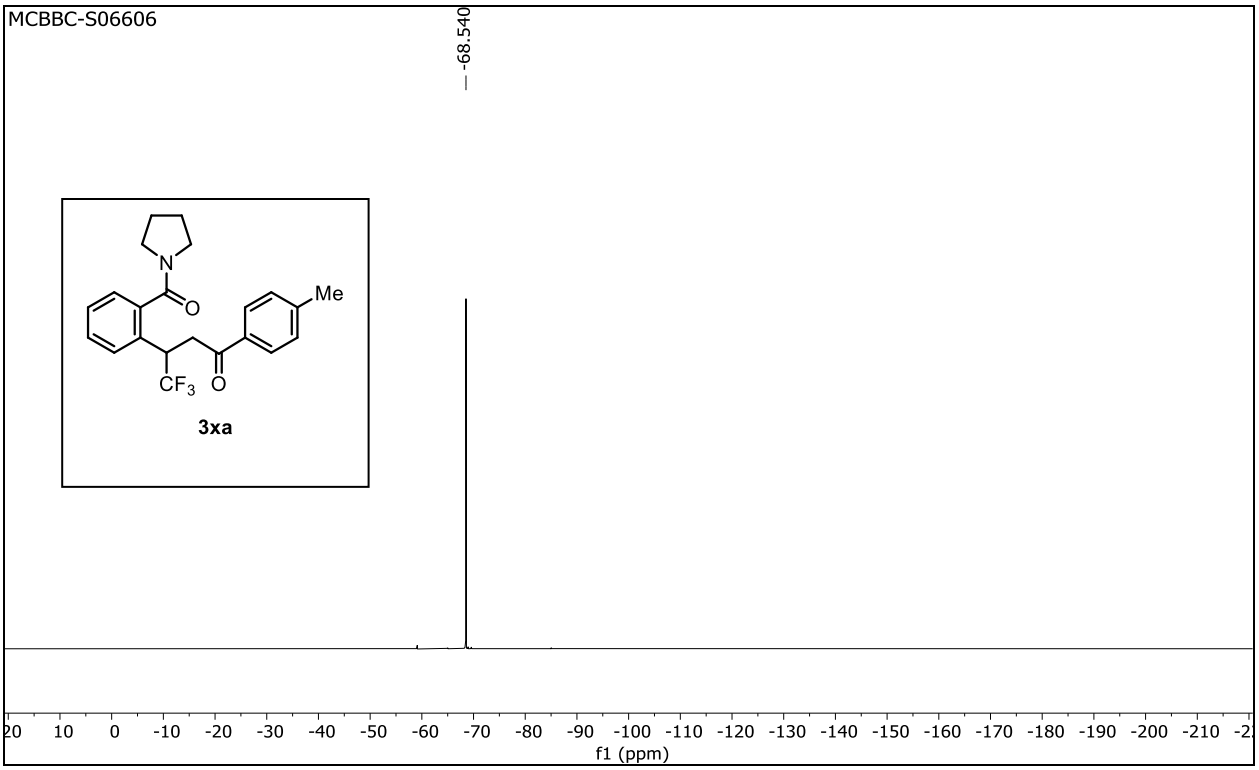

BBC-1278B
CDCl3
3wa
f1 (ppm)

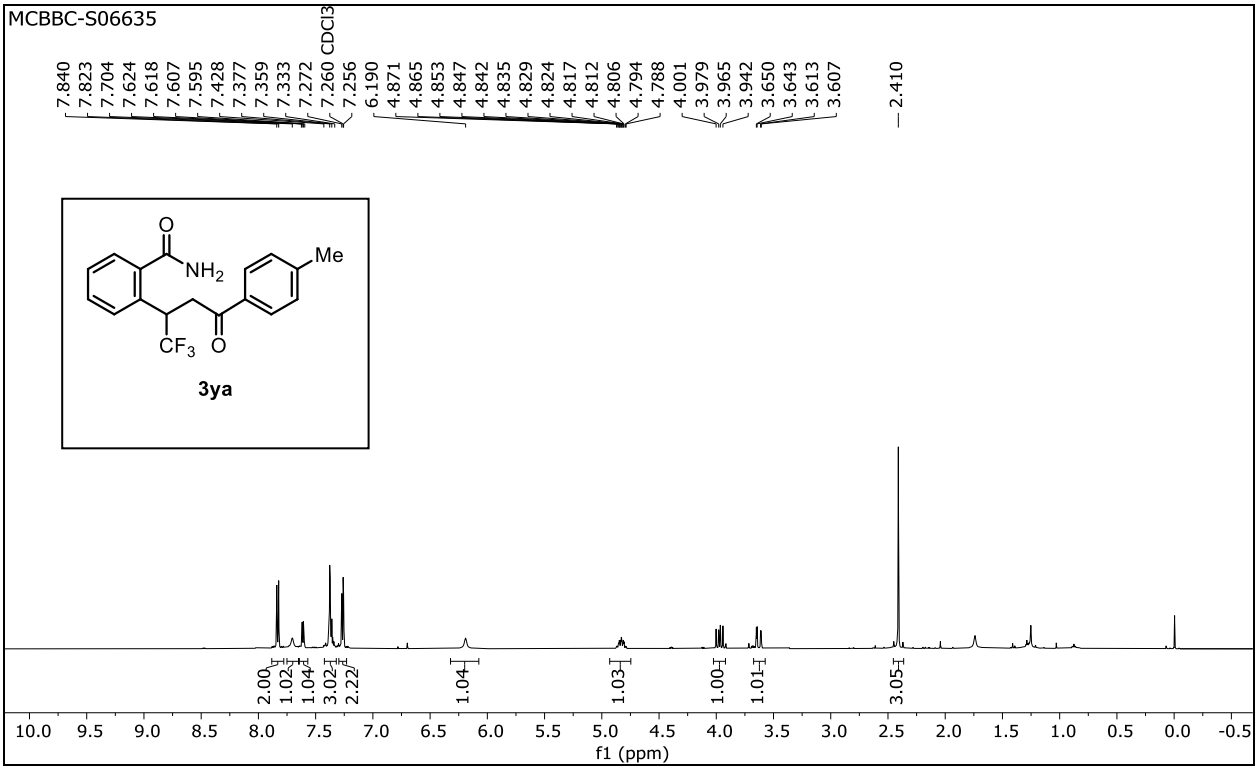

BBC-1278B
196.233
169.186
145.165
139.297
138.452
133.551
131.201
130.102
129.947
129.597
128.807
128.787
128.581
128.390
128.061
127.719
127.543
126.955
125.493
123.265
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
44.170
40.753
40.533
40.312
40.091
38.271
21.828
O
N
H
Bn
Me
CF3
O
3wa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

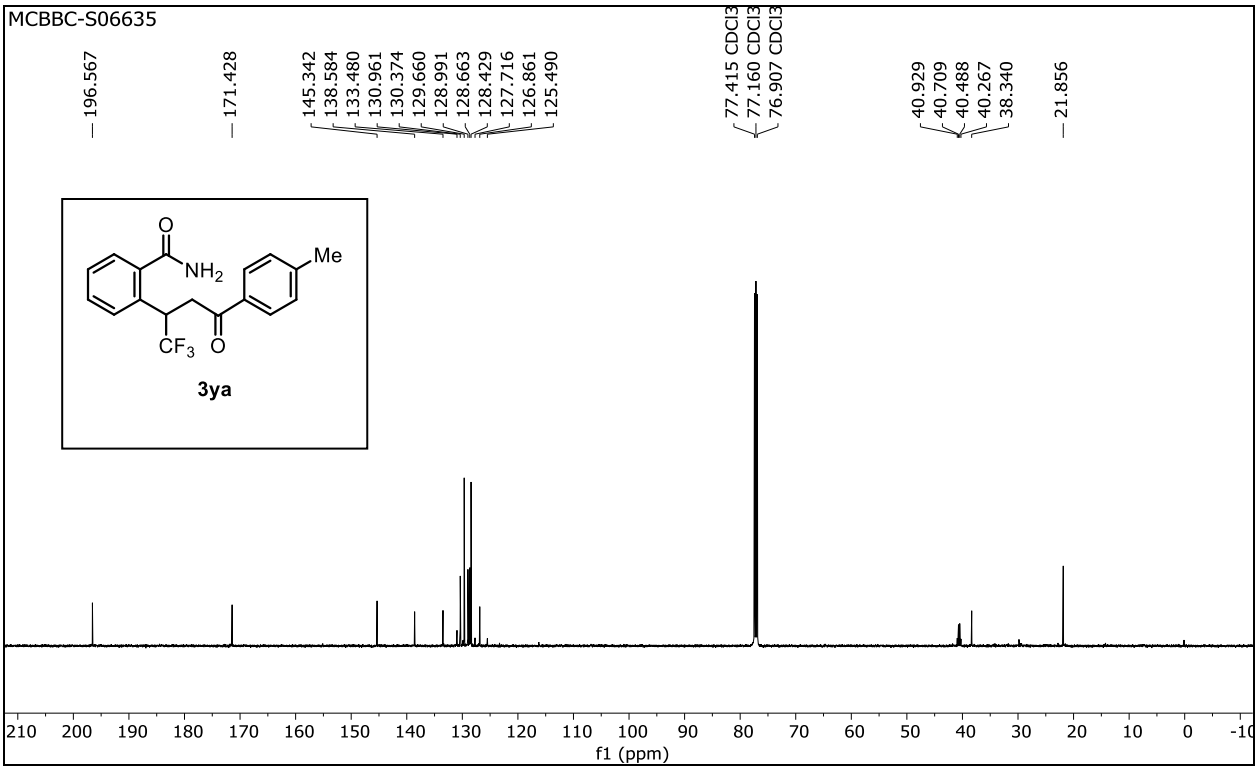

MCBBC-S06608
-69.272
O
N
H
Bn
Me
CF3
O
3wa
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

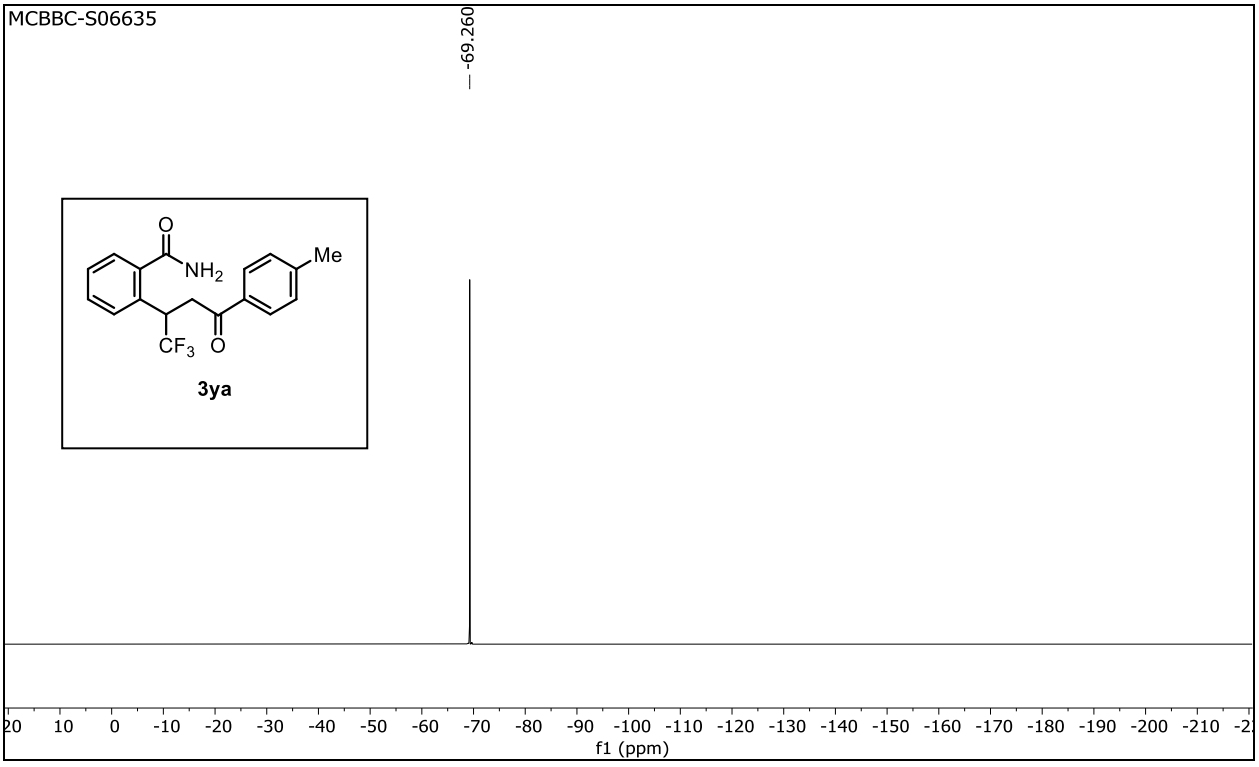

BBC-1276
7.824
7.807
7.515
7.500
7.379
7.374
7.367
7.362
7.358
7.352
7.346
7.322
7.320
7.312
7.307
7.305
7.299
7.294
7.284
7.279
7.260 CDCl3
7.246
7.230
4.752
4.668
3.762
3.670
3.652
3.555
3.242
3.165
2.392
2.040
1.926
1.880
1.825
Me
CF3
O
3xa
1.90
1.00
1.03
2.03
2.05
1.00
2.00
2.05
2.03
3.05
3.07
1.05
f1 (ppm)

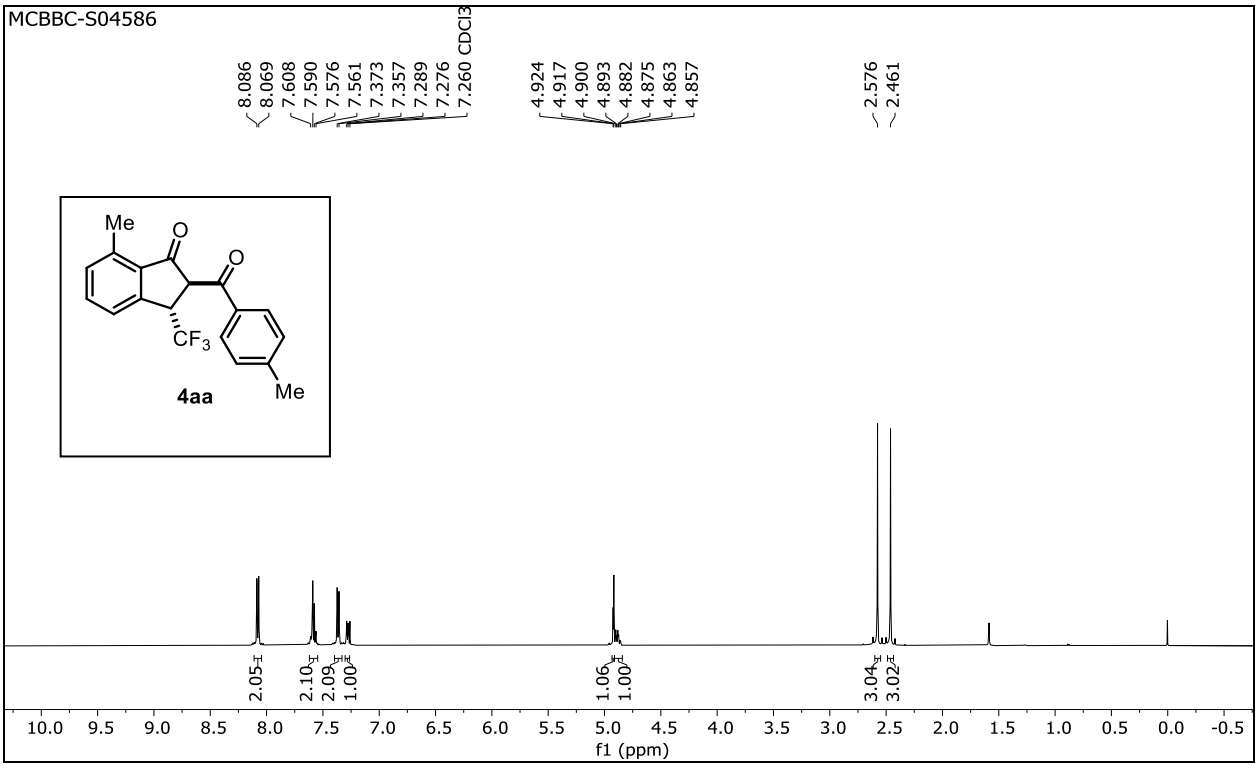

BBC-1276
194.795
168.819
144.455
139.200
133.893
132.593
129.497
129.409
128.425
128.318
128.251
127.967
127.098
126.022
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
49.354
45.906
41.184
40.966
40.745
40.528
39.186
26.224
24.719
21.777
Me
CF3
O
3xa
f1 (ppm)

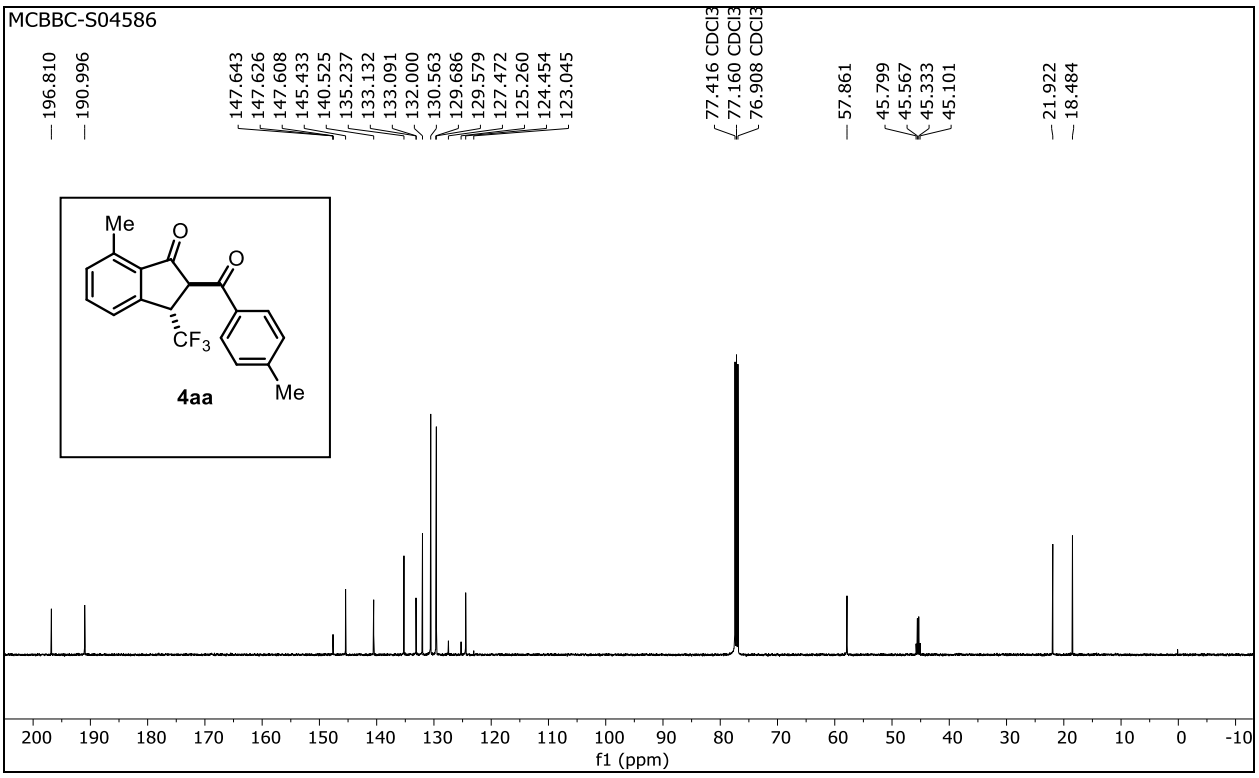

MCBBC-S06606
-68.540
N
O
Me
CF3
O
3xa
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

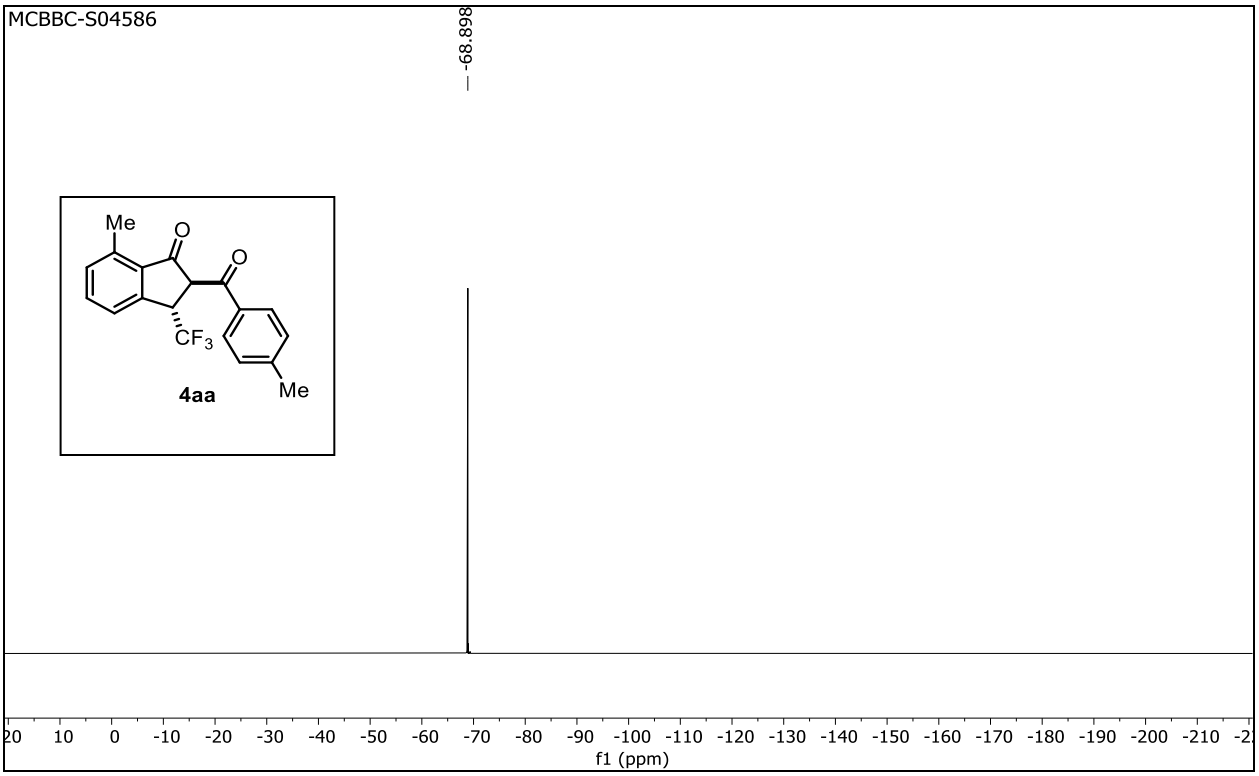

MCBBC-S06635
7.840 7.823 7.704 7.624 7.618 7.607 7.595 7.428 7.377 7.359 7.333 7.272 7.260 CDCl3 7.256 6.190 4.871 4.865 4.853 4.847 4.842 4.835 4.829 4.824 4.817 4.812 4.806 4.794 4.788 4.001 3.979 3.965 3.942 3.650 3.643 3.613 3.607 2.410
O
NH2
Me
CF3
O
3ya
2.00 1.02 1.04 3.02 2.22 1.04 1.03 1.00 1.01 3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

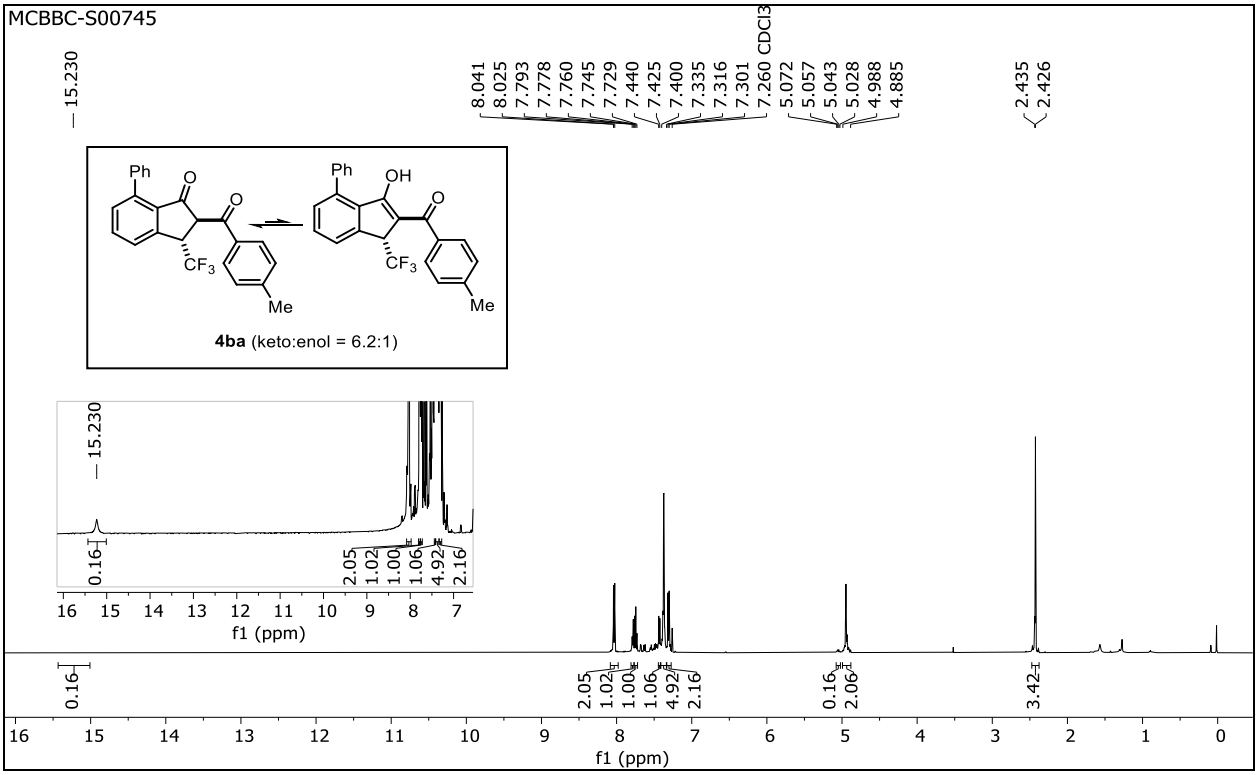

MCBBC-S06635
196.567
171.428
145.342
138.584
133.480
130.961
130.374
129.660
128.991
128.663
128.429
127.716
126.861
125.490
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
40.929
40.709
40.488
40.267
38.340
21.856
O
NH2
Me
CF3
O
3ya
f1 (ppm)

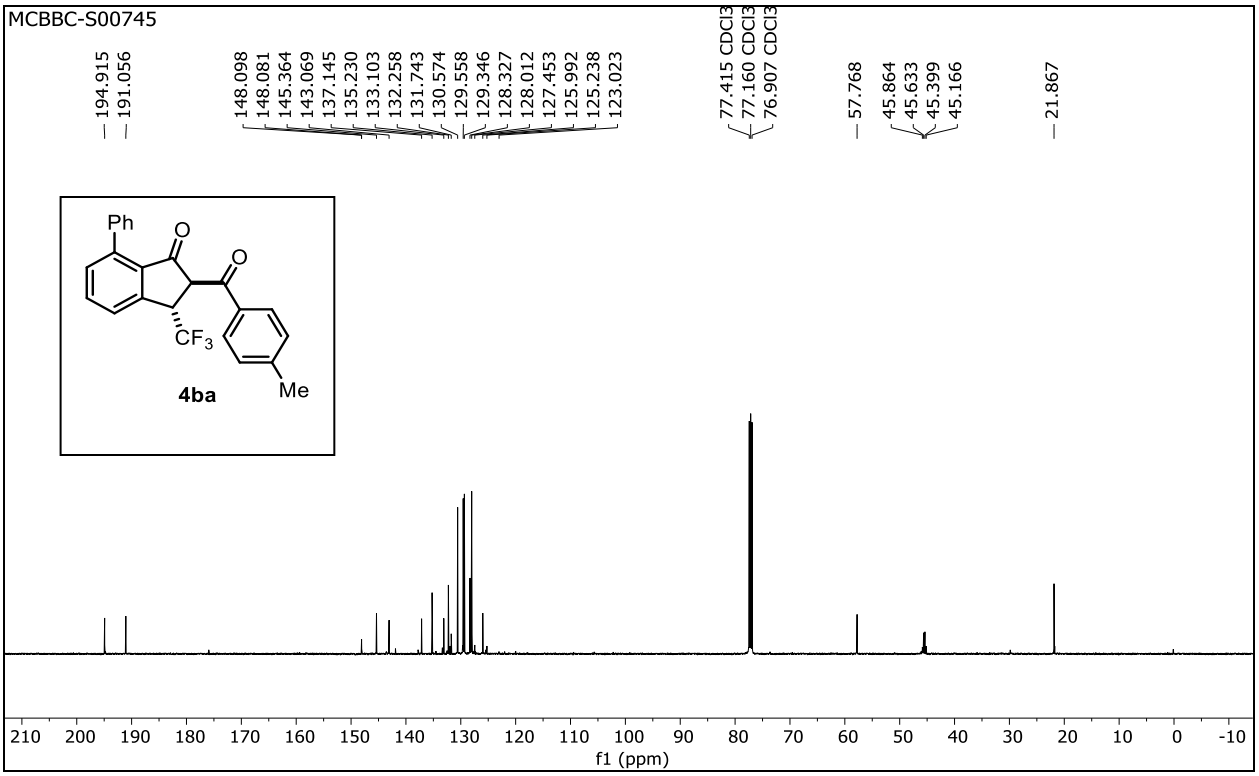

MCBBC-S06635
-69.260
O
NH2
Me
CF3
O
3ya
f1 (ppm)

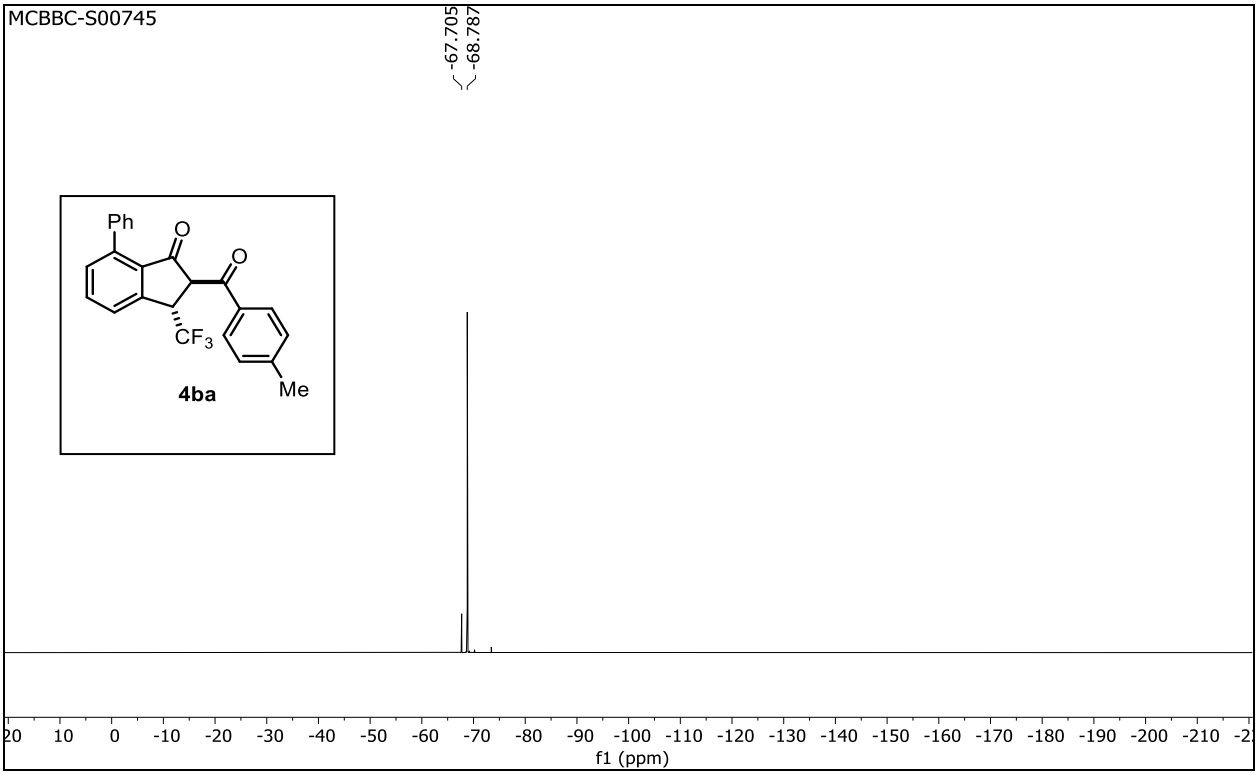

MCBBC-S04586
8.086
8.069
7.608
7.590
7.576
7.561
7.373
7.357
7.289
7.276
7.260 CDCl3
4.924
4.917
4.900
4.893
4.882
4.875
4.863
4.857
2.576
2.461
Me
O
O
CF3
Me
4aa
2.05
2.10
2.09
1.00
1.06
1.00
3.04
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

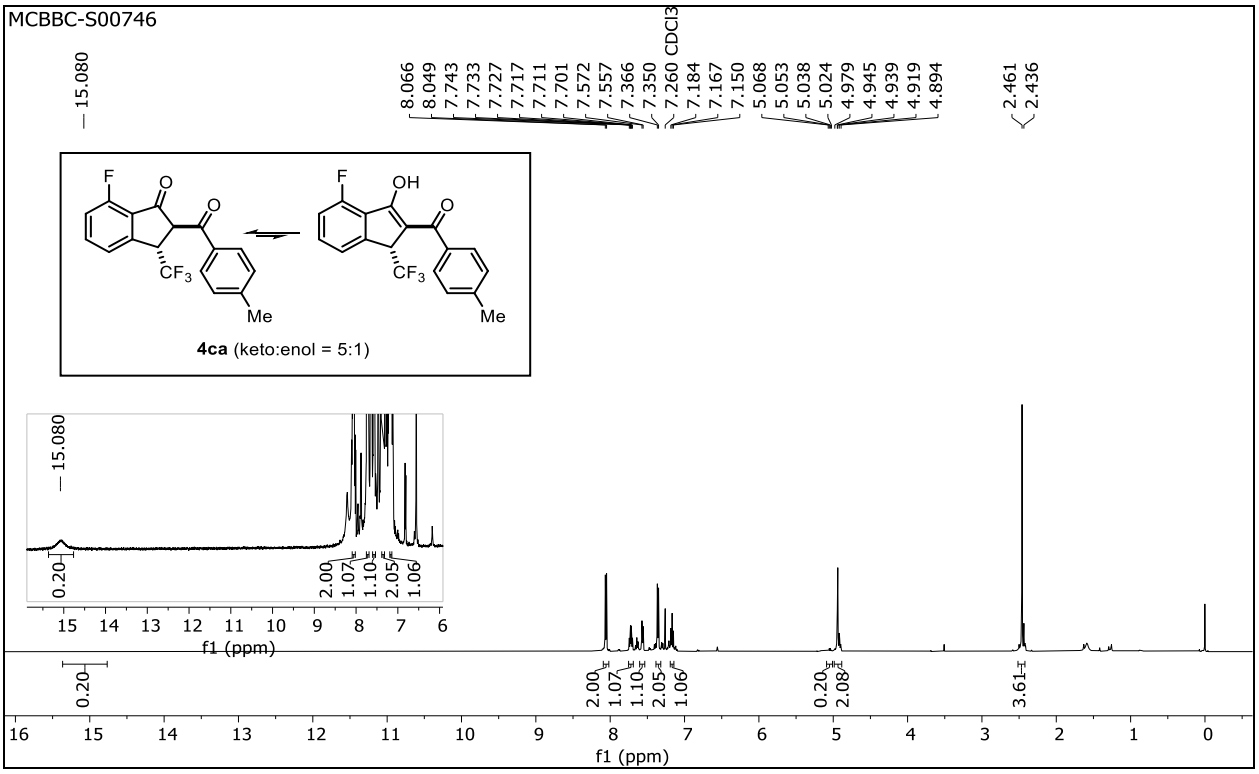

MCBBC-S04586
196.810
190.996
147.643
147.626
147.608
145.433
140.525
135.237
133.132
133.091
132.000
130.563
129.686
129.579
127.472
125.260
124.454
123.045
77.416 CDCl3
77.160 CDCl3
76.908 CDCl3
57.861
45.799
45.567
45.333
45.101
21.922
18.484
Me
O
O
CF3
Me
4aa
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

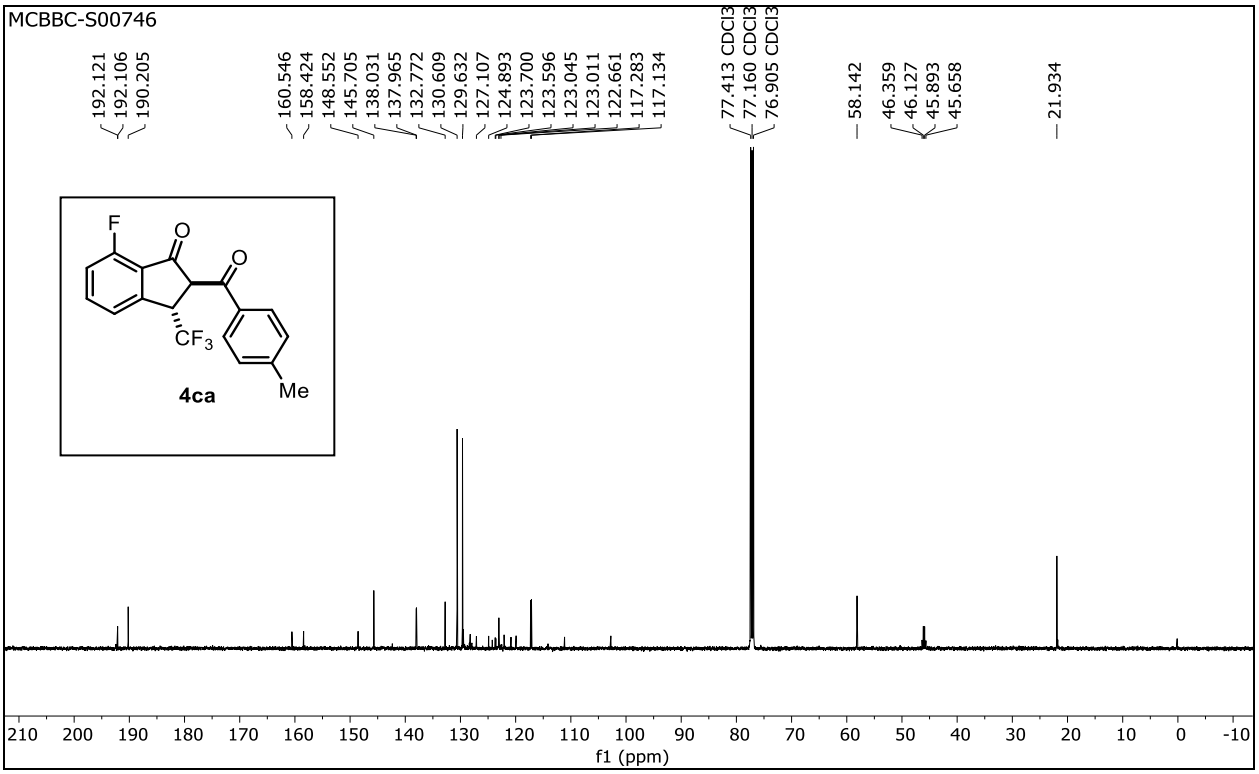

MCBBC-S04586
-68.898
Me
O
O
CF3
Me
4aa
f1 (ppm)

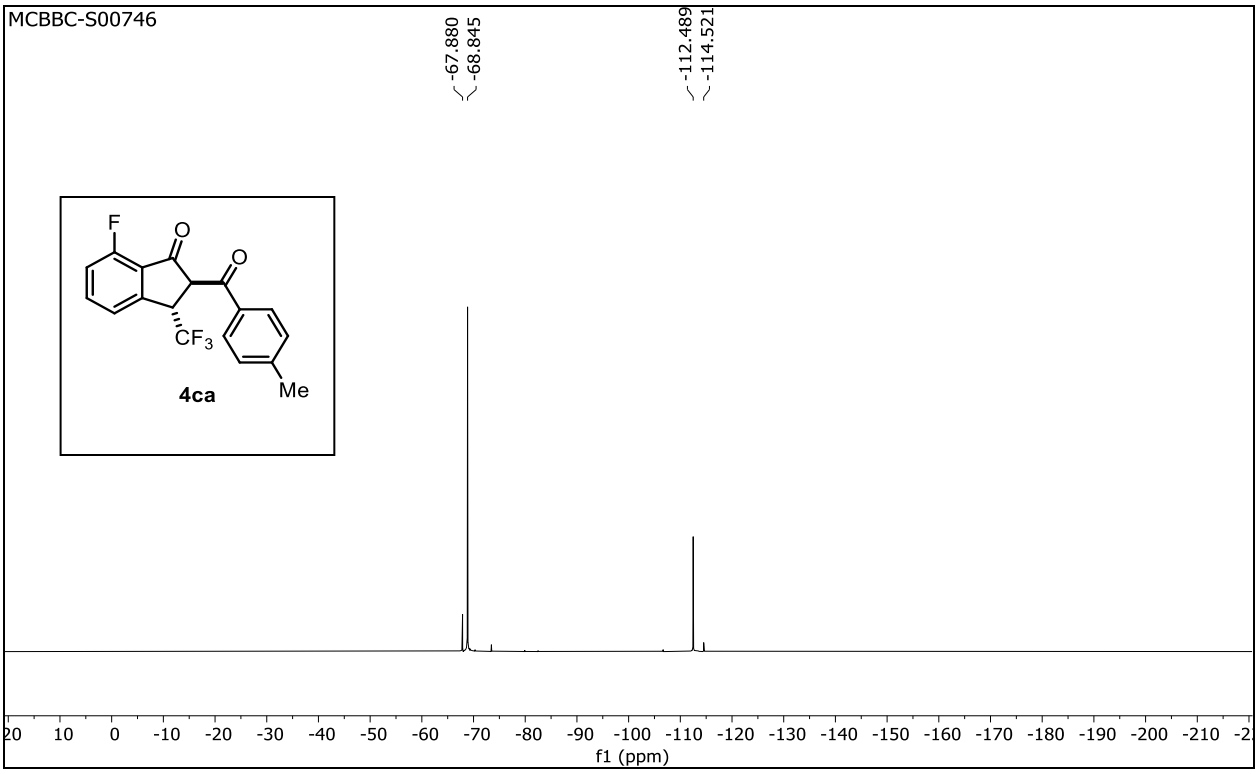

MCBBC-S00745
15.230
8.041
8.025
7.793
7.778
7.760
7.745
7.729
7.440
7.425
7.400
7.335
7.316
7.301
7.260 CDCl3
5.072
5.057
5.043
5.028
4.988
4.885
2.435
2.426
Ph
O
O
CF3
Me
Ph
OH
O
CF3
Me
4ba (keto:enol = 6.2:1)
0.16
2.05
1.02
1.00
1.06
4.92
2.16
0.16
2.06
3.42
f1 (ppm)

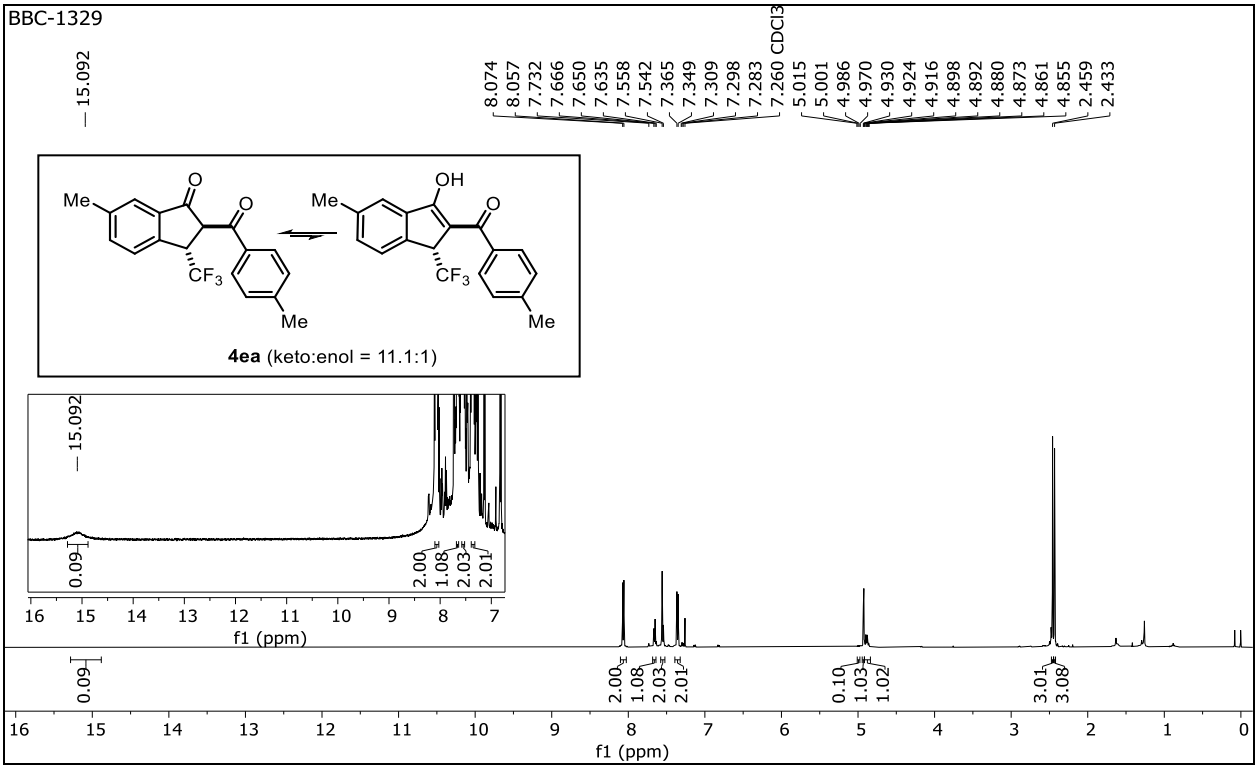

MCBBC-S00745
194.915
191.056
148.098
148.081
145.364
143.069
137.145
135.230
133.103
132.258
131.743
130.574
129.558
129.346
128.327
128.012
127.453
125.992
125.238
123.023
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
57.768
45.864
45.633
45.399
45.166
21.867
Ph
O
O
CF3
Me
4ba
f1 (ppm)

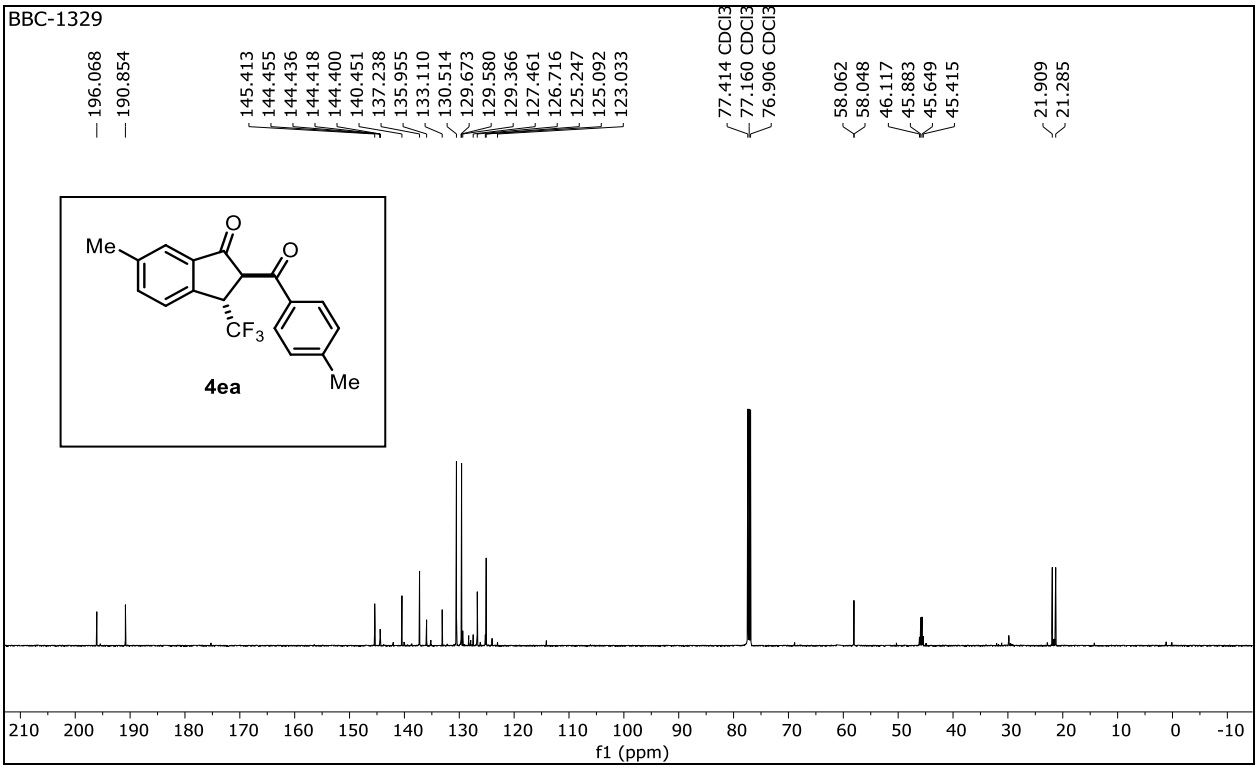

MCBBC-S00745
-67.705
-68.787
Ph
O
O
CF3
Me
4ba
f1 (ppm)

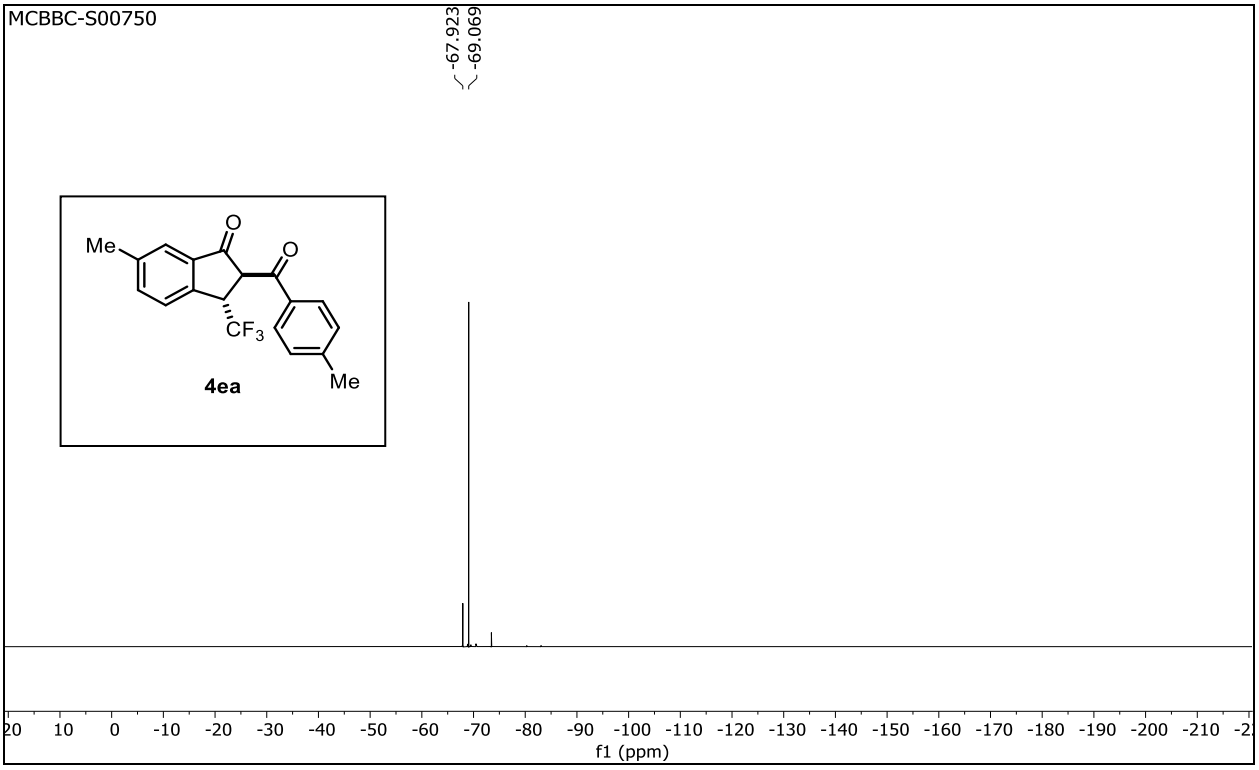

MCBBC-S00746
15.080
8.066
8.049
7.743
7.733
7.727
7.717
7.711
7.701
7.572
7.557
7.366
7.350
7.260 CDCl3
7.184
7.167
7.150
5.068
5.053
5.038
5.024
4.979
4.945
4.939
4.919
4.894
2.461
2.436
F
O
O
CF3
Me
OH
4ca (keto:enol = 5:1)
f1 (ppm)

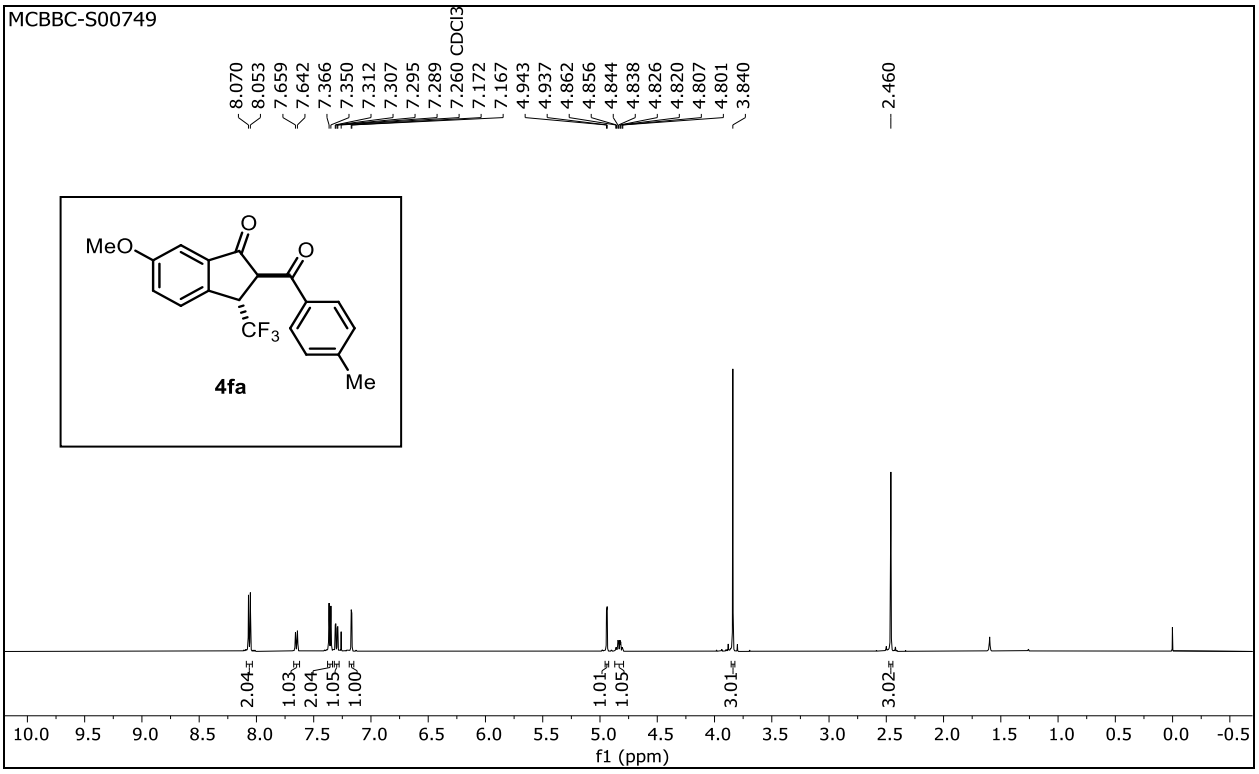

MCBBC-S00746
192.121
192.106
190.205
160.546
158.424
148.552
145.705
138.031
137.965
132.772
130.609
129.632
127.107
124.893
123.700
123.596
123.045
123.011
122.661
117.283
117.134
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
58.142
46.359
46.127
45.893
45.658
21.934
F
O
O
CF3
Me
4ca
f1 (ppm)

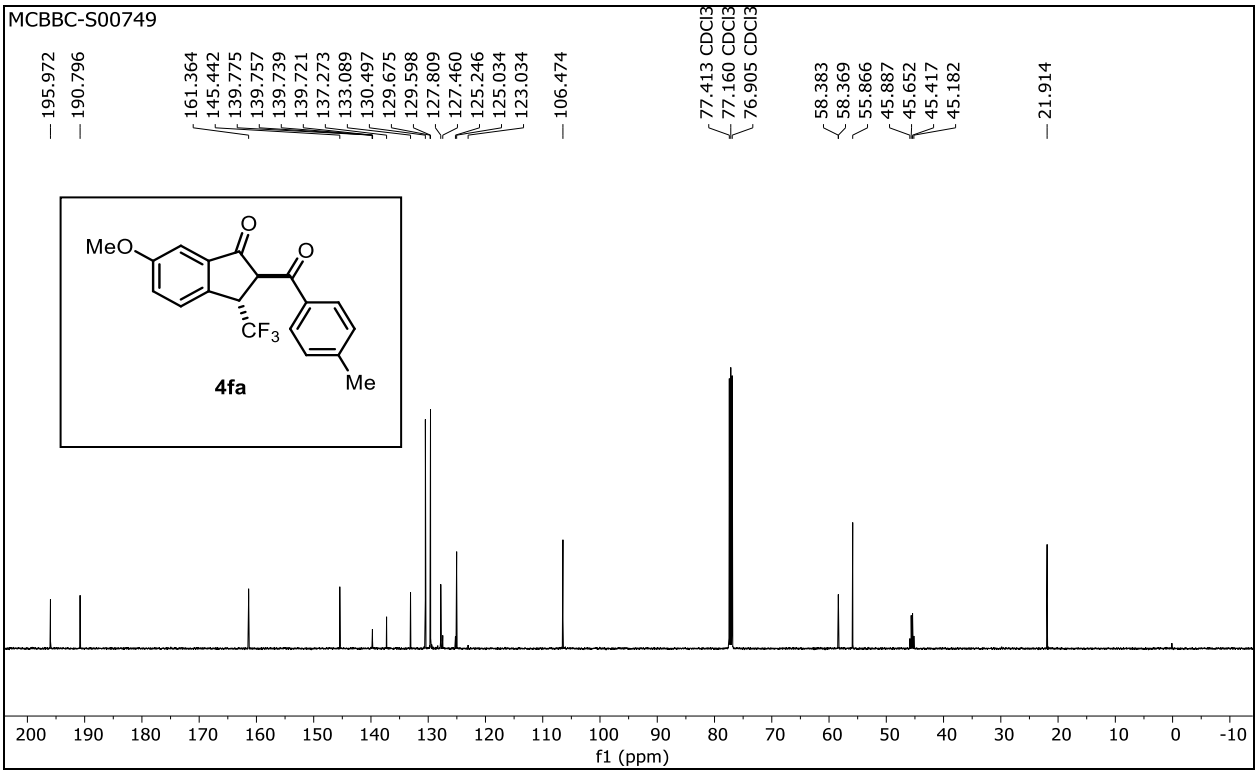

MCBBC-S00746
-67.880
-68.845
-112.489
-114.521
F
O
O
CF3
Me
4ca
f1 (ppm)

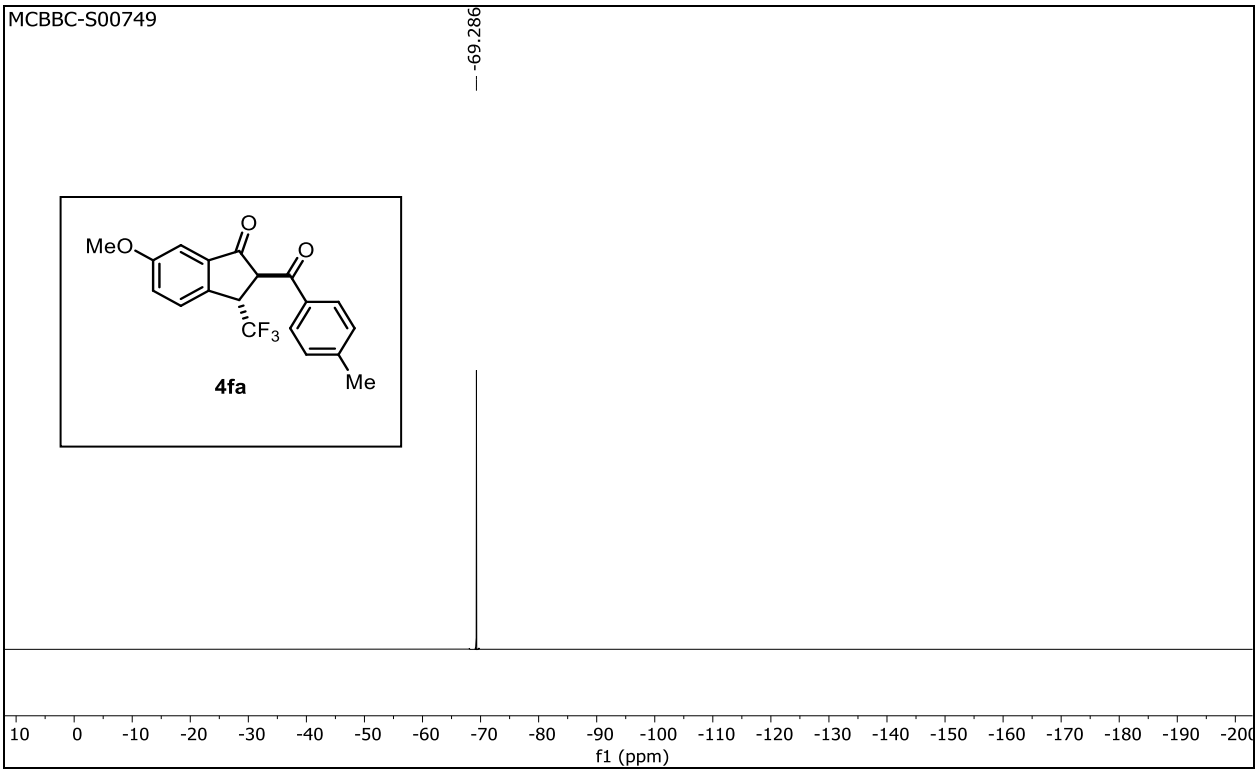

BBC-1329
15.092
8.074
8.057
7.732
7.666
7.650
7.635
7.558
7.542
7.365
7.349
7.309
7.298
7.283
7.260 CDCl3
5.015
5.001
4.986
4.970
4.930
4.924
4.916
4.898
4.892
4.880
4.873
4.861
4.855
2.459
2.433
Me
O
O
CF3
Me
OH
Me
O
CF3
Me
4ea (keto:enol = 11.1:1)
0.09
2.00
1.08
2.03
2.01
0.10
1.03
1.02
3.01
3.08
f1 (ppm)

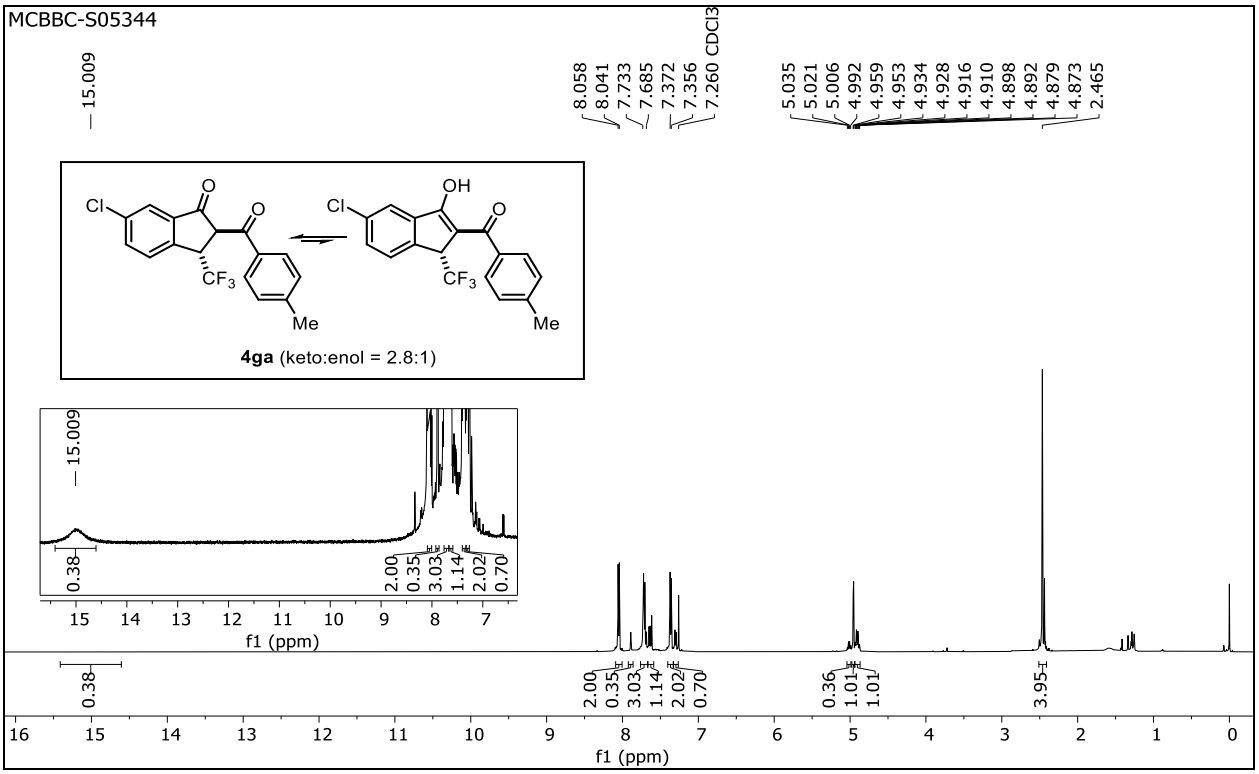

BBC-1329
196.068
190.854
145.413
144.455
144.436
144.418
144.400
140.451
137.238
135.955
133.110
130.514
129.673
129.580
129.366
127.461
126.716
125.247
125.092
123.033
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
58.062
58.048
46.117
45.883
45.649
45.415
21.909
21.285
Me
O
O
CF3
Me
4ea
f1 (ppm)

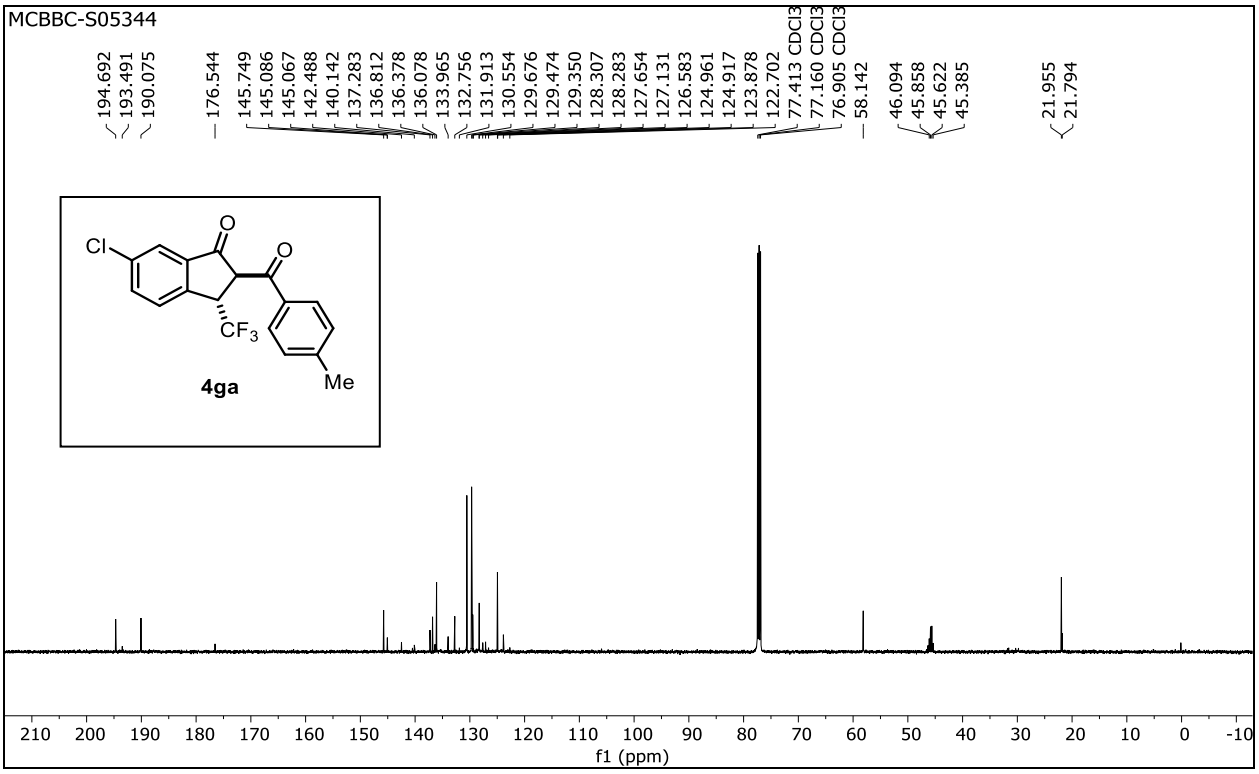

MCBBC-S00750
-67.923
-69.069
Me
O
O
CF3
Me
4ea
f1 (ppm)

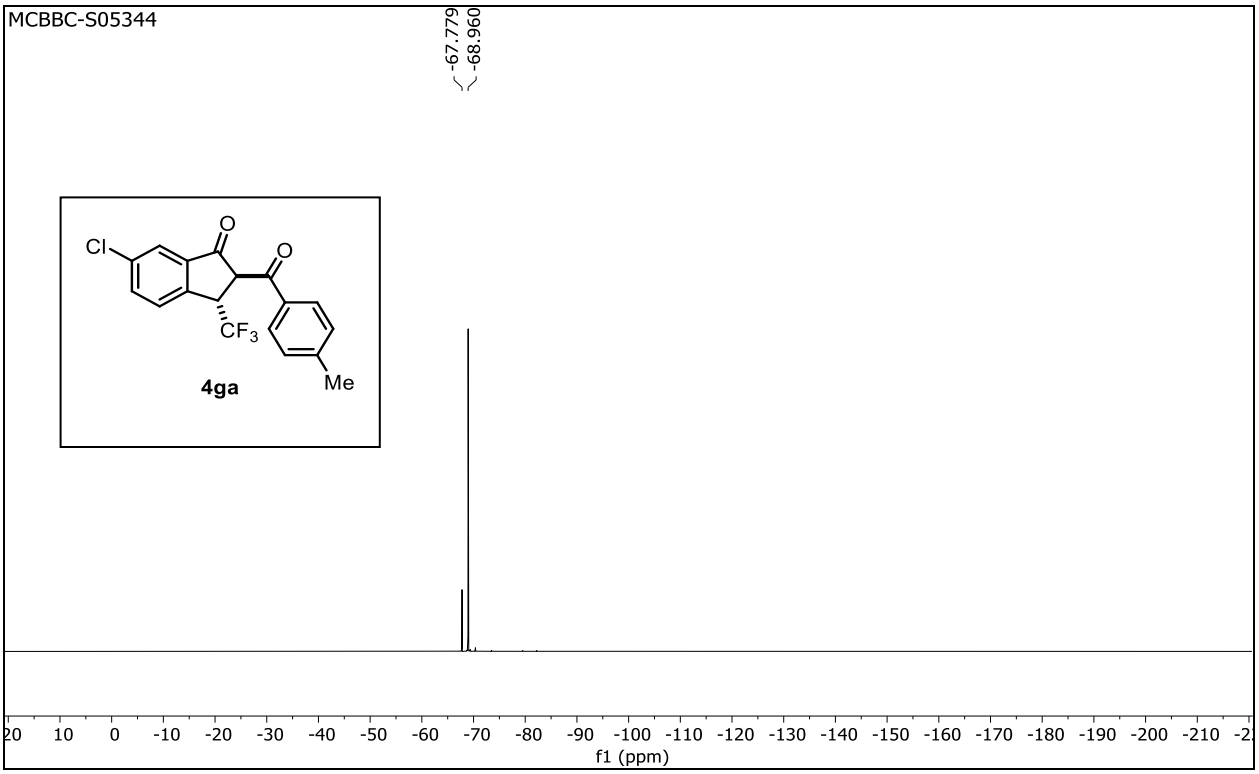

MCBBC-S00749
8.070
8.053
7.659
7.642
7.366
7.350
7.312
7.307
7.295
7.289
7.260 CDCl3
7.172
7.167
4.943
4.937
4.862
4.856
4.844
4.838
4.826
4.820
4.807
4.801
3.840
2.460
MeO
O
O
CF3
Me
4fa
2.04
1.03
2.04
1.05
1.00
1.01
1.05
3.01
3.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

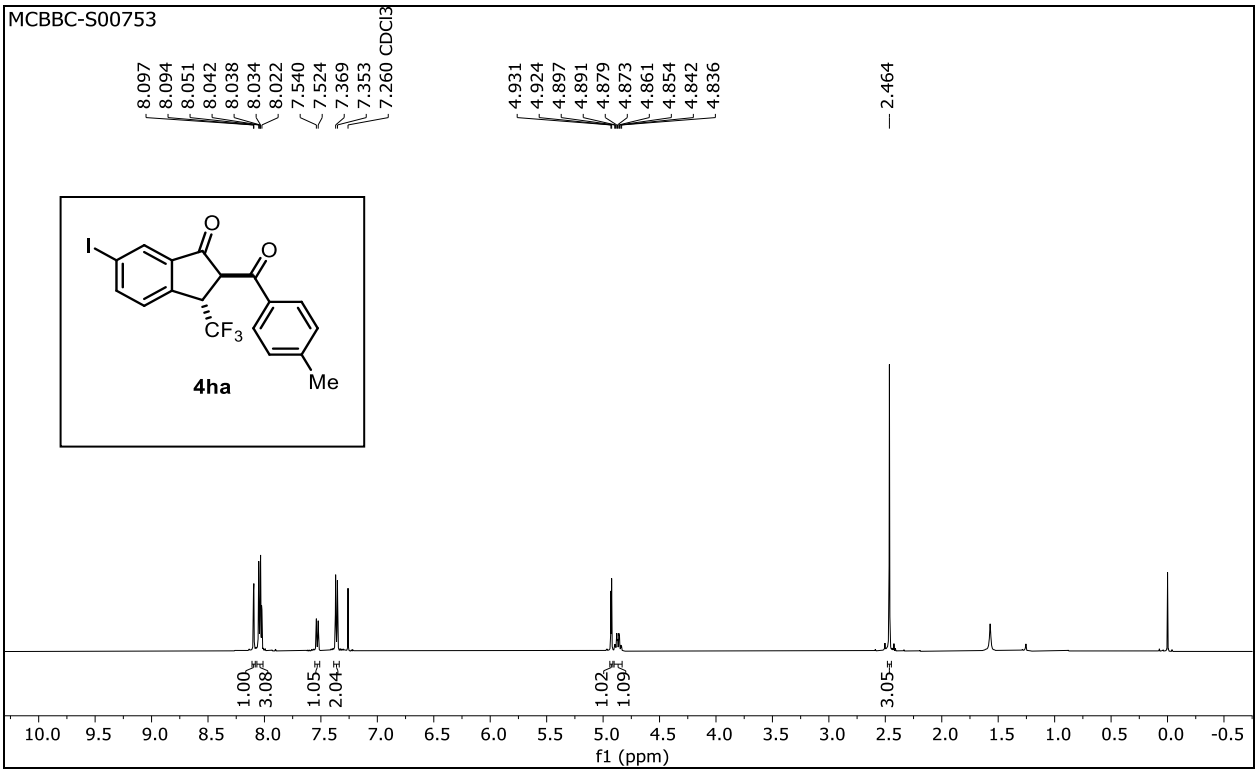

MCBBC-S00749
195.972
190.796
161.364
145.442
139.775
139.757
139.739
139.721
137.273
133.089
130.497
129.675
129.598
127.809
127.460
125.246
125.034
123.034
106.474
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
58.383
58.369
55.866
45.887
45.652
45.417
45.182
21.914
MeO
O
O
CF3
Me
4fa
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

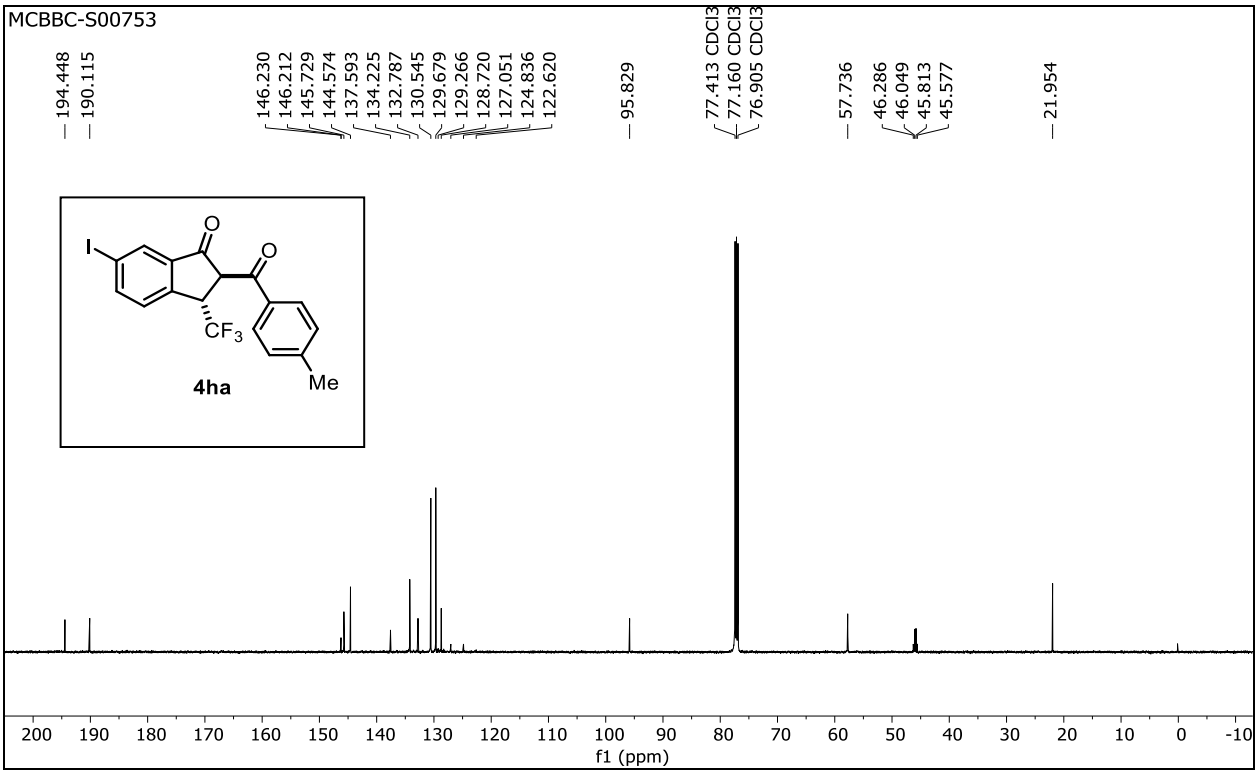

MCBBC-S00749
-69.286
MeO
O
O
CF3
Me
4fa
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

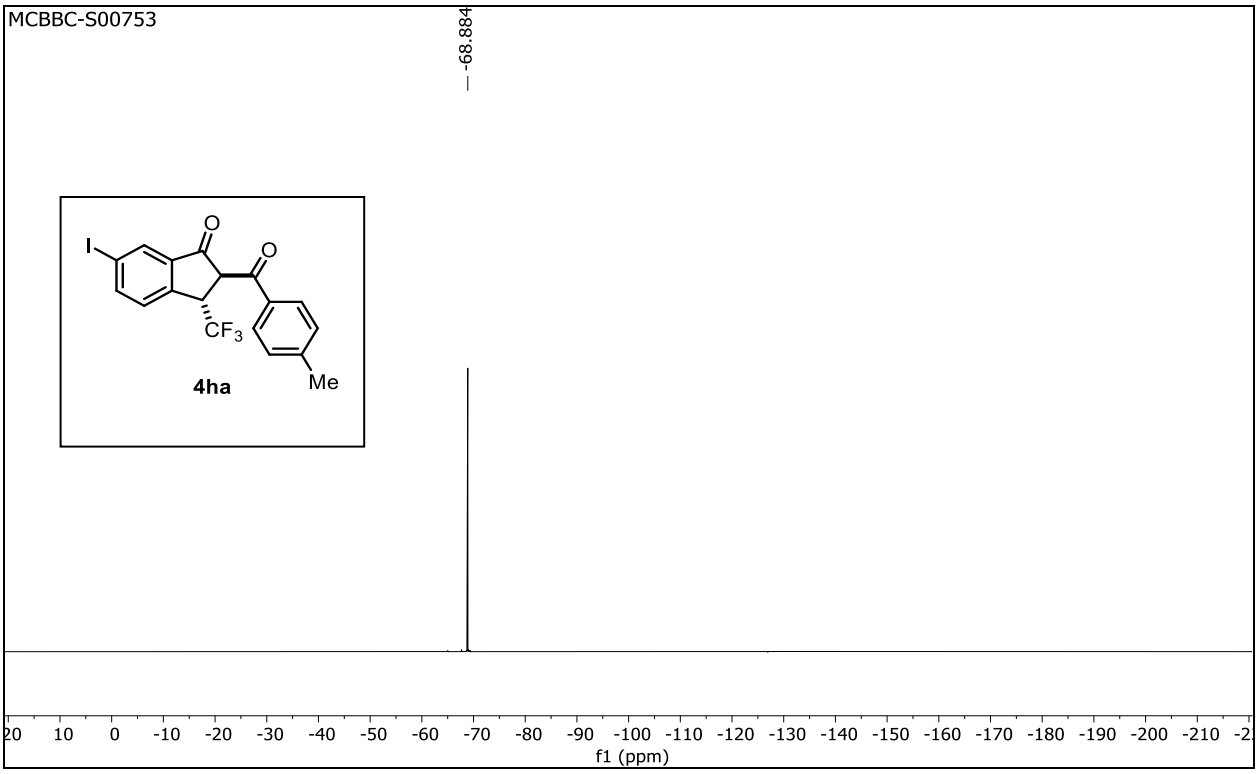

MCBBC-S05344
15.009
8.058
8.041
7.733
7.685
7.372
7.356
7.260 CDCl3
5.035
5.021
5.006
4.992
4.959
4.953
4.934
4.928
4.916
4.910
4.898
4.892
4.879
4.873
2.465
Cl
O
O
CF3
Me
OH
4ga (keto:enol = 2.8:1)
0.38
2.00
0.35
3.03
1.14
2.02
0.70
0.36
1.01
1.01
3.95
f1 (ppm)

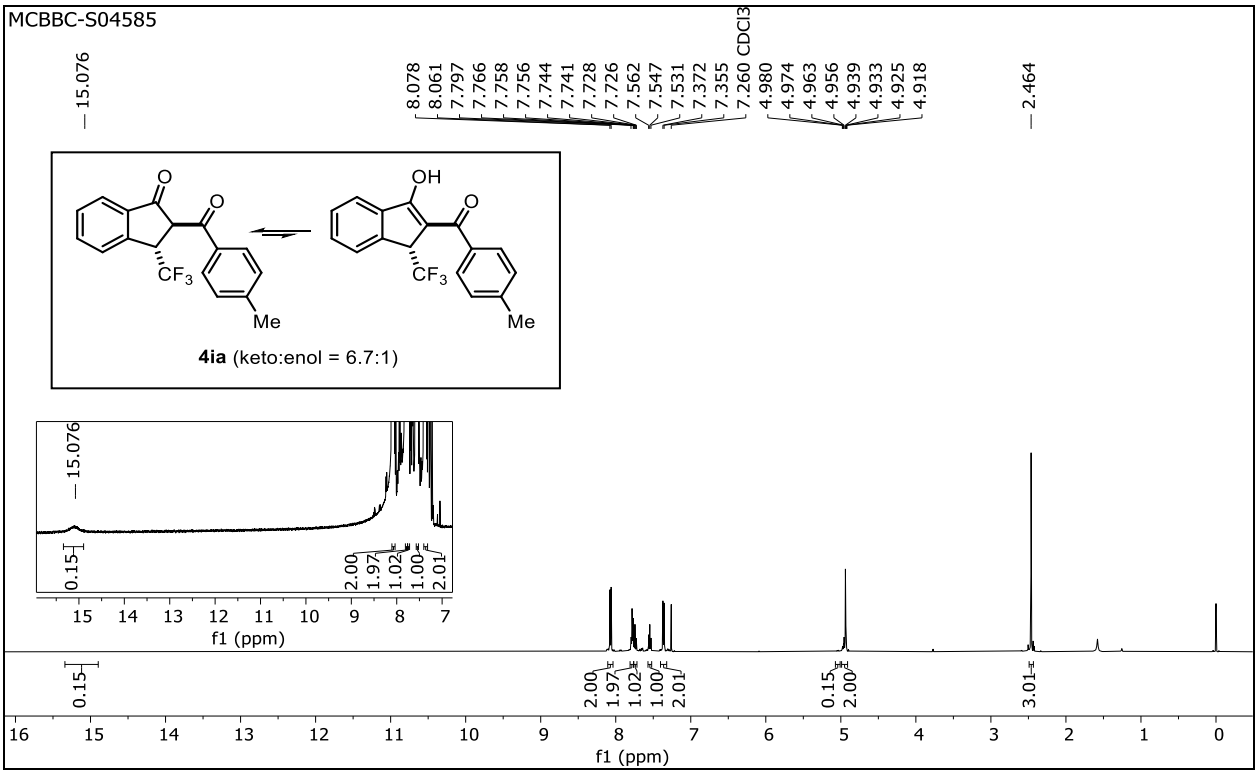

MCBBC-S05344
194.692
193.491
190.075
176.544
145.749
145.086
145.067
142.488
140.142
137.283
136.812
136.378
136.078
133.965
132.756
131.913
130.554
129.676
129.474
129.350
128.307
128.283
127.654
127.131
126.583
124.961
124.917
123.878
122.702
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
58.142
46.094
45.858
45.622
45.385
21.955
21.794
Cl
O
O
CF3
Me
4ga
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

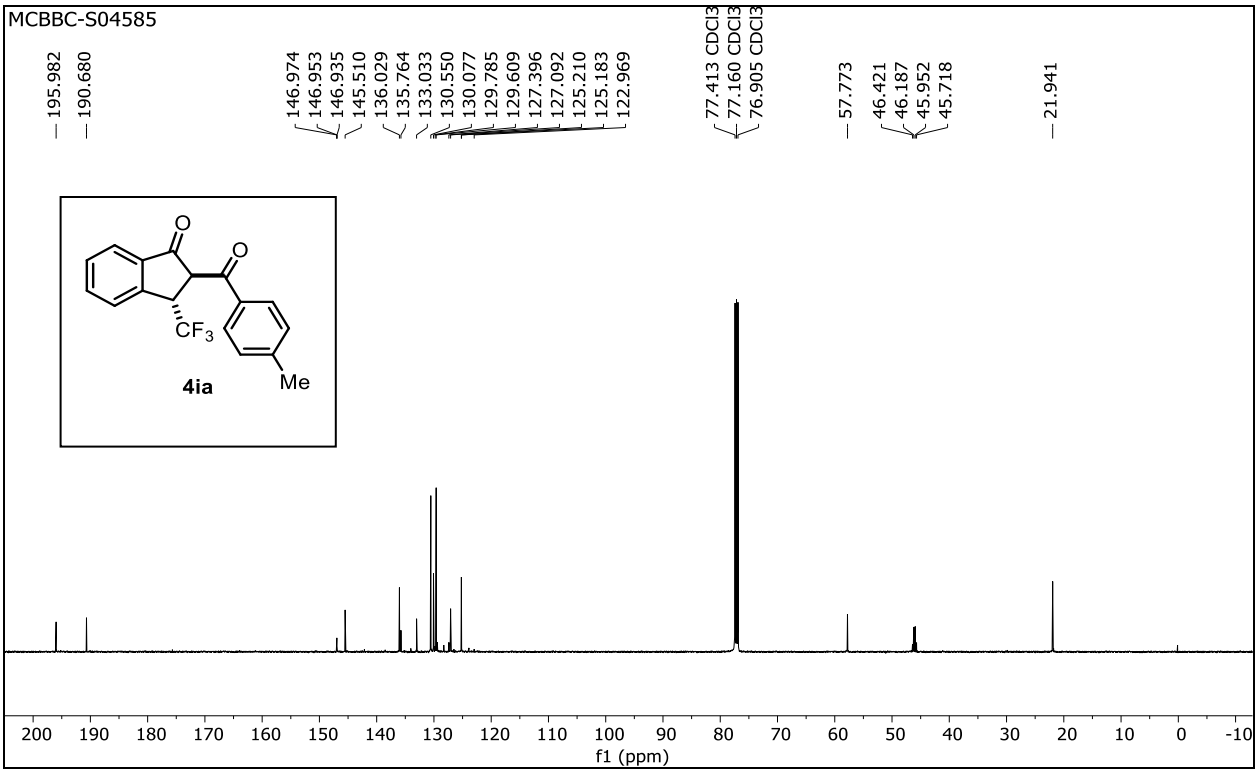

MCBBC-S05344
-67.779
-68.960
Cl
O
O
CF3
Me
4ga
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

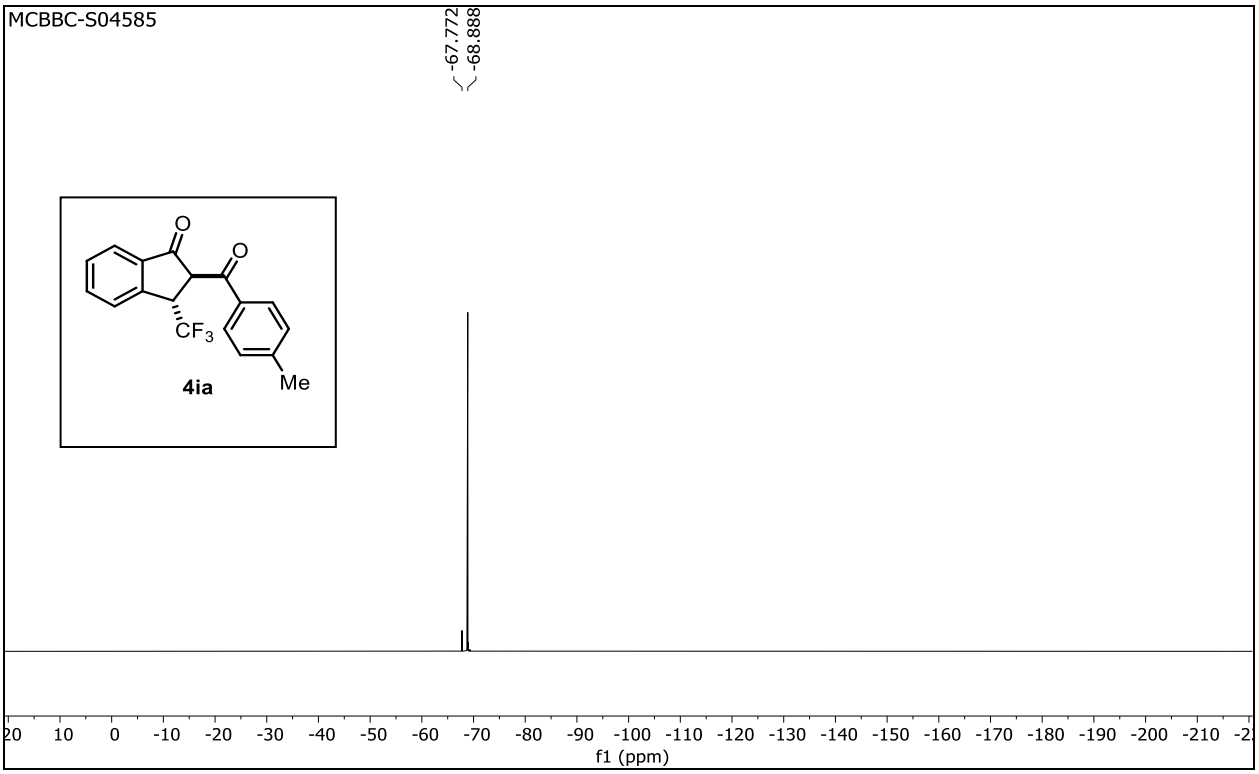

MCBBC-S00753
8.097
8.094
8.051
8.042
8.038
8.034
8.022
7.540
7.524
7.369
7.353
7.260 CDCl3
4.931
4.924
4.897
4.891
4.879
4.873
4.861
4.854
4.842
4.836
2.464
4ha
1.00
3.08
1.05
2.04
1.02
1.09
3.05
f1 (ppm)

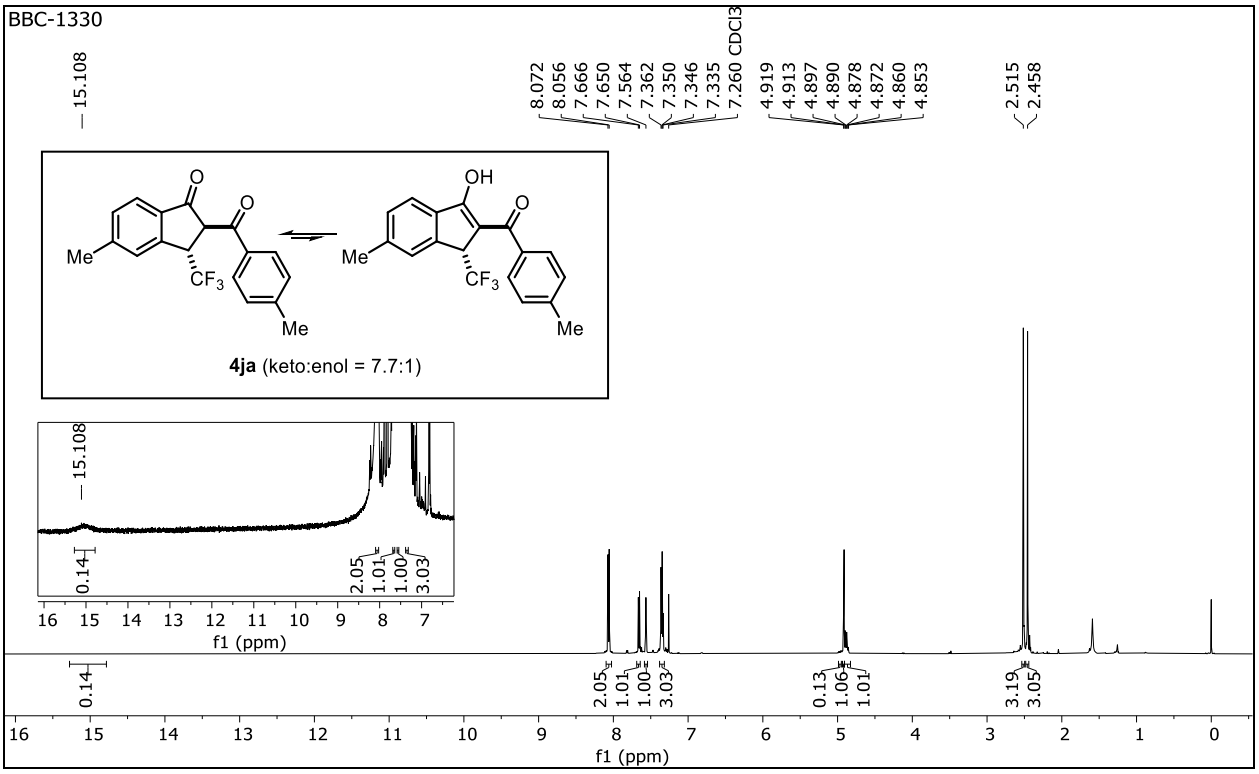

MCBBC-S00753
194.448
190.115
146.230
146.212
145.729
144.574
137.593
134.225
132.787
130.545
129.679
129.266
128.720
127.051
124.836
122.620
95.829
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
57.736
46.286
46.049
45.813
45.577
21.954
4ha
f1 (ppm)

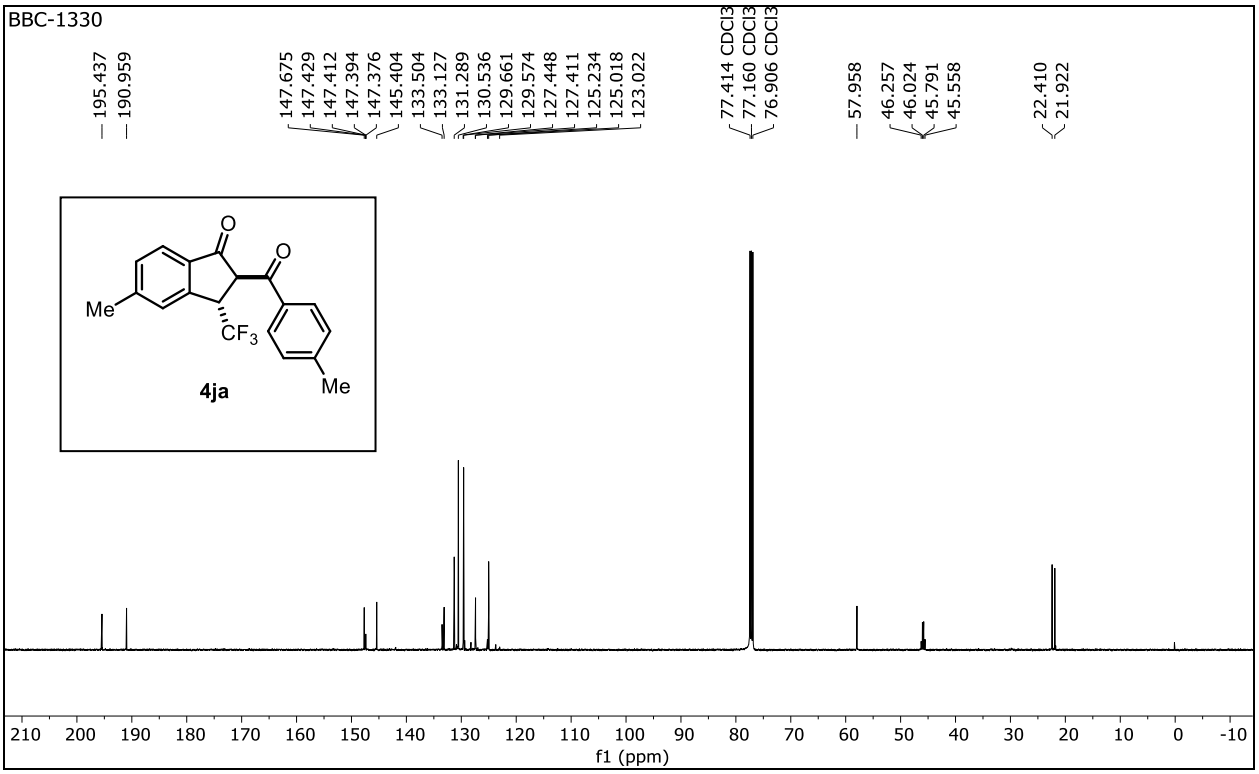

MCBBC-S00753
-68.884
4ha
f1 (ppm)

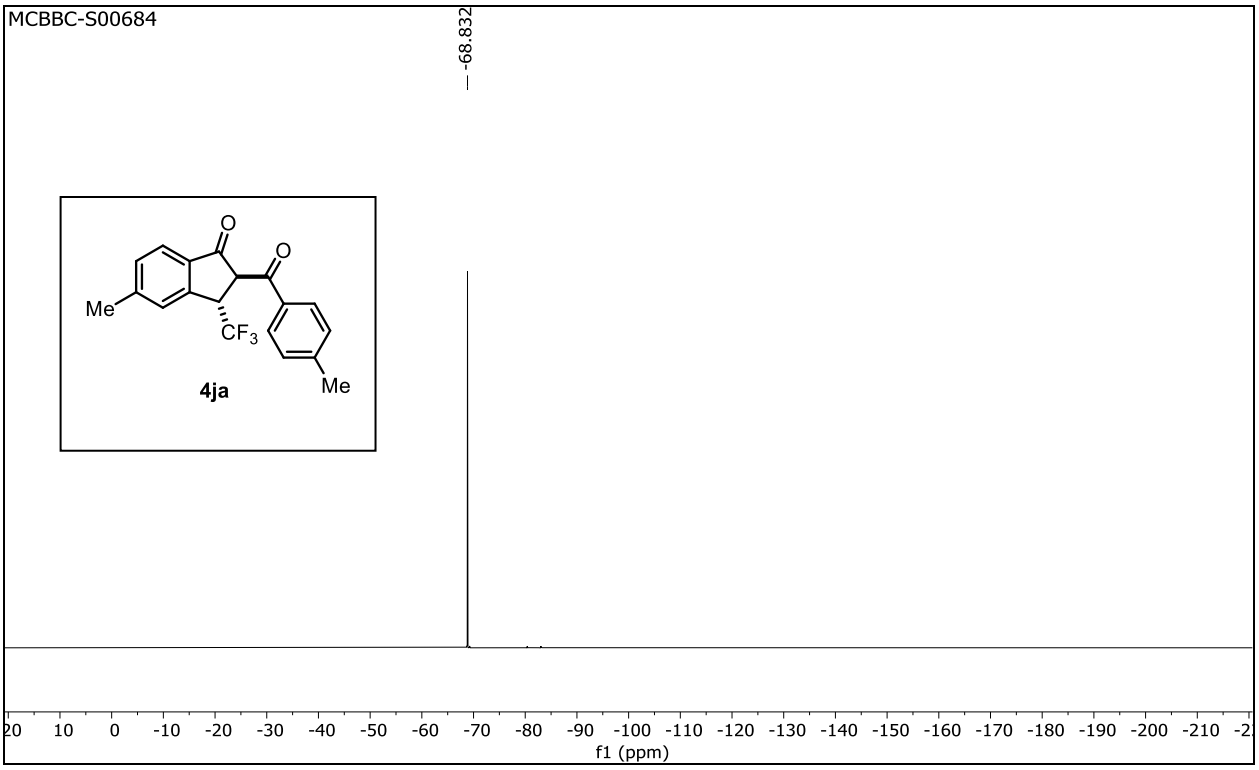

MCBBC-S04585
15.076
8.078
8.061
7.797
7.766
7.758
7.756
7.744
7.741
7.728
7.726
7.562
7.547
7.531
7.372
7.355
7.260 CDCl3
4.980
4.974
4.963
4.956
4.939
4.933
4.925
4.918
2.464
4ia (keto:enol = 6.7:1)
f1 (ppm)

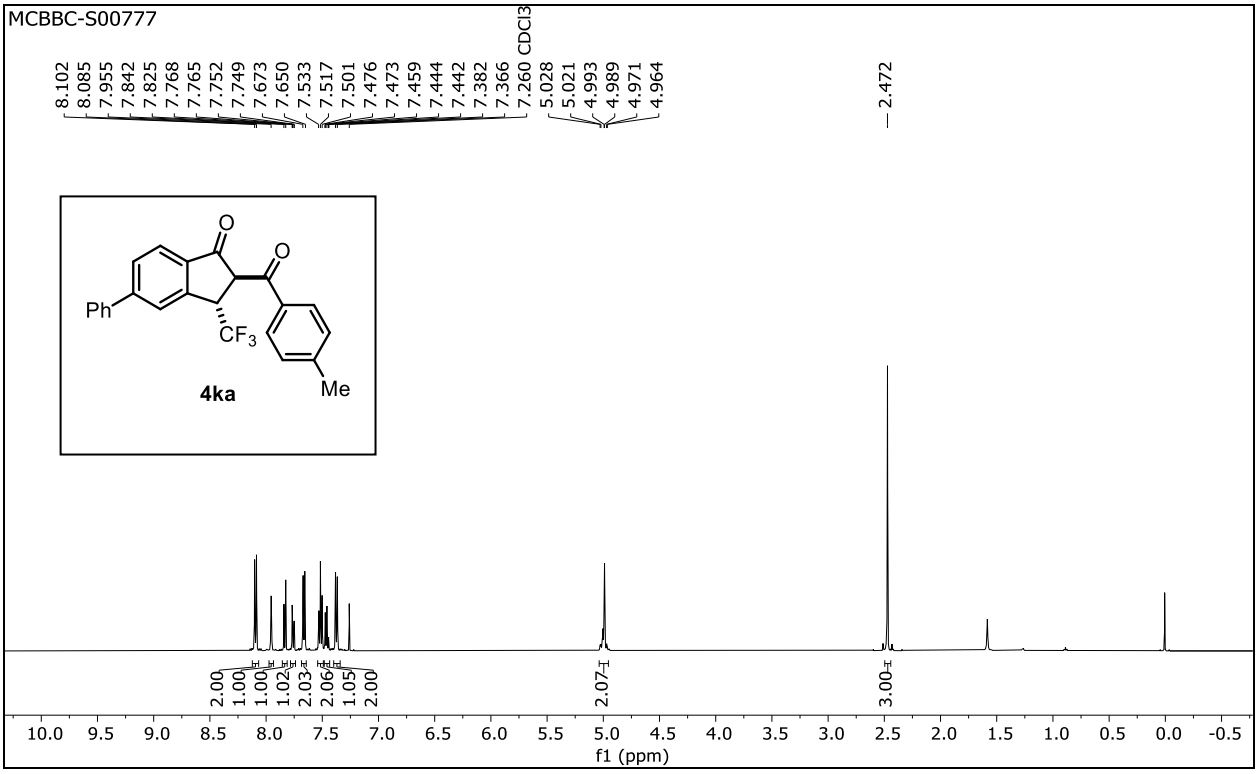

MCBBC-S04585
195.982
190.680
146.974
146.953
146.935
145.510
136.029
135.764
133.033
130.550
130.077
129.785
129.609
127.396
127.092
125.210
125.183
122.969
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
57.773
46.421
46.187
45.952
45.718
21.941
O
O
CF3
Me
4ia
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

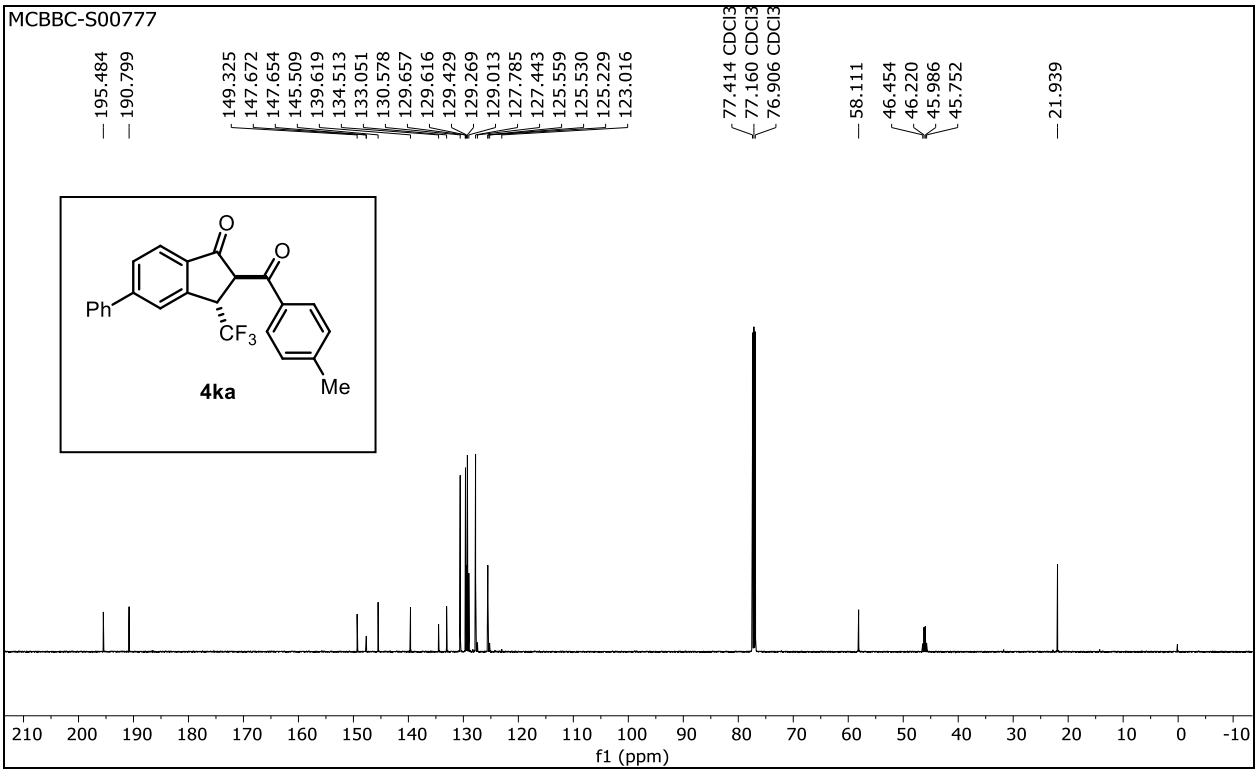

MCBBC-S04585
-67.772
-68.888
O
O
CF3
Me
4ia
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

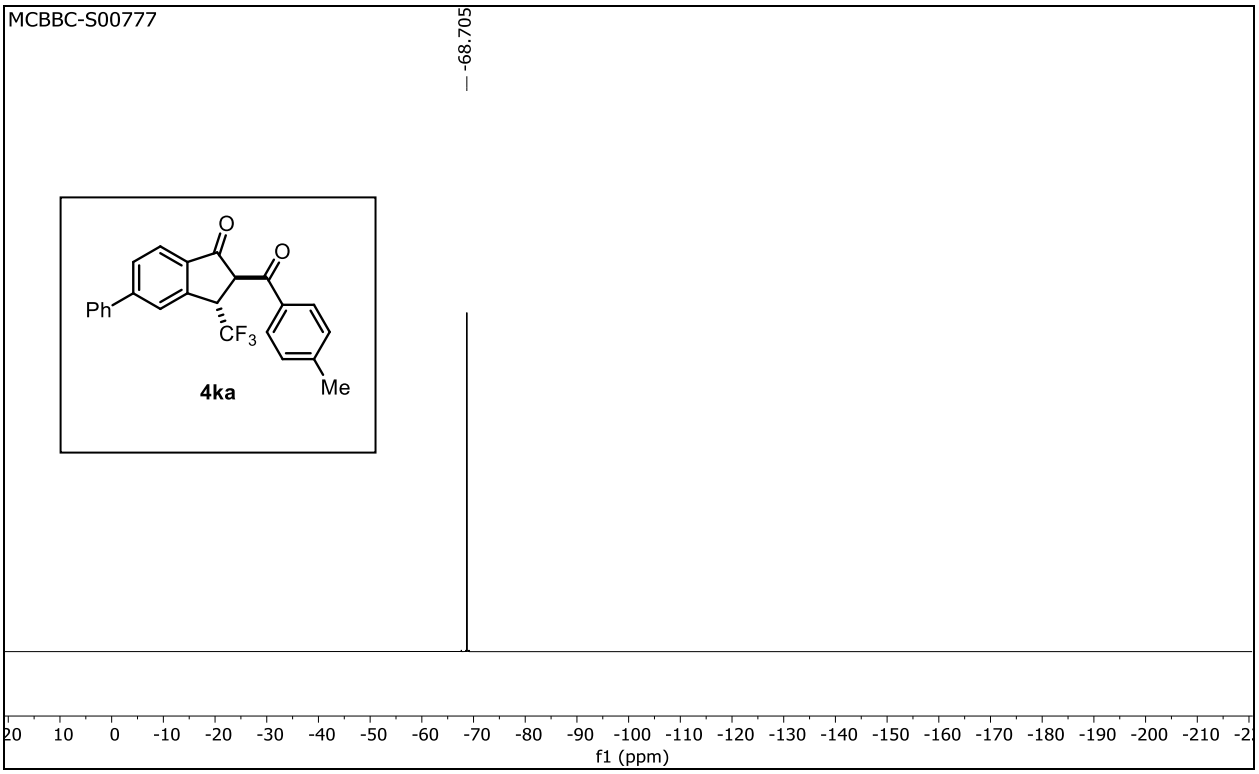

BBC-1330
15.108
8.072
8.056
7.666
7.650
7.564
7.362
7.350
7.346
7.335
7.260 CDCl3
4.919
4.913
4.897
4.890
4.878
4.872
4.860
4.853
2.515
2.458
4ja (keto:enol = 7.7:1)
f1 (ppm)

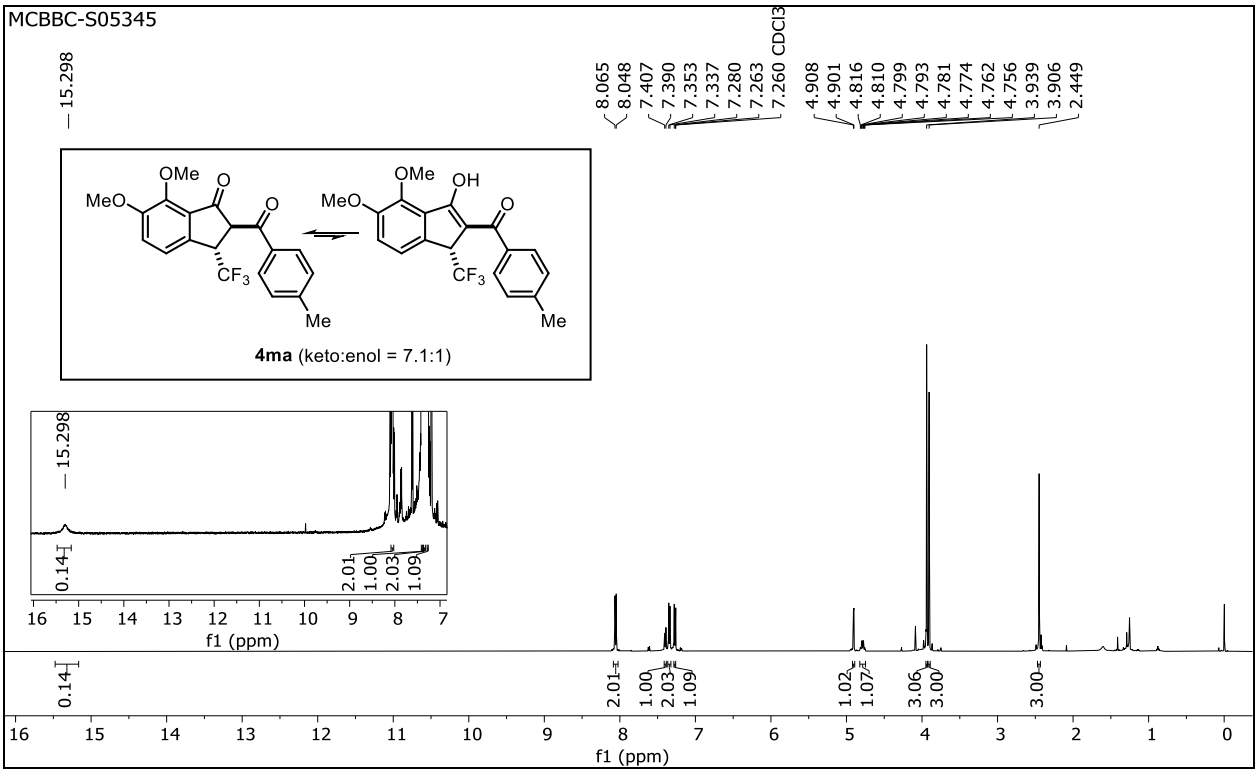

BBC-1330
195.437
190.959
147.675
147.429
147.412
147.394
147.376
145.404
133.504
133.127
131.289
130.536
129.661
129.574
127.448
127.411
125.234
125.018
123.022
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
57.958
46.257
46.024
45.791
45.558
22.410
21.922
4ja
f1 (ppm)

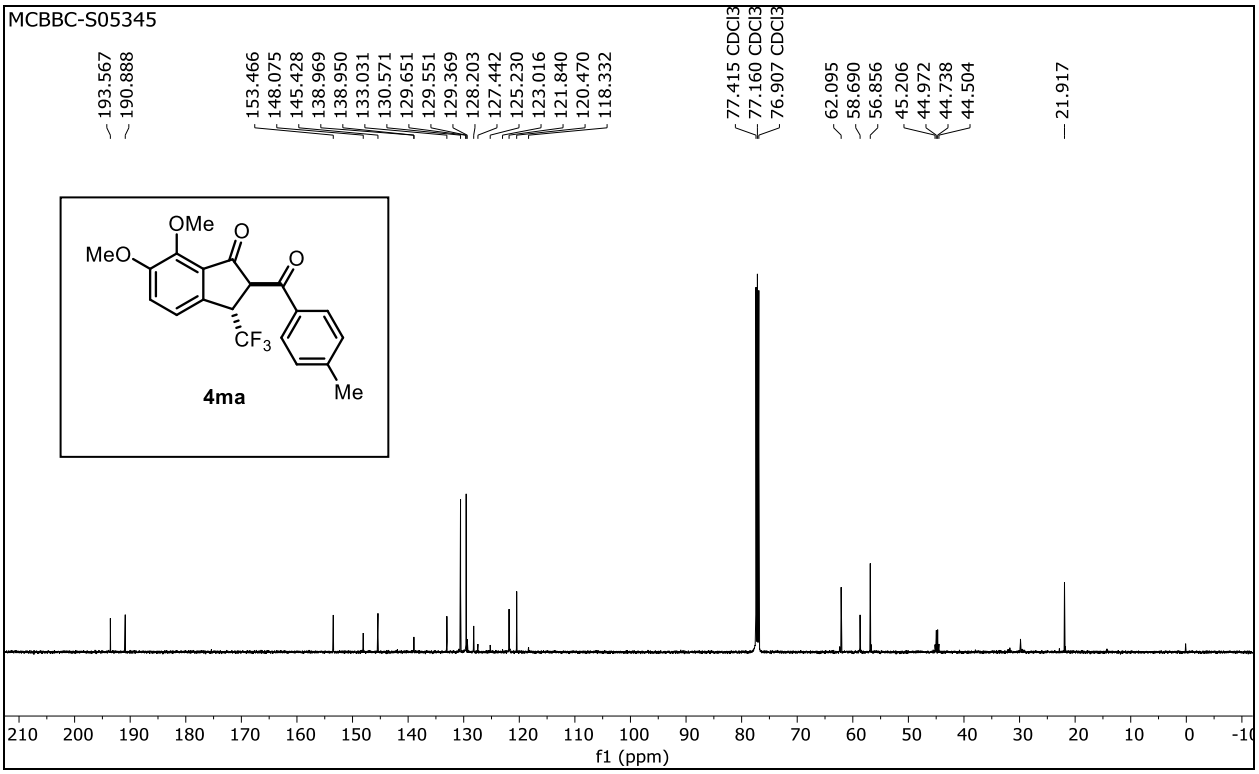

MCBBC-S00684
-68.832
O
O
Me
CF3
Me
4ja
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

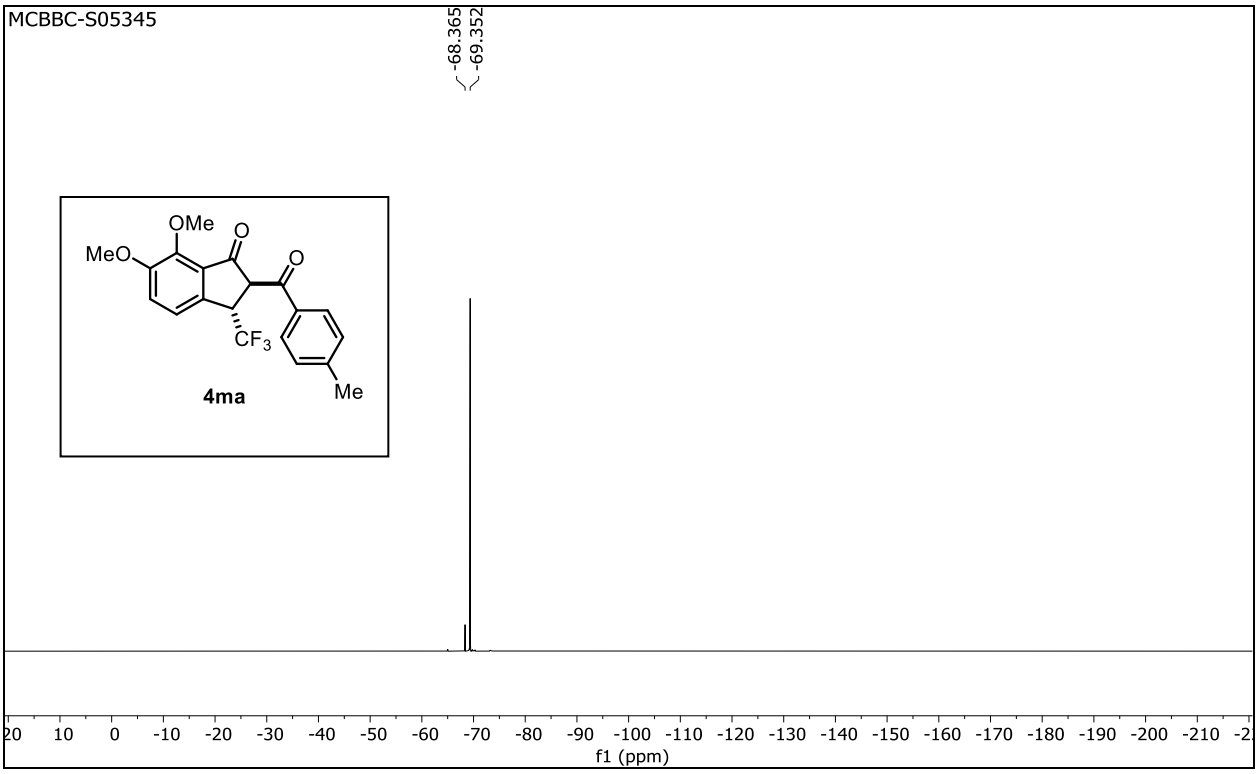

MCBBC-S00777
8.102
8.085
7.955
7.842
7.825
7.768
7.765
7.752
7.749
7.673
7.650
7.533
7.517
7.501
7.476
7.473
7.459
7.444
7.442
7.382
7.366
7.260 CDCl3
5.028
5.021
4.993
4.989
4.971
4.964
2.472
O
O
Ph
CF3
Me
4ka
2.00
1.00
1.00
1.02
2.03
2.06
1.05
2.00
2.07
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

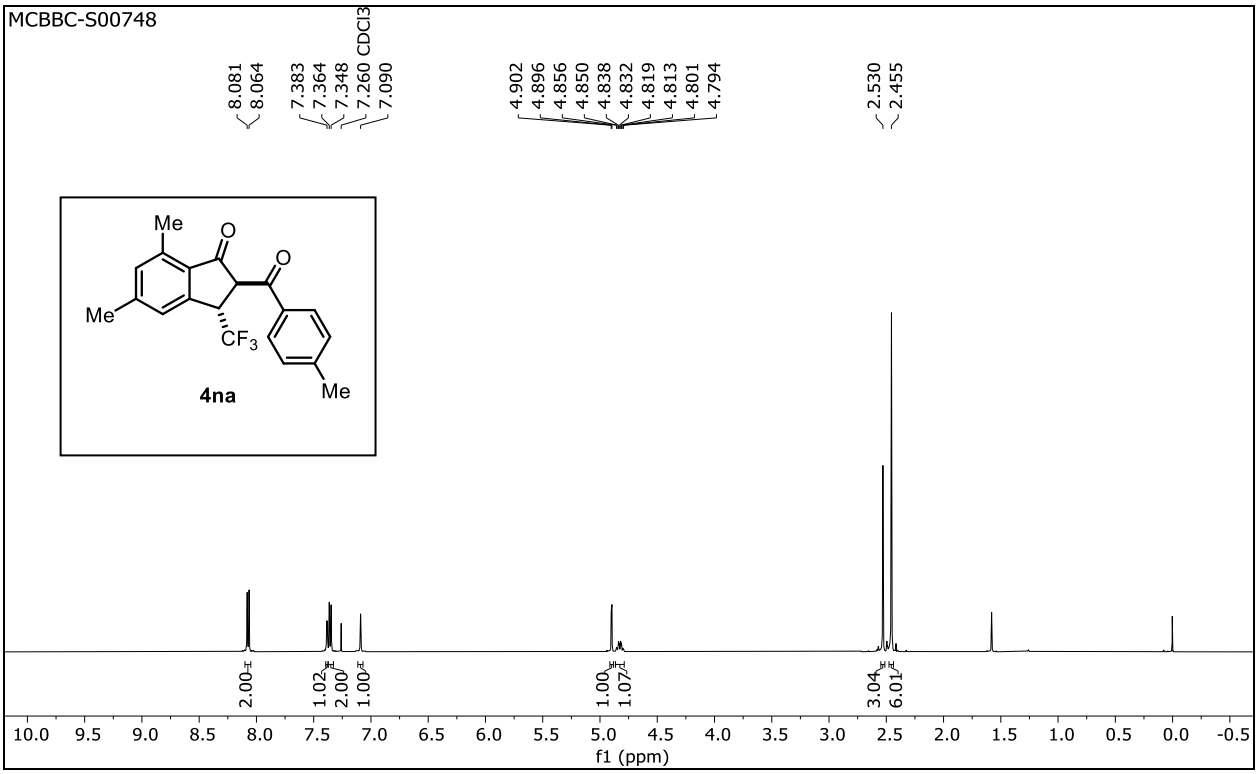

MCBBC-S00777
195.484
190.799
149.325
147.672
147.654
145.509
139.619
134.513
133.051
130.578
129.657
129.616
129.429
129.269
129.013
127.785
127.443
125.559
125.530
125.229
123.016
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
58.111
46.454
46.220
45.986
45.752
21.939
O
O
Ph
CF3
Me
4ka
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

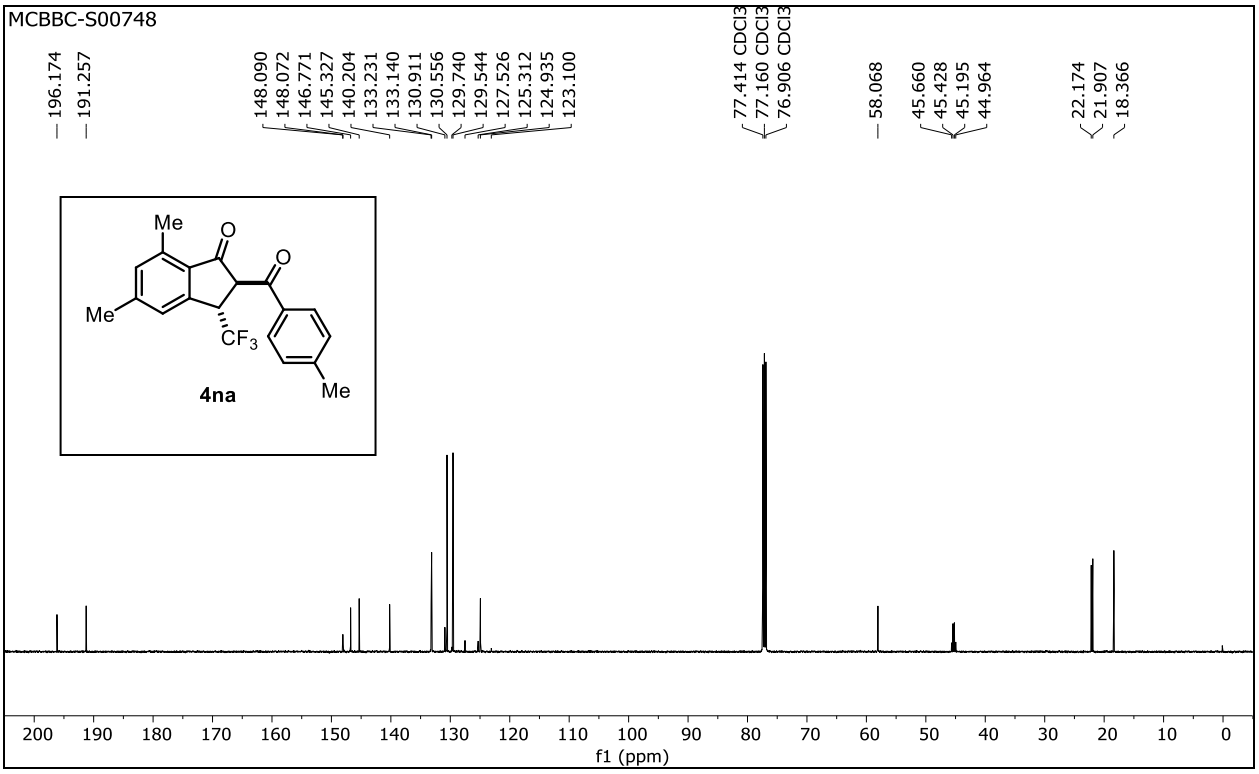

MCBBC-S00777
-68.705
O
O
Ph
CF3
Me
4ka
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

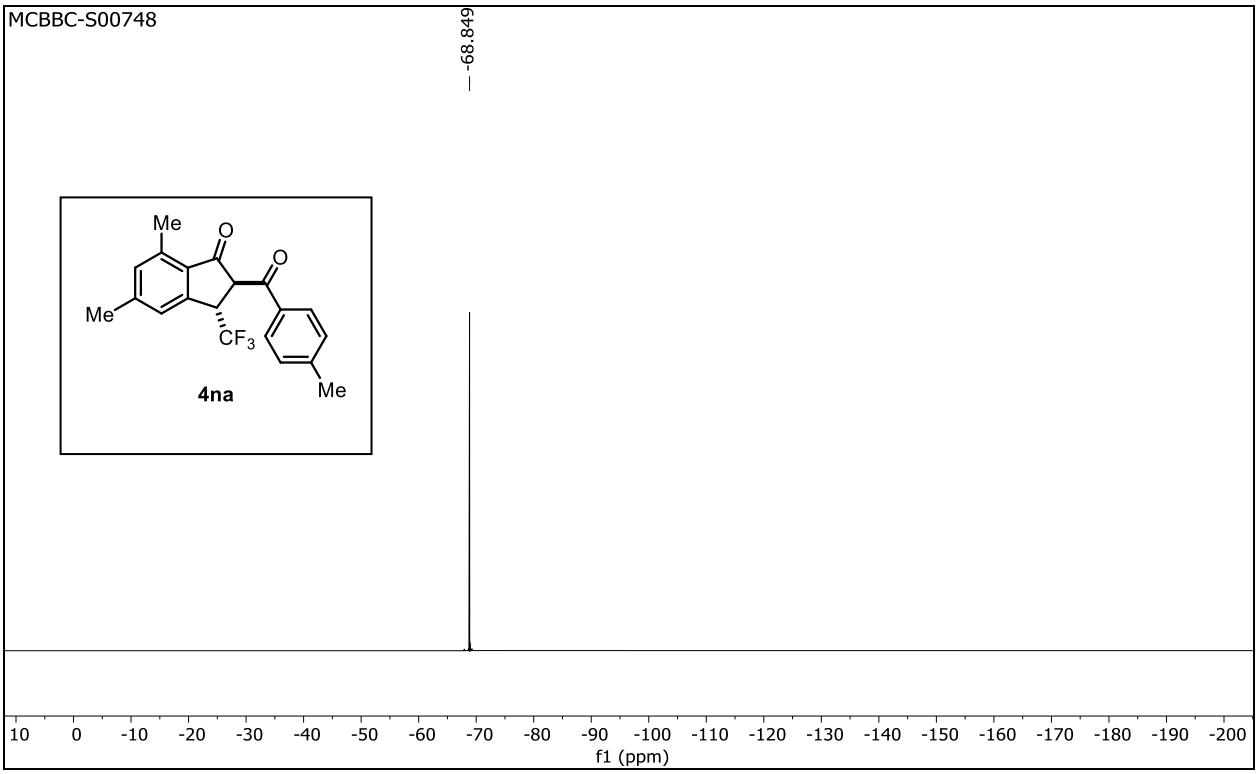

MCBBC-S05345
15.298
8.065
8.048
7.407
7.390
7.353
7.337
7.280
7.263
7.260 CDCl3
4.908
4.901
4.816
4.810
4.799
4.793
4.781
4.774
4.762
4.756
3.939
3.906
2.449
OMe
O
MeO
O
CF3
Me
OMe
OH
MeO
O
CF3
Me
4ma (keto:enol = 7.1:1)
0.14
2.01
1.00
2.03
1.09
1.02
1.07
3.06
3.00
3.00
f1 (ppm)

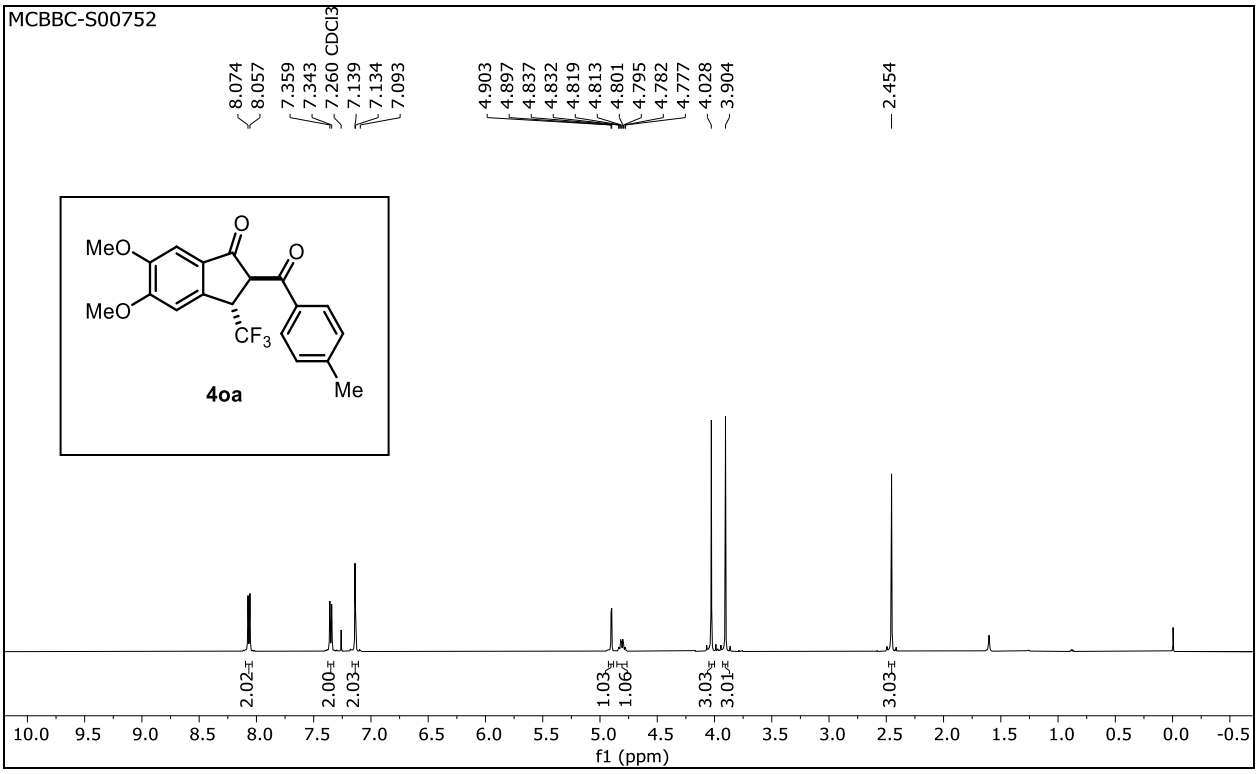

MCBBC-S05345
193.567
190.888
153.466
148.075
145.428
138.969
138.950
133.031
130.571
129.651
129.551
129.369
128.203
127.442
125.230
123.016
121.840
120.470
118.332
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
62.095
58.690
56.856
45.206
44.972
44.738
44.504
21.917
OMe
O
MeO
O
CF3
Me
4ma
f1 (ppm)

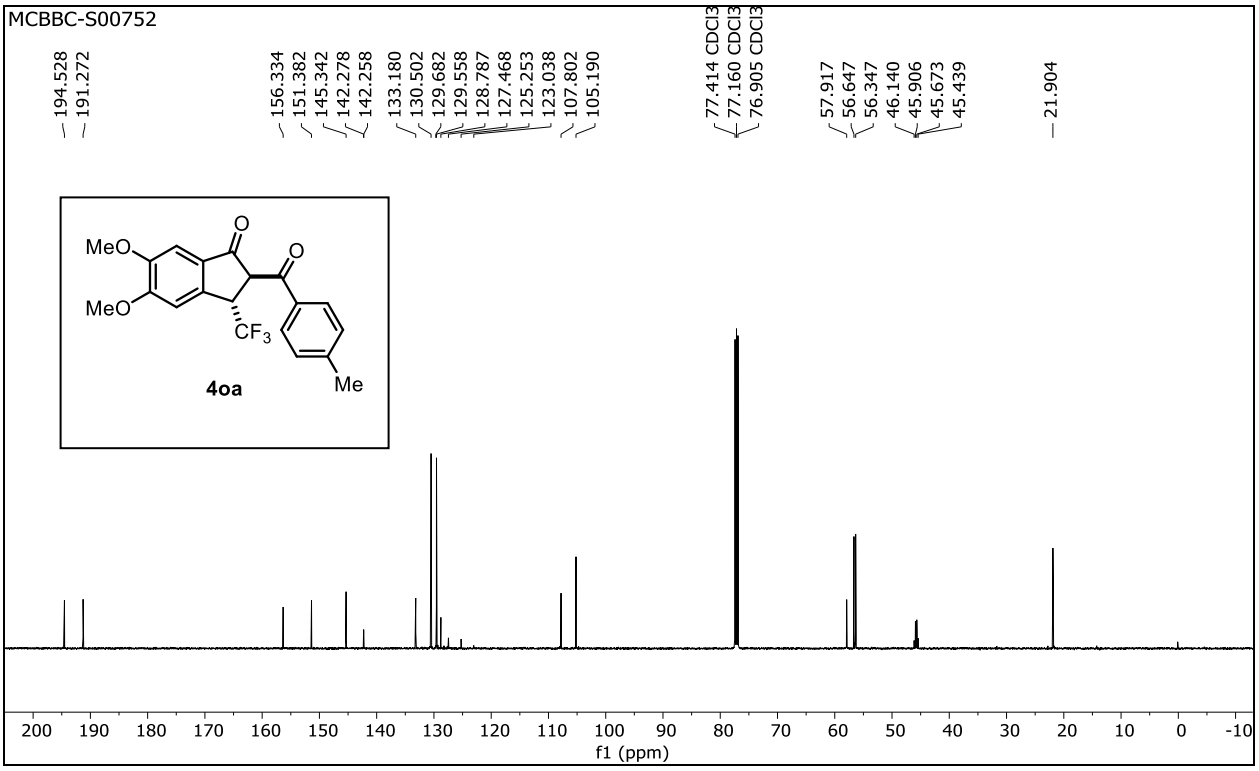

MCBBC-S05345
-68.365
-69.352
OMe
MeO
O
O
CF3
Me
4ma
f1 (ppm)

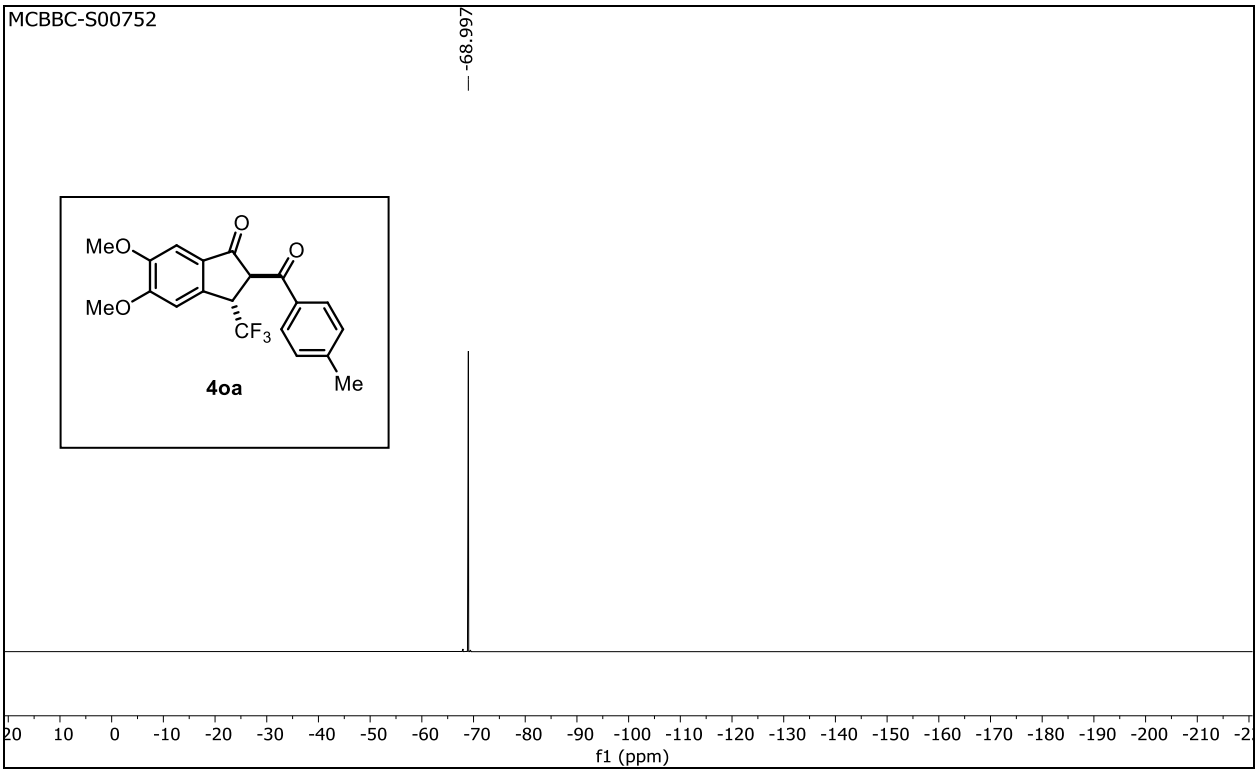

MCBBC-S00748
8.081
8.064
7.383
7.364
7.348
7.260 CDCl3
7.090
4.902
4.896
4.856
4.850
4.838
4.832
4.819
4.813
4.801
4.794
2.530
2.455
Me
O
O
Me
CF3
Me
4na
2.00
1.02
2.00
1.00
1.00
1.07
3.04
6.01
f1 (ppm)

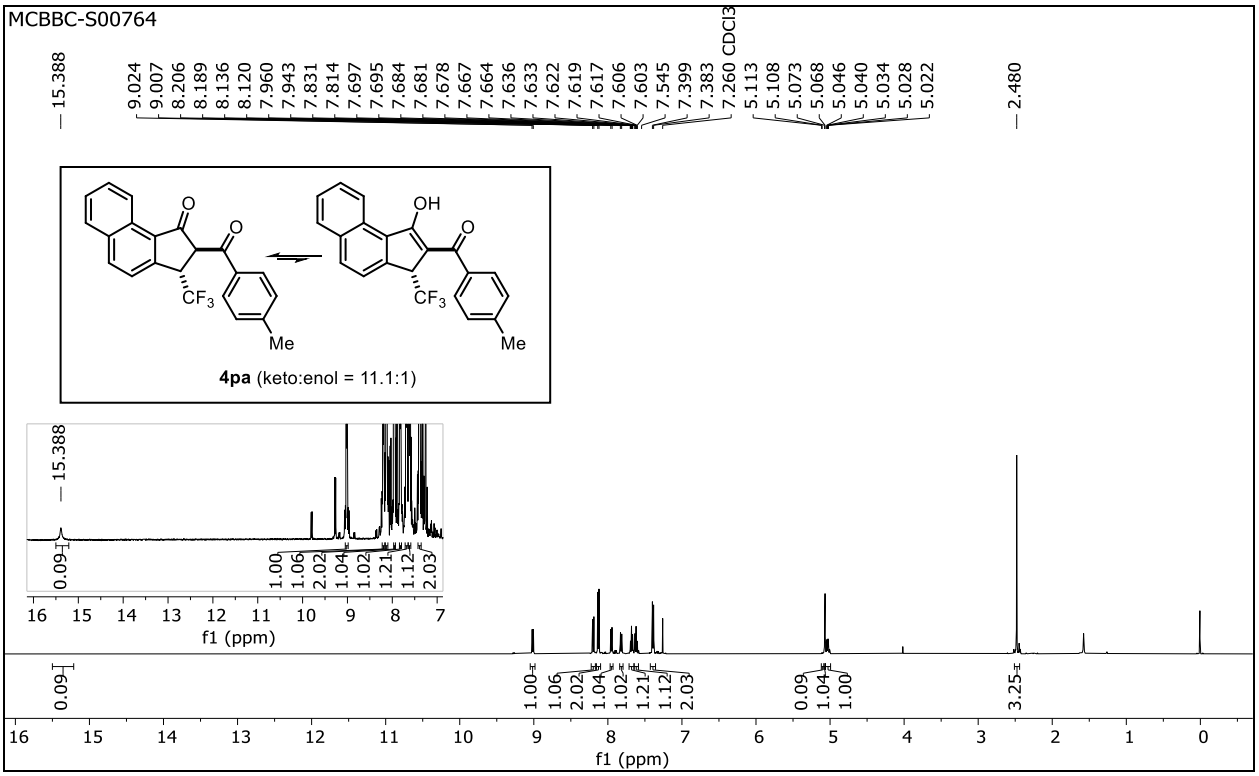

MCBBC-S00748
196.174
191.257
148.090
148.072
146.771
145.327
140.204
133.231
133.140
130.911
130.556
129.740
129.544
127.526
125.312
124.935
123.100
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
58.068
45.660
45.428
45.195
44.964
22.174
21.907
18.366
Me
O
O
Me
CF3
Me
4na
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

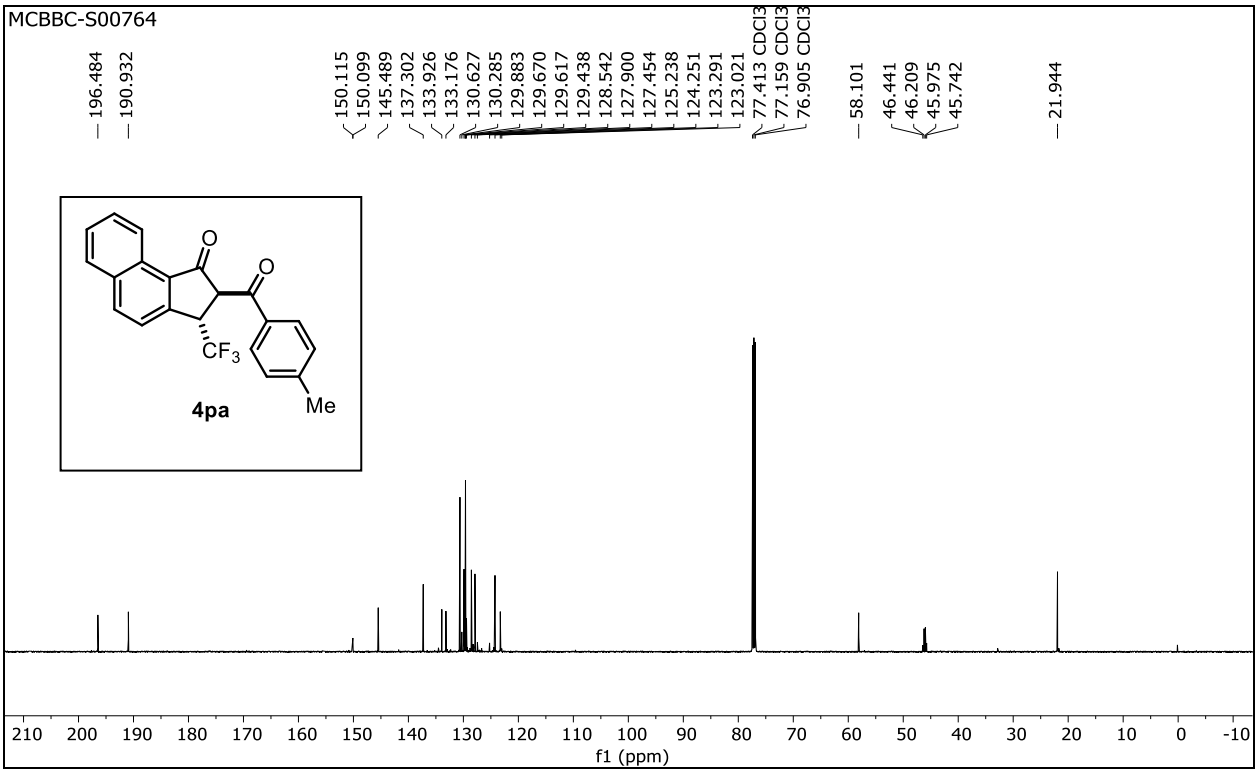

MCBBC-S00748
-68.849
Me
O
O
Me
CF3
Me
4na
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200
f1 (ppm)

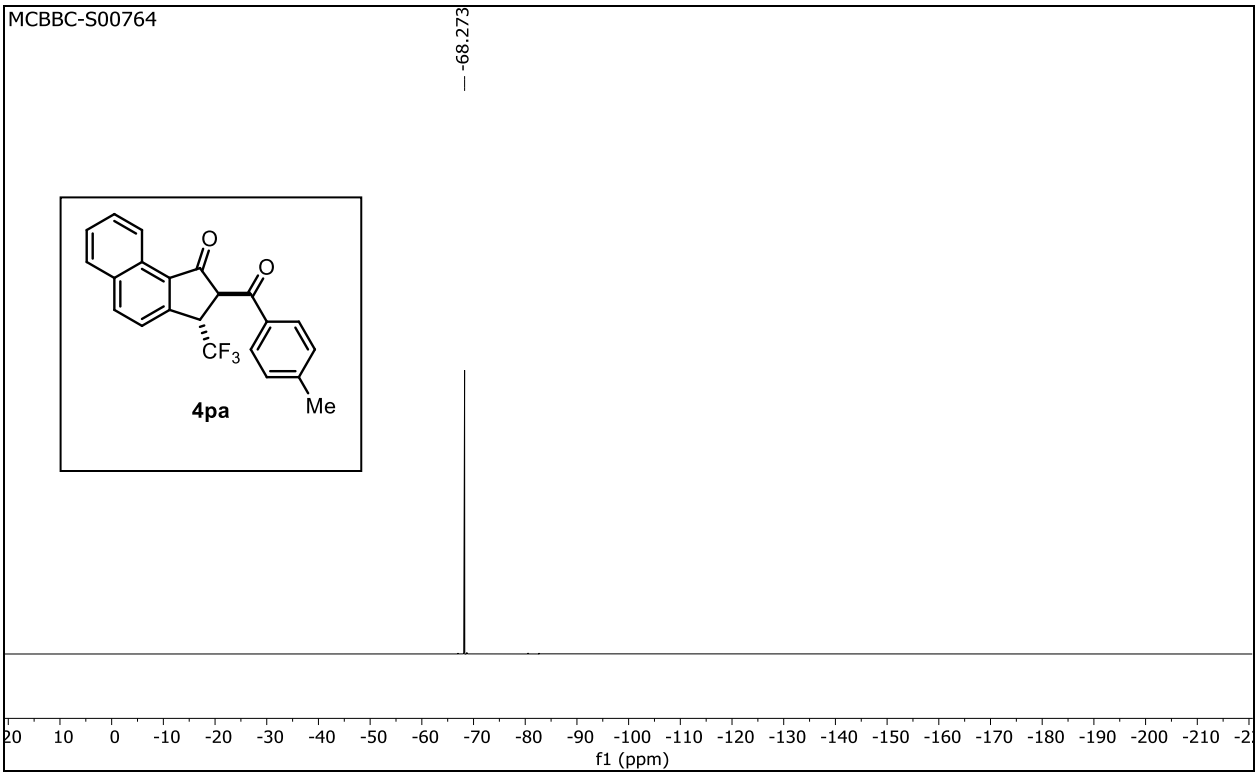

MCBBC-S00752
8.074
8.057
7.359
7.343
7.260 CDCl3
7.139
7.134
7.093
4.903
4.897
4.837
4.832
4.819
4.813
4.801
4.795
4.782
4.777
4.028
3.904
2.454
MeO
MeO
O
O
CF3
Me
4oa
2.02
2.00
2.03
1.03
1.06
3.03
3.01
3.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

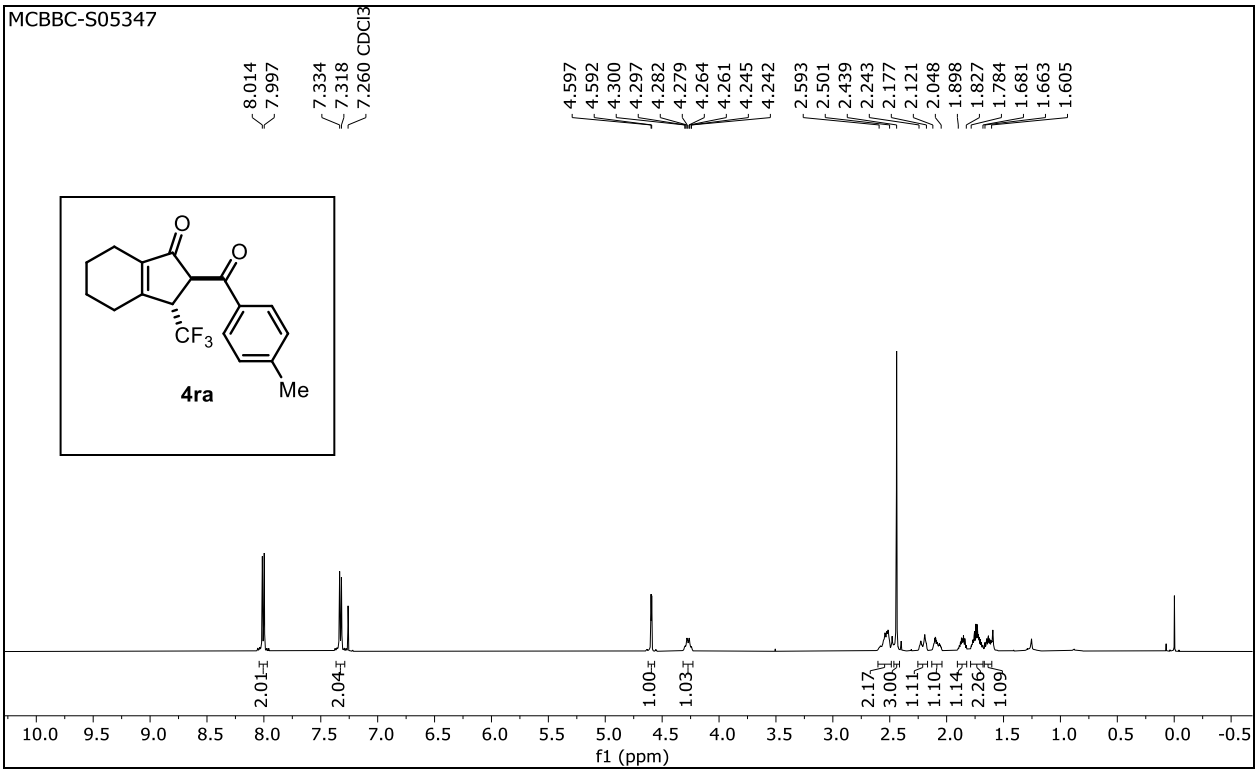

MCBBC-S00752
194.528
191.272
156.334
151.382
145.342
142.278
142.258
133.180
130.502
129.682
129.558
128.787
127.468
125.253
123.038
107.802
105.190
77.414 CDCl3
77.160 CDCl3
76.905 CDCl3
57.917
56.647
56.347
46.140
45.906
45.673
45.439
21.904
MeO
MeO
O
O
CF3
Me
4oa
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

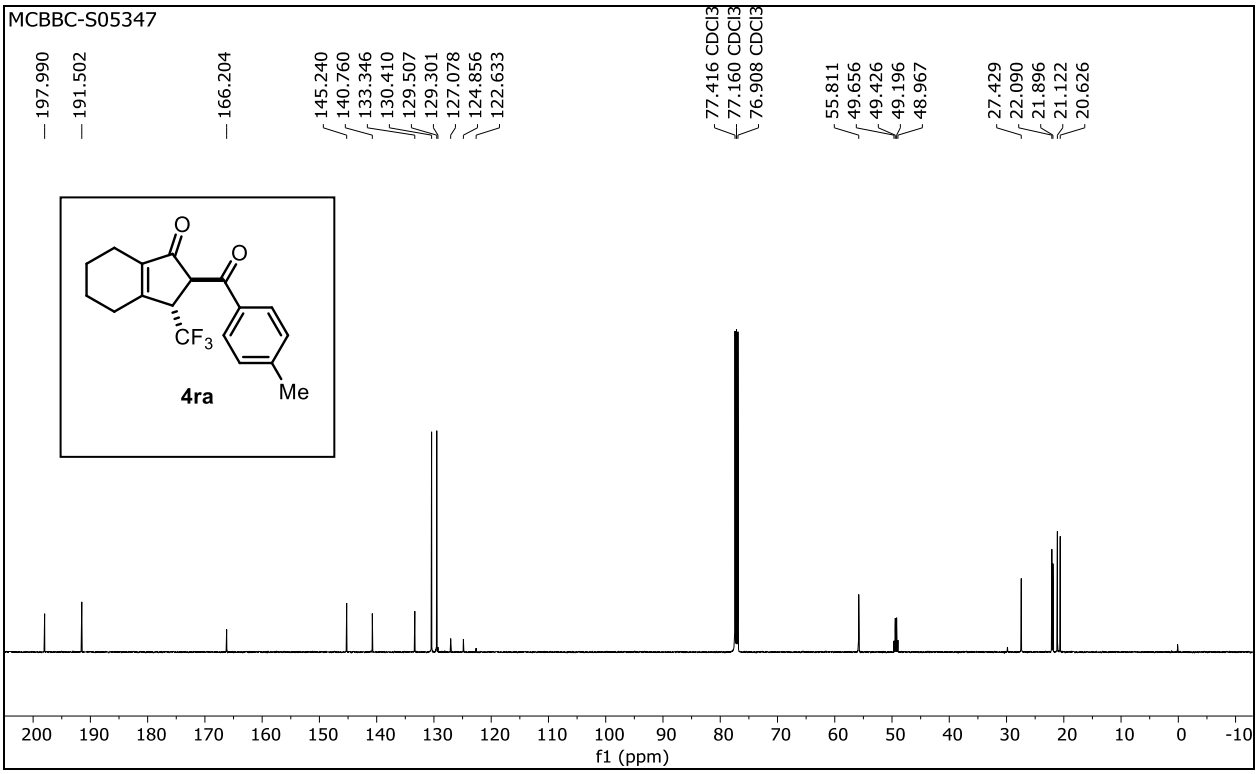

MCBBC-S00752
-68.997
MeO
MeO
O
O
CF3
Me
4oa
f1 (ppm)

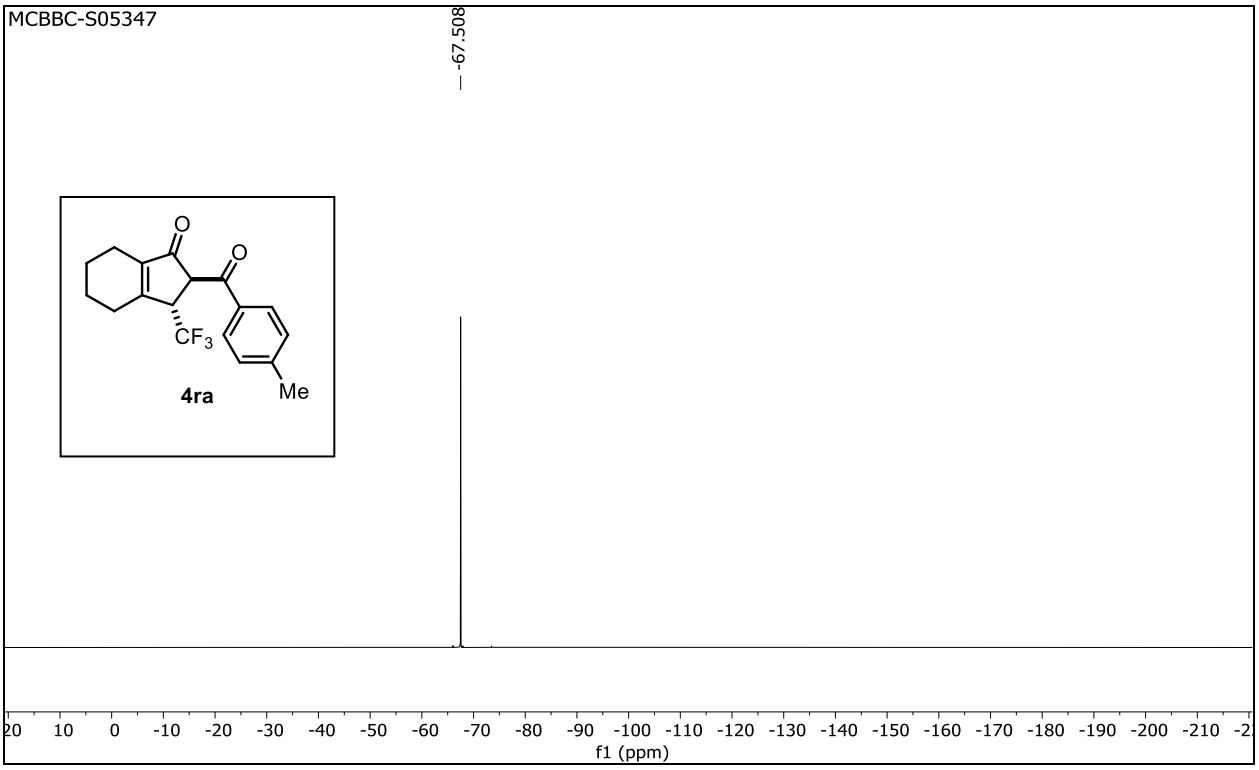

MCBBC-S00764
15.388
9.024
9.007
8.206
8.189
8.136
8.120
7.960
7.943
7.831
7.814
7.697
7.695
7.684
7.681
7.678
7.667
7.664
7.636
7.633
7.622
7.619
7.617
7.606
7.603
7.545
7.399
7.383
7.260 CDCl3
5.113
5.108
5.073
5.068
5.046
5.040
5.034
5.028
5.022
2.480
OH
CF3
Me
4pa (keto:enol = 11.1:1)
f1 (ppm)

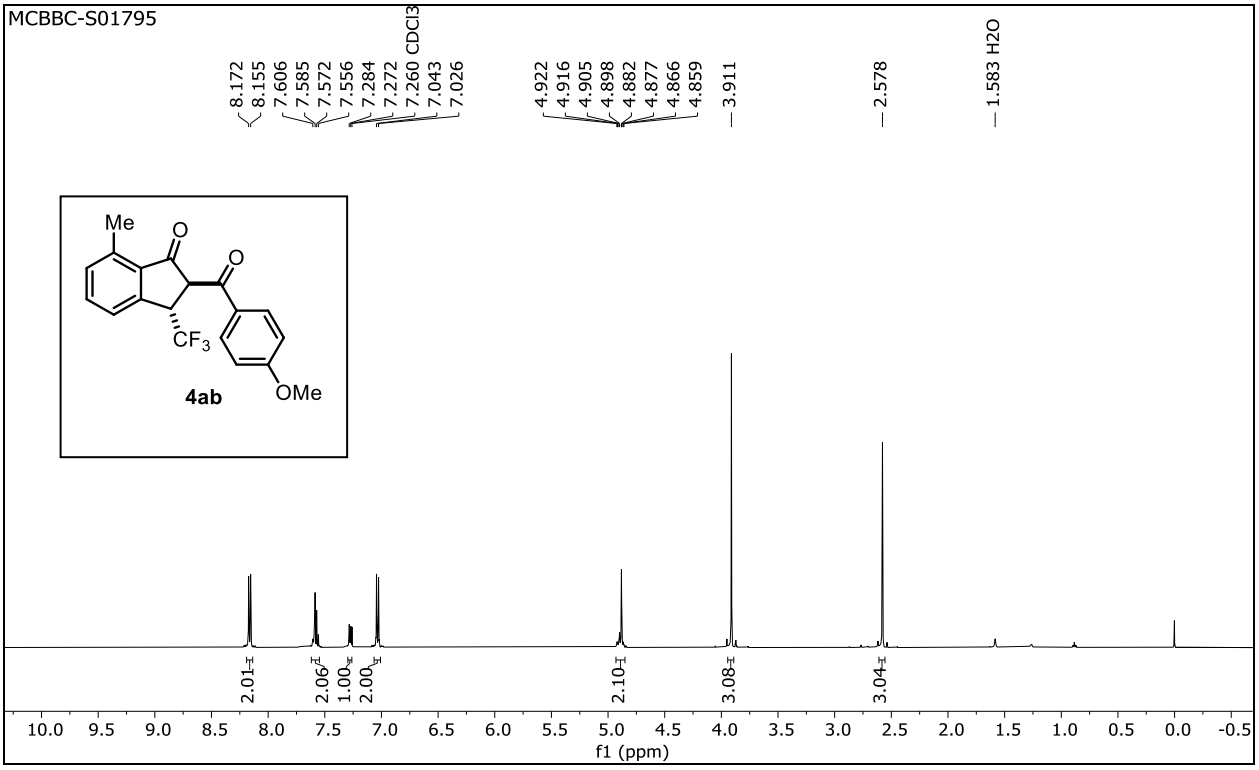

MCBBC-S00764
196.484
190.932
150.115
150.099
145.489
137.302
133.926
133.176
130.627
130.285
129.883
129.670
129.617
129.438
128.542
127.900
127.454
125.238
124.251
123.291
123.021
77.413 CDCl3
77.159 CDCl3
76.905 CDCl3
58.101
46.441
46.209
45.975
45.742
21.944
O
O
CF3
Me
4pa
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

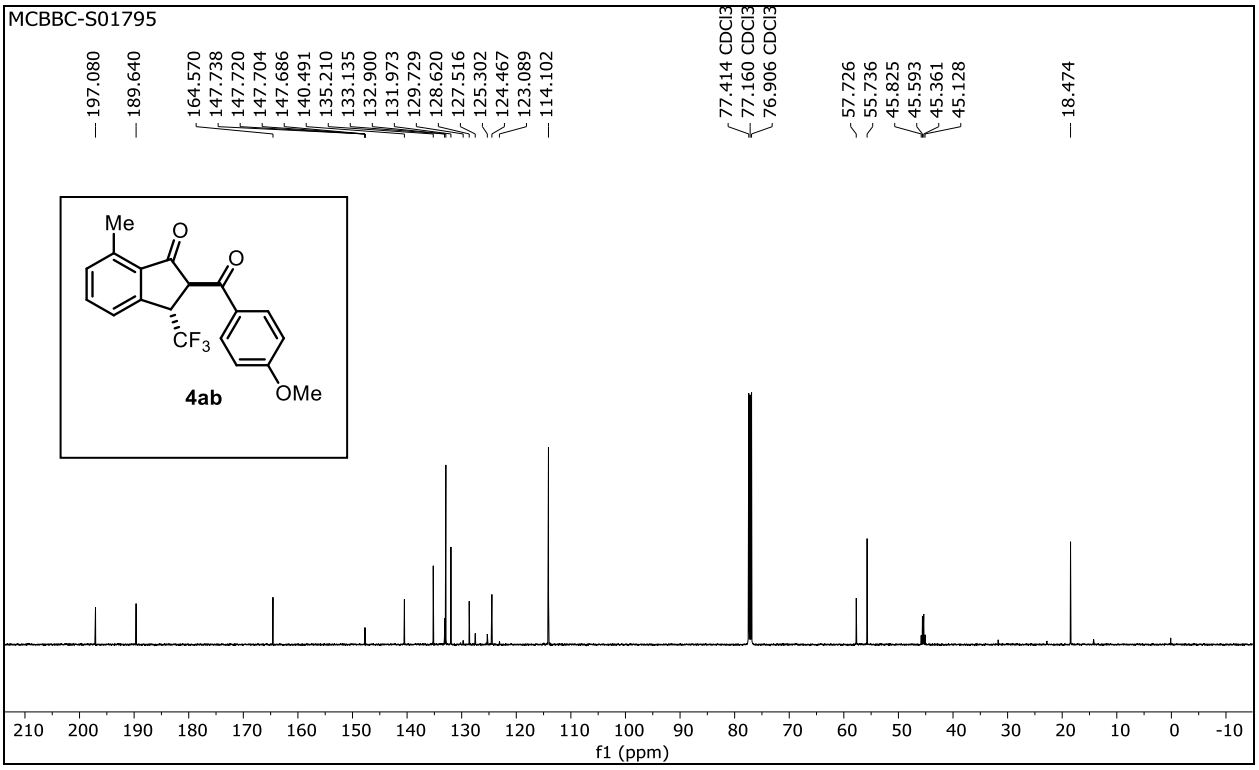

MCBBC-S00764
-68.273
O
O
CF3
Me
4pa
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

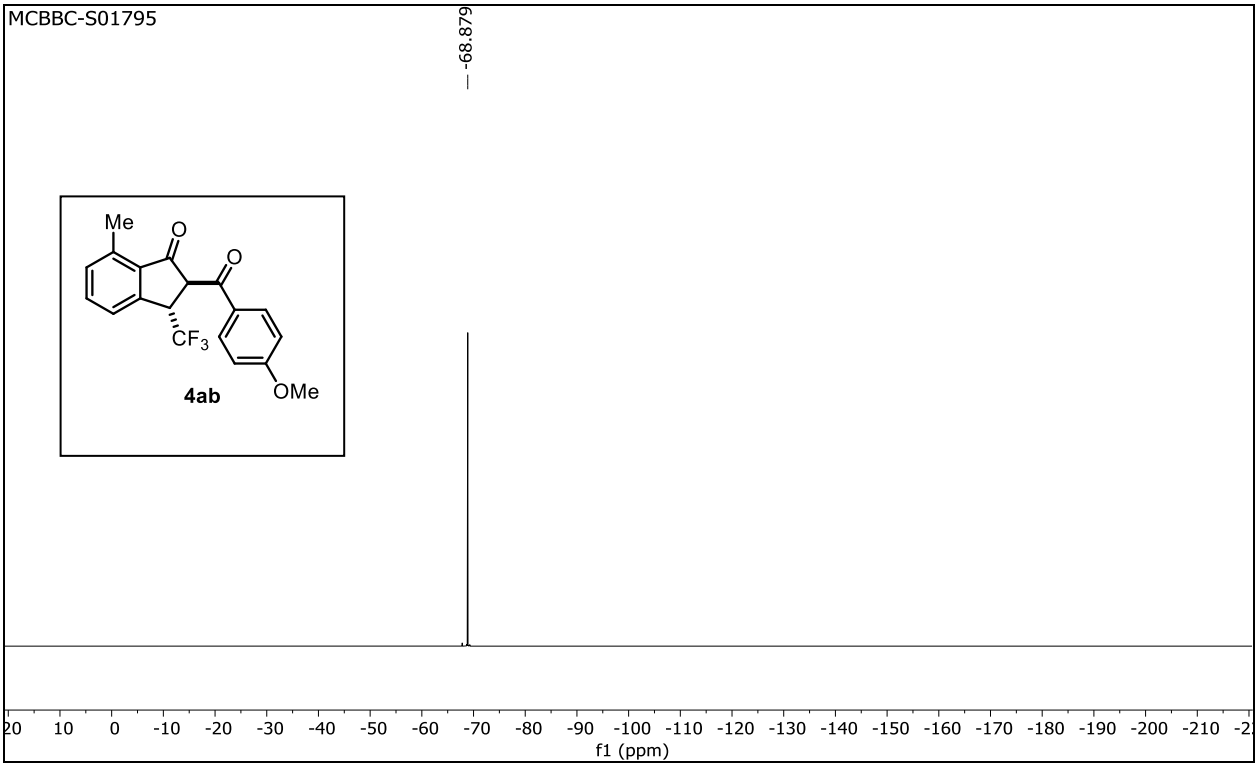

MCBBC-S05347
8.014
7.997
7.334
7.318
7.260 CDCl3
4.597
4.592
4.300
4.297
4.282
4.279
4.264
4.261
4.245
4.242
2.593
2.501
2.439
2.243
2.177
2.121
2.048
1.898
1.827
1.784
1.681
1.663
1.605
4ra
2.01
2.04
1.00
1.03
2.17
3.00
1.11
1.10
1.14
2.26
1.09
f1 (ppm)

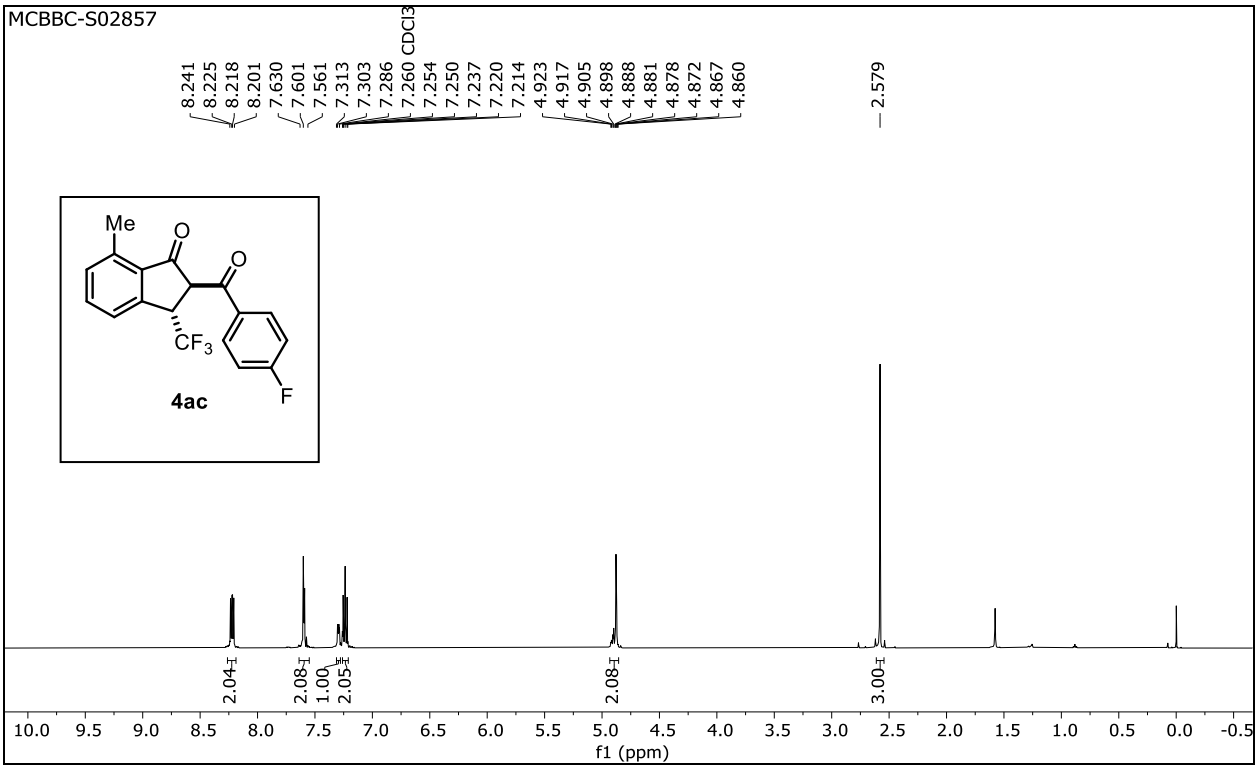

MCBBC-S05347
197.990
191.502
166.204
145.240
140.760
133.346
130.410
129.507
129.301
127.078
124.856
122.633
77.416 CDCl3
77.160 CDCl3
76.908 CDCl3
55.811
49.656
49.426
49.196
48.967
27.429
22.090
21.896
21.122
20.626
4ra
f1 (ppm)

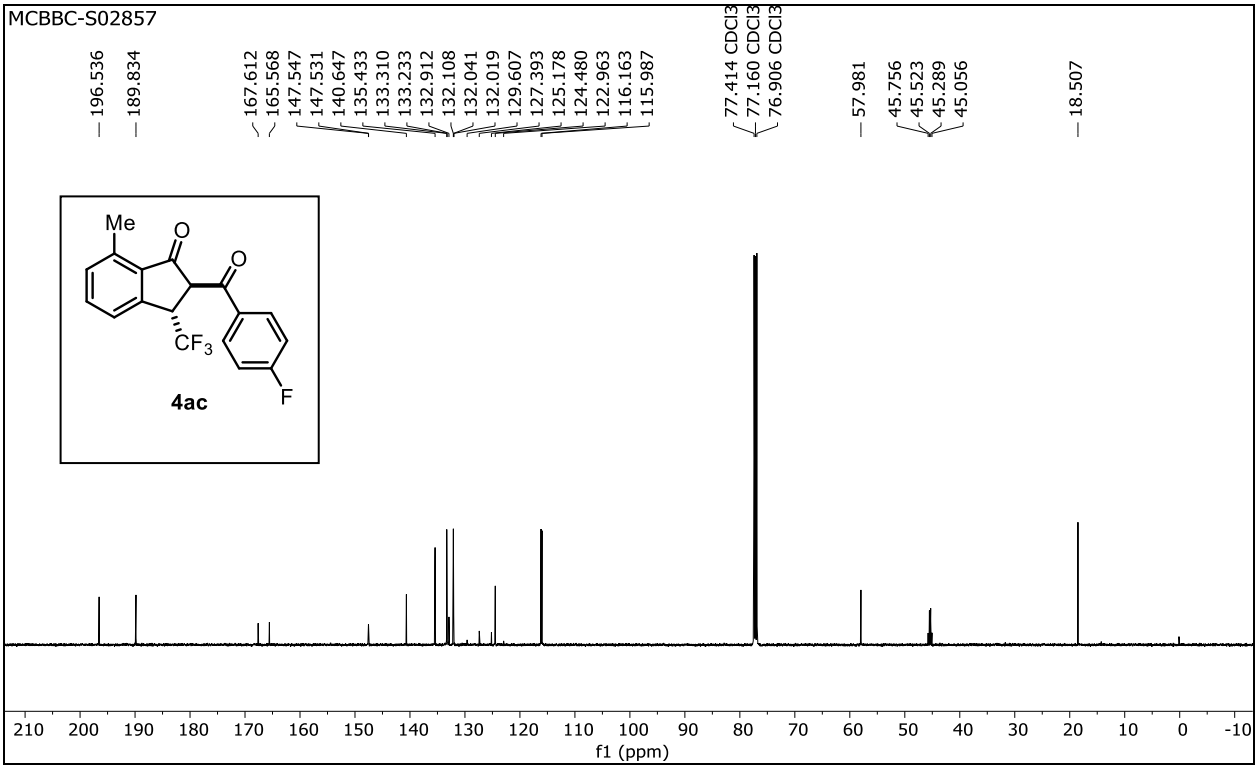

MCBBC-S05347
-67.508
O
O
CF3
Me
4ra
f1 (ppm)

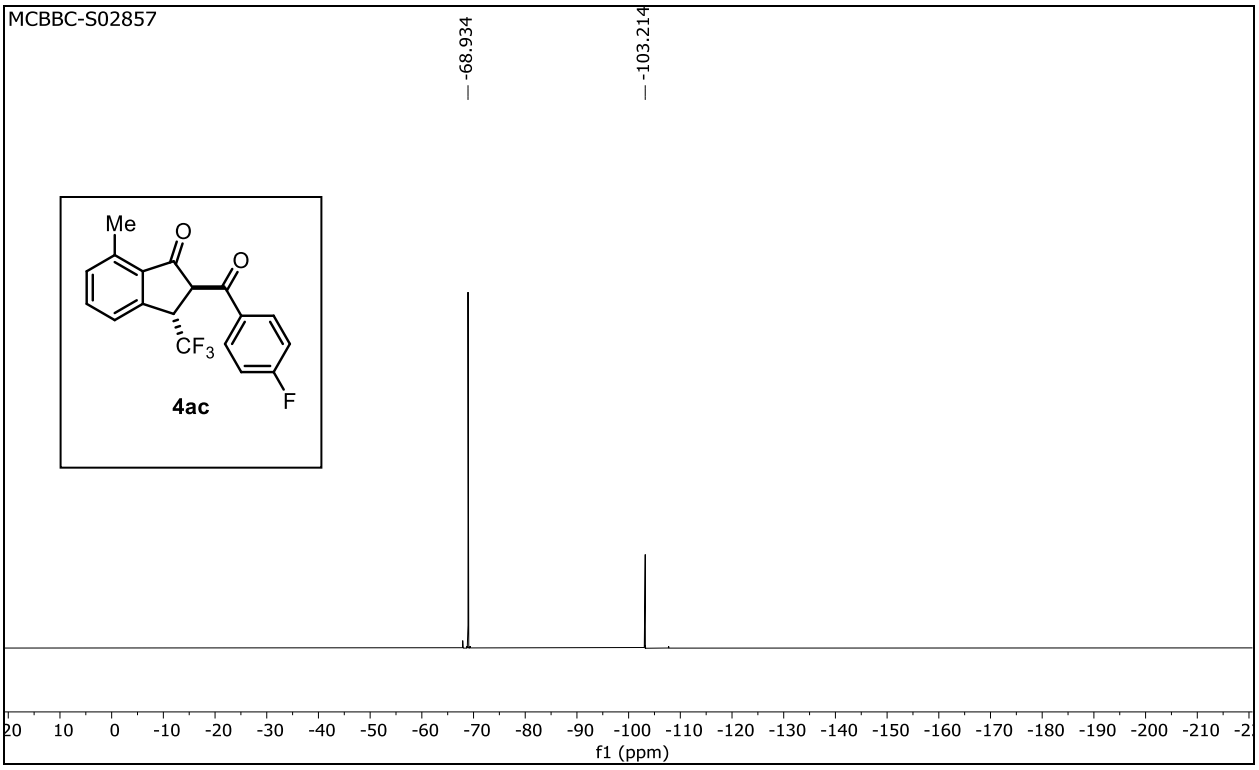

MCBBC-S01795
8.172
8.155
7.606
7.585
7.572
7.556
7.284
7.272
7.260 CDCl3
7.043
7.026
4.922
4.916
4.905
4.898
4.882
4.877
4.866
4.859
3.911
2.578
1.583 H2O
Me
O
O
CF3
OMe
4ab
2.01
2.06
1.00
2.00
2.10
3.08
3.04
f1 (ppm)

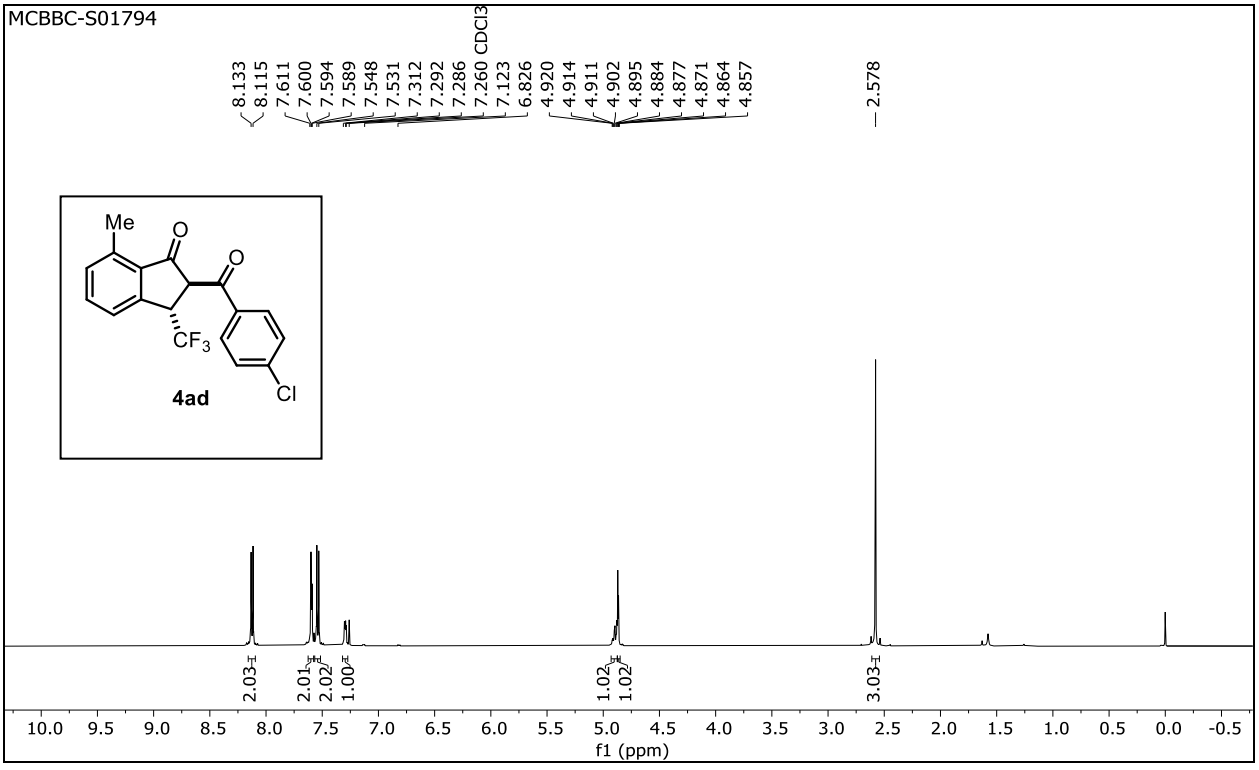

MCBBC-S01795
197.080
189.640
164.570
147.738
147.720
147.704
147.686
140.491
135.210
133.135
132.900
131.973
129.729
128.620
127.516
125.302
124.467
123.089
114.102
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
57.726
55.736
45.825
45.593
45.361
45.128
18.474
Me
O
O
CF3
OMe
4ab
f1 (ppm)

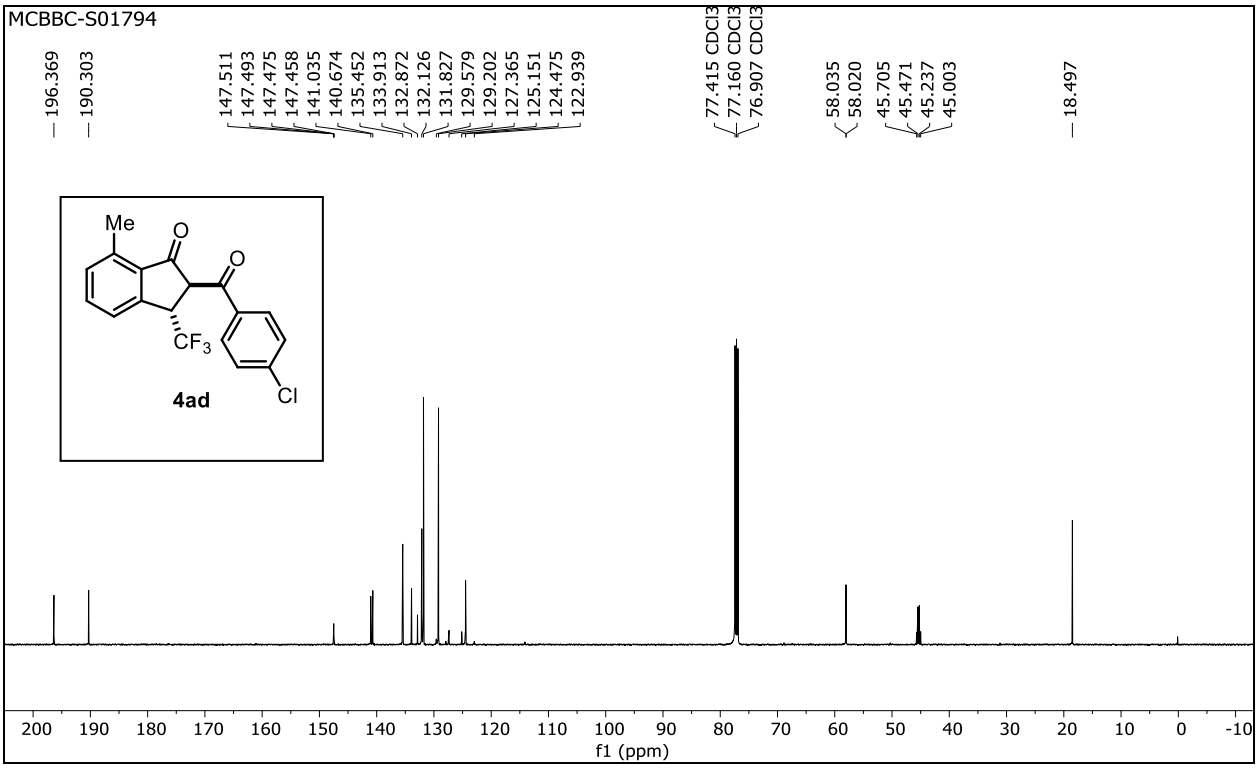

MCBBC-S01795
-68.879
Me
O
O
CF3
OMe
4ab
f1 (ppm)

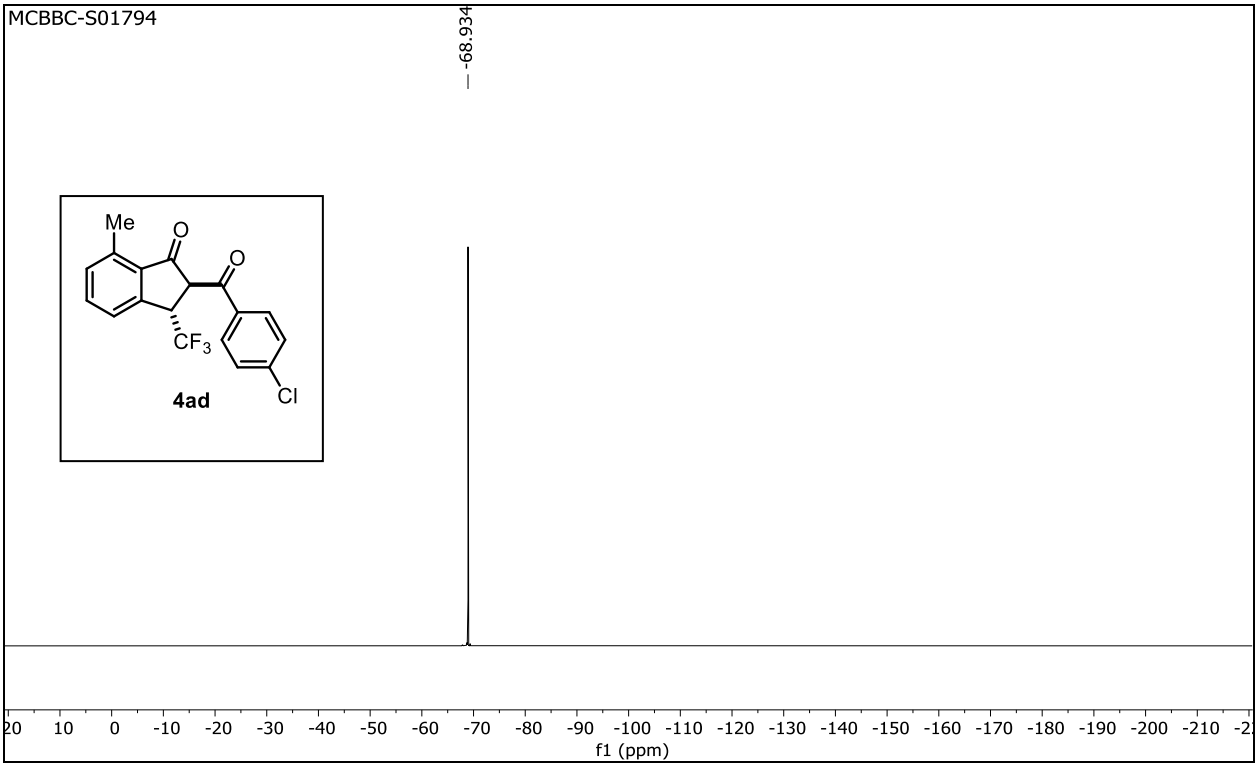

MCBBC-S02857
8.241
8.225
8.218
8.201
7.630
7.601
7.561
7.313
7.303
7.286
7.260 CDCl3
7.254
7.250
7.237
7.220
7.214
4.923
4.917
4.905
4.898
4.888
4.881
4.878
4.872
4.867
4.860
2.579
Me
O
O
CF3
F
4ac
2.04
2.08
1.00
2.05
2.08
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

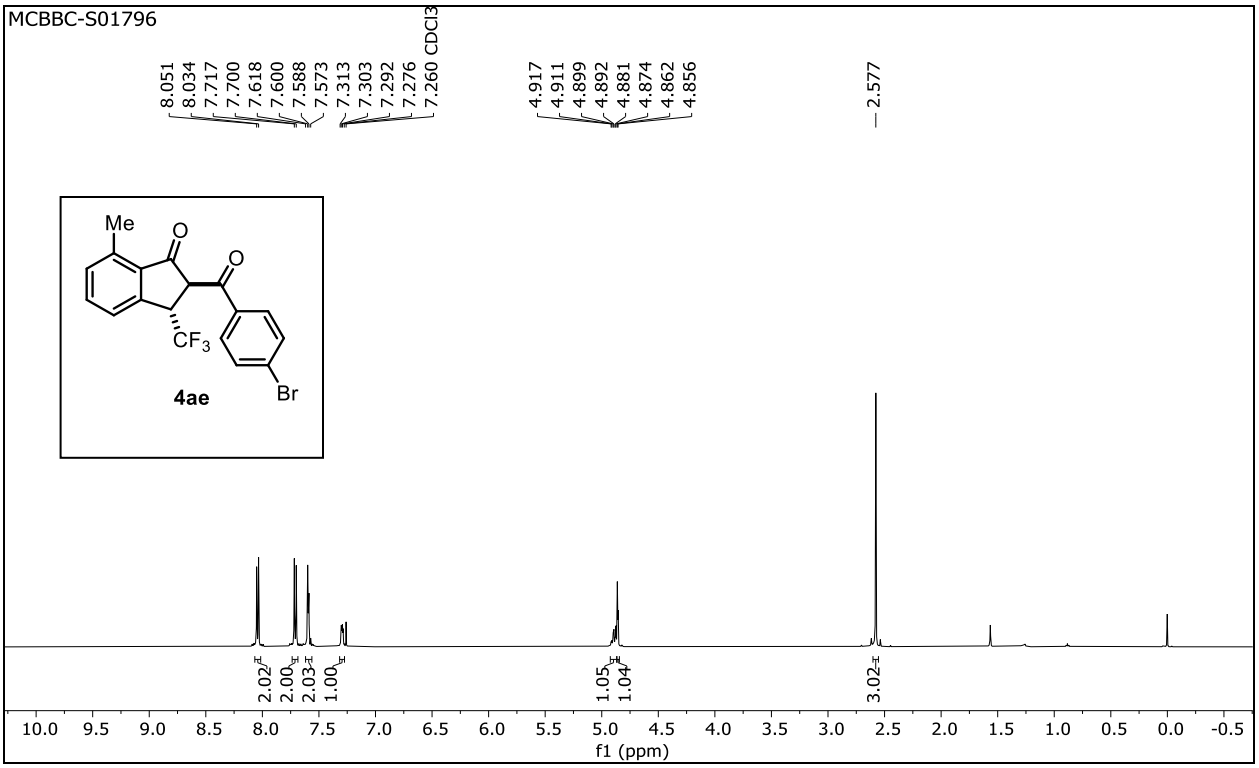

MCBBC-S02857
196.536
189.834
167.612
165.568
147.547
147.531
140.647
135.433
133.310
133.233
132.912
132.108
132.041
132.019
129.607
127.393
125.178
124.480
122.963
116.163
115.987
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
57.981
45.756
45.523
45.289
45.056
18.507
Me
O
O
CF3
F
4ac
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

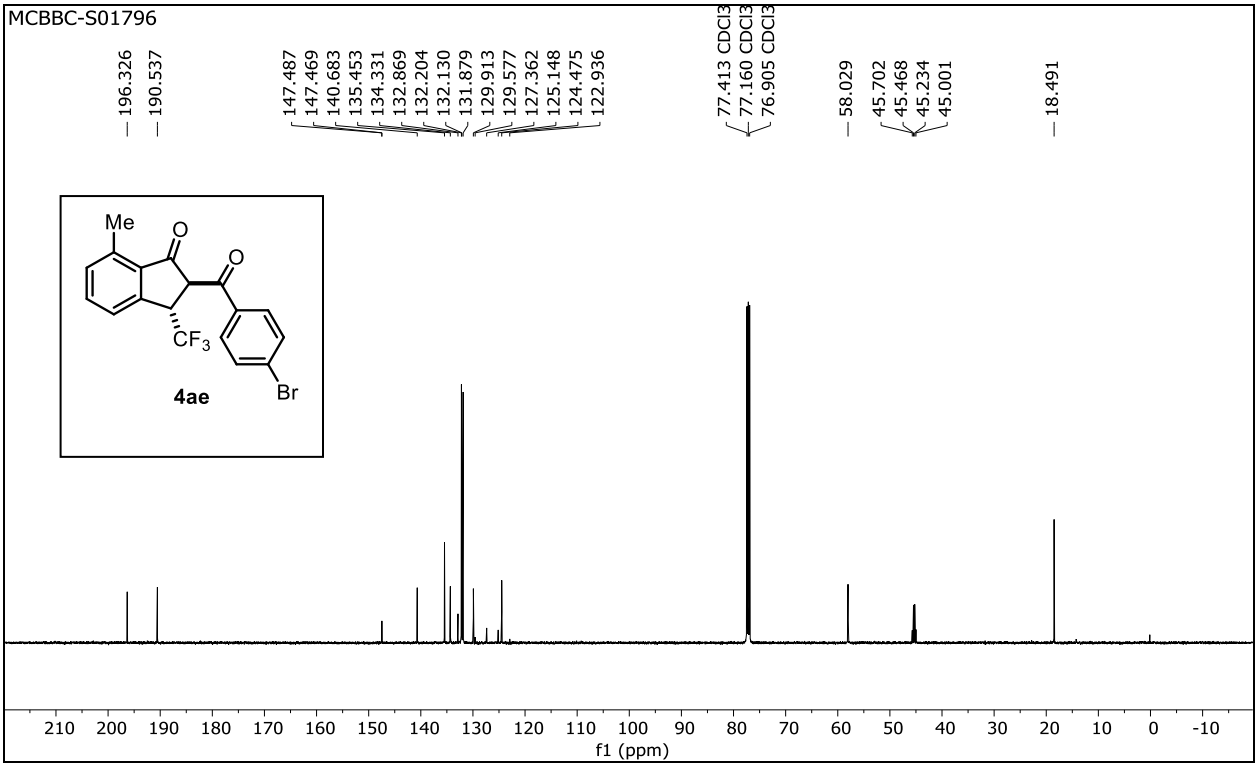

MCBBC-S02857
-68.934
-103.214
Me
O
O
CF3
F
4ac
f1 (ppm)

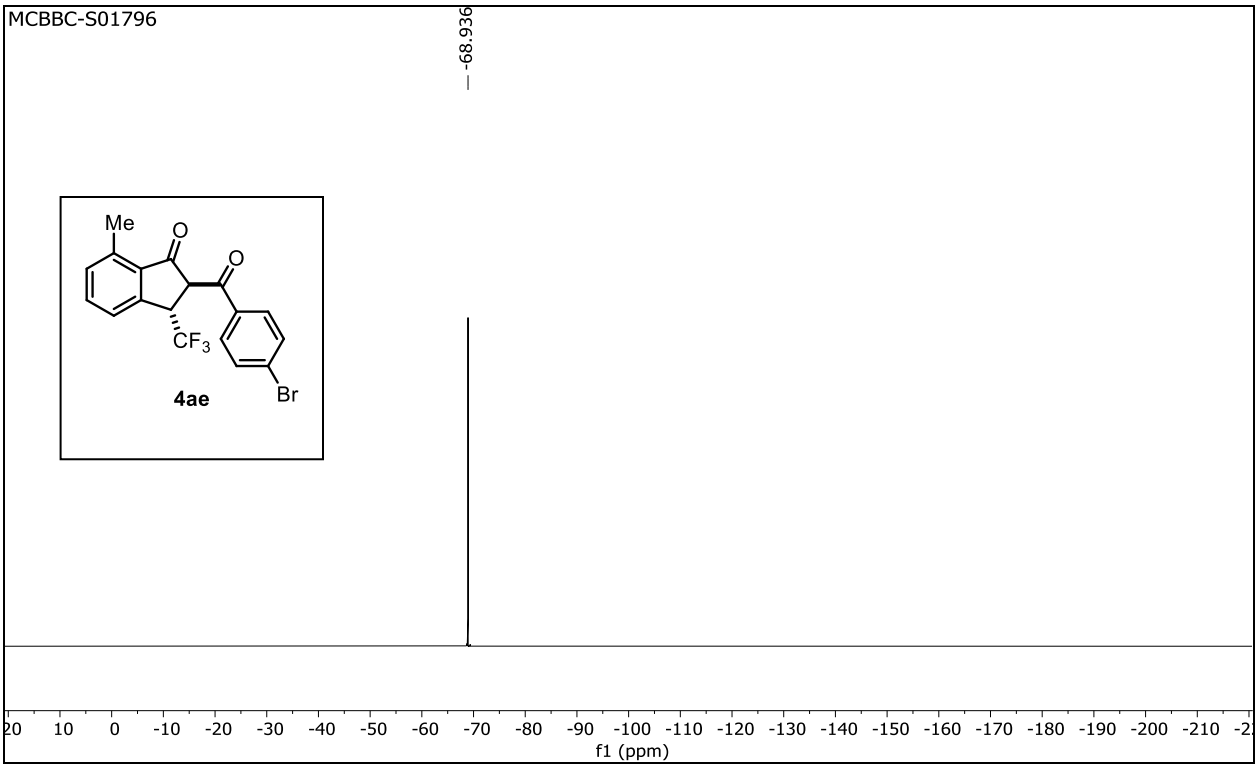

MCBBC-S01794
8.133
8.115
7.611
7.600
7.594
7.589
7.548
7.531
7.312
7.292
7.286
7.260 CDCl3
7.123
6.826
4.920
4.914
4.911
4.902
4.895
4.884
4.877
4.871
4.864
4.857
2.578
Me
O
O
CF3
Cl
4ad
2.03
2.01
2.02
1.00
1.02
1.02
3.03
f1 (ppm)

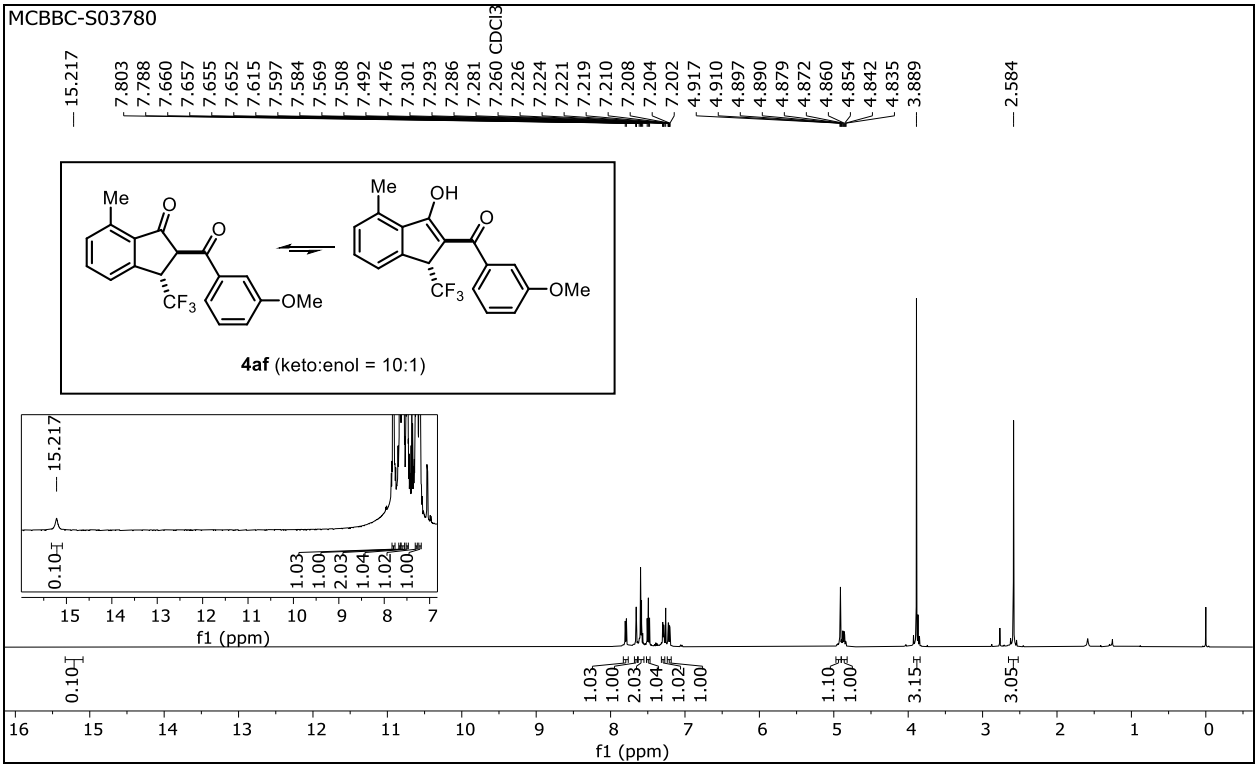

MCBBC-S01794
196.369
190.303
147.511
147.493
147.475
147.458
141.035
140.674
135.452
133.913
132.872
132.126
131.827
129.579
129.202
127.365
125.151
124.475
122.939
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
58.035
58.020
45.705
45.471
45.237
45.003
18.497
Me
O
O
CF3
Cl
4ad
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

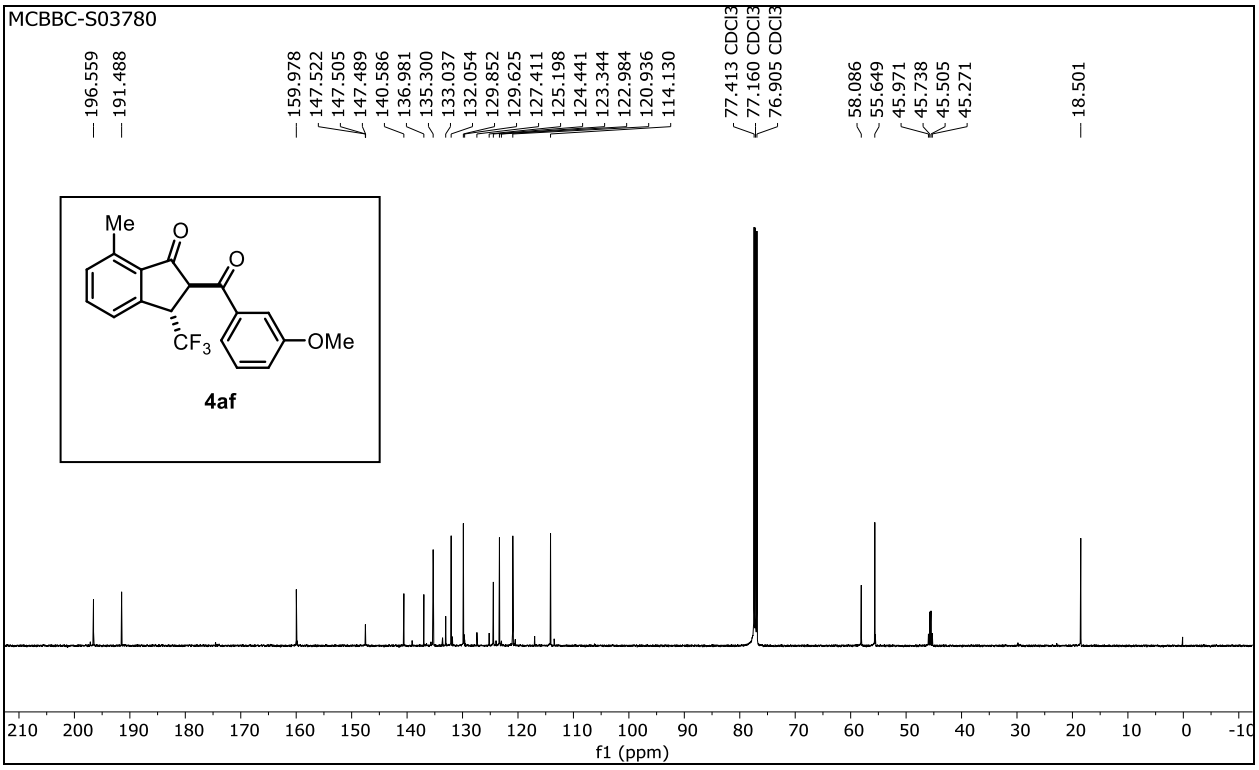

MCBBC-S01794
-68.934
Me
O
O
CF3
Cl
4ad
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

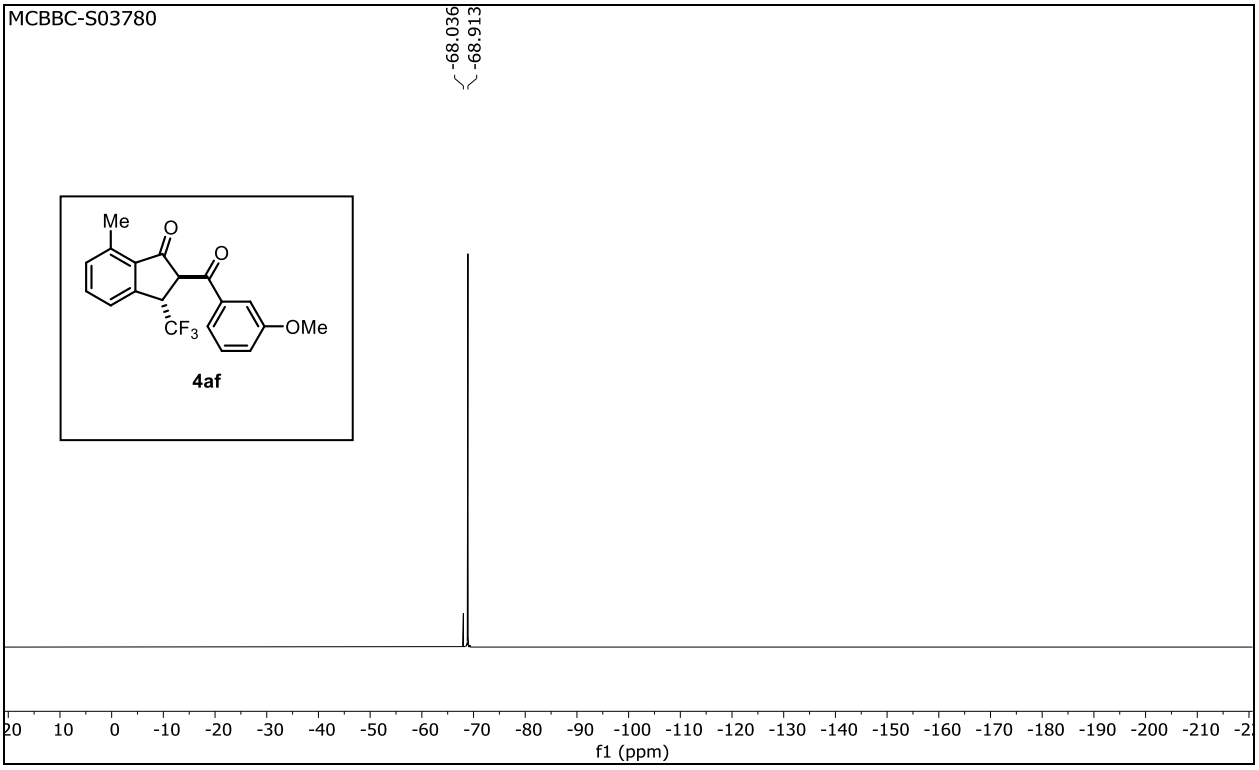

MCBBC-S01796
8.051
8.034
7.717
7.700
7.618
7.600
7.588
7.573
7.313
7.303
7.292
7.276
7.260 CDCl3
4.917
4.911
4.899
4.892
4.881
4.874
4.862
4.856
2.577
Me
O
O
CF3
Br
4ae
2.02
2.00
2.03
1.00
1.05
1.04
3.02
f1 (ppm)

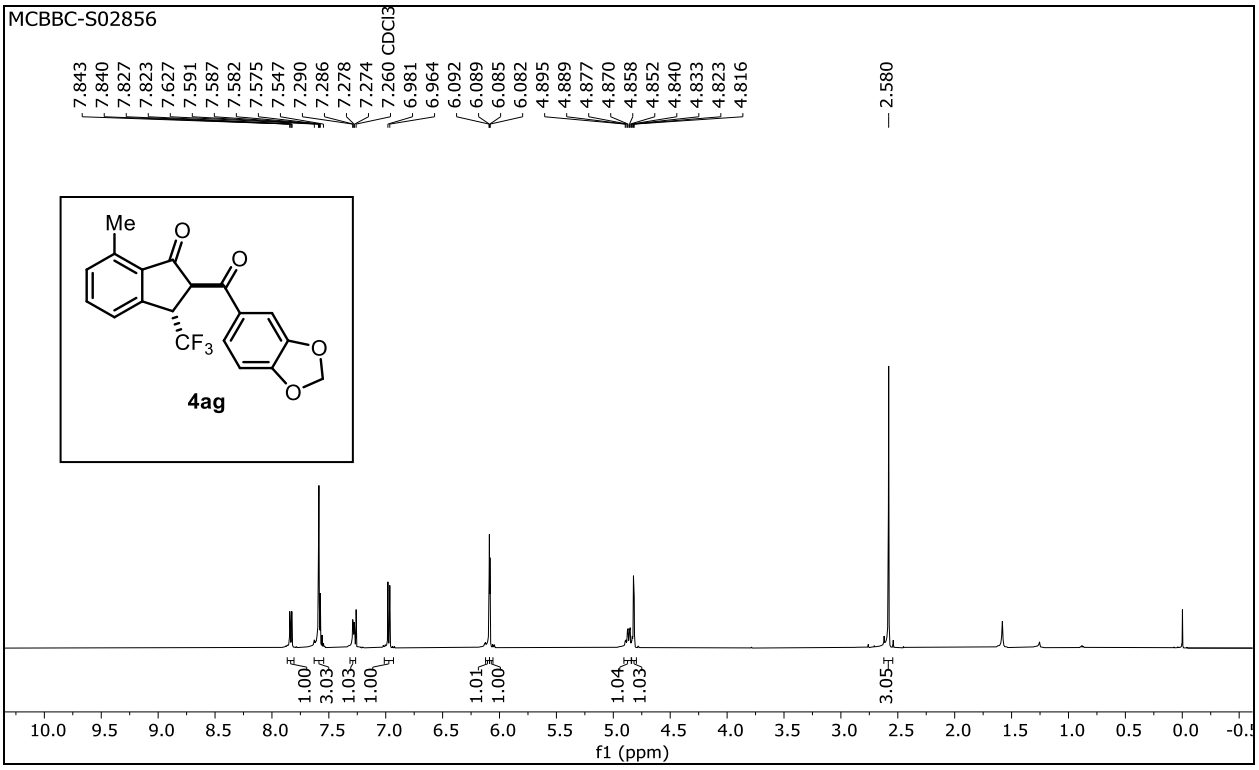

MCBBC-S01796
196.326
190.537
147.487
147.469
140.683
135.453
134.331
132.869
132.204
132.130
131.879
129.913
129.577
127.362
125.148
124.475
122.936
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
58.029
45.702
45.468
45.234
45.001
18.491
Me
O
O
CF3
Br
4ae
f1 (ppm)

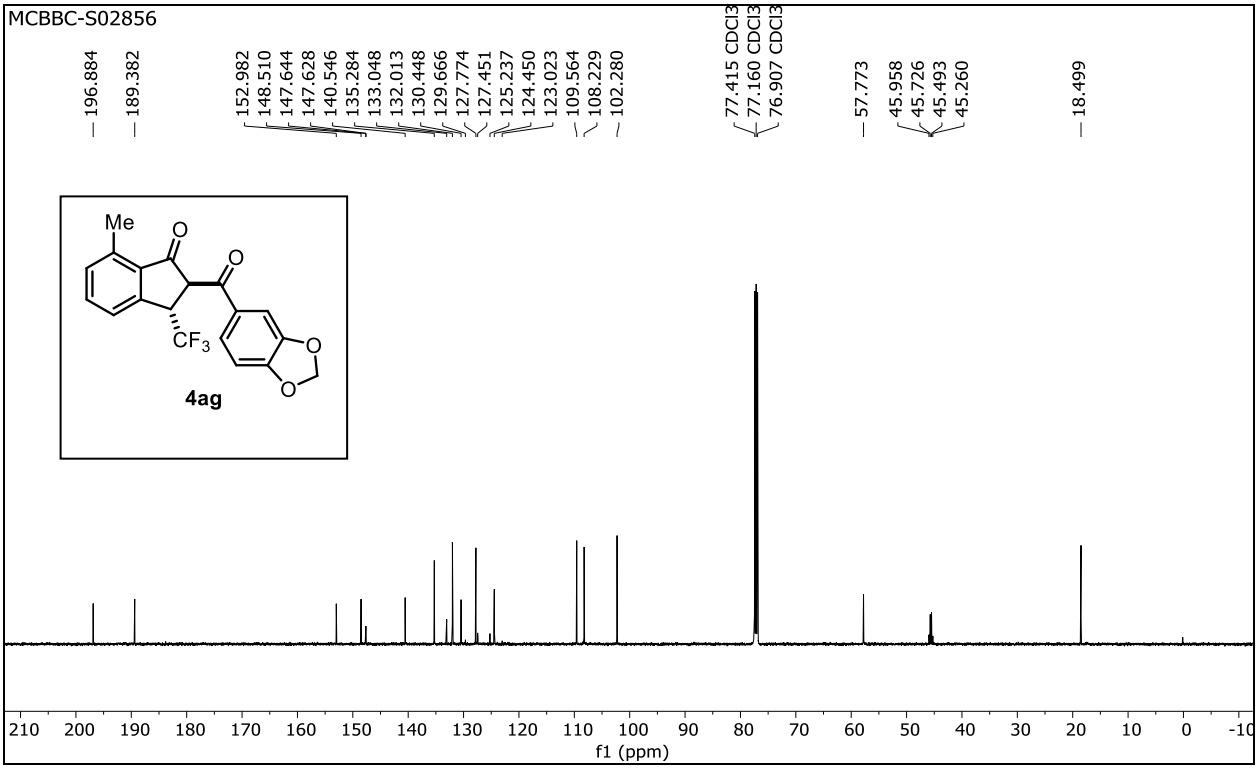

MCBBC-S01796
-68.936
Me
O
O
CF3
Br
4ae
f1 (ppm)

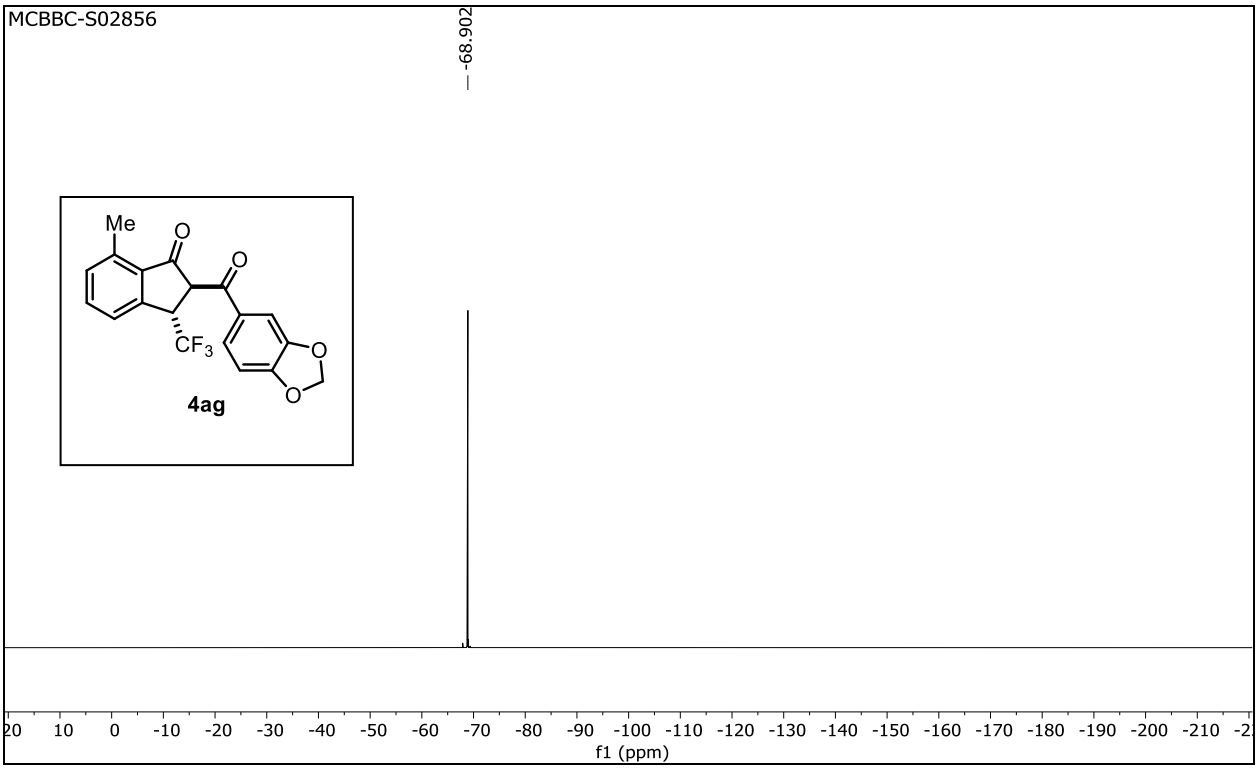

MCBBC-S03780
15.217
7.803
7.788
7.660
7.657
7.655
7.652
7.615
7.597
7.584
7.569
7.508
7.492
7.476
7.301
7.293
7.286
7.281
7.260 CDCl3
7.226
7.224
7.221
7.219
7.210
7.208
7.204
7.202
4.917
4.910
4.897
4.890
4.879
4.872
4.860
4.854
4.842
4.835
3.889
2.584
Me
O
O
CF3
OMe
Me
OH
O
CF3
OMe
4af (keto:enol = 10:1)
0.10
1.03
1.00
2.03
1.04
1.02
1.00
1.10
1.00
3.15
3.05
f1 (ppm)

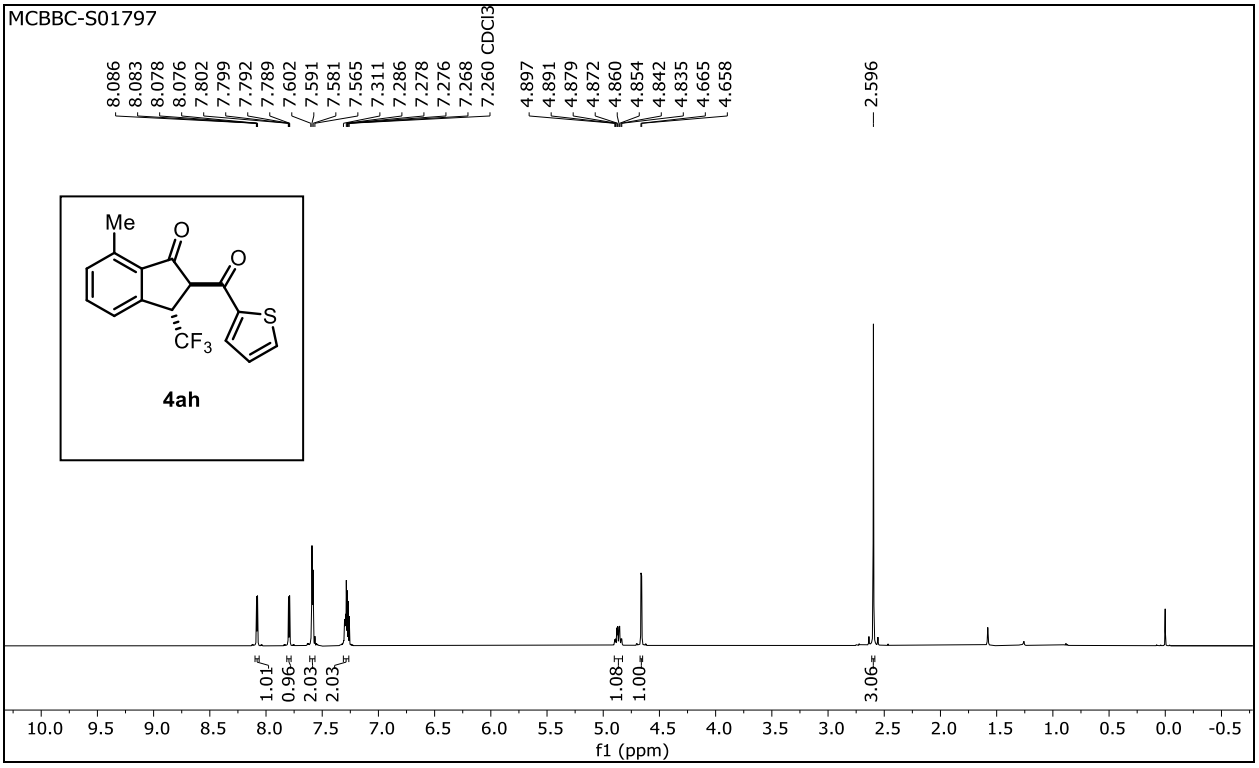

MCBBC-S03780
196.559
191.488
159.978
147.522
147.505
147.489
140.586
136.981
135.300
133.037
132.054
129.852
129.625
127.411
125.198
124.441
123.344
122.984
120.936
114.130
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
58.086
55.649
45.971
45.738
45.505
45.271
18.501
Me
O
O
CF3
OMe
4af
f1 (ppm)

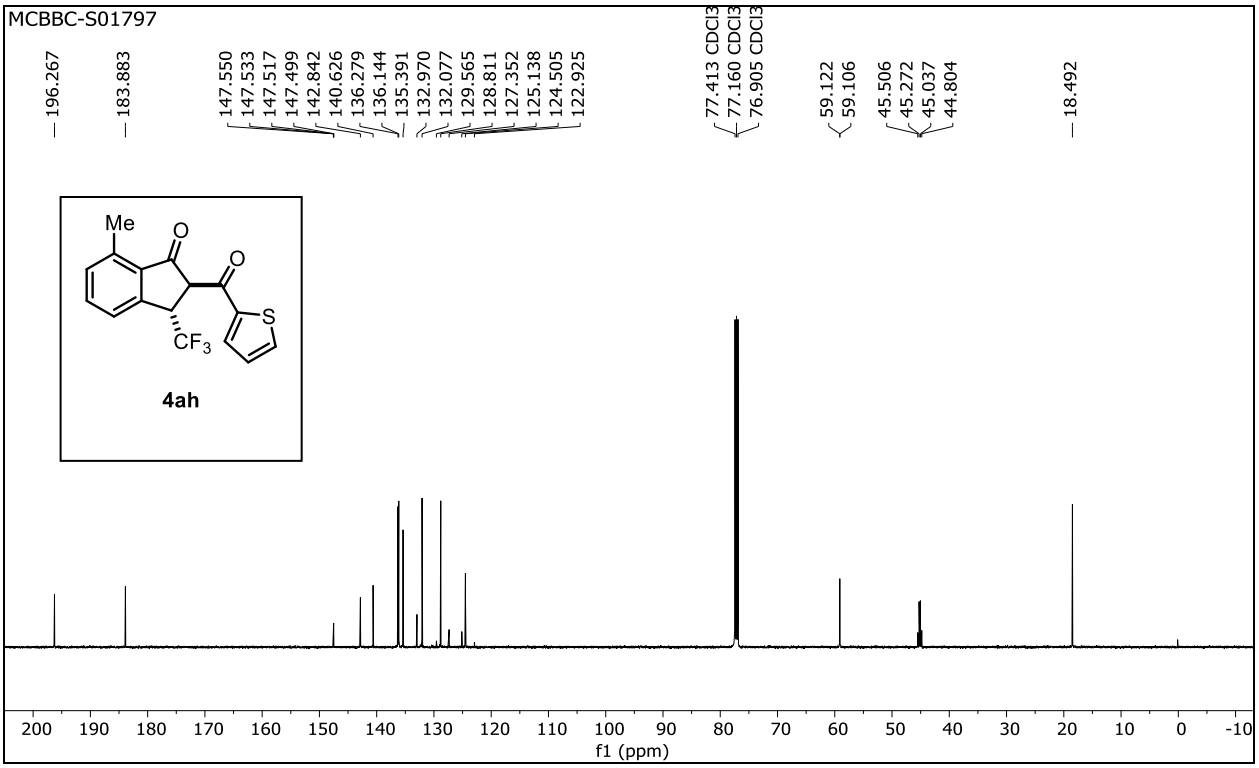

MCBBC-S03780
-68.036
-68.913
Me
O
O
CF3
OMe
4af
f1 (ppm)

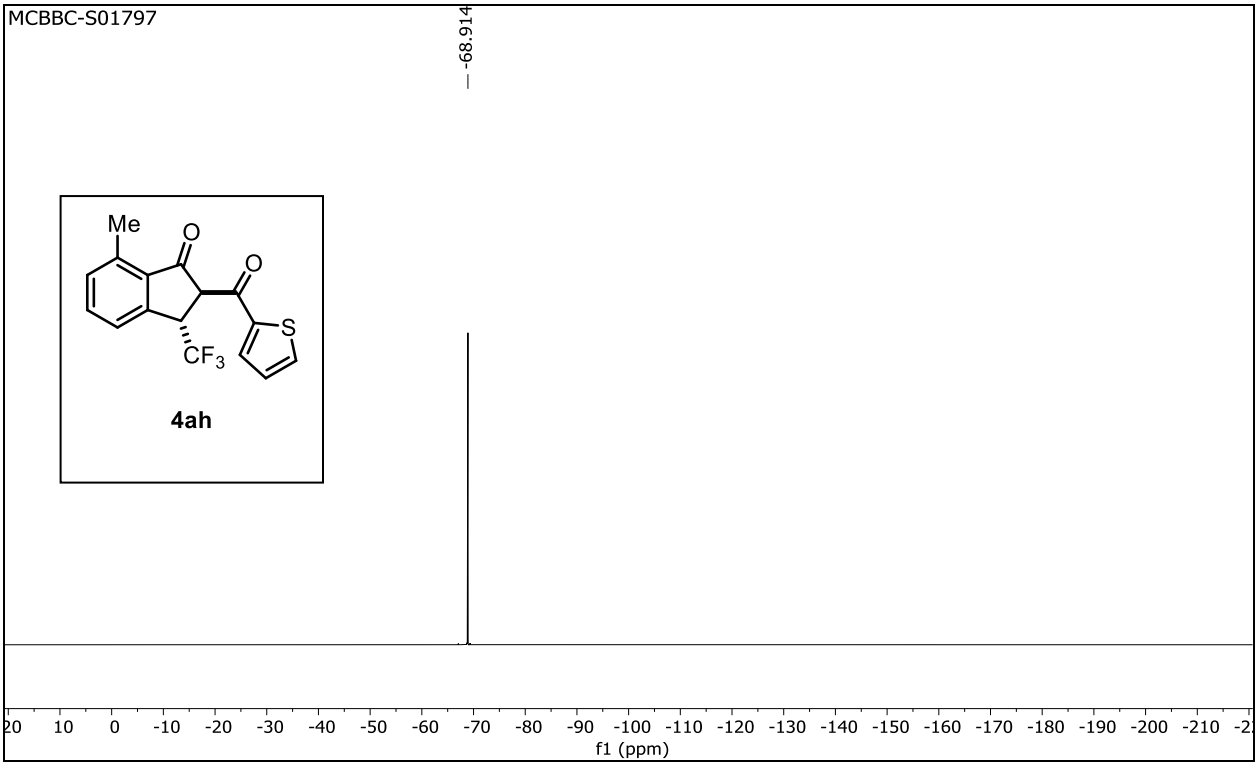

MCBBC-S02856
7.843
7.840
7.827
7.823
7.627
7.591
7.587
7.582
7.575
7.547
7.290
7.286
7.278
7.274
7.260 CDCl3
6.981
6.964
6.092
6.089
6.085
6.082
4.895
4.889
4.877
4.870
4.858
4.852
4.840
4.833
4.823
4.816
2.580
Me
O
O
CF3
O
O
4ag
1.00
3.03
1.03
1.00
1.01
1.00
1.04
1.03
3.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

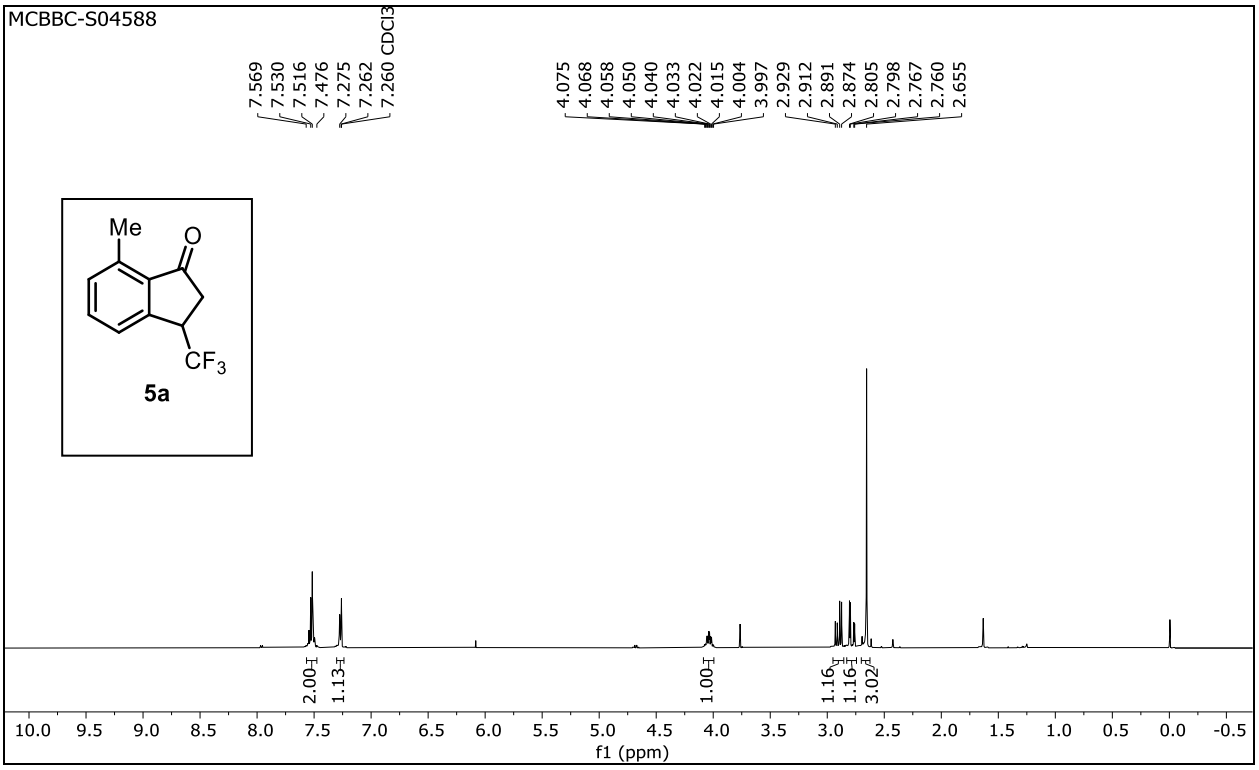

MCBBC-S02856
196.884
189.382
152.982
148.510
147.644
147.628
140.546
135.284
133.048
132.013
130.448
129.666
127.774
127.451
125.237
124.450
123.023
109.564
108.229
102.280
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
57.773
45.958
45.726
45.493
45.260
18.499
Me
O
O
CF3
O
O
4ag
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

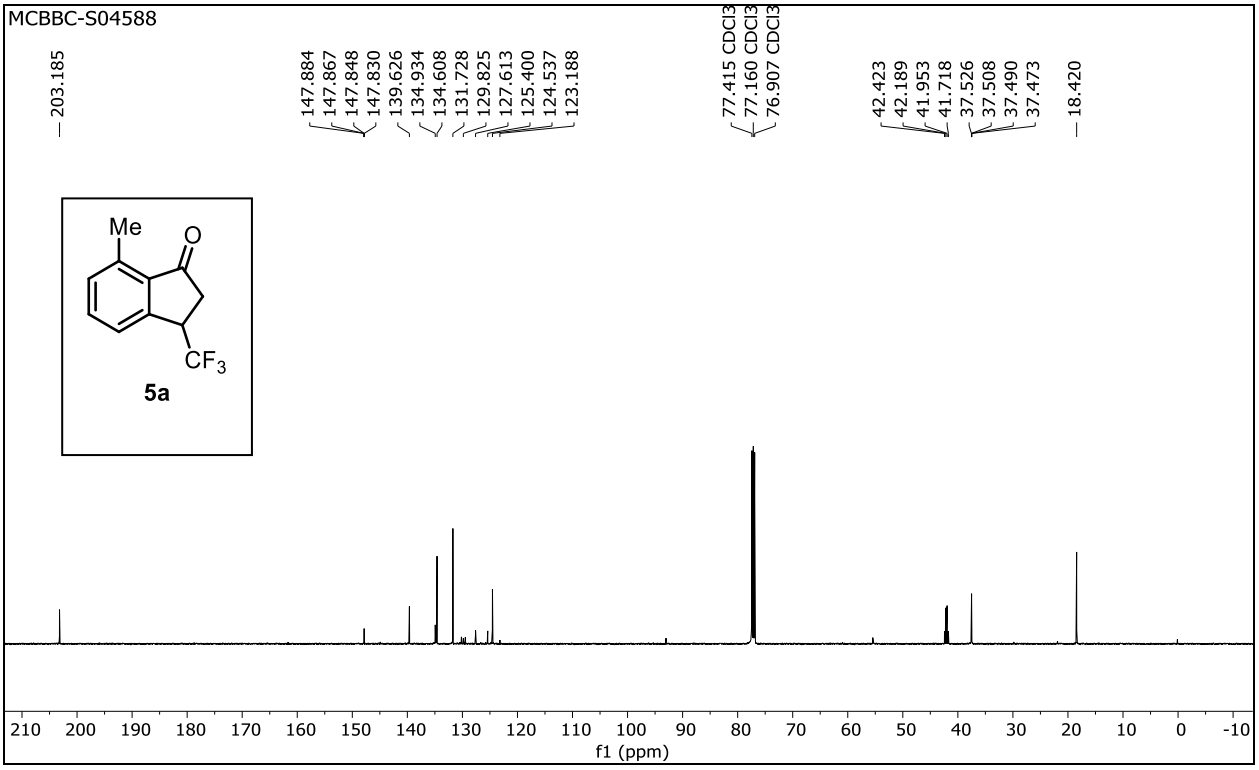

MCBBC-S02856
-68.902
Me
O
O
CF3
O
O
4ag
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

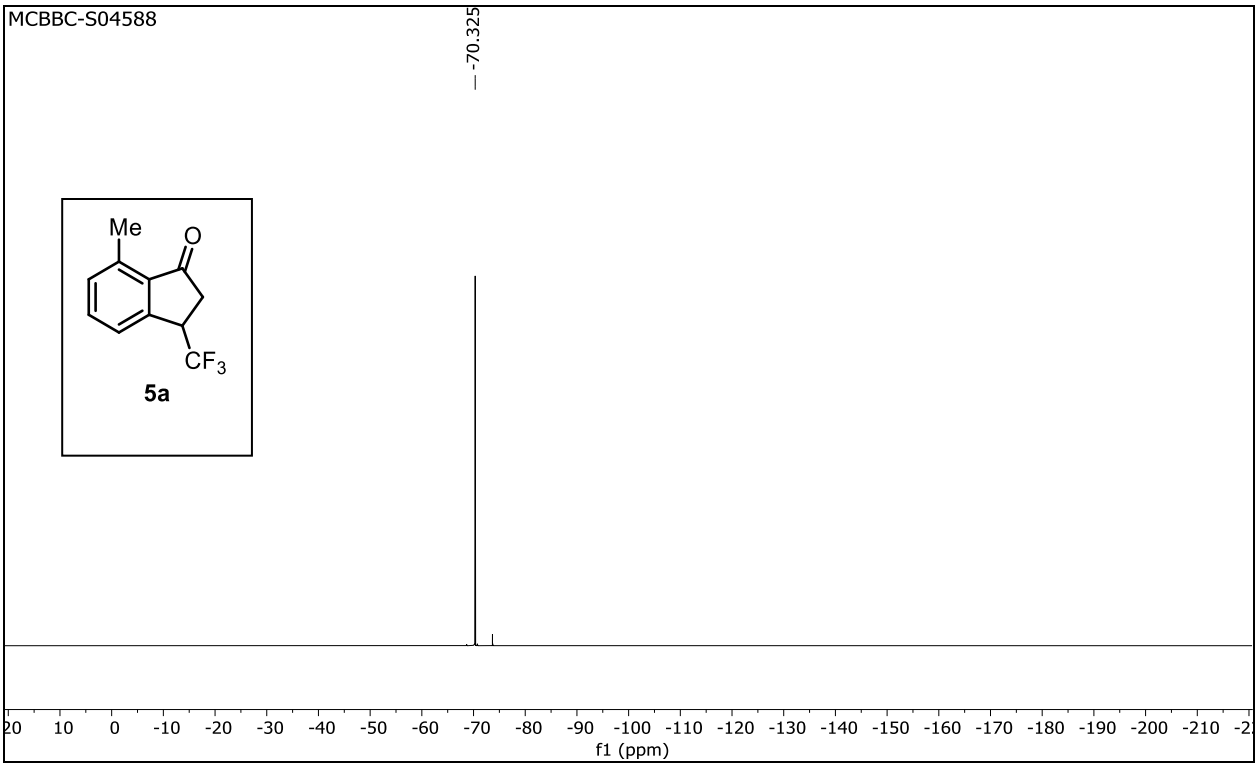

MCBBC-S01797
8.086
8.083
8.078
8.076
7.802
7.799
7.792
7.789
7.602
7.591
7.581
7.565
7.311
7.286
7.278
7.276
7.268
7.260 CDCl3
4.897
4.891
4.879
4.872
4.860
4.854
4.842
4.835
4.665
4.658
2.596
Me
O
O
CF3
S
4ah
1.01
0.96
2.03
2.03
1.08
1.00
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

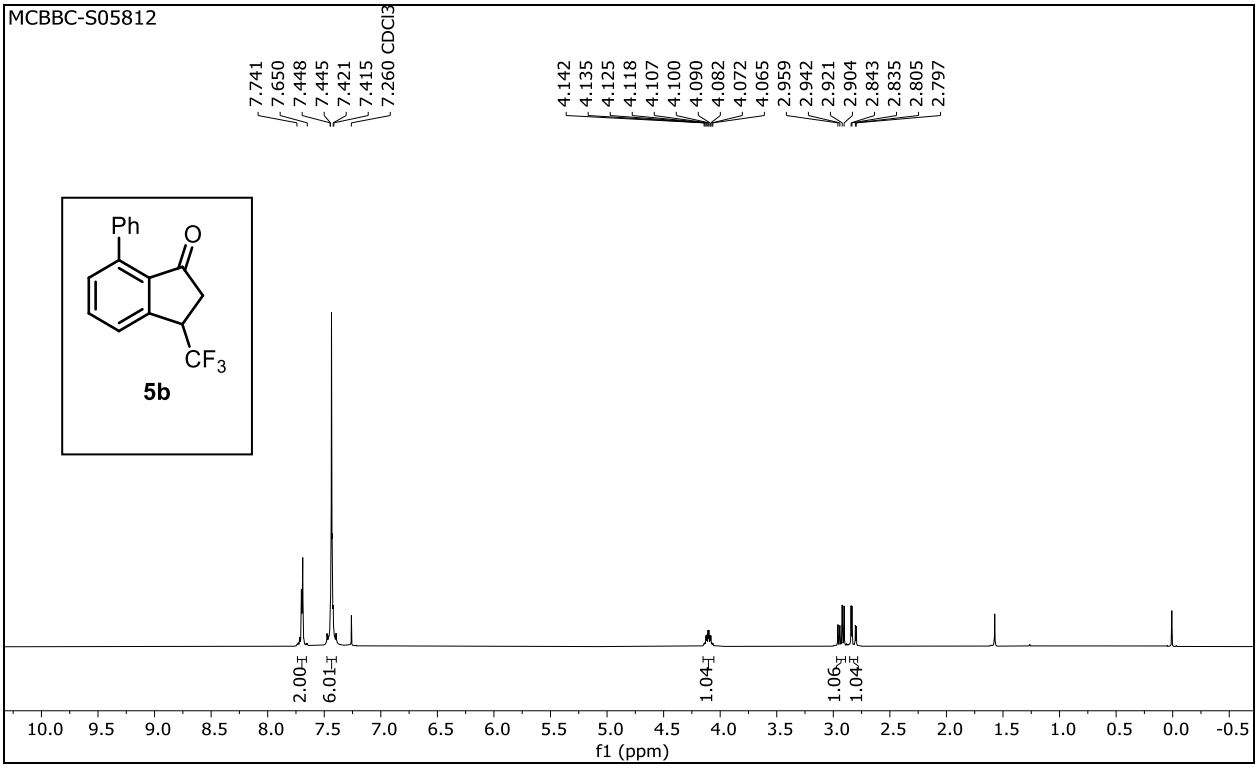

MCBBC-S01797
196.267
183.883
147.550
147.533
147.517
147.499
142.842
140.626
136.279
136.144
135.391
132.970
132.077
129.565
128.811
127.352
125.138
124.505
122.925
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
59.122
59.106
45.506
45.272
45.037
44.804
18.492
Me
O
O
S
CF3
4ah
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

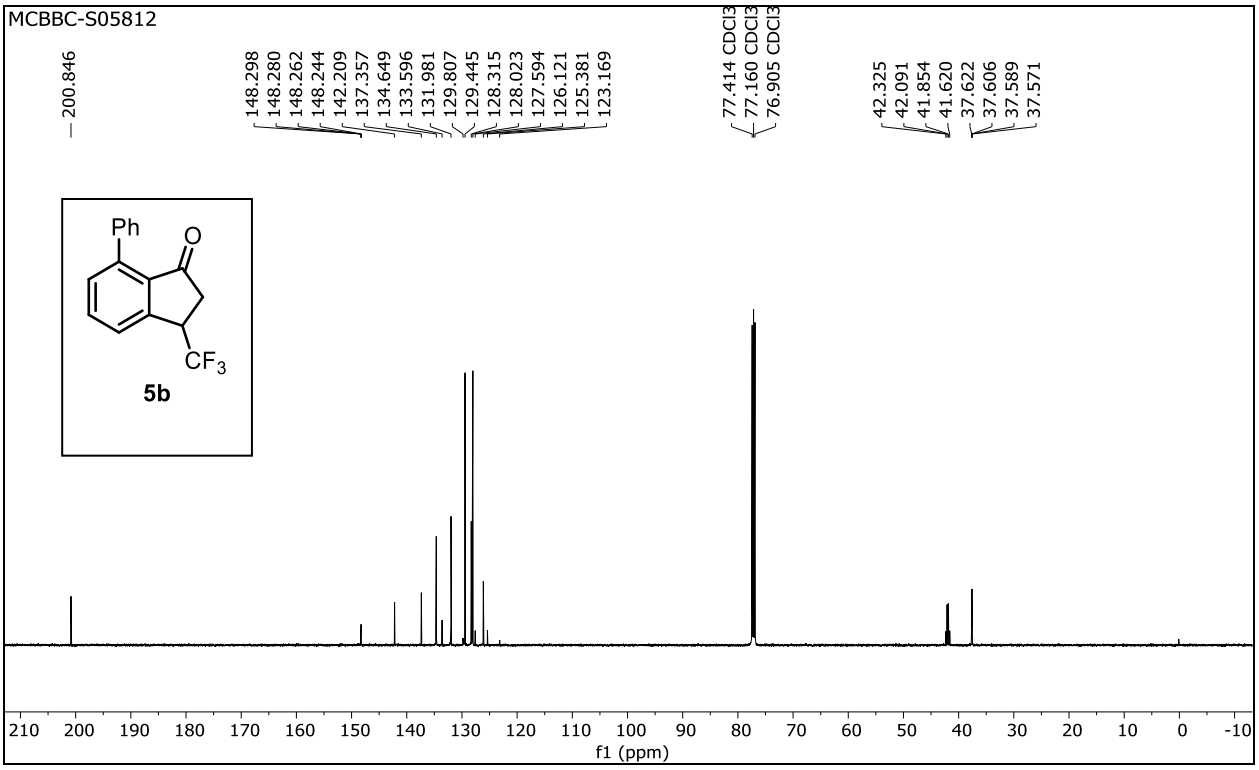

MCBBC-S01797
-68.914
Me
O
O
S
CF3
4ah
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

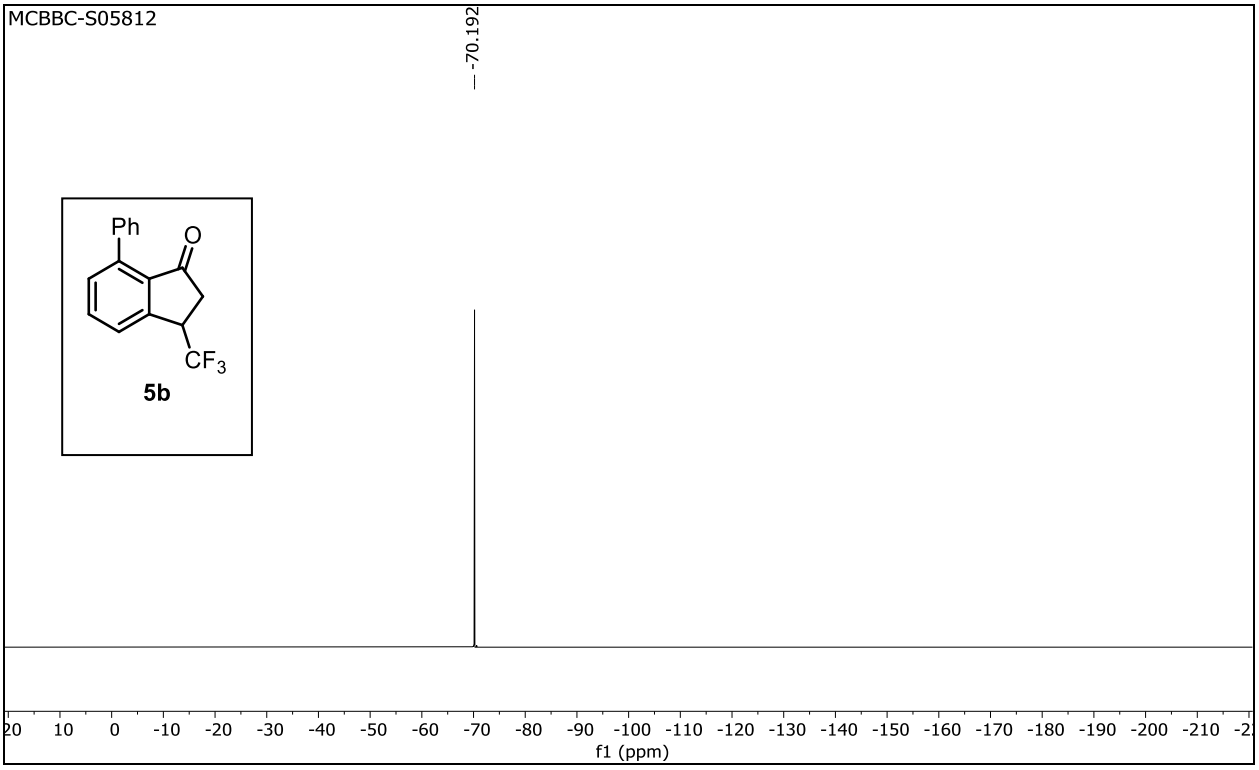

MCBBC-S04588
7.569
7.530
7.516
7.476
7.275
7.262
7.260 CDCl3
4.075
4.068
4.058
4.050
4.040
4.033
4.022
4.015
4.004
3.997
2.929
2.912
2.891
2.874
2.805
2.798
2.767
2.760
2.655
Me
O
CF3
5a
2.00
1.13
1.00
1.16
1.16
3.02
f1 (ppm)

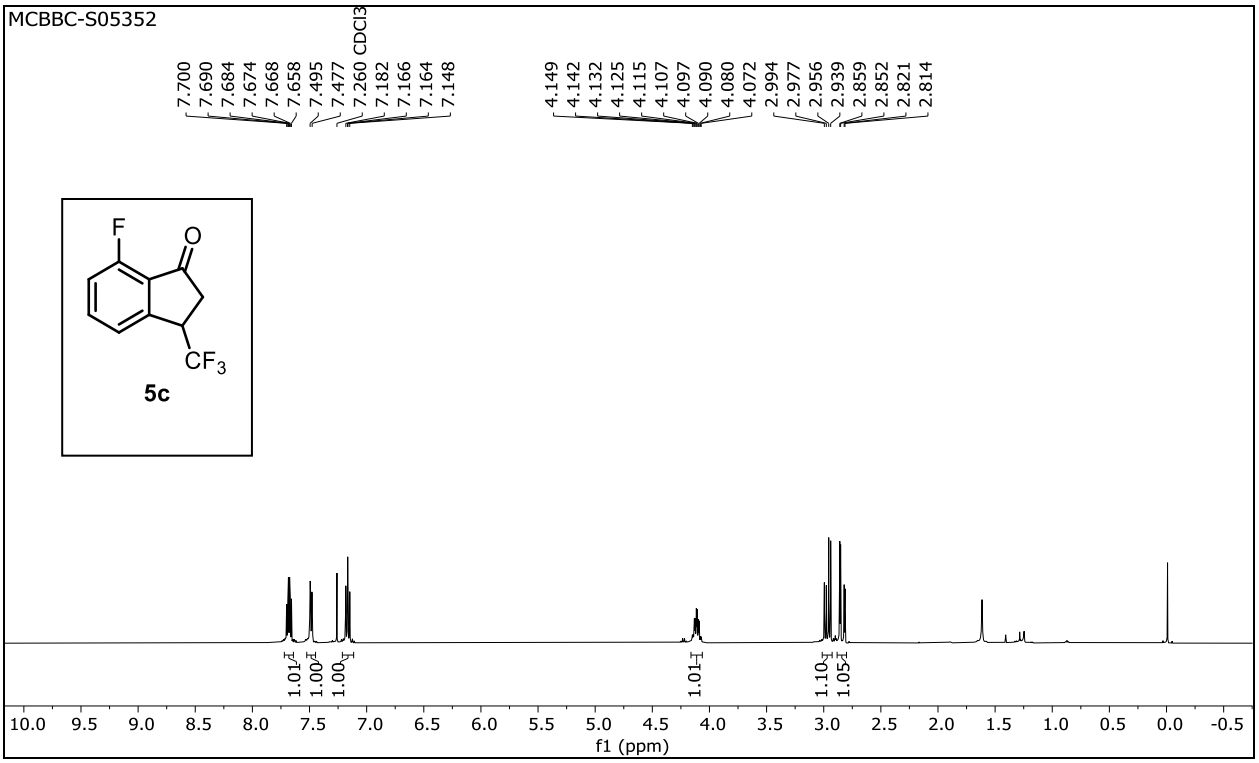

MCBBC-S04588
203.185
147.884
147.867
147.848
147.830
139.626
134.934
134.608
131.728
129.825
127.613
125.400
124.537
123.188
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
42.423
42.189
41.953
41.718
37.526
37.508
37.490
37.473
18.420
Me
O
CF3
5a
f1 (ppm)

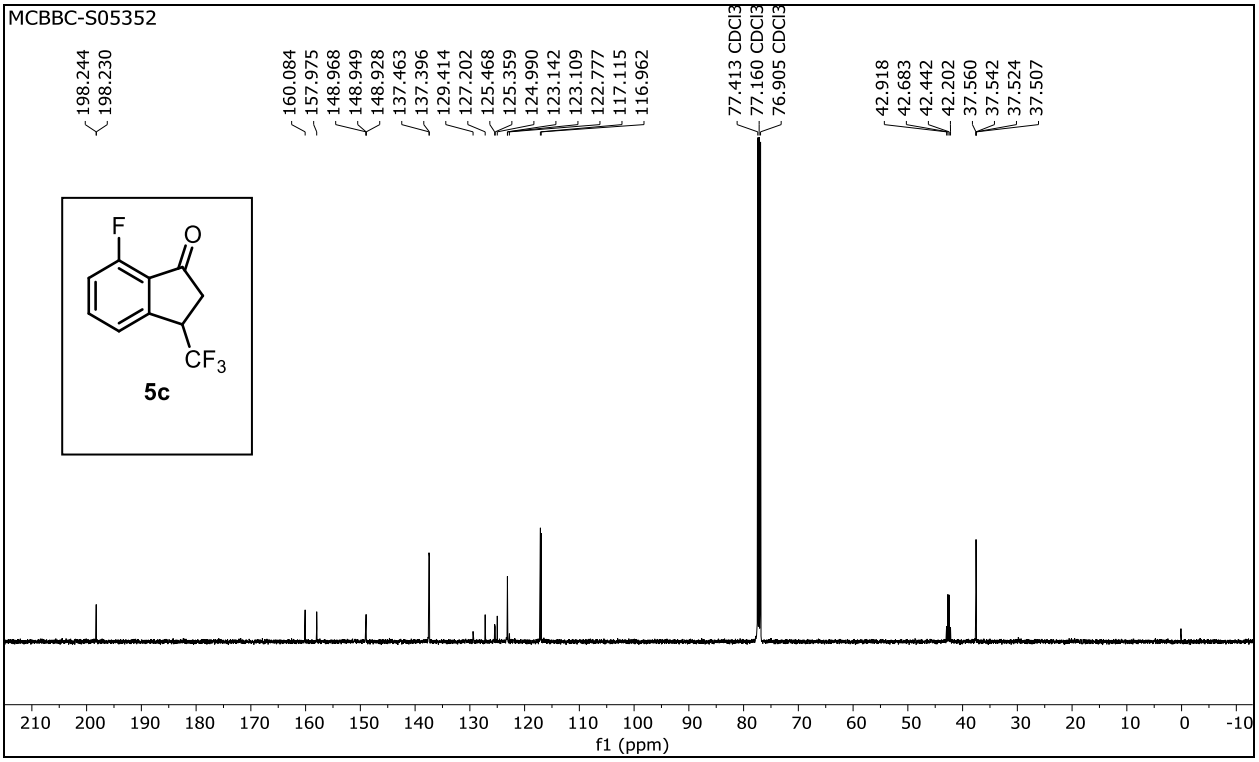

MCBBC-S04588
-70.325
Me
O
CF3
5a
f1 (ppm)

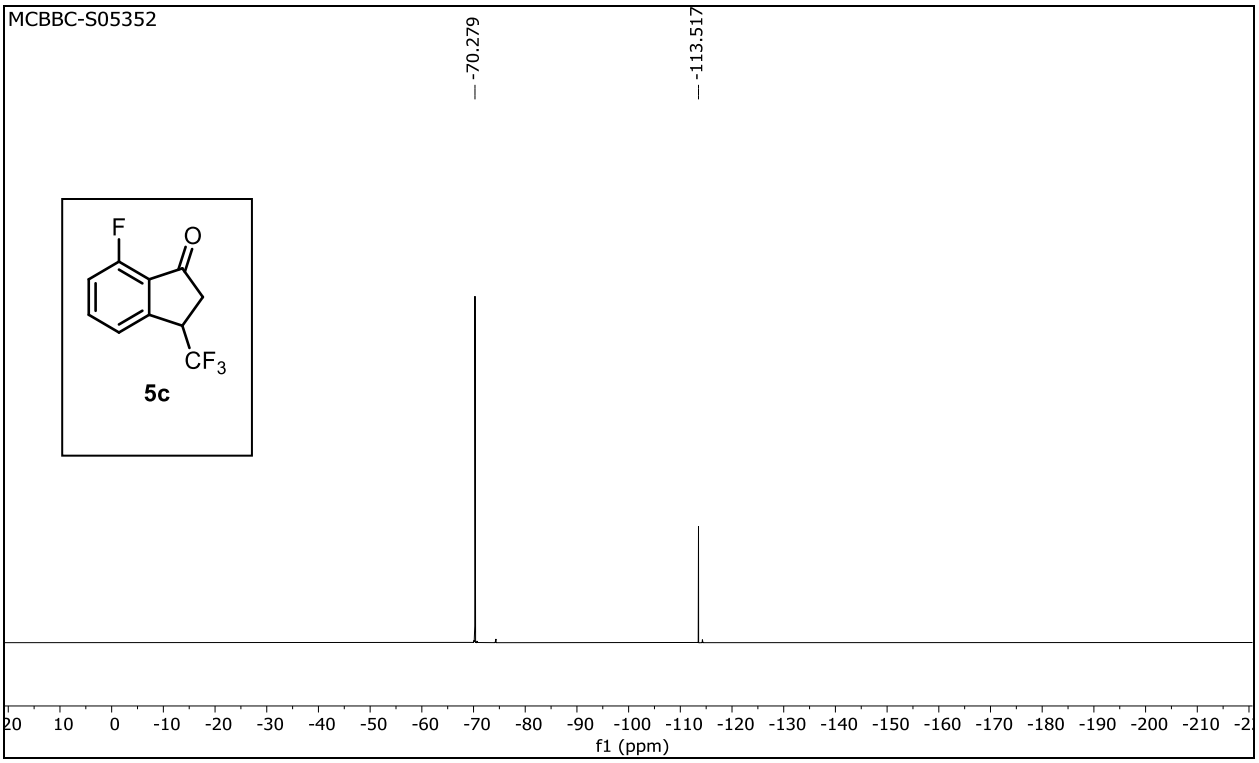

MCBBC-S05812
7.741
7.650
7.448
7.445
7.421
7.415
7.260 CDCl3
4.142
4.135
4.125
4.118
4.107
4.100
4.090
4.082
4.072
4.065
2.959
2.942
2.921
2.904
2.843
2.835
2.805
2.797
Ph
O
CF3
5b
2.00
6.01
1.04
1.06
1.04
f1 (ppm)

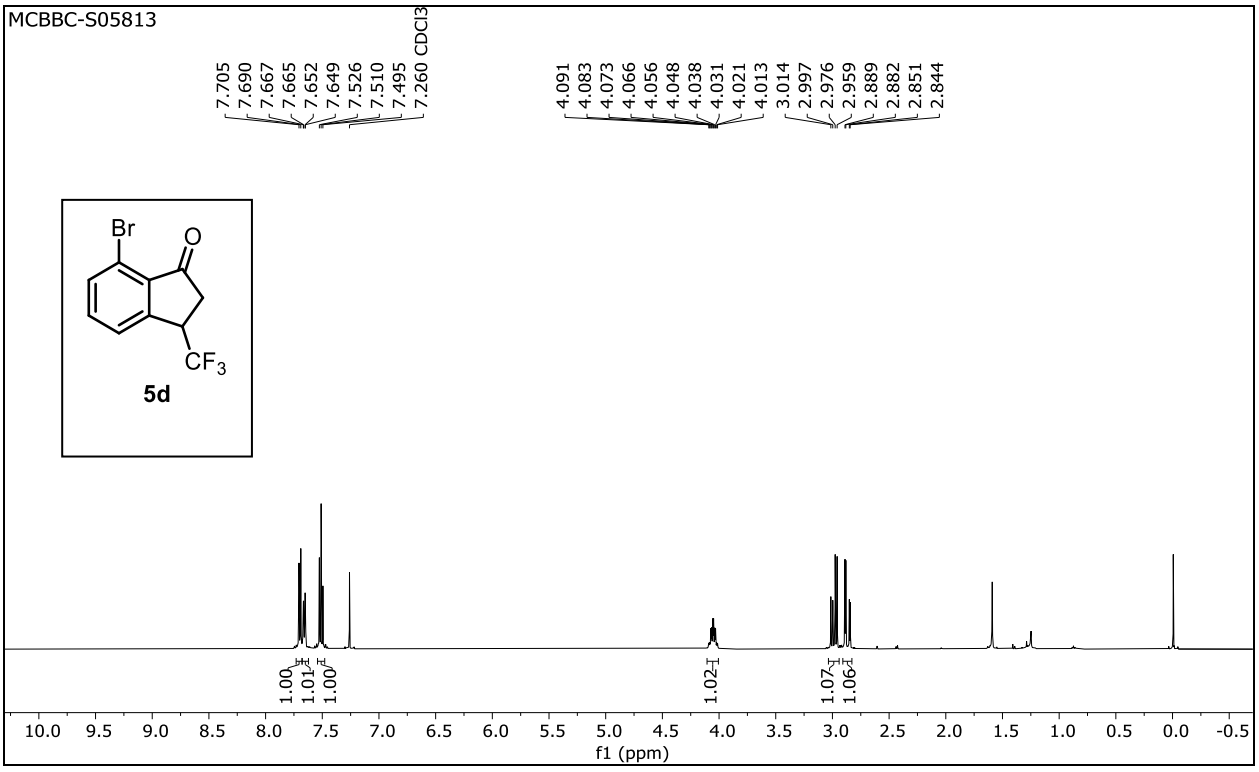

MCBBC-S05812
200.846
148.298
148.280
148.262
148.244
142.209
137.357
134.649
133.596
131.981
129.807
129.445
128.315
128.023
127.594
126.121
125.381
123.169
77.414 CDCl3
77.160 CDCl3
76.905 CDCl3
42.325
42.091
41.854
41.620
37.622
37.606
37.589
37.571
Ph
O
CF3
5b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

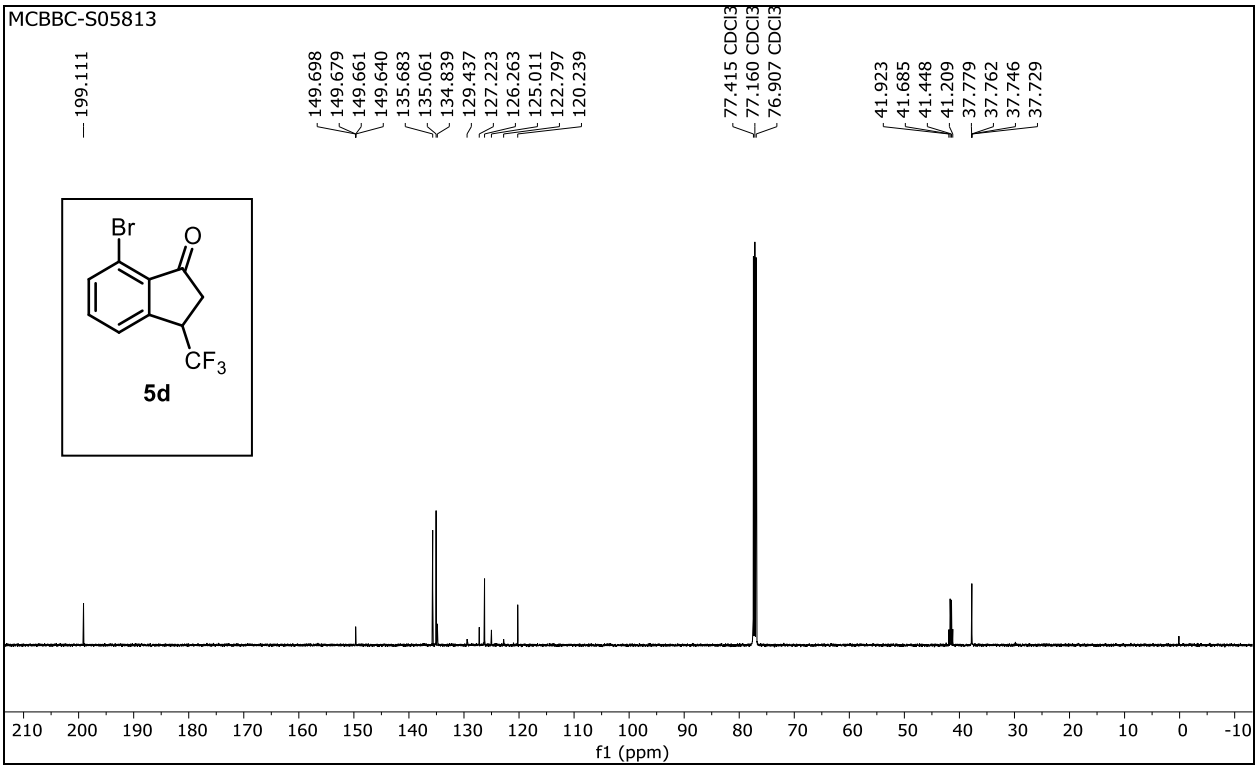

MCBBC-S05812
-70.192
Ph
O
CF3
5b
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

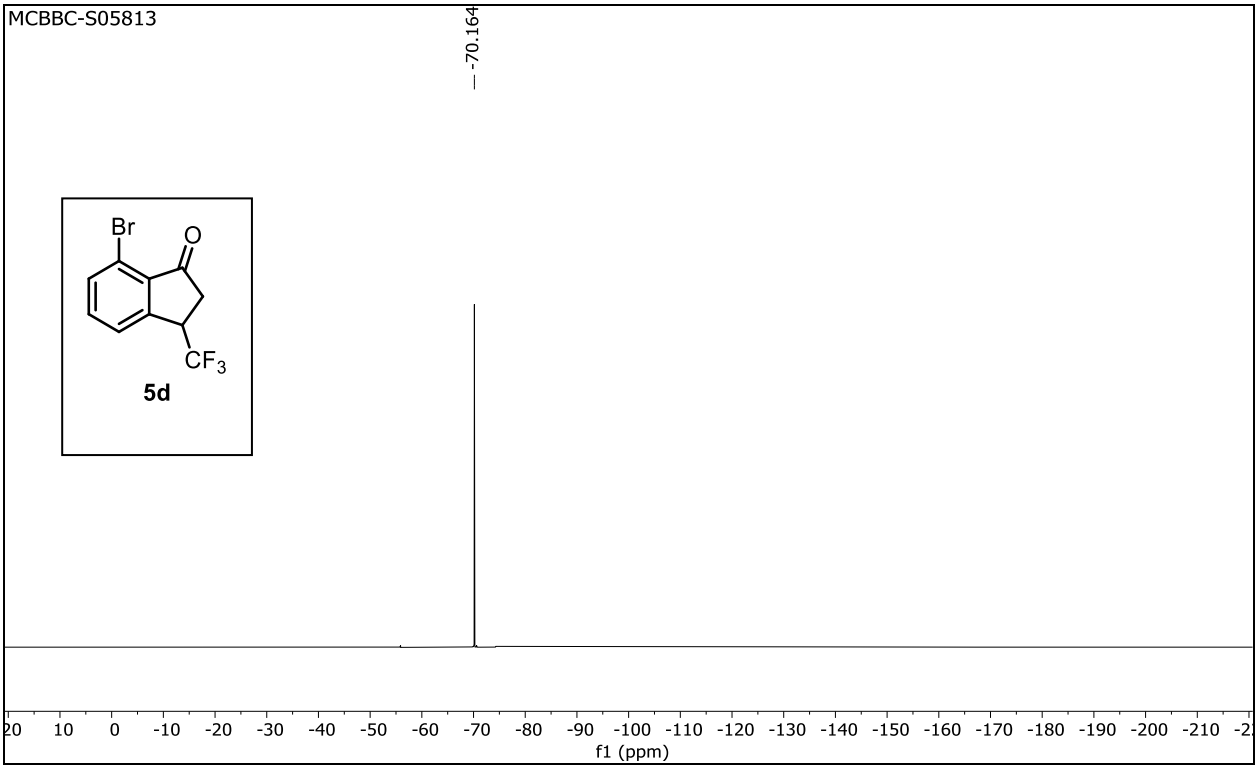

MCBBC-S05352
7.700
7.690
7.684
7.674
7.668
7.658
7.495
7.477
7.260 CDCl3
7.182
7.166
7.164
7.148
4.149
4.142
4.132
4.125
4.115
4.107
4.097
4.090
4.080
4.072
2.994
2.977
2.956
2.939
2.859
2.852
2.821
2.814
F
O
CF3
5c
1.01
1.00
1.00
1.01
1.10
1.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

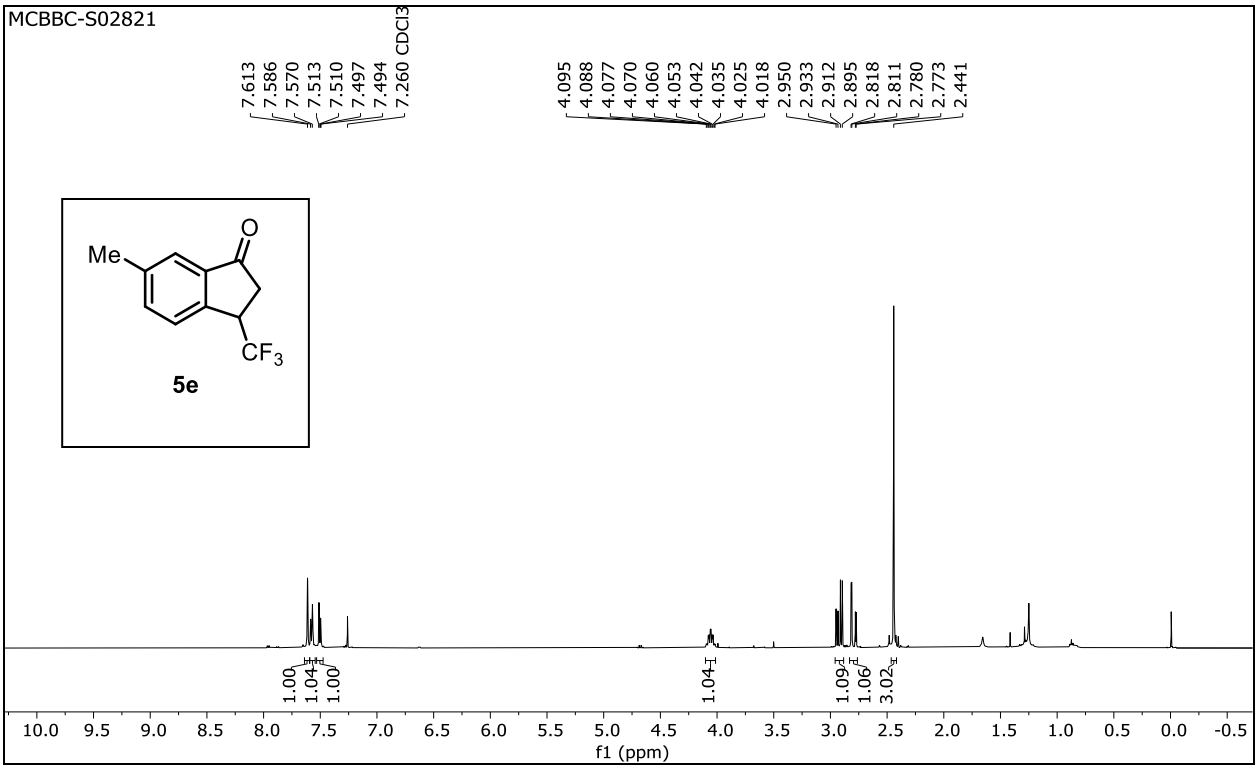

MCBBC-S05352
198.244
198.230
160.084
157.975
148.968
148.949
148.928
137.463
137.396
129.414
127.202
125.468
125.359
124.990
123.142
123.109
122.777
117.115
116.962
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
42.918
42.683
42.442
42.202
37.560
37.542
37.524
37.507
F
O
CF3
5c
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

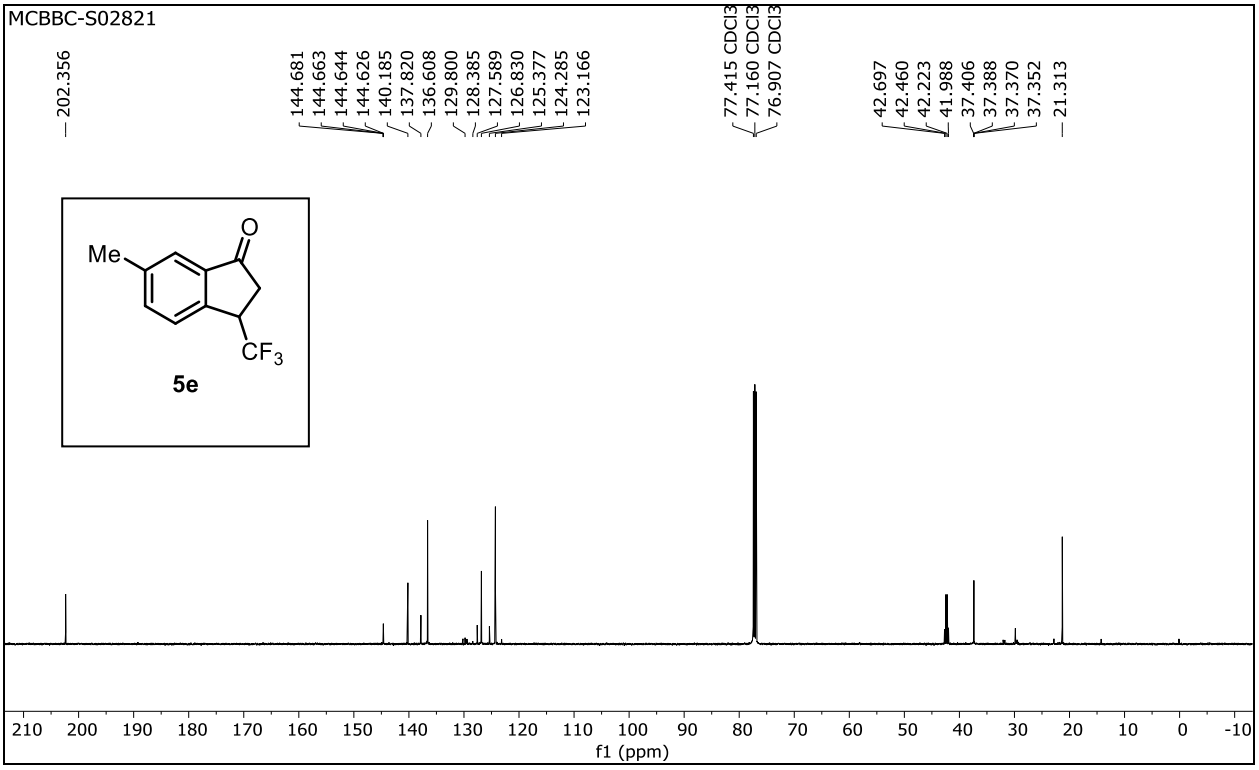

MCBBC-S05352
-70.279
-113.517
F
O
CF3
5c
f1 (ppm)

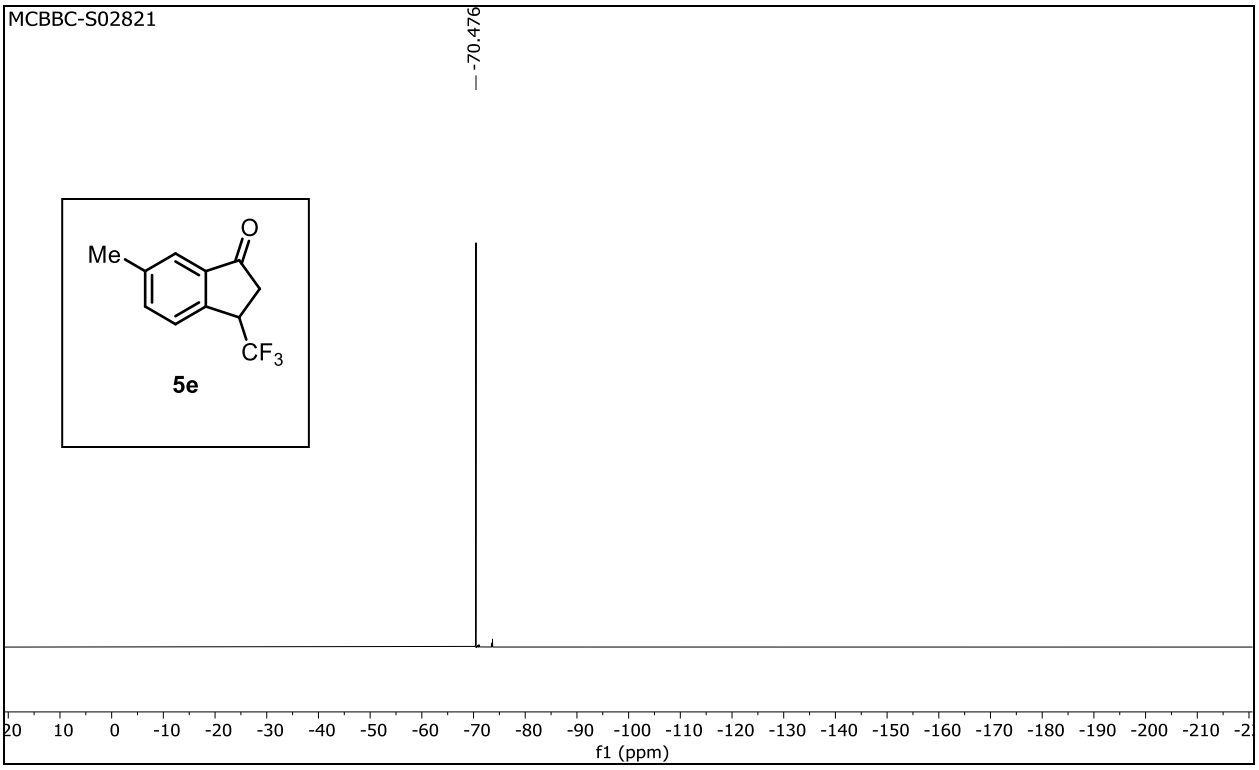

MCBBC-S05813
7.705
7.690
7.667
7.665
7.652
7.649
7.526
7.510
7.495
7.260 CDCl3
4.091
4.083
4.073
4.066
4.056
4.048
4.038
4.031
4.021
4.013
3.014
2.997
2.976
2.959
2.889
2.882
2.851
2.844
Br
O
CF3
5d
1.00
1.01
1.00
1.02
1.07
1.06
f1 (ppm)

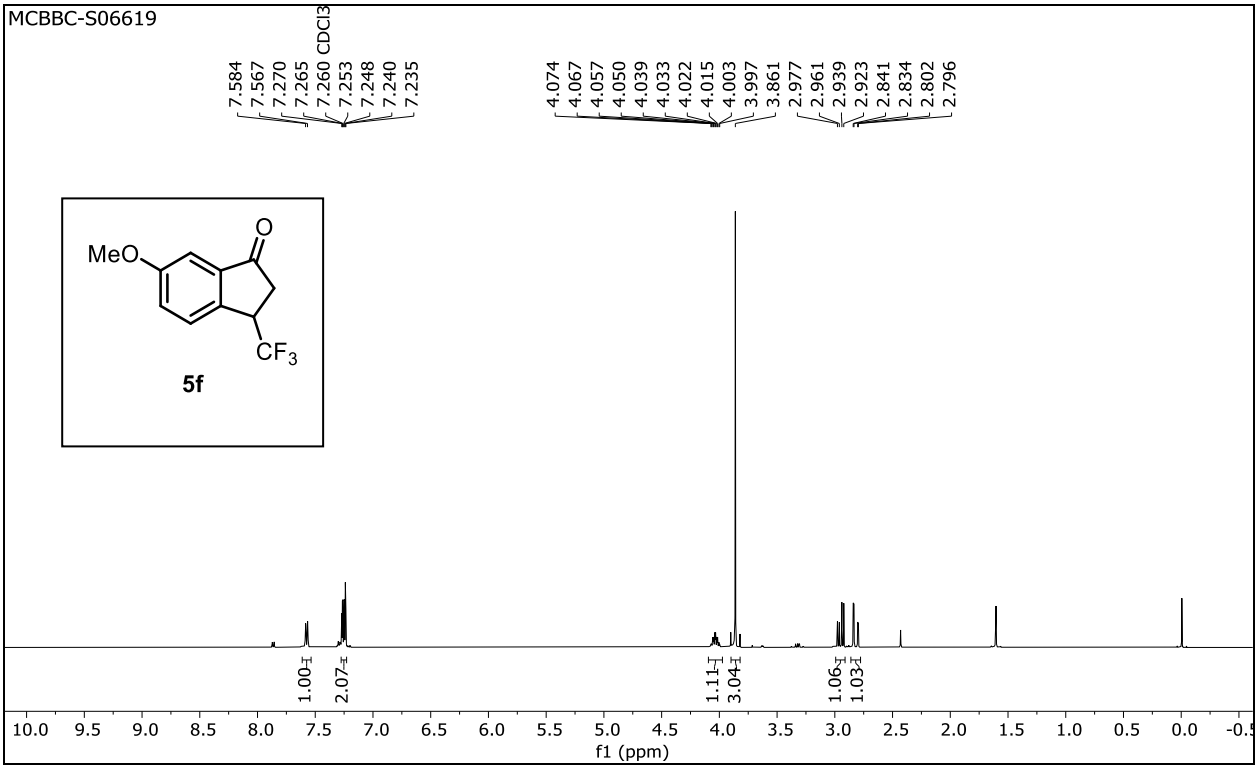

MCBBC-S05813
199.111
149.698
149.679
149.661
149.640
135.683
135.061
134.839
129.437
127.223
126.263
125.011
122.797
120.239
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
41.923
41.685
41.448
41.209
37.779
37.762
37.746
37.729
Br
O
CF3
5d
f1 (ppm)

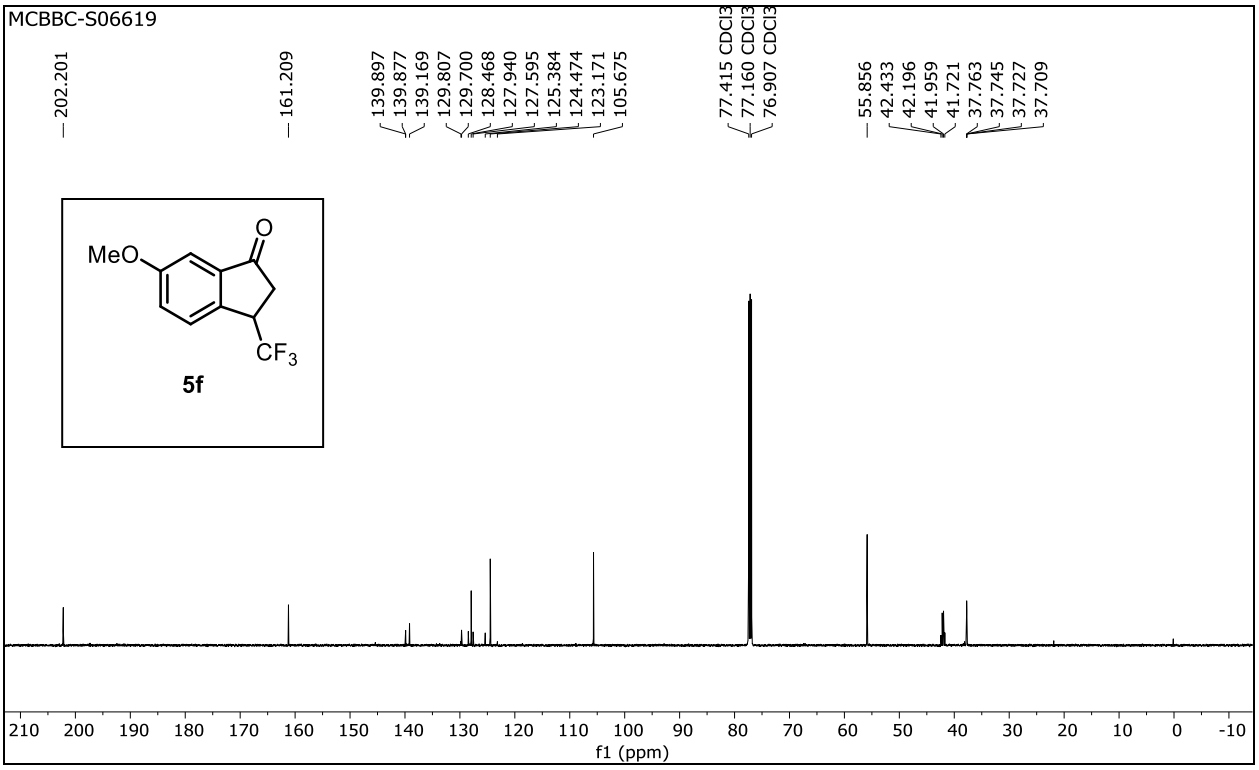

MCBBC-S05813
-70.164
Br
O
CF3
5d
f1 (ppm)

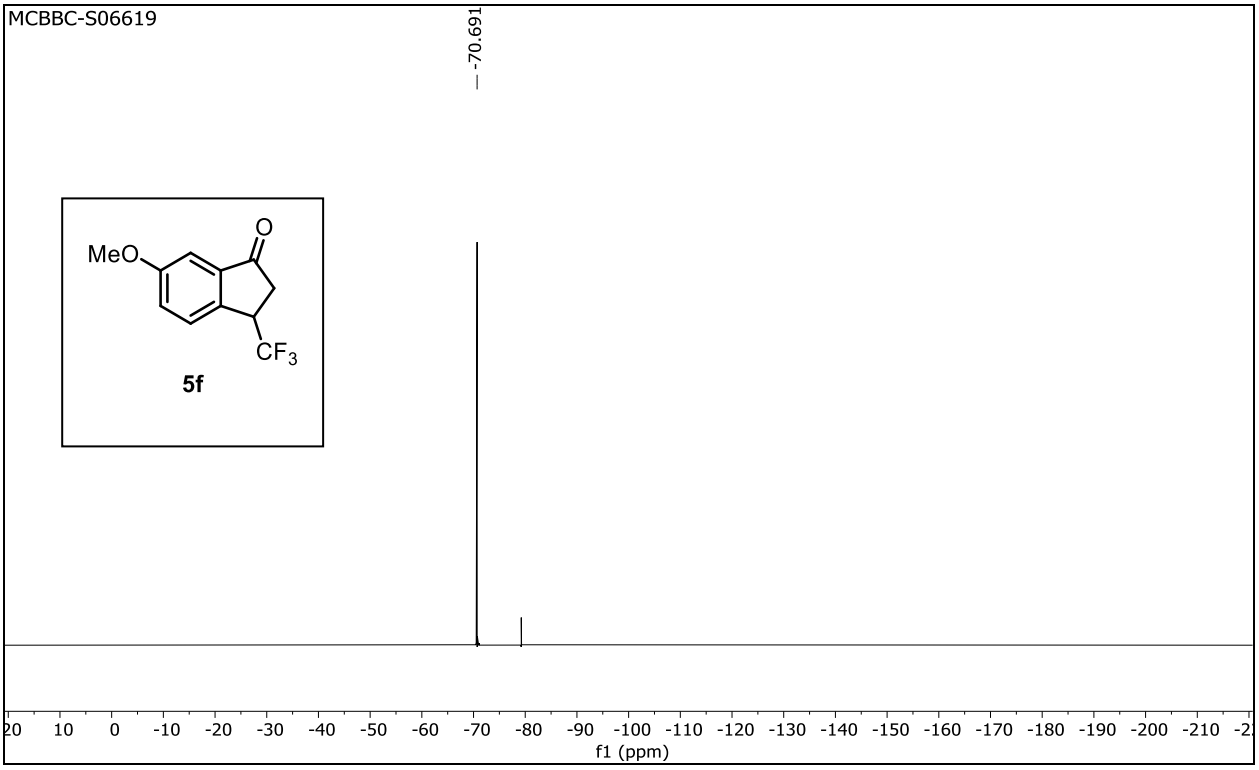

MCBBC-S02821
7.613
7.586
7.570
7.513
7.510
7.497
7.494
7.260 CDCl3
4.095
4.088
4.077
4.070
4.060
4.053
4.042
4.035
4.025
4.018
2.950
2.933
2.912
2.895
2.818
2.811
2.780
2.773
2.441
Me
O
CF3
5e
1.00
1.04
1.00
1.04
1.09
1.06
3.02
f1 (ppm)

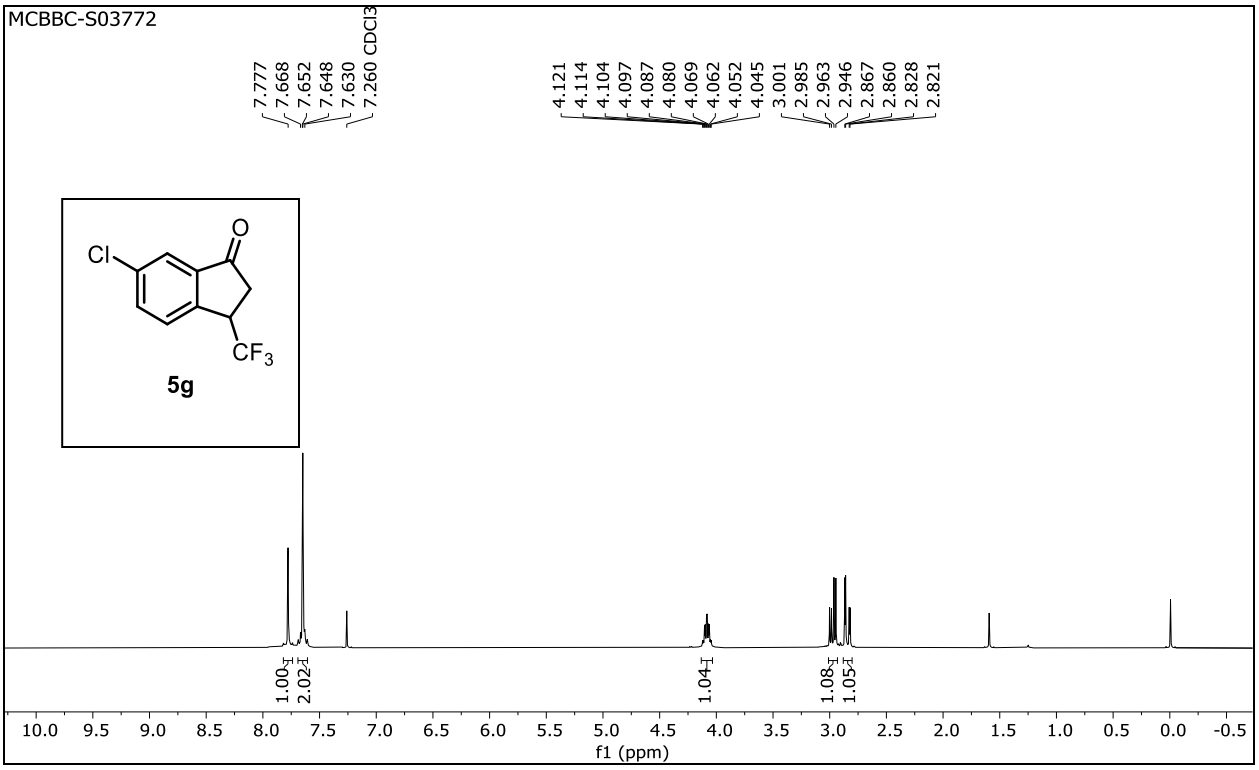

MCBBC-S02821
202.356
144.681
144.663
144.644
144.626
140.185
137.820
136.608
129.800
128.385
127.589
126.830
125.377
124.285
123.166
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
42.697
42.460
42.223
41.988
37.406
37.388
37.370
37.352
21.313
Me
O
CF3
5e
f1 (ppm)

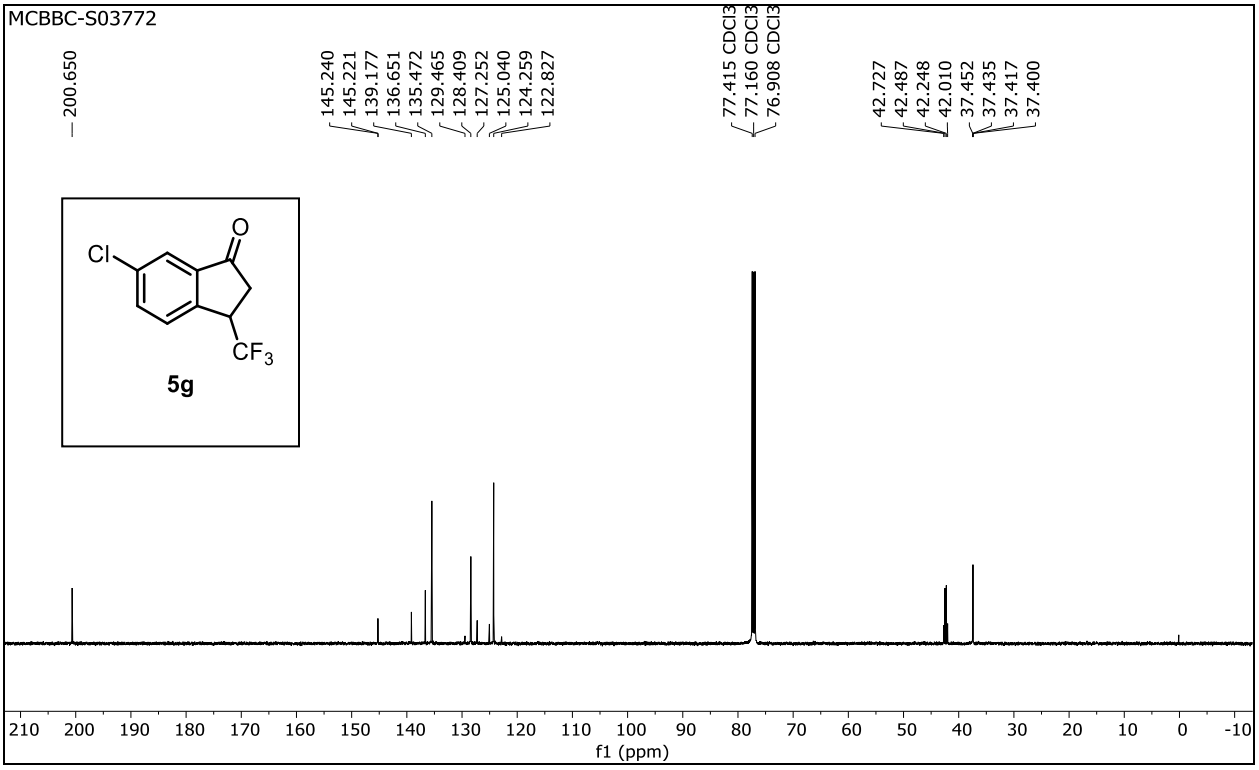

MCBBC-S02821
-70.476
Me
O
CF3
5e
f1 (ppm)

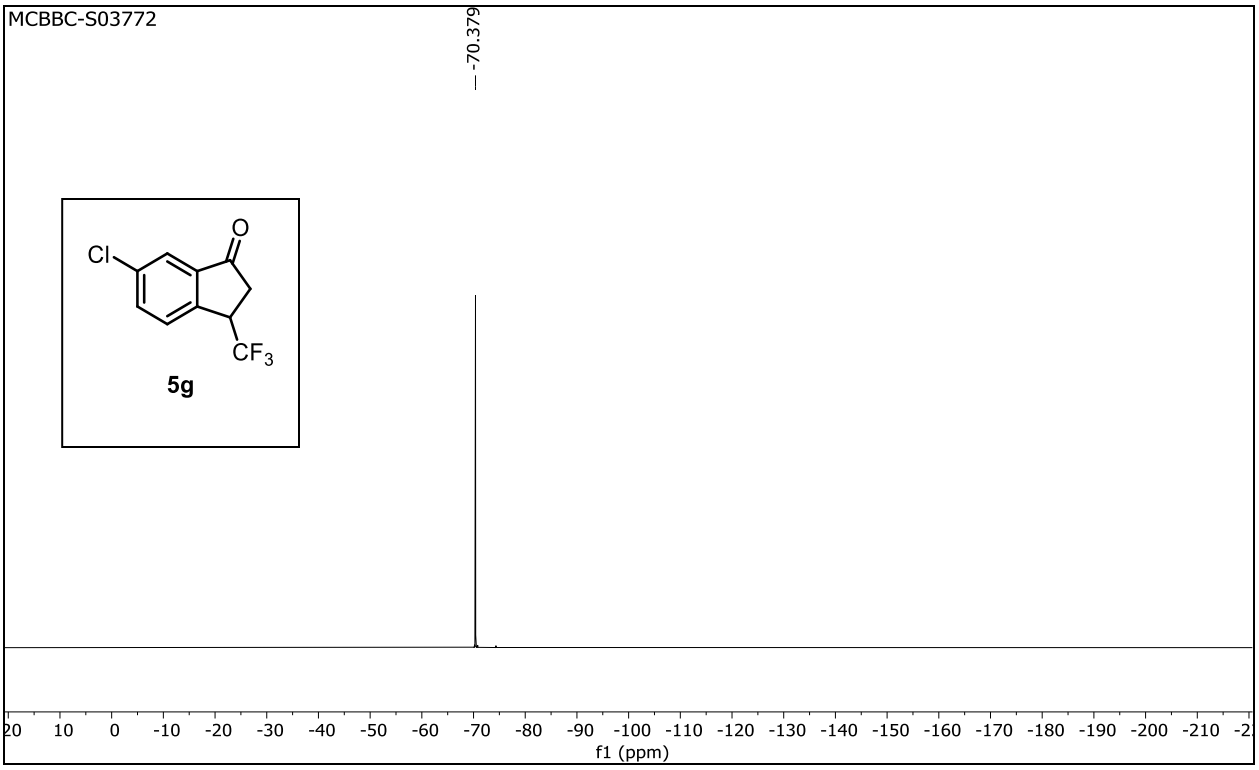

MCBBC-S06619
7.584
7.567
7.270
7.265
7.260 CDCl3
7.253
7.248
7.240
7.235
4.074
4.067
4.057
4.050
4.039
4.033
4.022
4.015
4.003
3.997
3.861
2.977
2.961
2.939
2.923
2.841
2.834
2.802
2.796
MeO
O
CF3
5f
1.00
2.07
1.11
3.04
1.06
1.03
f1 (ppm)

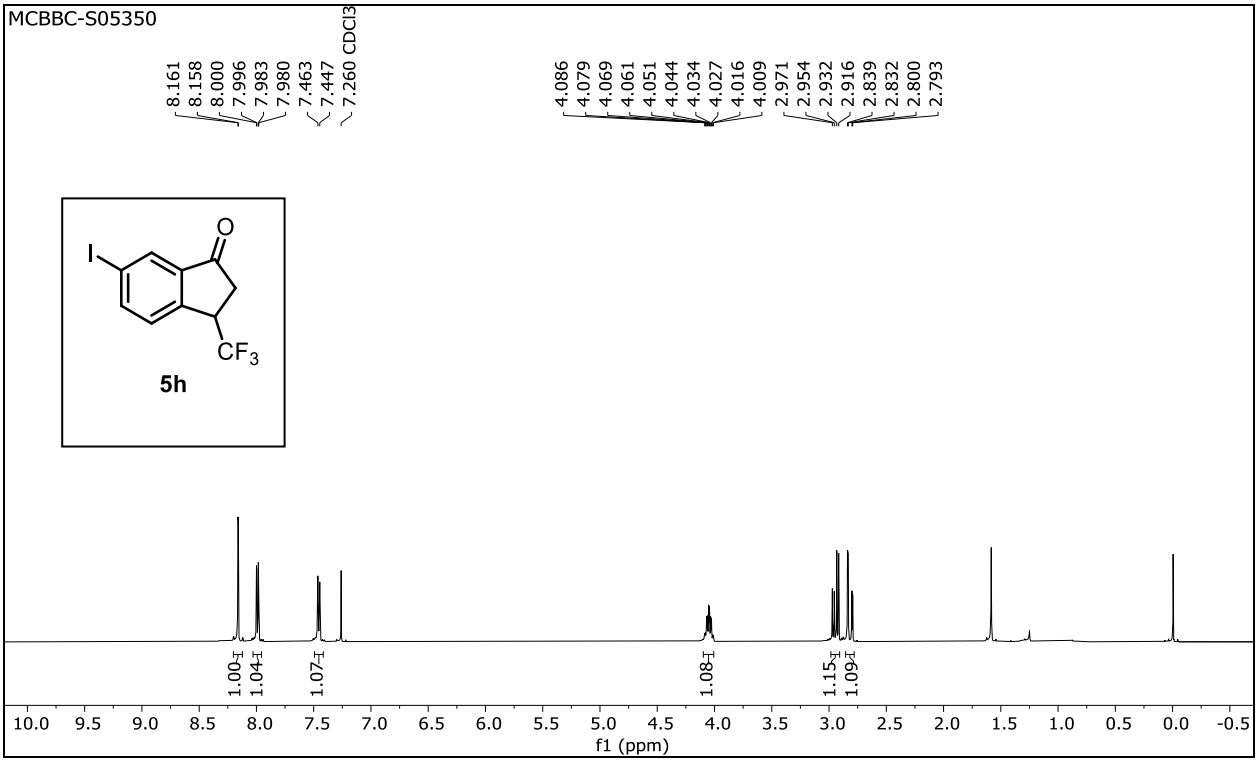

MCBBC-S06619
202.201
161.209
139.897
139.877
139.169
129.807
129.700
128.468
127.940
127.595
125.384
124.474
123.171
105.675
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
55.856
42.433
42.196
41.959
41.721
37.763
37.745
37.727
37.709
MeO
O
CF3
5f
f1 (ppm)

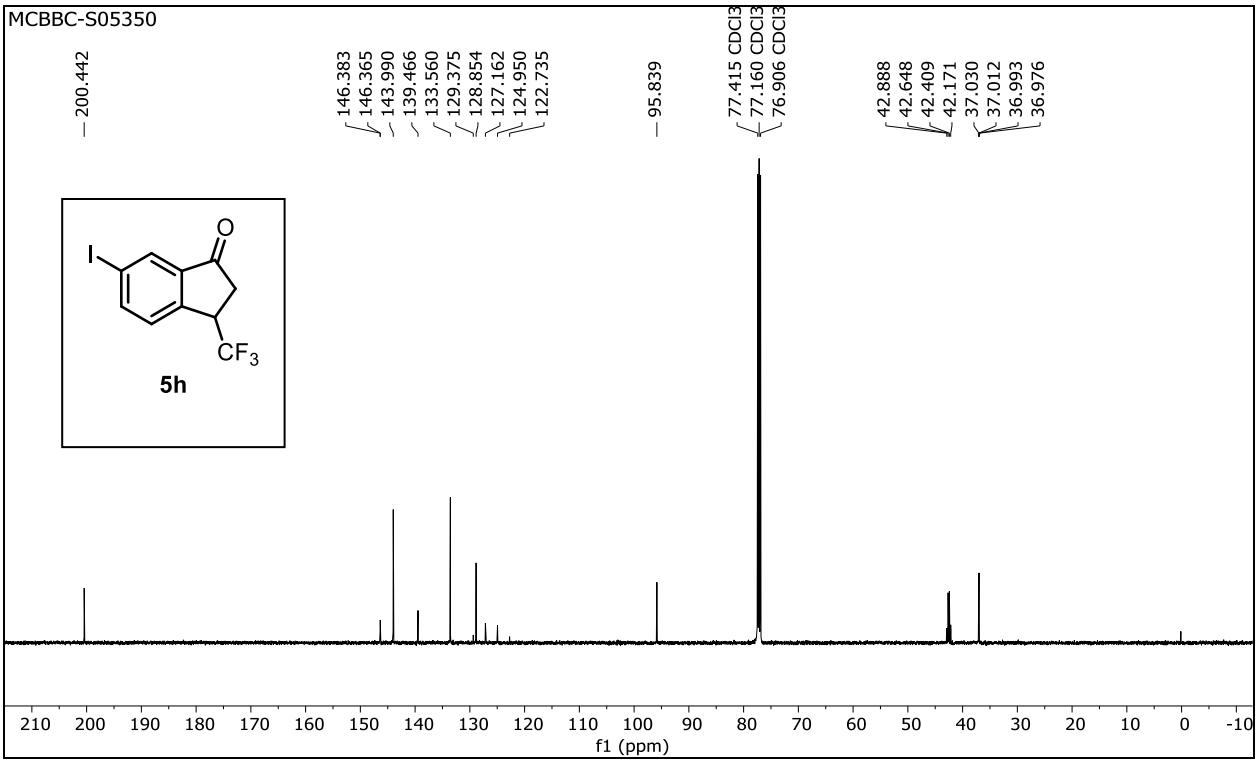

MCBBC-S06619
-70.691
MeO
O
CF3
5f
f1 (ppm)

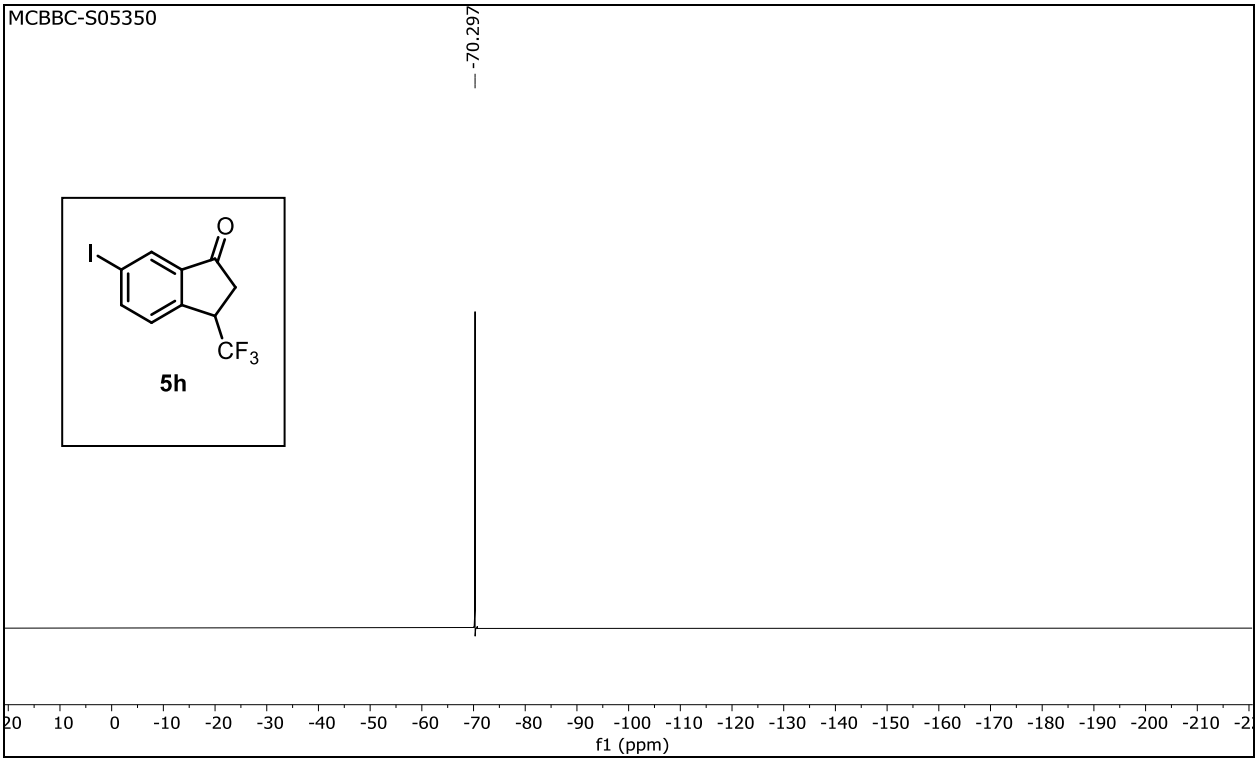

MCBBC-S03772
7.777
7.668
7.652
7.648
7.630
7.260 CDCl3
4.121
4.114
4.104
4.097
4.087
4.080
4.069
4.062
4.052
4.045
3.001
2.985
2.963
2.946
2.867
2.860
2.828
2.821
Cl
O
CF3
5g
1.00
2.02
1.04
1.08
1.05
f1 (ppm)

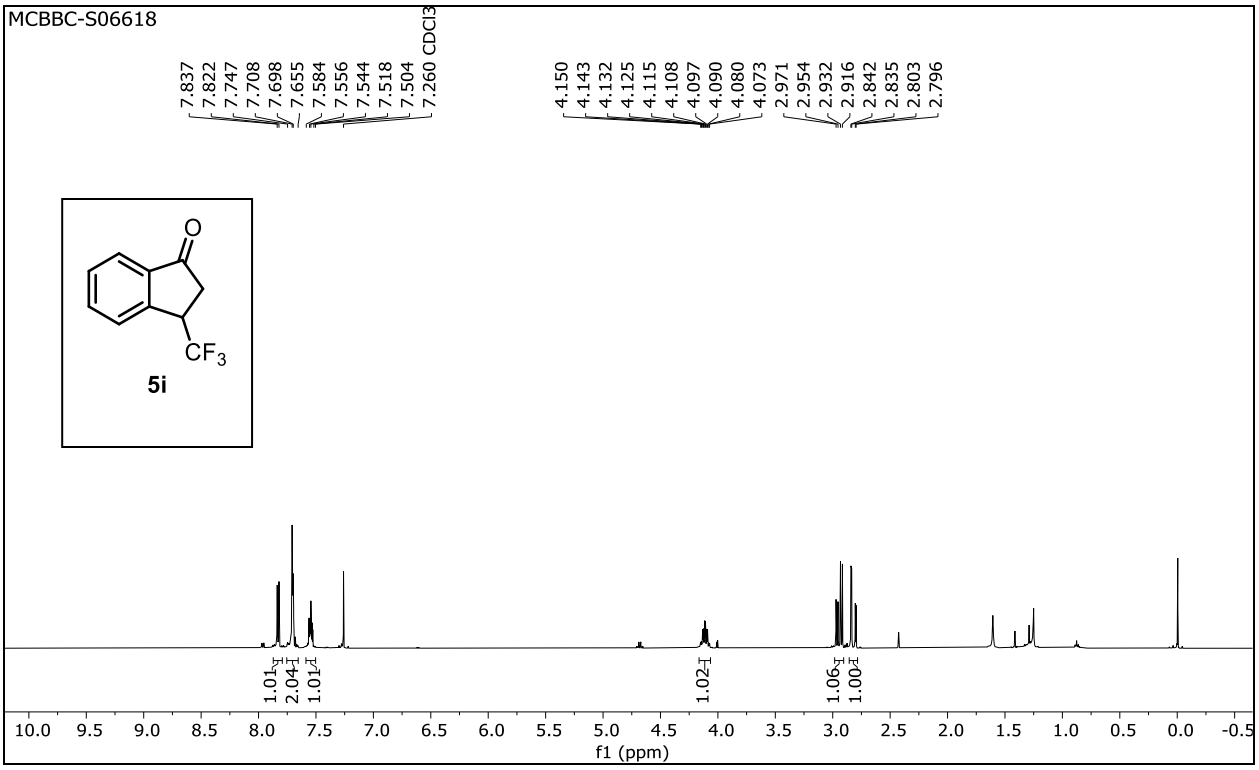

MCBBC-S03772
200.650
145.240
145.221
139.177
136.651
135.472
129.465
128.409
127.252
125.040
124.259
122.827
77.415 CDCl3
77.160 CDCl3
76.908 CDCl3
42.727
42.487
42.248
42.010
37.452
37.435
37.417
37.400
Cl
O
CF3
5g
f1 (ppm)

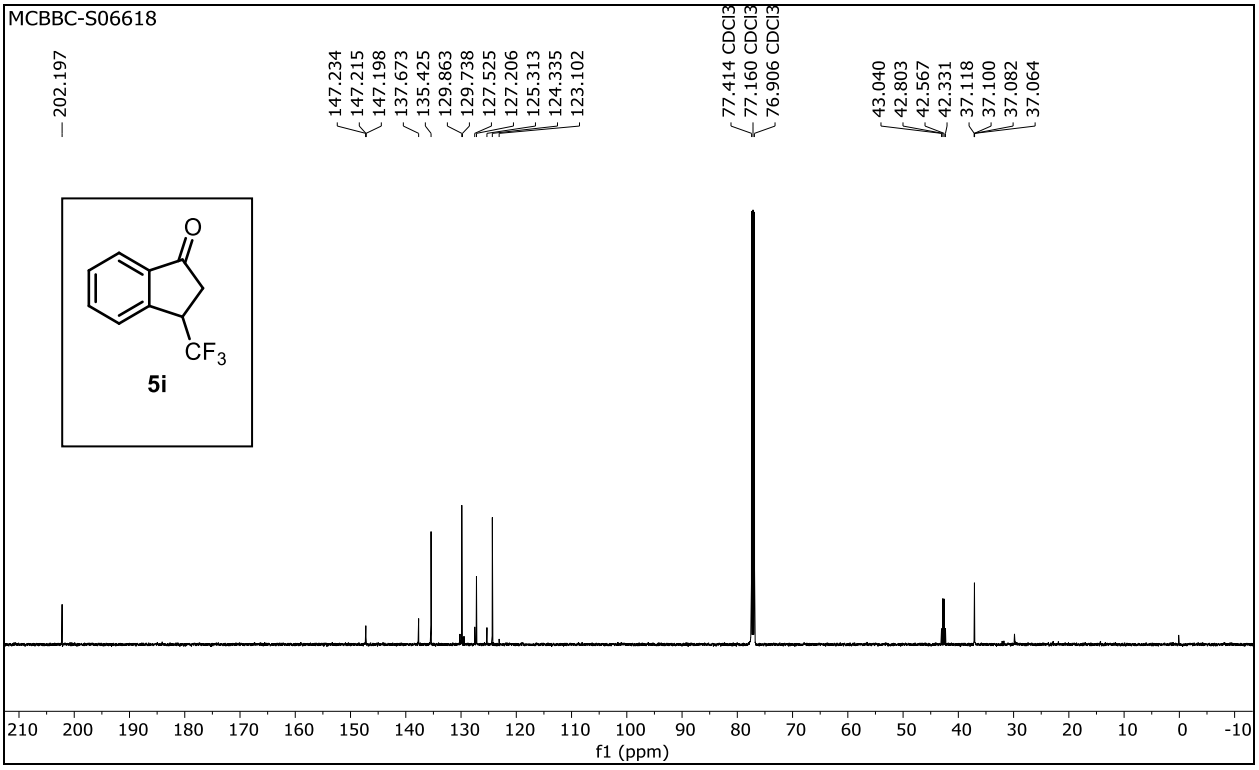

MCBBC-S03772
-70.379
Cl
O
CF3
5g
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

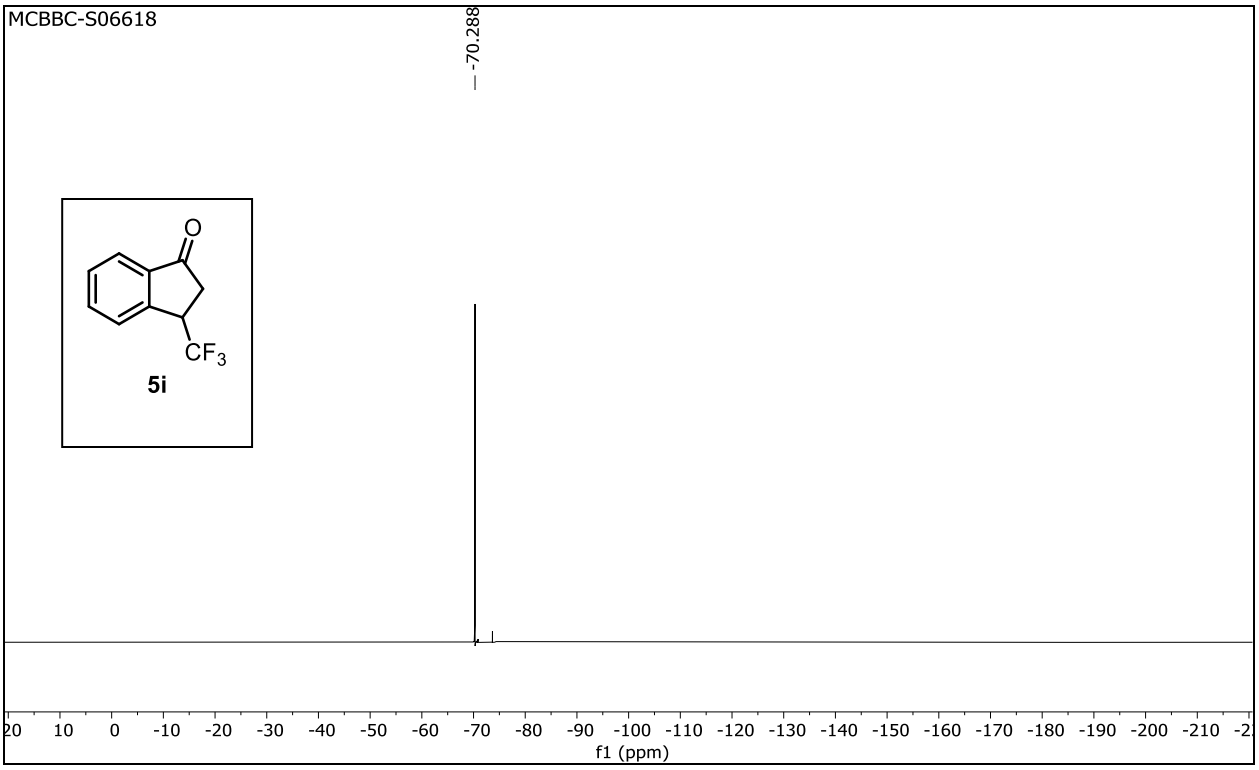

MCBBC-S05350
8.161
8.158
8.000
7.996
7.983
7.980
7.463
7.447
7.260 CDCl3
4.086
4.079
4.069
4.061
4.051
4.044
4.034
4.027
4.016
4.009
2.971
2.954
2.932
2.916
2.839
2.832
2.800
2.793
I
O
CF3
5h
1.00
1.04
1.07
1.08
1.15
1.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


MCBBC-S05350
200.442
146.383
146.365
143.990
139.466
133.560
129.375
128.854
127.162
124.950
122.735
95.839
77.415 CDCl3
77.160 CDCl3
76.906 CDCl3
42.888
42.648
42.409
42.171
37.030
37.012
36.993
36.976
O
I
CF3
5h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


MCBBC-S05350
-70.297
O
I
CF3
5h
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)


MCBBC-S06618
7.837
7.822
7.747
7.708
7.698
7.655
7.584
7.556
7.544
7.518
7.504
7.260 CDCl3
4.150
4.143
4.132
4.125
4.115
4.108
4.097
4.090
4.080
4.073
2.971
2.954
2.932
2.916
2.842
2.835
2.803
2.796
O
CF3
5i
1.01
2.04
1.01
1.02
1.06
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


MCBBC-S06618
202.197
147.234
147.215
147.198
137.673
135.425
129.863
129.738
127.525
127.206
125.313
124.335
123.102
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
43.040
42.803
42.567
42.331
37.118
37.100
37.082
37.064
O
CF3
5i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


MCBBC-S06618
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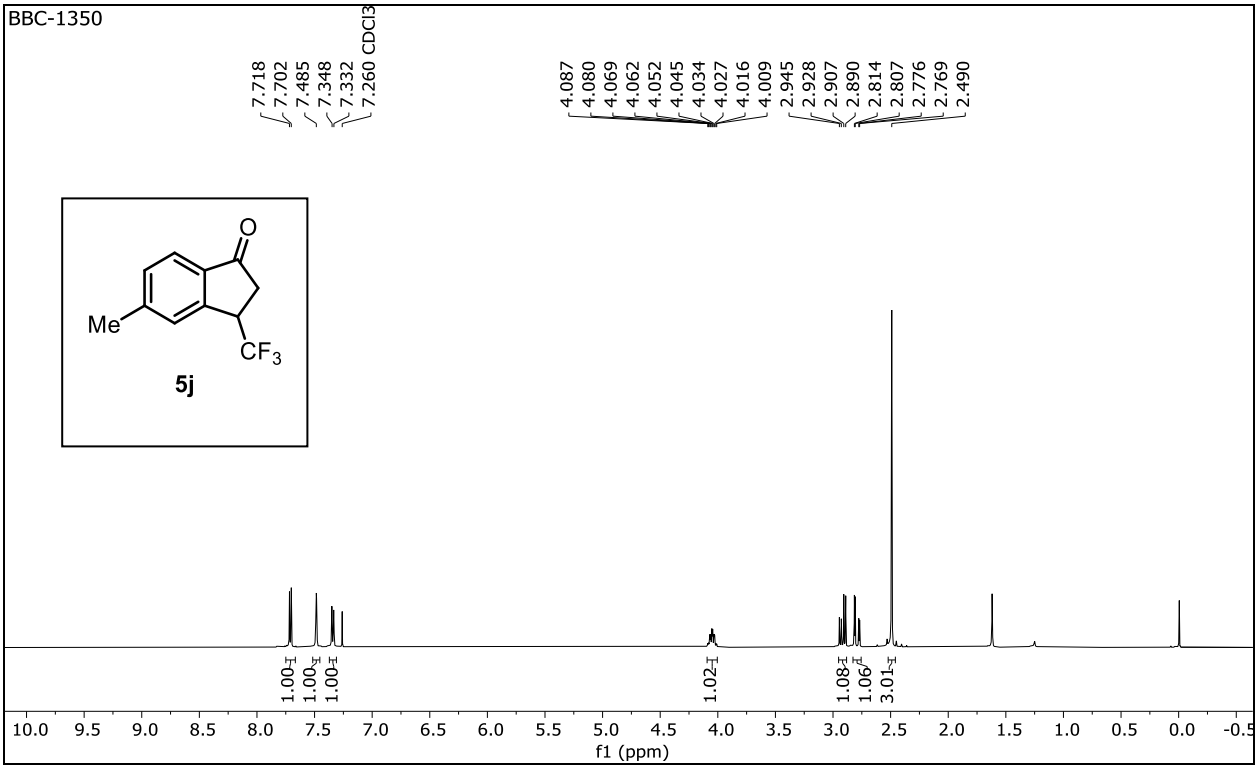
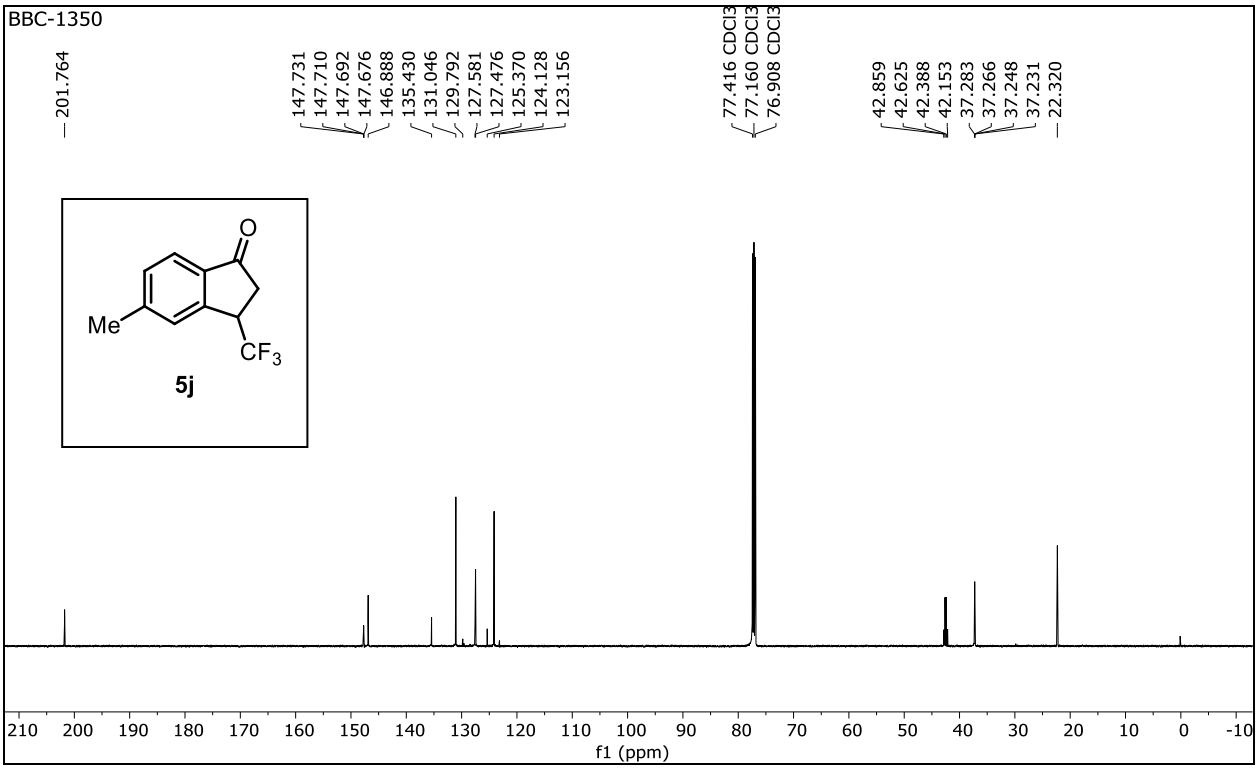
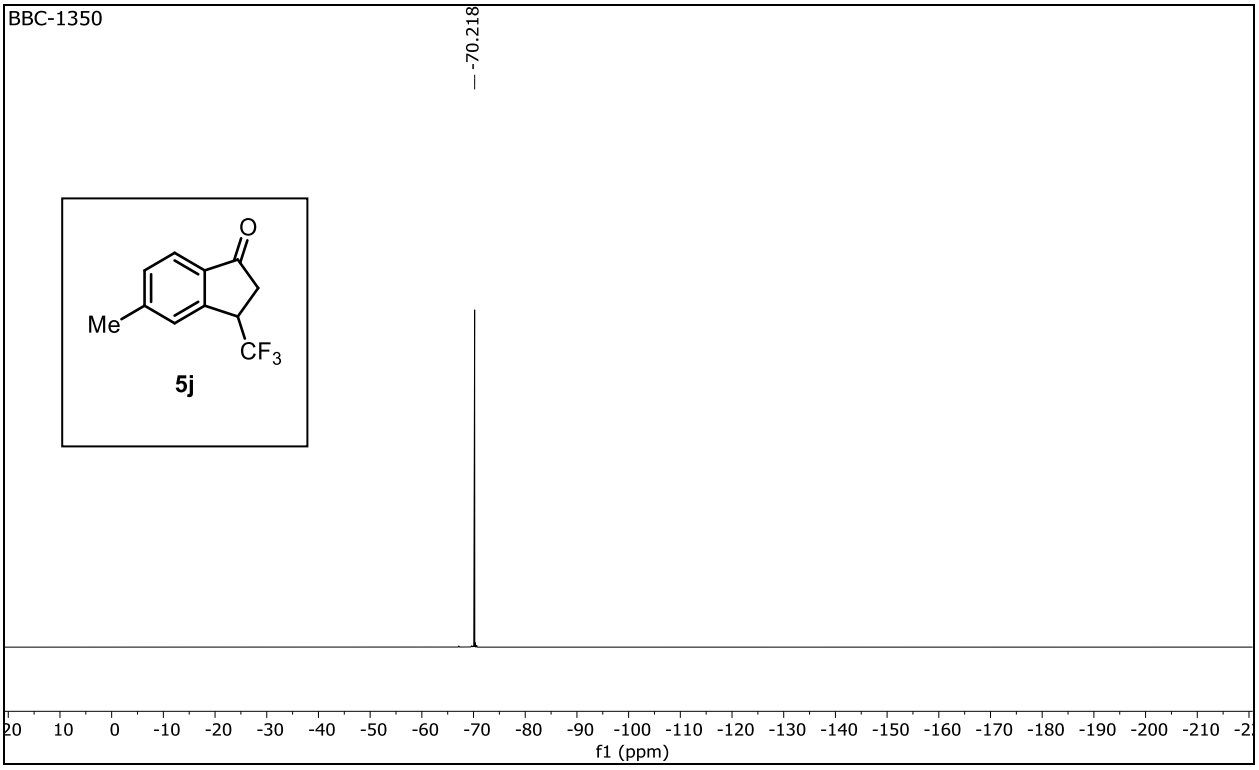
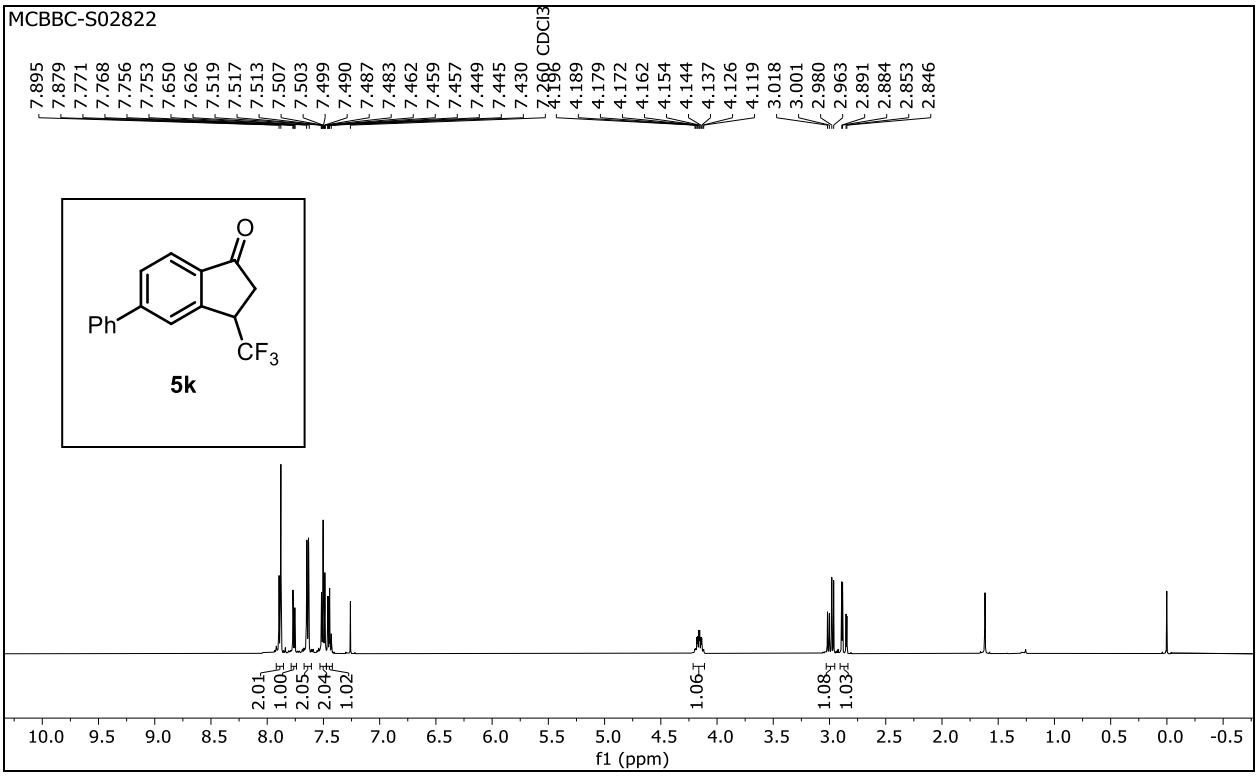
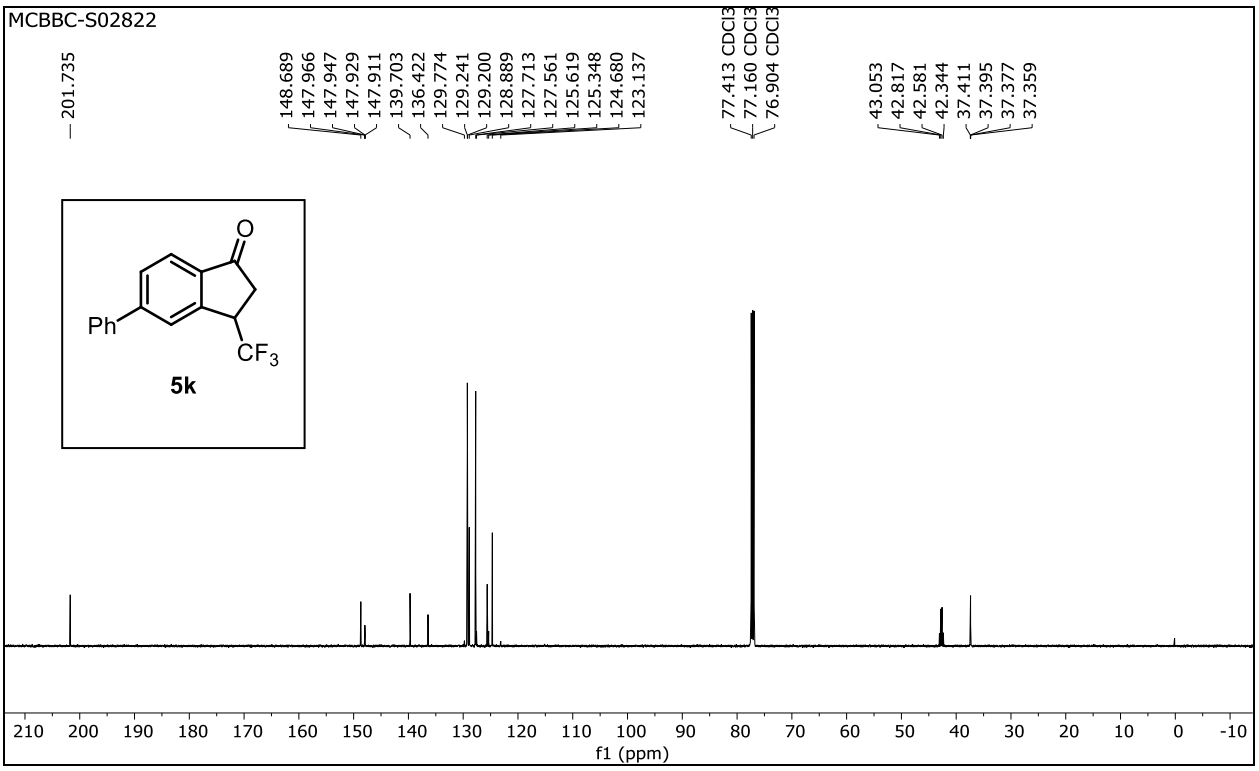
O
CF3
5i
f1 (ppm)

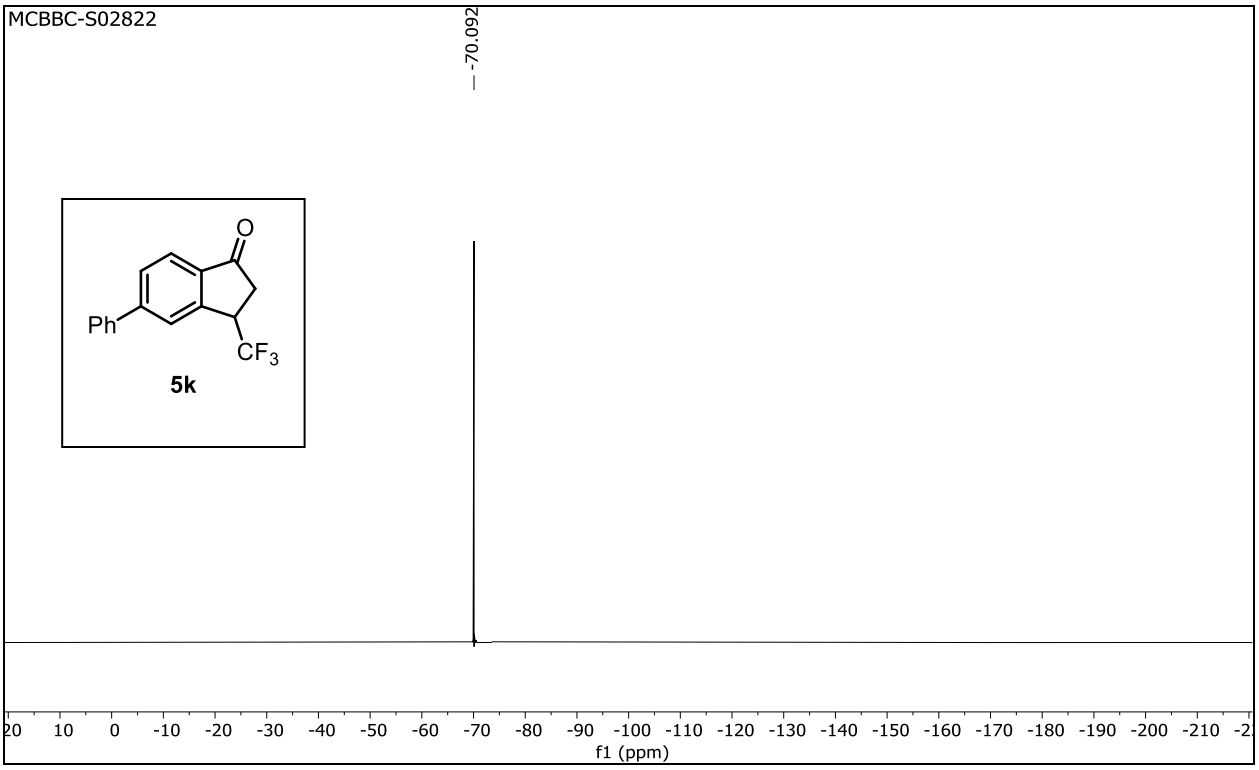

BBC-1350
7.718
7.702
7.485
7.348
7.332
7.260 CDCl3
4.087
4.080
4.069
4.062
4.052
4.045
4.034
4.027
4.016
4.009
2.945
2.928
2.907
2.890
2.814
2.807
2.776
2.769
2.490
O
Me
CF3
5j
1.00
1.00
1.00
1.02
1.08
1.06
3.01
f1 (ppm)

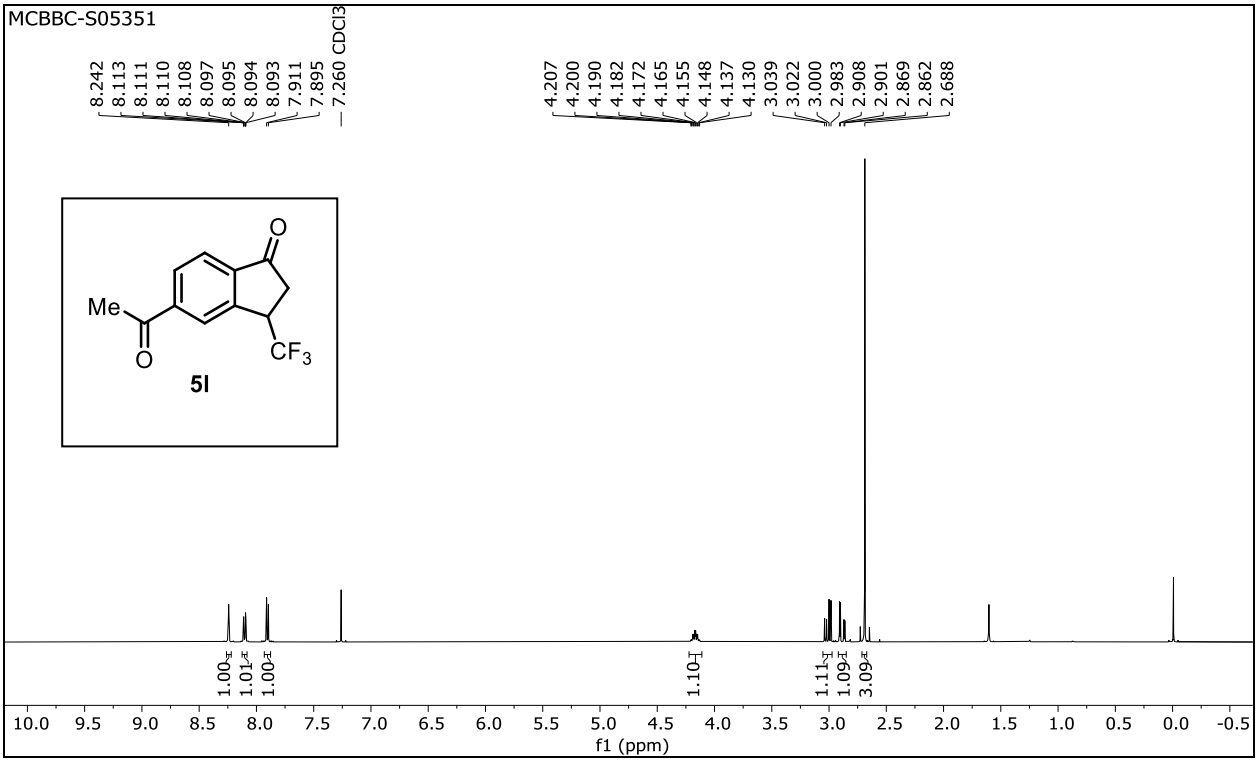

BBC-1350
201.764
147.731
147.710
147.692
147.676
146.888
135.430
131.046
129.792
127.581
127.476
125.370
124.128
123.156
77.416 CDCl3
77.160 CDCl3
76.908 CDCl3
42.859
42.625
42.388
42.153
37.283
37.266
37.248
37.231
22.320
O
Me
CF3
5j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

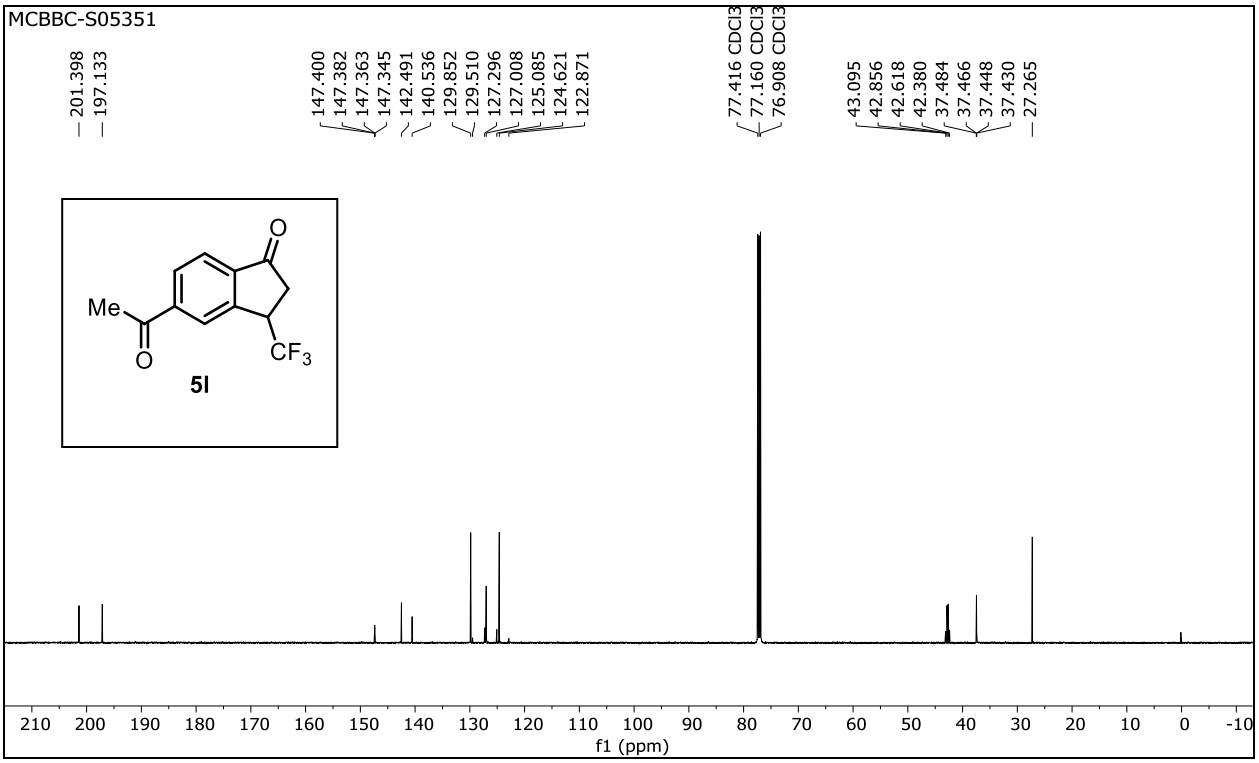

BBC-1350
-70.218
O
Me
CF3
5j
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

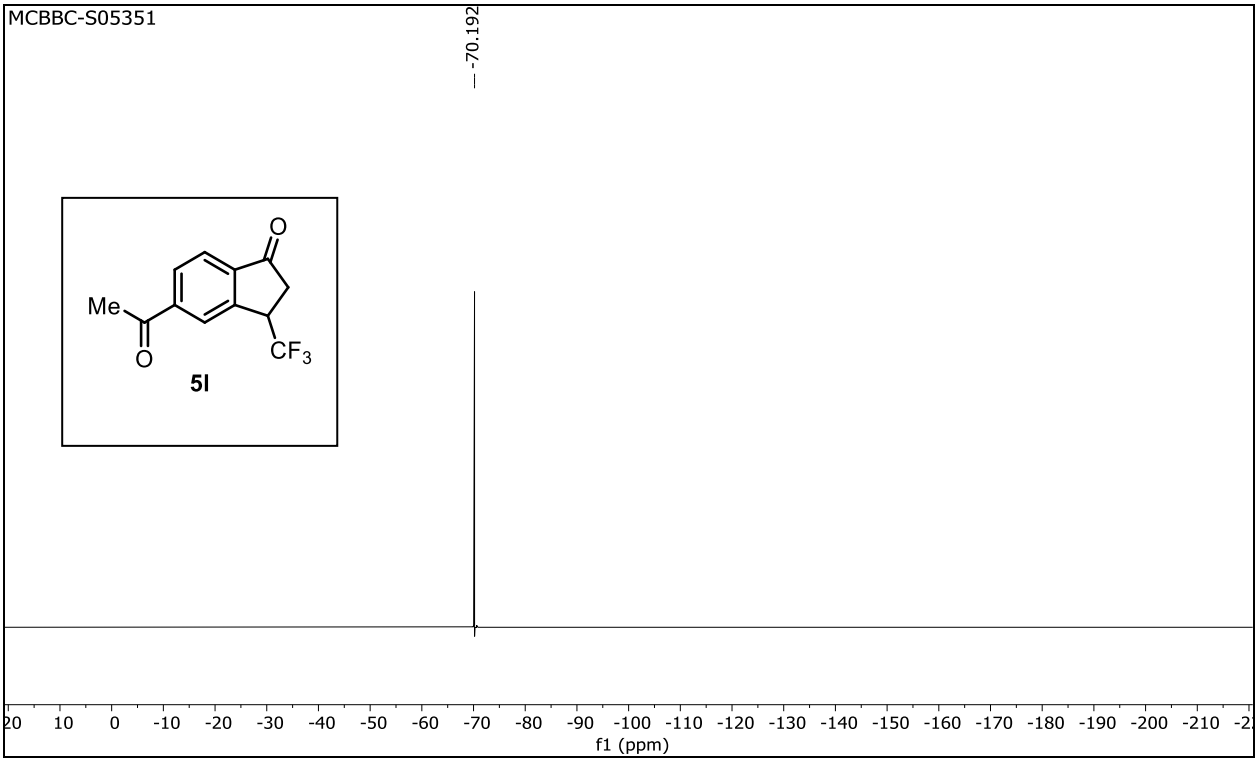

MCBBC-S02822
7.895
7.879
7.771
7.768
7.756
7.753
7.650
7.626
7.519
7.517
7.513
7.507
7.503
7.499
7.490
7.487
7.483
7.462
7.459
7.457
7.449
7.445
7.430
7.260 CDCl3
4.196
4.189
4.179
4.172
4.162
4.154
4.144
4.137
4.126
4.119
3.018
3.001
2.980
2.963
2.891
2.884
2.853
2.846
O
Ph
CF3
5k
2.01
1.00
2.05
2.04
1.02
1.06
1.08
1.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

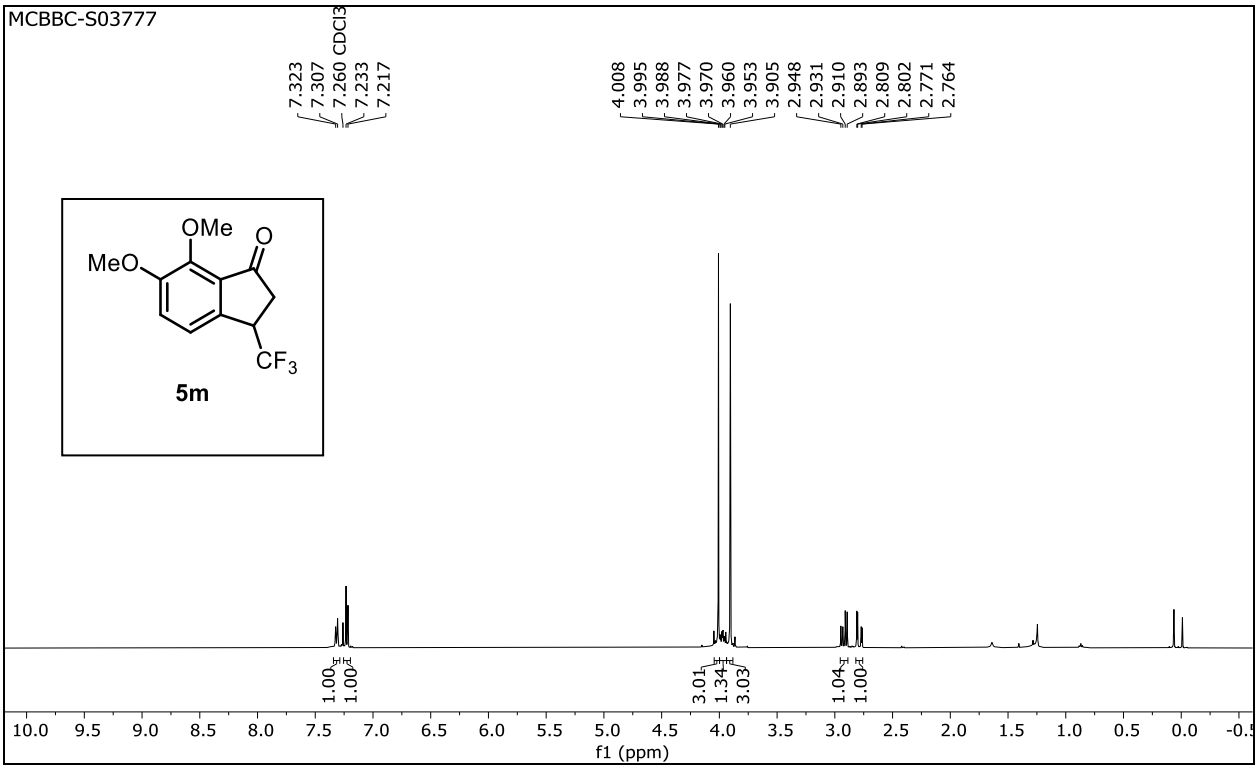

MCBBC-S02822
201.735
148.689
147.966
147.947
147.929
147.911
139.703
136.422
129.774
129.241
129.200
128.889
127.713
127.561
125.619
125.348
124.680
123.137
77.413 CDCl3
77.160 CDCl3
76.904 CDCl3
43.053
42.817
42.581
42.344
37.411
37.395
37.377
37.359
O
Ph
CF3
5k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

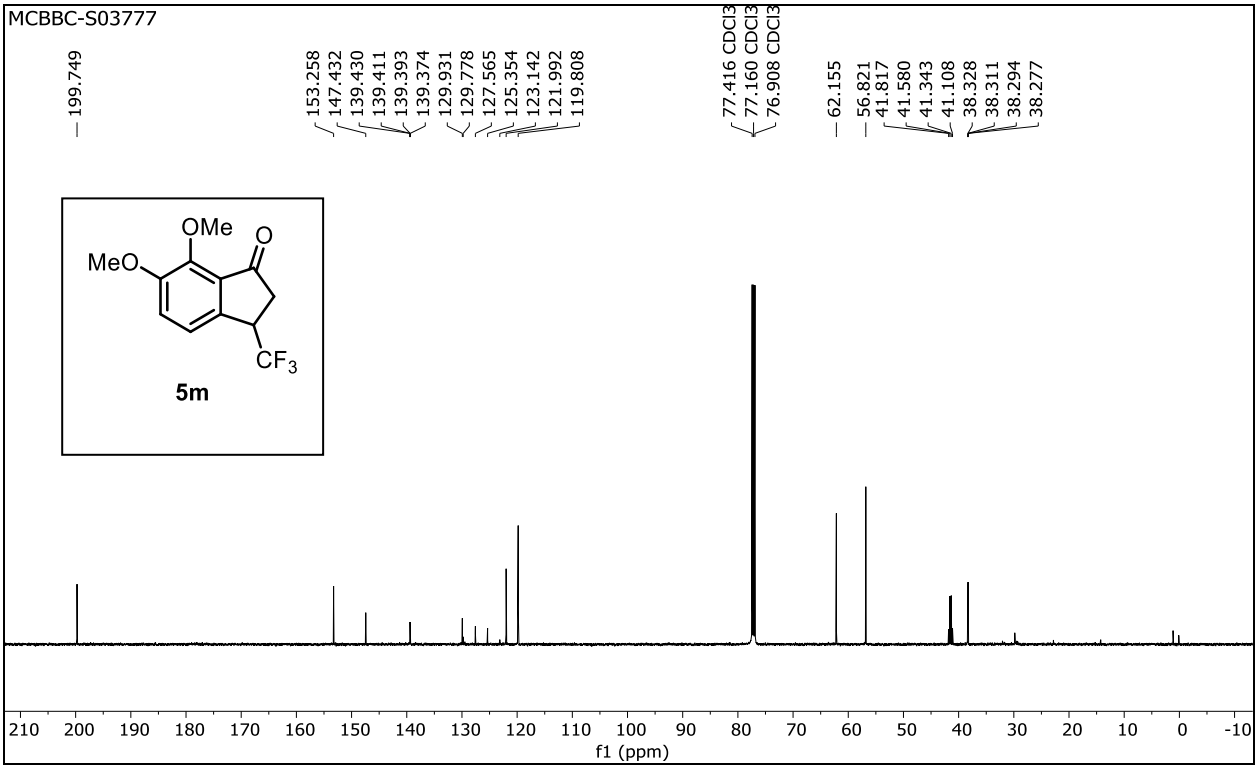

MCBBC-S02822
-70.092
O
Ph
CF3
5k
f1 (ppm)

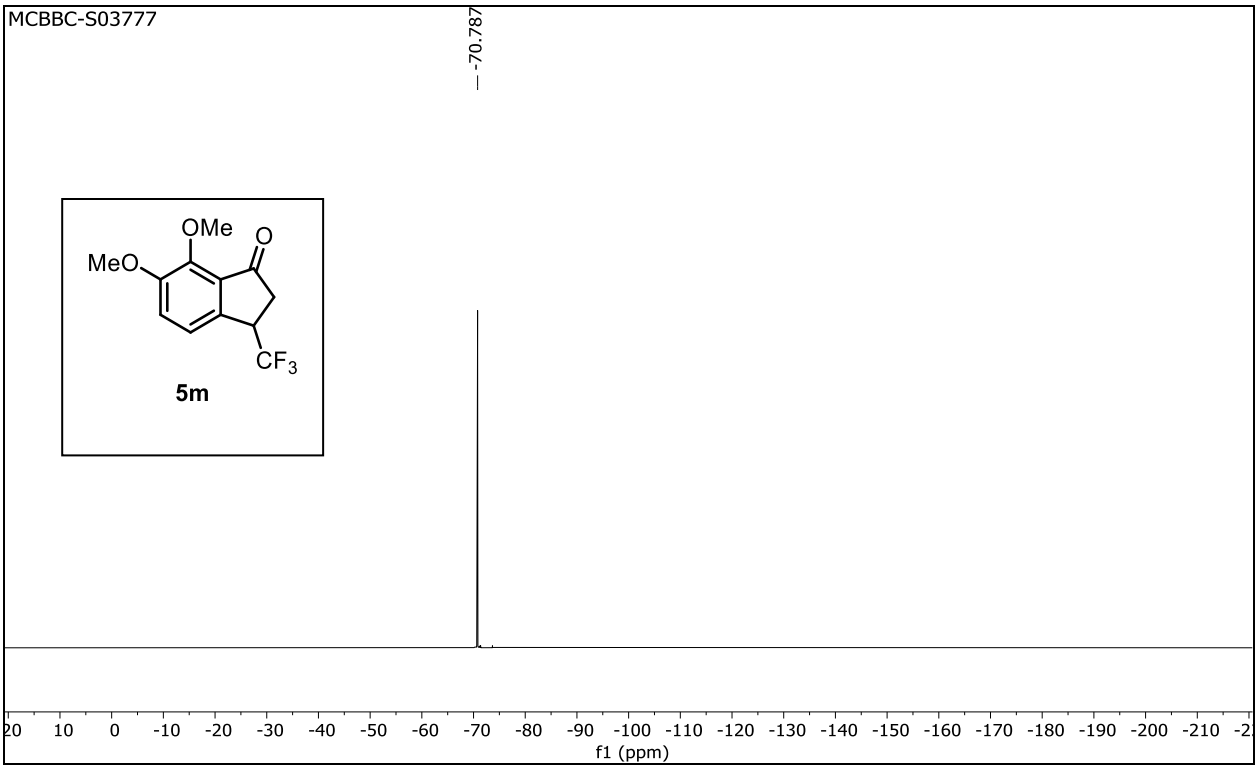

MCBBC-S05351
8.242
8.113
8.111
8.110
8.108
8.097
8.095
8.094
8.093
7.911
7.895
7.260 CDCl3
4.207
4.200
4.190
4.182
4.172
4.165
4.155
4.148
4.137
4.130
3.039
3.022
3.000
2.983
2.908
2.901
2.869
2.862
2.688
O
Me
O
CF3
5l
1.00
1.01
1.00
1.10
1.11
1.09
3.09
f1 (ppm)

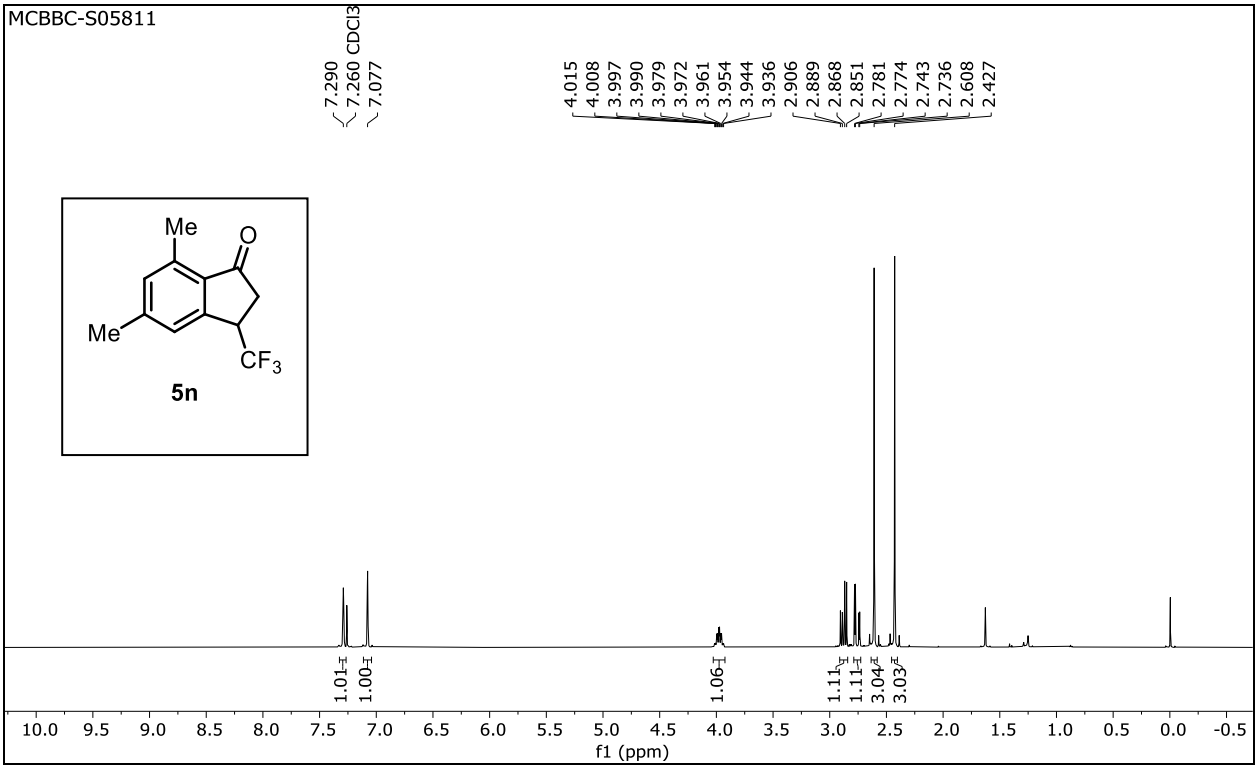

MCBBC-S05351
201.398
197.133
147.400
147.382
147.363
147.345
142.491
140.536
129.852
129.510
127.296
127.008
125.085
124.621
122.871
77.416 CDCl3
77.160 CDCl3
76.908 CDCl3
43.095
42.856
42.618
42.380
37.484
37.466
37.448
37.430
27.265
Me
O
O
CF3
5l
f1 (ppm)

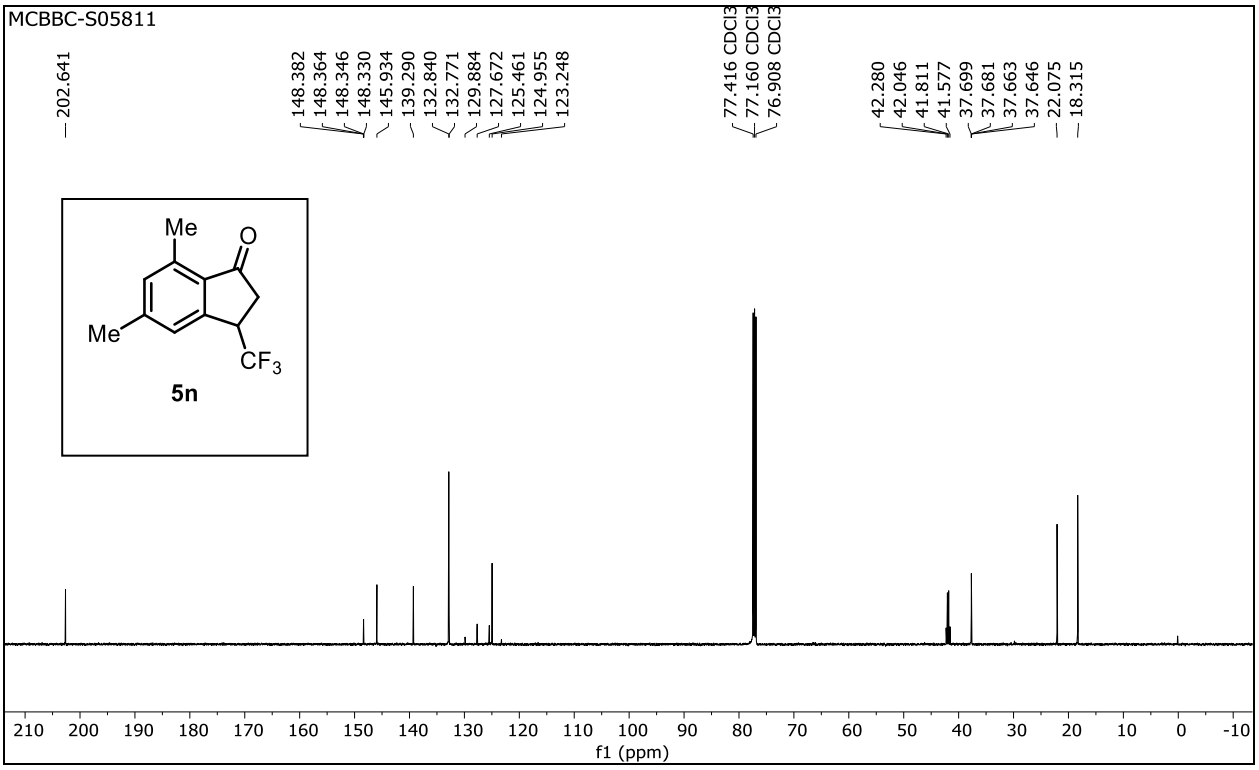

MCBBC-S05351
-70.192
Me
O
O
CF3
5l
f1 (ppm)

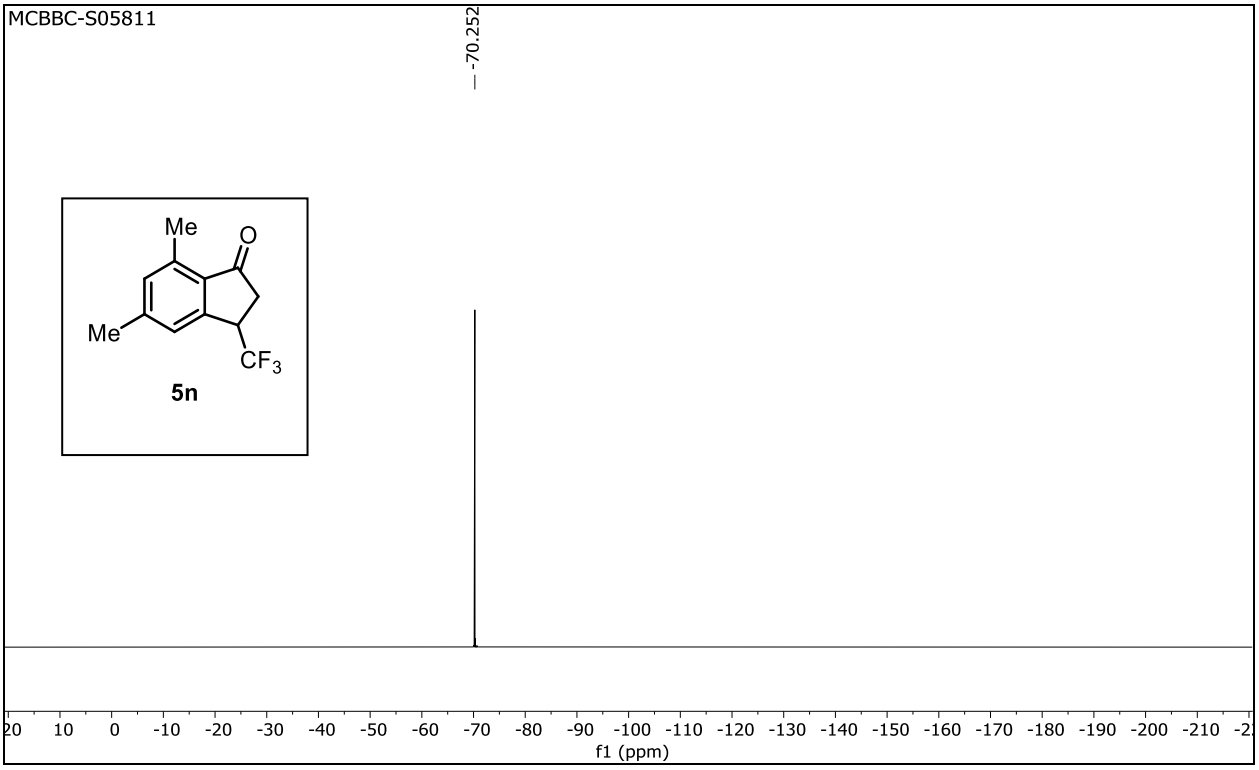

MCBBC-S03777
7.323
7.307
7.260 CDCl3
7.233
7.217
4.008
3.995
3.988
3.977
3.970
3.960
3.953
3.905
2.948
2.931
2.910
2.893
2.809
2.802
2.771
2.764
OMe
O
MeO
CF3
5m
1.00
1.00
3.01
1.34
3.03
1.04
1.00
f1 (ppm)

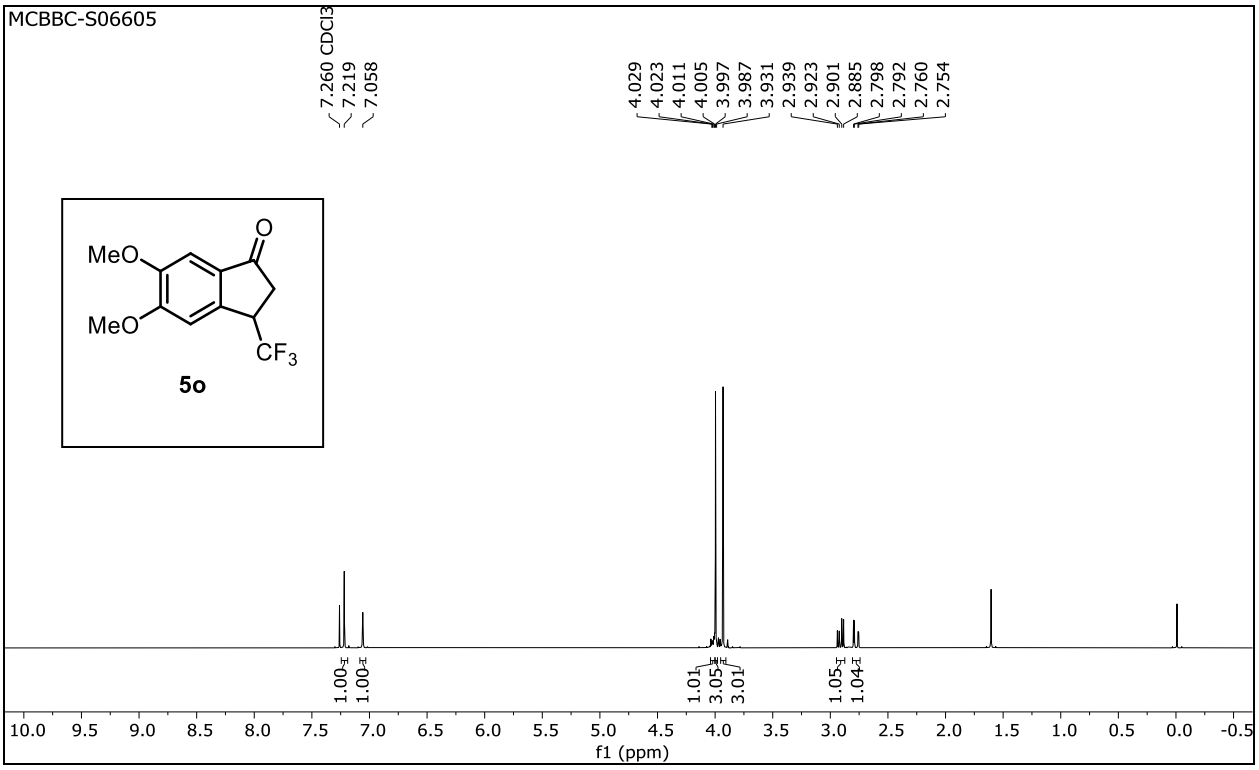

MCBBC-S03777
199.749
153.258
147.432
139.430
139.411
139.393
139.374
129.931
129.778
127.565
125.354
123.142
121.992
119.808
77.416 CDCl3
77.160 CDCl3
76.908 CDCl3
62.155
56.821
41.817
41.580
41.343
41.108
38.328
38.311
38.294
38.277
OMe
O
MeO
CF3
5m
f1 (ppm)

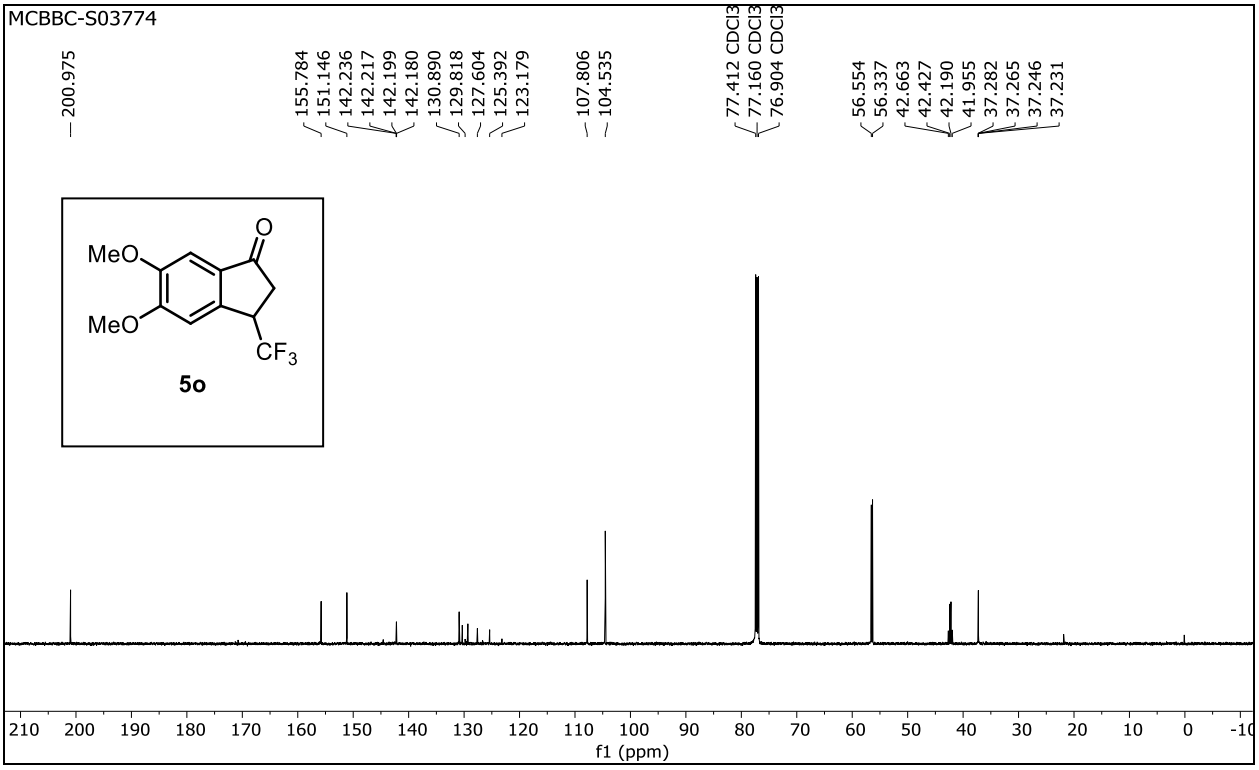

MCBBC-S03777
-70.787
OMe
O
MeO
CF3
5m
f1 (ppm)

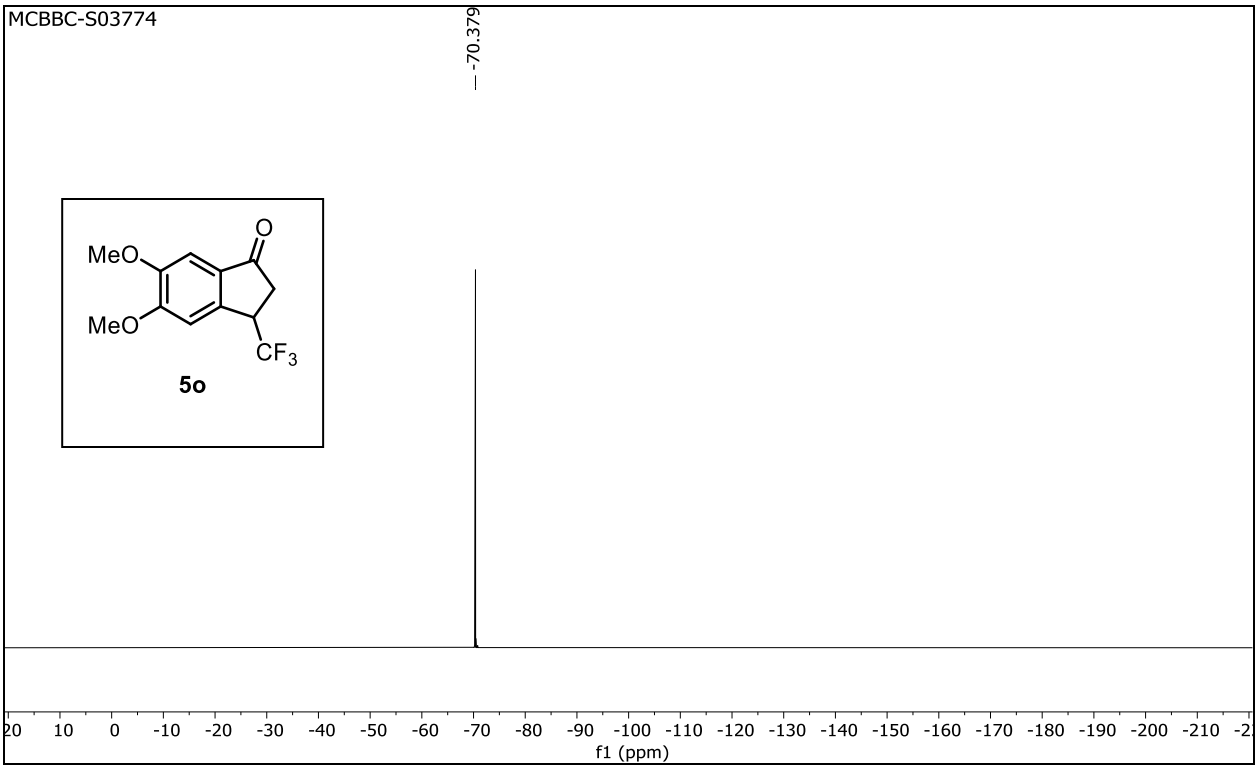

MCBBC-S05811
7.290
7.260 CDCl3
7.077
4.015
4.008
3.997
3.990
3.979
3.972
3.961
3.954
3.944
3.936
2.906
2.889
2.868
2.851
2.781
2.774
2.743
2.736
2.608
2.427
Me
O
Me
CF3
5n
1.01
1.00
1.06
1.11
1.11
3.04
3.03
f1 (ppm)

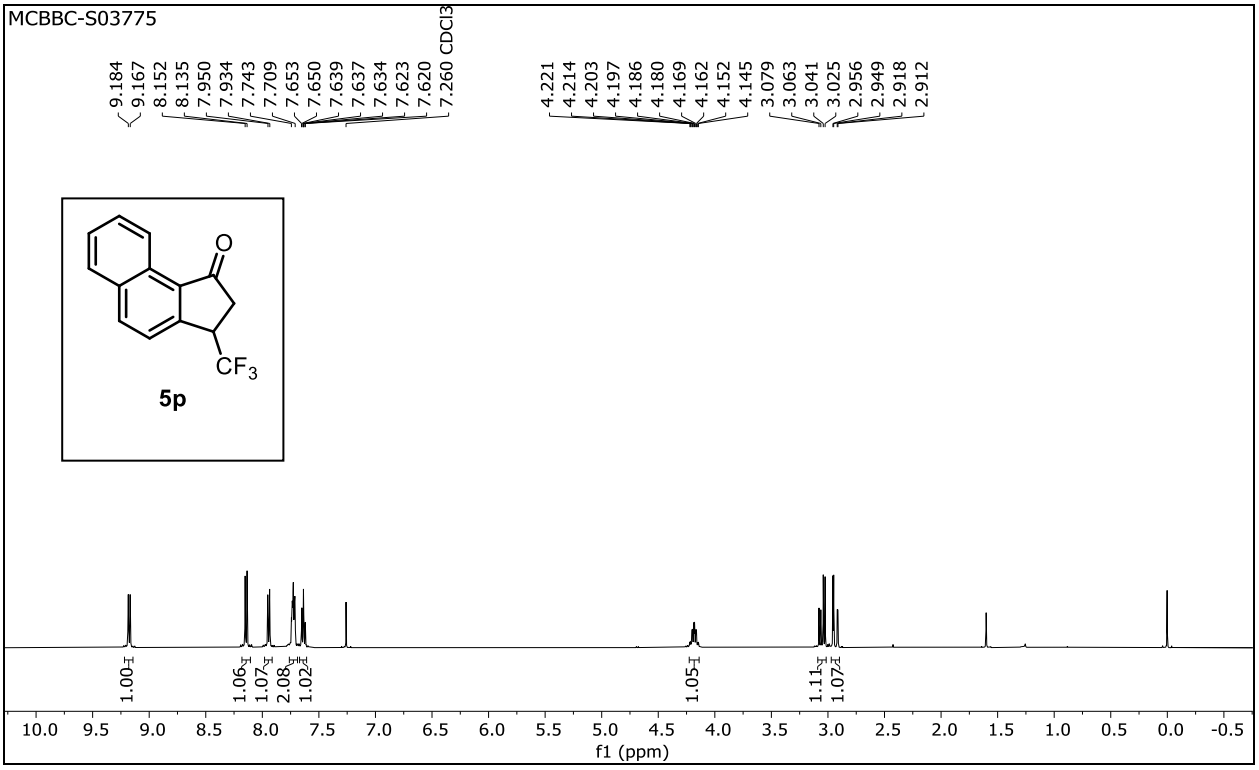

MCBBC-S05811
202.641
148.382
148.364
148.346
148.330
145.934
139.290
132.840
132.771
129.884
127.672
125.461
124.955
123.248
77.416 CDCl3
77.160 CDCl3
76.908 CDCl3
42.280
42.046
41.811
41.577
37.699
37.681
37.663
37.646
22.075
18.315
Me
O
Me
CF3
5n
f1 (ppm)

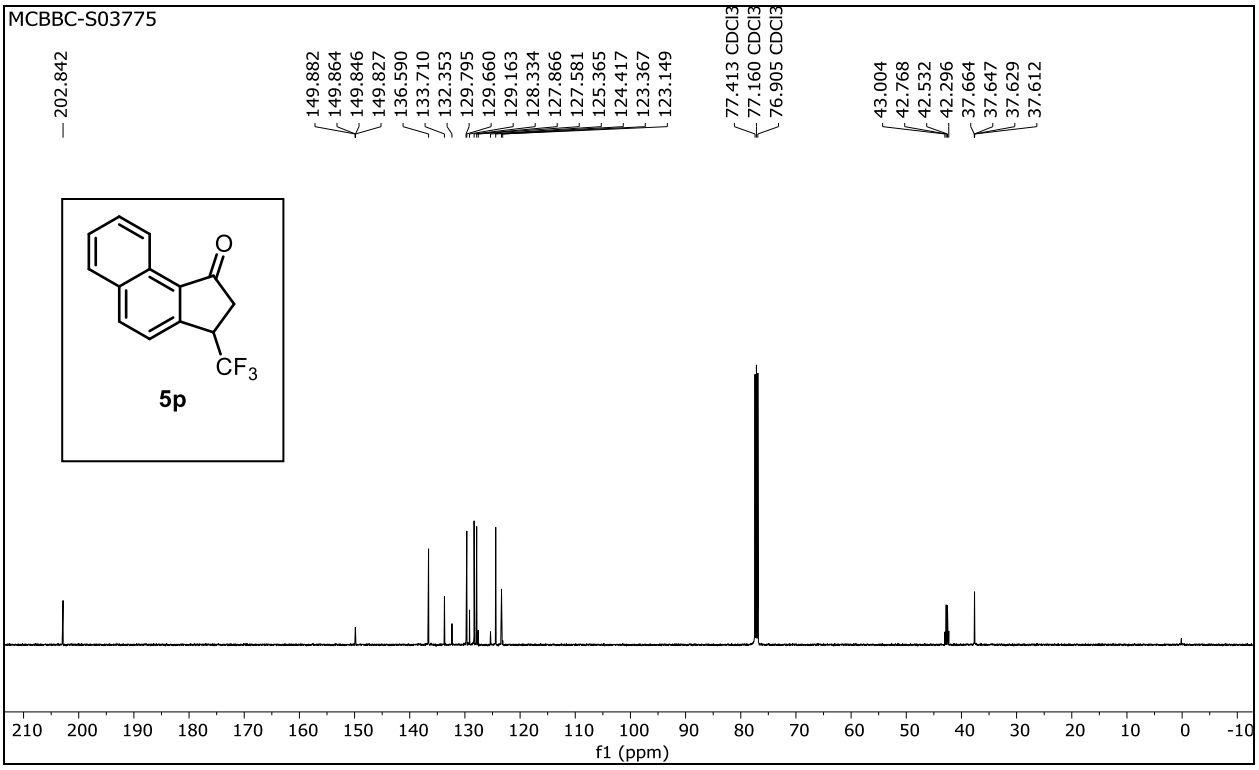

MCBBC-S05811
-70.252
Me
O
Me
CF3
5n
f1 (ppm)

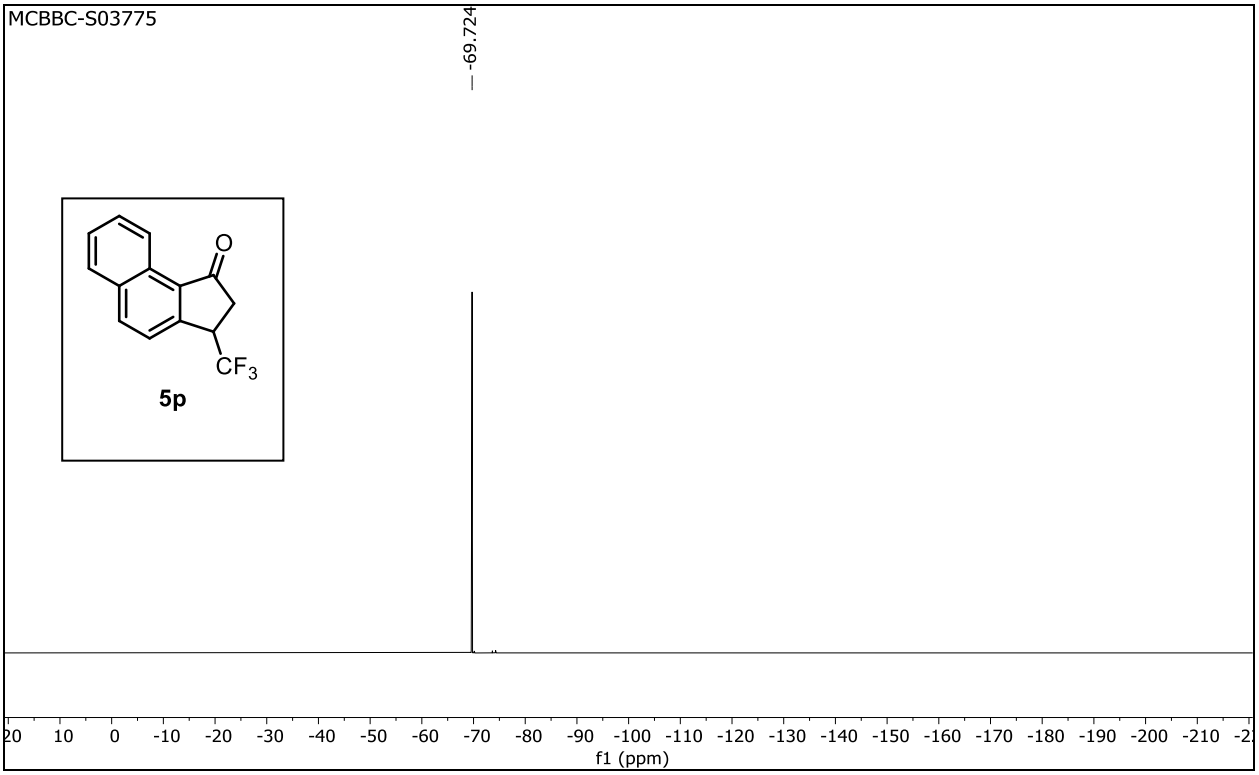

MCBBC-S06605
7.260 CDCl3
7.219
7.058
4.029
4.023
4.011
4.005
3.997
3.987
3.931
2.939
2.923
2.901
2.885
2.798
2.792
2.760
2.754
MeO
MeO
O
CF3
5o
1.00
1.00
1.01
3.05
3.01
1.05
1.04
f1 (ppm)

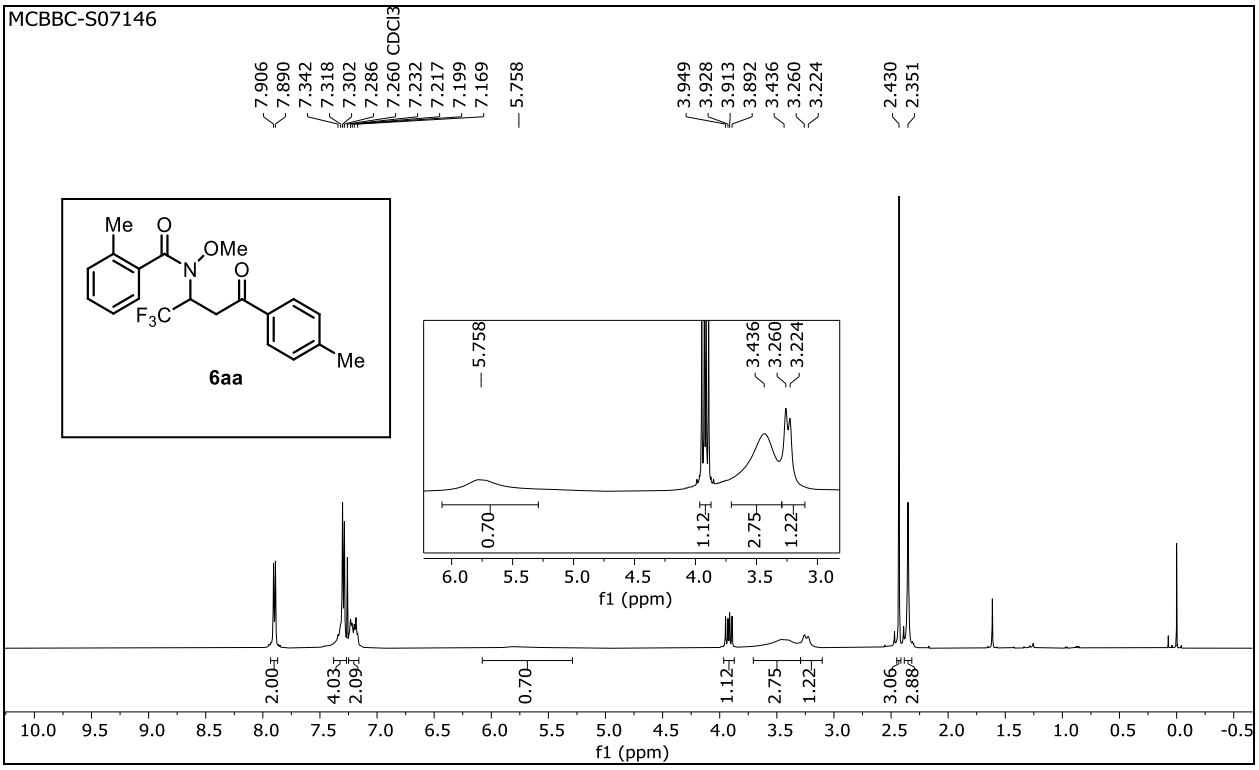

MCBBC-S03774
200.975
155.784
151.146
142.236
142.217
142.199
142.180
130.890
129.818
127.604
125.392
123.179
107.806
104.535
77.412 CDCl3
77.160 CDCl3
76.904 CDCl3
56.554
56.337
42.663
42.427
42.190
41.955
37.282
37.265
37.246
37.231
MeO
MeO
O
CF3
5o
f1 (ppm)

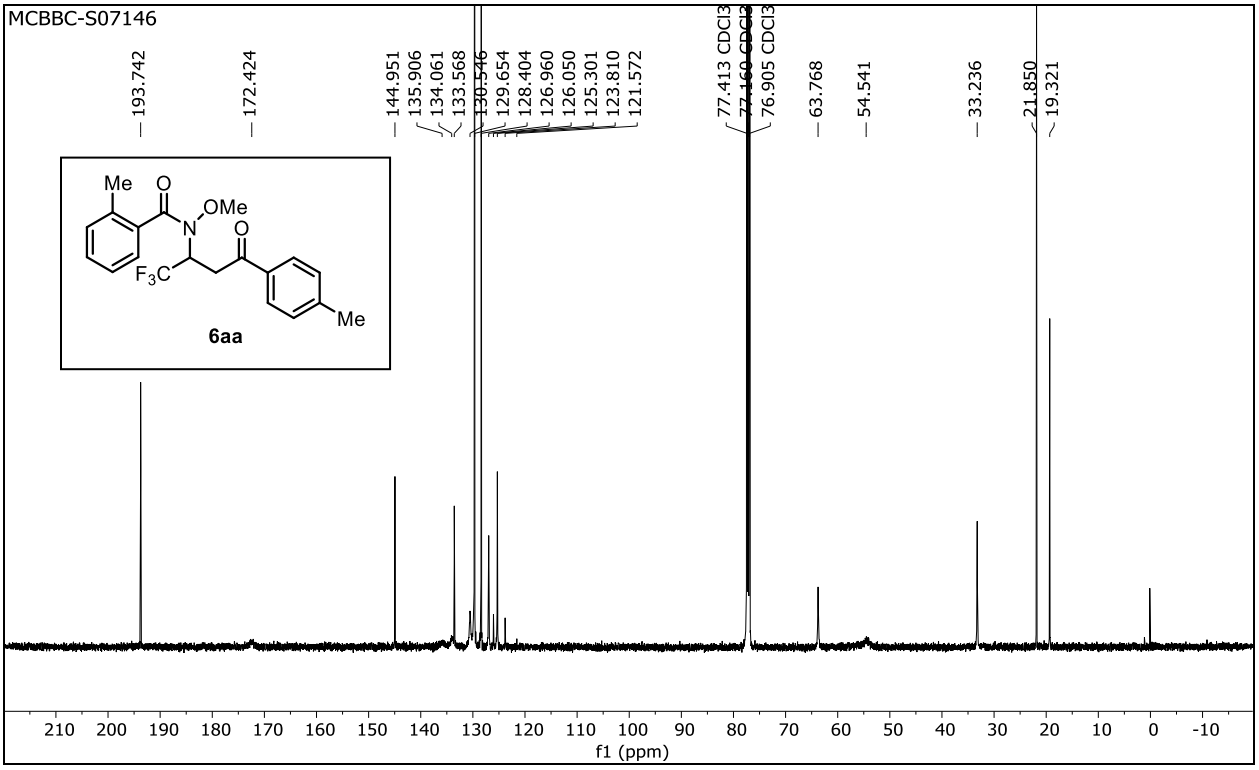

MCBBC-S03774
-70.379
MeO
MeO
O
CF3
5o
f1 (ppm)

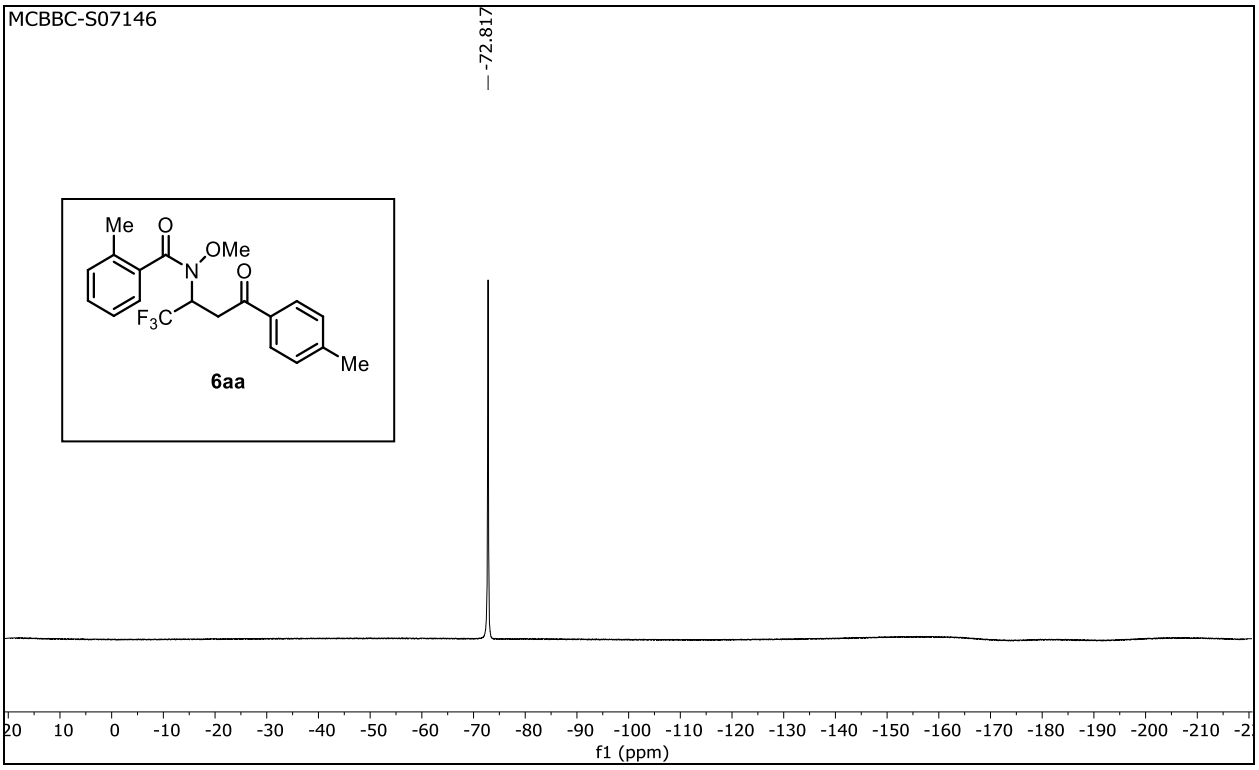

MCBBC-S03775
9.184
9.167
8.152
8.135
7.950
7.934
7.743
7.709
7.653
7.650
7.639
7.637
7.634
7.623
7.620
7.260 CDCl3
4.221
4.214
4.203
4.197
4.186
4.180
4.169
4.162
4.152
4.145
3.079
3.063
3.041
3.025
2.956
2.949
2.918
2.912
1.00
1.06
1.07
2.08
1.02
1.05
1.11
1.07
O
CF3
5p
f1 (ppm)

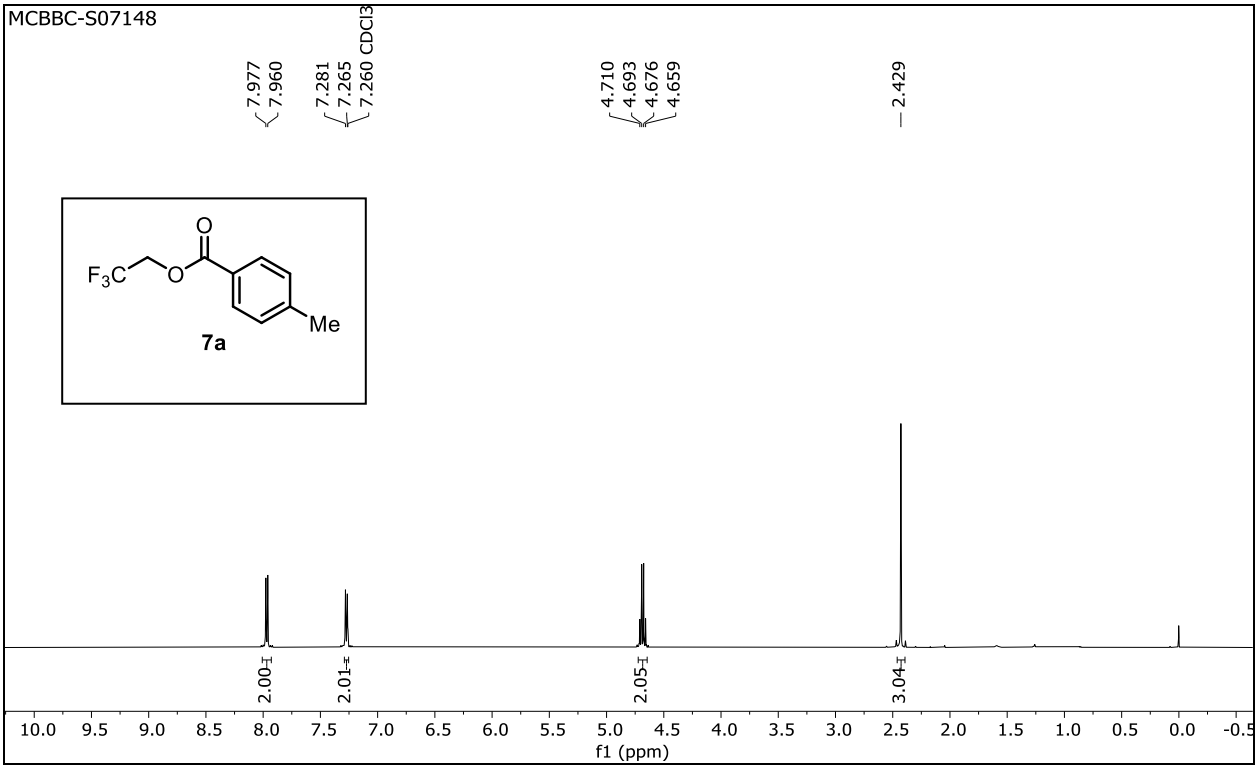

MCBBC-S03775
202.842
149.882
149.864
149.846
149.827
136.590
133.710
132.353
129.795
129.660
129.163
128.334
127.866
127.581
125.365
124.417
123.367
123.149
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
43.004
42.768
42.532
42.296
37.664
37.647
37.629
37.612
O
CF3
5p
f1 (ppm)

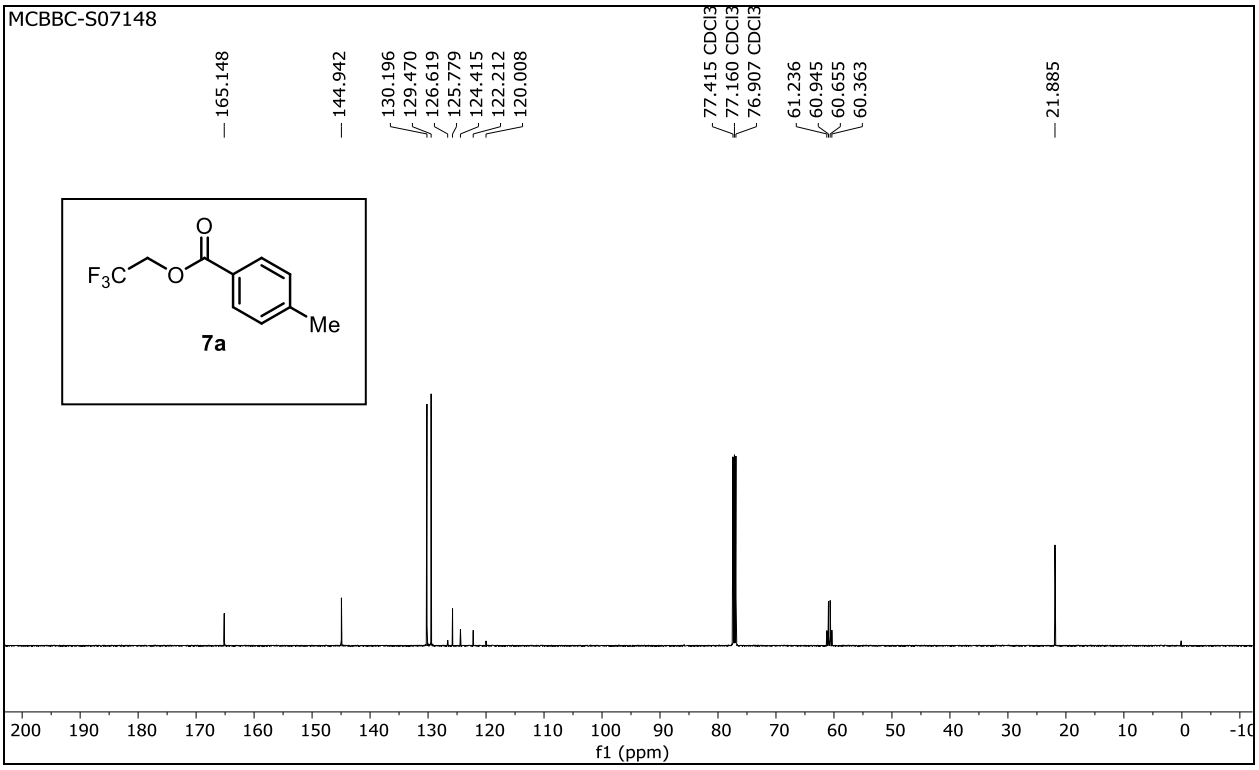

MCBBC-S03775
-69.724
O
CF3
5p
f1 (ppm)

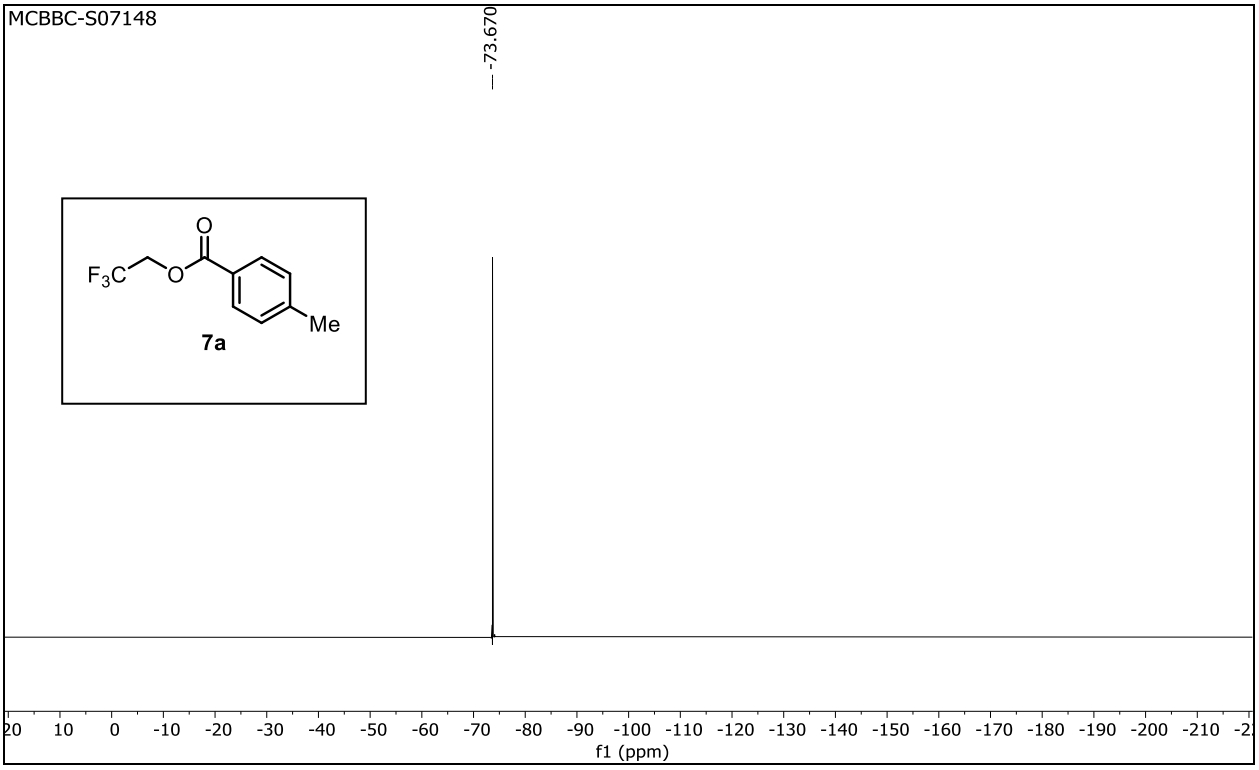

MCBBC-S07146
7.906
7.890
7.342
7.318
7.302
7.286
7.260 CDCl3
7.232
7.217
7.199
7.169
5.758
3.949
3.928
3.913
3.892
3.436
3.260
3.224
2.430
2.351
Me
O
OMe
N
O
F3C
Me
6aa
0.70
1.12
2.75
1.22
f1 (ppm)
2.00
4.03
2.09
0.70
1.12
2.75
1.22
3.06
2.88

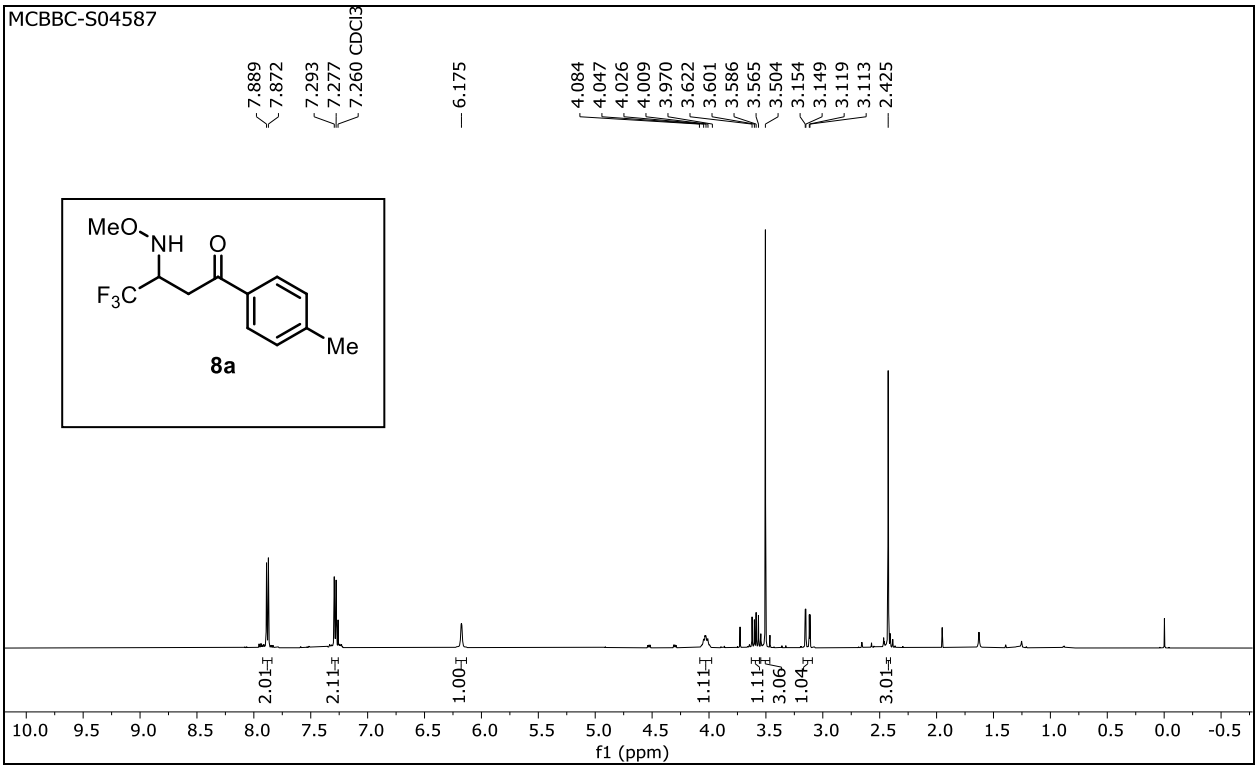

MCBBC-S07146
193.742
172.424
144.951
135.906
134.061
133.568
130.546
129.654
128.404
126.960
126.050
125.301
123.810
121.572
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
63.768
54.541
33.236
21.850
19.321
Me
O
OMe
N
O
F3C
Me
6aa
f1 (ppm)

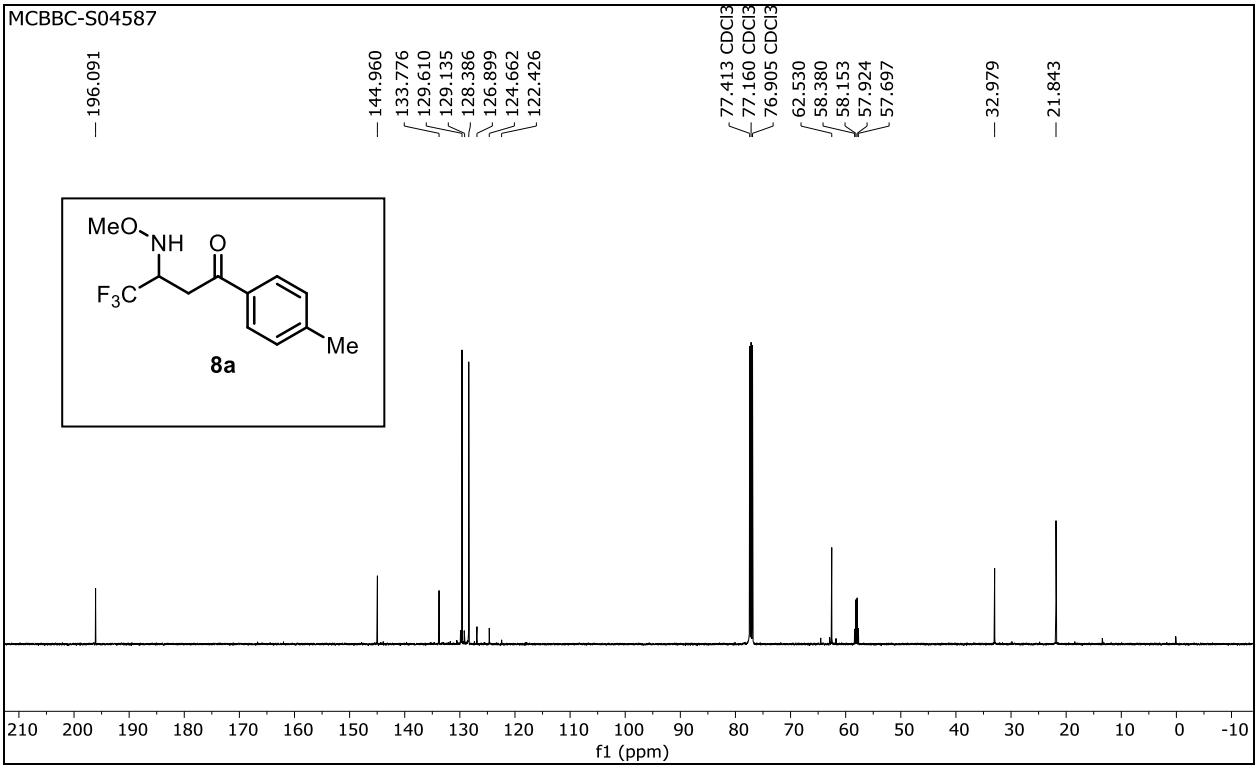

MCBBC-S07146
-72.817
Me
O
OMe
N
O
F3C
Me
6aa
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

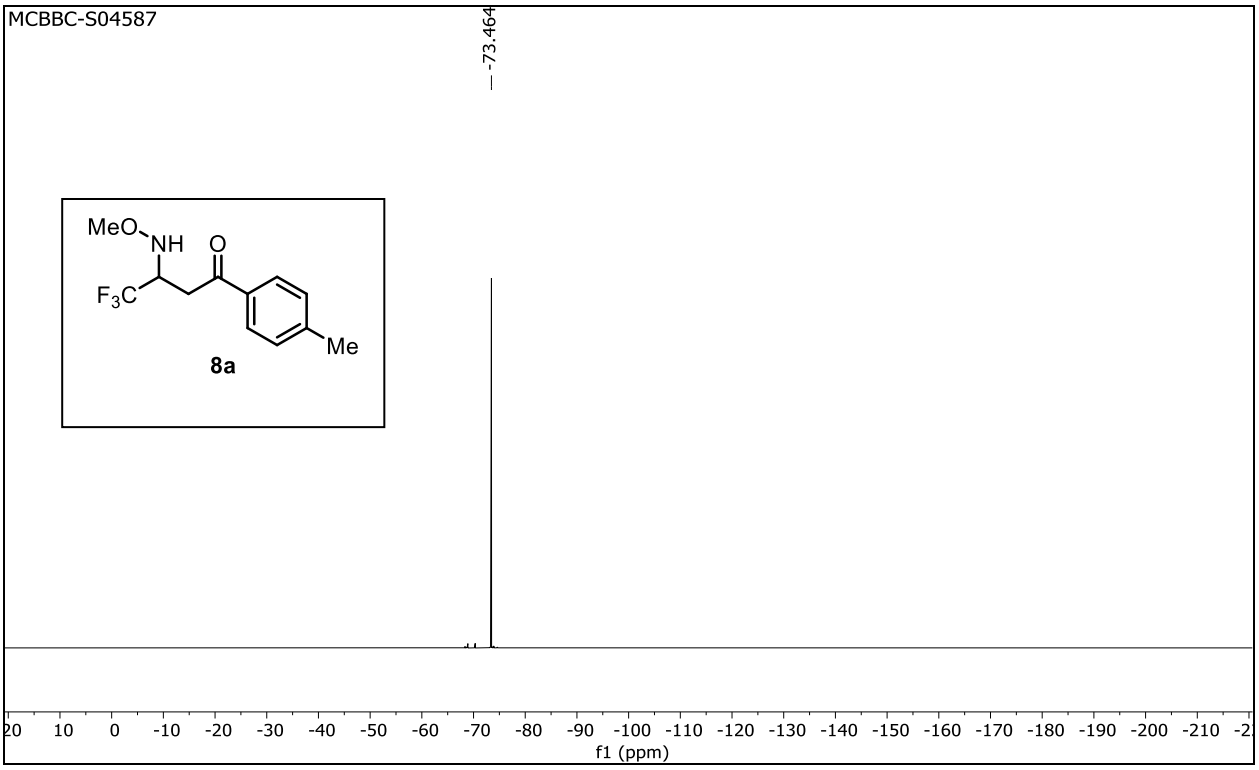

MCBBC-S07148
7.977
7.960
7.281
7.265
7.260 CDCl3
4.710
4.693
4.676
4.659
2.429
O
F3C
O
Me
7a
2.00
2.01
2.05
3.04
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

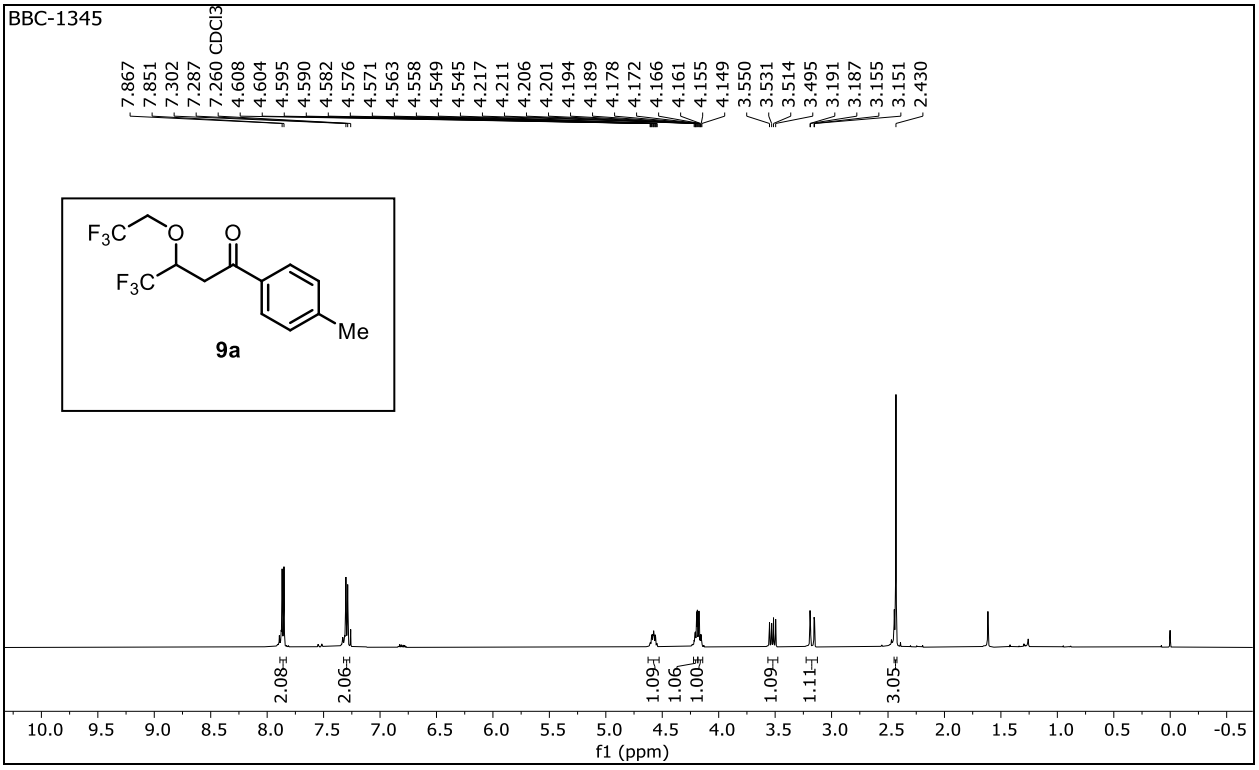

MCBBC-S07148
165.148
144.942
130.196
129.470
126.619
125.779
124.415
122.212
120.008
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
61.236
60.945
60.655
60.363
21.885
F3C
O
O
Me
7a
f1 (ppm)

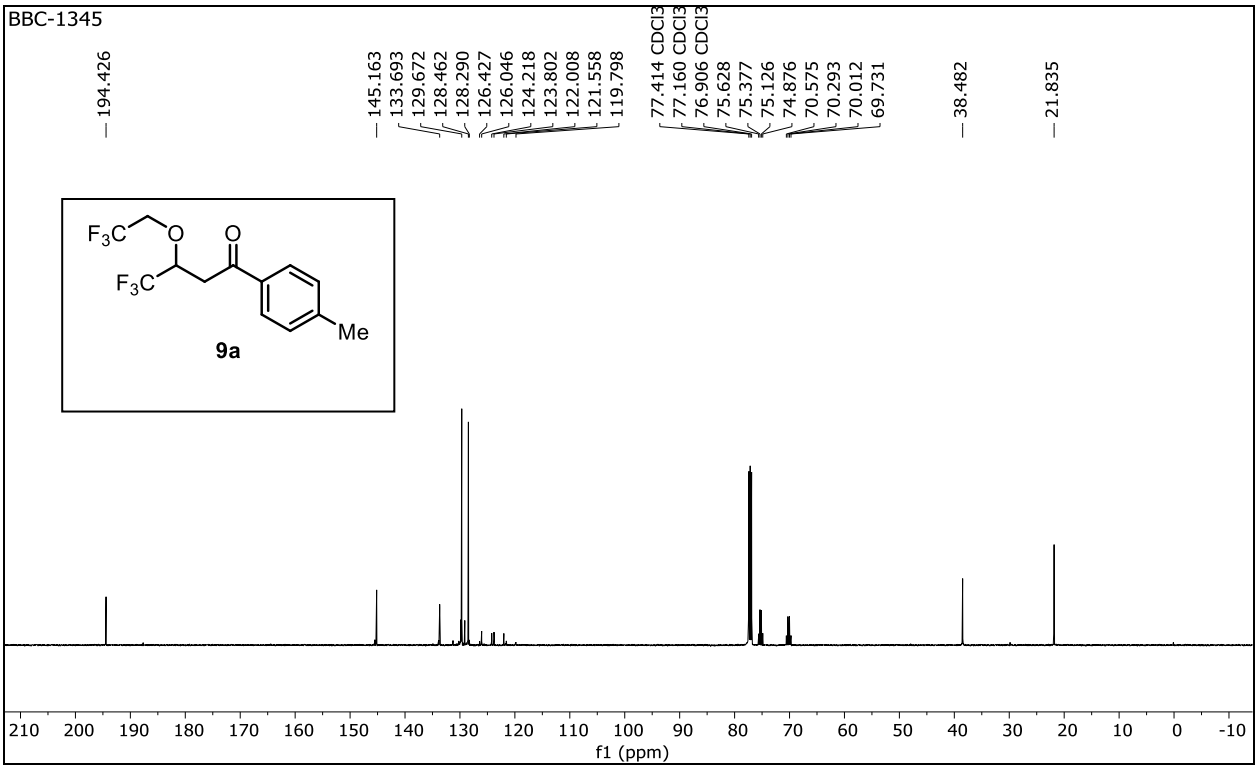

MCBBC-S07148
-73.670
F3C
O
O
Me
7a
f1 (ppm)

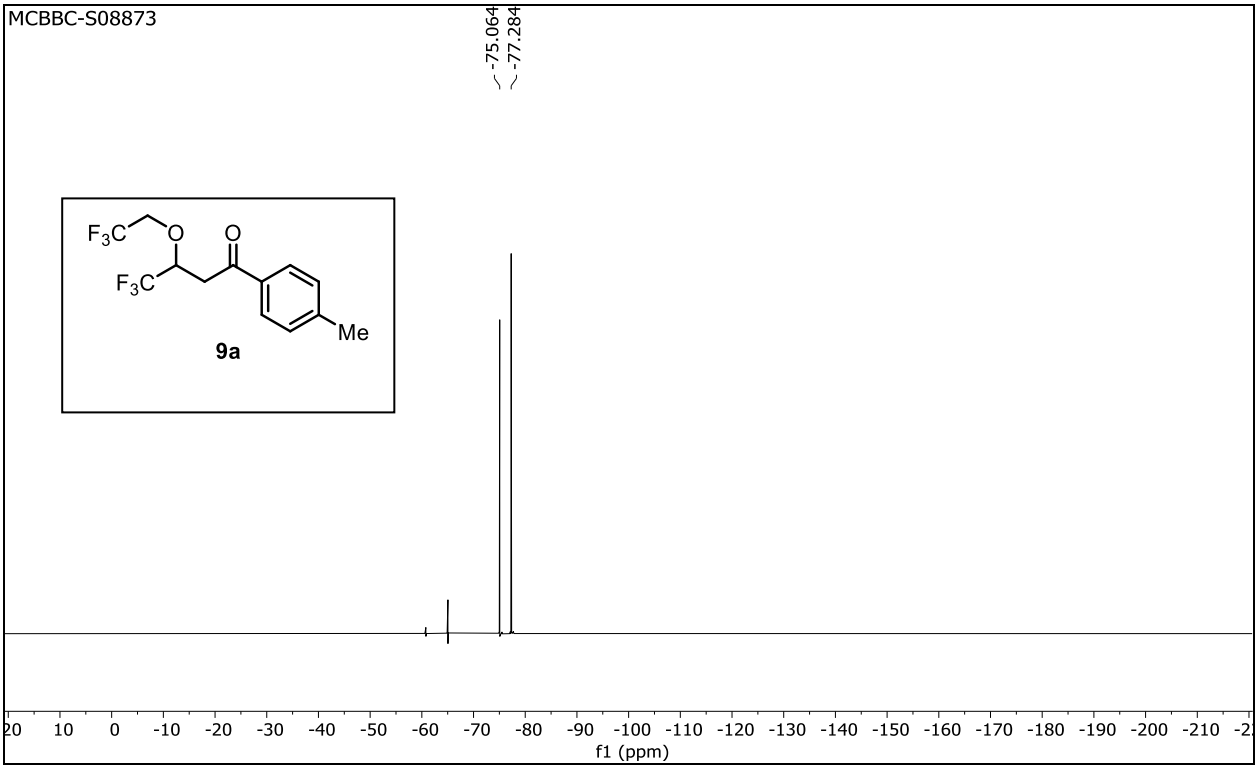

MCBBC-S04587
7.889
7.872
7.293
7.277
7.260 CDCl3
6.175
4.084
4.047
4.026
4.009
3.970
3.622
3.601
3.586
3.565
3.504
3.154
3.149
3.119
3.113
2.425
MeO
NH
O
F3C
Me
8a
2.01
2.11
1.00
1.11
1.11
3.06
1.04
3.01
f1 (ppm)

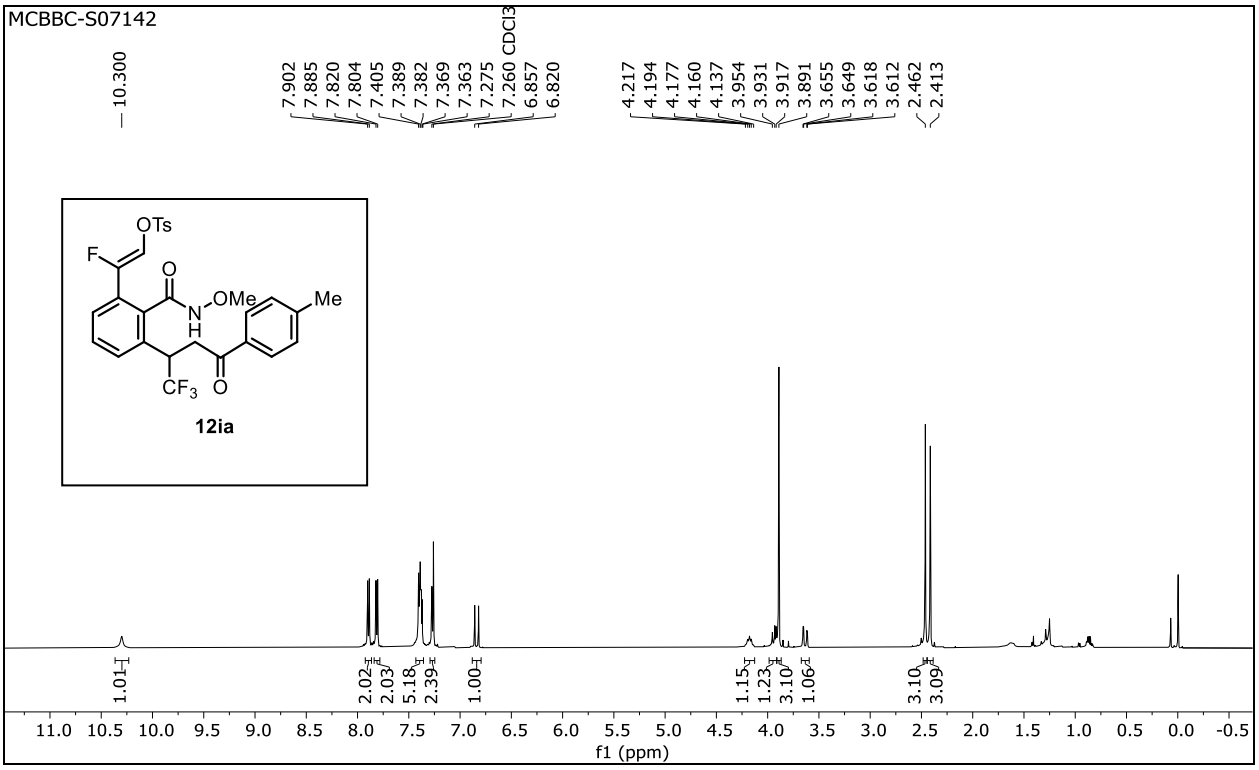

MCBBC-S04587
196.091
144.960
133.776
129.610
129.135
128.386
126.899
124.662
122.426
77.413 CDCl3
77.160 CDCl3
76.905 CDCl3
62.530
58.380
58.153
57.924
57.697
32.979
21.843
MeO
NH
O
F3C
Me
8a
f1 (ppm)

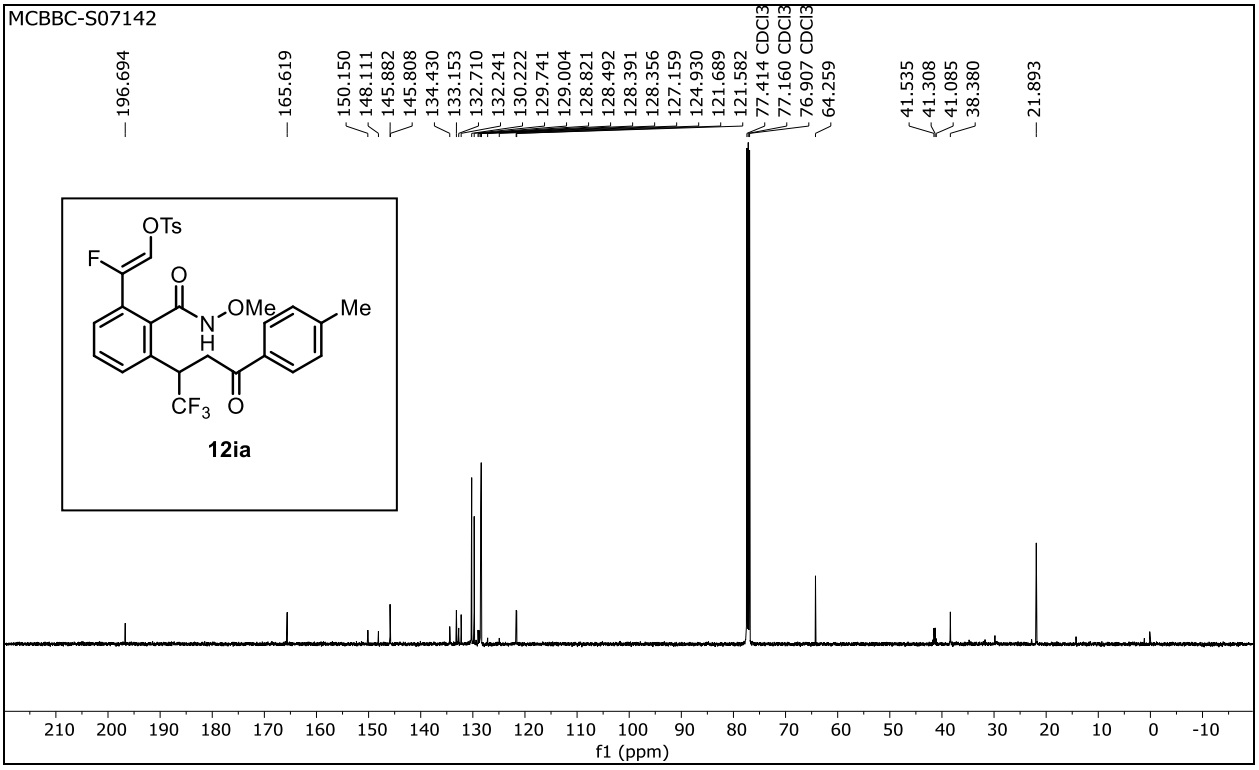

MCBBC-S04587
-73.464
MeO
NH
O
F3C
Me
8a
f1 (ppm)

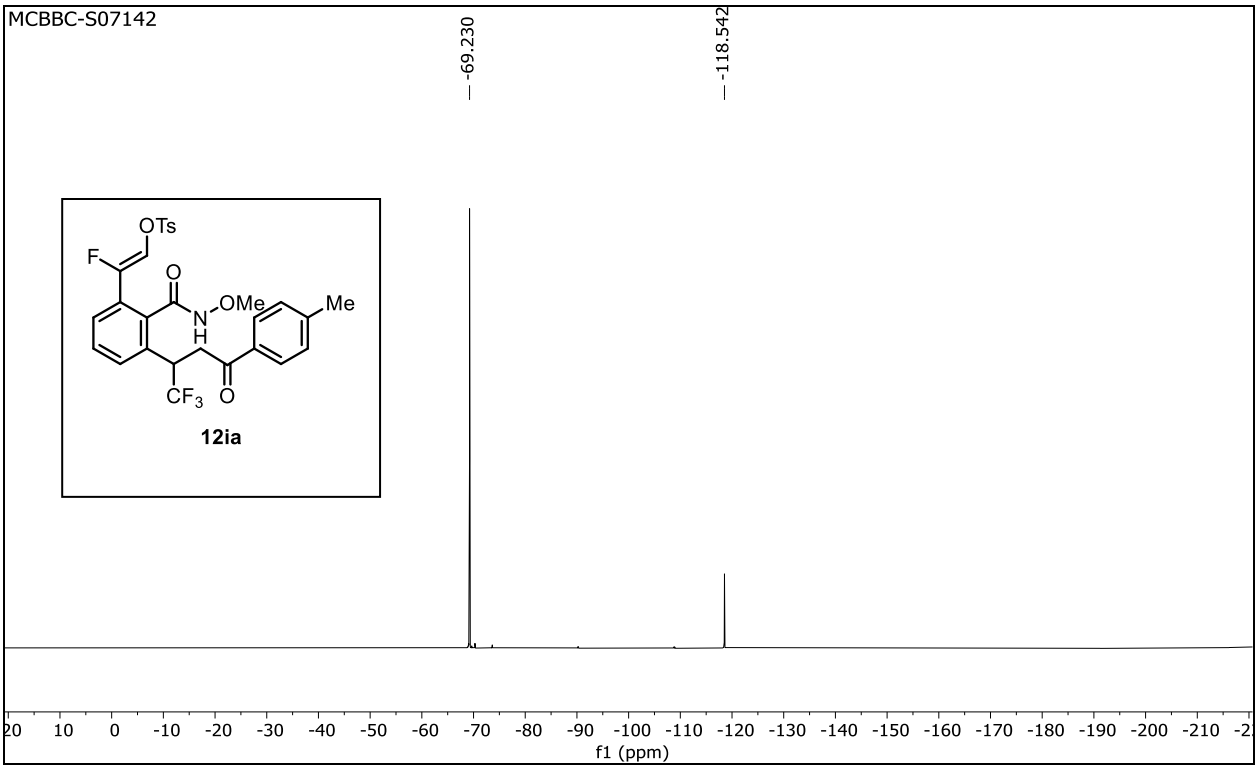

BBC-1345
7.867
7.851
7.302
7.287
7.260 CDCl3
4.608
4.604
4.595
4.590
4.582
4.576
4.571
4.563
4.558
4.549
4.545
4.217
4.211
4.206
4.201
4.194
4.189
4.178
4.172
4.166
4.161
4.155
4.149
3.550
3.531
3.514
3.495
3.191
3.187
3.155
3.151
2.430
F3C
O
O
F3C
Me
9a
2.08
2.06
1.09
1.06
1.00
1.09
1.11
3.05
f1 (ppm)

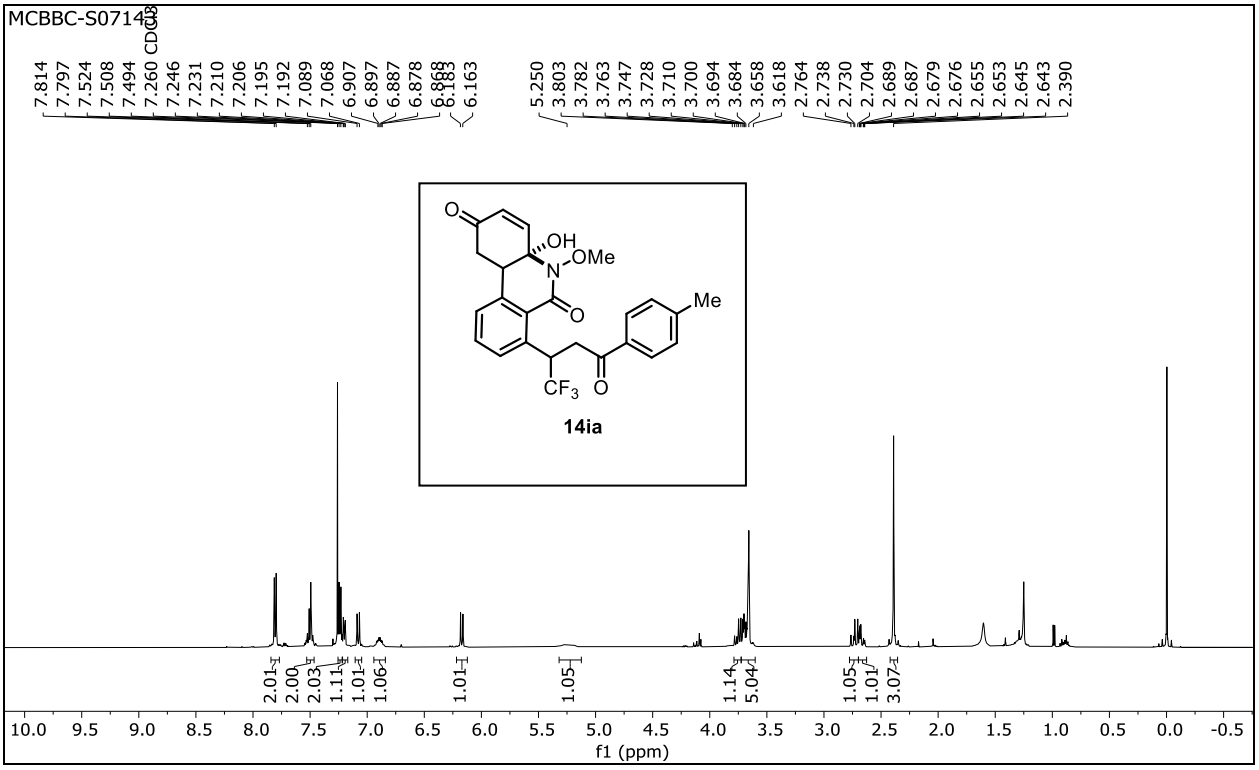

BBC-1345
194.426
145.163
133.693
129.672
128.462
128.290
126.427
126.046
124.218
123.802
122.008
121.558
119.798
77.414 CDCl3
77.160 CDCl3
76.906 CDCl3
75.628
75.377
75.126
74.876
70.575
70.293
70.012
69.731
38.482
21.835
F3C
O
O
F3C
Me
9a
f1 (ppm)

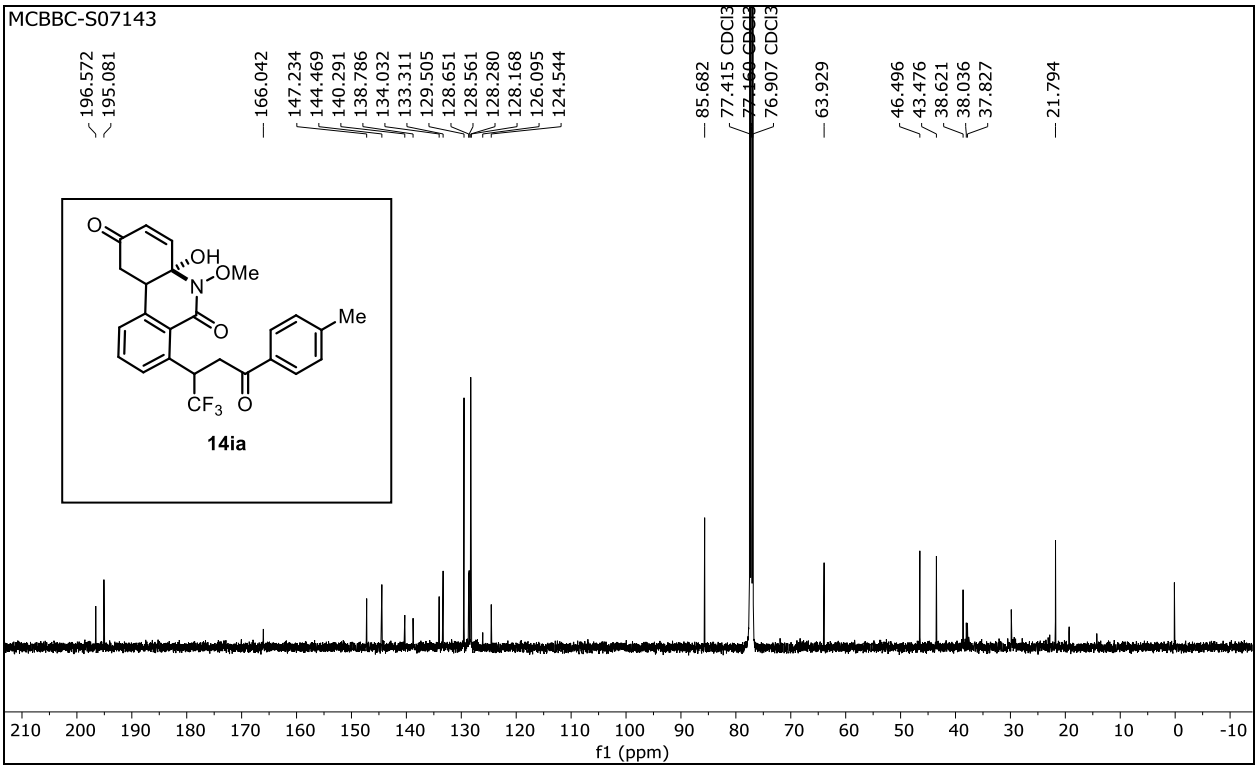

MCBBC-S08873
-75.064
-77.284
F3C
O
O
F3C
Me
9a
f1 (ppm)

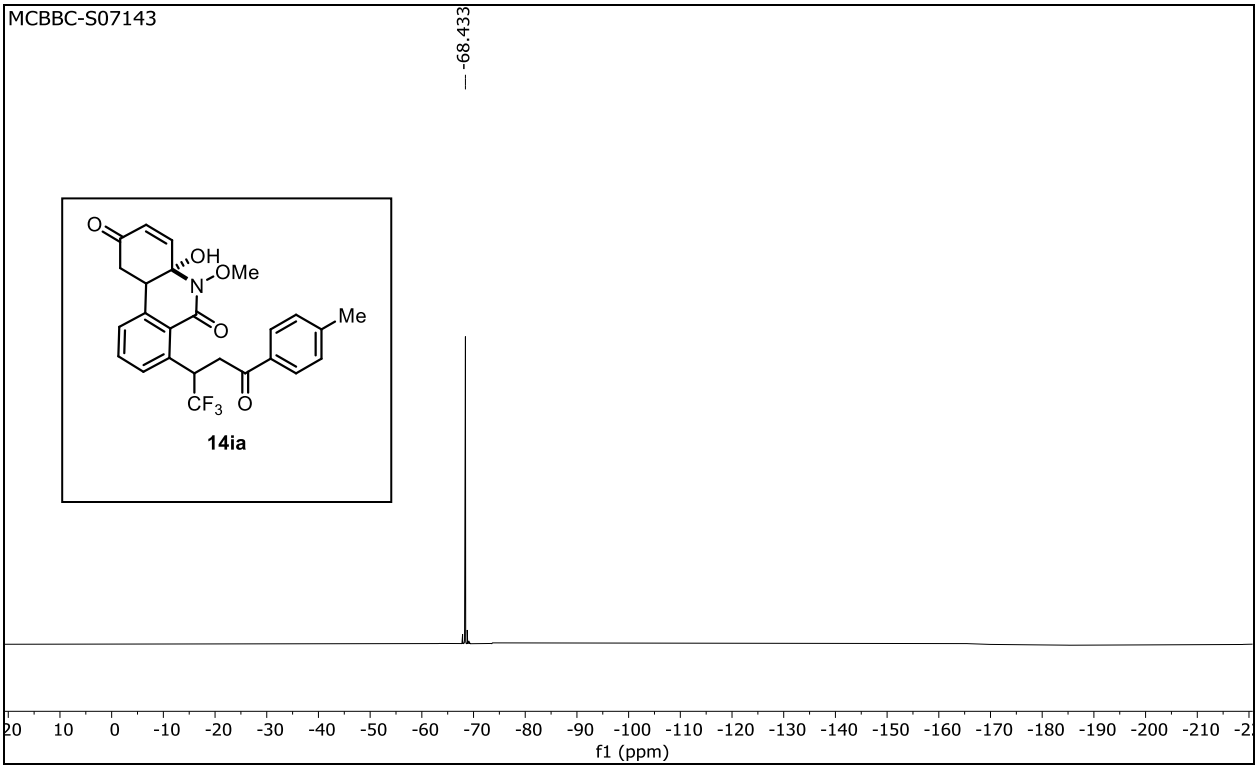

MCBBC-S07142
10.300
7.902
7.885
7.820
7.804
7.405
7.389
7.382
7.369
7.363
7.275
7.260 CDCl3
6.857
6.820
4.217
4.194
4.177
4.160
4.137
3.954
3.931
3.917
3.891
3.655
3.649
3.618
3.612
2.462
2.413
OTs
F
O
N
H
OMe
Me
CF3
O
12ia
1.01
2.02
2.03
5.18
2.39
1.00
1.15
1.23
3.10
1.06
3.10
3.09
f1 (ppm)

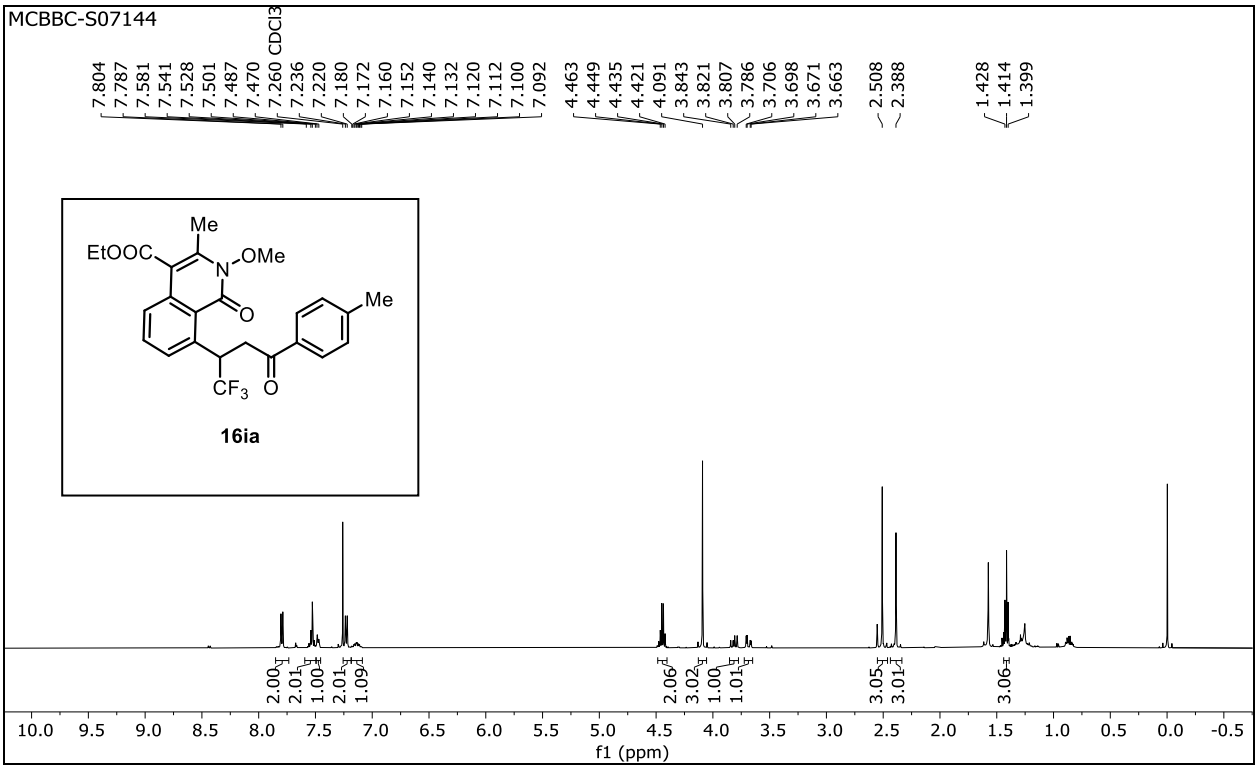

MCBBC-S07142
196.694
165.619
150.150
148.111
145.882
145.808
134.430
133.153
132.710
132.241
130.222
129.741
129.004
128.821
128.492
128.391
128.356
127.159
124.930
121.689
121.582
77.414 CDCl3
77.160 CDCl3
76.907 CDCl3
64.259
41.535
41.308
41.085
38.380
21.893
OTs
F
O
N
H
OMe
Me
CF3
O
12ia
f1 (ppm)

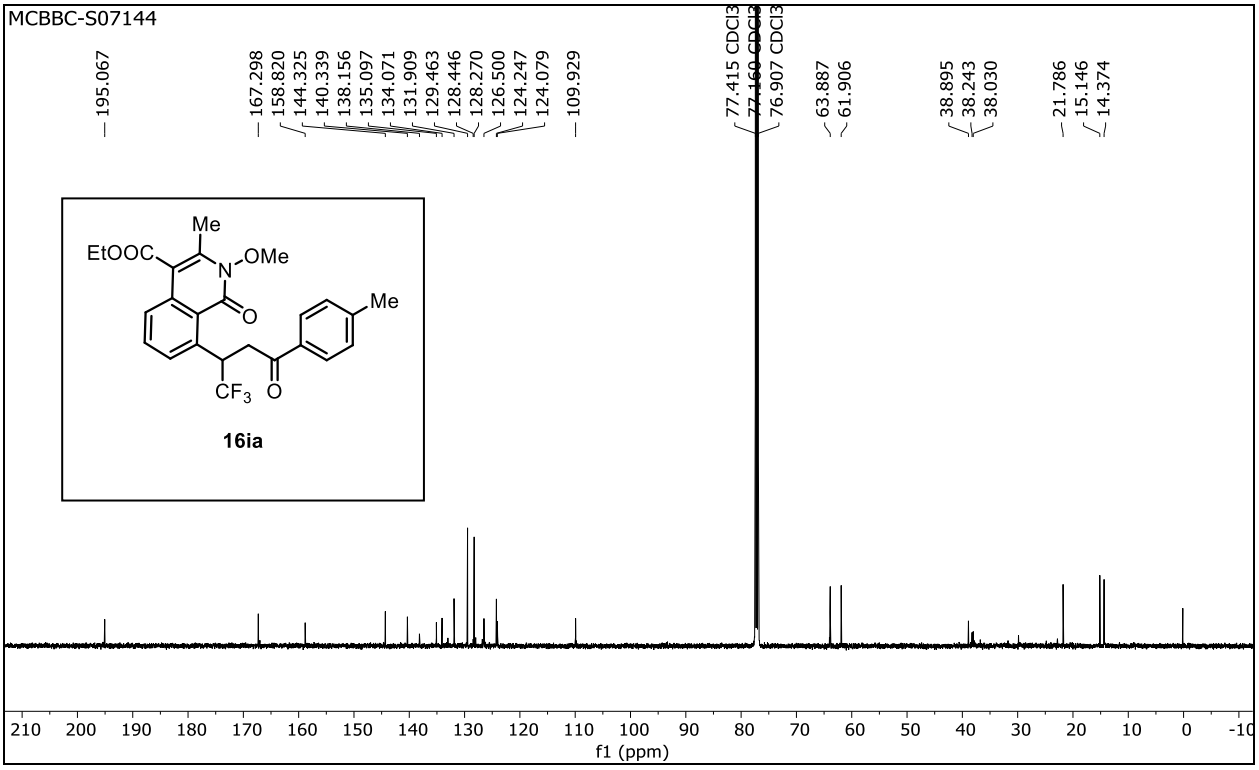

MCBBC-S07142
-69.230
-118.542
OTs
F
O
N
H
OMe
Me
CF3
O
12ia
f1 (ppm)

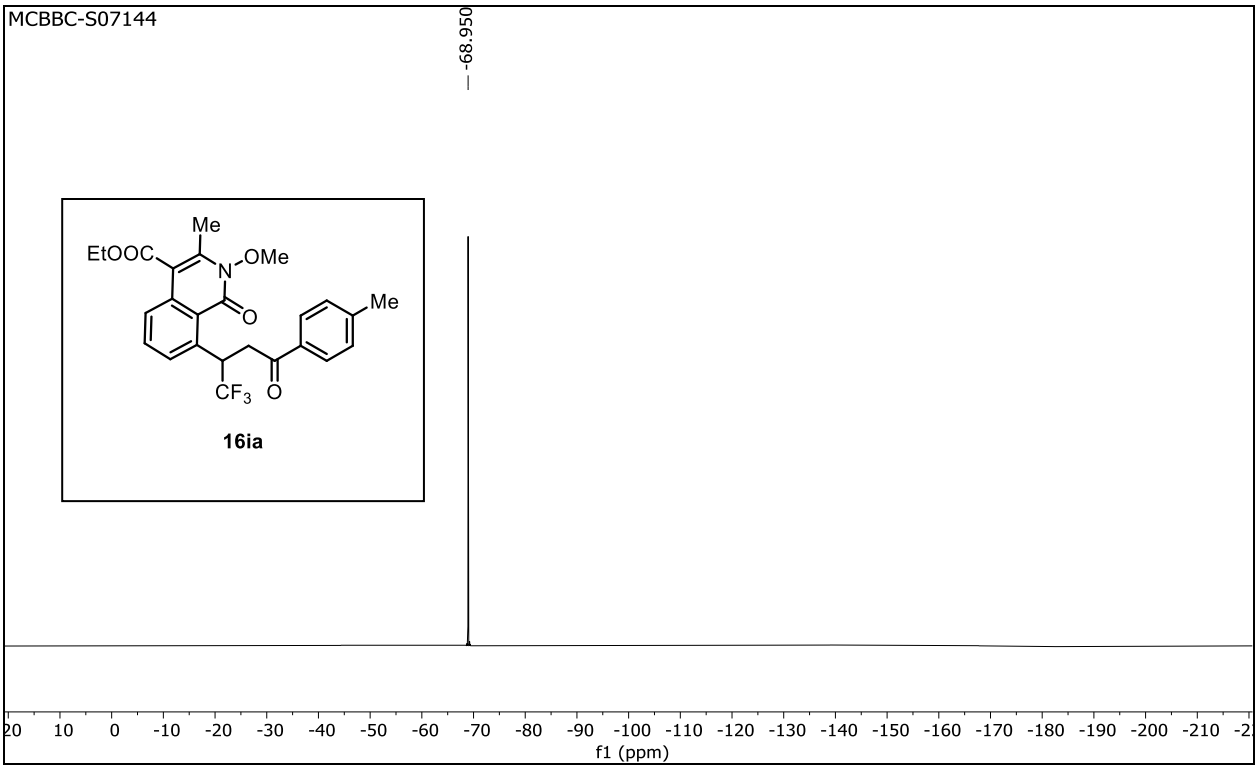

MCBBC-S07148
CDCl3
7.814
7.797
7.524
7.508
7.494
7.260
7.246
7.231
7.210
7.206
7.195
7.192
7.089
7.068
6.907
6.897
6.887
6.878
6.868
6.183
6.163
5.250
3.803
3.782
3.763
3.747
3.728
3.710
3.700
3.694
3.684
3.658
3.618
2.764
2.738
2.730
2.704
2.689
2.687
2.679
2.676
2.655
2.653
2.645
2.643
2.390
O
OH
N
OMe
O
Me
CF3
O
14ia
2.01
2.00
2.03
1.11
1.01
1.06
1.01
1.05
1.14
5.04
1.05
1.01
3.07
f1 (ppm)


MCBBC-S07143
196.572
195.081
166.042
147.234
144.469
140.291
138.786
134.032
133.311
129.505
128.651
128.561
128.280
128.168
126.095
124.544
85.682
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
63.929
46.496
43.476
38.621
38.036
37.827
21.794
OH
OMe
N
O
Me
CF3
O
14ia
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

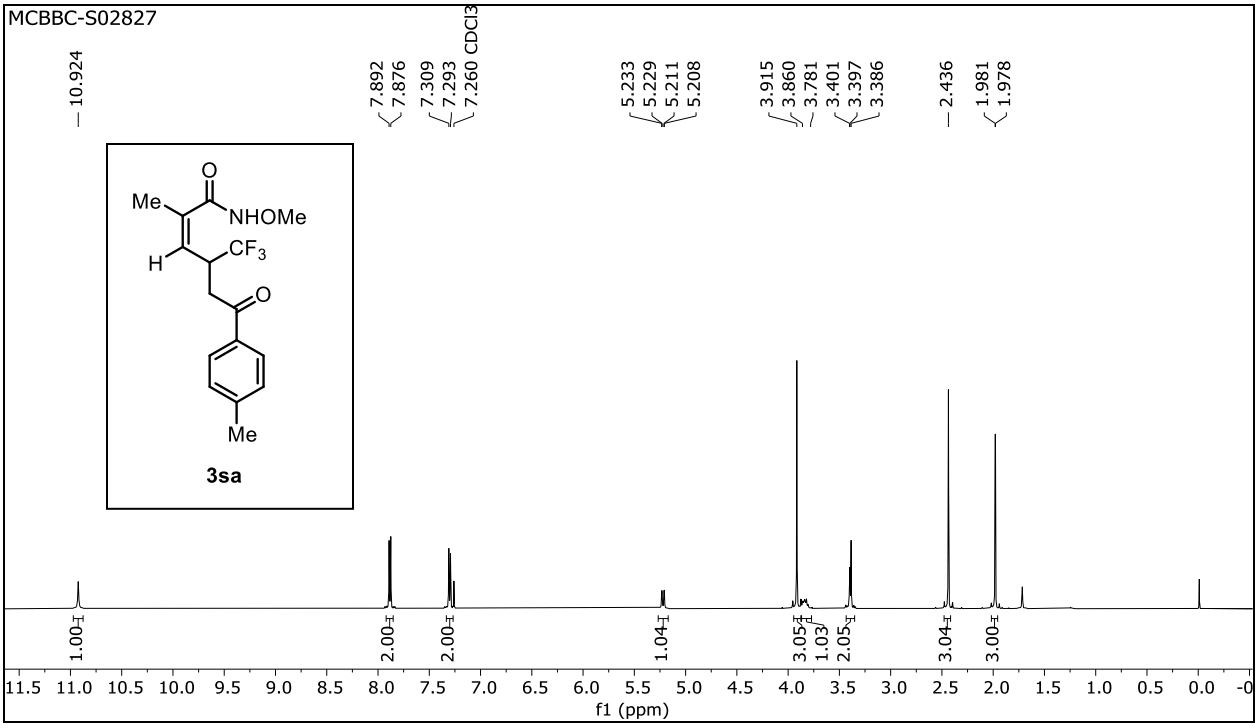

MCBBC-S07143
-68.433
OH
OMe
N
O
Me
CF3
O
14ia
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

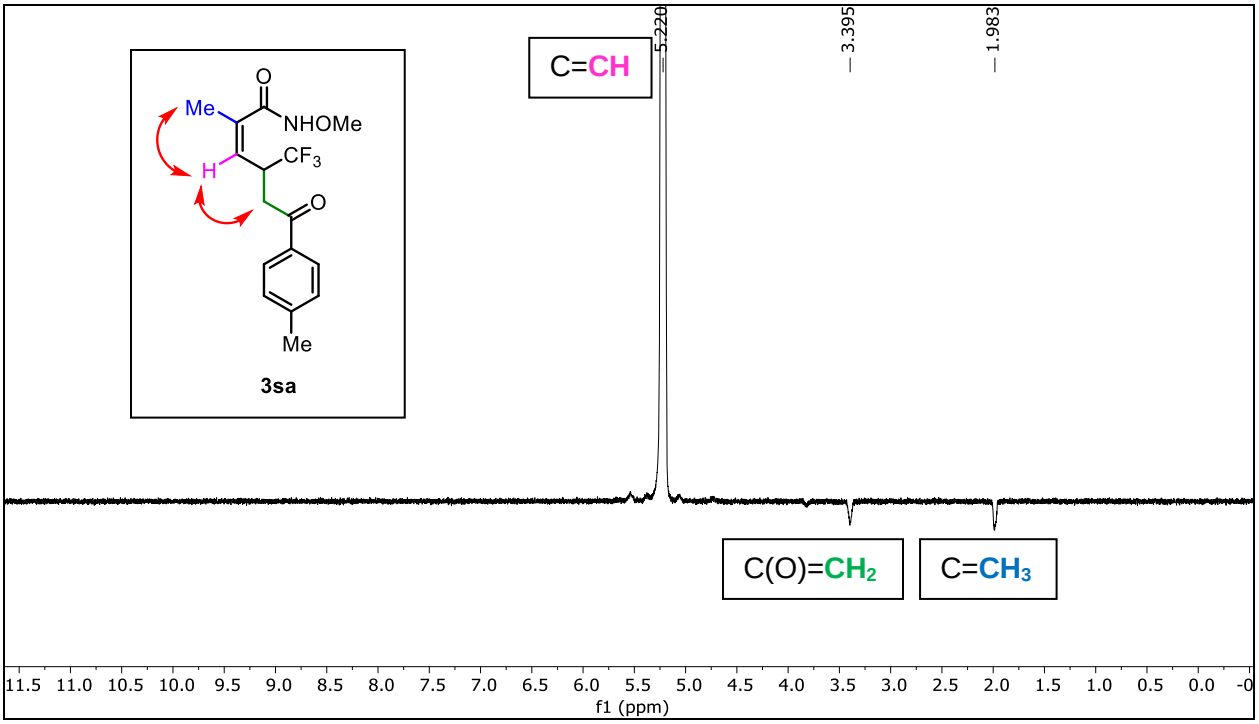

MCBBC-S07144
7.804
7.787
7.581
7.541
7.528
7.501
7.487
7.470
7.260 CDCl3
7.236
7.220
7.180
7.172
7.160
7.152
7.140
7.132
7.120
7.112
7.100
7.092
4.463
4.449
4.435
4.421
4.091
3.843
3.821
3.807
3.786
3.706
3.698
3.671
3.663
2.508
2.388
1.428
1.414
1.399
Me
EtOOC
N
OMe
O
Me
CF3
O
16ia
2.00
2.01
1.00
2.01
1.09
2.06
3.02
1.00
1.01
3.05
3.01
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


MCBBC-S07144
195.067
167.298
158.820
144.325
140.339
138.156
135.097
134.071
131.909
129.463
128.446
128.270
126.500
124.247
124.079
109.929
77.415 CDCl3
77.160 CDCl3
76.907 CDCl3
63.887
61.906
38.895
38.243
38.030
21.786
15.146
14.374
Me
EtOOC
N
OMe
O
Me
CF3
O
16ia
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


MCBBC-S07144
-68.950
Me
EtOOC
N
OMe
O
Me
CF3
O
16ia
20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

NOE data for Compound 3sa





NOE data for Compound 3ta