Supporting Information

Palladium-Catalyzed Oxidative Allylation of Sulfoxonium Ylides: Regioselective Synthesis of Conjugated Dienones

Chunsheng Li,[a] Meng Li,[a] Wentao Zhong,[a] Yangbin Jin,[a] Jianxiao Li,[a] Wanqing Wu,[a] and Huanfeng Jiang*,[a,b]

[a]Key Laboratory of Functional Molecular Engineering of Guangdong Province, Guangdong Engineering Research Center for Green Fine Chemicals, School of Chemistry and Chemical Engineering, South China University of Technology, Guangzhou 510640, China

[b]State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000, P. R. China

Table of Contents

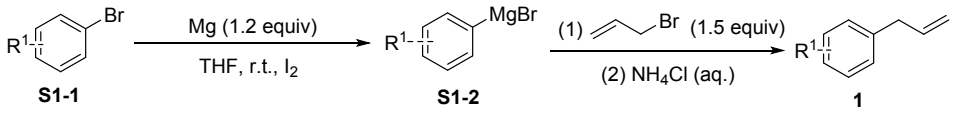
A. General Information

^{1}H and ^{13}C NMR spectra were recorded using a 400 MHz NMR spectrometer. Chemical shifts were reported in ppm from the solvent resonance as the internal reference ($CDCl_3$ δ_H = 7.26 ppm, downfield from TMS, δ_C = 77.0 ppm. Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet). IR spectra were obtained as potassium bromide pellets between two potassium bromide pellets with a spectrometer. GC-MS was obtained using electron ionization. HRMS was obtained with a LCMS-IT-TOF mass spectrometer or recorded on an EI-ion trap High Resolution mass spectrometer. TLC was performed by using commercially prepared 100-400 mesh silica gel plates and visualization was effected at 254 nm. X-ray structural analyses were conducted on an x-ray analysis instrument.

Materials. Toluene and tetrahydrofuran were distilled from sodium/benzophenone. Acetonitrile was distilled from phosphorus pentoxide. Other commercially available reagents were purchased and used without further purification. Analytical thin-layer chromatography was performed on 0.20 mm silica gel plates (GF_{254}) using UV light as a visualizing agent. Flash column chromatography was conducted using silica gel (200–300 mesh) with the indicated solvent system. All the reaction temperatures reported are oil bath temperatures. Bis[(pinacolato)boryl]methane were commercially available.

B. Typical Procedures for the Synthesis of Substrates

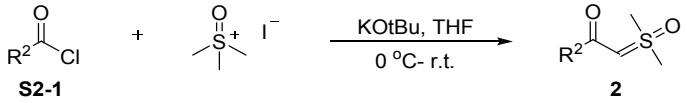
(a). General Procedure for the Synthesis of Allylbenzenes [1]



S1-1 S1-2 1

Aryl bromide (5 mmol) was reacted with magnesium (1.2 equiv) in 10 mL anhydrous THF using I_2 as initiator at room temperature. After the reaction was finished, the combined organics was added to the anhydrous THF solution of allyl bromide. After stirring for 1 h, NH_4Cl (aq.) was added to the reaction mixture, washing with water and then concentrated for further purification. Purification by column chromatography over silica gel (230-400 mesh) using petroleum ether as eluent afforded **1c**, **1d**, **1g**, **1j**, **1m**, **1n**, **1o**, **1q**, **1t** as a colorless oil.

(b). General Procedure for Synthesis of Sulfoxonium Ylides [2]



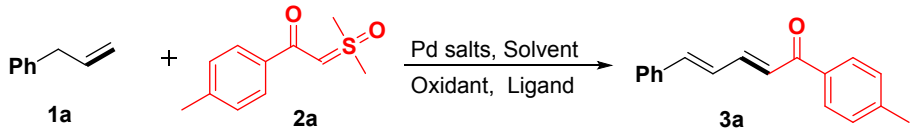
S2-1 2

Sulfoxonium ylides were prepared according to reported procedures. To a stirred solution of potassium *tert*-butoxide (3.0 g, 27.2 mmol) in THF (30 mL) was added trimethylsulfoxonium iodide (5.0 g, 20.6 mmol) at room temperature. The resulting mixture is refluxed for 2 h. Then reaction mixture was cooled to 0 °C, followed by addition of acyl chlorides **2** (7 mmol) in THF (5 mL). The reaction was allowed to stir at room temperature for 3 h. Next, the solvent was evaporated and water (15 mL) and ethyl acetate (20 mL) were added to the resulting slurry. The layers were separated and the aqueous layer was washed with ethyl acetate (2 x 30 mL) and the organic layers were combined. The organic solution was dried over anhydrous sodium sulfate (Na_2SO_4), filtered over a sintered funnel, and evaporated to dryness. The crude product was purified by flash chromatography over silica gel using EtOAc/MeOH (95:5) to afford the

corresponding sulfoxonium ylide

C. Optimization of Reaction Conditions [a]

In a 25 mL sealed test tube, a mixture of allylbenzene **1a** (0.2 mmol), sulfoxonium ylide **2a** (0.1 mmol), catalyst (10 mol %), ligand (20 mol %), oxidant (2 equiv) in 2 mL solvent was vigorously stirred together for 24 h. After completion of the reaction and quenched by saturated brines, the mixture was extracted with ethyl acetate (3 × 10 mL). The combined ethyl acetate layer was then dried over anhydrous sodium sulfate and concentrated in vacuum. Further purification by flash column chromatography on silica gel afforded the pure product **3a,** and calculated the isolated yield.

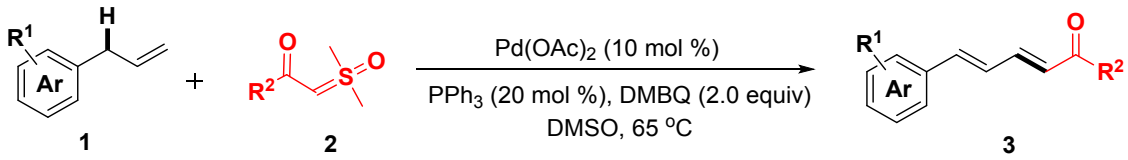


entr	catalyst	ligand	oxidant	solvent	temperature	yield[b] (%)
1	$Pd(OAc)_2$	PPh_3	NQ	DMSO	80	15
2	$Pd(OAc)_2$	PPh_3	BQ	DMSO	80	20
3	$Pd(OAc)_2$	PPh_3	DDQ	DMSO	80	Trace
4	$Pd(OAc)_2$	PPh_3	DMBQ	DMSO	80	62
5	$Pd(OAc)_2$	PPh_3	*o*-NQ	DMSO	80	N.D.
6	$Pd(OAc)_2$	PPh_3	DDQ:BQ=2:1	DMSO	80	N.D.
7	$Pd(OAc)_2$	PPh_3	DDQ:BQ=4:1	DMSO	80	N.D.
8	$Pd(OAc)_2$	PPh_3	O_2	DMSO	80	N.D.
9	$PdCl_2$	PPh_3	DMBQ	DMSO	80	N.D.
10	$Pd(TFA)_2$	PPh_3	DMBQ	DMSO	80	N.D.
11	$Pd(MeCN)_2Cl_2$	PPh_3	DMBQ	DMSO	80	N.D.
12	$Pd(PPh_3)_2Cl_2$	PPh_3	DMBQ	DMSO	80	N.D.
13	$Pd(PPh_3)_4$	PPh_3	DMBQ	DMSO	80	Trace
14	$Pd_3(dba)_2$	PPh_3	DMBQ	DMSO	80	21
15	$Pd(OAc)_2$	PPh_3	DMBQ	DMF	80	N.D.
16	$Pd(OAc)_2$	PPh_3	DMBQ	DMA	80	Trace
17	$Pd(OAc)_2$	PPh_3	DMBQ	Dioxane	80	Trace
18	$Pd(OAc)_2$	PPh_3	DMBQ	DCE	80	Trace
19	$Pd(OAc)_2$	PPh_3	DMBQ	DCM	80	Trace

20	$Pd(OAc)_2$	PPh_3	DMBQ	NMP	80	Trace
21	$Pd(OAc)_2$	PPh_3	DMBQ	THF	80	Trace
22	$Pd(OAc)_2$	PPh_3	DMBQ	DMSO	r.t.	Trace
23	$Pd(OAc)_2$	PPh_3	DMBQ	DMSO	55	52
24	$Pd(OAc)_2$	PPh_3	DMBQ	DMSO	60	70
25	$Pd(OAc)_2$	PPh_3	DMBQ	DMSO	65	89
26	$Pd(OAc)_2$	PPh_3	DMBQ	DMSO	70	77
27	$Pd(OAc)_2$	PPh_3	DMBQ	DMSO	75	70
28	$Pd(OAc)_2$	PPh_3	DMBQ	DMSO	85	60
29	$Pd(OAc)_2$	PPh_3	DMBQ	DMSO	90	55
30	$Pd(OAc)_2$	PPh_3	DMBQ	DMSO	95	50

[a] A mixture of **1a** (0.2 mmol, 2.0 equiv), **2a** (0.1 mmol, 1 equiv), catalyst (10 mol %), ligand (20 mol %), oxidant (2 equiv) and solvent (2 mL) was sealed in a 25 mL Schlenk tube at 65 °C for 24 h. NQ was 1,4-naphthoquinone; o-NQ was 1,2-naphthoquinone, DMBQ was 2,6-dimethylcyclohexa-2,5-diene-1,4-dione. [b] Determined by GC-MS using dodecane as the internal standard.

D. General Procedure for Synthesis of Dienones

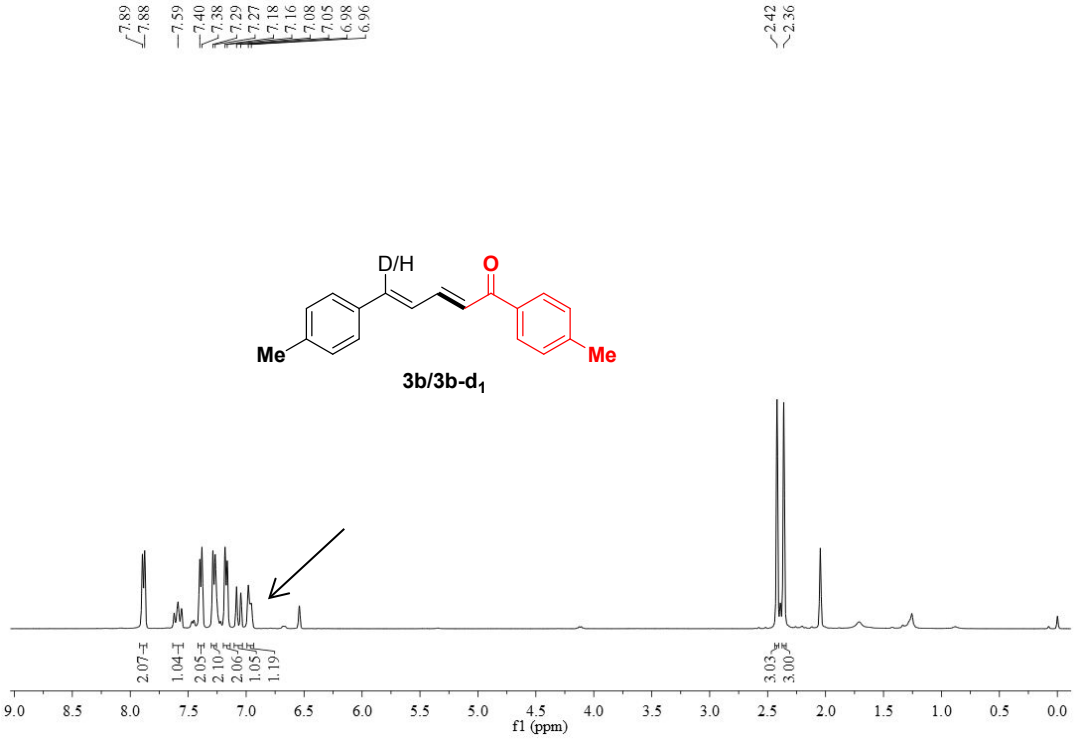


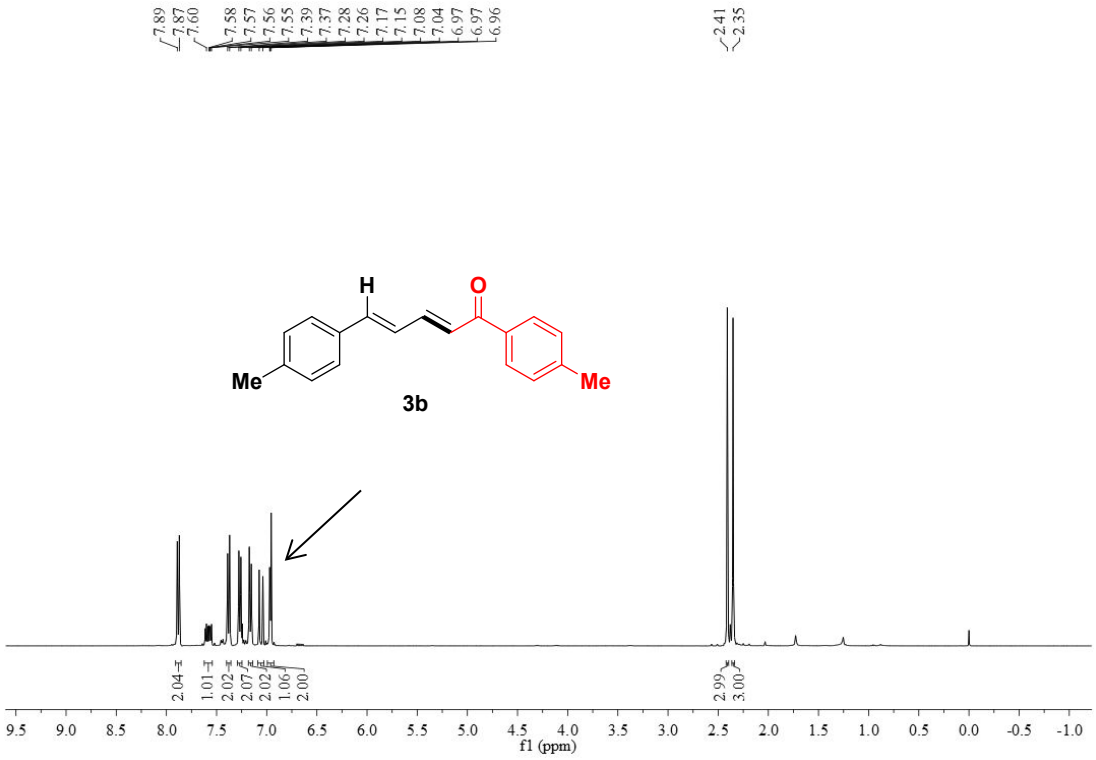
In a 25 mL sealed test tube, a mixture of olefins **1** (0.25 mmol), Sulfoxonium Ylides **2a** (0.1 mmol), $Pd(OAc)_2$ (10 mol %), DMBQ (2 equiv), PPh_3 (20 mol %) and 2 mL of anhydrous DMSO was vigorously stirred together at 65 °C for 24 h. After completion of the reaction and quenched by saturated brines, the mixture was extracted with ethyl acetate (3 × 10 mL). The combined ethyl acetate layer was then dried over anhydrous sodium sulfate and concentrated in vacuum. Further purification by flash column chromatography on silica gel (eluting with petroleum ether/ethyl acetate) afforded the pure product **3**.

E. Intramolecular Kinetic Isotope Effect Experiment

In a 25 mL sealed test tube, a mixture of 1-(allyl-1-d)-4-methylbenzene **1b-*d*$_1$** (0.2 mmol),

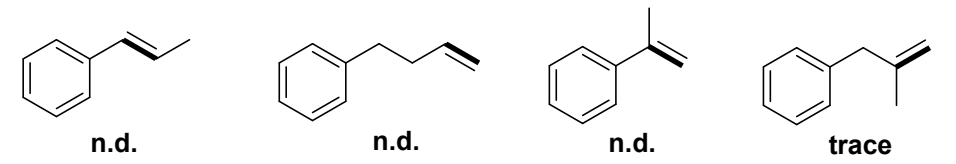
sulfoxonium ylides **2a** (0.1 mmol), $Pd(OAc)_2$ (10 mol %), DMBQ (2 equiv), PPh_3 (20 mol %) and 2 mL of anhydrous DMSO was vigorously stirred together at 65 °C for 24 h. After completion of the reaction and quenched by saturated brines, the mixture was extracted with ethyl acetate (3 × 10 mL). The combined ethyl acetate layer was then dried over anhydrous sodium sulfate and concentrated in vacuum. Further purification by flash column chromatography on silica gel (eluting with petroleum ether/ethyl acetate) afforded the pure product **3b-*d*$_1$** in 55% yield. The KIE value (K_H/K_D = 4) was determined on the basis of ^{1}H NMR analysis. Data for compounds **3b-d1**: Data for compounds **3b-d$_1$**: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 7.6 Hz, 2H), 7.62 - 7.56 (m, 1H), 7.39 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 7.06 (d, J = 12.0 Hz, 1H), 6.97 (d, J = 8.0 Hz, 1.19H).





F. The Investigation of Special Alkenes

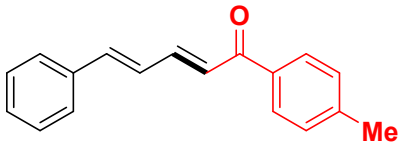
Unsuccessful Substrates



Reaction conditions: olefins **1** (0.25 mmol), sulfoxonium ylide **2a** (0.1 mmol), $Pd(OAc)_2$ (10 mol %), DMBQ (2 equiv), PPh_3 (20 mol %) and 2 mL of anhydrous DMSO was vigorously stirred together at 65 ^oC for 24 h.

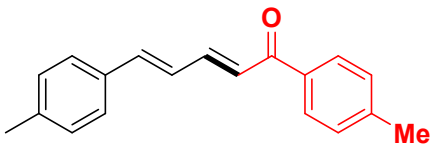
G. Analysis Data for the Products

(2*E*,4*E*)-5-Phenyl-1-(*p*-tolyl)penta-2,4-dien-1-one (3a)



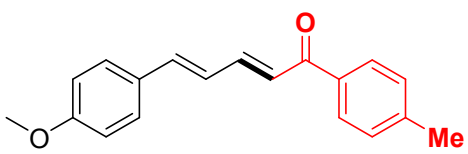
22.1 mg, 89% yield; yellow solid, Mp=88-89 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.0 Hz, 2H), 7.62 - 7.56 (m, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.36 (t, J = 6.0 Hz, 2H), 7.33 - 7.25 (m, 3H), 7.11 - 7.00 (m, 3H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 144.3, 143.4, 141.6, 136.1, 135.6, 129.3, 129.1, 128.8, 128.5, 127.2, 127.0, 125.5, 21.6; IR (KBr): 3919, 3740, 3646, 2907, 1645, 1495, 1249, 1012 cm^{-1}; HRMS (EI, m/z): $[M+Na]^+$ Calcd. for $C_{18}H_{16}NaO$, 271.1093, found, 271.1097.

(2*E*,4*E*)-1,5-Di-*p*-tolylpenta-2,4-dien-1-one (3b)



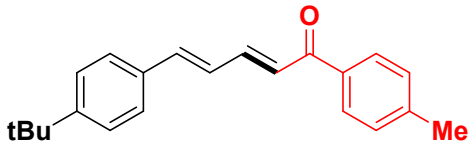
22.3 mg, 85% yield; yellow solid, Mp=124-125 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.0 Hz, 2H), 7.61 - 7.55 (m, 1H), 7.38 (d, J = 8.0 Hz, 2H), 7.27 (d, J = 8.0 Hz, 2H), 7.16 (d, J = 8.0 Hz, 2H), 7.06 (d, J = 16.0 Hz, 1H), 6.97 - 6.96 (m, 2H), 2.41 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 144.7, 143.3, 141.7, 139.4, 135.7, 133.4, 129.5, 129.2, 128.5, 127.2, 126.1, 124.9, 21.6, 21.3; IR (KBr): 3838, 3032, 2918, 1652, 1574, 999, 816, 725 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{19}H_{18}NaO$, 285.1250, found, 285.1255.

(2*E*,4*E*)-5-(4-Methoxyphenyl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3c)



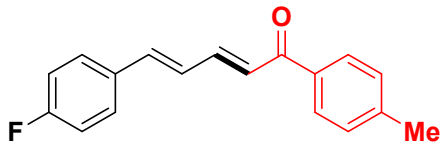
23.1 mg, 83% yield; yellow solid, Mp=96-97 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.0 Hz, 2H), 7.61 - 7.50 (m, 1H), 7.43 (d, J = 8.0 Hz, 2H), 7.28 - 7.25 (m, 2H), 7.04 (d, J = 16.0 Hz, 2H), 6.93 - 6.88 (m, 4H), 3.82 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 160.5, 144.9, 143.3, 141.4, 135.8, 130.3, 129.2, 128.7, 128.4, 124.9, 124.3, 114.3, 55.3, 21.6; IR (KBr): 3858, 3462, 2912, 1648, 1576, 1346, 999, 679 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{19}H_{18}NaO_2$, 301.1199,found, 301.1202.

(2*E*,4*E*)-5-(4-(*tert*-Butyl)phenyl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3d)



24.9 mg, 82% yield; yellow solid, Mp=83-84 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.0 Hz, 2H), 7.63 - 7.56 (m, 2H), 7.45 - 7.43 (m, 2H), 7.39 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 7.08 (d, J = 16.0 Hz, 1H), 7.00 - 7.68 (m, 2H), 2.42 (s, 3H), 1.33 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.0, 152.7, 144.8, 143.4, 141.7, 135.8, 133.5, 129.3, 128.5, 127.1, 126.3, 125.8, 125.0, 34.8, 31.2, 21.7; IR (KBr): 3842, 3462, 2916, 1645, 1458, 1169, 1003, 784 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{22}H_{24}NaO$, 327.1719, found, 327.1723.

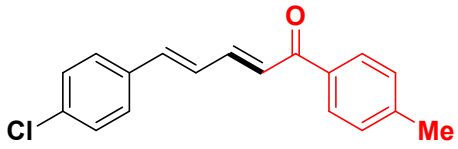
(2*E*,4*E*)-5-(4-Fluorophenyl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3e)



21.3 mg, 80% yield; yellow solid, Mp=102-103 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.0 Hz, 2H), 7.60 - 7.53 (m, 1H), 7.48 - 7.43 (m, 2H), 7.28 (d, J = 8.0 Hz, 2H), 7.10 - 7.03 (m, 3H), 6.94 - 6.92 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 163.2 (d, J = 250.0 Hz,), 144.2, 143.5, 140.2, 135.7, 132.5 (d, J = 3.4 Hz), 129.3, 128.9 (d, J = 8.2 Hz), 128.5, 126.8 (d, J =

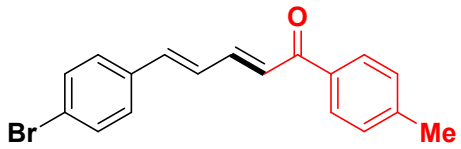
2.4 Hz), 125.5, 115.9 (d, J = 21.9 Hz), 21.7; IR (KBr): 3422, 3036, 2918, 1648, 1575, 1232, 996, 822 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{18}H_{16}FO$, 267.1180, found, 267.1183.

(2*E*,4*E*)-5-(4-Chlorophenyl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3f)



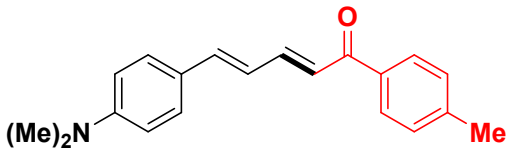
22.0 mg, 78% yield; yellow solid, Mp=133-134 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.0 Hz, 2H), 7.56 (dd, J = 15.2, 9.6 Hz, 1H), 7.40 (d, J = 12.0 Hz, 1H), 7.32 (d, J = 8.0 Hz, 1H), 7.29 - 7.26 (m, 2H), 7.10 (d, J = 12.0 Hz, 1H), 7.01 - 6.90 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8), 143.9, 143.5, 139.9, 135.5, 134.8, 134.6, 129.3, 129.0, 128.5, 128.3, 127.5, 125.7, 21.6; IR (KBr): 3840, 3481, 2909, 1650, 1584, 1250, 1002, 681 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{18}H_{16}ClO$, 283.0084, found, 283.0086.

(2*E*,4*E*)-5-(4-Bromophenyl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3g)



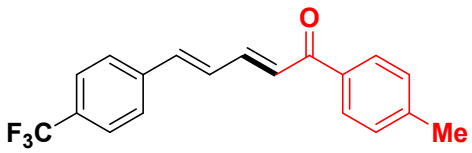
23.5 mg, 72% yield; yellow solid, Mp=142-143 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.0 Hz, 2H), 7.56 (dd, J = 15.0, 10.4 Hz, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.34 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.0 Hz, 1H), 7.11 (d, J = 16.0 Hz, 1H), 7.03 - 6.89 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8, 143.8, 143.6, 139.9, 135.5, 135.1, 131.9, 129.3, 128.6, 128.5, 127.6, 125.9, 123.1, 21.6; IR (KBr): 3463, 3030, 2916, 1649, 1575, 1253, 1001, 871 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{18}H_{16}BrO$, 327.0379, found, 327.0383.

(2*E*,4*E*)-5-(4-(Dimethylamino)phenyl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3h)



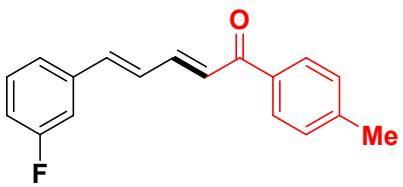
21.8 mg, 75% yield; yellow solid, Mp=126-127 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.0 Hz, 2H), 7.63 - 7.56 (m, 1H), 7.29 - 7.22 (m, 3H), 7.08 (d, J = 16.0 Hz, 1H), 7.00 (d, J = 8.3 Hz, 0H), 6.90 (d, J = 8.0 Hz, 2H), 6.81 (s, 1H), 6.72 (dd, J = 8.0, 2.4 Hz, 1H), 2.98 (s, 6H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.0, 144.7, 143.4, 142.8, 136.9, 135.7, 129.4, 129.2, 128.5, 126.6, 125.1, 113.7, 111.4, 40.6, 21.6; IR (KBr): 3024, 2918, 1655, 1587, 1346, 1269, 1004, 839 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{20}H_{22}NO$, 292.1696, found, 292.1700.

(2*E*,4*E*)-1-(p-Tolyl)-5-(4-(trifluoromethyl)phenyl)penta-2,4-dien-1-one



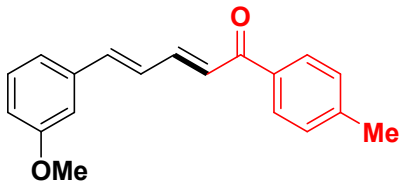
19.9 mg, 63% yield; yellow solid, Mp=116-117 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.90 (d, J = 6.6 Hz, 2H), 7.60 - 7.58 (m, 5H), 7.29 (d, J = 8.0 Hz, 2H), 7.18 - 6.97 (m, 3H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 143.7, 143.3, 139.5, 139.4, 135.4, 130.5 (q, J = 32.5 Hz), 129.3, 129.3, 128.5, 127.3, 126.8, 125.73 (q, J = 3.6 Hz), 123.9 (q, J = 272.0 Hz), 21.6; IR (KBr): 3050, 1659, 1588, 1324, 1255, 1119, 997 cm^{-1}; HRMS (ESI, m/z): [M+H]+ Calcd. for $C_{19}H_{16}F_3O$, 317.1148, found, 317.1151.

(2*E*,4*E*)-5-(3-Fluorophenyl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3j)



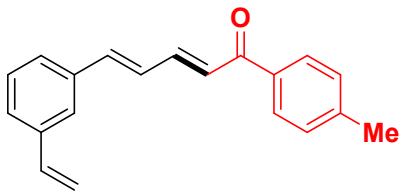
21.8 mg, 82% yield; yellow solid, Mp=97-98 °C; ^{1}H NMR (400 MHz, CDCl3) δ 7.89 (d, J = 8.0 Hz, 2H), 7.55 (dd, J = 14.4, 10.4 Hz, 1H), 7.34 - 7.30 (m, 1H), 7.27 (d, J = 8.0 Hz, 2H), 7.23 (d, J = 8.0 Hz, 1H), 7.19 - 7.16 (m, 1H), 7.11 (d, J = 16.0 Hz, 1H), 7.02 - 6.94 (m, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.7, 163.0 (d, J = 246.1 Hz), 143.6, 139.9 (d, J = 2.8 Hz), 138.4 (d, J = 7.7 Hz), 135.5, 130.3 (d, J = 8.4 Hz), 129.3, 128.5, 128.2, 126.2, 123.2 (d, J = 2.8 Hz), 115.8 (d, J = 21.5 Hz), 113.3 (d, J = 21.9 Hz), 21.6; IR (KBr): 3864, 3449, 3296, 2956, 1660, 1588, 1255, 1010, 825 cm^{-1}; HRMS (ESI, m/z): [M+ H]$^+$ Calcd. for $C_{18}H_{16}FO$, 267.1180, found, 267.1185.

(2*E*,4*E*)-5-(3-Methoxyphenyl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3k)



20.3 mg, 73% yield; yellow solid, Mp=88-89 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.0 Hz, 2H), 7.57 (dd, J = 14.4, 9.6 Hz, 1H), 7.26 (dd, J = 8.0, 2.4 Hz, 3H), 7.10 - 7.06 (m, 3H), 7.00 - 6.95 (m, 3H), 6.86 (dd, J = 8.0, 2.4 Hz, 1H), 3.82 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8, 159.8, 144.2, 143.4, 141.4, 137.5, 135.5, 129.7, 129.2, 128.4, 127.2, 125.5, 119.9, 114.9, 112.2, 55.2, 21.6; IR (KBr): 3884, 3033, 2955, 1644, 1585, 1181, 1010, 826 cm^{-1}; HRMS (ESI, m/z): [M+H]$^+$ Calcd. for $C_{19}H_{18}O_2$, 301.1199, found, 301.1204.

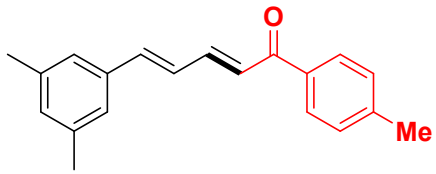
(2*E*,4*E*)-1-(*p*-Tolyl)-5-(3-vinylphenyl)penta-2,4-dien-1-one (3l)



21.1 mg, 77% yield; yellow solid, Mp=107-108 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.0

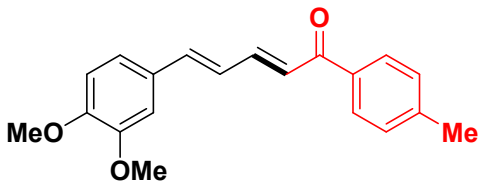
Hz, 2H), 7.59 (dd, J = 14.4, 9.6 Hz, 1H), 7.49 (s, 1H), 7.39 - 7.31 (m, 3H), 7.30 - 7.24 (m, 2H), 7.10 (d, J = 16.0 Hz, 1H), 6.99 (d, J = 4.0 Hz, 1H), 6.75 - 6.68 (m, 1H), 5.79 (d, J = 20.0 Hz, 1H), 5.29 (d, J = 12.0 Hz, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8, 144.2, 143.4, 141.3, 138.1, 136.4, 136.3, 135.6, 129.2, 128.9, 128.5, 127.2, 126.8, 126.5, 125.5, 125.2, 114.6, 21.6; IR (KBr): 3834, 3446, 2916, 1650, 1572, 1257, 1139, 1014 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{20}H_{18}O$, 275.1430; found, 275.1428.

(2*E*,4*E*)-5-(3,5-Dimethylphenyl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3m)



22.4 mg, 81% yield; yellow solid, Mp=89-90 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.0 Hz, 2H), 7.57 (dd, J = 14.4, 10.4 Hz, 1H), 7.26 (d, J = 8.0 Hz, 1H), 7.10 - 7.04 (m, 3H), 6.99 - 6.89 (m, 3H), 2.41 (s, 3H), 2.32 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 144.6, 143.3, 141.9, 138.2, 136.0, 135.7, 130.9, 129.2, 128.4, 126.6, 125.1, 125.0, 21.6, 21.2; IR (KBr): 3676, 2909, 2840, 1652, 1565, 1244, 1000, 814 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{20}H_{21}O$, 277.1587; found, 277.1585.

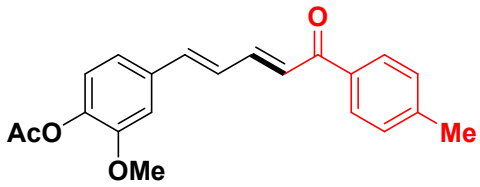
(2*E*,4*E*)-5-(3,4-Dimethoxyphenyl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3n)



22.2 mg, 72% yield; yellow solid, Mp=85-86 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.0 Hz, 2H), 7.59 (dd, J = 14.4, 9.6 Hz, 1H), 7.29 - .7.26 (m, 3H), 7.09 - 7.07 (m, 1H), 7.05 (d, J = 4.0 Hz, 2H), 6.94 - 6.89 (m, 2H), 6.86 (d, J = 8.0 Hz, 1H), 3.94 (s, 3H), 3.91 (s, 3H), 2.42 (s, 3H); ^{13}C

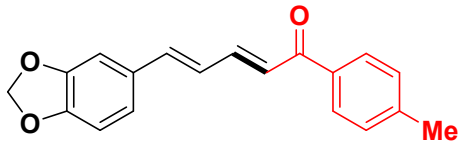
NMR (100 MHz, $CDCl_3$) δ 189.8, 150.2 149.1, 144.7, 143.2, 141.6, 135.7, 129.2, 129.2, 128.4, 125.1, 124.4, 121.3, 111.1, 109.1, 55.8, 55.8, 21.5; IR (KBr): 3468, 3620, 2912, 1648, 1580, 1254, 996, 699 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{20}H_{21}O_3$, 309.1485, found, 309.1488.

(2*E*,4*E*)-5-(Benzo[d][1,3]dioxol-5-yl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3o)



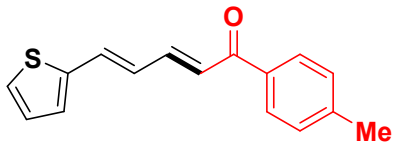
20.8 mg, 62% yield; yellow solid, Mp=94-95 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, J = 8.0 Hz, 2H), 7.61 - 7.54 (m, 1H), 7.29 - 7.26 (m, 3H), 7.13 - 7.07 (m, 3H), 6.97 - 6.95 (m, 2H), 3.88 (s, 3H), 2.42 (s, 3H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 168.9, 151.3, 144.1, 143.5, 140.8, 140.5, 135.6, 135.2, 129.3, 128.5, 127.3, 125.6, 123.1, 120.1, 110.6, 55.9, 21.6, 20.6; IR (KBr): 3842, 3431, 2917, 1652, 1576, 998, 818 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{21}H_{20}NaO_4$, 359.1254, found, 359.1259.

(2*E*,4*E*)-5-(Benzo[d][1,3]dioxol-5-yl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3p)



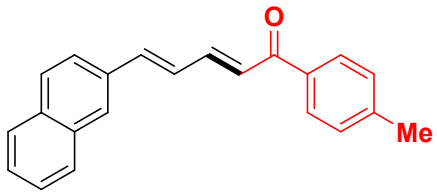
20.4 mg, 70% yield; yellow solid, Mp=116-117 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.0 Hz, 2H), 7.56 (dd, J = 14.4, 10.4 Hz, 1H), 7.27 (d, J = 8.0 Hz, 2H), 7.06 - 7.02 (m, 2H), 6.95 - 6.93 (m, 1H), 6.89 - 6.78 (m, 3H), 5.98 (s, 2H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 148.6, 148.3, 144.6, 143.3, 141.4, 135.7, 130.7, 129.2, 128.4, 125.3, 124.6, 123.1, 108.5, 105.8, 101.4, 21.6; IR (KBr): 3942, 3469, 1643, 1522, 1385, 1000, 788, 673 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{19}H_{17}O_3$, 293.1172, found, 293.1174.

(2*E*,4*E*)-5-(Thiophen-2-yl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3q)



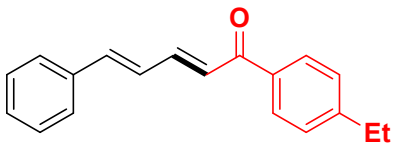
18.5 mg, 73% yield; yellow solid, Mp=111-112 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, J = 8.0 Hz, 2H), 7.53 (dd, J = 14.4, 11.2 Hz, 1H), 7.30 - 7.25 (m, 3H), 7.13 - 7.01 (m, 4H), 6.84 - 6.80 (m, 1H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.6, 143.8, 143.4, 141.6, 135.6, 133.9, 129.2, 128.7, 128.4, 127.9, 126.8, 126.5, 124.9, 21.6; IR (KBr): 3453, 3082, 1638, 1575, 1252, 1060, 788 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{16}H_{15}OS$, 255.0838, found, 255.0841.

(2*E*,4*E*)-5-(Naphthalen-2-yl)-1-(*p*-tolyl)penta-2,4-dien-1-one (3r)



25.3 mg, 85% yield; yellow solid, Mp=97-98 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (d, J = 8.0 Hz, 1H), 7.91 (d, J = 8.0 Hz, 2H), 7.84 - 7.70 (m, 5H), 7.55 - 7.46 (m, 3H), 7.28 (d, J = 8.0 Hz, 2H), 7.15 - 7.06 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.9, 144.5, 143.5, 138.2, 135.6, 133.7, 133.3, 131.1, 129.6, 129.5, 129.3, 128.7, 128.5, 126.6, 126.1, 125.6, 125.5, 124.1, 123.2, 21.6; IR (KBr): 3065, 1652, 1583, 1251, 1122, 1003, 884, 735 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{22}H_{18}NaO$, 321.1250, found, 321.1253.

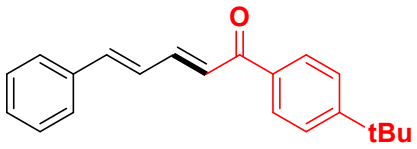
(*2E,4E*)-1-(4-(*tert*-butyl)phenyl)-5-phenylpenta-2,4-dien-1-one (4a)



22.0 mg, 84% yield; yellow solid, Mp=74-75 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.91 (d, J = 8.0 Hz, 2H), 7.61 - 7.55 (m, 1H), 7.47 (d, J = 8.0 Hz, 2H), 7.34 (t, J = 8.0 Hz, 2H), 7.20 - 7.27 (m, 3H), 7.08 (d, J = 16.0 Hz, 1H), 7.04 - 6.93 (m, 2H), 2.69 (q, J = 8.0 Hz, 2H), 1.25 (t, J = 8.0Hz,

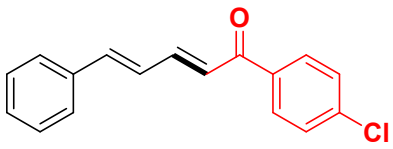
3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8, 149.5, 144.2, 141.5, 136.1, 135.8, 129.0, 128.7, 128.5, 128.0, 127.2, 126.9, 125.4, 28.8, 15.1; IR (KBr): 3782, 2910, 1762, 1583, 1257, 1060, 825 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{19}H_{19}O$, 263.1430, found, 263.1428.

(2*E*,4*E*)-1-(4-(*tert*-Butyl)phenyl)-5-phenylpenta-2,4-dien-1-one (4b)



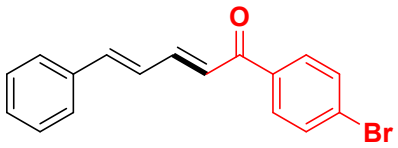
23.2 mg, 80% yield; yellow solid, Mp=87-88 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, J = 8.0 Hz, 2H), 7.59 (dd, J = 14.2, 9.2 Hz, 1H), 7.48 (dd, J = 8.0, 3.2 Hz, 4H), 7.37 - 7.30 (m, 3H), 7.10 (d, J = 16.0 Hz, 1H), 7.02 - 6.95 (m, 2H), 1.34 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.8, 156.3, 144.3, 141.5, 136.1, 135.5, 129.1, 128.8, 128.3, 127.2, 126.9, 125.5, 125.4, 35.0, 31.0; IR (KBr): 3841, 2915, 1762, 1588, 1265, 1196, 1020, 832 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{21}H_{22}NaO$, 313.1563, found, 313.1568.

(2*E*,4*E*)-1-(4-Chlorophenyl)-5-phenylpenta-2,4-dien-1-one(4c)



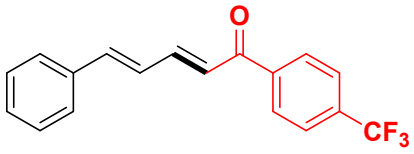
22.2 mg, 83% yield; yellow solid, Mp=131-132 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.92 (d, J = 8.0 Hz, 2H), 7.64 - 7.58 (m, 1H), 7.51 - 7.45 (m, 4H), 7.40 - 7.31 (m, 3H), 7.06 - 7.02 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.1, 145.3, 142.4, 139.1, 136.5, 135.9, 129.8, 129.3, 128.9, 127.3, 126.8, 124.8; IR (KBr): 3462, 1647, 1291, 1005, 678, 549 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{17}H_{13}ClNaO$, 291.0547, found, 291.0545.

(2*E*,4E)-1-(4-Bromophenyl)-5-phenylpenta-2,4-dien-1-one (4d)



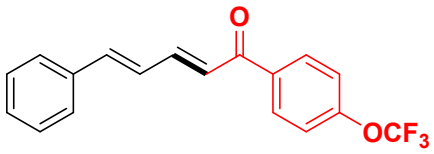
19.3mg, 62% yield; yellow solid, Mp=144-145 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 (d, J = 8.0 Hz, 2H), 7.64 - 7.59 (m, 3H), 7.50 (d, J = 8.0 Hz, 2H), 7.40 - 7.33 (m, 3H), 7.05 - 7.02 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.4, 145.4, 142.5, 137.0, 136.0, 131.2, 129.9, 129.4, 128.9, 127.7, 127.4, 126.8, 124.8; IR (KBr): 3782, 3469, 3026, 2919, 1649, 1588, 1090, 992 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{17}H_{13}BrNaO$, 335.0042, found, 335.0050.

(2*E*,4*E*)-5-Phenyl-1-(4-(trifluoromethyl)phenyl)penta-2,4-dien-1-one (4e)



21.8 mg, 72% yield; yellow solid, Mp=132-133 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (d, J = 8.0 Hz, 2H), 7.74 (d, J = 8.0 Hz, 2H), 7.65 - 7.59 (m, 1H), 7.50 (d, J = 8.0 Hz, 2H), 7.39 - 7.33 (m, 3H), 7.06 - 7.02 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.5, 146.0, 142.9, 141.1, 135.9, 133.8 (q, J = 32.6 Hz), 129.5, 128.9, 128.6, 127.4, 126.6, 125.6 (q, J = 3.7 Hz), 124.8, 123.7 (q, J = 273.4 Hz); IR (KBr): 3843, 3469, 2910, 1651, 1576, 997, 789, 674 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{18}H_{14}F_3O$, 303.0991, found, 303.0992.

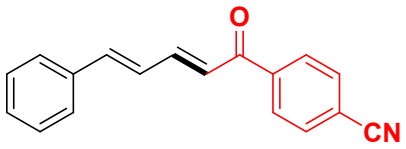
(2*E*,4*E*)-5-Phenyl-1-(4-(trifluoromethoxy)phenyl)penta-2,4-dien-1-one (4f)



21.9 mg, 69% yield; yellow solid, Mp=109-110 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.02 (d, J = 8.0 Hz, 2H), 7.64 - 7.58 (m, 1H), 7.50 (d, J = 8.0 Hz, 2H), 7.39 - 7.29 (m, 5H), 7.06 - 7.01 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.8, 152.2, 145.4, 142.5, 136.5, 135.9, 130.3, 129.3, 128.8,

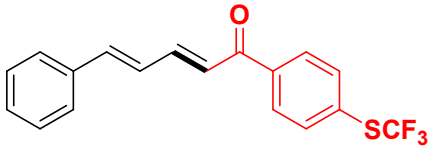
127.3, 126.7, 124.7, 120.4, 120.3 (q, J = 258.7 Hz); IR (KBr): 3844, 3672, 3005, 2873, 2813, 1594, 1359, 665 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{18}H_{13}F_3NaO_2$, 341.0760, found, 341.0766.

4-((2*E*,4*E*)-5-Phenylpenta-2,4-dienoyl)benzonitrile (4g)



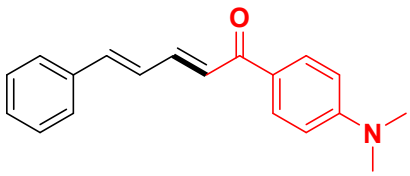
13.7mg, 53% yield; yellow solid, Mp=146-147 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, J = 8.0 Hz, 2H), 7.79 (d, J = 8.0 Hz, 2H), 7.63 (dd, J = 14.8, 9.2 Hz, 1H), 7.51 (d, J = 8.0 Hz, 2H), 7.41 - 7.33 (m, 3H), 7.10 - 6.99 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.0, 146.5, 143.4, 141.5, 135.8, 132.4, 129.6, 128.9, 128.7, 127.5, 126.5, 124.4, 118.1, 115.8; IR (KBr): 3473, 2913, 1650, 1581, 1282, 1125, 995 cm^{-1}; HRMS (ESI, m/z): $[M+ H]^+$ Calcd. for $C_{18}H_{14}NO$, 260.1070, found, 260.1069.

(2*E*,4*E*)-5-Phenyl-1-(4-((trifluoromethyl)thio)phenyl)penta-2,4-dien-1-one (4h)



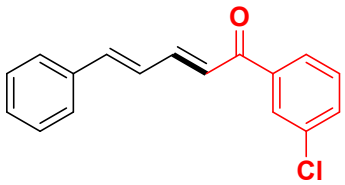
23.4mg, 70% yield; yellow solid, Mp=99-100 °C; ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, J = 8.0 Hz, 2H), 7.75 (d, J = 8.0 Hz, 2H), 7.65 - 7.58 (m, 1H), 7.50 (d, J = 8.0 Hz, 2H), 7.39 - 7.31 (m, 3H), 7.05 - 7.02 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 189.5, 145.9, 142.9, 139.9, 135.9, 135.8, 129.5, 129.3 (q, J = 308.4 Hz), 129.1, 128.9, 127.4, 126.7, 124.8, 120.5; IR (KBr): 3836, 3565, 3021, 2910, 1652, 1557, 1324, 1117 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{18}H_{14}F_3OS$, 335.0712, found, 335.0710.

(2*E*,4*E*)-1-(4-(Dimethylamino)phenyl)-5-phenylpenta-2,4-dien-1-one (4i)



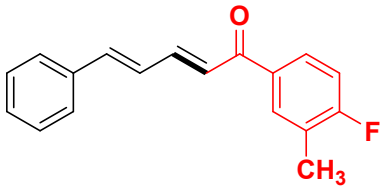
18.0mg, 65% yield; yellow solid, Mp=153-154 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, J = 8.0 Hz, 2H), 7.58 (dd, J = 14.8, 10.2 Hz, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.36 (t, J = 8.0 Hz, 2H), 7.31 (d, J = 8.0 Hz, 1H), 7.15 (d, J = 16.0 Hz, 1H), 7.06 - 6.98 (m, 2H), 6.70 (d, J = 8.0 Hz, 2H), 3.07 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 187.8, 153.3, 142.6, 140.4, 136.4, 130.7, 128.8, 128.8, 127.4, 127.1, 126.2, 125.7, 110.9, 40.1; IR (KBr): 3842, 3741, 2990, 2891, 1647, 1528, 938 cm^{-1}; HRMS (ESI, m/z): $[M+Na]^+$ Calcd. for $C_{19}H_{20}NO$, 278.1539, found, 278.1538.

(2*E*,4*E*)-1-(3-Chlorophenyl)-5-phenylpenta-2,4-dien-1-one (4j)



21.7mg, 81% yield; yellow solid, Mp=68-69 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 (t, J = 1.6 Hz, 1H), 7.83 (d, J = 8.0 Hz, 2H), 7.63 - 7.57 (m, 1H), 7.53 - 7.48 (m, 3H), 7.43 - 7.32 (m, 4H), 7.03 - 7.00 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.9, 145.6, 142.6, 139.8, 135.9, 134.8, 132.5, 129.9, 129.4, 128.8, 128.4, 127.3, 126.7, 126.4, 124.7; IR (KBr): 3488, 2960, 1655, 1590, 1262, 1006, 826 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{17}H_{14}ClO$, 269.0728, found, 269.0727.

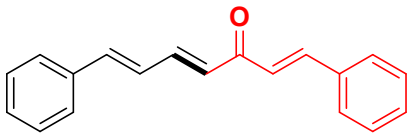
(2*E*,4*E*)-1-(4-Fluoro-3-methylphenyl)-5-phenylpenta-2,4-dien-1-one (4k)



22.6 mg, 85% yield; yellow solid, Mp=98-99 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.86 - 7.79 (m, 2H), 7.62 - 7.55 (m, 1H), 7.49 (d, J = 8.0 Hz, 2H), 7.38 - 7.31 (m, 3H), 7.10 - 7.04 (m, 2H), 7.01 -

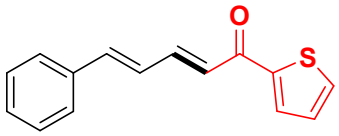
7.00 (m, 2H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.9, 164.1 (d, J = 253.0 Hz), 144.7, 141.9, 136.0, 134.2 (d, J = 3.3 Hz), 132.2 (d, J = 6.5 Hz), 129.2, 128.8, 128.19 (d, J = 9.2 Hz), 127.2, 126.8, 125.3 (d, J = 17.8 Hz), 125.0, 115.15 (d, J = 23.0 Hz) 14.5; IR (KBr): 3746, 3491, 2963, 1669, 1387, 1252, 998, 677 cm^{-1}; HRMS (ESI, m/z): $[M+H]^+$ Calcd. for $C_{18}H_{16}FO$, 267.1180, found, 267.1177.

(1*E*,4*E*,6*E*)-1,7-Diphenylhepta-1,4,6-trien-3-one (4l)



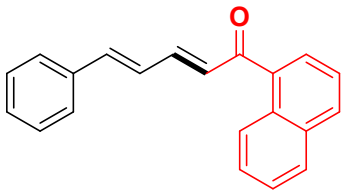
17.9 mg, 69% yield; yellow solid, Mp=109-110 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, J = 16.0 Hz, 1H), 7.61 - 7.59 (m, 2H), 7.54 - 7.49 (m, 3H), 7.41 - 7.31 (m, 7H), 7.00 (t, J = 13.6 Hz, 3H), 6.64 (d, J = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 188.9, 143.4, 142.9, 141.6, 136.1, 134.9, 130.4, 129.2, 128.9, 128.8, 128.3, 127.3, 126.9, 126.3, 125.5; IR (KBr): 3869, 3463, 1646, 1387, 1252, 998, 677 cm^{-1}; HRMS (EI, m/z): $[M+H]^+$ Calcd. for $C_{19}H_{17}O$, 261.1274, found, 261.1273.

(2*E*,4*E*)-5-Phenyl-1-(thiophen-2-yl)penta-2,4-dien-1-one (4m)



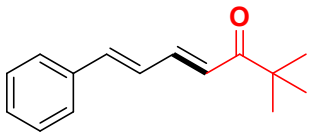
19.2 mg, 80% yield; yellow solid, Mp=80-81 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 4.0 Hz, 1H), 7.62 (dt, J = 16.0, 5.2 Hz, 2H), 7.48 (d, J = 8.0 Hz, 2H), 7.37 - 7.29 (m, 3H), 7.14 (t, J = 4.0 Hz, 1H), 7.00 - 6.96 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 181.9, 145.6, 143.9, 141.9, 135.9, 133.6, 131.5, 129.2, 128.8, 128.1, 127.2, 126.6, 124.9; IR (KBr): 3842, 2960, 2889, 1588, 1252, 980, 830cm^{-1}; HRMS (ESI, m/z): $[M+ Na]^+$ Calcd. for $C_{15}H_{12}NaOS$, 263.0501; found, 263.0506.

(2*E*,4*E*)-5-Phenyl-1-(thiophen-2-yl)penta-2,4-dien-1-one (4n)



21.9 mg, 77% yield; yellow solid, Mp=86-87 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, J = 4.0 Hz, 1H), 7.62 (dt, J = 16.0, 5.2 Hz, 2H), 7.48 (d, J = 8.0 Hz, 2H), 7.37 - 7.29 (m, 3H), 7.14 (t, J = 4.0 Hz, 1H), 7.00 - 6.96 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 190.3, 144.8, 141.9, 136.2, 135.6, 135.5, 132.6, 129.8, 129.5, 129.3, 128.9, 128.6, 128.3, 127.8, 127.3, 127.0, 126.8, 125.5, 124.5; IR (KBr): 3034, 2921, 1739, 1654, 1580, 1444, 987 cm^{-1}; HRMS (ESI, m/z): [M+ H]$^+$ Calcd. for $C_{21}H_{17}O$, 285.1274; found, 285.1279.

(4*E*,6*E*)-2,2-Dimethyl-7-phenylhepta-4,6-dien-3-one (4o)



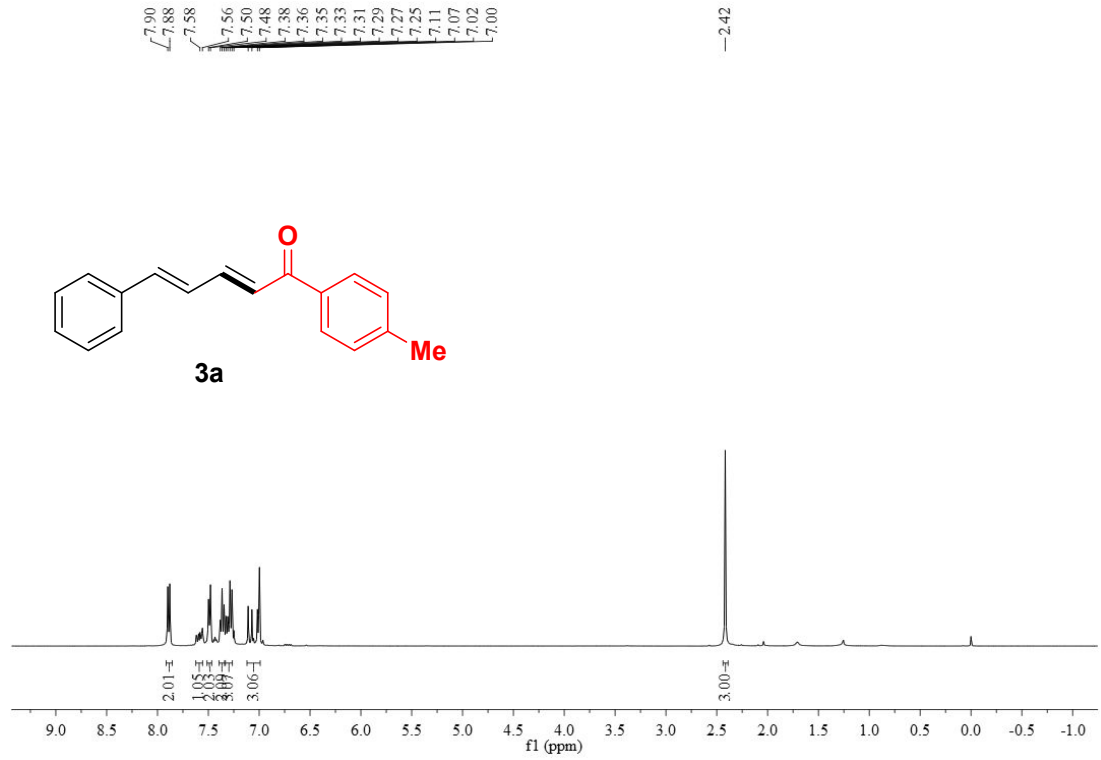
10.7 mg, 50% yield; yellow solid, Mp=56-57 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.47 (d, J = 8.0 Hz, 3H), 7.37 - 7.30 (m, 4H), 6.93 (d, J = 12.0 Hz, 1H), 6.68 (d, J = 16.0 Hz, 1H), 1.19 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 204.5, 142.8, 141.1, 136.3, 128.9, 128.8, 127.1, 126.9, 124.3, 43.0, 26.3; IR (KBr): 3461, 2919, 1739, 1654, 1459, 1325 1167, 1117 cm^{-1}; HRMS (ESI, m/z): [M+ Na]$^+$ Calcd. for $C_{15}H_{18}NaO$, 237.1250; found, 237.1247.

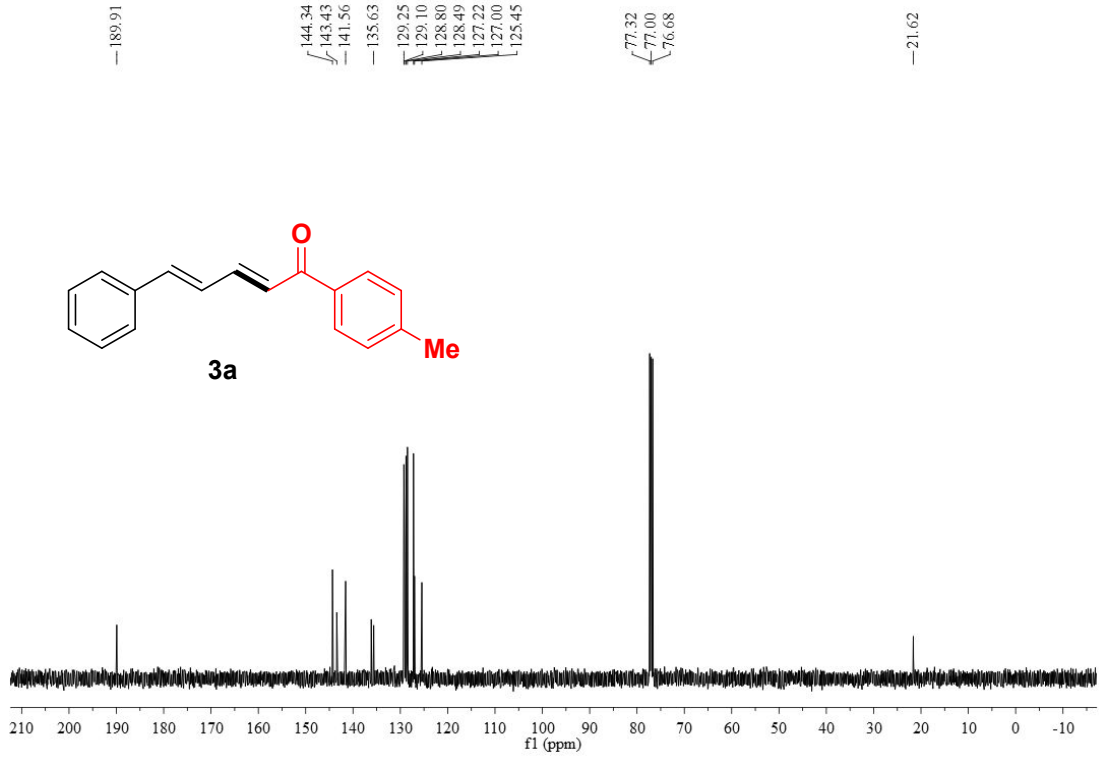
H. References

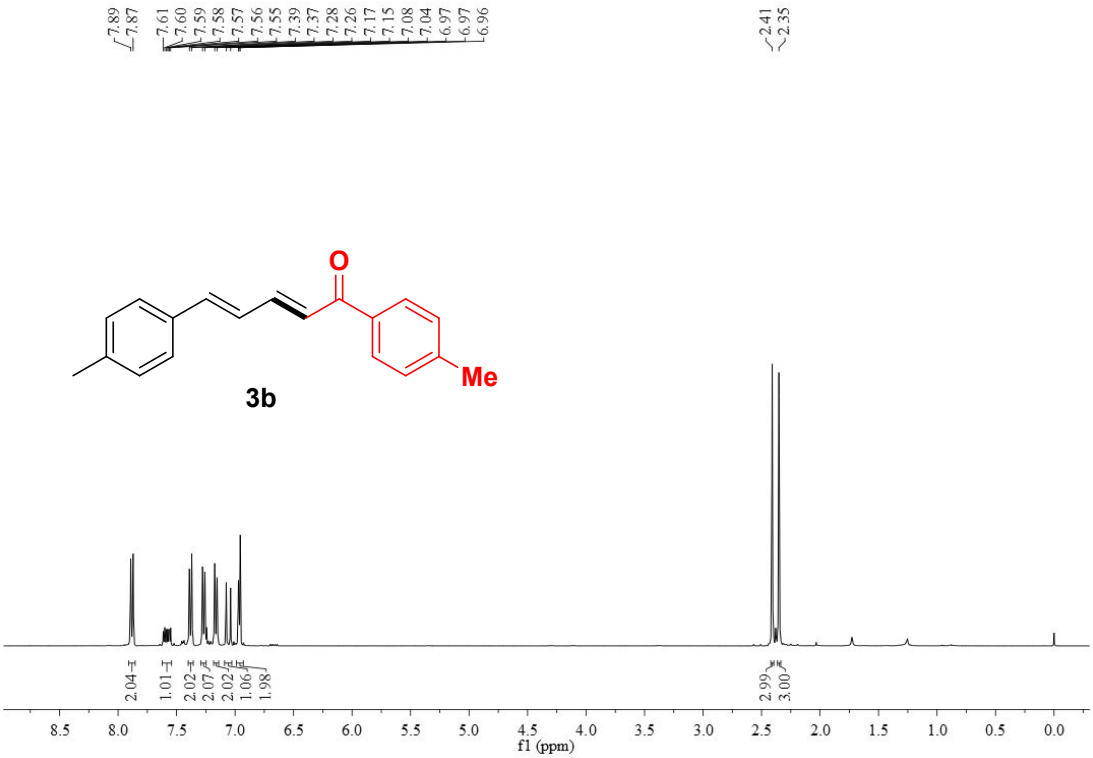
(1) Yang, W.; Chen, H.; Li, J.; Li, C.; Wu, W.; Jiang, H. *Chem. Commun.* **2015**, *51*, 9575.

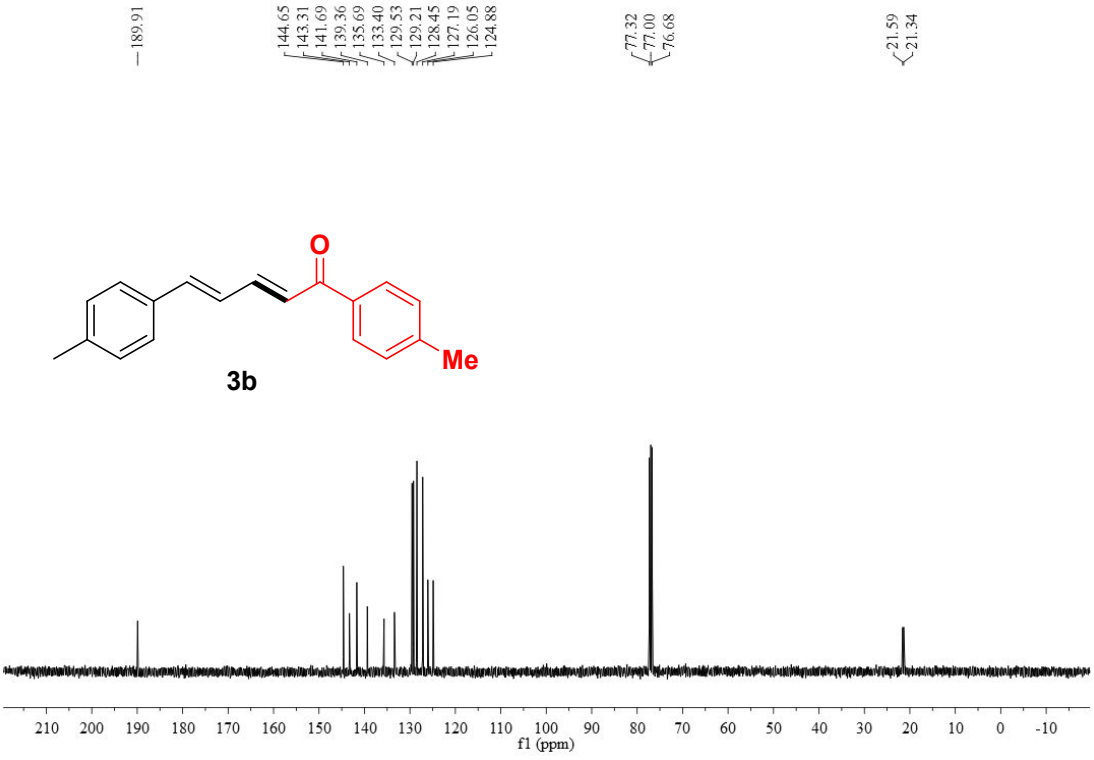
(2) Xu, Y.; Zhou, X.; Zheng, G.; Li, Xing. *Org. Lett.* **2017**, *19*, 5256.

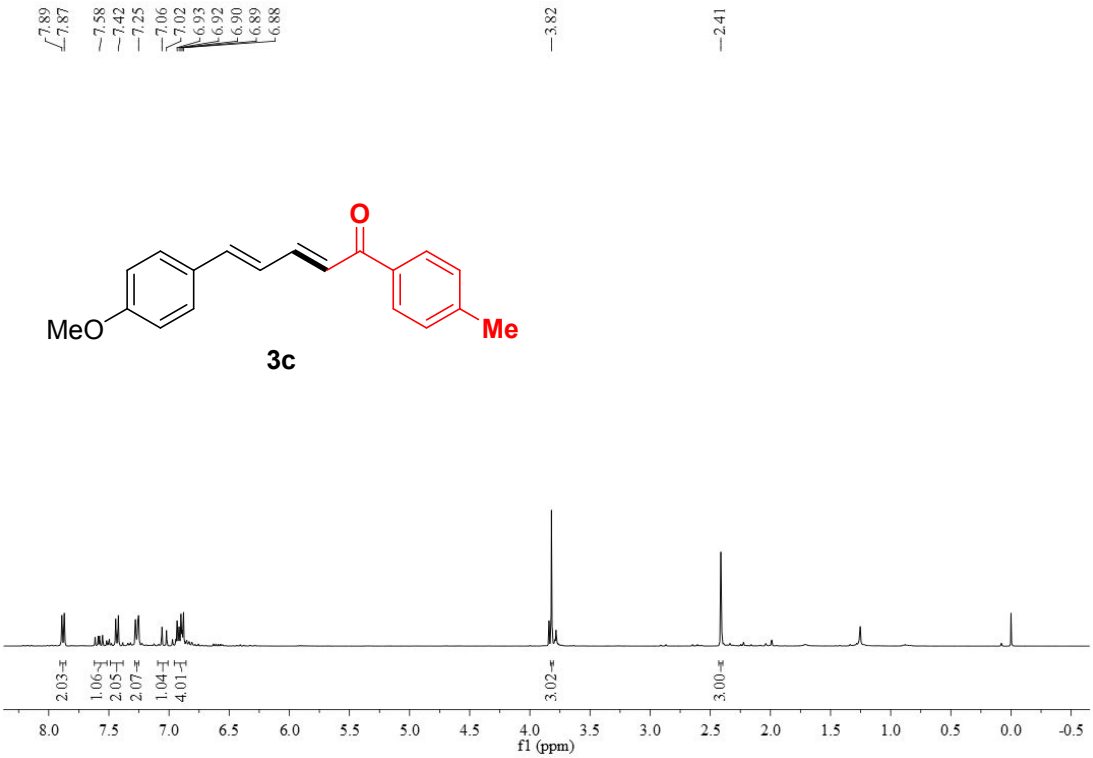
I. NMR Spectra of New Compounds

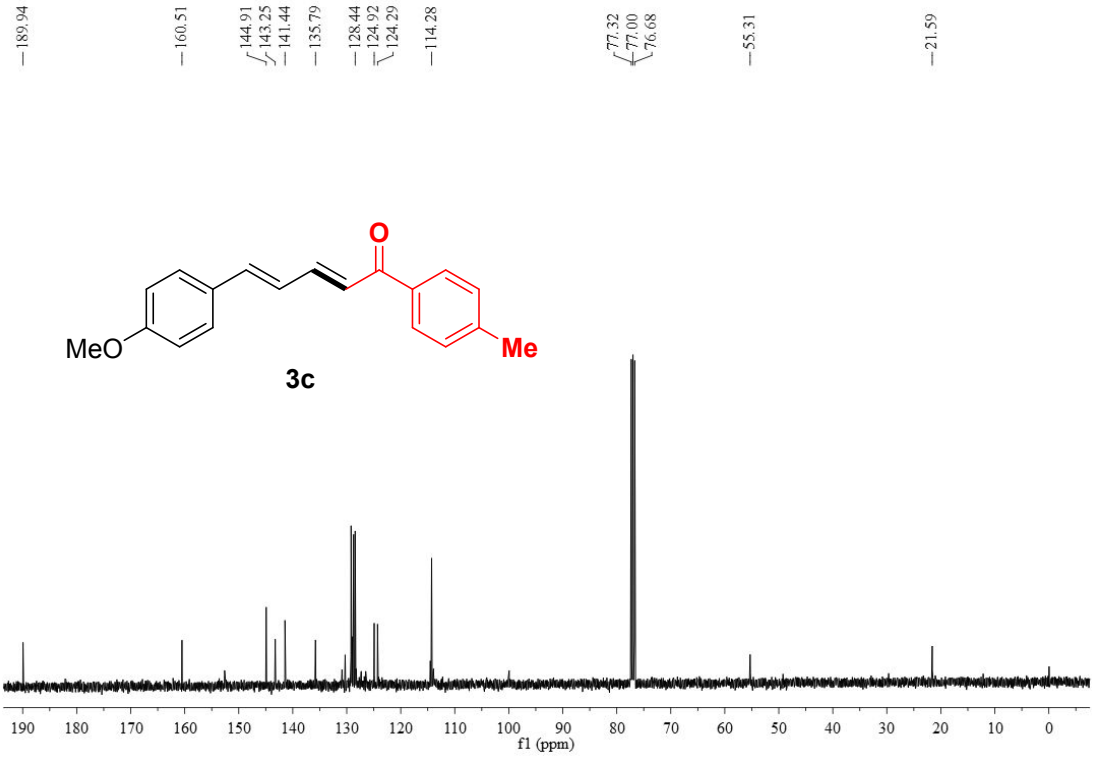


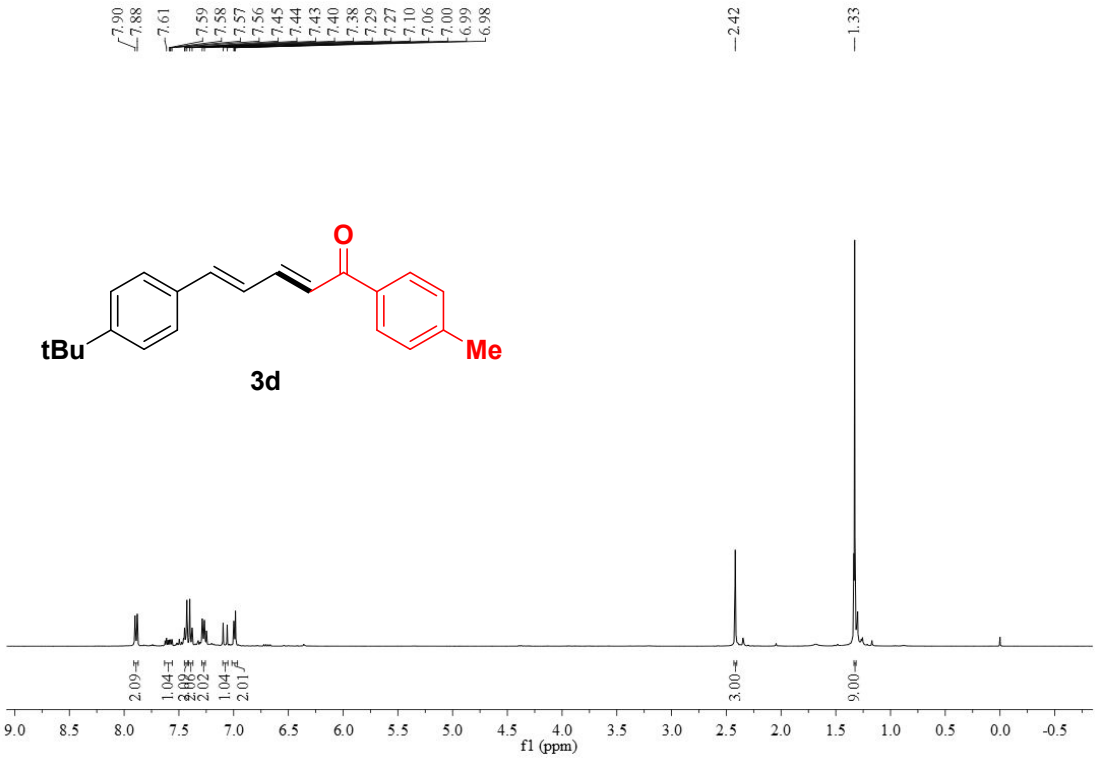


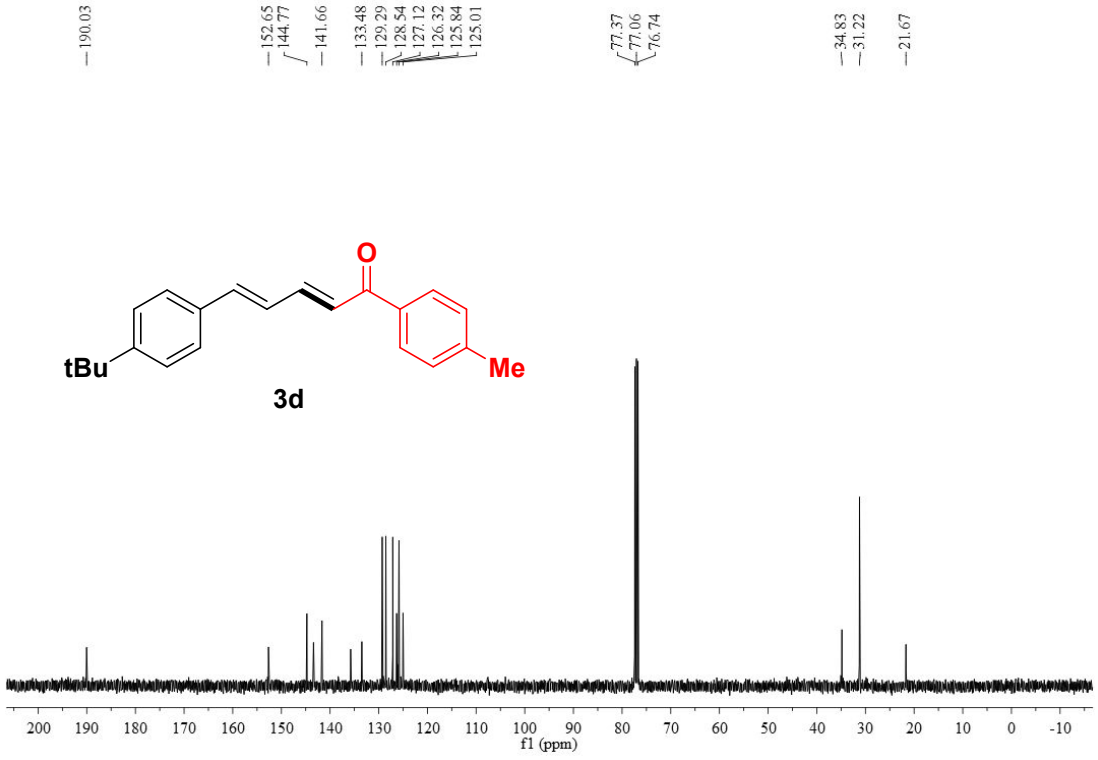

7.89
7.87
7.61
7.60
7.59
7.58
7.57
7.56
7.55
7.39
7.37
7.28
7.26
7.17
7.15
7.08
7.04
6.97
6.97
6.96
2.41
2.35
O
Me
3b
2.04
1.01
2.02
2.07
2.02
1.06
1.98
2.99
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

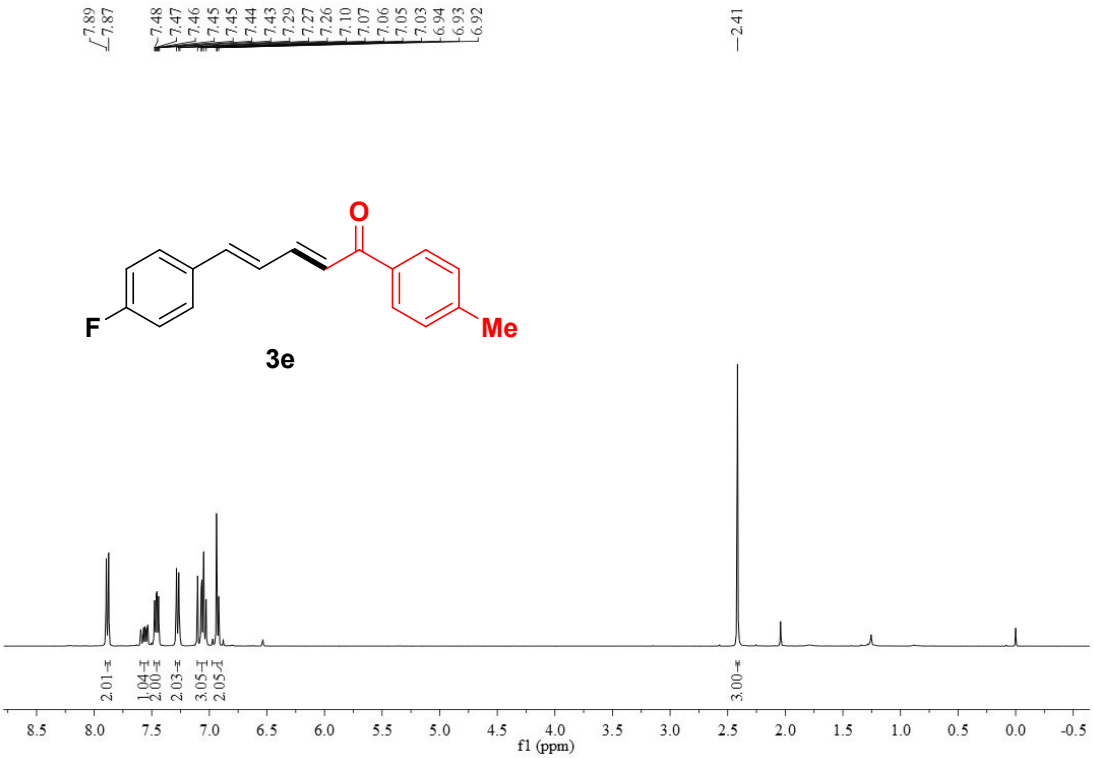

189.91
144.65
143.31
141.69
139.36
135.69
133.40
129.53
129.21
128.45
127.19
126.05
124.88
77.32
77.00
76.68
21.59
21.34
O
Me
3b
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

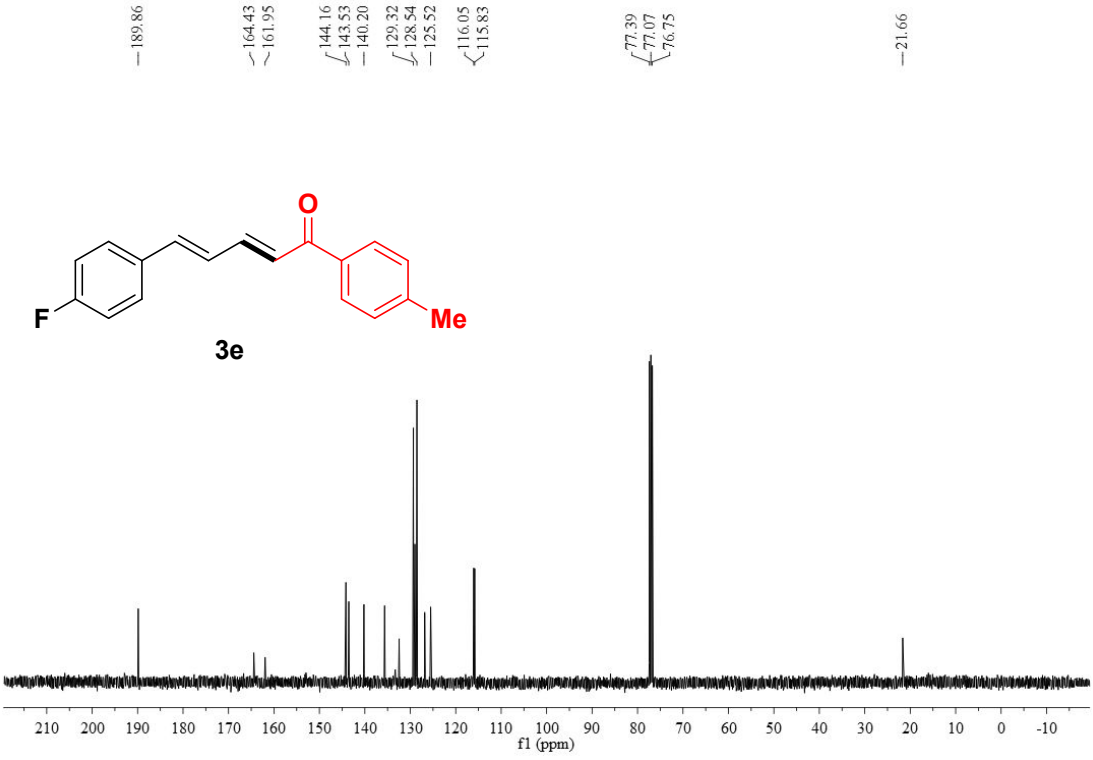

7.89
7.87
7.58
7.42
7.25
7.06
7.02
6.93
6.92
6.90
6.89
6.88
3.82
2.41
O
MeO
Me
3c
2.03
1.06
2.05
2.07
1.04
4.01
3.02
3.00
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

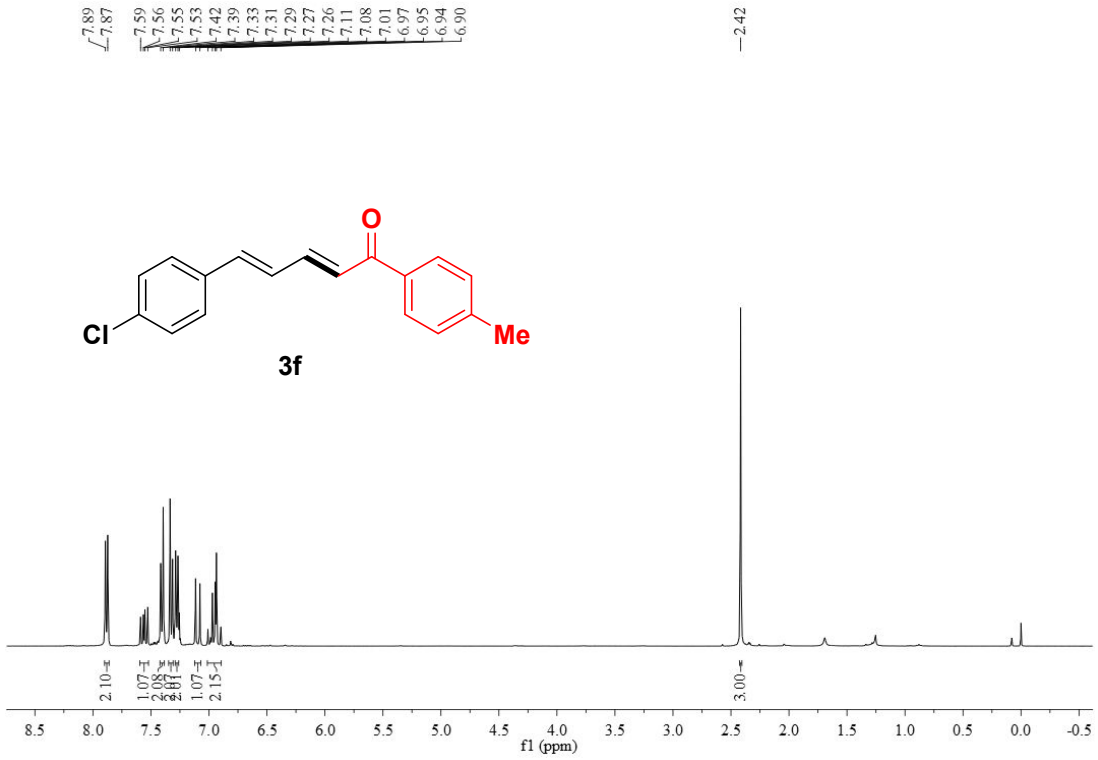

189.94
160.51
144.91
143.25
141.44
135.79
128.44
124.92
124.29
114.28
77.32
77.00
76.68
55.31
21.59
O
MeO
Me
3c
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

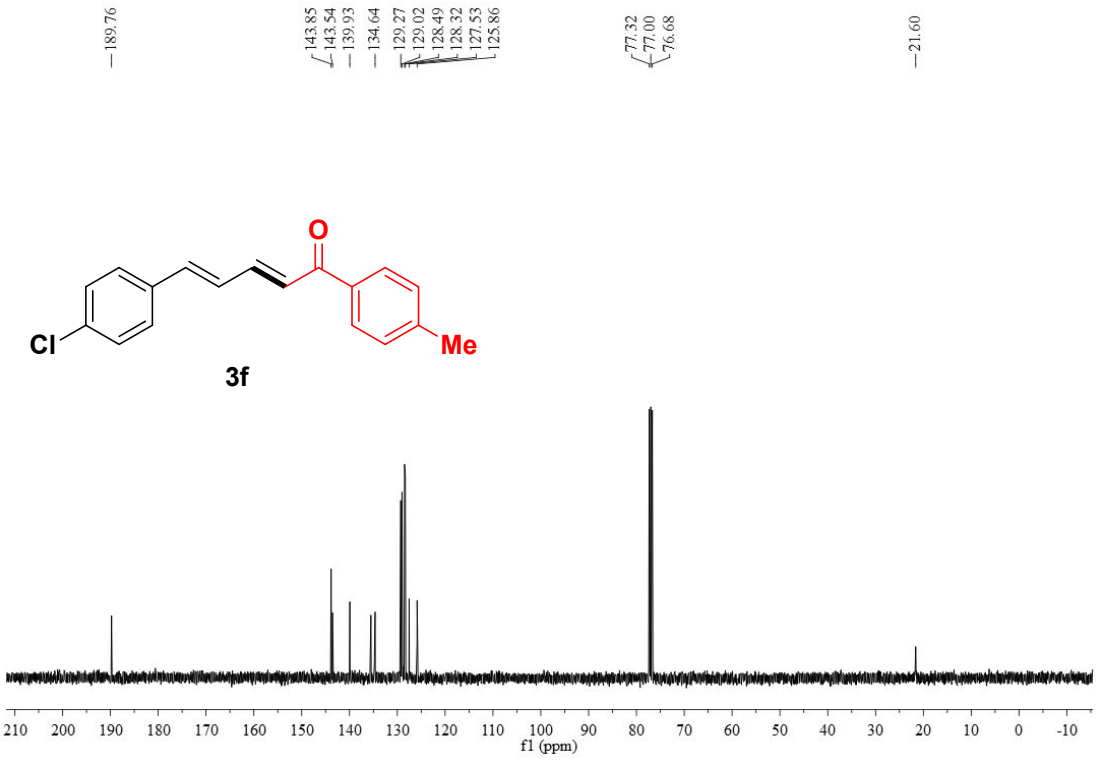

7.90
7.88
7.61
7.59
7.58
7.57
7.56
7.45
7.44
7.43
7.40
7.38
7.29
7.27
7.10
7.06
7.00
6.99
6.98
2.42
1.33
O
tBu
Me
3d
2.09
1.04
2.02
1.04
2.01
3.00
9.00
f1 (ppm)


190.03
152.65
144.77
141.66
133.48
129.29
128.54
127.12
126.32
125.84
125.01
77.37
77.06
76.74
34.83
31.22
21.67
O
tBu
Me
3d
f1 (ppm)

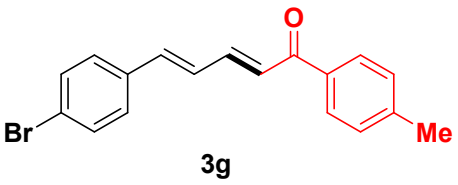

7.89
7.87
7.48
7.47
7.46
7.45
7.45
7.44
7.43
7.29
7.27
7.26
7.10
7.07
7.06
7.05
7.03
6.94
6.93
6.92
2.41
O
F
Me
3e
2.01
1.04
2.00
2.03
3.05
2.05
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


189.86
164.43
161.95
144.16
143.53
140.20
129.32
128.54
125.52
116.05
115.83
77.39
77.07
76.75
21.66
O
F
Me
3e
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)

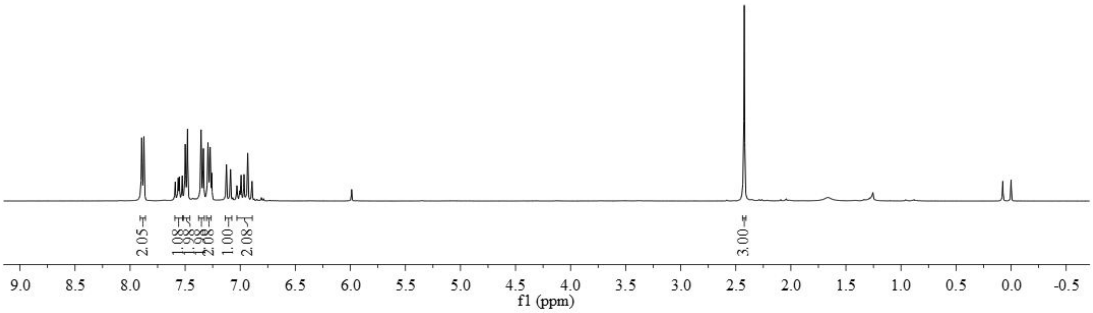

7.89
7.87
7.59
7.56
7.55
7.53
7.42
7.39
7.33
7.31
7.29
7.27
7.26
7.11
7.08
7.01
6.97
6.95
6.94
6.90
2.42
O
Cl
Me
3f
2.10
1.07
2.08
2.01
1.07
2.15
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


189.76
143.85
143.54
139.93
134.64
129.27
129.02
128.49
128.32
127.53
125.86
77.32
77.00
76.68
21.60
O
Cl
Me
3f
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)

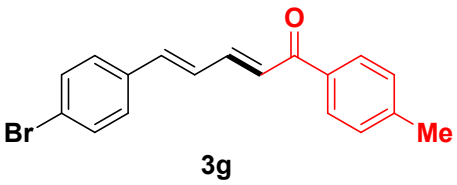

7.89
7.87
7.59
7.56
7.55
7.53
7.50
7.48
7.36
7.33
7.29
7.27
7.26
7.13
7.09
7.03
6.99
6.97
6.93
6.89
2.42


O
Br
Me

3g

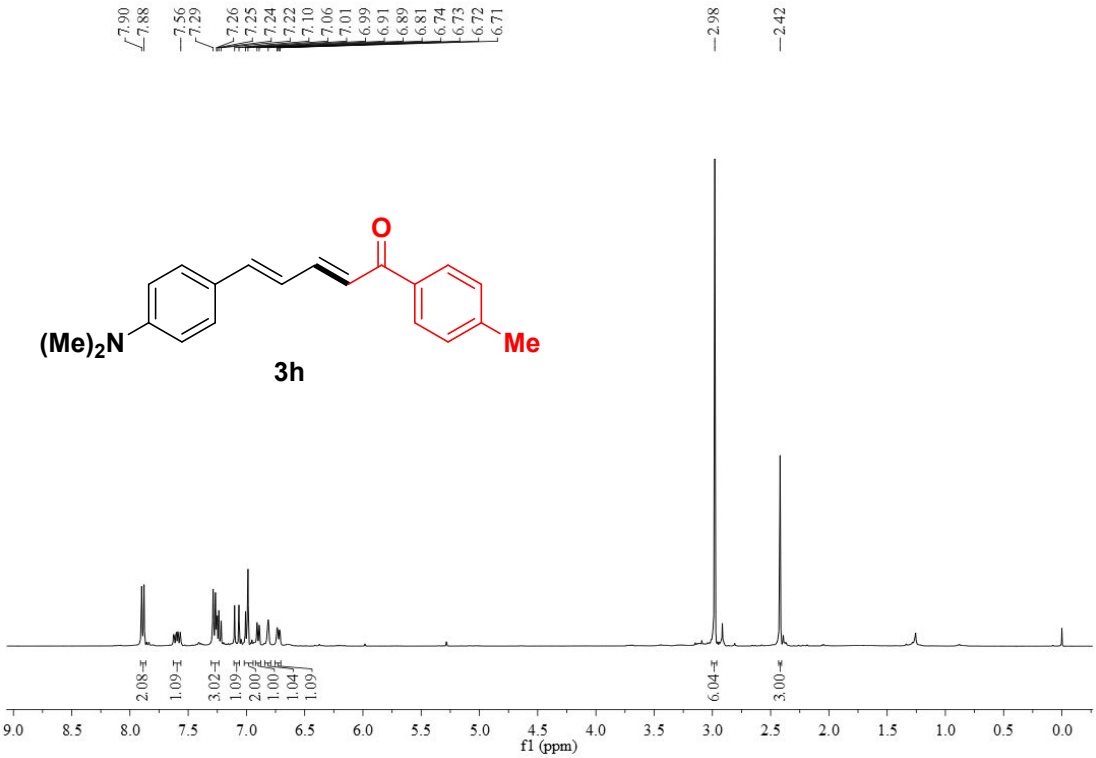

2.05
1.08
1.00
2.08
3.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

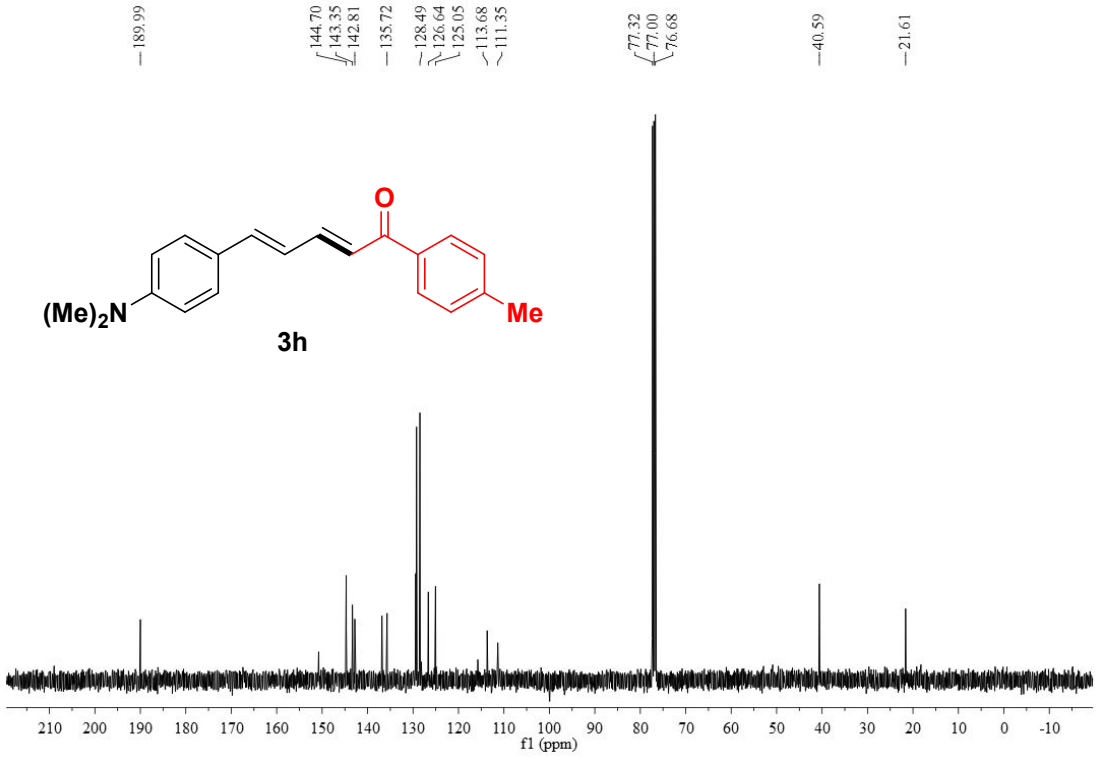

189.80
143.83
143.57
139.99
135.53
135.08
131.99
129.29
128.58
128.51
127.64
125.96
123.08
77.32
77.00
76.68
21.64

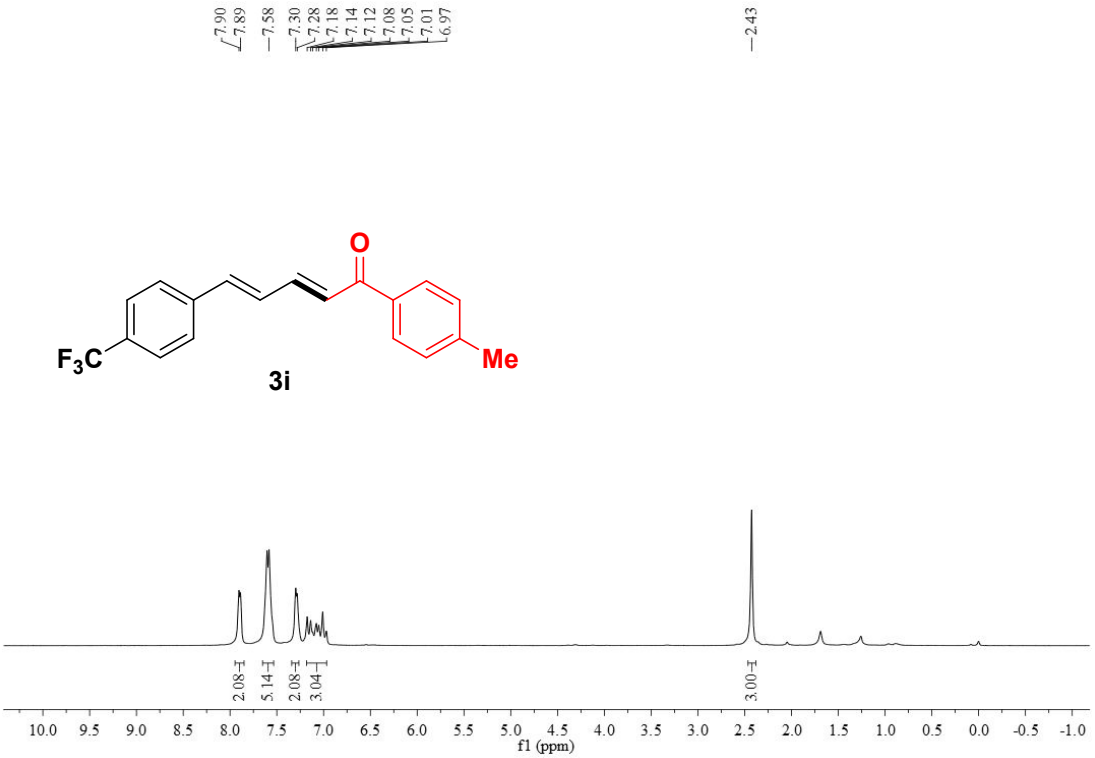

O
Br
Me

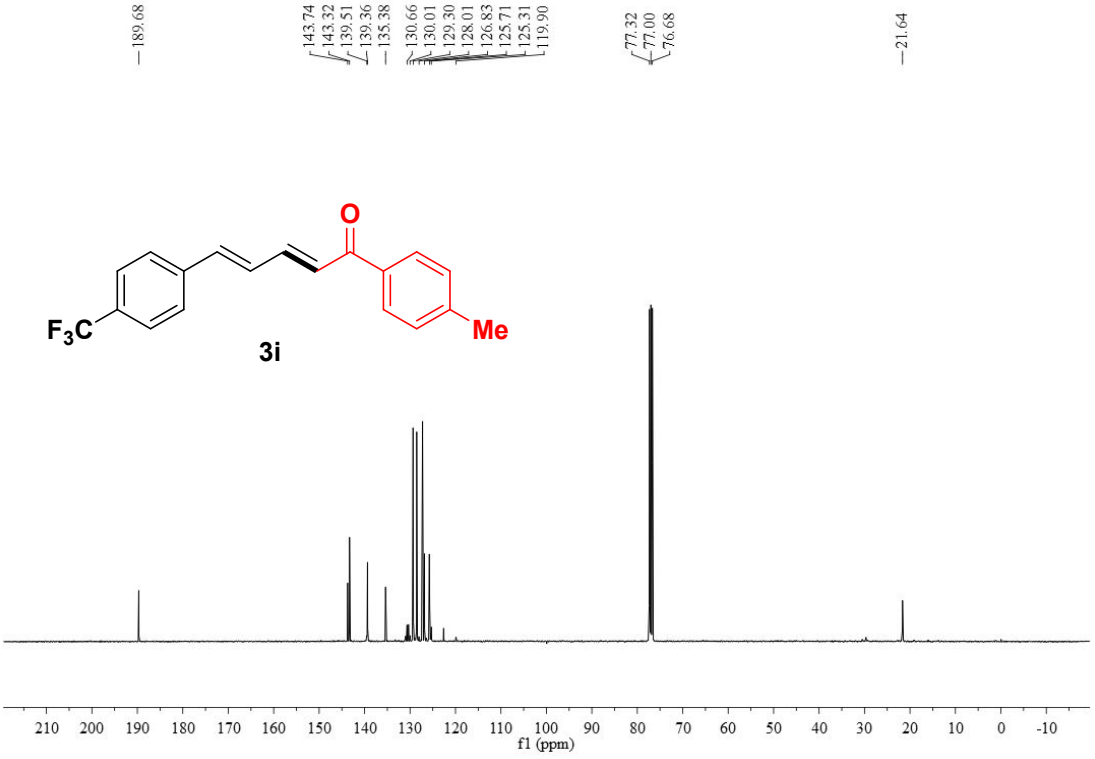
3g

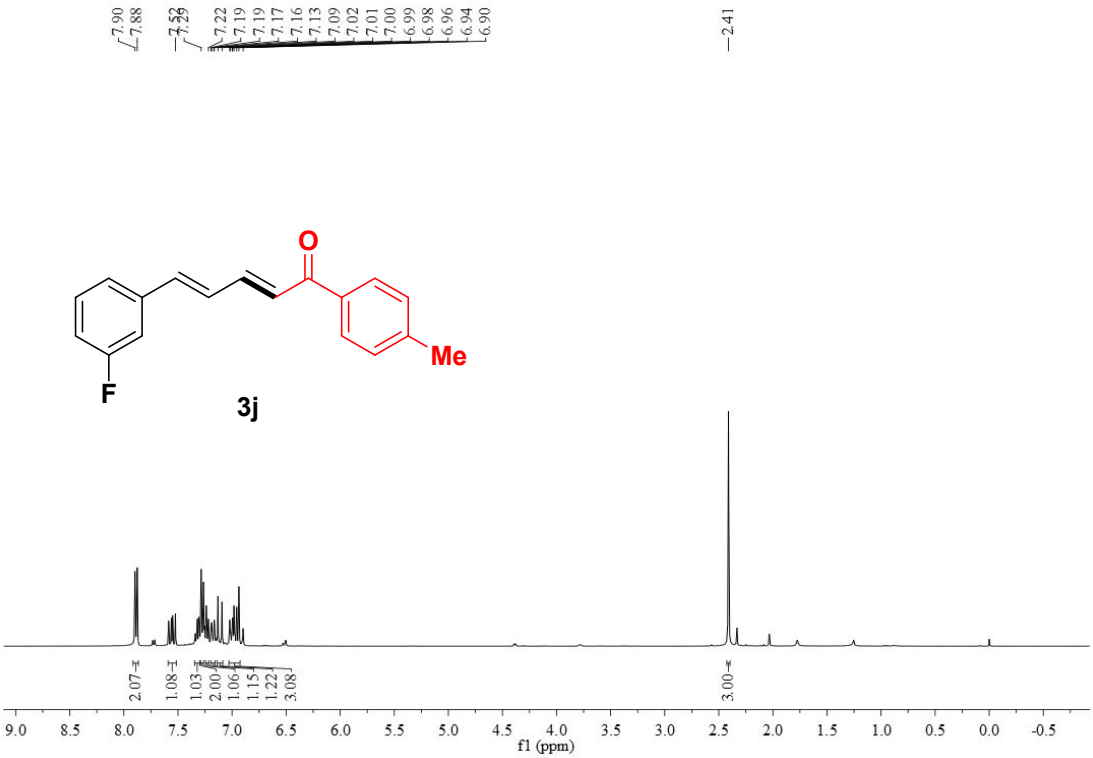
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

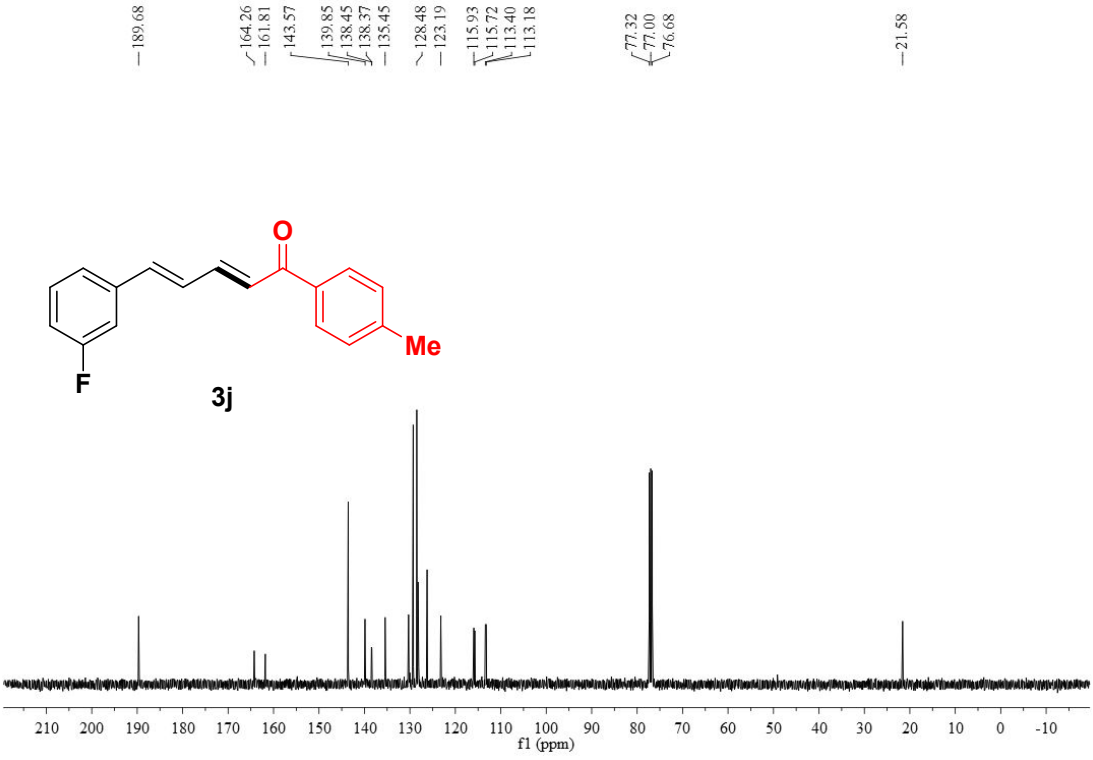

7.90
7.88
7.56
7.29
7.26
7.25
7.24
7.22
7.10
7.06
7.01
6.99
6.91
6.89
6.81
6.74
6.73
6.72
6.71
2.98
2.42
O
(Me)2N
Me
3h
2.08
1.09
3.02
1.09
2.00
1.00
1.04
1.09
6.04
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

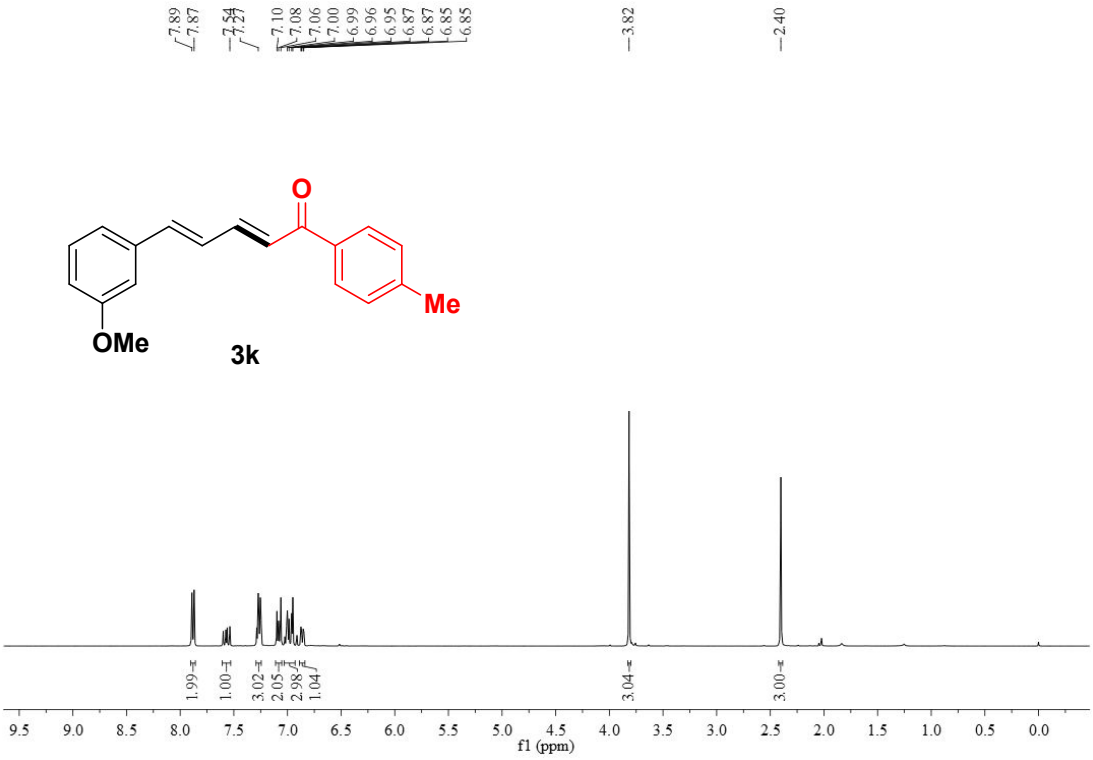

189.99
144.70
143.35
142.81
135.72
128.49
126.64
125.05
113.68
111.35
77.32
77.00
76.68
40.59
21.61
O
(Me)2N
Me
3h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

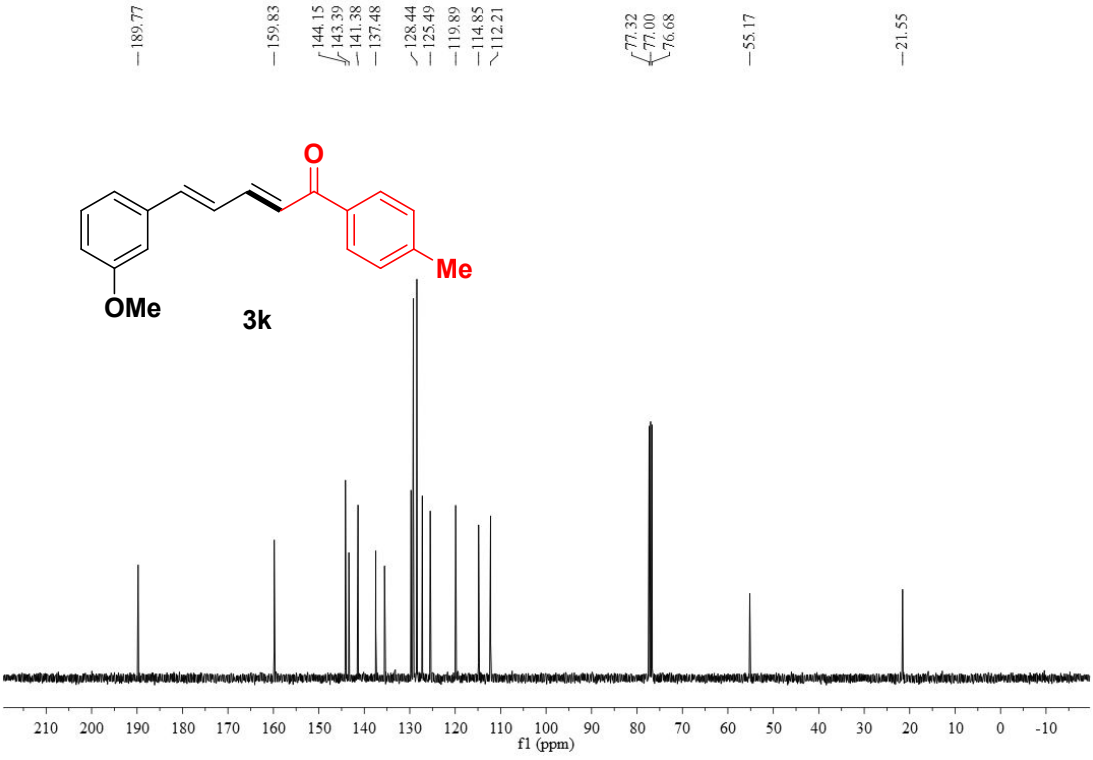

7.90
7.89
7.58
7.30
7.28
7.18
7.14
7.12
7.08
7.05
7.01
6.97
2.43
O
F3C
Me
3i
2.08
5.14
2.08
3.04
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

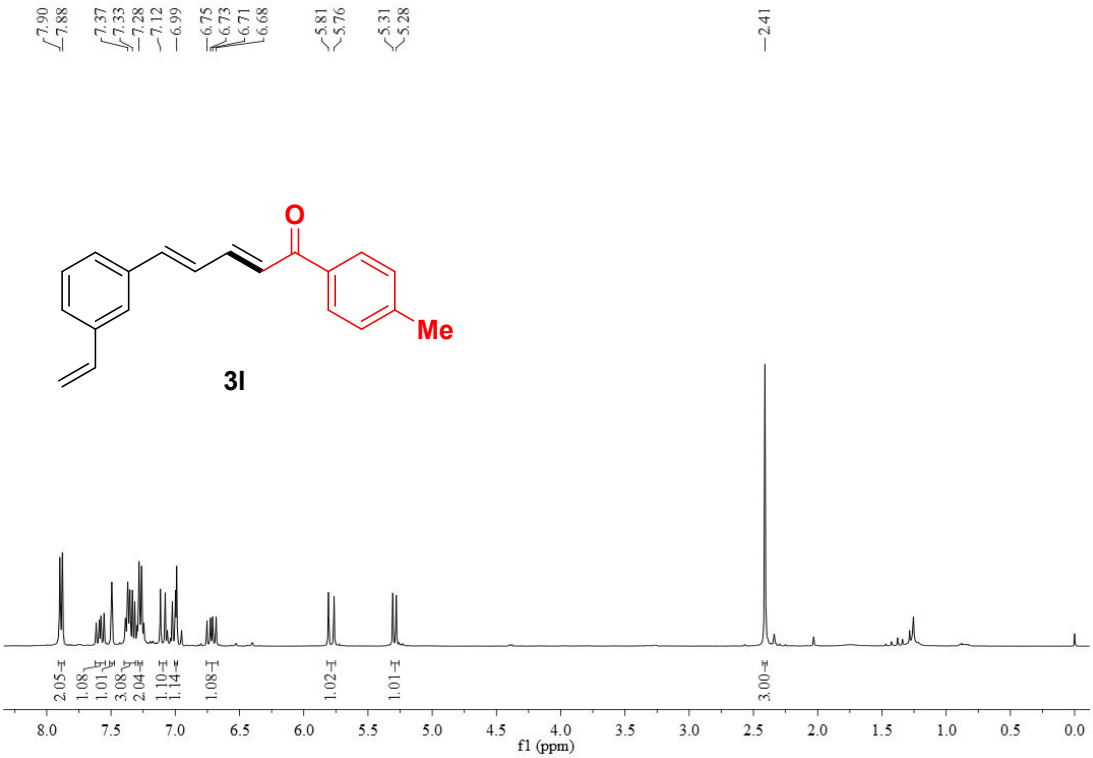

189.68
143.74
143.32
139.51
139.36
135.38
130.66
130.01
129.30
128.01
126.83
125.71
125.31
119.90
77.32
77.00
76.68
21.64
O
F3C
Me
3i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

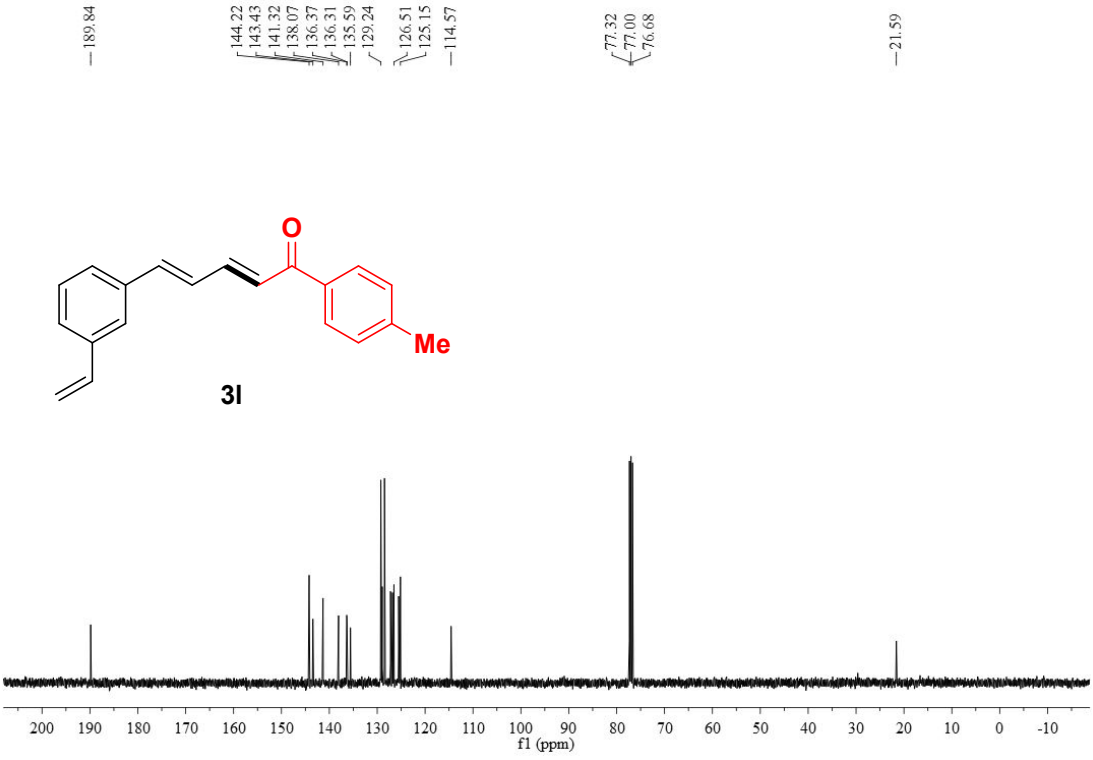

7.90
7.88
7.52
7.22
7.19
7.17
7.16
7.13
7.09
7.02
7.01
7.00
6.99
6.98
6.96
6.94
6.90
2.41
O
Me
F
3j
2.07
1.08
1.03
2.00
1.06
1.15
1.22
3.08
3.00
f1 (ppm)

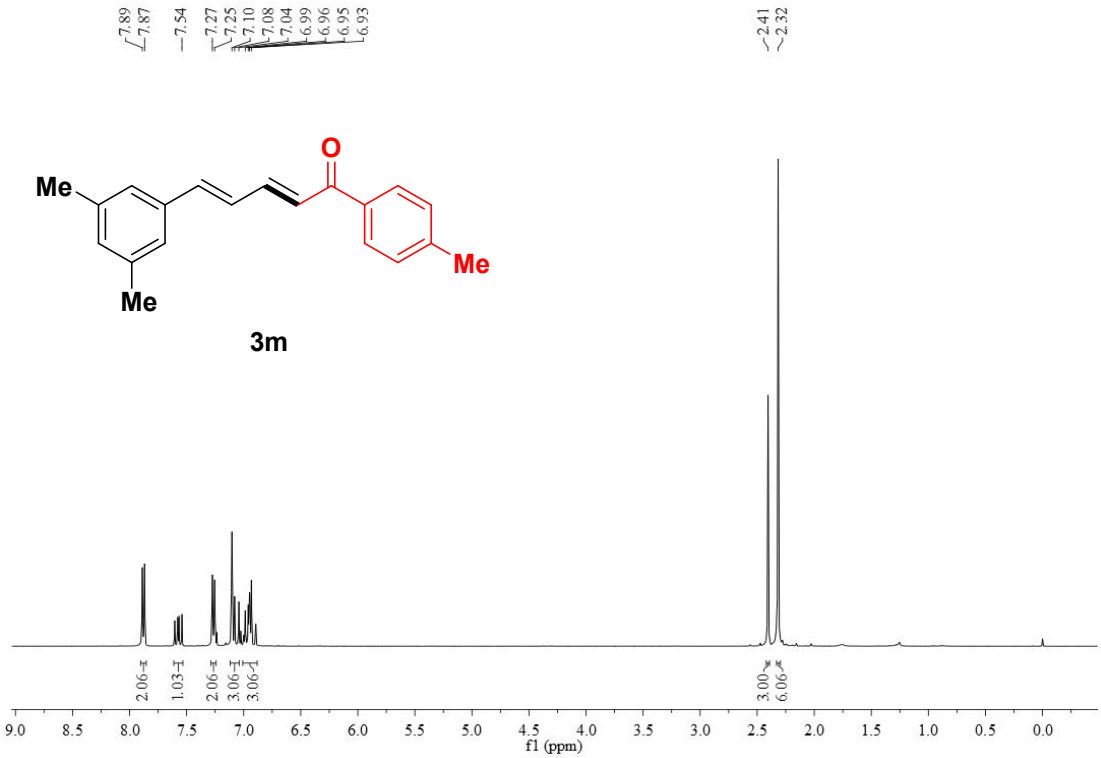

189.68
164.26
161.81
143.57
139.85
138.45
138.37
135.45
128.48
123.19
115.93
115.72
113.40
113.18
77.32
77.00
76.68
21.58
O
Me
F
3j
f1 (ppm)


7.89
7.87
7.54
7.52
7.10
7.08
7.06
7.00
6.99
6.96
6.95
6.87
6.87
6.85
6.85
3.82
2.40
O
Me
OMe
3k
1.99
1.00
3.02
2.05
2.98
1.04
3.04
3.00
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)

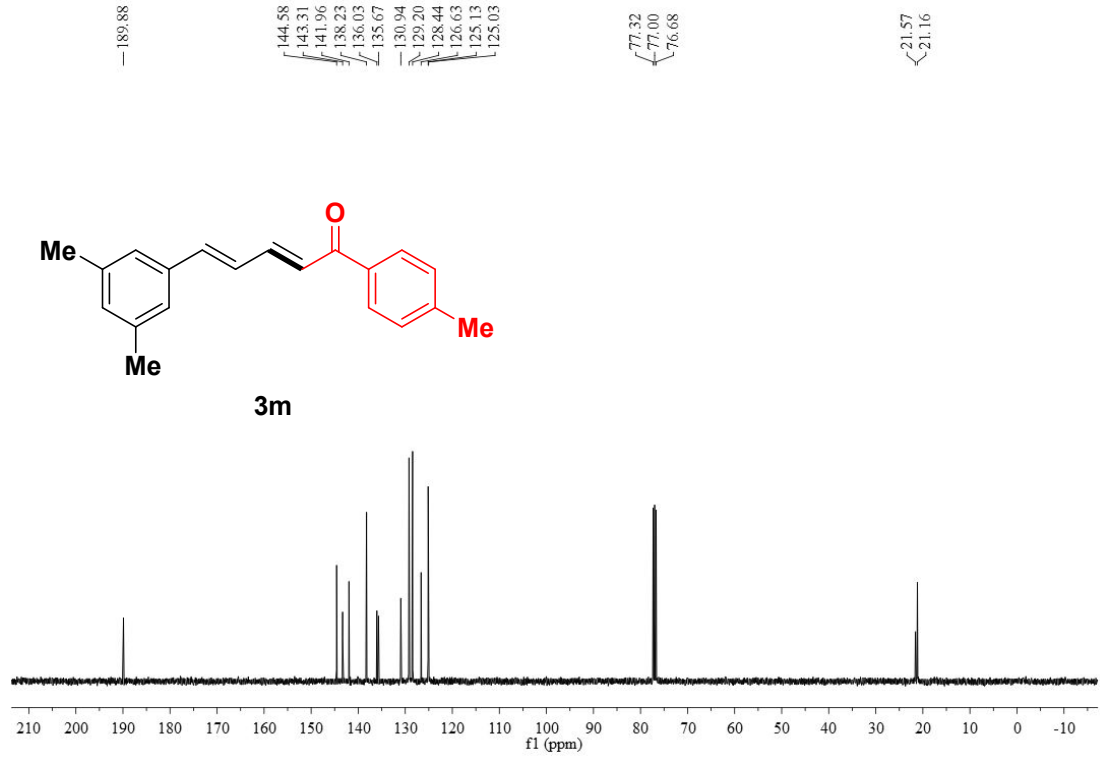

189.77
159.83
144.15
143.39
141.38
137.48
128.44
125.49
119.89
114.85
112.21
77.32
77.00
76.68
55.17
21.55
O
Me
OMe
3k
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.90
7.88
7.37
7.33
7.28
7.12
6.99
6.75
6.73
6.71
6.68
5.81
5.76
5.31
5.28
2.41
O
Me
3l
2.05
1.08
1.01
3.08
2.04
1.10
1.14
1.08
1.02
1.01
3.00
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)

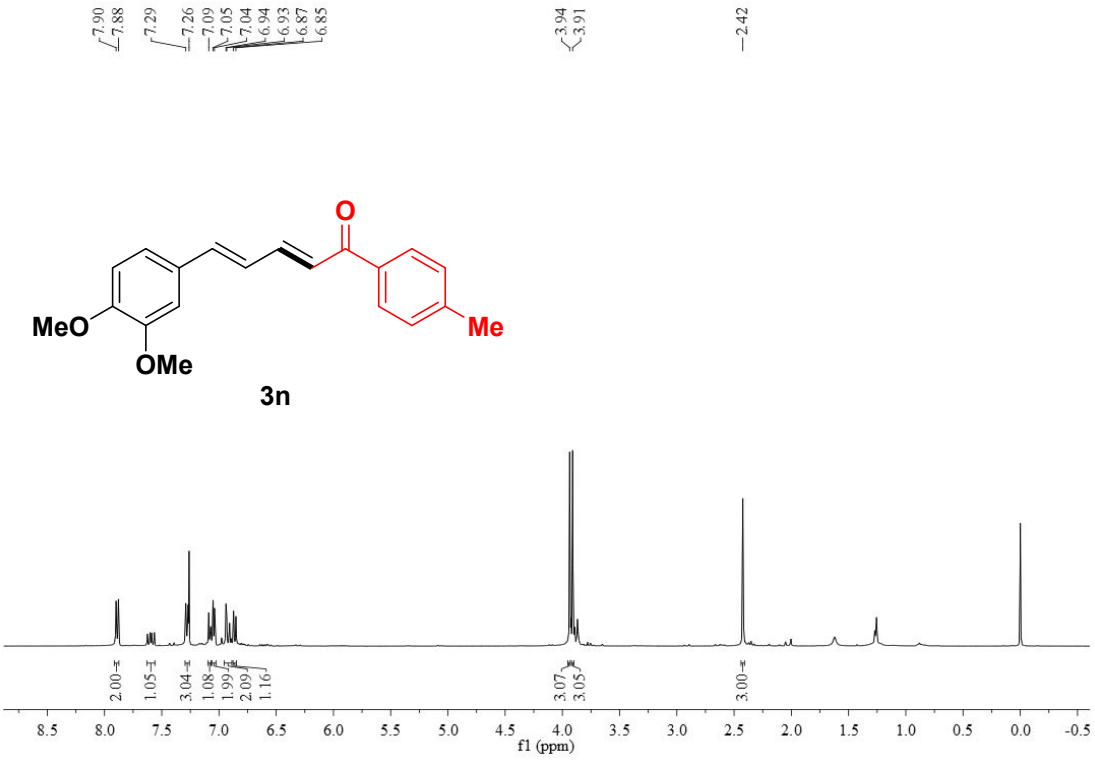

189.84
144.22
143.43
141.32
138.07
136.37
136.31
135.59
129.24
126.51
125.15
114.57
77.32
77.00
76.68
21.59
O
Me
3l
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

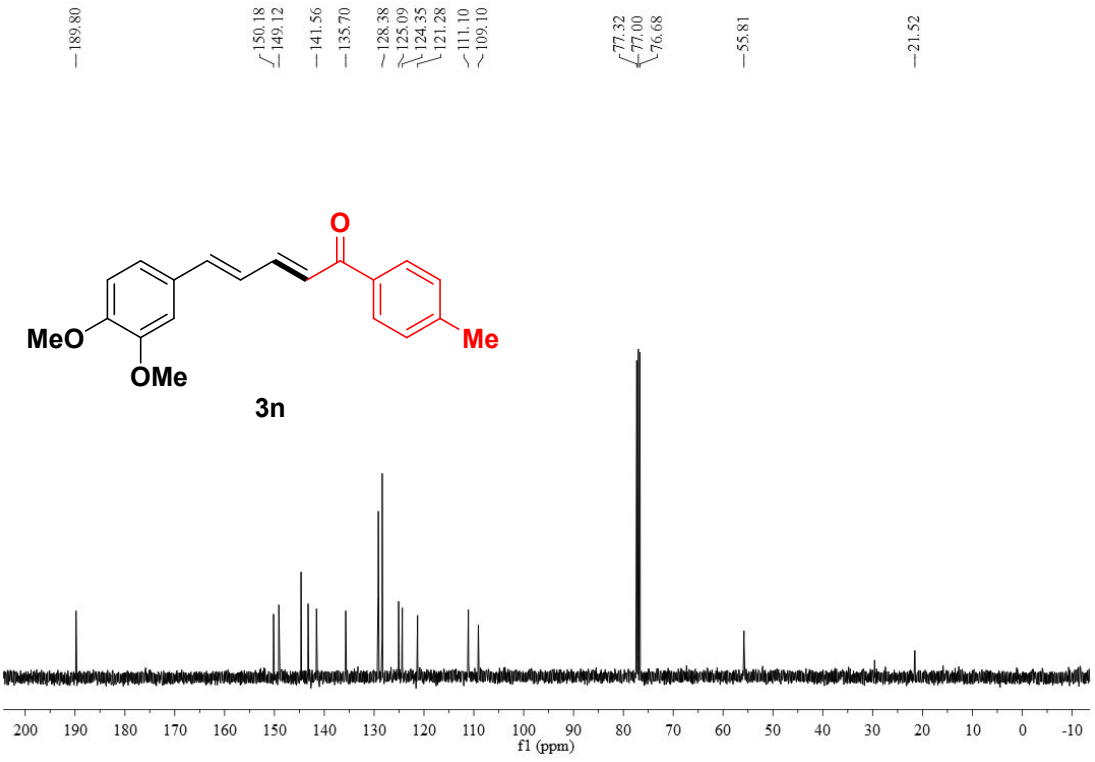

7.89
7.87
7.54
7.27
7.25
7.10
7.08
7.04
6.99
6.96
6.95
6.93
2.41
2.32
O
Me
Me
Me
2.06
1.03
2.06
3.06
3.06
3.00
6.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

3m

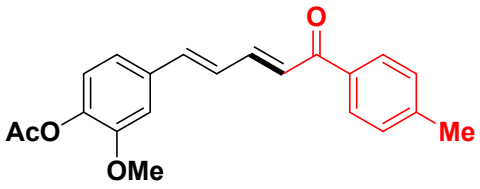

189.88
144.58
143.31
141.96
138.23
136.03
135.67
130.94
129.20
128.44
126.63
125.13
125.03
77.32
77.00
76.68
21.57
21.16
O
Me
Me
Me
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

3m

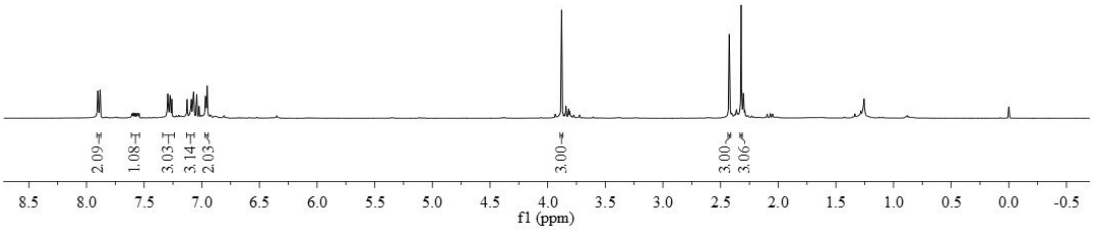

7.90
7.88
7.29
7.26
7.09
7.05
7.04
6.94
6.93
6.87
6.85
3.94
3.91
2.42
O
MeO
OMe
Me
3n
2.00
1.05
3.04
1.08
1.99
2.09
1.16
3.07
3.05
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


189.80
150.18
149.12
141.56
135.70
128.38
125.09
124.35
121.28
111.10
109.10
77.32
77.00
76.68
55.81
21.52
O
MeO
OMe
Me
3n
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

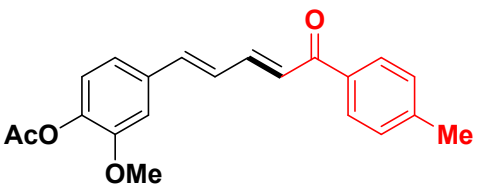

7.90
7.88
7.54
7.29
7.27
7.26
7.13
7.10
7.10
7.09
7.07
7.07
6.97
6.96
6.95
3.88
2.42
2.32


O
AcO
OMe
Me

3o

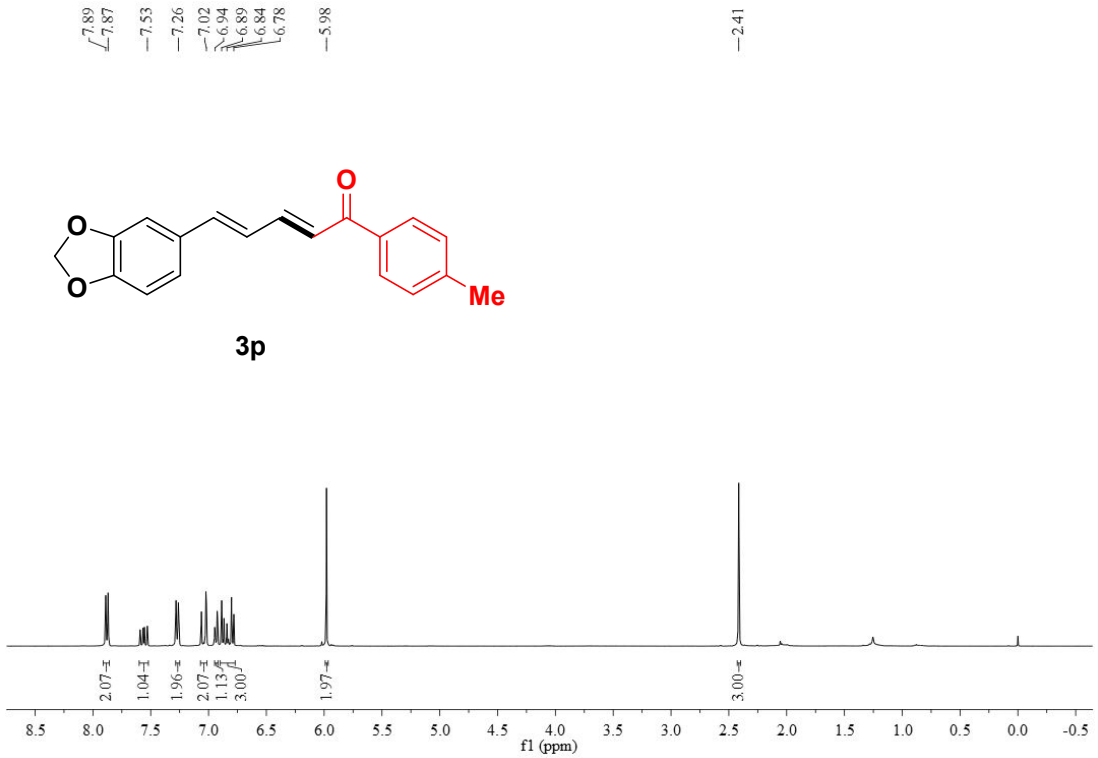

2.09
1.08
3.03
3.14
2.03
3.00
3.00
3.06
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


189.86
168.87
151.30
140.47
135.18
129.27
125.64
123.14
120.11
110.61
77.32
77.00
76.68
55.86
21.62
20.62

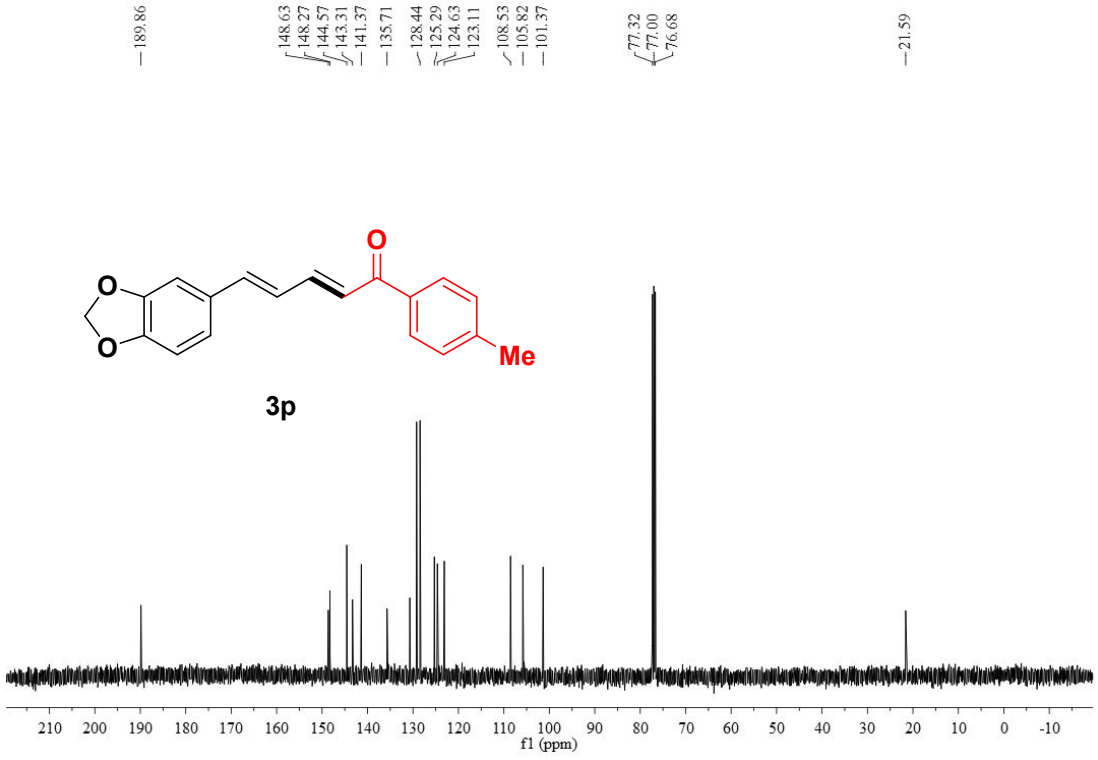

O
AcO
OMe
Me

3o

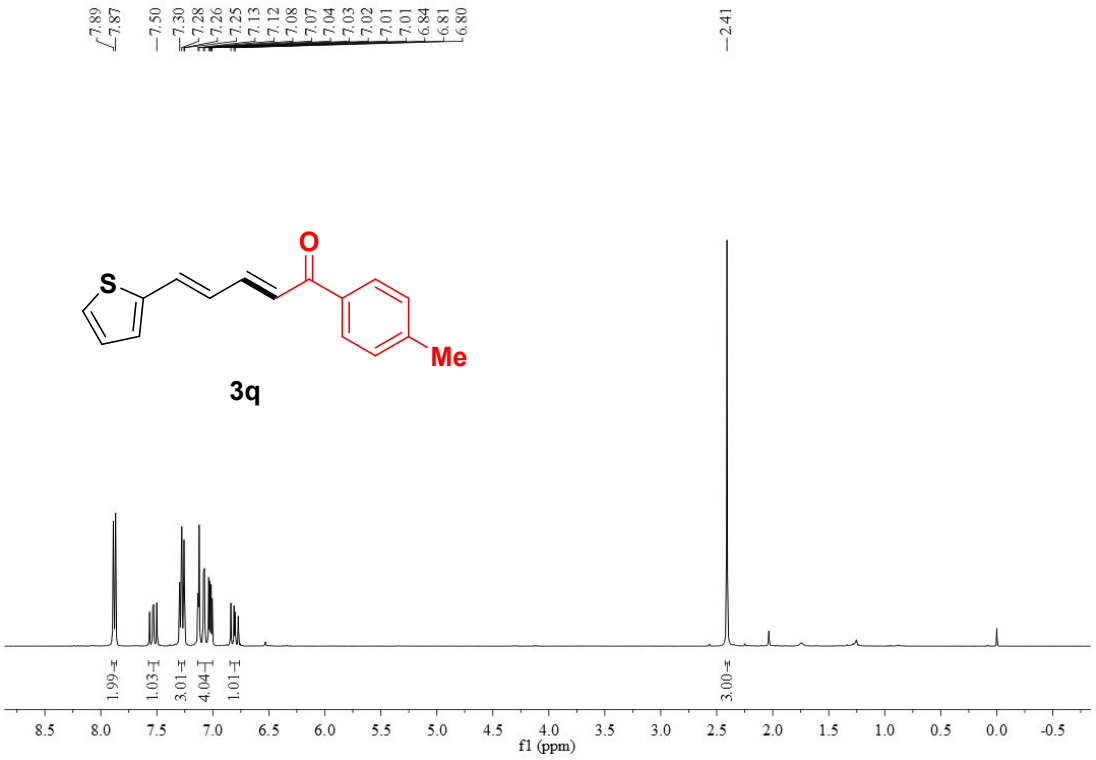
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

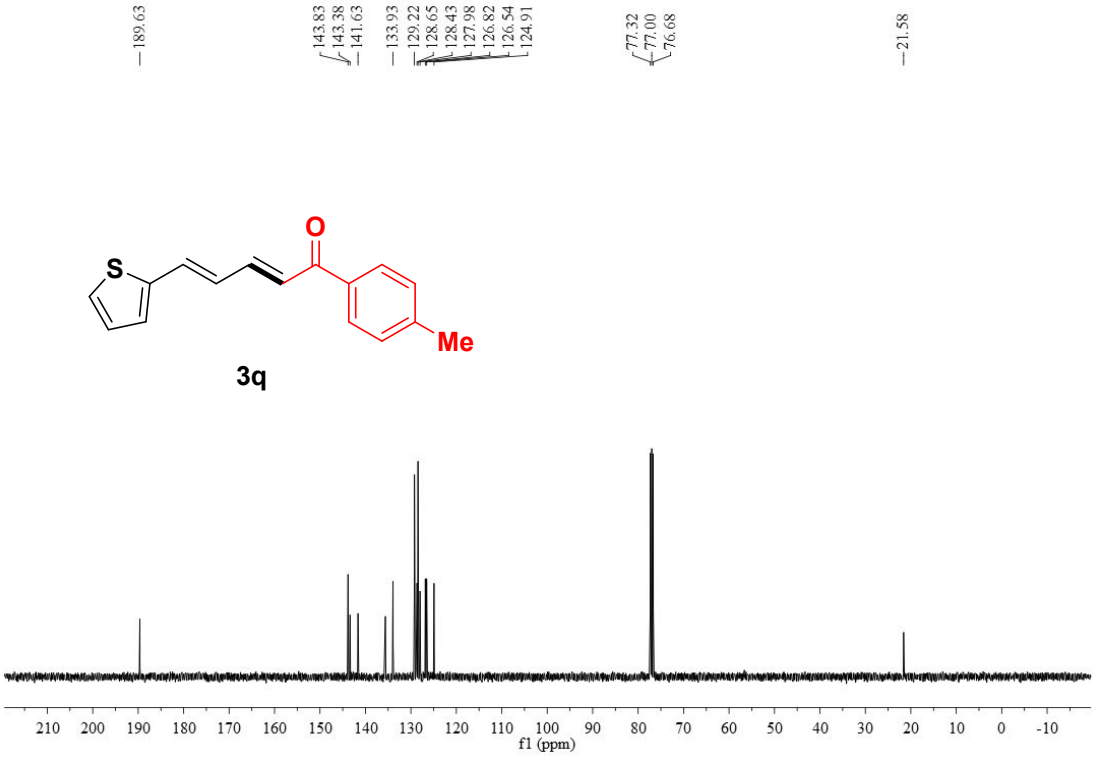

7.89
7.87
7.53
7.26
7.02
6.94
6.89
6.84
6.78
5.98
2.41
O
O
O
Me
2.07
1.04
1.96
2.07
1.13
3.00
1.97
3.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

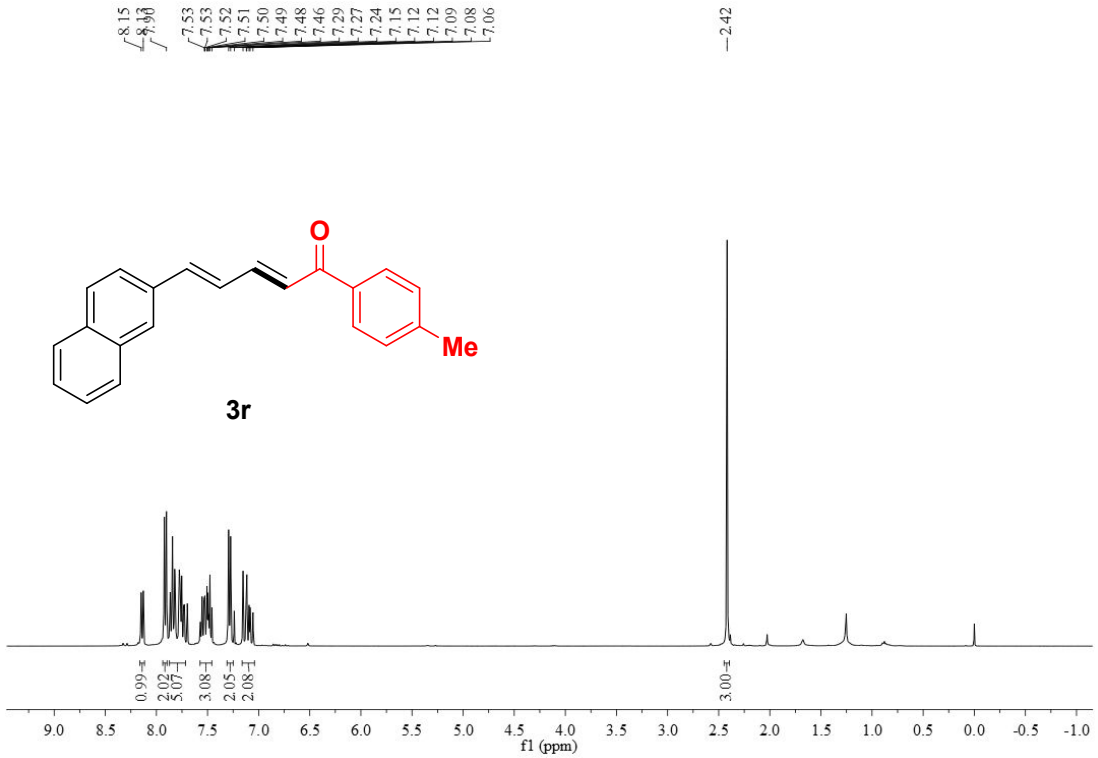
3p

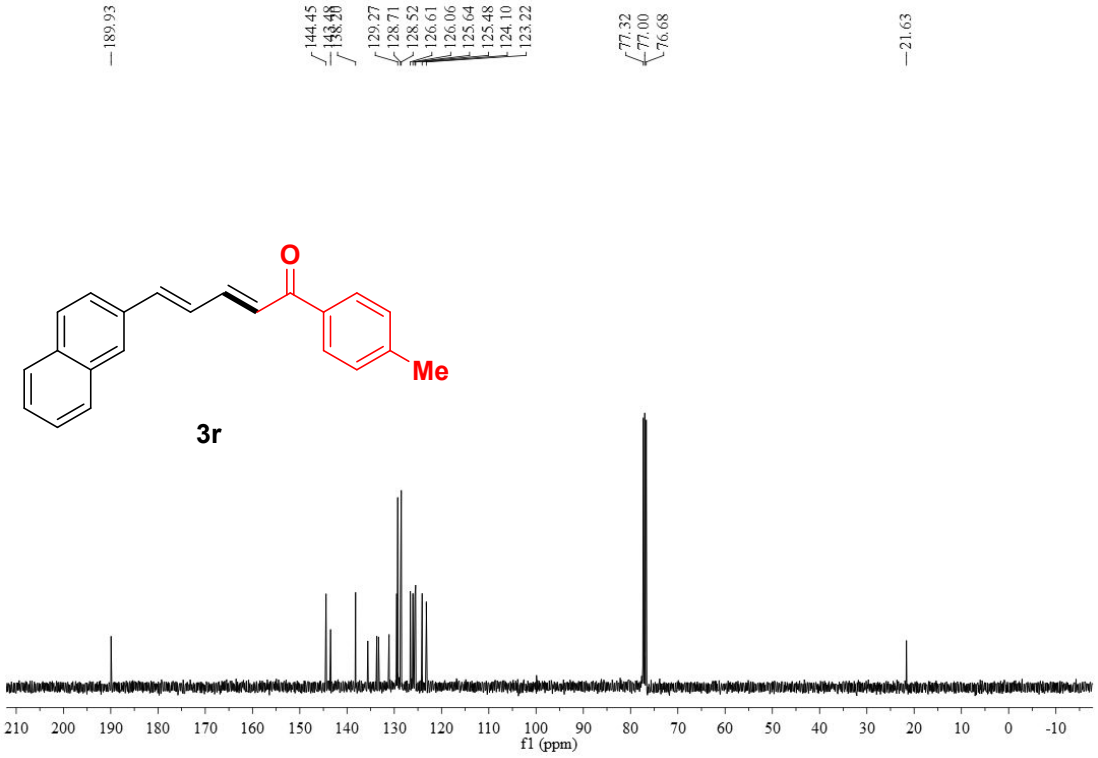

189.86
148.63
148.27
144.57
143.31
141.37
135.71
128.44
125.29
124.63
123.11
108.53
105.82
101.37
77.32
77.00
76.68
21.59
O
O
O
Me
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

3p

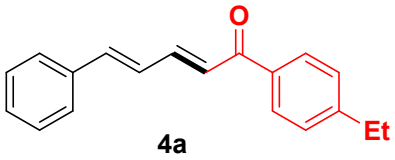

7.89
7.87
7.50
7.30
7.28
7.26
7.25
7.13
7.12
7.08
7.07
7.04
7.03
7.02
7.01
7.01
6.84
6.81
6.80
2.41
O
S
Me
3q
1.99
1.03
3.01
4.04
1.01
3.00
f1 (ppm)


189.63
143.83
143.38
141.63
133.93
129.22
128.65
128.43
127.98
126.82
126.54
124.91
77.32
77.00
76.68
21.58
O
S
Me
3q
f1 (ppm)

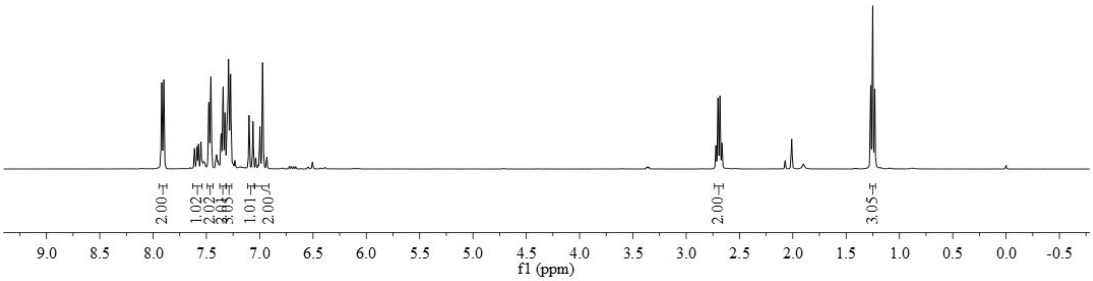

8.15
8.13
8.00
7.53
7.53
7.52
7.51
7.50
7.49
7.48
7.46
7.29
7.27
7.24
7.15
7.12
7.12
7.09
7.08
7.06
2.42
O
Me
3r
0.99
2.02
5.07
3.08
2.05
2.08
3.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

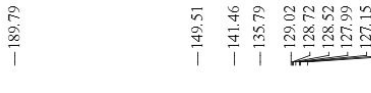

189.93
144.45
143.48
138.20
129.27
128.71
128.52
126.61
126.06
125.64
125.48
124.10
123.22
77.32
77.00
76.68
21.63
O
Me
3r
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

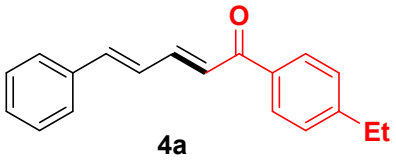

7.92
7.90
7.57
7.55
7.48
7.46
7.36
7.34
7.32
7.30
7.29
7.27
7.10
7.06
7.04
7.00
6.97
6.93
2.72
2.70
2.68
2.66
1.27
1.25
1.23


O
Et

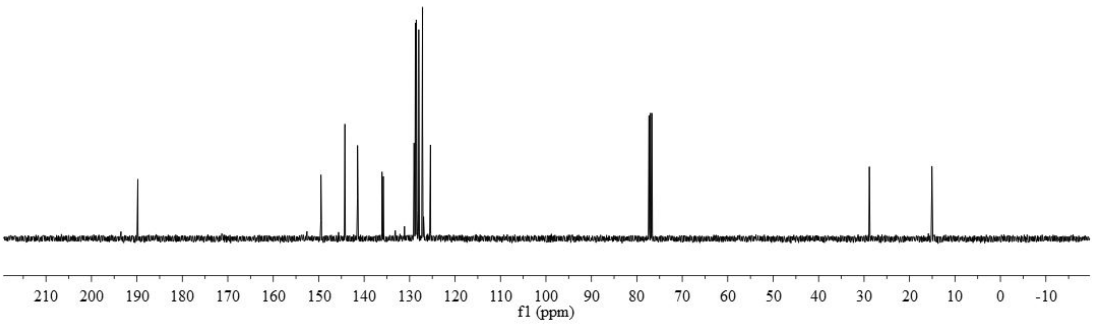
4a

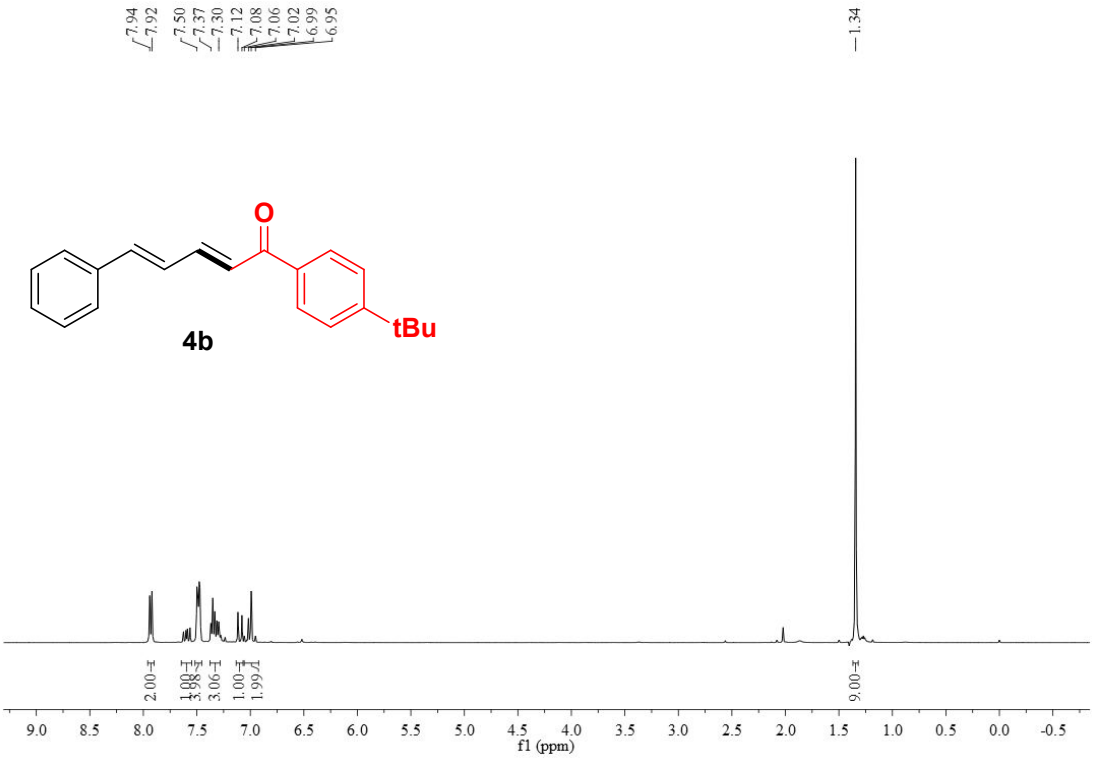

2.00
1.02
2.02
3.05
1.01
2.00
2.00
3.05
f1 (ppm)

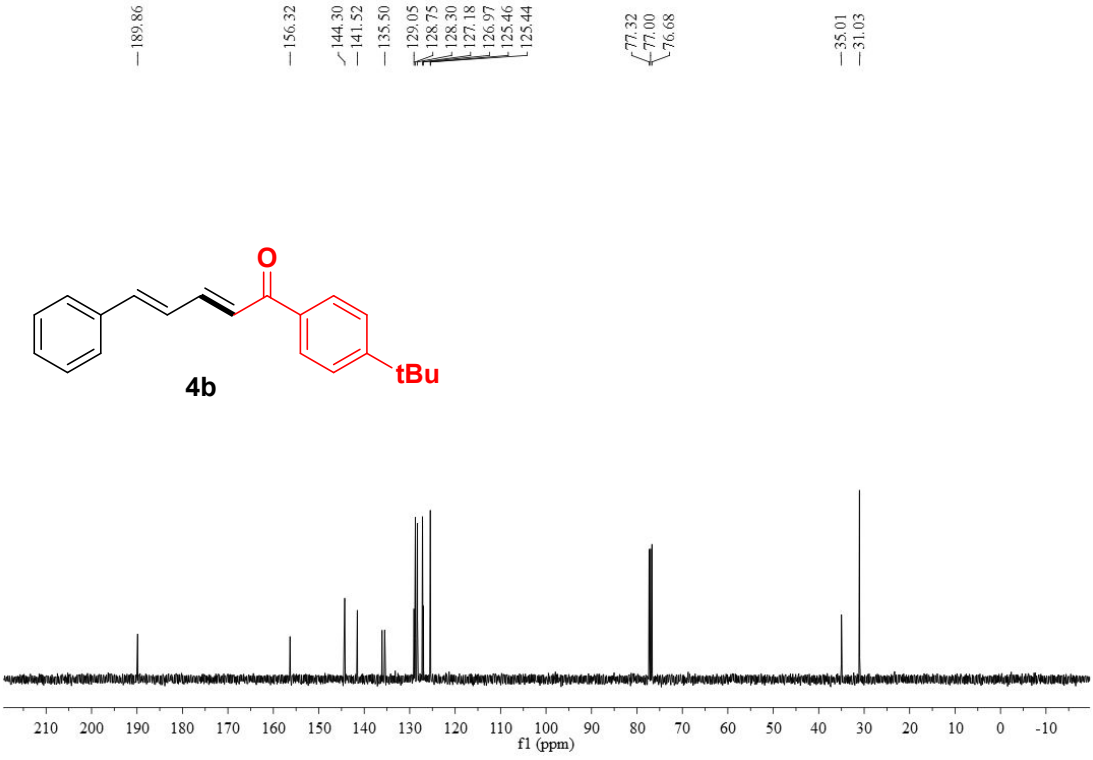

189.79
149.51
141.46
135.79
129.02
128.72
128.52
127.99
127.15
126.94
125.40
77.32
77.00
76.68
28.83
15.08

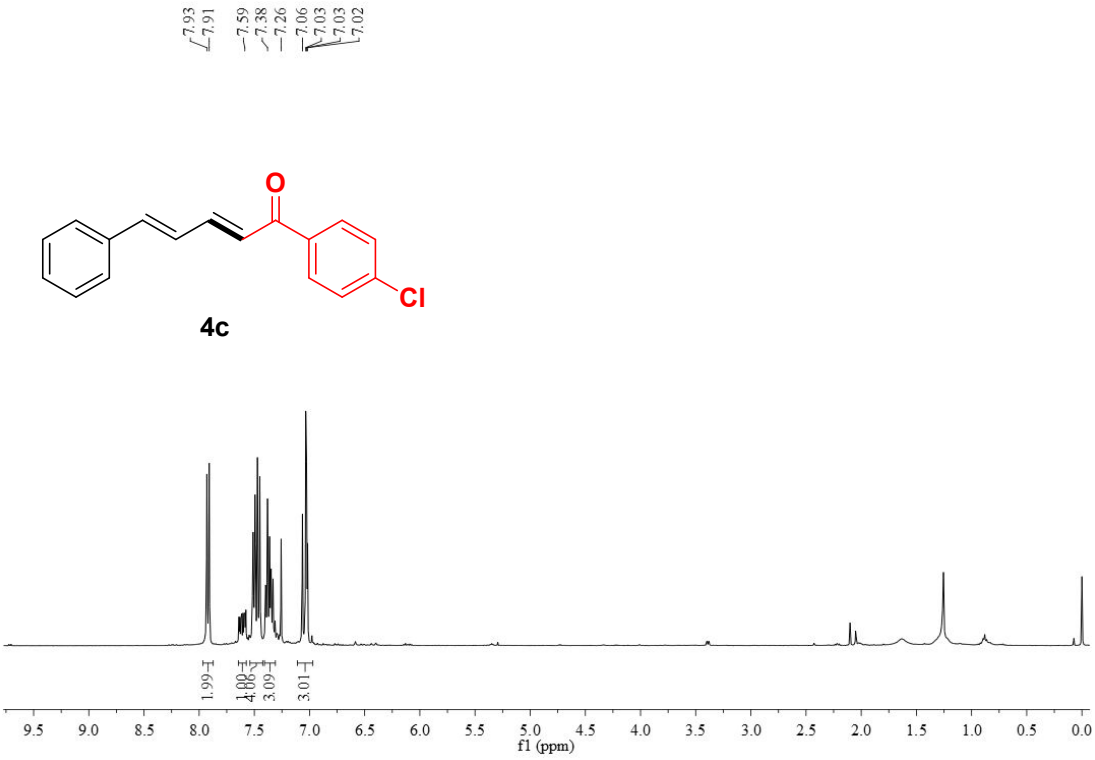

O
Et

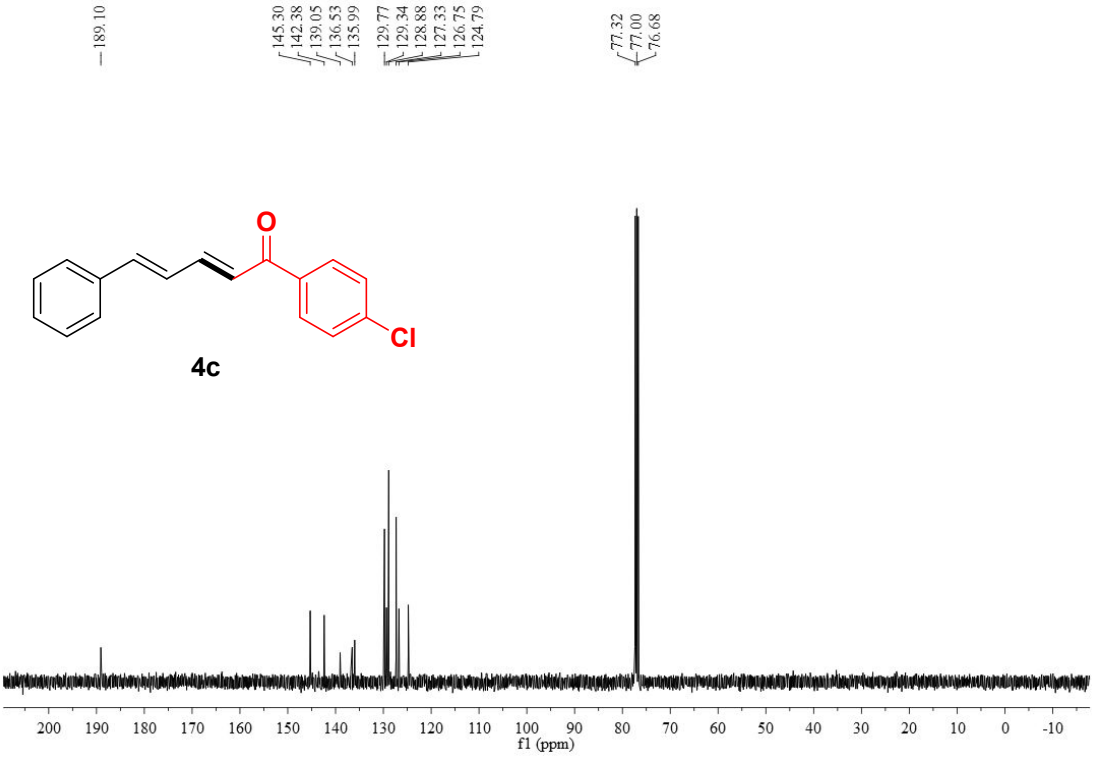
4a


f1 (ppm)

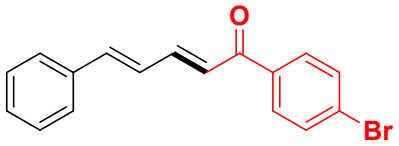

7.94
7.92
7.50
7.37
7.30
7.12
7.08
7.06
7.02
6.99
6.95
1.34
O
tBu
4b
2.00
1.00
3.06
1.00
1.99
9.00
f1 (ppm)


189.86
156.32
144.30
141.52
135.50
129.05
128.75
128.30
127.18
126.97
125.46
125.44
77.32
77.00
76.68
35.01
31.03
O
tBu
4b
f1 (ppm)

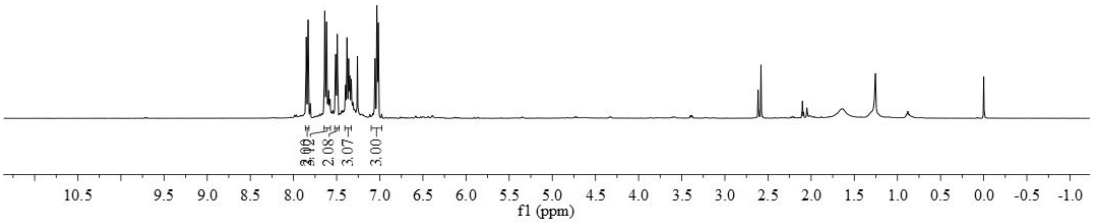

7.93
7.91
7.59
7.38
7.26
7.06
7.03
7.03
7.02
O
Cl
4c
1.99
1.00
1.08
3.09
3.01
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

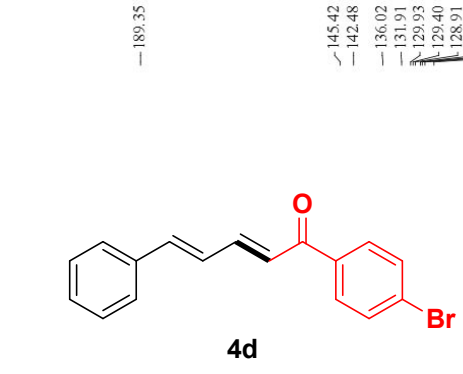

189.10
145.30
142.38
139.05
136.53
135.99
129.77
129.34
128.88
127.33
126.75
124.79
77.32
77.00
76.68
O
Cl
4c
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.85
7.83
7.64
7.62
7.59
7.51
7.49
7.40
7.38
7.36
7.35
7.33
7.05
7.03
7.03
7.02


O
Br

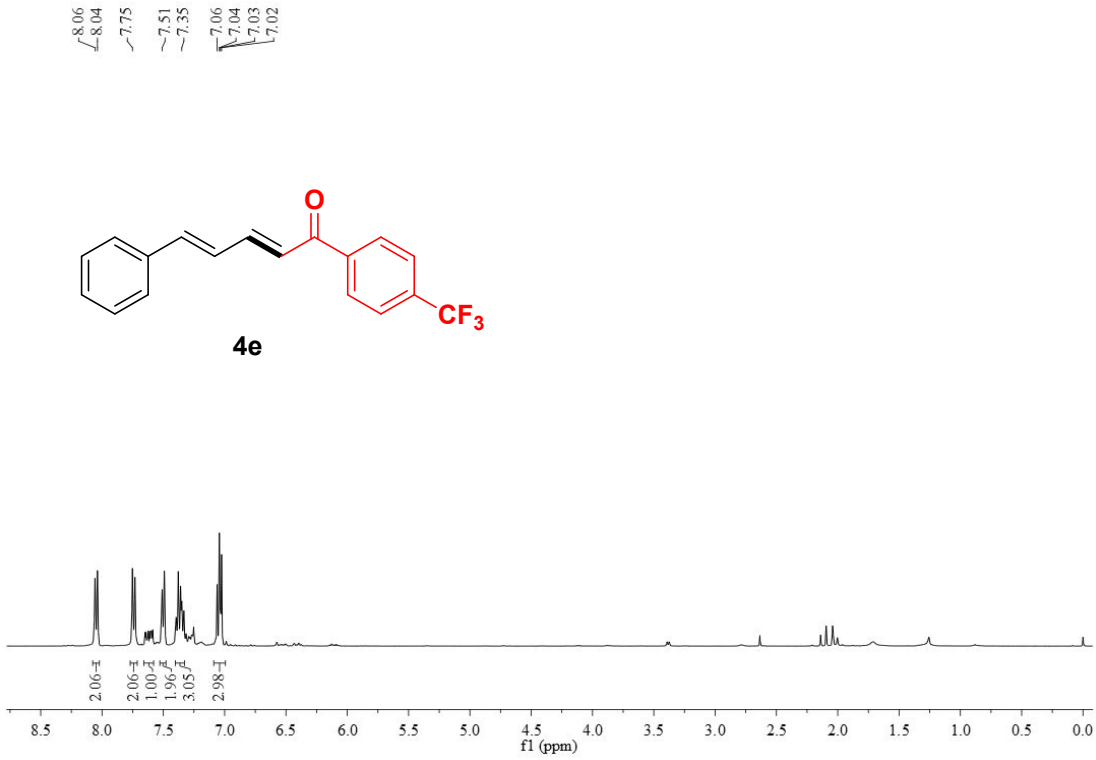
4d

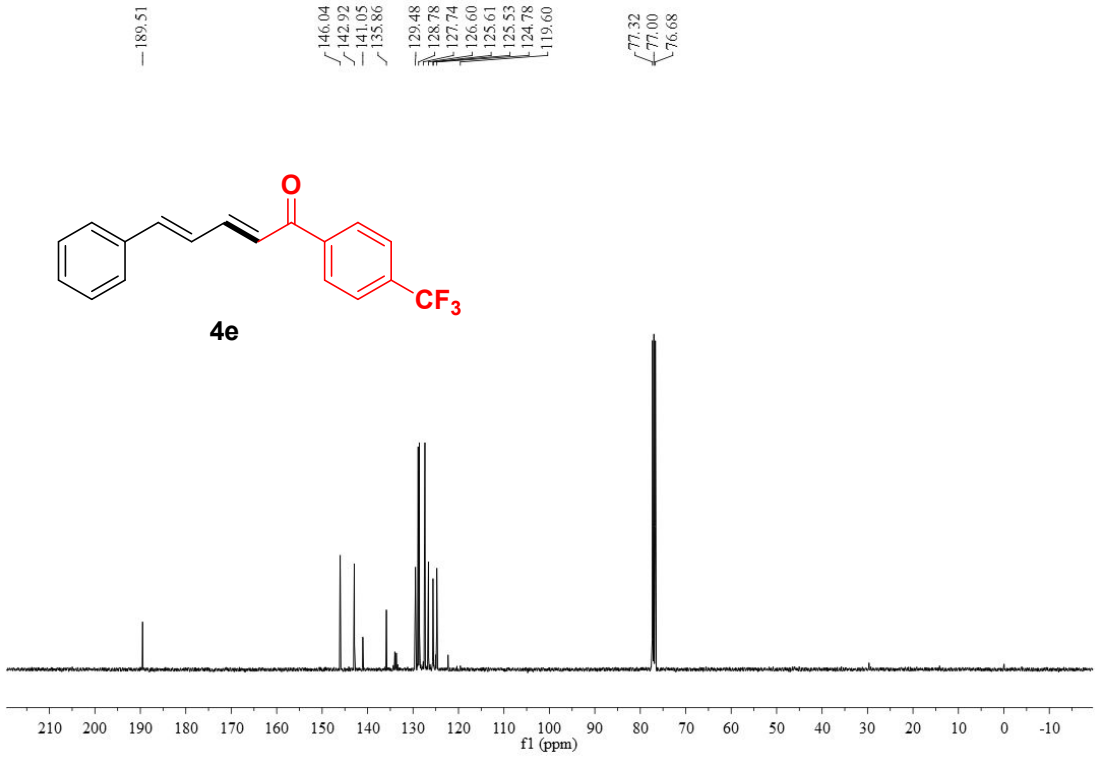

2.08
3.07
3.00
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

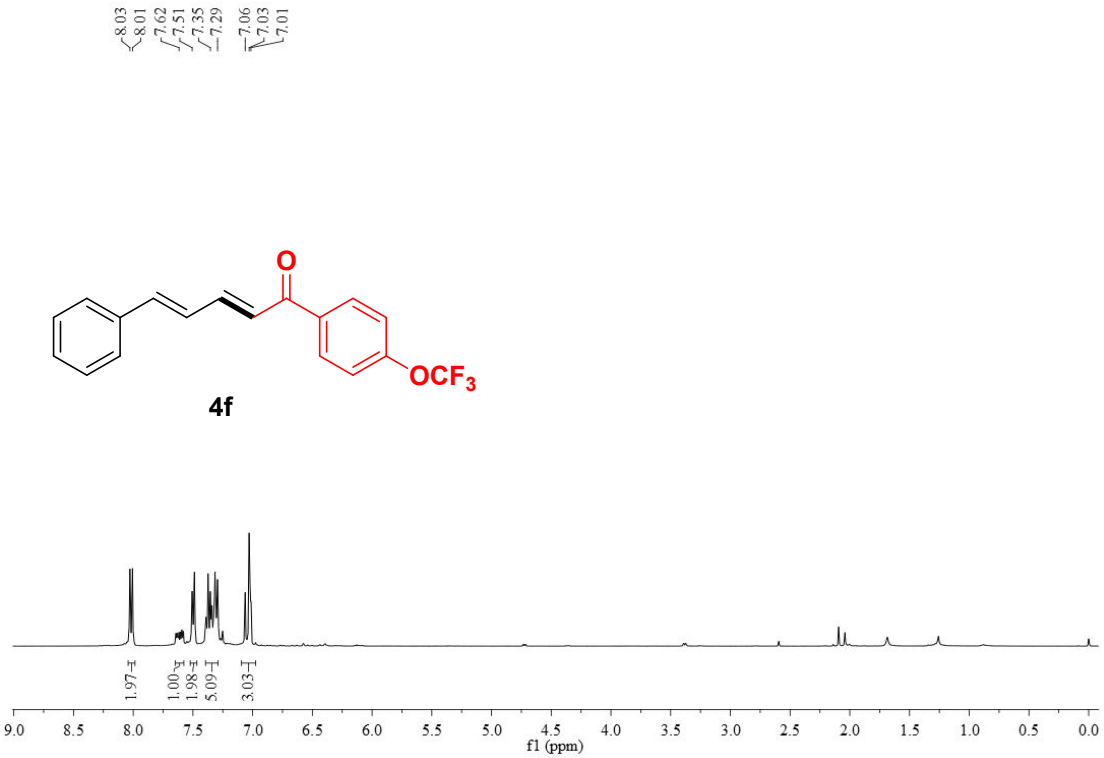

O
Br

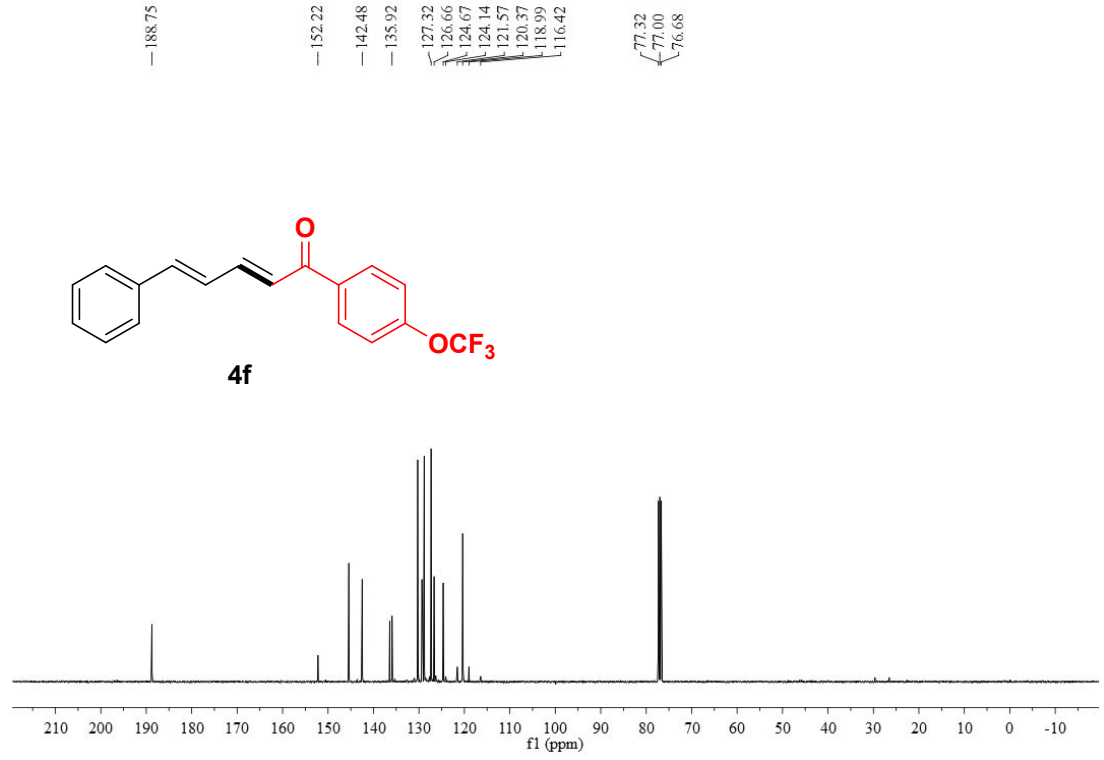
4d

189.35
145.42
142.48
136.02
131.91
129.93
129.40
128.91
127.76
127.37
126.78
124.79
77.36
77.04
76.72
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)

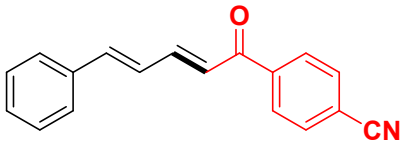

8.06
8.04
7.75
7.51
7.35
7.06
7.04
7.03
7.02
O
CF3
4e
2.06
2.06
1.00
1.96
3.05
2.98
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


189.51
146.04
142.92
141.05
135.86
129.48
128.78
127.74
126.60
125.61
125.53
124.78
119.60
77.32
77.00
76.68
O
CF3
4e
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)

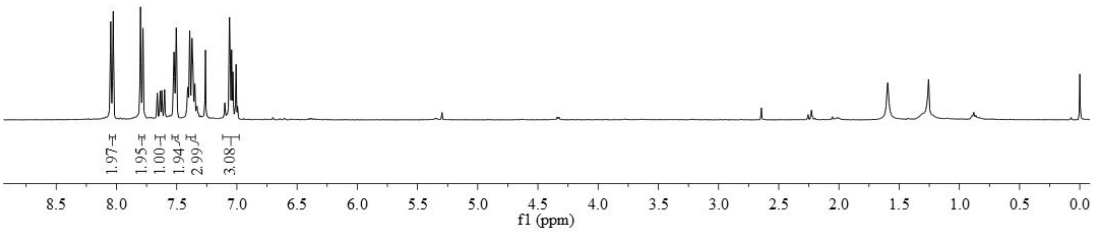

8.03
8.01
7.62
7.51
7.35
7.29
7.06
7.03
7.01
O
OCF3
4f
1.97
1.00
1.98
5.09
3.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

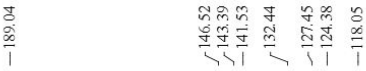

188.75
152.22
142.48
135.92
127.32
126.66
124.67
124.14
121.57
120.37
118.99
116.42
77.32
77.00
76.68
O
OCF3
4f
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

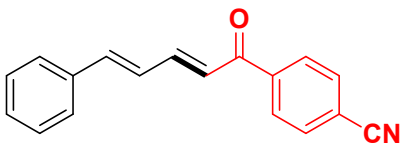

8.05
8.03
7.80
7.50
7.37
7.33
7.10
7.06
7.04
7.03
7.01
6.99


O
CN

4g

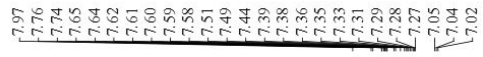

1.97
1.95
1.00
1.94
2.99
3.08
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

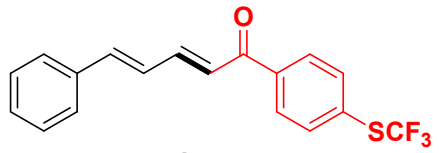

189.04
146.52
143.39
141.53
132.44
127.45
124.38
118.05
115.79
77.32
77.00
76.68


O
CN

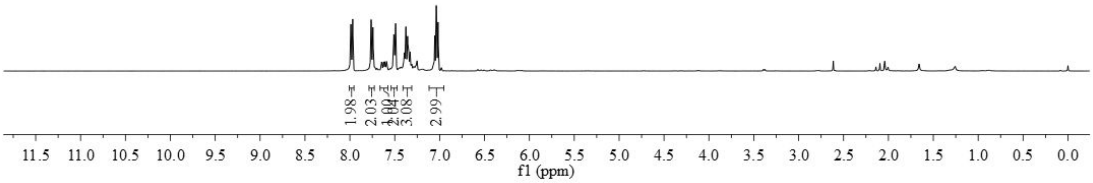
4g

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

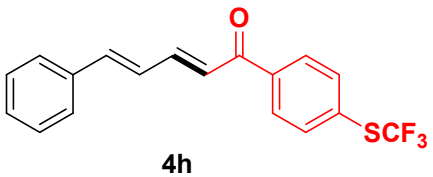

7.97
7.76
7.74
7.65
7.64
7.62
7.61
7.60
7.59
7.58
7.51
7.49
7.44
7.39
7.38
7.36
7.35
7.33
7.31
7.29
7.28
7.27
7.05
7.04
7.02


O
SCF3

4h

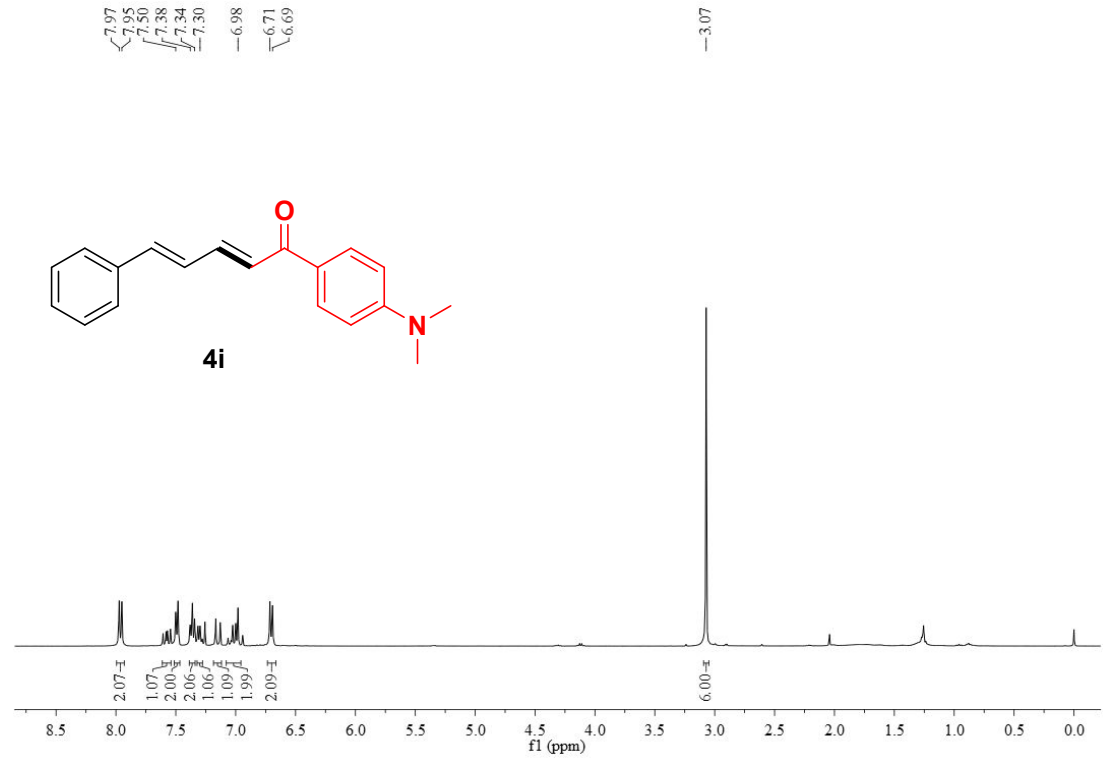

1.98
2.03
3.08
2.99
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

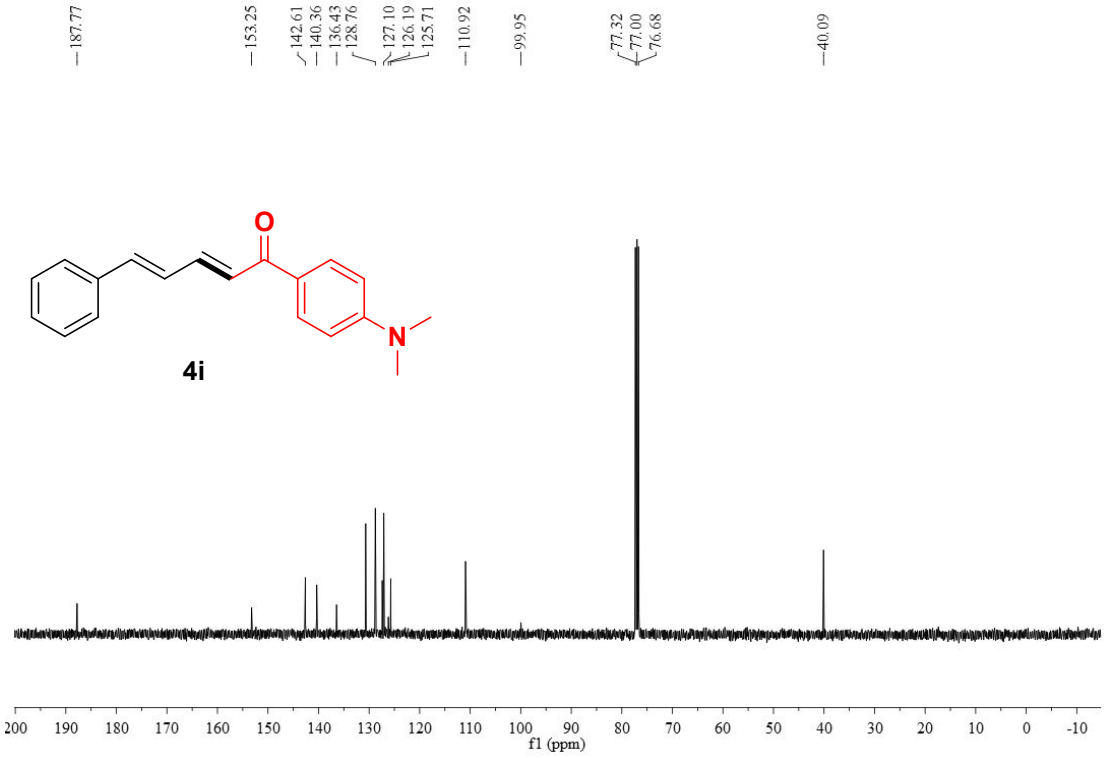

189.53
135.79
133.91
130.84
129.47
129.12
128.90
127.78
127.39
126.66
124.78
124.71
120.47
77.32
77.00
76.68

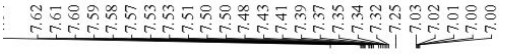

O
SCF3

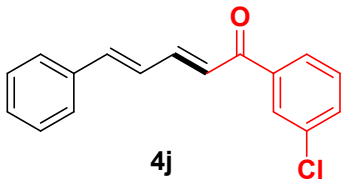
4h

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)

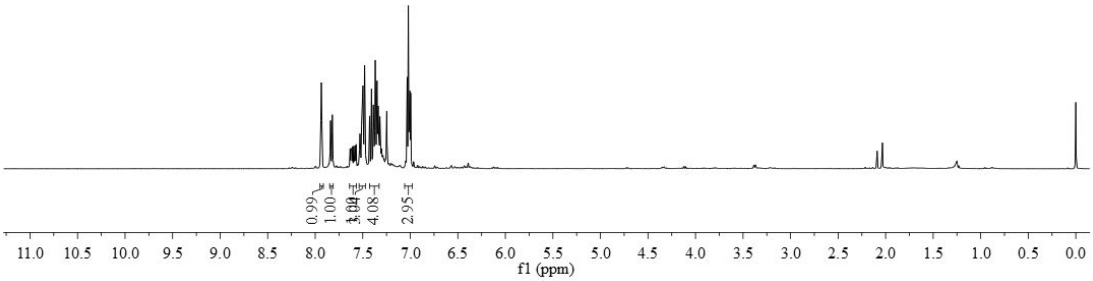

7.97
7.95
7.50
7.38
7.34
7.30
6.98
6.71
6.69
3.07
O
N
4i
2.07
1.07
2.00
2.06
1.06
1.09
1.99
2.09
6.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


187.77
153.25
142.61
140.36
136.43
128.76
127.10
126.19
125.71
110.92
99.95
77.32
77.00
76.68
40.09
O
N
4i
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

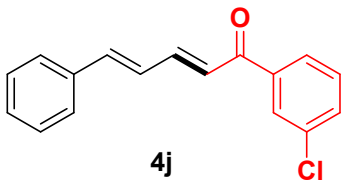

7.62
7.61
7.60
7.59
7.58
7.57
7.53
7.53
7.51
7.50
7.50
7.48
7.43
7.41
7.39
7.37
7.35
7.34
7.32
7.25
7.03
7.02
7.01
7.00
7.00


O
Cl

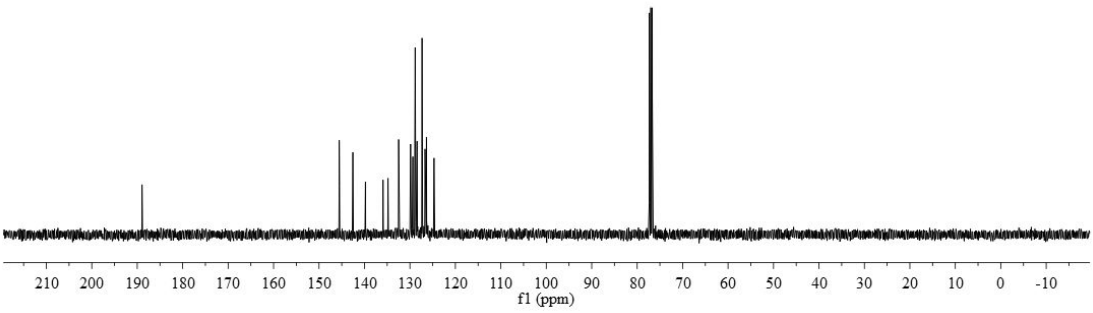
4j

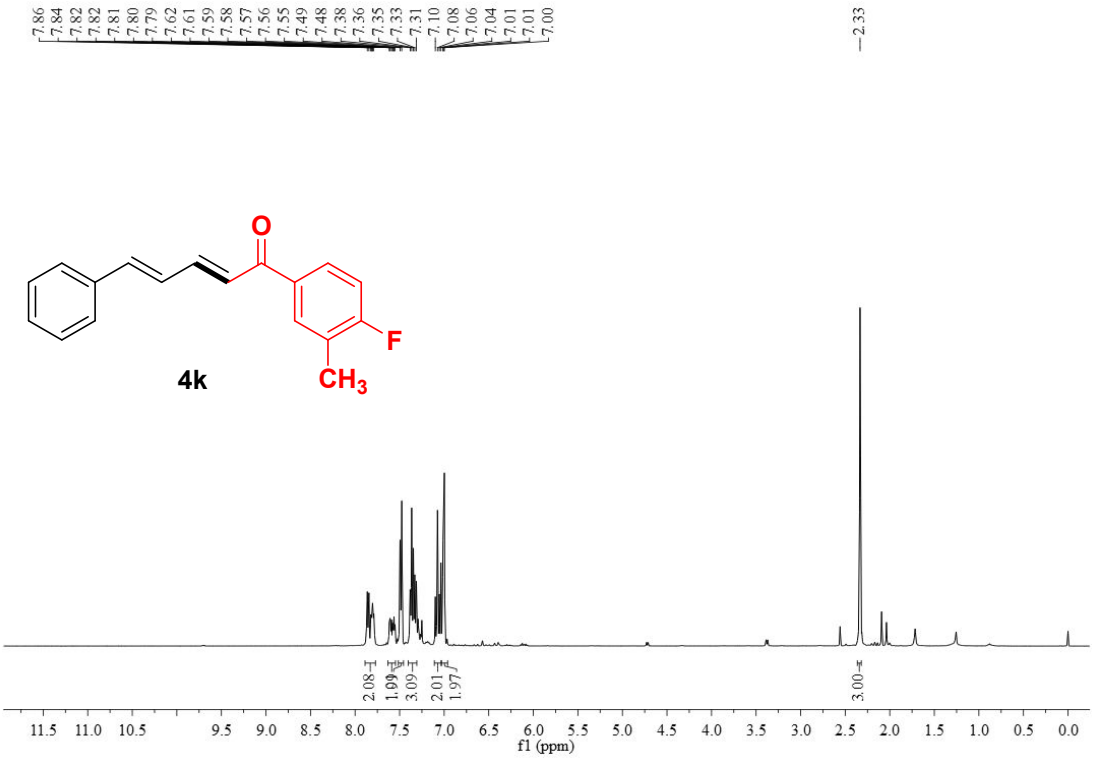

0.99
1.00
4.08
2.95
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

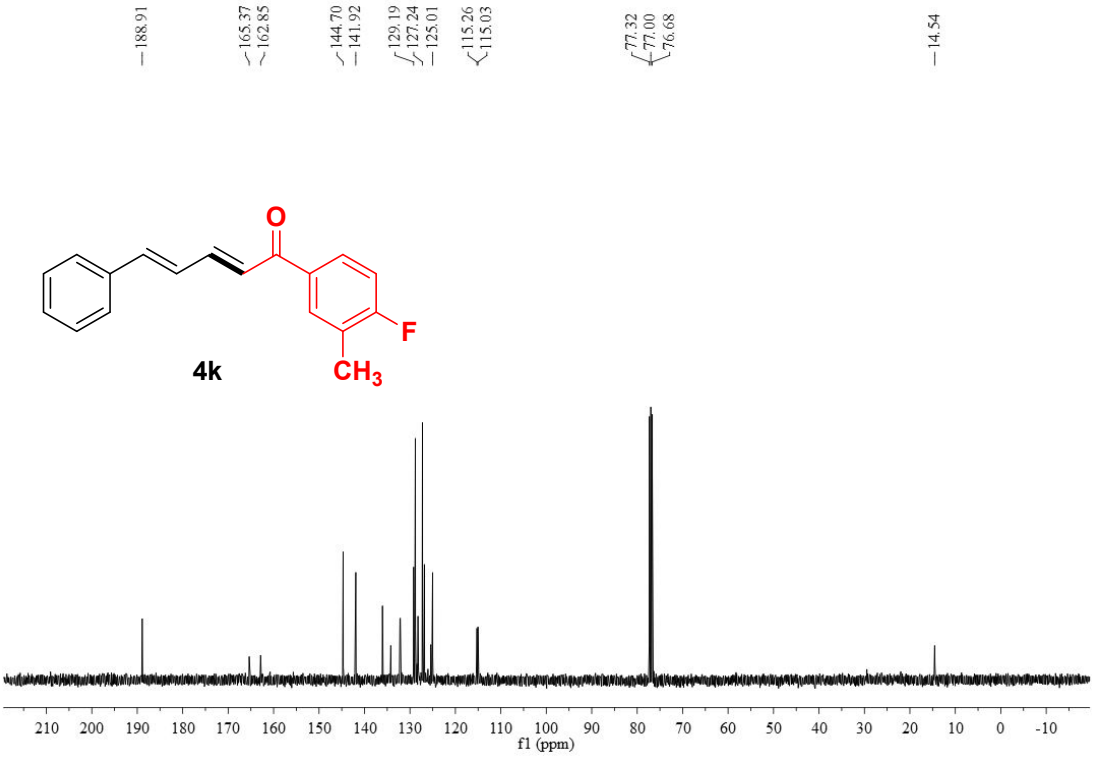

188.95
145.56
142.55
139.78
135.92
134.83
132.48
129.85
129.35
128.84
128.42
127.33
126.67
126.36
124.70
77.32
77.00
76.68


O
Cl

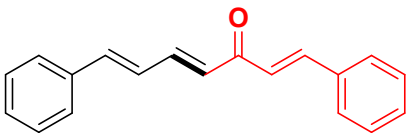
4j


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)

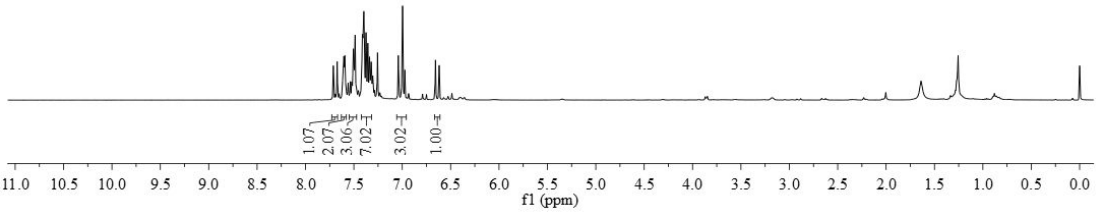

7.86
7.84
7.82
7.82
7.81
7.80
7.79
7.62
7.61
7.59
7.58
7.57
7.56
7.55
7.49
7.48
7.38
7.36
7.35
7.33
7.31
7.10
7.08
7.06
7.04
7.01
7.01
7.00
2.33
O
F
CH3
4k
2.08
1.09
3.09
2.01
1.97
3.00
11.5 11.0 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


188.91
165.37
162.85
144.70
141.92
129.19
127.24
125.01
115.26
115.03
77.32
77.00
76.68
14.54
O
F
CH3
4k
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)

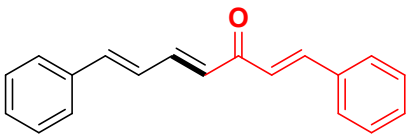

7.71
7.67
7.61
7.60
7.59
7.54
7.52
7.51
7.49
7.41
7.40
7.40
7.37
7.36
7.34
7.32
7.31
6.97
6.66
6.62


O

4l


1.07
2.07
3.06
7.02
3.02
1.00
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

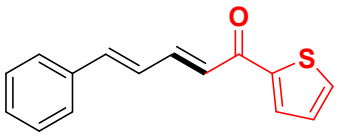

188.94
143.36
142.95
141.64
128.93
128.84
128.33
127.27
126.94
126.31
125.46
77.32
77.00
76.68


O

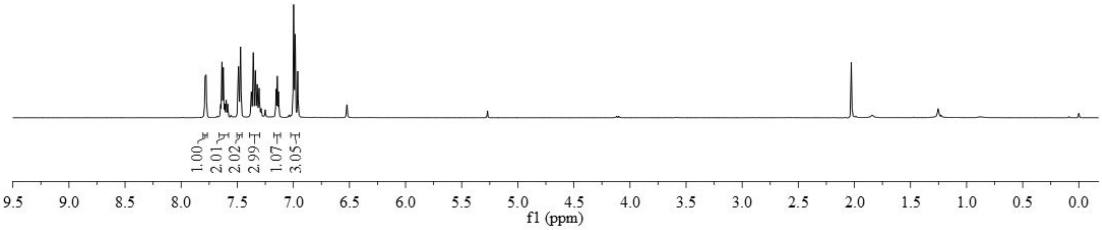
4l

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

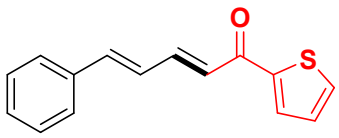

7.79
7.78
7.65
7.64
7.62
7.61
7.60
7.58
7.49
7.47
7.37
7.36
7.34
7.32
7.30
7.29
7.15
7.14
7.13
7.00
6.98
6.96


O
S

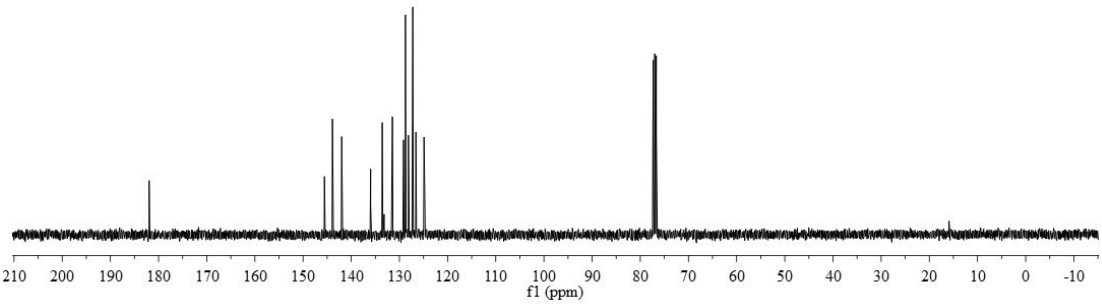
4m


1.00
2.01
2.02
2.99
1.07
3.05
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

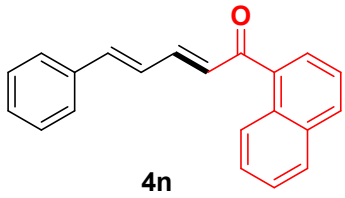

181.96
145.56
143.90
141.98
135.97
133.57
131.46
129.16
128.76
128.13
127.23
126.58
124.89
77.32
77.00
76.68


O
S

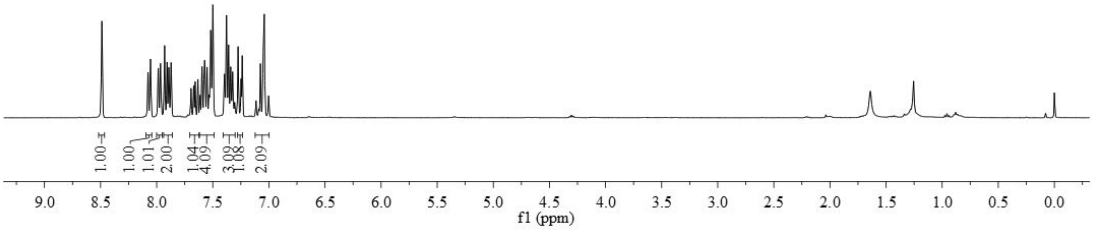
4m

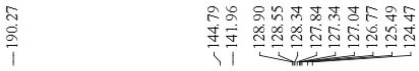

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

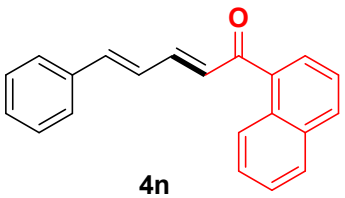

8.49
8.05
7.91
7.87
7.69
7.67
7.66
7.63
7.61
7.60
7.57
7.55
7.53
7.52
7.50
7.40
7.38
7.36
7.34
7.32
7.27
7.25
7.24
7.11
7.08
7.05
7.04


O

4n

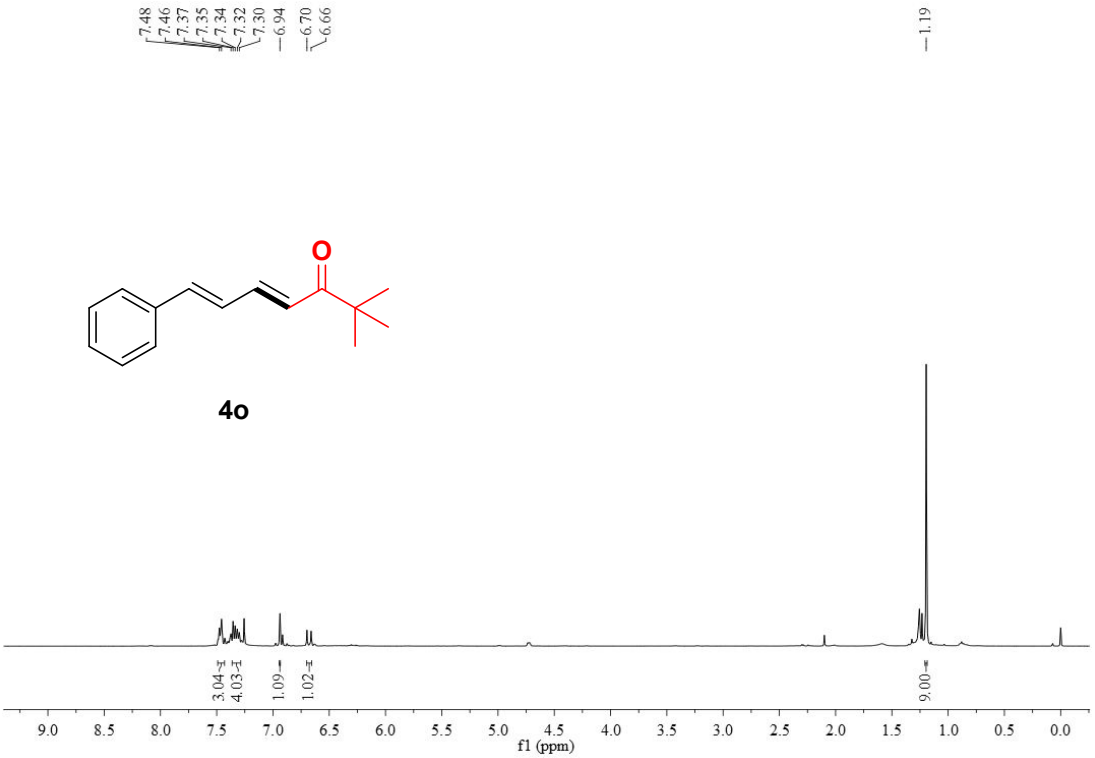

1.00
1.00
1.01
2.00
1.04
4.09
3.09
1.08
2.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

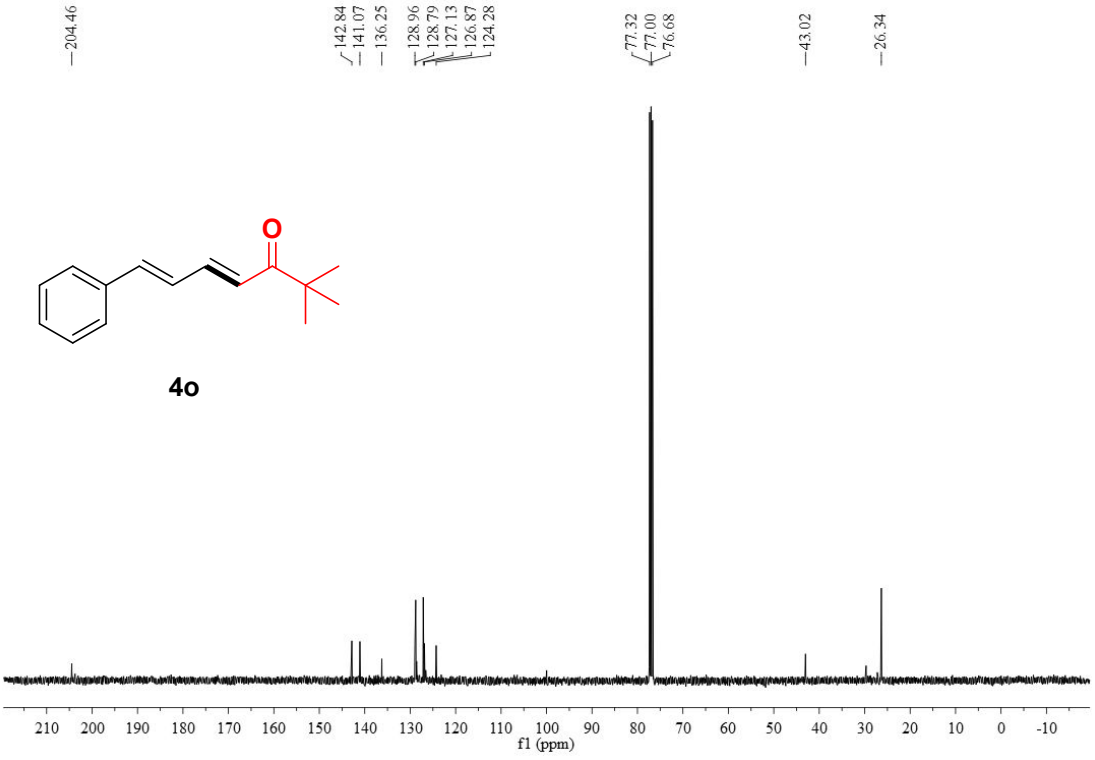

190.27
144.79
141.96
128.90
128.55
128.34
127.84
127.34
127.04
126.77
125.49
124.47
77.37
77.05
76.74


O

4n

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)


7.48
7.46
7.37
7.35
7.34
7.32
7.30
6.94
6.70
6.66
1.19
O
4o
3.04
4.03
1.09
1.02
9.00
f1 (ppm)


204.46
142.84
141.07
136.25
128.96
128.79
127.13
126.87
124.28
77.32
77.00
76.68
43.02
26.34
O
4o
f1 (ppm)