Electronic Supplementary Information

Visible-Light-Driven Regioselective Carbocarboxylation of 1,3-Dienes with Organic Halides and CO_2

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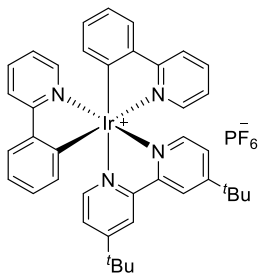
1. General Information

Unless otherwise noted, commercial available reagents were purchased from commercial suppliers (such as Strem, Alfa Aesar, J&K Chemical Co., Energy Chemical, Bide Pharmatech Ltd. and Adamas) and used as received. Solvents were generally dried over 4Å molecular sieves. Purification of products was performed by flash chromatography (FC) using silica gel or preparative thin layer chromatography. ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AVANCE III spectrometer (400 MHz and 101 MHz, respectively). Chemical shifts are reported parts per million (ppm) referenced to $CDCl_3$ (δ 7.26 ppm), tetramethylsilane (TMS, δ 0.00 ppm) for ^{1}H NMR; $CDCl_3$ (δ 77.16 ppm) for ^{13}C NMR. The following abbreviations (or combinations thereof) were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = doublet of doublet, td = triplet of doublet and m = multiplet,. To distinguish, some ^{13}C NMR chemical shifts retain two decimal places. High-resolution mass spectra (HRMS) were obtained on an Impact II UHR-TOF mass spectrometry equipped with an ESI source from Bruker at Fujian Institute of Research on the Structure of Matter. The Blue LED strips (1 meter, 30W) were purchased from Prime LED Co., Ltd. (China). CO_2 gas (Purity: 99.995%) was purchased from Linde.

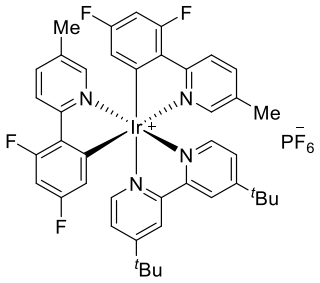
2. Experimental Section

2.1 Optimization of the reaction conditions

Photocatalysts:



PC1
$[Ir(ppy)_2(dtbbpy)]PF_6$



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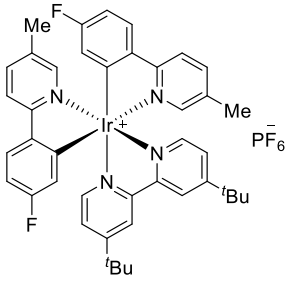
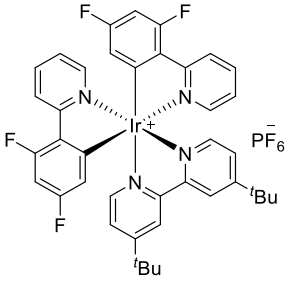
$[Ir(dF(Me)ppy)_2(dtbbpy)]PF_6$



PC3
$[Ir(FMppy)_2(dtbbpy)]PF_6$



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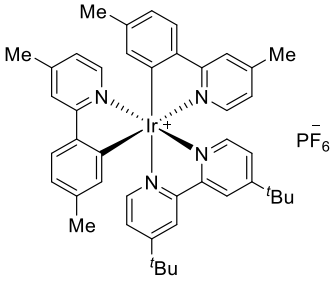
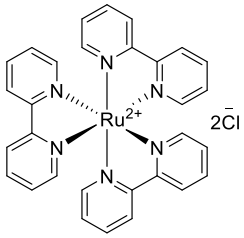
$[Ir(dFppy)_2(dtbbpy)]PF_6$

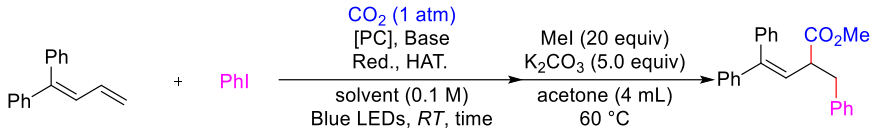


PC5
$[Ir(dMppy)_2(dtbbpy)]PF_6$



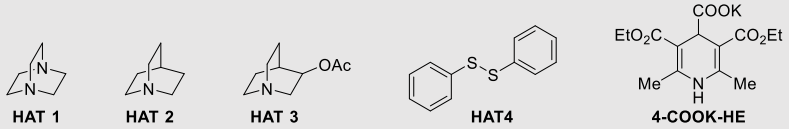
PC6
$Ru(bpy)_3Cl_2$

Table S1. Screening of the reaction conditions.



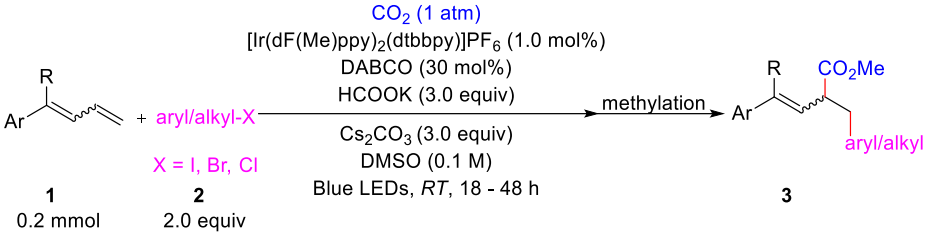
1a (0.2 mmo) **2a** (2.0 equiv) **3aa**

NO.	[PC] (2 mol%)	Base (3.0 eq.)	Red. (3.0 eq.)	HAT (0.5 eq.)	Solvent (0.1M)	time	Yield[a] (%)
1	**PC1**	K_2CO_3	HCOOK	**HAT 1**	DMSO	24 h	71
2	**PC2**	K_2CO_3	HCOOK	**HAT 1**	DMSO	24 h	74
3	**PC3**	K_2CO_3	HCOOK	**HAT 1**	DMSO	24 h	71
4	**PC4**	K_2CO_3	HCOOK	**HAT 1**	DMSO	24 h	71
5	**PC5**	K_2CO_3	HCOOK	**HAT 1**	DMSO	24 h	72
6	**PC6**	K_2CO_3	HCOOK	**HAT 1**	DMSO	24 h	74
7	**PC6**	^{t}BuOLi	HCOOK	**HAT 1**	DMSO	24 h	59
8	**PC6**	^{t}BuONa	HCOOK	**HAT 1**	DMSO	24 h	23
9	**PC6**	Na_2CO_3	HCOOK	**HAT 1**	DMSO	24 h	56
10	**PC6**	Cs_2CO_3	HCOOK	**HAT 1**	DMSO	24 h	75
11	**PC6**	Cs_2CO_3	HCOONa	**HAT 1**	DMSO	24 h	71
12	**PC6**	Cs_2CO_3	HCOOCs	**HAT 1**	DMSO	24 h	57
13	**PC6**	Cs_2CO_3	$(HCOO)_2Ca$	**HAT 1**	DMSO	24 h	7
14	**PC6**	Cs_2CO_3	4-COOK-HE	-	DMSO	24 h	67
15	**PC6**	Cs_2CO_3	DIPEA	-	DMSO	24 h	31
16	**PC6**	Cs_2CO_3	^{n}Bu$_3$N	-	DMSO	24 h	22
17	**PC6**	Cs_2CO_3	HCOOK	**HAT 2**	DMSO	24 h	trace
18	**PC6**	Cs_2CO_3	HCOOK	**HAT 3**	DMSO	24 h	n.d.
19	**PC6**	Cs_2CO_3	HCOOK	**HAT 4**	DMSO	24 h	trace
[c]**20**	**PC6**	Cs_2CO_3	HCOOK	**HAT 1**	DMSO	24 h	75
[c]**21**	**PC6**	Cs_2CO_3	HCOOK	**HAT 1**	DMF	24 h	8
[c]**22**	**PC6**	Cs_2CO_3	HCOOK	**HAT 1**	DMA	24 h	6
[c]**23**	**PC6**	Cs_2CO_3	HCOOK	**HAT 1**	MeCN	24 h	trace
[c]**24**	**PC6** (1mol%)	Cs_2CO_3	HCOOK	**HAT 1**	DMSO	24 h	75
[c]**25**	**PC6** (1mol%)	Cs_2CO_3	HCOOK	**HAT 1**	DMSO	12 h	71
[c]**26**	**PC6** (1mol%)	Cs_2CO_3	HCOOK	**HAT 1**	DMSO	18 h	80
[c]**27**	**PC1** (1mol%)	Cs_2CO_3	HCOOK	**HAT 1**	DMSO	18 h	80
[c]**28**	**PC2** (1mol%)	Cs_2CO_3	HCOOK	**HAT 1**	DMSO	18 h	93(79)[b]



[a]Yield was determined by ^{1}H NMR with CH_2Br_2 as internal standard. [b]Isolated yield. [c]30 mol% **HAT 1** (DABCO) was used.

2.2 General procedures for synthesis of products



General procedure A:

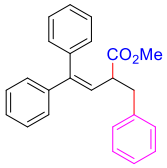
The oven-dried Schlenk tube (25 mL) containing a stirring bar was charged with substrates **1** (0.2 mmol, 1.0 equiv), **2** (0.4 mmol, 2.0 equiv) and Ir[(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$ (1 mol%) in the air. Then the tube was moved into a glovebox and charged with DABCO (30 mol%), HCOOK (3.0 equiv) and Cs_2CO_3 (3.0 equiv). The tube was sealed and evacuated and back-filled with CO_2 three times. Subsequently, the degassed anhydrous DMSO (2 mL, 0.1 M) was added into the tube via syringe. Then the tube was evacuated and back-filled with CO_2 for 10 times. Finally, the mixture was placed under a 30 W blue LEDs (λ_{max}=465 nm, 3.0 cm - 4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25 - 40 °C) light source and stirred at ambient temperature for 18 - 48 h. Upon completion of the reaction, all the solvent were removed under reduced pressure at high temperature. The residue was dissolved with acetone (4.0 mL), and CH_3I (20.0 equiv) was added to the tube. The mixture was stirred at 60 °C for 3 h and then cooled to room temperature. Upon completion of the methylation, the mixture was diluted with 5 mL EtOAc and filtered through a short pad of Celite and the Celite pad were washed with an additional EtOAc (10 mL x 4). Then the filtrate was concentrated *in vacuo* to give the crude product. The crude ^{1}H NMR spectrum was taken using CH_2Br_2 (0.2 mmol) as internal standard. Finally, the resulting residue was purified by preparative thin layer chromatography using PE/EtOAc as the eluent to afford the desired products.

General procedure B:

The oven-dried Schlenk tube (25 mL) containing a stirring bar was charged with substrates **1** (0.20 mmol, 1.0 equiv), **2** (0.40 mmol, 2.0 equiv) and Ir[(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$ (1 mol%) in the air. Then the tube was moved into a glovebox and charged with DABCO (30 mol%), HCOOK (3.0 equiv) and Cs_2CO_3 (3.0 equiv). The tube was sealed and evacuated and back-filled with CO_2 three times. Subsequently, the degassed anhydrous DMSO (2 mL, 0.1 M) was added into the tube via syringe. Then the tube was evacuated and back-filled with CO_2 for 10 times. Finally, the mixture was placed under a 30 W blue LEDs (λ_{max}=465 nm, 3.0 cm - 4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25 - 40 °C) light source and stirred at ambient temperature for 18 - 48 h. Upon completion of the reaction, AcOH (0.2 mL) was added and the system was stirred for 10 min at room temperature. Then all the solvent were removed under reduced pressure at high temperature. The residue was dissolved with MeOH (4.0 mL), then $SOCl_2$ (0.4 mL) was added dropwise to the tube at 0 °C in the ice bath. The mixture was stirred at 100 °C for 6 h and then

cooled to room temperature. Upon completion of the methylation, the mixture was diluted with 5 mL EtOAc and quenched with saturated aqueous $NaHCO_3$ at 0 °C in the ice bath. The organic phases were separated and the aqueous phase was extracted with ethyl acetate (15 mL x 3). The combined organic phases were dried with anhydrous Na_2SO_4 and concentrated *in vacuo* to give the crude product. The crude ^1H NMR spectrum was taken using CH_2Br_2 (0.2 mmol) as internal standard. Finally, the resulting residue was purified by preparative thin layer chromatography using PE/EtOAc as the eluent to afford the desired products.

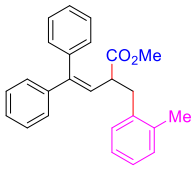
2.3 Characterization of products



3aa

methyl 2-benzyl-4,4-diphenylbut-3-enoate (3aa)

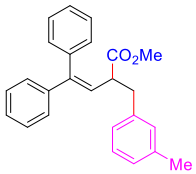
The general procedure A was followed. Yield: 79%, 54.0 mg. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.12 (m, 11H), 7.01 (d, *J* = 6.8 Hz, 2H), 6.88 (dd, *J* = 6.1, 2.6 Hz, 2H), 6.11 (d, *J* = 10.4 Hz, 1H), 3.65 (s, 3H), 3.47 (dt, *J* = 10.0, 7.5 Hz, 1H), 3.09 (dd, *J* = 13.6, 6.8 Hz, 1H), 2.88 (dd, *J* = 13.4, 8.2 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 144.7, 141.8, 139.2, 138.5, 129.7, 129.3, 128.4, 128.3, 128.2, 127.6, 127.4, 127.3, 126.5, 125.7, 52.0, 48.2, 39.4. HRMS (m/z, ESI): calcd for $C_{24}H_{22}O_2Na^+$ $(M+Na)^+$ 365.1512, found 365.1509.



3ab

methyl 2-(2-methylbenzyl)-4,4-diphenylbut-3-enoate (3ab)

The general procedure A was followed. Yield: 76%, 54.1 mg. ^1H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.12 (m, 8H), 7.12 – 6.93 (m, 4H), 6.79 (dd, *J* = 6.5, 2.7 Hz, 2H), 6.15 (d, *J* = 10.4 Hz, 1H), 3.64 (s, 3H), 3.54 – 3.38 (m, 1H), 3.11 (dd, *J* = 13.4, 6.6 Hz, 1H), 2.84 (dd, *J* = 13.6, 8.4 Hz, 1H), 1.98 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 144.6, 141.6, 139.1, 136.6, 130.4, 130.35, 129.7, 128.2, 127.5, 127.3, 127.27, 126.7, 125.8, 125.7, 52.0, 46.5, 36.8, 19.0. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_2Na^+$ $(M+Na)^+$ 379.1669, found 379.1669.

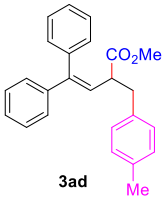


3ac

methyl 2-(3-methylbenzyl)-4,4-diphenylbut-3-enoate (3ac)

The general procedure A was followed. Yield: 78%, 55.6 mg. ^1H NMR (400 MHz,

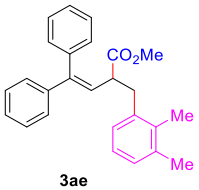
Chloroform-*d*) δ 7.34 – 7.14 (m, 8H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.98 (d, *J* = 7.6 Hz, 1H), 6.91 – 6.85 (m, 2H), 6.83 (d, *J* = 7.6 Hz, 1H), 6.80 (s, 1H), 6.09 (d, *J* = 10.4 Hz, 1H), 3.66 (s, 3H), 3.52 – 3.39 (m, 1H), 3.07 (dd, *J* = 13.4, 6.6 Hz, 1H), 2.84 (dd, *J* = 13.2, 8.4 Hz, 1H), 2.26 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 144.6, 141.9, 139.2, 138.4, 137.8, 130.0, 129.7, 128.23, 128.2, 127.5, 127.4, 127.3, 127.2, 126.4, 125.8, 52.0, 48.1, 39.3, 21.4. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_2Na^+$ $(M+Na)^+$ 379.1669, found 379.1670.



3ad

methyl 2-(4-methylbenzyl)-4,4-diphenylbut-3-enoate (3ad)

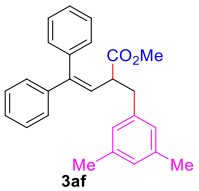
The general procedure A was followed. Yield: 72%, 51.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.12 (m, 8H), 7.01 (d, *J* = 7.6 Hz, 2H), 6.96 – 6.81 (m, 4H), 6.10 (d, *J* = 10.4 Hz, 1H), 3.64 (s, 3H), 3.44 (dt, *J* = 10.3, 7.4 Hz, 1H), 3.05 (dd, *J* = 13.6, 6.8 Hz, 1H), 2.84 (dd, *J* = 13.4, 7.8 Hz, 1H), 2.28 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 144.5, 141.8, 139.2, 135.9, 135.3, 129.7, 129.1, 129.0, 128.3, 128.2, 127.5, 127.4, 127.3, 125.9, 52.0, 48.3, 39.0, 21.2. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_2Na^+$ $(M+Na)^+$ 379.1669, found 379.1668.



3ae

methyl 2-(2,3-dimethylbenzyl)-4,4-diphenylbut-3-enoate (3ae)

The general procedure A was followed. Yield: 70%, 51.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.10 (m, 8H), 7.02 – 6.91 (m, 2H), 6.88 (d, *J* = 6.8 Hz, 1H), 6.72 (d, *J* = 7.6 Hz, 2H), 6.12 (d, *J* = 10.4 Hz, 1H), 3.66 (s, 3H), 3.53 – 3.39 (m, 1H), 3.17 (dd, *J* = 13.4, 5.8 Hz, 1H), 2.83 (dd, *J* = 13.1, 9.4 Hz, 1H), 2.16 (s, 3H), 1.78 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.5, 144.6, 141.7, 139.1, 136.9, 136.3, 135.2, 129.7, 128.6, 128.4, 128.2, 128.1, 127.5, 127.3, 127.1, 125.7, 125.2, 52.0, 46.4, 37.6, 20.7, 14.8. HRMS (m/z, ESI): calcd for $C_{26}H_{26}O_2Na^+$ $(M+Na)^+$ 393.1825, found 393.1826.

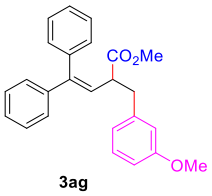


3af

methyl 2-(3,5-dimethylbenzyl)-4,4-diphenylbut-3-enoate (3af)

The general procedure A was followed. Yield: 72%, 53.4 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.08 (m, 8H), 6.86 (dd, *J* = 6.4, 2.9 Hz, 2H), 6.79 (s, 1H), 6.60 (s, 2H), 6.06 (d, *J* = 10.4 Hz, 1H), 3.66 (s, 3H), 3.51 – 3.34 (m, 1H), 3.02 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.79 (dd, *J* = 13.4, 8.6 Hz, 1H), 2.21 (s, 6H). ^{13}C NMR (101 MHz,

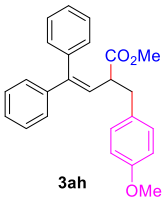
Chloroform-*d*) δ 174.4, 144.5, 142.0, 139.3, 138.3, 137.7, 129.8, 128.2, 128.2, 128.0, 127.5, 127.4, 127.3, 127.1, 126.0, 52.0, 48.0, 39.2, 21.3. HRMS (m/z, ESI): calcd for $C_{26}H_{26}O_2Na^+$ $(M+Na)^+$ 393.1825, found 393.1825.



3ag

methyl 2-(3-methoxybenzyl)-4,4-diphenylbut-3-enoate (3ag)

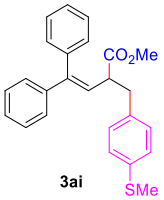
The general procedure A was followed. Yield: 70%, 52.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.15 (m, 8H), 7.12 (t, *J* = 7.9 Hz, 1H), 6.89 (dd, *J* = 6.5, 2.9 Hz, 2H), 6.72 (dd, *J* = 8.4, 2.4 Hz, 1H), 6.62 (d, *J* = 7.2 Hz, 1H), 6.52 (s, 1H), 6.10 (d, *J* = 10.4 Hz, 1H), 3.69 (s, 3H), 3.66 (s, 3H), 3.53 – 3.42 (m, 1H), 3.08 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.85 (dd, *J* = 13.4, 8.2 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 159.6, 144.7, 141.8, 140.0, 139.2, 129.7, 129.3, 128.3, 128.2, 127.6, 127.4, 127.3, 125.7, 121.7, 114.4, 112.3, 55.2, 52.0, 48.1, 39.4. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_3Na^+$ $(M+Na)^+$ 395.1618, found 395.1620.



3ah

methyl 2-(4-methoxybenzyl)-4,4-diphenylbut-3-enoate (3ah)

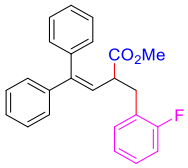
The general procedure A was followed. Yield: 53%, 39.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.13 (m, 8H), 6.99 – 6.84 (m, 4H), 6.75 (d, *J* = 8.4 Hz, 2H), 6.10 (d, *J* = 10.4 Hz, 1H), 3.75 (s, 3H), 3.64 (s, 3H), 3.43 (dt, *J* = 10.4, 7.4 Hz, 1H), 3.03 (dd, *J* = 13.6, 6.8 Hz, 1H), 2.82 (dd, *J* = 13.6, 8.0 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 158.3, 144.5, 141.8, 139.2, 130.5, 130.2, 129.7, 128.3, 128.2, 127.5, 127.4, 127.3, 125.8, 113.8, 55.3, 52.0, 48.4, 38.6. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_3Na^+$ $(M+Na)^+$ 395.1618, found 395.1618.



3ai

methyl 2-(4-(methylthio)benzyl)-4,4-diphenylbut-3-enoate (3ai)

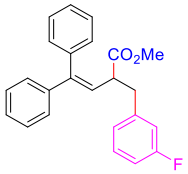
The general procedure A was followed. Yield: 56%, 43.4 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.14 (m, 8H), 7.10 (d, *J* = 7.9 Hz, 2H), 6.98 – 6.78 (m, 4H), 6.08 (d, *J* = 10.4 Hz, 1H), 3.65 (s, 3H), 3.44 (dt, *J* = 10.4, 7.4 Hz, 1H), 3.04 (dd, *J* = 13.6, 6.8 Hz, 1H), 2.82 (dd, *J* = 13.6, 8.0 Hz, 1H), 2.43 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 144.8, 141.7, 139.1, 136.2, 135.5, 129.8, 129.7, 128.3, 128.26, 127.6, 127.4, 127.4, 126.9, 125.5, 52.0, 48.1, 38.8, 16.3. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_2SNa^+$ $(M+Na)^+$ 411.1389, found 411.1388.



3aj

methyl 2-(2-fluorobenzyl)-4,4-diphenylbut-3-enoate (3aj)

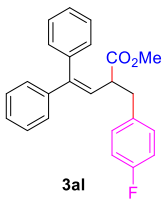
The general procedure A was followed. Yield: 48%, 34.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.09 (m, 9H), 7.05 – 6.87 (m, 3H), 6.87 – 6.76 (m, 2H), 6.10 (d, *J* = 10.4 Hz, 1H), 3.66 (s, 3H), 3.56 – 3.45 (m, 1H), 3.07 (dd, *J* = 13.4, 6.2 Hz, 1H), 2.97 (dd, *J* = 13.2, 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 161.4 (d, $J_{C\text{-}F}$ = 246.4 Hz), 145.0, 141.8, 139.0, 131.6 (d, $J_{C\text{-}F}$ = 4.6 Hz), 129.7, 128.4, 128.3, 128.2, 127.6, 127.4, 127.3, 125.5 (d, $J_{C\text{-}F}$ = 15.8 Hz), 125.3, 124.0 (d, $J_{C\text{-}F}$ = 3.6 Hz), 115.3 (d, $J_{C\text{-}F}$ = 22.1 Hz), 52.1, 46.8, 32.3 (d, $J_{C\text{-}F}$ = 1.7 Hz). HRMS (m/z, ESI): calcd for $C_{24}H_{21}FO_2Na^+$ $(M+Na)^+$ 383.1418, found 383.1418.



3ak

methyl 2-(3-fluorobenzyl)-4,4-diphenylbut-3-enoate (3ak)

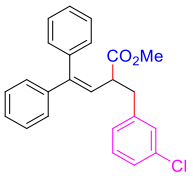
The general procedure A was followed. Yield: 61%, 43.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 (dd, *J* = 5.0, 1.9 Hz, 3H), 7.28 – 7.20 (m, 3H), 7.20 – 7.09 (m, 3H), 6.91 (dd, *J* = 6.6, 2.9 Hz, 2H), 6.86 (td, *J* = 8.5, 2.6 Hz, 1H), 6.79 (d, *J* = 7.6 Hz, 1H), 6.68 (d, *J* = 9.9 Hz, 1H), 6.07 (d, *J* = 10.4 Hz, 1H), 3.66 (s, 3H), 3.47 (dt, *J* = 10.3, 7.7 Hz, 1H), 3.08 (dd, *J* = 13.4, 6.6 Hz, 1H), 2.86 (dd, *J* = 13.6, 8.0 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.0, 162.8 (d, $J_{C\text{-}F}$ = 246.5 Hz), 145.1, 141.6, 141.0 (d, $J_{C\text{-}F}$ = 7.4 Hz), 139.1, 129.8 (d, $J_{C\text{-}F}$ = 8.3 Hz), 129.7, 128.4, 128.3, 127.7, 127.5, 127.4, 125.2, 125.0 (d, $J_{C\text{-}F}$ = 2.8 Hz), 116.1 (d, $J_{C\text{-}F}$ = 21.0 Hz), 113.4 (d, $J_{C\text{-}F}$ = 21.1 Hz), 52.1, 47.8, 38.9 (d, $J_{C\text{-}F}$ = 1.8 Hz). HRMS (m/z, ESI): calcd for $C_{24}H_{21}FO_2Na^+$ $(M+Na)^+$ 383.1418, found 383.1419.



3al

methyl 2-(4-fluorobenzyl)-4,4-diphenylbut-3-enoate (3al)

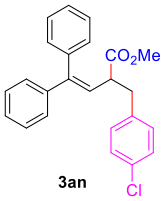
The general procedure A was followed. Yield: 60%, 43.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.19 (m, 6H), 7.16 (dd, *J* = 7.5, 2.1 Hz, 2H), 7.00 – 6.83 (m, 6H), 6.07 (d, *J* = 10.4 Hz, 1H), 3.65 (s, 3H), 3.44 (dt, *J* = 10.8, 7.5 Hz, 1H), 3.05 (dd, *J* = 13.5, 6.6 Hz, 1H), 2.83 (dd, *J* = 13.6, 8.0 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 161.7 (d, $J_{C\text{-}F}$ = 245.2 Hz), 144.9, 141.7, 139.1, 134.2 (d, $J_{C\text{-}F}$ = 3.3 Hz), 130.7 (d, $J_{C\text{-}F}$ = 7.9 Hz), 129.7, 128.3, 128.28, 127.7, 127.4, 127.36, 125.4, 115.1 (d, $J_{C\text{-}F}$ = 21.3 Hz), 52.1, 48.2, 38.5. HRMS (m/z, ESI): calcd for $C_{24}H_{21}FO_2Na^+$ $(M+Na)^+$ 383.1418, found 383.1418.



3am

methyl 2-(3-chlorobenzyl)-4,4-diphenylbut-3-enoate (3am)

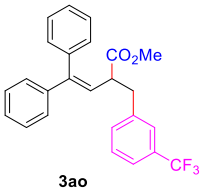
The general procedure A was followed. Yield: 52%, 38.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 3.28 (m, 3H), 7.28 – 7.20 (m, 3H), 7.19 – 7.07 (m, 4H), 6.97 (s, 1H), 6.93 – 6.82 (m, 3H), 6.05 (d, *J* = 10.4 Hz, 1H), 3.67 (s, 3H), 3.51 – 3.39 (m, 1H), 3.06 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.83 (dd, *J* = 13.6, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.0, 145.2, 141.6, 140.5, 139.0, 134.1, 129.63, 129.6, 129.4, 128.4, 128.3, 127.7, 127.55, 127.5, 127.4, 126.7, 125.1, 52.1, 47.8, 38.8. HRMS (m/z, ESI): calcd for $C_{24}H_{21}ClO_2Na^+$ $(M+Na)^+$ 399.1122, found 399.1123.



3an

methyl 2-(4-chlorobenzyl)-4,4-diphenylbut-3-enoate (3an)

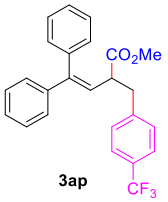
The general procedure A was followed. Yield: 60%, 45.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.20 (m, 6H), 7.16 (d, *J* = 8.0 Hz, 4H), 6.98 – 6.83 (m, 4H), 6.06 (d, *J* = 10.4 Hz, 1H), 3.65 (s, 3H), 3.44 (dt, *J* = 10.6, 7.3 Hz, 1H), 3.04 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.82 (dd, *J* = 13.6, 8.0 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 145.0, 141.6, 139.1, 137.0, 132.3, 130.6, 129.7, 128.5, 128.35, 128.3, 127.7, 127.5, 127.4, 125.2, 52.1, 48.0, 38.6. HRMS (m/z, ESI): calcd for $C_{24}H_{21}ClO_2Na^+$ $(M+Na)^+$ 399.1122, found 399.1123.



3ao

methyl 4,4-diphenyl-2-(3-(trifluoromethyl)benzyl)but-3-enoate (3ao)

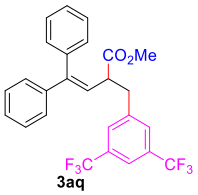
The general procedure A was followed. Yield: X = I, 53%, 43.3 mg; X = Br, 51%, 42.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.43 (d, *J* = 7.6 Hz, 1H), 7.37 – 7.10 (m, 11H), 6.83 (dd, *J* = 6.6, 3.0 Hz, 2H), 6.05 (d, *J* = 10.4 Hz, 1H), 3.68 (s, 3H), 3.47 (td, *J* = 9.4, 6.4Hz , 1H), 3.14 (dd, *J* = 13.6, 6.0 Hz, 1H), 2.92 (dd, *J* = 13.6, 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.9, 145.4, 141.6, 139.5, 139.0, 132.8, 130.7 (q, J_{C-F} = 32.3 Hz), 129.5, 128.8, 128.4, 128.3, 127.7, 127.5, 127.4, 126.0 (q, J_{C-F} = 3.8 Hz), 124.9, 124.2 (q, J_{C-F} = 273.3 Hz), 123.4 (q, J_{C-F} = 3.8 Hz), 52.2, 47.8, 38.9. HRMS (m/z, ESI): calcd for $C_{25}H_{21}F_3O_2Na^+$ $(M+Na)^+$ 433.1386, found 433.1387.



3ap

methyl 4,4-diphenyl-2-(4-(trifluoromethyl)benzyl)but-3-enoate (3ap)

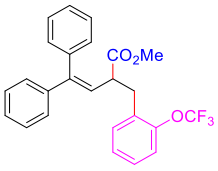
The general procedure A was followed. Yield: X = I, 56%, 46.1 mg; X = Br, 50%, 41.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 (d, *J* = 7.9 Hz, 2H), 7.32 – 7.20 (m, 6H), 7.20 – 7.13 (m, 2H), 7.09 (d, *J* = 7.9 Hz, 2H), 6.85 (dd, *J* = 6.7, 3.0 Hz, 2H), 6.07 (d, *J* = 10.4 Hz, 1H), 3.67 (s, 3H), 3.55 – 3.44 (m, 1H), 3.14 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.89 (dd, *J* = 13.2, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.9, 145.3, 142.7, 141.5, 138.9, 129.63, 129.57, 128.8 (q, J_{C-F} = 29.8 Hz), 128.4, 128.3, 127.8, 127.5, 127.4, 125.3 (q, J_{C-F} = 3.8 Hz), 124.9, 124.4(q, J_{C-F} = 272.8 Hz) 52.2, 47.9, 39.0. HRMS (m/z, ESI): calcd for $C_{25}H_{21}F_3O_2Na^+$ $(M+Na)^+$ 433.1386, found 433.1386.



3aq

methyl 2-(3,5-bis(trifluoromethyl)benzyl)-4,4-diphenylbut-3-enoate (3aq)

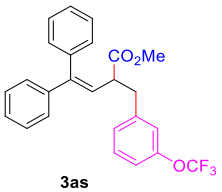
The general procedure A was followed. Yield: 50%, 48.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 (s, 1H), 7.44 (s, 2H), 7.35 – 7.18 (m, 6H), 7.13 (dd, *J* = 6.8, 2.9 Hz, 2H), 6.83 (dd, *J* = 6.6, 2.9 Hz, 2H), 6.02 (d, *J* = 10.8 Hz, 1H), 3.71 (s, 3H), 3.51 (td, *J* = 9.8, 6.0 Hz, 1H), 3.21 (dd, *J* = 13.6, 6.0 Hz, 1H), 2.98 (dd, *J* = 13.6, 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.6, 146.2, 141.3, 141.1, 138.8, 131.6 (q, J_{C-F} = 33.3 Hz), 129.5 (q, J_{C-F} = 2.6 Hz), 129.4, 128.5, 128.3, 128.0, 127.7, 127.4, 124.1, 123.4 (q, J_{C-F} = 273.6 Hz), 120.7 – 120.5 (m), 52.4, 47.5, 38.6. HRMS (m/z, ESI): calcd for $C_{26}H_{20}F_6O_2Na^+$ $(M+Na)^+$ 501.1260, found 501.1260.



3ar

methyl 4,4-diphenyl-2-(2-(trifluoromethoxy)benzyl)but-3-enoate (3ar)

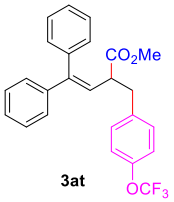
The general procedure A was followed. Yield: 55%, 45.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.02 (m, 12H), 6.86 (dd, *J* = 6.6, 3.0 Hz, 2H), 6.09 (d, *J* = 10.4 Hz, 1H), 3.65 (s, 3H), 3.58 – 3.48 (m, 1H), 3.12 (dd, *J* = 13.6, 6.8 Hz, 1H), 2.99 (dd, *J* = 13.6, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.0, 148.0, 145.1, 141.7, 139.0, 131.8, 130.9, 129.6, 128.3, 128.2, 128.1, 127.6, 127.4, 127.38, 126.5, 125.2, 120.6 (q, J_{C-F} = 258.6 Hz) 120.2 (q, J_{C-F} = 1.6 Hz), 52.1, 46.6, 33.2. HRMS (m/z, ESI): calcd for $C_{25}H_{21}F_3O_3Na^+$ $(M+Na)^+$ 449.1335, found 449.1334.



3as

methyl 4,4-diphenyl-2-(3-(trifluoromethoxy)benzyl)but-3-enoate (3as)

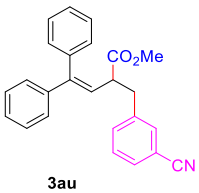
The general procedure A was followed. Yield: X = I, 48%, 41.0 mg; X = Br, 54%, 45.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.27 (m, 3H), 7.27 – 7.18 (m, 4H), 7.15 (dd, *J* = 7.4, 2.2 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 1H), 6.93 (d, *J* = 7.6 Hz, 1H), 6.93 – 6.83 (m, 3H), 6.06 (d, *J* = 10.4 Hz, 1H), 3.66 (s, 3H), 3.46 (dt, *J* = 9.1, 7.2 Hz, 1H), 3.10 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.88 (dd, *J* = 13.6, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.0, 149.3 (d, J_{C-F} = 1.7 Hz), 145.3, 141.6, 140.9, 139.0, 129.7, 129.6, 128.4, 128.3, 127.8, 127.7, 127.5, 127.4, 125.0, 121.8, 120.6 (q, J_{C-F} = 257.9 Hz), 119.0, 52.1, 47.9, 38.9. HRMS (m/z, ESI): calcd for $C_{25}H_{21}F_3O_3Na^+$ $(M+Na)^+$ 449.1335, found 449.1333.



3at

methyl 4,4-diphenyl-2-(4-(trifluoromethoxy)benzyl)but-3-enoate (3at)

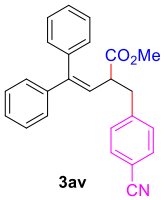
The general procedure A was followed. Yield: 57%, 48.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.20 (m, 6H), 7.16 (dd, *J* = 7.5, 2.1 Hz, 2H), 7.02 (q, *J* = 8.5 Hz, 4H), 6.89 – 6.78 (m, 2H), 6.07 (d, *J* = 10.4 Hz, 1H), 3.67 (s, 3H), 3.50 – 3.38 (m, 1H), 3.08 (dd, *J* = 13.4, 6.2 Hz, 1H), 2.85 (dd, *J* = 13.6, 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 147.9 (q, J_{C-F} = 1.7 Hz), 145.2, 141.6, 139.0, 137.4, 130.6, 129.6, 128.33, 128.3, 127.7, 127.5, 127.3, 125.1, 120.9, 120.6 (q, J_{C-F} = 257.7 Hz), 52.1, 48.1, 38.5. HRMS (m/z, ESI): calcd for $C_{25}H_{21}F_3O_3Na^+$ $(M+Na)^+$ 449.1335, found 449.1335.



3au

methyl 2-(3-cyanobenzyl)-4,4-diphenylbut-3-enoate (3au)

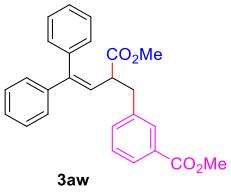
The general procedure A was followed. Yield: X = I, 40%, 29.4 mg; X = Br, 60%, 43.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 7.6 Hz, 1H), 7.37 – 7.18 (m, 9H), 7.18 – 7.10 (m, 2H), 6.88 (dd, *J* = 6.6, 3.0 Hz, 2H), 6.03 (d, *J* = 10.4 Hz, 1H), 3.68 (s, 3H), 3.49 (dt, *J* = 10.5, 7.4 Hz, 1H), 3.12 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.88 (dd, *J* = 13.8, 8.6 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.7, 145.6, 141.3, 140.0, 138.8, 133.9, 132.7, 130.3, 129.5, 129.1, 128.4, 128.3, 127.9, 127.7, 127.3, 124.5, 118.8, 112.4, 52.3, 47.5, 38.5. HRMS (m/z, ESI): calcd for $C_{25}H_{21}NO_2Na^+$ $(M+Na)^+$ 390.1464, found 390.1464.



3av

methyl 2-(4-cyanobenzyl)-4,4-diphenylbut-3-enoate (3av)

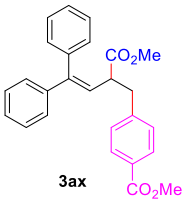
The general procedure A was followed. Yield: X = Br, 63%, 46.3 mg; X = Cl, 51%, 37.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 (d, *J* = 8.0 Hz, 2H), 7.37 – 7.28 (m, 3H), 7.28 – 7.19 (m, 3H), 7.19 – 7.12 (m, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.88 (dd, *J* = 6.4, 3.0 Hz, 2H), 6.05 (d, *J* = 10.4 Hz, 1H), 3.67 (s, 3H), 3.56 – 3.44 (m, 1H), 3.13 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.90 (dd, *J* = 13.6, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.7, 145.4, 144.2, 141.3, 138.8, 132.1, 130.1, 129.5, 128.4, 128.3, 127.9, 127.6, 127.3, 124.5, 119.0, 110.3, 52.2, 47.5, 39.1. HRMS (m/z, ESI): calcd for $C_{25}H_{21}NO_2Na^+$ $(M+Na)^+$ 390.1464, found 390.1464.



3aw

methyl 3-(2-(methoxycarbonyl)-4,4-diphenylbut-3-en-1-yl)benzoate (3aw)

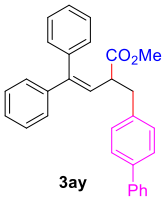
The general procedure A was followed. Yield: 57%, 45.4 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 (d, *J* = 7.6 Hz, 1H), 7.70 (s, 1H), 7.35 – 7.06 (m, 10H), 6.84 (dd, *J* = 6.7, 2.9 Hz, 2H), 6.07 (d, *J* = 10.4 Hz, 1H), 3.88 (s, 3H), 3.67 (s, 3H), 3.56 – 3.40 (m, 1H), 3.13 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.92 (dd, *J* = 13.6, 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.0, 167.1, 145.2, 141.7, 139.0, 138.8, 133.9, 130.5, 130.2, 129.6, 128.4, 128.3, 128.2, 127.8, 127.7, 127.4, 127.38, 125.2, 52.1, 52.1, 47.9, 39.0. HRMS (m/z, ESI): calcd for $C_{26}H_{24}O_4Na^+$ $(M+Na)^+$ 423.1567, found 423.1565.



3ax

methyl 4-(2-(methoxycarbonyl)-4,4-diphenylbut-3-en-1-yl)benzoate (3ax)

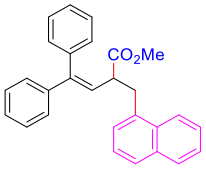
The general procedure A was followed. Yield: X = I, 55%, 43.9 mg; X = Br, 65%, 52.9 mg; X = Cl, 60%, 48.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.88 (d, *J* = 8.0 Hz, 2H), 7.34 – 7.26 (m, 3H), 7.26 – 7.19 (m, 3H), 7.18 – 7.11 (m, 2H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.87 (dd, *J* = 6.6, 3.0 Hz, 2H), 6.07 (d, *J* = 10.4 Hz, 1H), 3.88 (s, 3H), 3.66 (s, 3H), 3.54 – 3.44 (m, 1H), 3.13 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.92 (dd, *J* = 13.2, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.9, 167.1, 145.1, 144.0, 141.5, 139.0, 129.7, 129.6, 129.3, 128.4, 128.34, 128.27, 127.7, 127.5, 127.3, 125.1, 52.1, 47.7, 39.2. HRMS (m/z, ESI): calcd for $C_{26}H_{24}O_4Na^+$ $(M+Na)^+$ 423.1567, found 423.1566.



3ay

methyl 2-([1,1'-biphenyl]-4-ylmethyl)-4,4-diphenylbut-3-enoate (3ay)

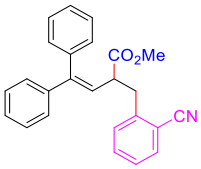
The general procedure A was followed. Yield: 62%, 51.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 7.6 Hz, 2H), 7.48 – 7.35 (m, 4H), 7.35 – 7.12 (m, 9H), 7.07 (d, *J* = 8.0 Hz, 2H), 6.95 – 6.82 (m, 2H), 6.12 (d, *J* = 10.4 Hz, 1H), 3.66 (s, 3H), 3.56 – 3.41 (m, 1H), 3.13 (dd, *J* = 13.6, 6.4 Hz, 1H), 2.90 (dd, *J* = 13.6, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 144.8, 141.8, 141.1, 139.4, 139.2, 137.6, 129.74, 129.7, 128.9, 128.3, 128.26, 127.6, 127.4, 127.36, 127.2, 127.1, 125.6, 52.1, 48.2, 39.0. HRMS (m/z, ESI): calcd for $C_{30}H_{26}O_2Na^+$ $(M+Na)^+$ 441.1825, found 441.1826.



3az

methyl 2-(naphthalen-1-ylmethyl)-4,4-diphenylbut-3-enoate (3az)

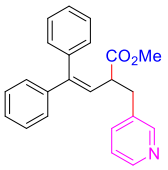
The general procedure A was followed. Yield: 55%, 43.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, *J* = 8.0 Hz, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.54 (d, *J* = 8.4 Hz, 1H), 7.39 (t, *J* = 7.6 Hz, 1H), 7.35 – 7.03 (m, 11H), 6.67 (d, *J* = 7.2 Hz, 2H), 6.21 (d, *J* = 10.0 Hz, 1H), 3.70 (dt, *J* = 10.0, 7.6 Hz, 1H), 3.60 (s, 3H), 3.56 (dd, *J* = 13.6, 7.2 Hz, 1H), 3.25 (dd, *J* = 13.6, 8.0 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 144.7, 141.6, 138.9, 134.4, 133.9, 132.0, 129.4, 128.7, 128.2, 128.1, 127.6, 127.5, 127.3, 127.1, 126.0, 125.8, 125.5, 125.3, 123.4, 52.0, 47.1, 36.7. HRMS (m/z, ESI): calcd for $C_{28}H_{24}O_2Na^+$ $(M+Na)^+$ 415.1668, found 415.1669.



3aaa

methyl 2-(2-cyanobenzyl)-4,4-diphenylbut-3-enoate (3aaa)

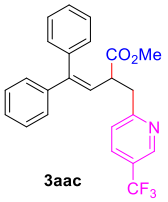
The general procedure A was followed. Yield: X = Cl, 67%, 49.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 (d, *J* = 7.7 Hz, 1H), 7.39 (t, *J* = 7.5 Hz, 1H), 7.33 – 7.14 (m, 9H), 7.08 (d, *J* = 8.0 Hz, 1H), 6.84 – 6.70 (m, 2H), 6.13 (d, *J* = 10.8 Hz, 1H), 3.71 (s, 3H), 3.61 (td, *J* = 10.0, 5.6 Hz, 1H), 3.29 (dd, *J* = 13.6, 5.6 Hz, 1H), 3.15 (dd, *J* = 13.6, 9.6 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.5, 145.7, 142.5, 141.3, 138.7, 132.8, 132.7, 130.6, 129.6, 128.3, 127.8, 127.5, 127.4, 127.1, 124.1, 117.9, 113.3, 52.3, 47.3, 37.1. HRMS (m/z, ESI): calcd for $C_{25}H_{21}NO_2Na^+$ $(M+Na)^+$ 390.1464, found 390.1462.



3aab

methyl 4,4-diphenyl-2-(pyridin-3-ylmethyl)but-3-enoate (3aab)

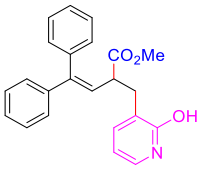
The general procedure B was followed. Yield: 50%, 33.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.45 (d, *J* = 4.8 Hz, 1H), 8.34 (s, 1H), 7.38 – 7.22 (m, 7H), 7.22 – 7.09 (m, 3H), 6.92 (dd, *J* = 6.5, 2.9 Hz, 2H), 6.09 (d, *J* = 10.4 Hz, 1H), 3.70 (s, 3H), 3.50 (dt, *J* = 10.2, 7.7 Hz, 1H), 3.11 (dd, *J* = 13.8, 6.6 Hz, 1H), 2.89 (dd, *J* = 13.7, 8.2 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.8, 150.4, 147.8, 145.5, 141.4, 138.9, 136.9, 134.1, 129.5, 128.4, 128.3, 127.8, 127.6, 127.3, 124.7, 123.4, 52.2, 47.6, 36.2. HRMS (m/z, ESI): calcd for $C_{23}H_{21}NO_2Na^+$ $(M+Na)^+$ 366.1464, found 366.1460.



3aac

methyl 4,4-diphenyl-2-((5-(trifluoromethyl)pyridin-2-yl)methyl)but-3-enoate (3aac)

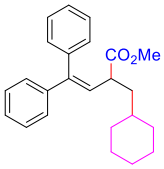
The general procedure B was followed. Yield: 50%, 41.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 8.64 (s, 1H), 7.74 (dd, *J* = 8.4, 2.4 Hz, 1H), 7.39 – 7.20 (m, 6H), 7.20 – 7.09 (m, 3H), 7.00 – 6.82 (m, 2H), 6.09 (d, *J* = 10.4 Hz, 1H), 3.87 – 3.76 (m, 1H), 3.71 (s, 3H), 3.36 (dd, *J* = 14.0, 6.0 Hz, 1H), 3.10 (dd, *J* = 13.6, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.0, 162.7 (q, J_{C-F} = 1.6 Hz), 146.2 (q, J_{C-F} = 4.1 Hz), 145.3, 141.7, 138.9, 133.2 (q, J_{C-F} = 3.5 Hz), 129.6, 128.34, 128.3, 127.8, 127.54, 127.5, 124.8, 124.5 (q, J_{C-F} = 33.1 Hz), 123.8 (q, J_{C-F} = 273.2 Hz), 123.3, 52.3, 45.9, 41.0. HRMS (m/z, ESI): calcd for $C_{24}H_{20}F_3NO_2Na^+$ $(M+Na)^+$ 434.1338, found 434.1339.



3aad

methyl 2-((2-hydroxypyridin-3-yl)methyl)-4,4-diphenylbut-3-enoate (3aad)

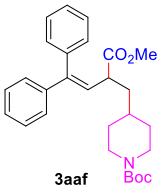
The general procedure B was followed. Yield: 46%, 32.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 13.05 (br, 1H), 7.25 – 7.13 (m, 9H), 7.09 (t, *J* = 7.4 Hz, 1H), 6.98 (d, *J* = 7.2 Hz, 2H), 6.17 (t, *J* = 6.6 Hz, 1H), 6.08 (d, *J* = 10.4 Hz, 1H), 3.83 – 3.74 (m, 1H), 3.69 (s, 3H), 3.04 (dd, *J* = 13.4, 5.8 Hz, 1H), 2.80 (dd, *J* = 13.2, 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 144.9, 142.0, 140.1, 139.2, 133.1, 129.7, 128.2, 128.1, 127.6, 127.5, 127.3, 125.8, 106.5, 52.1, 44.6, 34.0. HRMS (m/z, ESI): calcd for $C_{23}H_{21}NO_3Na^+$ $(M+Na)^+$ 382.1414, found 382.1406.



3aae

methyl 2-(cyclohexylmethyl)-4,4-diphenylbut-3-enoate (3aae)

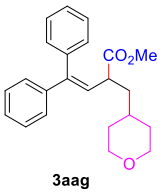
The general procedure A was followed. Yield: 44%, 30.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.48 – 7.14 (m, 10H), 6.08 (d, *J* = 10.4 Hz, 1H), 3.72 (s, 3H), 3.35 (td, *J* = 8.8, 6.5 Hz, 1H), 1.72 – 1.47 (m, 6H), 1.38 – 1.02 (m, 5H), 0.84 (qd, *J* = 12.4, 11.6, 3.8 Hz, 1H), 0.70 (qd, *J* = 12.1, 3.6 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.3, 143.8, 142.0, 139.5, 129.9, 128.4, 128.3, 127.5, 127.46, 127.4, 127.2, 52.0, 43.7, 41.0, 35.3, 33.6, 32.8, 26.6, 26.4, 26.2. HRMS (m/z, ESI): calcd for $C_{24}H_{28}O_2Na^+$ $(M+Na)^+$ 371.1982, found 371.1980.



3aaf

***tert*-butyl 4-(2-(methoxycarbonyl)-4,4-diphenylbut-3-en-1-yl)piperidine-1-carboxylate (3aaf)**

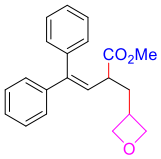
The general procedure A was followed. Yield: 50%, 45.7 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.23 (m, 3H), 7.23 – 7.13 (m, 5H), 7.13 – 7.07 (m, 2H), 5.97 (d, *J* = 10.4 Hz, 1H), 4.08 – 3.75 (m, 2H), 3.62 (s, 3H), 3.33 – 3.20 (m, 1H), 2.47 (dt, *J* = 35.7, 10.6 Hz, 2H), 1.60 (dt, *J* = 14.1, 7.1 Hz, 1H), 1.52 – 1.41 (m, 2H), 1.35 (s, 9H), 1.29 – 1.17 (m, 1H), 1.09 (dt, *J* = 13.5, 2.9 Hz, 1H), 0.91 (qd, *J* = 12.4, 4.3 Hz, 1H), 0.77 (qd, *J* = 12.4, 4.3 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.9, 154.9, 144.2, 141.7, 139.3, 129.8, 128.5, 128.3, 127.7, 127.6, 127.4, 126.5, 79.3, 52.1, 43.3, 39.9, 33.6, 32.3, 31.7, 28.5. HRMS (m/z, ESI): calcd for $C_{28}H_{35}NO_4Na^+$ $(M+Na)^+$ 472.2458, found 472.2462.



3aag

methyl 4,4-diphenyl-2-((tetrahydro-2H-pyran-4-yl)methyl)but-3-enoate (3aag)

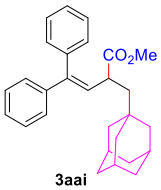
The general procedure A was followed. Yield: X = I, 50%, 35.1 mg; X = Br, 56%, 39.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.14 (m, 8H), 7.11 (d, *J* = 6.8 Hz, 2H), 5.98 (d, *J* = 10.4 Hz, 1H), 3.79 (dt, *J* = 11.4, 3.0 Hz, 1H), 3.75 – 3.67 (m, 1H), 3.62 (s, 3H), 3.32 – 3.16 (m, 2H), 3.11 (td, *J* = 11.4, 2.9 Hz, 1H), 1.76 – 1.55 (m, 1H), 1.52 – 1.28 (m, 3H), 1.23 – 0.88 (m, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.9, 144.2, 141.7, 139.3, 129.8, 128.4, 128.3, 127.65, 127.6, 127.4, 126.5, 68.0, 67.9, 52.1, 43.1, 40.3, 33.2, 32.6. HRMS (m/z, ESI): calcd for $C_{23}H_{26}O_3Na^+$ $(M+Na)^+$ 373.1774, found 373.1772.



3aah

methyl 2-(oxetan-3-ylmethyl)-4,4-diphenylbut-3-enoate (3aah)

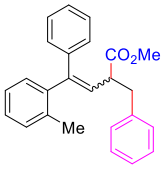
The general procedure A was followed. Yield: 60%, 38.7 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.23 (m, 3H), 7.23 – 7.02 (m, 7H), 5.95 (d, *J* = 10.8 Hz, 1H), 4.66 – 4.54 (m, 1H), 4.43 (m, *J* = 6.8 Hz, 1H), 4.21 (t, *J* = 6.2 Hz, 1H), 4.11 (t, *J* = 6.2 Hz, 1H), 3.62 (s, 3H), 3.07 (td, *J* = 10.1, 7.4 Hz, 1H), 2.84 (hept, *J* = 7.4 Hz, 1H), 2.06 (dt, *J* = 13.6, 7.0 Hz, 1H), 1.92 (dt, *J* = 13.6, 8.0 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 144.7, 141.5, 139.1, 129.7, 128.6, 128.3, 127.8, 127.7, 127.3, 125.3, 77.5, 77.2, 52.1, 44.3, 37.0, 33.3. HRMS (m/z, ESI): calcd for $C_{21}H_{22}O_3Na^+$ $(M+Na)^+$ 345.1461, found 345.1463.



3aai

methyl 2-((adamantan-1-yl)methyl)-4,4-diphenylbut-3-enoate (3aai)

The general procedure A was followed. Yield: 69%, 55.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.22 (m, 3H), 7.21 – 7.02 (m, 7H), 5.96 (d, *J* = 10.4 Hz, 1H), 3.59 (s, 3H), 3.28 (dt, *J* = 10.4, 6.7 Hz, 1H), 1.79 – 1.72 (m, 3H), 1.68 (dd, *J* = 14.1, 7.2 Hz, 1H), 1.60 – 1.37 (m, 6H), 1.35 – 1.13 (m, 7H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.7, 142.4, 142.1, 139.5, 129.9, 128.7, 128.4, 128.3, 127.5, 127.48, 127.4, 52.0, 47.8, 42.3, 41.7, 37.0, 33.0, 28.7. HRMS (m/z, ESI): calcd for $C_{28}H_{32}O_2Na^+$ $(M+Na)^+$ 423.2294, found 423.2294.

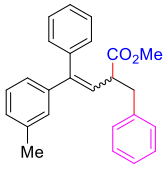


3ba

methyl 2-benzyl-4-phenyl-4-(o-tolyl)but-3-enoate (**3ba**, E/Z = 5.9/1)

The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 71%, 50.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.14 (m, 10H), 7.14 – 7.00 (m, 3H), 6.97 (dd, *J* = 7.3, 2.2 Hz, 0.33H), 6.42 (d, *J* = 7.5 Hz, 0.46H), 6.30 (d, *J* = 10.2 Hz, 0.46H), 6.24 (d, *J* = 10.1 Hz, 0.36H), 5.72 (d, *J* = 10.6 Hz, 0.14H), 3.90 – 3.79 (m, 0.16H), 3.74 (s, 0.44H), 3.69 (s, 1.06H), 3.65 (s, 1.42H), 3.38 (dt, *J* = 10.1, 7.3 Hz, 0.35H), 3.29 – 3.17 (m, 0.60H), 3.13 (dd, *J* = 13.3, 6.8 Hz, 1H), 3.01 – 2.82 (m, 1H), 2.08 (s, 1.37H), 2.01 (s, 0.46H), 1.58 (s, 1.09H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.31, 174.26, 174.1, 145.1, 144.4, 143.6, 143.1, 140.7, 140.2, 139.4, 138.63, 138.59, 138.51, 138.3, 138.1, 136.8, 136.6, 136.1, 130.7, 130.35, 130.33, 130.2, 129.9, 129.6, 129.4, 129.3, 129.2, 129.1, 128.5, 128.4, 128.2, 128.1, 127.8, 127.6, 127.56, 127.52, 127.48, 127.2, 126.6, 126.54, 126.51, 126.1, 125.7, 125.6,

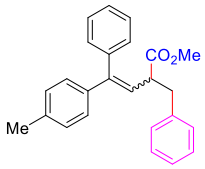
125.5, 52.1, 52.0, 51.9, 48.7, 48.3, 47.2, 39.4, 39.3, 39.1, 20.4, 19.5, 19.4. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_2Na^+$ $(M+Na)^+$ 379.1668, found 379.1669.



3ca

methyl 2-benzyl-4-phenyl-4-(m-tolyl)but-3-enoate (**3ca**, *E/Z* = 1.1/1)

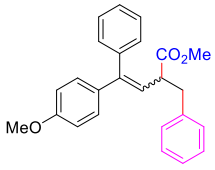
The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 59%, 42.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.03 (m, 11H), 7.01 (d, *J* = 7.8 Hz, 0.55H), 6.97 – 6.87 (m, 1H), 6.78 (d, *J* = 7.5 Hz, 0.52H), 6.61 (s, 0.48H), 6.14 (d, *J* = 10.4 Hz, 1H), 3.71 (s, 1.42H), 3.69 (s, 1.56H), 3.57 – 3.44 (m, 1H), 3.15 (dd, *J* = 13.5, 6.5 Hz, 1H), 3.00 – 2.86 (m, 1H), 2.34 (s, 1.51H), 2.33 (s, 1.59H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 174.3, 144.82, 144.75, 141.9, 141.8, 139.3, 139.1, 138.6, 138.5, 137.79, 137.77, 130.3, 129.7, 129.4, 129.3, 128.4, 128.3, 128.25, 128.21, 128.13, 128.09, 128.07, 128.0, 127.5, 127.l4, 127.3, 126.7, 126.5, 126.4, 125.6, 125.5, 124.6, 52.0, 48.23, 48.17, 39.4, 21.5. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_2Na^+$ $(M+Na)^+$ 379.1668, found 379.1668.



3da

methyl 2-benzyl-4-phenyl-4-(p-tolyl)but-3-enoate (**3da**, *E/Z* = 1.4/1)

The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 68%, 48.0 mg.^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.13 (m, 7H), 7.13 – 6.93 (m, 5H), 6.91 – 6.81 (m, 1H), 6.78 (d, *J* = 7.7 Hz, 1H), 6.07 (d, *J* = 10.4 Hz, 1H), 3.63 (s, 3H), 3.54 – 3.38 (m, 1H), 3.15 – 3.01 (m, 1H), 2.94 – 2.81 (m, 1H), 2.36 (s, 1.90H), 2.30 (s, 1.30H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 174.3, 144.6, 144.5, 142.0, 139.3, 139.0, 138.5, 137.4, 137.0, 136.2, 129.7, 129.6, 129.3, 129.0, 128.9, 128.4, 128.23, 128.2, 127.5, 127.4, 127.3, 126.5, 126.4, 125.6, 124.8, 52.0, 48.2, 39.4, 21.4, 21.2. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_2Na^+$ $(M+Na)^+$ 379.1668, found 379.1670.

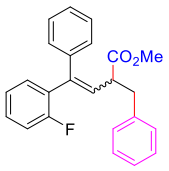


3ea

methyl 2-benzyl-4-(4-methoxyphenyl)-4-phenylbut-3-enoate (**3ea**, *E/Z* = 3.2/1)

The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 65%, 46.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 6.99 (m, 10H), 6.95 – 6.75 (m, 4H), 6.08 (d, *J* = 10.4 Hz, 0.76H), 6.05 (d, *J* = 10.4 Hz, 0.24H), 3.86 (s, 2.36H), 3.81 (s, 0.79H), 3.69 (s, 2.25H), 3.68 (s, 0.76H), 3.55 (dt, *J* = 10.3, 8.0 Hz, 0.79H), 3.46 (dt, *J* = 10.4, 7.9 Hz, 0.27H), 3.19 – 3.06 (m, 1H), 2.97 –

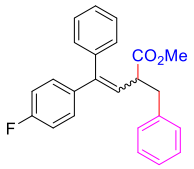
2.84 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.5, 174.4, 159.2, 158.9, 144.4, 144.1, 142.2, 139.4, 138.6, 138.5, 134.5, 131.5, 130.9, 129.7, 129.3, 128.5, 128.4, 128.3, 128.2, 127.52, 127.47, 127.3, 126.5, 126.4, 125.6, 123.9, 113.7, 113.6, 55.4, 55.3, 52.01, 51.98, 48.19, 48.17, 39.5, 39.4. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_3Na^+$ $(M+Na)^+$ 395.1618, found 395.1618.



3fa

methyl 2-benzyl-4-(2-fluorophenyl)-4-phenylbut-3-enoate (**3fa**, *E/Z* = 3.1/1)

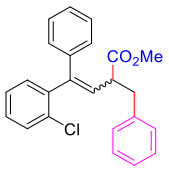
The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 71%, 51.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 7.12 (m, 9H), 7.12 – 6.57 (m, 5H), 6.27 (d, *J* = 10.4 Hz, 0.74H), 6.03 (d, *J* = 10.4 Hz, 0.24H), 3.66 (s, 0.75H), 3.61 (s, 2.44H), 3.32 (dt, *J* = 10.9, 7.4 Hz, 1H), 3.16 – 3.03 (m, 1H), 2.97 – 2.82 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 173.9, 160.2 (d, J_{C-F} = 250.3 Hz), 160.0 (d, J_{C-F} = 247.6 Hz), 140.5, 139.5, 139.1, 138.4, 138.3, 138.2, 131.9 (d, J_{C-F} = 3.5 Hz), 131.1 (d, J_{C-F} = 3.4 Hz), 129.8, 129.7, 129.6 (d, J_{C-F} = 8.0 Hz), 129.3, 129.2, 129.1(d, J_{C-F} = 8.4 Hz), 128.44, 128.4, 128.36, 128.2, 127.9, 127.8, 127.3, 126.7, 126.6, 126.5, 126.48, 126.3, 124.1 (d, J_{C-F} = 3.6 Hz), 123.8 (d, J_{C-F} = 3.4 Hz), 116.0 (d, J_{C-F} = 22.8 Hz), 115.8 (d, J_{C-F} = 22.1 Hz), 52.1, 52.0, 48.7, 47.9, 39.3. HRMS (m/z, ESI): calcd for $C_{24}H_{21}FO_2Na^+$ $(M+Na)^+$ 383.1418, found 383.1419.



3ga

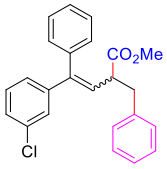
methyl 2-benzyl-4-(4-fluorophenyl)-4-phenylbut-3-enoate (**3ga**, *E/Z* = 1.6/1)

The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 55%, 39.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.12 (m, 8H), 7.10 – 6.92 (m, 4H), 6.89 (dd, *J* = 6.6, 3.0 Hz, 1H), 6.82 (dd, *J* = 8.3, 5.6 Hz, 1H), 6.13 (d, *J* = 10.4 Hz, 0.62H), 6.07 (d, *J* = 10.4 Hz, 0.38H), 3.71 (s, 1.82H), 3.70 (s, 1.17H), 3.55 – 3.39 (m, 1H), 3.20 – 3.08 (m, 1H), 2.98 – 2.84 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 174.1, 162.4 (d, J_{C-F} = 247.8 Hz), 162.1 (d, J_{C-F} = 247.1 Hz), 143.8, 143.7, 141.6, 139.0, 138.4, 138.0 (d, J_{C-F} = 3.3 Hz), 135.0 (d, J_{C-F} = 3.4 Hz), 131.4 (d, J_{C-F} = 7.9 Hz), 129.6, 129.34, 129.3, 129.0 (d, J_{C-F} = 8.0 Hz), 128.42, 128.4, 128.38, 128.3, 127.7, 127.5, 127.3, 126.5, 126.1, 125.5, 115.2 (d, J_{C-F} = 21.4 Hz), 115.1 (d, J_{C-F} = 21.4 Hz), 52.1, 52.0, 48.3, 48.1, 39.4, 39.3. HRMS (m/z, ESI): calcd for $C_{24}H_{21}FO_2Na^+$ $(M+Na)^+$ 383.1418, found 383.1420.



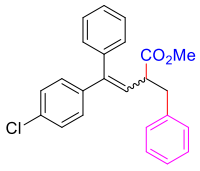
3ha

methyl 2-benzyl-4-(2-chlorophenyl)-4-phenylbut-3-enoate (**3ha**, *E/Z* = 1.2/1)
The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 66%, 50.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.55 – 7.41 (m, 1H), 7.41 – 7.17 (m, 10H), 7.17 – 6.95 (m, 2.70H), 6.42 – 6.26 (m, 1.42H), 3.68 (s, 1.51H), 3.63 (s, 1.29H), 3.33 (td, *J* = 9.3, 5.5 Hz, 0.43H), 3.27 – 3.08 (m, 1.50H), 3.02 (dd, *J* = 13.1, 5.7 Hz, 0.46H), 2.92 (dd, *J* = 13.2, 8.4 Hz, 0.54H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.85, 173.79, 141.6, 141.4, 139.8, 139.7, 138.5, 138.4, 137.7, 137.68, 133.9, 133.8, 132.1, 131.3, 130.0, 129.7, 129.5, 129.3, 129.26, 129.1, 128.9, 128.5, 128.4, 127.8, 127.7, 127.3, 127.0, 126.6, 126.57, 126.5, 52.0, 51.9, 48.7, 48.67, 39.5, 38.8. HRMS (m/z, ESI): calcd for $C_{24}H_{21}ClO_2Na^+$ $(M+Na)^+$ 399.1122, found 399.1124.



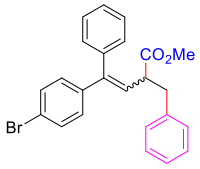
3ia

methyl 2-benzyl-4-(3-chlorophenyl)-4-phenylbut-3-enoate (**3ia**, *E/Z* = 2.0/1)
The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 47%, 35.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.11 (m, 9H), 7.05 (t, *J* = 7.4 Hz, 3H), 6.92 – 6.83 (m, 1.32H), 6.79 (d, *J* = 7.2 Hz, 0.35H), 6.73 (s, 0.34H), 6.13 (d, *J* = 10.4 Hz, 1H), 3.72 (s, 1H), 3.69 (s, 2H), 3.54 – 3.37 (m, 1H), 3.20 – 3.07 (m, 1H), 2.91 (dd, *J* = 13.4, 8.5 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.05, 174.02, 143.7, 143.6, 143.55, 141.1, 140.9, 138.4, 138.3, 138.26, 134.3, 134.2, 129.7, 129.6, 129.5, 129.46, 129.4, 129.3, 128.5, 128.45, 128.37, 127.9, 127.8, 127.65, 127.6, 127.58, 127.4, 127.3, 127.0, 126.7, 126.6, 126.4, 125.6, 52.2, 52.1, 48.3, 48.1, 39.3, 39.2. HRMS (m/z, ESI): calcd for $C_{24}H_{21}ClO_2Na^+$ $(M+Na)^+$ 399.1122, found 399.1123.



3ja

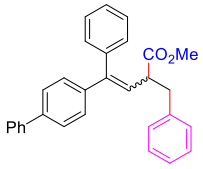
methyl 2-benzyl-4-(4-chlorophenyl)-4-phenylbut-3-enoate (**3ja**, *E/Z* = 1.2/1)
The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 60%, 43.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.15 (m, 9H), 7.12 (d, *J* = 8.5 Hz, 1H), 7.05 (t, *J* = 7.8 Hz, 2H), 6.88 (dd, *J* = 6.6, 3.0 Hz, 1H), 6.78 (d, *J* = 8.4 Hz, 1H), 6.13 (dd, *J* = 10.5, 6.9 Hz, 1H), 3.71 (s, 1.38H), 3.70 (s, 1.63H), 3.56 – 3.38 (m, 1H), 3.14 (dt, *J* = 13.6, 6.4 Hz, 1H), 2.91 (dd, *J* = 13.6, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 174.0, 143.7, 143.6, 141.4, 140.3, 138.7, 138.3, 137.6, 133.4, 133.3, 131.1, 129.6, 129.4, 129.3, 128.6, 128.5, 128.44, 128.4, 128.38, 128.3, 127.8, 127.6, 127.3, 126.6, 126.55, 126.2, 126.15, 52.1, 52.07, 48.2, 48.1, 39.4, 39.3. HRMS (m/z, ESI): calcd for $C_{24}H_{21}ClO_2Na^+$ $(M+Na)^+$ 399.1122, found 399.1122.



3ka

methyl 2-benzyl-4-(4-bromophenyl)-4-phenylbut-3-enoate (**3ka**, *E/Z* = 1.2/1)

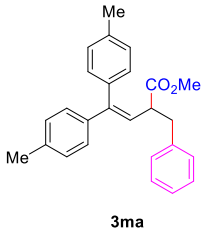
The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 70%, 57.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.23 (m, 2H), 7.24 – 6.98 (m, 7H), 6.98 – 6.84 (m, 3H), 6.75 (dd, *J* = 6.4, 2.9 Hz, 1H), 6.59 (d, *J* = 8.4 Hz, 1H), 6.01 (dd, *J* = 10.5, 4.2 Hz, 1H), 3.58 (s, 1.37H), 3.57 (s, 1.65H), 3.42 – 3.26 (m, 1H), 3.01 (dt, *J* = 13.6, 6.9 Hz, 1H), 2.78 (dd, *J* = 13.6, 8.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 174.0, 143.7, 143.66, 141.3, 140.7, 138.6, 138.3, 138.1, 131.4, 131.3, 129.6, 129.4, 129.3, 129.0, 128.44, 128.4, 128.3, 127.8, 127.6, 127.3, 126.6, 126.55, 126.2, 126.1, 121.7, 121.5, 52.1, 52.07, 48.2, 48.1, 39.3, 39.2. HRMS (m/z, ESI): calcd for $C_{24}H_{21}BrO_2Na^+$ $(M+Na)^+$ 443.0617, found 443.0620.



3la

methyl 4-([1,1'-biphenyl]-4-yl)-2-benzyl-4-phenylbut-3-enoate (**3la**, *E/Z* = 1.3/1)

The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 71%, 59.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.69 (d, *J* = 7.6 Hz, 1H), 7.60 (dd, *J* = 13.0, 7.8 Hz, 2H), 7.56 – 7.44 (m, 3H), 7.44 – 7.18 (m, 9H), 7.09 (t, *J* = 6.4 Hz, 2H), 7.03 – 6.90 (m, 2H), 6.23 (d, *J* = 10.4 Hz, 0.44H), 6.18 (d, *J* = 10.4 Hz, 0.56H), 3.73 (s, 1.57H), 3.71 (s, 1.38H), 3.67 – 3.48 (m, 1H), 3.17 (dt, *J* = 12.4, 6.0 Hz, 1H), 3.01 – 2.91 (m, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 174.25, 144.4, 144.2, 141.8, 140.8, 140.7, 140.67, 140.4, 140.1, 139.1, 138.5, 138.2, 130.2, 129.7, 129.34, 129.3, 128.9, 128.87, 128.4, 128.34, 128.27, 127.7, 127.6, 127.48, 127.45, 127.4, 127.1, 127.07, 127.0, 126.9, 126.5, 125.9, 125.7, 52.03, 52.01, 48.2, 39.4. HRMS (m/z, ESI): calcd for $C_{30}H_{26}O_2Na^+$ $(M+Na)^+$ 441.1825, found 441.1826.

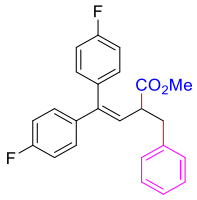


3ma

methyl 2-benzyl-4,4-di-p-tolylbut-3-enoate (3ma)

The general procedure A was followed. Yield: 60%, 44.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 – 7.17 (m, 3H), 7.17 – 6.99 (m, 8H), 6.81 (d, *J* = 7.6 Hz, 2H), 6.07 (d, *J* = 10.4 Hz, 1H), 3.68 (s, 3H), 3.51 (dt, *J* = 10.4, 7.2 Hz, 1H), 3.12 (dd, *J* = 13.5, 6.8 Hz, 1H), 2.91 (dd, *J* = 13.5, 8.0 Hz, 1H), 2.40 (s, 3H), 2.35 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.5, 144.5, 139.3, 138.6, 137.3, 136.9, 136.4, 129.6, 129.3, 129.0, 128.9, 128.4, 127.3, 126.4, 124.7, 52.0, 48.2, 39.5, 21.4, 21.2. HRMS

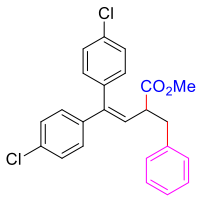
(m/z, ESI): calcd for $C_{26}H_{26}O_2Na^+$ $(M+Na)^+$ 393.1825, found 393.1826.



3na

methyl 2-benzyl-4,4-bis(4-fluorophenyl)but-3-enoate (3na)

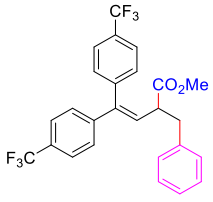
The general procedure A was followed. Yield: 65%, 49.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.30 – 7.17 (m, 3H), 7.17 – 7.09 (m, 2H), 7.09 – 6.92 (m, 6H), 6.80 (dd, *J* = 8.5, 5.7 Hz, 2H), 6.06 (d, *J* = 10.4 Hz, 1H), 3.71 (s, 3H), 3.49 – 3.39 (m, 1H), 3.14 (dd, *J* = 13.4, 6.2 Hz, 1H), 2.90 (dd, *J* = 13.4, 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 162.5 (d, J_{C-F} = 248.2 Hz), 162.2 (d, J_{C-F} = 247.5 Hz), 142.8, 138.3, 137.8 (d, J_{C-F} = 3.2 Hz), 134.8 (d, J_{C-F} = 3.3 Hz), 131.3 (d, J_{C-F} = 8.1 Hz), 129.3, 129.0 (d, J_{C-F} = 8.1 Hz), 128.4, 126.6, 125.9, 115.3 (d, J_{C-F} = 21.3 Hz), 115.2 (d, J_{C-F} = 21.6 Hz), 52.1, 48.2, 39.3. HRMS (m/z, ESI): calcd for $C_{24}H_{20}F_2O_2Na^+$ $(M+Na)^+$ 401.1324, found 401.1323.



3oa

methyl 2-benzyl-4,4-bis(4-chlorophenyl)but-3-enoate (3oa)

The general procedure A was followed. Yield: 65%, 52.4 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.16 (m, 7H), 7.13 – 6.98 (m, 4H), 6.73 (d, *J* = 8.0 Hz, 2H), 6.11 (d, *J* = 10.8 Hz, 1H), 3.71 (s, 3H), 3.42 (td, *J* = 9.7, 6.2 Hz, 1H), 3.14 (dd, *J* = 13.6, 6.0 Hz, 1H), 2.90 (dd, *J* = 13.4, 8.8 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.9, 142.6, 139.8, 138.2, 137.1, 133.7, 133.6, 131.0, 129.3, 128.63, 128.6, 128.5, 128.47, 126.6, 52.2, 48.2, 39.2. HRMS (m/z, ESI): calcd for $C_{24}H_{20}Cl_2O_2Na^+$ $(M+Na)^+$ 433.0733, found 433.0733.

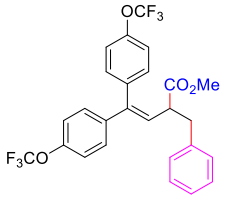


3pa

methyl 2-benzyl-4,4-bis(4-(trifluoromethyl)phenyl)but-3-enoate (3pa)

The general procedure A was followed. Yield: 50%, 48.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.56 (dd, *J* = 12.4, 8.4 Hz, 4H), 7.35 – 7.15 (m, 5H), 7.04 (dd, *J* = 7.1, 2.4 Hz, 2H), 6.90 (d, *J* = 8.0 Hz, 2H), 6.25 (d, *J* = 10.4 Hz, 1H), 3.74 (s, 3H), 3.41 (td, *J* = 10.0, 6.0 Hz, 1H), 3.17 (dd, *J* = 13.6, 5.6 Hz, 1H), 2.92 (dd, *J* = 13.6, 9.2 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.6, 144.4, 142.5, 142.1, 138.0, 130.1, 129.9 (q, J_{C-F} = 32.7 Hz), 129.88 (q, J_{C-F} = 32.6 Hz), 129.4, 128.7, 128.6, 127.6, 126.8, 125.4

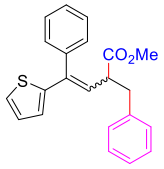
(q, $J_{C\text{-}F}$ = 3.9 Hz), 124.2 (q, $J_{C\text{-}F}$ = 273.1 Hz), 52.3, 48.3, 39.1. HRMS (m/z, ESI): calcd for $C_{26}H_{20}F_6O_2Na^+$ $(M+Na)^+$ 501.1260, found 501.1260.



3qa

methyl 2-benzyl-4,4-bis(4-(trifluoromethoxy)phenyl)but-3-enoate (3qa)

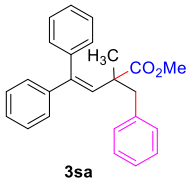
The general procedure A was followed. Yield: 65%, 64.7 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.19 (m, 3H), 7.19 – 7.07 (m, 6H), 7.06 – 6.97 (m, 2H), 6.81 (d, *J* = 8.4 Hz, 2H), 6.11 (d, *J* = 10.4 Hz, 1H), 3.71 (s, 3H), 3.41 (td, *J* = 9.2, 6.0 Hz, 1H), 3.13 (dd, *J* = 13.6, 6.0 Hz, 1H), 2.87 (dd, *J* = 13.6, 9.2 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.9, 148.9 (q, $J_{C\text{-}F}$ = 1.9 Hz), 148.7 (q, $J_{C\text{-}F}$ = 1.8 Hz), 142.4, 140.1, 138.2, 137.2, 131.1, 129.3, 128.7, 128.5, 127.2, 126.7, 120.9, 120.8, 120.6 (q, $J_{C\text{-}F}$ = 258.3 Hz), 120.58 (q, $J_{C\text{-}F}$ = 258.3 Hz), 52.2, 48.2, 39.2. HRMS (m/z, ESI): calcd for $C_{26}H_{20}F_6O_4Na^+$ $(M+Na)^+$ 533.1158, found 533.1160.



3ra

methyl 2-benzyl-4-phenyl-4-(thiophen-2-yl)but-3-enoate (**3ra**, *E/Z* = 2.1/1)

The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 60%, 40.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.17 (m, 8H), 7.17 – 7.10 (m, 1.43H), 7.08 – 6.99 (m, 1.32H), 6.97 – 6.86 (m, 1H), 6.79 (d, *J* = 3.6 Hz, 0.70H), 6.57 (d, *J* = 3.6 Hz, 0.29H), 6.18 (d, *J* = 10.4 Hz, 0.32H), 6.13 (d, *J* = 10.4 Hz, 0.68H), 3.85 (dt, *J* = 10.4, 7.4 Hz, 0.73H), 3.69 (s, 2H), 3.68 (s, 1H), 3.42 – 3.31 (m, 0.30H), 3.19 (dd, *J* = 13.6, 7.2 Hz, 0.71H), 3.10 (dd, *J* = 13.4, 6.6 Hz, 0.32H), 2.99 (dd, *J* = 13.6, 7.6 Hz, 0.71H), 2.89 (dd, *J* = 13.4, 8.2 Hz, 0.32H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.0, 173.97, 146.2, 142.1, 140.3, 138.7, 138.4, 138.3, 138.2, 137.5, 129.4, 129.35, 129.2, 128.6, 128.4, 128.39, 128.3, 128.25, 128.2, 127.9, 127.7, 127.6, 127.3, 126.9, 126.6, 126.5, 126.3, 126.0, 124.7, 124.2, 52.1, 52.0, 48.3, 48.0, 39.5, 39.3. HRMS (m/z, ESI): calcd for $C_{22}H_{20}O_2SNa^+$ $(M+Na)^+$ 371.1076, found 371.1075.

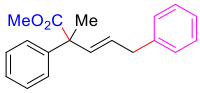


3sa

methyl 2-benzyl-2-methyl-4,4-diphenylbut-3-enoate (3sa)

The general procedure A was followed. Yield: 65%, 46.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.11 (m, 13H), 7.10 – 7.01 (m, 2H), 6.10 (s, 1H), 3.28 (s, 3H), 3.14 (d, *J* = 13.1 Hz, 1H), 2.99 (d, *J* = 13.1 Hz, 1H), 1.18 (s, 3H).^{13}C NMR (101 MHz,

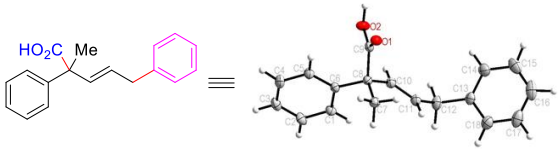
Chloroform-*d*) δ 175.7, 143.4, 142.0, 139.3, 137.1, 132.9, 130.7, 130.1, 128.2, 128.1, 128.0, 127.4, 127.34, 127.3, 126.8, 51.6, 49.0, 47.0, 23.8. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_2Na^+$ $(M+Na)^+$ 379.1669, found 379.1669.



5aa

methyl (*E*)-2-methyl-2,5-diphenylpent-3-enoate (5aa)

The general procedure A was followed. Yield: 49%, 27.4 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 – 7.03 (m, 10H), 6.04 (d, *J* = 15.6 Hz, 1H), 5.63 (dt, *J* = 15.6, 7.4 Hz, 1H), 3.62 (s, 3H), 3.40 (d, *J* = 6.8 Hz, 2H), 1.56 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.6, 144.2, 140.4, 134.5, 129.7, 128.6, 128.58, 128.5, 126.9, 126.5, 126.2, 53.3, 52.5, 39.2, 24.5. HRMS (m/z, ESI): calcd for $C_{19}H_{20}O_2Na^+$ $(M+Na)^+$ 303.1356, found 303.1355.

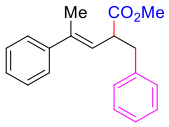


5aa'

X-Ray of 5aa'
CCDC(2116857)

(*E*)-2-methyl-2,5-diphenylpent-3-enoic acid (5aa')

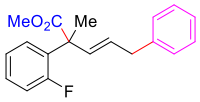
5aa' was obtained without methylation work-up of the reaction. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.14 (m, 10H), 6.12 (d, *J* = 15.6 Hz, 1H), 5.74 (dt, *J* = 14.9, 6.9 Hz, 1H), 3.47 (d, *J* = 6.9 Hz, 2H), 1.65 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 181.1, 143.4, 140.2, 134.0, 130.2, 128.7, 128.6, 128.6, 127.2, 126.7, 126.3, 53.1, 39.2, 24.1. HRMS (m/z, ESI): calcd for $C_{18}H_{18}O_2Na^+$ $(M+Na)^+$ 289.1199, found 289.1200.



6aa

methyl (*E*)-2-benzyl-4-phenylpent-3-enoate (6aa)

The general procedure A was followed. Yield: 15%, 8.7 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.36 – 6.97 (m, 10H), 5.71 (d, *J* = 10.0 Hz, 1H), 3.67 – 3.59 (m, 1H), 3.58 (s, 3H), 3.10 (dd, *J* = 13.4, 7.0 Hz, 1H), 2.79 (dd, *J* = 13.6, 8.0 Hz, 1H), 1.77 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 143.3, 138.9, 138.4, 129.3, 128.5, 128.3, 127.3, 126.5, 126.0, 125.0, 52.0, 47.8, 39.2, 16.3. HRMS (m/z, ESI): calcd for $C_{19}H_{20}O_2Na^+$ $(M+Na)^+$ 303.1356, found 303.1355.

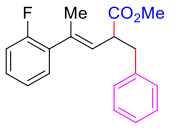


5ba

methyl (*E*)-2-(2-fluorophenyl)-2-methyl-5-phenylpent-3-enoate (5ba)

The general procedure A was followed. Yield: 46%, 27.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.20 (m, 7H), 7.16 (t, *J* = 7.4 Hz, 1H), 7.07 (dd, *J* = 10.8, 8.4 Hz, 1H), 6.10 (d, *J* = 15.2 Hz, 1H), 5.77 (dt, *J* = 15.6, 6.8 Hz, 1H), 3.76 (s, 3H), 3.53 (d, *J* = 6.8 Hz, 2H), 1.69 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.2, 160.5

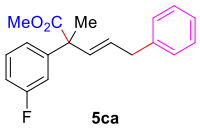
(d, $J_{C\text{-}F}$ = 247.7 Hz), 140.1, 133.0, 131.9 (d, $J_{C\text{-}F}$ = 13.3 Hz), 130.5, 128.9, 128.8, 128.6, 127.9 (d, $J_{C\text{-}F}$ = 4.3 Hz), 126.3, 124.1 (d, $J_{C\text{-}F}$ = 3.3 Hz), 115.8 (d, $J_{C\text{-}F}$ = 22.4 Hz), 52.6, 50.3, 39.0, 23.1. HRMS (m/z, ESI): calcd for $C_{19}H_{19}FO_2Na^+$ $(M+Na)^+$ 321.1261, found 321.1263.



6ba

methyl (*E*)-2-benzyl-4-(2-fluorophenyl)pent-3-enoate (6ba)

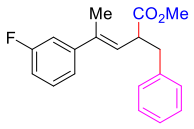
The general procedure A was followed. Yield: 17%, 10.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.05 (m, 7H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.95 (dd, *J* = 11.0, 8.2 Hz, 1H), 5.60 (d, *J* = 9.6 Hz, 1H), 3.71 – 3.58 (m, 4H), 3.13 (dd, *J* = 13.4, 7.0 Hz, 1H), 2.83 (dd, *J* = 13.2, 8.0 Hz, 1H), 1.76 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 159.9 (d, $J_{C\text{-}F}$ = 248.2 Hz), 138.7, 135.0, 132.0 (d, $J_{C\text{-}F}$ = 14.0 Hz), 129.8 (d, $J_{C\text{-}F}$ = 4.4 Hz), 129.3, 128.7 (d, $J_{C\text{-}F}$ = 8.3 Hz), 128.5, 128.1 (d, $J_{C\text{-}F}$ = 2.1 Hz), 126.6, 124.0 (d, $J_{C\text{-}F}$ = 3.4 Hz), 115.8 (d, $J_{C\text{-}F}$ = 22.6 Hz), 52.0, 47.4, 39.1, 17.2 (d, $J_{C\text{-}F}$ = 3.6 Hz). HRMS (m/z, ESI): calcd for $C_{19}H_{19}FO_2Na^+$ $(M+Na)^+$ 321.1261, found 321.1261.



5ca

methyl (*E*)-2-(3-fluorophenyl)-2-methyl-5-phenylpent-3-enoate (5ca)

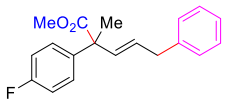
The general procedure A was followed. Yield: 50%, 30.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.08 (m, 6H), 6.97 (d, *J* = 7.6 Hz, 1H), 6.92 (dt, *J* = 10.4, 2.2 Hz, 1H), 6.87 (td, *J* = 8.3, 2.6 Hz, 1H), 6.01 (d, *J* = 15.6 Hz, 1H), 5.65 (dt, *J* = 15.6, 6.8 Hz, 1H), 3.64 (s, 3H), 3.41 (d, *J* = 6.8 Hz, 2H), 1.56 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.1, 162.9 (d, $J_{C\text{-}F}$ = 246.4 Hz), 146.7 (d, $J_{C\text{-}F}$ = 6.9 Hz), 140.1, 133.8, 130.2, 130.0, 129.9, 128.6, 126.3, 122.3 (d, $J_{C\text{-}F}$ = 2.9 Hz), 114.0 (d, $J_{C\text{-}F}$ = 2.1 Hz), 113.8, 53.1 (d, $J_{C\text{-}F}$ = 1.7 Hz), 52.6, 39.1, 24.3. HRMS (m/z, ESI): calcd for $C_{19}H_{19}FO_2Na^+$ $(M+Na)^+$ 321.1261, found 321.1261.



6ca

methyl (*E*)-2-benzyl-4-(3-fluorophenyl)pent-3-enoate (6ca)

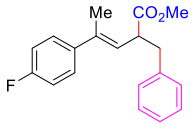
The general procedure A was followed. Yield: 14%, 8.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.16 (m, 6H), 7.13 (d, *J* = 8.0 Hz, 1H), 7.03 (dt, *J* = 10.4, 2.2 Hz, 1H), 6.96 (td, *J* = 8.4, 2.8 Hz, 1H), 5.83 (d, *J* = 9.6 Hz, 1H), 3.76 – 3.63 (m, 4H), 3.21 (dd, *J* = 13.4, 7.0 Hz, 1H), 2.89 (dd, *J* = 13.2, 8.0 Hz, 1H), 1.83 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 162.9 (d, $J_{C\text{-}F}$ = 245.9 Hz), 145.5 (d, $J_{C\text{-}F}$ = 7.5 Hz), 138.7, 137.3 (d, $J_{C\text{-}F}$ = 2.3 Hz), 129.7 (d, $J_{C\text{-}F}$ = 8.5 Hz), 129.3, 128.5, 126.6, 125.9, 121.6 (d, $J_{C\text{-}F}$ = 2.7 Hz), 114.0 (d, $J_{C\text{-}F}$ = 21.3 Hz), 112.9 (d, $J_{C\text{-}F}$ = 22.0 Hz), 52.1, 47.7, 39.2, 16.2. HRMS (m/z, ESI): calcd for $C_{19}H_{19}FO_2Na^+$ $(M+Na)^+$ 321.1261, found 321.1260.



5da

methyl (*E*)-2-(4-fluorophenyl)-2-methyl-5-phenylpent-3-enoate (5da)

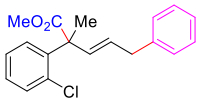
The general procedure A was followed. Yield: 34%, 20.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 (t, *J* = 7.4 Hz, 2H), 7.30 – 7.19 (m, 5H), 7.04 (t, *J* = 8.8 Hz, 2H), 6.12 (d, *J* = 15.6 Hz, 1H), 5.73 (dt, *J* = 15.7, 6.8 Hz, 2H), 3.74 (s, 3H), 3.51 (d, *J* = 6.8 Hz, 2H), 1.66 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.5, 161.7 (d, J_{C-F} = 246.4 Hz), 140.2, 139.8 (d, J_{C-F} = 3.3 Hz), 134.4, 129.9, 128.6, 128.3, 128.2, 126.3, 115.3 (d, J_{C-F} = 21.4 Hz), 52.8, 52.5, 39.1, 24.6. HRMS (m/z, ESI): calcd for $C_{19}H_{19}FO_2Na^+$ $(M+Na)^+$ 321.1261, found 321.1261.



6da

methyl (*E*)-2-benzyl-4-(4-fluorophenyl)pent-3-enoate (6da)

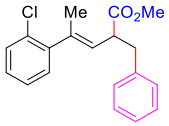
The general procedure A was followed. Yield: 8%, 6.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.33 – 7.24 (m, 4H), 7.24 – 7.15 (m, 3H), 6.99 (t, *J* = 8.8 Hz, 2H), 5.73 (d, *J* = 9.6 Hz, 1H), 3.75 – 3.61 (m, 4H), 3.18 (dd, *J* = 13.6, 7.2 Hz, 1H), 2.87 (dd, *J* = 13.4, 7.8 Hz, 1H), 1.82 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 162.2 (d, J_{C-F} = 246.9 Hz), 139.3 (d, J_{C-F} = 3.0 Hz), 138.8, 137.4, 129.3, 128.5, 127.5 (d, J_{C-F} = 7.9 Hz), 126.6, 124.9, 115.1 (d, J_{C-F} = 21.3 Hz), 52.0, 47.7, 39.2, 16.4. HRMS (m/z, ESI): calcd for $C_{19}H_{19}FO_2Na^+$ $(M+Na)^+$ 321.1261, found 321.1262.



5ea

methyl (*E*)-2-(2-chlorophenyl)-2-methyl-5-phenylpent-3-enoate (5ea)

The general procedure A was followed. Yield: 45%, 28.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.32 (ddd, *J* = 16.5, 7.6, 1.7 Hz, 2H), 7.25 – 7.09 (m, 7H), 6.11 (d, *J* = 15.7 Hz, 1H), 5.57 (dt, *J* = 15.7, 6.9 Hz, 1H), 3.65 (s, 3H), 3.41 (d, *J* = 6.8 Hz, 2H), 1.64 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.4, 141.6, 140.1, 133.8, 133.7, 130.7, 130.4, 128.6, 128.58, 128.56, 128.4, 126.9, 126.3, 53.1, 52.7, 39.1, 23.3. HRMS (m/z, ESI): calcd for $C_{19}H_{19}ClO_2Na^+$ $(M+Na)^+$ 337.0966, found 337.0965.

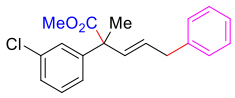


6ea

methyl (*E*)-2-benzyl-4-(2-chlorophenyl)pent-3-enoate (6ea)

The general procedure A was followed. Yield: 19%, 12.3 mg.^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.16 (m, 8H), 7.12 – 7.06 (m, 1H), 5.48 (d, *J* = 10.0 Hz, 1H), 3.76 – 3.66 (m, 4H), 3.20 (dd, *J* = 13.5, 6.8 Hz, 1H), 2.90 (dd, *J* = 13.6, 8.0 Hz, 1H), 1.83 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 143.6, 138.8, 138.4, 132.3,

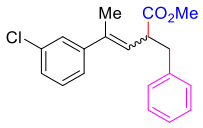
130.1, 129.6, 129.3, 128.5, 128.3, 127.8, 126.7, 126.6, 52.0, 47.2, 38.9, 17.7. HRMS (m/z, ESI): calcd for $C_{19}H_{19}ClO_2Na^+$ $(M+Na)^+$ 337.0966, found 337.0966.



5fa

methyl (*E*)-2-(3-chlorophenyl)-2-methyl-5-phenylpent-3-enoate (5fa)

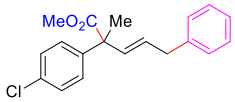
The general procedure A was followed. Yield: 43%, 27.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.24 (t, *J* = 7.0 Hz, 2H), 7.21 – 7.10 (m, 6H), 7.06 (dt, *J* = 7.1, 1.9 Hz, 1H), 6.00 (d, *J* = 15.6 Hz, 1H), 5.65 (dt, *J* = 15.6, 6.8 Hz, 2H), 3.64 (s, 3H), 3.41 (d, *J* = 6.8 Hz, 2H), 1.55 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.0, 146.2, 140.1, 134.4, 133.8, 130.4, 129.8, 128.64, 128.6, 127.2, 126.9, 126.3, 124.9, 53.2, 52.6, 39.1, 24.3. HRMS (m/z, ESI): calcd for $C_{19}H_{19}ClO_2Na^+$ $(M+Na)^+$ 337.0966, found 337.0966.



6fa

methyl 2-benzyl-4-(3-chlorophenyl)pent-3-enoate (6fa, *E/Z* = 6.9/1)

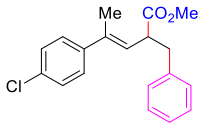
The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 17%, 10.8 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.34 – 7.10 (m, 9H), 5.79 (d, *J* = 9.8 Hz, 0.83H), 5.50 (d, *J* = 10.5 Hz, 0.12H), 3.65 (d, *J* = 10.9 Hz, 4H), 3.30 – 3.22 (m, 0.15H), 3.18 (dd, *J* = 13.5, 6.9 Hz, 0.84H), 3.00 (dd, *J* = 13.4, 6.3 Hz, 0.15H), 2.86 (dd, *J* = 13.4, 8.0 Hz, 0.84H), 2.73 (dd, *J* = 13.5, 8.5 Hz, 0.14H), 1.95 (s, 0.40H), 1.80 (s, 2.43H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 174.1, 145.1, 143.0, 139.4, 138.6, 138.5, 137.2, 134.2, 129.55, 129.49, 129.3, 129.2, 128.5, 128.4, 127.8, 127.2, 127.1, 126.6, 126.5, 126.2, 126.04, 125.97, 124.8, 124.1, 52.1, 52.0, 47.7, 47.65, 39.7, 39.2, 25.8, 16.1. HRMS (m/z, ESI): calcd for $C_{19}H_{19}ClO_2Na^+$ $(M+Na)^+$ 337.0966, found 337.0966.



5ga

methyl (*E*)-2-(4-chlorophenyl)-2-methyl-5-phenylpent-3-enoate (5ga)

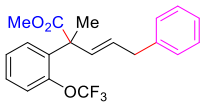
The general procedure A was followed. Yield: 42%, 26.2 mg.^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.27 (m, 4H), 7.25 – 7.13 (m, 5H), 6.08 (d, *J* = 15.6 Hz, 1H), 5.70 (dt, *J* = 15.6, 6.9 Hz, 1H), 3.71 (s, 3H), 3.48 (d, *J* = 6.8 Hz, 2H), 1.63 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.2, 142.6, 140.2, 134.1, 132.8, 130.2, 128.64, 128.63, 128.61, 128.1, 126.3, 52.9, 52.6, 39.1, 24.4. HRMS (m/z, ESI): calcd for $C_{19}H_{19}ClO_2Na^+$ $(M+Na)^+$ 337.0966, found 337.0966.



6ga

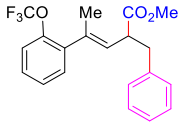
methyl (*E*)-2-benzyl-4-(4-chlorophenyl)pent-3-enoate (6ga)

The general procedure A was followed. Yield: 8%, 5.7 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.13 (m, 9H), 5.77 (d, *J* = 10.0 Hz, 1H), 3.74 – 3.63 (m, 4H), 3.18 (dd, *J* = 13.6, 6.8 Hz, 1H), 2.87 (dd, *J* = 13.2, 8.0 Hz, 1H), 1.81 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 141.6, 138.7, 137.3, 133.1, 129.3, 128.5, 128.45, 127.3, 126.6, 125.4, 52.1, 47.7, 39.2, 16.2. HRMS (m/z, ESI): calcd for $C_{19}H_{19}ClO_2Na^+$ $(M+Na)^+$ 337.0966, found 337.0966.



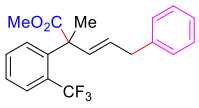
5ha

methyl (*E*)-2-methyl-5-phenyl-2-(2-(trifluoromethoxy)phenyl)pent-3-enoate (5ha)
The general procedure A was followed. Yield: 39%, 28.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.39 (dd, *J* = 7.6, 2.0 Hz, 1H), 7.35 – 7.27 (m, 3H), 7.27 – 7.16 (m, 5H), 6.07 (d, *J* = 15.6 Hz, 1H), 5.70 (dt, *J* = 15.6, 6.8 Hz, 1H), 3.70 (s, 3H), 3.48 (d, *J* = 6.8 Hz, 2H), 1.63 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.0, 147.4, 140.1, 135.3, 133.4, 130.7, 128.6, 128.63, 128.61, 128.55, 126.3, 125.9, 120.5 (q, J_{C-F} = 260.1 Hz), 117.7 (q, J_{C-F} = 2.1 Hz), 52.4, 50.9, 39.1, 23.2. HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_3Na^+$ $(M+Na)^+$ 387.1178, found 387.1177.



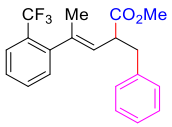
6ha

methyl (*E*)-2-benzyl-4-(2-(trifluoromethoxy)phenyl)pent-3-enoate (6ha)
The general procedure A was followed. Yield: 24%, 17.7 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.09 (m, 9H), 5.53 (d, *J* = 10.0 Hz, 1H), 3.75 – 3.60 (m, 4H), 3.17 (dd, *J* = 13.6, 6.8 Hz, 1H), 2.86 (dd, *J* = 13.6, 8.0 Hz, 1H), 1.82 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.0, 146.2 (q, J_{C-F} = 1.8 Hz), 138.8, 138.2, 135.6, 130.3, 129.2, 128.6, 128.5, 128.4, 126.9, 126.6, 121.0 (q, J_{C-F} = 1.6 Hz), 120.6 (q, J_{C-F} = 257.2 Hz), 52.0, 47.3, 38.7, 17.5. HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_3Na^+$ $(M+Na)^+$ 387.1178, found 387.1178.



5ia

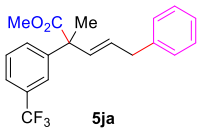
methyl (*E*)-2-methyl-5-phenyl-2-(2-(trifluoromethyl)phenyl)pent-3-enoate (5ia)
The general procedure A was followed. Yield: 14%, 9.7 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 (d, *J* = 8.0 Hz, 1H), 7.58 – 7.49 (m, 2H), 7.41 (t, *J* = 7.6 Hz, 1H), 7.33 – 7.24 (m, 2H), 7.24 – 7.11 (m, 3H), 6.24 (d, *J* = 15.6 Hz, 1H), 5.44 (dt, *J* = 15.6, 6.8 Hz, 1H), 3.68 (s, 3H), 3.43 (d, *J* = 6.8 Hz, 2H), 1.74 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.2, 141.1, 140.1, 135.7, 131.7, 129.9, 128.9, 128.8 (q, J_{C-F} = 5.2 Hz), 128.6, 128.55, 128.5, 127.5, 126.2, 124.6 (q, J_{C-F} = 275.1 Hz), 53.3, 52.4, 39.0, 26.4. HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_2Na^+$ $(M+Na)^+$ 371.1229, found 371.1229.



6ia

methyl (*E*)-2-benzyl-4-(2-(trifluoromethyl)phenyl)pent-3-enoate (6ia)

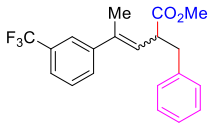
The general procedure A was followed. Yield: 50%, 35.2 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.63 (d, *J* = 8.0 Hz, 1H), 7.46 (t, *J* = 7.6 Hz, 1H), 7.37 – 7.28 (m, 3H), 7.24 (t, *J* = 7.2 Hz, 3H), 7.10 (d, *J* = 7.6 Hz, 1H), 5.39 (d, *J* = 10.0 Hz, 1H), 3.77 – 3.68 (m, 1H), 3.68 (s, 3H), 3.18 (dd, *J* = 13.6, 7.2 Hz, 1H), 2.88 (dd, *J* = 13.6, 7.6 Hz, 1H), 1.85 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.9, 144.0 (q, J_{C-F} = 2.0 Hz), 138.9, 137.2, 131.5, 130.1, 129.2, 128.4, 127.8 (d, J_{C-F} = 30.0 Hz), 127.5 (q, J_{C-F} = 1.8 Hz), 127.0, 126.5, 126.1 (q, J_{C-F} = 5.3 Hz), 124.3 (q, J_{C-F} = 274.9 Hz), 51.9, 47.3, 38.5, 19.1 (q, J_{C-F} = 2.1 Hz). HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_2Na^+$ $(M+Na)^+$ 371.1229, found 371.1230.



5ja

methyl (*E*)-2-methyl-5-phenyl-2-(3-(trifluoromethyl)phenyl)pent-3-enoate (5ja)

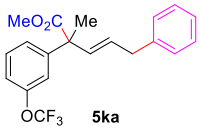
The general procedure A was followed. Yield: 43%, 30.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.59 – 7.38 (m, 4H), 7.33 (t, *J* = 7.4 Hz, 2H), 7.27 – 7.15 (m, 3H), 6.09 (d, *J* = 15.6 Hz, 1H), 5.75 (dt, *J* = 15.6, 6.8 Hz, 1H), 3.73 (s, 3H), 3.50 (d, *J* = 7.2 Hz, 2H), 1.67 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.0, 145.2, 140.0, 133.7, 130.8 (q, J_{C-F} = 32.1 Hz), 130.77, 130.2, 129.0, 128.7, 128.6, 126.4, 124.1 (q, J_{C-F} = 265.6 Hz), 123.9 (q, J_{C-F} = 3.8 Hz), 123.5 (q, J_{C-F} = 3.9 Hz), 53.3, 52.7, 39.1, 24.4. HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_2Na^+$ $(M+Na)^+$ 371.1229, found 371.1230.



6ja

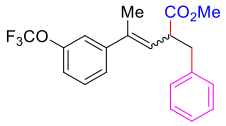
methyl 2-benzyl-4-(3-(trifluoromethyl)phenyl)pent-3-enoate (6ja, *E/Z* = 14.3/1)

The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 17%, 12.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.57 (s, 1H), 7.55 – 7.48 (m, 2H), 7.44 (t, *J* = 7.7 Hz, 1H), 7.35 – 7.28 (m, 2H), 7.28 – 7.16 (m, 3H), 5.85 (d, *J* = 9.6 Hz, 1H), 5.57 (d, *J* = 10.8 Hz, 0.07H), 3.79 – 3.64 (m, 4H), 3.23 (dd, *J* = 13.4, 6.9 Hz, 1H), 3.04 (dd, *J* = 13.4, 6.3 Hz, 0.11H), 2.91 (dd, *J* = 13.4, 8.0 Hz, 1H), 2.77 (dd, *J* = 13.4, 8.7 Hz, 0.10H), 2.01 (s, 0.27H), 1.88 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 144.0, 138.6, 137.3, 130.7 (q, J_{C-F} = 32.5 Hz), 129.3, 129.2, 128.8, 128.5, 126.7, 126.5, 124.3 (q, J_{C-F} = 273.2 Hz), 123.9 (q, J_{C-F} = 11.4 Hz), 122.8 (q, J_{C-F} = 11.4 Hz), 52.1, 47.7, 39.2, 16.2. HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_2Na^+$ $(M+Na)^+$ 371.1229, found 371.1230.



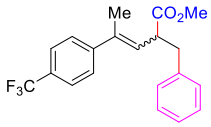
5ka

methyl (*E*)-2-methyl-5-phenyl-2-(3-(trifluoromethoxy)phenyl)pent-3-enoate (5ka)
The general procedure A was followed. Yield: 39%, 28.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.38 – 7.28 (m, 3H), 7.26 – 7.17 (m, 4H), 7.16 – 7.08 (m, 2H), 6.07 (d, *J* = 16.0 Hz, 1H), 5.74 (dt, *J* = 16.0, 7.0 Hz, 1H), 3.72 (s, 3H), 3.49 (d, *J* = 6.8 Hz, 2H), 1.64 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.0, 149.4 (q, $J_{C\text{-}F}$ = 1.6 Hz), 146.6, 140.1, 133.7, 130.6, 129.8, 128.7, 128.6, 126.4, 125.0, 120.6 (q, $J_{C\text{-}F}$ = 258.2 Hz), 119.6, 119.3, 53.2, 52.6, 39.2, 24.4. HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_3Na^+$ $(M+Na)^+$ 387.1178, found 387.1177.



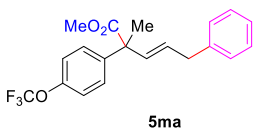
6ka

methyl 2-benzyl-4-(3-(trifluoromethoxy)phenyl)pent-3-enoate (6ka, *E/Z* = 12.5/1)
The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 20%, 14.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.21 (m, 7H), 7.20 (s, 1H), 7.15 (d, *J* = 8.0 Hz, 1H), 7.06 – 7.00 (m, 0.18H), 6.83 (d, *J* = 7.6 Hz, 0.08H), 6.73 (s, 0.07H), 5.87 (d, *J* = 10.0 Hz, 1H), 5.57 (d, *J* = 10.4 Hz, 0.08H), 3.80 – 3.67 (m, 4H), 3.37 – 3.28 (m, 0.12H), 3.25 (dd, *J* = 13.6, 6.8 Hz, 1H), 3.07 (dd, *J* = 13.6, 6.4 Hz, 0.11H), 2.93 (dd, *J* = 13.4, 8.0 Hz, 1H), 2.80 (dd, *J* = 13.4, 8.6 Hz, 0.09H), 2.03 (s, 0.26H), 1.87 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 174.1, 149.4 (q, $J_{C\text{-}F}$ = 2.0 Hz), 145.3, 143.3, 139.2, 138.6, 137.1, 129.6, 129.3, 129.2, 128.5, 128.3, 126.7, 126.5, 126.3, 126.2, 125.1, 124.4, 120.6 (q, $J_{C\text{-}F}$ = 257.9 Hz), 120.4, 119.5, 118.7, 52.1, 51.9, 47.7, 47.6, 39.15, 39.07, 25.7, 16.2. HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_3Na^+$ $(M+Na)^+$ 387.1178, found 387.1177.



6la

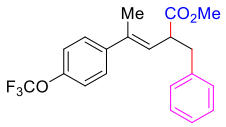
methyl 2-benzyl-4-(4-(trifluoromethyl)phenyl)pent-3-enoate (6la) (*E/Z* = 5.9/1)
The corresponding substrate contained inseparable *E/Z* isomers. The general procedure A was followed. Yield: 50%, 35.7 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.58 (d, *J* = 8.2 Hz, 2H), 7.52 (d, *J* = 8.0 Hz, 0.47H), 7.44 (d, *J* = 8.1 Hz, 2H), 7.34 – 7.28 (m, 2H), 7.28 – 7.17 (m, 3H), 7.04 – 6.98 (m, 0.36H), 6.92 (d, *J* = 7.9 Hz, 0.34H), 5.88 (d, *J* = 9.6 Hz, 1H), 5.58 (d, *J* = 10.4 Hz, 0.17H), 3.82 – 3.69 (s, 4H), 3.68 (s, 0.58H), 3.23 (dd, *J* = 13.2, 6.8 Hz, 1H), 3.04 (dd, *J* = 13.2, 6.4 Hz, 0.20H), 2.91 (dd, *J* = 13.6, 8.0 Hz, 1H), 2.77 (dd, *J* = 13.4, 8.6 Hz, 0.19H), 2.01 (s, 0.53H), 1.86 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.3, 174.0, 146.7, 145.0, 139.5, 138.6, 138.5, 137.4, 129.3, 129.26, 129.2 (q, $J_{C\text{-}F}$ = 32.5 Hz), 128.5, 128.4, 128.1, 126.9, 126.7, 126.5, 126.3, 125.3 (q, $J_{C\text{-}F}$ = 3.8 Hz), 125.2, 125.1 ,124.4 (q, $J_{C\text{-}F}$ = 272.8 Hz), 52.1, 52.0, 47.7, 47.66, 39.2, 39.1, 25.7, 16.1. HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_2Na^+$ $(M+Na)^+$ 371.1229, found 371.1230.



5ma

methyl (*E*)-2-methyl-5-phenyl-2-(4-(trifluoromethoxy)phenyl)pent-3-enoate (5ma)

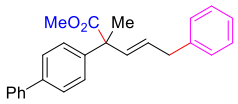
The general procedure A was followed. Yield: 50%, 36.1 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.27 (m, 4H), 7.26 – 7.14 (m, 5H), 6.10 (d, *J* = 15.6 Hz, 1H), 5.74 (dt, *J* = 15.6, 6.8 Hz, 1H), 3.73 (s, 3H), 3.49 (d, *J* = 6.8 Hz, 2H), 1.65 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.2, 148.1 (q, J_{C-F} = 1.9 Hz), 142.8, 140.1, 134.0, 130.3, 128.7, 128.6, 128.1, 126.3, 120.9, 120.6 (q, J_{C-F} = 258.1 Hz), 52.9, 52.6, 39.2, 24.5. HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_3Na^+$ $(M+Na)^+$ 387.1178, found 387.1180.



6ma

methyl (*E*)-2-benzyl-4-(4-(trifluoromethoxy)phenyl)pent-3-enoate (6ma)

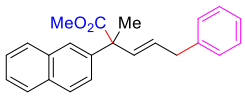
The general procedure A was followed. Yield: 11%, 8.5 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.35 – 7.24 (m, 4H), 7.24 – 7.11 (m, 5H), 5.77 (d, *J* = 9.7 Hz, 1H), 3.73 – 3.63 (m, 4H), 3.19 (dd, *J* = 13.6, 6.8 Hz, 1H), 2.87 (dd, *J* = 13.6, 8.0 Hz, 1H), 1.82 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.2, 148.4 (J_{C-F} = 1.9 Hz), 142.0, 138.7, 137.2, 129.3, 128.5, 127.3, 126.6, 125.8, 120.8, 120.6 (q, J_{C-F} = 256.9 Hz), 52.1, 47.7, 39.2, 16.3. HRMS (m/z, ESI): calcd for $C_{20}H_{19}F_3O_3Na^+$ $(M+Na)^+$ 387.1178, found 387.1178.



5na

methyl (*E*)-2-([1,1'-biphenyl]-4-yl)-2-methyl-5-phenylpent-3-enoate (5na)

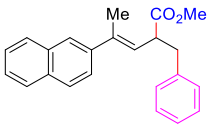
The general procedure A was followed. Yield: 57%, 40.9 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.53 (dd, *J* = 11.0, 7.8 Hz, 4H), 7.39 (t, *J* = 7.5 Hz, 2H), 7.34 – 7.27 (m, 5H), 7.22 – 7.13 (m, 3H), 6.12 (d, *J* = 15.6 Hz, 1H), 5.71 (dt, *J* = 15.6, 6.8 Hz, 1H), 3.69 (s, 3H), 3.46 (d, *J* = 6.8 Hz, 2H), 1.64 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.6, 143.2, 140.8, 140.3, 139.8, 134.4, 129.8, 128.9, 128.7, 128.6, 127.4, 127.3, 127.2, 127.0, 126.3, 53.1, 52.5, 39.2, 24.4. HRMS (m/z, ESI): calcd for $C_{25}H_{24}O_2Na^+$ $(M+Na)^+$ 379.1668, found 379.1668.



5oa

methyl (*E*)-2-methyl-2-(naphthalen-2-yl)-5-phenylpent-3-enoate (5oa)

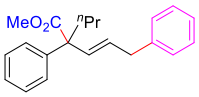
The general procedure A was followed. Yield: 45%, 29.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.85 (d, *J* = 8.0 Hz, 3H), 7.77 (s, 1H), 7.58 – 7.47 (m, 2H), 7.47 – 7.33 (m, 3H), 7.29 (d, *J* = 7.2 Hz, 3H), 6.29 (d, *J* = 15.6 Hz, 1H), 5.81 (dt, *J* = 15.6, 6.5 Hz, 1H), 3.78 (s, 3H), 3.57 (d, *J* = 6.4 Hz, 2H), 1.80 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.7, 141.5, 140.4, 134.4, 133.3, 132.4, 130.1, 128.7, 128.6, 128.19, 128.15, 127.6, 126.27, 126.25, 126.0, 125.3, 124.9, 53.4, 52.5, 39.2, 24.4. HRMS (m/z, ESI): calcd for $C_{23}H_{22}O_2Na^+$ $(M+Na)^+$ 353.1512, found 353.1512.



6oa

methyl (*E*)-2-benzyl-4-(naphthalen-2-yl)pent-3-enoate (6oa)

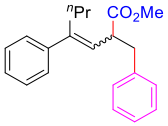
The general procedure A was followed. Yield: 7%, 5.0 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.87 – 7.79 (m, 3H), 7.77 (s, 1H), 7.59 – 7.44 (m, 4H), 7.36 – 7.21 (m, 4H), 5.99 (d, *J* = 9.6 Hz, 1H), 3.80 (dt, *J* = 9.6, 7.4 Hz, 1H), 3.72 (s, 3H), 3.25 (dd, *J* = 13.6, 7.2 Hz, 1H), 2.95 (dd, *J* = 13.4, 7.8 Hz, 1H), 1.99 (s, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.4, 140.4, 138.9, 138.2, 133.5, 132.8, 129.3, 128.5, 128.2, 127.8, 127.6, 126.6, 126.3, 125.9, 125.5, 124.6, 124.5, 52.1, 47.9, 39.3, 16.3. HRMS (m/z, ESI): calcd for $C_{23}H_{22}O_2Na^+$ $(M+Na)^+$ 353.1512, found 353.1512.



5pa

methyl (*E*)-2,5-diphenyl-2-propylpent-3-enoate (5pa)

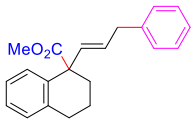
The general procedure A was followed. Yield: 50%, 31.3 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.22 (t, *J* = 7.8 Hz, 4H), 7.19 – 7.14 (m, 3H), 7.11 (t, *J* = 7.3 Hz, 3H), 6.05 (d, *J* = 16.0 Hz, 1H), 5.50 (dt, *J* = 16.0, 6.9 Hz, 1H), 3.61 (s, 3H), 3.38 (d, *J* = 7.2 Hz, 2H), 2.12 – 1.90 (m, 2H), 1.24 – 1.02 (m, 2H), 0.82 (t, *J* = 7.4 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 175.4, 142.8, 140.4, 133.7, 130.5, 128.6, 128.5, 128.3, 127.3, 126.8, 126.2, 57.1, 52.3, 39.8, 39.3, 18.3, 14.7. HRMS (m/z, ESI): calcd for $C_{21}H_{24}O_2Na^+$ $(M+Na)^+$ 331.1668, found 331.1665.



6pa

methyl 2-benzyl-4-phenylhept-3-enoate (**6pa**, *E*/*Z* = 7.1/1)

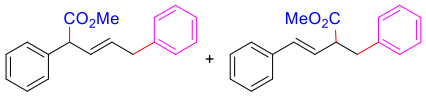
The corresponding substrate contained inseparable *E*/*Z* isomers. The general procedure A was followed. Yield: 15%, 9.7 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.11 (m, 10H), 6.95 (d, *J* = 6.6 Hz, 0.29H), 6.78 – 6.73 (m, 0.26H), 5.62 (d, *J* = 10.0 Hz, 1H), 5.43 (d, *J* = 10.4 Hz, 0.14H), 3.71 – 3.62 (m, 1H), 3.61 (s, 3H), 3.57 (s, 0.43H), 3.24 (dt, *J* = 10.3, 7.4 Hz, 0.16H), 3.13 (dd, *J* = 13.4, 7.2 Hz, 1H), 2.95 (dd, *J* = 13.4, 6.8 Hz, 0.16H), 2.83 (dd, *J* = 13.4, 7.6 Hz, 1H), 2.71 (dd, *J* = 13.4, 8.0 Hz, 0.15H), 2.29 (t, *J* = 7.7 Hz, 2H), 2.21 (t, *J* = 7.5 Hz, 0.30H), 1.26 – 1.12 (m, 2H), 1.08 – 0.99 (m, 1H), 0.79 (t, *J* = 7.4 Hz, 0.53H), 0.72 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.8, 174.4, 143.6, 142.6, 138.9, 138.8, 129.4, 129.3, 128.5, 128.31, 128.27, 128.2, 128.1, 127.4, 127.2, 126.8, 126.7, 126.6, 126.4, 125.5, 123.8, 52.0, 51.8, 47.6, 47.5, 41.7, 39.5, 39.4, 32.1, 21.6, 20.9, 14.0, 13.7. HRMS (m/z, ESI): calcd for $C_{21}H_{24}O_2Na^+$ $(M+Na)^+$ 331.1668, found 331.1668.



5qa

methyl (*E*)-1-(3-phenylprop-1-en-1-yl)-1,2,3,4-tetrahydronaphthalene-1-carboxylate (5qa)

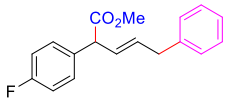
The general procedure A was followed. Yield: 32%, 19.6 mg. ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.29 – 7.20 (m, 2H), 7.19 – 7.02 (m, 7H), 5.91 (d, *J* = 15.6 Hz, 1H), 5.15 (dt, *J* = 15.6, 6.9 Hz, 1H), 3.67 (s, 3H), 3.37 (d, *J* = 6.8 Hz, 2H), 2.87 – 2.65 (m, 2H), 2.39 – 2.27 (m, 1H), 1.93 – 1.83 (m, 1H), 1.83 – 1.70 (m, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 176.3, 140.5, 137.2, 136.7, 136.0, 130.9, 130.4, 129.3, 128.6, 128.5, 126.9, 126.1, 125.6, 53.9, 52.5, 39.0, 33.9, 29.6, 19.1. HRMS (m/z, ESI): calcd for $C_{21}H_{22}O_2Na^+$ $(M+Na)^+$ 329.1512, found 329.1511.



5ra 6ra

methyl (*E*)-2,5-diphenylpent-3-enoate (5ra), methyl (*E*)-2-benzyl-4-phenylbut-3-enoate (6ra) (5ra/6ra = 8.3/1)

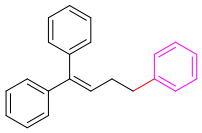
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.46 – 7.07 (m, 11H), 6.40 (d, *J* = 15.8 Hz, 0.12H), 6.23 (dd, *J* = 15.9, 8.6 Hz, 0.13H), 5.95 (dd, *J* = 15.3, 8.3 Hz, 1H), 5.71 (dt, *J* = 14.6, 6.8 Hz, 1H), 4.32 (d, *J* = 8.2 Hz, 1H), 3.68 (s, 3H), 3.64 (s, 0.40H), 3.51 – 3.45 (m, 0.19H), 3.39 (d, *J* = 6.8 Hz, 2H), 3.17 (dd, *J* = 13.6, 7.9 Hz, 0.14H), 2.93 (dd, *J* = 13.6, 7.1 Hz, 0.12H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.3, 140.0, 138.7, 132.8, 132.4, 129.2, 128.9, 128.8, 128.6, 128.55, 128.5, 128.0, 127.8, 127.4, 126.9, 126.6, 126.5, 126.2, 54.7, 52.3, 51.5, 39.1, 39.0. HRMS (m/z, ESI): calcd for $C_{18}H_{18}O_2Na^+$ $(M+Na)^+$ 289.1199, found 289.1199.



5sa

methyl (*E*)-5-phenyl-2-(4-(trifluoromethyl)phenyl)pent-3-enoate (5sa)

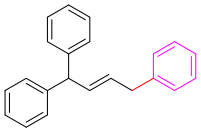
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.31 – 7.23 (m, 4H), 7.22 – 7.12 (m, 3H), 7.01 (t, *J* = 8.6 Hz, 2H), 5.90 (dd, *J* = 15.3, 8.1 Hz, 1H), 5.71 (dt, *J* = 15.2, 6.8 Hz, 1H), 4.30 (d, *J* = 8.1 Hz, 1H), 3.69 (s, 3H), 3.40 (d, *J* = 6.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 173.1, 162.2 (d, J_{C-F} = 245.7 Hz), 139.9, 134.4 (d, J_{C-F} = 3.3 Hz), 132.6, 129.6 (d, J_{C-F} = 8.1 Hz), 128.7, 128.64, 128.6, 126.3, 115.7 (d, J_{C-F} = 21.5 Hz), 53.9, 52.4, 38.9. HRMS (m/z, ESI): calcd for $C_{18}H_{17}FO_2Na^+$ $(M+Na)^+$ 307.1105, found 307.1106.



BP1

but-1-ene-1,1,4-triyltribenzene (BP1)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.37 – 7.10 (m, 13H), 7.10 – 7.03 (m, 2H), 6.10 (t, *J* = 7.4 Hz, 1H), 2.74 (t, *J* = 7.7 Hz, 2H), 2.42 (q, *J* = 7.6 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.8, 142.4, 141.8, 140.2, 129.9, 128.9, 128.7, 128.4, 128.3, 128.2, 127.3, 127.0, 127.0, 126.0, 36.3, 31.8.



BP2

(*E*)-but-2-ene-1,1,4-triyltribenzene (BP2)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.41 – 7.27 (m, 7H), 7.25 – 7.15 (m, 8H), 6.02 (dd, *J* = 15.2, 7.6 Hz, 1H), 5.61 (dt, *J* = 14.2, 6.8 Hz, 1H), 4.75 (d, *J* = 7.5 Hz, 1H), 3.44 (d, *J* = 6.7 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.1, 140.6, 134.1, 131.0, 128.7, 128.54, 128.53, 128.5, 126.4, 126.1, 54.0, 39.1.

2.4 Mechanistic Studies

Stern-Volmer fluorescence quenching experiments:

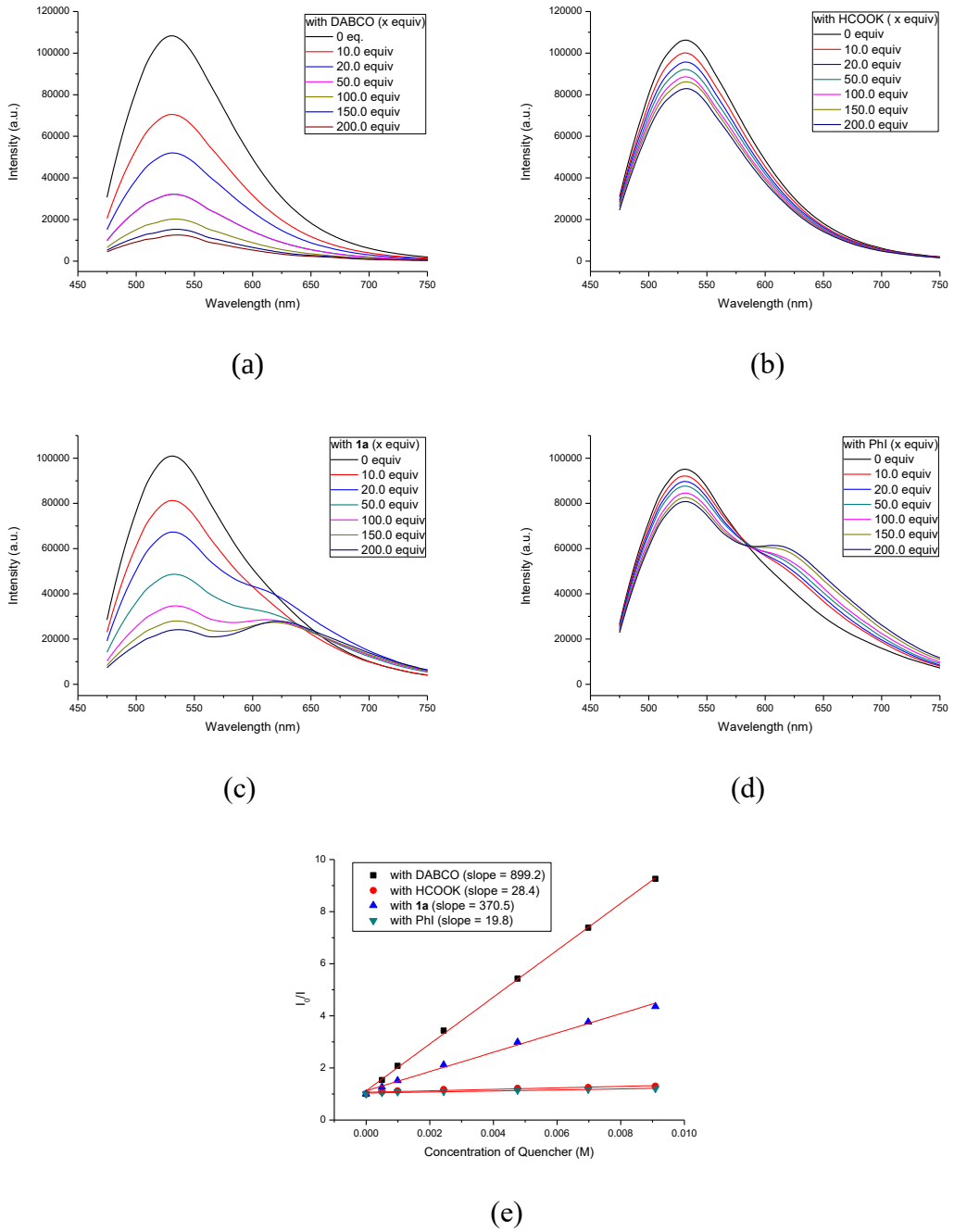


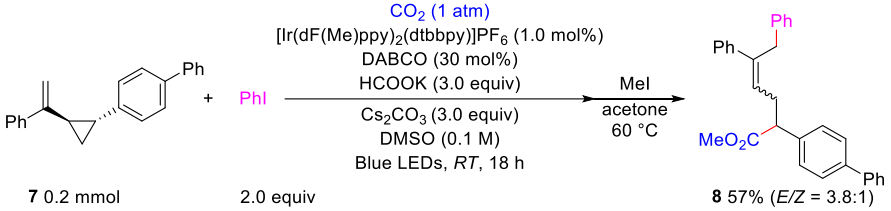
Figure S1. (a) Stern-Volmer quenching by DABCO. (b) Stern-Volmer quenching by HCOOK. (c) Stern-Volmer quenching by substrate **1a**. (d) Stern-Volmer quenching by PhI. (e) Stern-Volmer quenching plot of DABCO, HCOOK, **1a** and PhI.

Fluorescence spectra were collected on FLS1000 spectrofluorimeter. Samples for the quenching experiments were prepared in a 4.0 mL glass cuvette with a septum screw cap. Photocatalyst $[Ir(dF(Me)ppy)_2(dtbbpy)]PF_6$ (**PC**) was irradiated at 465 nm and the emission intensity at 531 nm was observed. In a typical experiment, the emission

spectrum of a 5.0 x 10^{-5} M solution of **PC** in DMSO was collected.

A stock solution of quenchers DABCO (0.5 mmol), HCOOK (0.5 mmol), **1a** (0.5 mmol) and PhI (0.5 mmol) in 5.0 mL of DMSO were prepared respectively. Then, different amounts of this stock solution were added to a solution of the photocatalyst [Ir(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$ (**PC**) in DMSO (5.0 x 10^{-5} M). As shown in **Figure S1**, the stock solution of HCOOK or PhI were added to the solution of **PC**, a less decrease of [Ir(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$ (**PC**) luminescence with a slope of 28.4 and 19.8 were observed respectively. While the stock solution of DABCO or substrate **1a** were added to the solution of PC, a significant decrease of **PC** luminescence were observed, but the slope of DABCO (= 899.2) is much larger than the slope of **1a** (= 370.5). These results suggested that DABCO had the priority to undergo SET with excited [Ir(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$ (**PC***).

Radical clock experiment:

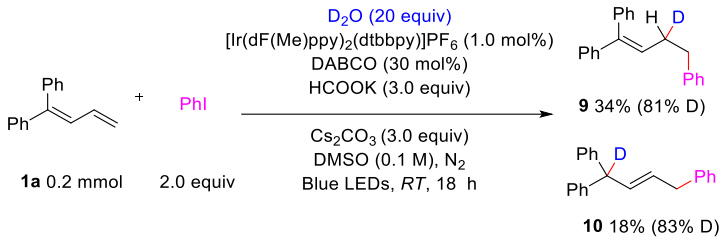


The oven-dried Schlenk tube (25 mL) containing a stirring bar was charged with substrates **7** (0.2 mmol, 1.0 equiv) and Ir[(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$ (1 mol%) in the air. Then the tube was moved into a glovebox and charged with DABCO (30 mol%), HCOOK (3.0 equiv) and Cs_2CO_3 (3.0 equiv). The tube was sealed and evacuated and back-filled with CO_2 three times. Subsequently, PhI (0.4 mmol, 2.0 equiv) and the degassed anhydrous DMSO (2 mL, 0.1M) was added into the tube via syringe. Then the tube was evacuated and back-filled with CO_2 for 10 times. Finally, the mixture was placed under a 30 W blue LEDs (λ_{max}=465 nm, 3.0 cm - 4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25 - 40 °C) light source and stirred at ambient temperature for 18 h. Upon completion of the reaction, all the solvent were removed under reduced pressure at high temperature. The residue was dissolved with acetone (4.0 mL), and CH_3I (20.0 equiv) was added to the tube. The mixture was stirred at 60 °C for 3 h and then cooled to room temperature. Upon completion of the methylation, the mixture was diluted with 5 mL EtOAc and filtered through a short pad of Celite and the Celite pad were washed with an additional EtOAc (10 mL x 4). Then the filtrate was concentrated *in vacuo* to give the crude product. The resulting residue was purified by preparative thin layer chromatography using petroleum ether/EtOAc (30:1) as the eluent to afford the product **8** in 57% (*E*/*Z* = 3.8/1) yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.67 – 7.46 (m, 5H), 7.46 – 7.28 (m, 6H), 7.28 – 7.02 (m, 12H), 6.99 (dd, *J* = 5.5, 3.6 Hz, 0.61H), 6.94 – 6.86 (m, 0.55H), 5.88 (t, *J* = 7.2 Hz, 1H), 5.37 (t, *J* = 7.1 Hz, 0.26H), 3.86 (q, *J* = 16.0 Hz, 2H), 3.73 (t, *J* = 7.6 Hz, 1H), 3.66 (s, 3H), 3.61 (s, 1H), 3.54 (s, 0.59H), 3.05 (dt, *J* = 15.5, 7.9 Hz, 1H), 2.74 (tt, *J* = 19.2, 7.0 Hz, 1.34H), 2.52 (dt, *J* = 15.0, 7.9 Hz, 0.33H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 174.1, 174.0, 142.9, 142.7, 140.9, 140.8, 140.5, 140.4, 140.3, 139.9,

139.5, 139.4, 137.7, 137.6, 129.1, 128.9, 128.6, 128.5, 128.48, 128.4, 128.3, 128.26, 128.2, 128.1, 127.5, 127.4, 127.38, 127.3, 127.2, 127.1, 127.0, 126.8, 126.4, 126.1, 126.0, 125.5, 52.3, 52.1, 51.6, 51.4, 45.9, 36.0, 33.2, 32.9. HRMS (m/z, ESI): calcd for $C_{31}H_{28}O_2Na^+$ $(M+Na)^+$ 455.1982, found 455.1982.

Isotope-labelling experiment with D_2O:

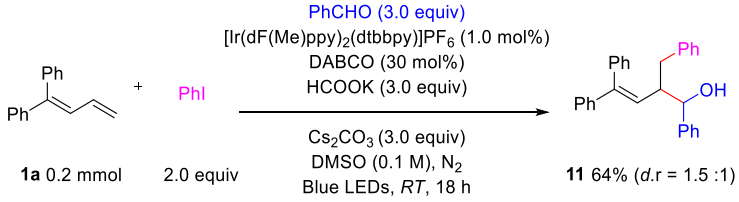


The oven-dried Schlenk tube (25 mL) containing a stirring bar was charged with substrates **1a** (0.2 mmol, 1.0 equiv) and Ir[(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$ (1 mol%) in the air. Then the tube was moved into a glovebox and charged with DABCO (30 mol%), HCOOK (3.0 equiv) and Cs_2CO_3 (3.0 equiv). The tube was sealed and evacuated and back-filled with N_2 three times. Subsequently, PhI (0.4 mmol, 2.0 equiv), D_2O (20.0 equiv) and the degassed anhydrous DMSO (2 mL, 0.1M) was added into the tube via syringe. Then the tube was evacuated and back-filled with N_2 for 3 times. Finally, the mixture was placed under a 30 W blue LEDs (λ_{max}=465 nm, 3.0 cm - 4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25 - 40 °C) light source and stirred at ambient temperature for 18 h. Upon completion of the reaction, the mixture was quenched with water (15 ml) and diluted with 5 mL EtOAc. The organic phases were separated and the aqueous phase was extracted with ethyl acetate (10 mL x 4). The combined organic phases were dried with anhydrous Na_2SO_4 and concentrated *in vacuo* to give the crude product. The resulting residue was purified by preparative thin layer chromatography using petroleum ether as the eluent to afford the 3,4-adduct **9** in 34% (81% D) yield and 1,4-adduct **10** in 18% (83% D) yield.

Characterization of 3,4-adduct **9**: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.52 – 6.94 (m, 15H), 6.10 (d, *J* = 7.3 Hz, 1H), 2.73 (d, *J* = 7.6 Hz, 2H), 2.41 (p, *J* = 7.8 Hz, 1.19H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.8, 142.4, 141.8, 140.2, 129.9, 128.9, 128.7, 128.4, 128.3, 128.2, 127.3, 127.0, 127.0, 126.0, 36.3, 36.2, 31.8, 31.6, 31.4, 31.2. HRMS (m/z, ESI): calcd for $C_{22}H_{19}DNa^+$ $(M+Na)^+$ 308.1520, found 308.1521.

Characterization of 1,4-adduct **10**: ^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.44 – 7.27 (m, 6H), 7.25 – 7.13 (m, 9H), 6.02 (d, *J* = 15.1 Hz, 1H), 5.62 (dt, *J* = 15.3, 6.8 Hz, 1H), 4.75 (d, *J* = 7.5 Hz, 0.17H), 3.44 (d, *J* = 6.8 Hz, 2H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.1, 140.6, 134.1, 131.0, 128.7, 128.6, 128.54, 128.5, 126.4, 126.1, 54.0, 39.1. HRMS (m/z, ESI): calcd for $C_{22}H_{19}DNa^+$ $(M+Na)^+$ 308.1520, found 308.1521.

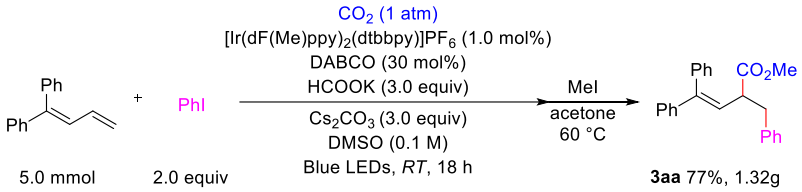
Investigation of using aldehyde as the electrophile:



The oven-dried Schlenk tube (25 mL) containing a stirring bar was charged with substrates **1a** (0.2 mmol, 1.0 equiv) and Ir[(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$ (1 mol%) in the air. Then the tube was moved into a glovebox and charged with DABCO (30 mol%), HCOOK (3.0 equiv) and Cs_2CO_3 (3.0 equiv). The tube was sealed and evacuated and back-filled with N_2 three times. Subsequently, PhI (0.4 mmol, 2.0 equiv), PhCHO (3.0 equiv) and the degassed anhydrous DMSO (2 mL, 0.1M) was added into the tube via syringe. Then the tube was evacuated and back-filled with N_2 for 3 times. Finally, the mixture was placed under a 30 W blue LEDs (λ_{max}=465 nm, 3.0 cm - 4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25 - 40 °C) light source and stirred at ambient temperature for 18 h. Upon completion of the reaction, the mixture was quenched with water (15 ml) and diluted with 5 mL EtOAc. The organic phases were separated and the aqueous phase was extracted with ethyl acetate (10 mL x 4). The combined organic phases were dried with anhydrous Na_2SO_4 and concentrated *in vacuo* to give the crude product. The resulting residue was purified by preparative thin layer chromatography using PE/EA (12:1) as the eluent to afford the product **11** in 64% (*d.r.* = 1.5:1) yield.

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.51 – 7.02 (m, 16H), 6.97 (dd, *J* = 13.4, 6.6 Hz, 2H), 6.28 (d, *J* = 7.0 Hz, 1.30H), 6.22 (d, *J* = 7.0 Hz, 0.75H), 6.09 (d, *J* = 10.2 Hz, 0.58H), 5.80 (d, *J* = 10.5 Hz, 0.38H), 4.64 (dd, *J* = 10.3, 5.5 Hz, 1H), 3.04 (dd, *J* = 12.8, 3.2 Hz, 0.38H), 2.84 – 2.59 (m, 2.74H), 2.07 (br, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.9, 143.8, 143.1, 143.0, 142.3, 142.2, 140.1, 140.0, 139.7, 139.6, 129.9, 129.6, 129.55, 129.5, 128.9, 128.3, 128.25, 128.23, 128.2, 128.15, 128.1, 127.8, 127.78, 127.7, 127.6, 127.58, 127.14, 127.1, 127.04, 127.0, 126.7, 126.63, 126.0, 49.9, 49.3, 38.9, 37.8. HRMS (m/z, ESI): calcd for $C_{29}H_{26}ONa^+$ $(M+Na)^+$ 413.1876, found 413.1875.

2.5 Gram-scale reaction

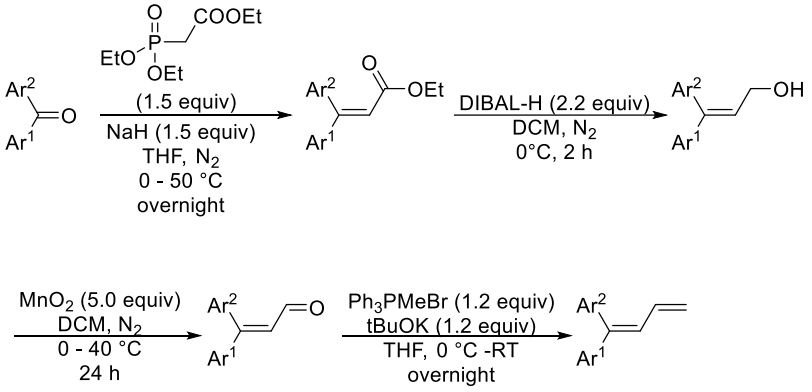


The oven-dried Schlenk tube (350 mL) containing a stirring bar was charged with substrates **1** (5.0 mmol, 1.0 equiv) and Ir[(dF(Me)ppy)$_2$(dtbbpy)]PF$_6$ (1 mol%) in the air. Then the tube was moved into a glovebox and charged with DABCO (30 mol%), HCOOK (3.0 equiv) and Cs_2CO_3 (3.0 equiv). The tube was sealed and evacuated and back-filled with CO_2 three times. Subsequently, PhI (10.0 mmol, 2.0 equiv) and the degassed anhydrous DMSO (50 mL, 0.1M) was added into the tube via syringe. Then the tube was evacuated and back-filled with CO_2 for 10 times. Finally, the mixture was placed under a 30 W blue LEDs (λ_{max}=465 nm, 3.0 cm - 4.5 cm away from the LEDs, with cooling fan to keep the reaction temperature at 25 - 40 °C) light source and stirred at ambient temperature for 18 h. Upon completion of the reaction, all the solvent were removed under reduced pressure at high temperature. The residue was dissolved with

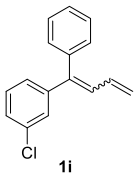
acetone (30 mL), and CH_3I (20.0 equiv) was added to the tube. The mixture was stirred at 60 °C for 3 h and then cooled to room temperature. Upon completion of the methylation, the mixture was diluted with 10 mL EtOAc and filtered through a short pad of Celite and the Celite pad were washed with an additional EtOAc (15 mL x 4). Then the filtrate was concentrated *in vacuo* to give the crude product. The crude ^1H NMR spectrum was taken using CH_2Br_2 (5.0 mmol) as internal standard. Finally, the resulting residue was purified by preparative thin layer chromatography using PE to PE/EtOAc (40:1) as the eluent to afford the desired product **3aa** in 77% (1.32g) isolated yiled.

2.6 General procedures for the synthesis of substrates

All the 1,1-disubstituted conjugated dienes were prepared according to the reported literatures[S1] and the NMR spectrum of substrates **1a – h, 1j, 1l – o, 1r – s, 4a - s** are accordance with the reported literatures.[S2]



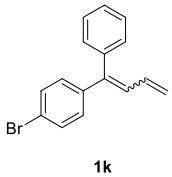
Characterization of substrates 1i, 1k, 1p and 1q:



1i

1-chloro-3-(1-phenylbuta-1,3-dien-1-yl)benzene (1i)

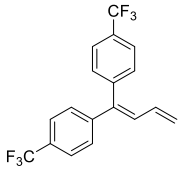
^1H NMR (400 MHz, Chloroform-*d*) δ 7.42 – 7.14 (m, 8H), 7.14 – 7.05 (m, 1H), 6.70 (dd, *J* = 11.0, 9.2 Hz, 1H), 6.50 – 6.32 (m, 1H), 5.41 (dd, *J* = 16.9, 1.8 Hz, 1H), 5.16 (dt, *J* = 10.2, 2.4 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.1, 141.9, 141.7, 141.6, 141.5, 139.0, 134.7, 134.5, 134.34, 134.27, 130.44, 130.4, 129.64, 129.6, 129.5, 129.3, 128.8, 128.4, 127.9, 127.8, 127.7, 127.63, 127.6, 127.56, 125.9, 119.7, 119.66.



1k

1-bromo-4-(1-phenylbuta-1,3-dien-1-yl)benzene (1k)

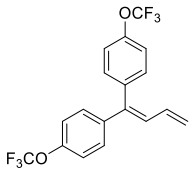
^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.60 – 7.42 (m, 1H), 7.41 – 6.98 (m, 8H), 6.68 (dd, *J* = 11.7, 9.4 Hz, 1H), 6.52 – 6.27 (m, 1H), 5.39 (d, *J* = 16.9 Hz, 1H), 5.14 (dd, *J* = 10.0, 2.7 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 142.1, 141.9, 141.7, 141.1, 139.2, 138.6, 134.8, 134.6, 132.2, 131.5, 131.4, 130.4, 129.2, 129.0, 128.98, 128.4, 127.8, 127.7, 127.6, 121.7, 119.5, 119.4.



1p

4,4'-(buta-1,3-diene-1,1-diyl)bis((trifluoromethyl)benzene) (1p)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.70 (d, *J* = 8.1 Hz, 2H), 7.57 (d, *J* = 8.3 Hz, 2H), 7.37 (dd, *J* = 8.0, 5.3 Hz, 4H), 6.85 (d, *J* = 11.0 Hz, 1H), 6.41 (dt, *J* = 16.8, 10.5 Hz, 1H), 5.54 (d, *J* = 16.8 Hz, 1H), 5.30 (d, *J* = 10.3 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 144.9, 142.8, 140.4, 134.0, 131.4, 130.9, 130.1 (q, J_{C-F} = 32.6 Hz), 129.8 (q, J_{C-F} = 32.6 Hz), 127.8, 125.6 (q, J_{C-F} = 3.7 Hz), 125.5 (q, J_{C-F} = 3.8 Hz), 124.3 (q, J_{C-F} = 273.0 Hz), 124.28 (q, J_{C-F} = 273.2 Hz), 121.5.



1q

4,4'-(buta-1,3-diene-1,1-diyl)bis((trifluoromethoxy)benzene) (1q)

^{1}H NMR (400 MHz, Chloroform-*d*) δ 7.40 – 7.22 (m, 6H), 7.17 (d, *J* = 8.3 Hz, 2H), 6.74 (d, *J* = 11.0 Hz, 1H), 6.43 (dt, *J* = 16.9, 10.5 Hz, 1H), 5.48 (d, *J* = 16.8 Hz, 1H), 5.24 (d, *J* = 10.1 Hz, 1H). ^{13}C NMR (101 MHz, Chloroform-*d*) δ 148.9 (q, J_{C-F} = 2.6 Hz), 148.88 (q, J_{C-F} = 2.0 Hz), 140.53, 140.40, 137.93, 134.35, 131.96, 130.02, 128.98, 120.97, 120.91, 120.7 (q, J_{C-F} = 258.3 Hz), 120.66 (q, J_{C-F} = 258.2 Hz), 120.30.

3. References

[S1] (a) J. Takaya, K. Sasano, N. Iwasawa. *Org. Lett.* 2011, **13**, 1698-1701. (b) C. Liu, J. Yuan, J. Zhang, Z. Wang, Z. Zhang, W. Zhang. *Org. Lett.* 2018, **20**, 108-111.

[S2] (a) K. Wang, S. Chen, H. Zhang, S. Xu, F. Ye, Y. Zhang, J. Wang. *Org. Biomol. Chem.*, 2016, **14**, 3809-3820. (b) L. Zhou, F. Ye, Y. Zhang, J. Wang. *Org. Lett.* 2012, **14**, 922-925. (c) Q. Yang, H. Chai, T. Liu, Z. Yu. *Tetrahedron Lett.,* 2013, **54**, 6485-6489.

4. X-Ray Crystallographic Spectrum of 3aai and 5aa' (the acid of 5aa)

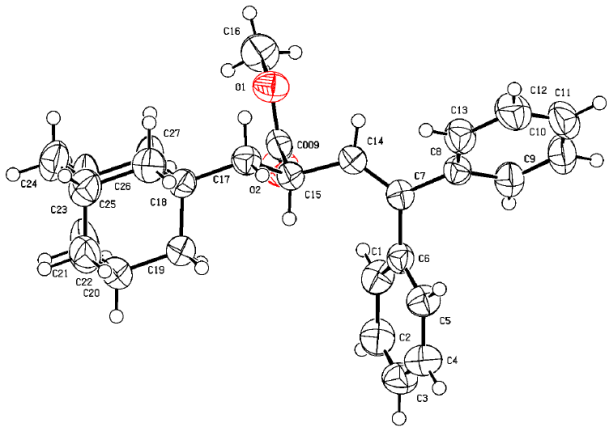


Figure S2. The crystal structure of **3aai** (CCDC 2116858).

Table S2. Crystal data and structure refinement for **3aai**.

Identification code	19-12-4tm_auto	
Empirical formula	$C_{28}H_{32}O_2$	
Formula weight	400.53	
Temperature	293(2) K	
Wavelength	1.3405 Å	
Crystal system	Monoclinic	
Space group	$P2_1/c$	
Unit cell dimensions	a = 9.5909(4) Å	α = 90 °.
	b = 23.7105(9) Å	β = 106.352(4) °.
	c = 10.2921(4) Å	γ = 90 °.
Volume	2245.80(16) $Å^3$	
Z	4	
Density (calculated)	1.185 g/cm^3	
Absorption coefficient	0.360 mm^{-1}	
F(000)	864	
Crystal size	0.230 x 0.039 x 0.025 mm^3	
Theta range for data collection	3.241 to 61.562 °.	
Index ranges	-12<=h<=11, -30<=k<=31, -13<=l<=13	
Reflections collected	31933	
Independent reflections	5141 [R(int) = 0.0327]	
Completeness to theta = 53.543 °	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5141 / 0 / 272	
Goodness-of-fit on F^2	1.106	
Final R indices [I>2sigma(I)]	R1 = 0.0451, wR2 = 0.1212	
R indices (all data)	R1 = 0.0572, wR2 = 0.1295	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.160 and -0.162 e.$Å^{-3}$	

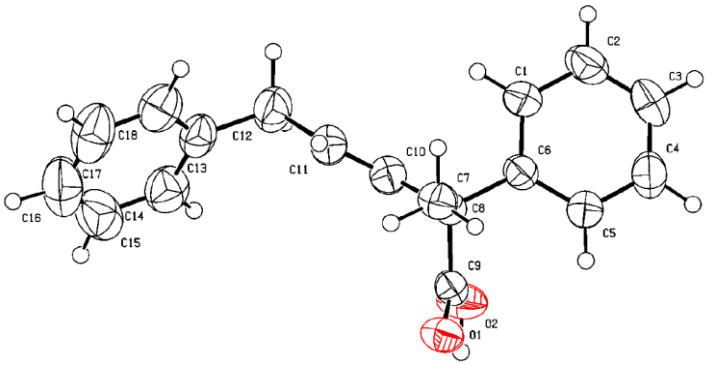
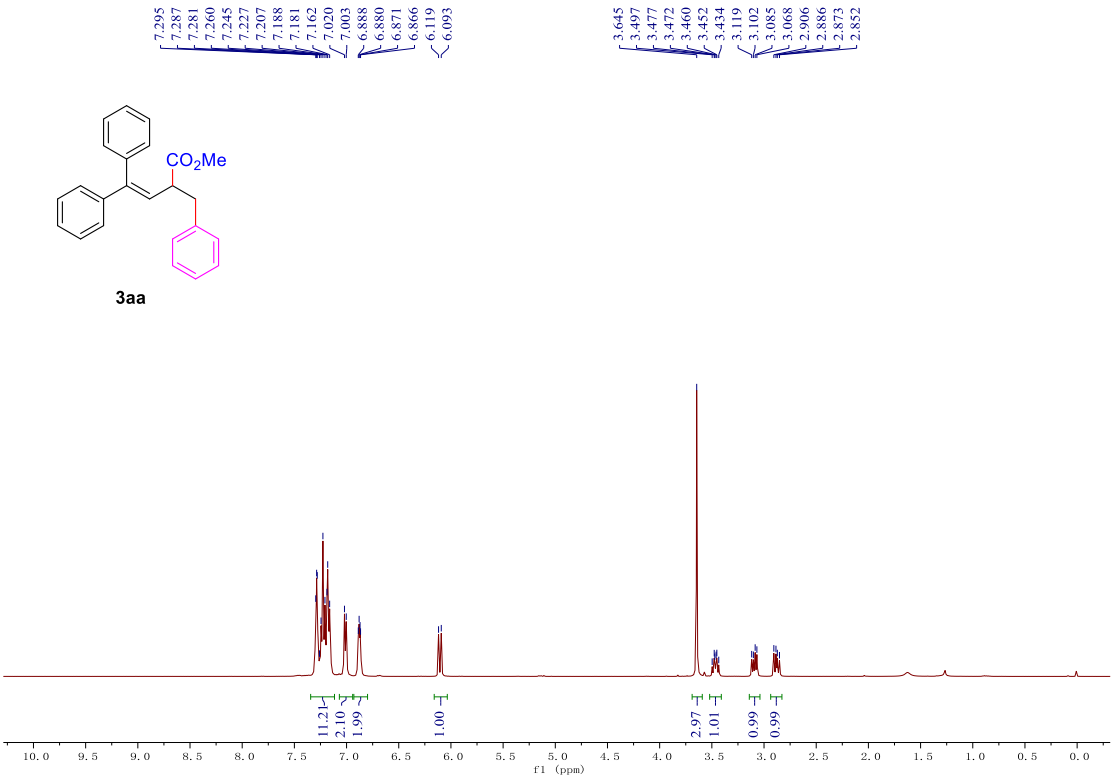


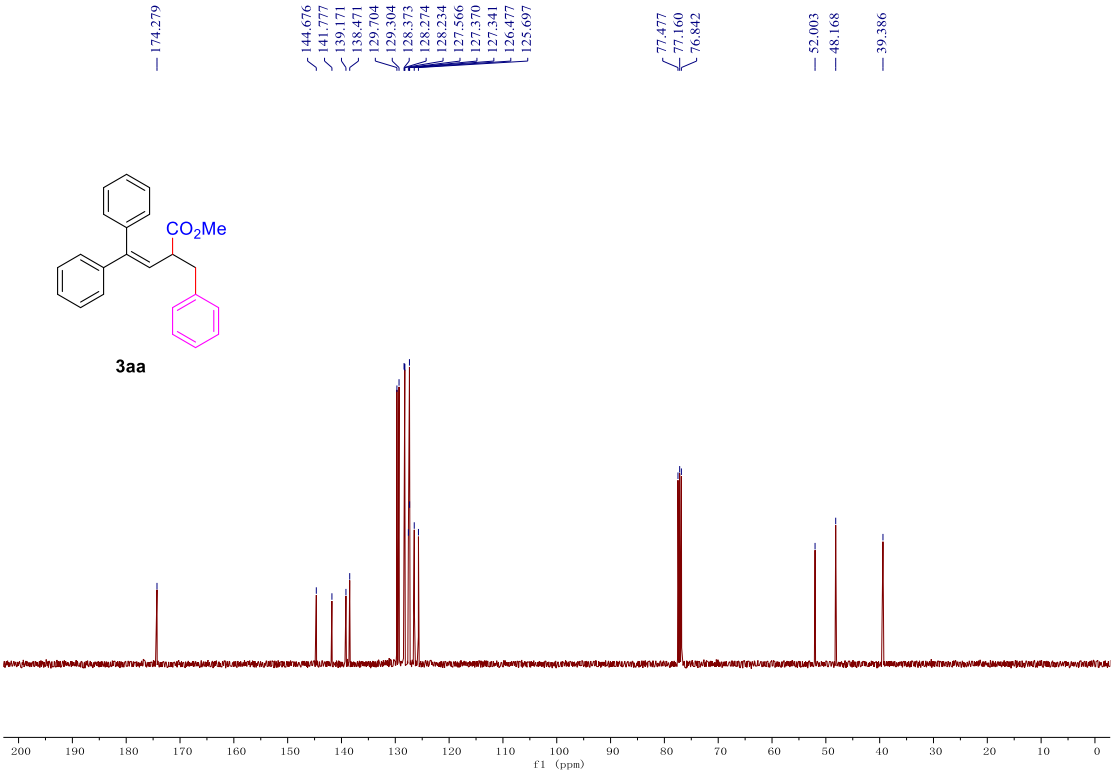
Figure S3. The crystal structure of **5aa'** (CCDC 2116857)

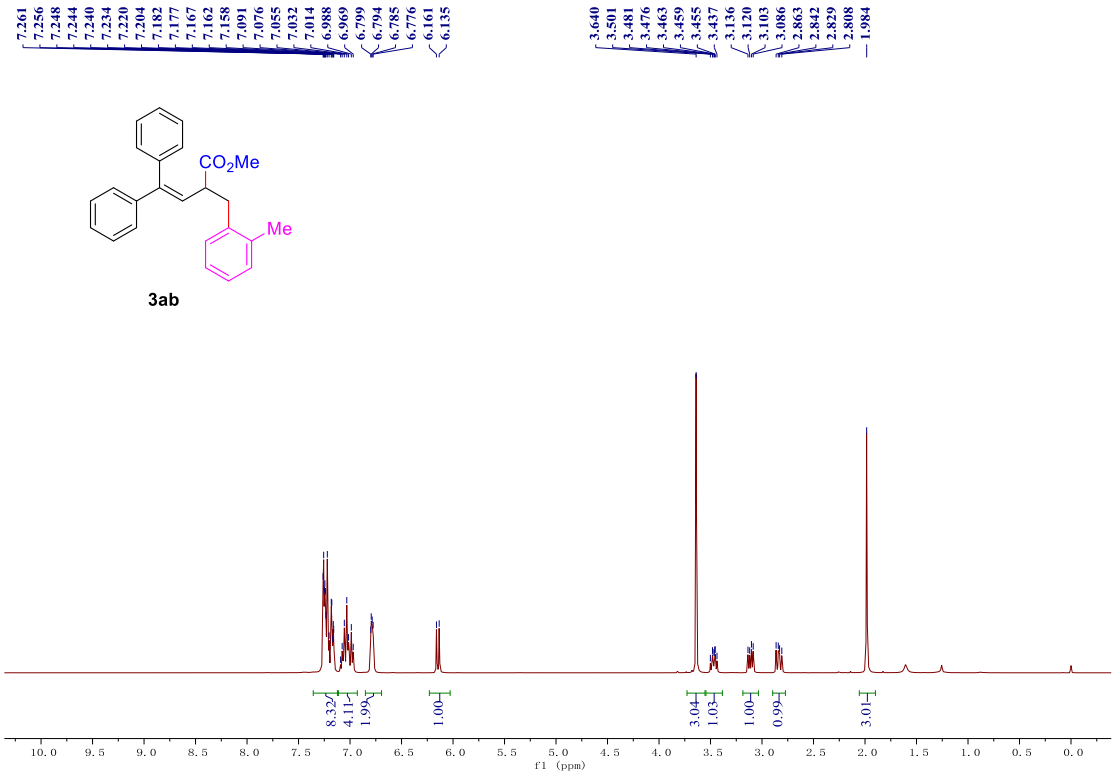
Table S3. Crystal data and structure refinement for **5aa'**.

Identification code	18-16-3A_auto	
Empirical formula	$C_{18}H_{18}O_2$	
Formula weight	266.34	
Temperature	293.0 K	
Wavelength	1.3405 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.8580(2) Å	α = 101.608(2) °.
	b = 9.5201(2) Å	β = 109.911(2) °.
	c = 9.7104(2) Å	γ = 92.242(2) °.
Volume	749.00(3) $Å^3$	
Z	2	
Density (calculated)	1.1809 g/cm^3	
Absorption coefficient	0.383 mm^{-1}	
F(000)	284.6713	
Crystal size	0.033 x 0.028 x 0.025 mm^3	
Theta range for data collection	4.15 to 60.64 °.	
Index ranges	-11<=h<=11, -12<=k<=12, -12<=l<=12	
Reflections collected	19649	
Independent reflections	3409 [R(int) = 0.0340]	
Completeness to theta = 60.6394 °	98.64 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.70352	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3409 / 0 / 253	
Goodness-of-fit on F^2	1.0649	
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1139	
R indices (all data)	R1 = 0.0556, wR2 = 0.1197	
Largest diff. peak and hole	0.2958 and -0.2085 $e.Å^{-3}$	

5. NMR spectrum of compounds



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7.076
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7.014
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6.969
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6.776
6.161
6.135
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3.437
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3.120
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2.808
1.984
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1.00
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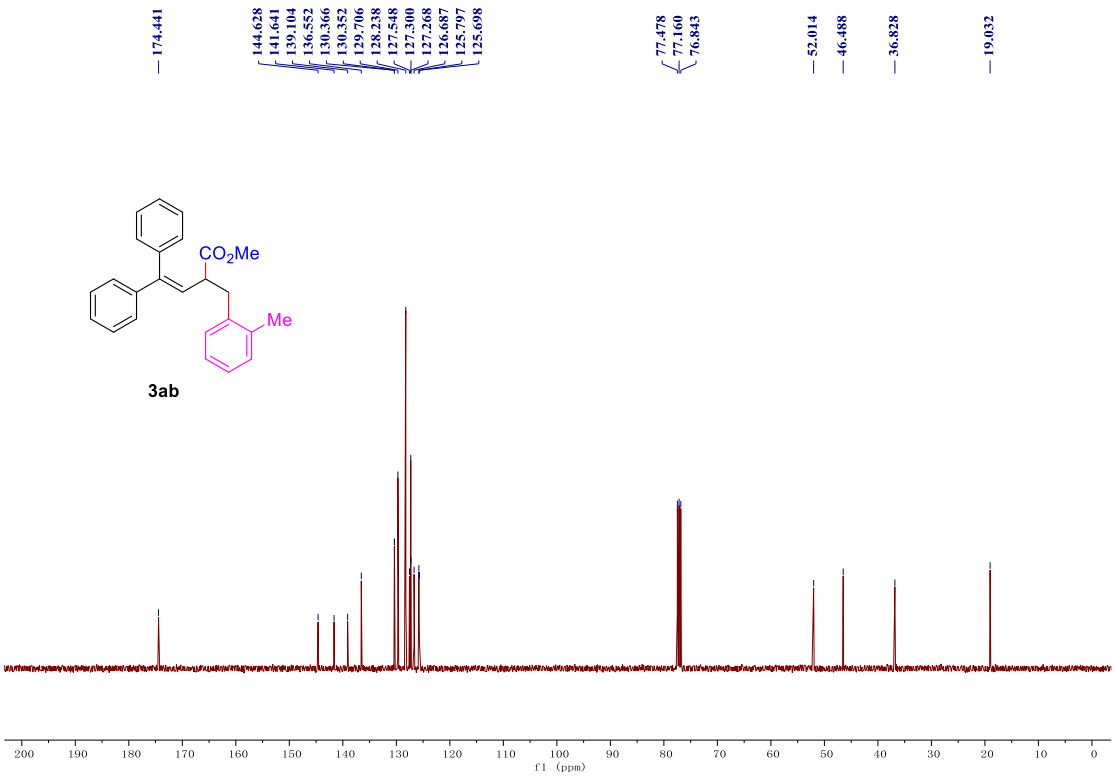
3.01
f1 (ppm)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125.797
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77.160
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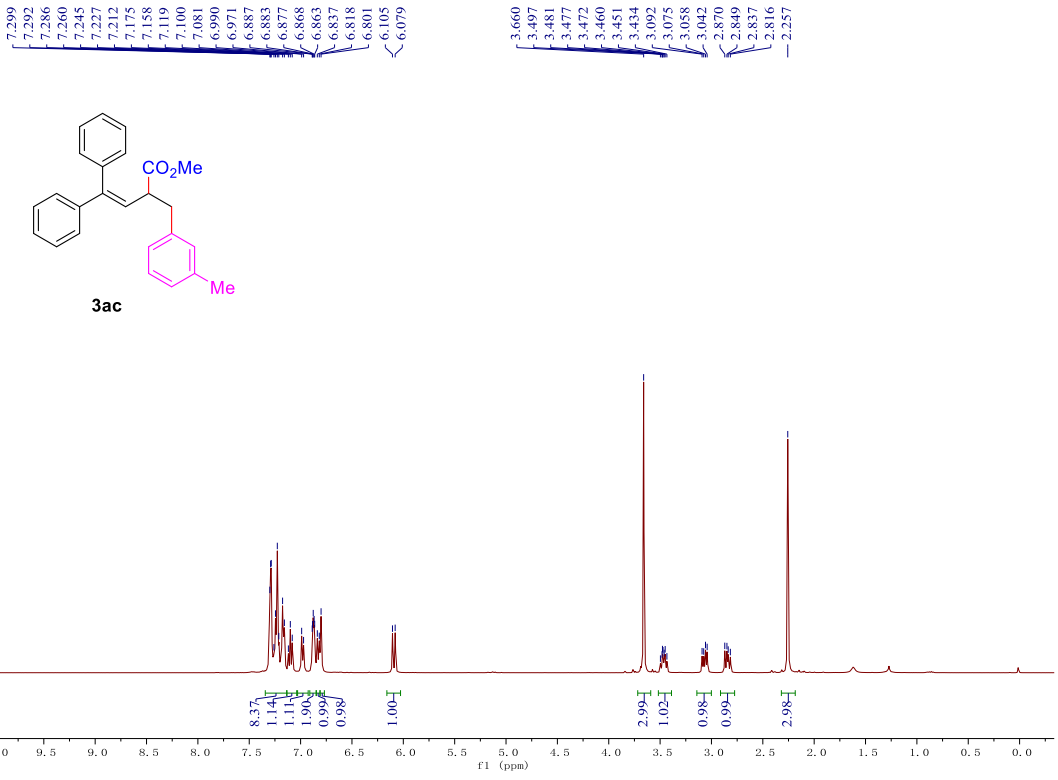
19.032
CO2Me
Me
3ab
f1 (ppm)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3.472
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3.042
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2.849
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2.816
2.257
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Me
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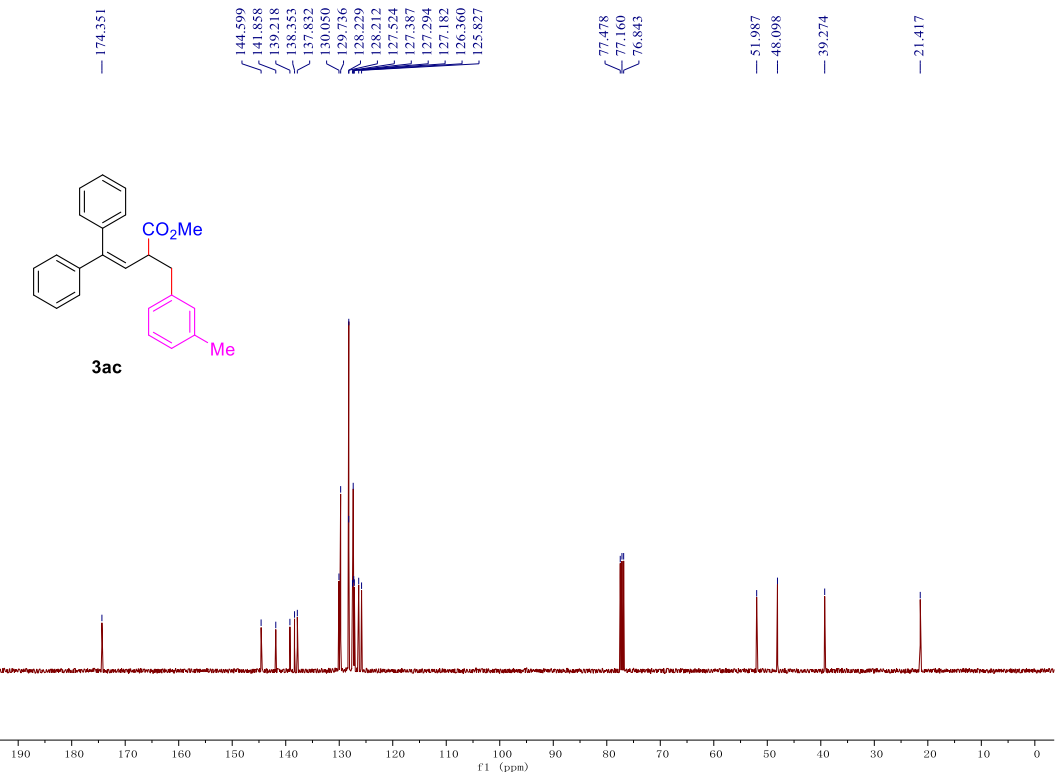
f1 (ppm)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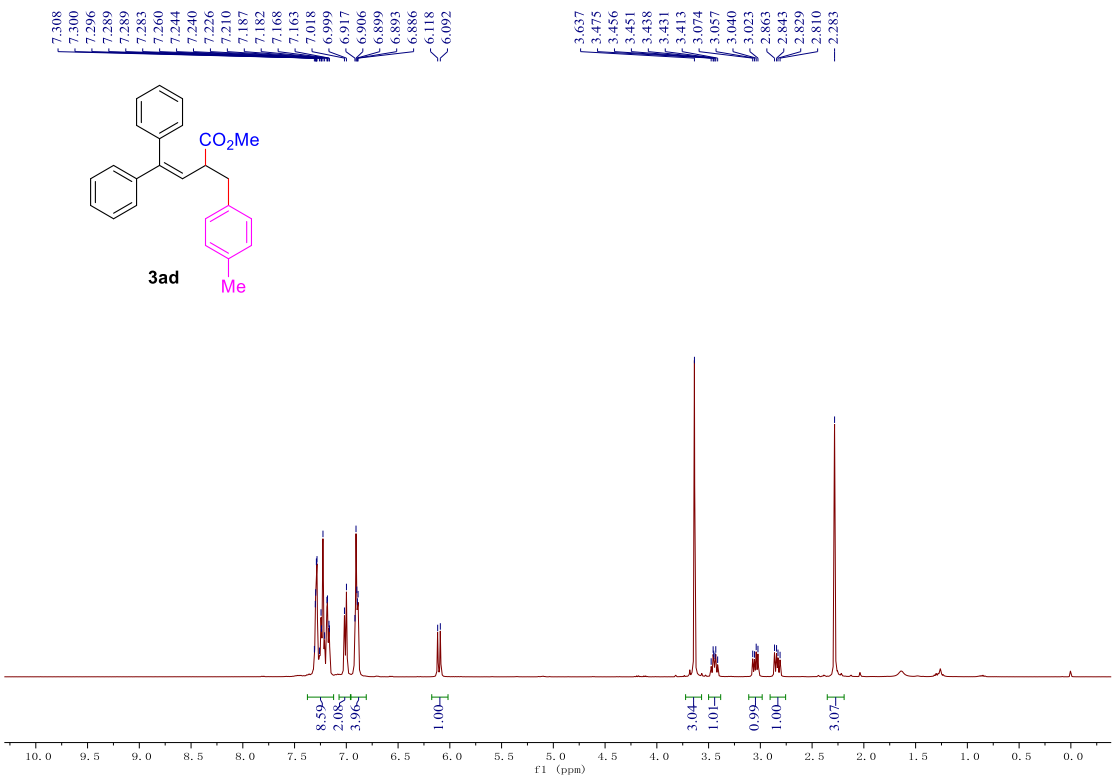
f1 (ppm)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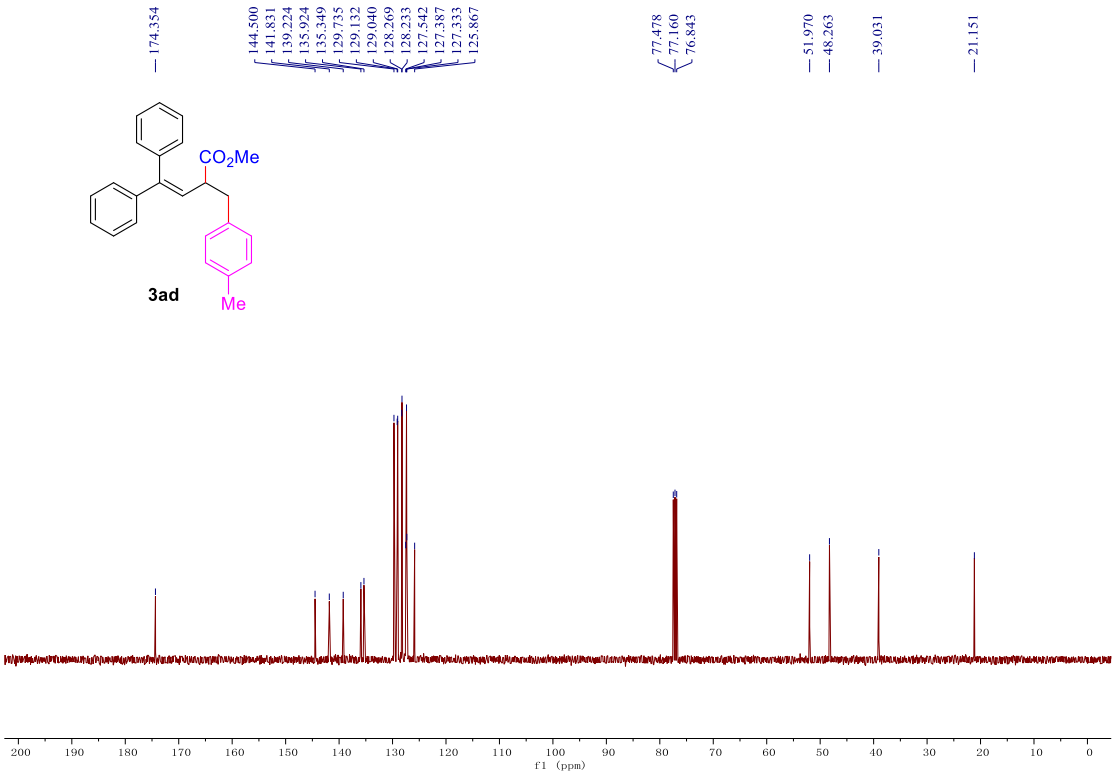
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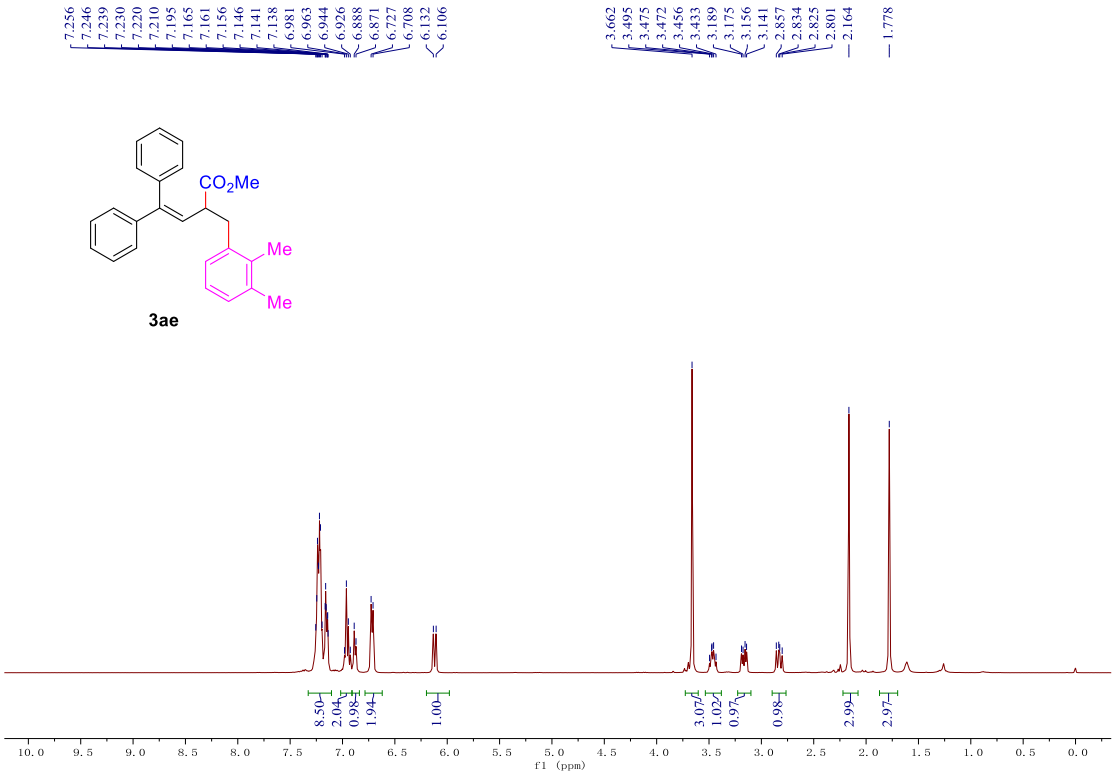
f1 (ppm)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1.02
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2.99
2.97
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
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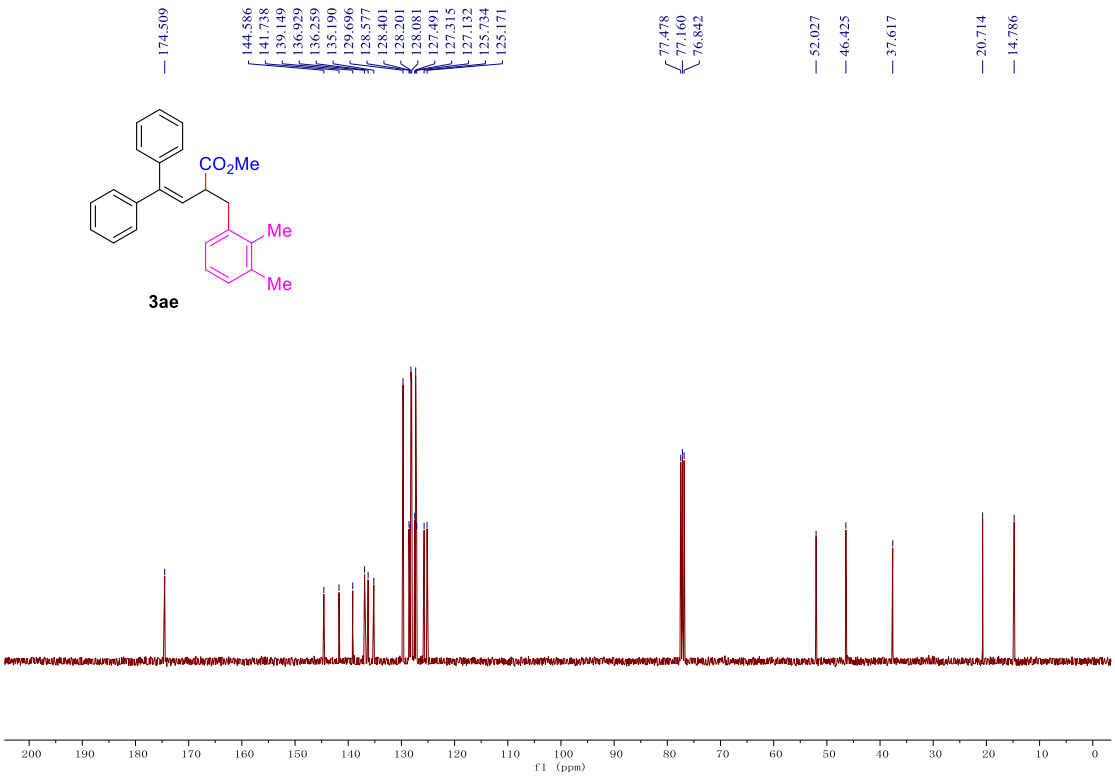
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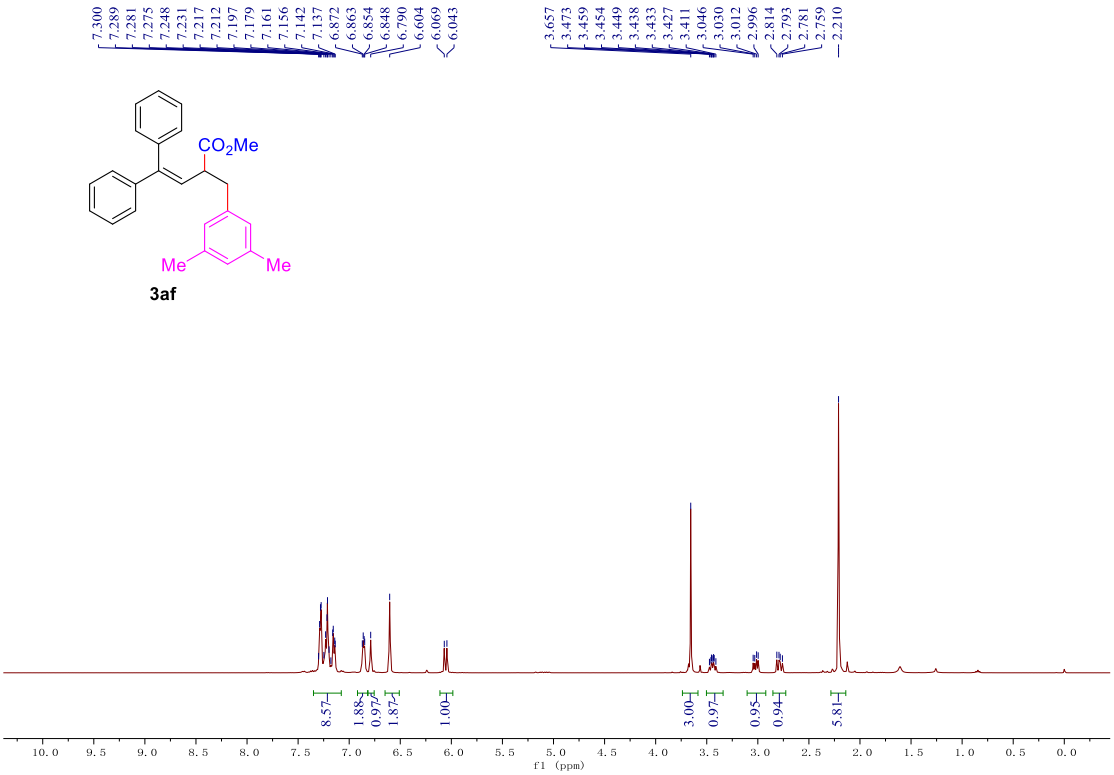
f1 (ppm)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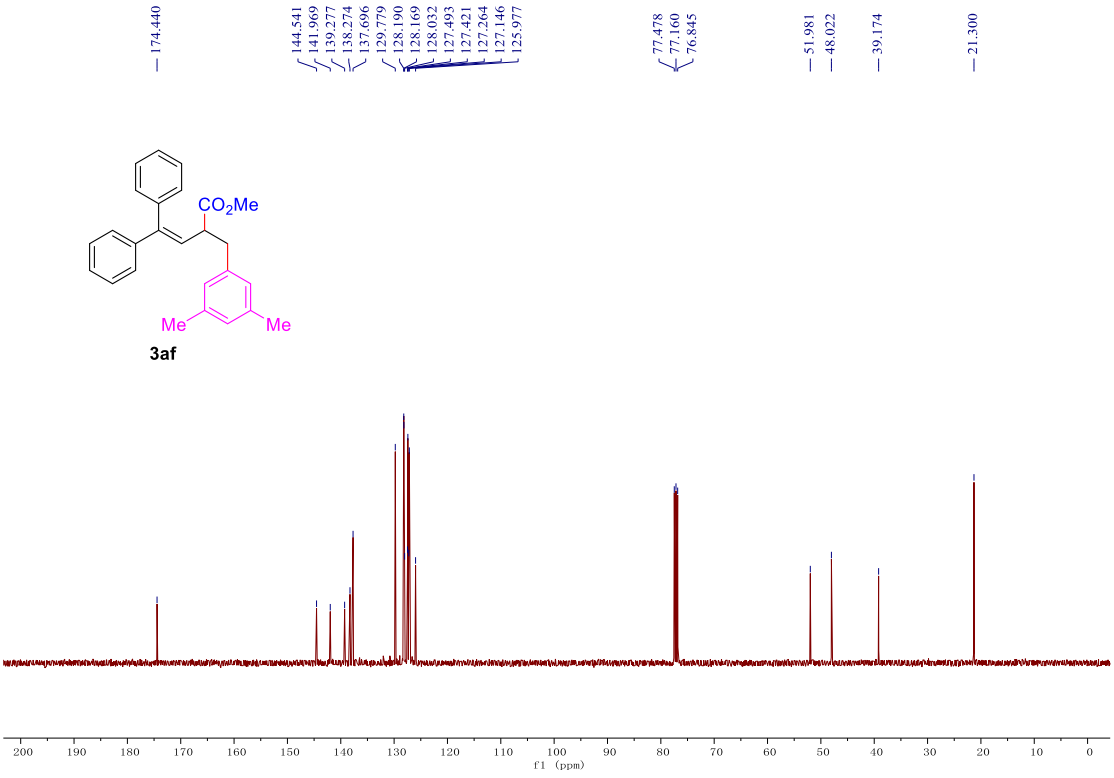
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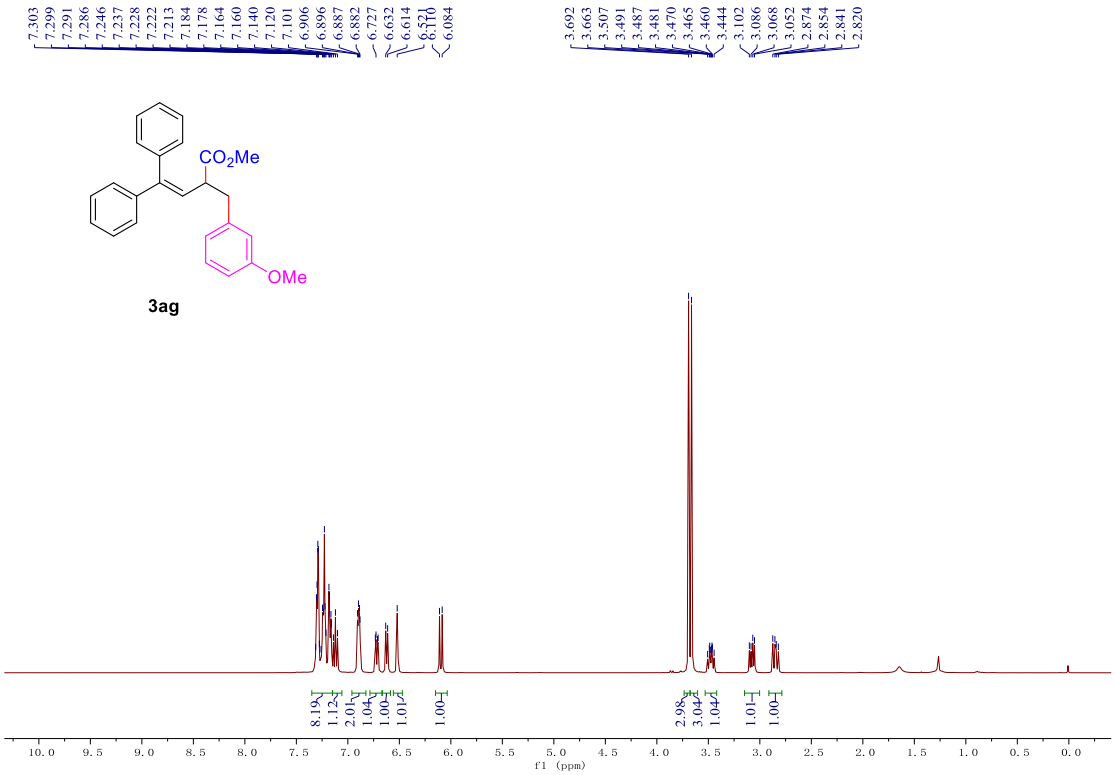
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2.874
2.854
2.841
2.820
CO2Me
OMe
3ag
8.19
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1.00
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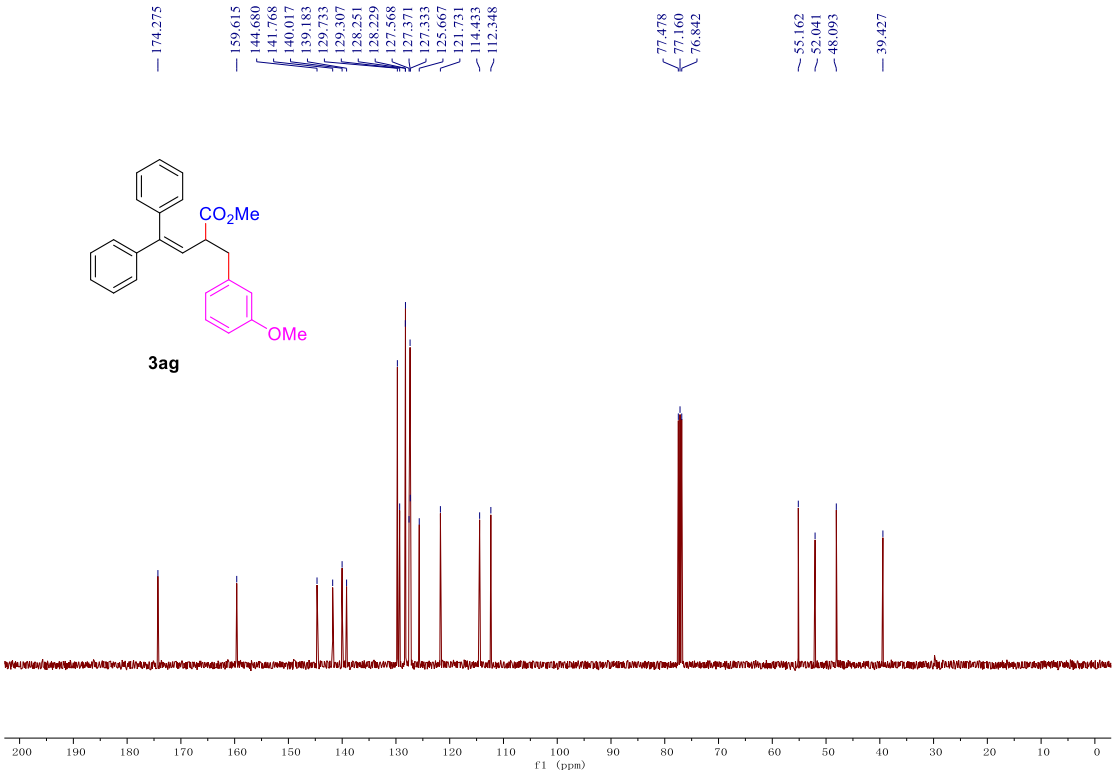
1.01
1.00
f1 (ppm)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52.041
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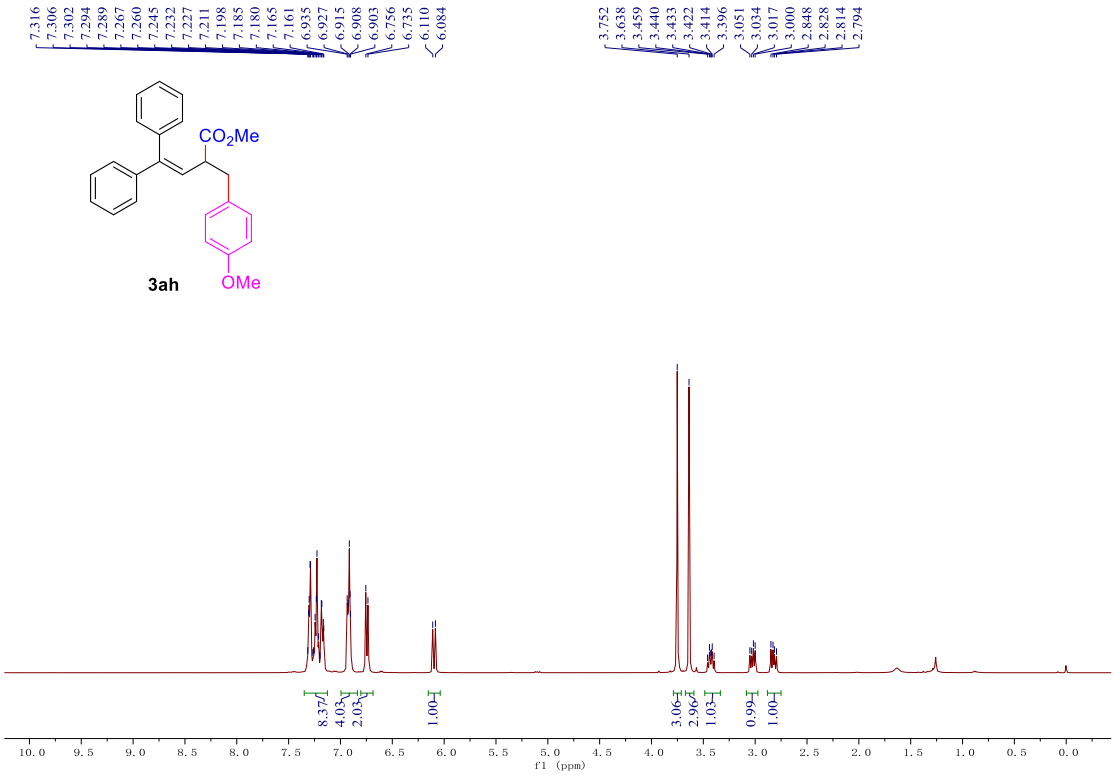
39.427
CO2Me
OMe
3ag
f1 (ppm)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6.915
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6.903
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6.735
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6.084
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3.638
3.459
3.440
3.433
3.422
3.414
3.396
3.051
3.034
3.017
3.000
2.848
2.828
2.814
2.794
CO2Me
OMe
3ah
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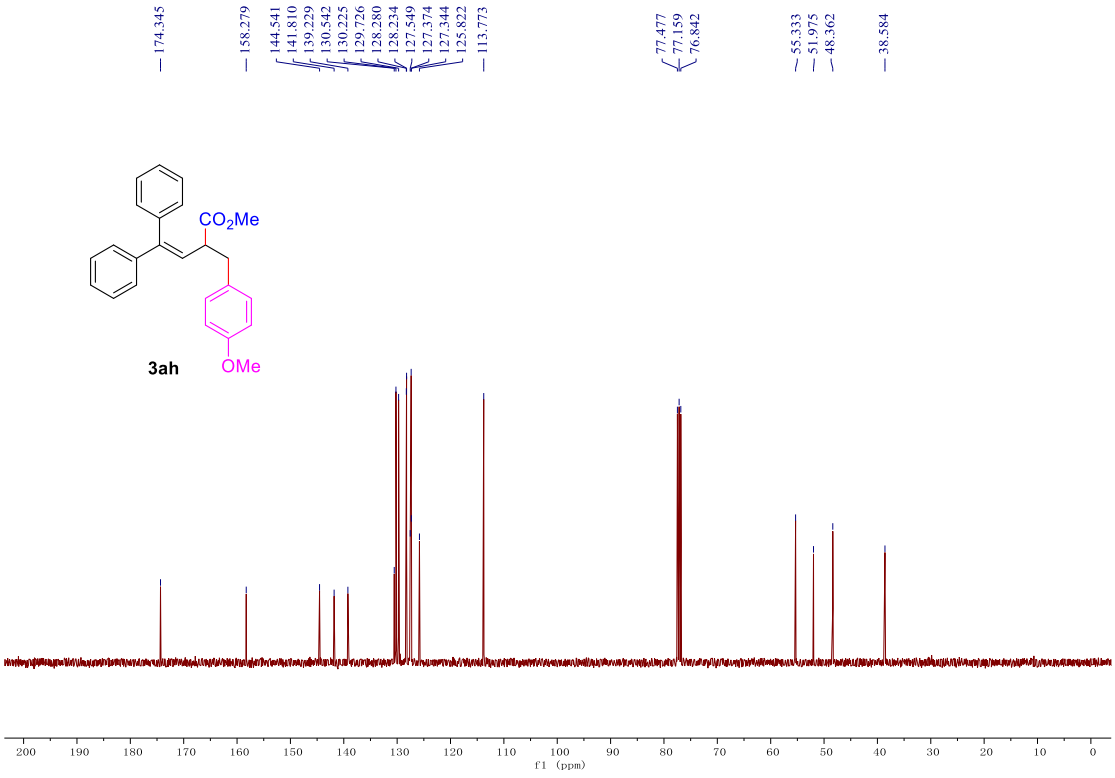
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125.822
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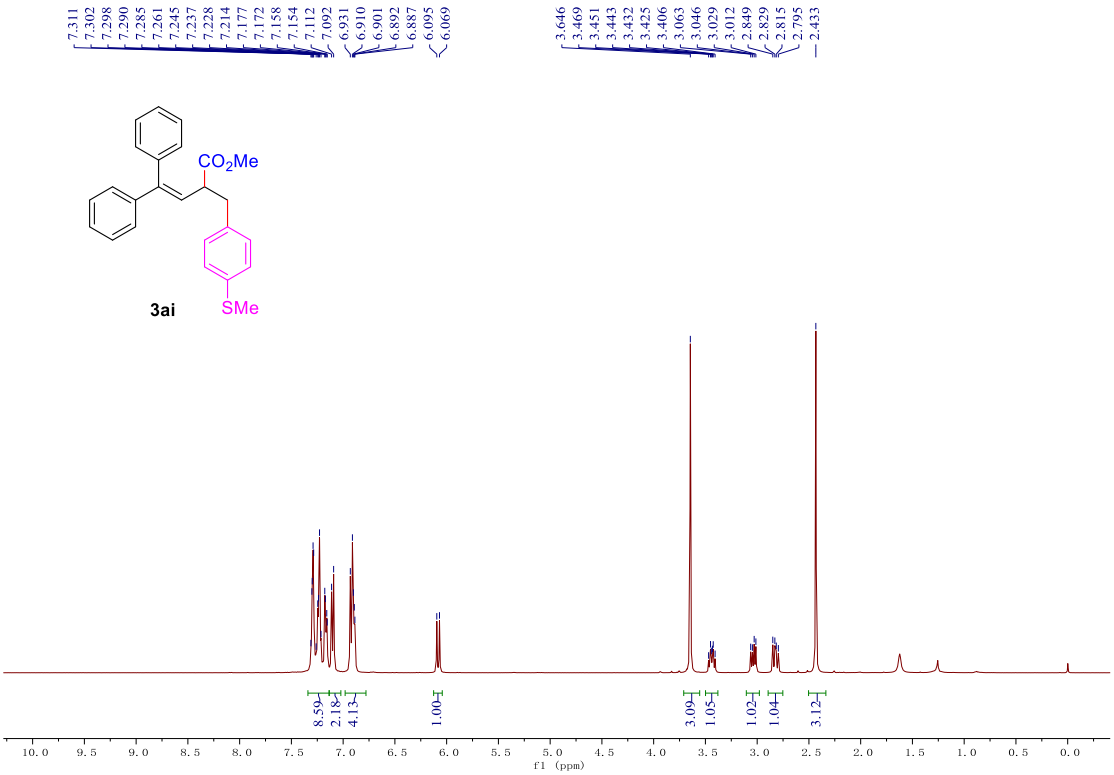
38.584
CO2Me
OMe
3ah
f1 (ppm)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7.158
7.154
7.112
7.092
6.931
6.910
6.901
6.892
6.887
6.095
6.069
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3.469
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3.443
3.432
3.425
3.406
3.063
3.046
3.029
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2.849
2.829
2.815
2.795
2.433
CO2Me
SMe
3ai
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1.02
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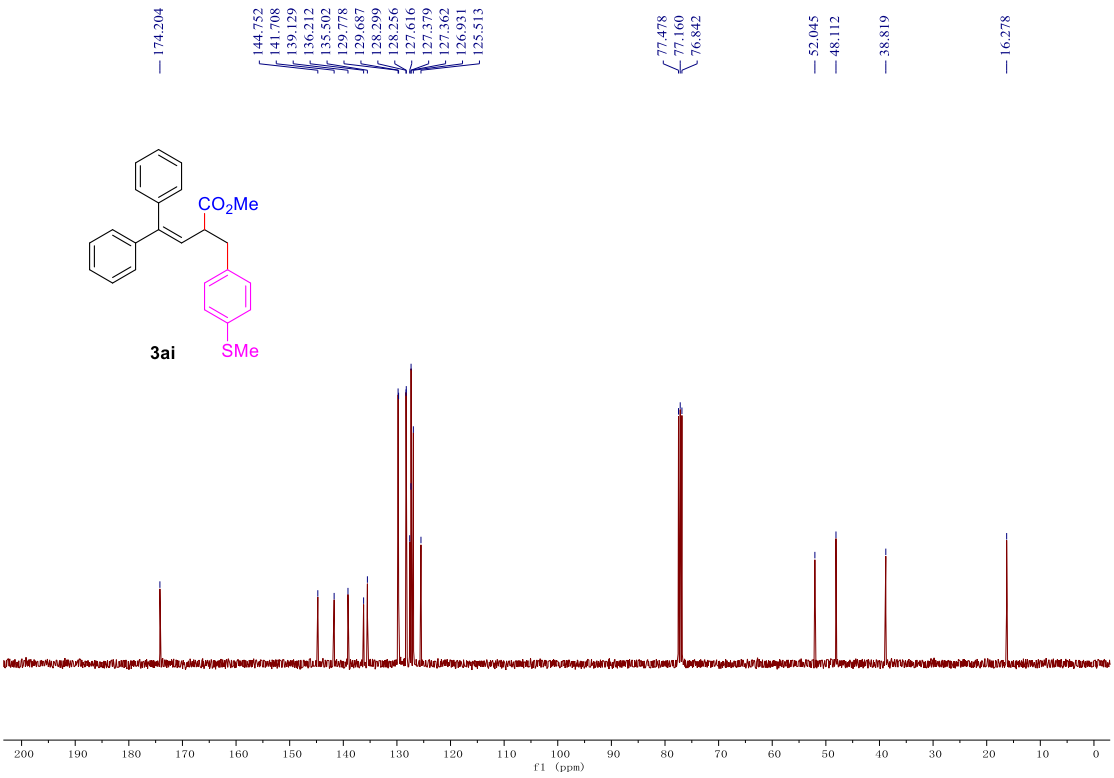
3.12
f1 (ppm)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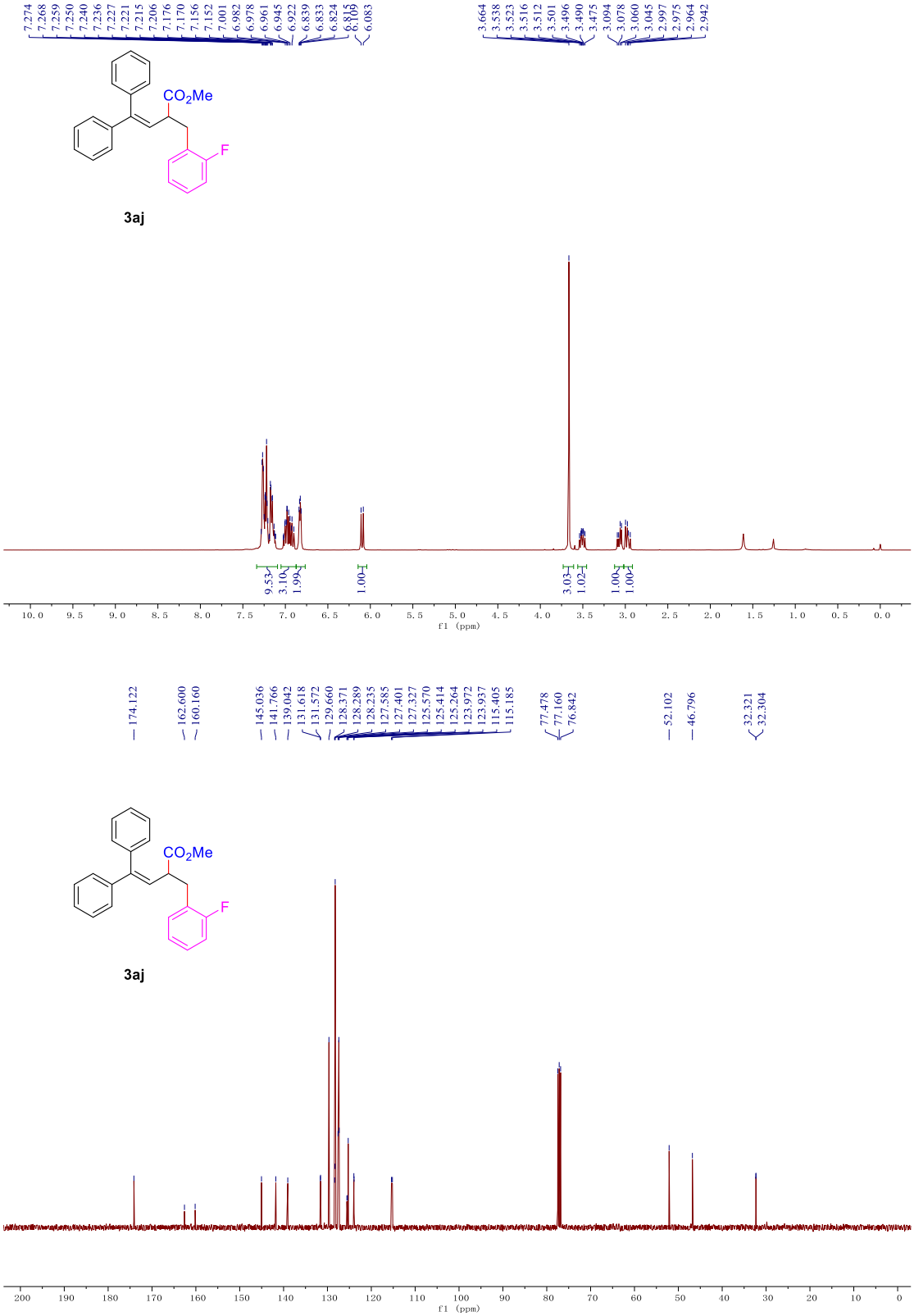
CO2Me
SMe
3ai
f1 (ppm)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7.152
7.001
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3.512
3.501
3.496
3.490
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3.078
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3.045
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2.964
2.942
CO2Me
F
3aj
9.53
3.10
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1.00
3.03
1.02
1.00
1.00
f1 (ppm)
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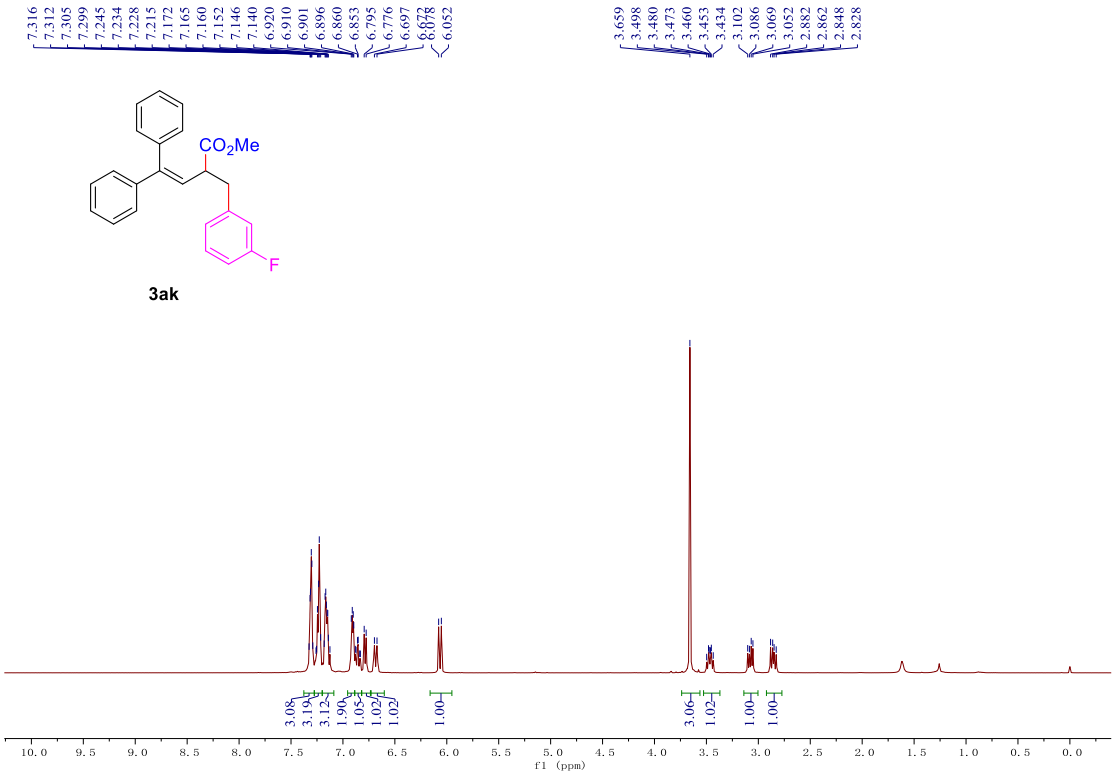
32.304
CO2Me
F
3aj
f1 (ppm)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7.140
6.920
6.910
6.901
6.896
6.860
6.853
6.795
6.776
6.697
6.672
6.052
3.659
3.498
3.480
3.473
3.460
3.453
3.434
3.102
3.086
3.069
3.052
2.882
2.862
2.848
2.828
CO2Me
F
3.08
3.19
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1.02
1.02
1.00
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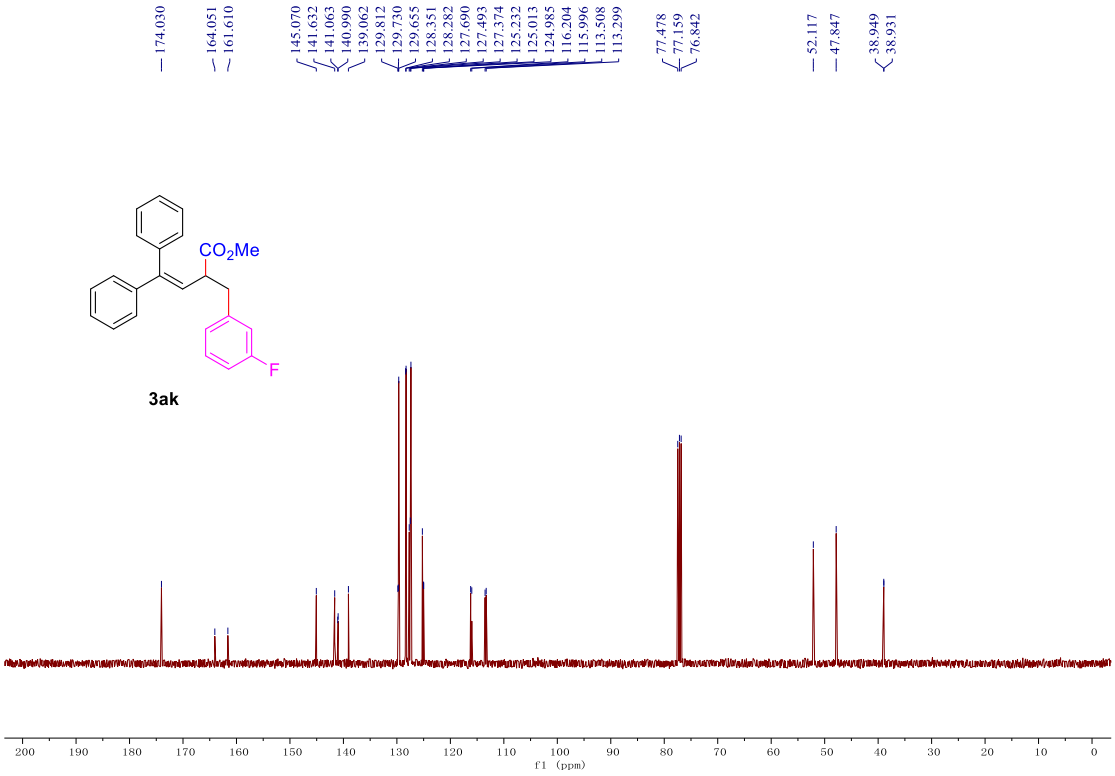
1.00
1.00
f1 (ppm)

3ak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127.493
127.374
125.232
125.013
124.985
116.204
115.996
113.508
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76.842
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47.847
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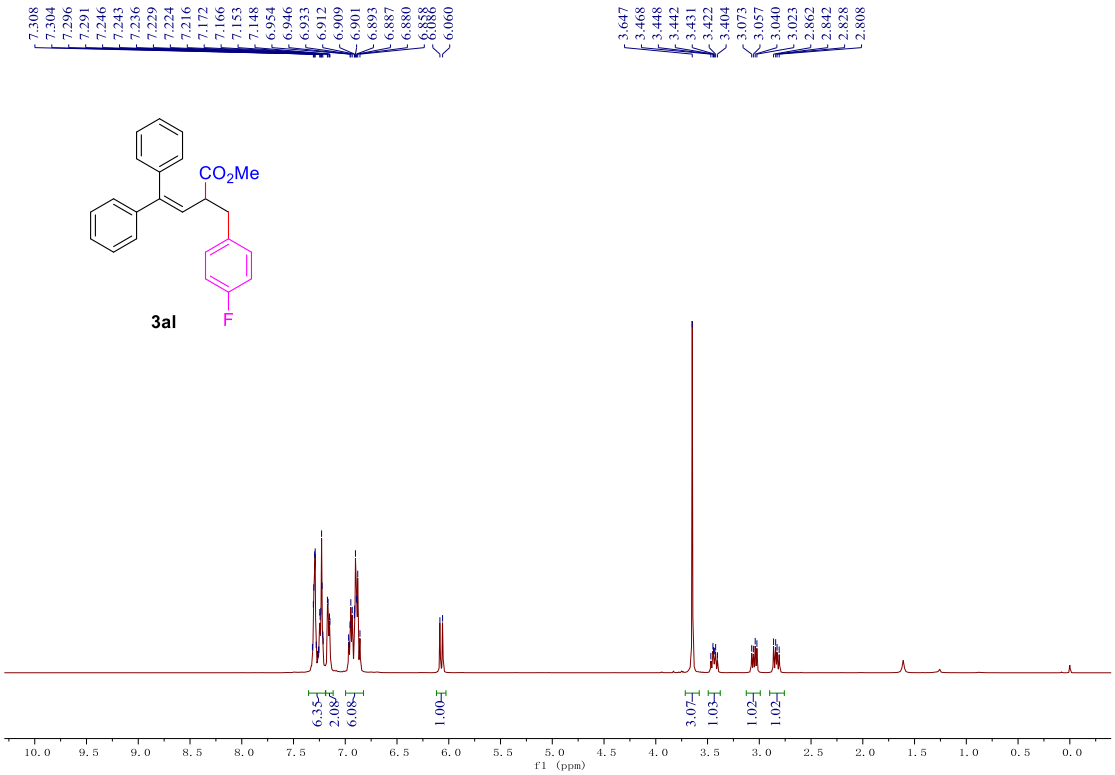
38.931
CO2Me
F
f1 (ppm)

3ak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7.153
7.148
6.954
6.946
6.933
6.912
6.909
6.901
6.893
6.887
6.880
6.858
6.060
3.647
3.468
3.448
3.442
3.431
3.422
3.404
3.073
3.057
3.040
3.023
2.862
2.842
2.828
2.808
CO2Me
F
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6.08
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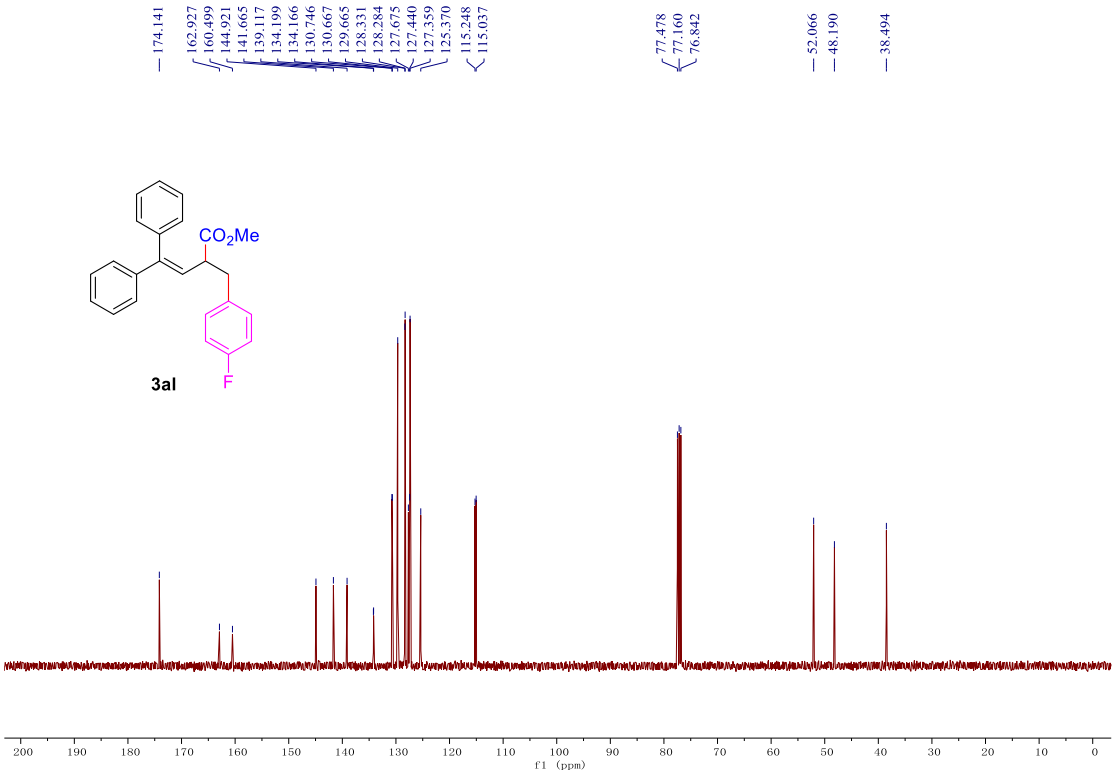
1.03
1.02
1.02
f1 (ppm)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139.117
134.199
134.166
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130.667
129.665
128.331
128.284
127.675
127.440
127.359
125.370
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77.160
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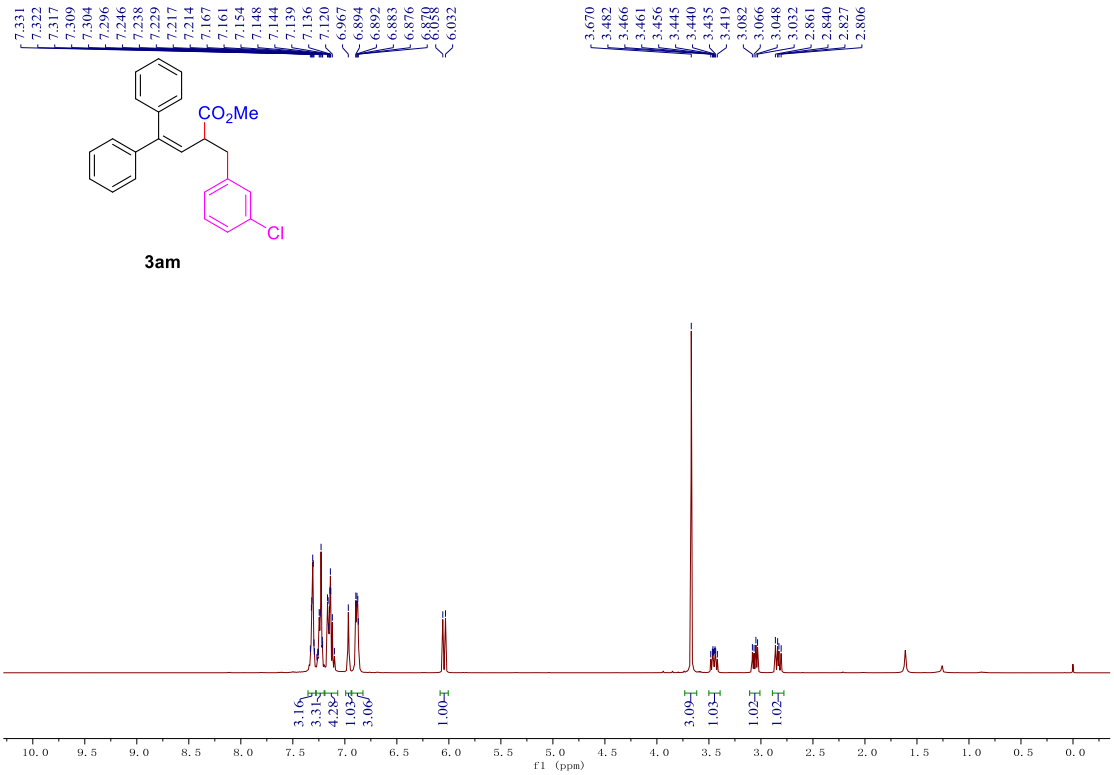
48.190
38.494
CO2Me
F
3al
f1 (ppm)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7.154
7.148
7.144
7.139
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7.120
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6.876
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6.858
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3.461
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3.435
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3.082
3.066
3.048
3.032
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2.840
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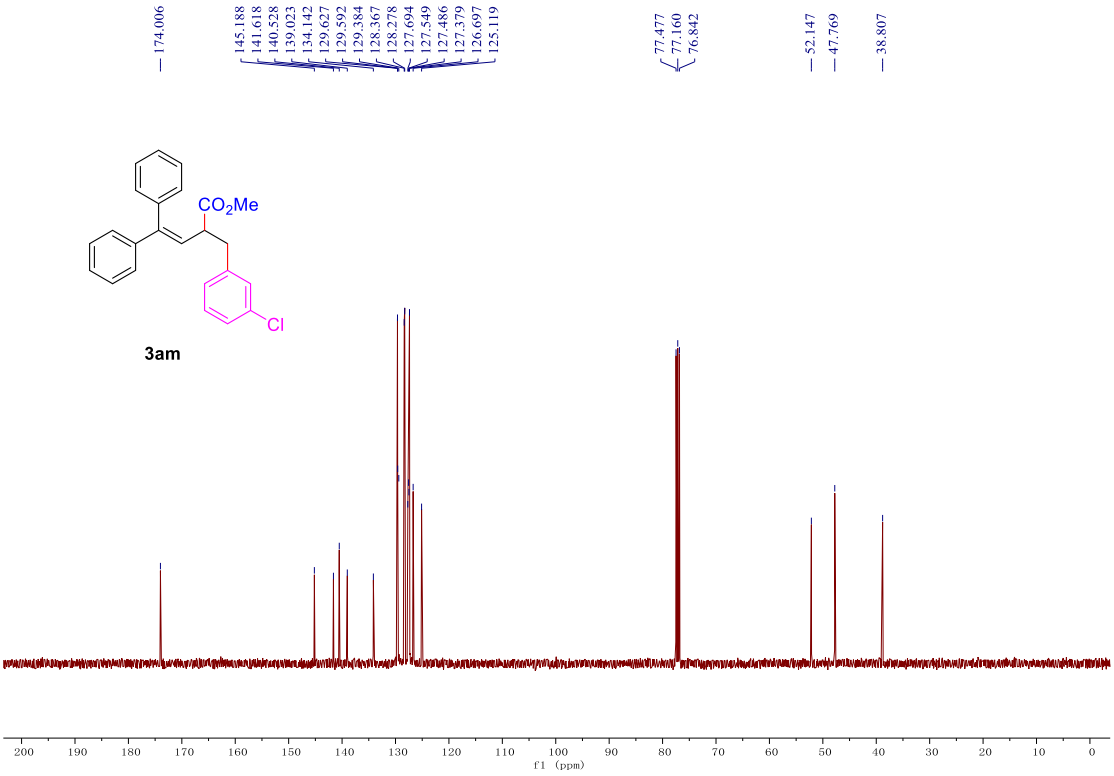
2.806
CO2Me
Cl
3am
3.16
3.31
4.28
1.03
3.06
1.00
3.09
1.03
1.02
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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127.379
126.697
125.119
77.477
77.160
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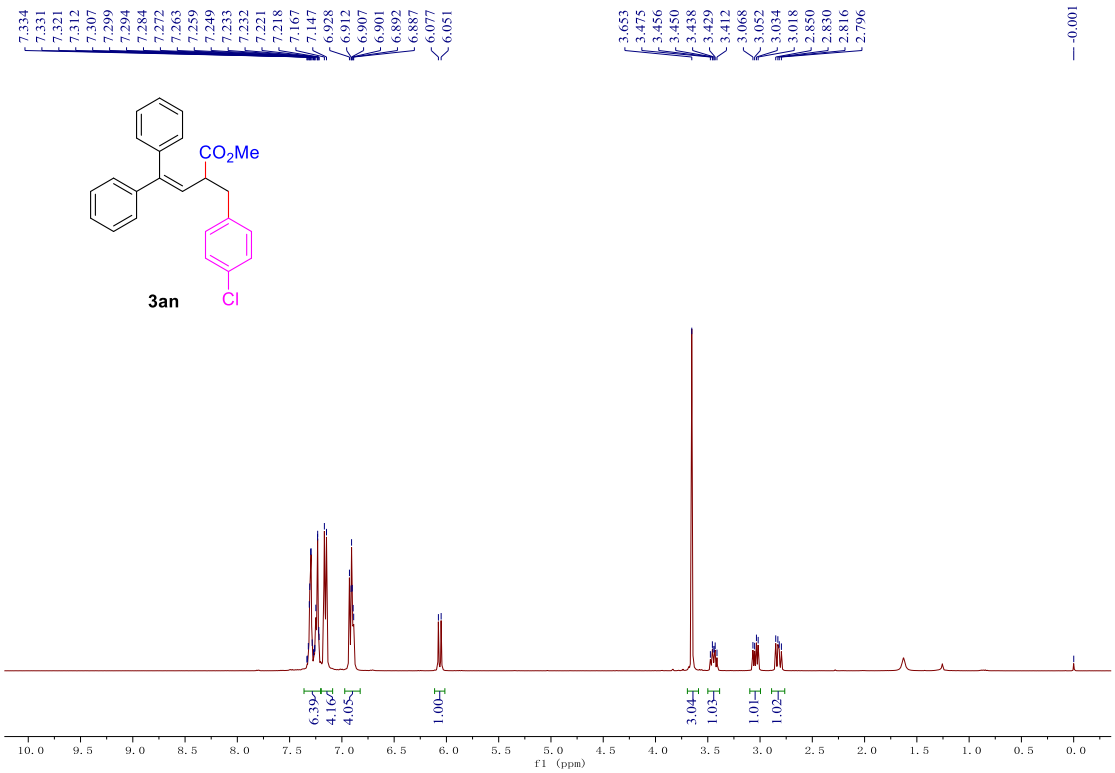
38.807
CO2Me
Cl
3am
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.232
7.221
7.218
7.167
7.147
6.928
6.912
6.907
6.901
6.892
6.887
6.077
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3.450
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-0.001
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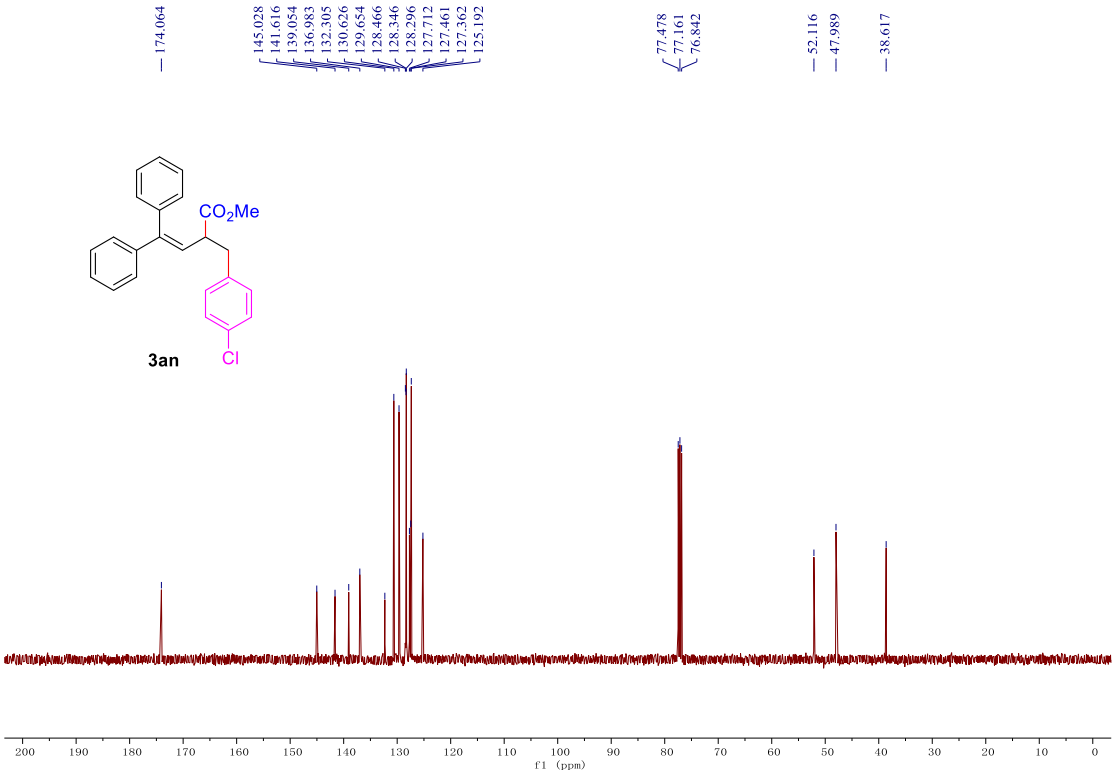
1.02
f1 (ppm)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Cl
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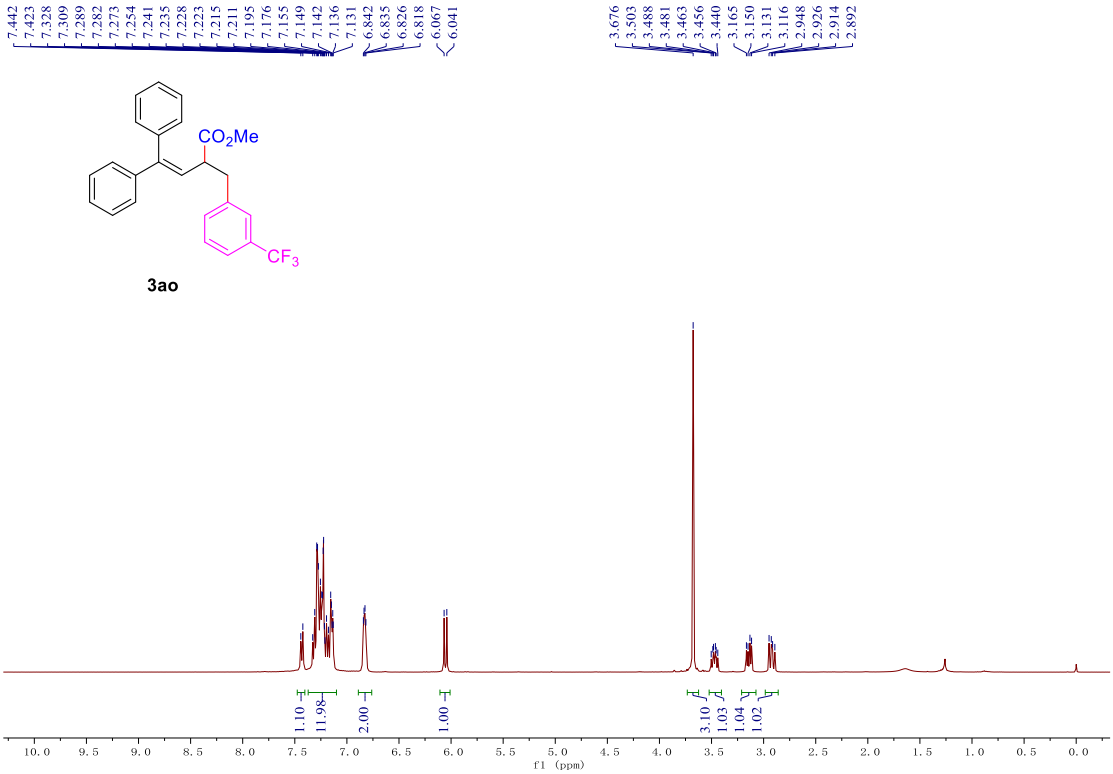
f1 (ppm)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3.456
3.440
3.165
3.150
3.131
3.116
2.948
2.926
2.914
2.892
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CF3
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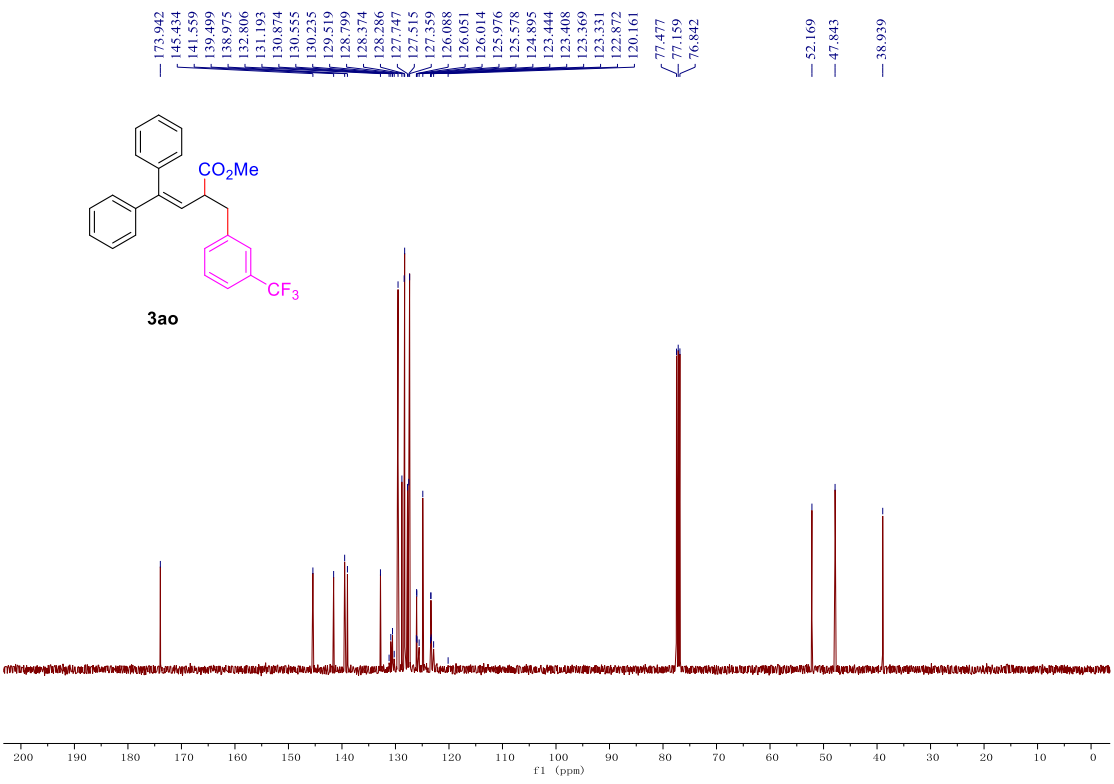
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128.374
128.286
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127.359
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123.408
123.369
123.331
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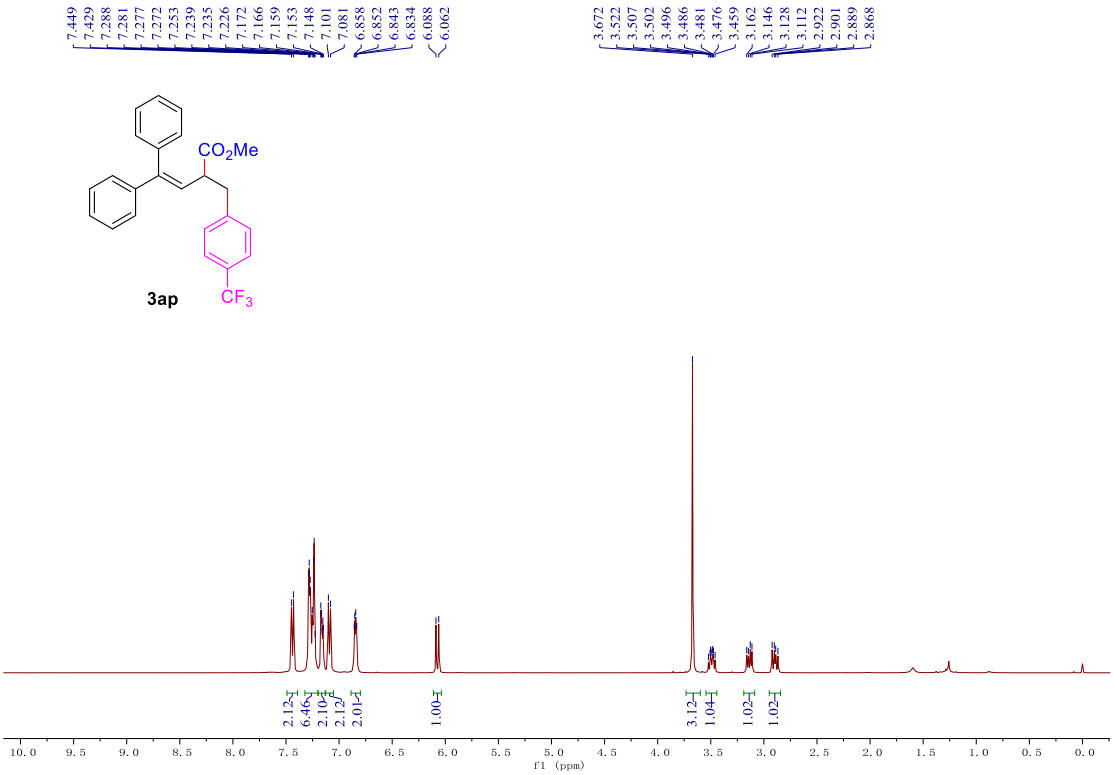
CO2Me
CF3
3ao
f1 (ppm)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7.153
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CF3
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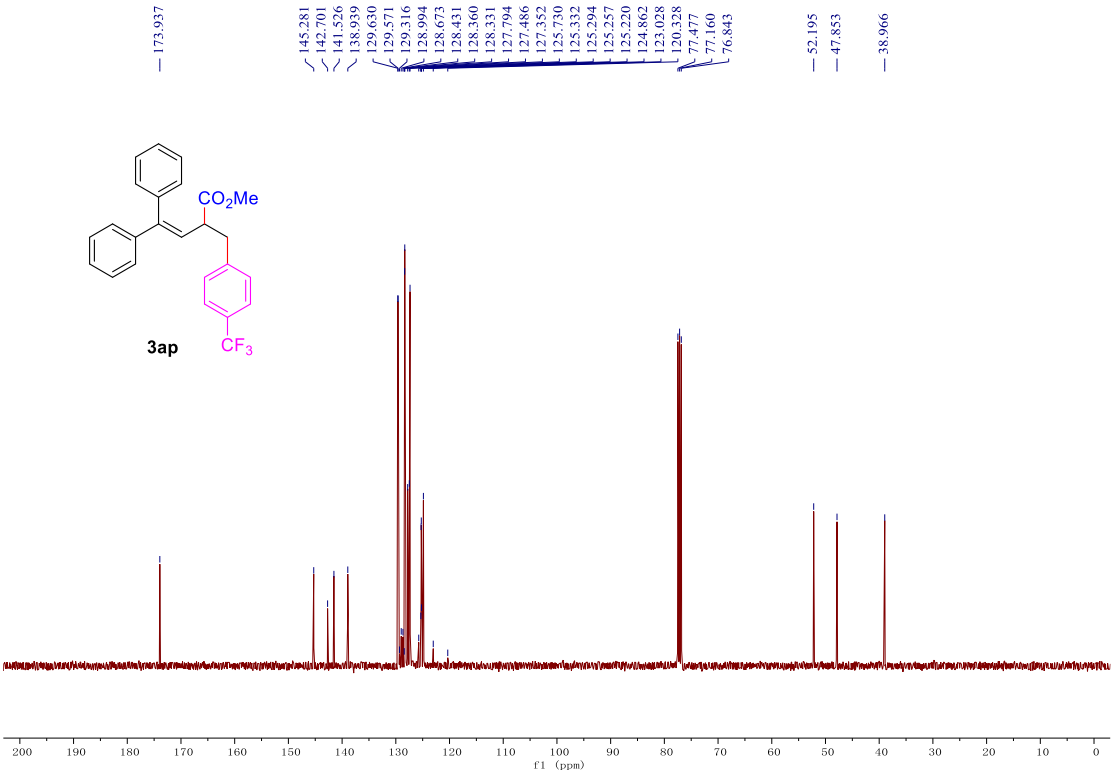
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127.486
127.352
125.730
125.332
125.294
125.257
125.220
124.862
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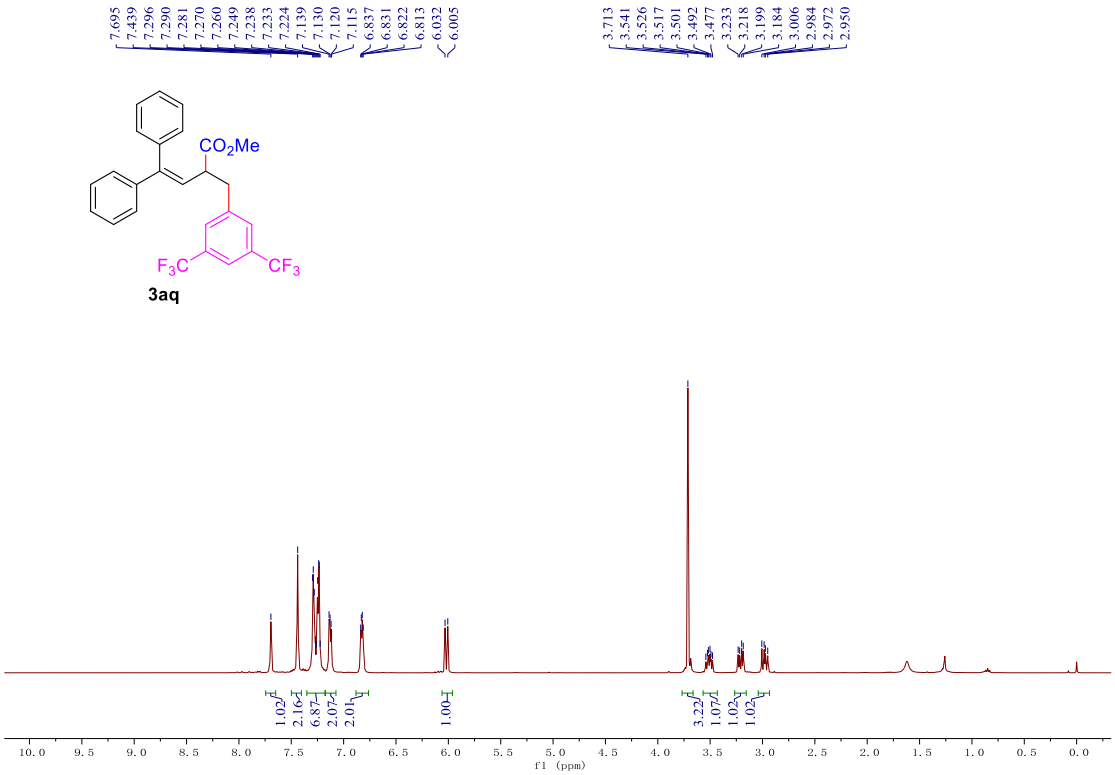
52.195
47.853
38.966
CO2Me
CF3
3ap
f1 (ppm)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7.115
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6.032
6.005
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3.541
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3.517
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3.492
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CO2Me
F3C
CF3
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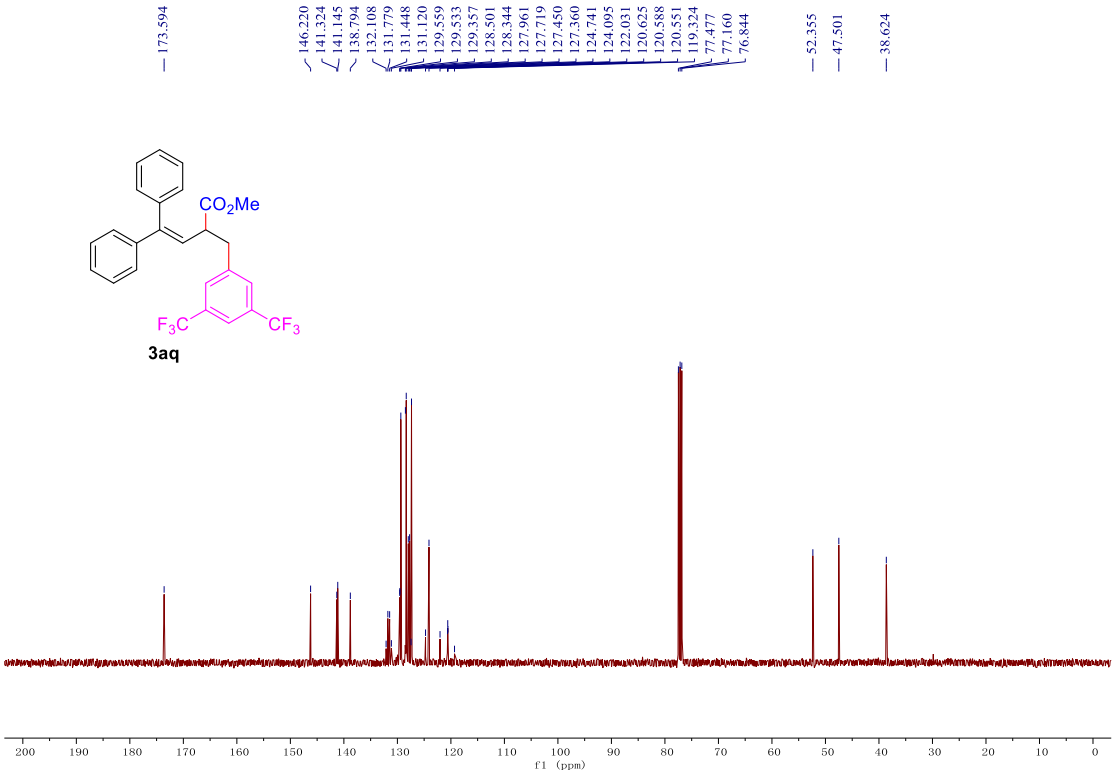
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127.360
124.741
124.095
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120.551
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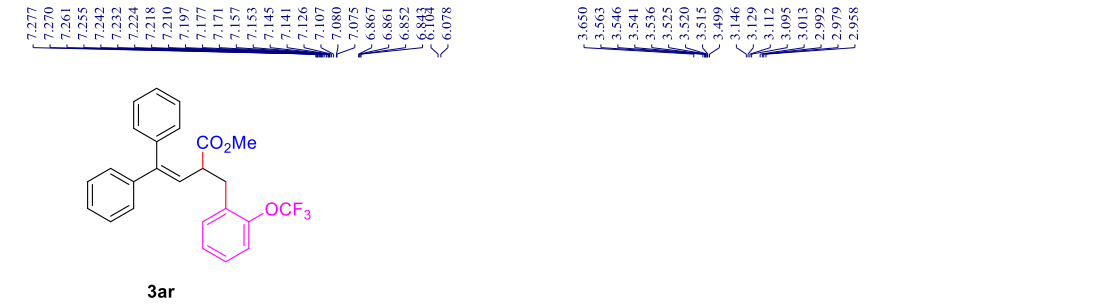
CO2Me
F3C
CF3
3aq
f1 (ppm)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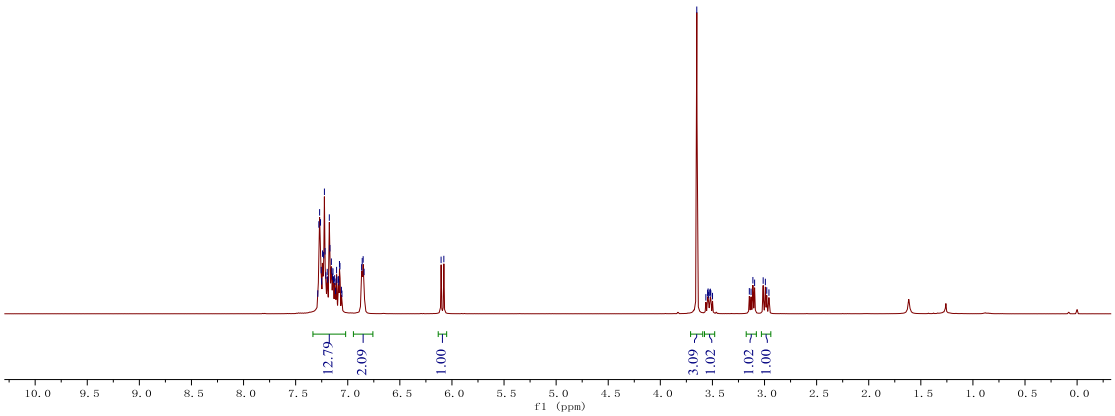
CO2Me
OCF3

3ar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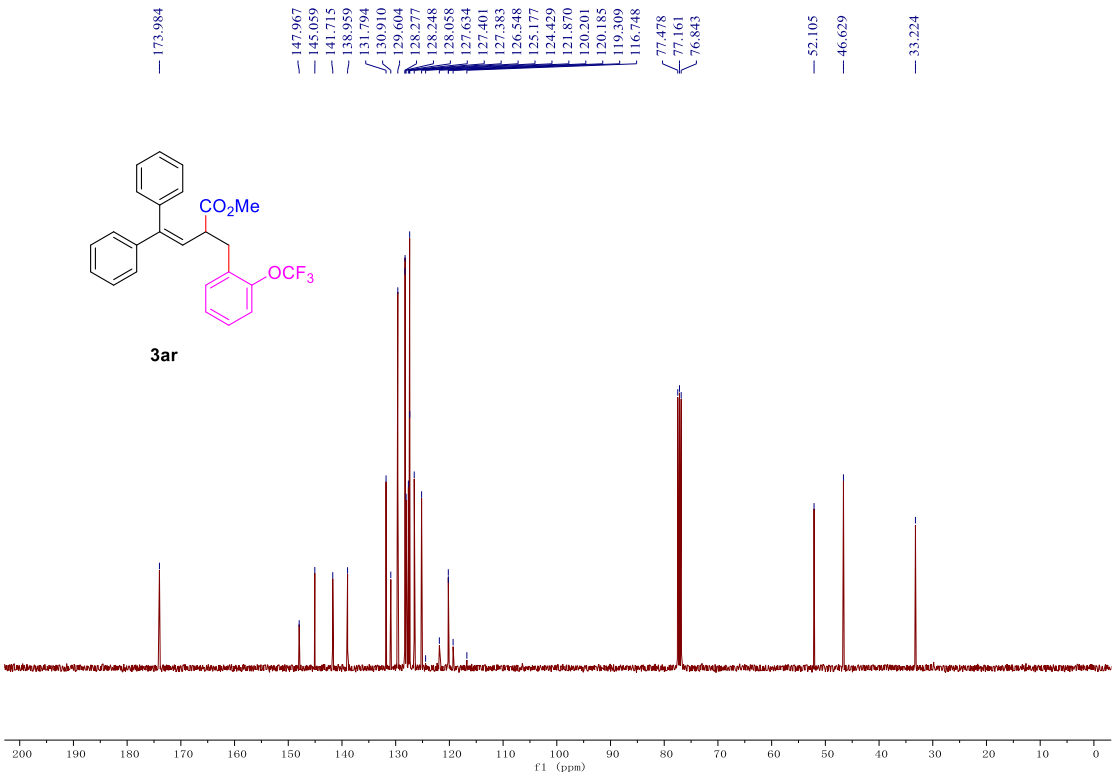
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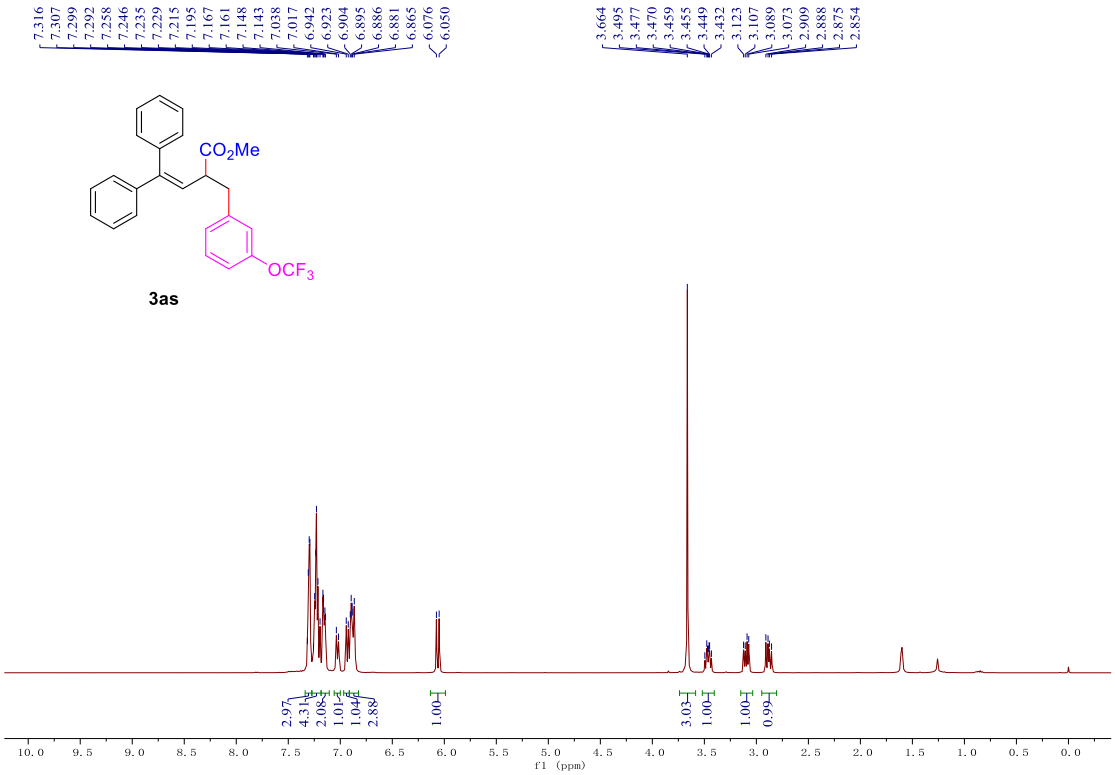
120.185
119.309
116.748
77.478
77.161
76.843
52.105
46.629
33.224
CO2Me
OCF3
f1 (ppm)

3ar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7.161
7.148
7.143
7.038
7.017
6.942
6.923
6.904
6.895
6.886
6.881
6.865
6.076
6.050
3.664
3.495
3.477
3.470
3.459
3.455
3.449
3.432
3.123
3.107
3.089
3.073
2.909
2.888
2.875
2.854
CO2Me
OCF3
3as
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1.04
2.88
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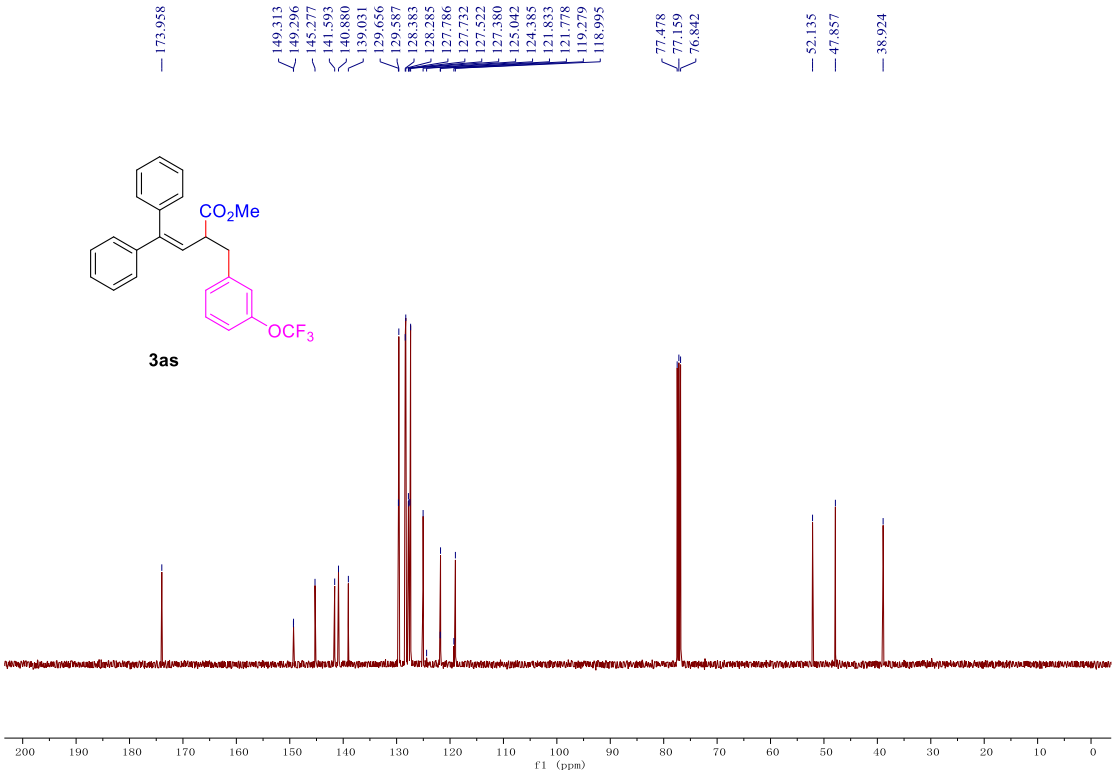
3.03
1.00
1.00
0.99
f1 (ppm)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128.285
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127.732
127.522
127.380
125.042
124.385
121.833
121.778
119.279
118.995
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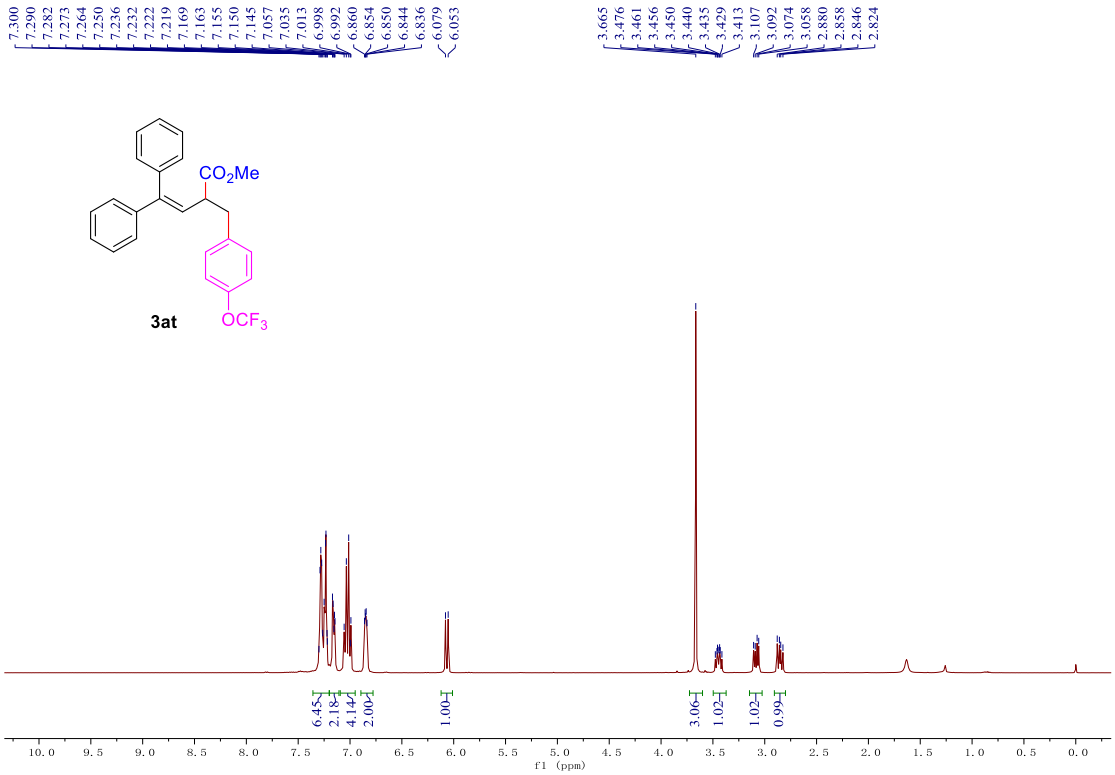
77.159
76.842
52.135
47.857
38.924
CO2Me
OCF3
3as
f1 (ppm)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7.155
7.150
7.145
7.057
7.035
7.013
6.998
6.992
6.860
6.854
6.850
6.844
6.836
6.079
6.053
3.665
3.476
3.461
3.456
3.450
3.440
3.435
3.429
3.413
3.107
3.092
3.074
3.058
2.880
2.858
2.846
2.824
CO2Me
OCF3
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1.00
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1.02
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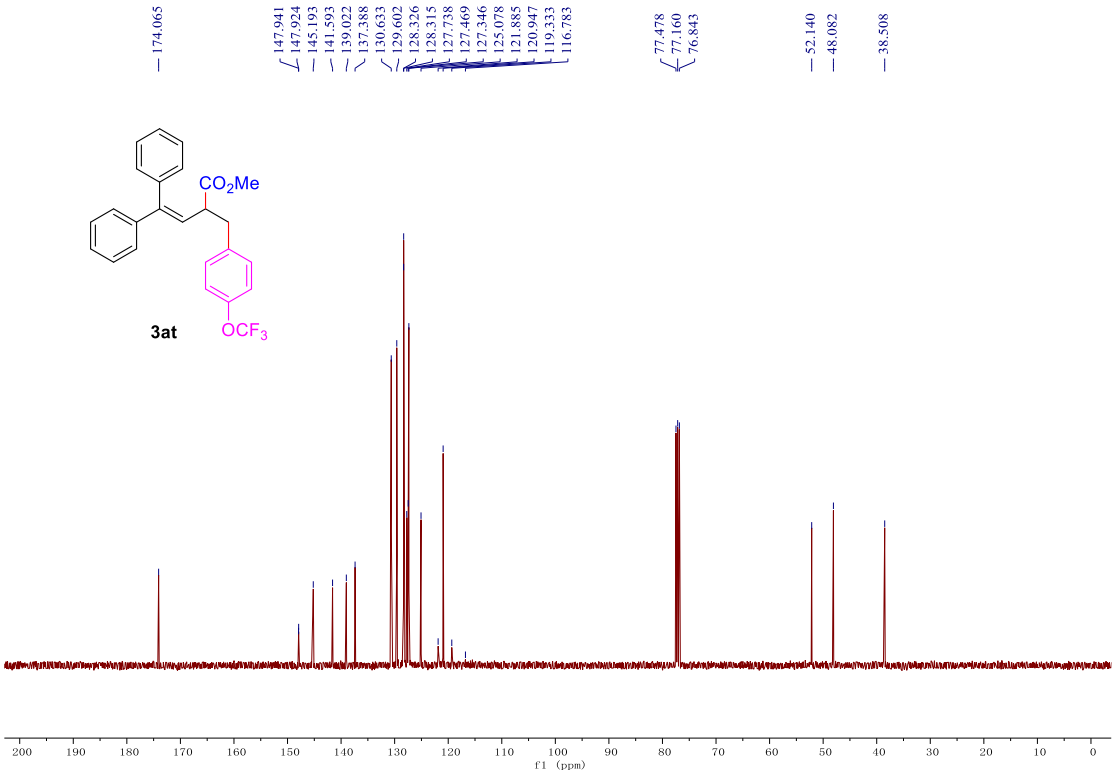
0.99
f1 (ppm)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147.924
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130.633
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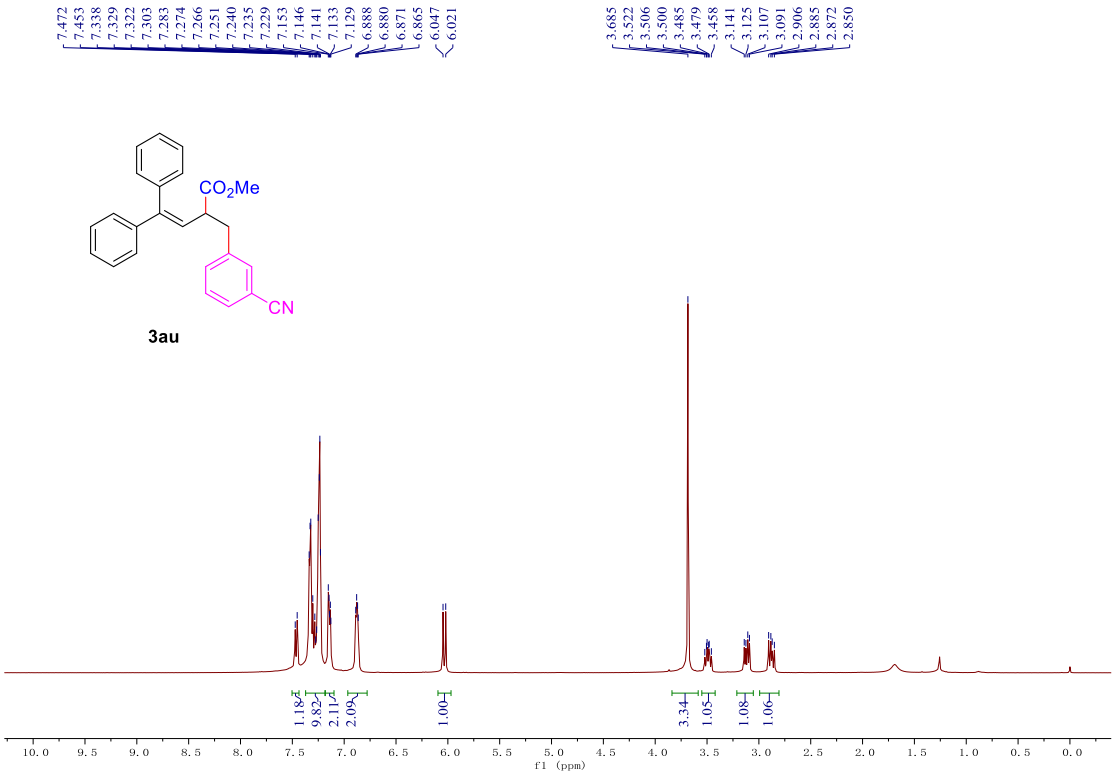
127.469
127.346
125.078
121.885
120.947
119.333
116.783
77.478
77.160
76.843
52.140
48.082
38.508
CO2Me
OCF3
3at
f1 (ppm)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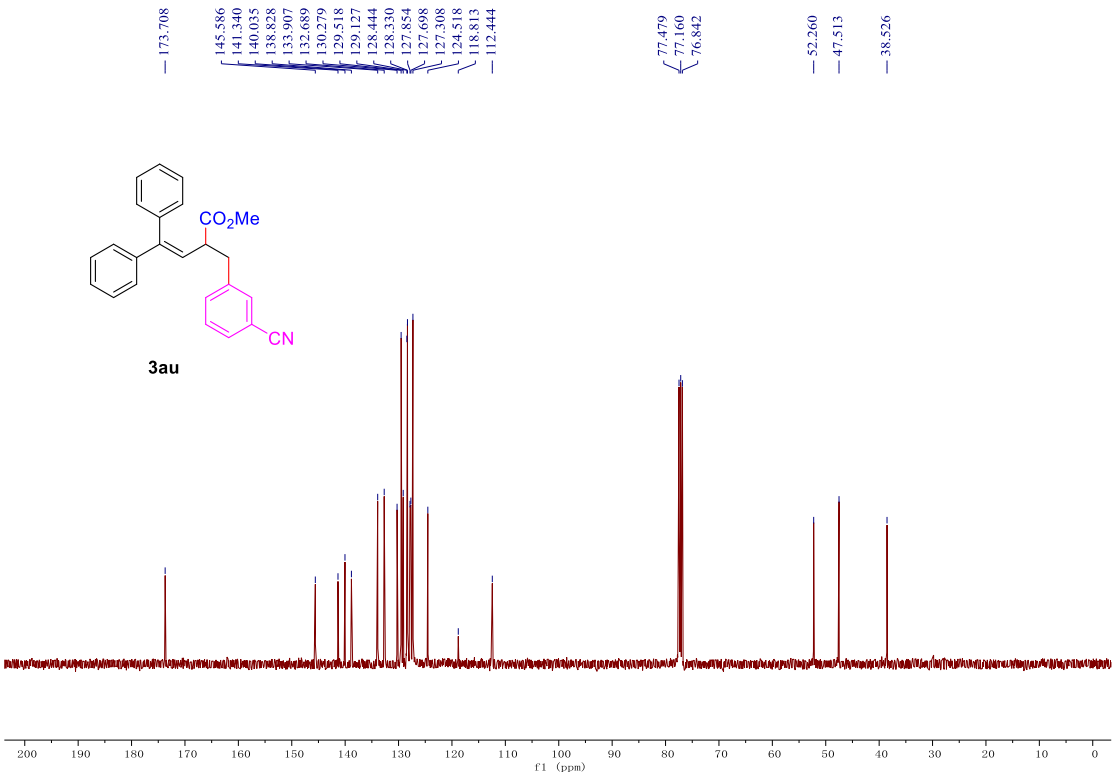
7.229
7.153
7.146
7.141
7.133
7.129
6.888
6.880
6.871
6.865
6.047
6.021
3.685
3.522
3.506
3.500
3.485
3.479
3.458
3.141
3.125
3.107
3.091
2.906
2.885
2.872
2.850
CO2Me
CN
3au
1.18
9.82
2.11
2.09
1.00
3.34
1.05
1.08
1.06
f1 (ppm)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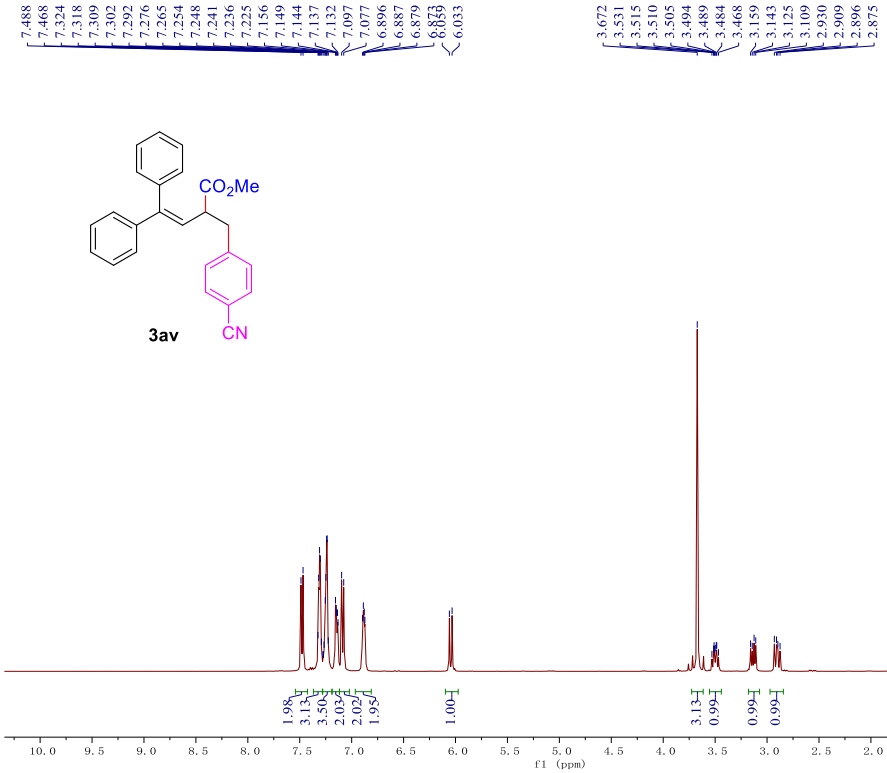
138.828
133.907
132.689
130.279
129.518
129.127
128.444
128.330
127.854
127.698
127.308
124.518
118.813
112.444
77.479
77.160
76.842
52.260
47.513
38.526
CO2Me
CN
3au
f1 (ppm)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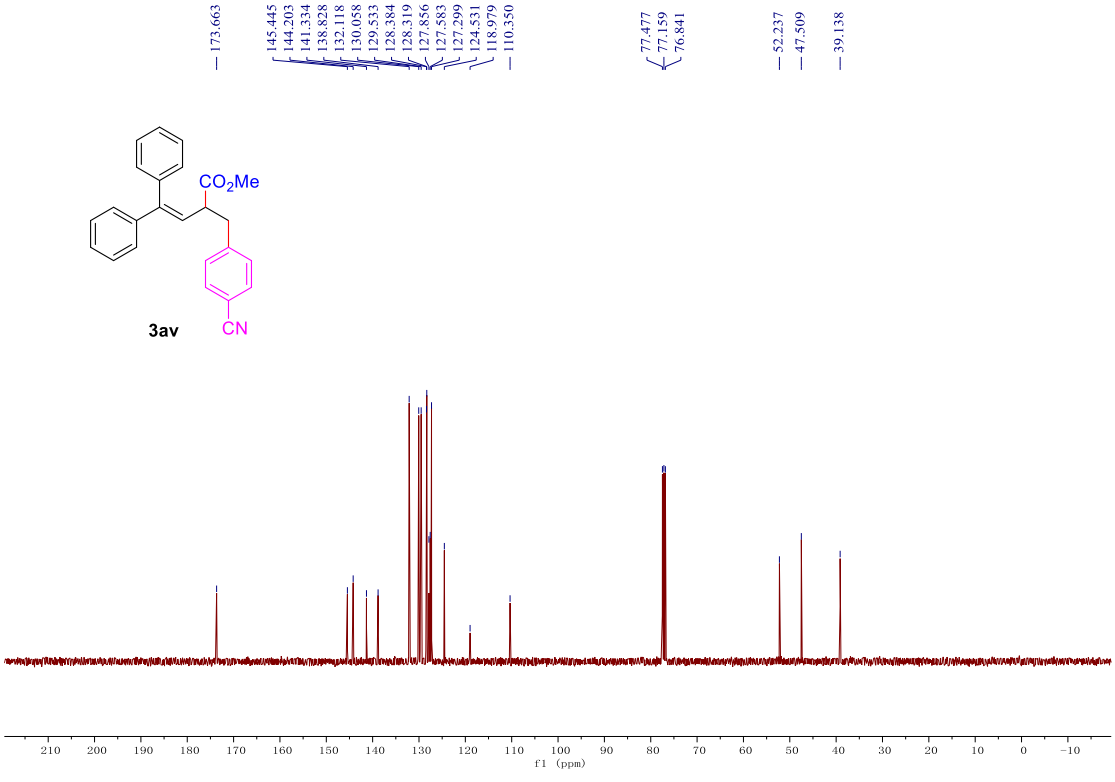
7.318
7.309
7.302
7.292
7.276
7.265
7.254
7.248
7.241
7.236
7.225
7.156
7.149
7.144
7.137
7.132
7.097
7.077
6.896
6.887
6.879
6.873
6.059
6.033
3.672
3.531
3.515
3.510
3.505
3.494
3.489
3.484
3.468
3.159
3.143
3.125
3.109
2.930
2.909
2.896
2.875
CO2Me
CN
3av
1.98
3.13
3.56
2.02
2.02
1.95
1.00
3.13
0.99
0.99
0.99
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)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141.334
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130.058
129.533
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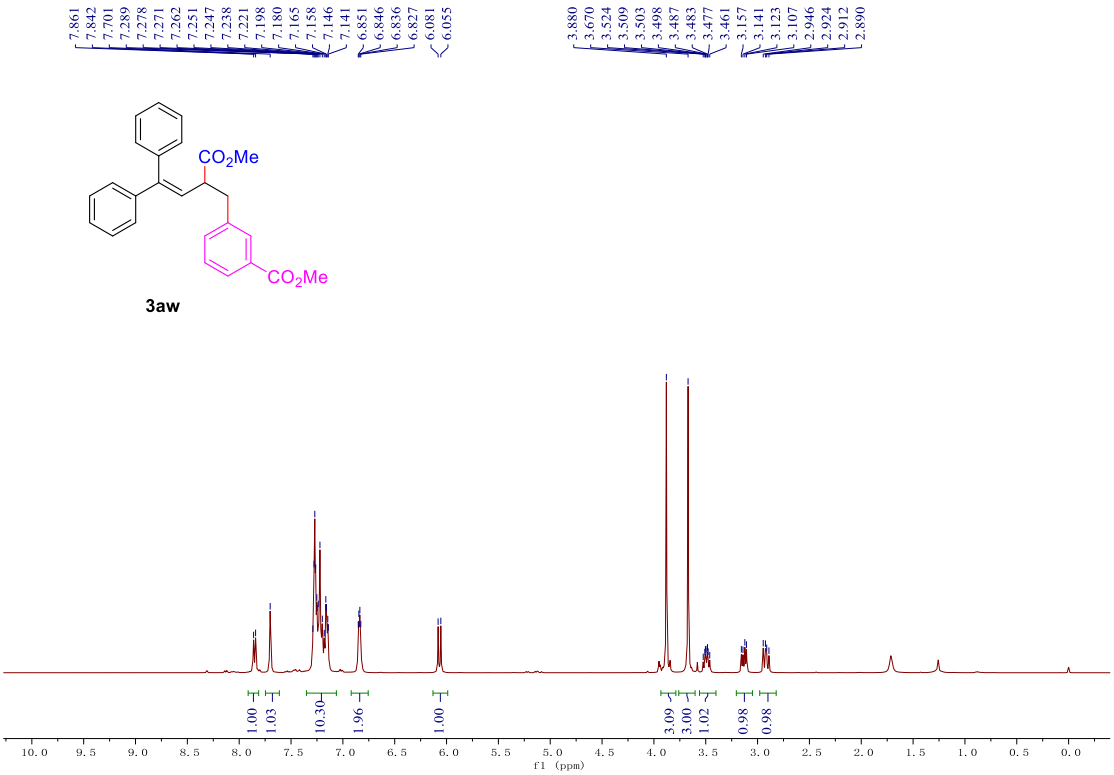
128.319
127.856
127.583
127.299
124.531
118.979
110.350
77.477
77.159
76.841
52.237
47.509
39.138
CO2Me
CN
3av
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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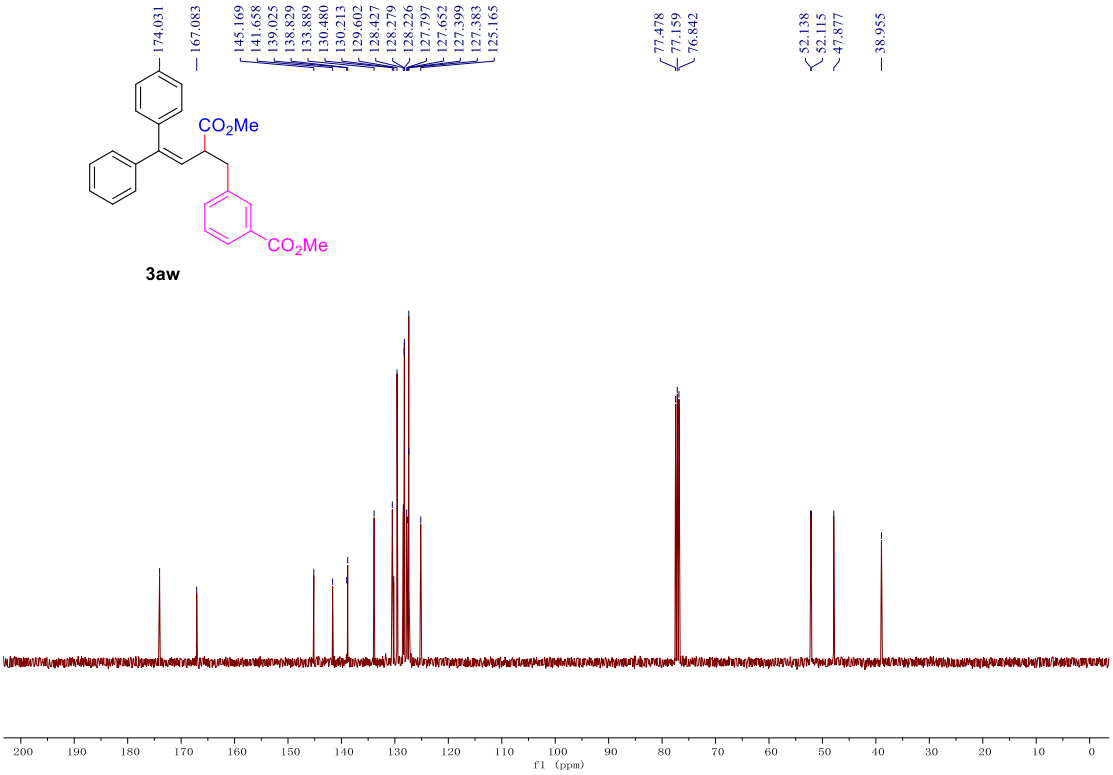
7.289
7.278
7.271
7.262
7.251
7.247
7.238
7.221
7.198
7.180
7.165
7.158
7.146
7.141
6.851
6.846
6.836
6.827
6.081
6.055
3.880
3.670
3.524
3.509
3.503
3.498
3.487
3.483
3.477
3.461
3.157
3.141
3.123
3.107
2.946
2.924
2.912
2.890
CO2Me
CO2Me
1.00
1.03
10.30
1.96
1.00
3.09
3.00
1.02
0.98
0.98
f1 (ppm)

3aw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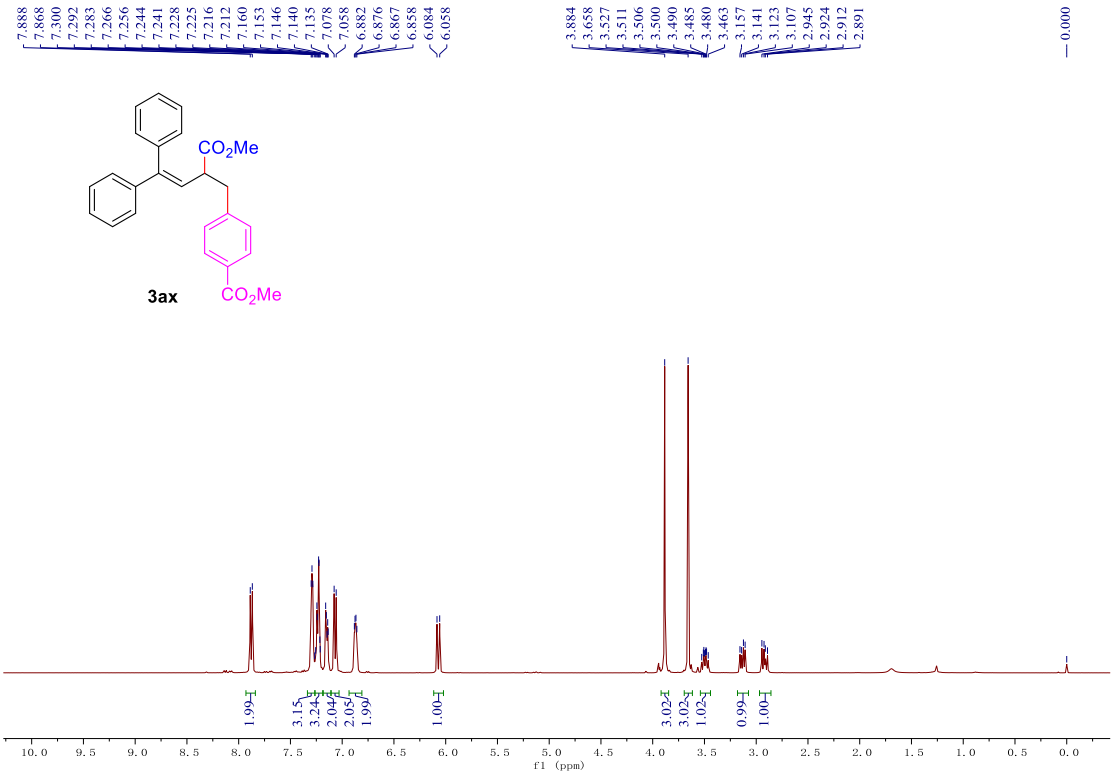
145.169
141.658
139.025
138.829
133.889
130.480
130.213
129.602
128.427
128.279
128.226
127.797
127.652
127.399
127.383
125.165
77.478
77.159
76.842
52.138
52.115
47.877
38.955
CO2Me
CO2Me
f1 (ppm)

3aw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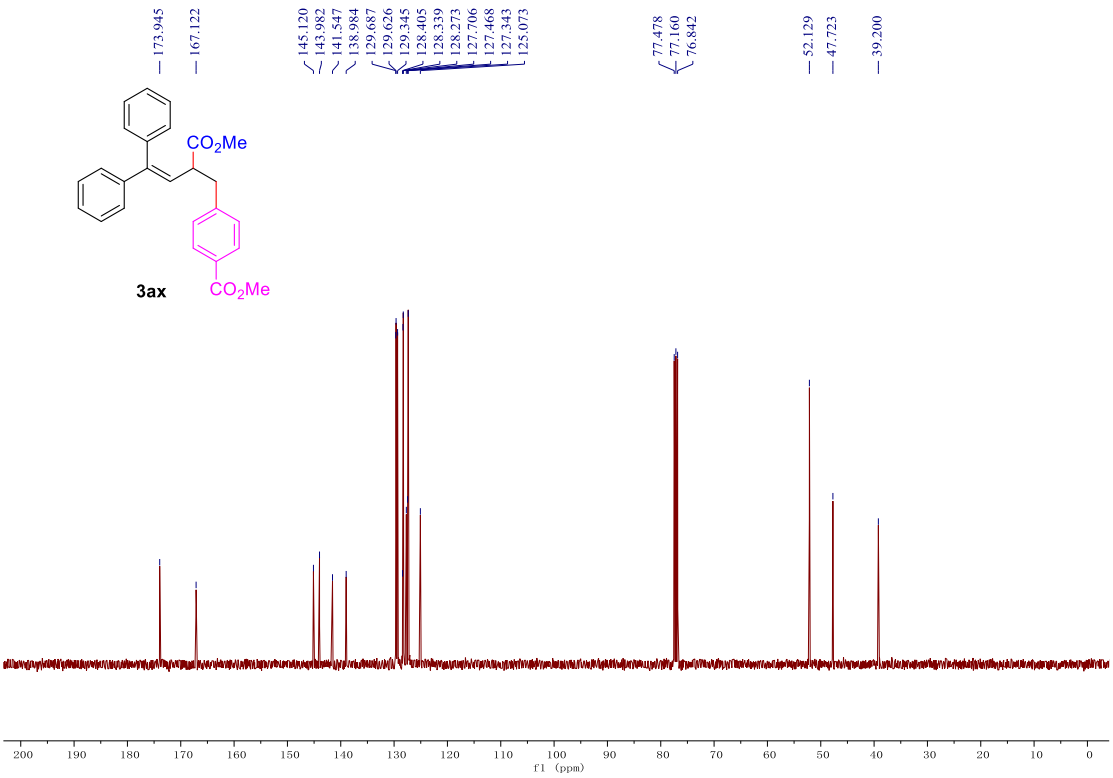
7.266
7.256
7.244
7.241
7.228
7.225
7.216
7.212
7.160
7.153
7.146
7.140
7.135
7.078
7.058
6.882
6.876
6.867
6.858
6.084
6.058
3.884
3.658
3.527
3.511
3.506
3.500
3.490
3.485
3.480
3.463
3.157
3.141
3.123
3.107
2.945
2.924
2.912
2.891
0.000
CO2Me
CO2Me
3ax
1.99
3.15
3.24
2.04
2.05
1.99
1.00
3.02
3.02
1.02
0.99
1.00
f1 (ppm)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167.122
145.120
143.982
141.547
138.984
129.687
129.626
129.345
128.405
128.339
128.273
127.706
127.468
127.343
125.073
77.478
77.160
76.842
52.129
47.723
39.200
CO2Me
CO2Me
3ax
f1 (ppm)


7.557
7.538
7.441
7.437
7.421
7.416
7.405
7.402
7.385
7.306
7.285
7.280
7.276
7.273
7.269
7.264
7.241
7.237
7.222
7.217
7.208
7.189
7.184
7.179
7.170
7.165
7.080
7.060
6.897
6.894
6.890
6.886
6.879
6.862
3.536
3.530
3.520
3.515
3.509
3.500
3.494
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3.117
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2.932
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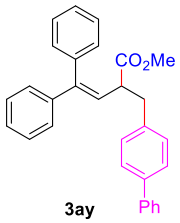
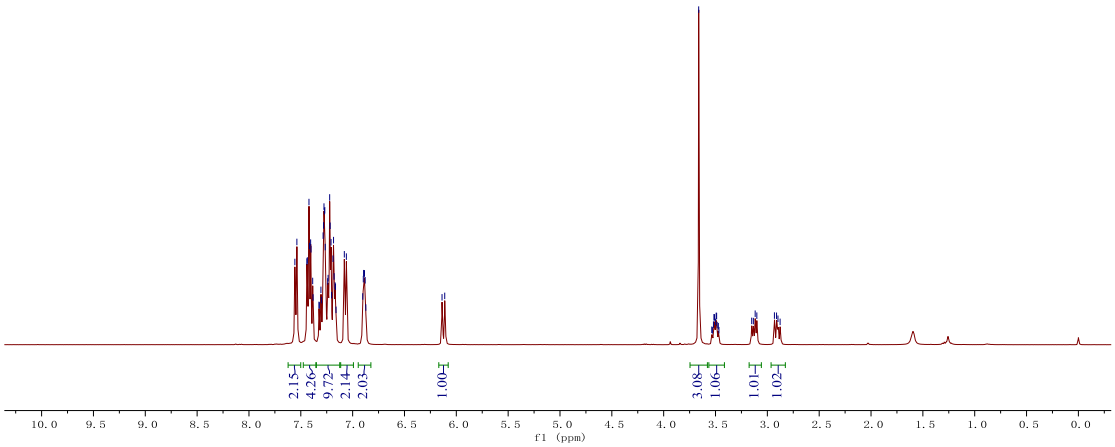
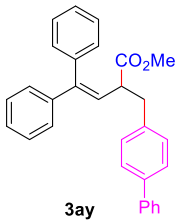
2.898
2.877


CO2Me
Ph

3ay

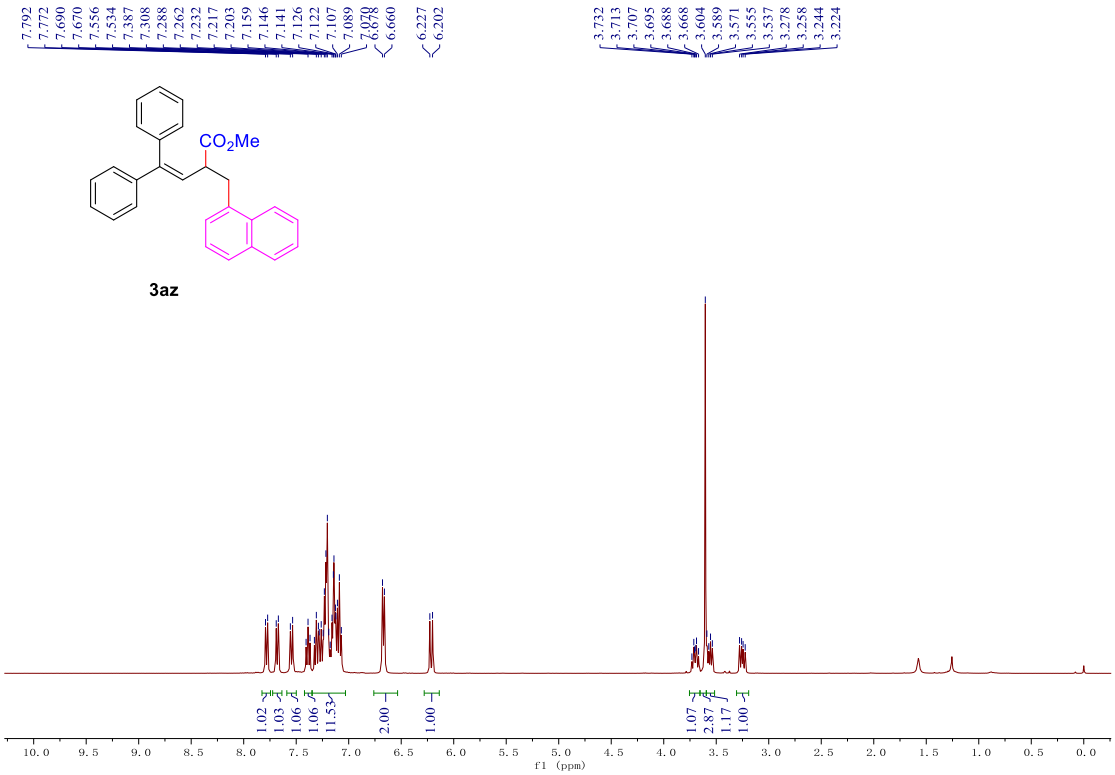

2.15
4.26
9.72
2.14
2.03
1.00
3.08
1.06
1.01
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


174.291
144.792
141.768
141.071
139.378
139.162
137.621
129.743
129.711
128.853
128.285
128.263
127.610
127.388
127.356
127.232
127.074
125.581
77.477
77.160
76.842
52.069
48.177
39.006


CO2Me
Ph

3ay

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.232
7.217
7.203
7.159
7.146
7.141
7.126
7.122
7.107
7.089
7.070
6.678
6.660
6.227
6.202
3.732
3.713
3.707
3.695
3.688
3.668
3.604
3.589
3.571
3.555
3.537
3.278
3.258
3.244
3.224
CO2Me
3az
1.02
1.03
1.06
1.06
11.53
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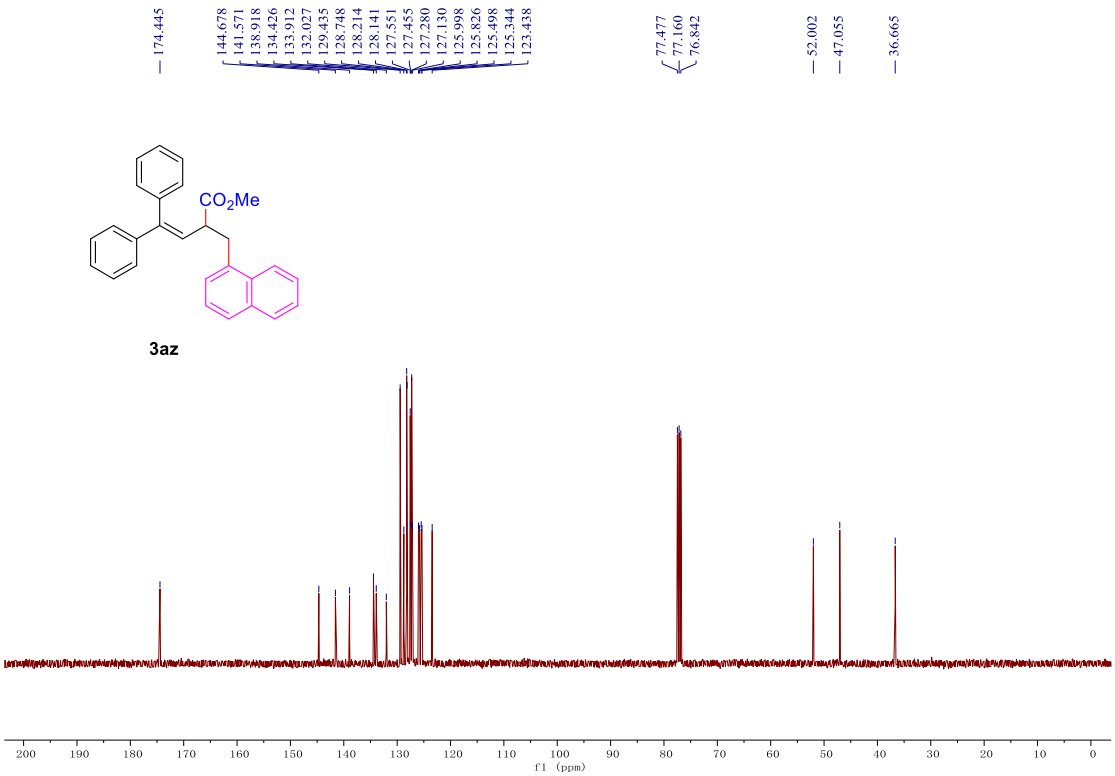
1.00
1.07
2.87
1.17
1.00
f1 (ppm)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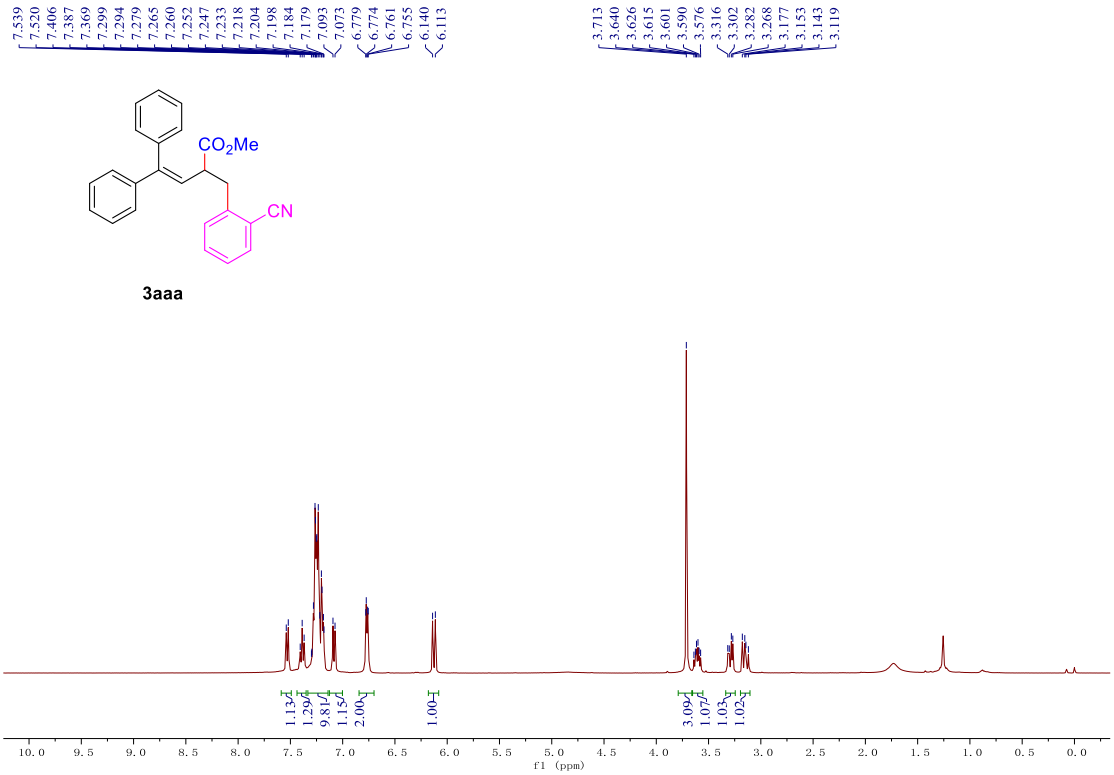
141.571
138.918
134.426
133.912
132.027
129.435
128.748
128.214
128.141
127.551
127.455
127.280
127.130
125.998
125.826
125.498
125.344
123.438
77.477
77.160
76.842
52.002
47.055
36.665
CO2Me
3az
f1 (ppm)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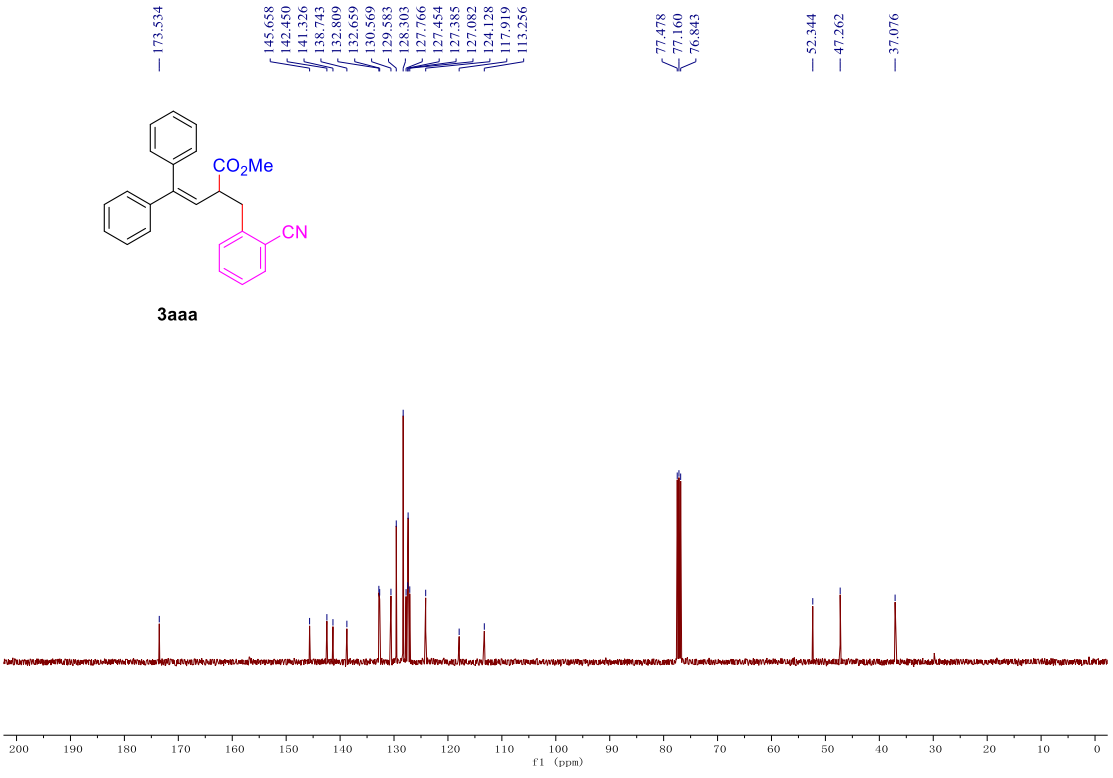
7.265
7.260
7.252
7.247
7.233
7.218
7.204
7.198
7.184
7.179
7.093
7.073
6.779
6.774
6.761
6.755
6.140
6.113
3.713
3.640
3.626
3.615
3.601
3.590
3.576
3.316
3.302
3.282
3.268
3.177
3.153
3.143
3.119
CO2Me
CN
1.13
1.29
9.81
1.15
2.00
1.00
3.09
1.07
1.03
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3aaa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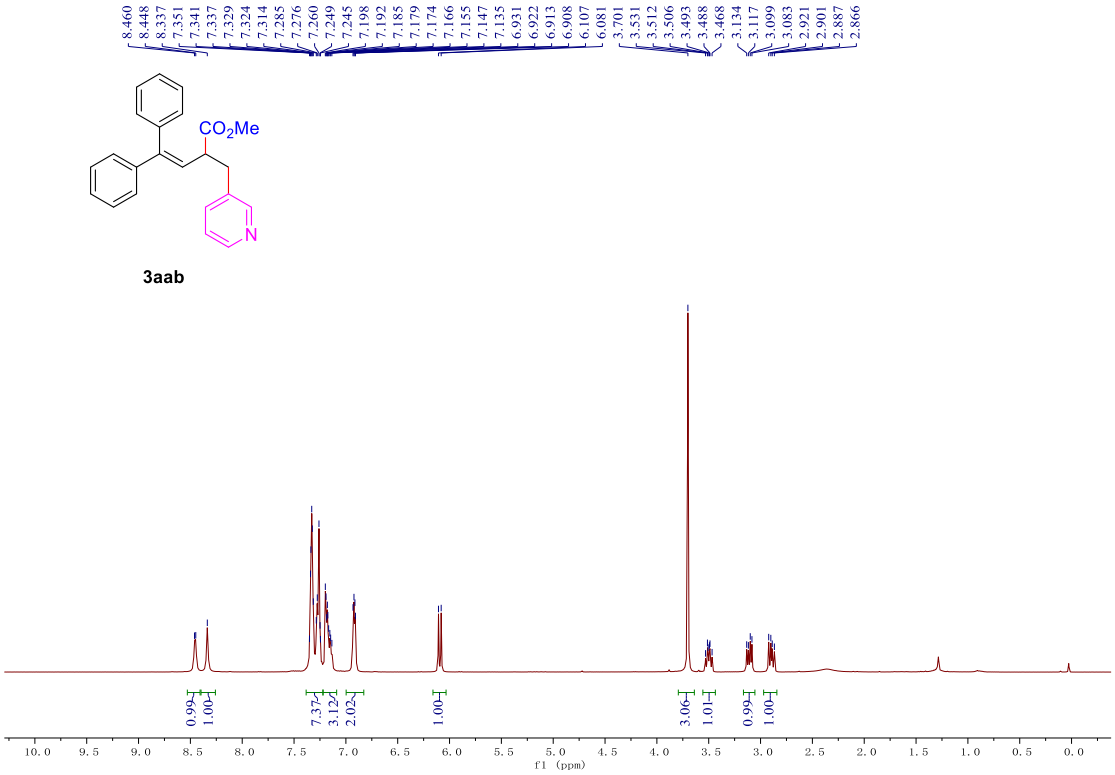
130.569
129.583
128.303
127.766
127.454
127.385
127.082
124.128
117.919
113.256
77.478
77.160
76.843
52.344
47.262
37.076
CO2Me
CN
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3aaa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7.249
7.245
7.198
7.192
7.185
7.179
7.174
7.166
7.155
7.147
7.135
6.931
6.922
6.913
6.908
6.107
6.081
3.701
3.531
3.512
3.506
3.493
3.488
3.468
3.134
3.117
3.099
3.083
2.921
2.901
2.887
2.866
CO2Me
N
3aab
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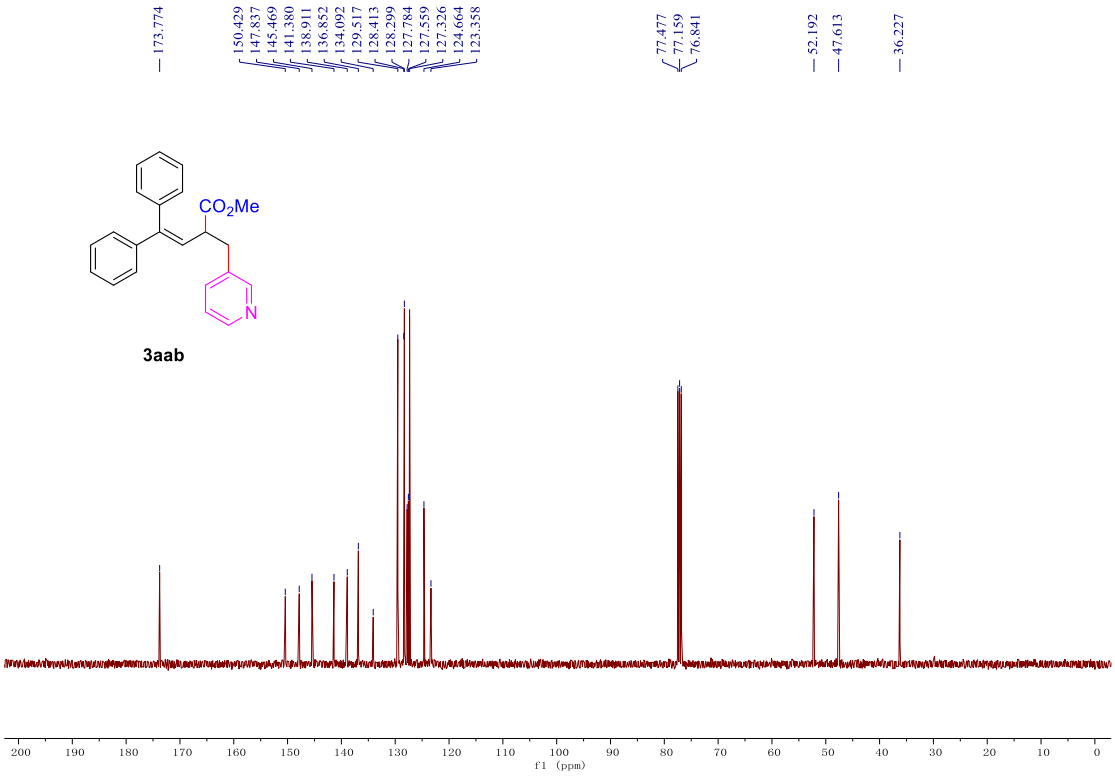
1.00
7.37
3.12
2.02
1.00
3.06
1.01
0.99
1.00
f1 (ppm)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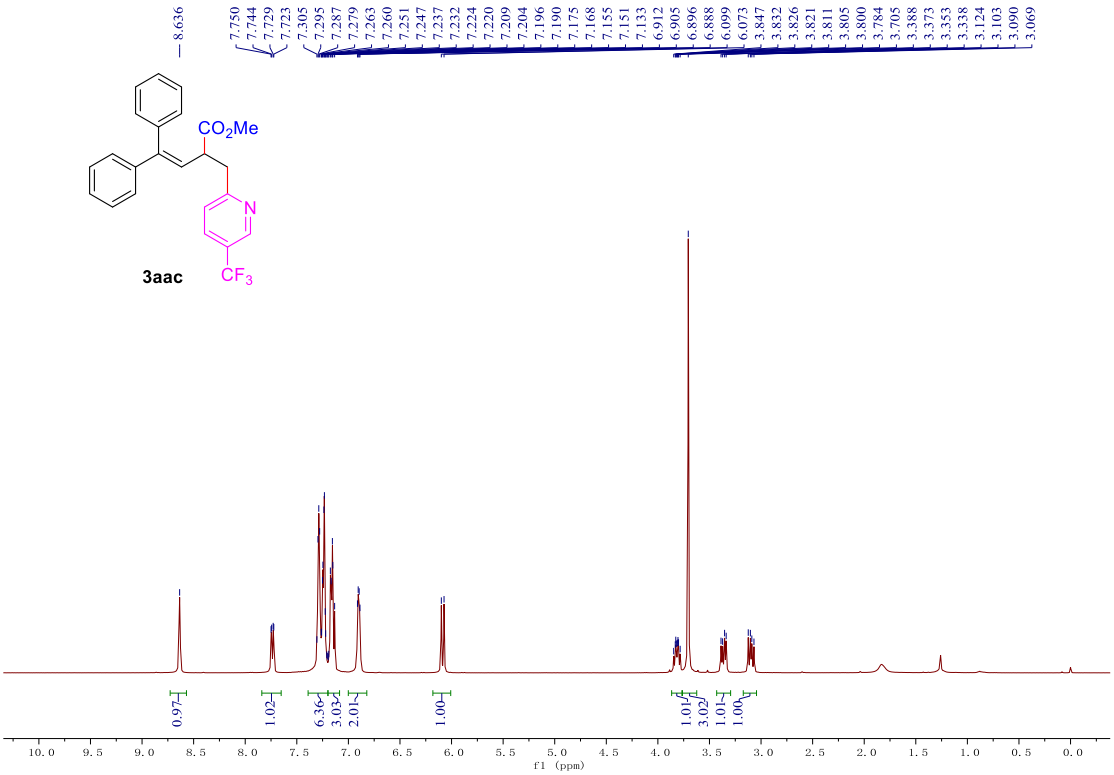
136.852
134.092
129.517
128.413
128.299
127.784
127.559
127.326
124.664
123.358
77.477
77.159
76.841
52.192
47.613
36.227
CO2Me
N
3aab
f1 (ppm)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7.263
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7.251
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7.237
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7.224
7.220
7.209
7.204
7.196
7.190
7.175
7.168
7.155
7.151
7.133
6.912
6.905
6.896
6.888
6.099
6.073
3.847
3.832
3.826
3.821
3.811
3.805
3.800
3.784
3.705
3.388
3.373
3.353
3.338
3.124
3.103
3.090
3.069
CO2Me
N
CF3
3aac
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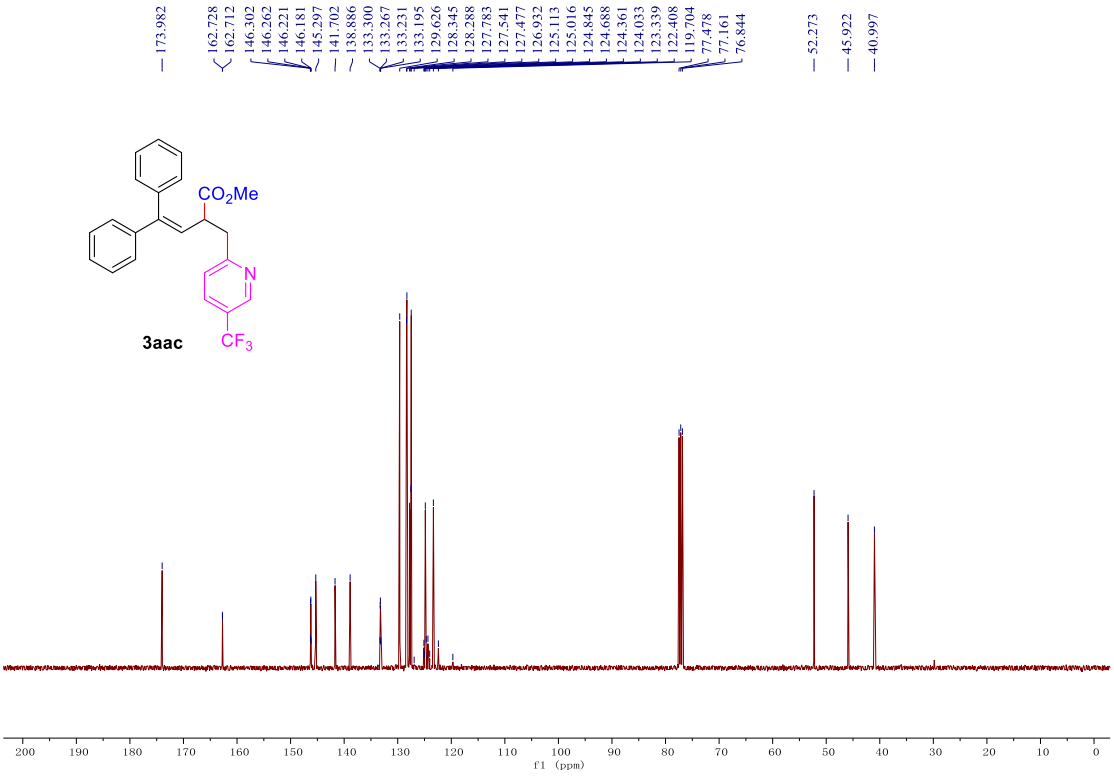
6.36
3.03
2.01
1.00
1.01
3.02
1.01
1.00
f1 (ppm)


173.982
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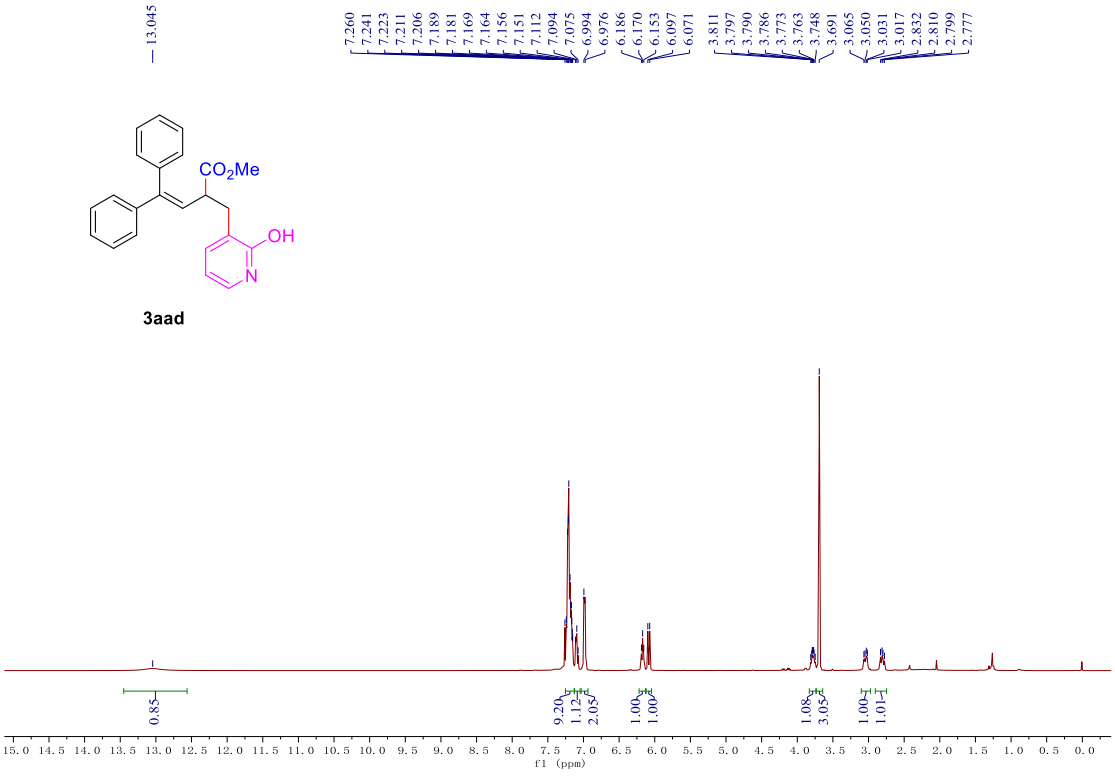
162.712
146.302
146.262
146.221
146.181
145.297
141.702
138.886
133.300
133.267
133.231
133.195
129.626
128.345
128.288
127.783
127.541
127.477
126.932
125.113
125.016
124.845
124.688
124.361
124.033
123.339
122.408
119.704
77.478
77.161
76.844
52.273
45.922
40.997
CO2Me
N
CF3
3aac
f1 (ppm)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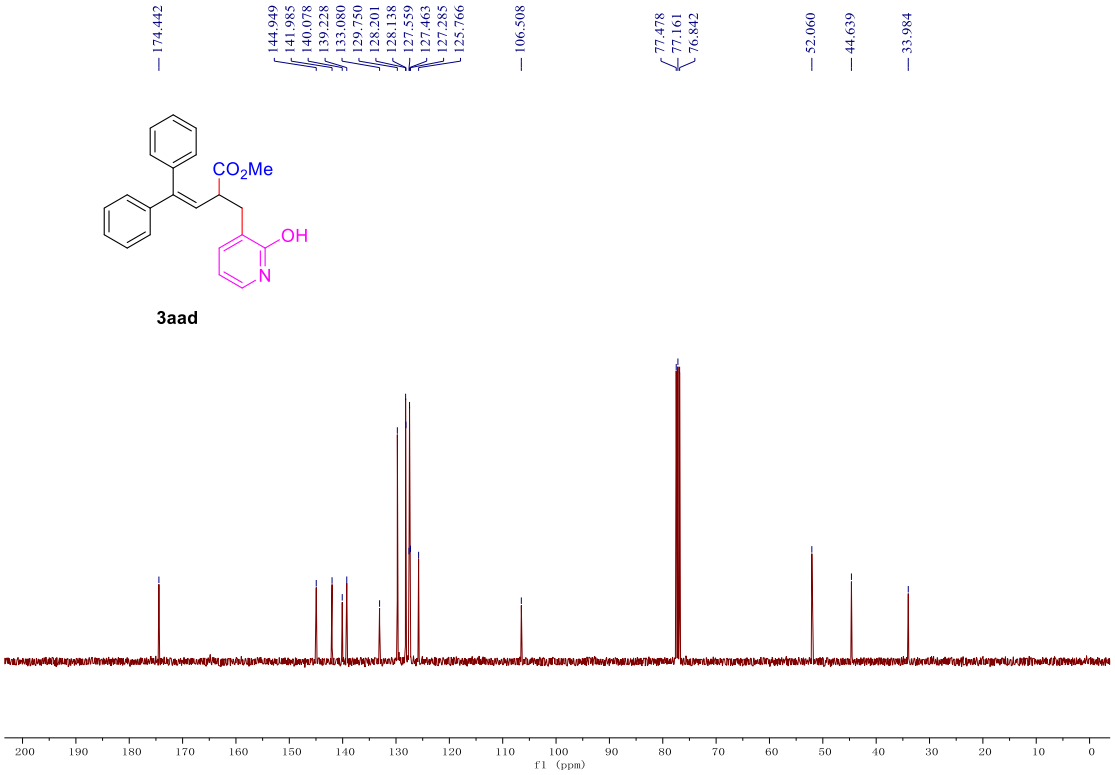
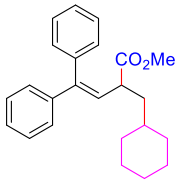
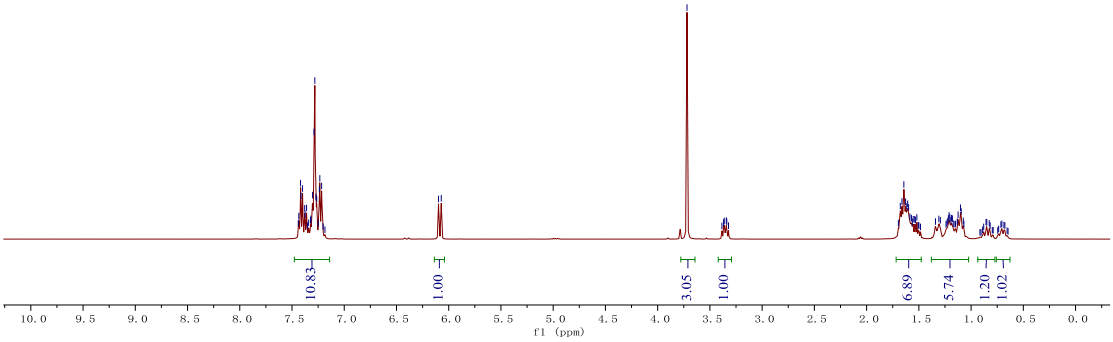
7.260
7.241
7.223
7.211
7.206
7.189
7.181
7.169
7.164
7.156
7.151
7.112
7.094
7.075
6.994
6.976
6.186
6.170
6.153
6.097
6.071
3.811
3.797
3.790
3.786
3.773
3.763
3.748
3.691
3.065
3.050
3.031
3.017
2.832
2.810
2.799
2.777
CO2Me
OH
N
3aad
0.85
9.20
1.12
2.05
1.00
1.00
1.08
3.05
1.00
1.01
f1 (ppm)


174.442
144.949
141.985
140.078
139.228
133.080
129.750
128.201
128.138
127.559
127.463
127.285
125.766
106.508
77.478
77.161
76.842
52.060
44.639
33.984
CO2Me
OH
N
3aad
f1 (ppm)

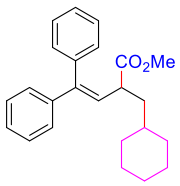

7.440
7.435
7.418
7.414
7.399
7.378
7.374
7.360
7.341
7.323
7.319
7.303
7.289
7.282
7.271
7.263
7.248
7.238
7.234
7.216
6.097
6.071
3.719
3.369
3.363
3.343
3.338
1.696
1.677
1.662
1.643
1.627
1.615
1.607
1.598
1.586
1.571
1.562
1.554
1.539
1.533
1.519
1.506
1.341
1.308
1.294
1.240
1.231
1.223
1.217
1.210
1.203
1.194
1.187
1.179
1.171
1.155
1.149
1.132
1.124
1.102
1.094
1.075
1.069
0.857
0.850
0.826
0.818
0.715
0.705
0.686
0.676


CO2Me

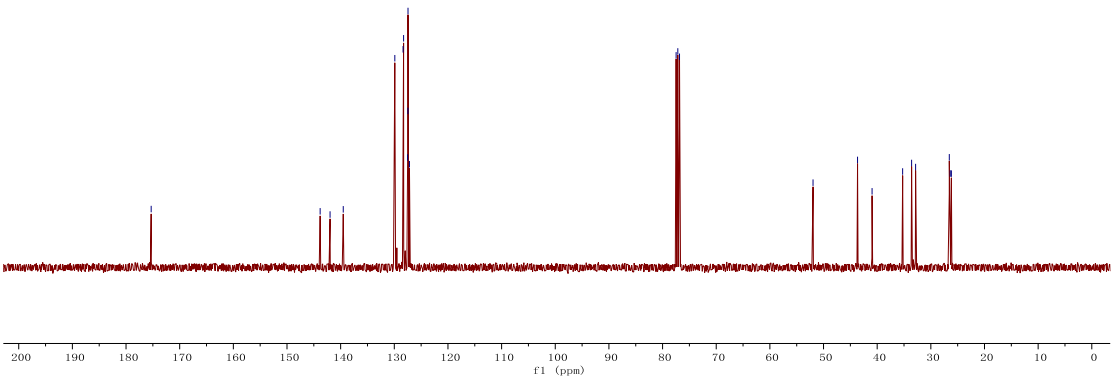
3aae

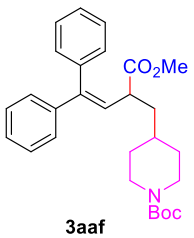

10.83
1.00
3.05
1.00
6.89
5.74
1.20
1.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


175.314
143.821
141.973
139.515
129.904
128.367
128.268
127.518
127.459
127.444
127.176
77.477
77.160
76.842
51.957
43.660
40.952
35.255
33.584
32.839
26.559
26.384
26.172

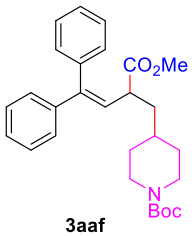

CO2Me

3aae

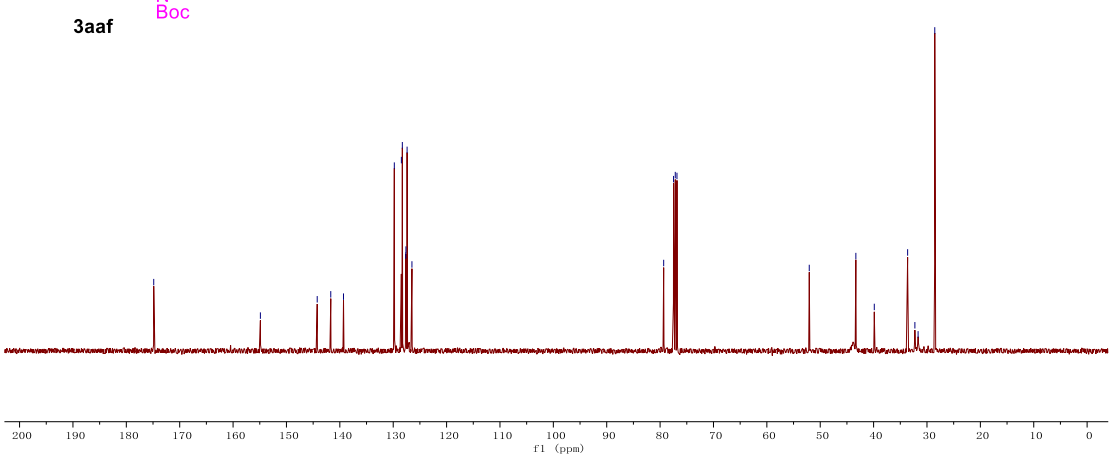

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

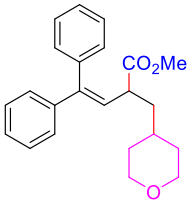


3aaf

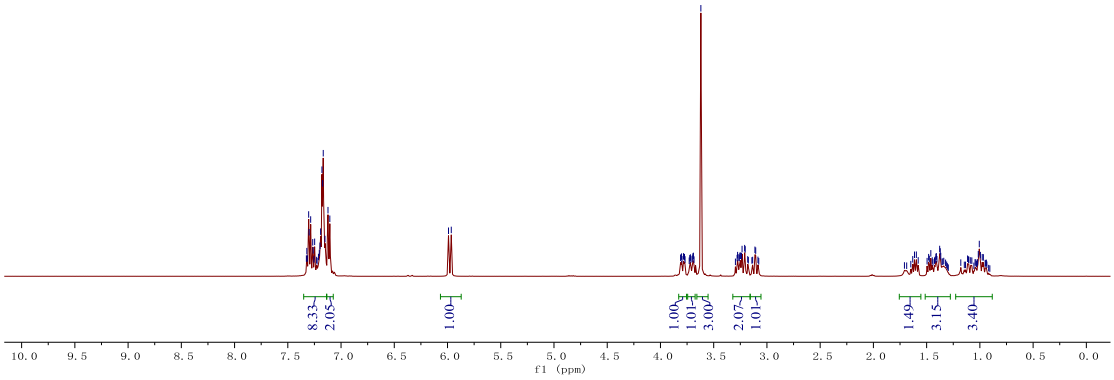


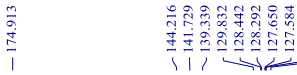
3aaf

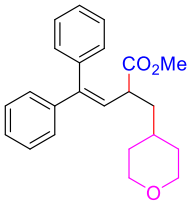



CO2Me
O

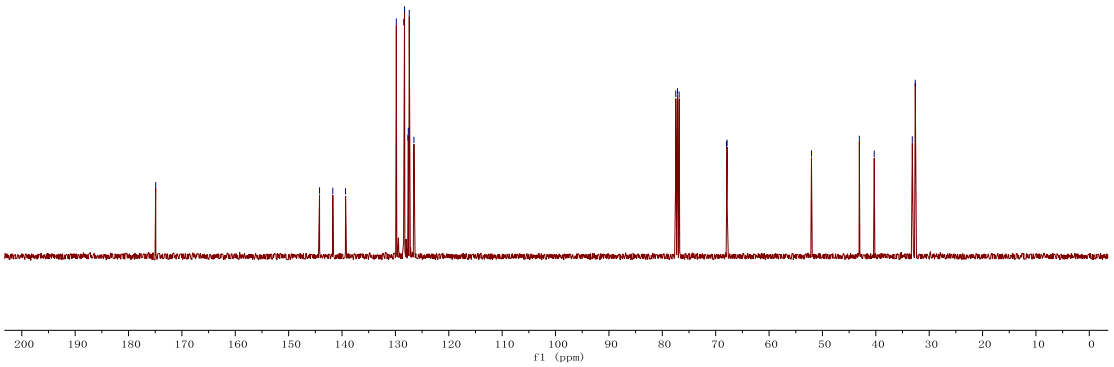
3aag


8.33
2.05
1.00
1.00
1.01
3.00
2.07
1.01
1.49
3.15
3.40
f1 (ppm)

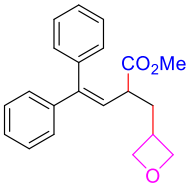

174.913
144.216
141.729
139.339
129.832
128.442
128.292
127.650
127.584
127.408
126.534
77.478
77.161
76.843
67.970
67.864
52.053
43.084
40.297
33.163
32.606


CO2Me
O

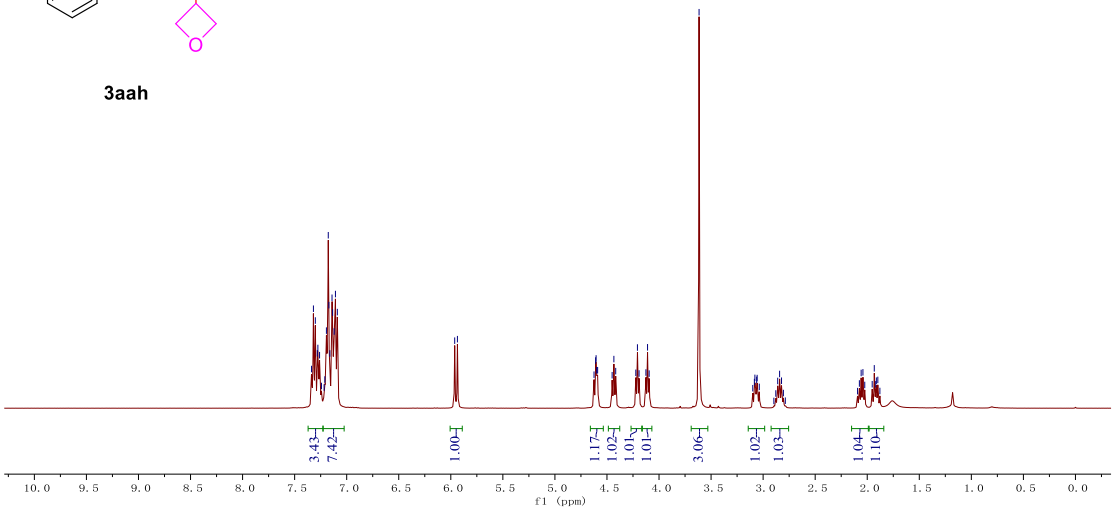
3aag


f1 (ppm)

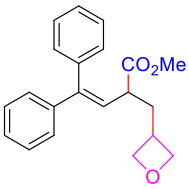

7.338
7.320
7.301
7.282
7.277
7.261
7.243
7.217
7.210
7.195
7.177
7.171
7.162
7.141
7.135
7.120
7.108
7.090
5.963
5.936
4.624
4.609
4.604
4.599
4.590
4.450
4.434
4.416
4.223
4.207
4.192
4.126
4.110
4.095
3.615
3.099
3.084
3.079
3.062
3.058
3.037
2.897
2.878
2.860
2.842
2.823
2.805
2.787
2.093
2.075
2.059
2.041
2.024
1.952
1.932
1.918
1.912
1.898
1.878


CO2Me
O

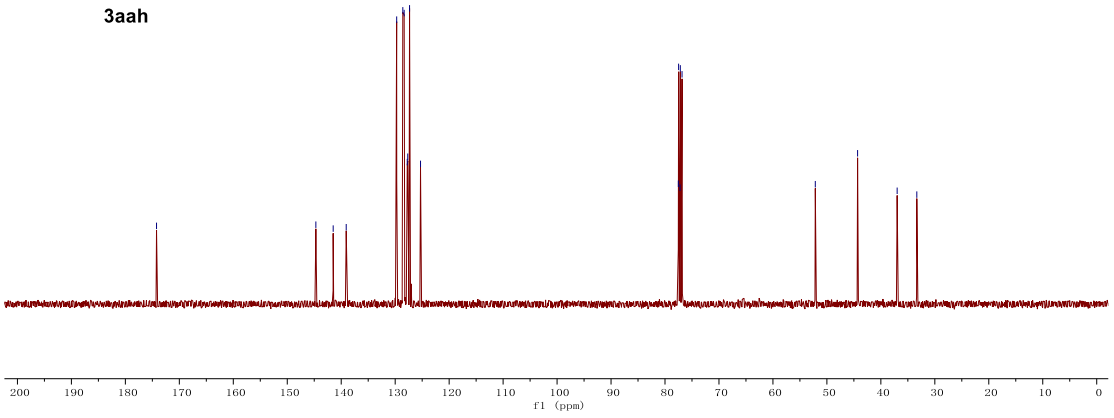
3aah


3.43
7.42
1.00
1.17
1.02
1.01
1.01
3.06
1.02
1.03
1.04
1.10
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
f1 (ppm)

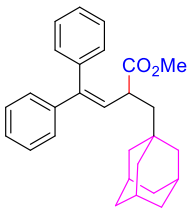

174.225
144.701
141.491
139.075
129.723
128.586
128.337
127.767
127.670
127.336
125.305
77.524
77.479
77.220
77.160
76.843
52.148
44.310
36.979
33.338


CO2Me
O

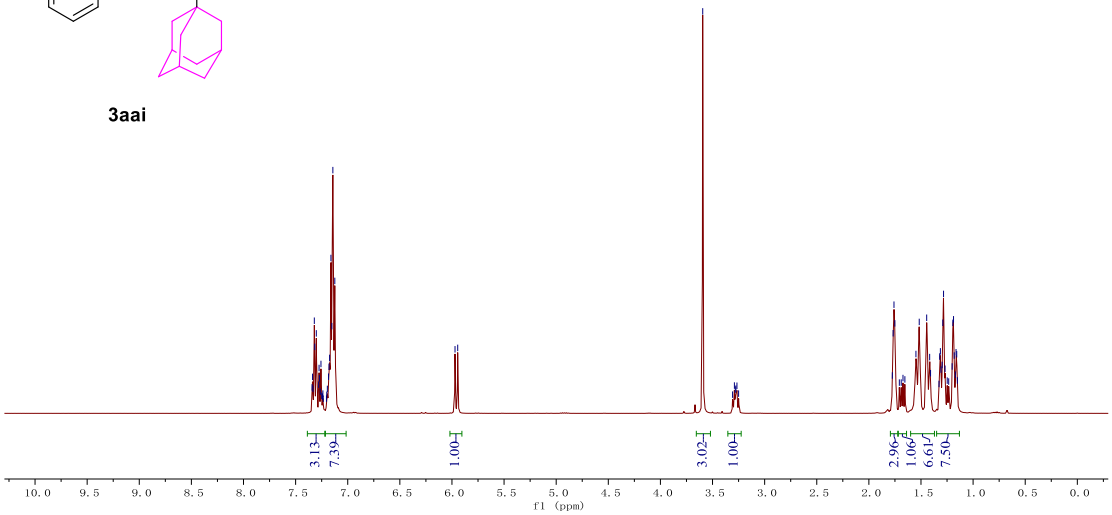
3aah


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

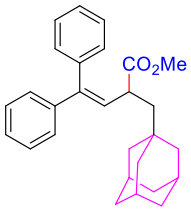

7.342
7.338
7.334
7.321
7.317
7.301
7.279
7.275
7.271
7.263
7.257
7.250
7.242
7.238
7.235
7.204
7.201
7.195
7.184
7.180
7.174
7.161
7.152
7.143
7.124
5.971
5.945
3.594
3.308
3.290
3.282
3.276
3.266
3.250
1.775
1.767
1.759
1.751
1.708
1.690
1.673
1.655
1.549
1.517
1.445
1.417
1.408
1.327
1.321
1.314
1.308
1.297
1.291
1.284
1.269
1.248
1.234
1.201
1.194
1.188
1.181
1.170
1.164
1.157
1.151


CO2Me

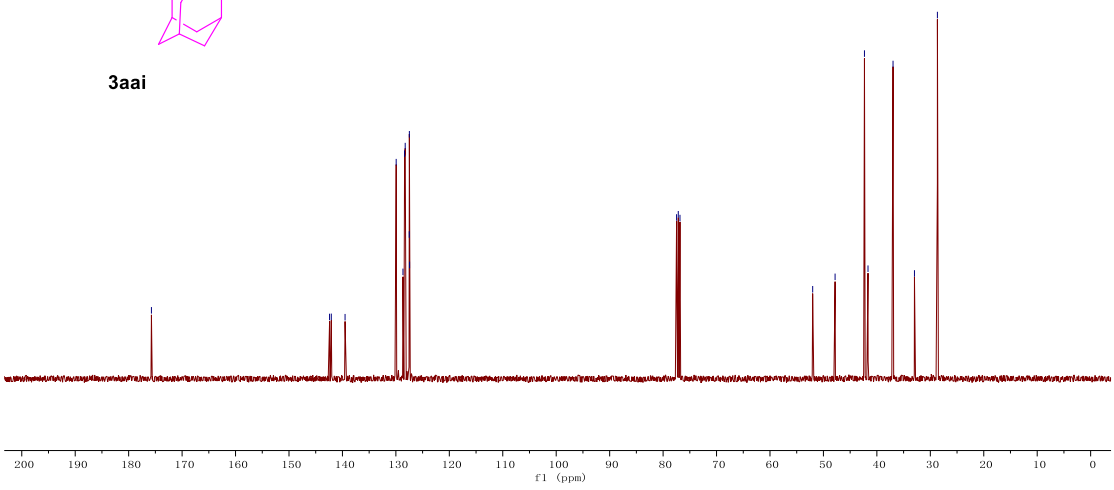
3aai

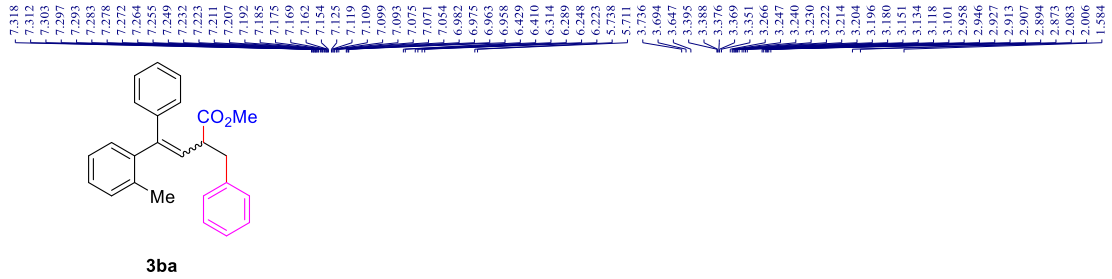

3.13
7.39
1.00
3.02
1.00
2.96
1.06
6.61
7.50
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


175.73
142.40
142.08
139.50
129.94
128.67
128.37
128.25
127.49
127.47
127.43
77.477
77.160
76.842
52.012
47.820
42.323
41.659
36.975
32.968
28.673


CO2Me

3aai


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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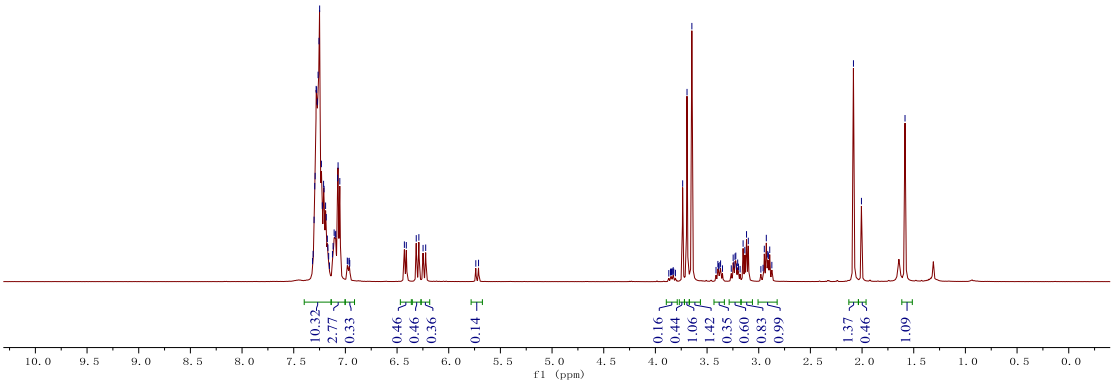
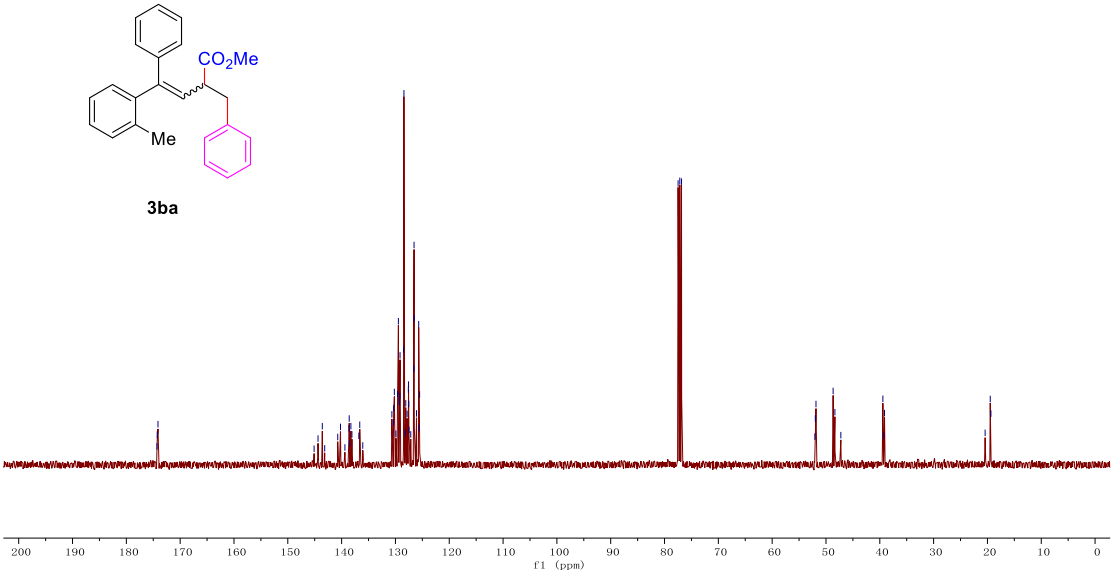
7.272
7.264
7.255
7.249
7.232
7.223
7.211
7.207
7.192
7.185
7.175
7.169
7.162
7.154
7.125
7.119
7.109
7.099
7.093
7.075
7.071
7.054
6.982
6.975
6.963
6.958
6.429
6.410
6.314
6.289
6.248
6.223
5.738
5.711
3.736
3.694
3.647
3.395
3.388
3.376
3.369
3.351
3.266
3.247
3.240
3.230
3.222
3.214
3.204
3.196
3.180
3.151
3.134
3.118
3.101
2.958
2.946
2.927
2.913
2.907
2.894
2.873
2.083
2.006
1.584
CO2Me
Me

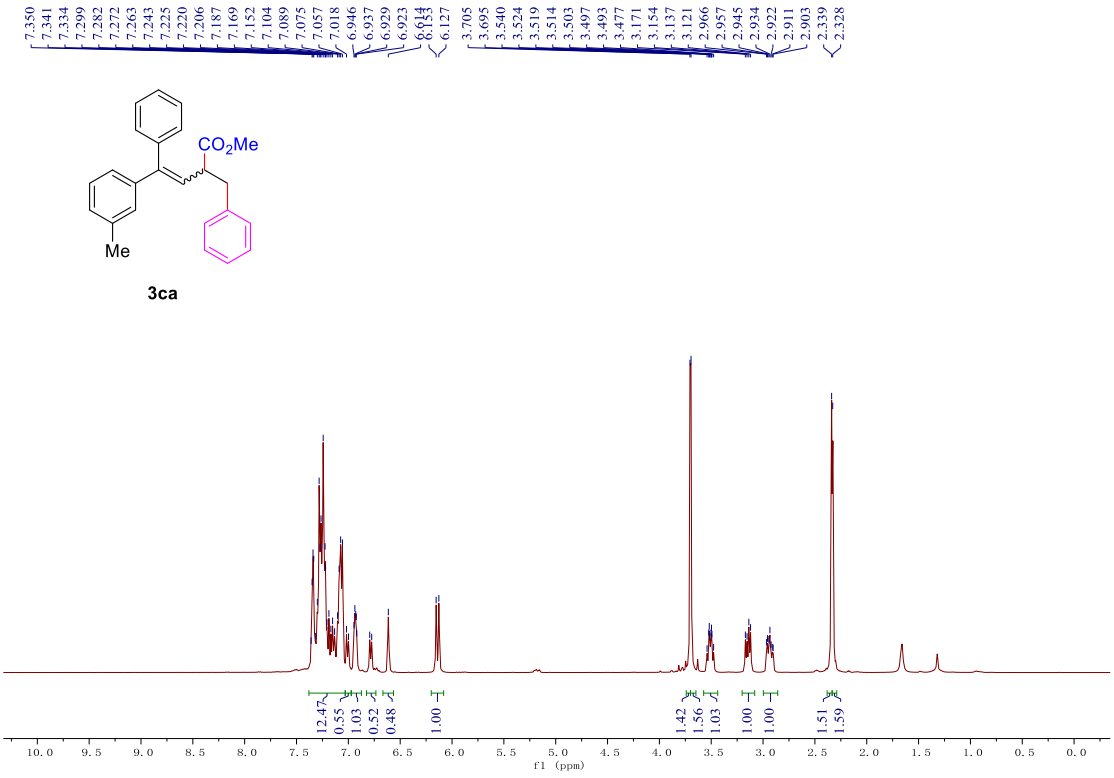
3ba


10.32
2.77
2.71
0.33
0.46
0.46
0.36
0.14
0.16
0.44
1.06
1.42
0.35
0.60
0.83
0.99
1.37
0.46
1.09
f1 (ppm)


174.305
174.264
174.119
145.111
144.383
143.589
143.142
140.720
140.212
139.388
138.628
138.591
138.515
138.277
138.085
136.797
136.630
136.068
130.660
130.348
130.328
130.202
129.914
129.605
129.448
129.298
129.178
129.145
128.482
128.420
128.153
128.081
127.838
127.600
127.564
127.523
127.481
127.150
126.560
126.538
126.510
126.083
125.675
125.614
125.509
77.477
77.160
76.841
52.059
51.982
51.857
48.676
48.341
47.238
39.429
39.252
39.124
20.428
19.479
19.354


CO2Me
Me
f1 (ppm)

3ba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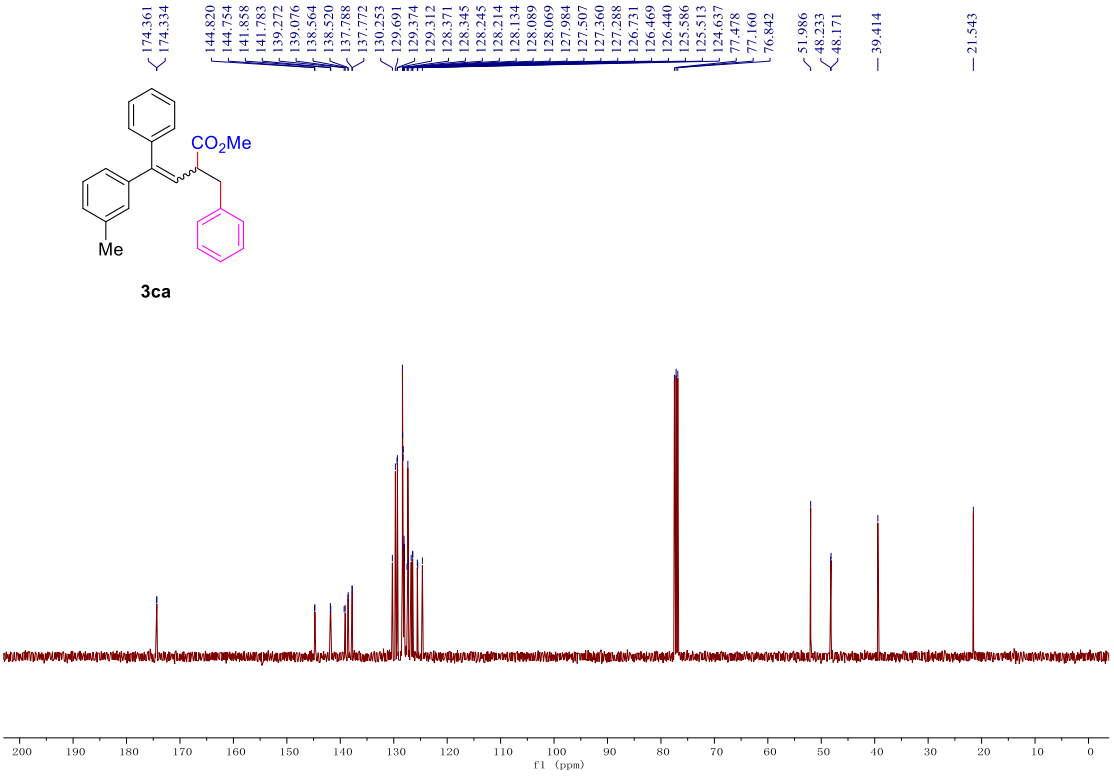
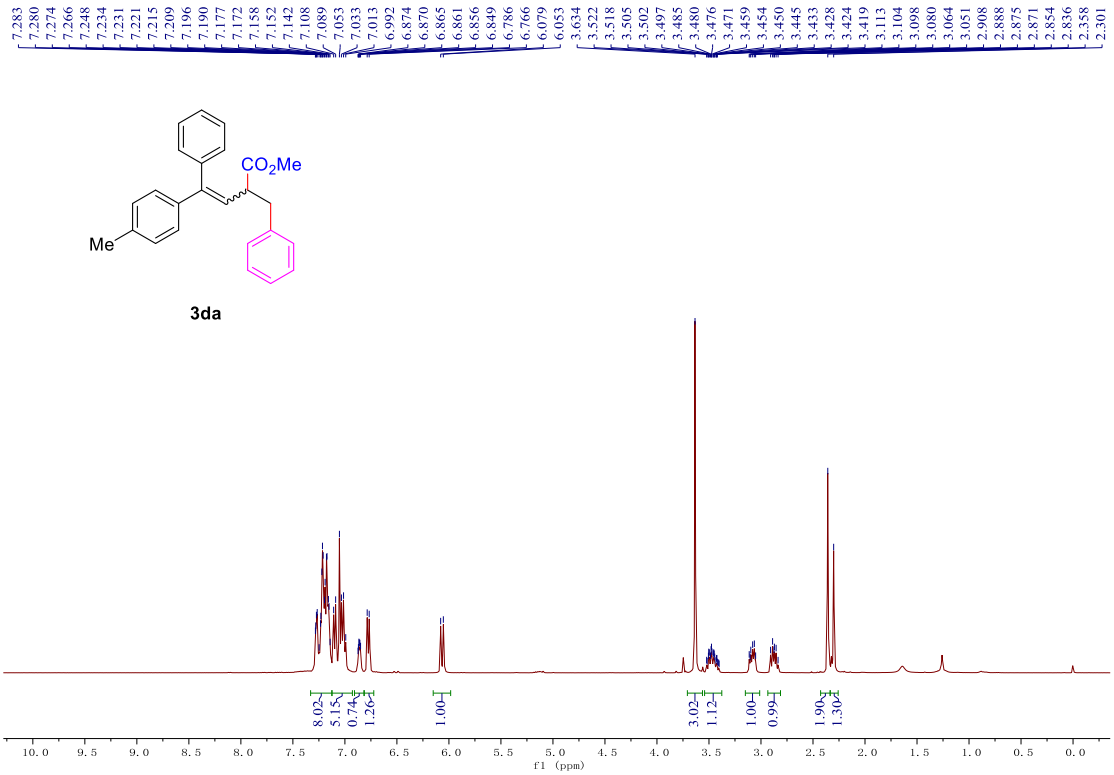
7.272
7.263
7.243
7.225
7.220
7.206
7.187
7.169
7.152
7.104
7.089
7.075
7.057
7.018
6.946
6.937
6.929
6.923
6.614
6.153
6.127
3.705
3.695
3.540
3.524
3.519
3.514
3.503
3.497
3.493
3.477
3.171
3.154
3.137
3.121
2.966
2.957
2.945
2.934
2.922
2.911
2.903
2.339
2.328
CO2Me
Me
3ca
12.47
0.55
1.03
0.52
0.48
1.00
1.42
1.56
1.03
1.00
1.00
1.51
1.59
f1 (ppm)


174.361
174.334
144.820
144.754
141.858
141.783
139.272
139.076
138.564
138.520
137.788
137.772
130.253
129.691
129.374
129.312
128.371
128.345
128.245
128.214
128.134
128.089
128.069
127.984
127.507
127.360
127.288
126.731
126.469
126.440
125.586
125.513
124.637
77.478
77.160
76.842
51.986
48.233
48.171
39.414
21.543
CO2Me
Me
3ca
f1 (ppm)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7.266
7.248
7.234
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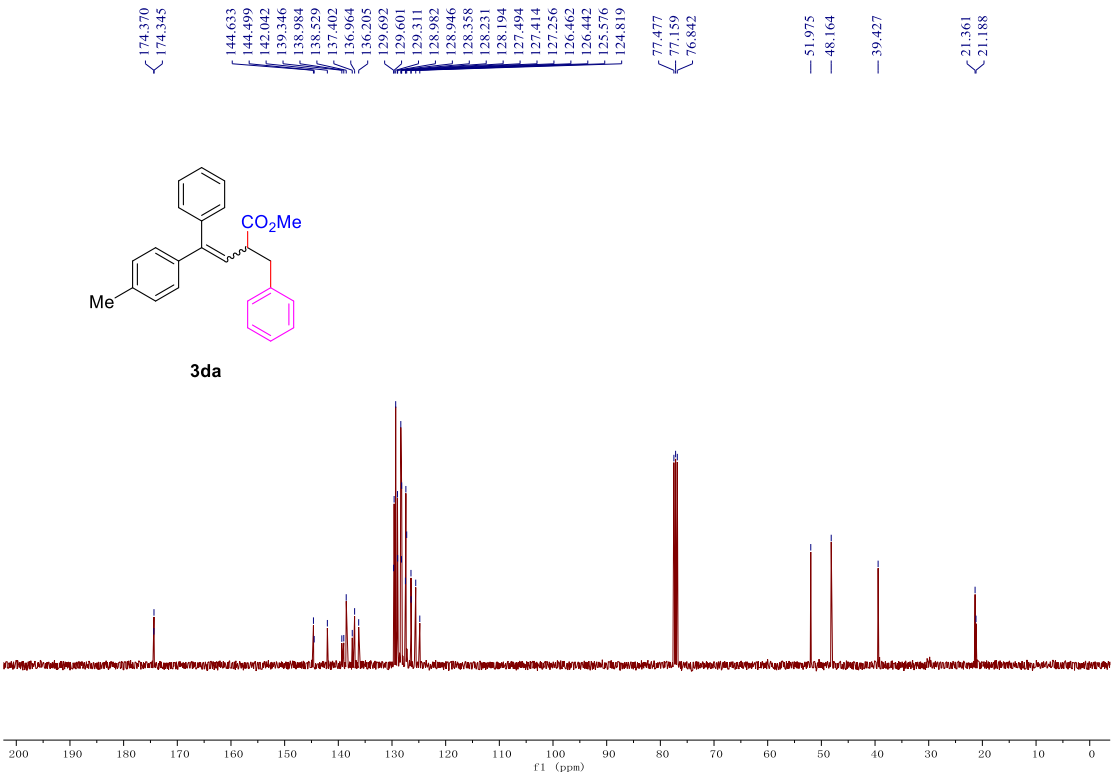
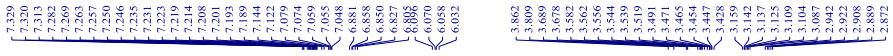
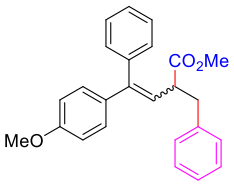
7.196
7.190
7.177
7.172
7.158
7.152
7.142
7.108
7.089
7.053
7.033
7.013
6.992
6.874
6.870
6.865
6.861
6.856
6.849
6.786
6.766
6.079
6.053
3.634
3.522
3.518
3.505
3.502
3.497
3.485
3.480
3.476
3.471
3.459
3.454
3.450
3.445
3.433
3.428
3.424
3.419
3.113
3.104
3.098
3.080
3.064
3.051
2.908
2.888
2.875
2.871
2.854
2.836
2.358
2.301
CO2Me
Me
8.02
5.15
0.74
1.26
1.00
3.02
1.12
1.00
0.99
1.90
1.30
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)

3da

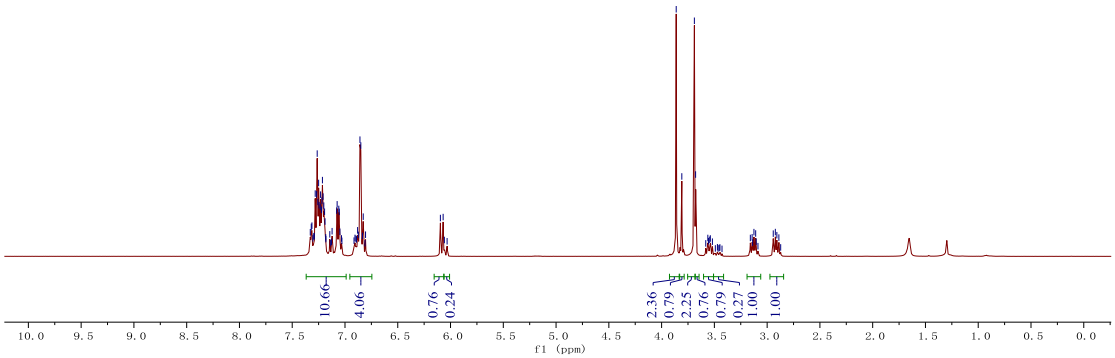

174.370
174.345
144.633
144.499
142.042
139.346
138.984
138.529
137.402
136.964
136.205
129.692
129.601
129.311
128.982
128.946
128.358
128.231
128.194
127.494
127.414
127.256
126.462
126.442
125.576
124.819
77.477
77.159
76.842
51.975
48.164
39.427
21.361
21.188
CO2Me
Me
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

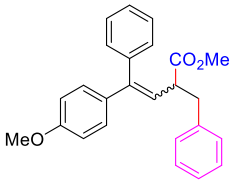
3da



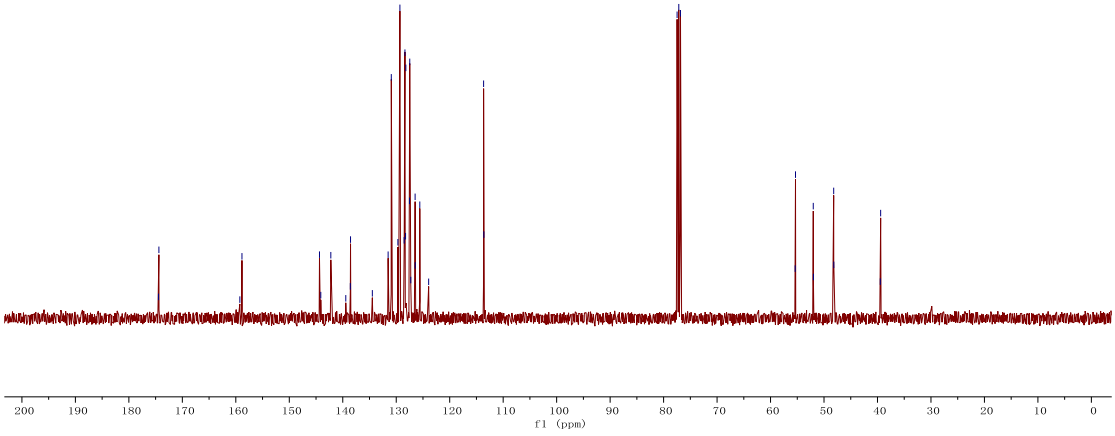

CO2Me
MeO

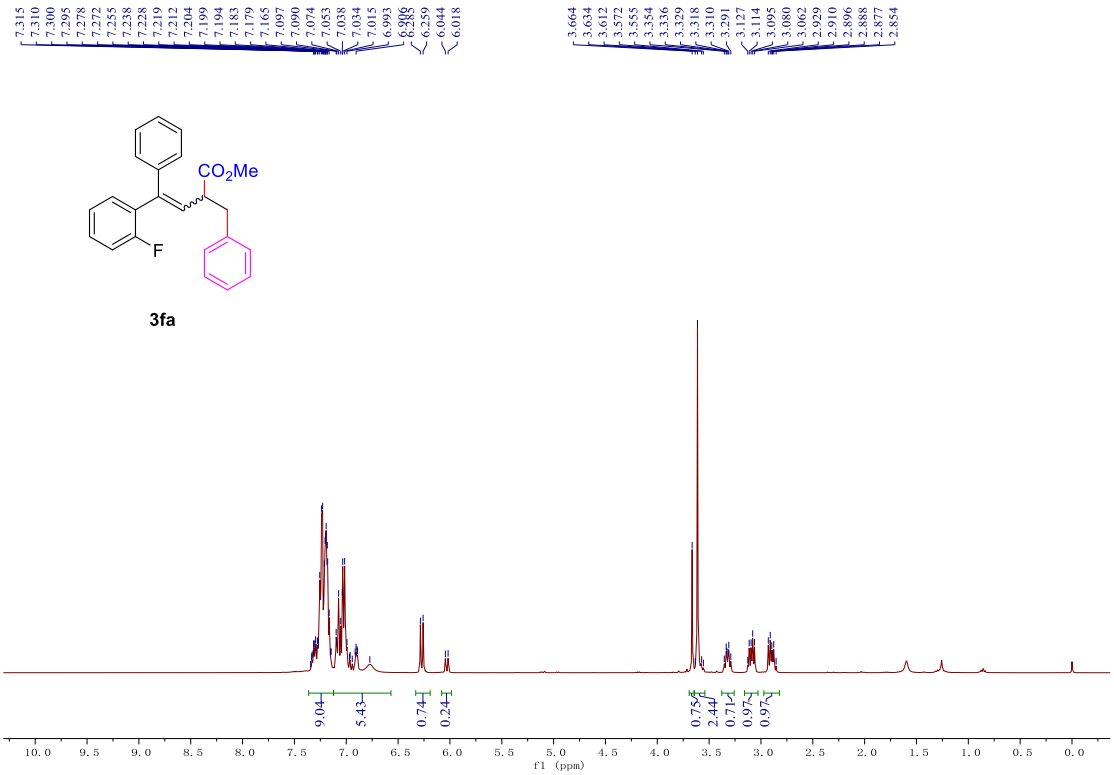
3ea


10.66
4.06
0.76
0.24
2.36
0.79
2.25
0.76
0.79
0.27
1.00
1.00
f1 (ppm)


CO2Me
MeO

3ea


f1 (ppm)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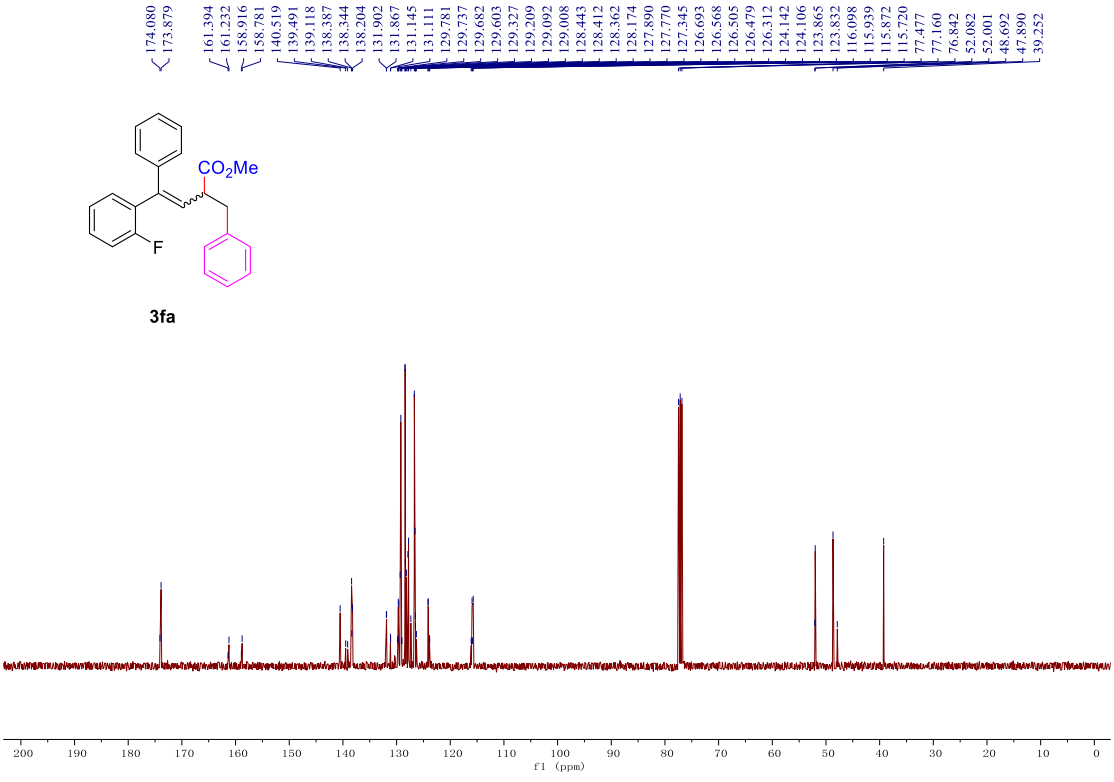
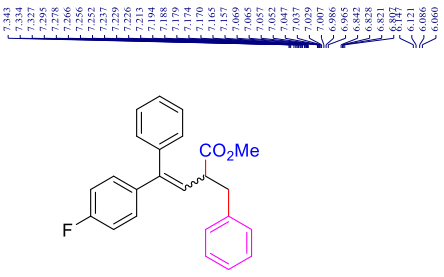
7.300
7.295
7.278
7.272
7.255
7.238
7.228
7.219
7.212
7.204
7.199
7.194
7.183
7.179
7.165
7.097
7.090
7.074
7.053
7.038
7.034
7.015
6.993
6.306
6.285
6.259
6.044
6.018
3.664
3.634
3.612
3.572
3.555
3.354
3.336
3.329
3.318
3.310
3.291
3.127
3.114
3.095
3.080
3.062
2.929
2.910
2.896
2.888
2.877
2.854
CO2Me
F
9.04
5.43
0.74
0.24
0.75
2.44
0.71
0.97
0.97
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)

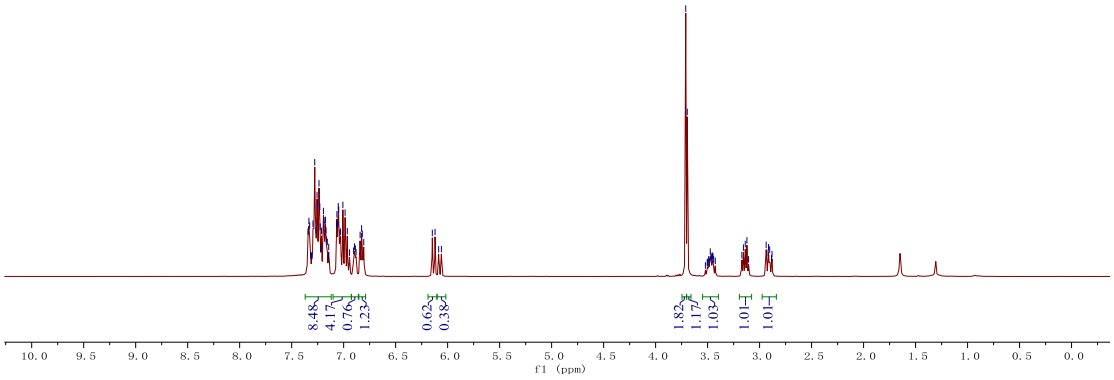
3fa

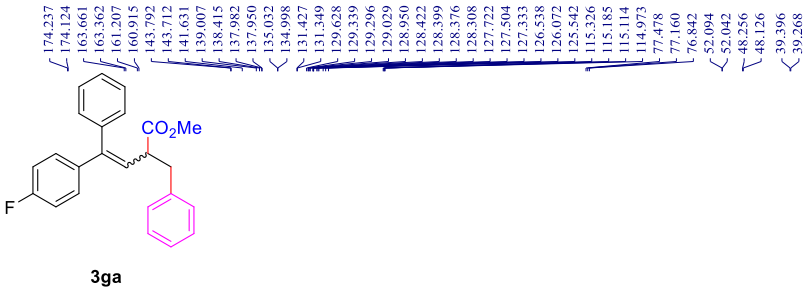

174.080
173.879
161.394
161.232
158.916
158.781
140.519
139.491
139.118
138.387
138.344
138.204
131.902
131.867
131.145
131.111
129.781
129.737
129.682
129.603
129.327
129.209
129.092
129.008
128.443
128.412
128.362
128.174
127.890
127.770
127.345
126.693
126.568
126.505
126.479
126.312
124.142
124.106
123.865
123.832
116.098
115.939
115.872
115.720
77.477
77.160
76.842
52.082
52.001
48.692
47.890
39.252
CO2Me
F
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

3fa

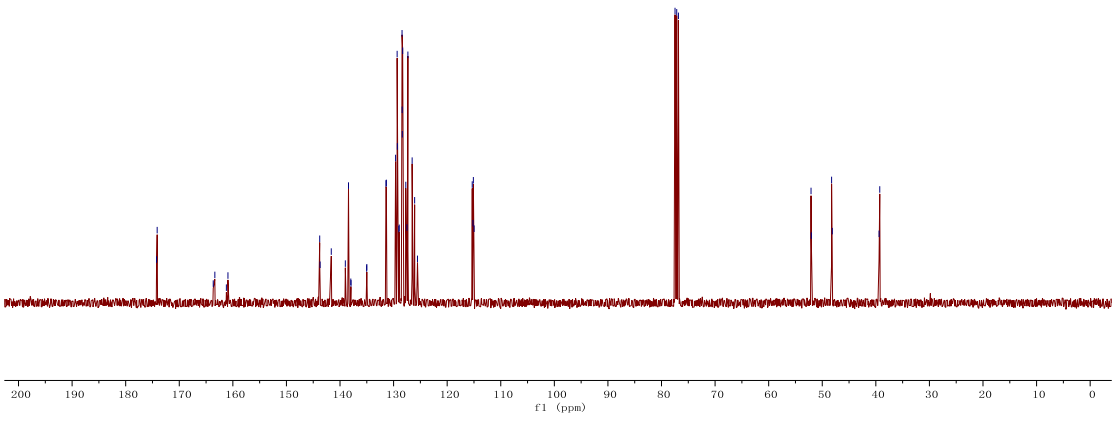

CO2Me
F

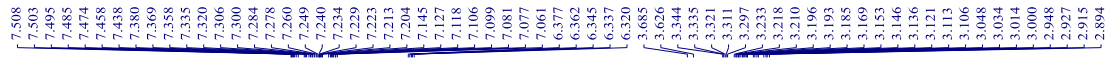
3ga


8.48
4.17
0.76
1.23
0.62
0.38
1.82
1.17
1.03
1.01
1.01
f1 (ppm)


CO2Me
F

3ga


f1 (ppm)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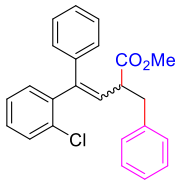
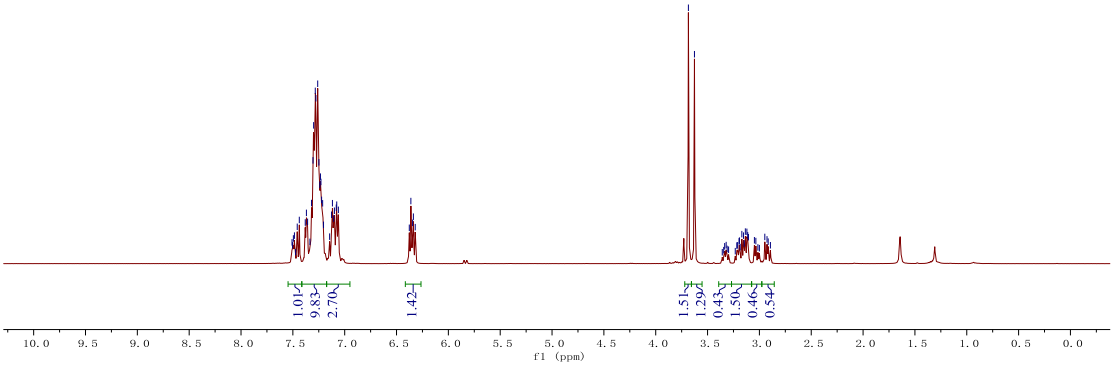
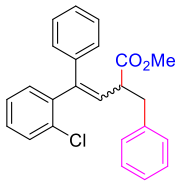
7.503
7.495
7.485
7.474
7.458
7.438
7.380
7.369
7.358
7.335
7.320
7.306
7.300
7.284
7.278
7.260
7.249
7.240
7.234
7.229
7.223
7.213
7.204
7.145
7.127
7.118
7.106
7.099
7.081
7.077
7.061
6.377
6.362
6.345
6.337
6.320
3.685
3.626
3.344
3.335
3.321
3.311
3.297
3.233
3.218
3.210
3.196
3.193
3.185
3.169
3.153
3.146
3.136
3.121
3.113
3.106
3.048
3.034
3.014
3.000
2.948
2.927
2.915
2.894


CO2Me
Cl

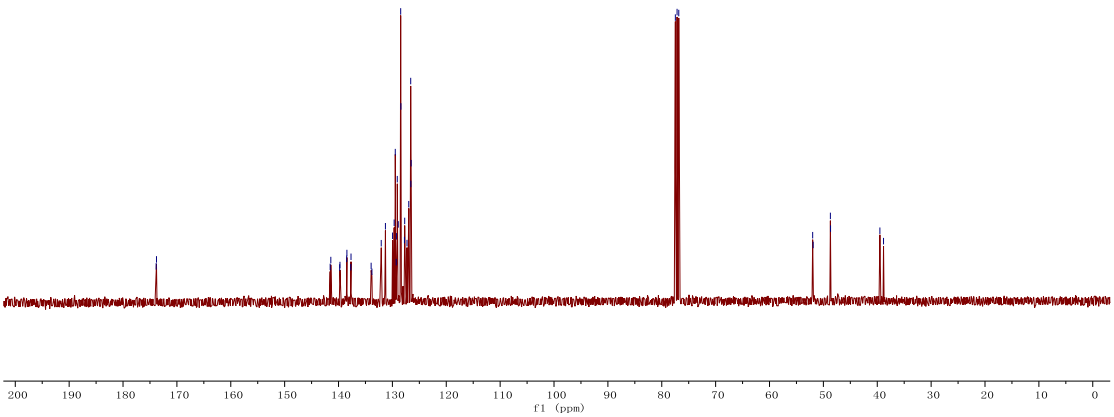
3ha


1.01
9.83
2.70
1.42
1.51
1.29
0.43
1.50
0.46
0.54
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)


173.849
173.789
141.552
141.429
139.789
139.733
138.487
138.443
137.722
137.681
133.946
133.798
132.071
131.293
129.970
129.675
129.466
129.292
129.258
129.093
128.917
128.461
128.426
127.764
127.716
127.290
126.963
126.602
126.577
126.525
77.477
77.159
76.842
51.990
51.903
48.702
48.669
39.512
38.836

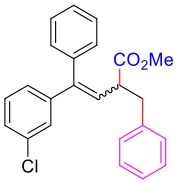

CO2Me
Cl

3ha

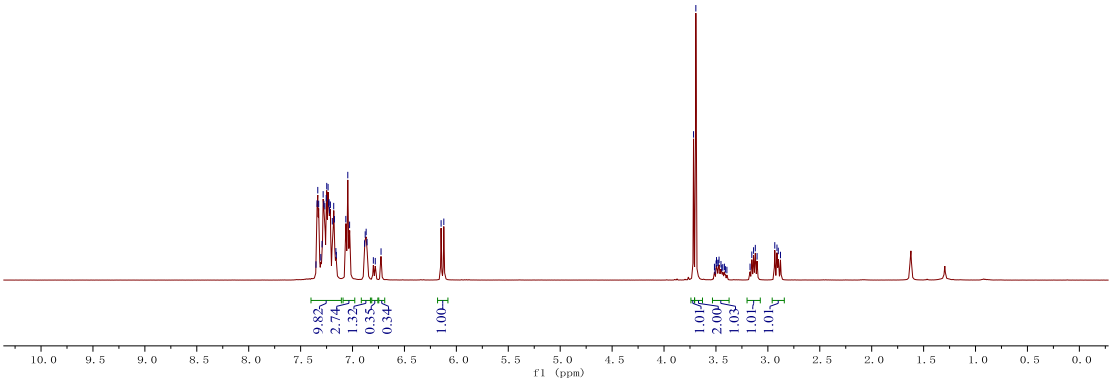

200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.352
7.342
7.335
7.326
7.305
7.294
7.283
7.276
7.267
7.253
7.248
7.236
7.229
7.226
7.221
7.213
7.195
7.181
7.175
7.160
7.156
7.065
7.046
7.028
6.884
6.878
6.869
6.860
6.799
6.791
6.725
6.447
6.121

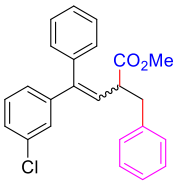

3.716
3.694
3.514
3.509
3.499
3.495
3.489
3.478
3.470
3.452
3.444
3.414
3.410
3.409
3.395
3.172
3.155
3.138
3.121
3.104
2.933
2.912
2.900
2.879


CO2Me
Cl

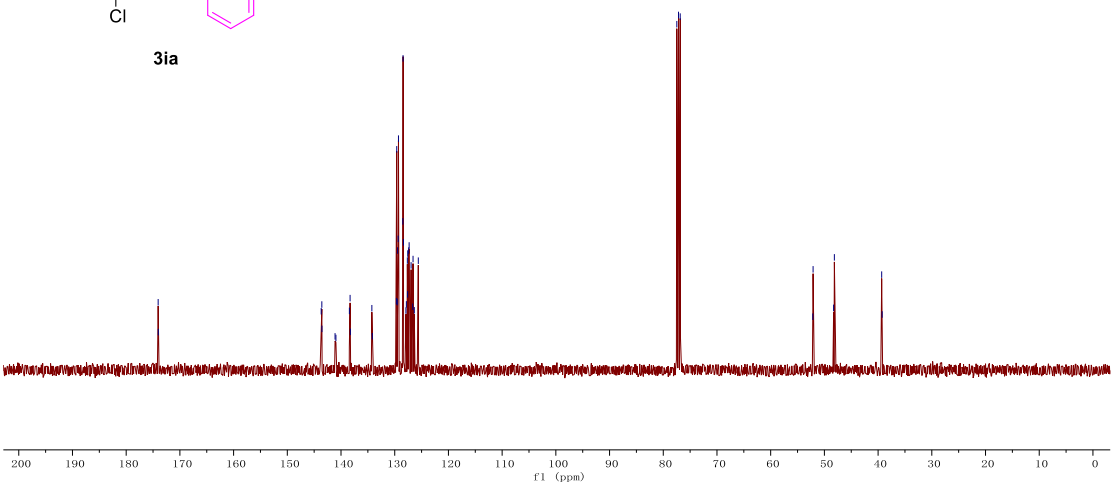
3ia

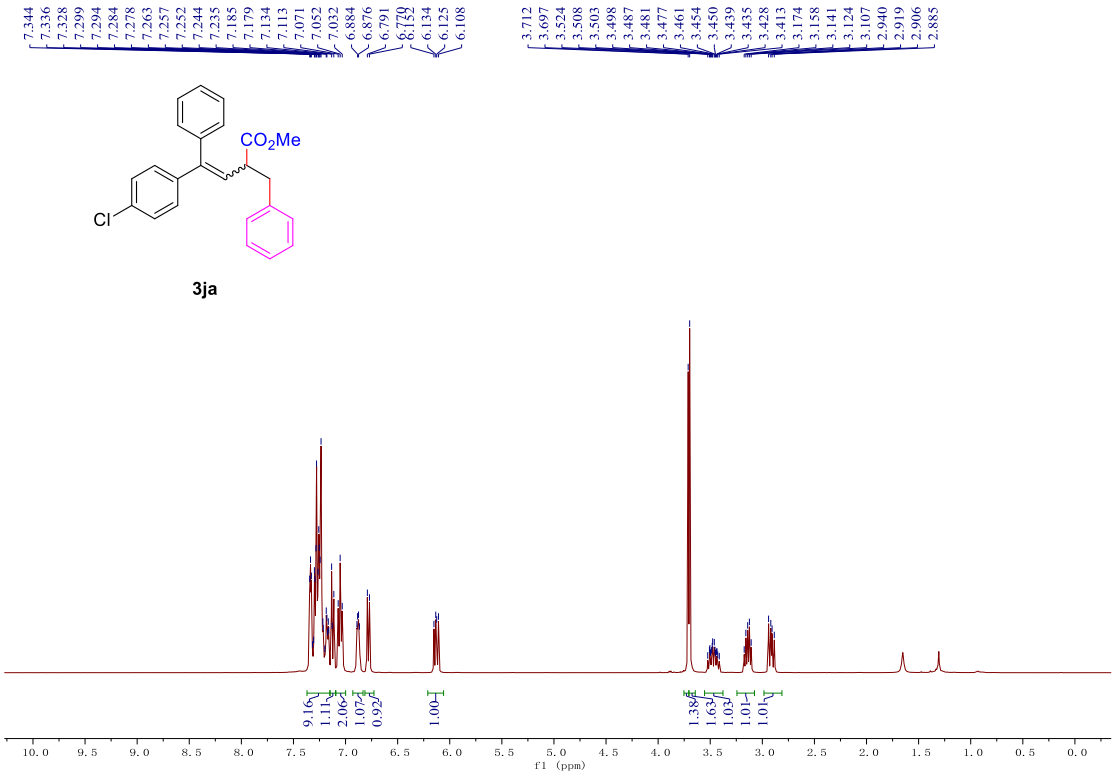

9.82
2.74
1.32
0.35
0.34
1.00
1.01
2.00
1.03
1.01
1.01
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

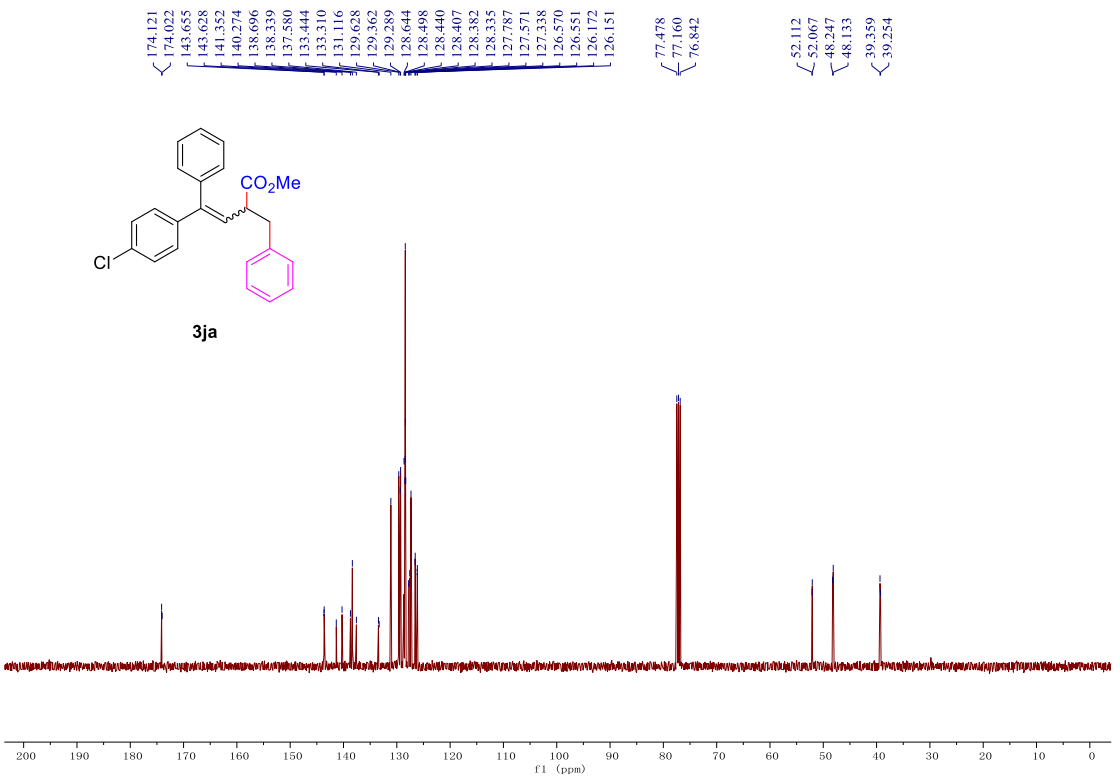

174.046
174.018
143.690
143.571
143.552
141.110
140.949
138.441
138.309
138.259
134.258
134.175
129.681
129.626
129.519
129.460
129.356
129.301
128.488
128.448
128.372
127.917
127.831
127.648
127.601
127.579
127.404
127.318
126.953
126.650
126.591
126.352
125.610
77.478
77.160
76.842
52.151
52.104
48.283
48.143
39.334
39.246


CO2Me
Cl

3ia


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


7.344
7.336
7.328
7.299
7.294
7.284
7.278
7.263
7.257
7.252
7.244
7.235
7.185
7.179
7.134
7.113
7.071
7.052
7.032
6.884
6.876
6.791
6.770
6.152
6.134
6.125
6.108
3.712
3.697
3.524
3.508
3.503
3.498
3.487
3.481
3.477
3.461
3.454
3.450
3.439
3.435
3.428
3.413
3.174
3.158
3.141
3.124
3.107
2.940
2.919
2.906
2.885
CO2Me
Cl
3ja
9.16
1.11
2.06
1.07
0.92
1.00
1.38
1.63
1.03
1.01
1.01
f1 (ppm)


174.121
174.022
143.655
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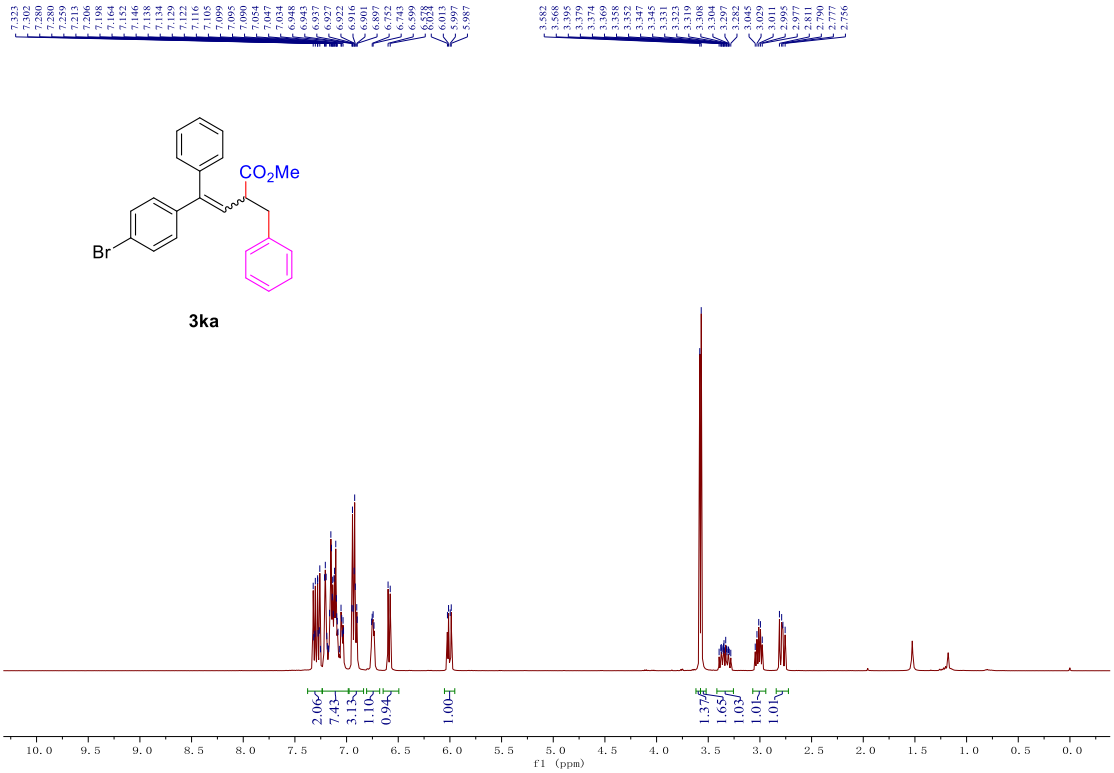
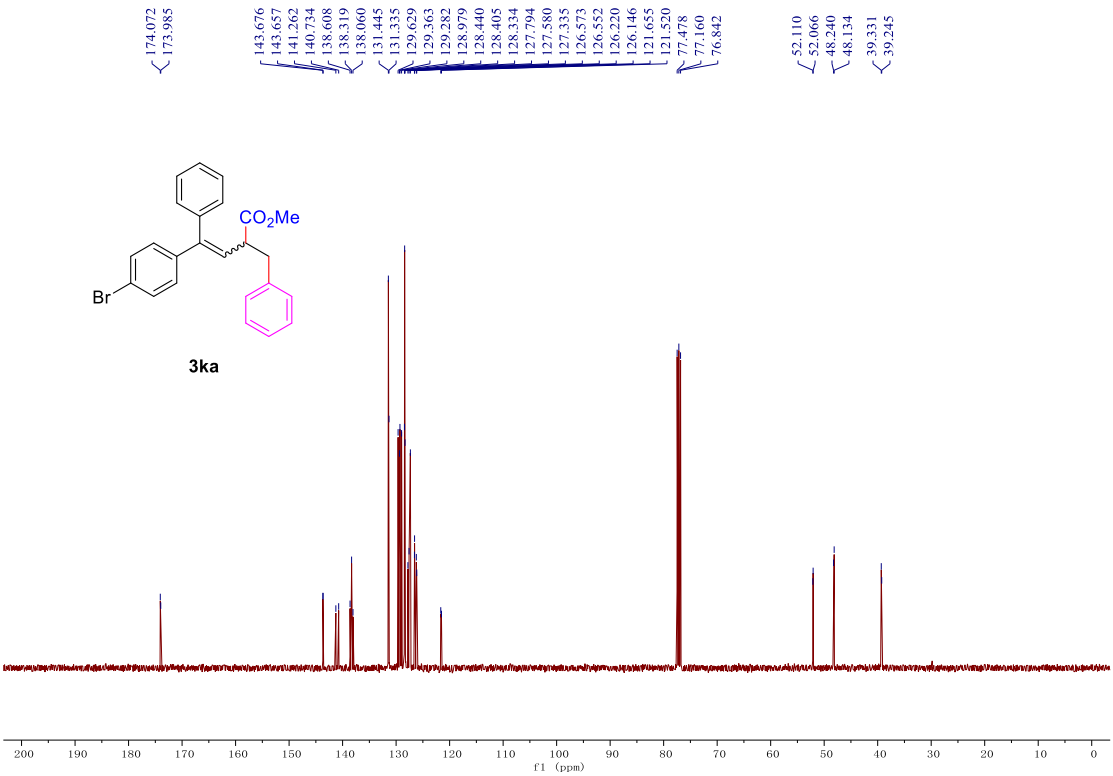
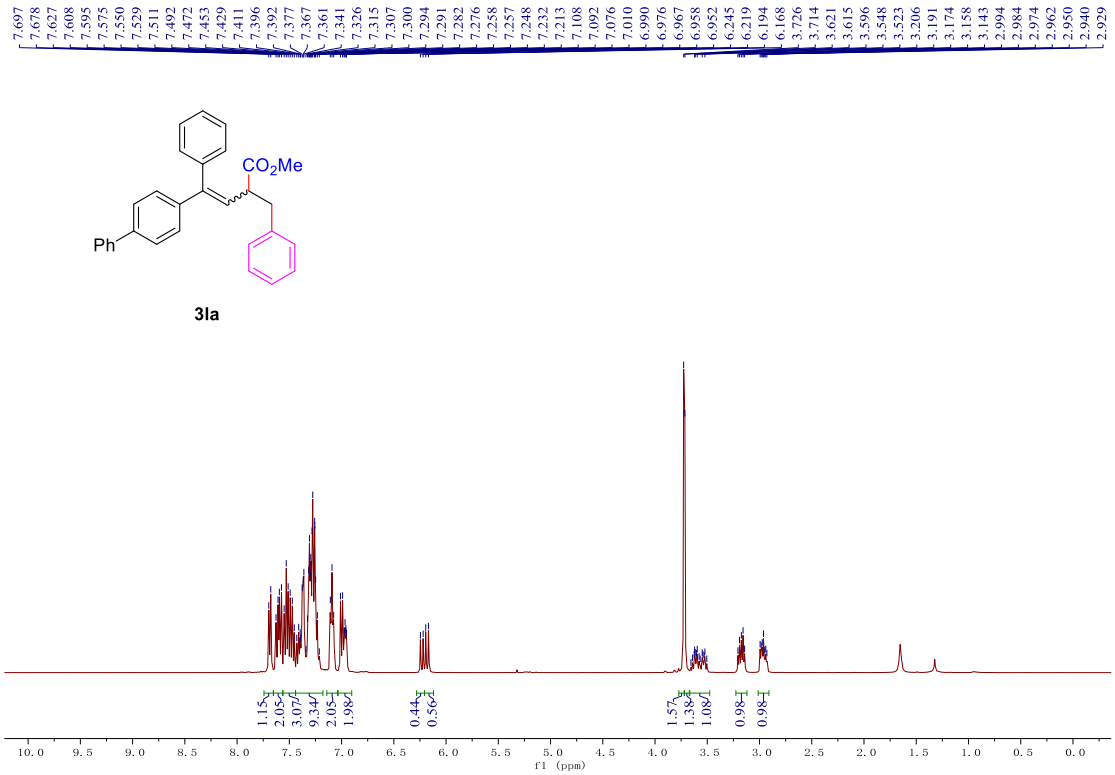
141.352
140.274
138.696
138.339
137.580
133.444
133.310
131.116
129.628
129.362
129.289
128.644
128.498
128.440
128.407
128.382
128.335
127.787
127.571
127.338
126.570
126.551
126.172
126.151
77.478
77.160
76.842
52.112
52.067
48.247
48.133
39.359
39.254
CO2Me
Cl
3ja
f1 (ppm)


CO2Me
Br
3ka
2.06
7.43
3.13
1.10
0.94
1.00
1.37
1.65
1.03
1.01
1.01
f1 (ppm)


CO2Me
Br
3ka
f1 (ppm)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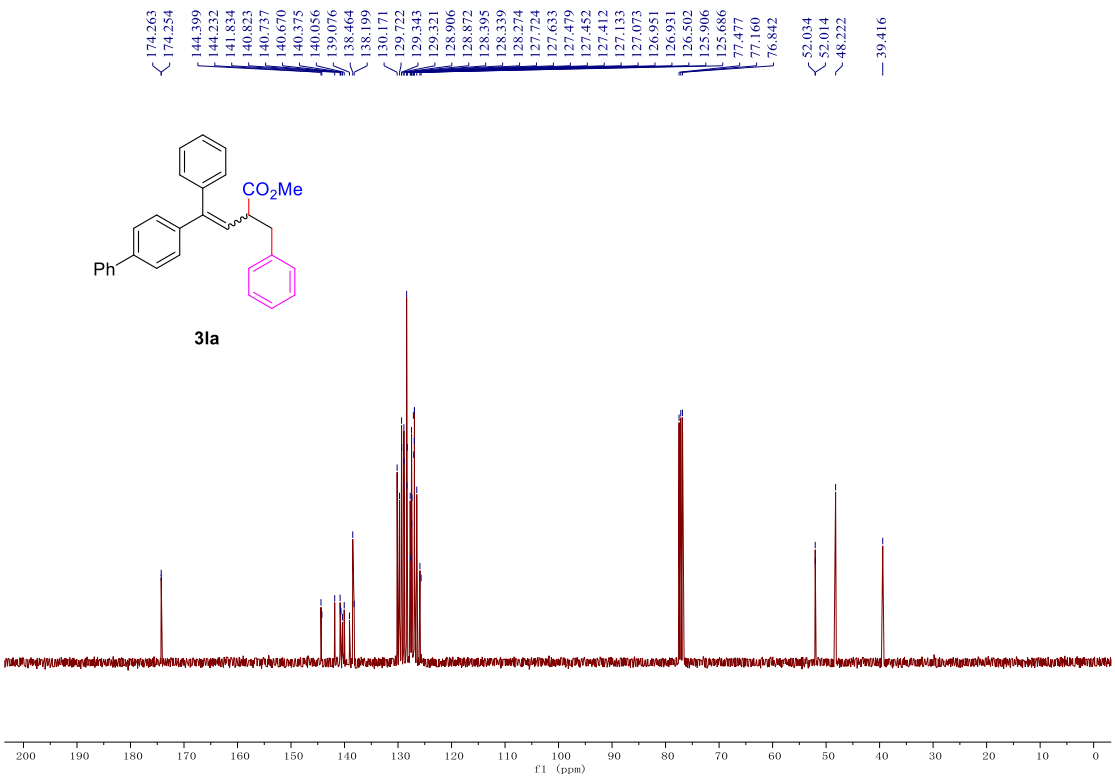
7.575
7.550
7.529
7.511
7.492
7.472
7.453
7.429
7.411
7.396
7.392
7.377
7.367
7.361
7.341
7.326
7.315
7.307
7.300
7.294
7.291
7.282
7.276
7.258
7.257
7.248
7.232
7.213
7.108
7.092
7.076
7.010
6.990
6.976
6.967
6.958
6.952
6.245
6.219
6.194
6.168
3.726
3.714
3.621
3.615
3.596
3.548
3.523
3.206
3.191
3.174
3.158
3.143
2.994
2.984
2.974
2.962
2.950
2.940
2.929
CO2Me
Ph
3la
1.15
2.05
3.07
9.34
2.05
1.98
0.44
0.56
1.57
1.38
1.08
0.98
0.98
f1 (ppm)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174.254
144.399
144.232
141.834
140.823
140.737
140.670
140.375
140.056
139.076
138.464
138.199
130.171
129.722
129.343
129.321
128.906
128.872
128.395
128.339
128.274
127.724
127.633
127.479
127.452
127.412
127.133
127.073
126.951
126.931
126.502
125.906
125.686
77.477
77.160
76.842
52.034
52.014
48.222
39.416
CO2Me
Ph
3la
f1 (ppm)


7.283
7.269
7.264
7.260
7.248
7.243
7.229
7.221
7.217
7.213
7.206
7.200
7.145
7.126
7.117
7.110
7.096
7.092
7.075
7.071
7.055
7.051
6.817
6.788
6.059
3.675
3.540
3.522
3.514
3.503
3.496
3.477
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3.127
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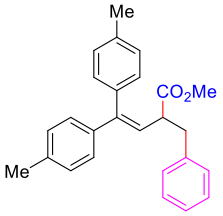
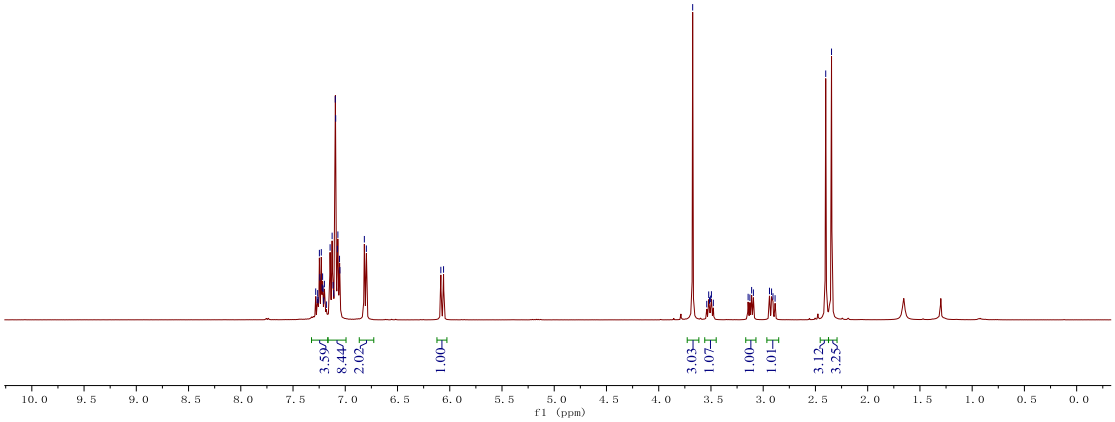
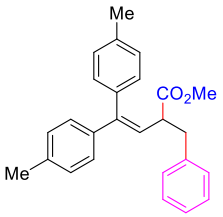
2.886
2.402
2.346


Me
CO2Me
Me

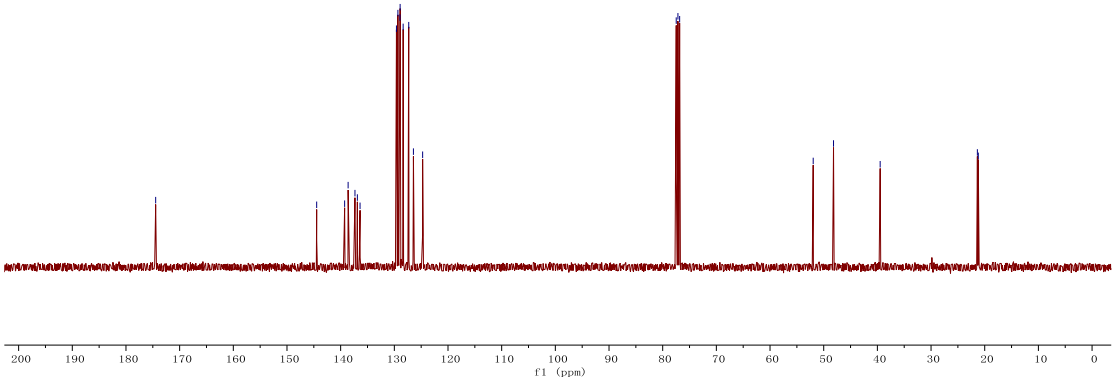
3ma


3.59
8.44
2.02
1.00
3.03
1.07
1.00
1.01
3.12
3.25
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)


174.467
144.469
139.261
138.609
137.336
136.888
136.388
129.605
129.333
128.954
128.919
128.356
127.314
126.443
124.726
77.479
77.161
76.842
51.958
48.171
39.479
21.369
21.196


Me
CO2Me
Me

3ma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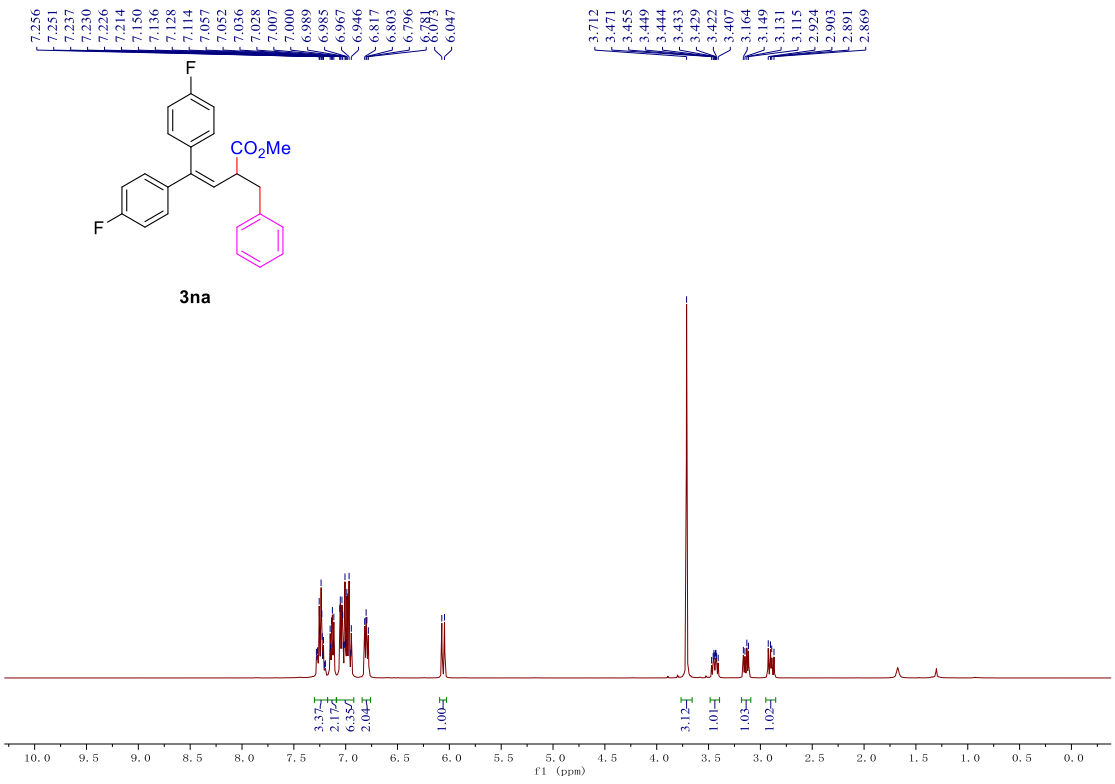
f1 (ppm)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7.136
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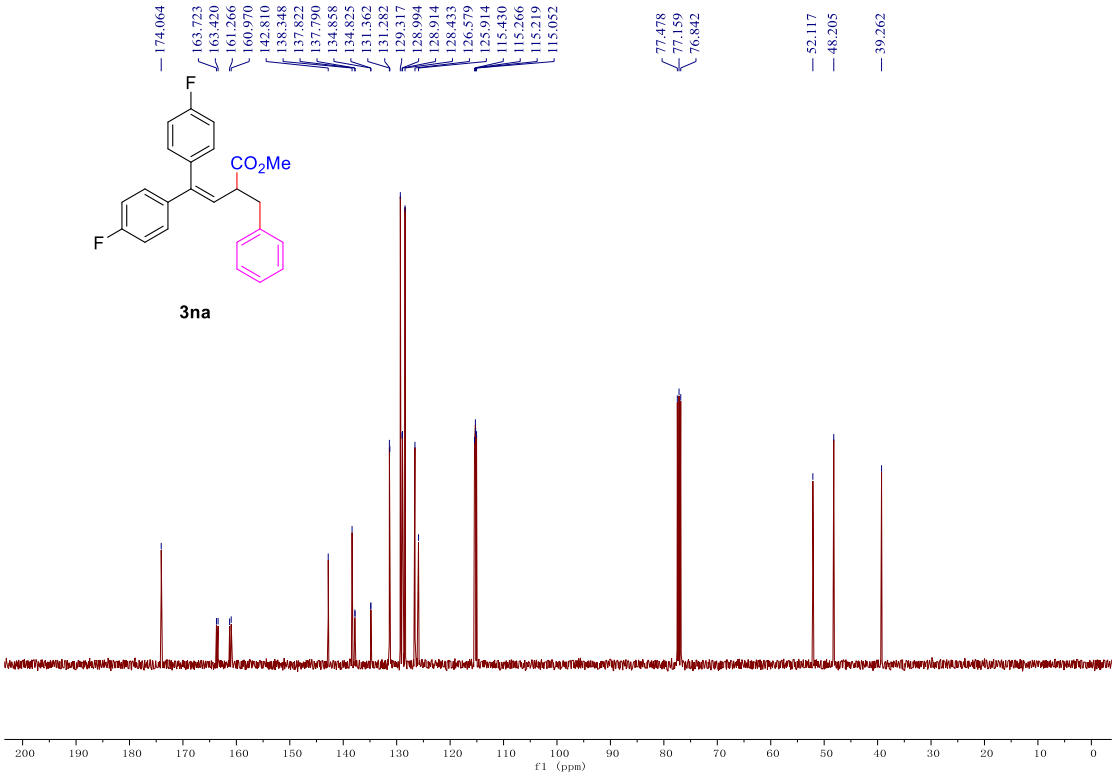
7.114
7.057
7.052
7.036
7.028
7.007
7.000
6.989
6.985
6.967
6.946
6.817
6.803
6.796
6.047
3.712
3.471
3.455
3.449
3.444
3.433
3.429
3.422
3.407
3.164
3.149
3.131
3.115
2.924
2.903
2.891
2.869
F
CO2Me
F
3.37
2.17
6.35
2.04
1.00
3.12
1.01
1.03
1.02
f1 (ppm)

3na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161.266
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142.810
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137.822
137.790
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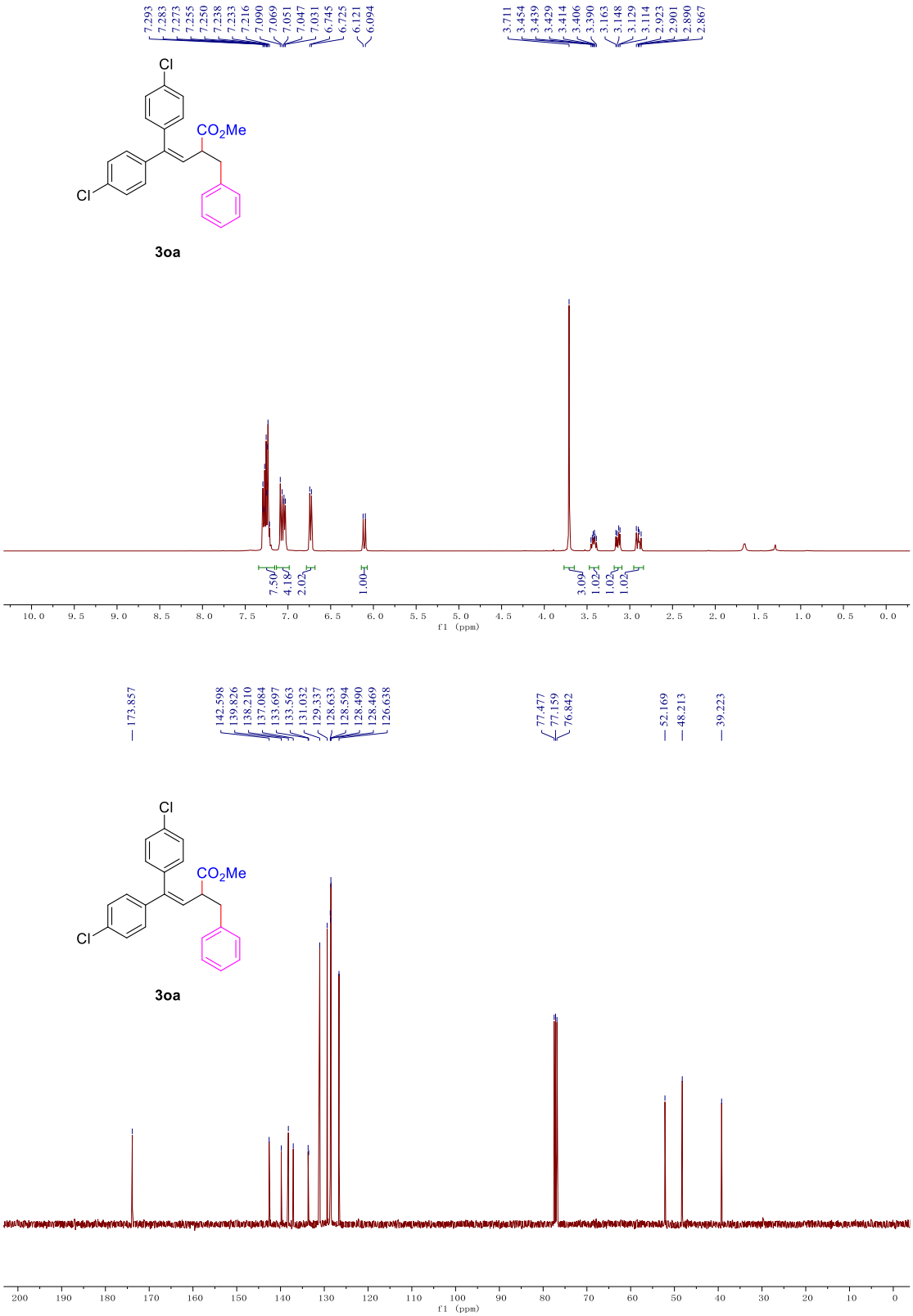
134.825
131.362
131.282
129.317
128.994
128.914
128.433
126.579
125.914
115.430
115.266
115.219
115.052
77.478
77.159
76.842
52.117
48.205
39.262
F
CO2Me
F
f1 (ppm)

3na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7.238
7.233
7.216
7.090
7.069
7.051
7.047
7.031
6.745
6.725
6.121
6.094
3.711
3.454
3.439
3.429
3.414
3.406
3.390
3.163
3.148
3.129
3.114
2.923
2.901
2.890
2.867
Cl
CO2Me
Cl
3oa
7.50
4.18
2.02
1.00
3.09
1.02
1.02
1.02
f1 (ppm)
173.857
142.598
139.826
138.210
137.084
133.697
133.563
131.032
129.337
128.633
128.594
128.490
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77.159
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52.169
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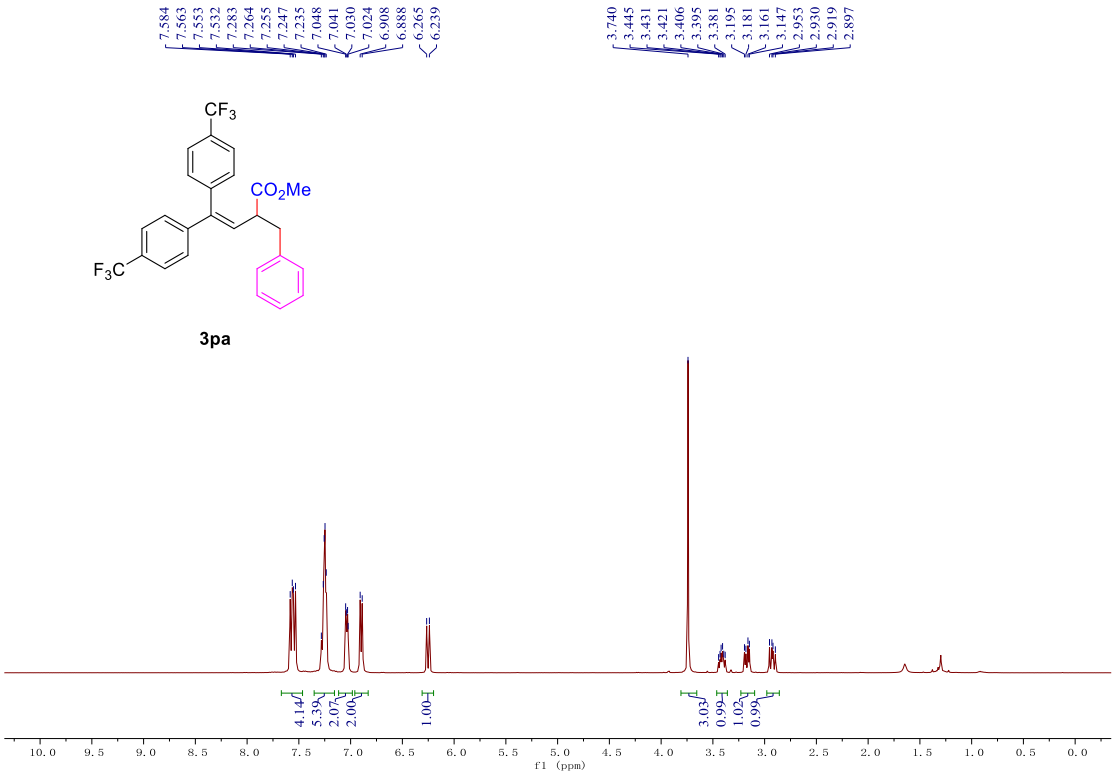
39.223
Cl
CO2Me
Cl
3oa
f1 (ppm)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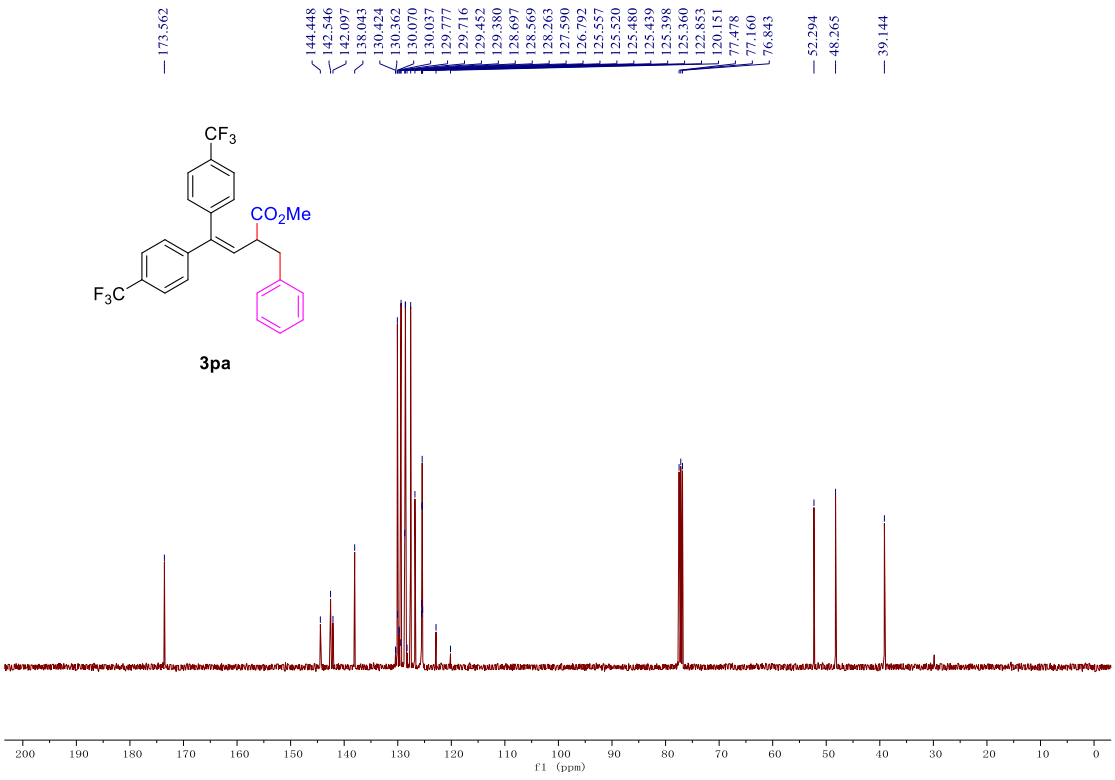
7.553
7.532
7.283
7.264
7.255
7.247
7.235
7.048
7.041
7.030
7.024
6.908
6.888
6.265
6.239
3.740
3.445
3.431
3.421
3.406
3.395
3.381
3.195
3.181
3.161
3.147
2.953
2.930
2.919
2.897
CF3
CO2Me
F3C
3pa
4.14
5.39
2.07
2.00
1.00
3.03
0.99
1.02
0.99
f1 (ppm)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129.380
128.697
128.569
128.263
127.590
126.792
125.557
125.520
125.480
125.439
125.398
125.360
122.853
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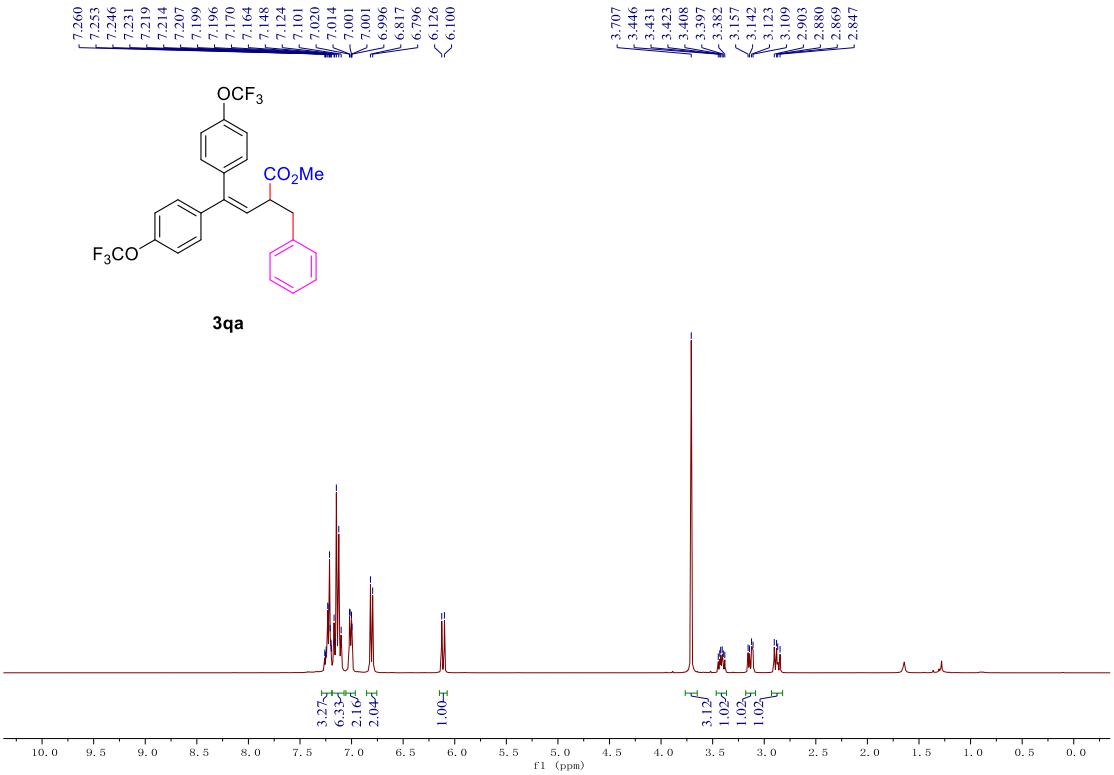
CF3
CO2Me
F3C
3pa
f1 (ppm)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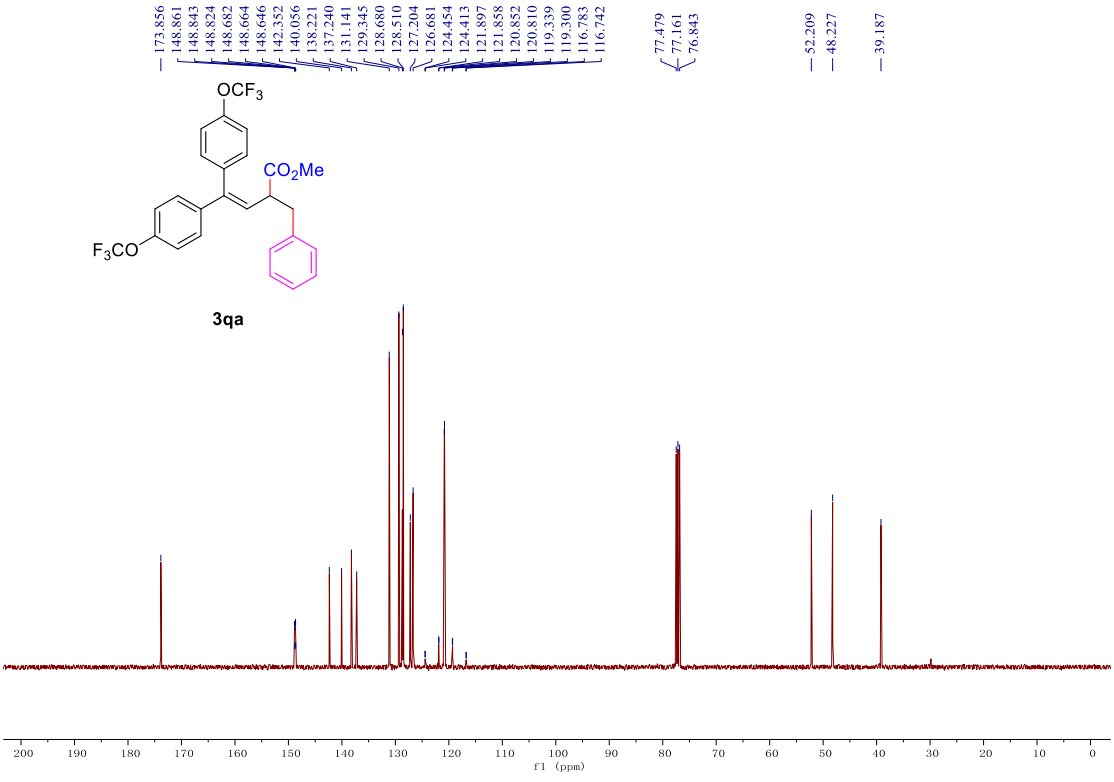
7.214
7.207
7.199
7.196
7.170
7.164
7.148
7.124
7.101
7.020
7.014
7.001
7.001
6.996
6.817
6.796
6.126
6.100
3.707
3.446
3.431
3.423
3.408
3.397
3.382
3.157
3.142
3.123
3.109
2.903
2.880
2.869
2.847
OCF3
CO2Me
F3CO
3qa
3.27
6.33
2.16
2.04
1.00
3.12
1.02
1.03
1.02
f1 (ppm)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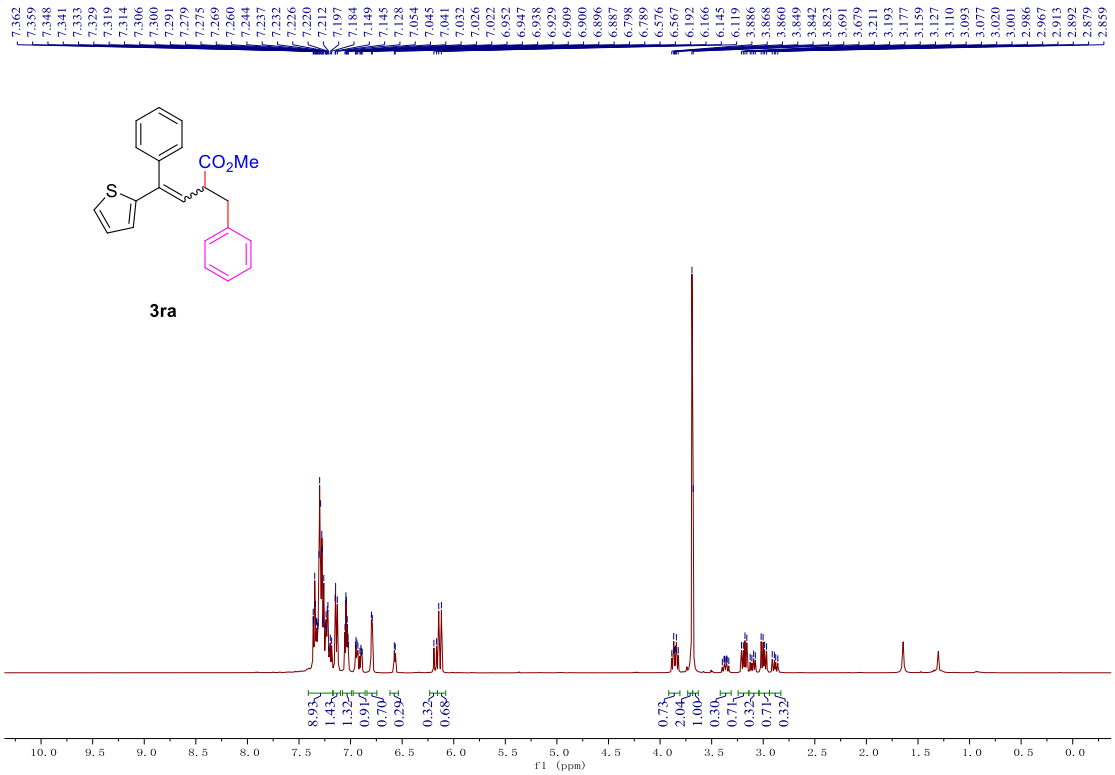
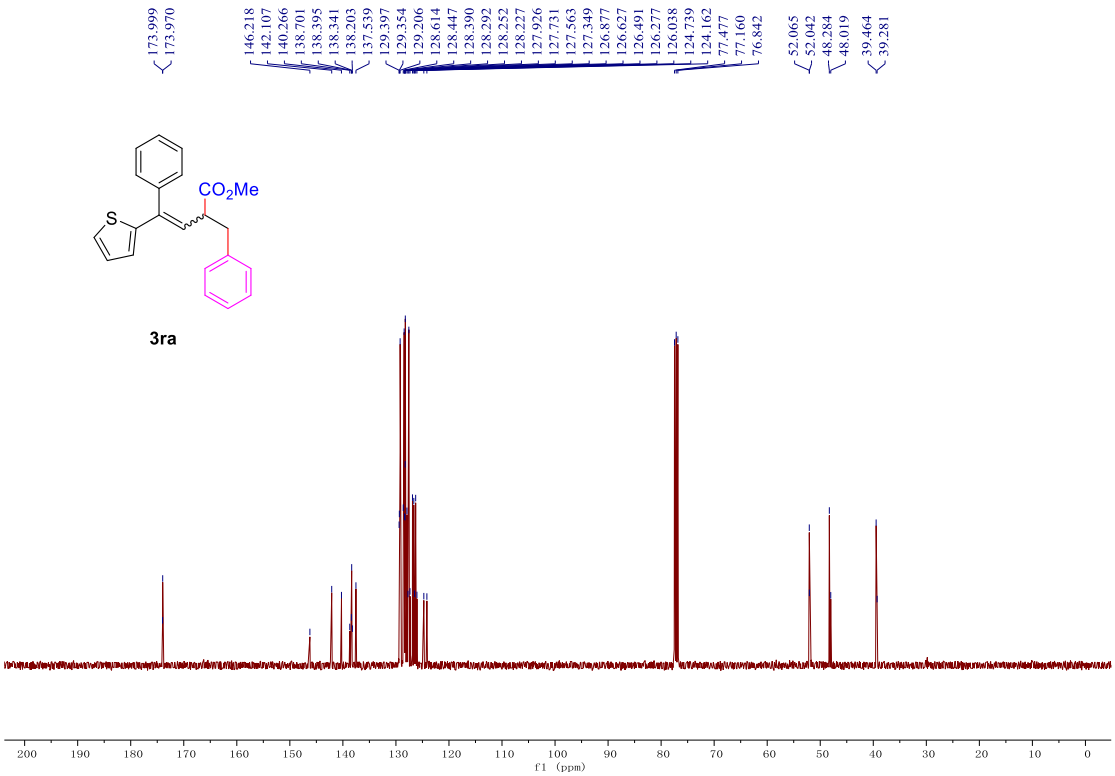
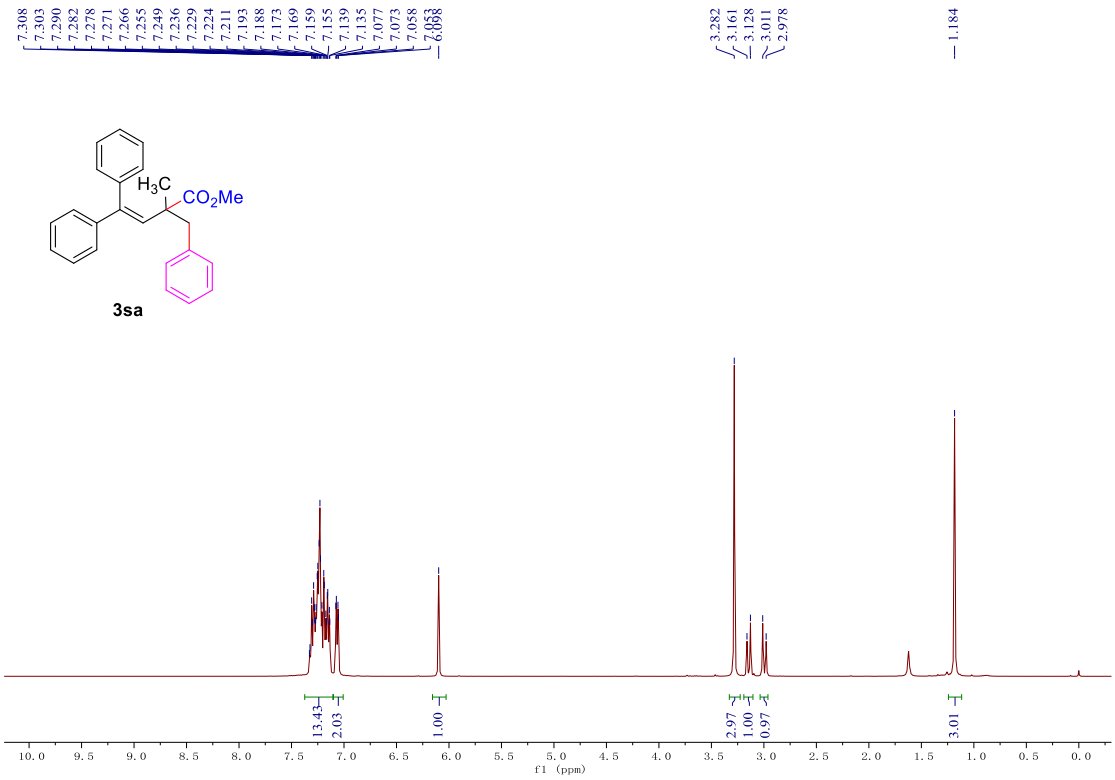
148.843
148.824
148.682
148.664
148.646
142.352
140.056
138.221
137.240
131.141
129.345
128.680
128.510
127.204
126.681
124.454
124.413
121.897
121.858
120.852
120.810
119.339
119.300
116.783
116.742
77.479
77.161
76.843
52.209
48.227
39.187
OCF3
CO2Me
F3CO
3qa
f1 (ppm)


CO2Me
S
3ra
f1 (ppm)


CO2Me
S
3ra
f1 (ppm)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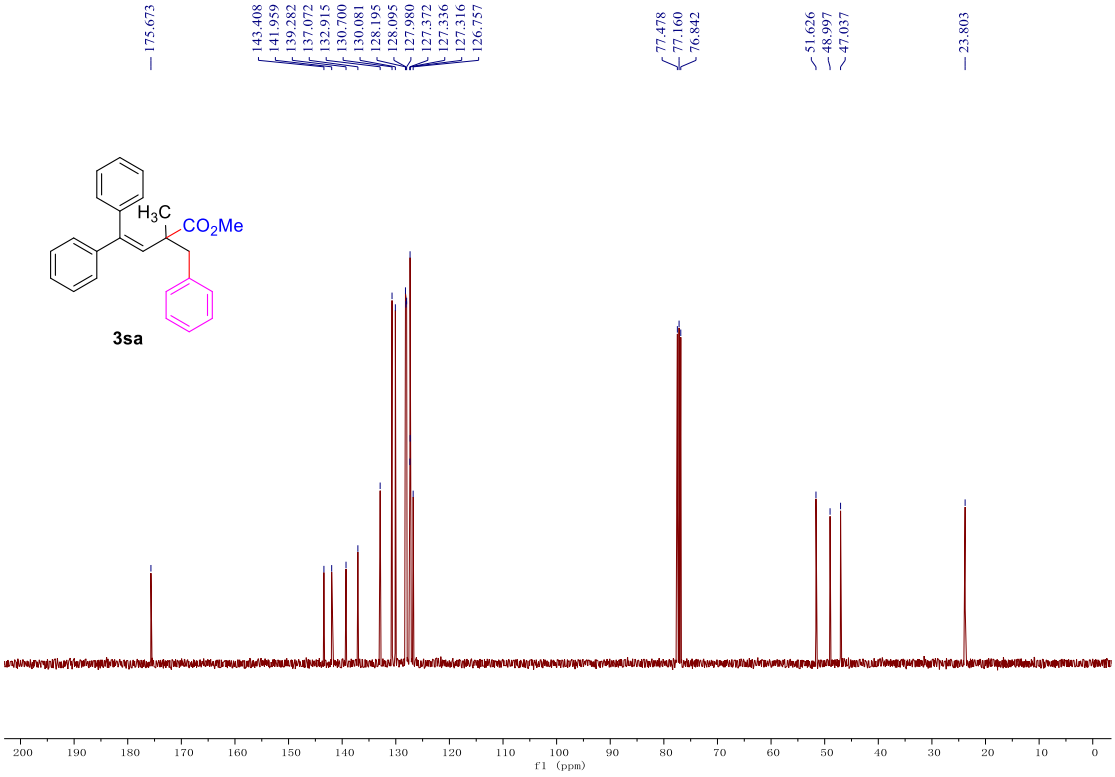
7.290
7.282
7.278
7.271
7.266
7.255
7.249
7.236
7.229
7.224
7.211
7.193
7.188
7.173
7.169
7.159
7.155
7.139
7.135
7.077
7.073
7.058
6.098
3.282
3.161
3.128
3.011
2.978
1.184
H3C
CO2Me
3sa
13.43
2.03
1.00
2.97
1.00
0.97
3.01
f1 (ppm)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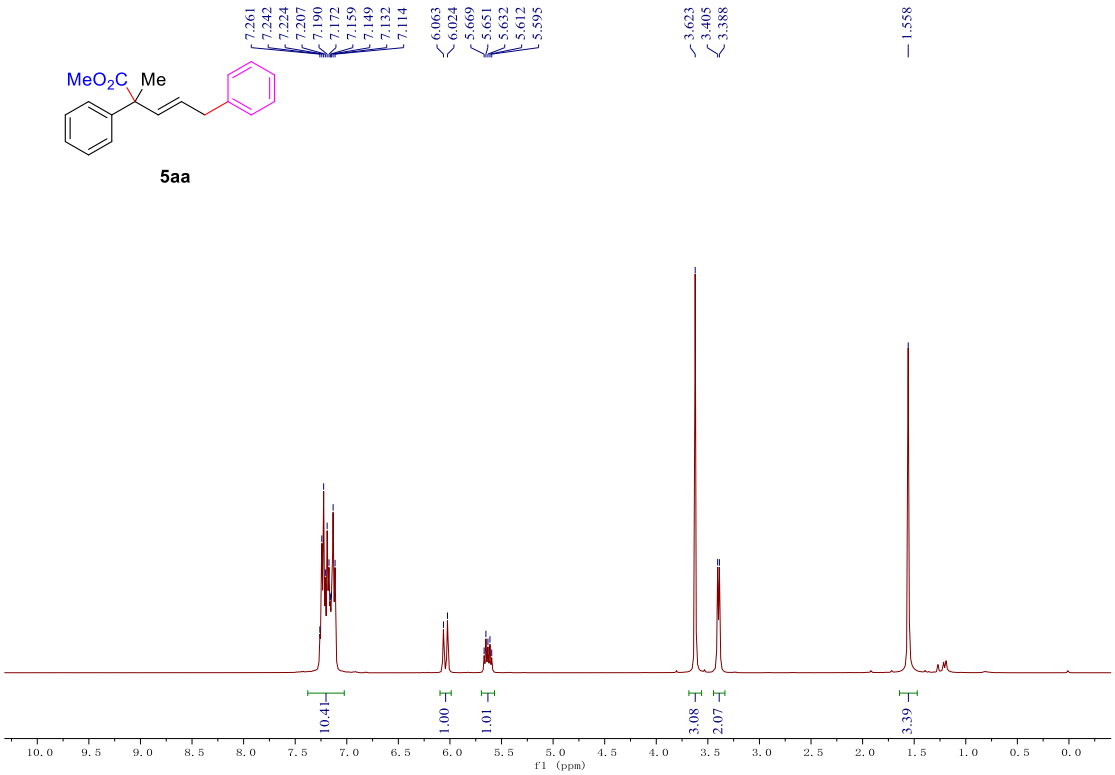
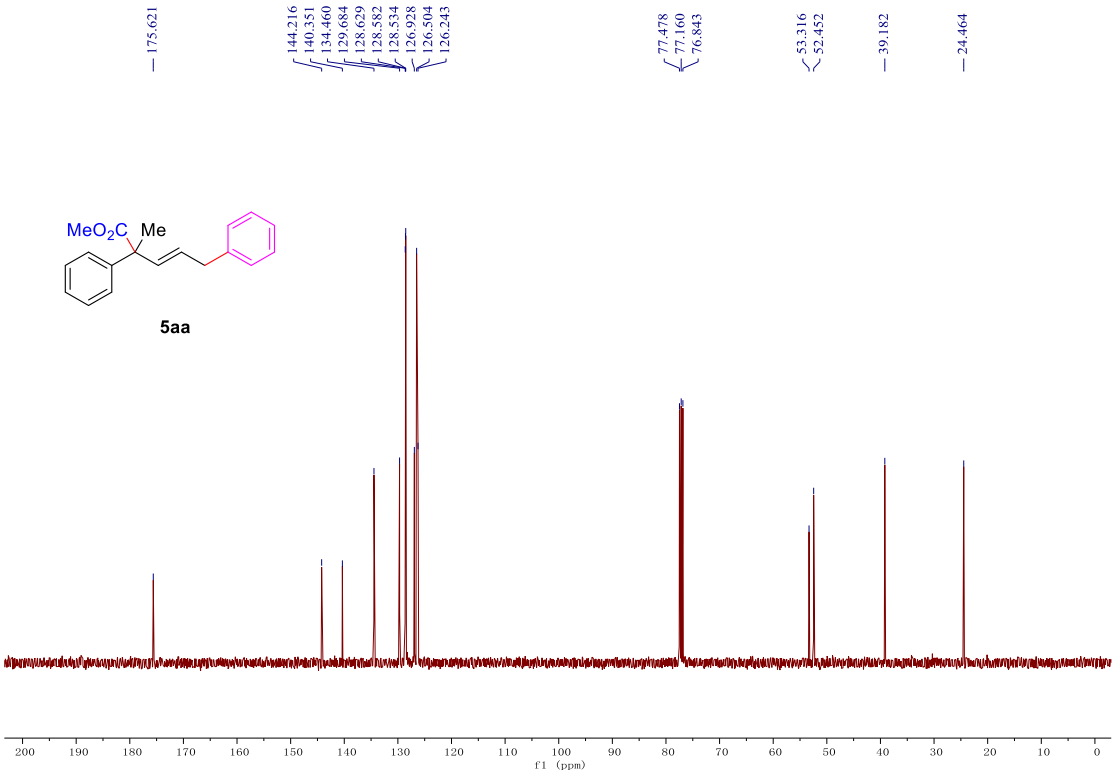
141.959
139.282
137.072
132.915
130.700
130.081
128.195
128.095
127.980
127.372
127.336
127.316
126.757
77.478
77.160
76.842
51.626
48.997
47.037
23.803
H3C
CO2Me
3sa
f1 (ppm)


7.261
7.242
7.224
7.207
7.190
7.172
7.159
7.149
7.132
7.114
6.063
6.024
5.669
5.651
5.632
5.612
5.595
3.623
3.405
3.388
1.558
MeO2C Me
5aa
10.41
1.00
1.01
3.08
2.07
3.39
f1 (ppm)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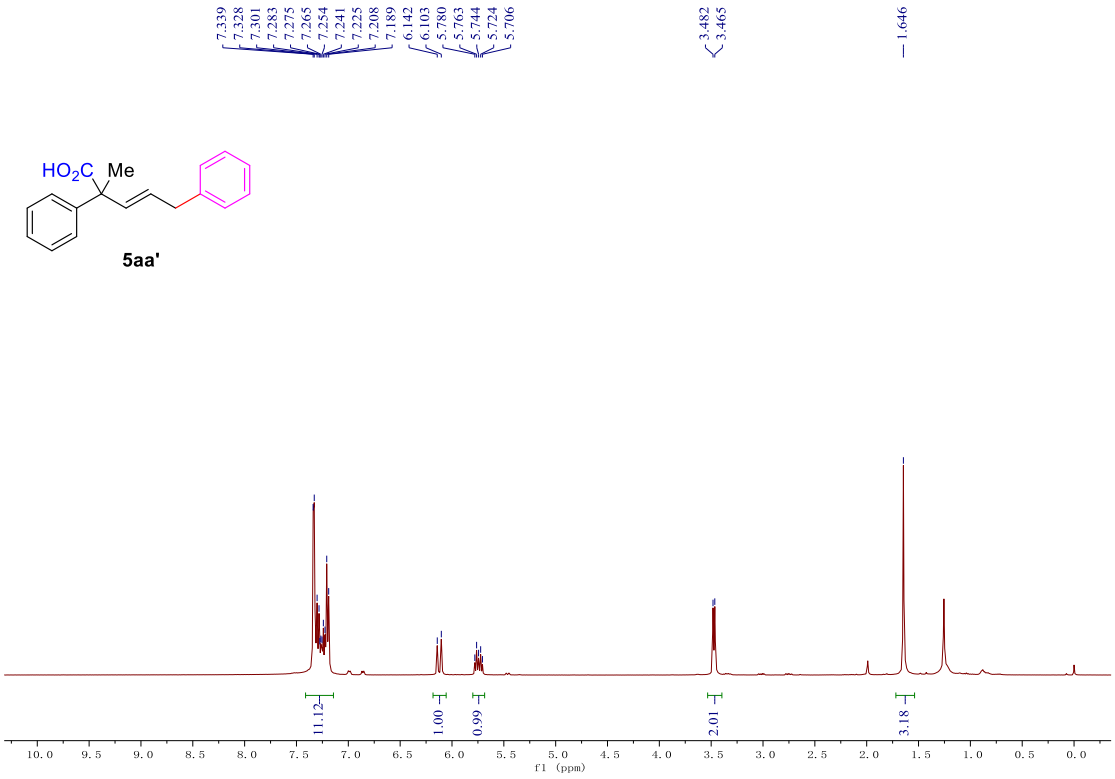
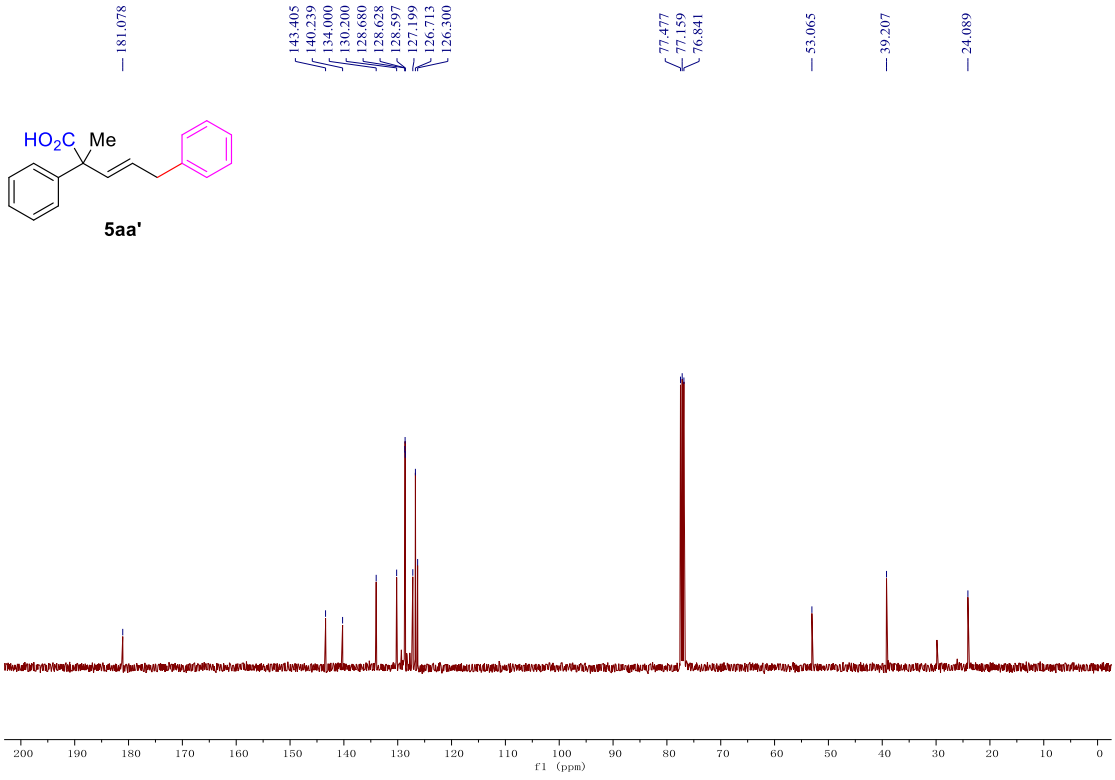
140.351
134.460
129.684
128.629
128.582
128.534
126.928
126.504
126.243
77.478
77.160
76.843
53.316
52.452
39.182
24.464
MeO2C Me
5aa
f1 (ppm)


7.339
7.328
7.301
7.283
7.275
7.265
7.254
7.241
7.225
7.208
7.189
6.142
6.103
5.780
5.763
5.744
5.724
5.706
3.482
3.465
1.646
HO2C Me
5aa'
11.12
1.00
0.99
2.01
3.18
f1 (ppm)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140.239
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128.680
128.628
128.597
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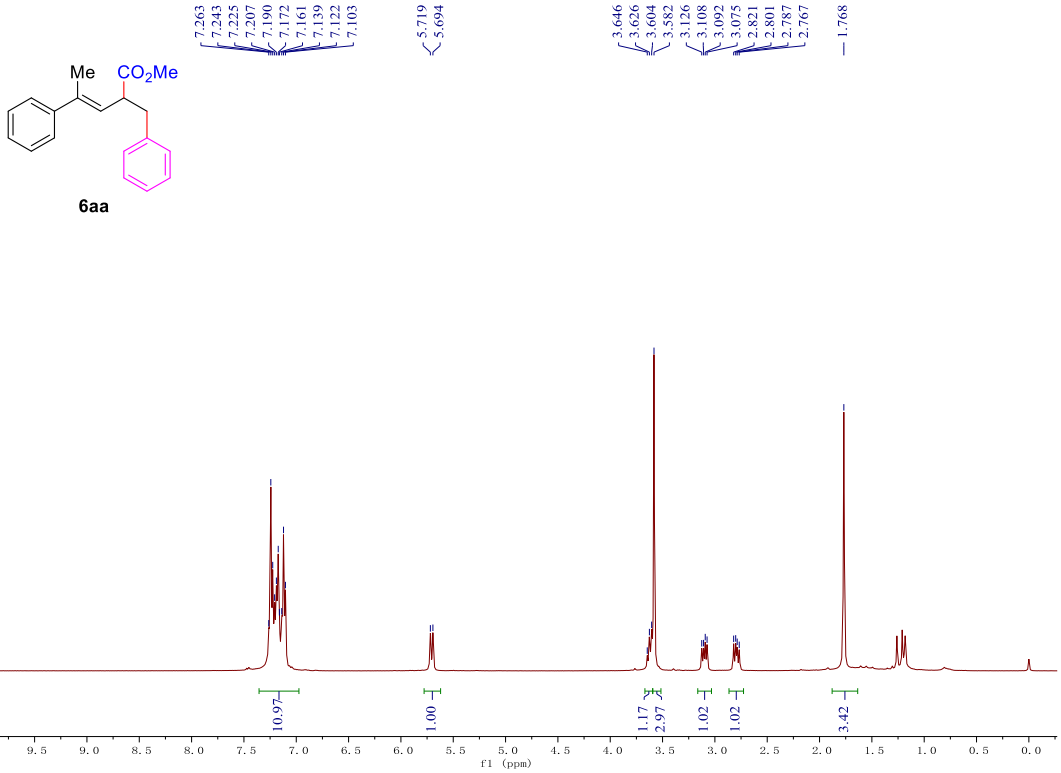
126.713
126.300
77.477
77.159
76.841
53.065
39.207
24.089
HO2C Me
5aa'
f1 (ppm)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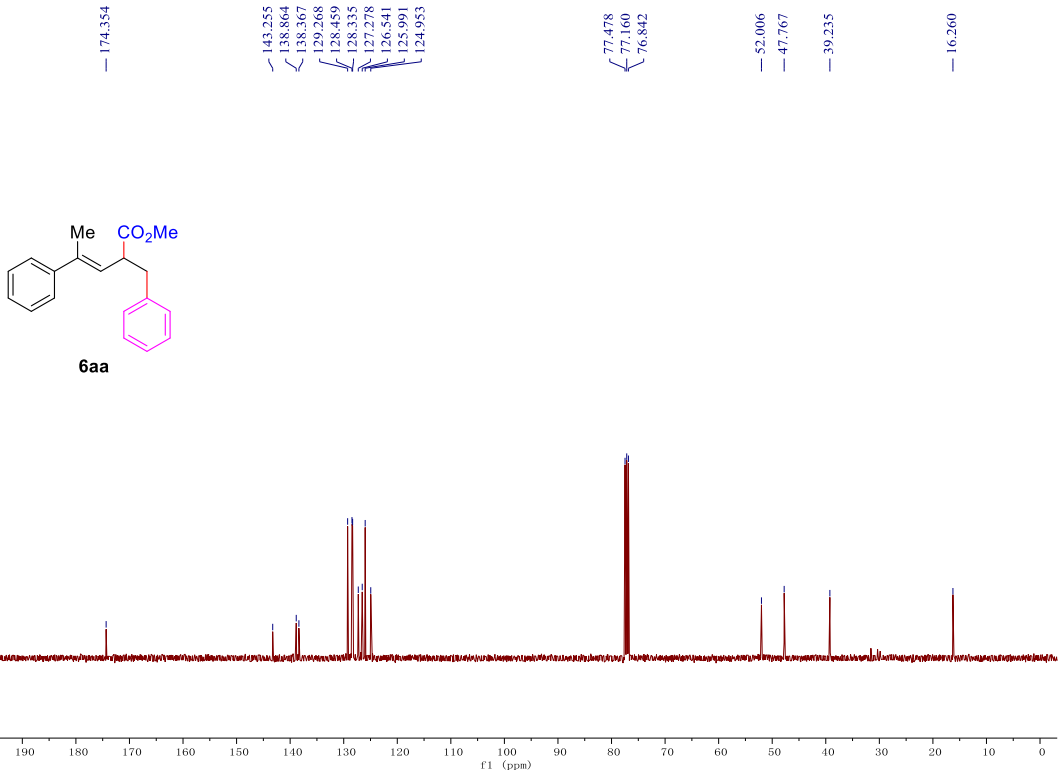
7.243
7.225
7.207
7.190
7.172
7.161
7.139
7.122
7.103
5.719
5.694
3.646
3.626
3.604
3.582
3.126
3.108
3.092
3.075
2.821
2.801
2.787
2.767
1.768
Me
CO2Me
6aa
10.97
1.00
1.17
2.97
1.02
1.02
3.42
f1 (ppm)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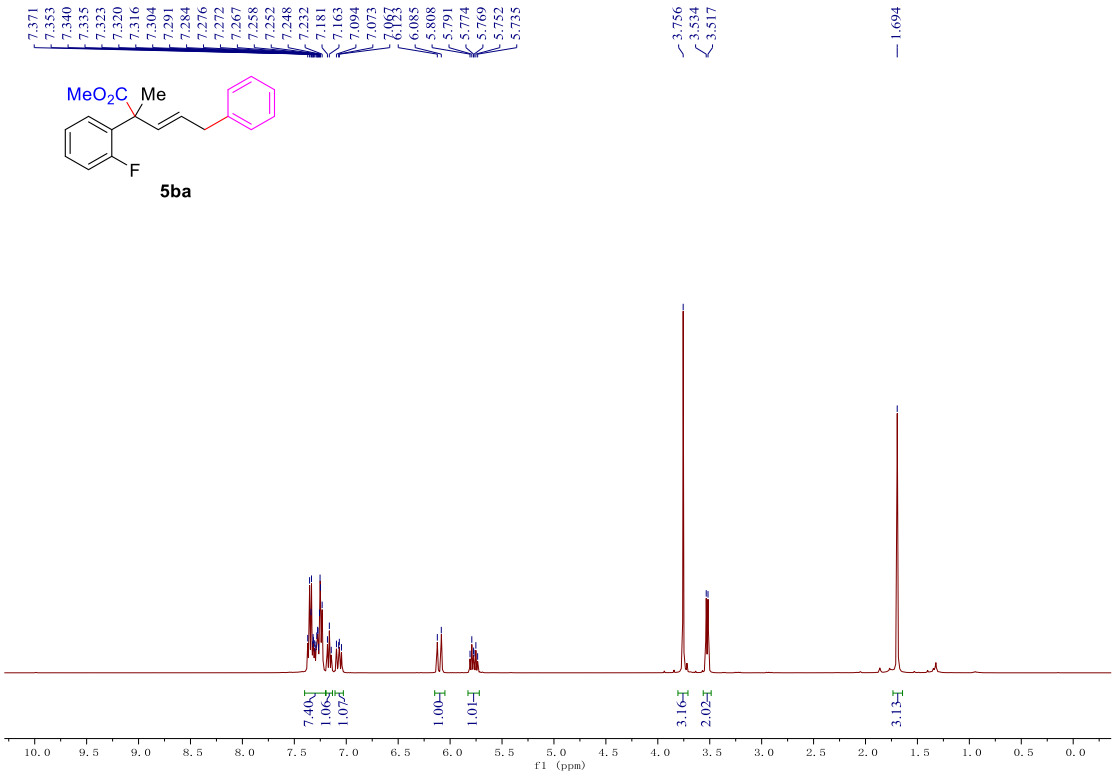
128.335
127.278
126.541
125.991
124.953
77.478
77.160
76.842
52.006
47.767
39.235
16.260
Me
CO2Me
6aa
f1 (ppm)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7.353
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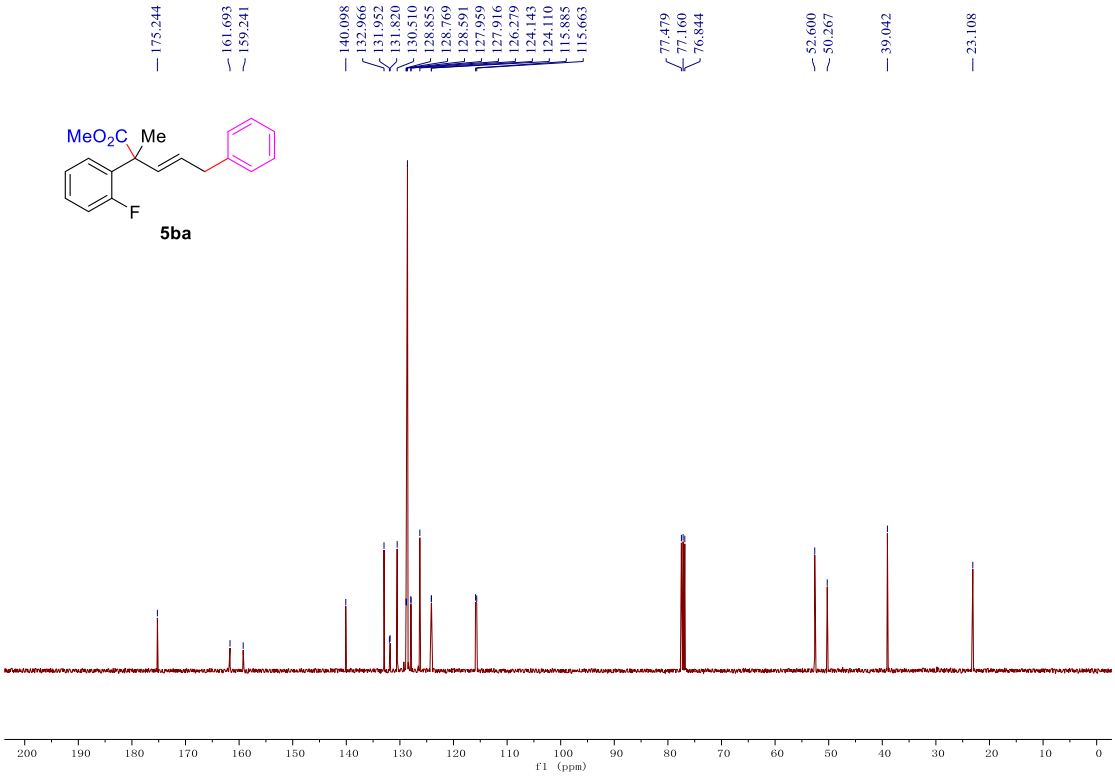
7.320
7.316
7.304
7.291
7.284
7.276
7.272
7.267
7.258
7.252
7.248
7.232
7.181
7.163
7.094
7.073
7.067
6.123
6.085
5.808
5.791
5.774
5.769
5.752
5.735
3.756
3.534
3.517
1.694
MeO2C
Me
F
5ba
7.40
1.06
1.07
1.00
1.01
3.16
2.02
3.13
f1 (ppm)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130.510
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128.769
128.591
127.959
127.916
126.279
124.143
124.110
115.885
115.663
77.479
77.160
76.844
52.600
50.267
39.042
23.108
MeO2C
Me
F
5ba
f1 (ppm)


7.260
7.241
7.223
7.212
7.185
7.177
7.168
7.158
7.154
7.148
7.140
7.135
7.130
7.125
7.111
7.106
7.092
7.087
7.036
7.017
6.999
6.979
6.958
6.951
6.931
5.610
5.586
3.673
3.666
3.654
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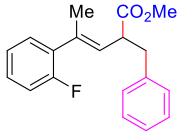
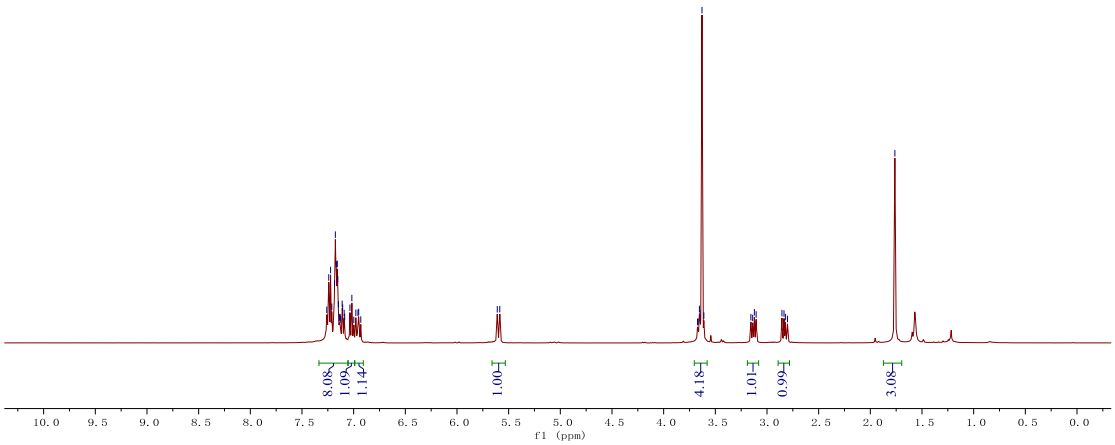
1.762


Me
CO2Me
F

6ba


8.08
1.09
1.14
1.00
4.18
1.01
0.99
3.08
f1 (ppm)


174.182
161.118
158.661
138.746
134.954
132.028
131.889
129.788
129.744
129.299
128.729
128.647
128.470
128.066
128.046
126.579
124.039
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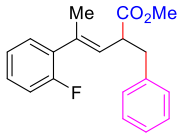
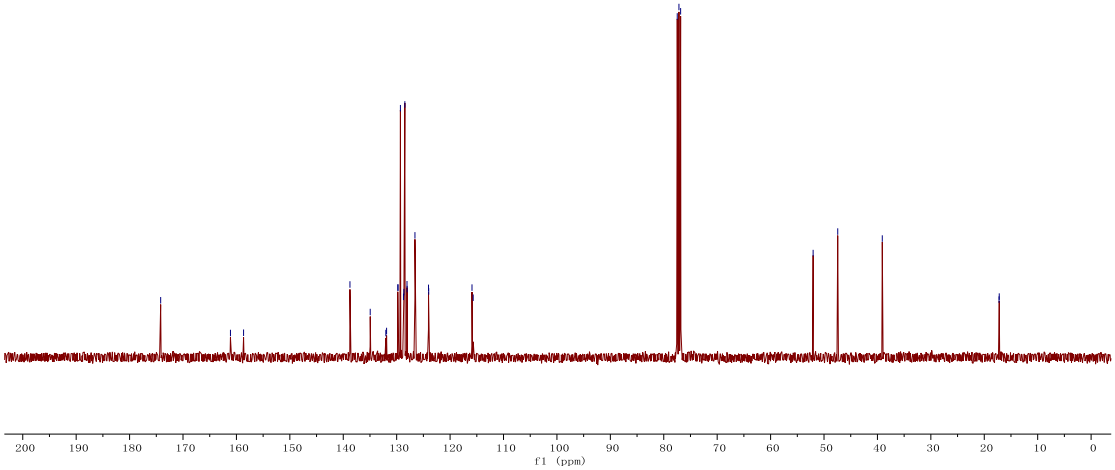
52.039
47.433
39.092
17.232
17.196


Me
CO2Me
F

6ba


f1 (ppm)


7.260
7.247
7.241
7.236
7.222
7.214
7.199
7.194
7.167
7.164
7.161
7.146
7.141
7.137
7.120
6.975
6.956
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6.929
6.908
6.903
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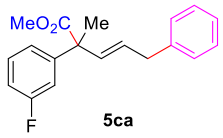
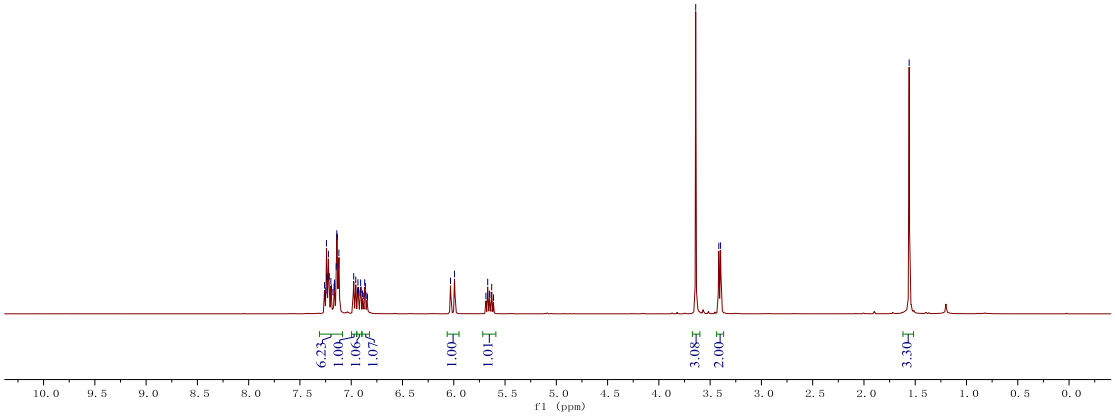
1.559


MeO2C
Me
F

5ca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1.00
1.06
1.07
1.00
1.01
3.08
2.00
3.30
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)


175.069
164.105
161.665
146.763
146.695
140.138
133.834
130.250
129.974
129.892
128.618
126.313
122.266
122.237
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53.156
53.140
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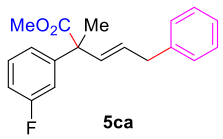
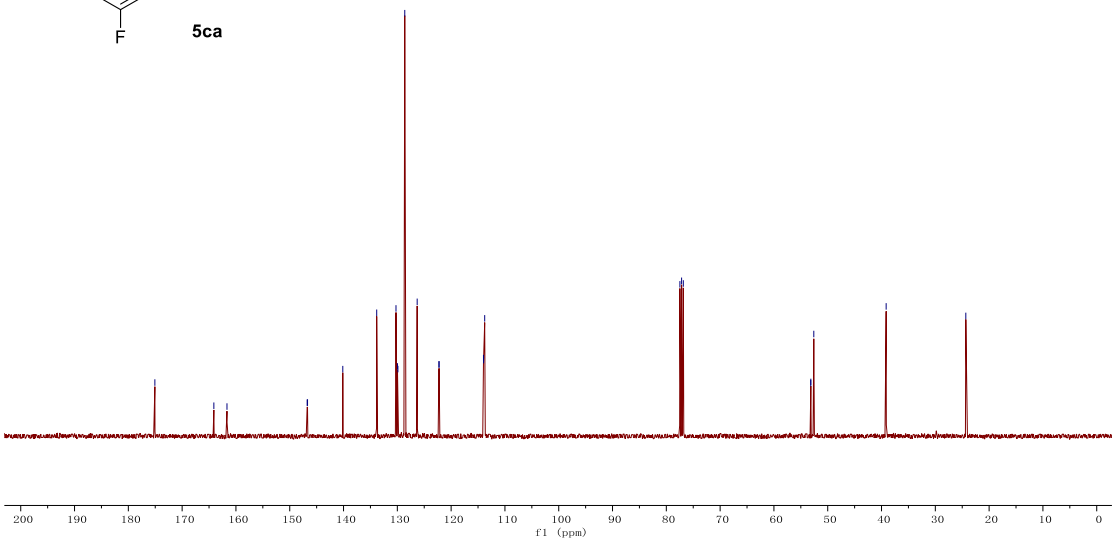
39.139
24.331


MeO2C
Me
F

5ca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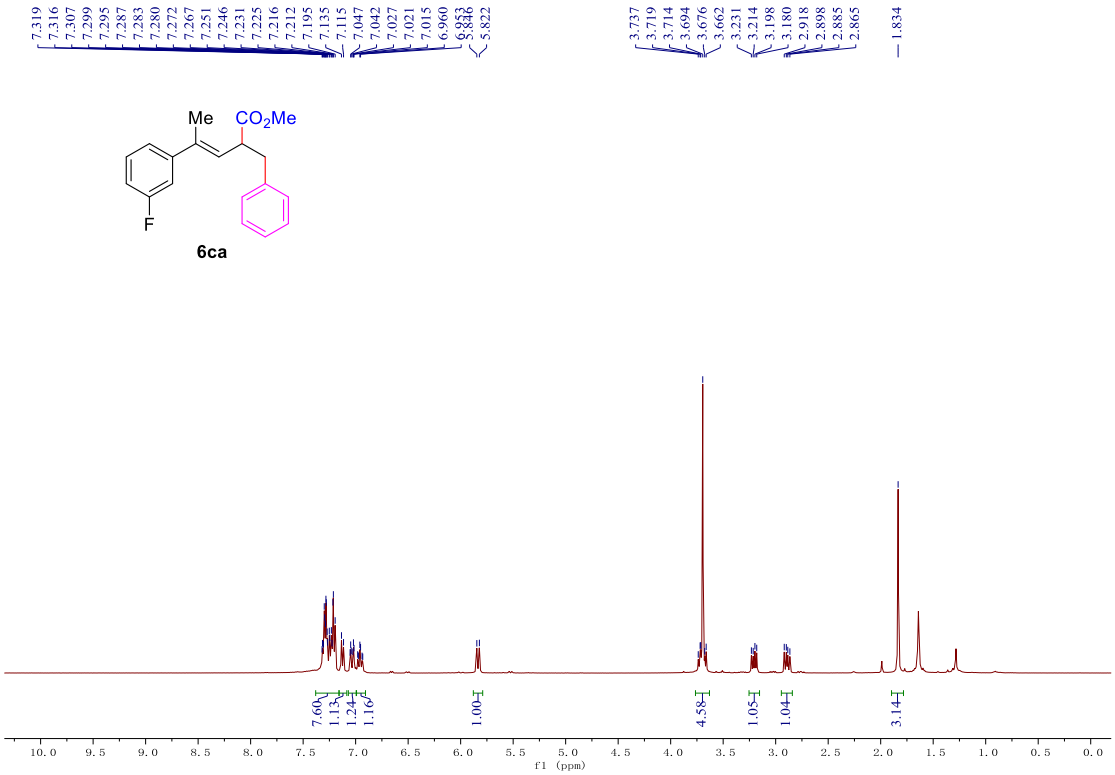
f1 (ppm)


7.319
7.316
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7.231
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7.216
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7.195
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7.115
7.047
7.042
7.027
7.021
7.015
6.960
6.953
5.846
5.822
3.737
3.719
3.714
3.694
3.676
3.662
3.231
3.214
3.198
3.180
2.918
2.898
2.885
2.865
1.834
Me
CO2Me
F
6ca
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1.24
1.16
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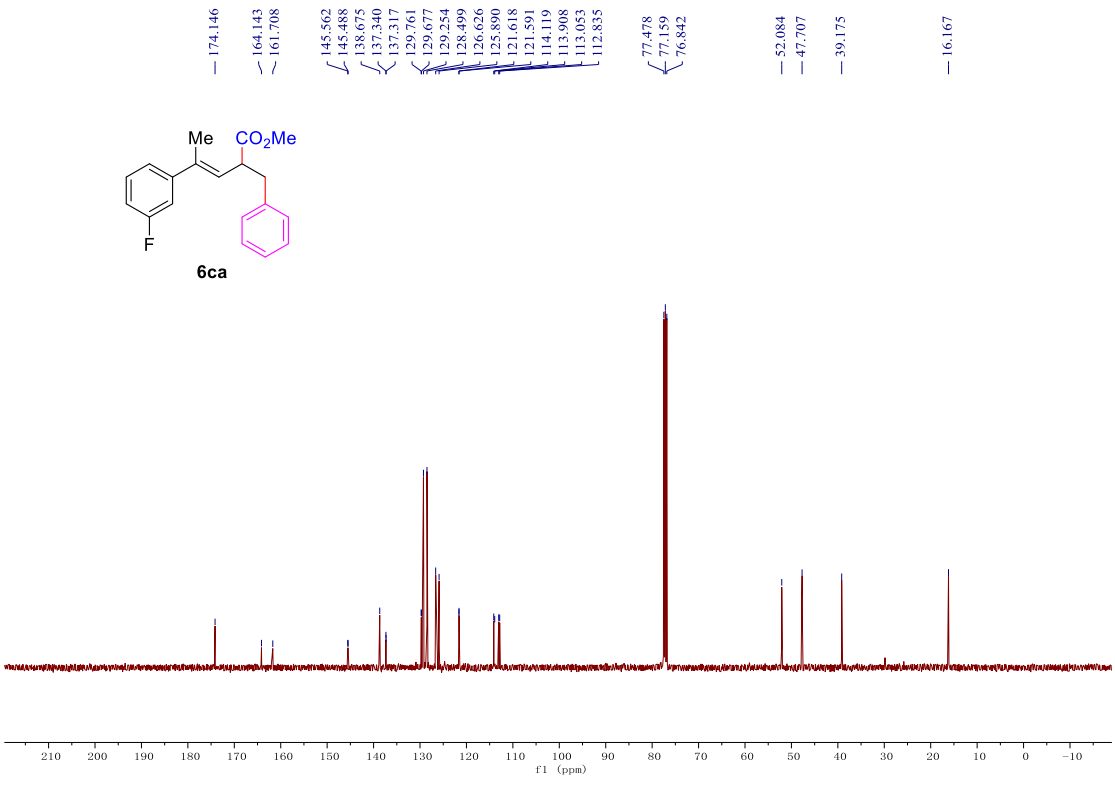
1.05
1.04
3.14
f1 (ppm)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125.890
121.618
121.591
114.119
113.908
113.053
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47.707
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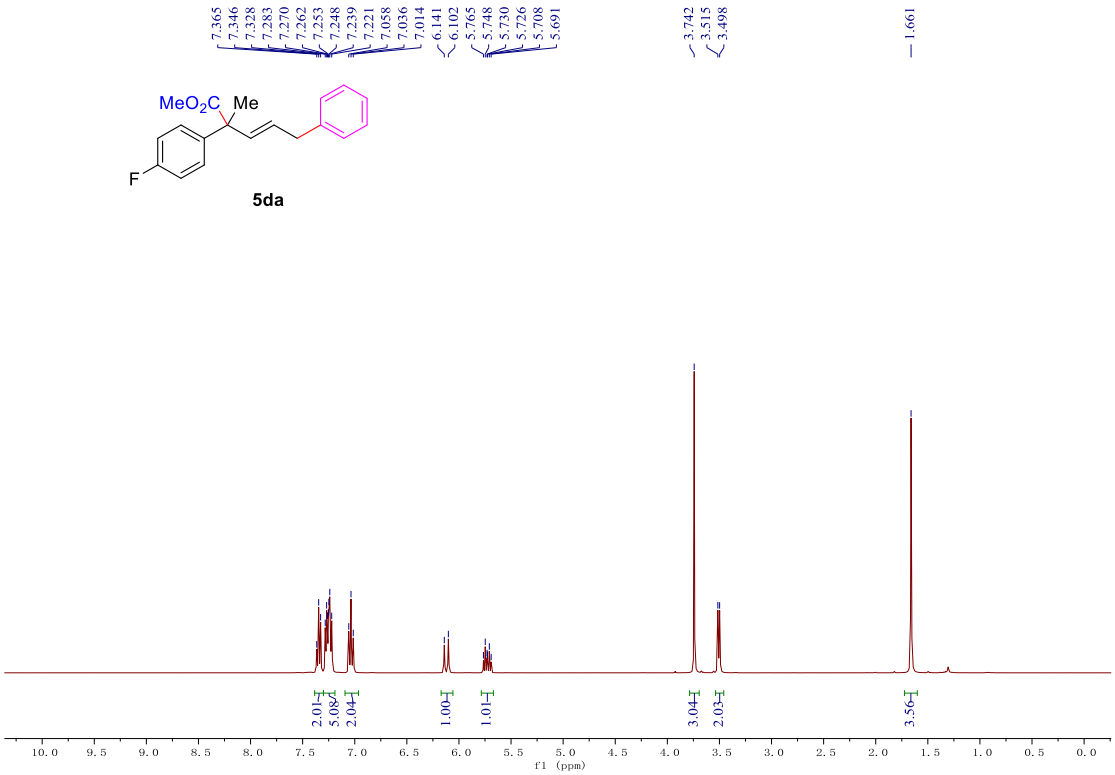
Me
CO2Me
F
6ca
f1 (ppm)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6.141
6.102
5.765
5.748
5.730
5.726
5.708
5.691
3.742
3.515
3.498
1.661
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Me
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2.04
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1.01
3.04
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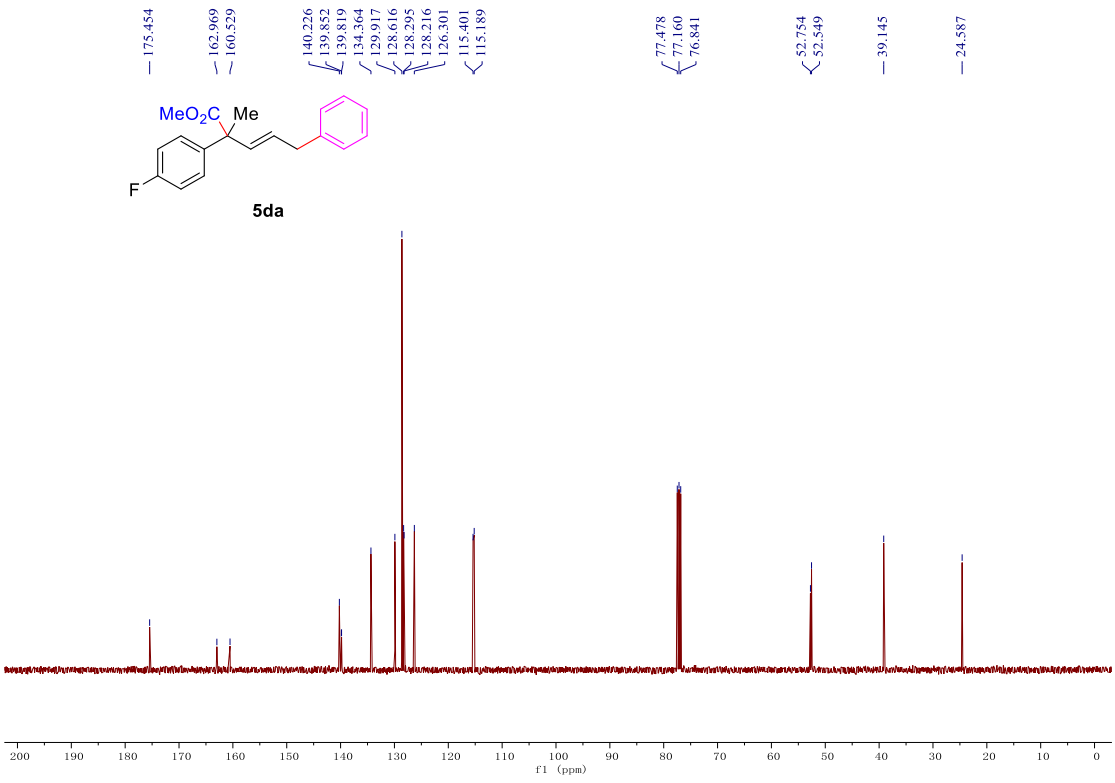
3.56
f1 (ppm)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76.841
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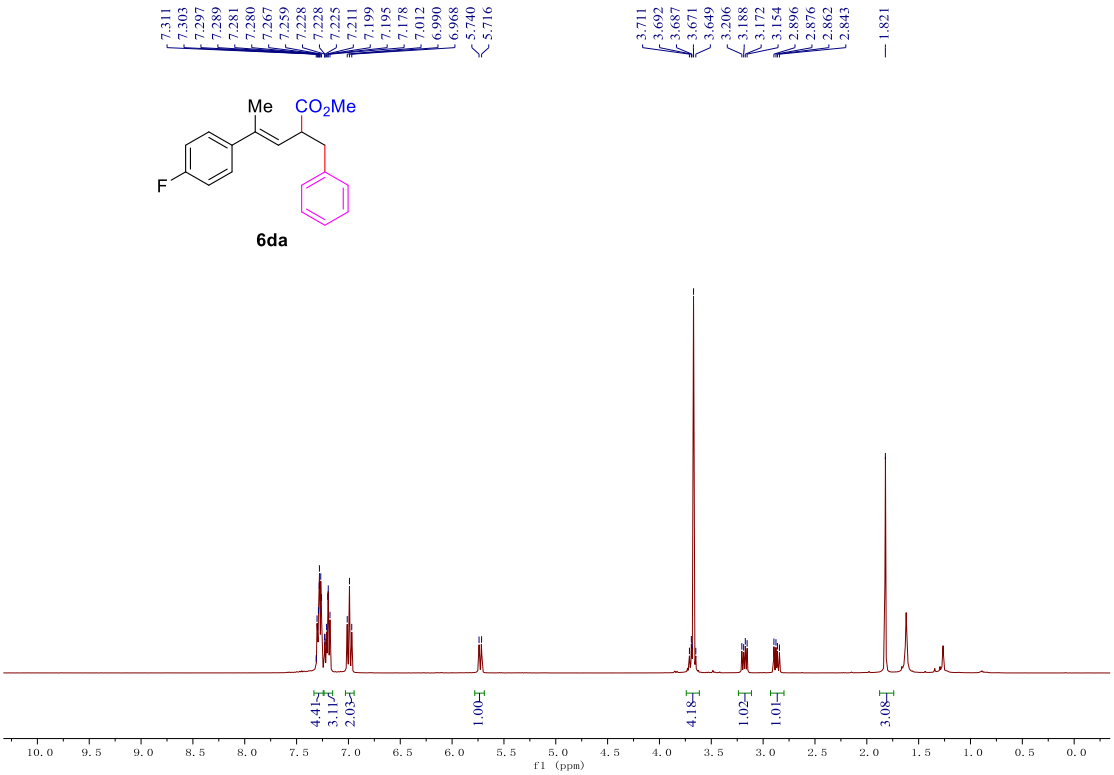
MeO2C
Me
F
5da
f1 (ppm)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7.259
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7.228
7.225
7.211
7.199
7.195
7.178
7.012
6.990
6.968
5.740
5.716
3.711
3.692
3.687
3.671
3.649
3.206
3.188
3.172
3.154
2.896
2.876
2.862
2.843
1.821
Me
CO2Me
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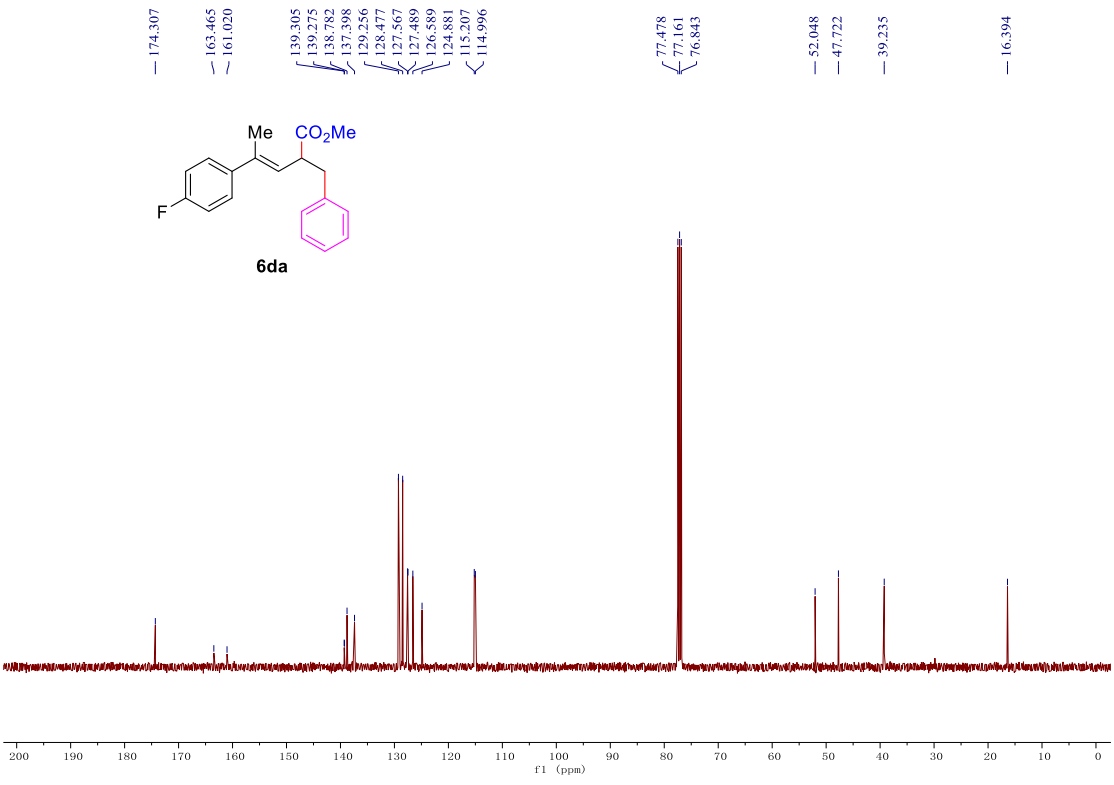
2.03
1.00
4.18
1.02
1.01
3.08
f1 (ppm)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124.881
115.207
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76.843
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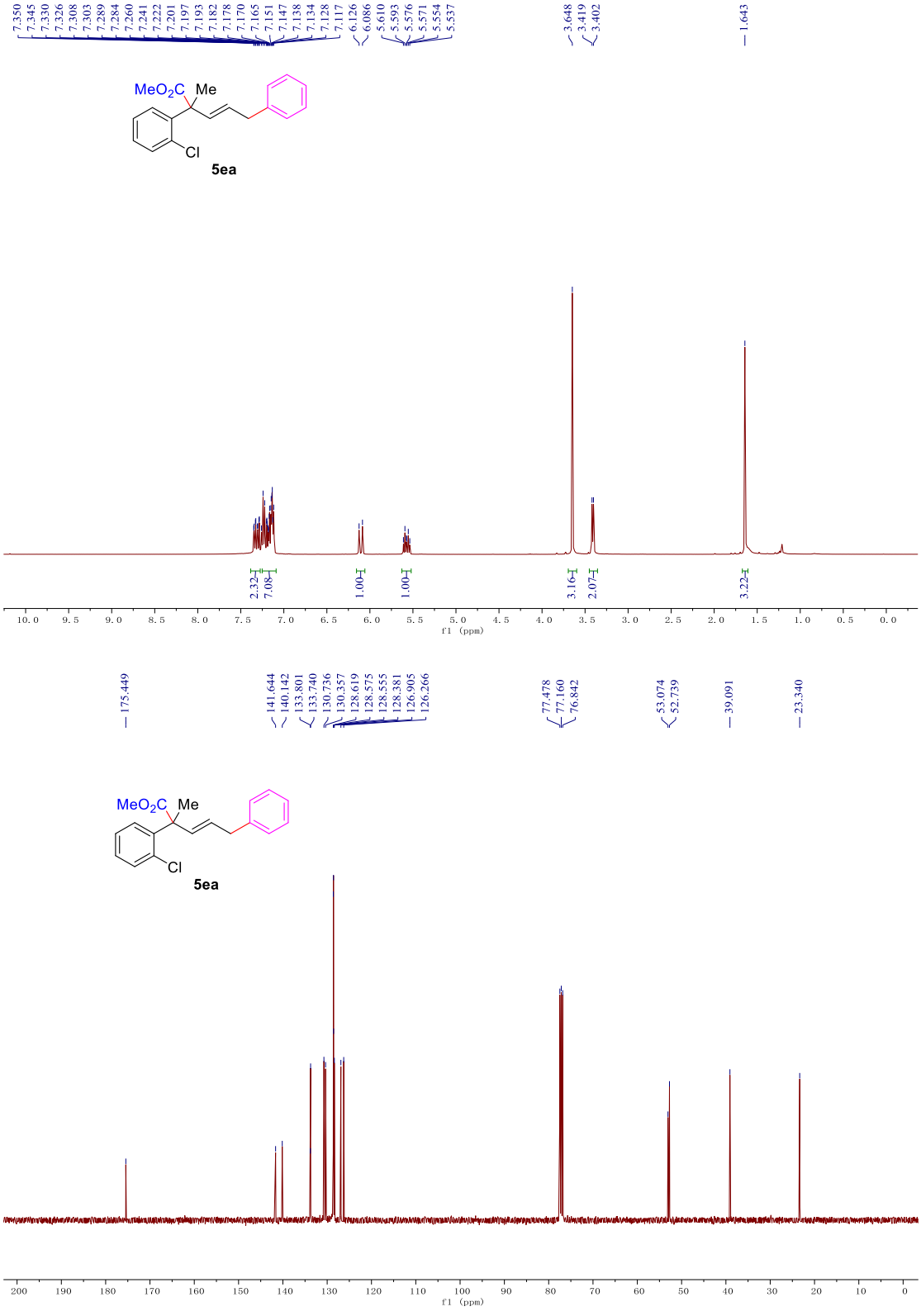
Me
CO2Me
F
6da
f1 (ppm)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7.197
7.193
7.182
7.178
7.170
7.165
7.151
7.147
7.138
7.134
7.128
7.117
6.126
6.086
5.610
5.593
5.576
5.571
5.554
5.537
3.648
3.419
3.402
1.643
MeO2C
Me
Cl
5ea
2.32
7.08
1.00
1.00
3.16
2.07
3.22
f1 (ppm)
175.449
141.644
140.142
133.801
133.740
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130.357
128.619
128.575
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128.381
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126.266
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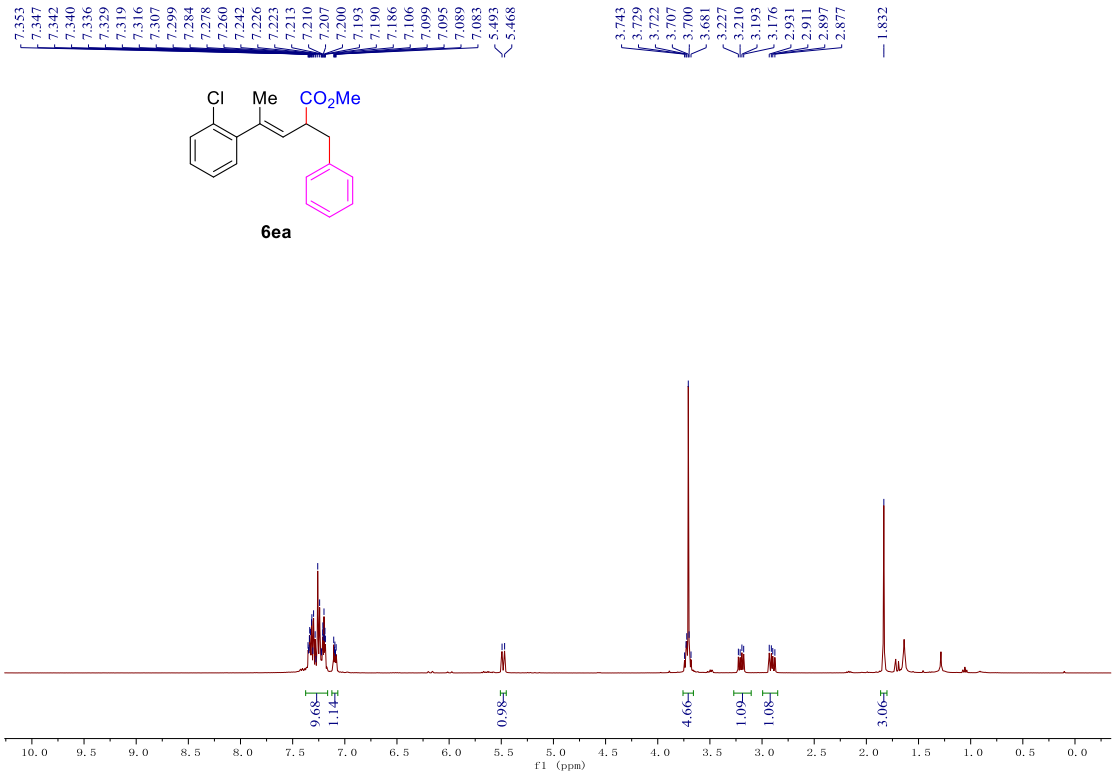
MeO2C
Me
Cl
5ea
f1 (ppm)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7.316
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7.278
7.260
7.242
7.226
7.223
7.213
7.210
7.207
7.200
7.193
7.190
7.186
7.106
7.099
7.095
7.089
7.083
5.493
5.468
3.743
3.729
3.722
3.707
3.700
3.681
3.227
3.210
3.193
3.176
2.931
2.911
2.897
2.877
1.832
Cl
Me
CO2Me
6ea
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1.14
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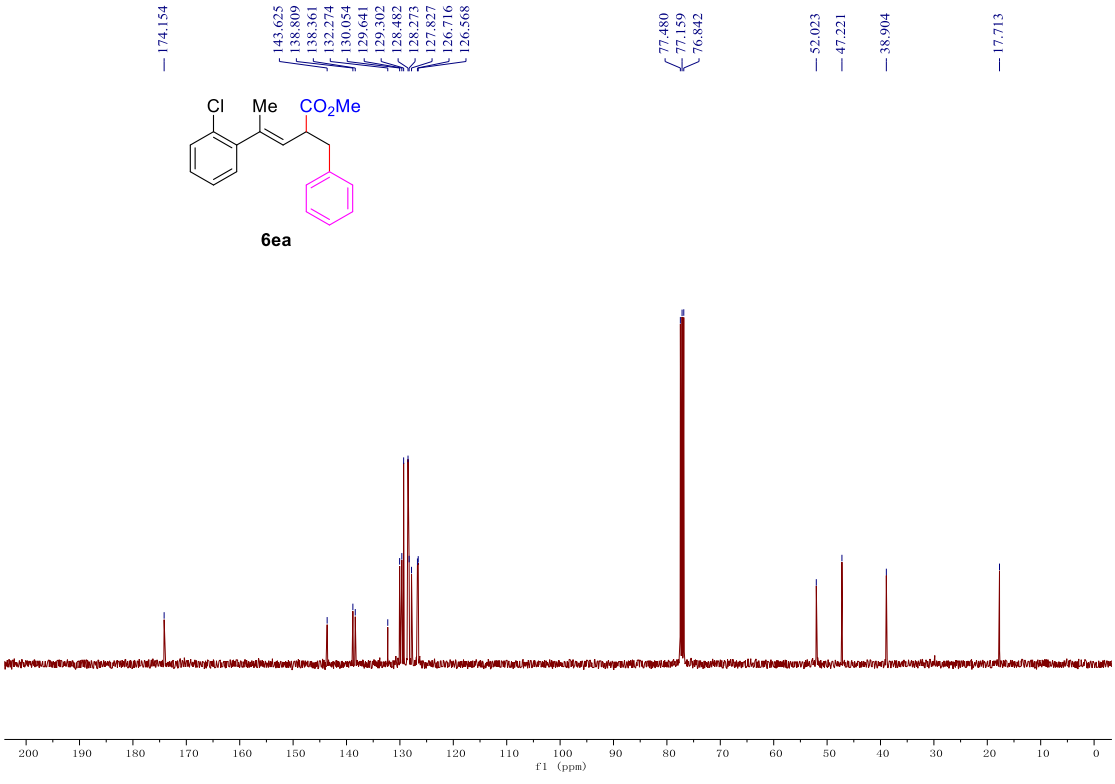
4.66
1.09
1.08
3.06
f1 (ppm)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130.054
129.641
129.302
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128.273
127.827
126.716
126.568
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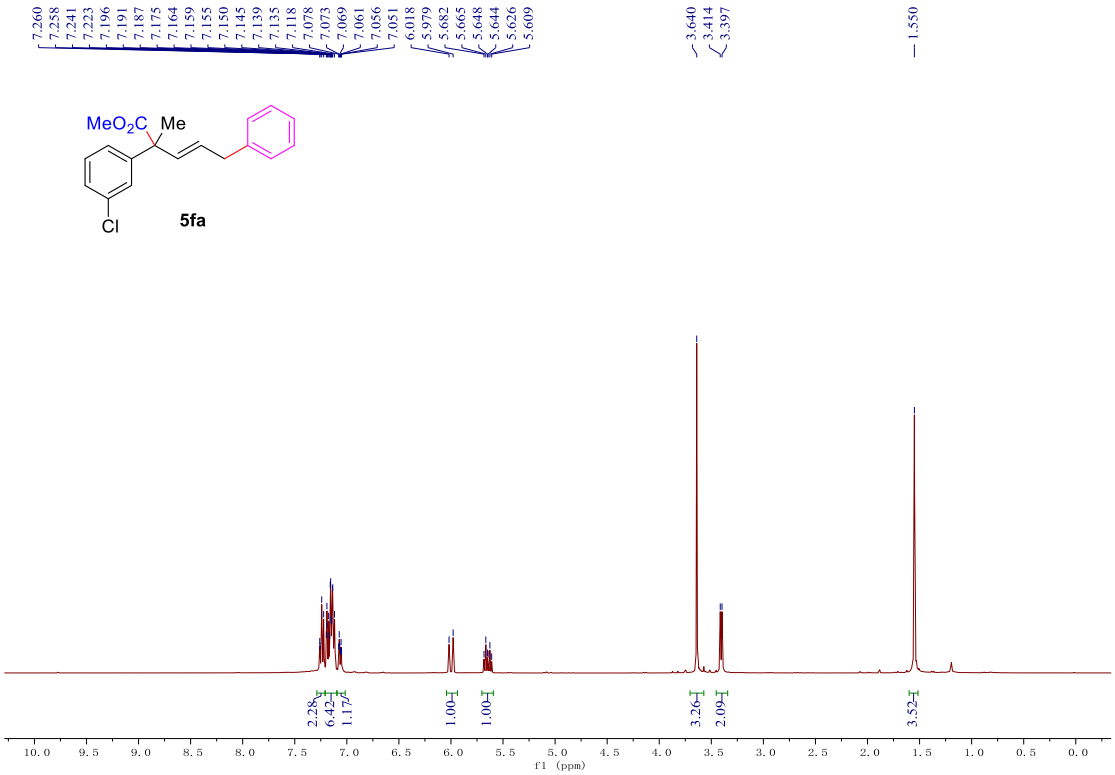
76.842
52.023
47.221
38.904
17.713
Cl
Me
CO2Me
6ea
f1 (ppm)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7.258
7.241
7.223
7.196
7.191
7.187
7.175
7.164
7.159
7.155
7.150
7.145
7.139
7.135
7.118
7.078
7.073
7.069
7.061
7.056
7.051
6.018
5.979
5.682
5.665
5.648
5.644
5.626
5.609
3.640
3.414
3.397
1.550
MeO2C
Me
Cl
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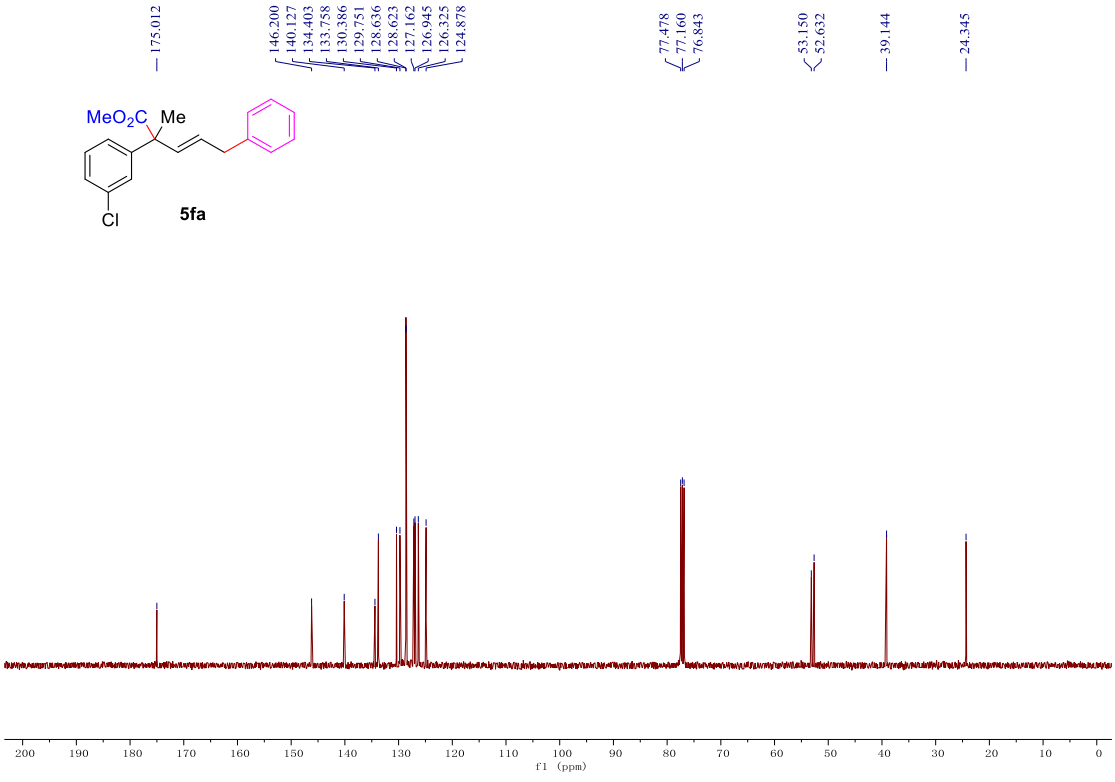
1.17
1.00
1.00
3.26
2.09
3.52
f1 (ppm)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129.751
128.636
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127.162
126.945
126.325
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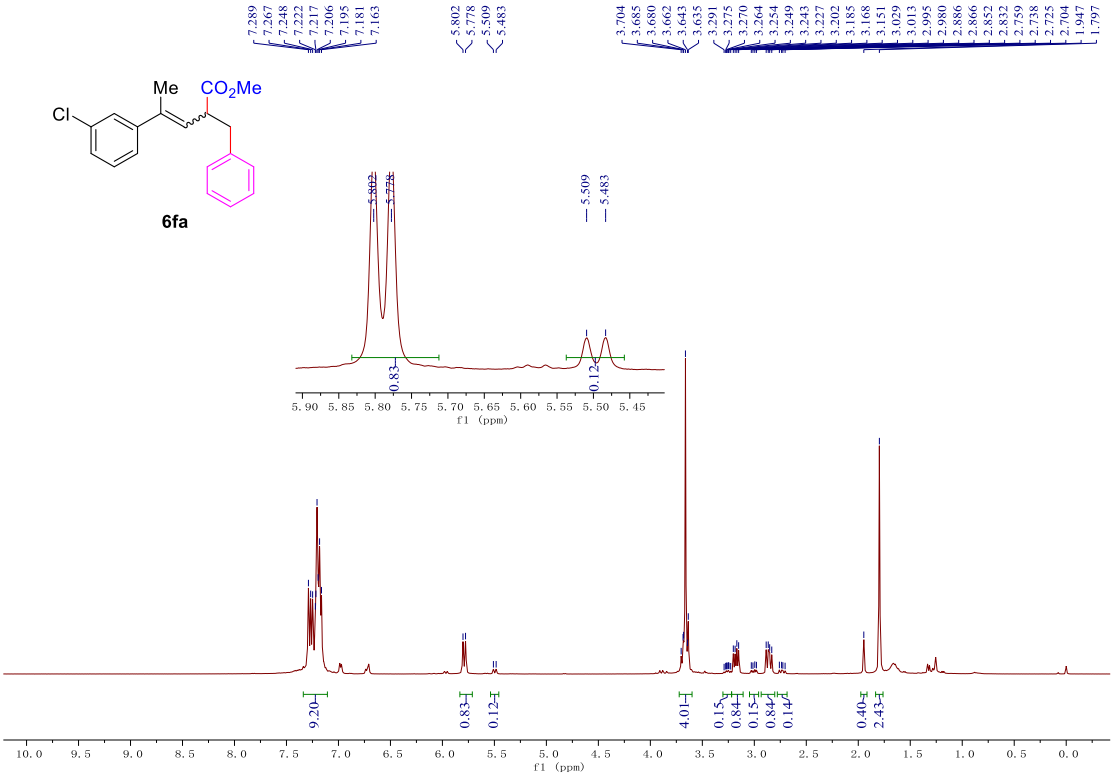
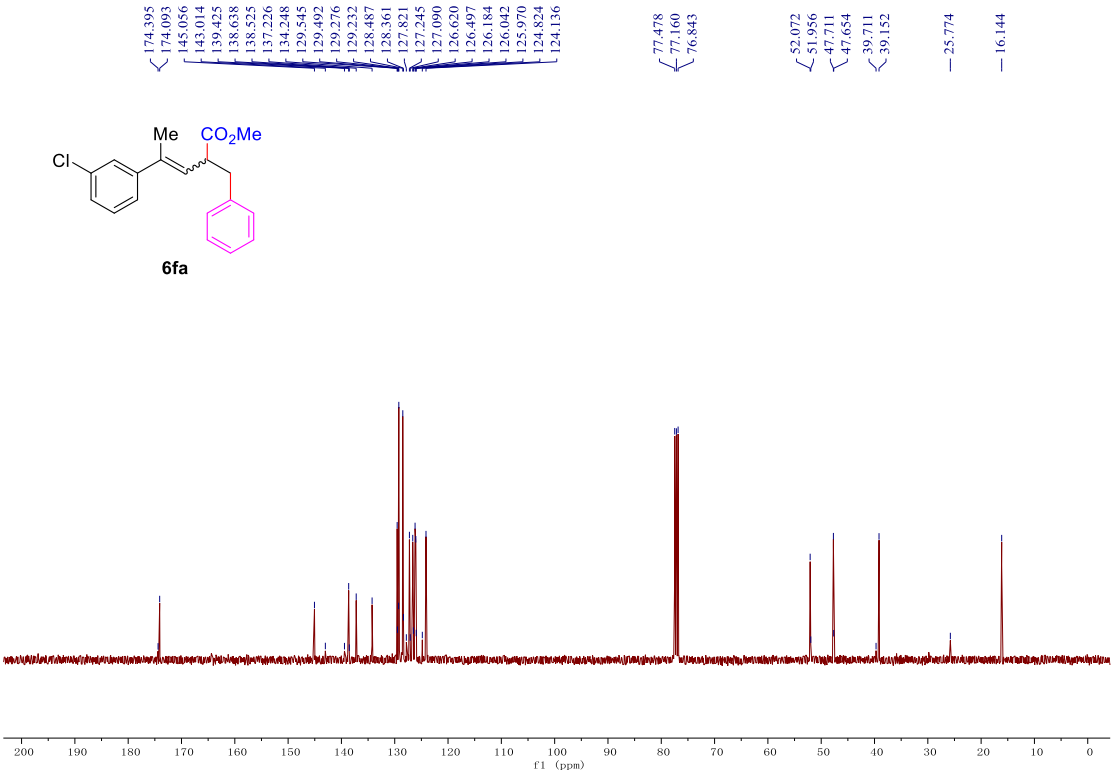
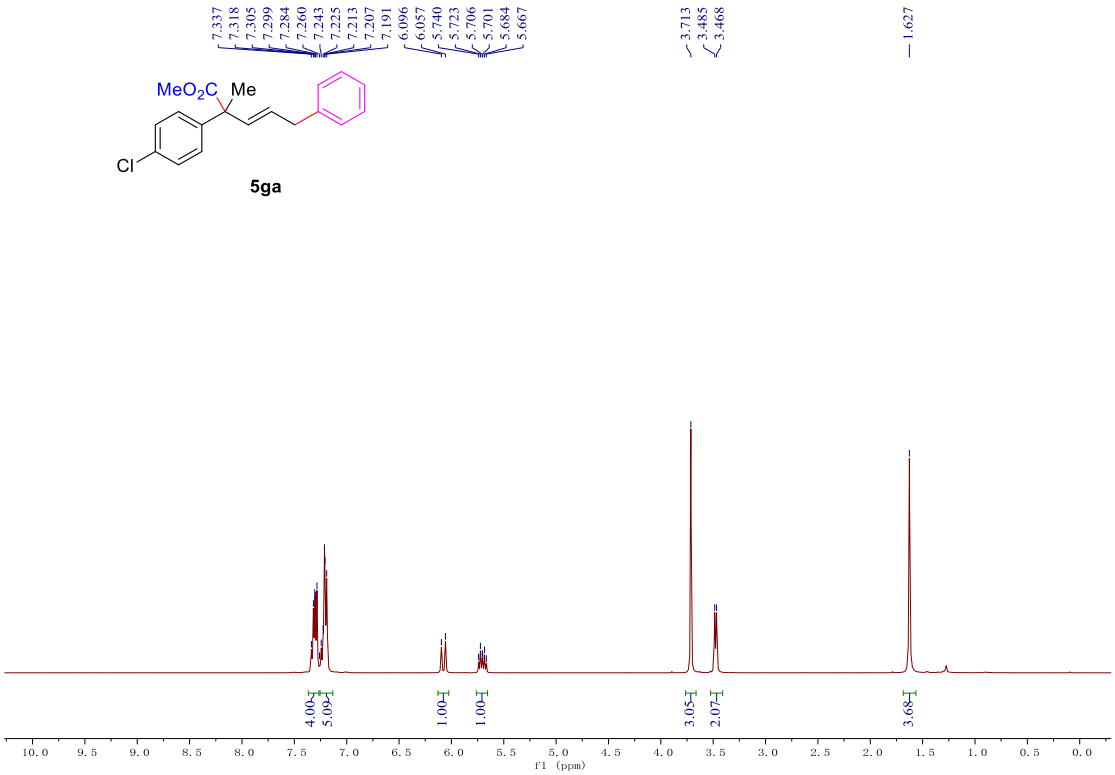
77.160
76.843
53.150
52.632
39.144
24.345
MeO2C
Me
Cl
5fa
f1 (ppm)


Me
CO2Me
Cl
6fa
f1 (ppm)


Me
CO2Me
Cl
6fa
f1 (ppm)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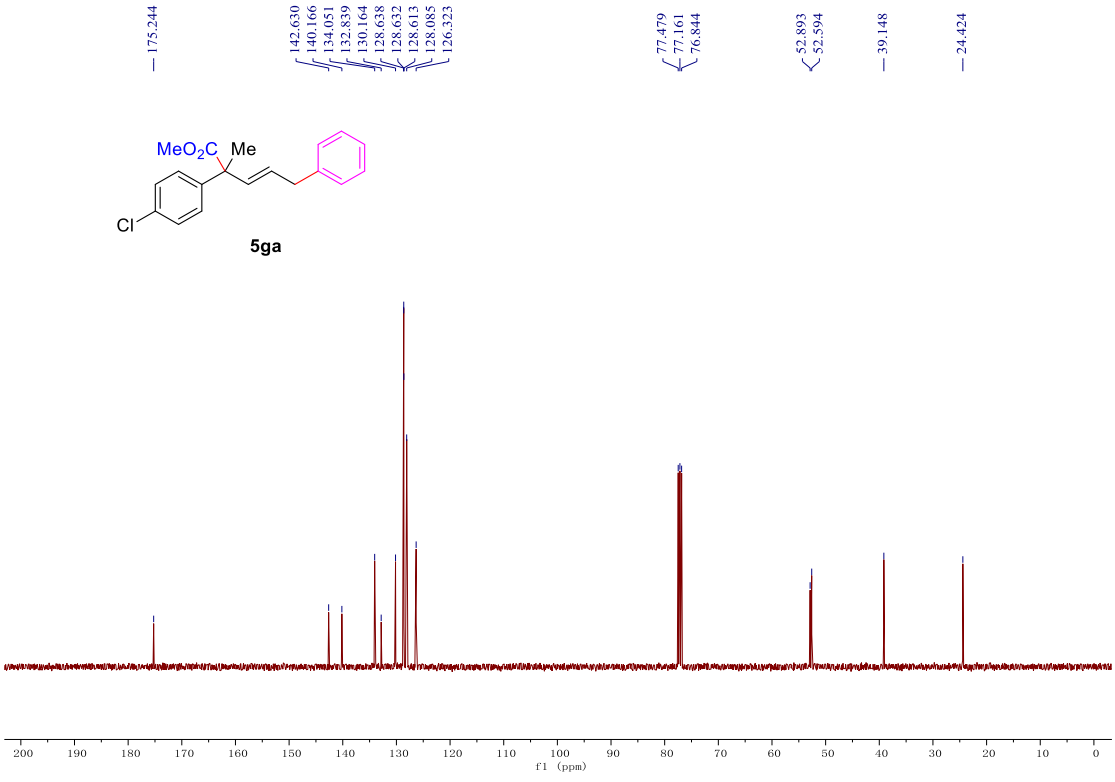
7.260
7.243
7.225
7.213
7.207
7.191
6.096
6.057
5.740
5.723
5.706
5.701
5.684
5.667
3.713
3.485
3.468
1.627
MeO2C
Me
Cl
5ga
4.00
5.09
1.00
1.00
3.05
2.07
3.68
f1 (ppm)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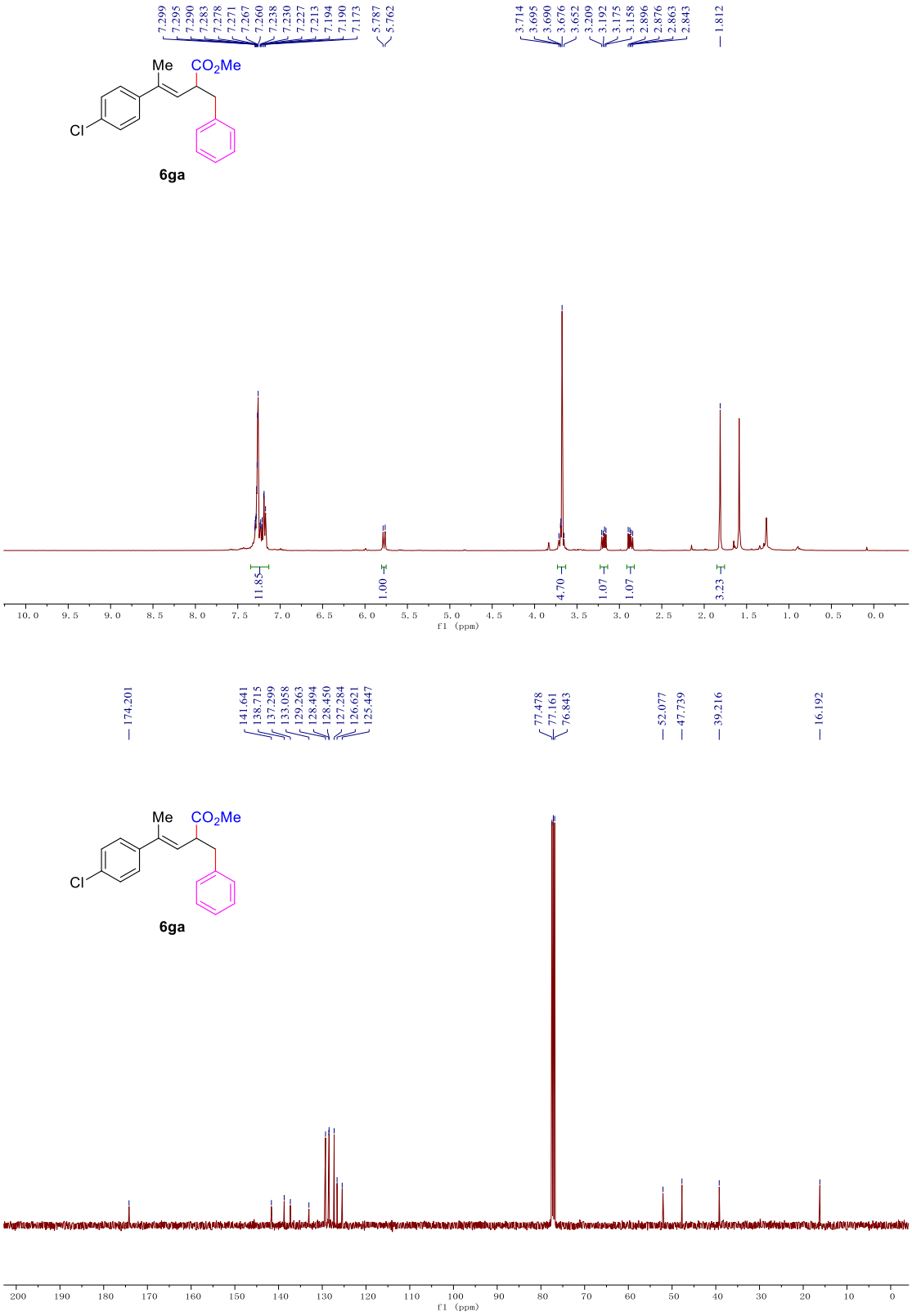
130.164
128.638
128.632
128.613
128.085
126.323
77.479
77.161
76.844
52.893
52.594
39.148
24.424
MeO2C
Me
Cl
5ga
f1 (ppm)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7.283
7.278
7.271
7.267
7.260
7.238
7.230
7.227
7.213
7.194
7.190
7.173
5.787
5.762
3.714
3.695
3.690
3.676
3.652
3.209
3.192
3.175
3.158
2.896
2.876
2.863
2.843
1.812
Me
CO2Me
Cl
6ga
11.85
1.00
4.70
1.07
1.07
3.23
f1 (ppm)
174.201
141.641
138.715
137.299
133.058
129.263
128.494
128.450
127.284
126.621
125.447
77.478
77.161
76.843
52.077
47.739
39.216
16.192
Me
CO2Me
Cl
6ga
f1 (ppm)


7.401
7.396
7.382
7.377
7.329
7.325
7.312
7.308
7.304
7.291
7.285
7.261
7.254
7.247
7.237
7.233
7.229
7.225
7.218
7.211
7.204
7.200
7.183
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6.054
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5.715
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5.676
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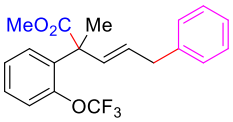
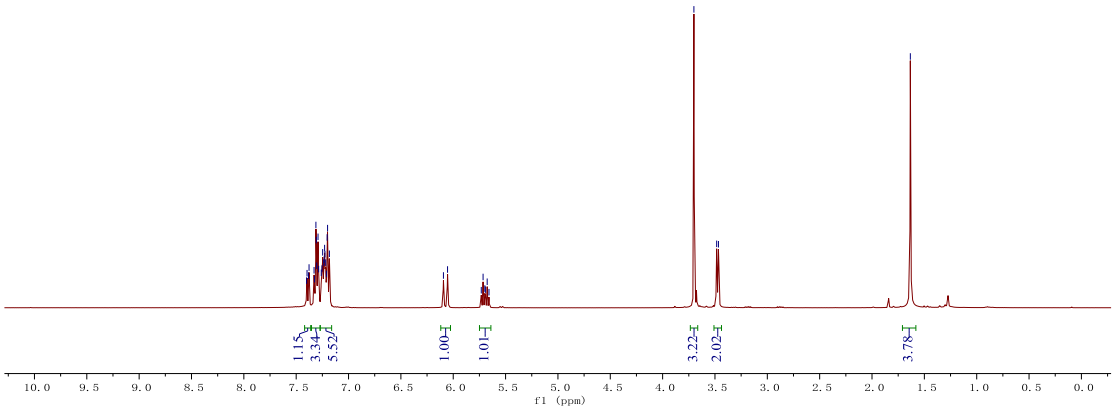
3.467
1.634


MeO2C
Me
OCF3

5ha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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)


175.049
147.383
140.107
135.278
133.362
130.660
128.630
128.613
128.551
126.311
125.907
124.411
121.835
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117.648
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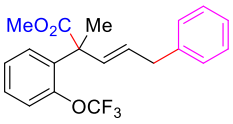
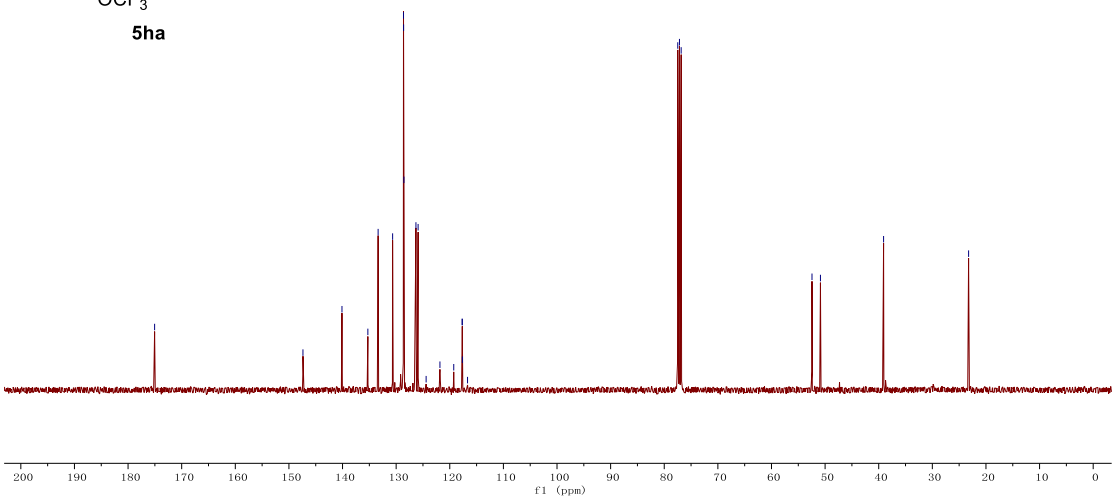
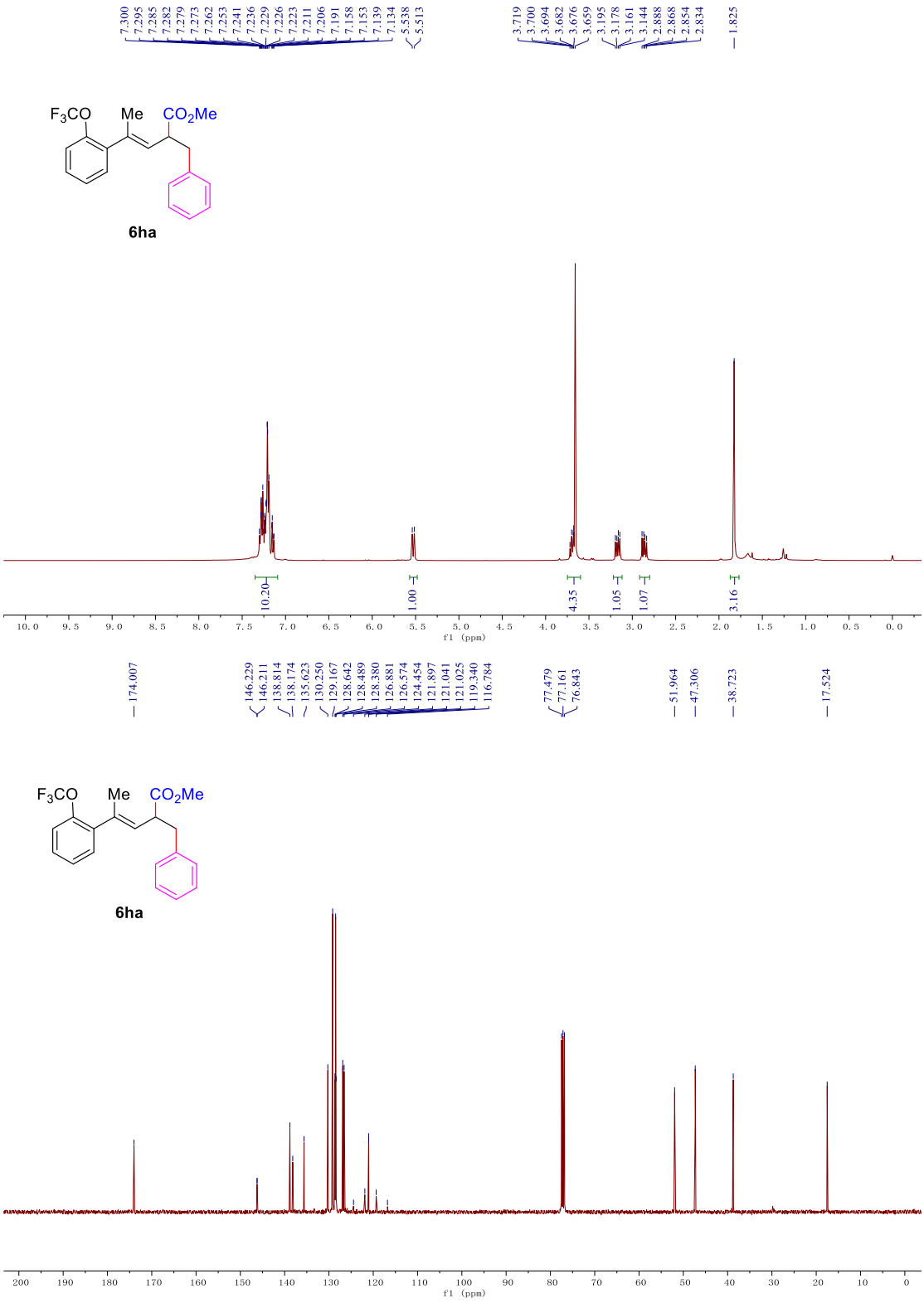
23.238


MeO2C
Me
OCF3

5ha


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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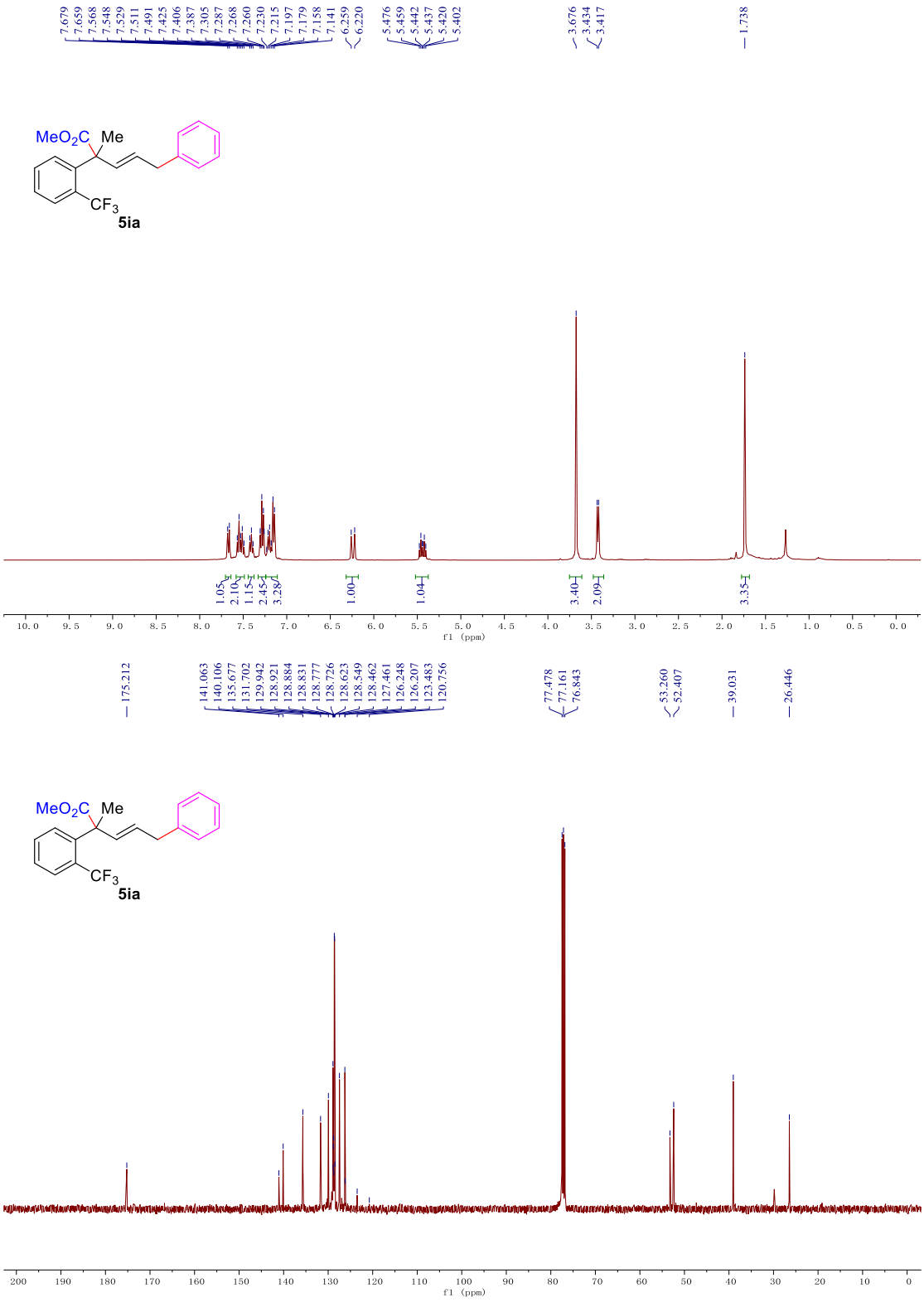
7.273
7.262
7.253
7.241
7.236
7.229
7.226
7.223
7.211
7.206
7.191
7.158
7.153
7.139
7.134
5.538
5.513
3.719
3.700
3.694
3.682
3.676
3.659
3.195
3.178
3.161
3.144
2.888
2.868
2.854
2.834
1.825
F3CO
Me
CO2Me
6ha
10.20
1.00
4.35
1.05
1.07
3.16
f1 (ppm)
174.007
146.229
146.211
138.814
138.174
135.623
130.250
129.167
128.642
128.489
128.380
126.881
126.574
124.454
121.897
121.041
121.025
119.340
116.784
77.479
77.161
76.843
51.964
47.306
38.723
17.524
F3CO
Me
CO2Me
6ha
f1 (ppm)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7.260
7.230
7.215
7.197
7.179
7.158
7.141
6.259
6.220
5.476
5.459
5.442
5.437
5.420
5.402
3.676
3.434
3.417
1.738
MeO2C
Me
CF3
5ia
1.05
2.10
1.15
2.45
3.28
1.00
1.04
3.40
2.09
3.35
f1 (ppm)
175.212
141.063
140.106
135.677
131.702
129.942
128.921
128.884
128.831
128.777
128.726
128.623
128.549
128.462
127.461
126.248
126.207
123.483
120.756
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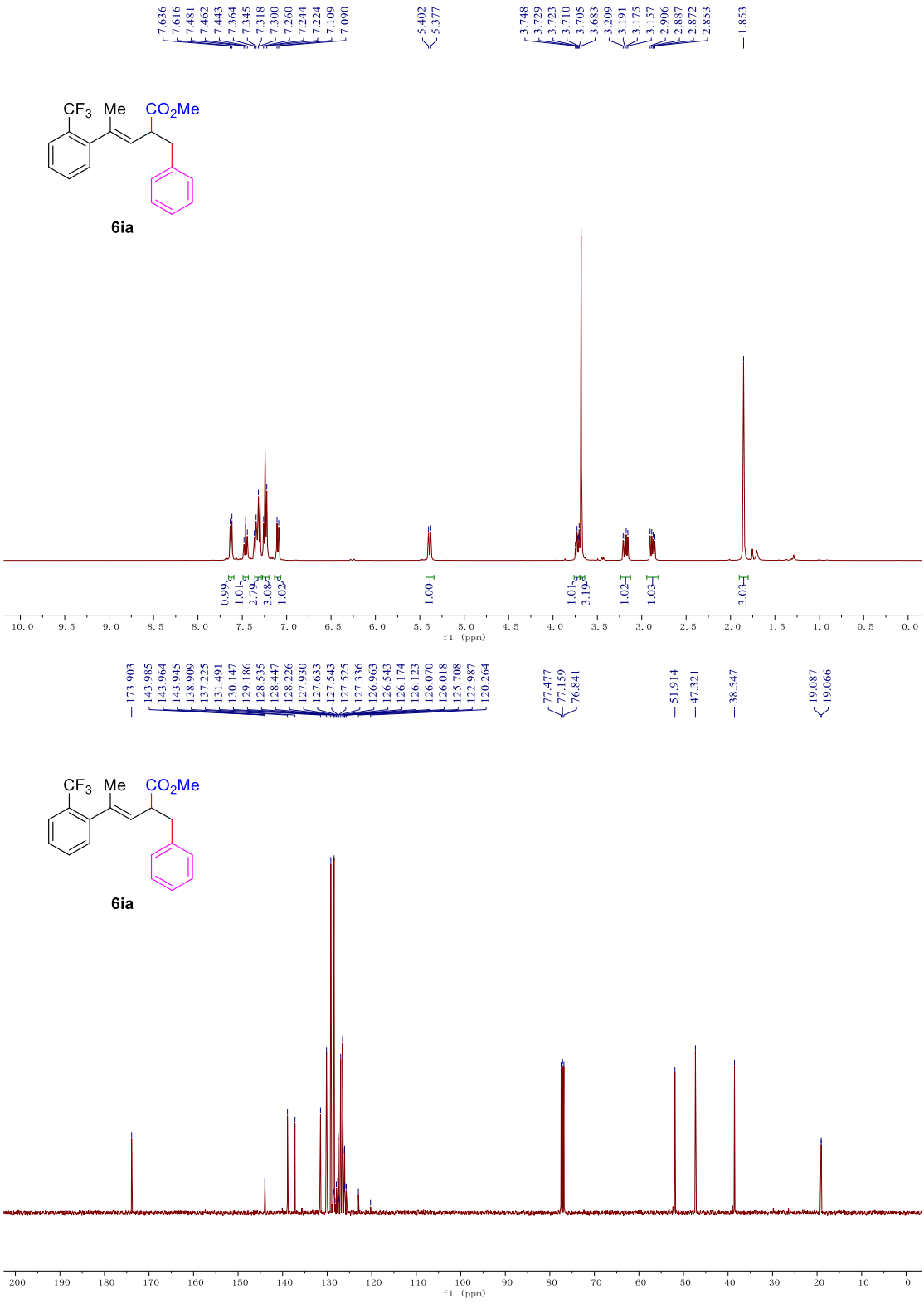
MeO2C
Me
CF3
5ia
f1 (ppm)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7.318
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7.260
7.244
7.224
7.109
7.090
5.402
5.377
3.748
3.729
3.723
3.710
3.705
3.683
3.209
3.191
3.175
3.157
2.906
2.887
2.872
2.853
1.853
CF3 Me CO2Me
6ia
0.99
1.01
2.79
3.08
1.02
1.00
1.01
3.19
1.02
1.03
3.03
f1 (ppm)
173.903
143.985
143.964
143.945
138.909
137.225
131.491
130.147
129.186
128.535
128.447
128.226
127.930
127.633
127.543
127.525
127.336
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126.543
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126.123
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126.018
125.708
122.987
120.264
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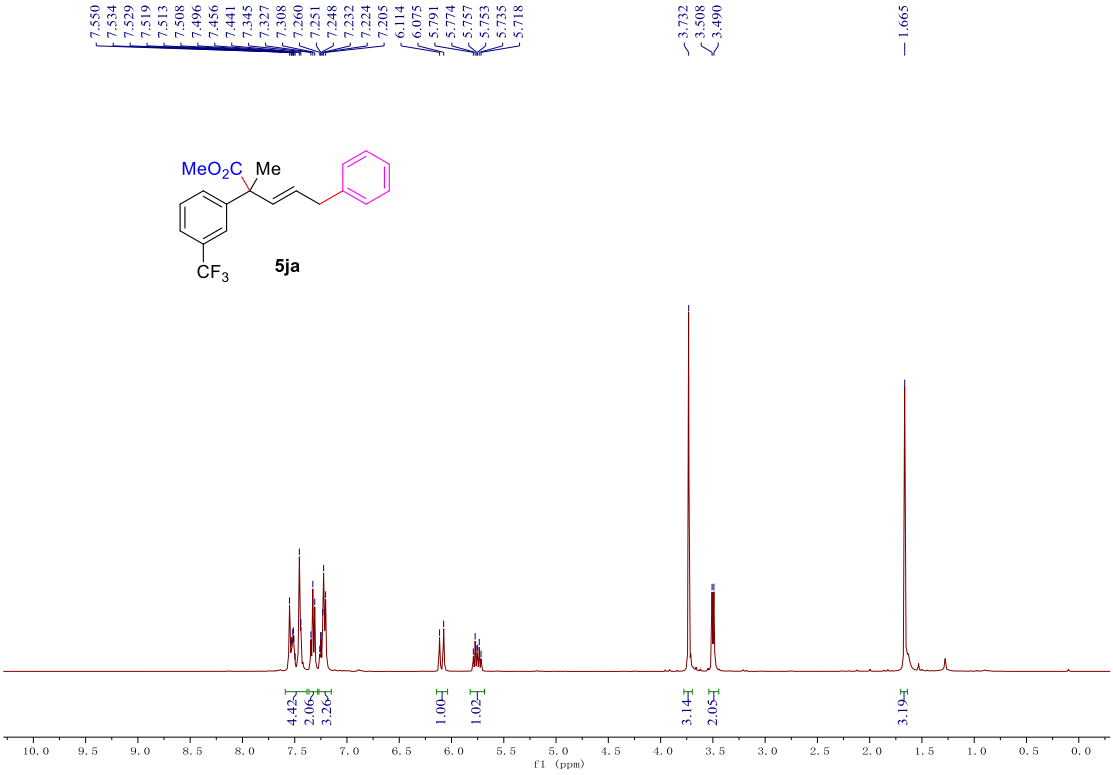
51.914
47.321
38.547
19.087
19.066
CF3 Me CO2Me
6ia
f1 (ppm)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7.251
7.248
7.232
7.224
7.205
6.114
6.075
5.791
5.774
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5.718
3.732
3.508
3.490
1.665
MeO2C
Me
CF3
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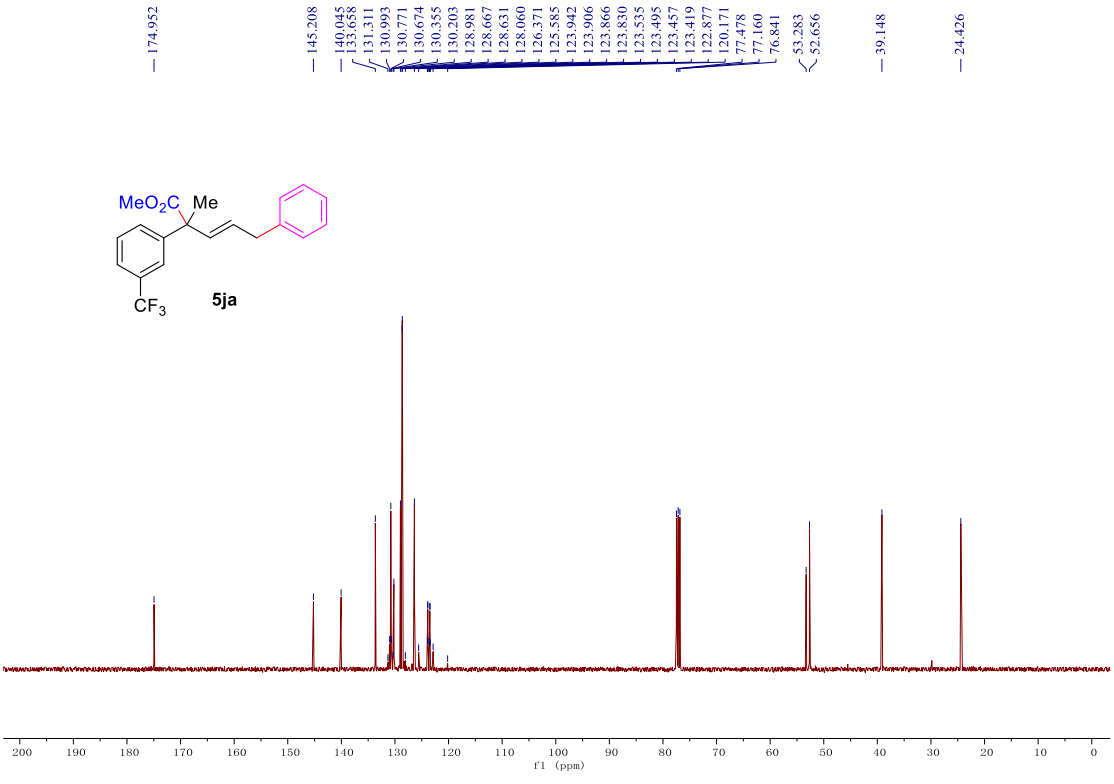
2.06
3.26
1.00
1.02
3.14
2.05
3.19
f1 (ppm)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128.060
126.371
125.585
123.942
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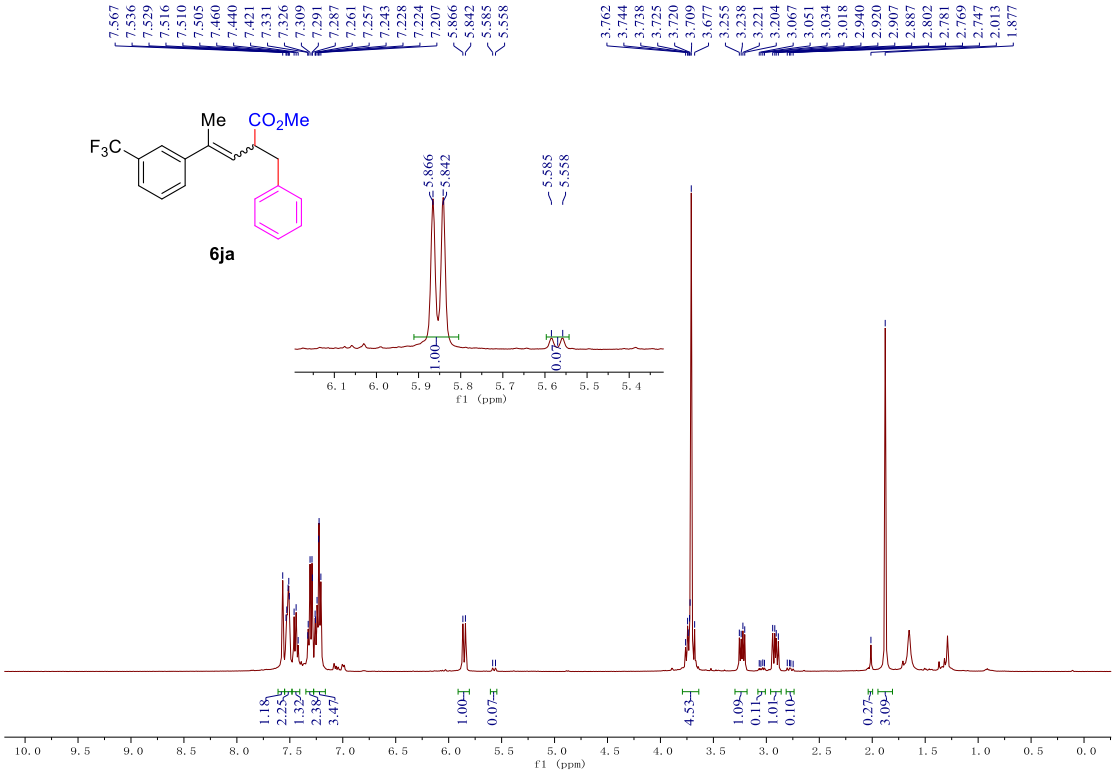
123.866
123.830
123.535
123.495
123.457
123.419
122.877
120.171
77.478
77.160
76.841
53.283
52.656
39.148
24.426
MeO2C
Me
CF3
5ja
f1 (ppm)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7.505
7.460
7.440
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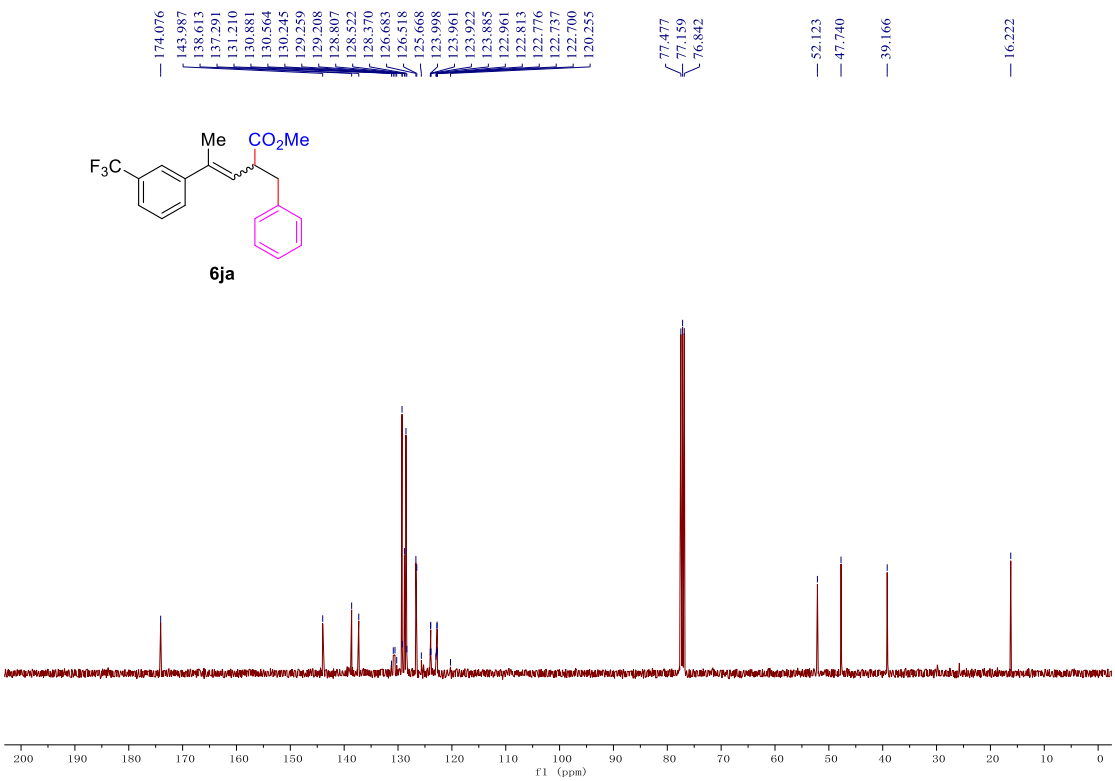
7.331
7.326
7.309
7.291
7.287
7.261
7.257
7.243
7.228
7.224
7.207
5.866
5.842
5.585
5.558
3.762
3.744
3.738
3.725
3.720
3.709
3.677
3.255
3.238
3.221
3.204
3.067
3.051
3.034
3.018
2.940
2.920
2.907
2.887
2.802
2.781
2.769
2.747
2.013
1.877
Me
CO2Me
F3C
6ja
1.18
2.25
1.32
2.38
3.47
1.00
0.07
4.53
1.09
0.11
1.01
0.10
0.27
3.09
f1 (ppm)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138.613
137.291
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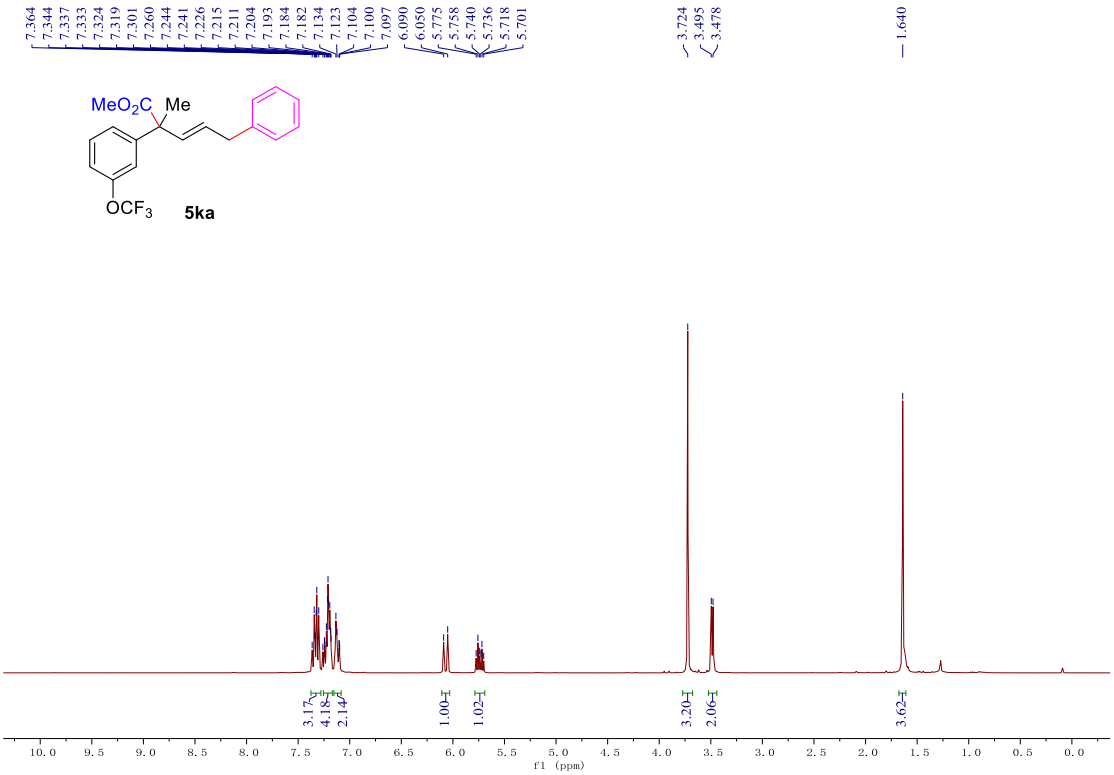
130.564
130.245
129.259
129.208
128.807
128.522
128.370
126.683
126.518
125.668
123.998
123.961
123.922
123.885
122.961
122.813
122.776
122.737
122.700
120.255
77.477
77.159
76.842
52.123
47.740
39.166
16.222
Me
CO2Me
F3C
6ja
f1 (ppm)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7.319
7.301
7.260
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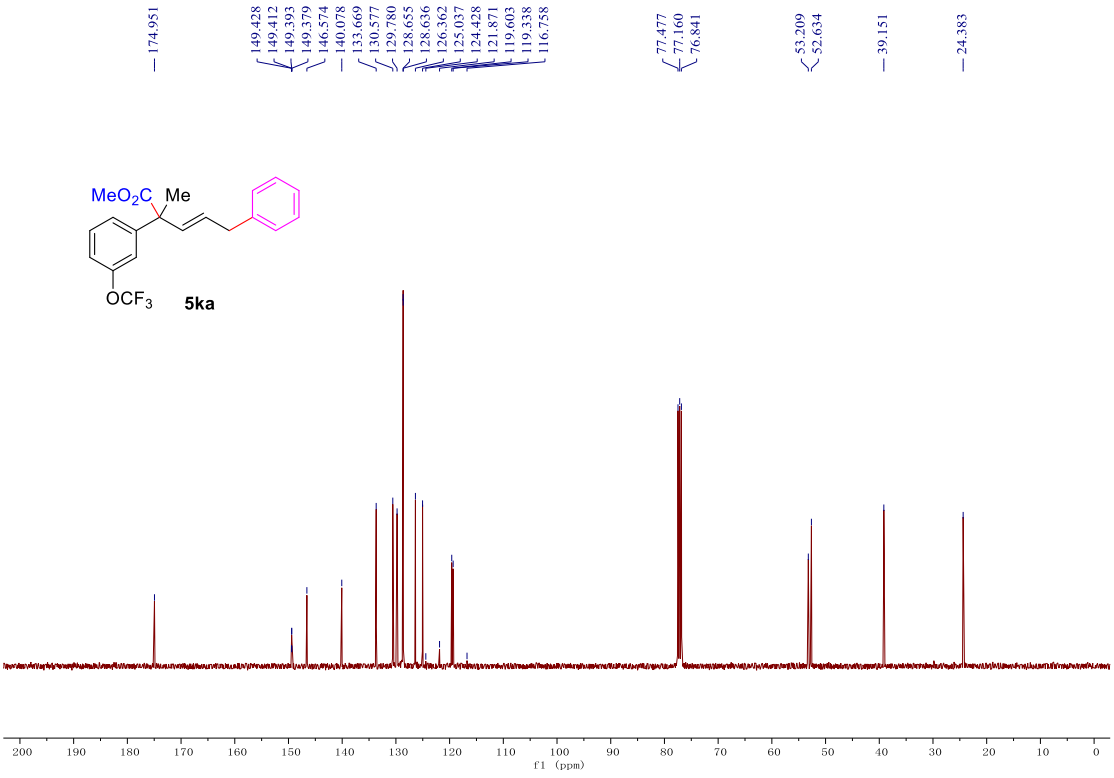
7.241
7.226
7.215
7.211
7.204
7.193
7.184
7.182
7.134
7.123
7.104
7.100
7.097
6.090
6.050
5.775
5.758
5.740
5.736
5.718
5.701
3.724
3.495
3.478
1.640
MeO2C
Me
OCF3
5ka
3.17
4.18
2.14
1.00
1.02
3.20
2.06
3.62
f1 (ppm)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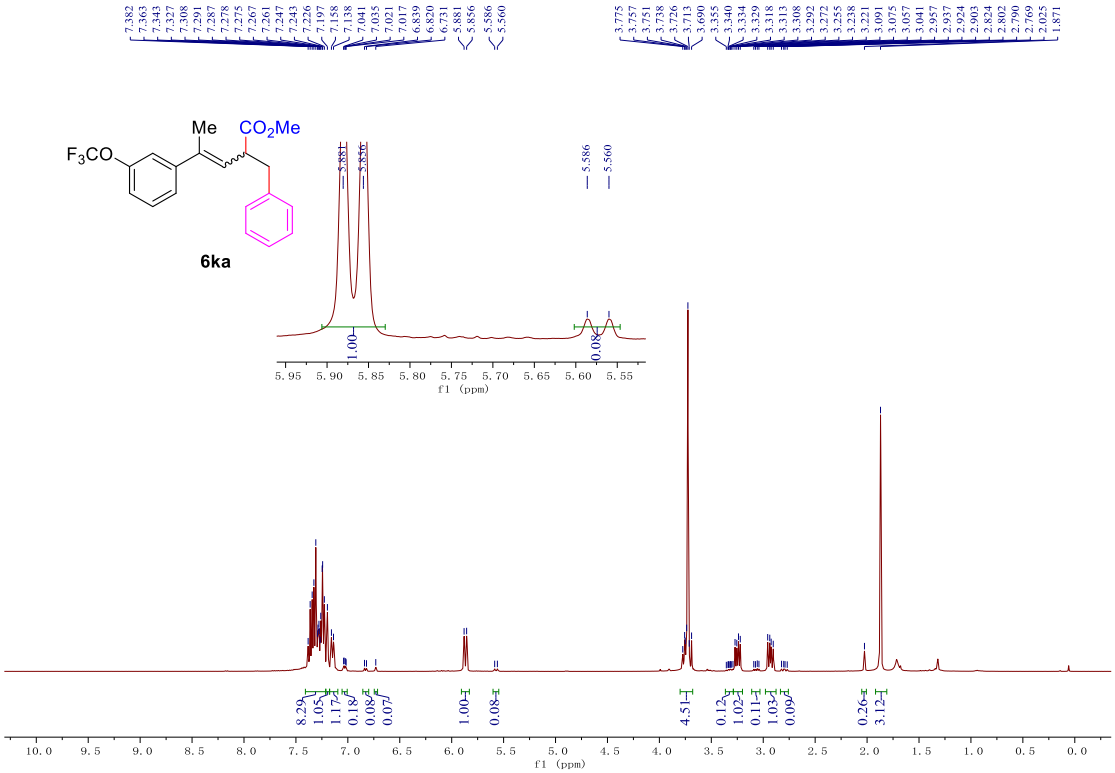
149.412
149.393
149.379
146.574
140.078
133.669
130.577
129.780
128.655
128.636
126.362
125.037
124.428
121.871
119.603
119.338
116.758
77.477
77.160
76.841
53.209
52.634
39.151
24.383
MeO2C
Me
OCF3
5ka
f1 (ppm)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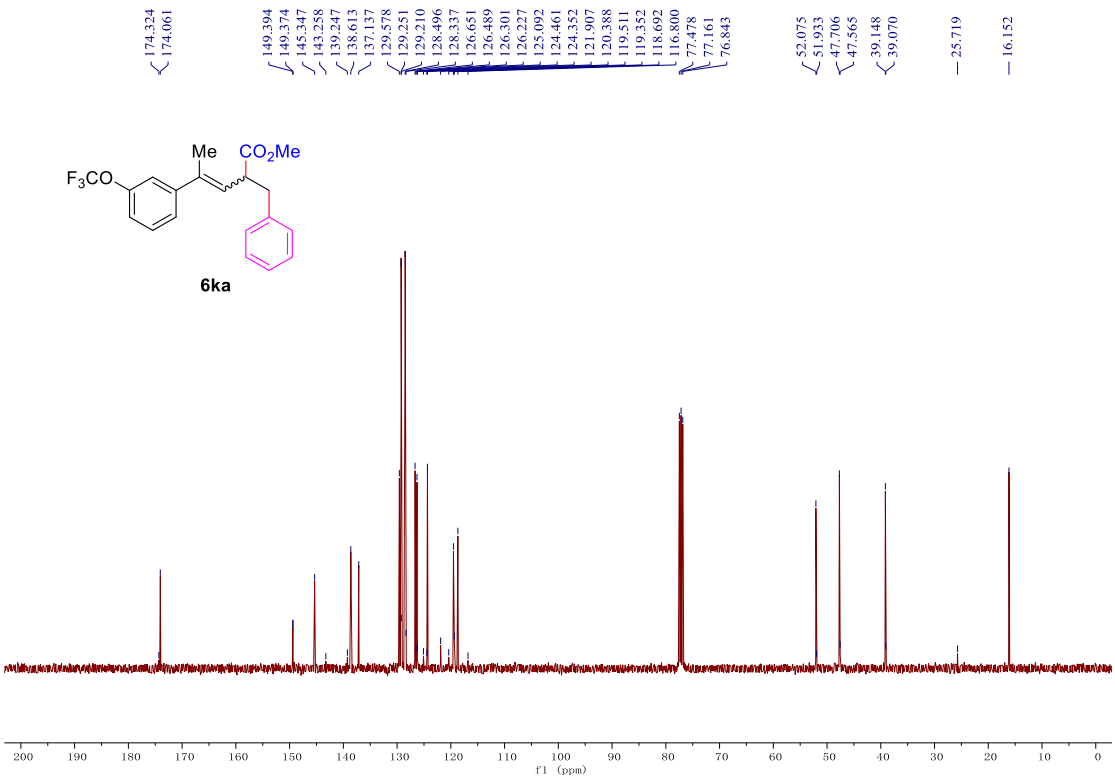
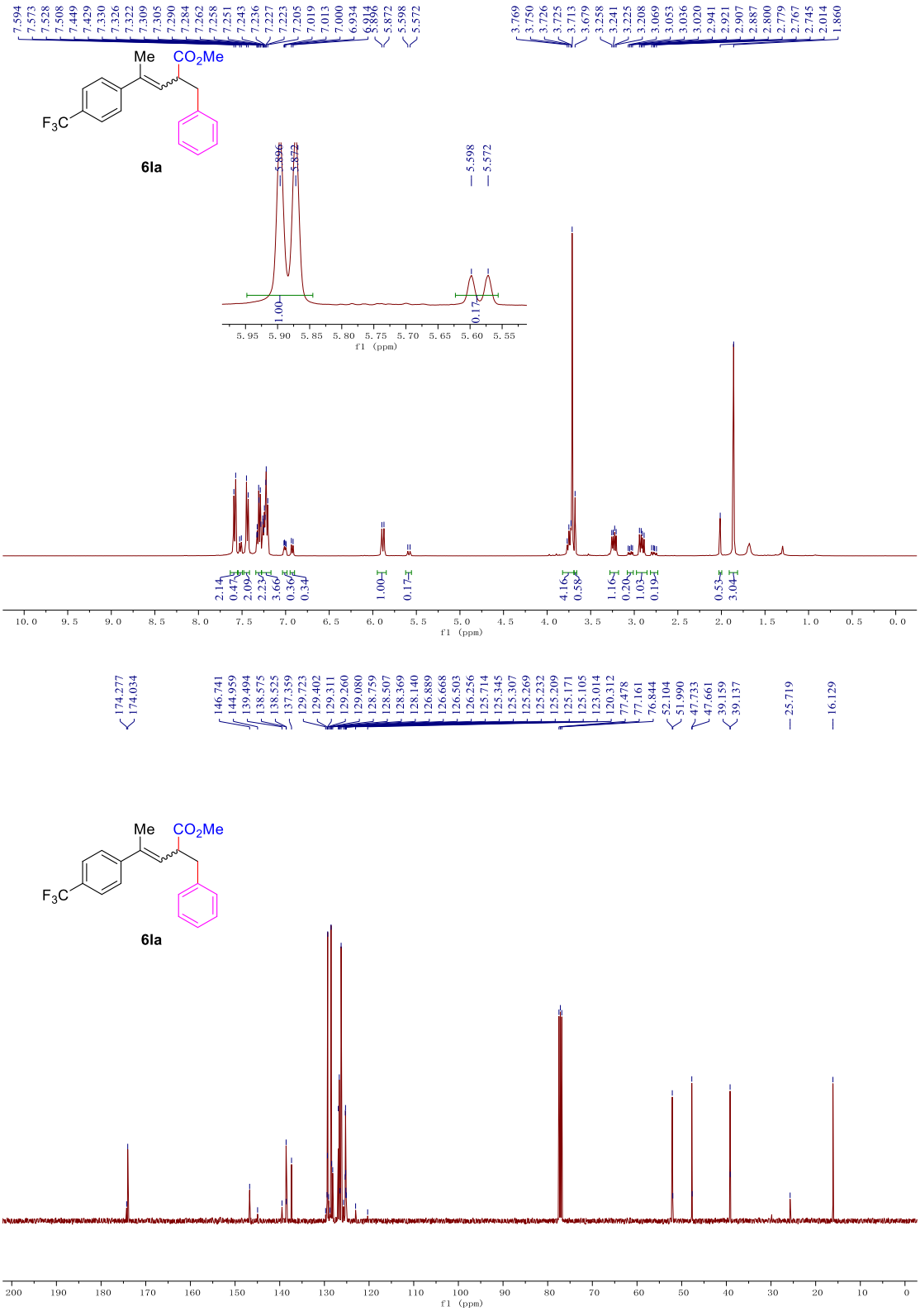
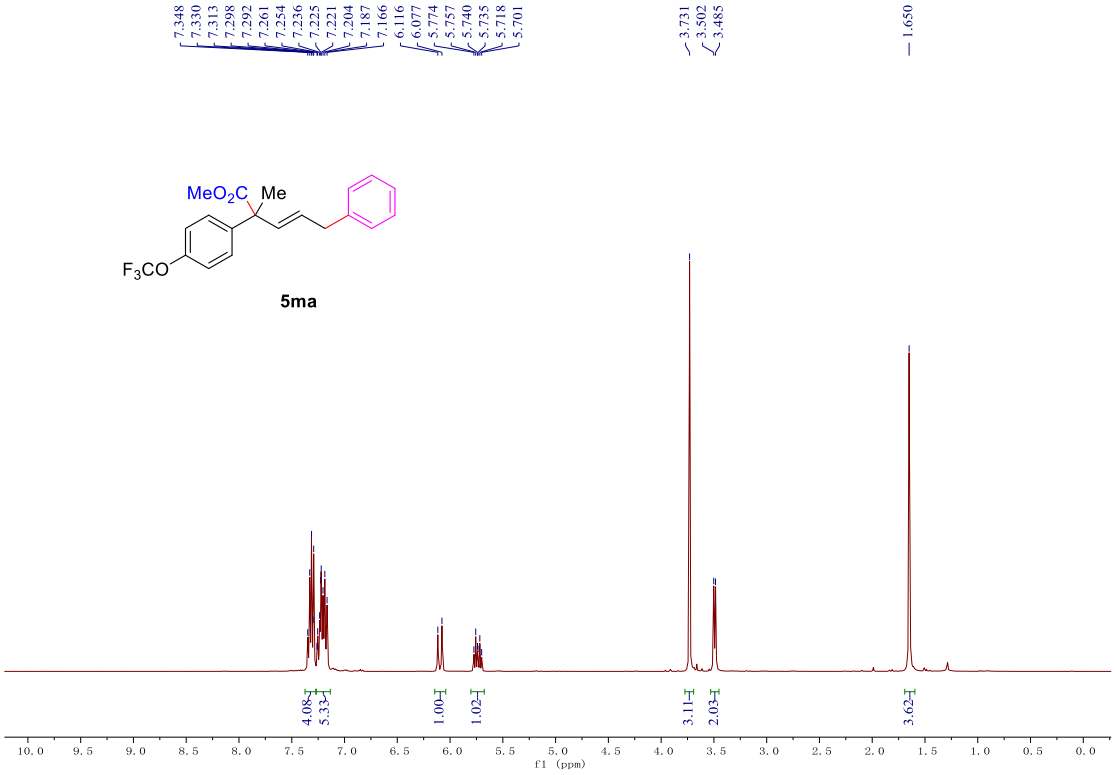
CO2Me
F3CO
6ka
f1 (ppm)


Me
CO2Me
F3CO
6ka
f1 (ppm)


Me
CO2Me
F3C
6la
f1 (ppm)
Me
CO2Me
F3C
6la
f1 (ppm)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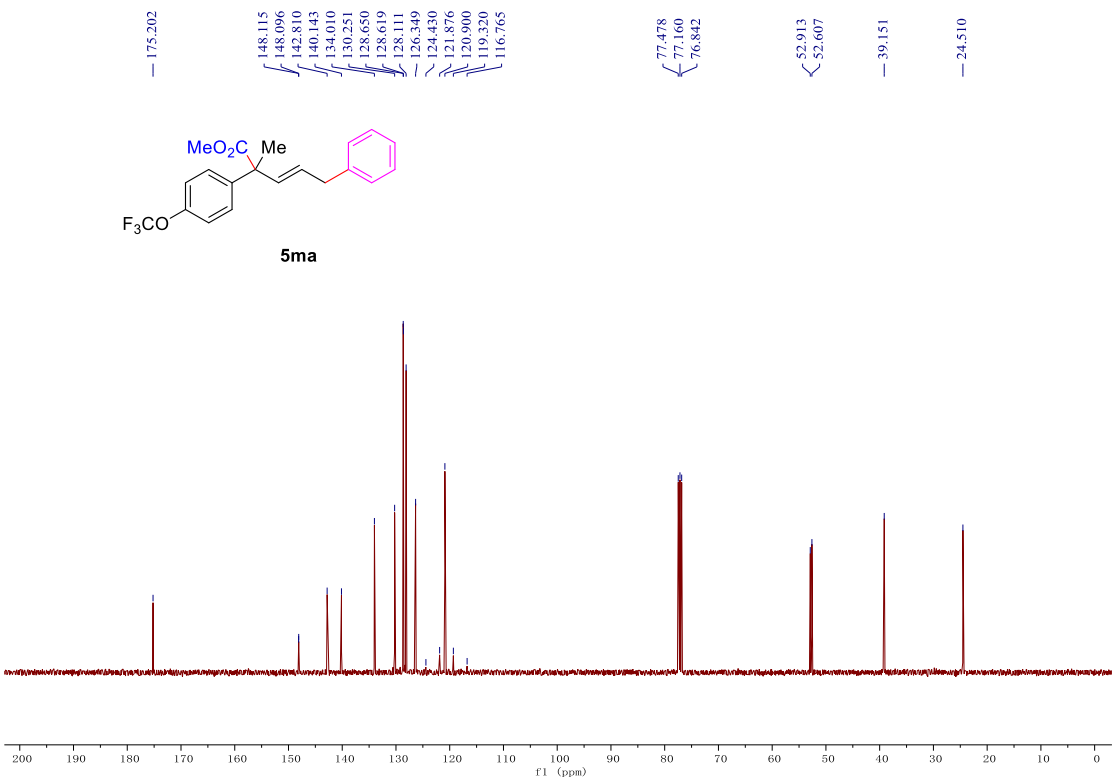
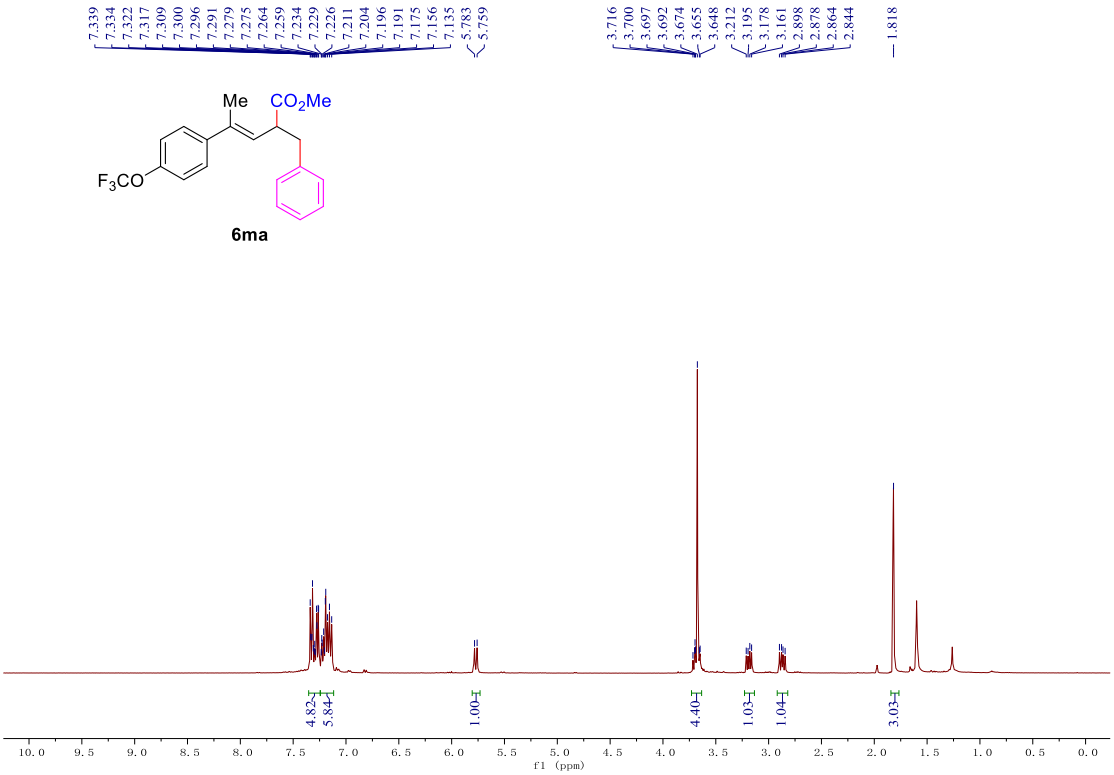
7.313
7.298
7.292
7.261
7.254
7.236
7.225
7.221
7.204
7.187
7.166
6.116
6.077
5.774
5.757
5.740
5.735
5.718
5.701
3.731
3.502
3.485
1.650
MeO2C Me
F3CO
5ma
4.08
5.33
1.00
1.02
3.11
2.03
3.62
f1 (ppm)


175.202
148.115
148.096
142.810
140.143
134.010
130.251
128.650
128.619
128.111
126.349
124.430
121.876
120.900
119.320
116.765
77.478
77.160
76.842
52.913
52.607
39.151
24.510
MeO2C Me
F3CO
5ma
f1 (ppm)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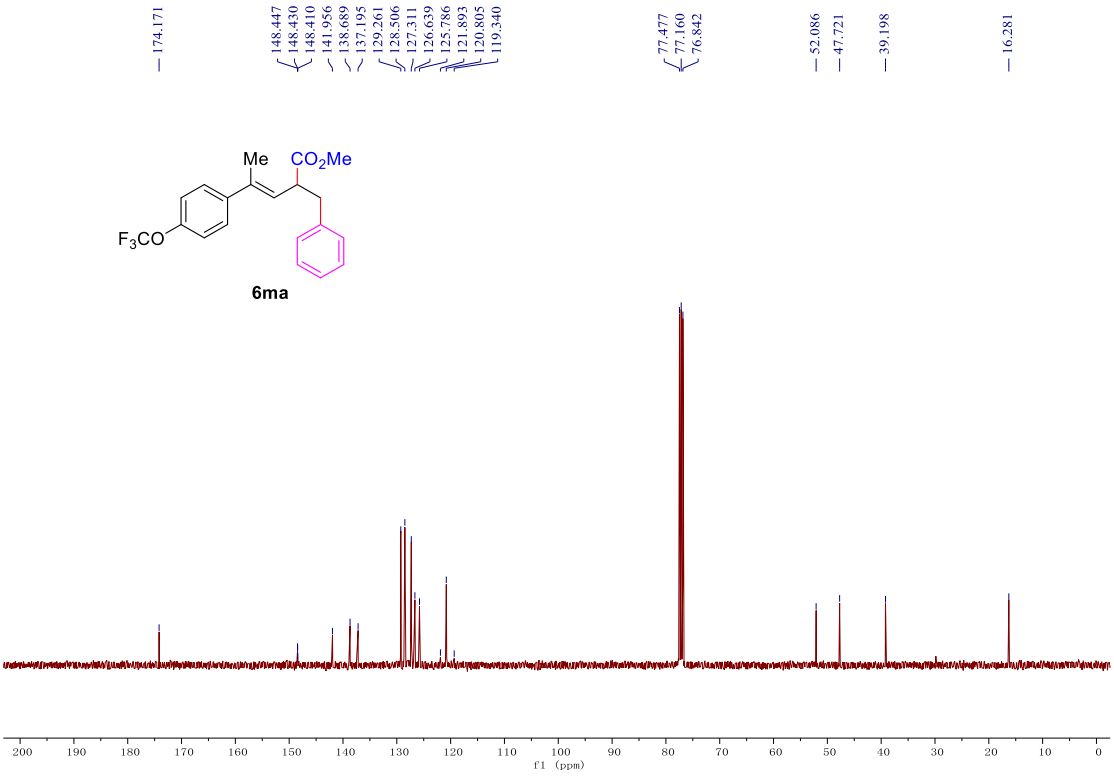
7.334
7.322
7.317
7.309
7.300
7.296
7.291
7.279
7.275
7.264
7.259
7.234
7.229
7.226
7.211
7.204
7.196
7.191
7.175
7.156
7.135
5.783
5.759
3.716
3.700
3.697
3.692
3.674
3.655
3.648
3.212
3.195
3.178
3.161
2.898
2.878
2.864
2.844
1.818
Me
CO2Me
F3CO
6ma
4.82
5.84
1.00
4.40
1.03
1.04
3.03
f1 (ppm)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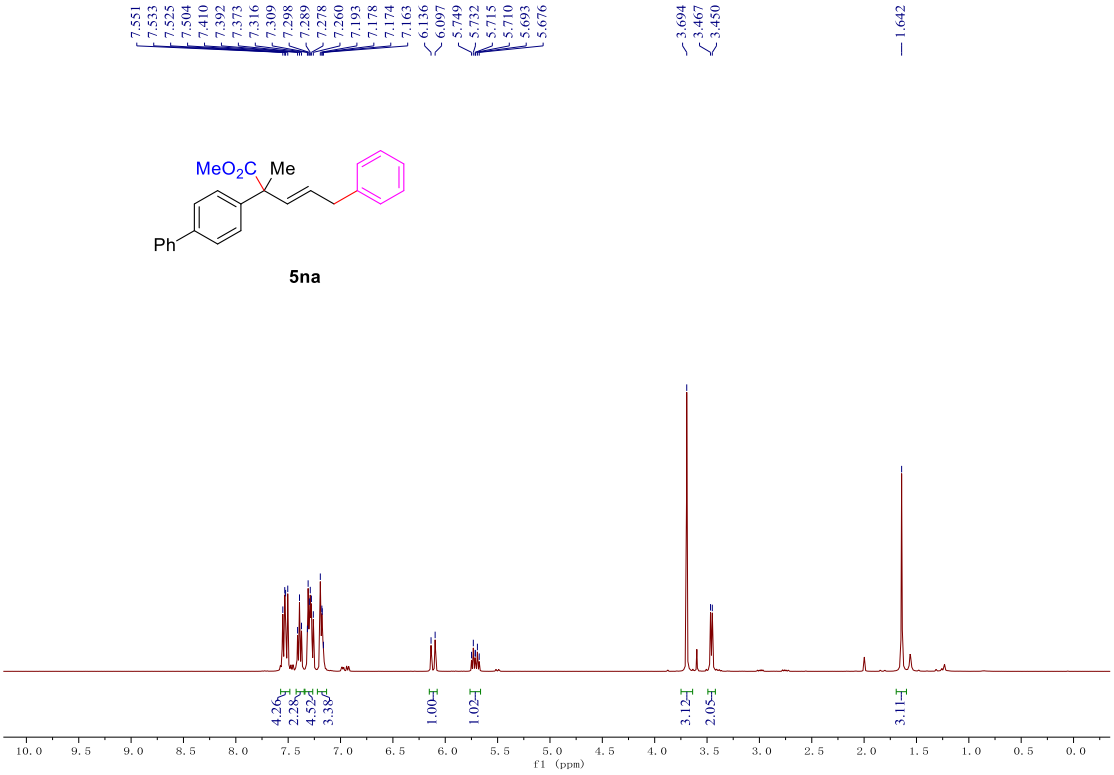
148.430
148.410
141.956
138.689
137.195
129.261
128.506
127.311
126.639
125.786
121.893
120.805
119.340
77.477
77.160
76.842
52.086
47.721
39.198
16.281
Me
CO2Me
F3CO
6ma
f1 (ppm)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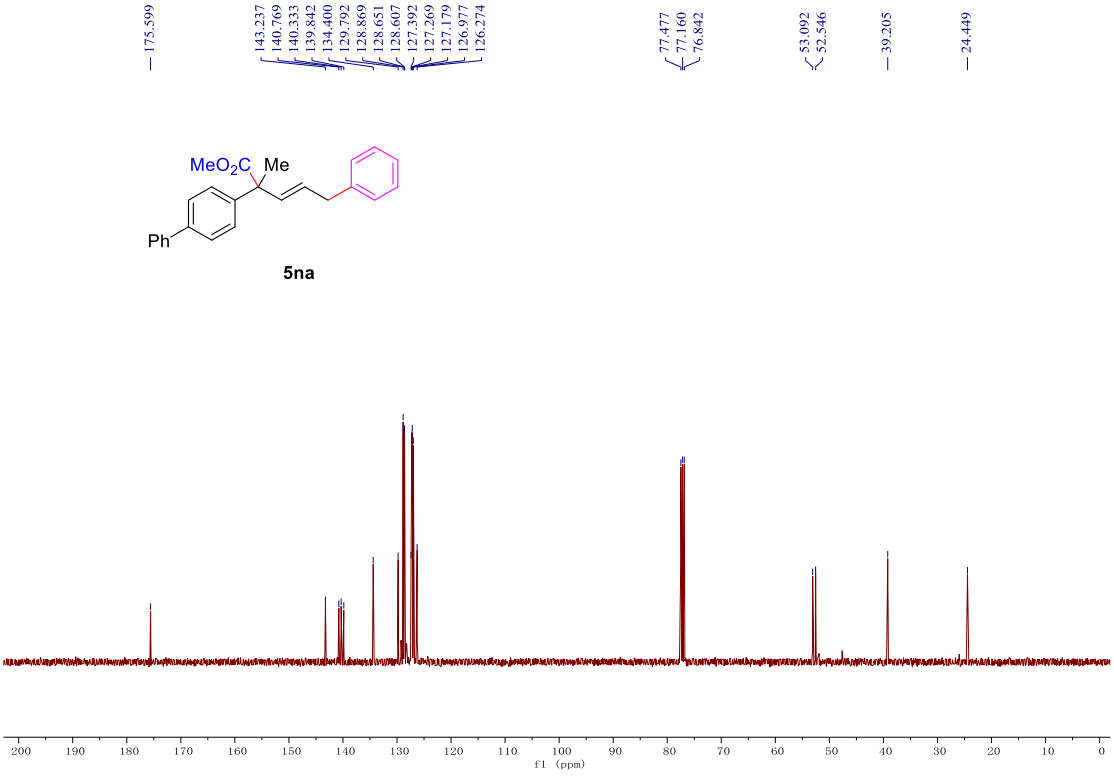
7.533
7.525
7.504
7.410
7.392
7.373
7.316
7.309
7.298
7.289
7.278
7.260
7.193
7.178
7.174
7.163
6.136
6.097
5.749
5.732
5.715
5.710
5.693
5.676
3.694
3.467
3.450
1.642
MeO2C
Me
Ph
4.26
2.28
4.52
3.38
1.00
1.02
3.12
2.05
3.11
f1 (ppm)

5na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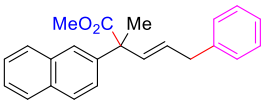
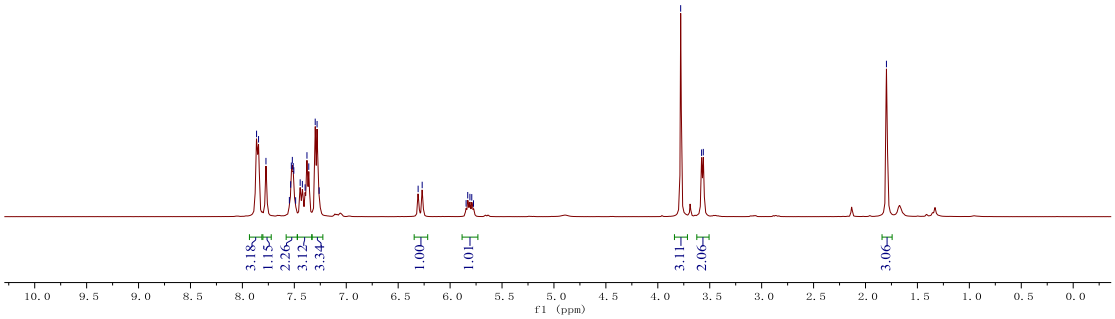
140.769
140.333
139.842
134.400
129.792
128.869
128.651
128.607
127.392
127.269
127.179
126.977
126.274
77.477
77.160
76.842
53.092
52.546
39.205
24.449
MeO2C
Me
Ph
f1 (ppm)

5na

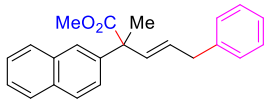

7.864
7.844
7.773
7.548
7.535
7.529
7.519
7.511
7.505
7.488
7.444
7.422
7.396
7.378
7.361
7.299
7.281
7.261
6.308
6.269
5.846
5.830
5.809
5.791
5.775
3.780
3.578
3.562
1.798


MeO2C
Me

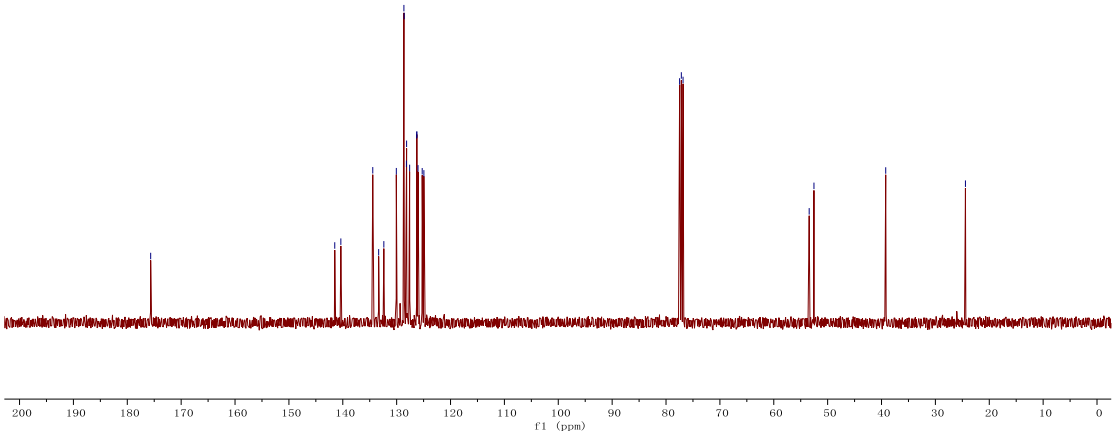
5oa

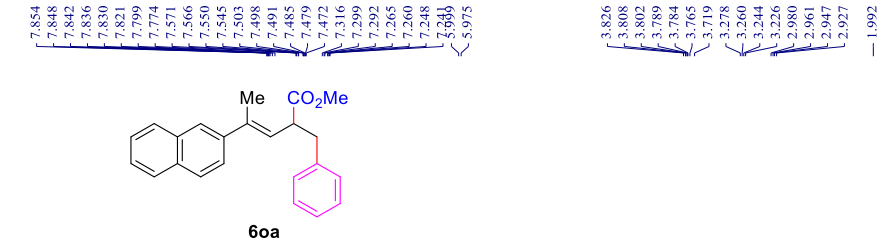

3.18
1.15
2.26
3.12
3.34
1.00
1.01
3.11
2.06
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


175.659
141.489
140.360
134.435
133.340
132.378
130.062
128.653
128.604
128.186
128.153
127.590
126.272
126.252
126.038
125.257
124.948
77.479
77.159
76.842
53.428
52.542
39.221
24.423


MeO2C
Me

5oa


200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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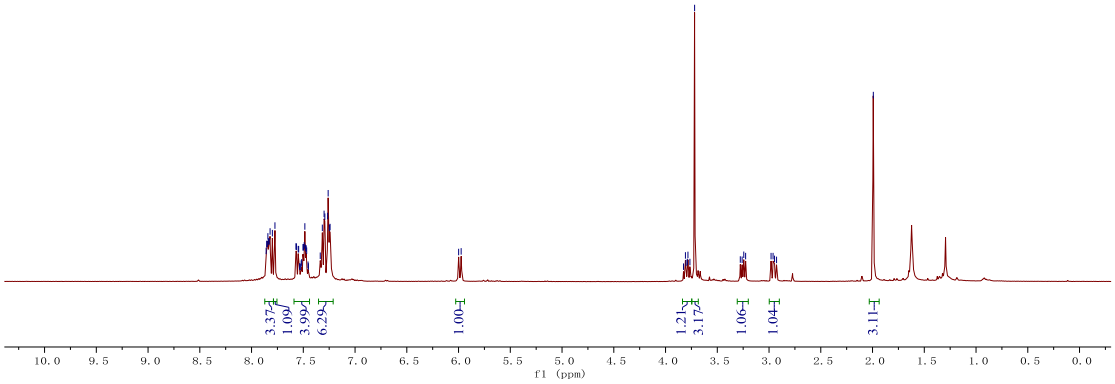
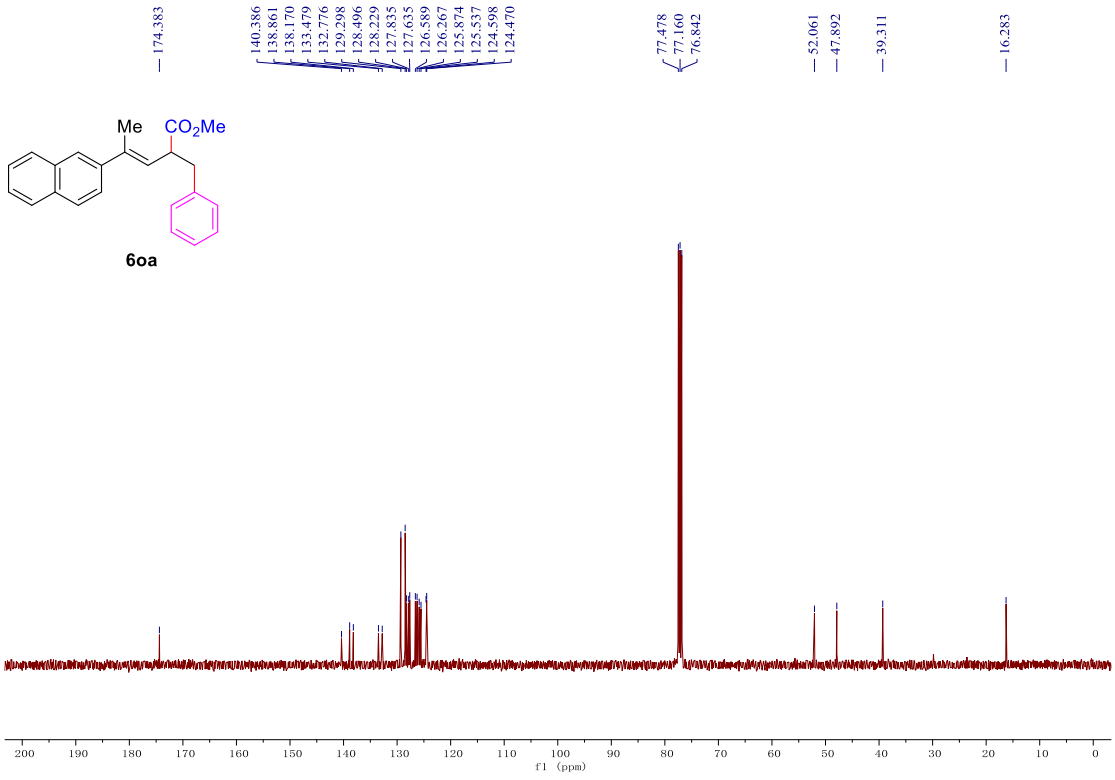
7.848
7.842
7.836
7.830
7.821
7.799
7.774
7.571
7.566
7.550
7.545
7.503
7.498
7.491
7.485
7.479
7.472
7.316
7.299
7.292
7.265
7.260
7.248
5.999
5.975
3.826
3.808
3.802
3.789
3.784
3.765
3.719
3.278
3.260
3.244
3.226
2.980
2.961
2.947
2.927
1.992

Me
CO2Me

6oa


3.37
1.09
3.99
6.29
1.00
1.21
3.17
1.06
1.04
3.11
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)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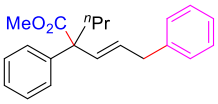
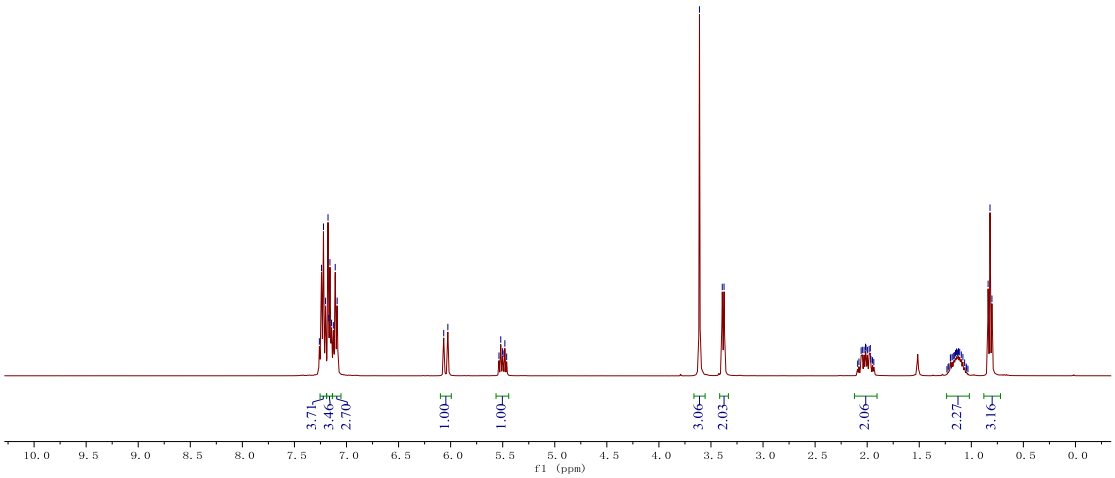
138.861
138.170
133.479
132.776
129.298
128.496
128.229
127.835
127.635
126.589
126.267
125.874
125.537
124.598
124.470
77.478
77.160
76.842
52.061
47.892
39.311
16.283
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

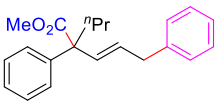
Me
CO2Me

6oa

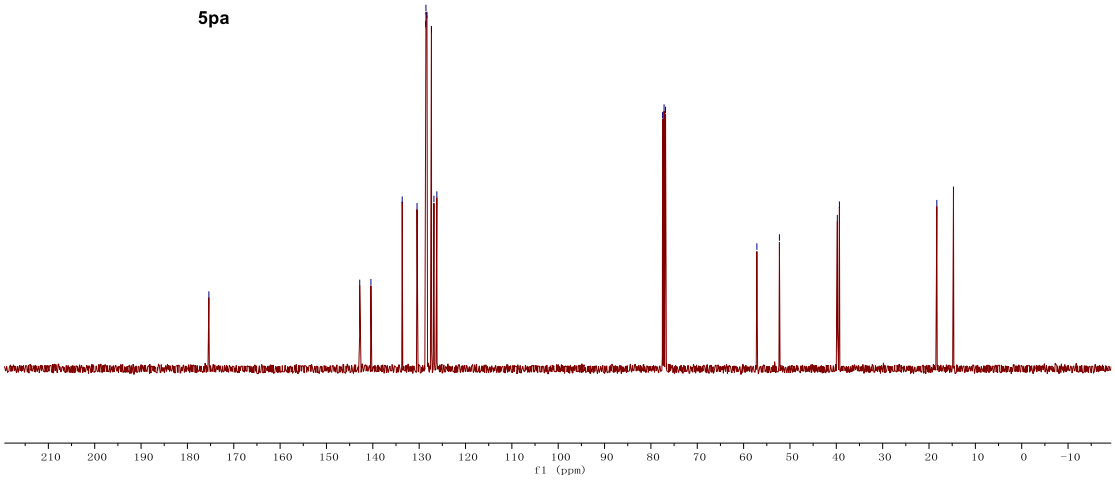


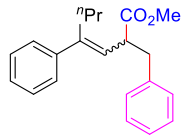
5pa



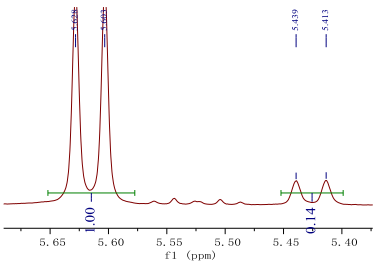


5pa




nPr
CO2Me

6pa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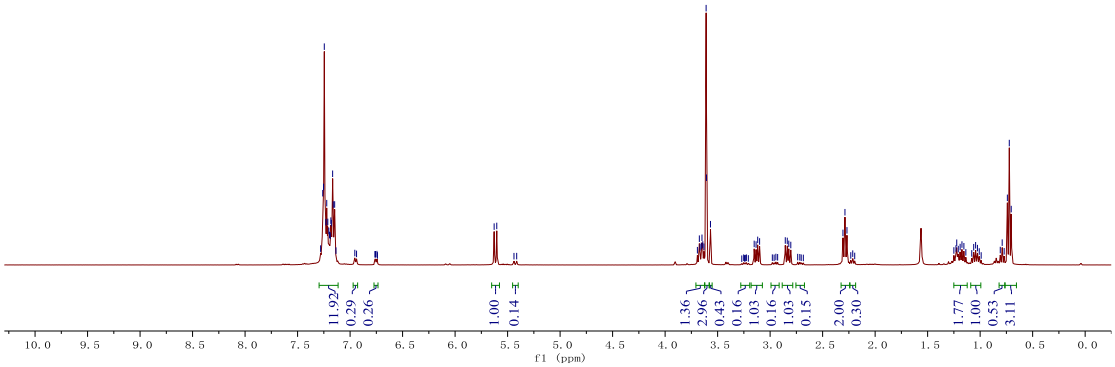
0.14
f1 (ppm)


11.92
0.29
0.26
1.00
0.14
1.36
2.96
0.43
0.16
1.03
0.16
1.03
0.15
2.00
0.30
1.77
1.00
0.53
3.11
f1 (ppm)


174.770
174.365
143.607
142.594
138.918
138.828
129.352
129.257
128.468
128.313
128.279
128.203
128.088
127.356
127.187
126.791
126.692
126.578
126.367
125.528
123.776
77.478
77.161
76.842
51.969
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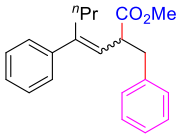
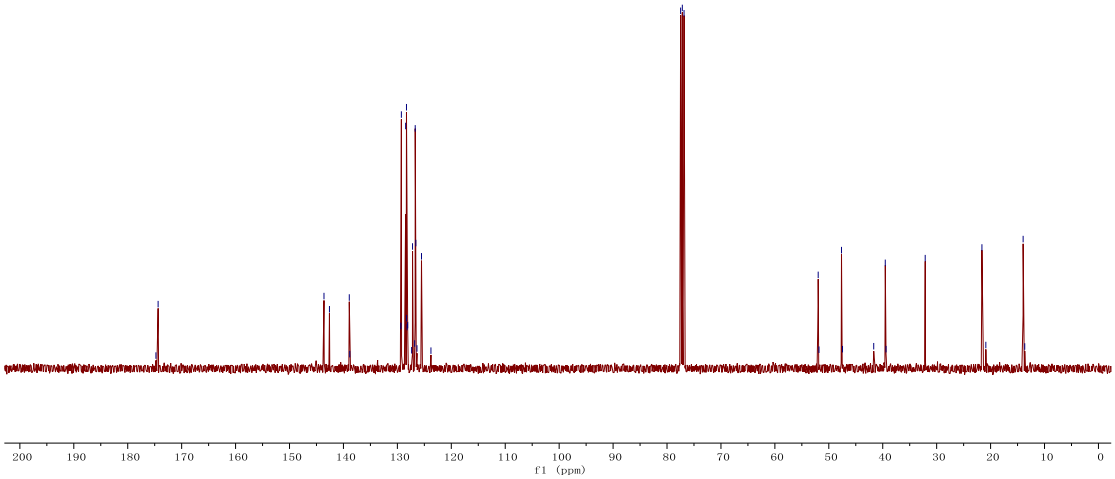
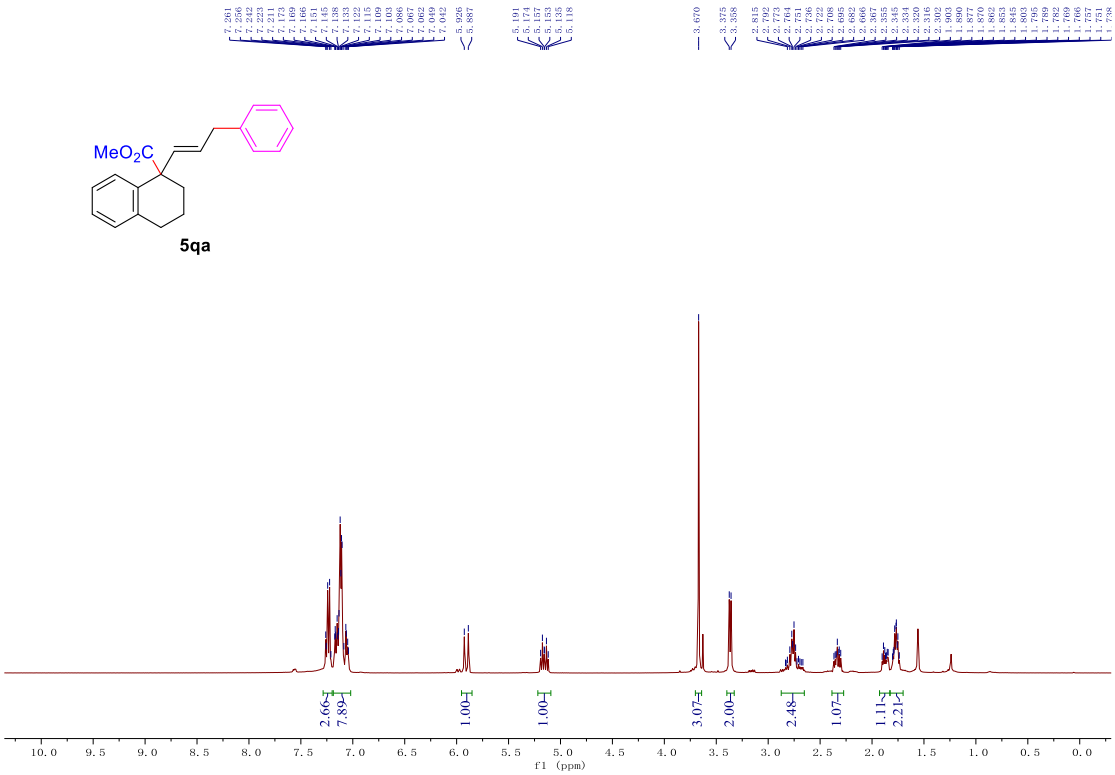
39.529
39.389
32.124
21.607
20.881
13.966
13.667


nPr
CO2Me

6pa


f1 (ppm)


MeO2C
5qa
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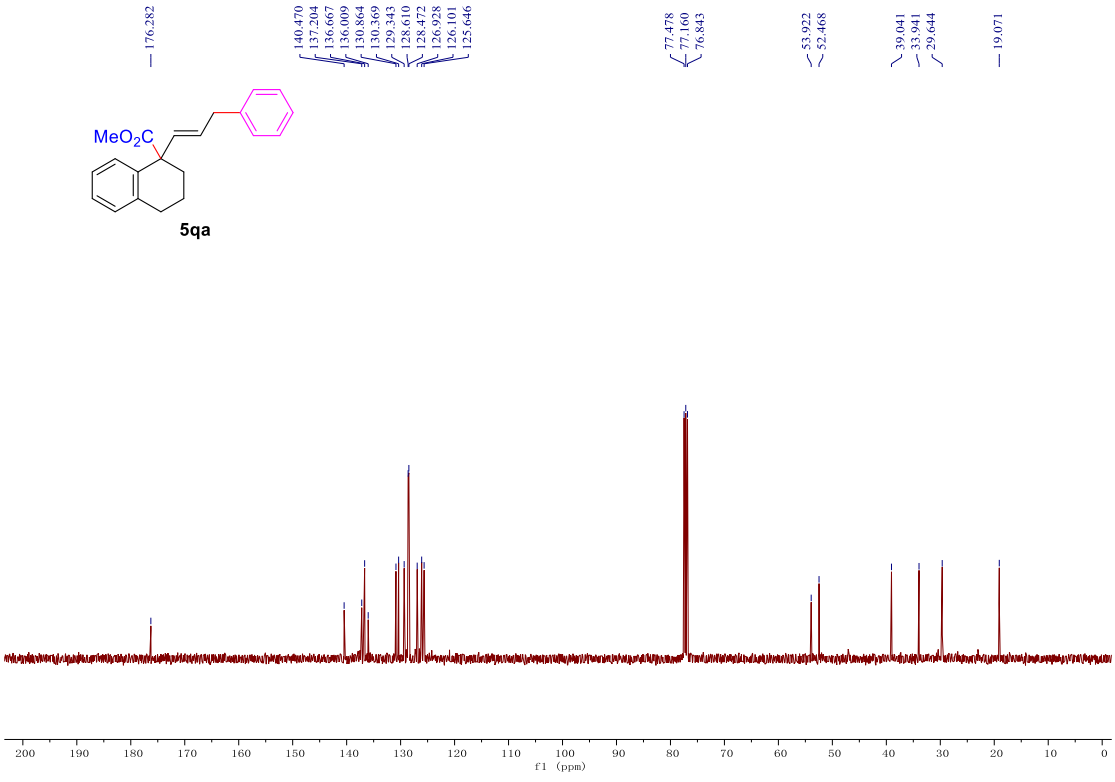
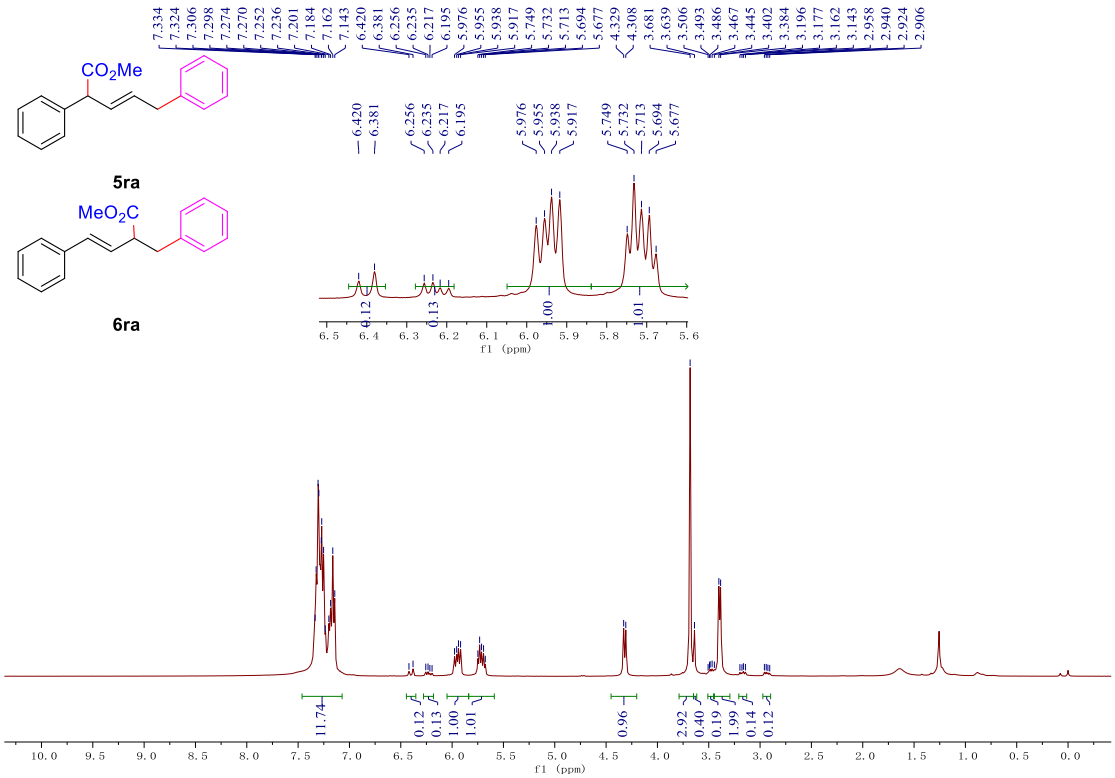
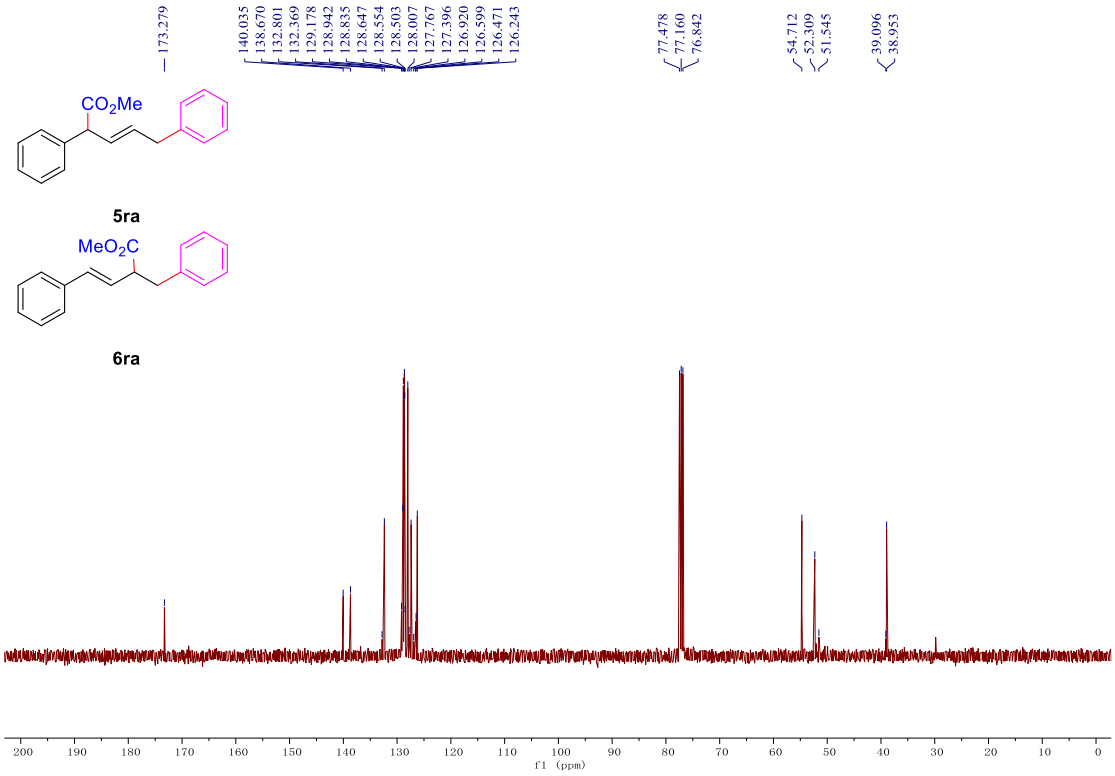
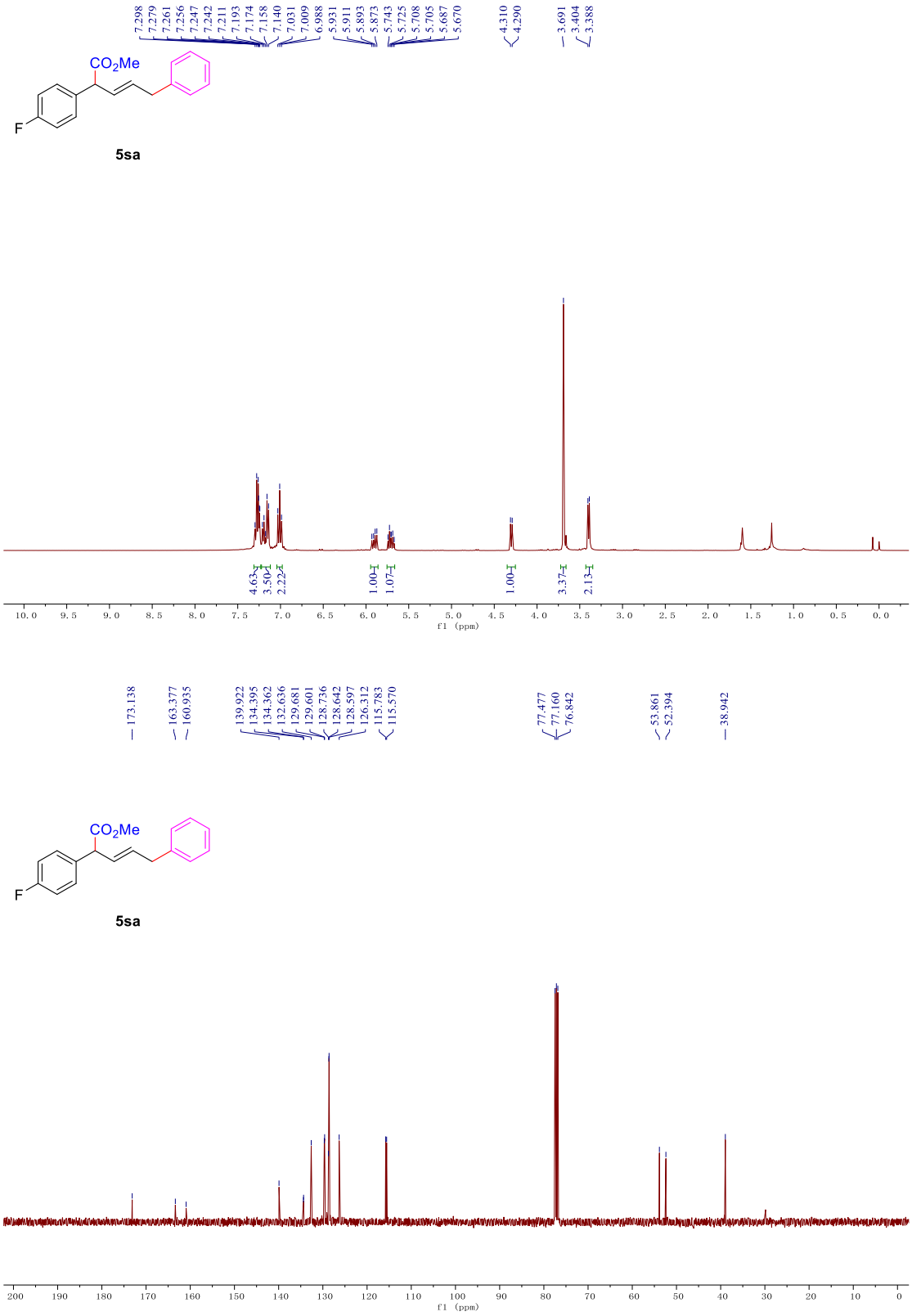
1.00
1.00
3.07
2.00
2.48
1.07
1.11
2.21
f1 (ppm)

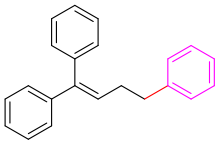

MeO2C
5qa
f1 (ppm)


7.334
7.324
7.306
7.298
7.274
7.270
7.252
7.236
7.201
7.184
7.162
7.143
6.420
6.381
6.256
6.235
6.217
6.195
5.976
5.955
5.938
5.917
5.749
5.732
5.713
5.694
5.677
4.329
4.308
3.681
3.639
3.506
3.493
3.486
3.467
3.445
3.402
3.384
3.196
3.177
3.162
3.143
2.958
2.940
2.924
2.906
CO2Me
5ra
MeO2C
6ra
6.12
0.13
1.00
1.01
f1 (ppm)
11.74
0.12
0.13
1.00
1.01
0.96
2.92
0.40
0.19
1.99
0.14
0.12
f1 (ppm)

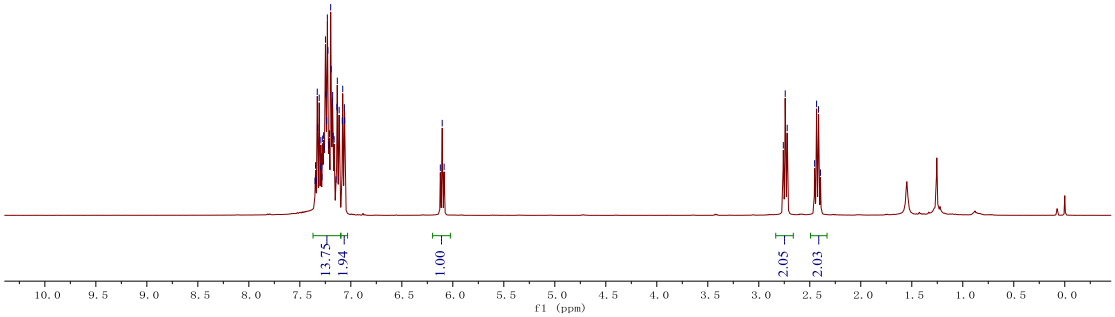

173.279
140.035
138.670
132.801
132.369
129.178
128.942
128.835
128.647
128.554
128.503
128.007
127.767
127.396
126.920
126.599
126.471
126.243
77.478
77.160
76.842
54.712
52.309
51.545
39.096
38.953
CO2Me
5ra
MeO2C
6ra
f1 (ppm)


7.298
7.279
7.261
7.256
7.247
7.242
7.211
7.193
7.174
7.158
7.140
7.031
7.009
6.988
5.931
5.911
5.893
5.873
5.743
5.725
5.708
5.705
5.687
5.670
4.310
4.290
3.691
3.404
3.388
CO2Me
F
5sa
4.63
3.50
2.22
1.00
1.07
1.00
3.37
2.13
f1 (ppm)
173.138
163.377
160.935
139.922
134.395
134.362
132.636
129.681
129.601
128.736
128.642
128.597
126.312
115.783
115.570
77.477
77.160
76.842
53.861
52.394
38.942
CO2Me
F
5sa
f1 (ppm)

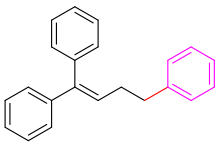

7.329
7.325
7.310
7.276
7.267
7.249
7.243
7.237
7.230
7.225
7.209
7.198
7.193
7.182
7.178
7.174
7.164
7.136
7.132
7.115
7.084
7.079
7.063
7.060
6.122
6.104
6.085
2.759
2.741
2.721
2.452
2.433
2.414
2.395



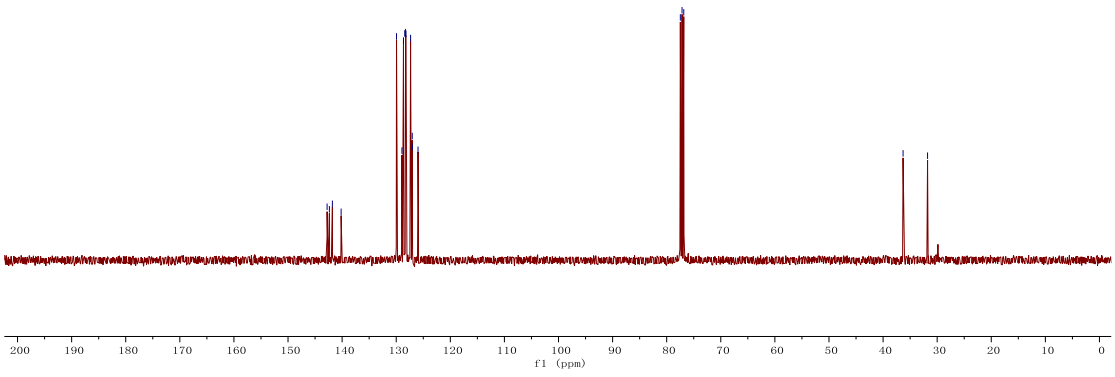
BP1

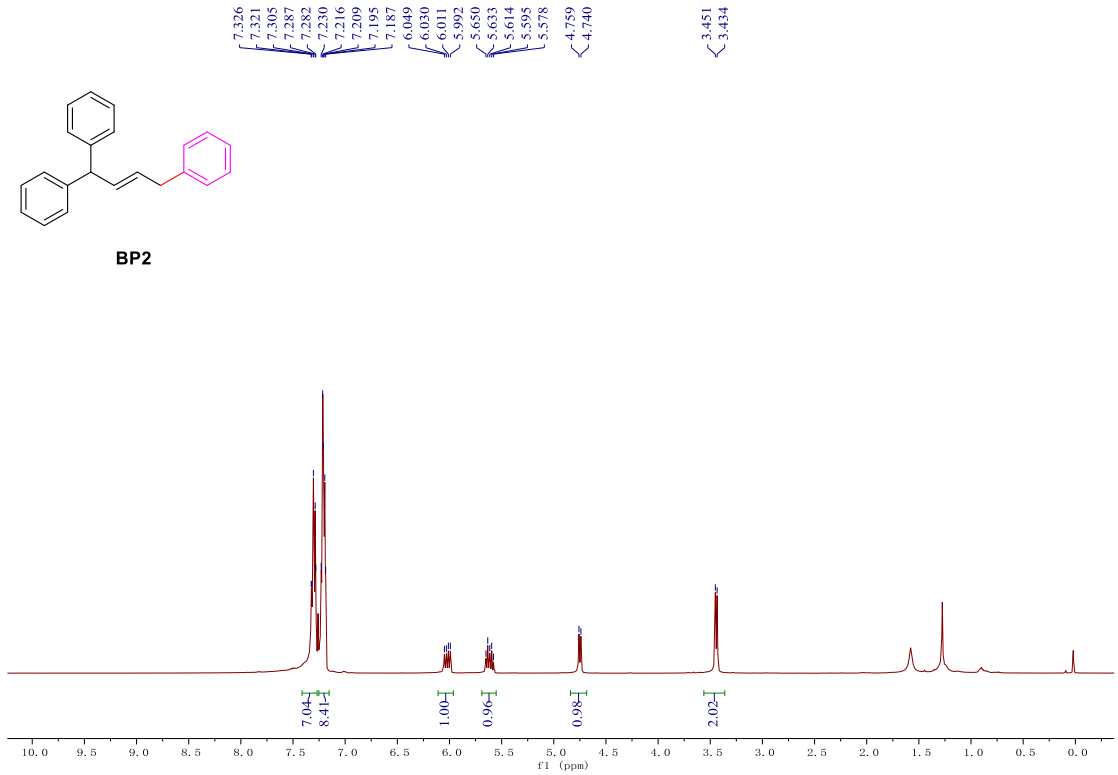

13.75
1.94
1.00
2.05
2.03
f1 (ppm)

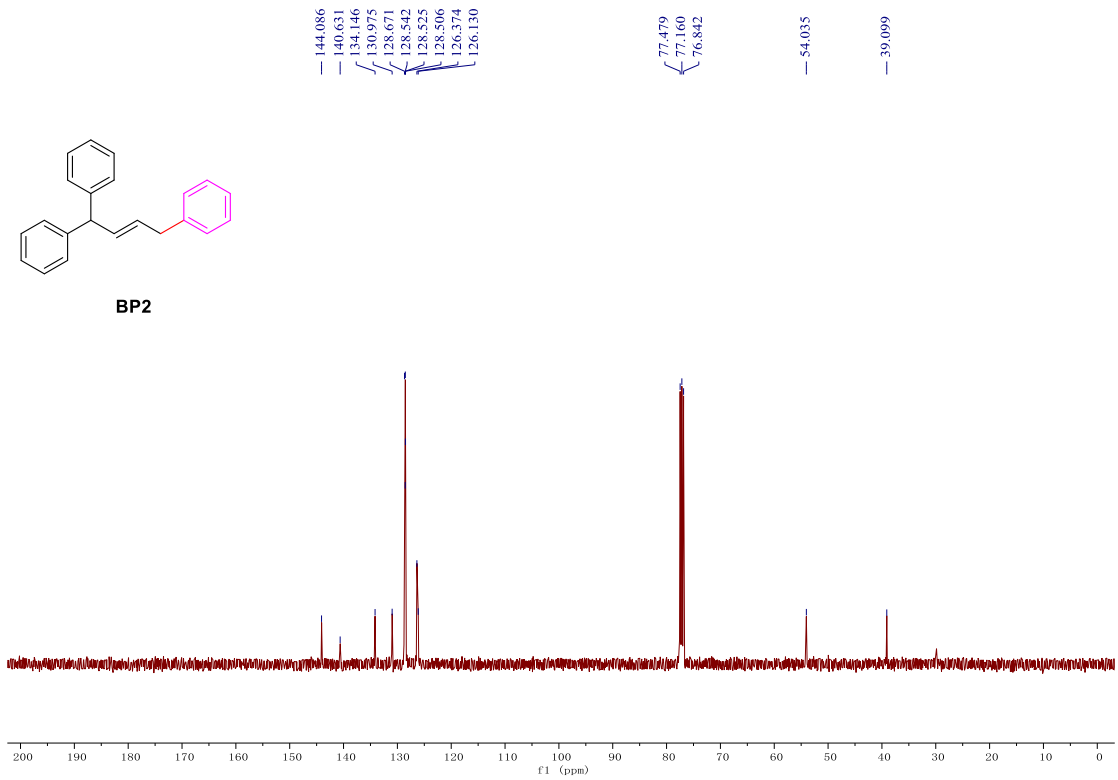

142.777
142.353
141.801
140.186
129.944
128.941
128.656
128.423
128.267
128.202
127.344
127.035
127.007
125.969
77.478
77.160
76.842
36.304
31.779

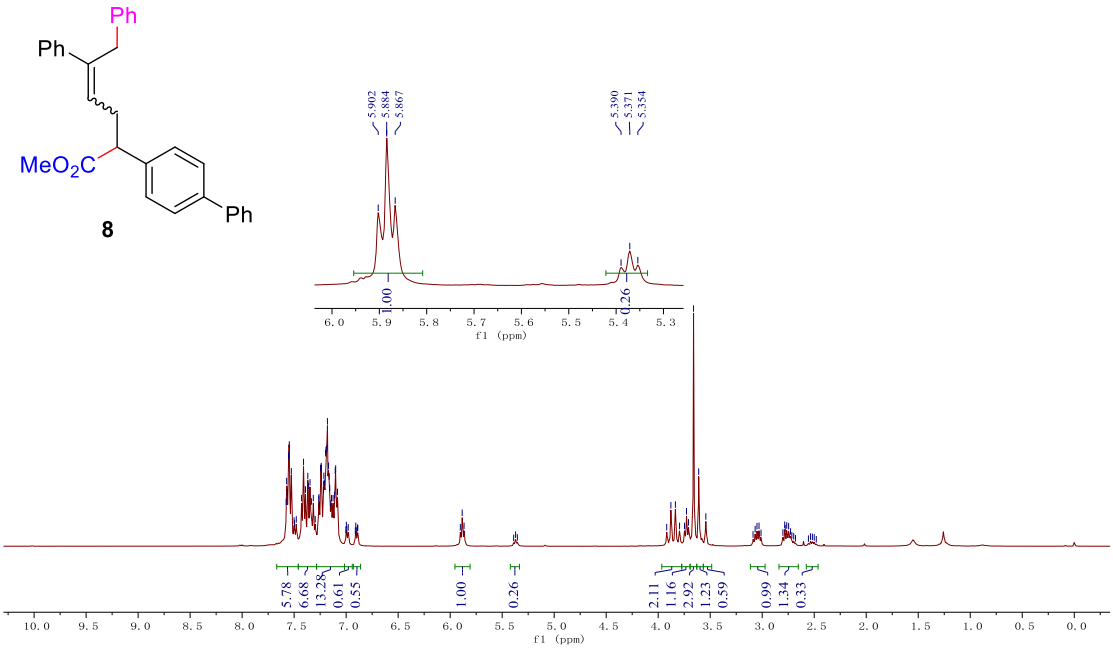


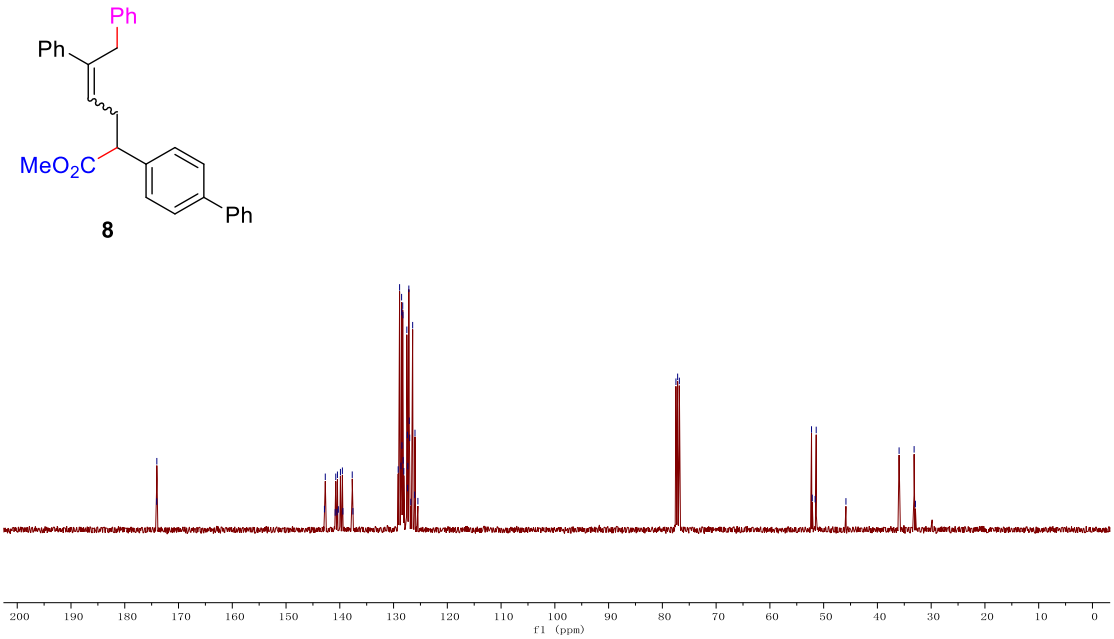
BP1


f1 (ppm)


7.326
7.321
7.305
7.287
7.282
7.230
7.216
7.209
7.195
7.187
6.049
6.030
6.011
5.992
5.650
5.633
5.614
5.595
5.578
4.759
4.740
3.451
3.434
BP2
7.04
8.41
1.00
0.96
0.98
2.02
f1 (ppm)

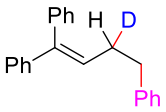

144.086
140.631
134.146
130.975
128.671
128.542
128.525
128.506
126.374
126.130
77.479
77.160
76.842
54.035
39.099
BP2
f1 (ppm)


Ph
Ph
MeO2C
Ph
8
5.902
5.884
5.867
5.390
5.371
5.354
1.00
0.26
f1 (ppm)
5.78
6.68
13.28
0.61
0.55
1.00
0.26
2.11
1.16
2.92
1.23
0.59
0.99
1.34
0.33
f1 (ppm)

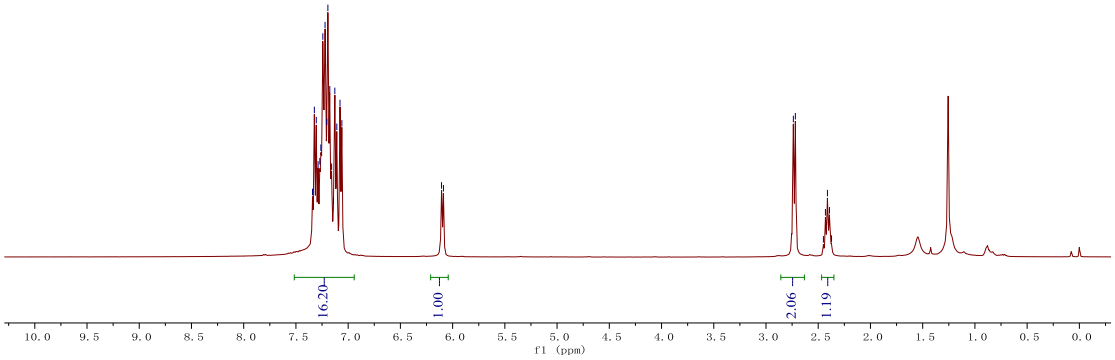

Ph
Ph
MeO2C
Ph
8
f1 (ppm)


7.341
7.324
7.305
7.288
7.271
7.261
7.243
7.221
7.205
7.194
7.176
7.158
7.141
7.128
7.109
7.078
7.060
6.106
6.088


2.738
2.719
2.450
2.431
2.412
2.392
2.373


Ph
H
D
Ph
Ph

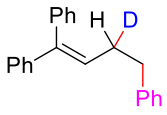
9


16.20
1.00
2.06
1.19
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)

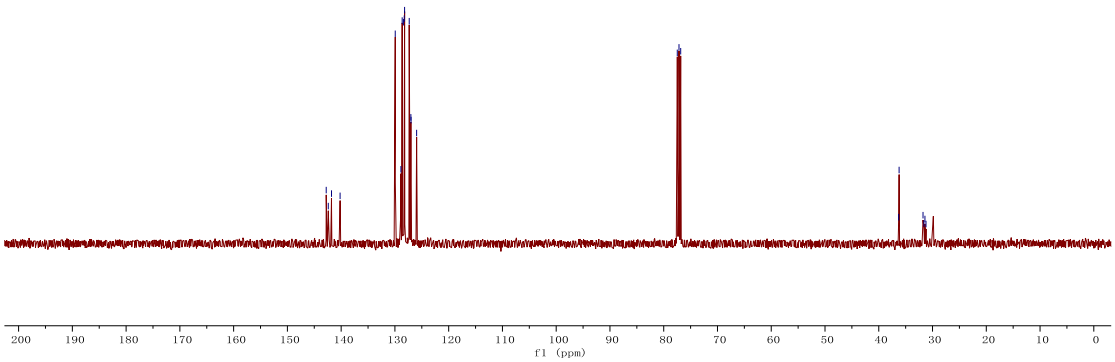

142.780
142.394
141.794
140.197
129.940
128.884
128.650
128.418
128.264
128.198
127.340
127.031
127.002
125.962

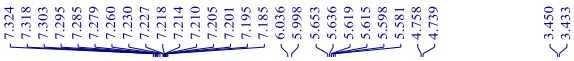

77.477
77.160
76.842

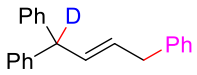

36.302
36.216
31.767
31.607
31.411
31.216


Ph
H
D
Ph
Ph

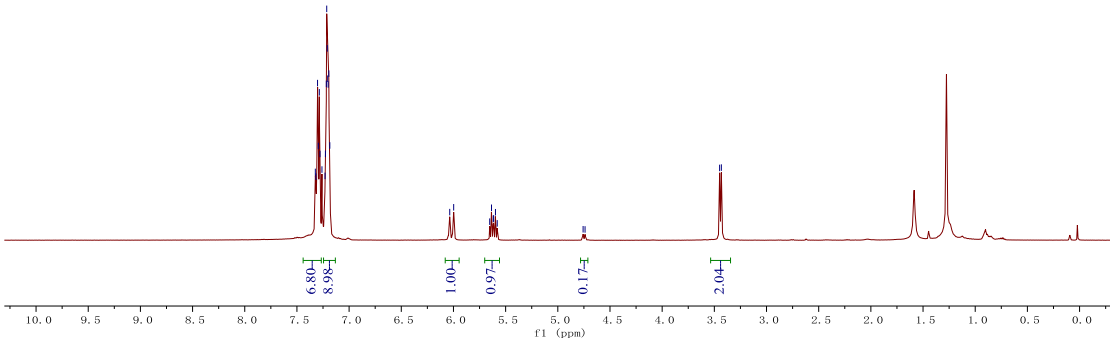
9


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

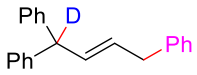

7.324
7.318
7.303
7.295
7.285
7.279
7.260
7.230
7.227
7.218
7.214
7.210
7.205
7.201
7.195
7.185
6.036
5.998
5.653
5.636
5.619
5.615
5.598
5.581
4.758
4.739
3.450
3.433


Ph
D
Ph
Ph

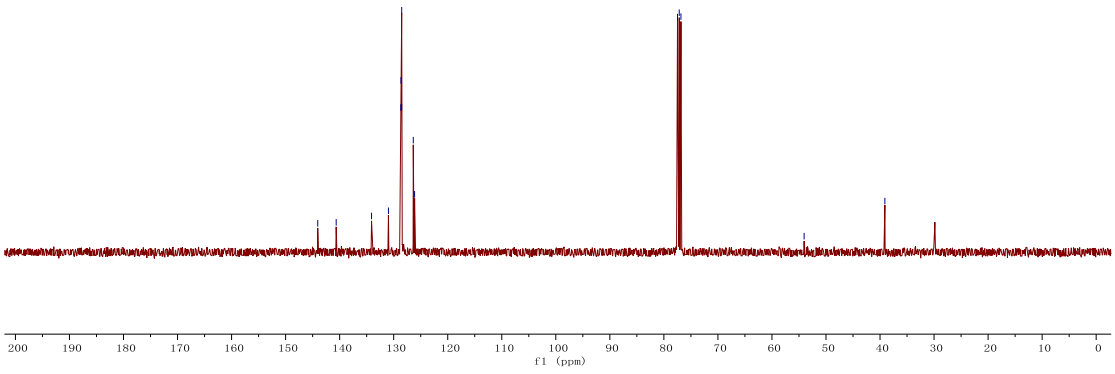
10


6.80
8.98
1.00
0.97
0.17
2.04
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
f1 (ppm)

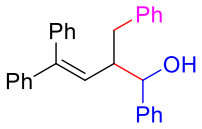

144.055
140.642
134.101
130.974
128.676
128.649
128.535
128.518
126.376
126.131
77.478
77.160
76.843
54.047
39.105


Ph
D
Ph
Ph

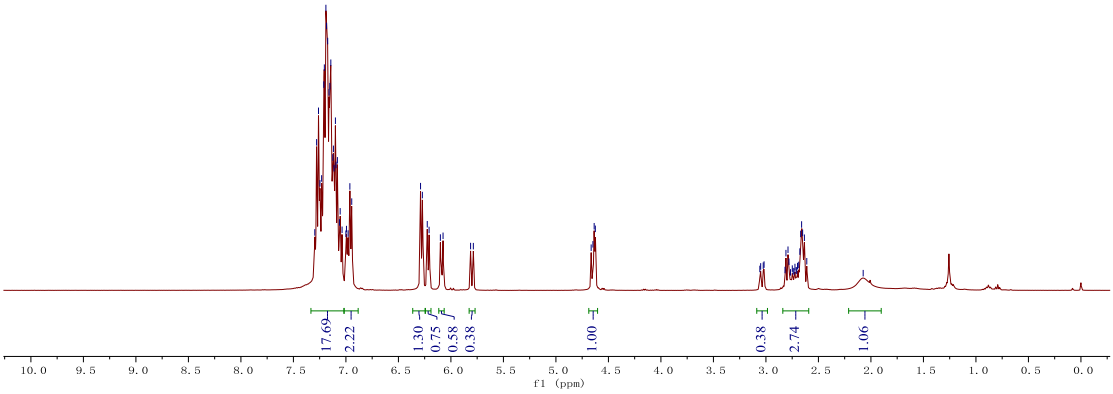
10


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

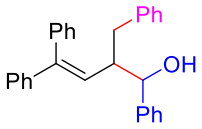

7.279
7.261
7.247
7.231
7.211
7.205
7.191
7.184
7.174
7.161
7.153
7.144
7.125
7.119
7.113
7.100
7.094
7.081
7.061
7.055
6.962
6.345
6.289
6.272
6.225
6.208
6.100
6.075
5.813
5.786
4.664
4.648
4.636
4.625
3.058
3.050
3.026
3.018
2.818
2.809
2.790
2.781
2.766
2.749
2.741
2.732
2.724
2.713
2.706
2.699
2.688
2.677
2.669
2.660
2.650
2.634
2.611
2.074


Ph
Ph
Ph
OH
Ph

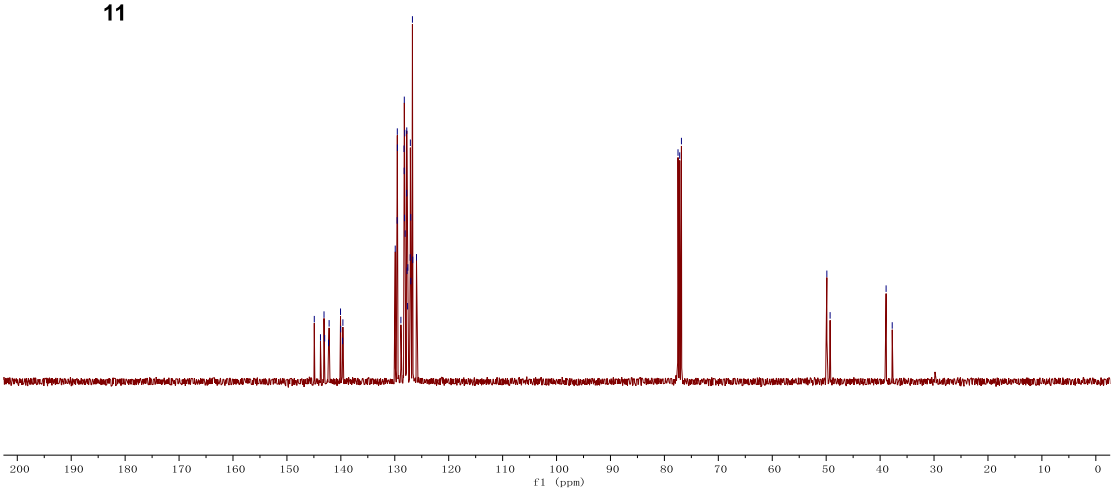
11

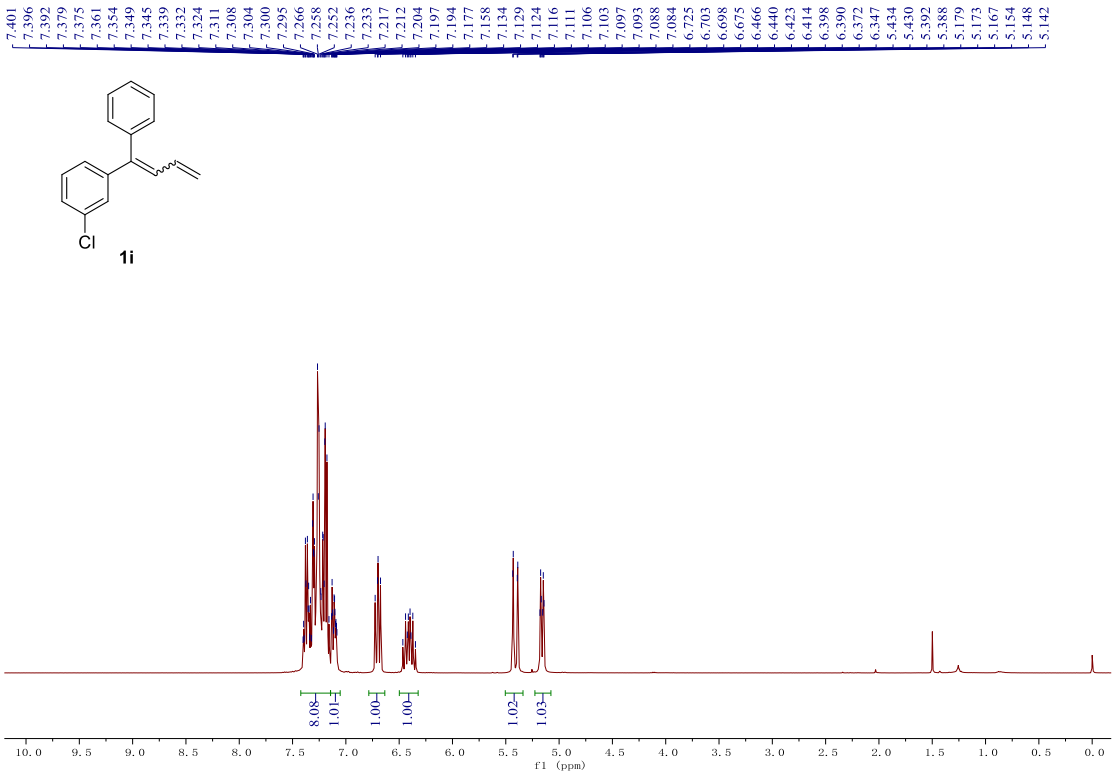

17.69
2.22
1.30
0.75
0.58
0.38
1.00
0.38
2.74
1.06
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

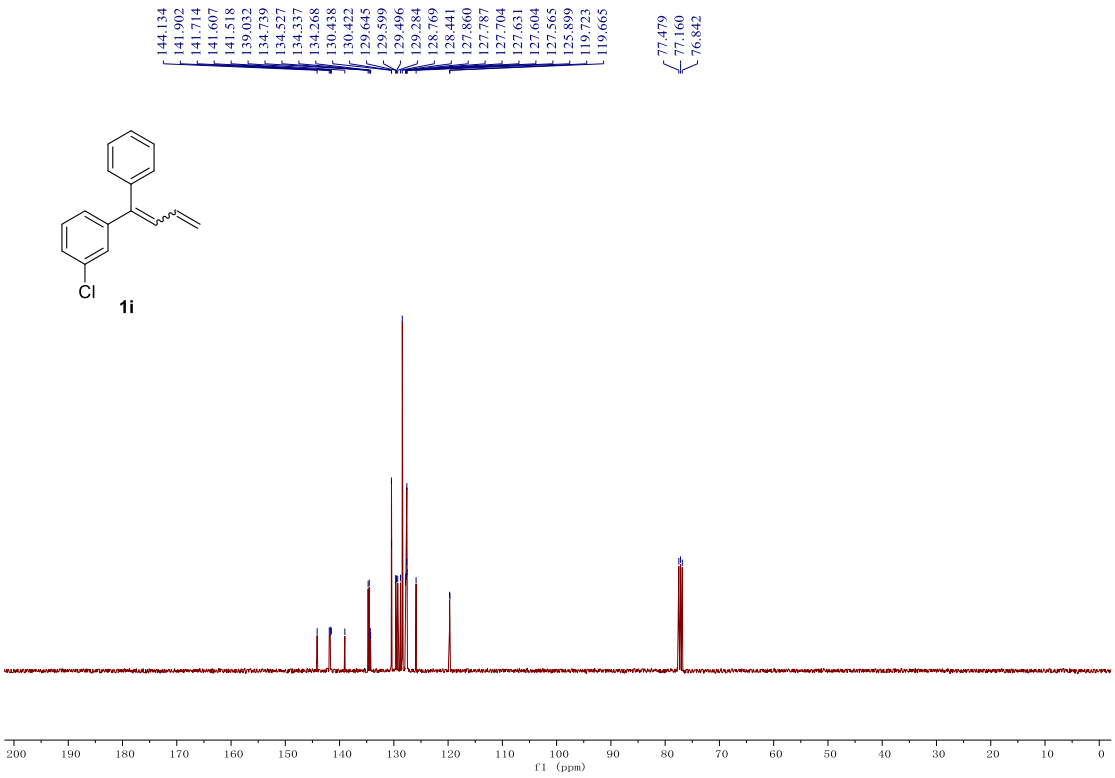

144.927
143.778
143.120
142.999
142.290
142.173
140.061
140.033
139.683
139.620
129.914
129.552
129.529
129.502
128.863
128.281
128.249
128.233
128.194
128.149
128.080
127.794
127.779
127.723
127.627
127.579
127.139
127.106
127.043
127.027
126.723
126.673
125.971
77.478
77.160
76.843
49.877
49.271
38.889
37.753

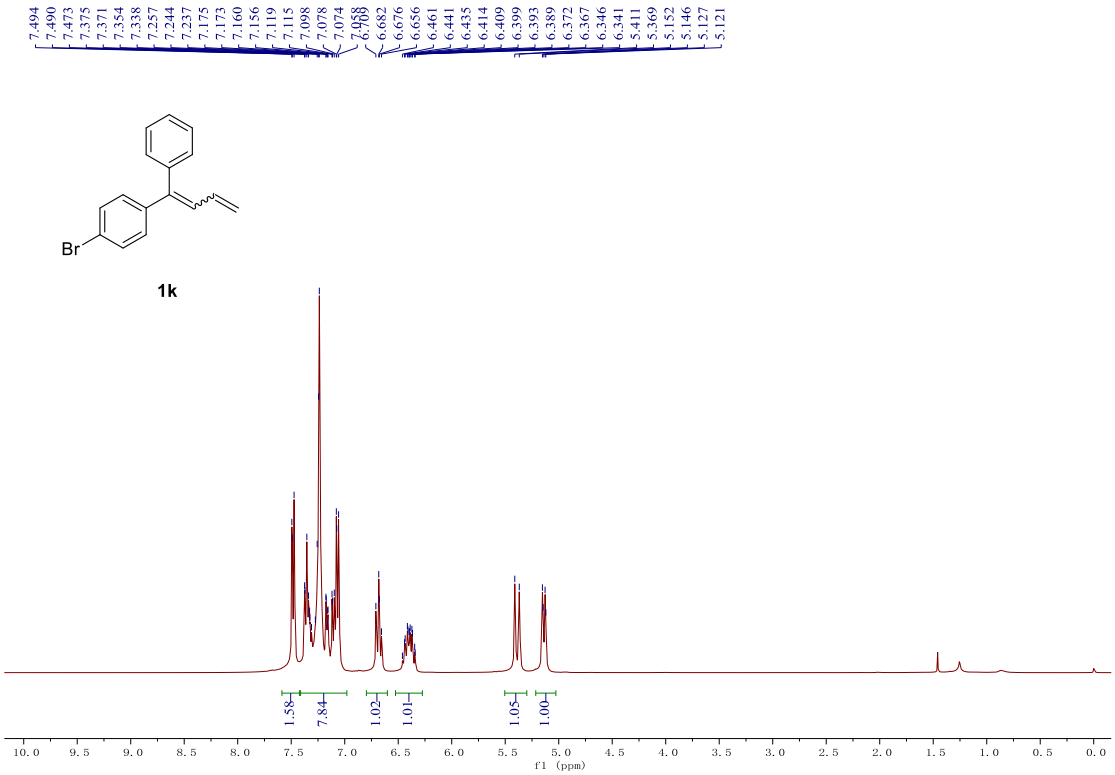

Ph
Ph
Ph
OH
Ph

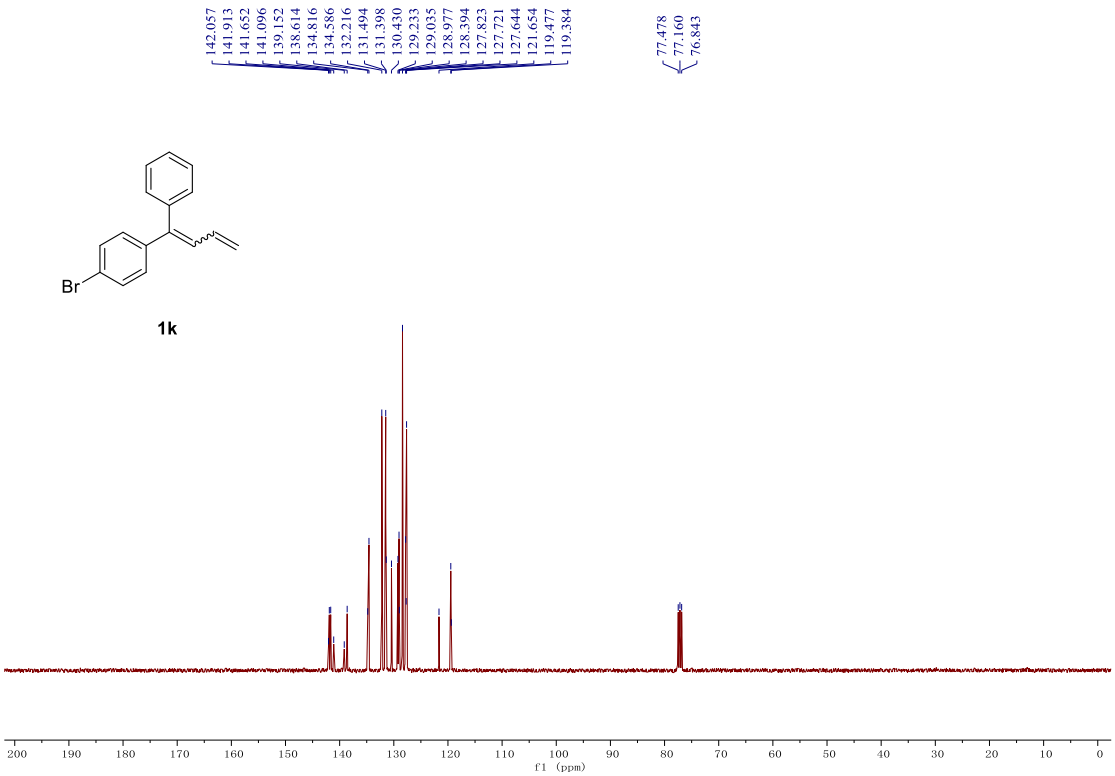
11


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


7.401
7.396
7.392
7.379
7.375
7.361
7.354
7.349
7.345
7.339
7.332
7.324
7.311
7.308
7.304
7.300
7.295
7.266
7.258
7.252
7.236
7.233
7.217
7.212
7.204
7.197
7.194
7.177
7.158
7.134
7.129
7.124
7.116
7.111
7.106
7.103
7.097
7.093
7.088
7.084
6.725
6.703
6.698
6.675
6.466
6.440
6.423
6.414
6.398
6.390
6.372
6.347
5.434
5.430
5.392
5.388
5.179
5.173
5.167
5.154
5.148
5.142
Cl
1i
8.08
1.01
1.00
1.00
1.02
1.03
f1 (ppm)


144.134
141.902
141.714
141.607
141.518
139.032
134.739
134.527
134.337
134.268
130.438
130.422
129.645
129.599
129.496
129.284
128.769
128.441
127.860
127.787
127.704
127.631
127.604
127.565
125.899
119.723
119.665
77.479
77.160
76.842
Cl
1i
f1 (ppm)


7.494
7.490
7.473
7.375
7.371
7.354
7.338
7.257
7.244
7.237
7.175
7.173
7.160
7.156
7.119
7.115
7.098
7.078
7.074
6.682
6.676
6.656
6.461
6.441
6.435
6.414
6.409
6.399
6.393
6.389
6.372
6.367
6.346
6.341
5.411
5.369
5.152
5.146
5.127
5.121
Br
1k
1.58
7.84
1.02
1.01
1.05
1.00
f1 (ppm)


142.057
141.913
141.652
141.096
139.152
138.614
134.816
134.586
132.216
131.494
131.398
130.430
129.233
129.035
128.977
128.394
127.823
127.721
127.644
121.654
119.477
119.384
77.478
77.160
76.843
Br
1k
f1 (ppm)


7.710
7.690
7.585
7.564
7.384
7.370
7.363
7.351
7.260
6.861
6.834
6.463
6.436
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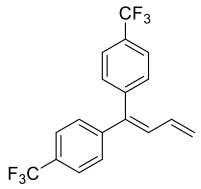
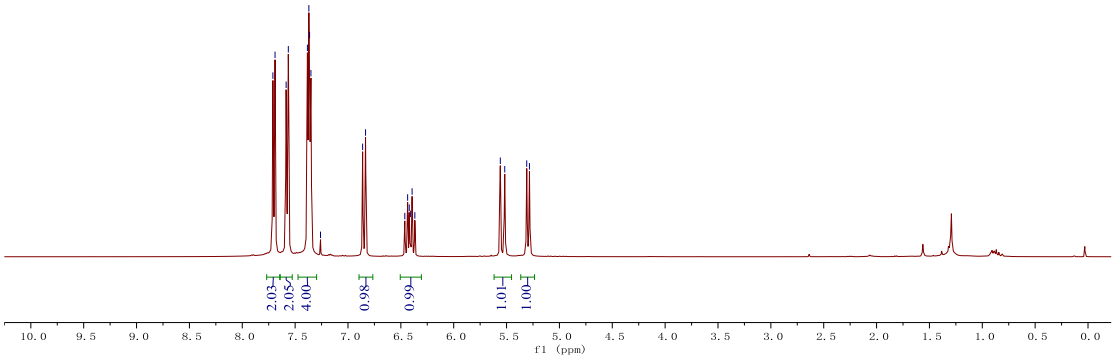
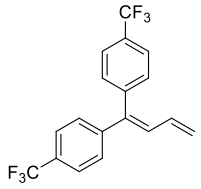
6.394
6.368
5.559
5.517
5.309
5.284


CF3
F3C

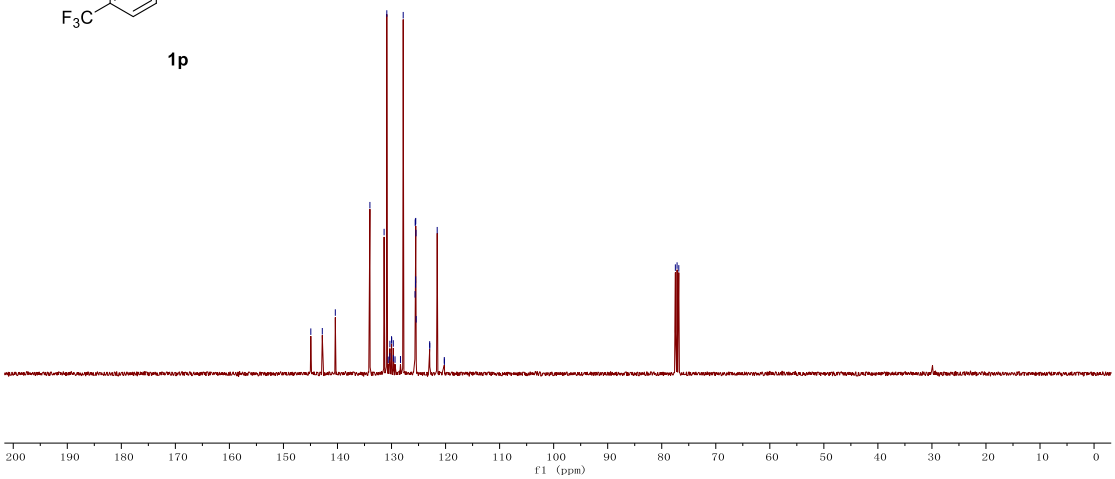
1p

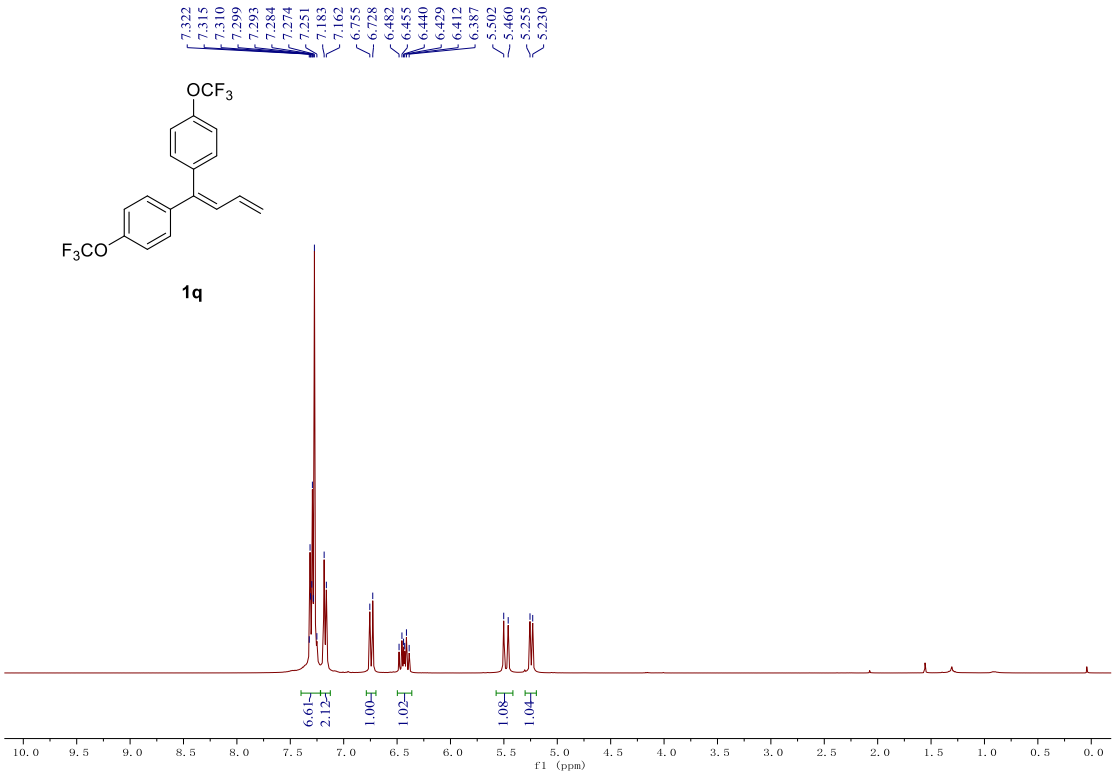

2.03
2.05
4.00
0.98
0.99
1.01
1.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

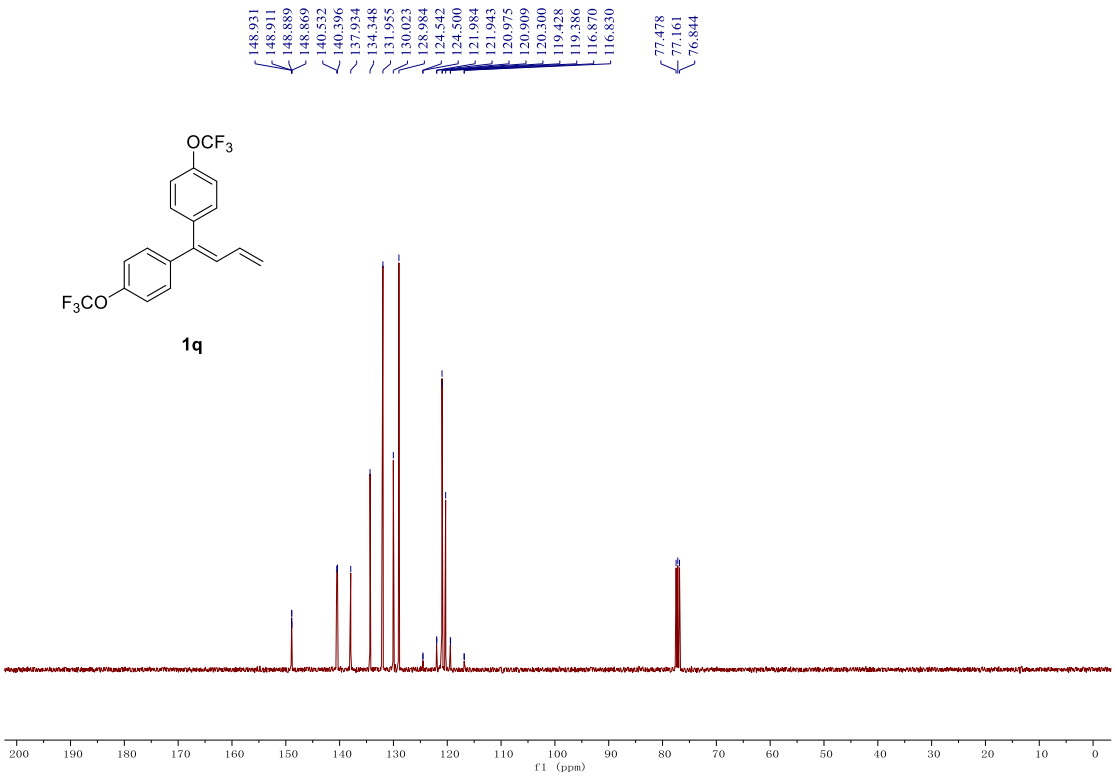

144.937
142.810
140.403
134.001
131.377
130.873
130.621
130.317
130.297
129.995
129.973
129.671
129.653
129.349
128.346
128.335
127.840
125.647
125.613
125.576
125.556
125.537
125.518
125.481
125.443
122.941
122.925
121.549
120.236
120.221
77.478
77.161
76.843


CF3
F3C

1p


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


7.322
7.315
7.310
7.299
7.293
7.284
7.274
7.251
7.183
7.162
6.755
6.728
6.482
6.455
6.440
6.429
6.412
6.387
5.502
5.460
5.255
5.230
OCF3
F3CO
1q
6.61
2.12
1.00
1.02
1.08
1.04
f1 (ppm)


148.931
148.911
148.889
148.869
140.532
140.396
137.934
134.348
131.955
130.023
128.984
124.542
124.500
121.984
121.943
120.975
120.909
120.300
119.428
119.386
116.870
116.830
77.478
77.161
76.844
OCF3
F3CO
1q
f1 (ppm)