Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

A Convenient Access to Allylic Triflones with Allenes and Triflyl chloride in the Presence of $(EtO)_2P(O)H$

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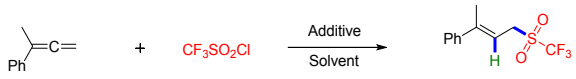
General remark

^{1}H NMR, and ^{13}C NMR spectra were recorded on Bruker 400M and Mercury 300M in $CDCl_3$. All ^{1}H NMR and ^{13}C NMR chemical shifts were given as δ value (ppm) with reference to tetramethylsilane (TMS) as an internal standard. All compounds were further characterized by HRMS; copies of their ^{1}H NMR and ^{13}C NMR spectra were provided. Products were purified by flash chromatography on 200–300 mesh silica gels. All melting points were determined without correction. All reactions were carried out under argon atmosphere in oven-dried glassware, unless otherwise noted. Tetrahydrofuran (THF) was distilled prior to use and stored over activated molecular sieves. All reagents were purchased commercially and used as received, unless otherwise noted.

Table S1. Optimization of reaction conditions [a]



1a **2a** **3aa**

Entry	Additive (equiv)	Solvent	Temp. (°C)	Yield (%) [b]
1	$(EtO)_2P(O)H$ (2.0)	MeCN	100/Ar	39
2	$(EtO)_2P(O)H$ (2.0)	THF	100/Ar	20
3	$(EtO)_2P(O)H$ (2.0)	toluene	100/Ar	61
4	$(EtO)_2P(O)H$ (2.0)	DCE	100/Ar	5
5	$(EtO)_2P(O)H$ (2.0)	DMF	100/Ar	-
6	$(EtO)_2P(O)H$ (2.0)	PhCl	100/Ar	55
7	Ph_3P (2.0)	toluene	100/Ar	10
8	$Ph_2P(O)H$ (2.0)	toluene	100/Ar	12
9	*i*PrOH (2.0)	toluene	100/Ar	-
10	$(EtO)_2P(O)H$ (2.0)	toluene	rt/Ar	-
11	$(EtO)_2P(O)H$ (2.0)	toluene	80/Ar	45
12	$(EtO)_2P(O)H$ (2.0)	toluene	120/Ar	50
13	$(EtO)_2P(O)H$ (2.0)	toluene	100/O_2	-
14	**$(EtO)_2P(O)H$ (2.0)**	**toluene**	**100/air**	**75**
15	$(EtO)_2P(O)H$ (3.0)	toluene	100/Ar	54
16	$(EtO)_2P(O)H$ (1.0)	toluene	100/Ar	43
17	$(EtO)_2P(O)H$ (0.6)	toluene	100/Ar	26

[a] Reaction conditions: **1a** (0.3 mmol), **2a** (0.9 mmol), additive (0.6 mmol), solvent (2 mL). [b] Yields of isolated products. Entry in bold highlights optimized reaction conditions, and the reaction time was monitored by TLC.

General procedure for the GC-MS experiment

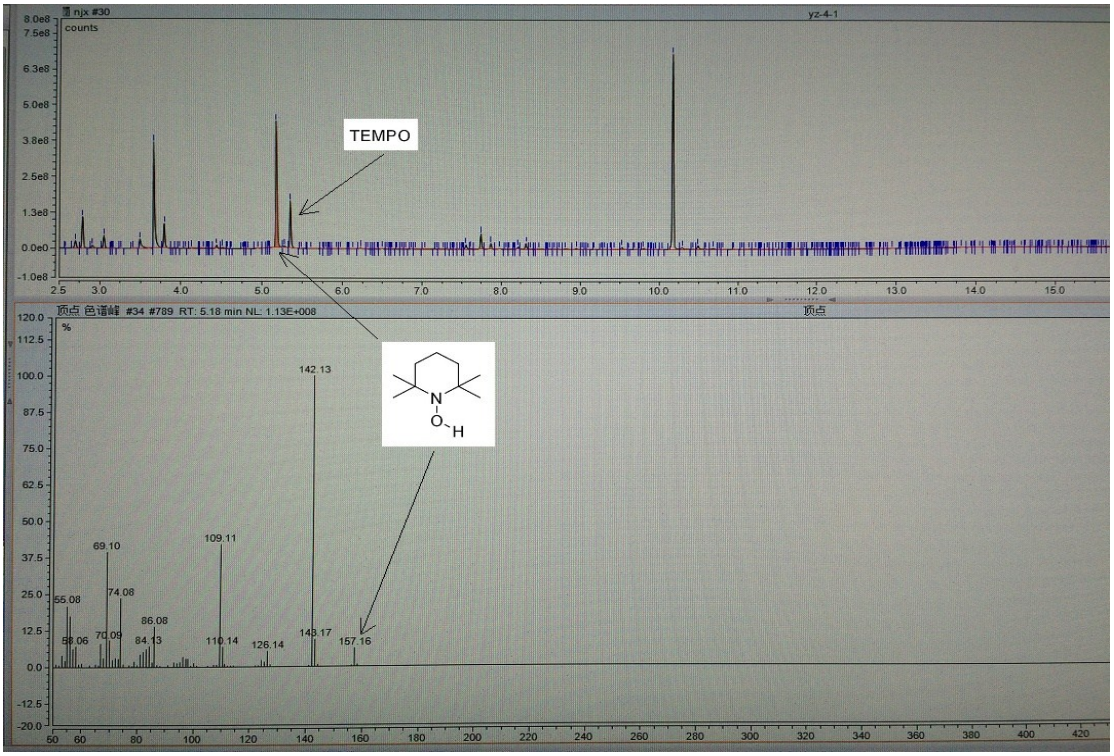


Figure S1

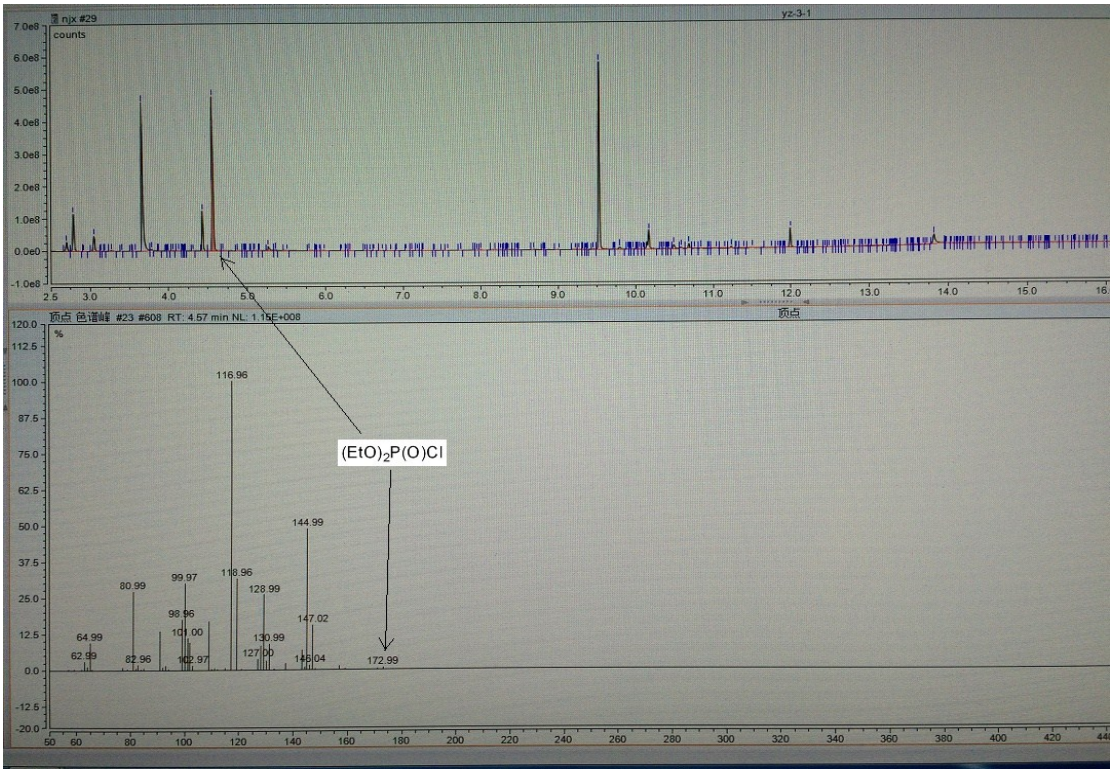
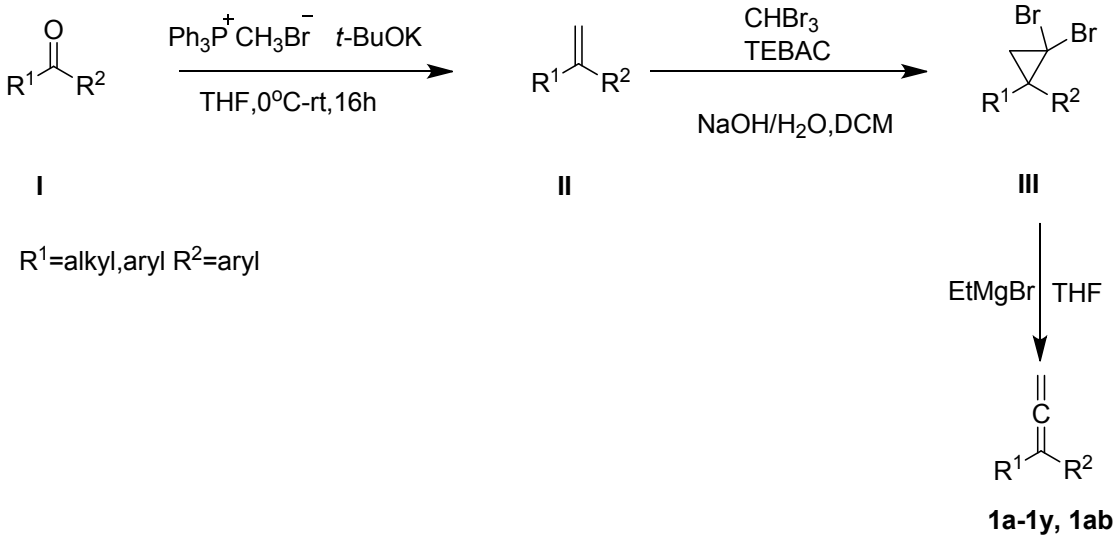


Figure S2

General procedure for synthesis of substituted allenes [1-3]



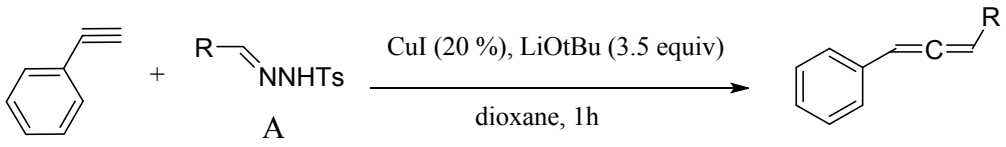
Step 1: In an oven dried flask, methyl triphenylphosphonium bromide (1.2 equiv.) was taken and to this abs. THF (1.6 mL/mmol) was added. The suspension was cooled to 0 °C, *t*-BuOK (1.2 equiv.) was added and the resulting yellow suspension was stirred at 0 °C for 45 min. To this suspension, a solution of ketone **I** (1.0 equiv., 10.0 mmol) in THF (0.7 mL/mmol) was added dropwise and the resulting mixture was warmed gradually to rt. and stirred at rt for 16 h. Reaction mixture was concentrated under reduced pressure and filtered over Celite®. The filtrate was concentrated under reduced pressure to afford yellow oil. Purification by column chromatography over silica gel (200-300 mesh) using petroleumether as eluent afforded **II**.

Step 2: To a solution of alkene **II** (1.0 equiv.), bromoform (1.6 equiv.), TEBAC (0.85 mol%) in dichloromethane (4 mL/mmol **II**), was added dropwise a solution of 50% NaOH (2.86mL/mmol **II**) and left stirring at 30-35 °C until full conversion was observed by TLC (1-3days). Water and DCM were added. The aqueous phase was extracted with DCM (30 mL×3). The combined organic phases were washed with saturated NaCl solution, dried over Na_2SO_4 and the solvent removed under reduced pressure. The reaction mixture was purified by flash column chromatography using hexanes as eluent afforded **III**.

Step 3: EtMgBr (2.0 M in THF, 1.5 equiv, 7.6 mL) was added dropwise to a solution

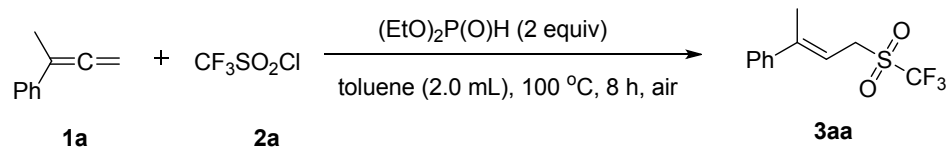
of **III** (10 mmol) in dry THF (20 ml) under nitrogen atmosphere at room temperature. The resulting mixture was allowed to stir at room temperature for an additional 30 minutes. Then the reaction was quenched by saturated NH_4Cl solution (30 ml), and extracted with petroleum ether (30 mL×3). The combined organic layers was washed with brine (30 mL×3), and dried with anhydrous Na_2SO_4. After removing the solvent under reduced pressure, the crude product was purified by flash column chromatography on silica gel afforded **1a-1y, 1ab.**

Typical Procedure for the Cross-Coupling of *N*-Tosylhydrazones and Terminal Alkynes [4]



Under a nitrogen atmosphere, ethynylbenzene (1020.0 mg, 10.0 mmol) was added to a mixture of CuI (382.5 mg, 2.0 mmol), LitOBu (2.8 g, 35.0 mmol), and the N-tosylhydrazone A (6.0 g, 22.0 mmol) in 1,4-dioxane (50 mL). The solution was stirred at 90 °C for 1 h, and the progress of the reaction was monitored by TLC. Upon completion of the reaction, the mixture was cooled to room temperature and was filtered through a short silica gel column eluting with EtOAc. The solvent was removed in vacuum to leave a crude mixture, which was purified by column chromatography on silica gel (eluting with petroleum ether) to afford pure **1z** as a colorless oil.

General procedure for the synthesis of allylic triflones:

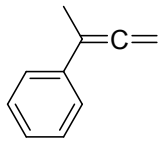


1a **2a** **3aa**

A mixture of buta-2,3-dien-2-ylbenzene **1a** (1 equiv, 0.3 mmol), trifluoromethyl sulfonyl chloride **2a** (3.0 equiv, 0.9 mmol), diethyl phosphate (2.0 equiv, 0.6 mmol), toluene (2 mL) were stirred at 100 °C under air atmosphere for 8 h (TLC monitored).

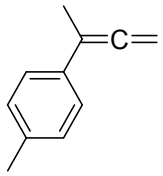
Upon completion of the reaction, the reaction mixture was cooled to room temperature. The solvent was evaporated in vacuo and the crude product was purified by column chromatography, eluting with petroleum ether/EtOAc (20:1) to afford the desired product (*E*)-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene **3aa.**

The data of products:



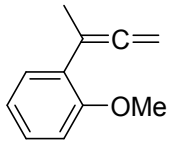
buta-2,3-dien-2-ylbenzene (1a) [5-9]

Yellow oil (702.0 mg, 54% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.41-7.39 (d, J = 8.0 Hz, 2 H), 7.33-7.29 (m, 2 H), 7.21-7.17 (m, 1 H), 5.02-5.00 (m, 2 H), 2.10-2.08 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.0, 136.7, 128.3, 126.6, 125.7, 99.8, 77.1, 16.7.



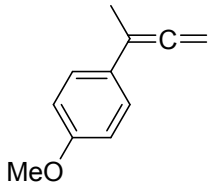
1-(buta-2,3-dien-2-yl)-4-methylbenzene (1b) [5, 8]

Yellow oil (720.0 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.29-7.27 (d, J = 8.0 Hz, 2 H), 7.13-7.11 (d, J = 8.0 Hz, 2 H), 5.00-4.97 (m, 2 H), 2.32 (s, 3 H), 2.07-2.06 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 208.8, 136.3, 133.7, 129.1, 125.6, 99.6, 76.8, 21.1, 16.8.



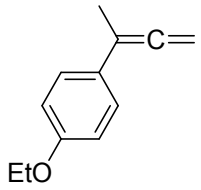
1-(buta-2,3-dien-2-yl)-2-methoxybenzene (1c) [8-11]

Yellow oil (768.0 mg, 48% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.24-7.21 (m, 2 H), 6.95-6.87 (m, 2 H), 4.80-4.78 (m, 2 H), 3.84 (s, 3 H), 2.10-2.08 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.2, 156.9, 129.2, 128.2, 127.2, 120.7, 111.3, 97.8, 73.6, 55.5, 19.2.



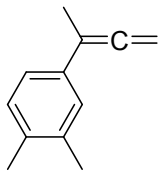
1-(buta-2,3-dien-2-yl)-4-methoxybenzene (1d) [5, 8, 11]

Yellow oil (816.0 mg, 51% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.35-7.32 (d, J = 8.8 Hz, 2 H), 6.88-6.85 (m, 2 H), 5.01-5.00 (m, 2 H), 3.80 (s, 3 H), 2.08-2.07 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 208.6, 158.5, 129.0, 126.8, 113.8, 110.7, 99.3, 76.9, 55.3, 16.9.



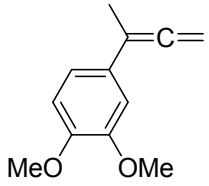
1-(buta-2,3-dien-2-yl)-4-ethoxybenzene (1e) [8]

Yellow solid (713.4 mg, 41% yield), mp: 49-51 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.32-7.29 (m, 2 H), 6.87-6.83 (m, 2 H), 5.00-4.98 (m, 2 H), 4.04-3.99 (m, 2 H), 2.07-2.05 (t, J = 3.2 Hz, 3 H), 1.42-1.38 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 208.6, 157.8, 128.8, 126.7, 114.4, 99.3, 76.8, 63.4, 16.9, 14.9.



4-(buta-2,3-dien-2-yl)-1,2-dimethylbenzene (1f) [8]

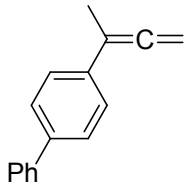
Yellow oil (695.2 mg, 44% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.20 (s, 1 H), 7.17-7.06 (m, 2 H), 5.00-4.98 (m, 2 H), 2.25 (s, 3 H), 2.23 (s, 3 H), 2.07-2.06 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 208.8, 136.4, 135.0, 134.2, 129.7, 127.0, 123.1, 99.7, 76.8, 19.9, 19.4, 16.8.



4-(buta-2,3-dien-2-yl)-1,2-dimethoxybenzene (1g) [10]

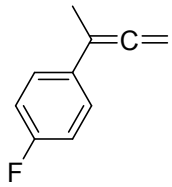
Yellow oil (950.0 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.98-6.97 (d, J = 2.0 Hz, 1 H), 6.91-6.89 (d, J = 8.8 Hz, 1 H), 6.82-6.80 (d, J = 8.4 Hz, 1 H),

5.02-5.00 (m, 2 H), 3.87 (s, 3 H), 3.85 (s, 3 H), 2.08-2.06 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 208.7, 148.9, 148.2, 129.4, 117.7, 111.0, 109.3, 99.7, 77.1, 55.9, 55.8, 16.9.



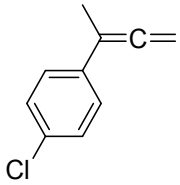
4-(buta-2,3-dien-2-yl)-1,1'-biphenyl (1h) [8]

white solid (824.0 mg, 40% yield), mp: 84-86 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.60-7.55 (m, 4 H), 7.48-7.40 (m, 4 H), 7.34-7.30 (m, 1 H), 5.06-5.04 (m, 2 H), 2.13-2.11 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.2, 140.8, 139.4, 135.8, 128.8, 127.2, 127.1, 127.0, 126.1, 99.6, 77.4, 16.7.



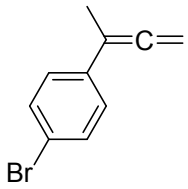
1-(buta-2,3-dien-2-yl)-4-fluorobenzene (1i) [5, 8]

colorless oil (710.4 mg, 48% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.36-7.32 (m, 2 H), 7.02-6.97 (m, 2 H), 5.01-5.00 (d, J = 4.0 Hz, 2 H), 2.07-2.05 (t, J=3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 208.8 (J = 2 Hz, 1 C), 163.0 (J = 244 Hz, 1 C), 132.7 (J = 3 Hz, 1 C), 127.2 (J = 8 Hz, 2 C), 115.3 (J = 21 Hz, 2 C), 99.0, 77.4, 16.8.



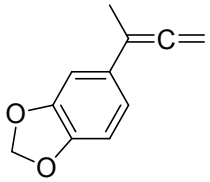
1-(buta-2,3-dien-2-yl)-4-chlorobenzene (1j) [5, 8]

Yellow oil (623.2 mg, 38% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.33-7.25 (m, 4 H), 5.04-5.02 (m, 2 H), 2.08-2.06 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 208.9, 135.2, 132.2, 128.4, 126.9, 99.0, 77.3, 16.6.



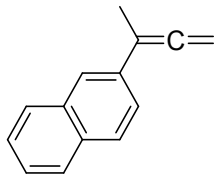
1-bromo-4-(buta-2,3-dien-2-yl)benzene (1k) [5, 8-9, 11]

Yellow solid (728.0 mg, 35% yield), mp: 54-56 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.45-7.42 (d, J = 8.8 Hz, 2 H), 7.28-7.26 (d, J = 8.8 Hz, 2 H), 5.04-5.02 (m, 2 H), 2.08-2.06 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 208.9, 135.8, 131.3, 127.3, 120.4, 99.1, 77.4, 16.6.



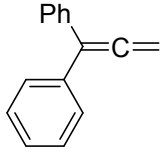
5-(buta-2,3-dien-2-yl)benzo[*d*][1,3]dioxole (1l) [5]

Yellow oil (1131.0 mg, 65% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.99-6.93 (m, 1 H), 6.83-6.74 (m, 2 H), 5.96-5.90 (m, 2 H), 5.05-4.98 (m, 2 H), 2.04-2.03 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 208.6, 147.8, 146.4, 130.8, 118.7, 108.0, 106.4, 101.0, 99.6, 77.0, 17.0.



2-(buta-2,3-dien-2-yl)naphthalene (1m) [5, 6, 8, 9, 11, 13]

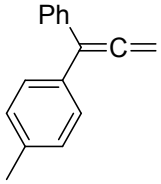
Yellow solid (918.0 mg, 51% yield), mp: 59-61 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.82-7.78 (m, 2 H), 7.77-7.72 (m, 2 H), 7.65-7.63 (m, 1 H), 7.48-7.40 (m, 2 H), 5.12-5.10 (m, 2 H), 2.22-2.21 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.7, 134.1, 133.6, 132.3, 128.0, 127.7, 127.6, 126.1, 125.6, 124.9, 123.3, 100.1, 77.3, 16.8.



propa-1,2-diene-1,1-diyldibenzene (1n) [6-9, 13]

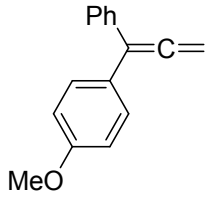
Yellow oil (1152.0 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.38-7.32

(m, 8 H), 7.29-7.25 (m, 2 H), 5.26 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.9, 136.3, 128.5, 127.3, 109.2, 78.1.



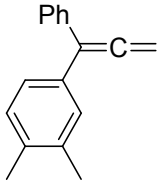
1-methyl-4-(1-phenylpropa-1,2-dien-1-yl)benzene (1o) [5, 6, 8]

Yellow oil (1071.2 mg, 52% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.38-7.31 (m, 4 H), 7.27-7.24 (m, 3 H), 7.17-7.14 (m, 2 H), 5.24 (s, 2 H), 2.36 (s, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 209.7, 137.0, 136.3, 133.2, 129.1, 128.4, 128.3, 127.1, 108.9, 78.0, 21.2.



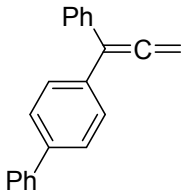
1-methoxy-4-(1-phenylpropa-1,2-dien-1-yl)benzene (1p) [7, 12]

Yellow solid (1021.2 mg, 46% yield), mp: 90-91 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.40-7.34 (m, 4 H), 7.32-7.27 (m, 3 H), 6.92-6.88 (m, 2 H), 5.26 (s, 2 H) , 3.83 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.6, 158.9, 136.5, 129.5, 128.3, 127.1, 113.8, 108.6, 77.9, 55.3.



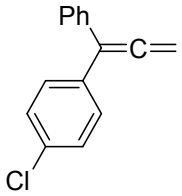
1,2-dimethyl-4-(1-phenylpropa-1,2-dien-1-yl)benzene (1q) [7, 8]

Yellow solid (990.0 mg, 45% yield), mp: 94-96 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.39-7.31 (m, 4 H), 7.29-7.26 (m, 1 H), 7.14-7.13 (m, 1 H), 7.11-7.05 (m, 2 H), 5.24 (s, 2 H), 2.27 (s, 3 H), 2.25 (s, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 209.7, 136.6, 136.4, 135.7, 133.6, 129.7, 129.5, 128.4, 128.3, 127.1, 125.8, 108.9, 77.8, 19.8, 19.5.



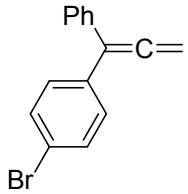
4-(1-phenylpropa-1,2-dien-1-yl)-1,1'-biphenyl (1r) [7]

Yellow solid (964.8 mg, 36% yield), mp: 99-101 °C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.58-7.54 (m, 4 H), 7.43-7.34 (m, 10 H), 5.26 (s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 209.9, 140.6, 140.0, 136.1, 135.1, 128.7, 128.4, 127.3, 127.1, 127.0, 108.9, 77.4.



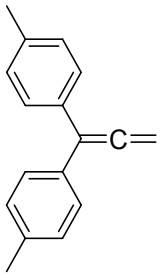
1-chloro-4-(1-phenylpropa-1,2-dienyl)benzene (1s) [6-8, 19]

Yellow solid (904.0 mg, 40% yield), mp: 115-117 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.36-7.22 (m, 9 H), 5.26 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.8, 135.9, 134.9, 133.0, 129.7, 128.6, 128.5, 128.4, 127.5, 108.4, 78.5.



1-bromo-4-(1-phenylpropa-1,2-dien-1-yl)benzene (1t) [20]

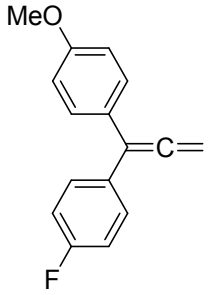
Yellow solid (1053.0 mg, 39% yield), mp: 110-112 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.46-7.44 (d, J = 8.4 Hz, 2 H), 7.35-731 (m, 4 H), 7.30-7.28 (m, 1 H), 7.23-7.21 (m, J = 8.4 Hz, 2H), 5.26 (s, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.7, 135.7, 135.3, 131.5, 130.0, 128.5, 128.3, 127.4, 121.1, 108.4, 78.5.



4,4'-(propa-1,2-diene-1,1-diyl)bis(methylbenzene) (1u) [7, 21]

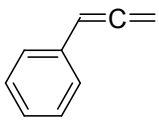
Colorless solid (1320.0 mg, 60% yield), mp: 92-94 °C. ^{1}H NMR (400 MHz, $CDCl_3$,

ppm): δ = 7.26-7.24 (d, J = 8.0 Hz, 4 H), 7.15-7.13 (d, J = 8.0 Hz, 4 H), 5.21 (s, 2 H), 2.34 (s, 6 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.6, 136.9, 133.4, 129.1, 128.3, 108.8, 77.8, 21.1.



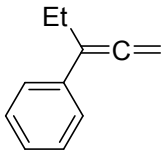
1-fluoro-4-(1-(4-methoxyphenyl)propa-1,2-dien-1-yl)benzene (1v)

Yellow solid (1608.0 mg, 67% yield), mp: 97-98 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.33-7.30 (m, 2 H), 7.27-7.23 (m, 2 H), 7.05-7.00 (m, 2 H), 6.90-6.88 (m, 2 H), 5.23 (s, 2 H), 3.81 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.5, 163.2-160.8 (d, J = 245.0 Hz, 1C), 159.0, 132.5-132.4 (d, J = 3.0 Hz, 1C), 130.0-129.8 (d, J = 8.0 Hz, 1C), 128.2, 115.4-115.1 (d, J = 84.0 Hz, 1C), 113.9, 107.8, 78.1, 55.3. $C_{16}H_{14}FO$ $[M+H]^+$ 241.1023; found: 241.1026.



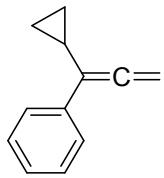
propa-1,2-dien-1-ylbenzene (1w) [13]

Yellow oil (777.2 mg, 67% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.33-7.30 (m, 4 H), 7.23-7.17 (m, 1 H), 6.18-6.15 (t, J = 6.8 Hz, 1 H), 5.15-5.14 (d, J = 6.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 209.8, 139.9, 128.6, 126.9, 126.7, 94.0, 78.9.



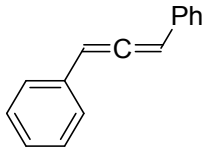
penta-1,2-dien-3-ylbenzene (1x) [5, 6, 8, 14]

Yellow oil (878.4 mg, 61% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.40 (d, J = 7.6 Hz, 2 H), 7.33-7.29 (m, 2 H), 7.25-7.17 (m, 1 H), 5.10-5.09 (t, J = 3.6 Hz, 2 H), 2.46-2.39 (m, 2 H), 1.17-1.13 (t, J = 3.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 208.4, 136.6, 128.4, 126.6, 125.9, 106.7, 78.8, 22.4, 12.5.



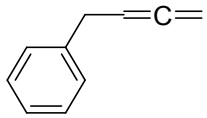
(1-cyclopropylpropa-1,2-dien-1-yl)benzene (1y) [5, 8, 15, 16]

Yellow oil (546.0 mg, 35% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.59-7.57 (m, 2 H), 7.35-7.32 (m, 2 H), 7.23-7.19 (m, 1 H), 5.10-5.09 (d, J = 2.8 Hz, 2 H), 1.60-1.52 (m, 1 H), 0.89-0.85 (m, 2 H), 0.57-0.53 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 207.9, 136.8, 128.3, 126.8, 126.2, 108.3, 79.3, 10.4, 6.9.



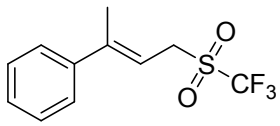
1,3-diphenylpropa-1,2-diene (1z) [8, 13, 17]

colorless oil (960.0 mg, 50% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.12-7.37 (m, 10 H), 6.60 (s, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 207.8, 133.6, 128.7, 127.3, 127.0, 98.4.



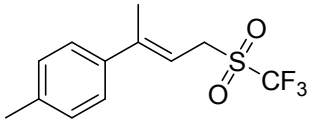
buta-2,3-dien-1-ylbenzene (1ab) [18-21]

colorless oil (650.0 mg, 50% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.21 (m, 5 H), 5.33 (m, 1 H), 4.76 (m, 2 H), 3.41 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 209.4, 140.7, 128.9, 128.8, 126.6, 90.0, 75.5, 35.5.



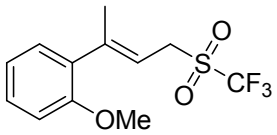
(*E*)-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene (3aa)

Yellow solid (59.4 mg, 75% yield), mp: 35-37 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.42-7.31 (m, 5 H), 5.78-5.74 (m, 1 H), 4.20-4.18 (d, J = 8.0 Hz, 2 H), 2.19 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.9, 141.6, 128.5, 128.4, 126.0, 119.7 (q, J = 327.0 Hz, 1C), 108.0, 50.7, 16.9; HRMS calcd for $C_{11}H_{12}F_3O_2S$ $[M+H]^+$ 265.0505; found: 265.0511.



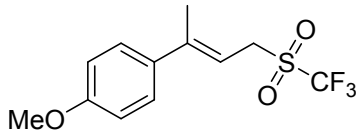
(*E*)-1-methyl-4-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene (3ba)

Yellow solid (59.2 mg, 71% yield), mp: 48-50 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.32-7.30 (d, J = 8.0 Hz, 2 H), 7.18-7.16 (d, J = 8.0 Hz, 2 H), 5.76-5.72 (m, 1 H), 4.19-4.17 (d, J = 8.0 Hz, 2 H), 2.36 (s, 3 H) , 2.17 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.7, 138.7, 138.5, 129.2, 125.9, 119.7 (q, J = 327.0 Hz, 1C), 107.1, 50.8, 21.1, 16.9; HRMS calcd for $C_{12}H_{14}F_3O_2S$ $[M+H]^+$ 279.0661; found: 279.0653.



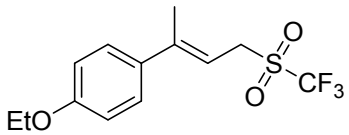
(*E*)-1-methoxy-2-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene (3ca)

Yellow oil (37.9 mg, 43% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.31-7.27 (m, 1 H), 7.14-7.11 (m, 1 H), 6.95-6.88 (m, 2 H), 5.55-5.51 (m, 1 H), 4.17-4.15 (d, J = 8.0 Hz, 2 H), 3.81 (s, 3 H), 2.12 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 156.3, 148.1, 132.3, 129.3, 129.2, 120.7, 119.7 (q, J = 326.0 Hz, 1C), 110.9, 110.1, 55.4, 50.5, 17.9; HRMS calcd for $C_{12}H_{14}F_3O_3S$ $[M+H]^+$ 295.0574; found: 295.0580.



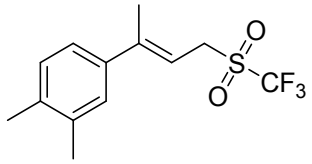
(*E*)-1-methoxy-4-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene (3da)

Yellow solid (70.6 mg, 80% yield), mp: 76-78 °C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.39-7.34 (m, 2 H), 6.90-6.87 (m, 2 H), 5.72-5.67 (m, 1 H), 4.20-4.17 (m, 2 H), 3.82 (s, 3 H), 2.16 (s, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 159.9, 147.2, 133.9, 127.2, 119.7 (q, J = 326.3 Hz, 1C), 113.8, 106.1, 55.3, 50.8, 16.8; HRMS calcd for $C_{12}H_{14}F_3O_3S$ $[M+H]^+$ 295.0574; found: 295.0570.



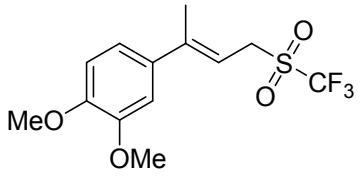
(*E*)-1-ethoxy-4-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene (3ea)

Yellow solid (64.7 mg, 70% yield), mp: 70-72 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.37-7.33 (m, 2 H), 6.90-6.85 (m, 2 H), 5.71-5.67 (m, 1 H), 4.19-4.17 (d, J = 8.0 Hz, 2 H), 4.07-4.02 (m, 2 H), 2.16 (s, 3 H) , 1.44-1.40 (m, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 159.3, 147.2, 133.8, 127.2, 119.8 (q, J = 327.0 Hz, 1C), 114.4, 106.0, 63.5, 50.8, 16.8, 14.8; HRMS calcd for $C_{13}H_{16}F_3O_3S$ $[M+H]^+$ 309.0767; found: 309.0770.



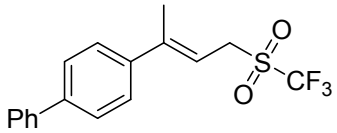
(*E*)-1,2-dimethyl-4-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene (3fa)

Yellow solid (63.1 mg, 72% yield), mp: 50-52 °C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.18 (s, 1 H), 7.16-7.10 (m, 2 H), 5.75-5.71 (m, 1 H), 4.19-4.17 (d, J = 8.0 Hz, 2 H), 2.28 (s, 3 H), 2.27 (s, 3 H), 2.16 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.8, 139.2, 137.2, 136.7, 129.7, 127.3, 123.5, 119.8 (q, J = 327.0 Hz, 1C), 106.9, 50.8, 19.9, 19.5, 16.9; HRMS calcd for $C_{13}H_{16}F_3O_2S$ $[M+H]^+$ 293.0818; found: 293.0825.



(*E*)-1,2-dimethoxy-4-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene (3ga)

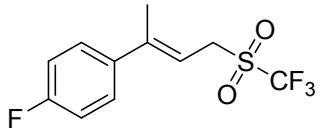
Yellow oil (58.3 mg, 60% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.01-6.98 (m, 1 H), 6.93-6.92 (d, J = 2.0 Hz, 1 H), 6.86-6.84 (d, J = 8.8 Hz, 1 H), 5.73-5.69 (t, J = 7.6 Hz, 1 H), 4.20-4.18 (d, J = 8.0 Hz, 2 H), 3.91 (s, 3 H), 3.90 (s, 3 H), 2.18 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 149.6, 148.9, 147.6, 134.4, 119.8(q, J = 326.0 Hz, 1C), 118.8, 111.0, 109.3, 106.4, 56.0, 50.8, 17.1; HRMS calcd for $C_{13}H_{16}F_3O_4S$ $[M+H]^+$ 325.0716; found: 325.0720.



(*E*)-4-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)-1,1'-biphenyl (3ha)

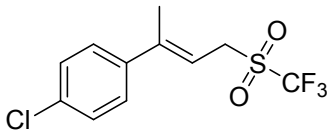
Yellow solid (74.5 mg, 73% yield), mp: 136-139 °C. ^{1}H NMR (400 MHz, $CDCl_3$,

ppm): δ = 7.61-7.58 (m, 4 H), 7.50-7.43 (m, 4 H), 7.38-7.34 (m, 1 H), 5.85-5.81 (m, 1 H), 4.23-4.21 (d, J = 8.0 Hz, 2 H), 2.22 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.4, 141.4, 140.4, 140.3, 128.9, 127.6, 127.2, 127.0, 126.5, 119.8 (q, J = 326.0 Hz, 1C), 107.9, 50.8, 16.9; HRMS calcd for $C_{17}H_{16}F_3O_2S$ $[M+H]^+$ 341.0818; found: 341.0824.



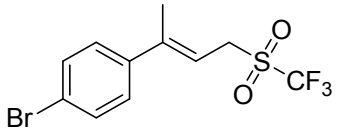
(*E*)-1-fluoro-4-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene (3ia)

Yellow solid (42.3 mg, 50% yield), mp: 40-42 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.41-7.36 (m, 2 H), 7.08-7.02 (m, 2 H), 5.74-5.70 (m, 1 H), 4.20-4.18 (d, J = 8.0 Hz, 2 H), 2.18 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.9, 137.6-137.5 (d, J = 4.0 Hz, 1C), 127.8-127.7 (d, J = 8.0 Hz, 1C), 119.6 (q, J = 327.0 Hz, 1C), 115.5-115.3 (d, J = 21.0 Hz, 1C), 107.9, 50.5, 17.1; HRMS calcd for $C_{11}H_{11}F_4O_2S$ $[M+H]^+$ 283.0411; found: 283.0408.



(*E*)-1-chloro-4-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene (3ja)

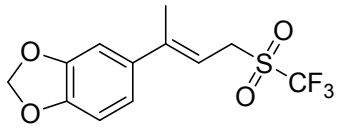
Yellow solid (38.4 mg, 43% yield), mp: 34-36 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.34 (s, 4 H), 5.77-5.73 (m, 1 H), 4.19-4.17 (d, J = 8.0 Hz, 2 H), 2.17 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 146.8, 140.0, 134.5, 128.7, 127.4, 119.7 (q, J = 327.0 Hz, 1C), 108.6, 50.6, 16.9; HRMS calcd for $C_{11}H_{11}ClF_3O_2S$ $[M+H]^+$ 299.0115; found: 299.0120.



(*E*)-1-bromo-4-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzene (3ka)

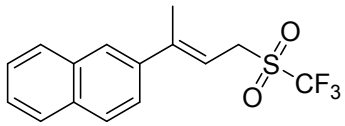
Yellow solid (41.0 mg, 40% yield), mp: 28-30 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.51-7.48 (d, J = 8.4 Hz, 2 H), 7.30-7.27 (m, 8.7 Hz, 2 H), 5.79-5.73 (m, 1 H), 4.21-4.18 (d, J = 8.1 Hz, 2 H), 2.18 (s, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 140.3, 131.6, 127.6, 122.6, 108.5, 50.5, 16.9; HRMS calcd for $C_{11}H_{11}BrF_3O_2S$

$[M+H]^+$ 342.9610; found: 342.9617.



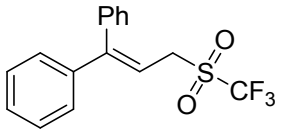
(*E*)-5-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)benzo[d][1,3]dioxole (3la)

Yellow oil (48.0 mg, 52% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 6.91-6.89 (m, 2 H), 6.80-6.77 (m, 1 H), 5.97 (s, 2 H), 5.69-5.65 (t, J = 8.0 Hz, 1 H), 4.18-4.16 (d, J = 8.0 Hz, 2 H), 2.14 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.8, 147.3, 135.8, 119.9, 119.7 (q, J = 326.0 Hz, 1C), 108.1, 106.8, 106.5, 101.3, 100.8, 50.7, 17.0; HRMS calcd for $C_{12}H_{12}F_3O_4S$ $[M+H]^+$ 309.0403; found: 309.0400



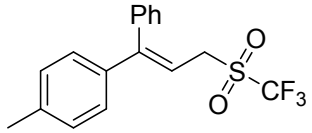
(*E*)-2-(4-((trifluoromethyl)sulfonyl)but-2-en-2-yl)naphthalene (3ma)

Yellow solid (52.8 mg, 56% yield), mp: 98-100 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.87-7.81 (m, 4 H), 7.56-7.53 (m, 1 H), 7.52-7.47 (m, 2 H), 5.93-5.89 (m, 1 H), 4.26-4.24 (d, J = 8.0 Hz, 2 H), 2.30 (s, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 147.7, 138.8, 133.2, 128.3, 128.2, 127.6, 126.5, 126.4, 125.2, 123.9, 119.8 (q, J = 327.0 Hz, 1C), 108.4, 50.8, 16.9; HRMS calcd for $C_{15}H_{14}F_3O_2S$ $[M+H]^+$ 315.0661; found: 315.0669.



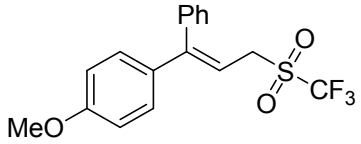
(3-((trifluoromethyl)sulfonyl)prop-1-ene-1,1-diyl)dibenzene (3na)

Yellow oil (79.2 mg, 81% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.46-7.41 (m, 3 H), 7.34-7.31 (m, 3 H), 7.28-7.24 (m, 2 H), 7.23-7.20 (m, 2 H), 6.14-6.10 (m, 1 H), 4.11-4.09 (d, J = 7.6 Hz, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.6, 140.3, 137.3, 129.4, 128.8, 128.7, 128.5, 128.4, 127.7, 108.9, 51.8; HRMS calcd for $C_{16}H_{14}F_3O_2S$ $[M+H]^+$ 327.0661; found: 327.0655.



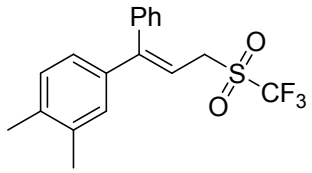
(*E/Z*)-1-methyl-4-(1-phenyl-3-((trifluoromethyl)sulfonyl)prop-1-en-1-yl)benzene (3oa)

Colorless oil (71.4 mg, 70% yield). (*E/Z* = 61/39) ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.45-7.09 (m, 9 H, Ar), 6.10-6.06 (m, 1 H), 4.09-4.07 (d, *J* = 8.0 Hz, 2 H), 2.35 (s, 3 H); δ = 7.45-7.09 (m, 9 H, Ar), 6.10-6.06 (m, 1 H), 4.13-4.11 (d, *J* = 8.0 Hz, 2 H), 2.40 (s, 3 H);^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.7, 152.5, 140.6, 138.9, 138.4, 137.5, 137.4, 134.3, 129.5, 129.4, 129.3, 129.1, 128.7, 128.4, 128.3, 127.7, 127.6, 119.5 (q, *J* = 326.0 Hz, 1C), 108.9, 107.9, 51.9, 21.3, 21.2; HRMS calcd for $C_{17}H_{16}F_3O_2S$ $[M+H]^+$ 341.0818; found: 341.0822.



(*E/Z*)-1-methoxy-4-(1-phenyl-3-((trifluoromethyl)sulfonyl)prop-1-en-1-yl)benzene (3pa)

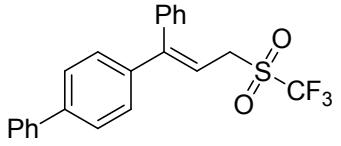
Colorless oil (65.1 mg, 61% yield). (*E/Z* = 72/28) ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.45-6.82 (m, 9 H, Ar), 6.07-6.01 (m, 1 H), 4.08-4.06 (d, *J* = 8.0 Hz, 2H), 3.80 (s, 3H); 7.45-6.82 (m, 9 H, Ar), 6.07-6.01 (m, 1 H), 4.15-4.13 (d, *J* = 8.0 Hz, 2H), 3.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 160.1, 159.7, 152.5, 152.1, 140.8, 137.5, 132.8, 130.8, 129.5, 129.4, 129.0, 128.7, 128.4, 128.3, 127.8, 119.5 (q, *J* = 327.0 Hz, 1C), 114.1, 113.7, 108.4, 106.7, 55.3, 51.9; HRMS calcd for $C_{17}H_{16}F_3O_3S$ $[M+H]^+$ 357.0767; found: 357.0759.



(*E/Z*)-1,2-dimethyl-4-(1-phenyl-3-((trifluoromethyl)sulfonyl)prop-1-en-1-yl)benzene (3qa)

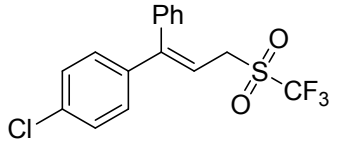
Colorless oil (66.9 mg, 63% yield). (*E/Z* = 65/35) ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.45-6.93 (m, 8 H, Ar), 6.09-6.04 (m, 1 H), 4.09-4.07 (d, *J* = 8.0 Hz, 2H), 2.25 (s, 3H), 2.22 (s, 3H); 7.45-6.93 (m, 8 H, Ar), 6.09-6.04 (m, 1 H), 4.14-4.12 (d, *J* = 7.6 Hz, 2H), 2.30 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ =152.7, 152.6, 140.6, 137.9, 137.6, 137.5, 137.1, 137.0, 136.7, 134.7, 130.4, 129.9, 129.6, 129.4,

128.7, 128.6, 128.4, 128.3, 127.7, 126.8, 126.8, 125.2, 119.5 (q, J = 326.0 Hz, 1C), 108.5, 107.7, 52.0, 51.8, 19.8, 19.7, 19.6, 19.5; HRMS calcd for $C_{18}H_{18}F_3O_2S$ $[M+H]^+$ 355.0974; found: 355.0982.



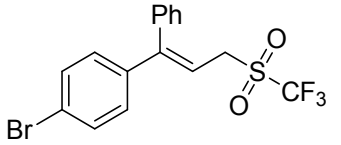
(*E/Z*)-4-(1-phenyl-3-((trifluoromethyl)sulfonyl)prop-1-en-1-yl)-1,1'-biphenyl (3ra)

Colorless oil (69.9 mg, 58% yield). (*E/Z* = 65/35) ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.67-7.26 (m, 14 H, Ar), 6.20-6.12 (m, 1 H), 4.13-4.11 (d, J = 7.6 Hz, 2H); 7.67-7.26 (m, 14 H, Ar), 6.20-6.12 (m, 1 H), 4.18-4.16 (d, J = 8.0 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.4, 152.2, 141.6, 141.3, 140.4, 140.2, 140.1, 139.1, 137.2, 136.2, 129.9 129.4, 128.9, 128.8, 128.6, 128.5, 128.1, 127.8, 127.7, 127.6, 127.4, 127.1, 127.0, 126.9, 119.5 (q, J = 326.0 Hz, 1C), 108.9, 108.7, 51.8; HRMS calcd for $C_{22}H_{18}F_3O_2S$ $[M+H]^+$ 403.0974; found: 403.0977.



(*E/Z*)-1-chloro-4-(1-phenyl-3-((trifluoromethyl)sulfonyl)prop-1-en-1-yl)benzene (3sa)

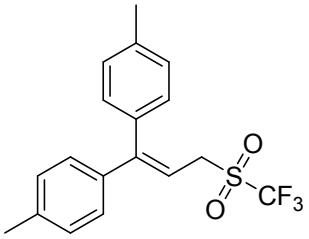
Colorless oil (44.3 mg, 41% yield). (*E/Z* = 50/50) ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.67-7.25 (m, 9 H, Ar), 6.20-6.12 (m, 1 H), 4.13-4.11 (m, 2 H); 7.67-7.25 (m, 9 H, Ar), 6.20-6.12 (m, 1 H), 4.18-4.16 (m, 2 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 152.4, 152.2, 141.6, 141.3, 140.4, 140.2, 140.1, 139.1, 137.2, 136.2, 129.9, 129.4, 128.9, 128.8, 128.6, 128.5, 128.1, 127.8, 127.7, 127.6, 127.4, 127.09, 127.06, 127.00, 119.5 (q, J = 326.0 Hz, 1C), 108.9, 108.7, 51.8; HRMS calcd for $C_{16}H_{13}ClF_3O_2S$ $[M+H]^+$ 361.0272; found: 361.0266.



(*E/Z*)-1-bromo-4-(1-phenyl-3-((trifluoromethyl)sulfonyl)prop-1-en-1-yl)benzene (3ta)

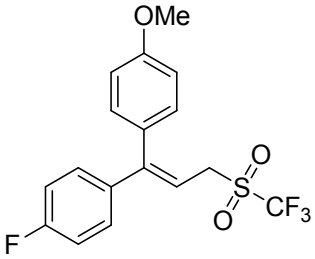
Colorless oil (48.4 mg, 40% yield). (*E/Z* = 49/51) ^{1}H NMR (400 MHz, $CDCl_3$, ppm):

δ = 7.60-7.10 (m, 9 H, Ar), 6.15-6.09 (m, 1 H), 4.07-4.06 (m, 2 H); 7.60-7.10 (m, 9 H, Ar), 6.15-6.09 (m, 1 H), 4.09-4.08 (m, 2 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 151.7, 151.6, 139.8, 139.2, 136.7, 136.1, 132.2, 132.1, 131.6, 131.1, 129.3, 129.2, 129.1, 128.9, 128.8, 128.5, 127.6, 123.1, 122.9, 109.4, 109.2, 51.7; HRMS calcd for $C_{16}H_{13}BrF_3O_2S$ $[M+H]^+$ 404.9766; found: 404.9473.



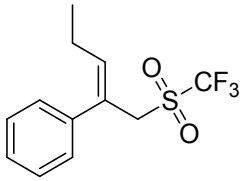
4,4'-(3-((trifluoromethyl)sulfonyl)prop-1-ene-1,1-diyl)bis(methylbenzene) (3ua)

Colorless oil (73.3 mg, 69% yield). ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.24-7.21 (d, J = 6.9 Hz, 2 H), 7.17-7.07 (m, 6 H), 6.07-6.02 (m, 1 H), 4.11-4.09 (d, J = 7.8 Hz, 2 H), 2.40 (s, 3 H), 2.34 (s, 3 H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 152.5, 138.8, 138.3, 137.7, 134.4, 129.4, 129.3, 129.0, 127.6, 119.5 (q, J = 326.3 Hz, 1C), 107.6, 51.9, 21.2, 21.1; HRMS calcd for $C_{18}H_{18}F_3O_2S$ $[M+H]^+$ 355.0974; found: 355.0966.



(*E/Z*)-1-fluoro-4-(1-(4-methoxyphenyl)-3-((trifluoromethyl)sulfonyl)prop-1-en-1-yl)benzene (3va)

Colorless oil (56.1 mg, 50% yield). (*E/Z* = 65/35) ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ = 7.24-7.10 (m, 5 H), 7.07-6.93 (m, 2 H), 6.87-6.81 (m, 1 H), 6.05-6.00 (m, 1 H), 4.14-4.05 (m, 2 H), 3.86-3.81 (m, 3H); ^{13}C NMR (75 MHz, $CDCl_3$, ppm): δ = 164.6, 164.3, 161.0, 160.2, 159.7, 151.4, 151.3, 133.4, 133.3, 132.7, 131.3, 131.2, 130.7, 129.6, 129.5, 129.2, 128.9, 119.5 (q, J = 326.3 Hz, 1C), 116.0, 115.7, 115.4, 115.2, 114.2, 113.8, 108.2, 106.9, 55.3, 51.8; HRMS calcd for $C_{17}H_{15}F_4O_3S$ $[M+H]^+$ 375.0673; found: 375.0678.



(*E*)-(1-((trifluoromethyl)sulfonyl)pent-2-en-2-yl)benzene (5aa)

Yellow oil (33.4 mg, 40% yield). ^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ = 7.40-7.37 (m, 2 H), 7.33-7.29 (m, 2 H), 7.26-7.23 (m, 1 H), 5.79-5.75 (m, 1 H), 3.62-3.59 (t, J = 7.2 Hz, 1 H), 2.71-2.66 (m, 2H), 2.06 (d, J = 1.2 Hz, 3 H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm): δ = 143.4, 138.0, 128.3, 127.1, 125.8, 123.6, 44.2, 32.3, 16.2; HRMS calcd for $C_{12}H_{14}F_3O_2S$ $[M+H]^+$ 279.0661; found: 279.0655.

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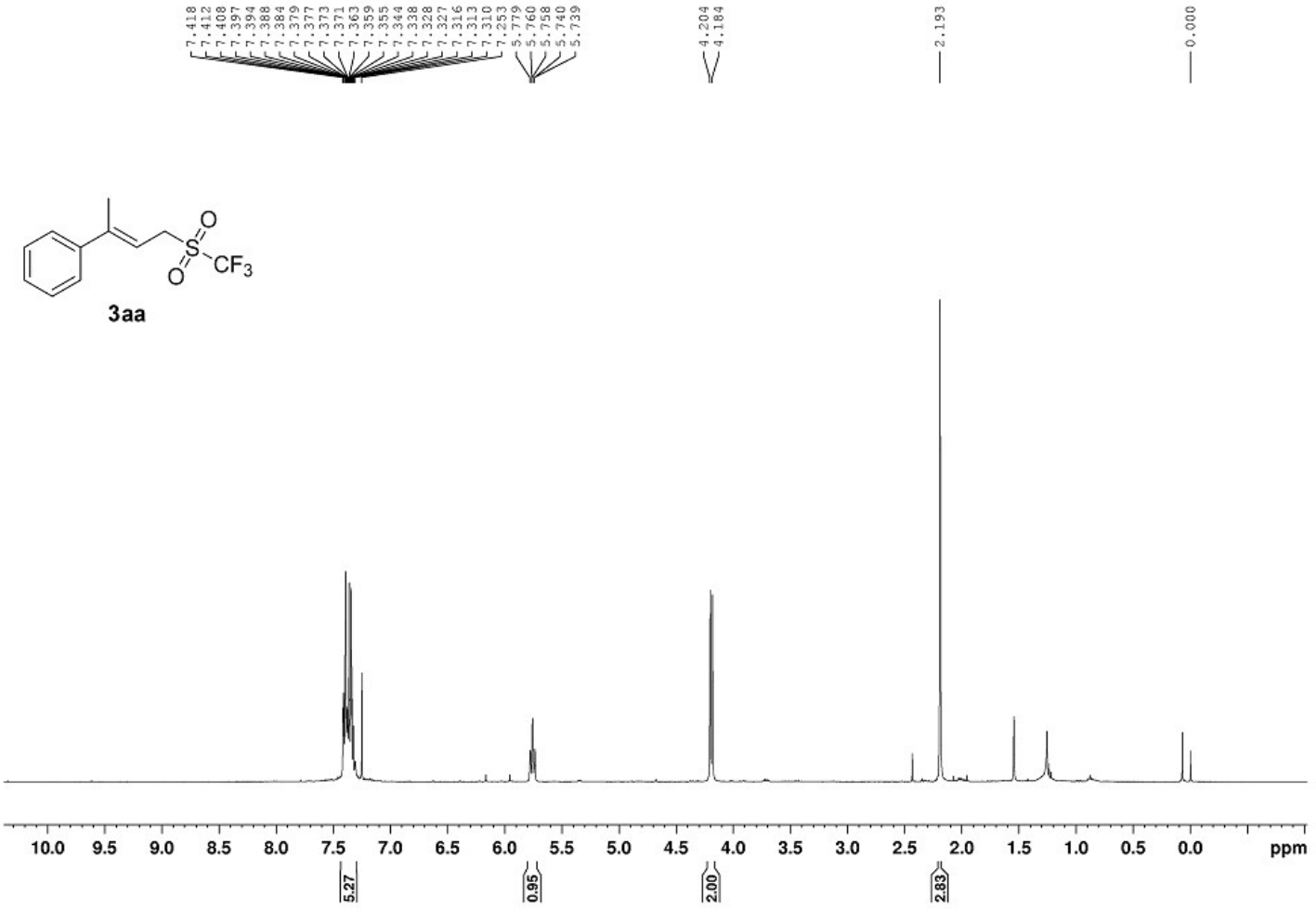
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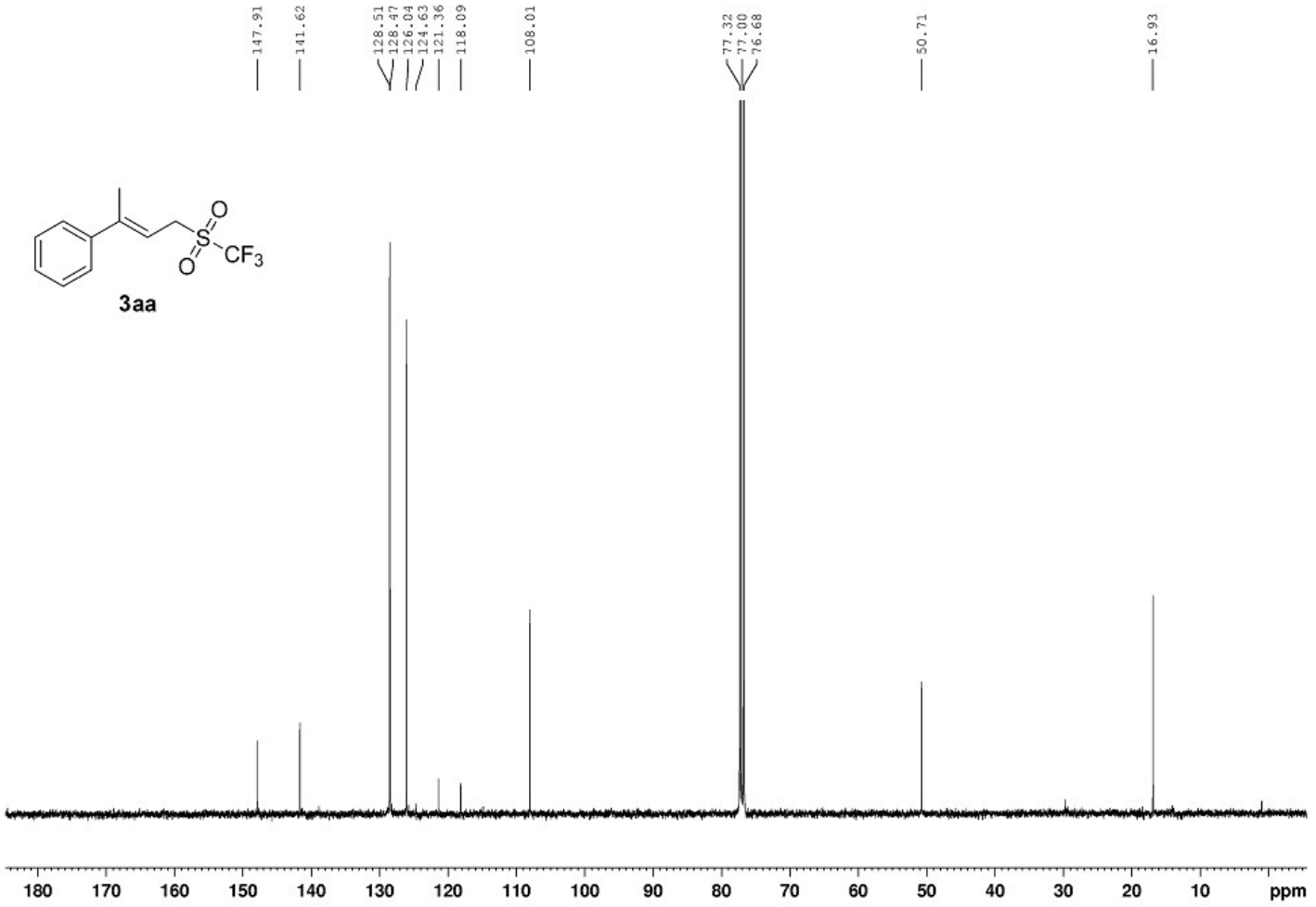
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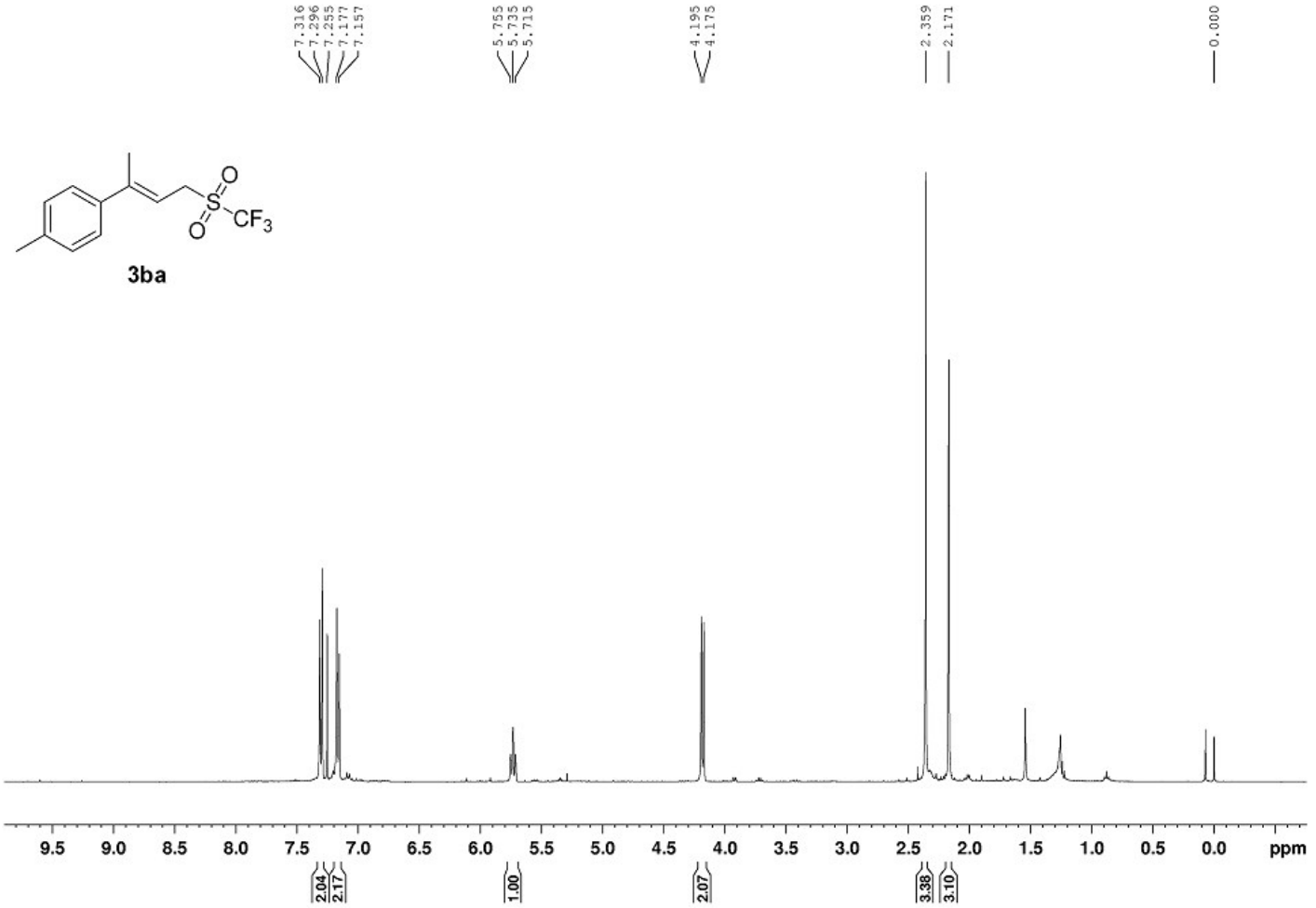
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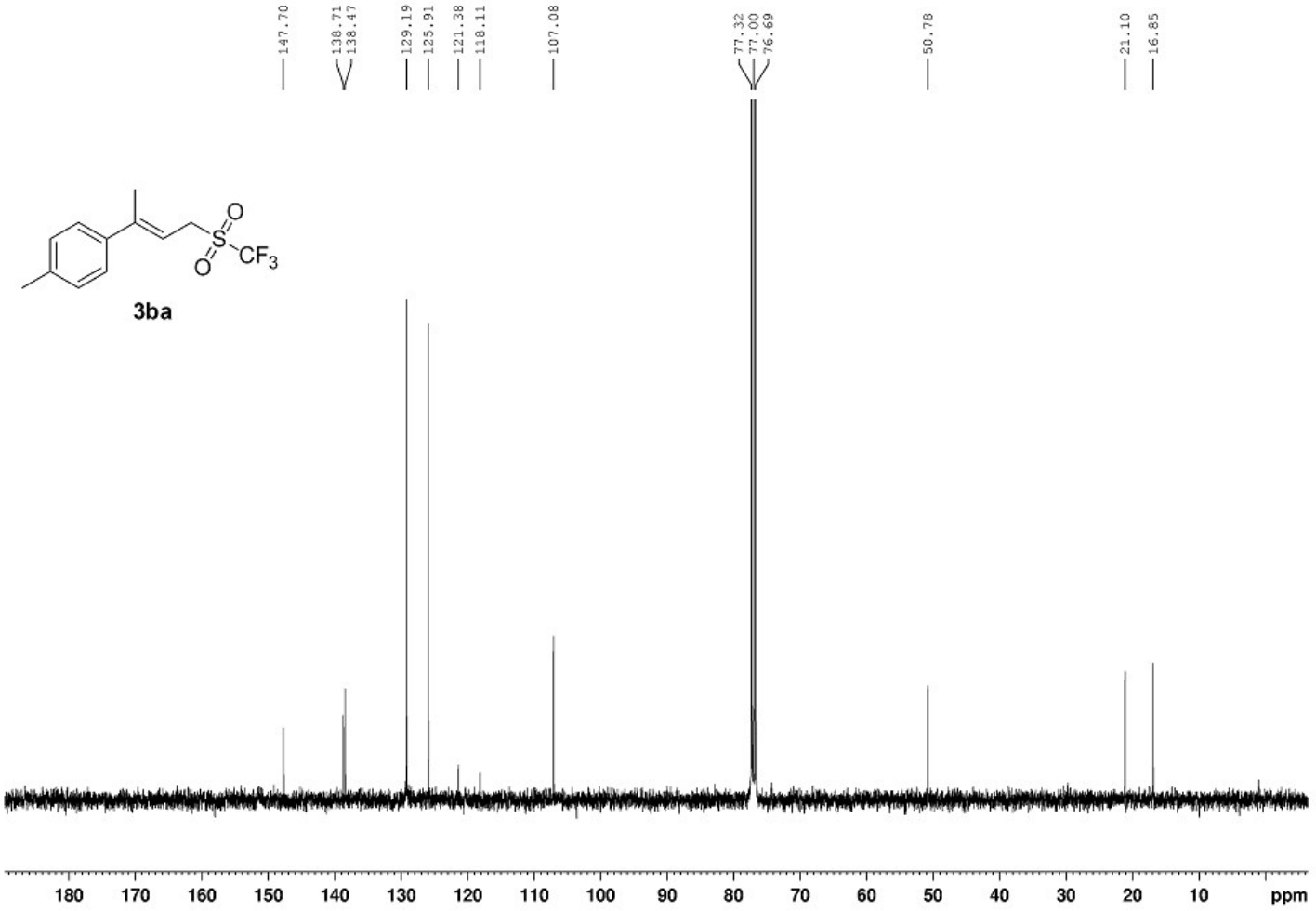
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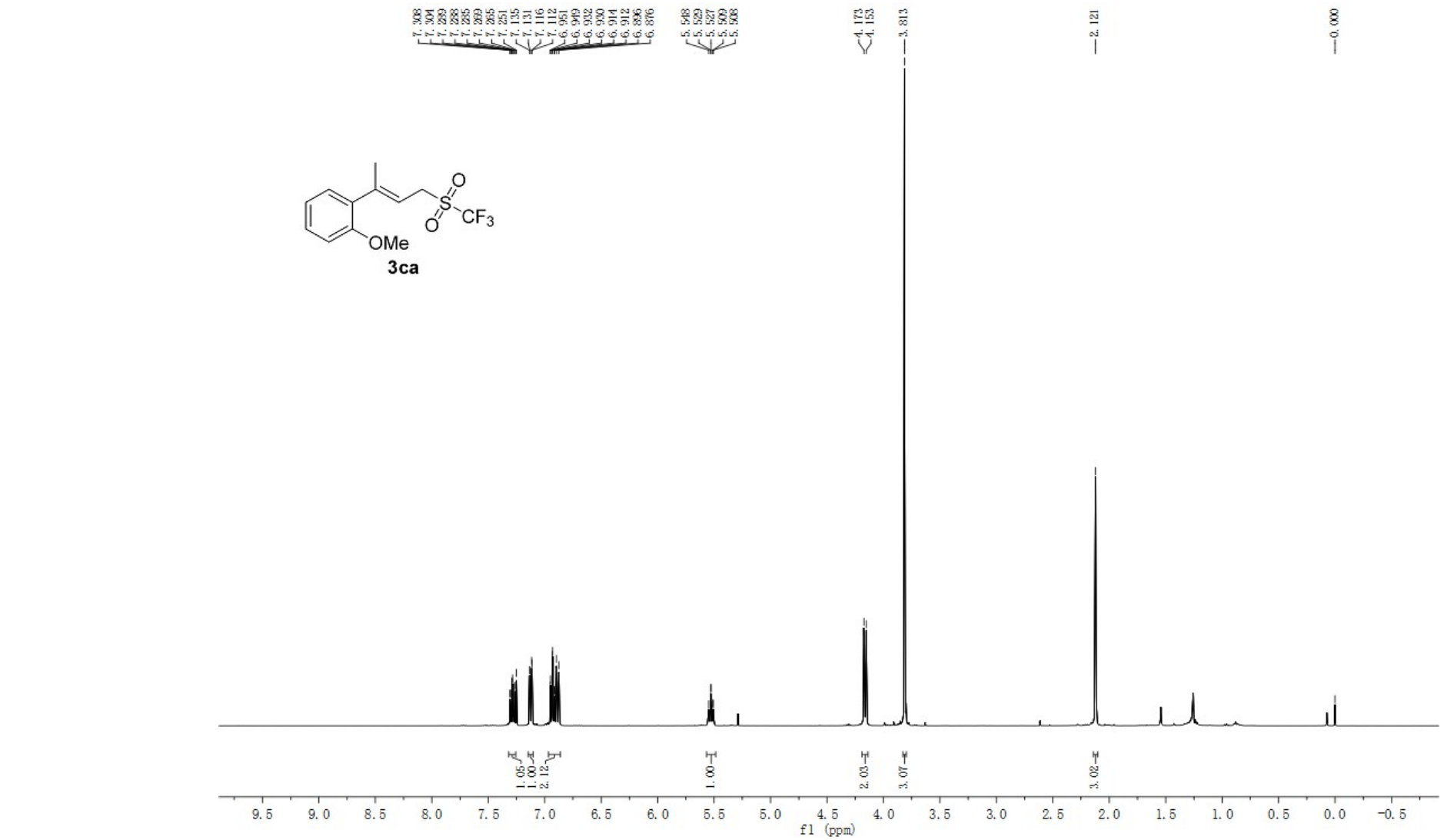
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6.930
6.914
6.912
6.896
6.876
5.548
5.529
5.527
5.509
5.508
4.173
4.153
3.813
2.121
0.000
O
O
S
CF3
OMe
3ca
1.05
1.00
2.12
1.00
2.03
3.07
3.02
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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3.0
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2.0
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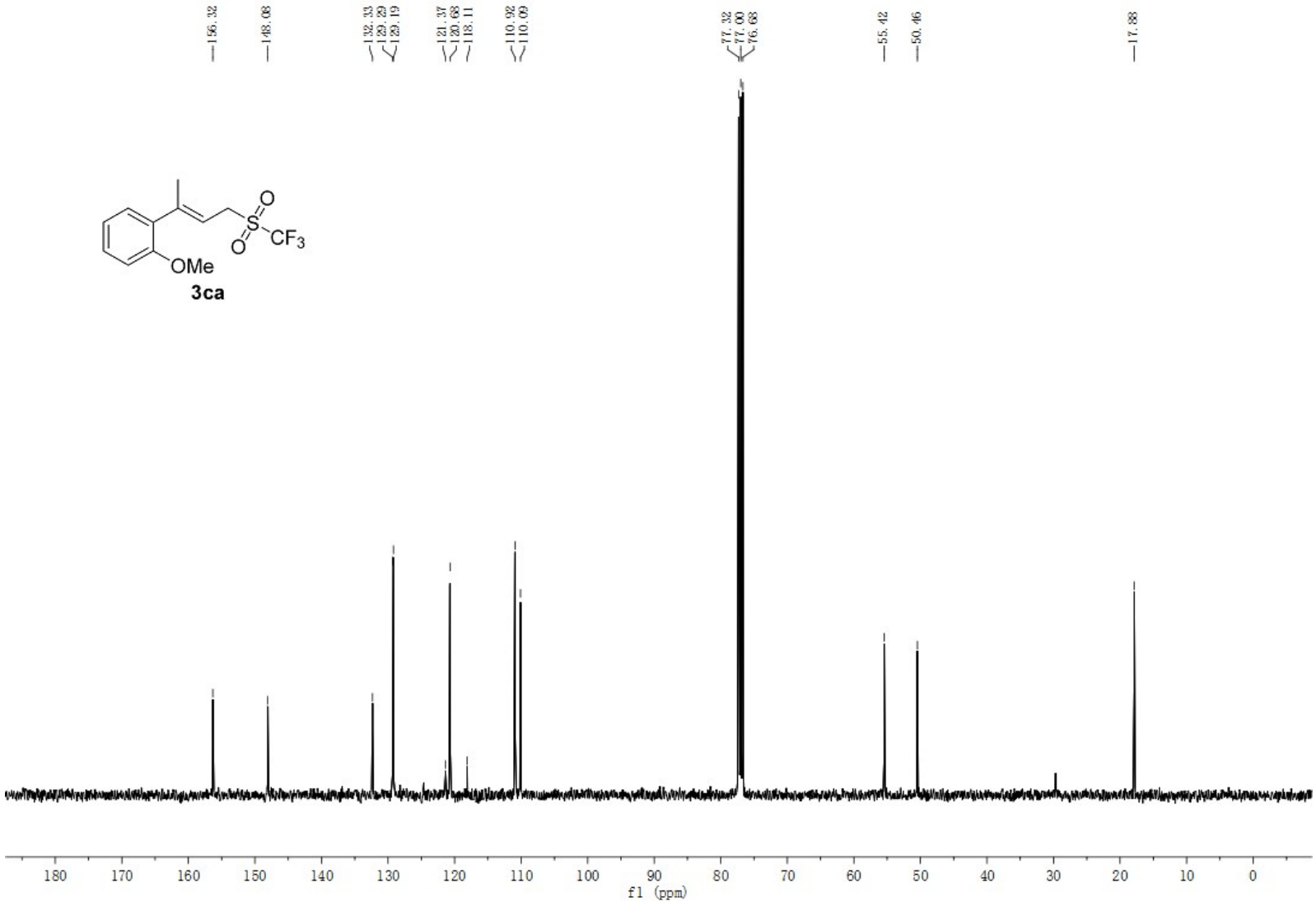
f1 (ppm)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121.37
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118.11
110.92
110.09
77.32
77.00
76.68
55.42
50.46
17.88
OMe
3ca
180
170
160
150
140
130
120
110
100
90
80
70
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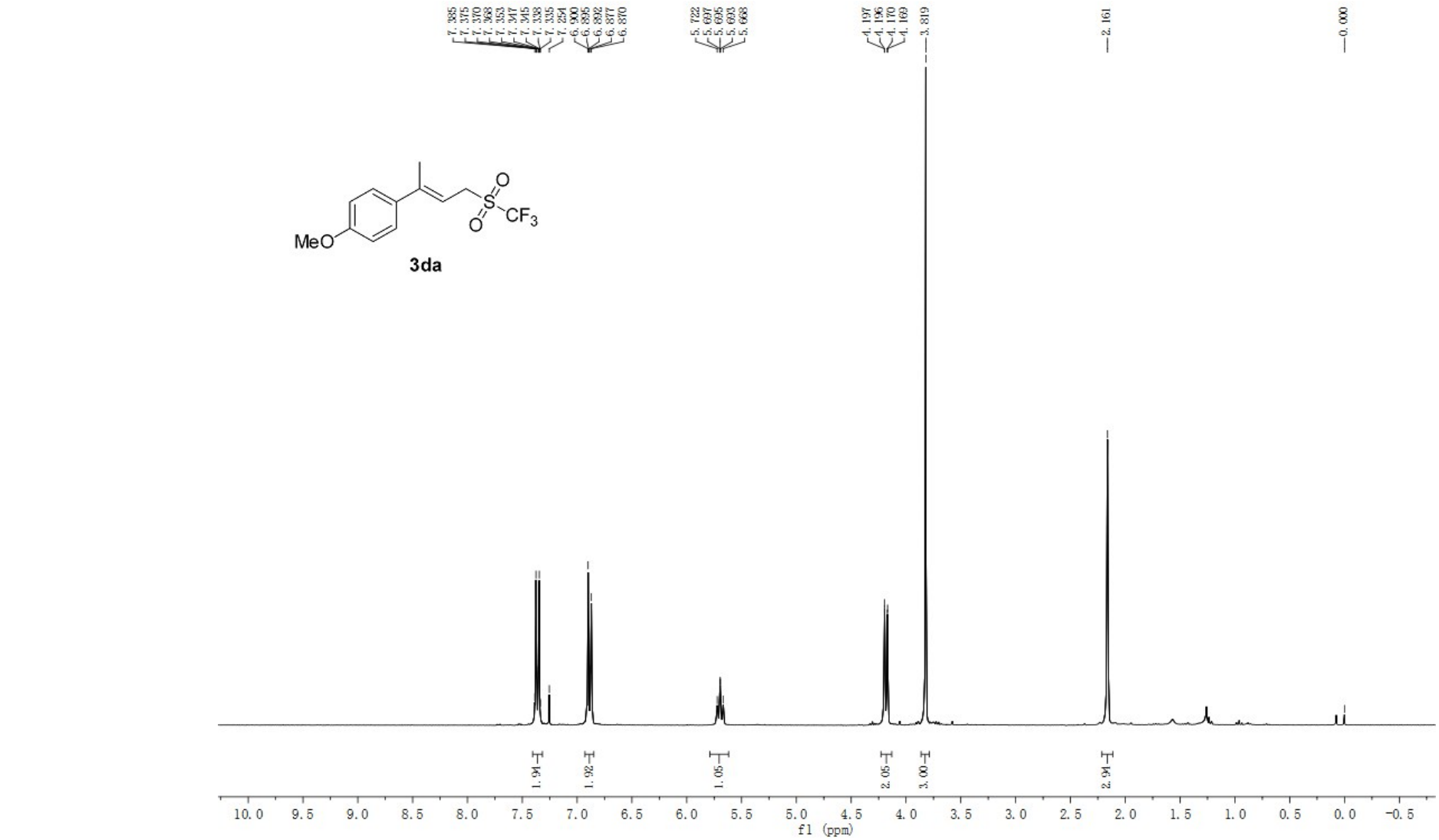
50
40
30
20
10
0
f1 (ppm)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7.254
6.900
6.895
6.892
6.877
6.870
5.722
5.697
5.695
5.693
5.668
4.197
4.196
4.170
4.169
3.819
2.161
0.000
MeO
O=S=O
CF3
3da
1.94
1.92
1.05
2.05
3.00
2.94
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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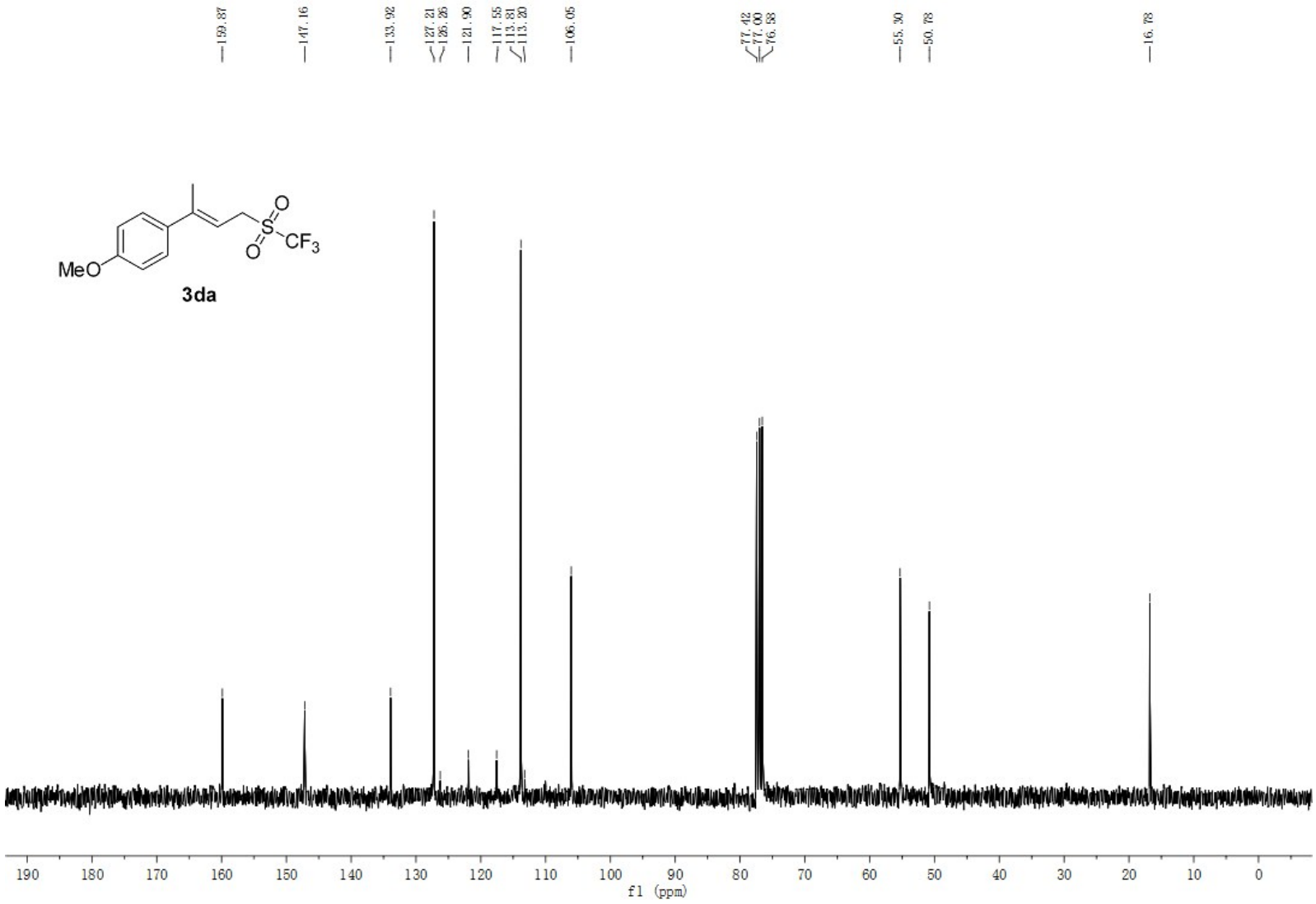
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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121.90
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113.81
113.20
106.05
77.42
77.00
76.58
55.30
50.78
16.78
MeO
O
O
S
CF3
3da
190
180
170
160
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130
120
110
100
90
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70
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50
40
30
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10
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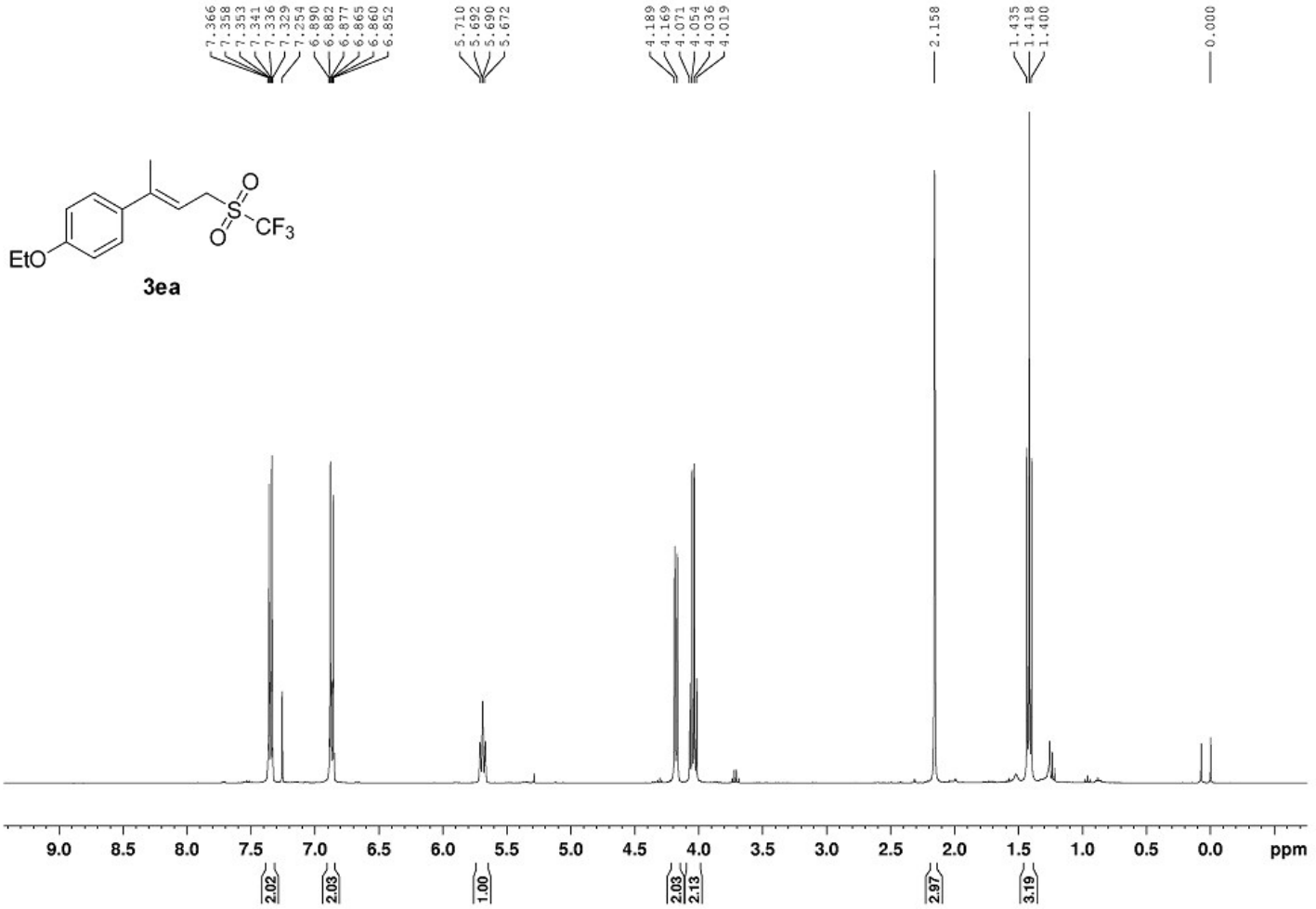
f1 (ppm)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7.254
6.890
6.882
6.877
6.865
6.860
6.852
5.710
5.692
5.690
5.672
4.189
4.169
4.071
4.054
4.036
4.019
2.158
1.435
1.418
1.400
0.000
EtO
O
S
O
CF3
3ea
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
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ppm
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2.03
1.00
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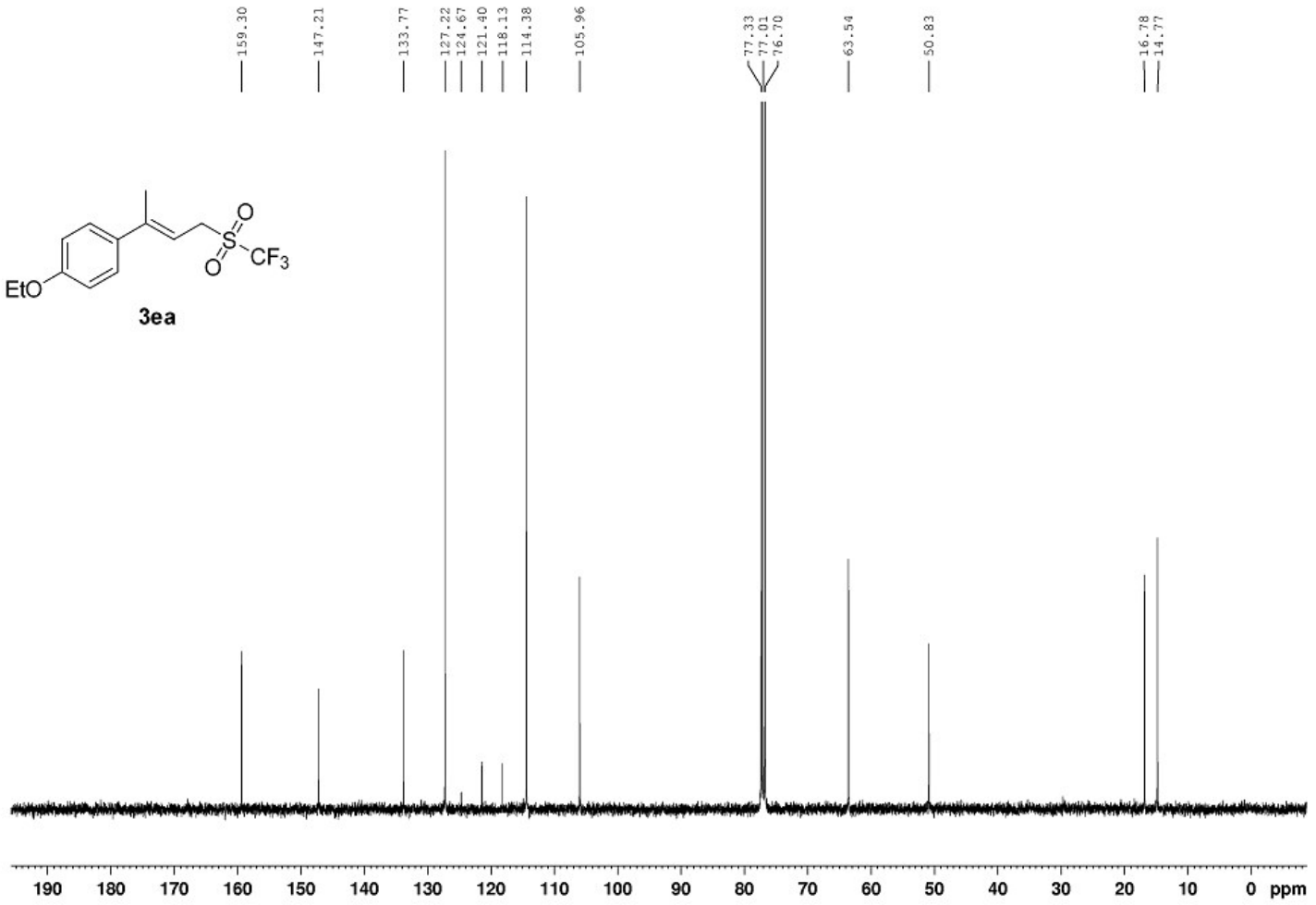
2.97
3.19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121.40
118.13
114.38
105.96
77.33
77.01
76.70
63.54
50.83
16.78
14.77
EtO
O
O
S
CF3
3ea
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180
170
160
150
140
130
120
110
100
90
80
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60
50
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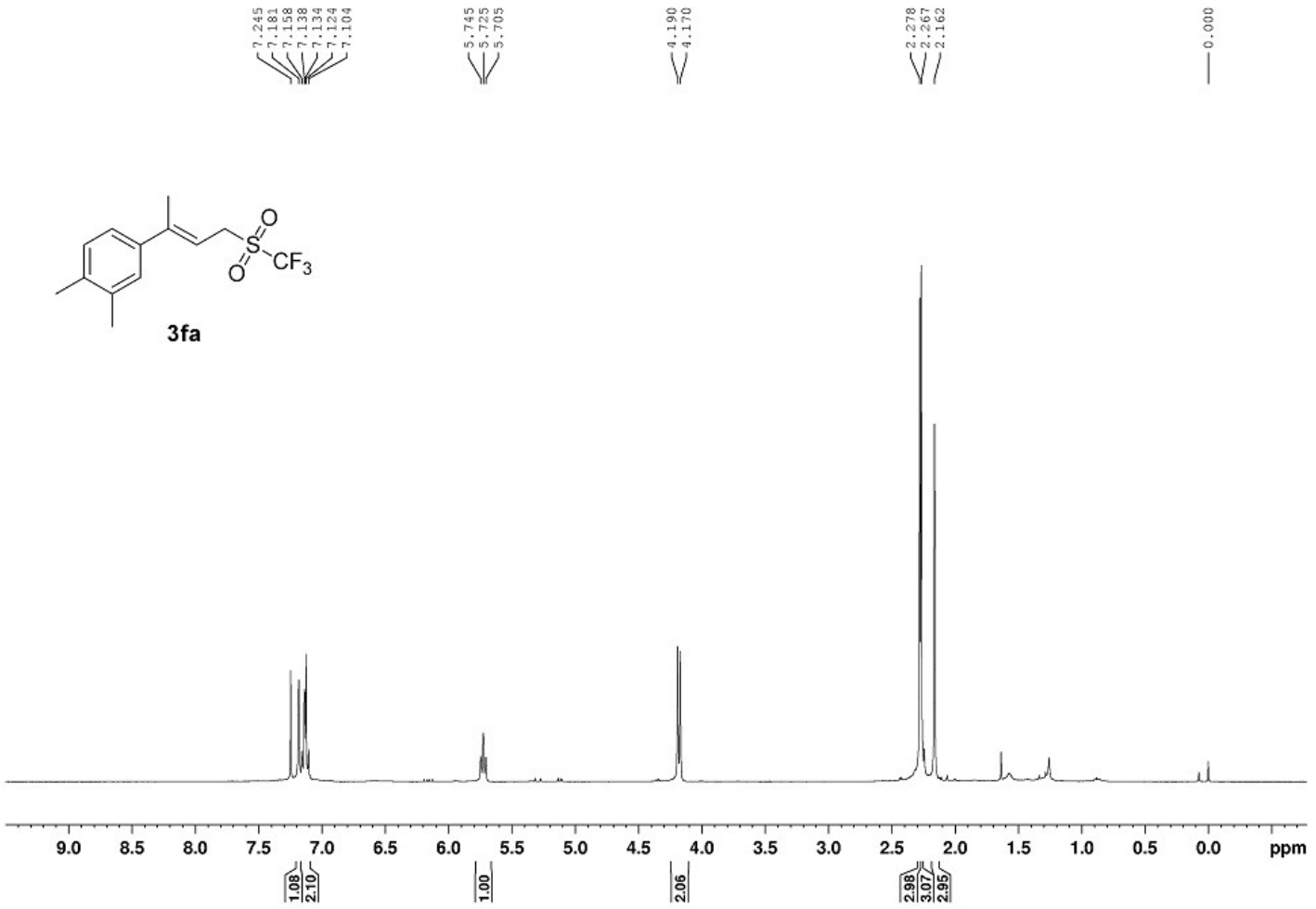
30
20
10
0
ppm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7.124
7.104
5.745
5.725
5.705
4.190
4.170
2.278
2.267
2.162
0.000
O
O
S
O
CF3
3fa
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
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0.5
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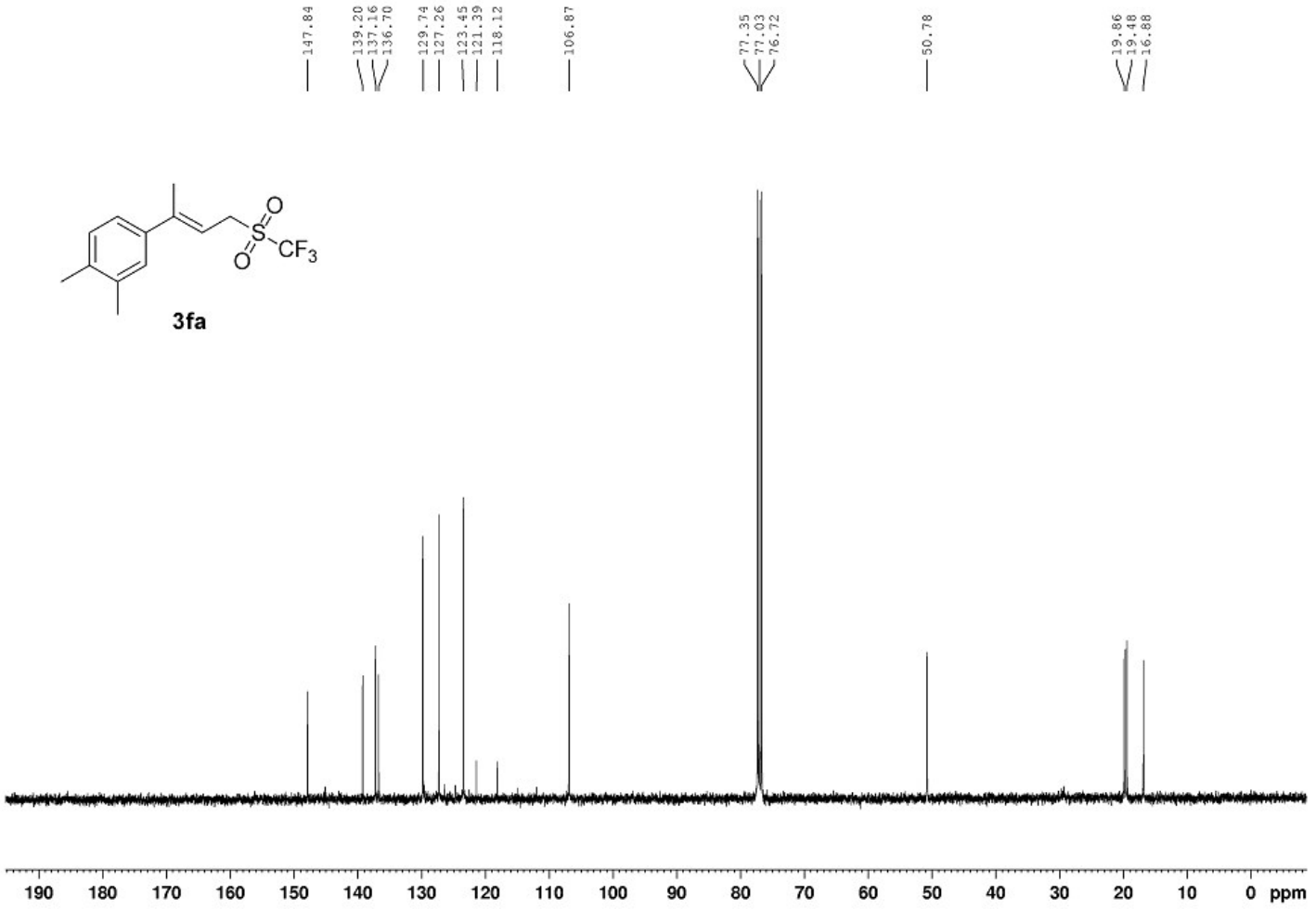
1.00
2.06
2.98
3.07
2.95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127.26
123.45
121.39
118.12
106.87
77.35
77.03
76.72
50.78
19.86
19.48
16.88
O
S
O
CF3
3fa
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180
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160
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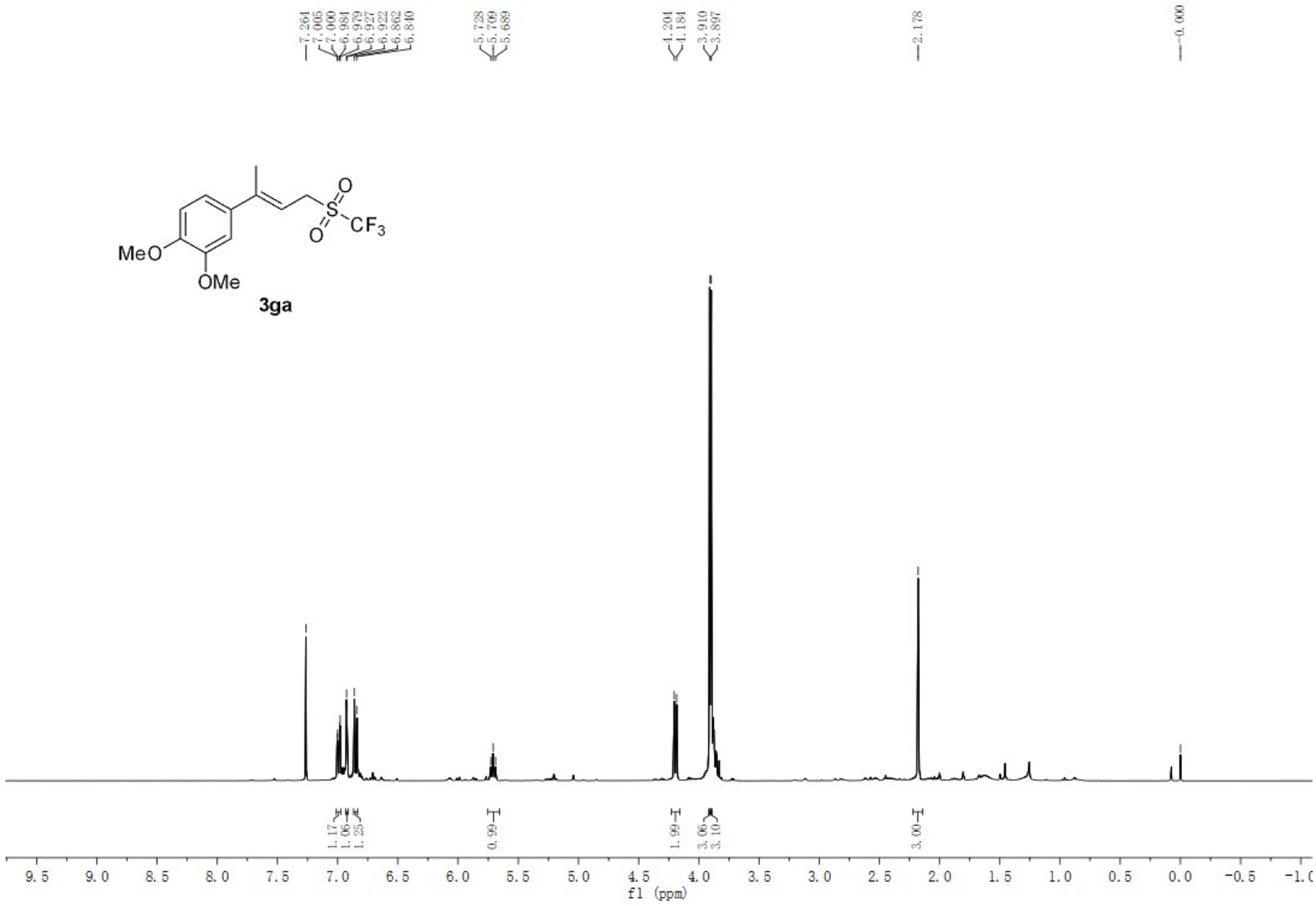
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.000
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6.927
6.922
6.862
6.840
5.728
5.709
5.689
4.201
4.184
3.910
3.897
2.178
0.000
MeO
OMe
O
S
O
CF3
3ga
1.17
1.06
1.25
0.99
1.99
3.06
3.10
3.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
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4.0
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3.0
2.5
2.0
1.5
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0.5
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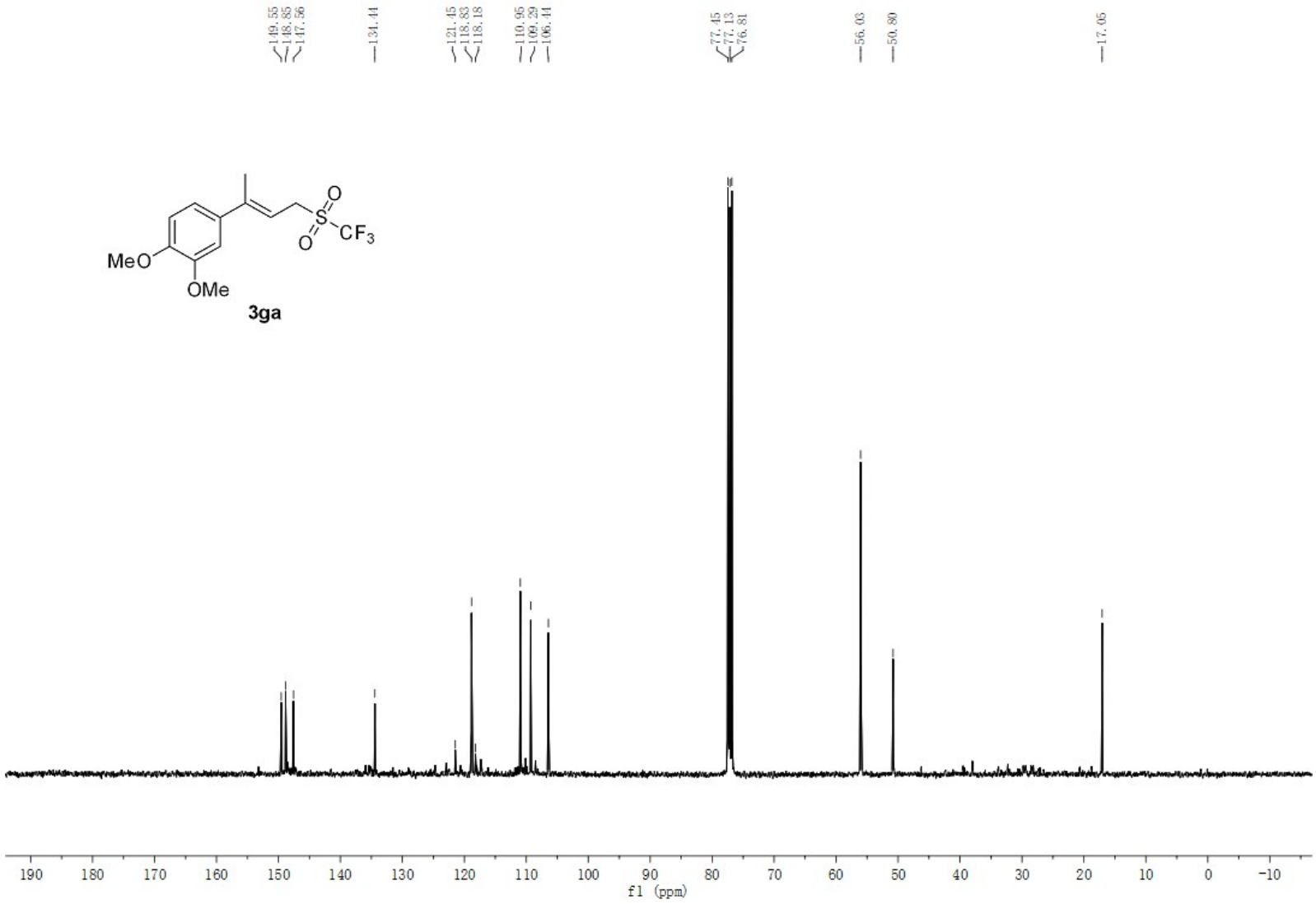
-0.5
f1 (ppm)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147.56
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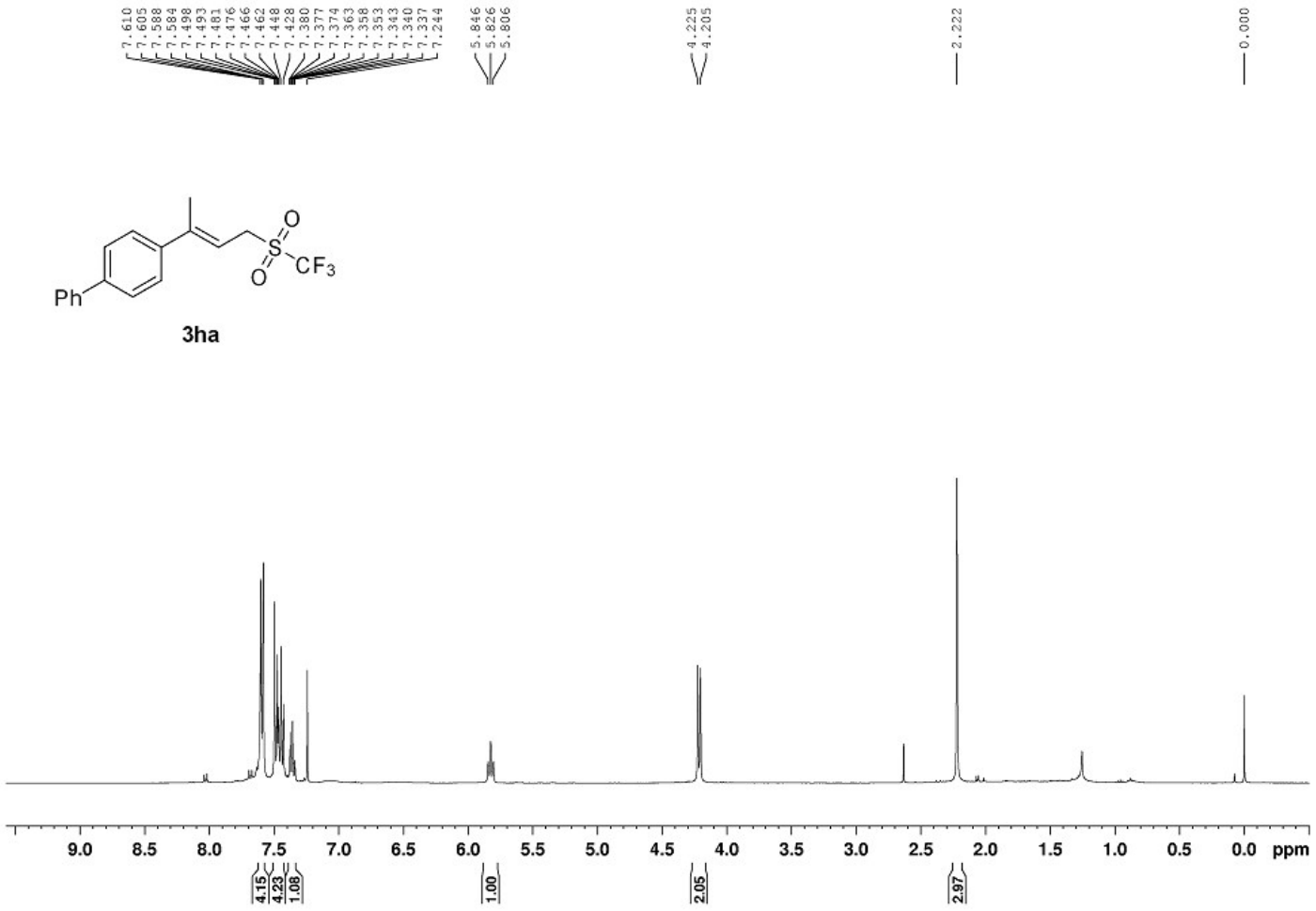
118.18
110.95
109.29
106.44
77.45
77.13
76.81
56.03
50.80
17.05
MeO
OMe
O
O
S
CF3
3ga
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)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7.476
7.466
7.462
7.448
7.428
7.380
7.377
7.374
7.363
7.358
7.353
7.343
7.340
7.337
7.244
5.846
5.826
5.806
4.225
4.205
2.222
0.000
Ph
O
S
O
CF3
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
ppm
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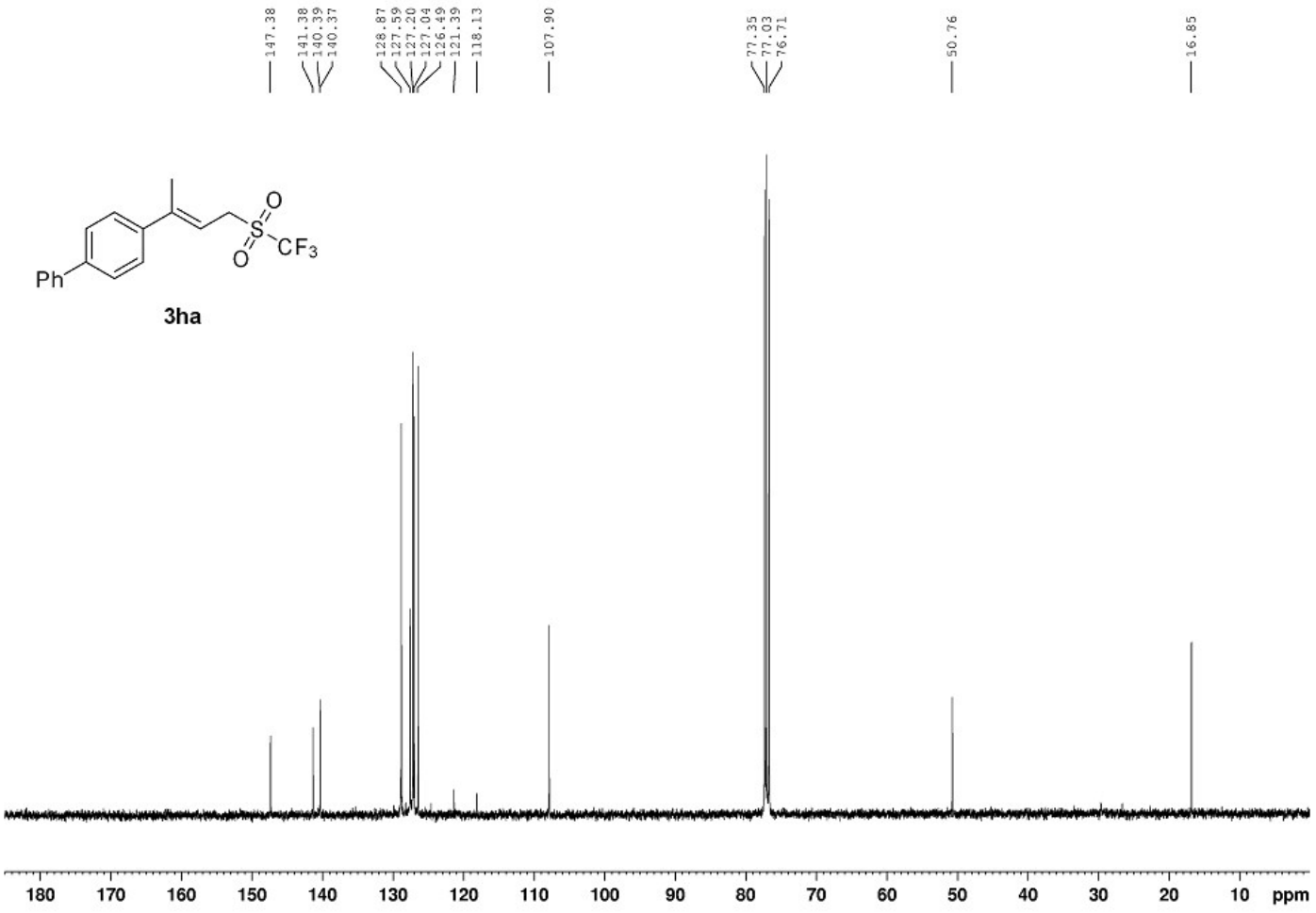
4.23
1.08
1.00
2.05
2.97

3ha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141.38
140.39
140.37
128.87
127.59
127.20
127.04
126.49
121.39
118.13
107.90
77.35
77.03
76.71
50.76
16.85
Ph
O
S
O
CF3
3ha
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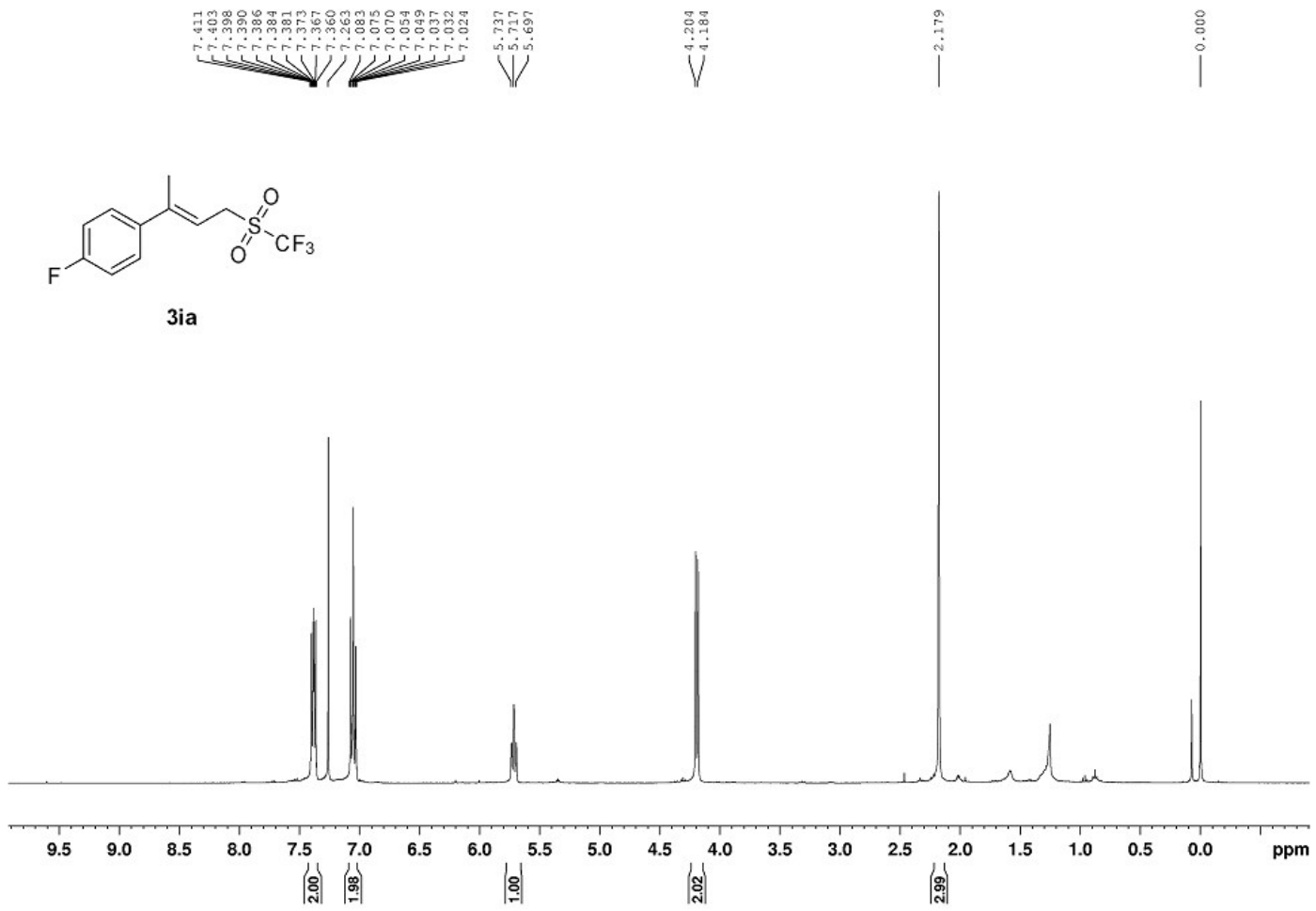
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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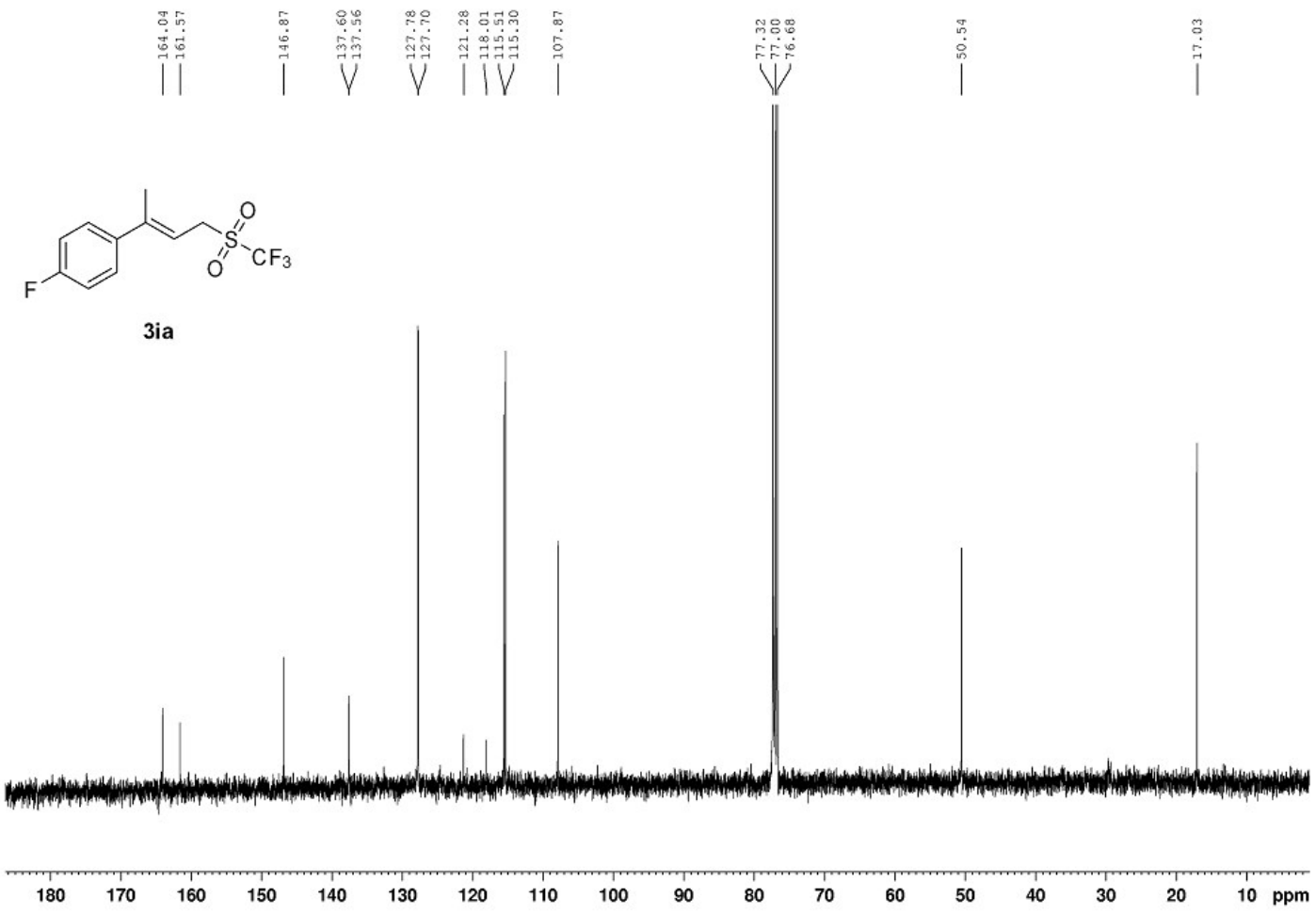
7.386
7.384
7.381
7.373
7.367
7.360
7.263
7.083
7.075
7.070
7.054
7.049
7.037
7.032
7.024
5.737
5.717
5.697
4.204
4.184
2.179
0.000
F
O
S
O
CF3
3ia
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm
2.00
1.98
1.00
2.02
2.99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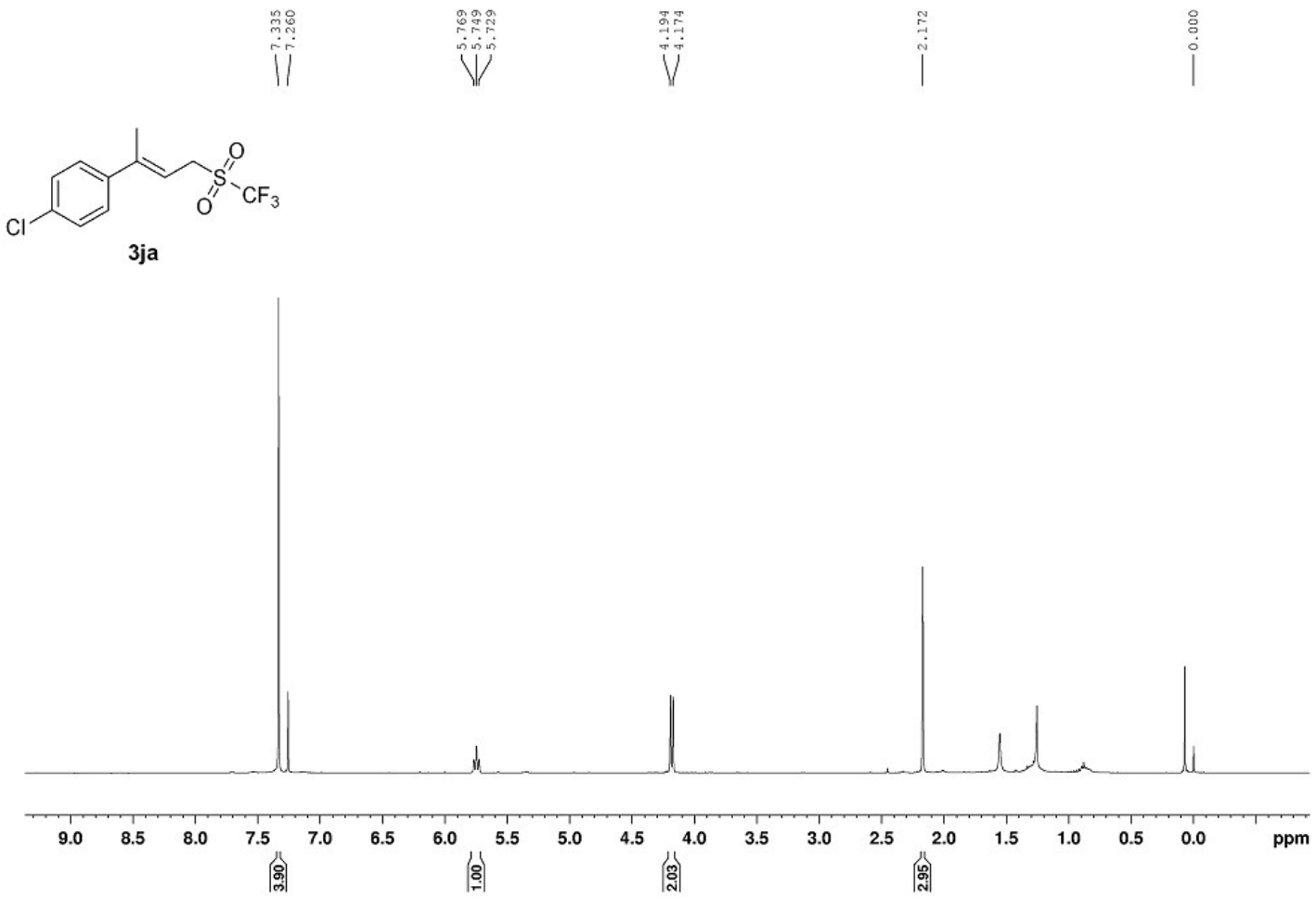
161.57
146.87
137.60
137.56
127.78
127.70
121.28
118.01
115.51
115.30
107.87
77.32
77.00
76.68
50.54
17.03
F
O
S
O
CF3
3ia
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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5.749
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2.172
0.000
Cl
O
S
O
CF3
3ja
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
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2.0
1.5
1.0
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ppm
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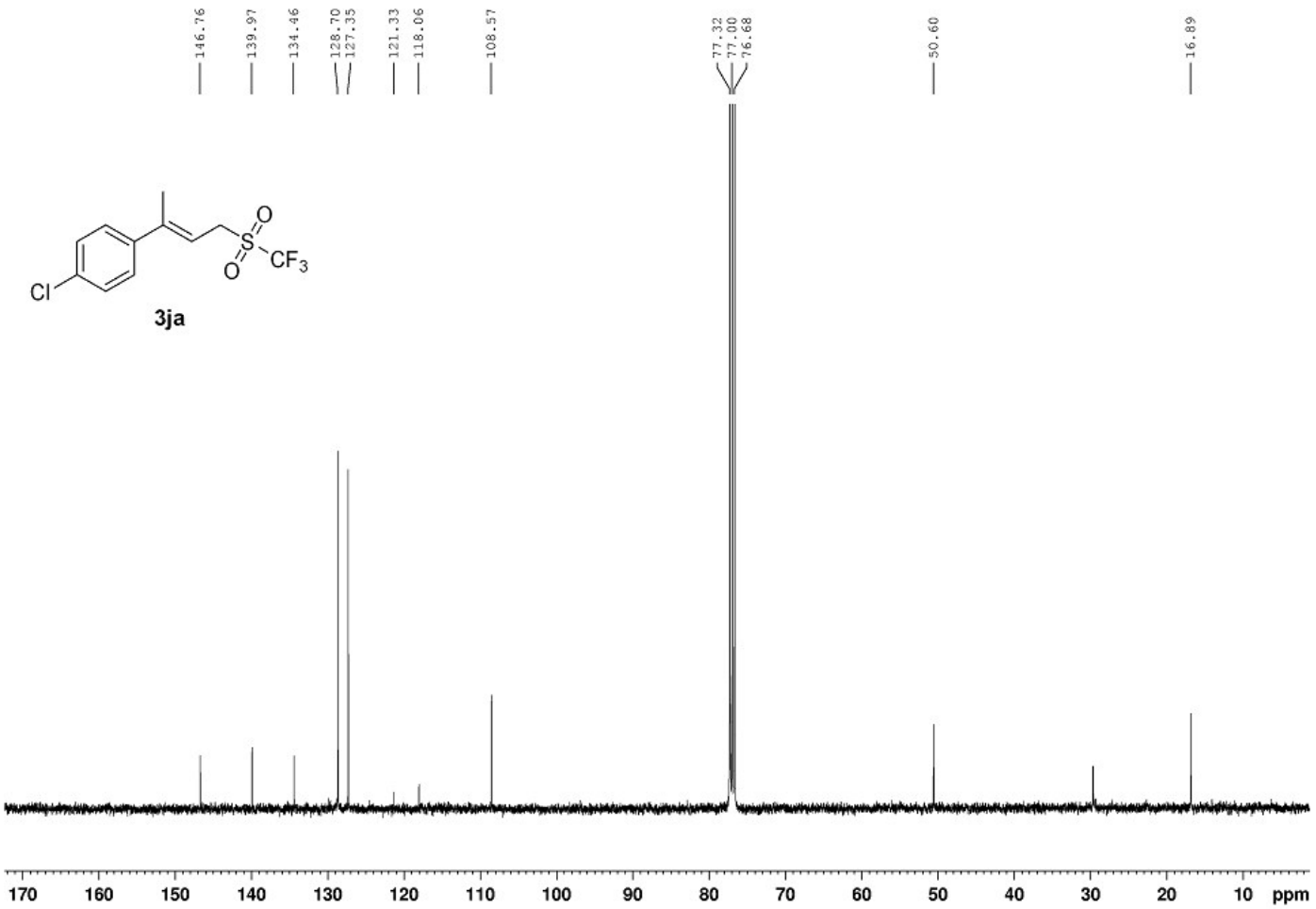
1.00
2.03
2.95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127.35
121.33
118.06
108.57
77.32
77.00
76.68
50.60
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Cl
O
O
S
CF3
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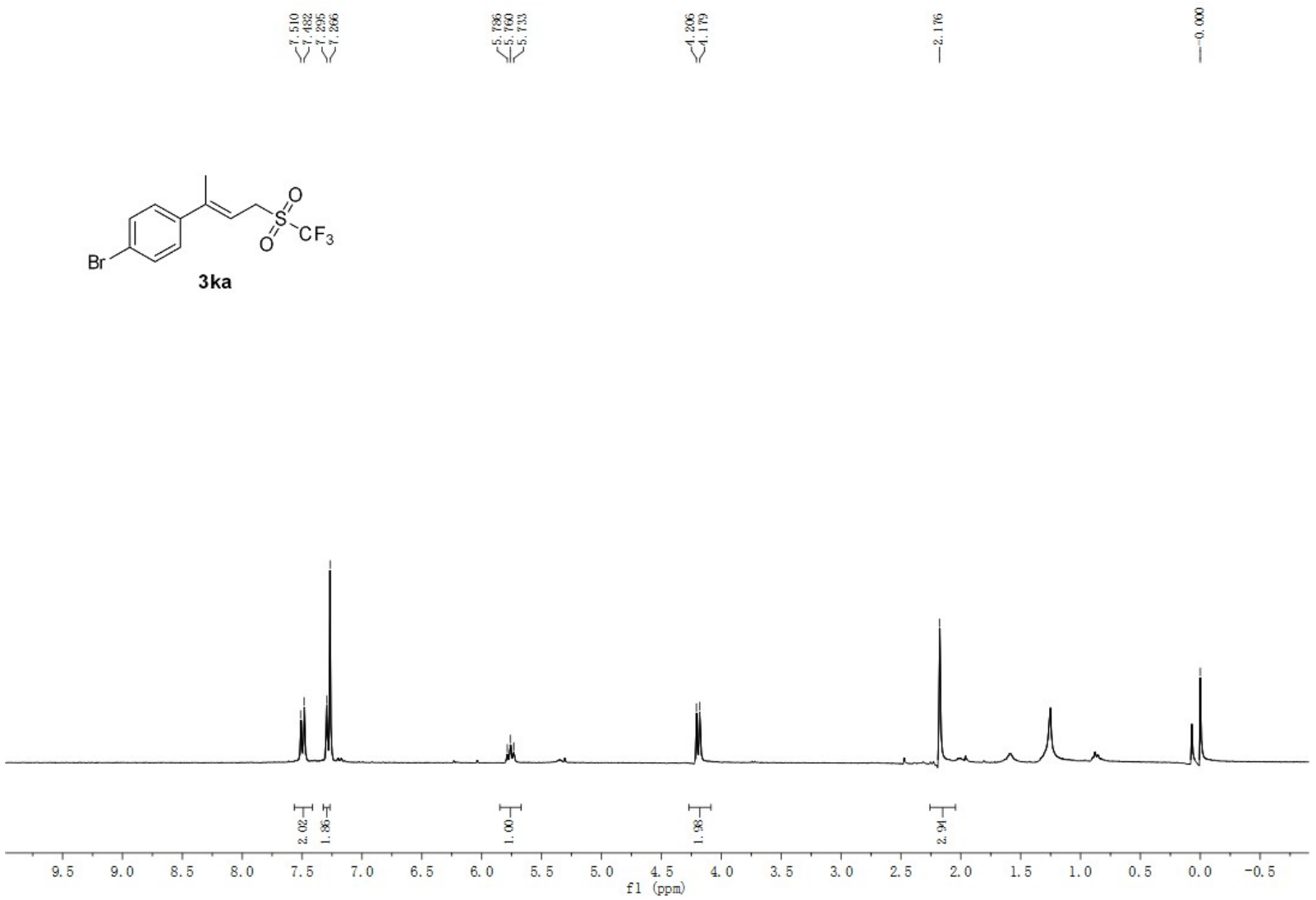
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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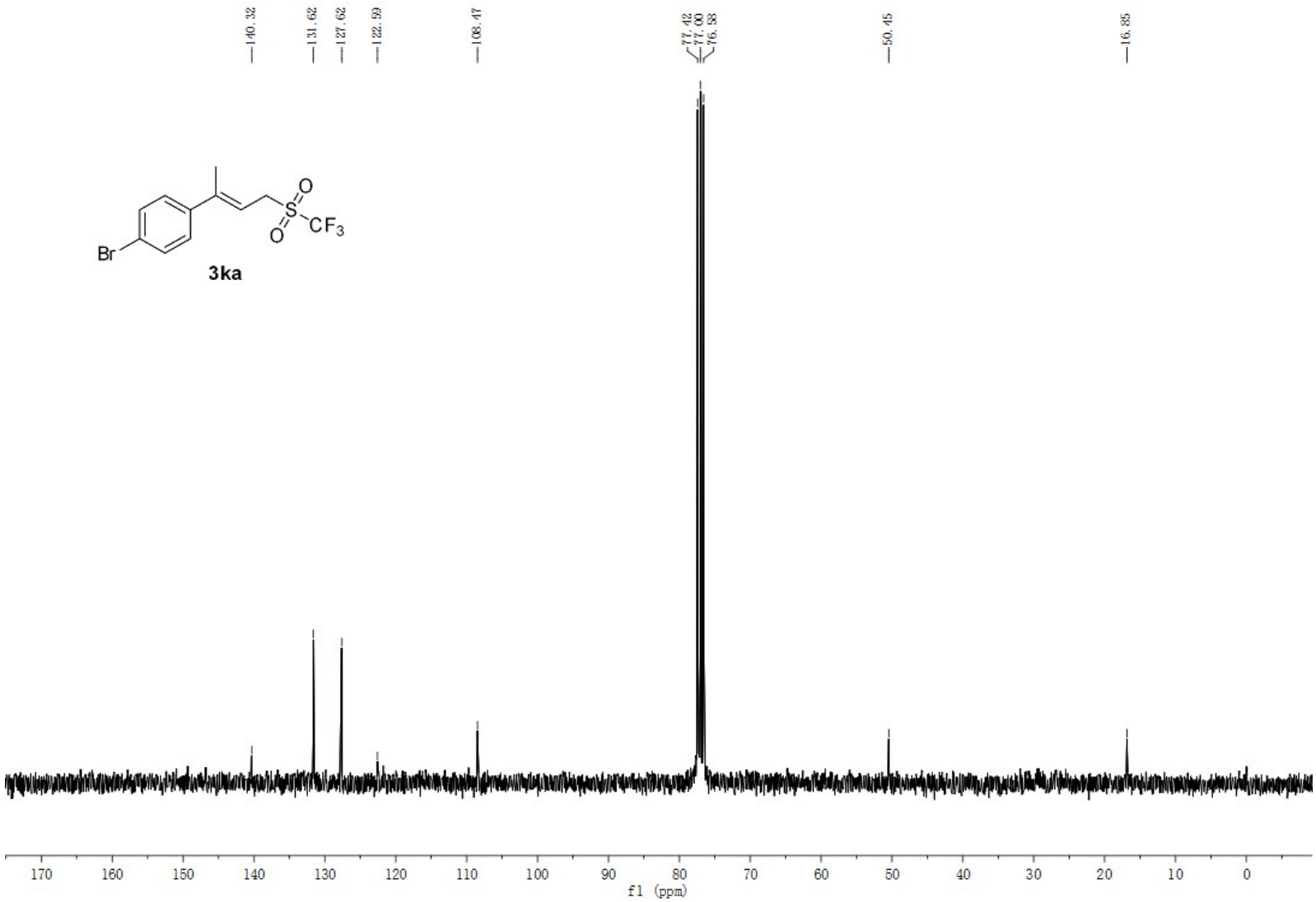
Br
O
S
O
CF3
3ka
2.02
1.86
1.00
1.98
2.94
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)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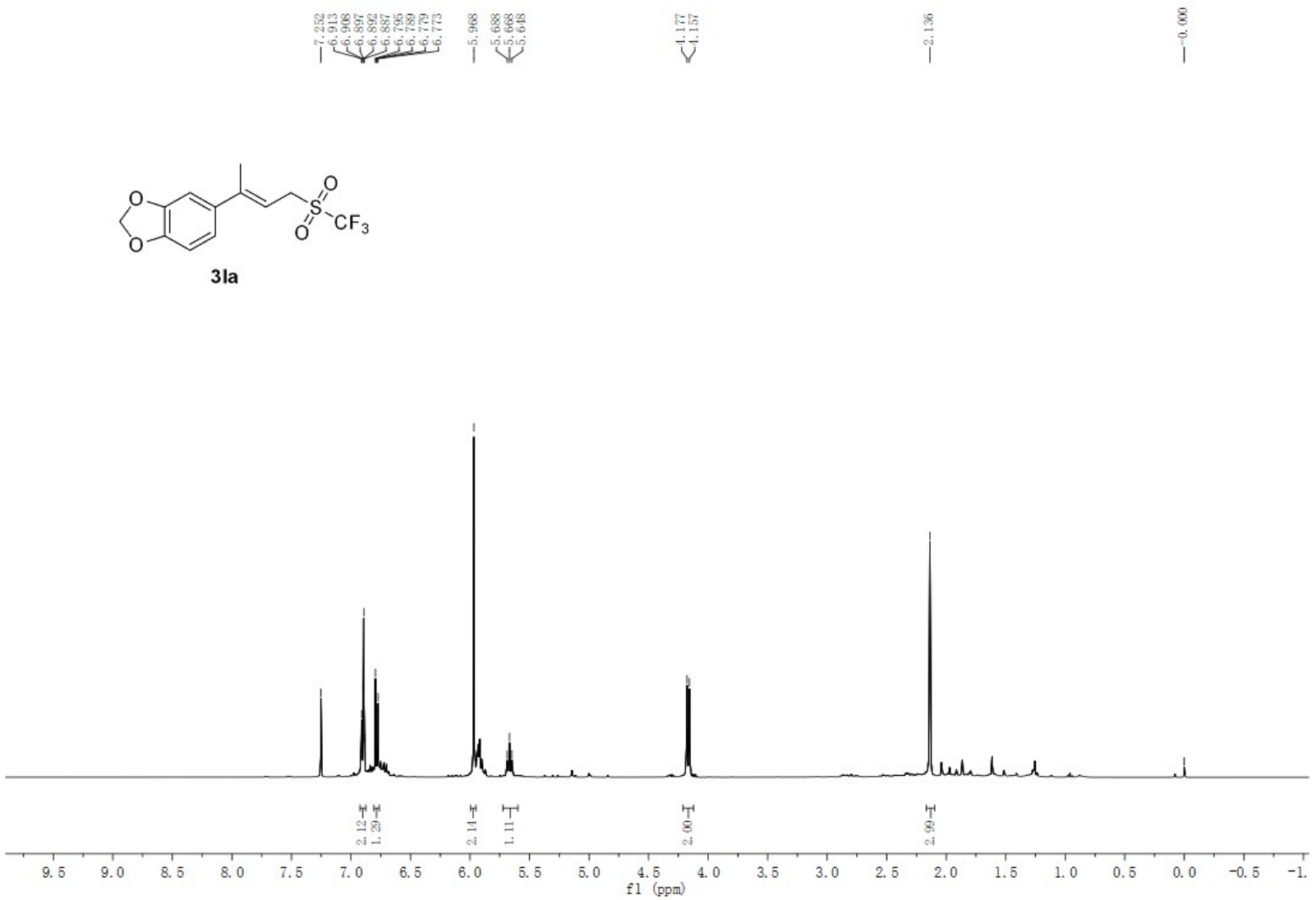
77.42
77.00
76.58
50.45
16.85
Br
O
S
O
CF3
3ka
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.789
6.779
6.773
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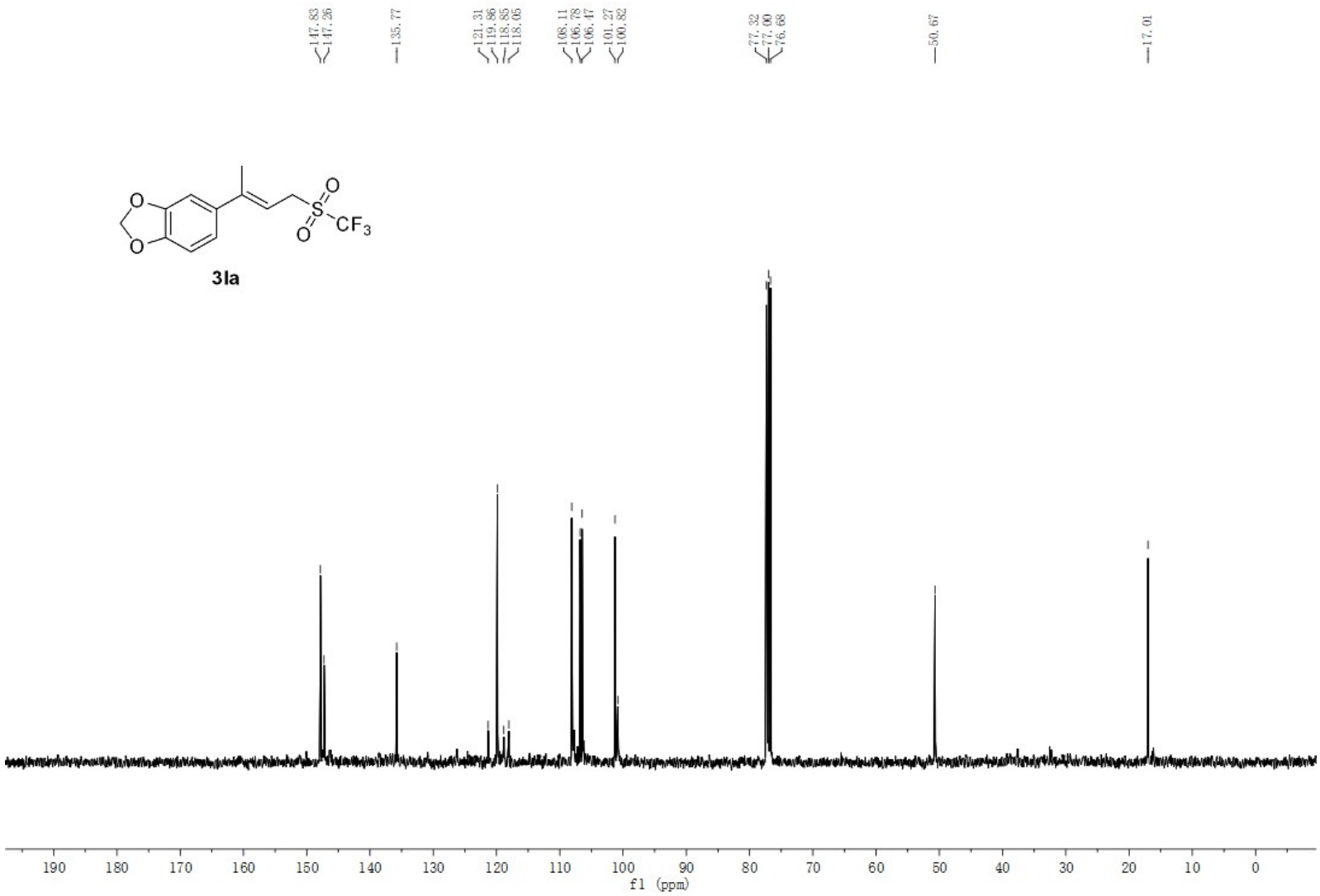
5.688
5.668
5.648
1.177
1.157
2.136
0.000
O
O
O
S
O
CF3
3la
2.12
1.29
2.14
1.11
2.00
2.99
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.
f1 (ppm)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108.11
106.78
106.47
101.27
100.82
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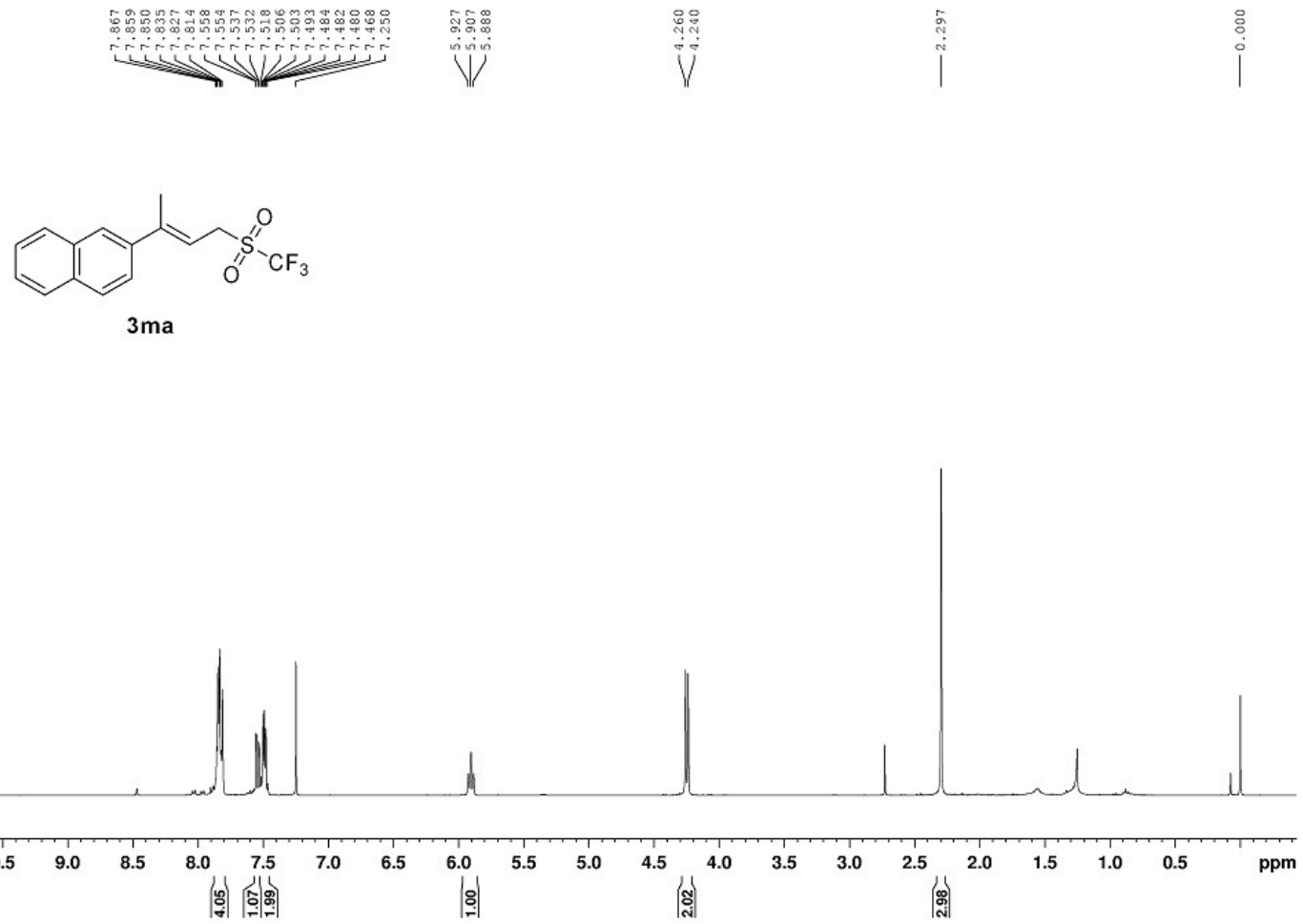
77.00
76.68
50.67
17.01
O
O
O
S
O
CF3
3la
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.537
7.532
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7.506
7.503
7.493
7.484
7.482
7.480
7.468
7.250
5.927
5.907
5.888
4.260
4.240
2.297
0.000
O
O
S
CF3
3ma
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
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1.5
1.0
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ppm
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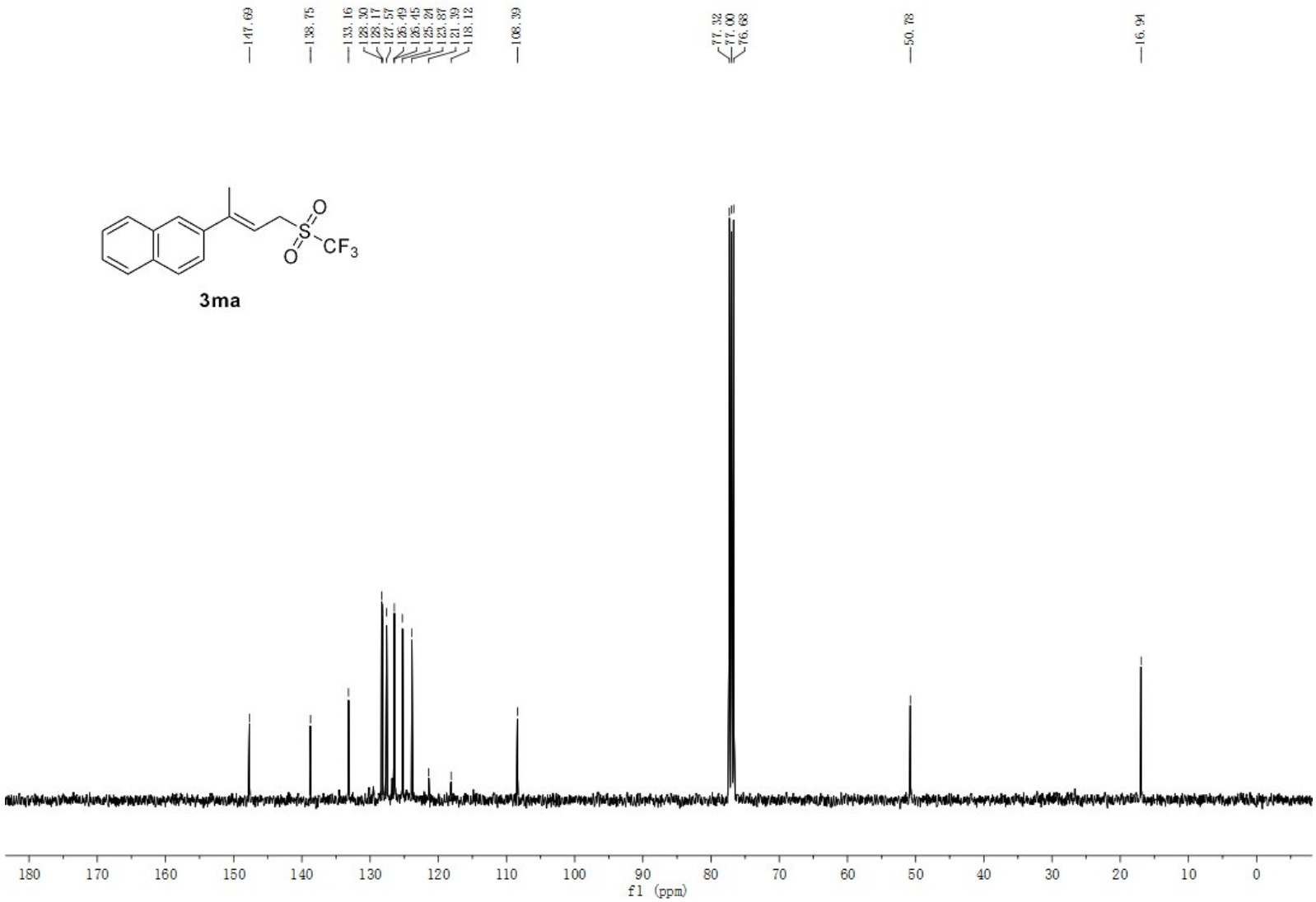
1.07
1.99
1.00
2.02
2.98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126.45
125.24
123.87
121.39
118.12
108.39
77.32
77.00
76.68
50.78
16.94
O
S
O
CF3
3ma
180
170
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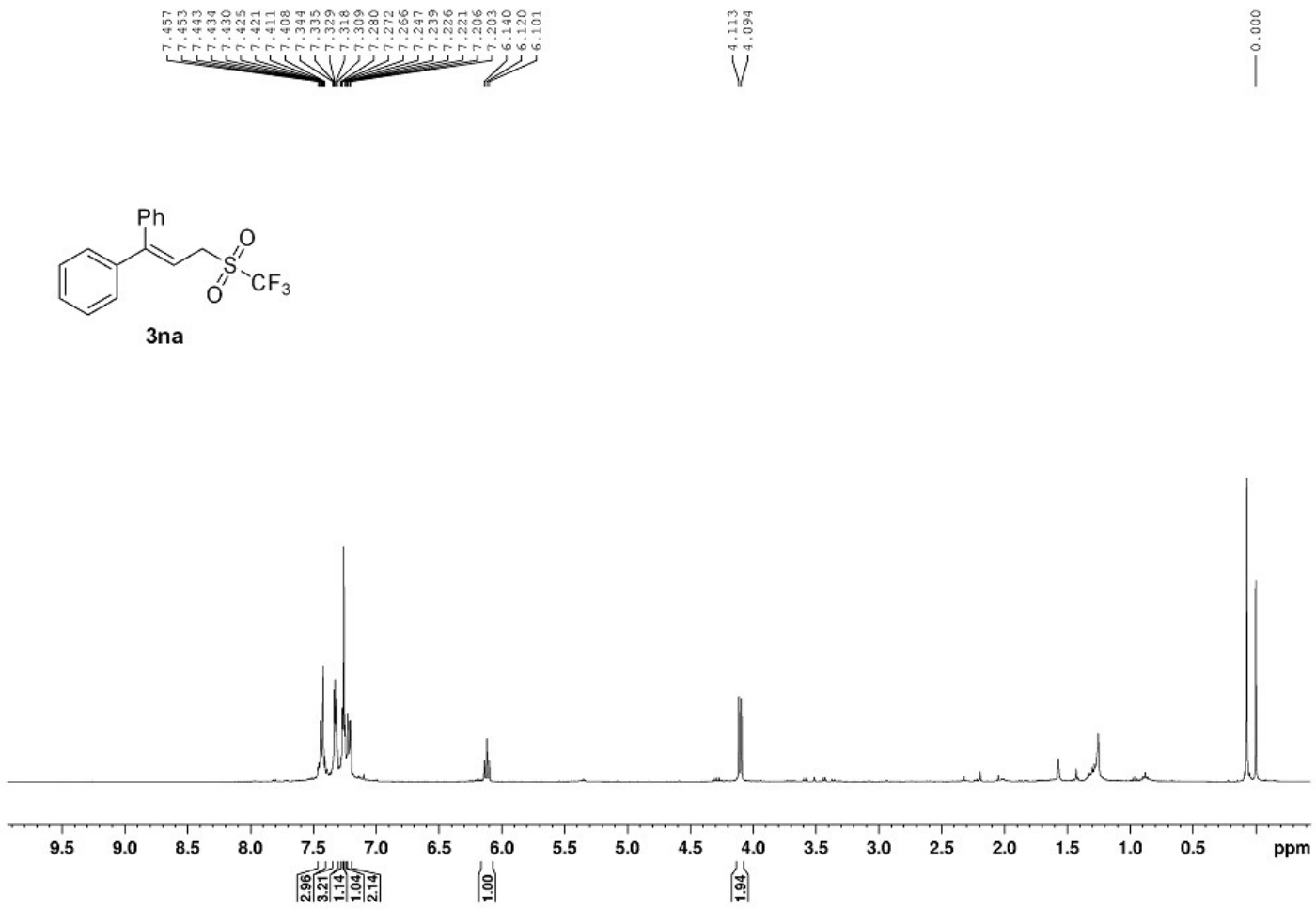
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.318
7.309
7.280
7.272
7.266
7.247
7.239
7.226
7.221
7.206
7.203
6.140
6.120
6.101
4.113
4.094
0.000
Ph
O
S
O
CF3
3na
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
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1.0
0.5
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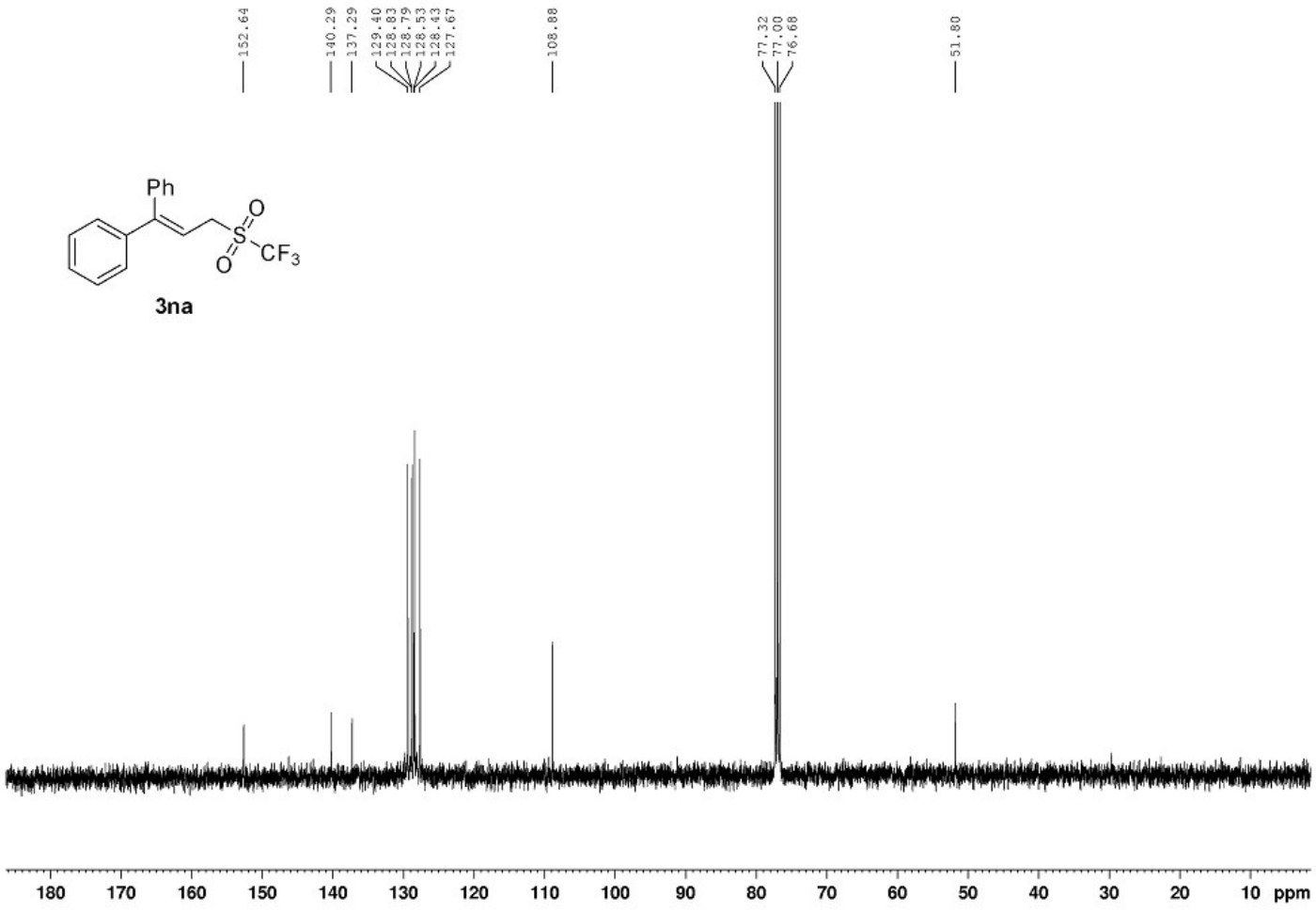
1.04
2.14
1.00
1.94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128.79
128.53
128.43
127.67
108.88
77.32
77.00
76.68
51.80
Ph
O
S
O
CF3
3na
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170
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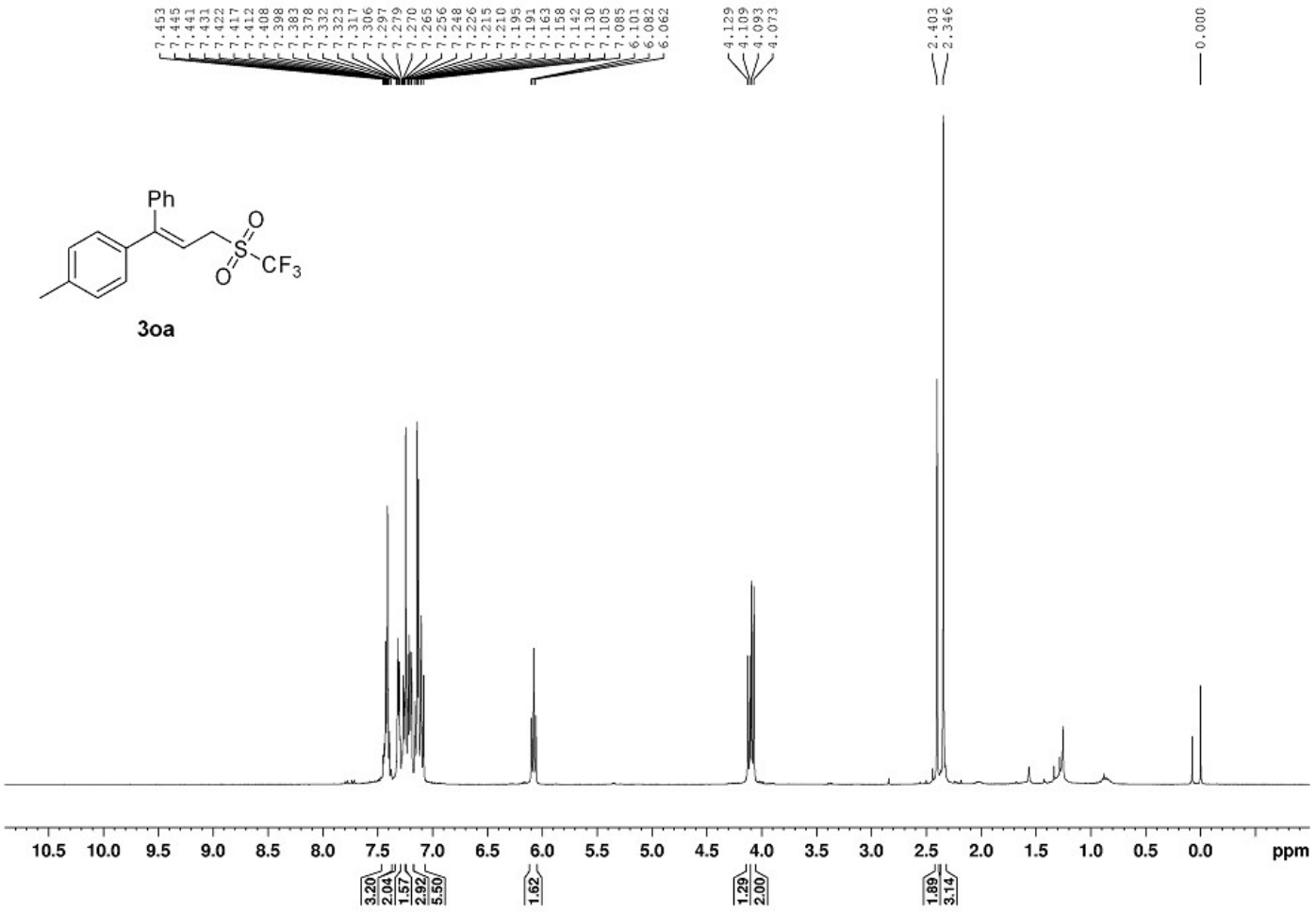
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.417
7.412
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7.398
7.383
7.378
7.332
7.323
7.317
7.306
7.297
7.279
7.270
7.265
7.256
7.248
7.226
7.215
7.210
7.195
7.191
7.163
7.158
7.142
7.130
7.105
7.085
6.101
6.082
6.062
4.129
4.109
4.093
4.073
2.403
2.346
0.000
Ph
O
S
O
CF3
3oa
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 ppm
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1.62
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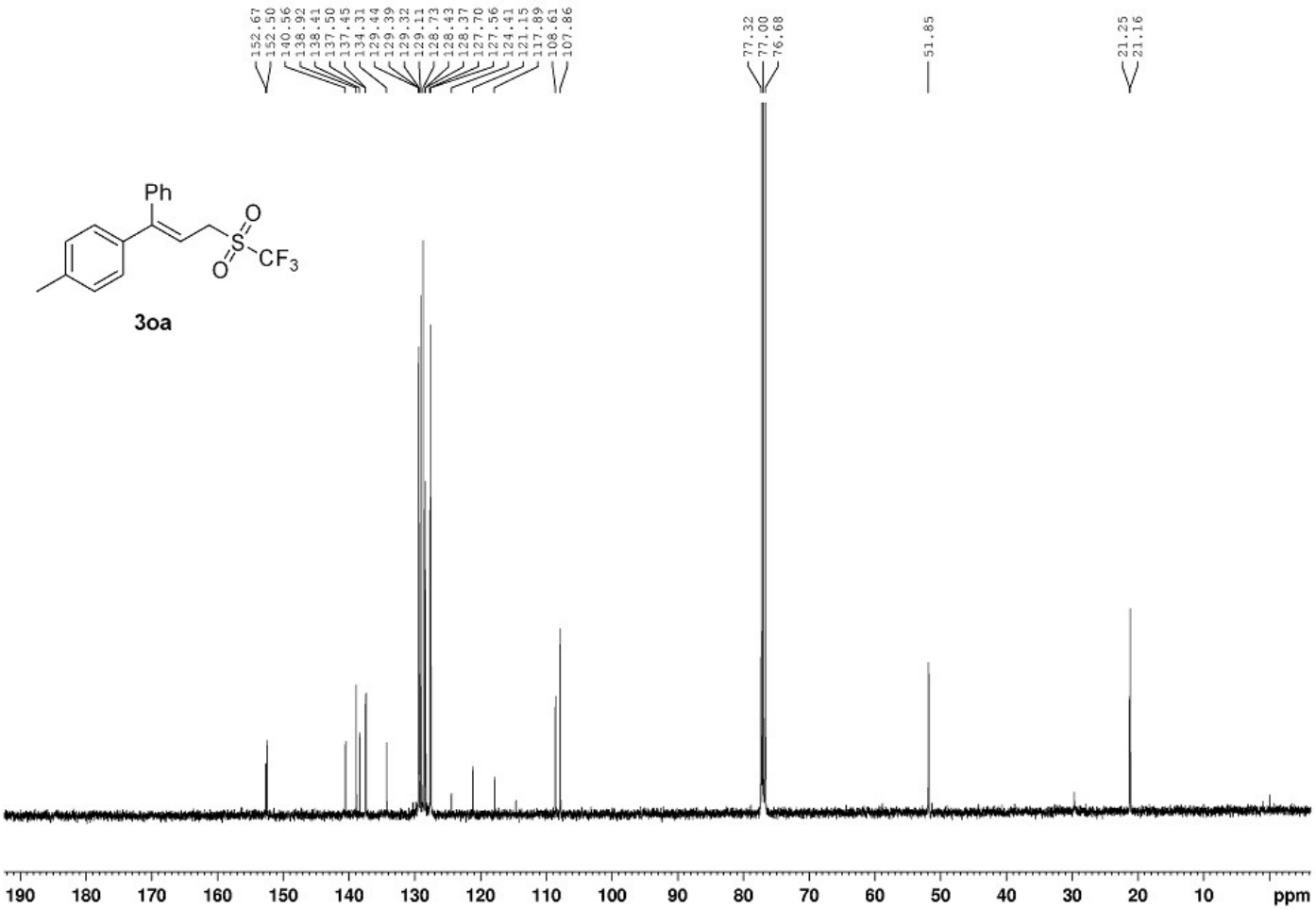
1.89
3.14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134.31
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128.43
128.37
127.70
127.56
124.41
121.15
117.89
108.61
107.86
77.32
77.00
76.68
51.85
21.25
21.16
Ph
O
S
O
CF3
3oa
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150
140
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120
110
100
90
80
70
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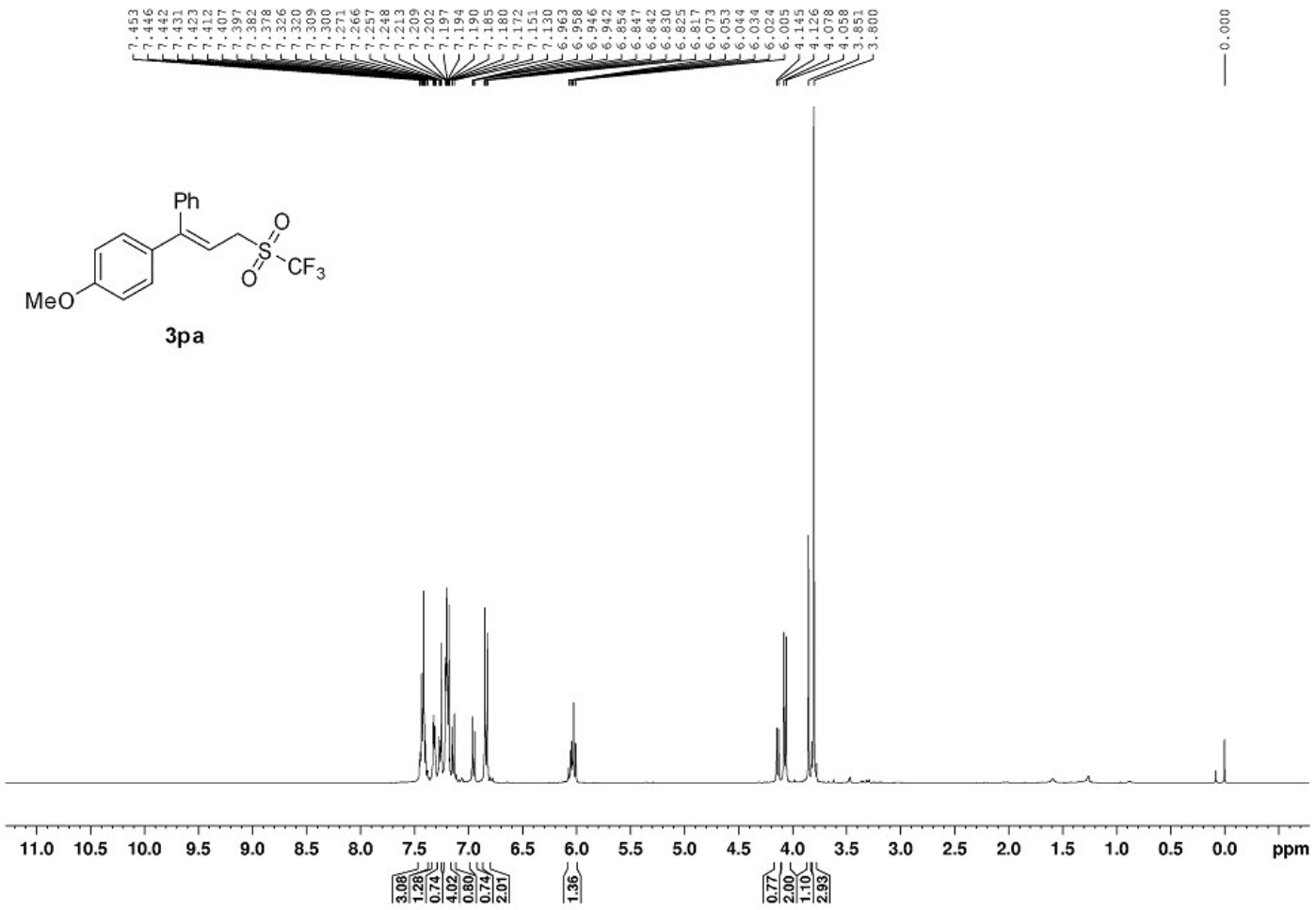
30
20
10
ppm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7.397
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7.320
7.309
7.300
7.271
7.266
7.257
7.248
7.213
7.209
7.202
7.197
7.194
7.190
7.185
7.180
7.172
7.151
7.130
6.963
6.958
6.946
6.942
6.854
6.847
6.842
6.830
6.825
6.817
6.073
6.053
6.044
6.034
6.024
6.005
4.145
4.126
4.078
4.058
3.851
3.800
0.000
Ph
MeO
O
O
S
CF3
3pa
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 ppm
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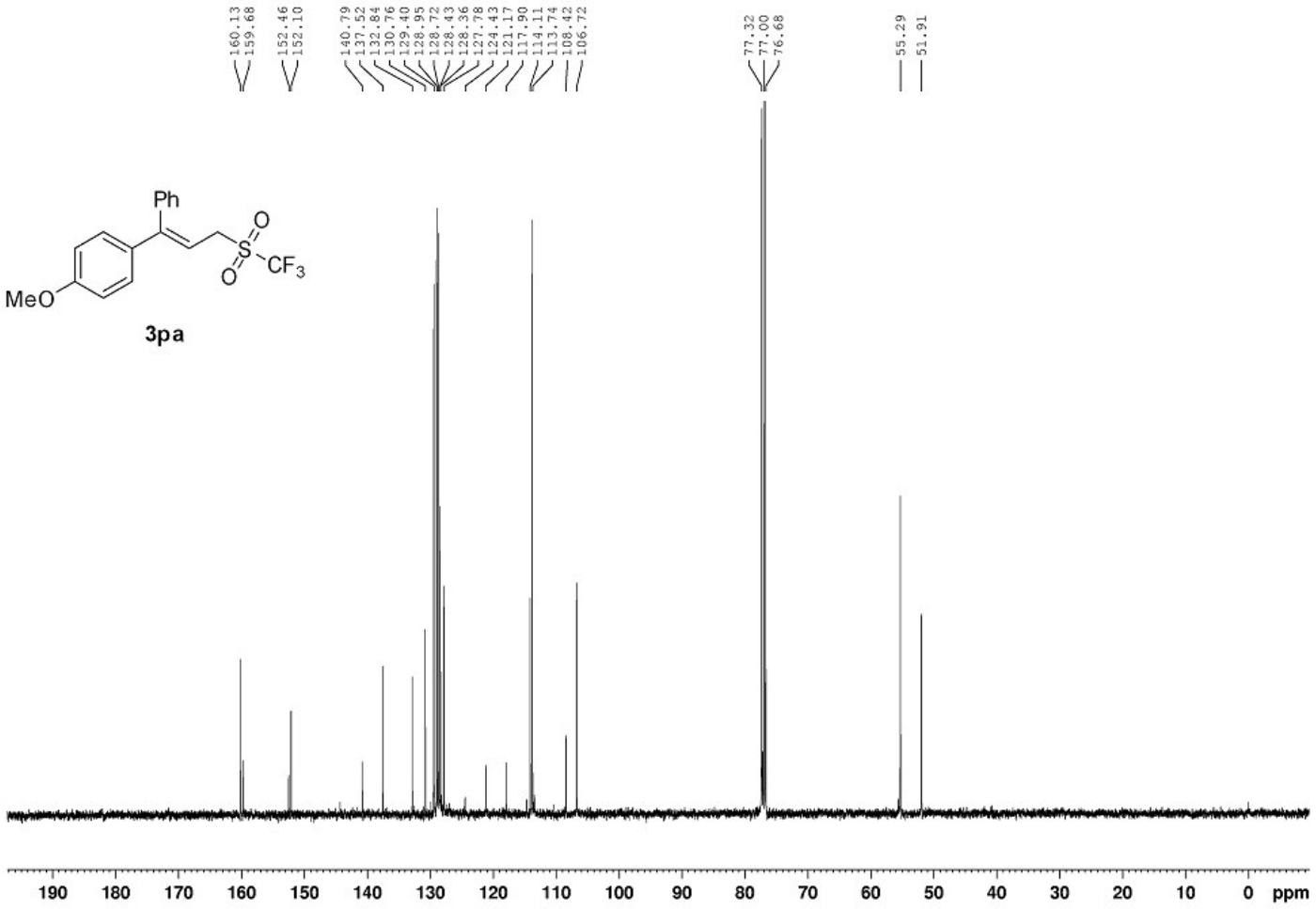
0.74
4.02
0.80
0.74
2.01
1.36
0.77
2.00
1.10
2.93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128.43
128.36
127.78
124.43
121.17
117.90
114.11
113.74
108.42
106.72
77.32
77.00
76.68
55.29
51.91
Ph
O
S
O
CF3
MeO
3pa
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180
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140
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120
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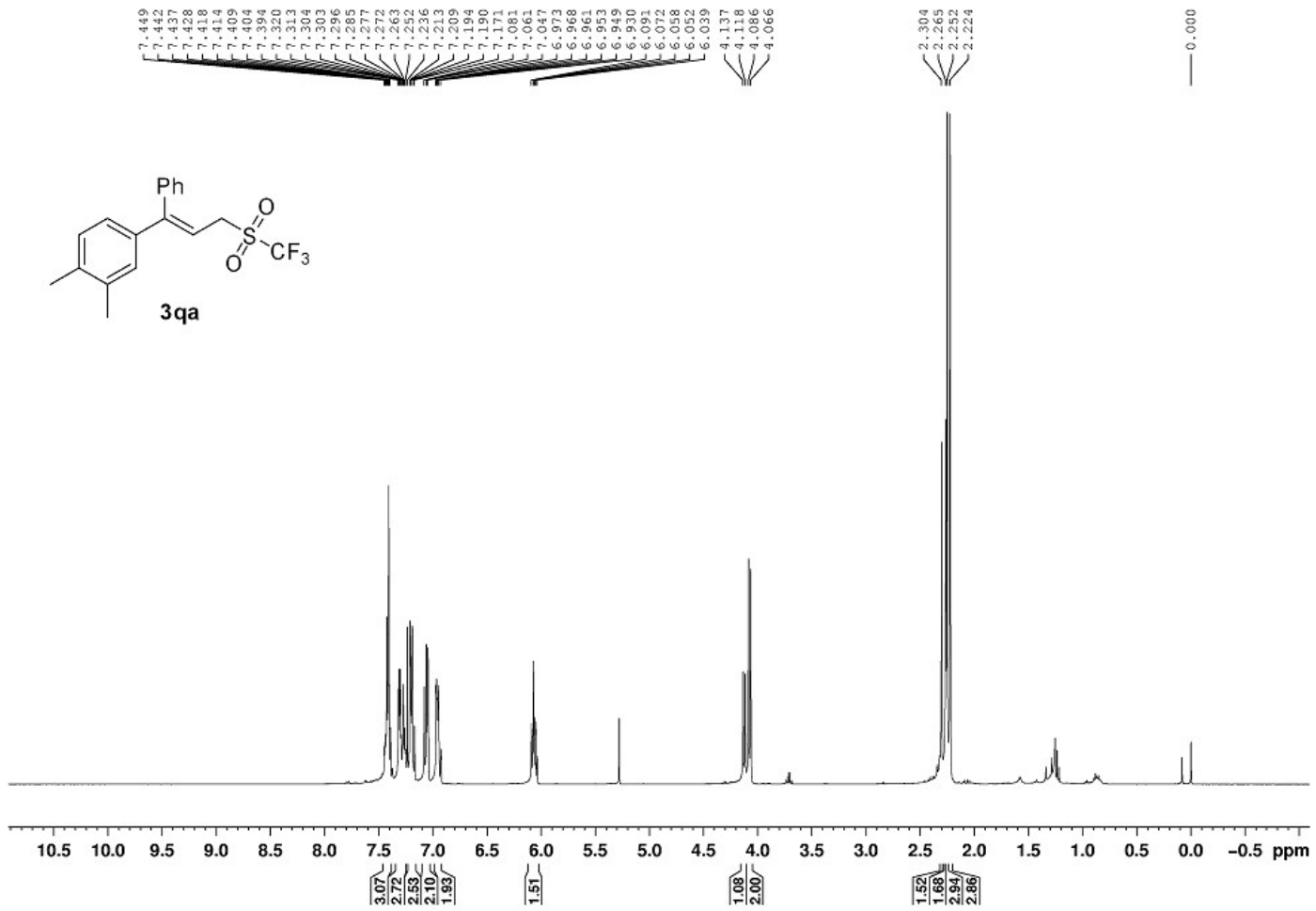
20
10
0
ppm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7.409
7.404
7.394
7.320
7.313
7.304
7.303
7.296
7.285
7.277
7.272
7.263
7.252
7.236
7.213
7.209
7.194
7.190
7.171
7.081
7.061
7.047
6.973
6.968
6.961
6.953
6.949
6.930
6.091
6.072
6.058
6.052
6.039
4.137
4.118
4.086
4.066
2.304
2.265
2.252
2.224
0.000
Ph
O
S
O
CF3
3qa
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 ppm
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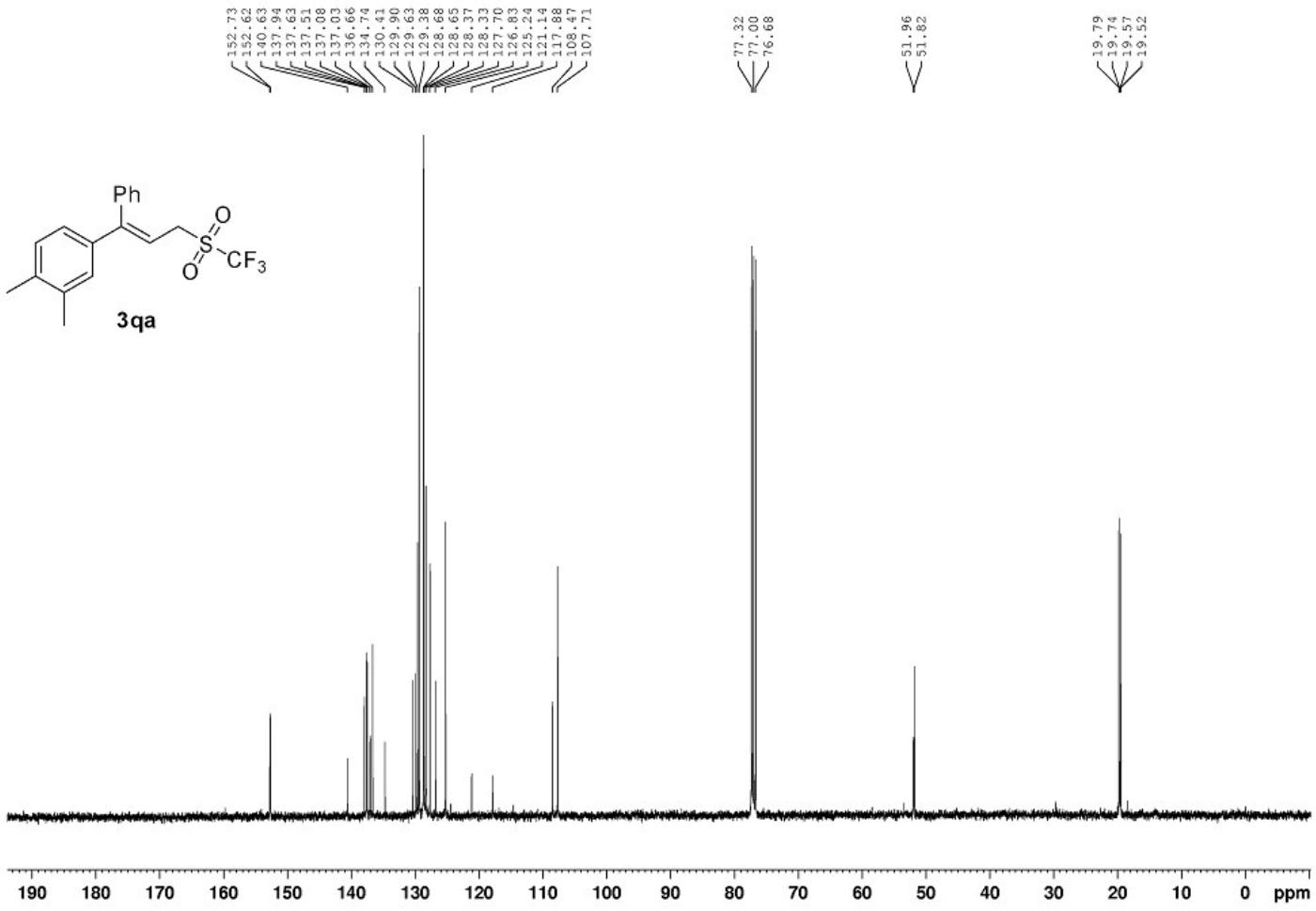
2.72
2.53
2.10
1.93
1.51
1.08
2.00
1.52
1.68
2.94
2.86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137.51
137.08
137.03
136.66
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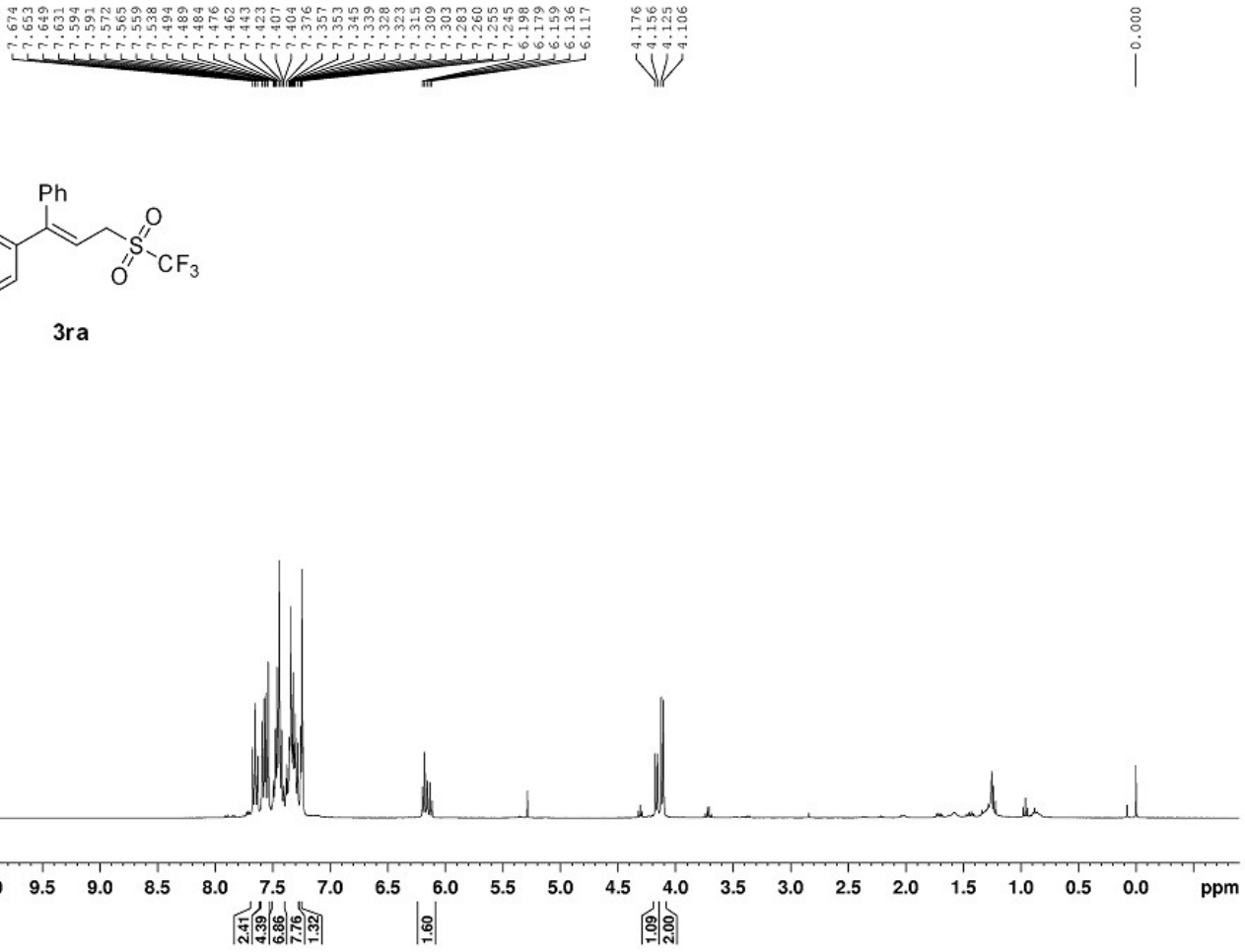
130.41
129.90
129.63
129.38
128.68
128.65
128.37
128.33
127.70
126.83
125.24
121.14
117.88
108.47
107.71
77.32
77.00
76.68
51.96
51.82
19.79
19.74
19.57
19.52
Ph
O
O
S
O
CF3
3qa
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm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7.631
7.594
7.591
7.572
7.565
7.559
7.538
7.494
7.489
7.484
7.476
7.462
7.443
7.423
7.407
7.404
7.376
7.357
7.353
7.345
7.339
7.328
7.323
7.315
7.309
7.303
7.283
7.260
7.255
7.245
6.198
6.179
6.159
6.136
6.117
4.176
4.156
4.125
4.106
0.000
Ph
Ph
O
S
O
CF3
3ra
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
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0.0
ppm
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4.39
6.86
7.76
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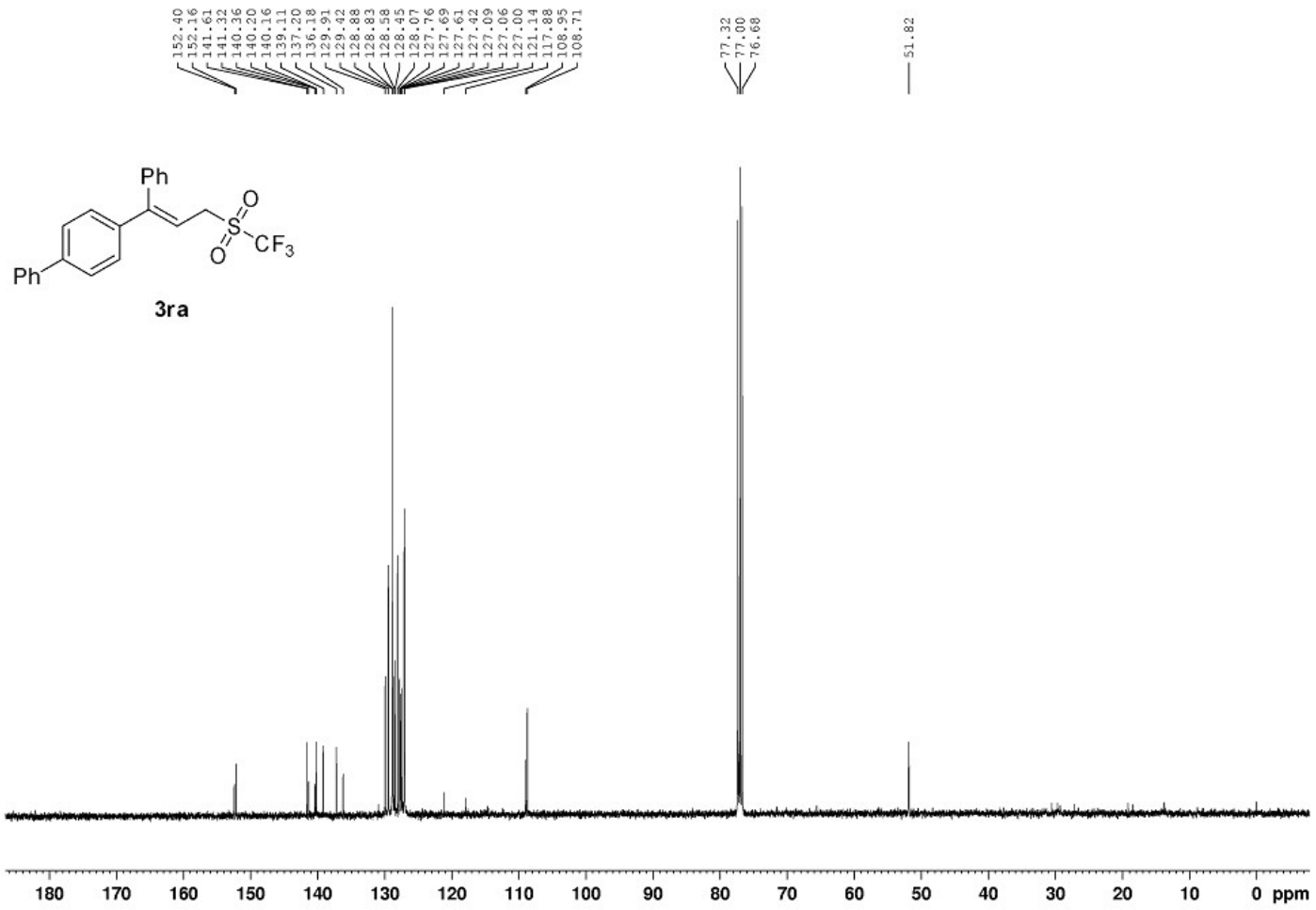
1.60
1.09
2.00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152.16
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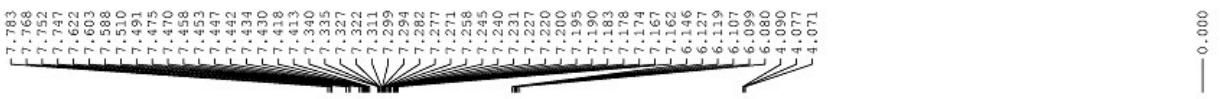
140.20
140.16
139.11
137.20
136.18
129.91
129.42
128.88
128.83
128.58
128.45
128.07
127.76
127.69
127.61
127.42
127.09
127.06
127.00
121.14
117.88
108.95
108.71
77.32
77.00
76.68
51.82
Ph
O
S
O
CF3
Ph
3ra
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm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7.622
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7.588
7.510
7.491
7.475
7.470
7.458
7.453
7.447
7.442
7.434
7.430
7.418
7.413
7.340
7.335
7.327
7.322
7.311
7.299
7.294
7.282
7.277
7.271
7.258
7.245
7.240
7.231
7.227
7.220
7.200
7.195
7.190
7.183
7.178
7.174
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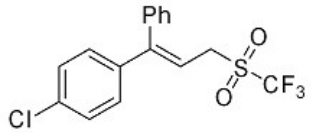
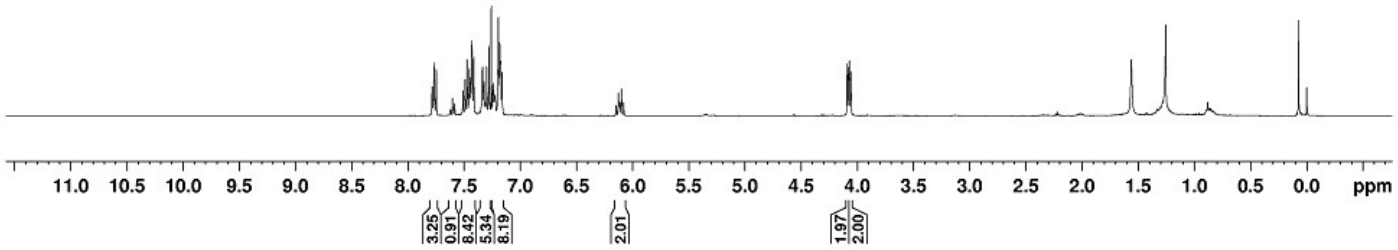
7.162
6.146
6.127
6.119
6.107
6.099
6.080
4.090
4.077
4.071
0.000


Ph
O
S
O
CF3
Cl

3sa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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
ppm
3.25
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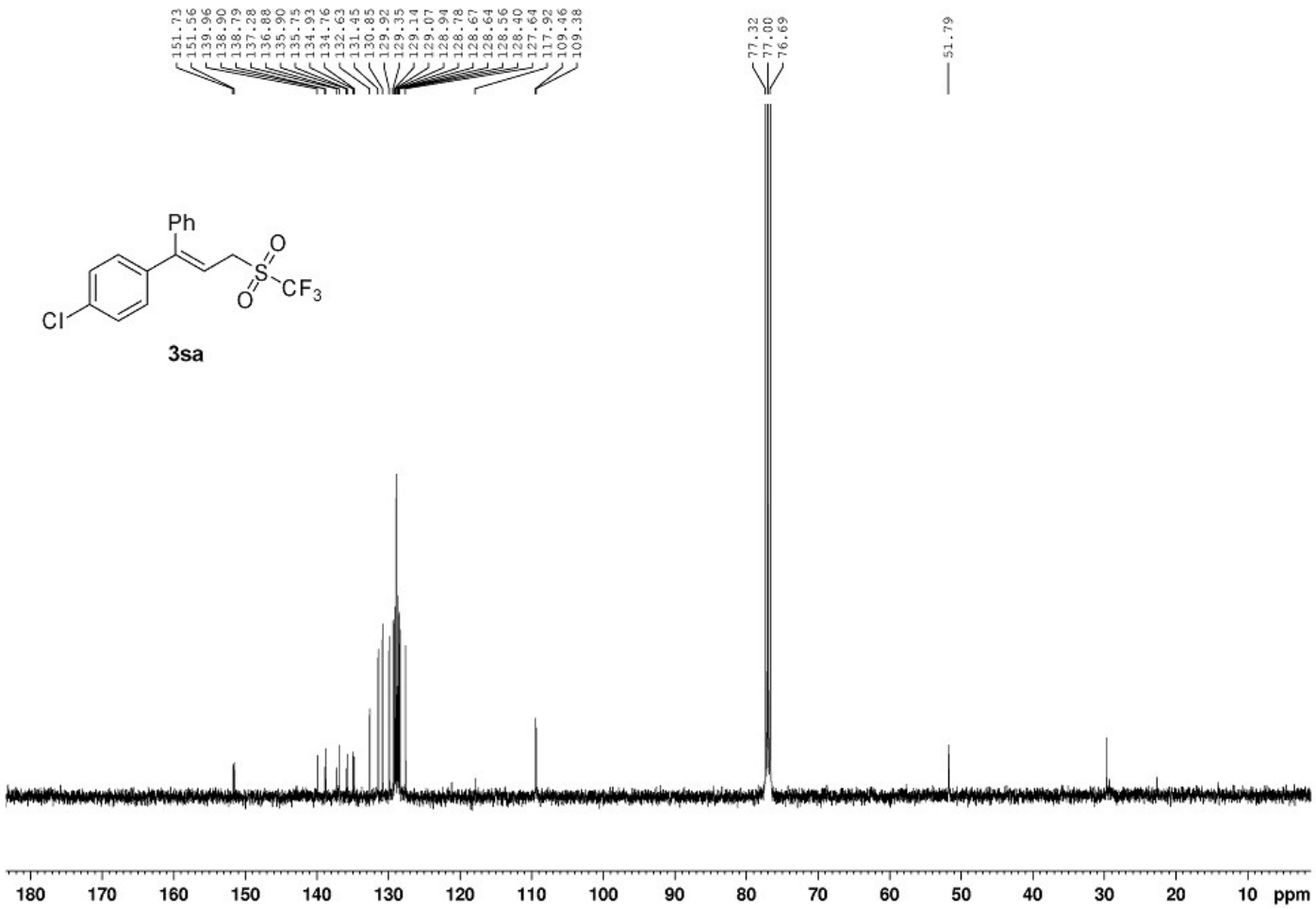
5.34
8.19
2.01
1.97
2.00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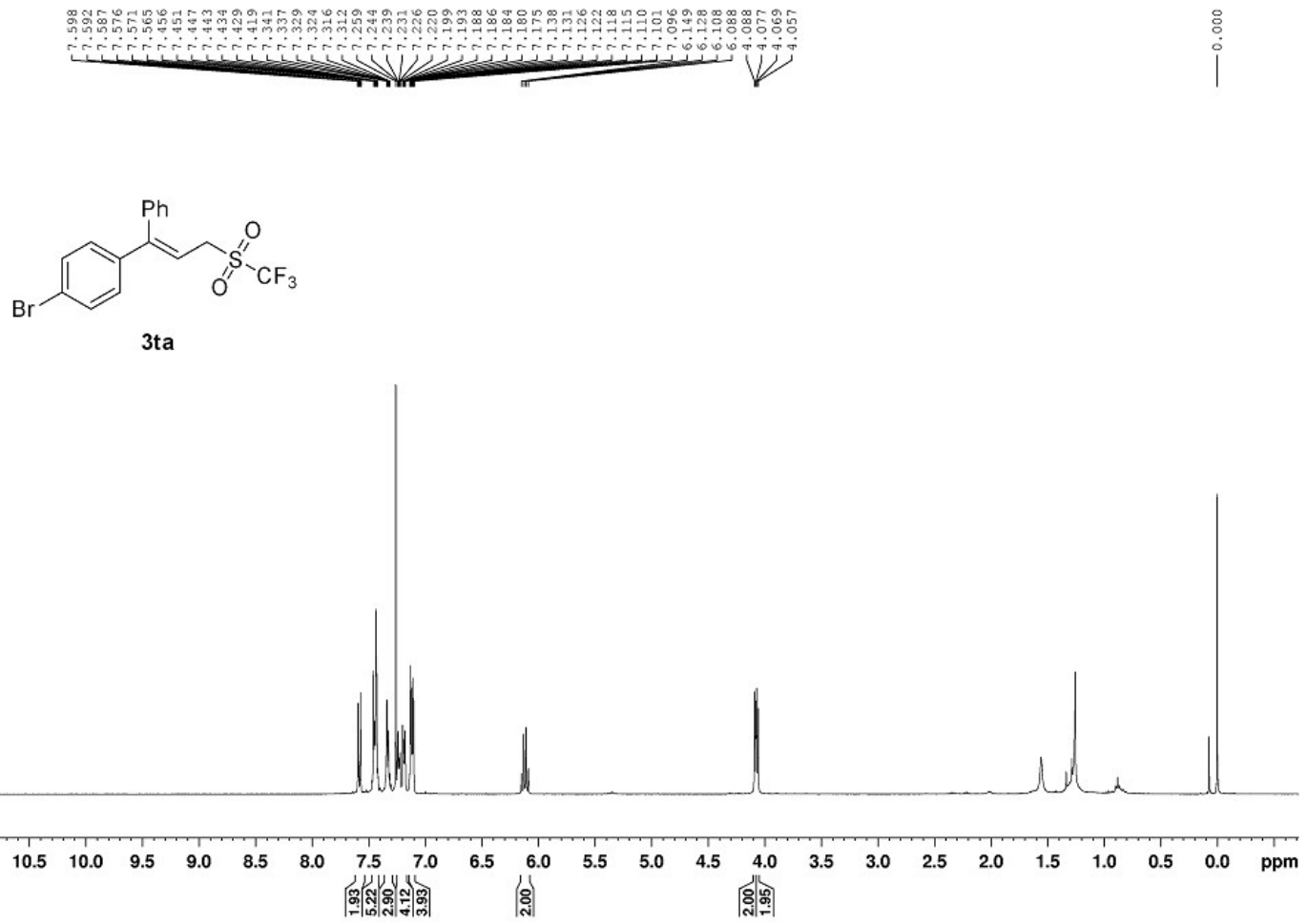
151.56
139.96
138.90
138.79
137.28
136.88
135.90
135.75
134.93
134.76
132.63
131.45
130.85
129.92
129.35
129.14
129.07
128.94
128.78
128.67
128.64
128.56
128.40
127.64
117.92
109.46
109.38
77.32
77.00
76.69
51.79
Ph
O
S
O
CF3
Cl
3sa
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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7.565
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7.451
7.447
7.443
7.434
7.429
7.419
7.341
7.337
7.329
7.324
7.316
7.312
7.259
7.244
7.239
7.231
7.226
7.220
7.199
7.193
7.188
7.186
7.184
7.180
7.175
7.138
7.131
7.126
7.122
7.118
7.115
7.110
7.101
7.096
6.149
6.128
6.108
6.088
4.088
4.077
4.069
4.057
0.000
Ph
O
S
O
CF3
Br
3ta
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
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0.0
ppm
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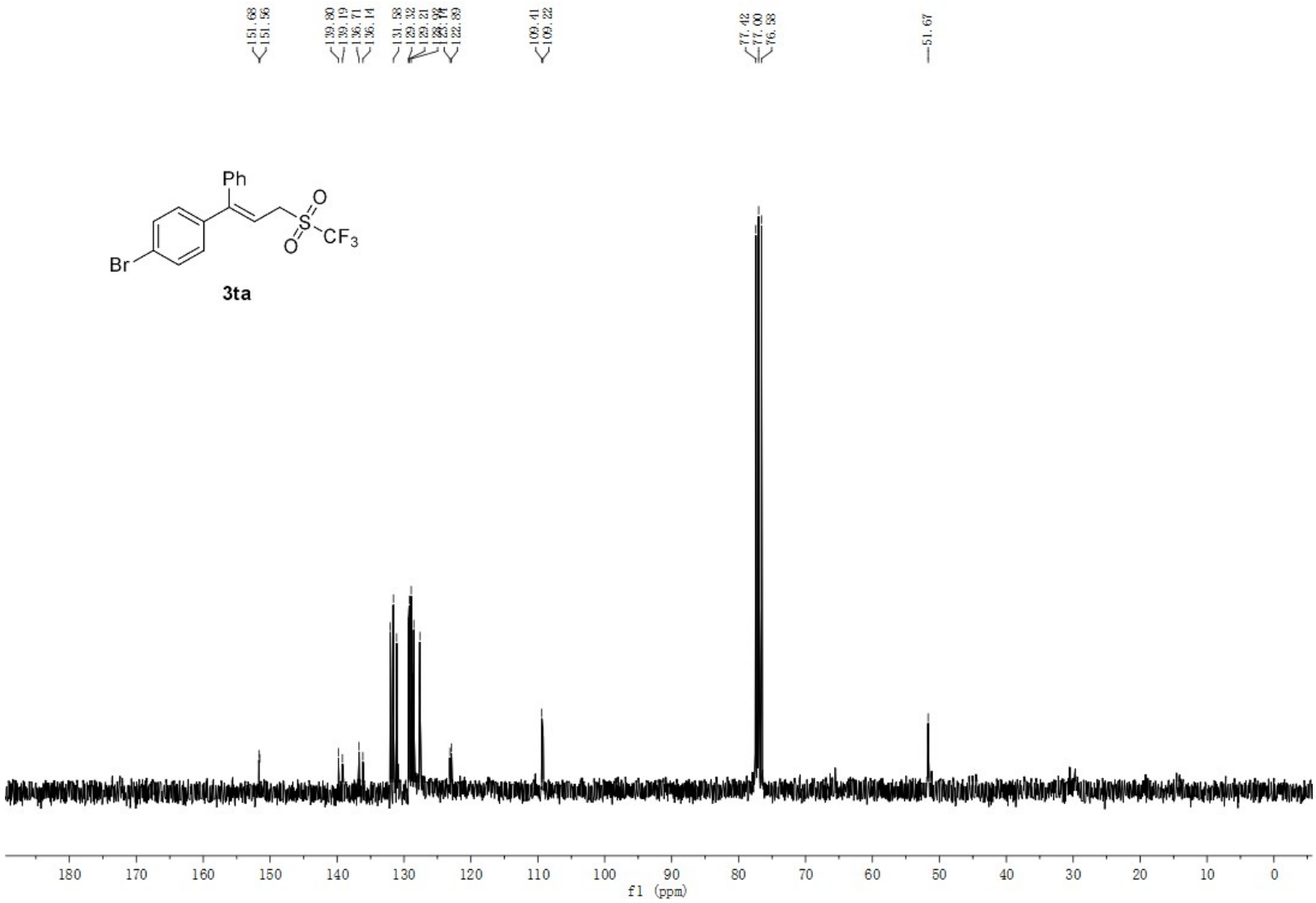
2.90
4.12
3.93
2.00
2.00
1.95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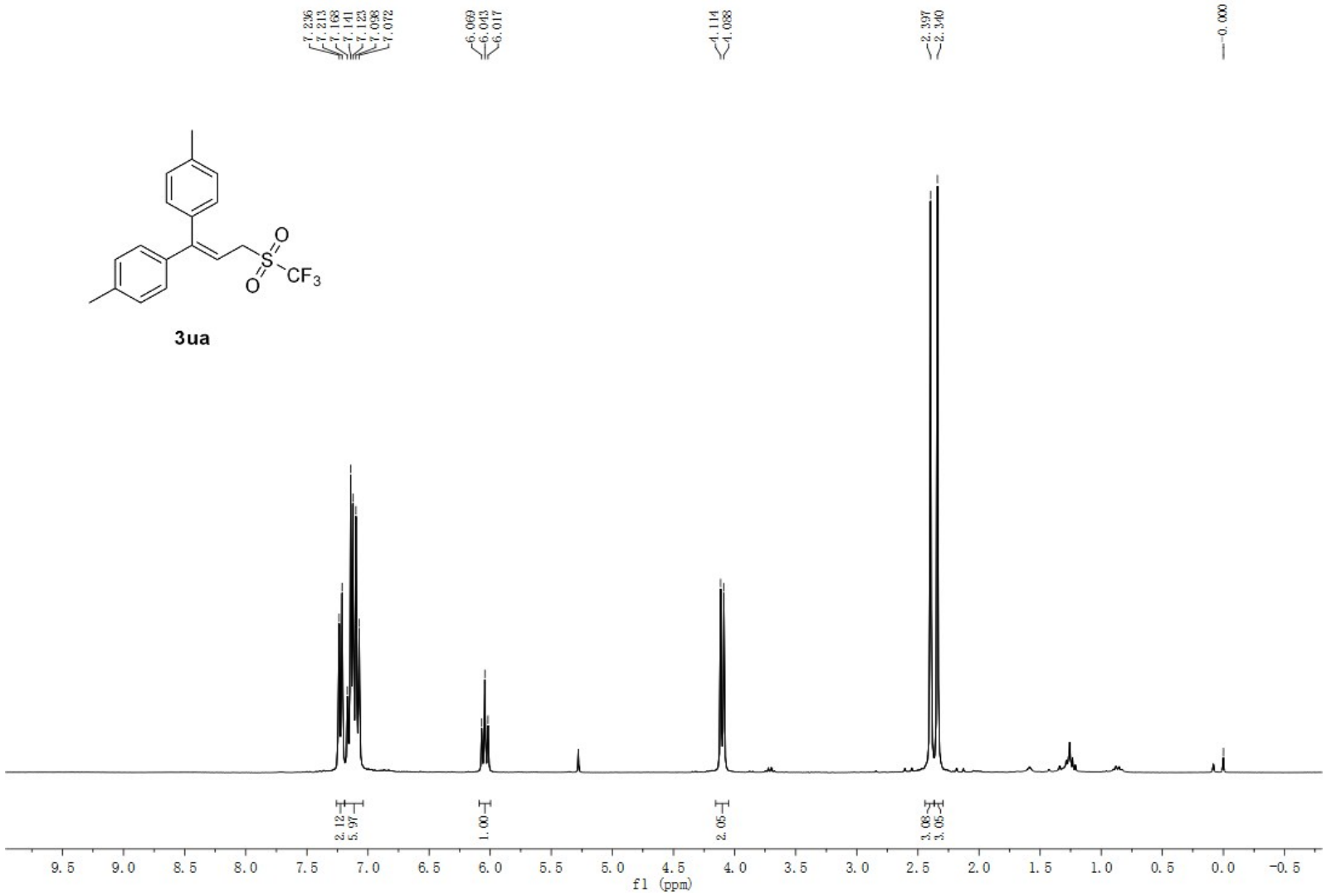
136.14
131.58
129.32
129.21
122.89
109.41
109.22
77.42
77.00
76.58
51.67
Ph
O
S
O
CF3
Br
3ta
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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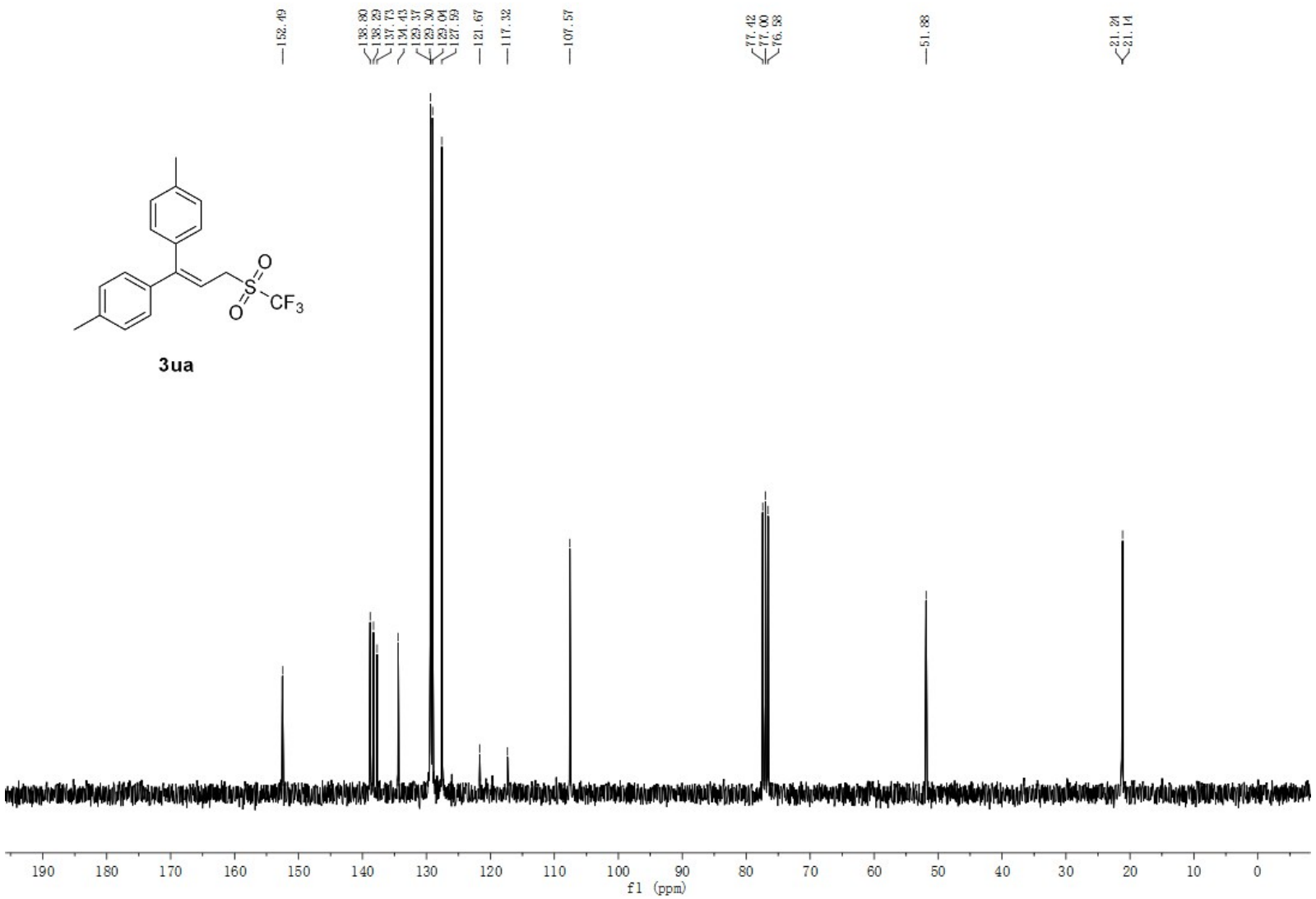
7.072
6.069
6.043
6.017
4.114
4.088
2.397
2.340
0.000
O
O
S
CF3
3ua
2.12
5.97
1.00
2.05
3.08
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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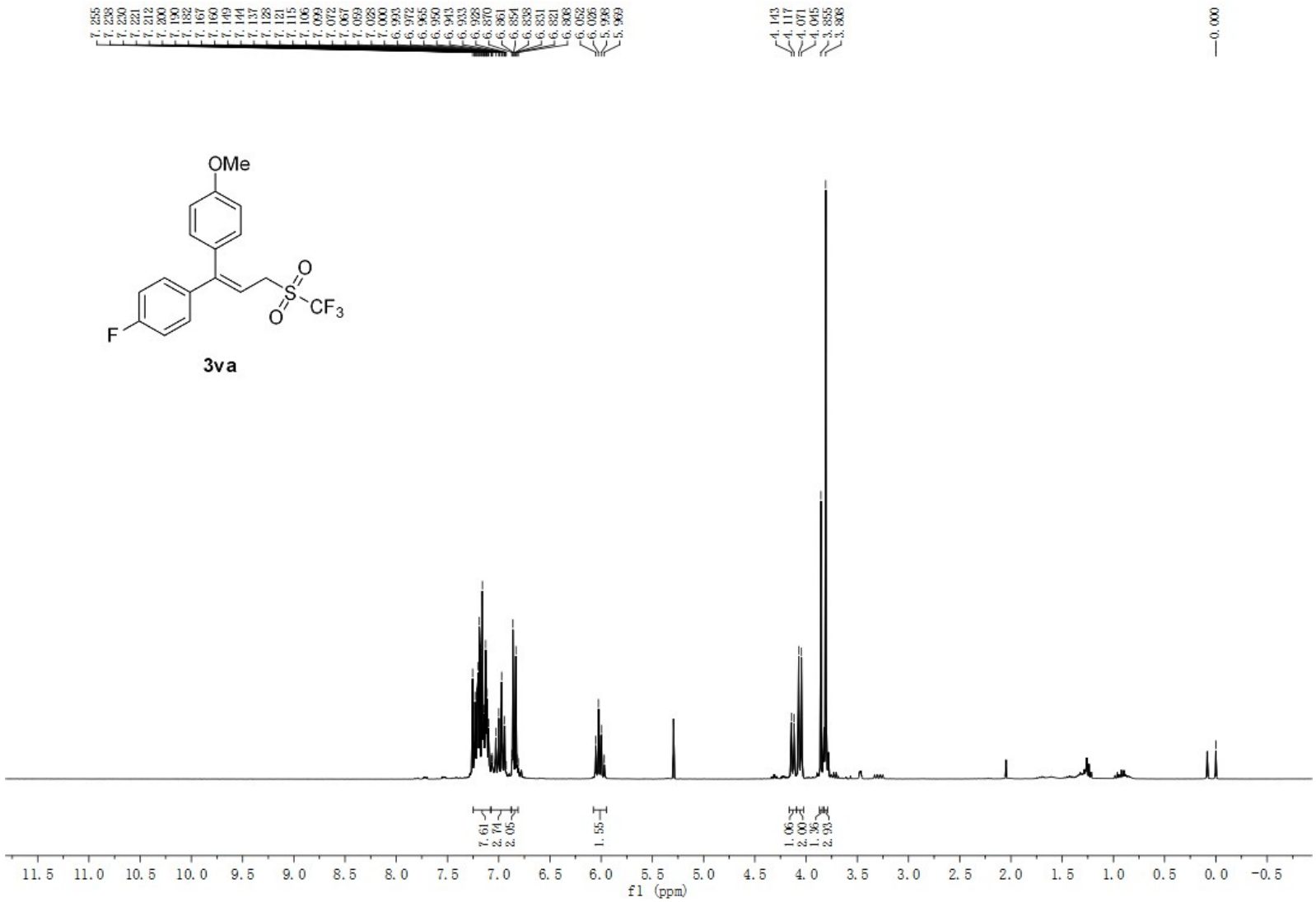
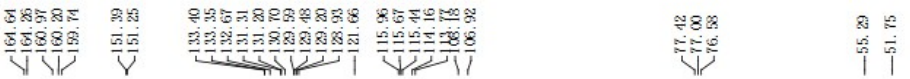
137.13
134.43
129.37
129.30
129.04
127.59
121.67
117.32
107.57
77.42
77.00
76.58
51.88
21.21
21.14
O
O
S
CF3
3ua
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


OMe
F
O
O
S
CF3
3va
fl (ppm)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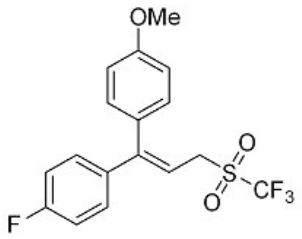
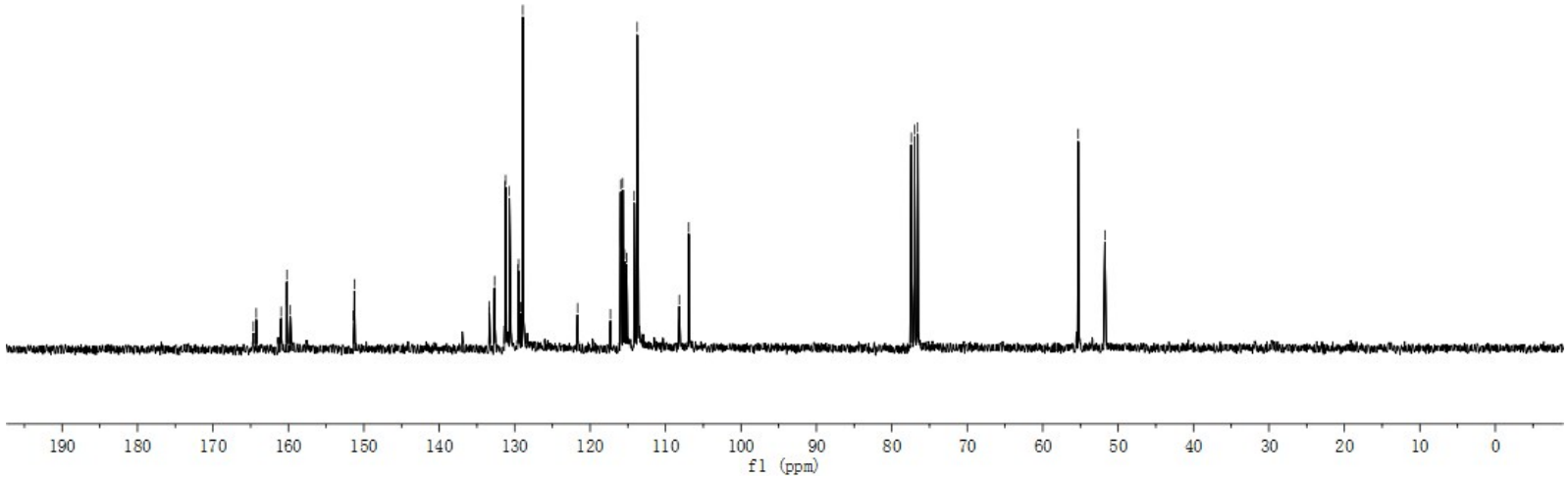
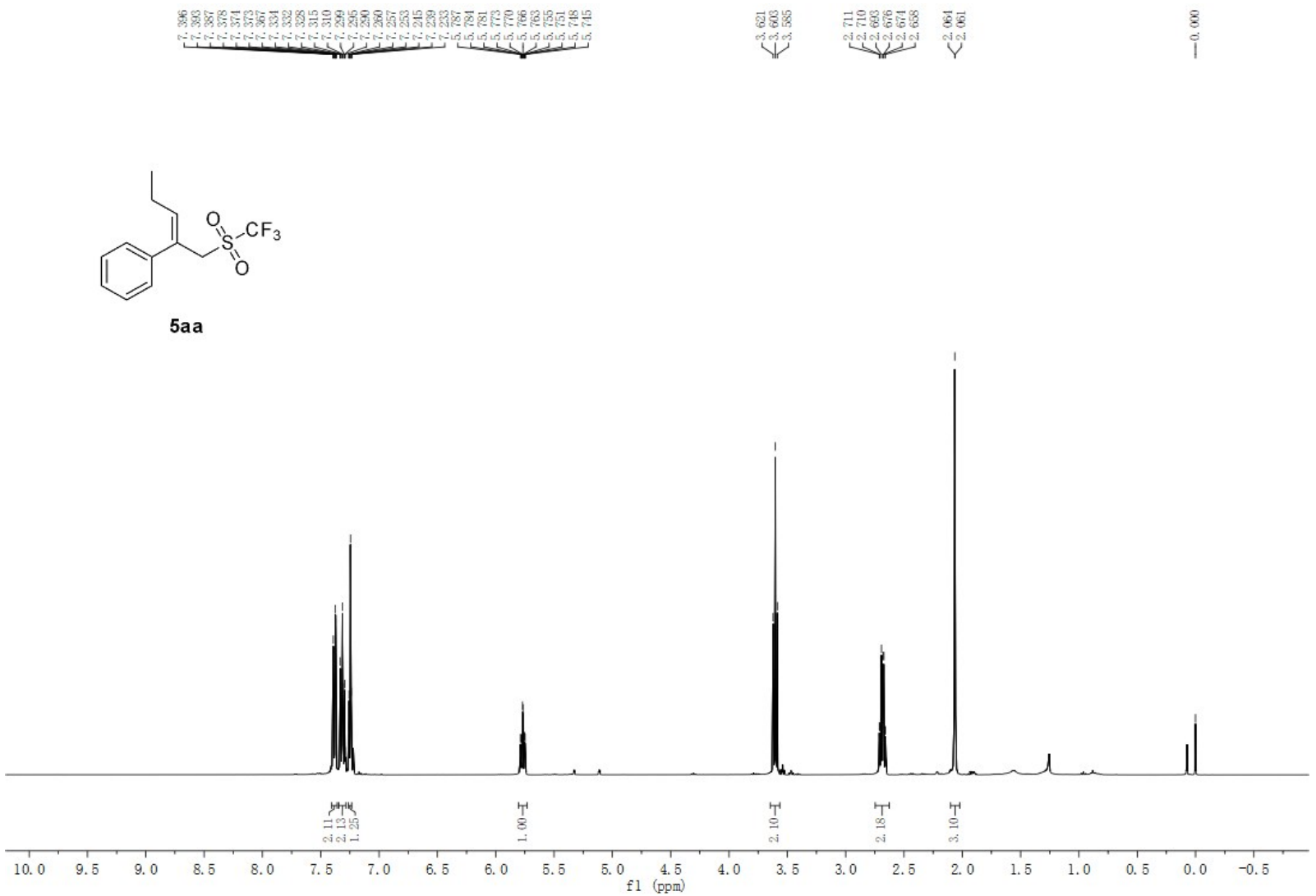
159.74
151.39
151.25
133.40
133.35
132.67
131.31
131.20
130.70
129.59
129.48
129.20
128.93
121.66
115.96
115.67
115.44
114.16
113.73
113.18
106.92
77.42
77.00
76.58
55.29
51.75


OMe
O
S
O
CF3
F

3va


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.374
7.373
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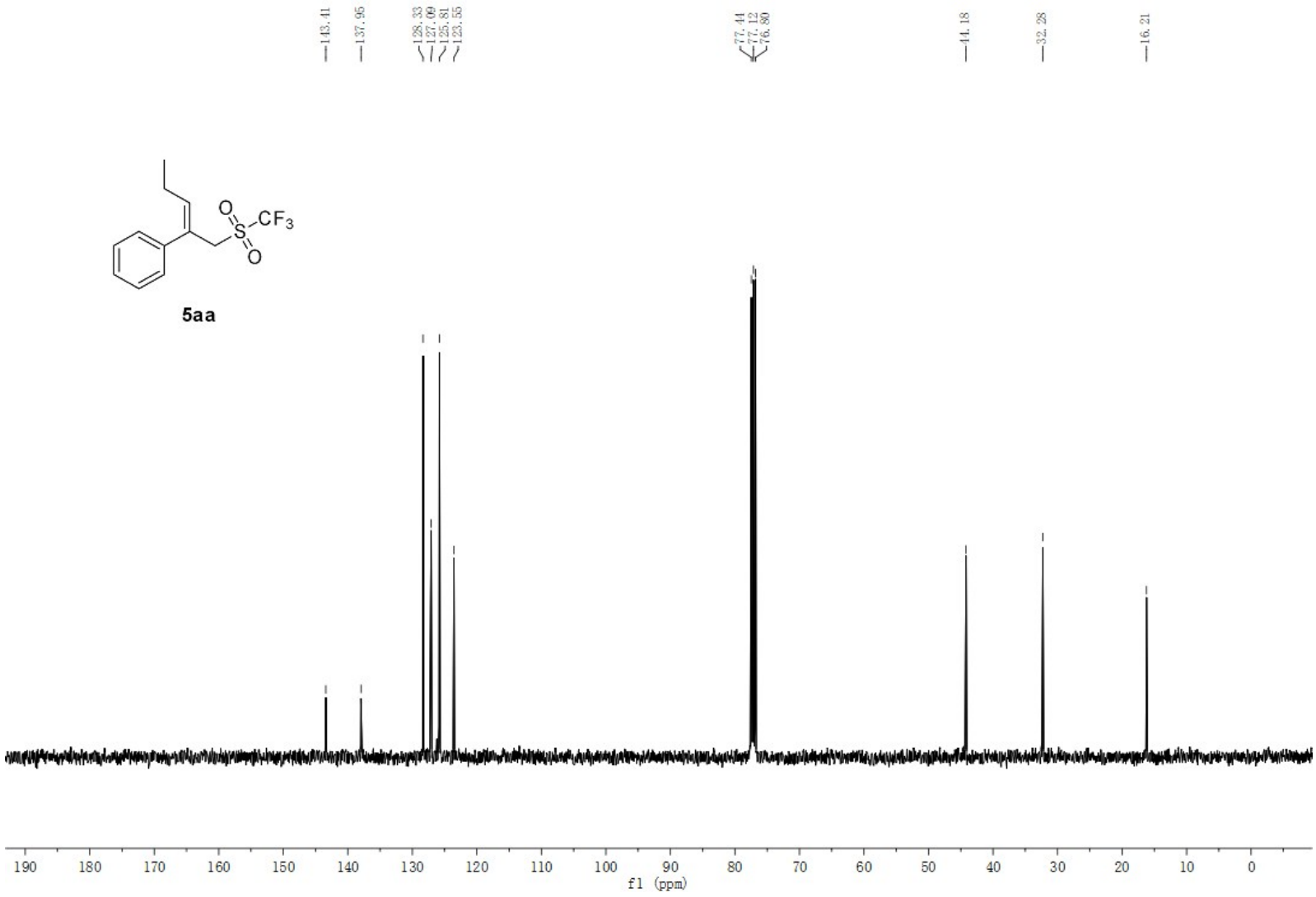
7.334
7.332
7.328
7.315
7.310
7.299
7.295
7.290
7.260
7.257
7.253
7.245
7.239
7.233
5.787
5.784
5.781
5.773
5.770
5.766
5.763
5.755
5.751
5.748
5.745
3.621
3.603
3.585
2.711
2.710
2.693
2.676
2.674
2.658
2.064
2.061
0.000
O
S
CF3
O
5aa
2.11
2.13
1.25
1.00
2.10
2.18
3.10
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
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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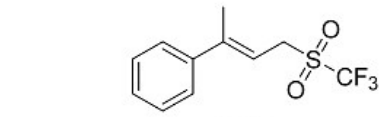
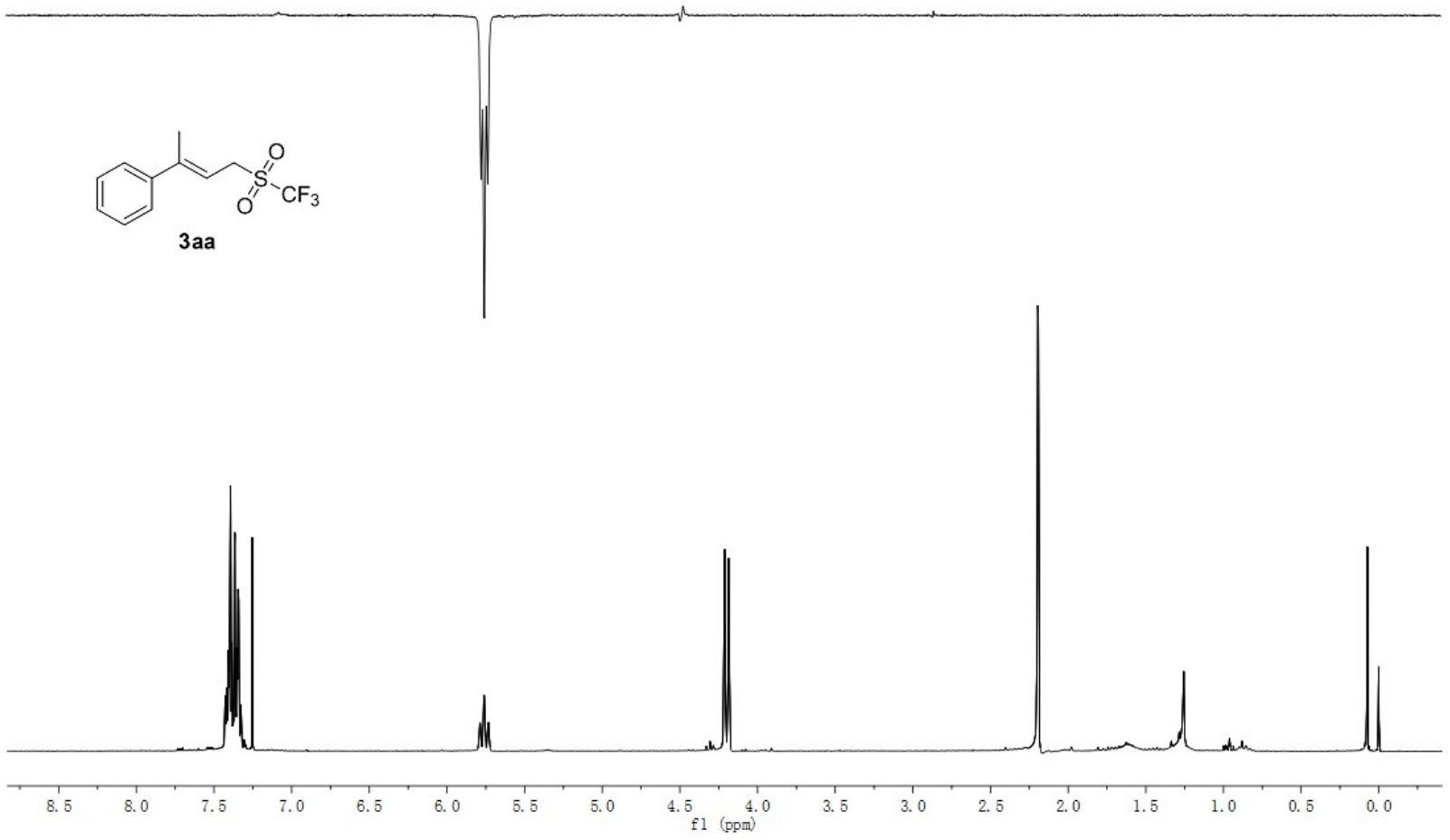
137.95
128.33
127.09
125.81
123.55
77.44
77.12
76.80
44.18
32.28
16.21
O
S
CF3
O
5aa
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



3aa


O
S
O
CF3
3aa
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)