Supplementary Information

$InCl_3$-Catalyzed Intramolecular Carbonyl−Olefin Metathesis

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1. General Information

General Laboratory Procedures: Unless the preparation procedure is indicated, the compounds used were obtained from commercial sources and used without further purification. Potassium α-oxocarboxylates were obtained by the reaction of the corresponding α-oxocarboxylic acids with potassium *tert*-butoxide in ethanol.[1] α-Bromoacetophenones **8c**, **8f**, **8h** and **8i** were obtained by bromination with *N*-bromosuccinimide and *p*-toluenesulfonic acid from the corresponding acetophenones. Solvents used as eluents in chromatographic techniques (TLC or column chromatography) were purified by distillation.

Instruments and conditions:

Nuclear Magnetic Resonance: NMR spectra were recorded with Bruker spectrometer brand model Avance-300 DPX at 300 MHz for ^{1}H NMR (using the Me_4Si signal as internal reference standard, δ = 0.00 ppm) and at 75 MHz for ^{13}C NMR (using the solvent signal as internal reference standard). Measurements were made with sample dissolved in $CDCl_3$. ^{1}H NMR spectra are informed indicating the chemical shifts of the signals (δ) and then, in parentheses, the multiplicity of the signal, the coupling constants (*J*) and integration. The ^{13}C NMR spectra are reported indicating the chemical shifts of the signals. Abbreviations used to indicate the multiplicities of the signals are s: singlet; brs: broad singlet; d: doublet; dd: doublet of doublets; td: triplet of doublets; dt: doublet of triplets; t: triplet; sept: septet and m: multiplet.

Mass Spectrometry: HRMS spectra were performed at the Unit of Microanalysis and Physical Methods Applied to Organic Chemistry (UMYMFOR-UBA), using a Bruker mass spectrometer micrOTOF-Q II. The detection of ions was carried out by electrospray ionization (ESI), positive mode.

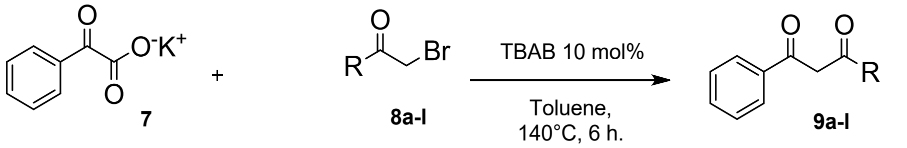
Chromatography: TLCs were performed on commercial aluminum plates covered with Merck silica gel (60 F_{254}). Chromatographic plates were analyzed by UV radiation (254 nm) and/or spraying with irreversible development methods. Preparative separations were carried out by liquid column chromatography using Merck 60 H silica gel (70-230 mesh and 230-400 mesh).

Microwave: Microwave reactions were carried out in 10 mL microwave vials on Biotage® Initiator+ Microwave or 10 mL vials on Discover 2.0 Microwave Synthesizer.

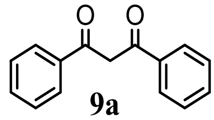
2. Preparation of Starting Materials

2.1. General Procedure for the Synthesis of Starting Materials 1a-l

2.1.1. General Procedure to Prepare 1,3-Diketones 9a-l[2]

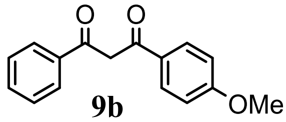


A flame-dried schlenk tube with a magnetic stirring bar was charged with potassium α-oxocarboxylate **7** (1 equiv.), α-bromoketone **8a-l** (1 equiv.), 10 mol% TBAB and toluene (0.25 M). The reaction was stirred at 140 ºC for 6 h under N_2 atmosphere. After cooled down to room temperature, the mixture was diluted with 15 mL of CH_2Cl_2, filtered through a celite pad. The solvent was then evaporated and the residue was purified by column chromatography using hexane/EtOAc as the eluent to provide the corresponding 1,3-diketone **9a-l**.



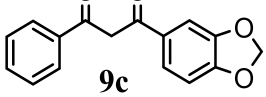
9a

1,3-diphenylpropane-1,3-dione (9a).[1] General procedure to prepare 1,3-diketones was followed employing 2-bromoacetophenone (**8a**) (99.5 mg, 0.5 mmol) and compound **7** (94 mg, 0.5 mmol) in 2 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **9a** with 56% yield (63 mg), as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 – 7.89 (m, 4H), 7.62 – 7.35 (m, 6H), 6.86 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.8, 135.6, 132.5, 128.7, 127.2, 93.2.



9b

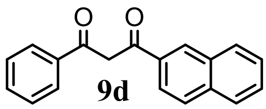
1-(4-methoxyphenyl)-3-phenylpropane-1,3-dione (9b).[1] General procedure to prepare 1,3-diketones was followed employing 2-bromo-4'-methoxyacetophenone (**8b**) (183 mg, 0.8 mmol) and compound **7** (150 mg, 0.8 mmol) in 3.2 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **9b** with 50% yield (101.6 mg), as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 – 7.90 (m, 4H), 7.60 – 7.40 (m, 3H), 6.97 (d, J = 9.0 Hz, 2H), 6.79 (s, 1H), 3.96 – 3.73 (m, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 186.2, 184.0, 163.3, 135.6, 132.2, 129.3, 128.6, 128.2, 127.0, 114.0, 92.4, 55.5.



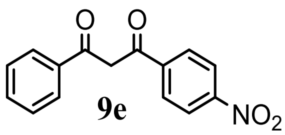
9c

1-(benzo[d][1,3]dioxol-5-yl)-3-phenylpropane-1,3-dione (9c).[1] General procedure to prepare 1,3-diketones was followed employing 1-(1,3-benzodioxol-5-yl)-2-bromoethan-

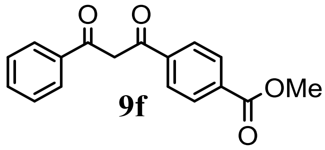
1-one (**8c**) (194.4 mg, 0.8 mmol) and compound **7** (150 mg, 0.8 mmol) in 3.2 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (90:10) provided **9c** with 66% yield, as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (d, J = 8.2 Hz, 2H), 7.65 – 7.34 (m, 5H), 6.86 (d, J = 8.2 Hz, 1H), 6.72 (s, 1H), 6.03 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 186.1, 183.7, 151.4, 148.2, 135.3, 132.2, 130.2, 128.6, 127.0, 122.9, 108.2



1-(naphthalen-2-yl)-3-phenylpropane-1,3-dione (9d).[3] General procedure to prepare 1,3-diketones was followed employing 2-bromo-2′-acetonaphthone (**8d**) (380 mg, 2 mmol) and compound **7** (503 mg, 2 mmol) in 8 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **9d** with 87% yield (477 mg), as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.54 (s, 1H), 8.12 – 7.73 (m, 6H), 7.68 – 7.38 (m, 5H), 7.01 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.8, 185.6, 135.6, 135.3, 132.81 132.8, 132.5, 129.4, 128.7, 128.5, 128.3, 128.2, 127.8, 127.2, 126.8, 123.3, 93.5.

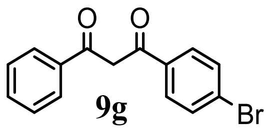


1-(4-nitrophenyl)-3-phenylpropane-1,3-dione (9e).[1] General procedure to prepare 1,3-diketones was followed employing 2-bromo-4-nitroacetophenone (**8e**) (519 mg, 2.13 mmol) and compound **7** (400 mg, 2.13 mmol) in 8.5 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **9e** with 60% yield (344 mg), as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.34 (d, J = 8.8 Hz, 2H), 8.14 (d, J = 8.8 Hz, 2H), 8.01 (d, J = 7.6 Hz, 2H), 7.61 (t, J = 7.2 Hz, 1H), 7.53 (t, J = 7.2 Hz, 2H), 6.90 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$): δ = 188.0, 181.8, 150.0, 141.1, 135.3, 133.3, 129.0, 128.2, 127.6, 124.0, 94.4.



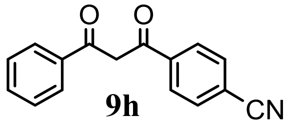
9f

methyl 4-(3-oxo-3-phenylpropanoyl)benzoate (9f).[1] General procedure to prepare 1,3-diketones was followed employing methyl 4-(2-bromoacetyl)benzoate (**8f**) (360 mg, 1.4 mmol) and compound **7** (263 mg, 1.4 mmol) in 6 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **9f** with 50% yield (197 mg), as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.13 (d, J = 8.5 Hz, 2H), 8.01 (d, J = 8.5 Hz, 2H), 7.62 – 7.41 (m, 4H), 6.88 (s, 1H), 3.95 (s, 3H). ^{13}C NMR (100 MHz, CDCl3): δ = 187.3, 183.7, 166.4, 139.4, 135.6, 133.4, 132.9, 130.0, 128.9, 127.5, 127.2, 94.1, 52.6.



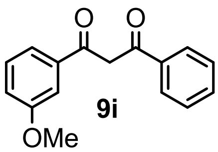
9g

1-(4-bromophenyl)-3-phenylpropane-1,3-dione (9g).[1] General procedure to prepare 1,3-diketones was followed employing 2-bromo-4'-bromoacetophenone (**8g**) (740 mg, 2.7 mmol) and compound **7** (500 mg, 2.7 mmol) in 10 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (98:2) provided **9g** with 83% yield (681 mg), as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 (d, J = 6.9 Hz, 2H), 7.83 (d, J = 8.5 Hz, 2H), 7.61 (d, J = 8.5 Hz, 2H), 7.57 – 7.43 (m, 3H), 6.80 (s, 1H).^{13}C NMR (75 MHz, $CDCl_3$) δ 185.9, 184.6, 135.3, 134.4, 132.6, 131.9, 128.7, 128.7, 127.3, 127.2, 93.0.



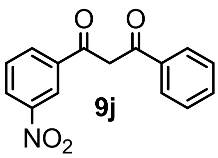
9h

4-(3-oxo-3-phenylpropanoyl)benzonitrile (9h).[1] General procedure to prepare 1,3-diketones was followed employing 4-(2-bromoacetyl) benzonitrile (**8h**) (473 mg, 2.1 mmol) and compound **7** (400 mg, 2.1 mmol) in 8.5 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (98:2) provided **9h** with 66% yield (346.5 mg), as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 (d, J = 8.4 Hz, 2H), 8.00 (d, J = 7.2 Hz, 2H), 7.79 (d, J = 7.2 Hz, 2H), 7.66 – 7.56 (m, 2H), 7.56 – 7.46 (m, 2H), 6.86 (s, 1H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 187.5, 182.2, 139.3, 135.2, 133.1, 132.5, 128.8, 127.6, 127.4, 118.1, 115.5, 93.9.



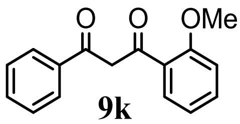
9i

1-(3-methoxyphenyl)-3-phenylpropane-1,3-dione (9i).[1] General procedure to prepare 1,3-diketones was followed employing 2-bromo-1-(3-methoxyphenyl)ethanone (365.1 mg, 1.6 mmol) and compound **7** (300 mg, 1.6 mmol) in 4.0 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **9i** with 72% yield (290.0 mg), as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 – 7.94 (m, 2H), 7.57 – 7.42 (m, 5H), 7.37 (t, J = 8.0 Hz, 1H), 7.08 (d, J = 8.0 Hz, 1H), 6.82 (s, 1H), 3.85 (s, 3H).^{13}C NMR (75 MHz, $CDCl_3$) δ 185.9, 185.4, 159.9, 137.1, 132.5, 129.7, 128.7, 127.2, 119.6, 118.6, 112.0, 93.4, 55.5.



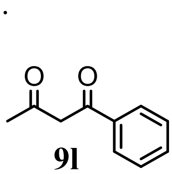
9j

1-(3-nitrophenyl)-3-phenylpropane-1,3-dione (9j).[1] General procedure to prepare 1,3-diketones was followed employing 2-bromo-1-(3-nitrophenyl)ethanone (194.4 mg, 0.8 mmol) and compound **7** (150 mg, 0.8 mmol) in 3.2 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **9j** with 50% yield (108 mg), as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.80 (t, J = 2.1 Hz, 1H), 8.40 (ddd, J = 8.0, 2.0, 1.1 Hz, 1H), 8.33 (ddd, J = 8.0, 2.0, 1.1 Hz, 1H), 8.05 – 8.00 (m, 2H), 7.70 (t, J = 8.0 Hz, 1H), 7.64 – 7.57 (m, 1H), 7.57 – 7.49 (m, 2H), 6.91 (s, 1H).^{13}C NMR (75 MHz, $CDCl_3$) δ 186.8, 182.6, 148.5, 137.3, 134.9, 133.1, 132.8, 129.9, 128.9, 127.4, 126.6, 122.0, 93.4.



9k

1-(2-methoxyphenyl)-3-phenylpropane-1,3-dione (9k).[1] General procedure to prepare 1,3-diketones was followed employing 2-bromo-1-(2-methoxyphenyl)ethanone (365.1 mg, 1.6 mmol) and compound **7** (300 mg, 1.6 mmol) in 4.0 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **9k** with 35% yield (140.0 mg), as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.04 – 7.93 (m, 3H), 7.57 – 7.45 (m, 4H), 7.14 (s, 1H), 7.09 – 7.05 (m, 1H), 7.02 – 6.97 (m, 1H), 3.95 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 185.8, 184.2, 158.5, 136.0, 133.1, 132.2, 130.3, 128.3, 127.2, 124.9, 120.8, 111.7, 98.5, 55.8.

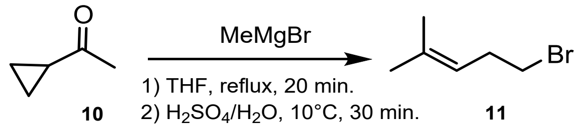


9l

1-phenylbutane-1,3-dione (9l).[1] General procedure to prepare 1,3-diketones was followed employing 1-bromopropan-2-one (**8l**) (411.7 mg, 2.2 mmol) and compound **7** (300 mg, 2.2 mmol) in 8.8 mL of toluene. Purification by column chromatography eluting with hexane/EtOAc (98:2) provided **9l** with 29% yield (103 mg), as a white solid. ^{1}H

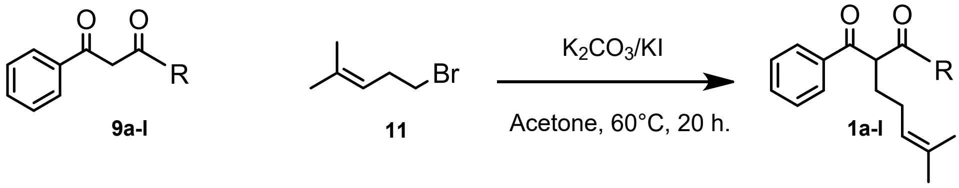
NMR (300 MHz, $CDCl_3$) δ 7.88 (d, *J* =7.2 Hz, 2H), 7.58 – 7.39 (m, 3H), 6.18 (s, 1H), 2.20 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 193.8, 183.3, 134.9, 132.3, 128.6, 127.0, 96.7, 25.9.

2.1.2. Synthesis of 5-bromo-2-methylpent-2-ene (11)[4]



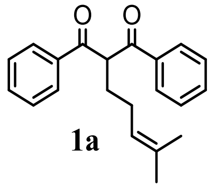
A solution of cyclopropylmethyl ketone (**10**) (5g, 59.5 mmol, 1.0 equiv.) in anhydrous THF (8 mL) was added dropwise to a solution of methylmagnesium bromide (3M in Et_2O, 71.4 mmol, 1.2 equiv.) at room temperature. The mixture was then heated at reflux for 30 minutes. The reaction mixture was cooled to 0°C, and slowly added to a cooled solution of concentrate sulphuric acid in water (1:2). After completion of the addition, the mixture was stirred for 30 minutes. The organic layer was then separated and the aqueous phase was extracted with diethyl ether (3×10 mL). The combined organic extracts were washed with saturated $NaHCO_3$ and brine, dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was distilled under vacuum to give 5-bromo-2-methylpent-2-ene (**11**) as a colorless oil (7.76g, 80% yield). ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.17 – 5.07 (m, 1H), 3.34 (t, *J* = 7.3 Hz, 2H), 2.56 (q, *J* = 7.3 Hz, 2H), 1.72 (s, 3H), 1.63 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 135.2, 121.1, 33.0, 32.0, 25.8, 18.1.

2.1.3. General Alkylation Procedure for the Synthesis of Compounds 1a-l[5]



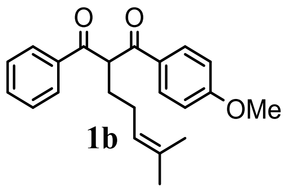
A round bottom flask equipped with a magnetic stir bar was charged with K_2CO_3 (2.5 equiv.) and KI (1.5 equiv). Dry acetone (0.2 M) was then added, followed by the 1,3-

diketone **9a-l** (1 equiv.) and 5-bromo-2-methylpent-2-ene (**11**) (1.2 equiv). The resulting mixture was heated at reflux and stirred overnight. The reaction was then cooled to room temperature, quenched with H_2O and extracted with Et_2O (3x10 mL). The combined organic extracts were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated under reduced pressure by rotary evaporation. Purification by column chromatography using hexane/ethyl acetate as the eluent provided compound **1a-l**.



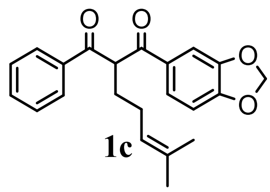
1a

2-(4-Methylpent-3-en-1-yl)-1,3-diphenylpropane-1,3-dione (1a).[6] General procedure 2.1.3. was followed employing compound **9a** (300 mg, 1.34 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (262 mg, 1.60 mmol) in 6.7 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (98:2) provided **1a** with 60% yield (246 mg), as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.2 Hz, 2H), 7.61 – 7.48 (m, 2H), 7.43 (td, *J* = 7.5, 7.1, 1.5 Hz, 5H), 5.27-5.23 (m, 1H), 5.19-5.15 (m, 1H), 2.25 – 2.04 (m, 4H), 1.69 (s, 3H), 1.50 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.2, 136.2, 133.7, 133.4, 128.8, 128.5, 123.2, 56.0, 29.4, 26.5, 25.7, 17.7. HRMS (ESI+) calcd. for $[C_{21}H_{22}O_2 + H]$: 307.1685, found: 307.1693.



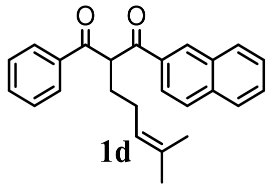
1b

1-(4-Methoxyphenyl)-2-(4-methylpent-3-en-1-yl)-3-phenylpropane-1,3-dione (1b). General procedure 2.1.3. was followed employing compound **9b** (274.6 mg, 1.08 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (211.5 mg, 1.30 mmol) in 5.4 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (98:2) provided **1b** with 70% yield (255.5 mg), as an orange solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.06 – 7.66 (m, 4H), 7.69 – 7.49 (m, 1H), 7.50 – 7.38 (m, 2H), 7.00 – 6.82 (m, 2H), 5.24 – 5.06 (m, 2H), 3.86 (s, 3H), 2.39 – 1.86 (m, 4H), 1.70 (d, *J* = 1.3 Hz, 3H), 1.50 (d, *J* = 1.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.3, 194.7, 163.7, 136.3, 133.6, 133.3, 130.9, 129.1, 128.8, 128.5, 123.3, 114.0, 56.2, 55.5, 29.5, 26.5, 25.7, 17.7. HRMS (ESI+) calcd. for $[C_{22}H_{24}O_3 + Na]$: 359.1607, found: 359.1618.



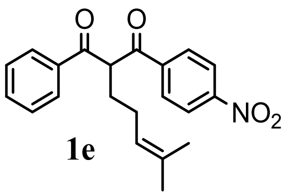
1c

1-(Benzo[d][1,3]dioxol-5-yl)-2-(4-methylpent-3-en-1-yl)-3-phenylpropane-1,3-dione (1c). General procedure 2.1.3. was followed employing compound **9c** (274 mg, 1.02 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (200 mg, 1.23 mmol) in 6 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (98:2) provided **1c** with yields of 56% (200 mg), as a white solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.99 – 7.90 (m, 2H), 7.59 – 7.51 (m, 2H), 7.47 – 7.40 (m, 3H), 6.82 (d, *J* = 8.2 Hz, 1H), 6.03 (s, 2H), 5.20 – 5.13 (m, 1H), 5.13 – 5.07 (m, 1H), 2.20 – 2.07 (m, 4H), 1.70 (d, *J* = 1.4 Hz, 3H), 1.51 (d, *J* = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.2, 194.3, 152.1, 148.4, 136.17, 133.7, 133.4, 130.9, 128.8, 128.5, 124.9, 123.2, 108.4, 108.0, 101.9, 56.2, 29.5, 26.5, 25.7, 17.7. HRMS (ESI+) calcd. for $[C_{22}H_{22}O_4 + Na]$: 373.1426, found: 373.1410.



1d

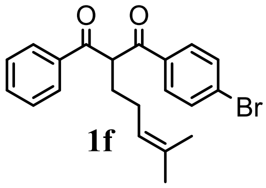
2-(4-Methylpent-3-en-1-yl)-1-(naphthalen-2-yl)-3-phenylpropane-1,3-dione (1d). General procedure 2.1.3. was followed employing compound **9d** (400 mg, 1.46 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (285.5 mg, 1.75 mmol) in 7 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (98:2) provided **1d** with 46% yield (240 mg), as a yellow solid. ^{1}H NMR (300 MHz $CDCl_3$) δ 8.49 (s, 1H), 8.07 – 7.95 (m, 3H), 7.94 – 7.81 (m, 3H), 7.65 – 7.48 (m, 3H), 7.47 – 7.39 (m, 2H), 5.37 (t, J = 4.9 Hz, 1H), 5.28 – 5.13 (m, 1H), 2.43 – 2.07 (m, 4H), 1.73 (d, J = 1.4 Hz, 3H), 1.51 (d, J = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.3, 196.2, 136.3, 135.7, 133.7, 133.5, 133.4, 132.5, 130.4, 129.7, 128.9, 128.8, 128.7, 128.5, 127.8, 126.9, 124.2, 123.3, 56.3, 29.5, 26.5, 25.8, 17.8. HRMS (ESI+) calcd. for $[C_{25}H_{24}O_2 + Na]$: 379.1687, found: 379.1669.



1e

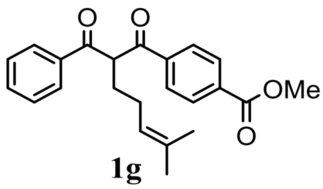
2-(4-Methylpent-3-en-1-yl)-1-(4-nitrophenyl)-3-phenylpropane-1,3-dione (1e). General procedure 2.1.3. was followed employing compound **9e** (400 mg, 1.49 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (291 mg, 1.78 mmol) in 7 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **1e** with 15% yield (78.4 mg), as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.31 – 8.23 (m, 2H), 8.10 – 8.04 (m, 2H), 7.99 – 7.93 (m, 2H), 7.66 – 7.57 (m, 1H), 7.56 – 7.44 (m, 2H), 5.26 – 5.07 (m, 2H), 2.32 – 2.05 (m, 4H), 1.70 (d, J = 1.4 Hz, 3H), 1.50 (d, J = 1.4

Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.0, 194.7, 150.3, 140.8, 135.6, 134.1, 133.9, 129.4, 129.1, 128.6, 124.0, 122.9, 113.8, 94.3, 56.7, 29.2, 26.3, 25.7, 17.8. HRMS (ESI+) calcd. for [$C_{21}H_{21}NO_4$ + Na]: 374.1348, found: 374.1363.



1f

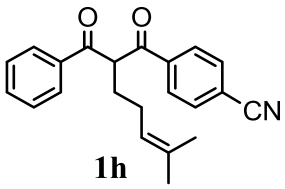
1-(4-Bromophenyl)-2-(4-methylpent-3-en-1-yl)-3-phenylpropane-1,3-dione (1f). General procedure 2.1.3. was followed employing compound **9f** (400 mg, 1.32 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (257 mg, 1.58 mmol) in 6.6 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **1f** with 25% yield (127.4 mg), as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.97 – 7.91 (m, 2H), 7.83 – 7.77 (m, 2H), 7.61 – 7.53 (m, 3H), 7.49 – 7.40 (m, 2H), 5.21 – 5.09 (m, 2H), 2.23 – 2.07 (m, 3H), 1.70 (d, J = 1.4 Hz, 3H), 1.50 (d, J = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.0, 195.2, 135.9, 134.9, 133.9, 133.6, 132.1, 130.0, 128.9, 128.7, 128.6, 123.0, 56.3, 29.3, 26.4, 25.7, 17.8. HRMS (ESI+) calcd. for [$C_{21}H_{19}BrO_2$ + H]: 383.0652, found: 383.0641.



1g

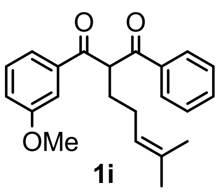
Methyl 4-(2-benzoyl-6-methylhept-5-enoyl)benzoate (1g). General procedure 2.1.3. was followed employing compound **9g** (100 mg, 0.35 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (68.5 mg, 0.42 mmol) in 1.75 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (98:2) provided **1g** with 59% yield (75.16

mg), as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.12 – 8.06 (m, 2H), 8.00 – 7.93 (m, 4H), 7.62 – 7.54 (m, 1H), 7.49 – 7.43 (m, 2H), 5.26 – 5.10 (m, 2H), 3.93 (s, 3H), 2.28 – 2.05 (m, 4H), 1.70 (d, J = 1.4 Hz, 3H), 1.49 (d, J = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.1, 195.7, 166.1, 139.5, 135.9, 133.9, 133.6, 130.0, 128.9, 128.6, 128.4, 123.0, 56.4, 52.5, 29.3, 26.4, 25.7, 17.8. HRMS (ESI+) calcd. for [$C_{23}H_{24}O_4$ + H]: 365.1732, found: 365.1747.



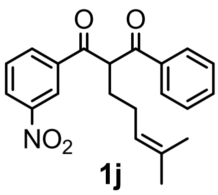
1h

4-(2-Benzoyl-6-methylhept-5-enoyl) benzonitrile (1h). General procedure 2.1.3. was followed employing compound **9h** (184 mg, 0.74 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (144 mg, 0.88 mmol) in 3.7 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **1h** with 30% yield (73.7 mg), as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 – 7.91 (m, 4H), 7.76 – 7.69 (m, 2H), 7.65 – 7.56 (m, 1H), 7.55 – 7.43 (m, 2H), 5.42 – 4.90 (m, 2H), 2.34 – 2.02 (m, 4H), 1.69 (s, 3H), 1.49 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 195.9, 194.9, 139.3, 135.6, 134.1, 133.9, 132.6, 132.5, 132.5, 129.0, 128.8, 128.8, 128.7, 128.6, 122.9, 117.7, 116.6, 56.5, 29.2, 26.4, 25.7, 17.7. HRMS (ESI+) calcd. for [$C_{22}H_{21}NO_2$ + Na]: 354.1466, found: 354.1464.



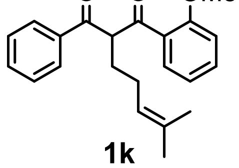
1i

1-(3-methoxyphenyl)-2-(4-methylpent-3-en-1-yl)-3-phenylpropane-1,3-dione (1i). General procedure 2.1.3. was followed employing compound **9i** (100 mg, 0.393 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (96 mg, 0.590 mmol) in 3 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **1i** with 49% yield (49.0 mg), as a yellow oil. ^{1}H NMR (300 MHz, CDCl$_3$) δ 7.98 – 7.92 (m, 2H), 7.59 – 7.48 (m, 3H), 7.48 – 7.40 (m, 2H), 7.34 (t, *J* = 8.0 Hz, 1H), 7.09 (ddd, *J* = 8.0, 2.7, 1.0 Hz, 1H), 5.25 – 5.13 (m, 2H), 3.79 (s, 3H), 2.20 – 2.10 (m, 4H), 1.70 (d, *J* = 1.3 Hz, 3H), 1.50 (d, *J* = 1.3 Hz, 3H).^{13}C NMR (75 MHz, CDCl$_3$) δ 196.2, 196.0, 160.0, 137.5, 136.2, 133.7, 133.4, 129.8, 128.8, 128.5, 123.2, 121.0, 120.1, 112.7, 56.1, 55.4, 29.4, 26.5, 25.7, 17.8. HRMS (ESI+) calcd. for [$C_{22}H_{24}O_3$ + Na]: 359.1618, found: 359.1631.



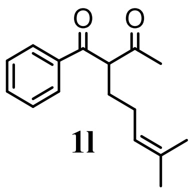
1j

2-(4-methylpent-3-en-1-yl)-1-(3-nitrophenyl)-3-phenylpropane-1,3-dione (1j). General procedure 2.1.3. was followed employing compound **9j** (100 mg, 0.371 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (91 mg, 0.557 mmol) in 3 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **1j** with 29% yield (38.0 mg), as a yellow solid. ^{1}H NMR (300 MHz, CDCl$_3$) δ 8.77 (t, *J* = 2.1 Hz, 1H), 8.40 (ddd, *J* = 8.2, 2.1, 1.1 Hz, 1H), 8.25 (ddd, *J* = 7.8, 1.7, 1.1 Hz, 1H), 8.00 – 7.92 (m, 2H), 7.70 – 7.56 (m, 2H), 7.54 – 7.44 (m, 2H), 5.28 – 5.13 (m, 2H), 2.29 – 2.08 (m, 4H), 1.72 (d, *J* = 1.4 Hz, 3H), 1.50 (d, *J* = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, CDCl$_3$) δ 195.9, 194.1, 148.5, 137.5, 135.7, 134.3, 134.0, 133.9, 130.1, 129.1, 128.6, 127.6, 123.3, 122.8, 56.3, 29.3, 26.3, 25.7, 17.8. HRMS (ESI+) calcd. for [$C_{21}H_{21}NO_4$ + Na]: 374.1363, found: 374.1378.



1k

1-(2-methoxyphenyl)-2-(4-methylpent-3-en-1-yl)-3-phenylpropane-1,3-dione (1k). General procedure 2.1.3. was followed employing compound **9k** (100 mg, 0.393 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (96 mg, 0.590 mmol) in 3 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **1k** with 19% yield (25.0 mg), as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.02 – 7.97 (m, 2H), 7.85 (dd, *J* = 7.9, 1.8 Hz, 1H), 7.60 – 7.53 (m, 1H), 7.51 – 7.41 (m, 3H), 7.01 (ddd, *J* = 7.9, 7.3, 1.0 Hz, 1H), 6.87 (dd, *J* = 7.9, 1.0 Hz, 1H), 5.35 (dd, *J* = 7.9, 4.6 Hz, 1H), 5.18 – 5.10 (m, 1H), 3.50 (s, 3H), 2.28 – 2.16 (m, 1H), 2.11 (q, *J* = 7.1 Hz, 2H), 1.94 – 1.83 (m, 1H), 1.68 (d, *J* = 1.4 Hz, 3H), 1.50 (d, *J* = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.9, 196.7, 158.3, 136.4, 134.0, 133.1, 132.9, 131.3, 128.6, 128.5, 126.9, 123.6, 121.0, 111.4, 59.6, 54.9, 28.9, 26.7, 25.7, 17.7. HRMS (ESI+) calcd. for [$C_{22}H_{24}O_3$ + Na]: 359.1618, found: 359.1608.

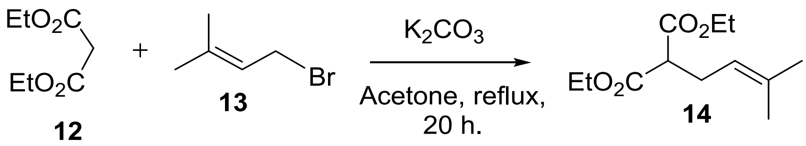


1l

2-(4-Methylpent-3-en-1-yl)-1-phenylbutane-1,3-dione (1l). General procedure 2.1.3. was followed employing compound **9l** (186 mg, 1.15 mmol) and 5-bromo-2-methylpent-2-ene (**11**) (225 mg, 1.38 mmol) in 3.7 mL of dry acetone. Purification by column chromatography eluting with hexane/EtOAc (99:1) provided **1l** with 29% yield (81.4 mg), as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.07 – 7.88 (m, 2H), 7.67 – 7.52 (m, 1H), 7.52 – 7.44 (m, 2H), 5.16 – 4.93 (m, 1H), 4.45 (t, *J* = 6.6 Hz, 1H), 2.14 (s, 3H), 2.13 – 1.81 (m, 4H), 1.65 (d, *J* = 1.4 Hz, 3H), 1.49 (d, *J* = 1.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 204.5, 196.6, 136.5, 133.6, 133.4, 128.8, 128.7, 122.9, 62.70 29.2, 27.9, 26.0, 25.7, 17.6. HRMS (ESI+) calcd. for [$C_{16}H_{20}O_2$ + Na]: 267.1350, found: 267.1356.

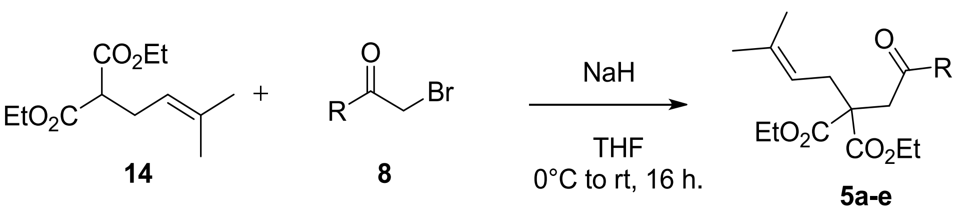
2.2. General Procedure for the Synthesis of Starting Materials 5a-e

2.2.1 Synthesis of diethyl 2-(3-methylbut-2-en-1-yl)malonate (14).

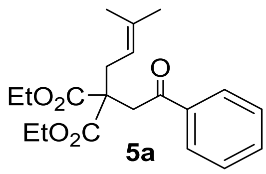


1-Bromo-3-methylbut-2-ene (**13**) (820 mg, 5.5 mmol, 1.1 equiv.) and K_2CO_3 (1.38 g, 10 mmol, 2.0 equiv.), were sequentially added to a stirred solution of dimethyl malonate (**12**) (800 mg, 5 mmol, 1 equiv.) in acetone (12,5 mL). The resulting mixture was stirred at room temperature overnight. Then K_2CO_3 was removed by filtration though a funnel. The resulting mixture was then extracted with ethyl ether (3×10 mL), washed with saturated brine, dried over Na_2SO_4, and evaporated under reduced pressure. The residue was purified by column chromatography (hexane/EtOAc, 95:5) to afford diethyl 2-(3-methylbut-2-en-1-yl)malonate (**14**) with 89% yield (1.2 g). ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.17 – 4.95 (m, 1H), 4.19 (q, J = 7.1 Hz, 4H), 3.32 (t, J = 7.6 Hz, 1H), 2.58 (t, J = 7.6 Hz, 2H), 1.68 (s, 3H), 1.63 (s, 3H), 1.26. (t, J = 7.1 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 169.3, 134.8, 119.7, 61.3, 52.2, 27.5, 25.8, 17.7, 14.1.

2.2.2 General Alkylation Procedure for the Synthesis of Compounds 5a-e.

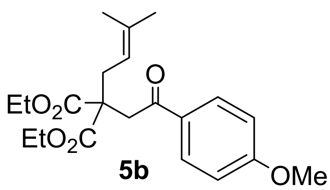


A round bottom flask was charged with NaH (2 equiv.) followed by THF (0.1 M) under a nitrogen atmosphere. The resulting suspension was then cooled to 0 °C and a solution of diethyl 2-(3-methylbut-2-en-1-yl)malonate (**14**) (1.0 equiv.) in THF (0.5 M) was added dropwise over 20 min. The cooling bath was removed and the reaction mixture was allowed to warm to rt over 45 min. A solution of the corresponding α-bromoacetophenone (**8**) (1.1 equiv.) in THF (0.6 M) was rapidly added. The resulting mixture was stirred at room temperature for 16 h. Then 1M hydrochloric acid was added, and the resulting mixture was stirred for 10 min and extracted with EtOAc (3x10mL). The combined organic extracts were dried over $MgSO_4$ and concentrated under reduced pressure. The residue was purified by column chromatography (hexane/ethyl acetate) affording products **5a-e**.



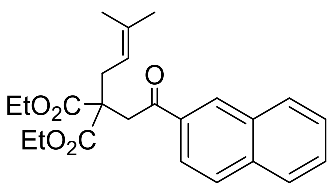
5a

Diethyl 2-(3-methylbut-2-en-1-yl)-2-(2-oxo-2-phenylethyl)malonate (5a). General procedure 2.2.2. was followed with diethyl 2-(3-methylbut-2-en-1-yl) malonate (**14**) (200 mg, 0.88 mmol) and 2-bromoacetophenone (**8a**) (286.3 mg, 0.96 mmol). Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **5a** with 29% yield (88.3 mg), as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.03 – 7.88 (m, 2H), 7.64 – 7.51 (m, 1H), 7.51 – 7.36 (m, 2H), 4.96 (t, J = 6.7 Hz, 1H), 4.21 (q, J = 7.1 Hz, 4H), 3.65 (s, 2H), 2.84 (d, J = 7.8 Hz, 2H), 1.62 (d, J = 1.5 Hz, 3H), 1.42 (d, J = 1.5 Hz, 3H), 1.24 (td, J = 7.1, 1.2 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 197.0, 170.8, 136.7, 136.3, 133.2, 128.6, 128.0, 118.2, 61.5, 55.5, 40.9, 31.6, 25.9, 17.7, 14.0. HRMS (ESI+) calcd. for [$C_{20}H_{26}O_5$ + Na]: 369.1672, found: 369.1680.



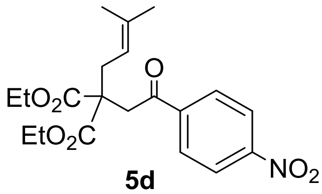
5b

Diethyl 2-(2-(4-methoxyphenyl)-2-oxoethyl)-2-(3-methylbut-2-en-1-yl)malonate (5b). General procedure 2.2.2. was followed with diethyl 2-(3-methylbut-2-en-1-yl) malonate (**14**) (150 mg, 0.66 mmol) and 2-bromo-4'-methoxyacetophenone (**8b**) (166 mg, 0.72 mmol). Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **5b** with 46% yield (114 mg), as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (d, J = 8.9 Hz, 2H), 6.93 (d, J = 8.9 Hz, 2H), 4.96 (t, J = 7.8 Hz, 1H), 4.21 (q, J = 7.1 Hz, 4H), 3.87 (s, 3H), 3.60 (s, 2H), 2.84 (d, J = 7.8 Hz, 2H), 1.62 (d, J = 1.5 Hz, 3H), 1.42 (d, J = 1.5 Hz, 3H), 1.24 (t, J = 7.1 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 195.5, 170.8, 163.5, 136.2, 130.3, 129.8, 118.2, 113.7, 61.4, 55.5, 40.4, 31.5, 25.9, 17.8, 14.0. HRMS (ESI+) calcd. for [$C_{21}H_{28}O_6$ + Na]: 399.1778, found: 399.1780.



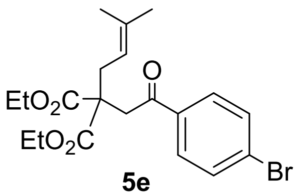
5c

Diethyl 2-(3-methylbut-2-en-1-yl)-2-(2-(naphthalen-2-yl)-2-oxoethyl)malonate (5c). General procedure 2.2.2. was followed with diethyl 2-(3-methylbut-2-en-1-yl) malonate (**14**) (200 mg, 0.88 mmol) and 2-bromo-2′-acetonaphthone (**8d**) (240 mg, 0.96 mmol). Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **5c** with yields of 35% (111.5 mg), as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.56 – 8.41 (m, 1H), 8.06 – 7.94 (m, 2H), 7.94 – 7.81 (m, 2H), 7.65 – 7.50 (m, 2H), 5.00 (t, J = 7.8 Hz, 1H), 4.24 (q, J = 7.1 Hz, 4H), 3.80 (s, 2H), 2.90 (d, J = 7.8 Hz, 2H), 1.62 (d, J = 1.4 Hz, 3H), 1.42 (d, J = 1.4 Hz, 3H), 1.26 (t, J = 7.1 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.9, 170.8, 136.4, 135.6, 134.1, 132.5, 129.8, 129.6, 128.5, 128.4, 127.8, 126.8, 123.7, 118.2, 61.6, 55.5, 40.9, 31.5, 25.9, 17.8, 14.0. HRMS (ESI+) calcd. for [$C_{24}H_{28}O_5$ + Na]: 419.1829, found: 419.1821.



5d

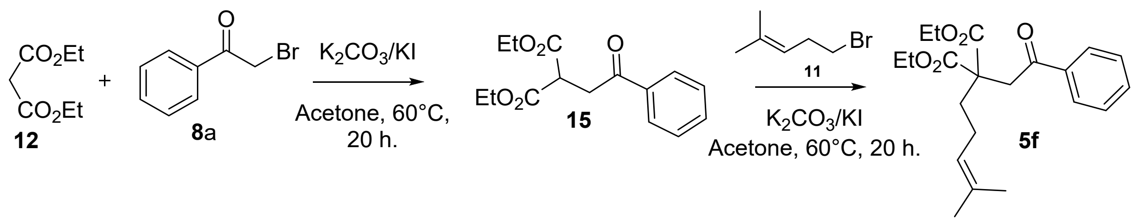
Diethyl 2-(3-methylbut-2-en-1-yl)-2-(2-(4-nitrophenyl)-2-oxoethyl)malonate (5d). General procedure 2.2.2. was followed with diethyl 2-(3-methylbut-2-en-1-yl) malonate (**14**) (200 mg, 0.88 mmol) and 2-bromo-4-nitroacetophenone (**8e**) (235 mg, 0.96 mmol). Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **5d** with 27% yield (93 mg), as a yellow solid. ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.31 (d, *J* = 8.9 Hz, 2H), 8.11 (d, *J* = 8.9 Hz, 2H), 4.96 (t, *J* = 7.8 Hz, 1H), 4.22 (q, *J* = 7.1 Hz, 4H), 3.65 (s, 2H), 2.85 (d, *J* = 7.8 Hz, 2H), 1.63 (d, *J* = 1.5 Hz, 3H), 1.44 (d, *J* = 1.5 Hz, 3H), 1.37 – 1.11 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.5, 171.2, 151.2, 141.9, 137.4, 129.8, 124.6, 118.7, 62.5, 56.4, 42.2, 32.5, 26.7, 18.6, 14.8. HRMS (ESI+) calcd. for [$C_{20}H_{25}NO_7$ + Na]: 414.1523, found: 414.1525.



5e

Diethyl 2-(2-(4-bromophenyl)-2-oxoethyl)-2-(3-methylbut-2-en-1-yl)malonate (5e). General procedure 2.2.2. was followed with diethyl 2-(3-methylbut-2-en-1-yl) malonate (**14**) (200 mg, 0.88 mmol) and 2-bromo-4'-bromoacetophenone (**8g**) (286 mg, 0.96 mmol). Purification by column chromatography eluting with hexane/EtOAc (95:5) provided **5e** with 28% yield (104.7 mg), as a colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.82 (d, *J* = 8.6 Hz, 2H), 7.60 (d, *J* = 8.6 Hz, 2H), 4.94 (t, *J* = 6.4 Hz, 1H), 4.21 (q, *J* = 7.1 Hz, 4H), 3.59 (s, 2H), 2.83 (d, *J* = 7.8 Hz, 2H), 1.63 (d, *J* = 1.4 Hz, 3H), 1.43 (d, *J* = 1.4 Hz, 3H), 1.24 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.1, 170.7, 136.5, 135.5, 131.9, 129.5, 128.5, 118.1, 61.6, 55.5, 40.8, 31.6, 26.0, 17.8, 14.0. HRMS (ESI+) calcd. for [$C_{20}H_{25}BrO_5$ + Na]: 447.0778, found: 447.0784

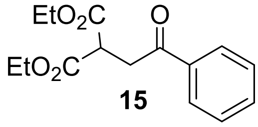
2.3. General Procedure for the Synthesis of Starting Material 5f



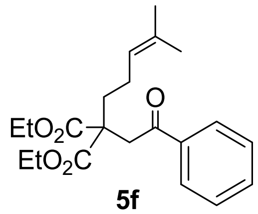
A round bottom flask was charged with K_2CO_3 (1.1 g, 7.8 mmol, 2.5 equiv.) and KI (777 mg, 4.68 mmol, 1.5 equiv). Dry acetone (0.2 M) was then added, followed by diethyl malonate (**12**) (500 mg, 3.12 mmol, 1 equiv.) and 2-bromoacetophenone (**8a**) (750 mg, 3.75 mmol, 1.2 equiv). The resulting mixture was heated at reflux and stirred overnight. The reaction was then cooled to room temperature, quenched with H_2O and extracted with AcOEt (3x15mL). The combined organic extracts were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated under reduced pressure by rotary evaporation. Purification by column chromatography using hexane/ EtOAc (95:5) as the eluent to provide diethyl 2-(2-oxo-2-phenylethyl) malonate (**15)** with 60% yields (520 mg), as a yellow oil.

A round bottom flask was charged with K_2CO_3 (1.1 g, 7.8 mmol, 2.5 equiv.) and KI (777 mg, 4.68 mmol, 1.5 equiv.). Dry acetone (0.2 M) was then added, followed by compound **15** (407 mg, 1.46 mmol, 1 equiv.) and 5-bromo-2-methylpent-2-ene (**11**) (352 mg, 2.16 mmol, 1.2 equiv). The resulting mixture was heated at reflux and stirred overnight. The reaction was then cooled to room temperature, quenched with H_2O and extracted with AcOEt (3x15mL). The combined organic extracts were washed with H_2O and brine, dried over $MgSO_4$, filtered and concentrated under reduced pressure by rotary evaporation.

Purification by column chromatography using hexane/ EtOAc (95:5) as the eluent to provide **5f** with 19% yield (99.8 mg), as a colorless oil.

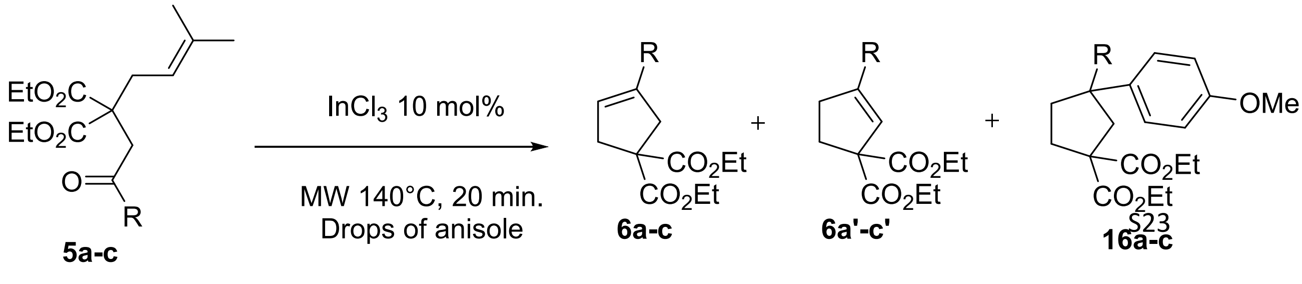


Diethyl 2-(2-oxo-2-phenylethyl) malonate (15). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.05 – 7.93 (m, 2H), 7.66 – 7.54 (m, 1H), 7.50 – 7.39 (m, 2H), 4.33 – 4.15 (m, 4H), 4.06 (t, *J* = 7.1 Hz, 1H), 3.62 (d, *J* = 7.1 Hz, 2H), 1.28 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.5, 169.0, 136.1, 133.5, 128.6, 128.1, 61.7, 47.2, 37.7, 14.0.

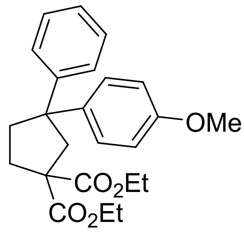


Diethyl 2-(4-methylpent-3-en-1-yl)-2-(2-oxo-2-phenylethyl) malonate (5f). ^{1}H NMR (300 MHz, $CDCl_3$) δ 8.15 – 7.83 (m, 1H), 7.63 – 7.53 (m, 1H), 7.52 – 7.41 (m, 2H), 5.03 (t, *J* = 7.1 Hz, 1H), 4.21 (q, *J* = 7.1 Hz, 4H), 3.72 (s, 2H), 2.22 – 2.11 (m, 2H), 1.93 (q, *J* = 7.7, 7.1 Hz, 2H), 1.59 (t, *J* = 1.5 Hz, 3H), 1.53 (d, *J* = 1.5 Hz, 3H), 1.25 (td, *J* = 7.1, 1.2 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 196.7, 171.0, 136.7, 133.3, 132.5, 128.6, 128.0, 123.2, 61.5, 55.3, 41.3, 32.9, 25.5, 23.5, 17.6, 14.2. HRMS (ESI+) calcd. for [$C_{21}H_{28}O_5$ + Na]: 383.1829, found: 383.1821.

3. In(III)-catalyzed metathesis/hydroarylation by-reaction from malonates 5a-c

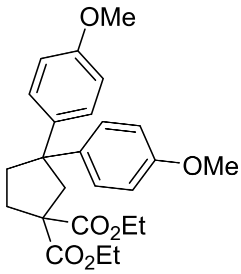


A microwave vessel was charged with compound **5a-c**, $InCl_3$ (10 mol%) and drops of anisole to facilitate stirring. The reaction mixture was heated to 140 °C in a microwave reactor (holding time 20 min). The reaction mixture was purified by column chromatography eluting with hexane/EtOAc to afford the desired metathesis products (**6a-c** and **6a'-c'**) and product **16a-c**, obtained by hydroarylation of the alkene with anisole.



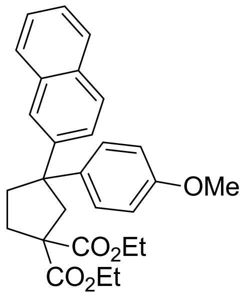
16a

Diethyl 3-(4-methoxyphenyl)-3-phenylcyclopentane-1,1-dicarboxylate (16a). General procedure 3.2.3 was followed with compound **5a** (14 mg, 0.043 mmol). Purification by column chromatography eluting with hexane/EtOAc (95:5) provided products **6a, 6a'** and **16a** with 95% yield. Specifically, product **16a** was obtained with 52% yield (8.9 mg), as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.31 – 7.15 (m, 6H), 7.15 – 7.07 (m, 1H), 6.81 – 6.73 (m, 2H), 4.08 (q, *J* = 7.1 Hz, 4H), 3.74 (s, 3H), 3.23 – 3.04 (m, 2H), 2.47 (t, *J* = 6.8 Hz, 2H), 2.32 (t, *J* = 6.8 Hz, 2H), 1.18 (td, *J* = 7.1, 1.3 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.6, 172.5, 157.8, 147.9, 139.5, 128.4, 128.1, 126.9, 126.0, 113.7, 61.7, 59.6, 55.4, 55.3, 45.6, 38.5, 32.8, 14.2. HRMS (ESI+) calcd. for [$C_{24}H_{28}O_5$ + Na]: 419.1825, found: 419.1829.



16b

Diethyl 3,3-bis(4-methoxyphenyl)cyclopentane-1,1-dicarboxylate (16b). General procedure 3.2.3 was followed with compound **5b** (30.1 mg, 0.087 mmol). Purification by column chromatography eluting with hexane/EtOAc (95:5) provided products **6b**, **6b´** and **16b** with 87% yield. Specifically, product **16b** was obtained with 32% yield (11.85 mg), as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.20 – 7.08 (m, 4H), 6.79 – 6.69 (m, 4H), 4.08 (q, *J* = 7.1 Hz, 4H), 3.75 (s, 6H), 3.10 (s, 2H), 2.44 (t, *J* = 6.7 Hz, 2H), 2.31 (t, *J* = 6.7 Hz, 2H), 1.19 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.3, 157.5, 139.7, 127.8, 113.5, 61.5, 59.5, 55.2, 54.5, 45.6, 38.5, 32.6, 13.9. HRMS (ESI+) calcd. for [$C_{25}H_{30}O_6$ + Na]: 449.1935, found: 449.1918.

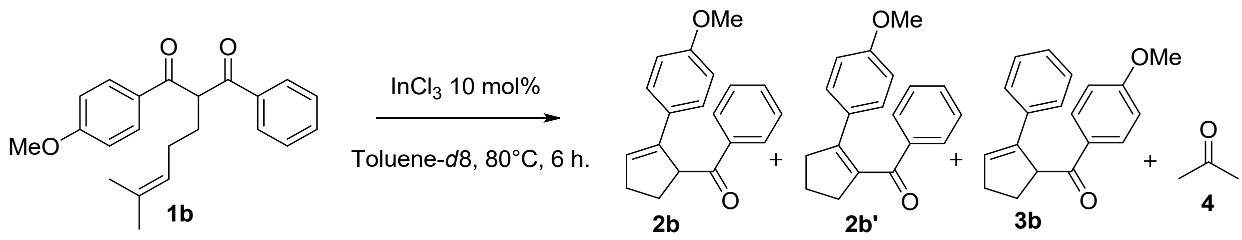


16c

Diethyl 3-(4-methoxyphenyl)-3-(naphthalen-2-yl)cyclopentane-1,1-dicarboxylate (16c). General procedure 3.2.3 was followed with compound **5c** (42.5 mg, 0.107 mmol). Purification by column chromatography eluting with hexane/EtOAc (95:5) provided products **6c**, **6c’** and **16c** with 72% yield. Specifically, product **16c** was obtained with 14% yield (6.7 mg), as a yellow oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 – 7.63 (m, 5H), 7.51 – 7.36 (m, 2H), 7.23 (d, *J* = 8.8 Hz, 2H), 6.77 (d, *J* = 8.8 Hz, 2H), 4.17 – 3.98 (m, 4H), 3.74 (s, 3H), 3.33 – 3.11 (m, 2H), 2.65 – 2.51 (m, 2H), 2.41 – 2.30 (m, 2H), 1.25 –

1.08 (m, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 172.3, 157.7, 144.9, 139.1, 133.1, 131.7, 128.1, 127.9, 127.8, 127. 126.4, 125.9, 125.6, 124.1, 113.5, 61.5, 59.5, 55.3, 55.2, 45.3, 38.3, 32.6, 14.0, 13.9. HRMS (ESI+) calcd. for [$C_{28}H_{30}O_5$+ Na]: 469.1985, found: 469.1967.

4. *In Situ* ^{1}H-NMR Experiment for Intramolecular Carbonyl-Olefin Metathesis



An NMR tube containing $InCl_3$ (0.7 mg, 0.0032 mmol) was charged with **1b** (10.9 mg, 0.032 mmol) and toluene-*d*8 (0.5 mL). Then, the reaction mixture was measured in a 400 MHz NMR at regular time points (15 minutes) at 80°C. An abbreviated series of spectra is shown in the paper, including time points at 0 min., 30 min., 90 min., 3 h, 4.5 h, 6 h. As indicated in the **Figure S1**, the disappearance of **2b** is accompanied by the emergence of **2b'** over time, which confirmed that the direct metathesis product is formed first and this isomerized to give the more stable by conjugation, product **2b'**. The reaction was very clean and completed after ca. 3 h at 80 °C.

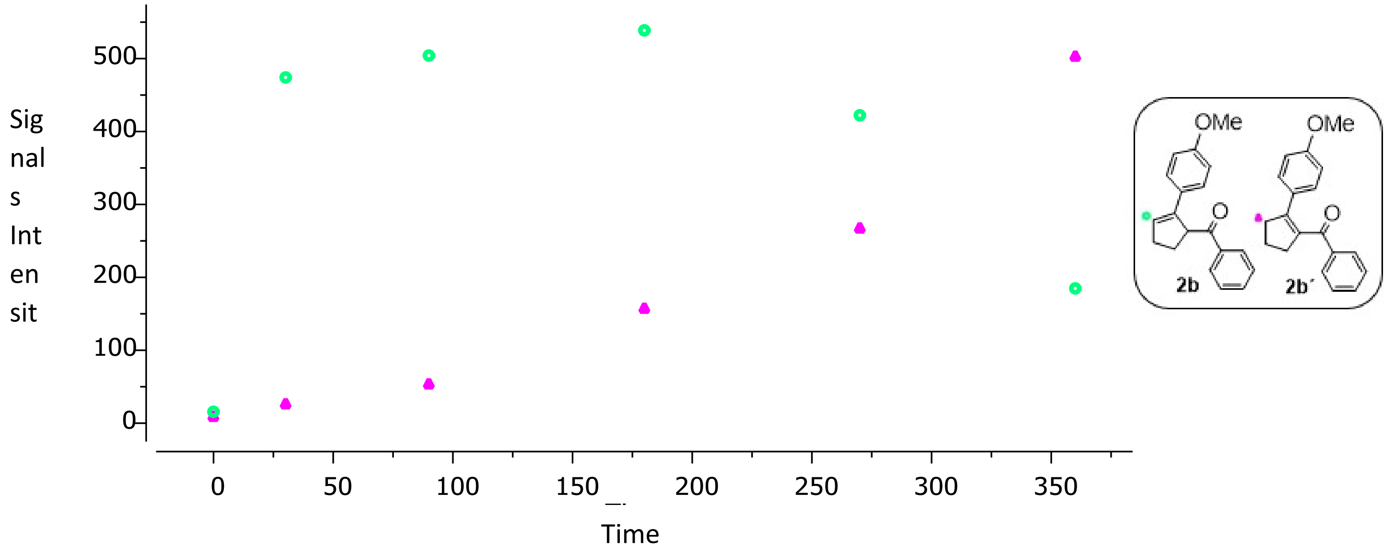


Figure S1. Signals intensity of the characteristic protons of **2b** and **2b'** vs reaction time (minutes).

5. Computational Details

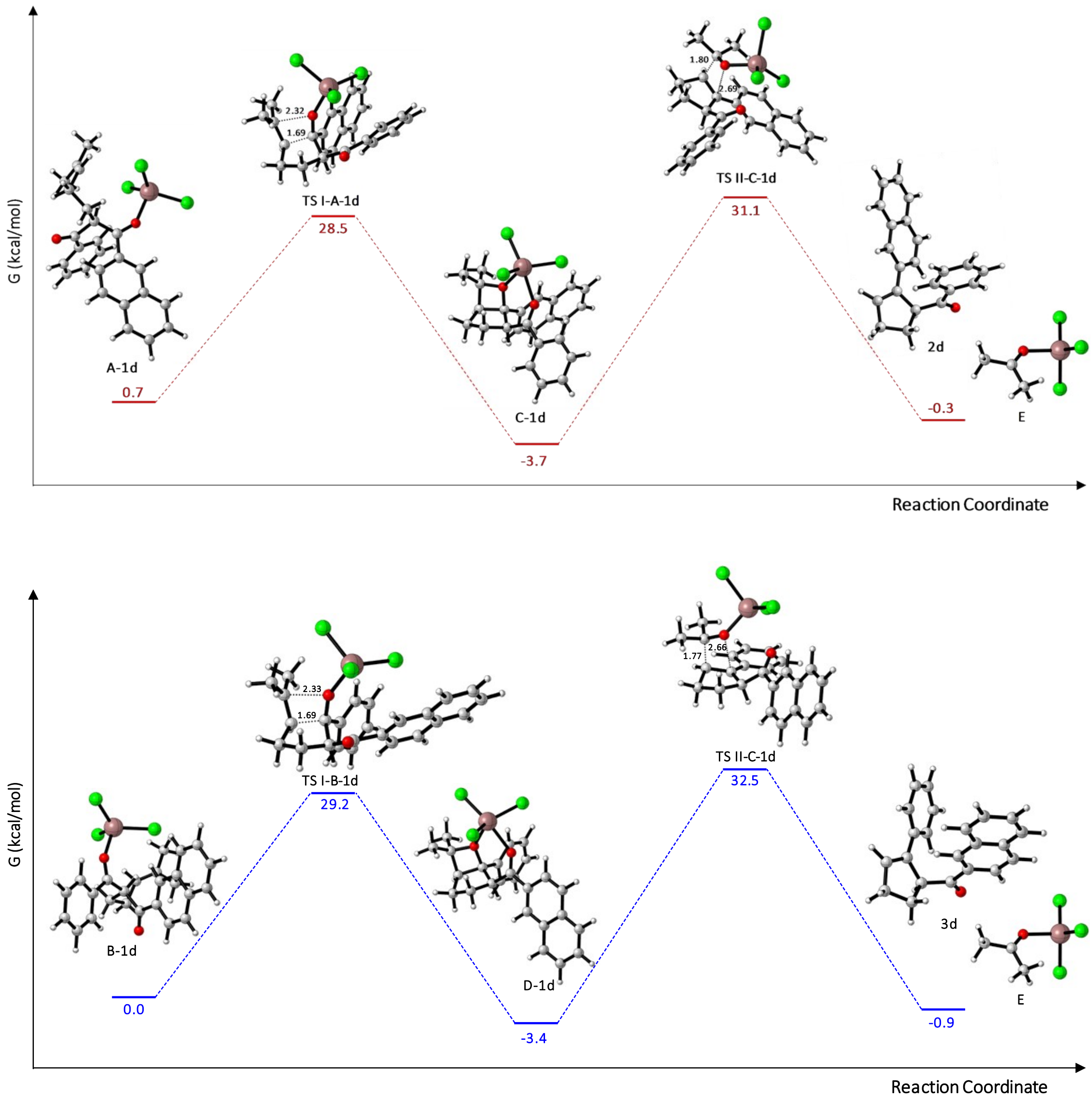


Figure S2. Global minima structures found for the **2d** (top) and **3d** (bottom) paths at the M06-2X/6-311+G** level of theory. Gibbs free energies (relative to **B-1d**) and selected distances are given in kcal/mol, and Å, respectively.

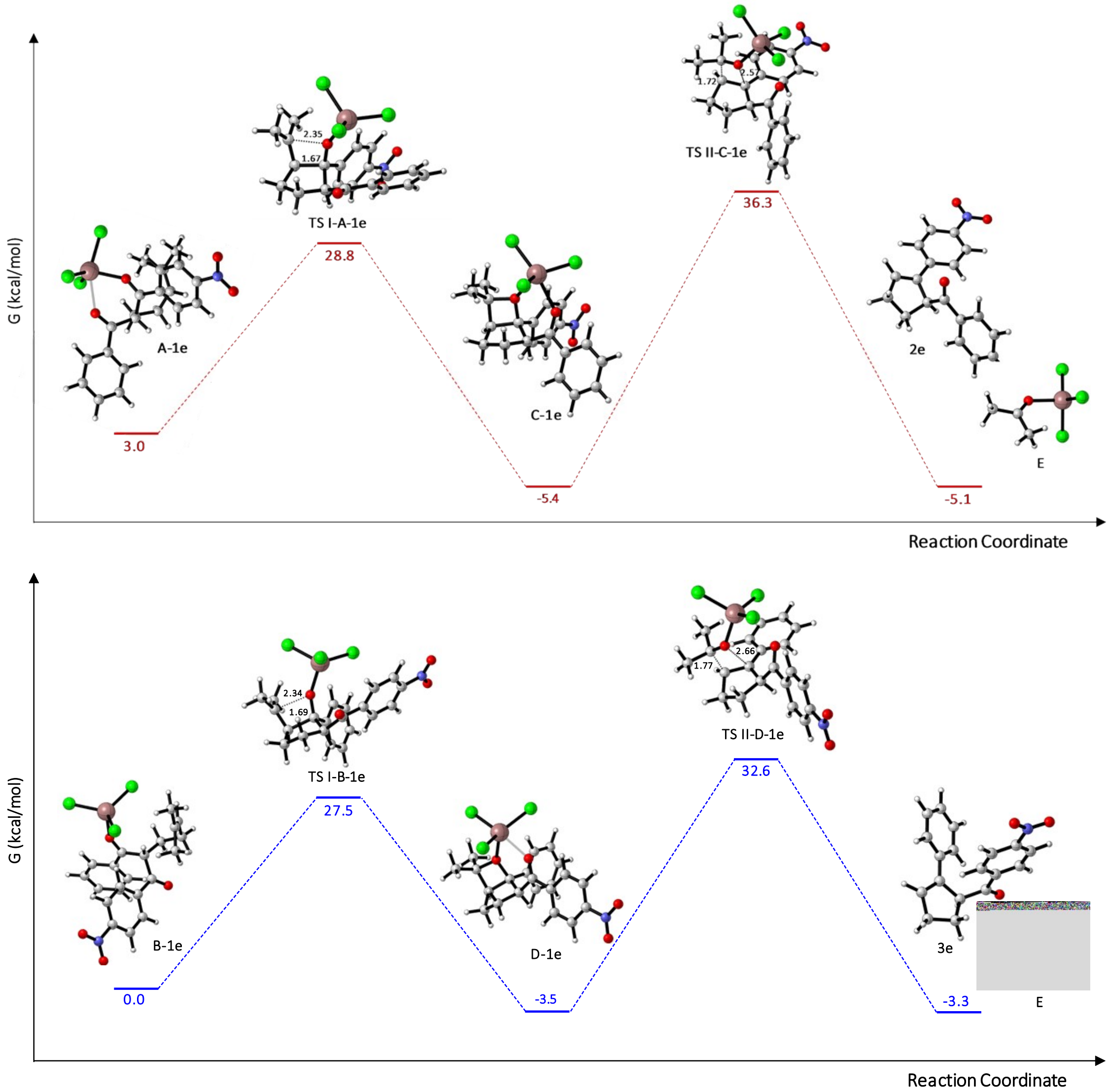


Figure S3. Global minima structures found for the **2e** (top) and **3e** (bottom) paths at the M06-2X/6-311+G** level of theory. Gibbs free energies (relative to **B-1e**) and selected distances are given in kcal/mol, and Å, respectively.

Table S1. M06-2X/6-31G* energies (E), zero-point corrected energies (ZPE), enthalpies (H) and Gibbs free energies (G), in au, computed for all structures shown in Figures S1 and S2.

	E	ZPE	H	G
A_1d	-2500.064873	-2499.634687	-2499.601968	-2499.702741
TS_IA_1d	-2500.023655	-2499.595599	-2499.564310	-2499.658372
C_1d	-2500.080871	-2499.647172	-2499.616576	-2499.709787
TS_IIC_1d	-2500.022632	-2499.592454	-2499.561814	-2499.654277
2d	-924.251419	-923.913654	-923.894716	-923.961661
B_1d	-2500.066669	-2499.636193	-2499.603582	-2499.703864
TS_IB_1d	-2500.021417	-2499.593856	-2499.562343	-2499.657295
D_1d	-2500.079922	-2499.646322	-2499.615772	-2499.709207
TS_IID_1d	-2500.020170	-2499.590337	-2499.559700	-2499.652137
3d	-924.252303	-923.914589	-923.895640	-923.962558
A_1e	-2550.927859	-2550.542102	-2550.509544	-2550.611194
TS_IA_1e	-2550.890320	-2550.506281	-2550.475059	-2550.570043
C_1e	-2550.949794	-2550.560497	-2550.529975	-2550.624589
TS_IIC_1e	-2550.881917	-2550.495708	-2550.465289	-2550.558046
2e	-975.125503	-974.832248	-974.813315	-974.881299
B_1e	-2550.932653	-2550.546926	-2550.514161	-2550.615930
TS_IB_1e	-2550.892375	-2550.508739	-2550.477473	-2550.572044
D_1e	-2550.946350	-2550.557399	-2550.526789	-2550.621478
TS_IID_1e	-2550.888133	-2550.501739	-2550.471263	-2550.563973
3e	-975.123365	-974.829781	-974.810914	-974.878500
E	-1575.789197	-1575.700080	-1575.686411	-1575.742708

Cartesian Coordinates

2d

C	-2.066797	-1.509808	0.660446
C	-3.208817	-2.010488	-0.256949
C	-2.538099	-3.045853	-1.184106
C	-1.087957	-2.637766	-1.155273
C	-0.819207	-1.771504	-0.173161
C	0.487480	-1.181256	0.161669
C	2.986099	-0.060183	0.860802
C	0.787649	-0.847510	1.512795
C	1.426442	-0.925812	-0.812108
C	2.688616	-0.370239	-0.493752
C	2.000095	-0.311250	1.848956
C	-2.278712	-0.093921	1.186284
O	-2.554504	0.060651	2.355376
C	-2.170623	1.100445	0.278698
C	-1.993400	3.412218	-1.278430
C	-2.355626	2.360494	0.855985
C	-1.894998	1.011297	-1.088198
C	-1.809519	2.163980	-1.861800
C	-2.266102	3.509168	0.084078
C	3.666407	-0.105941	-1.489168
C	4.879348	0.432269	-1.152212
C	5.175905	0.737649	0.198416
C	4.250648	0.497408	1.179141
H	-2.024409	-2.127910	1.564589
H	-3.595524	-1.178928	-0.850875
H	-4.039266	-2.419808	0.317864
H	-2.963506	-3.044226	-2.190709
H	-2.651175	-4.064456	-0.794511
H	-0.340788	-3.058825	-1.818383
H	0.047134	-1.028241	2.284367
H	1.195799	-1.133957	-1.852647
H	2.221320	-0.067276	2.882651
H	-1.924112	4.309170	-1.882998
H	-2.567903	2.413341	1.916800
H	-1.738090	0.049042	-1.557293
H	-1.595001	2.085543	-2.920849
H	-2.407723	4.481067	0.541877
H	3.435820	-0.341472	-2.522921
H	5.619764	0.626293	-1.919284
H	6.139455	1.163716	0.451290
H	4.471256	0.731343	2.215348

SCF Energy (M06-2X/6-311+G**)= -924.251418870

Gibbs Energy (M06-2X/6-311+G**)= -923.961661

Number of imaginary frequencies = 0

2e

C	-1.174608	1.183672	-0.526998

C -2.034131 2.461983 -0.723190
C -1.374684 3.507464 0.196205
C 0.041764 3.012519 0.301449
C 0.167133 1.745077 -0.103657
C 1.388298 0.927287 -0.096950
C 3.685331 -0.625264 -0.084888
C 2.656602 1.523318 -0.037901
C 1.309147 -0.469017 -0.164844
C 2.453389 -1.253821 -0.156127
C 3.808194 0.756666 -0.026166
C -1.799301 0.323099 0.572968
O -1.418707 0.396328 1.716898
C -2.933332 -0.589135 0.198766
C -5.038823 -2.321353 -0.385757
C -3.429747 -1.451719 1.179813
C -3.503875 -0.598575 -1.075869
C -4.555918 -1.460521 -1.365404
C -4.474125 -2.316655 0.887683
H -1.101240 0.598155 -1.446598
H -3.090436 2.300989 -0.500345
H -1.952277 2.782524 -1.764022
H -1.836723 3.515869 1.190194
H -1.447954 4.521273 -0.203199
H 0.839632 3.610156 0.725906
H 2.740822 2.602803 -0.017859
H 0.343504 -0.958357 -0.212799
H 2.403228 -2.333237 -0.201182
H 4.791336 1.205187 0.018184
H -5.855884 -2.995744 -0.613799
H -2.979176 -1.426238 2.164825
H -3.142748 0.070920 -1.847652
H -4.997129 -1.460133 -2.354707
H -4.851069 -2.987722 1.650140
N 4.908024 -1.449285 -0.081555
O 5.973215 -0.871872 -0.030607
O 4.774501 -2.653405 -0.130165
SCF Energy (M06-2X/6-311+G**)= -975.125503207
Gibbs Energy (M06-2X/6-311+G**)= -974.881299
Number of imaginary frequencies = 0

3d

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C 1.571181 -2.843596 -0.835267
C 2.250746 -2.429956 -2.156846
C 2.370391 -0.934123 -2.020677
C 2.157608 -0.515095 -0.769067
C 2.218868 0.869269 -0.270246
C 2.335008 3.499627 0.687090
C 2.572086 1.128996 1.058015
C 1.905455 1.947596 -1.105516

C	1.966809	3.251121	-0.632606
C	2.635107	2.435460	1.529844
C	0.880435	-1.538686	1.267165
O	1.183993	-1.863747	2.394308
C	-0.501490	-1.020137	0.991873
C	-3.127607	-0.046840	0.662021
C	-0.915753	-0.577713	-0.242513
C	-1.406858	-0.982175	2.088434
C	-2.678146	-0.512686	1.927253
C	-2.229588	-0.080854	-0.436640
C	-2.667760	0.386144	-1.702874
C	-3.941076	0.862793	-1.868448
C	-4.836120	0.895115	-0.773190
C	-4.439163	0.451270	0.461203
H	2.840490	-1.934918	0.683053
H	0.489016	-2.893372	-0.978552
H	1.901953	-3.813188	-0.463486
H	1.677685	-2.735732	-3.035650
H	3.245466	-2.880733	-2.255033
H	2.665297	-0.287844	-2.839642
H	2.376231	4.516706	1.058068
H	2.805541	0.307158	1.726334
H	1.591220	1.755530	-2.125770
H	1.714383	4.074993	-1.289761
H	2.914408	2.620442	2.560315
H	-0.246895	-0.589341	-1.094405
H	-1.054544	-1.334335	3.049756
H	-3.364604	-0.486264	2.766732
H	-1.974670	0.359197	-2.537140
H	-4.268867	1.217805	-2.838124
H	-5.840817	1.275175	-0.915816
H	-5.123044	0.475992	1.302721

SCF Energy (M06-2X/6-311+G**)= -924.252302533

Gibbs Energy (M06-2X/6-311+G**)= -923.962558

Number of imaginary frequencies = 0

3e

C	1.962001	-1.594315	0.458092
C	1.852449	-2.870529	-0.411528
C	2.717018	-2.569302	-1.653521
C	2.739167	-1.063321	-1.694262
C	2.300073	-0.511959	-0.558127
C	2.204259	0.921612	-0.234349
C	2.014843	3.645178	0.396395
C	2.284566	1.353421	1.093671
C	2.011526	1.875878	-1.240327
C	1.921891	3.225199	-0.928184
C	2.195096	2.705793	1.405006
C	0.746234	-1.379038	1.347674
O	0.830638	-1.598072	2.533639

C -0.577356 -0.924113 0.776152
C -3.047169 -0.080216 -0.105743
C -1.615503 -0.706924 1.686739
C -0.800574 -0.712752 -0.586741
C -2.044158 -0.288147 -1.037202
C -2.860947 -0.281254 1.254112
H 2.795783 -1.695854 1.162006
H 0.813441 -3.023190 -0.715050
H 2.169184 -3.759387 0.133352
H 2.310820 -3.015873 -2.564154
H 3.734746 -2.959291 -1.536423
H 3.134118 -0.502486 -2.533616
H 2.430011 0.631976 1.890603
H 1.911926 1.550665 -2.270129
H 1.767714 3.951406 -1.717587
H 2.264532 3.024330 2.438268
H -1.423992 -0.876745 2.738653
H -0.010767 -0.869490 -1.308349
H -2.241454 -0.116532 -2.086400
H -3.676389 -0.104772 1.942042
H 1.938312 4.698160 0.639347
N -4.373192 0.375487 -0.582935
O -5.240035 0.536231 0.247067
O -4.506370 0.557766 -1.773100
SCF Energy (M06-2X/6-311+G**)= -975.123365409
Gibbs Energy (M06-2X/6-311+G**)= -974.878500
Number of imaginary frequencies = 0

A_1d

C 4.045592 0.753232 -1.667162
C 4.777986 -0.273973 -1.014566
C 4.077476 -1.224347 -0.221187
C 2.676528 -1.121288 -0.110457
C 1.986201 -0.103089 -0.741341
C 2.689854 0.849159 -1.533479
C 0.529336 -0.058793 -0.561549
O -0.026413 -1.064785 -0.089515
C -0.313894 1.122197 -0.971020
C 0.308590 2.486766 -0.627266
O 0.513673 3.303353 -1.493772
C 0.642533 2.767096 0.799744
C 1.420809 3.894388 1.080606
C 0.205166 1.949079 1.843211
C 0.542740 2.256436 3.156712
C 1.325825 3.372193 3.428922
C 1.764582 4.192083 2.389882
C -0.676837 0.994997 -2.466537
C -1.899193 1.862081 -2.822838
C -3.162050 1.380810 -2.163776
C -3.721210 1.851977 -1.043958

C -5.012865 1.278390 -0.524974
C -3.156442 2.974749 -0.213993
In -1.886768 -1.893405 0.424229
Cl -2.902012 -2.156963 -1.637740
Cl -1.156350 -3.792044 1.516292
Cl -2.722607 -0.218311 1.815115
C 4.800588 -2.255896 0.435652
C 6.159750 -2.336621 0.305905
C 6.857059 -1.390509 -0.484246
C 6.185660 -0.384896 -1.128888
H 4.582865 1.467804 -2.280351
H 2.131102 -1.845555 0.484891
H 2.159921 1.637767 -2.050266
H -1.246236 1.043177 -0.395729
H 1.744148 4.520778 0.257947
H -0.429133 1.091331 1.657615
H 0.186745 1.625616 3.962071
H 1.591299 3.608939 4.452765
H 2.371824 5.062667 2.606699
H 0.180530 1.288978 -3.075589
H -0.908528 -0.052753 -2.683964
H -1.681502 2.903284 -2.583925
H -2.025565 1.810532 -3.907856
H -3.651192 0.542544 -2.653751
H -4.926791 1.023598 0.534250
H -5.814998 2.018604 -0.616859
H -5.302464 0.382753 -1.076910
H -2.295293 3.464131 -0.671149
H -3.921653 3.736230 -0.035008
H -2.857113 2.593327 0.769758
H 4.254451 -2.975027 1.035931
H 6.709132 -3.124522 0.806446
H 7.934009 -1.467088 -0.577566
H 6.721786 0.338300 -1.733088
SCF Energy (M06-2X/6-311+G**)= -2500.06487325
Gibbs Energy (M06-2X/6-311+G**)= -2499.702741
Number of imaginary frequencies = 0

A_1e

C 4.080616 1.622865 -0.047581
C 4.636277 0.613089 -0.818048
C 3.925017 -0.504023 -1.225051
C 2.597899 -0.612728 -0.838245
C 2.005646 0.388418 -0.060309
C 2.751983 1.504656 0.329097
C 0.576303 0.193170 0.314377
O 0.044224 -0.859346 -0.028381
C -0.248145 1.276698 0.970590
C -1.430882 1.611505 0.051748
O -2.020476 0.727273 -0.534273

C	-1.878938	3.021268	-0.074287
C	-2.770586	3.317031	-1.110656
C	-1.467256	4.029602	0.801283
C	-1.945271	5.323687	0.640629
C	-2.818705	5.616501	-0.402450
C	-3.228957	4.614412	-1.278491
C	-0.867271	0.817366	2.319106
C	0.179748	0.694364	3.434857
C	1.348758	-0.170633	3.035135
C	1.288194	-1.485055	2.783158
C	2.471389	-2.225335	2.231158
C	0.049196	-2.314321	2.952333
In	-1.822459	-1.724223	-0.712682
Cl	-2.165052	-1.190996	-2.945257
Cl	-0.725058	-3.808441	-0.609736
Cl	-3.371397	-1.648338	1.030790
N	6.059279	0.737474	-1.221932
O	6.655869	1.723346	-0.851171
O	6.524613	-0.154230	-1.892692
H	4.683946	2.471954	0.242735
H	4.407774	-1.262148	-1.826681
H	2.007499	-1.472670	-1.132650
H	2.319990	2.282991	0.943873
H	0.355904	2.165858	1.127961
H	-3.083268	2.518849	-1.773595
H	-0.799257	3.813544	1.627136
H	-1.637473	6.102305	1.327445
H	-3.183444	6.628695	-0.530854
H	-3.908848	4.845639	-2.089028
H	-1.643557	1.533722	2.605825
H	-1.371963	-0.135502	2.147269
H	0.538205	1.691803	3.706202
H	-0.322540	0.295986	4.321792
H	2.305208	0.327397	2.896898
H	2.757838	-3.052944	2.886351
H	2.197844	-2.670309	1.265771
H	3.334472	-1.571780	2.089059
H	0.290885	-3.234992	3.490634
H	-0.749711	-1.802335	3.487787
H	-0.332261	-2.630842	1.974504

SCF Energy (M06-2X/6-311+G**)= -2550.92785853
Gibbs Energy (M06-2X/6-311+G**)= -2550.611194
Number of imaginary frequencies = 0

B_1d

C	2.057415	4.630842	0.187356
C	2.097769	4.979790	-1.158724
C	1.420204	4.214853	-2.106798
C	0.701484	3.101143	-1.708034
C	0.670648	2.733866	-0.354519

C	1.352071	3.506799	0.594287
C	-0.105786	1.540639	0.017062
O	-0.877187	1.071552	-0.834950
C	-0.049881	0.909275	1.384787
C	1.369803	0.792728	1.972656
O	1.645400	1.340043	3.014723
C	2.376687	-0.015300	1.232922
C	2.040823	-0.775979	0.137553
C	3.721742	0.007326	1.695300
C	4.682612	-0.714949	1.049351
C	4.361296	-1.510156	-0.086190
C	3.017270	-1.543431	-0.543129
C	-1.017457	1.655570	2.329443
C	-1.385687	0.788252	3.548067
C	-2.198348	-0.418660	3.170543
C	-1.760314	-1.669308	2.990240
C	-2.715508	-2.775415	2.628319
C	-0.325135	-2.103453	3.133468
In	-2.329934	-0.408387	-1.192139
Cl	-4.061941	0.240061	0.194699
Cl	-2.584584	-0.127799	-3.468113
Cl	-1.135541	-2.318990	-0.581159
C	2.676980	-2.346408	-1.662112
C	3.641105	-3.075956	-2.305723
C	4.982475	-3.036861	-1.857590
C	5.335169	-2.274428	-0.773988
H	2.576486	5.233017	0.922306
H	2.658100	5.853479	-1.470956
H	1.452579	4.490711	-3.153484
H	0.163695	2.499224	-2.430328
H	1.325420	3.252554	1.645341
H	-0.433643	-0.111855	1.260624
H	1.020787	-0.842863	-0.220325
H	3.956849	0.607898	2.565299
H	5.710022	-0.695358	1.396674
H	-0.556630	2.588068	2.660974
H	-1.930398	1.901777	1.777403
H	-0.475627	0.522414	4.086288
H	-1.976046	1.414290	4.222976
H	-3.255815	-0.230184	3.002116
H	-2.362861	-3.318581	1.747733
H	-2.784242	-3.497369	3.449024
H	-3.714204	-2.387350	2.422171
H	0.336104	-1.317361	3.500810
H	-0.253482	-2.952383	3.820271
H	0.054830	-2.450640	2.165293
H	1.642749	-2.375600	-1.988697
H	3.379391	-3.688492	-3.160017
H	5.734874	-3.618769	-2.376718
H	6.362628	-2.248748	-0.427716

SCF Energy (M06-2X/6-311+G**)= -2500.06666854
Gibbs Energy (M06-2X/6-311+G**)= -2499.703864
Number of imaginary frequencies = 0

B_1e

C	2.174639	4.019986	1.884951
C	2.182825	4.889644	0.798760
C	1.443228	4.597596	-0.346298
C	0.692802	3.435951	-0.404270
C	0.692865	2.547090	0.680627
C	1.437745	2.844964	1.829236
C	-0.125236	1.330023	0.569339
O	-0.952343	1.275458	-0.351839
C	-0.040905	0.183755	1.548586
C	1.387196	-0.185250	1.972212
O	1.710866	-0.179488	3.134413
C	2.372157	-0.567348	0.907788
C	3.713563	-0.686110	1.282466
C	1.989999	-0.802963	-0.413190
C	2.940710	-1.156094	-1.363369
C	4.261572	-1.253405	-0.961833
C	4.673129	-1.027751	0.344856
C	-0.958596	0.473848	2.756508
C	-1.316300	-0.822389	3.508362
C	-2.174451	-1.742015	2.685078
C	-1.779172	-2.801466	1.971214
C	-2.777849	-3.633025	1.211145
C	-0.353468	-3.274983	1.858993
In	-2.474601	0.113840	-1.246874
Cl	-4.126321	0.144806	0.368590
Cl	-2.808660	1.344547	-3.164960
Cl	-1.277839	-1.868390	-1.532484
N	5.285384	-1.618201	-1.971645
O	6.433062	-1.697554	-1.594180
O	4.906131	-1.809509	-3.104334
H	2.741048	4.257520	2.776659
H	2.766518	5.801668	0.844088
H	1.451475	5.277912	-1.188535
H	0.104773	3.196217	-1.281956
H	1.430298	2.185034	2.686661
H	-0.455249	-0.689524	1.025580
H	3.984912	-0.506661	2.315342
H	0.953120	-0.753689	-0.720598
H	2.668406	-1.357813	-2.390674
H	5.719268	-1.121999	0.601972
H	-0.465520	1.176762	3.431252
H	-1.880151	0.938369	2.391115
H	-0.400428	-1.306280	3.848573
H	-1.868399	-0.532843	4.406636
H	-3.231135	-1.487921	2.658103

H -2.450396 -3.784186 0.179659
H -2.871891 -4.622753 1.670509
H -3.761346 -3.160679 1.198620
H 0.335817 -2.743838 2.517333
H -0.288865 -4.341469 2.094701
H -0.006993 -3.162540 0.824371
SCF Energy (M06-2X/6-311+G**)= -2550.93265301
Gibbs Energy (M06-2X/6-311+G**)= -2550.615930
Number of imaginary frequencies = 0

C_1d

C 2.616238 0.397099 2.103360
C 1.655367 -0.134981 1.201249
C 2.064172 -0.655409 0.002668
C 3.437531 -0.664383 -0.355873
C 4.396301 -0.139090 0.549394
C 3.946255 0.390630 1.788050
C 0.205366 -0.065160 1.592711
C -0.394053 1.346961 1.525531
C -1.672063 1.251433 2.382908
C -1.216761 0.368313 3.557077
C -0.238580 -0.649769 2.958510
C -0.839597 -1.827189 2.156485
C 0.052795 -3.051411 2.159298
O -0.614432 -1.052056 0.894696
In -1.562246 -1.134493 -1.057922
Cl -1.764269 -3.490453 -0.868127
C -2.297782 -2.162008 2.366574
Cl -0.261825 -0.935673 -3.000750
Cl -3.690293 -0.246967 -0.616346
C -0.631378 1.835025 0.119893
O -0.863881 1.032704 -0.773363
C -0.600220 3.280315 -0.197884
C -0.497704 4.259280 0.794083
C -0.694490 3.655254 -1.542582
C -0.674449 4.997013 -1.887937
C -0.574129 5.970070 -0.895429
C -0.490218 5.603172 0.444062
C 3.870680 -1.188558 -1.600579
C 5.202317 -1.194700 -1.921341
C 6.160315 -0.679256 -1.016026
C 5.767639 -0.162815 0.190627
H 2.287564 0.797196 3.058384
H 1.357191 -1.075022 -0.703524
H 4.676829 0.787202 2.485101
H 0.326355 2.003504 2.022875
H -2.036355 2.228903 2.701605
H -2.462668 0.774623 1.797897
H -0.683974 0.982387 4.288910
H -2.052745 -0.104169 4.075109

H	0.558396	-0.949598	3.637808
H	-0.010241	-3.527831	3.141466
H	-0.274042	-3.758911	1.397080
H	1.092086	-2.774045	1.971113
H	-2.415096	-2.556619	3.379866
H	-2.947192	-1.293888	2.252574
H	-2.618706	-2.929153	1.660795
H	-0.435095	3.983351	1.840110
H	-0.777331	2.880263	-2.295507
H	-0.739162	5.288081	-2.929076
H	-0.561601	7.019090	-1.167694
H	-0.415950	6.362311	1.212867
H	3.127312	-1.576564	-2.289142
H	5.529420	-1.594243	-2.873773
H	7.210251	-0.693696	-1.283943
H	6.498562	0.235388	0.886438

SCF Energy (M06-2X/6-311+G**)= -2500.08087066
Gibbs Energy (M06-2X/6-311+G**)= -2499.709787
Number of imaginary frequencies = 0

C_1e

C	2.929041	0.283549	1.500152
C	1.851530	-0.277515	0.807702
C	2.066330	-0.880143	-0.429547
C	3.341054	-0.910014	-0.983455
C	4.384198	-0.339815	-0.275703
C	4.206113	0.256236	0.964830
C	0.477699	-0.174963	1.416974
C	-0.076878	1.256500	1.462539
C	-1.205269	1.189492	2.511255
C	-0.605900	0.269238	3.587109
C	0.228639	-0.769508	2.828704
C	-0.530369	-1.911902	2.111861
C	0.303903	-3.168132	1.975077
O	-0.459302	-1.126682	0.837512
In	-1.683901	-1.139752	-0.978487
Cl	-1.959344	-3.481966	-0.756297
C	-1.955849	-2.192159	2.524534
Cl	-0.659631	-0.960134	-3.070541
Cl	-3.653940	-0.133253	-0.197343
C	-0.532064	1.784189	0.126627
O	-0.826544	1.001598	-0.765407
C	-0.667266	3.239638	-0.101264
C	-0.358601	4.182276	0.884099
C	-1.141797	3.663725	-1.347776
C	-1.300269	5.016376	-1.603150
C	-0.991264	5.951621	-0.617828
C	-0.522730	5.536338	0.625077
N	5.743863	-0.368855	-0.857568
O	6.631380	0.160214	-0.223817

O	5.882139	-0.916979	-1.927122
H	2.771732	0.737936	2.473621
H	1.253406	-1.334276	-0.980450
H	3.523768	-1.365438	-1.947715
H	5.054823	0.680637	1.483564
H	0.731701	1.885121	1.848264
H	-1.475266	2.174138	2.893956
H	-2.096951	0.756100	2.051259
H	0.056323	0.850660	4.235166
H	-1.366537	-0.186163	4.222896
H	1.109418	-1.108999	3.372586
H	0.354075	-3.663869	2.948323
H	-0.147341	-3.846781	1.251588
H	1.321030	-2.928001	1.657565
H	-1.948670	-2.572837	3.549680
H	-2.581403	-1.300361	2.484067
H	-2.396119	-2.952088	1.878245
H	0.004724	3.871007	1.856140
H	-1.378330	2.918134	-2.097437
H	-1.665971	5.345348	-2.567882
H	-1.117301	7.008975	-0.819061
H	-0.286362	6.266255	1.389330

SCF Energy (M06-2X/6-311+G**)= -2550.94979444
Gibbs Energy (M06-2X/6-311+G**)= -2550.624589
Number of imaginary frequencies = 0

D_1d

C	0.285638	3.722362	-0.385379
C	0.836224	2.445399	-0.517532
C	1.357374	2.049219	-1.745809
C	1.320572	2.919815	-2.831433
C	0.771465	4.188956	-2.696789
C	0.254341	4.591136	-1.468032
C	0.809097	1.523196	0.672513
C	-0.584034	0.971156	1.007344
C	-0.456230	0.481495	2.463810
C	0.416250	1.572375	3.106356
C	1.404827	2.009733	2.019269
C	2.600674	1.074155	1.723403
C	3.797841	1.815230	1.165261
O	1.823134	0.475545	0.592792
In	1.928012	-1.472605	-0.382741
Cl	4.290053	-1.451621	-0.160847
C	2.974741	0.045308	2.764265
Cl	1.669111	-1.692878	-2.699015
Cl	1.106168	-2.886873	1.302639
C	-1.066597	-0.092049	0.055267
O	-0.255412	-0.781602	-0.547668
C	-2.509676	-0.346907	-0.137403
C	-3.473090	0.339341	0.567211

C -2.887017 -1.359627 -1.063298
C -4.205221 -1.650083 -1.257678
C -5.220533 -0.958313 -0.541304
C -4.846462 0.050922 0.386381
C -5.855373 0.743897 1.104649
C -7.176848 0.445164 0.909248
C -7.549488 -0.559949 -0.014369
C -6.596166 -1.243876 -0.722571
H -0.108556 4.044513 0.574656
H 1.798371 1.068747 -1.875839
H 1.725640 2.596708 -3.782751
H 0.749196 4.864817 -3.543058
H -0.168122 5.582211 -1.352124
H -1.259504 1.831065 0.974464
H -1.425842 0.367853 2.950369
H 0.037028 -0.493917 2.474361
H -0.210157 2.426901 3.378432
H 0.913719 1.230324 4.015158
H 1.680867 3.062085 2.071228
H 4.285919 2.360093 1.977877
H 4.506513 1.111121 0.729127
H 3.486901 2.531376 0.401549
H 3.376285 0.570053 3.635781
H 2.122078 -0.556300 3.079656
H 3.745957 -0.623365 2.379541
H -3.206268 1.111042 1.281291
H -2.105644 -1.883052 -1.600405
H -4.498106 -2.419677 -1.963209
H -5.561298 1.513807 1.810017
H -7.943724 0.976450 1.459669
H -8.598842 -0.787007 -0.160057
H -6.881278 -2.014738 -1.429874
SCF Energy (M06-2X/6-311+G**)= -2500.07992217
Gibbs Energy (M06-2X/6-311+G**)= -2499.709207
Number of imaginary frequencies = 0

D_1e

C 0.349470 3.738314 -0.254713
C 0.842293 2.446272 -0.452811
C 1.238772 2.052555 -1.727434
C 1.135596 2.941215 -2.794330
C 0.645184 4.225288 -2.594033
C 0.252787 4.624681 -1.318770
C 0.896320 1.508169 0.723962
C -0.481801 1.038533 1.214641
C -0.216948 0.511505 2.639840
C 0.788983 1.537778 3.187701
C 1.671496 1.933349 1.998079
C 2.765922 0.934142 1.556055
C 3.933165 1.617029 0.873648

O	1.825657	0.401792	0.514927
In	1.734284	-1.534192	-0.477520
Cl	4.096531	-1.650317	-0.525358
C	3.196090	-0.132896	2.535027
Cl	1.167883	-1.653556	-2.741912
Cl	0.988270	-2.911206	1.267876
C	-1.137789	0.034131	0.307167
O	-0.461716	-0.718439	-0.371549
C	-2.621857	-0.074734	0.234498
C	-3.459032	0.612112	1.115603
C	-3.162361	-0.912449	-0.745692
C	-4.535769	-1.058016	-0.854243
C	-5.340470	-0.363859	0.037229
C	-4.836052	0.465614	1.025319
N	-6.813577	-0.514792	-0.069413
O	-7.493226	0.118967	0.706422
O	-7.234326	-1.259328	-0.924113
H	0.052793	4.058095	0.740500
H	1.635964	1.061292	-1.906159
H	1.444834	2.621200	-3.781834
H	0.571499	4.915981	-3.425245
H	-0.123430	5.627194	-1.153694
H	-1.100363	1.939370	1.272275
H	-1.126156	0.447352	3.239291
H	0.214393	-0.490786	2.579677
H	0.251027	2.423401	3.538074
H	1.363627	1.151415	4.030812
H	2.015104	2.966385	2.028950
H	4.532624	2.126388	1.633022
H	4.554893	0.884415	0.359463
H	3.581239	2.359007	0.153620
H	3.711439	0.355141	3.367207
H	2.354143	-0.701634	2.930019
H	3.891280	-0.827995	2.062559
H	-3.049775	1.256220	1.883797
H	-2.491277	-1.437562	-1.414861
H	-4.986318	-1.693442	-1.604480
H	-5.513131	0.977508	1.695129

SCF Energy (M06-2X/6-311+G**)= -2550.94635048
Gibbs Energy (M06-2X/6-311+G**)= -2550.621478
Number of imaginary frequencies = 0

E

C	2.407710	0.555537	-0.058922
C	2.741631	-0.898938	0.025291
O	1.240436	0.945713	-0.081340
In	-0.663302	-0.045839	0.006685
Cl	-0.321954	-1.148071	2.025325
C	3.508244	1.559097	-0.110246
Cl	-0.417495	-1.387198	-1.875293

Cl -2.151456 1.701884 -0.068005
H 3.812553 -1.075364 -0.047608
H 2.365333 -1.285143 0.978979
H 2.213064 -1.437603 -0.767180
H 4.123433 1.358848 -0.992463
H 3.110240 2.570024 -0.142150
H 4.153561 1.423021 0.762362
SCF Energy (M06-2X/6-311+G**)= -1575.78919746
Gibbs Energy (M06-2X/6-311+G**)= -1575.742708
Number of imaginary frequencies = 0

TS_IA_1d

C -2.284003 1.943794 1.395966
C -1.325430 1.322156 0.543844
C -1.764683 0.597859 -0.529988
C -3.149945 0.396965 -0.769190
C -4.099448 0.994770 0.098556
C -3.623605 1.787085 1.180188
C 0.152633 1.440096 0.854365
C 0.561669 1.075814 2.315784
C 1.740239 1.990165 2.647822
C 1.338804 3.357842 2.101264
C 0.523998 3.092123 0.834154
C 1.166571 3.126719 -0.460428
C 0.347031 3.239350 -1.672867
O 0.974163 0.843670 -0.066216
In 1.646737 -0.734493 -1.066226
Cl 2.201910 0.452636 -3.051152
C 2.626564 3.084188 -0.615191
Cl -0.011002 -2.295652 -1.605702
Cl 3.547916 -1.479848 0.040916
C 0.979241 -0.394091 2.522530
O 2.056136 -0.616845 3.019719
C 0.084738 -1.523666 2.130338
C -1.304173 -1.406247 2.052128
C 0.689982 -2.761632 1.883733
C -0.084035 -3.854053 1.523127
C -1.466598 -3.725451 1.425289
C -2.077084 -2.506550 1.700064
C -3.600306 -0.412400 -1.841731
C -4.942584 -0.603753 -2.045511
C -5.890417 0.002682 -1.188822
C -5.479428 0.784144 -0.139364
H -1.950355 2.545798 2.236539
H -1.065154 0.122133 -1.201560
H -4.344000 2.260677 1.838861
H -0.279030 1.285514 2.987928
H 1.963568 2.005349 3.713807
H 2.626669 1.595917 2.145288
H 0.688877 3.872351 2.813739

H	2.196137	4.011620	1.925052
H	-0.420559	3.631357	0.796703
H	0.682790	4.123717	-2.230064
H	0.587043	2.380326	-2.315043
H	-0.719534	3.296707	-1.469432
H	2.948871	4.138690	-0.609120
H	3.117125	2.580702	0.215639
H	2.913533	2.644691	-1.571690
H	-1.795339	-0.470174	2.286185
H	1.768151	-2.838495	1.963152
H	0.391587	-4.802034	1.303596
H	-2.069211	-4.577100	1.131740
H	-3.154561	-2.407746	1.637460
H	-2.862607	-0.884249	-2.482196
H	-5.282989	-1.226953	-2.863711
H	-6.947668	-0.157344	-1.364226
H	-6.204247	1.245372	0.523016

SCF Energy (M06-2X/6-311+G**)= -2500.02365476
Gibbs Energy (M06-2X/6-311+G**)= -2499.658372
Number of imaginary frequencies = 1 (-289.8)

TS_IA_1e

C	2.707791	-1.332635	1.155501
C	1.592418	-0.957253	0.393781
C	1.789571	-0.322923	-0.827477
C	3.074460	-0.030798	-1.277324
C	4.149480	-0.393532	-0.487893
C	3.992421	-1.050489	0.727181
C	0.185422	-1.239423	0.908057
C	-0.105345	-0.737308	2.360019
C	-1.052953	-1.772293	2.965292
C	-0.494603	-3.119055	2.516283
C	0.078839	-2.897794	1.112196
C	-0.739772	-3.229313	-0.044932
C	-0.106103	-3.431247	-1.347908
O	-0.803071	-0.881017	0.032703
In	-1.892738	0.409364	-1.018887
Cl	-2.439078	-1.134157	-2.746141
C	-2.195613	-3.372622	0.040155
Cl	-0.597992	2.115779	-1.944533
Cl	-3.747588	0.956603	0.262566
C	-0.754388	0.658721	2.432944
O	-1.810479	0.770918	3.004947
C	-0.102399	1.850510	1.815223
C	1.272770	1.936137	1.591418
C	-0.924967	2.939153	1.502245
C	-0.379307	4.079778	0.933647
C	0.990165	4.152393	0.694901
C	1.817217	3.086821	1.033939
N	5.518899	-0.083873	-0.952573

O	5.634964	0.457637	-2.028496
O	6.437259	-0.392395	-0.223874
H	2.573959	-1.844570	2.103687
H	0.947228	-0.016126	-1.428904
H	3.238147	0.478810	-2.217638
H	4.863590	-1.323125	1.307407
H	0.831896	-0.708322	2.927853
H	-1.126608	-1.680705	4.048414
H	-2.053629	-1.592839	2.566087
H	0.330066	-3.422551	3.166269
H	-1.235962	-3.920654	2.551058
H	1.073313	-3.320252	0.984875
H	-0.591640	-4.244585	-1.894617
H	-0.367095	-2.521133	-1.918132
H	0.973700	-3.549759	-1.302805
H	-2.366321	-4.453438	0.182522
H	-2.627250	-2.843348	0.886322
H	-2.671187	-3.086338	-0.900774
H	1.930232	1.124061	1.875830
H	-1.988728	2.860694	1.696044
H	-1.022265	4.908342	0.663413
H	1.413938	5.041491	0.243172
H	2.885657	3.150673	0.865514

SCF Energy (M06-2X/6-311+G**)= -2550.89031972
Gibbs Energy (M06-2X/6-311+G**)= -2550.570043
Number of imaginary frequencies = 1 (-227.7)

TS_IB_1d

C	1.567394	3.437617	0.021841
C	1.329012	2.110316	-0.356195
C	0.722507	1.864132	-1.582061
C	0.311171	2.919743	-2.394528
C	0.519882	4.232008	-1.997065
C	1.162674	4.489639	-0.785474
C	1.733770	0.963129	0.557340
C	1.300425	1.092849	2.051978
C	2.422816	0.447387	2.863462
C	3.712193	0.938484	2.210942
C	3.418957	1.055044	0.714372
C	3.756260	-0.035184	-0.173501
C	3.849972	0.205876	-1.618060
O	1.449117	-0.281155	0.060617
In	0.183839	-1.660860	-0.616668
Cl	1.717226	-2.626531	-2.162554
C	4.037178	-1.390658	0.316943
Cl	-1.625539	-0.803557	-1.819586
Cl	-0.259705	-3.130207	1.131183
C	-0.034376	0.395094	2.378000
O	-0.046772	-0.448843	3.240840
C	-1.283765	0.742238	1.640239

C	-1.486620	1.995425	1.004851
C	-2.280622	-0.209106	1.614463
C	-3.485370	0.021310	0.914506
C	-3.675021	1.267226	0.258338
C	-2.653690	2.248476	0.338782
C	-4.494329	-0.972295	0.825575
C	-5.642124	-0.732877	0.119792
C	-5.835656	0.512382	-0.525792
C	-4.877478	1.488826	-0.457770
H	2.066953	3.655559	0.961896
H	0.542979	0.852615	-1.913548
H	-0.182374	2.702209	-3.334177
H	0.194876	5.053204	-2.624671
H	1.344642	5.510886	-0.472055
H	1.206185	2.153255	2.312188
H	2.360799	0.693396	3.923013
H	2.316651	-0.636920	2.785379
H	3.965796	1.936086	2.578211
H	4.567387	0.293766	2.426868
H	3.727098	2.002960	0.279137
H	4.840532	-0.123594	-1.957141
H	3.137020	-0.471841	-2.110545
H	3.671936	1.241527	-1.898433
H	5.129886	-1.426346	0.459836
H	3.564974	-1.592335	1.276022
H	3.767211	-2.143340	-0.426072
H	-0.729101	2.766088	1.061545
H	-2.119333	-1.156030	2.119004
H	-2.809114	3.208649	-0.141641
H	-4.329074	-1.926479	1.314023
H	-6.405910	-1.497539	0.044803
H	-6.749491	0.687983	-1.081229
H	-5.022041	2.440913	-0.956933

SCF Energy (M06-2X/6-311+G**)= -2500.02141664
Gibbs Energy (M06-2X/6-311+G**)= -2499.657295
Number of imaginary frequencies = 1 (-291.6)

TS_IB_1e

C	0.582017	3.615556	-0.000054
C	0.660085	2.268759	-0.376008
C	0.033837	1.864123	-1.548798
C	-0.699364	2.773563	-2.310080
C	-0.799004	4.099521	-1.913966
C	-0.144000	4.522963	-0.756782
C	1.395916	1.267355	0.500950
C	1.004638	1.282259	2.013931
C	2.286271	0.932174	2.770174
C	3.379342	1.737899	2.074067
C	2.998722	1.786819	0.592648
C	3.575645	0.830007	-0.329033

C 3.526479 1.089549 -1.771396
O 1.418857 -0.006968 0.000559
In 0.586382 -1.711202 -0.592825
Cl 2.231777 -2.261812 -2.208061
C 4.237153 -0.397207 0.129266
Cl -1.468788 -1.395640 -1.659071
Cl 0.648519 -3.117750 1.256968
C -0.103675 0.291955 2.411976
O 0.105375 -0.476750 3.316236
C -1.433123 0.267609 1.718158
C -1.969825 1.374612 1.059745
C -2.161009 -0.925110 1.793536
C -3.399731 -1.027646 1.181659
C -3.891833 0.082219 0.513042
C -3.212256 1.286661 0.446907
N -5.209683 -0.018208 -0.156543
O -5.592866 0.946395 -0.782545
O -5.820884 -1.055328 -0.033580
H 1.083147 3.961125 0.900233
H 0.080523 0.833232 -1.866755
H -1.200943 2.429969 -3.206911
H -1.376567 4.803682 -2.500616
H -0.203721 5.559107 -0.445261
H 0.668751 2.288947 2.290200
H 2.209404 1.147235 3.835108
H 2.453384 -0.143455 2.676432
H 3.388914 2.764047 2.449930
H 4.378259 1.329417 2.243356
H 3.038552 2.785625 0.163457
H 4.541144 0.997557 -2.178340
H 2.961513 0.261063 -2.224733
H 3.088222 2.051183 -2.027686
H 5.296992 -0.120786 0.259237
H 3.861129 -0.736726 1.092580
H 4.180778 -1.186328 -0.621817
H -1.439101 2.316870 1.030874
H -1.730187 -1.768252 2.319791
H -3.971567 -1.945148 1.198207
H -3.650747 2.125781 -0.075298
SCF Energy (M06-2X/6-311+G**)= -2550.89237511
Gibbs Energy (M06-2X/6-311+G**)= -2550.572044
Number of imaginary frequencies = 1 (-279.1)

TS_IIC_1d

C -1.678833 -1.872902 0.371547
C -1.558590 -1.019594 1.471257
C -2.758916 -0.452475 2.023807
C -3.969539 -0.691879 1.457153
C -4.087506 -1.513558 0.298613
C -2.918995 -2.124811 -0.233691

C	-0.280899	-0.705650	2.006582
C	1.007607	-1.397061	1.620122
C	2.096493	-0.753653	2.517503
C	1.295177	-0.176289	3.683191
C	-0.004794	0.269903	3.015508
C	1.444841	-1.399604	0.147096
O	0.838913	-0.818835	-0.718785
C	2.696194	-2.151078	-0.172306
C	3.196511	-3.171689	0.640642
C	4.342823	-3.860944	0.267035
C	5.002847	-3.521343	-0.910219
C	4.510771	-2.501161	-1.719907
C	3.355028	-1.821380	-1.360801
C	-3.015832	-2.938236	-1.393546
C	-4.228434	-3.138397	-1.994234
C	-5.390408	-2.536794	-1.457606
C	-5.325099	-1.744818	-0.337196
H	-0.807120	-2.337794	-0.066510
H	-2.699180	0.174499	2.902562
H	-4.867434	-0.252696	1.876506
H	0.864114	-2.447098	1.916120
H	2.855524	-1.470269	2.826450
H	2.581159	0.048366	1.957510
H	1.069134	-0.956553	4.417920
H	1.812489	0.624339	4.207393
H	-0.818230	0.543589	3.680107
H	2.694580	-3.450228	1.560013
H	4.721233	-4.659567	0.893215
H	5.902455	-4.053839	-1.196064
H	5.028315	-2.234491	-2.633271
H	2.954719	-1.022874	-1.976220
H	-2.111535	-3.374378	-1.802844
H	-4.302652	-3.746617	-2.886923
H	-6.344659	-2.698513	-1.945274
H	-6.219109	-1.280105	0.062356
C	0.230972	1.769502	2.047816
C	-1.169560	2.356144	1.912615
O	0.841579	1.464522	0.890897
In	0.319443	1.885917	-0.998492
Cl	0.043068	4.241362	-0.883270
C	1.111450	2.658956	2.915246
Cl	-1.808064	0.950790	-1.477744
Cl	2.100702	1.476125	-2.463840
H	-1.640181	2.510902	2.886157
H	-1.070187	3.330661	1.425403
H	-1.815996	1.744654	1.281619
H	0.726052	2.782874	3.929956
H	2.135534	2.287881	2.939686
H	1.127462	3.633978	2.418494

SCF Energy (M06-2X/6-311+G**)= -2500.02263200

Gibbs Energy (M06-2X/6-311+G**)= -2499.654277
Number of imaginary frequencies = 1 (-302.3)

TS_IIC_1e

C	-1.467758	-2.229773	-0.139774
C	-1.486868	-1.457517	1.042430
C	-2.729688	-0.993382	1.530679
C	-3.896918	-1.224302	0.831731
C	-3.813750	-1.950253	-0.347445
C	-2.632071	-2.476438	-0.841914
C	-0.275201	-1.125776	1.725962
C	1.077458	-1.656931	1.352342
C	2.045111	-1.090659	2.420876
C	1.118661	-0.765000	3.591170
C	-0.160076	-0.282258	2.897871
C	1.582728	-1.409642	-0.090116
O	0.926032	-0.834136	-0.917012
C	2.948215	-1.922886	-0.405798
C	3.549453	-2.975143	0.290014
C	4.801551	-3.436254	-0.096057
C	5.463399	-2.834755	-1.163060
C	4.868121	-1.783781	-1.854983
C	3.608037	-1.333425	-1.488073
N	-5.070833	-2.206642	-1.104166
O	-4.989186	-2.908317	-2.084067
O	-6.081246	-1.700042	-0.676540
H	-0.541188	-2.625304	-0.525746
H	-2.779590	-0.443679	2.459290
H	-4.854388	-0.856970	1.173850
H	-2.635569	-3.044772	-1.761337
H	0.993724	-2.750548	1.468992
H	2.835218	-1.791862	2.680927
H	2.502305	-0.181633	2.025860
H	0.894631	-1.670104	4.165053
H	1.530672	-0.033010	4.282184
H	-1.037956	-0.231141	3.536554
H	3.045249	-3.456149	1.120636
H	5.261317	-4.261496	0.433942
H	6.444876	-3.188591	-1.455953
H	5.384542	-1.314820	-2.683535
H	3.123615	-0.518992	-2.014919
C	0.007983	1.284984	2.221742
C	-1.401535	1.868757	2.135659
O	0.635669	1.154348	1.014729
In	0.194175	1.969880	-0.753492
Cl	-0.226005	4.243247	-0.249186
C	0.853134	2.115516	3.180335
Cl	-1.839931	0.963546	-1.458905
Cl	2.040586	1.881411	-2.185607
H	-1.915216	1.836241	3.099868

H -1.309532 2.916380 1.837463
H -2.007863 1.379435 1.371725
H 0.447571 2.136489 4.195182
H 1.886103 1.769038 3.195720
H 0.853630 3.133063 2.778953
SCF Energy (M06-2X/6-311+G**)= -2550.88191736
Gibbs Energy (M06-2X/6-311+G**)= -2550.558046
Number of imaginary frequencies = 1 (-249.3)

TS_IID_1d

C -1.328053 -2.509724 -1.757320
C -1.979499 -2.391482 -0.507930
C -3.386244 -2.543868 -0.467165
C -4.108451 -2.737072 -1.626030
C -3.443403 -2.807387 -2.850402
C -2.055122 -2.714138 -2.912771
C -1.247166 -2.117147 0.682361
C 0.258184 -2.067027 0.754544
C 0.585070 -1.819921 2.249179
C -0.681906 -2.287369 2.964352
C -1.792733 -1.888430 1.990024
C 0.996625 -1.069405 -0.156906
O 0.417886 -0.314604 -0.898037
C 2.483330 -1.058895 -0.052202
C 3.242282 -2.166767 0.414655
C 4.607063 -2.097092 0.457804
C 5.289270 -0.913969 0.066669
C 4.530019 0.197853 -0.388732
C 3.122145 0.092546 -0.453541
C 5.198677 1.390751 -0.769501
C 6.563781 1.468135 -0.705103
C 7.320998 0.358252 -0.258558
C 6.701322 -0.804275 0.118864
H -0.254297 -2.417680 -1.825207
H -3.907331 -2.503816 0.479238
H -5.186149 -2.829291 -1.585750
H -4.012629 -2.944225 -3.762634
H -1.547588 -2.776000 -3.866542
H 0.593379 -3.075261 0.465051
H 1.482028 -2.346145 2.570864
H 0.735124 -0.749315 2.400866
H -0.679899 -3.376721 3.076732
H -0.803171 -1.857589 3.956034
H -2.773955 -2.306825 2.193769
H 2.750879 -3.084020 0.718431
H 5.188788 -2.948473 0.794052
H 2.529086 0.930750 -0.806125
H 4.604207 2.233759 -1.104706
H 7.072270 2.379969 -0.993719
H 8.401138 0.434219 -0.214291

H	7.282237	-1.653213	0.462803
C	-2.081098	-0.138786	2.003524
C	-3.502148	0.031312	1.476222
O	-1.125350	0.473028	1.274552
In	-1.286478	1.791719	-0.222712
Cl	-2.707307	3.439735	0.727690
C	-2.000787	0.281491	3.465712
Cl	-2.469213	0.780460	-2.012100
Cl	0.764106	2.845369	-0.654662
H	-4.222235	-0.558215	2.048590
H	-3.766566	1.086984	1.584675
H	-3.583693	-0.207222	0.414564
H	-2.653467	-0.305565	4.116401
H	-0.973121	0.244342	3.825696
H	-2.319806	1.327812	3.489733

SCF Energy (M06-2X/6-311+G**)= -2500.02016983

Gibbs Energy (M06-2X/6-311+G**)= -2499.652137

Number of imaginary frequencies = 1 (-283.3)

TS_IID_1e

C	0.929556	2.664854	-1.601521
C	1.562889	2.565893	-0.340383
C	2.929803	2.925105	-0.246741
C	3.641765	3.287022	-1.370762
C	3.003086	3.326263	-2.610415
C	1.644490	3.038156	-2.721101
C	0.858418	2.101218	0.805273
C	-0.623933	1.813964	0.828785
C	-0.937437	1.409492	2.291834
C	0.226062	2.015047	3.075825
C	1.405394	1.866792	2.111796
C	-1.182234	0.791639	-0.173097
O	-0.496708	0.194483	-0.958722
C	-2.664170	0.550988	-0.126759
C	-3.565876	1.486530	0.387250
C	-4.929754	1.234942	0.352907
C	-5.358173	0.031721	-0.184760
C	-4.488813	-0.919283	-0.696342
C	-3.128480	-0.647275	-0.675291
N	-6.815252	-0.244705	-0.213813
O	-7.553416	0.621514	0.201511
O	-7.169973	-1.315159	-0.650034
H	-0.118158	2.427209	-1.708284
H	3.428649	2.910252	0.712204
H	4.692148	3.535744	-1.291700
H	3.568423	3.594254	-3.495599
H	1.155445	3.082183	-3.685401
H	-1.102723	2.779977	0.604011
H	-1.910886	1.765496	2.624693
H	-0.919912	0.320546	2.364626

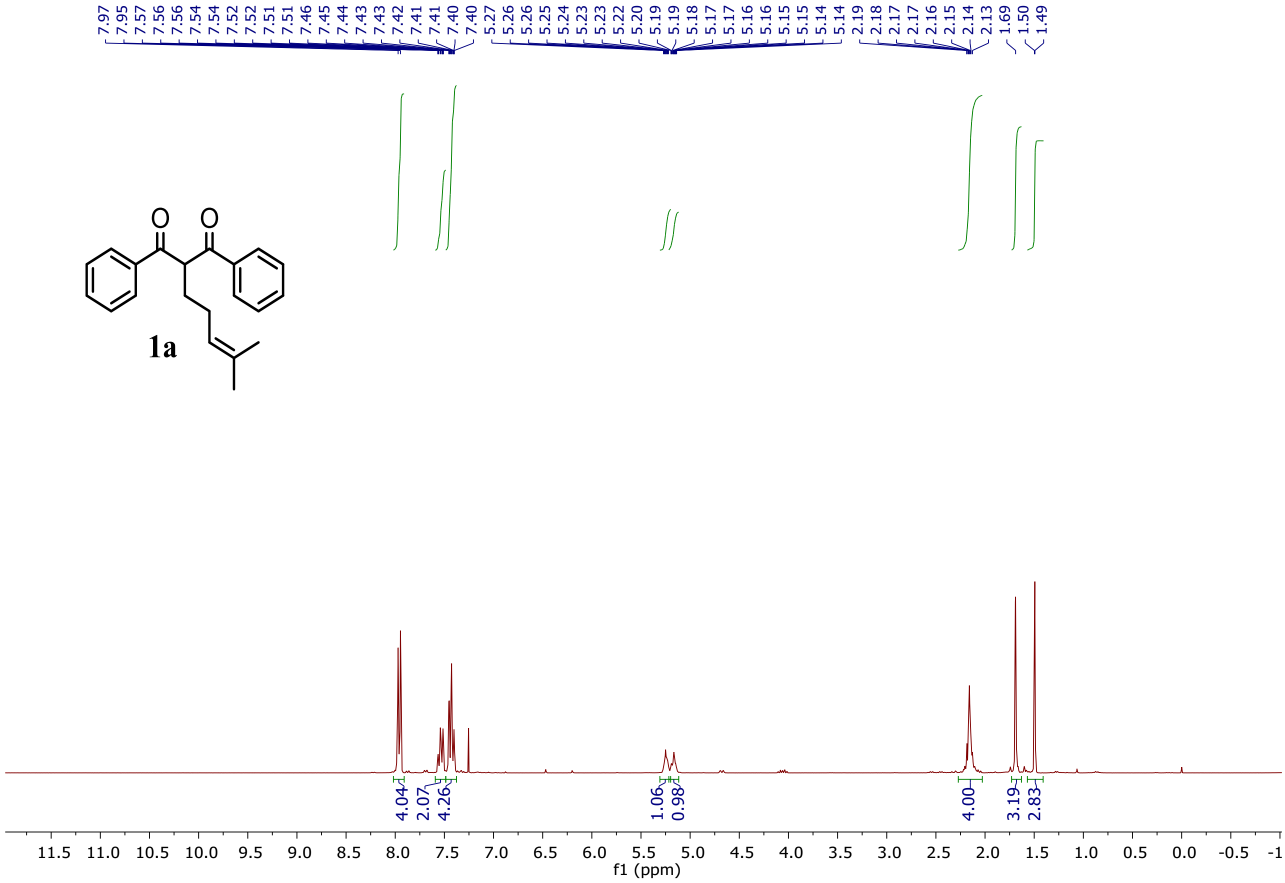
H	0.048967	3.079587	3.261699
H	0.391677	1.539508	4.039934
H	2.302088	2.419869	2.375238
H	-3.222219	2.425254	0.804536
H	-5.653384	1.944098	0.730573
H	-4.877221	-1.844468	-1.100377
H	-2.411340	-1.359346	-1.068243
C	1.971448	0.191275	2.016376
C	3.407570	0.285354	1.513399
O	1.136998	-0.513284	1.222487
In	1.555034	-1.722164	-0.316673
Cl	3.183507	-3.182443	0.584724
C	1.939106	-0.336203	3.445273
Cl	2.568467	-0.419472	-2.016340
Cl	-0.350465	-2.977024	-0.843552
H	4.019693	0.935243	2.143167
H	3.833984	-0.721255	1.554127
H	3.462162	0.611216	0.473683
H	2.475133	0.303910	4.150068
H	0.914759	-0.495042	3.780729
H	2.427646	-1.314705	3.410606

SCF Energy (M06-2X/6-311+G**)= -2550.88813346

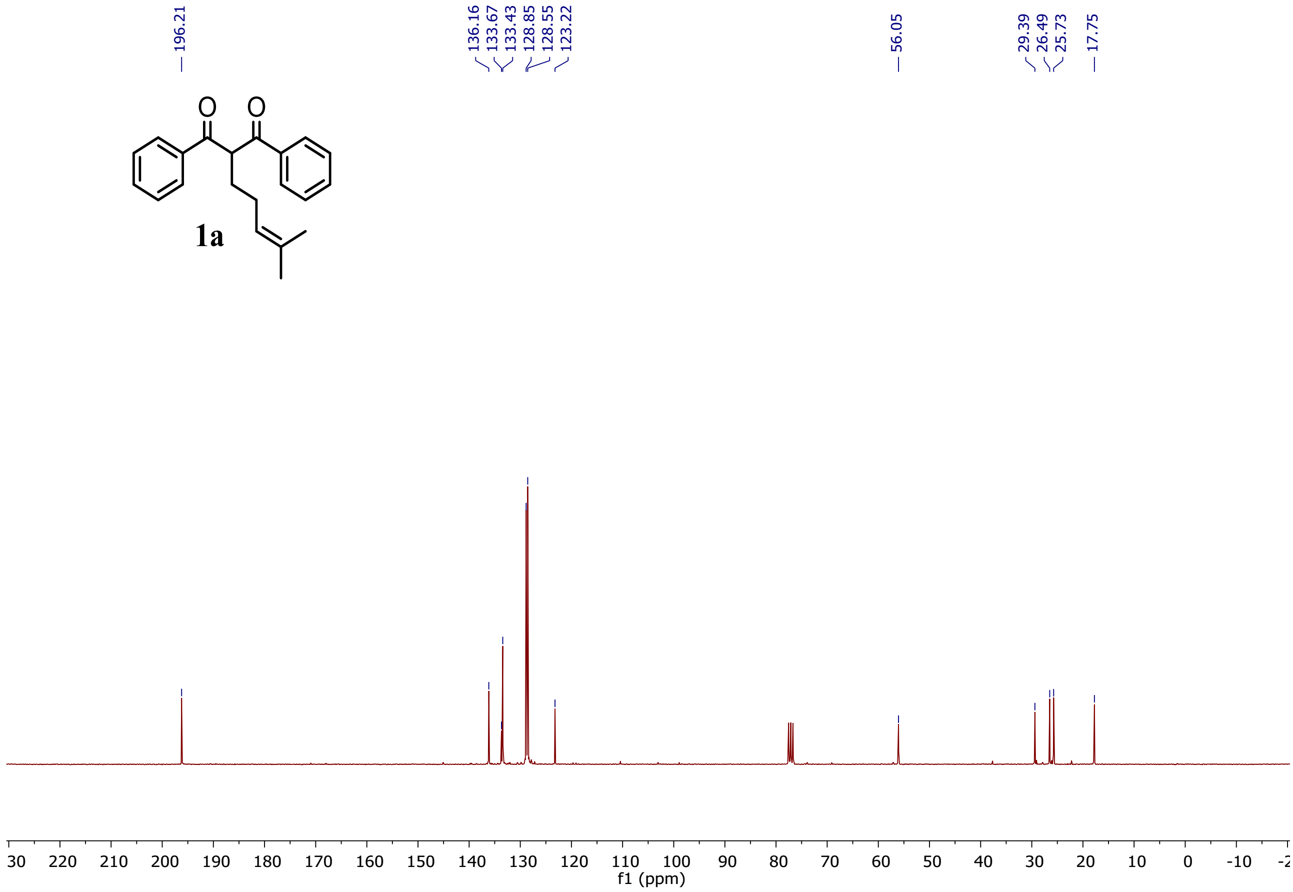
Gibbs Energy (M06-2X/6-311+G**)= -2550.563973

Number of imaginary frequencies = 1 (-266.9)

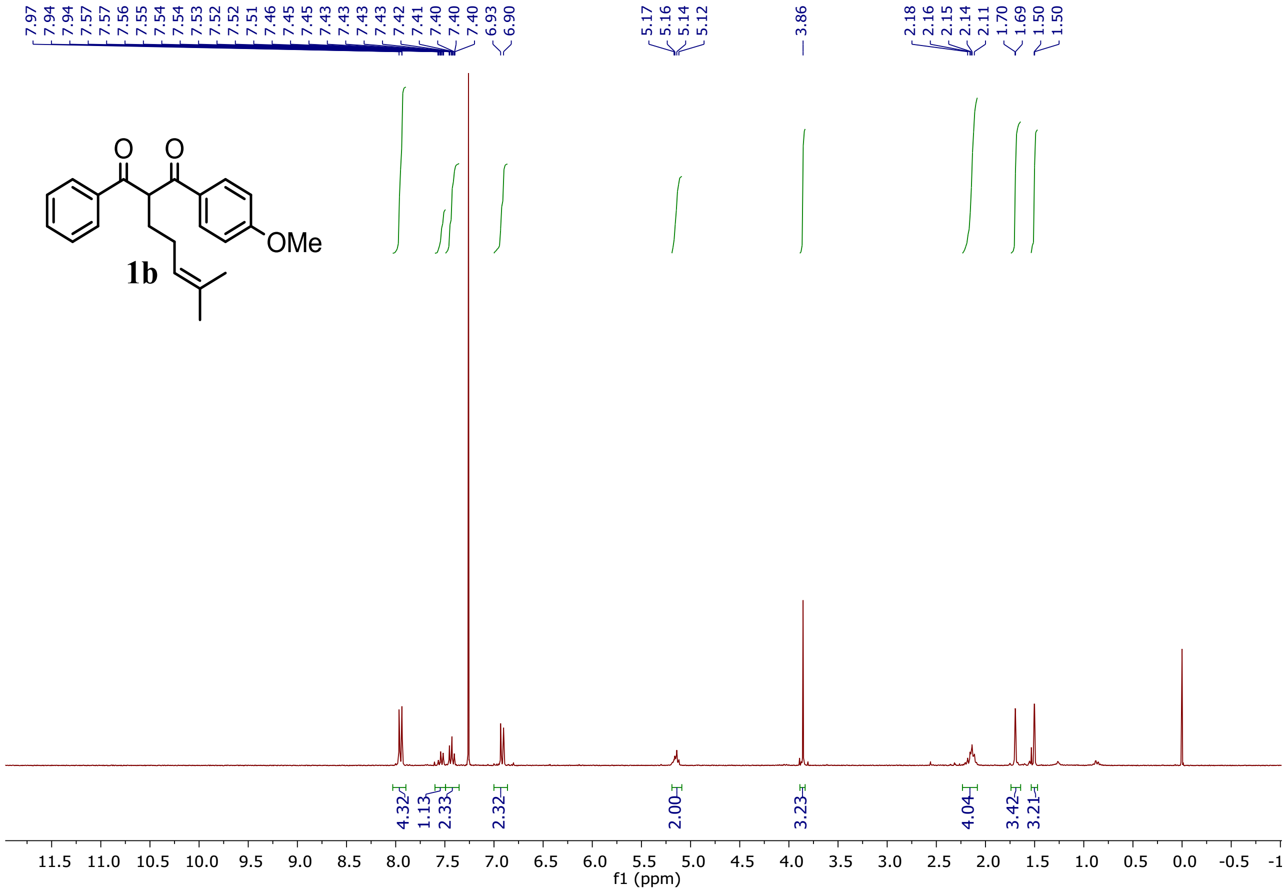
6. ^{1}H NMR and ^{13}C NMR

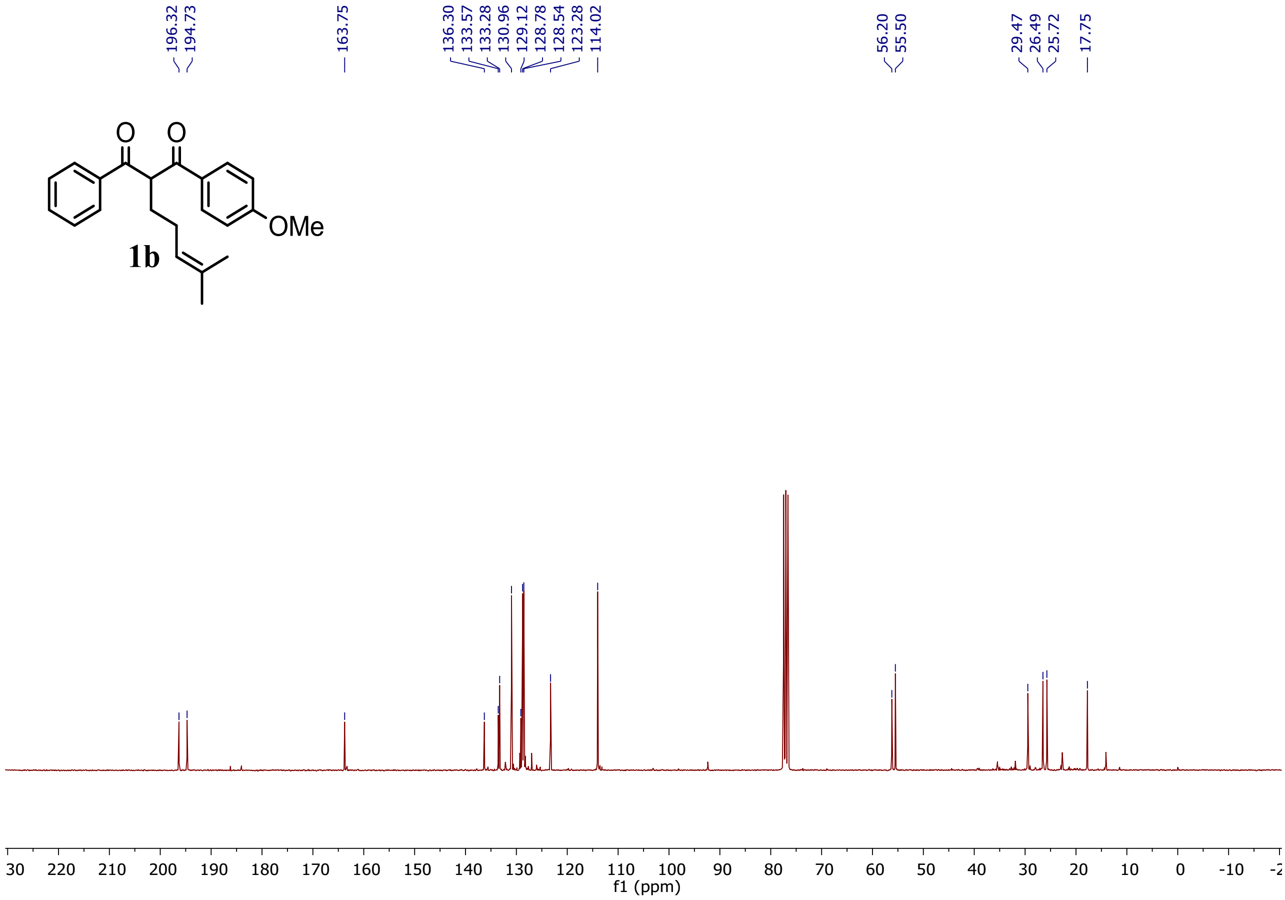


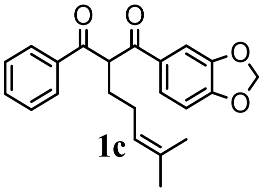
1a


196.21
136.16
133.67
133.43
128.85
128.55
123.22
56.05
29.39
26.49
25.73
17.75
f1 (ppm)

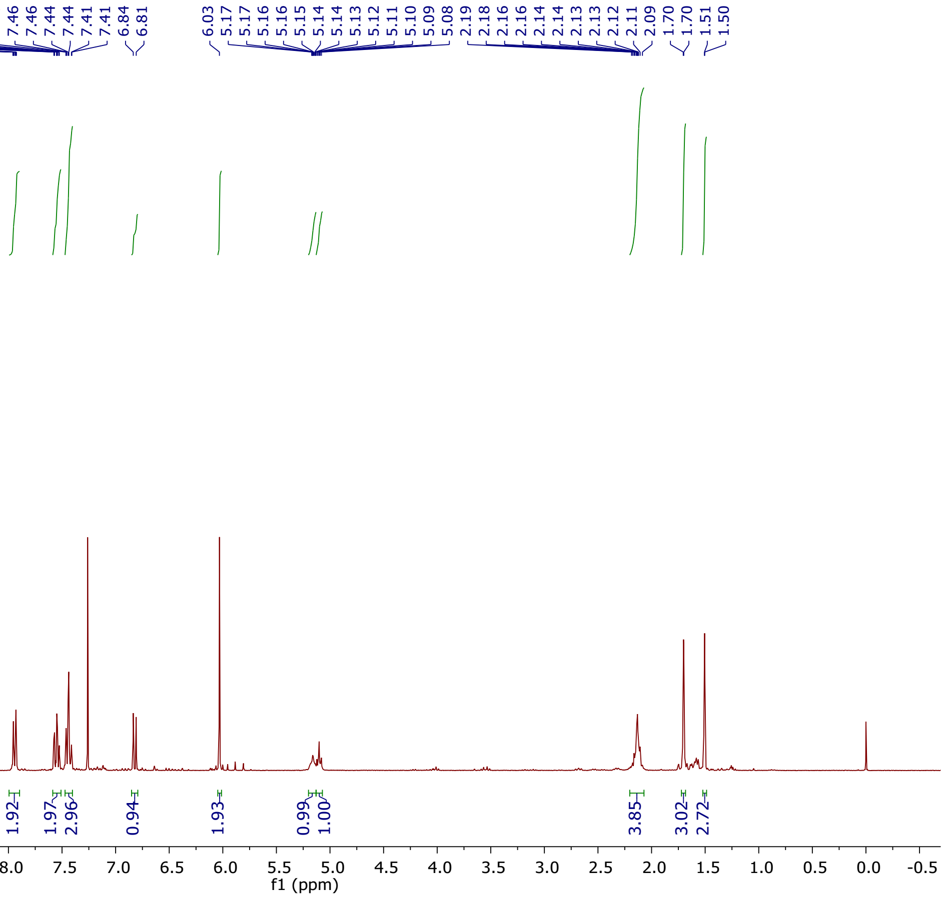
1a

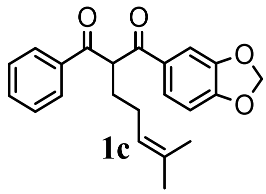

1b
OMe
f1 (ppm)


196.32
194.73
163.75
136.30
133.57
133.28
130.96
129.12
128.78
128.54
123.28
114.02
56.20
55.50
29.47
26.49
25.72
17.75
OMe
1b
f1 (ppm)

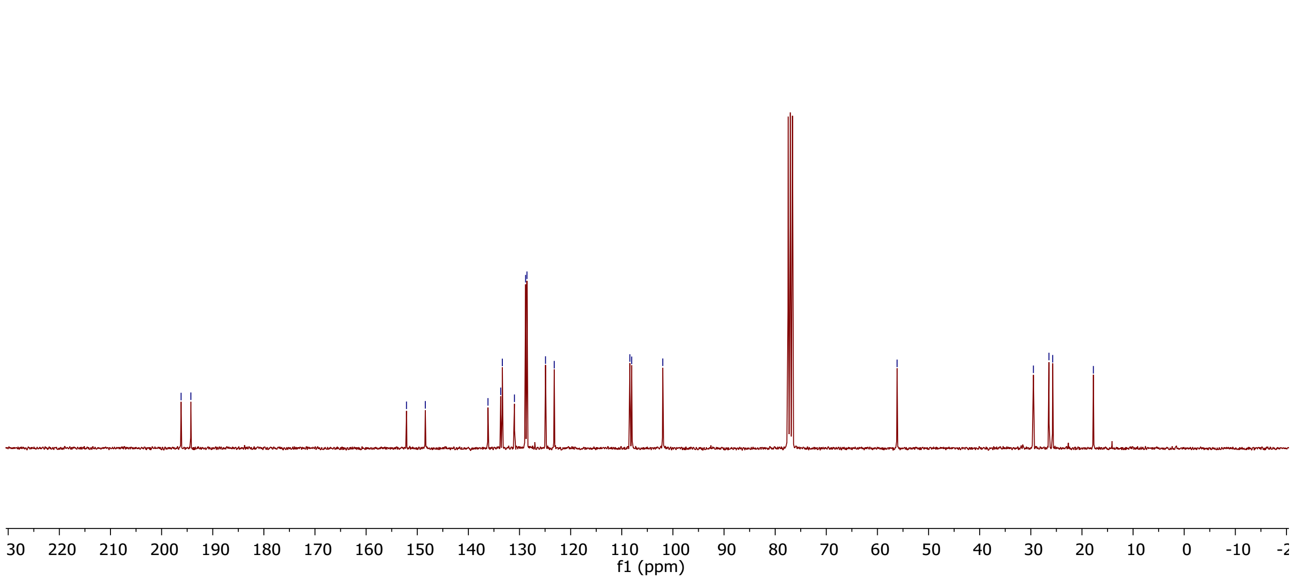


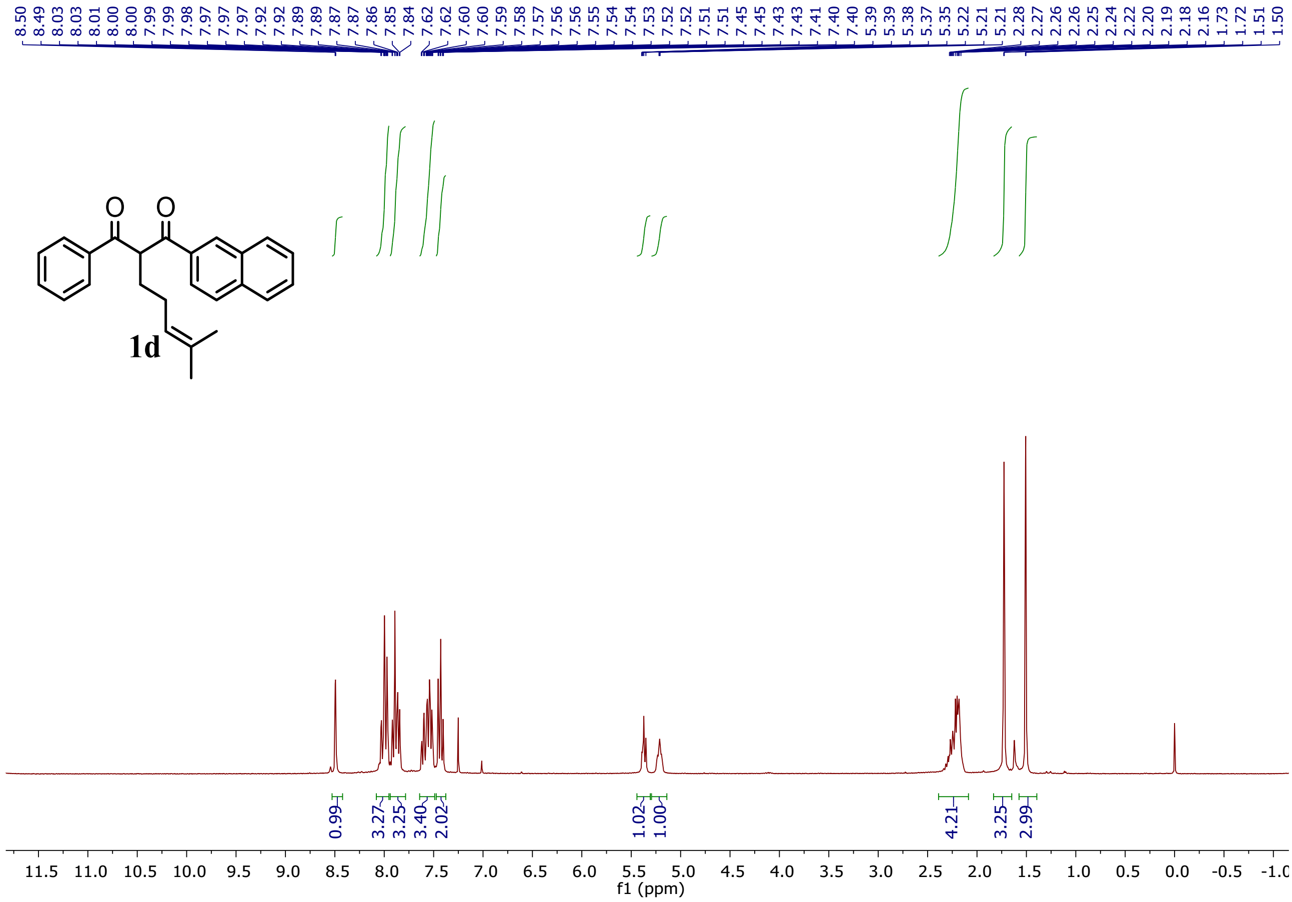
1c

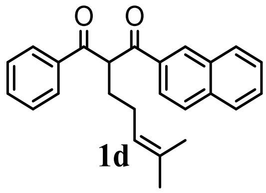

7.96
7.95
7.95
7.94
7.93
7.93
7.58
7.57
7.55
7.55
7.54
7.53
7.53
7.46
7.46
7.44
7.44
7.41
7.41
6.84
6.81
6.03
5.17
5.17
5.16
5.16
5.15
5.14
5.14
5.13
5.12
5.11
5.10
5.09
5.08
2.19
2.18
2.16
2.16
2.14
2.14
2.13
2.13
2.12
2.11
2.09
1.70
1.70
1.51
1.50
1.92
1.97
2.96
0.94
1.93
0.99
1.00
3.85
3.02
2.72
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)



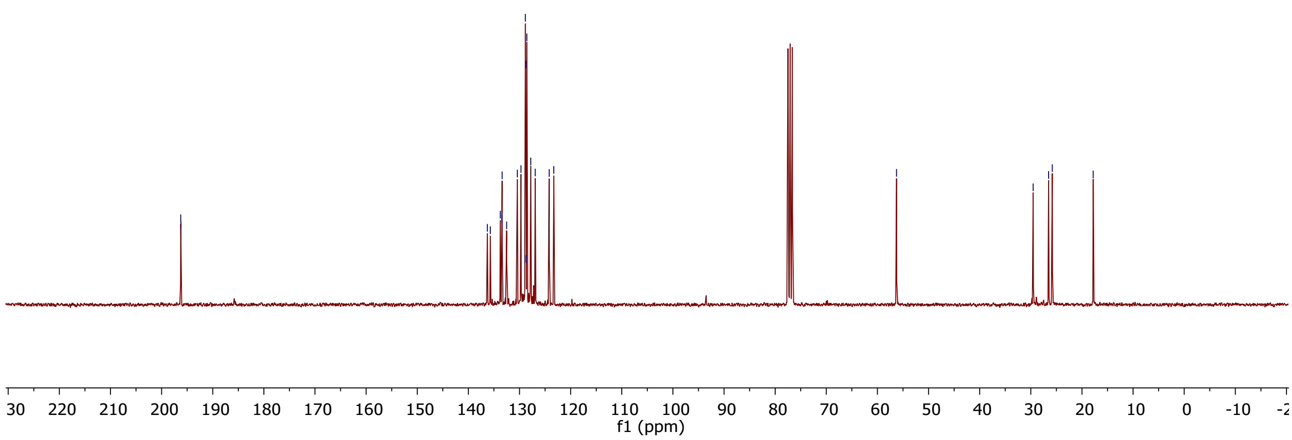
1c

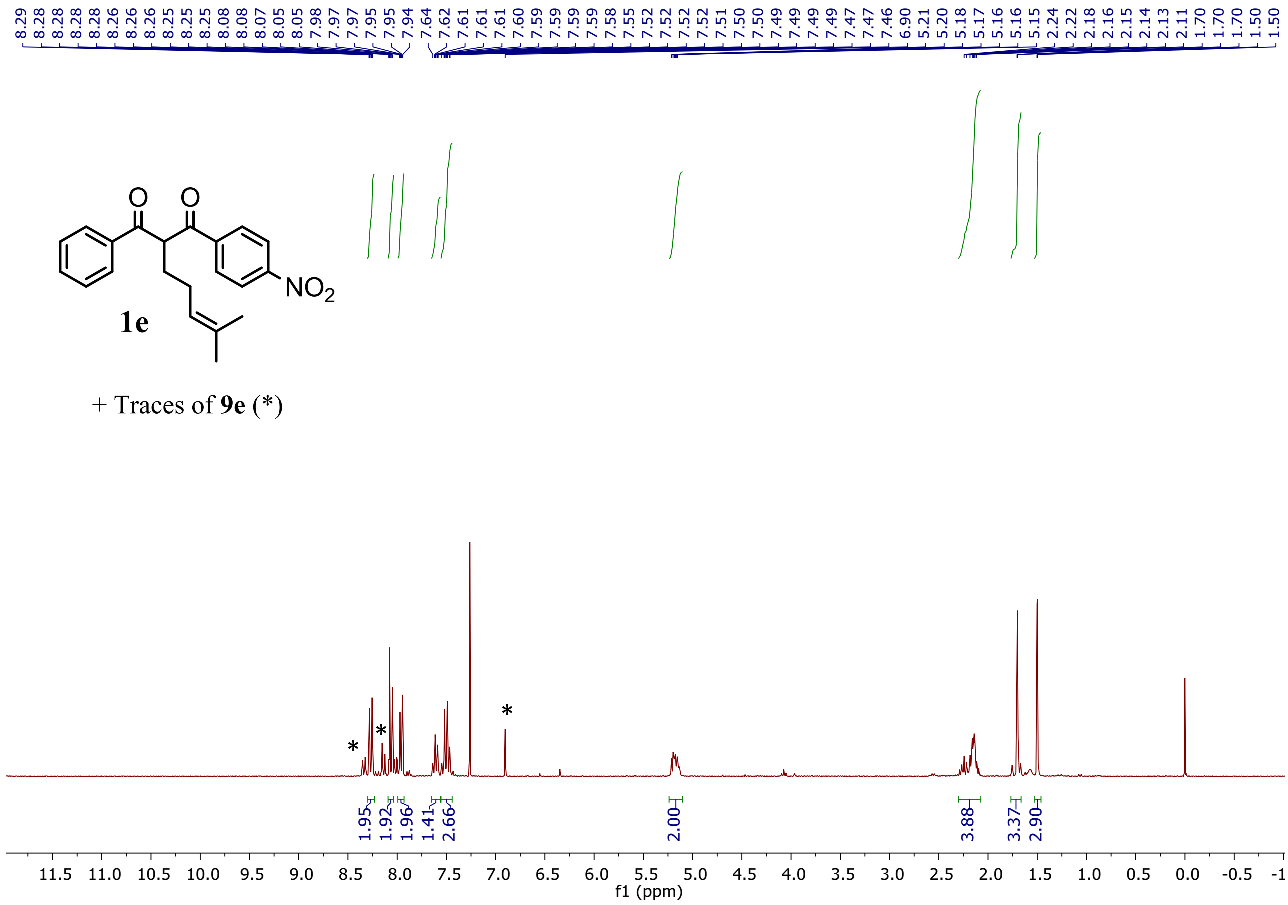

196.19
194.28
152.10
148.43
136.17
133.68
133.36
130.99
128.81
128.54
124.92
123.21
108.41
108.06
101.97
56.16
29.49
26.46
25.72
17.76
30 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


1d
f1 (ppm)



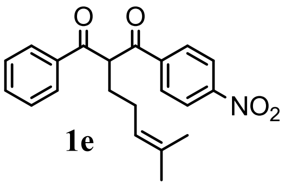
1d


196.26
196.22
136.29
135.71
133.77
133.47
133.40
132.52
130.42
129.71
128.86
128.80
128.73
128.56
127.80
126.93
124.20
123.30
56.27
29.54
26.52
25.80
17.80
f1 (ppm)



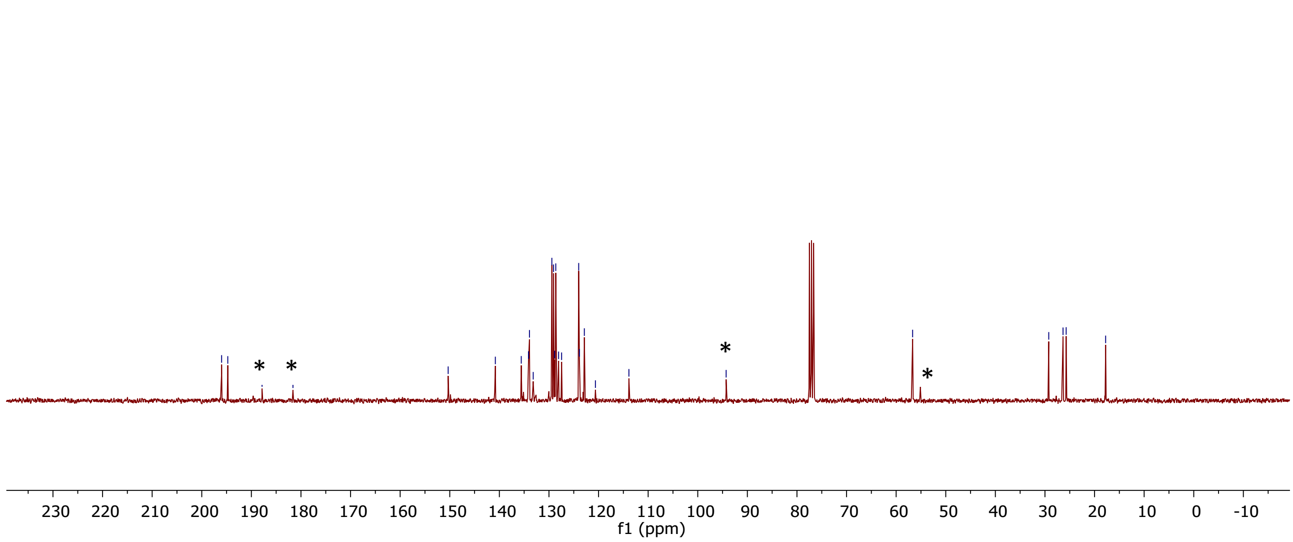
1e

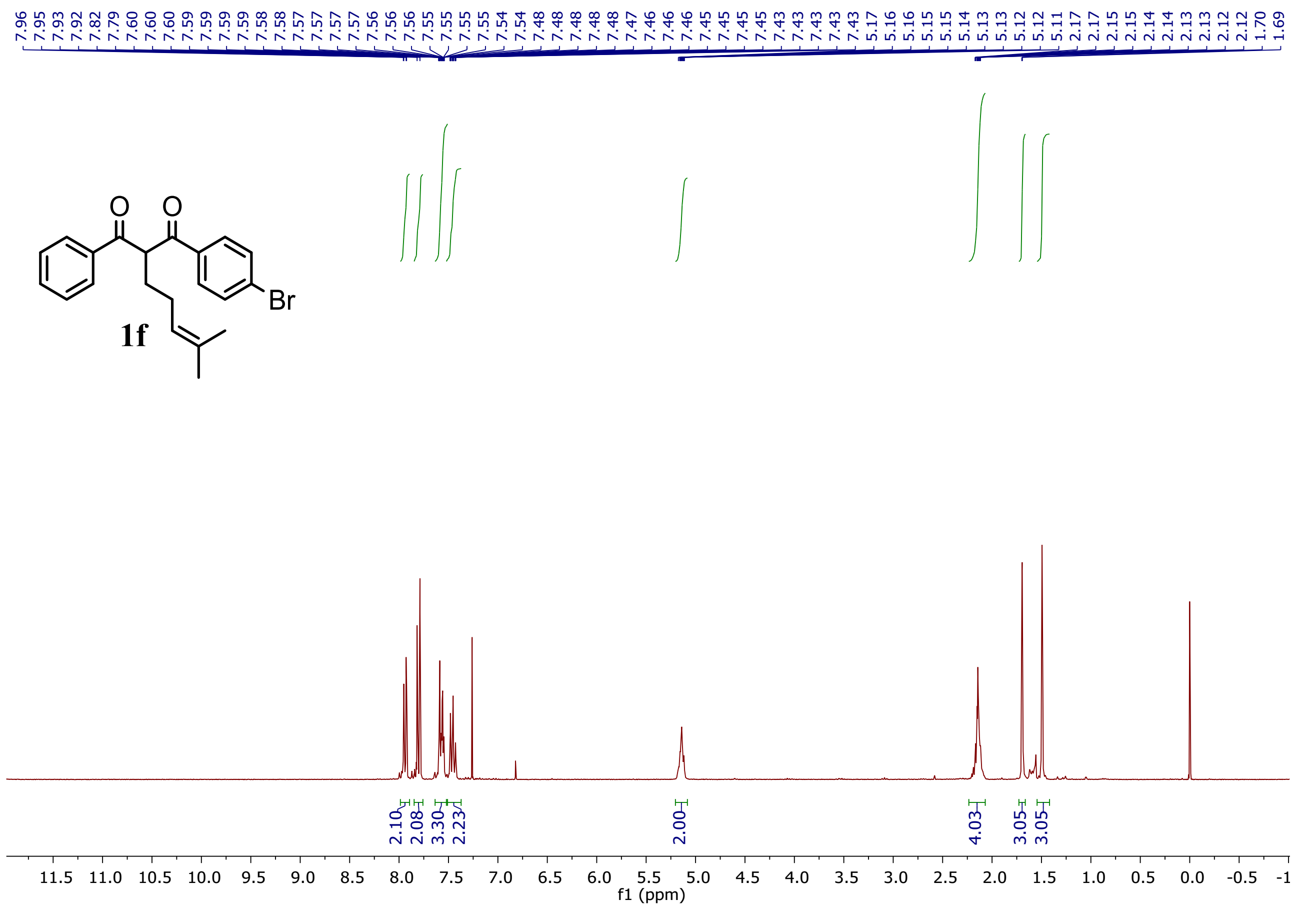
+ Traces of **9e** (*)

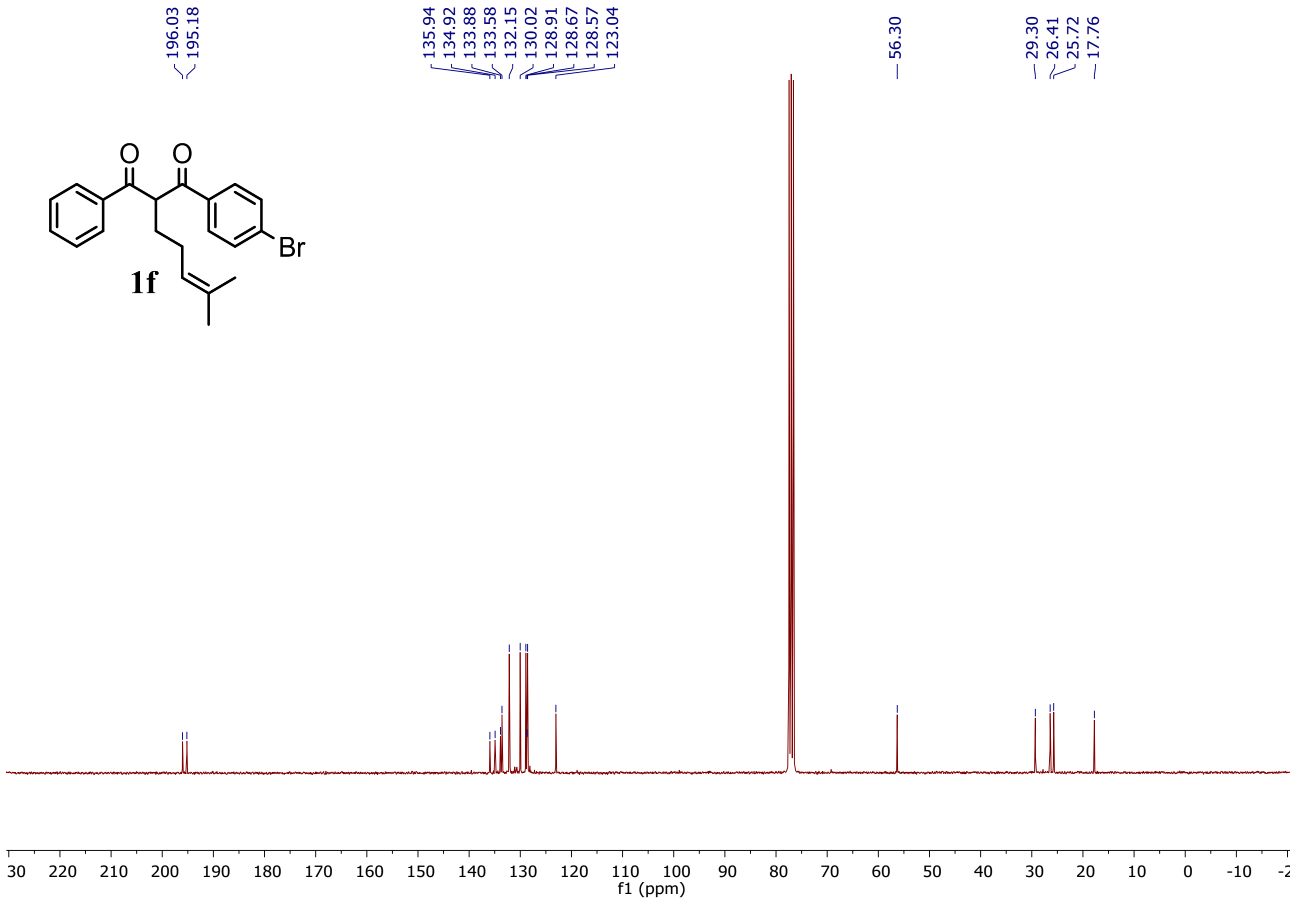


1e

+ Traces of **9e** (*)



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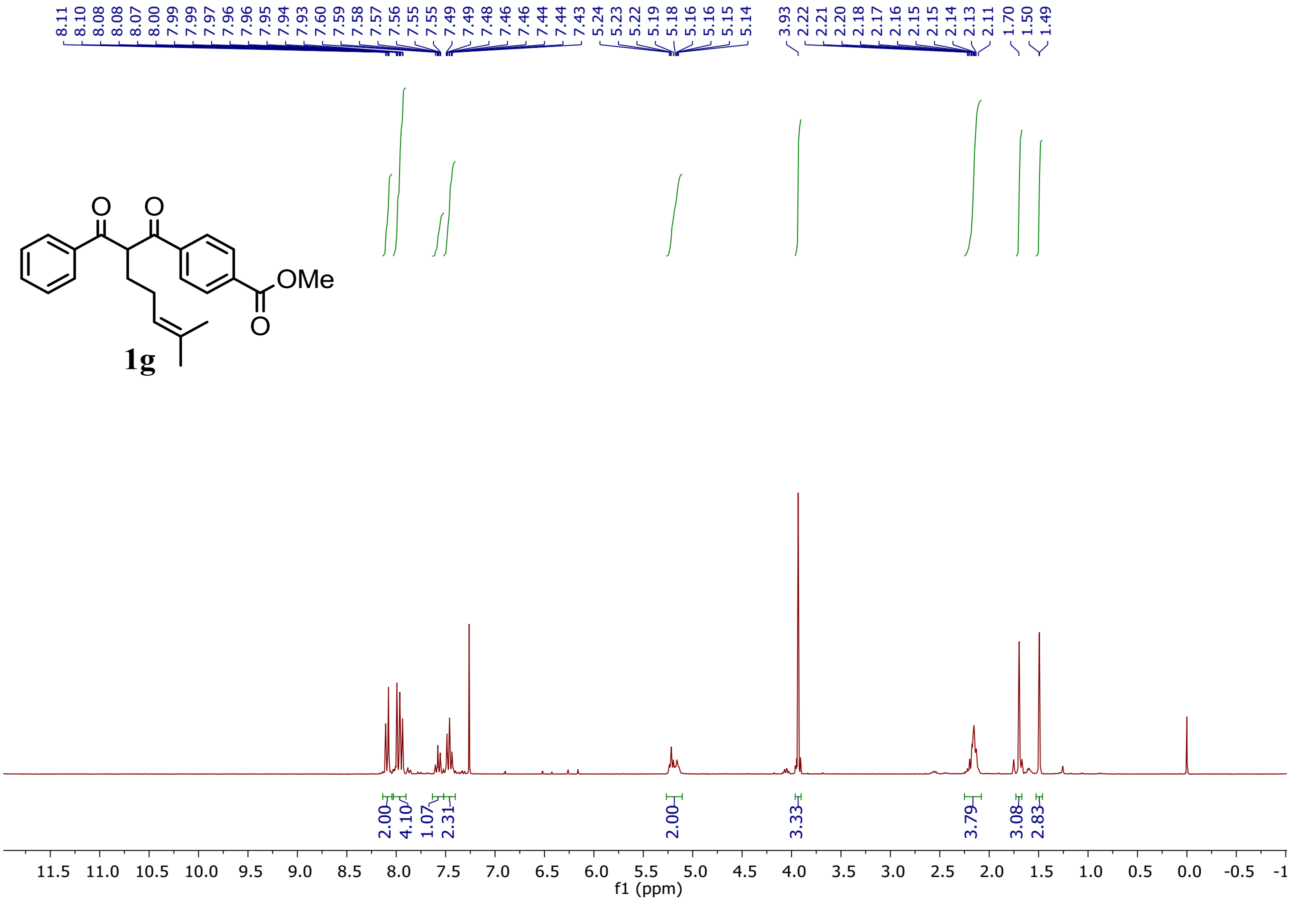
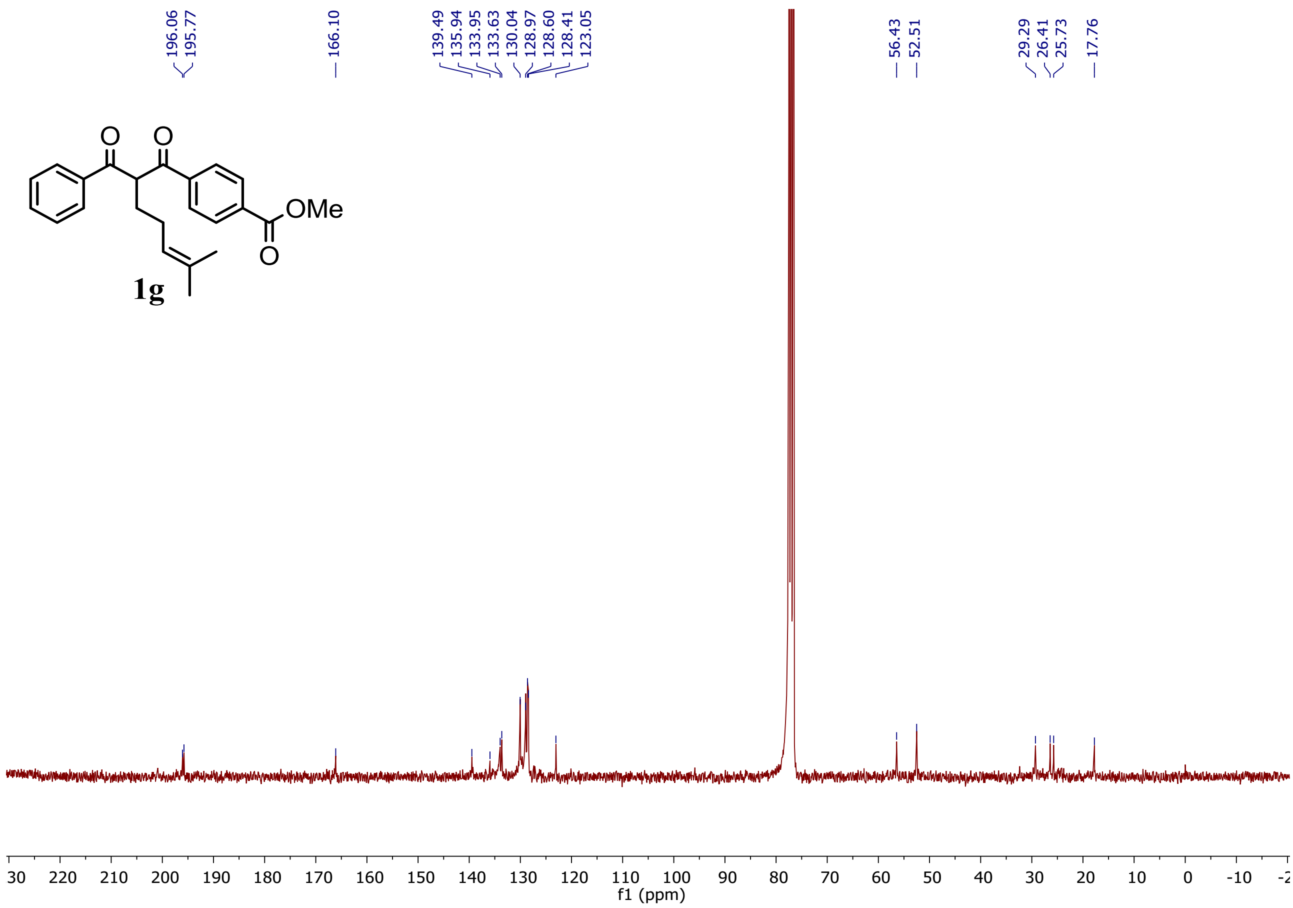
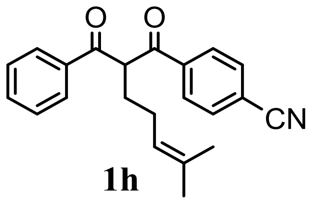
195.18
135.94
134.92
133.88
133.58
132.15
130.02
128.91
128.67
128.57
123.04
56.30
29.30
26.41
25.72
17.76
1f
Br
f1 (ppm)

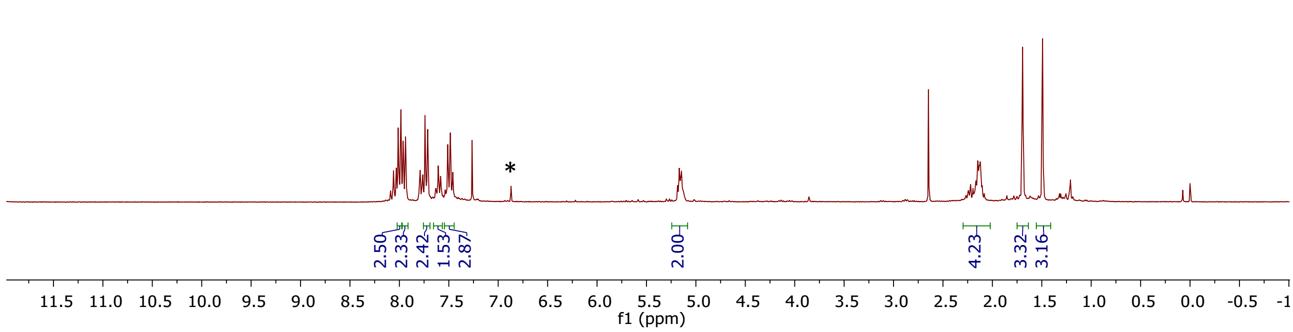

OMe
1g

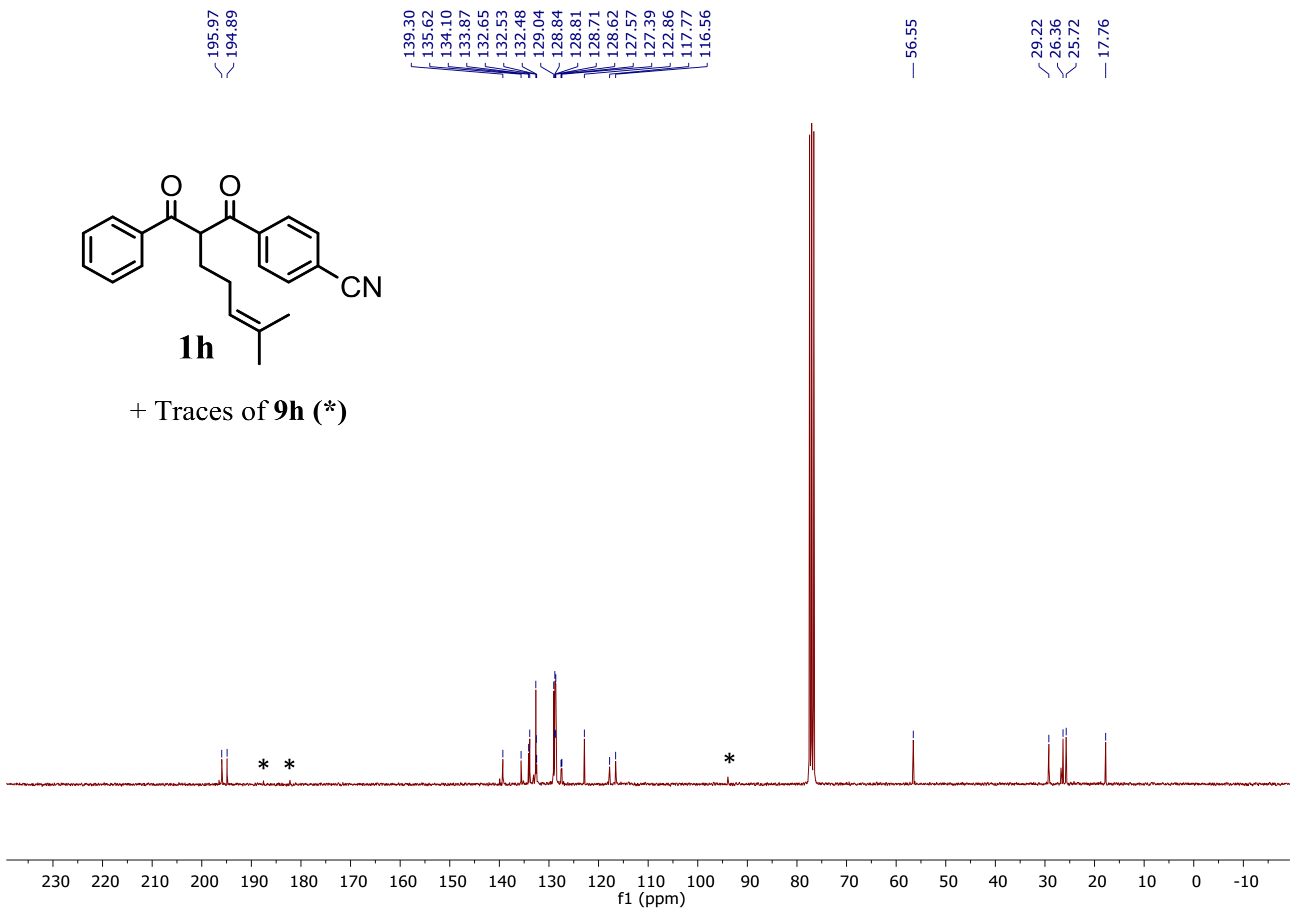

196.06
195.77
166.10
139.49
135.94
133.95
133.63
130.04
128.97
128.60
128.41
123.05
56.43
52.51
29.29
26.41
25.73
17.76
OMe
1g
30
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)



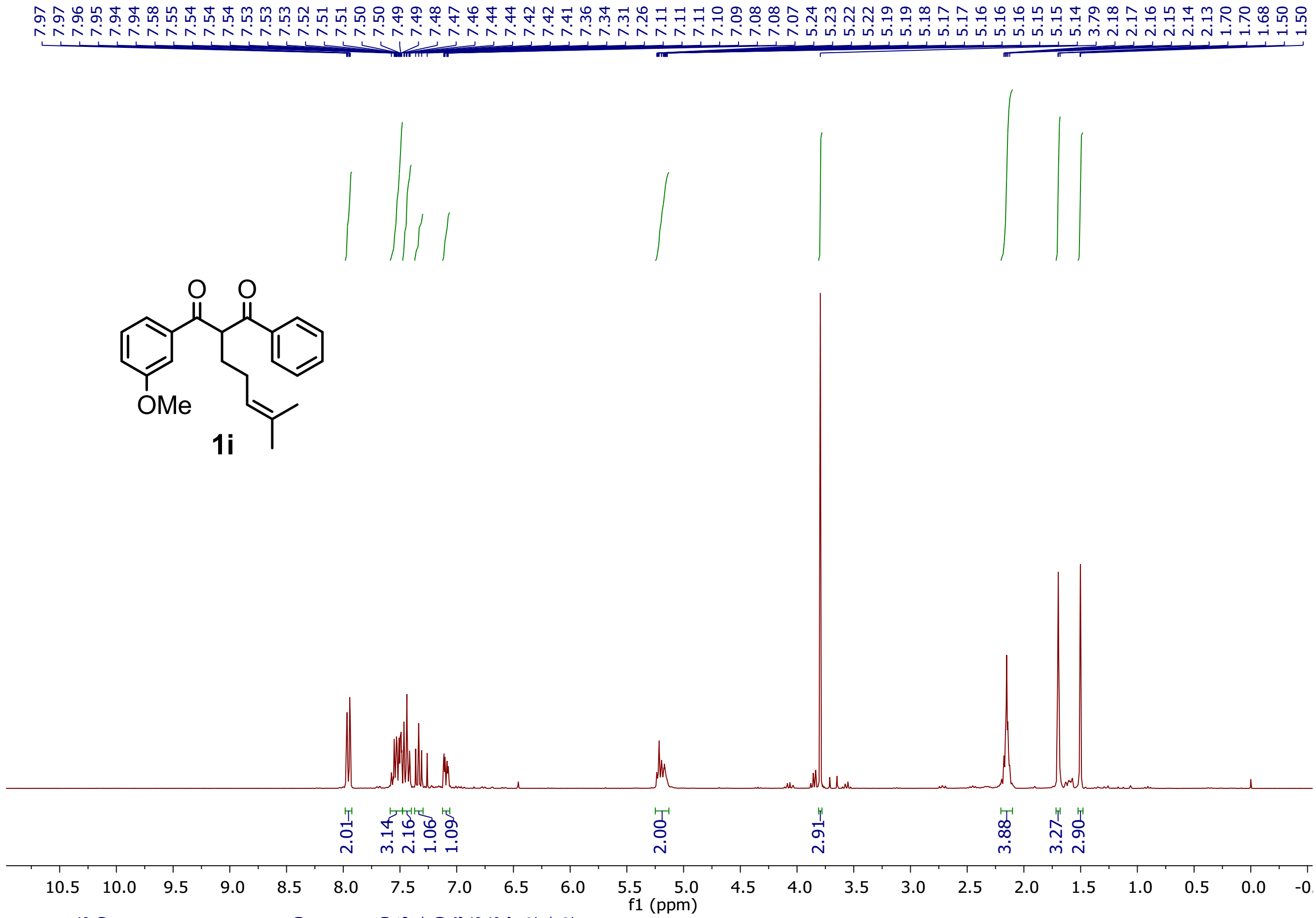
1h

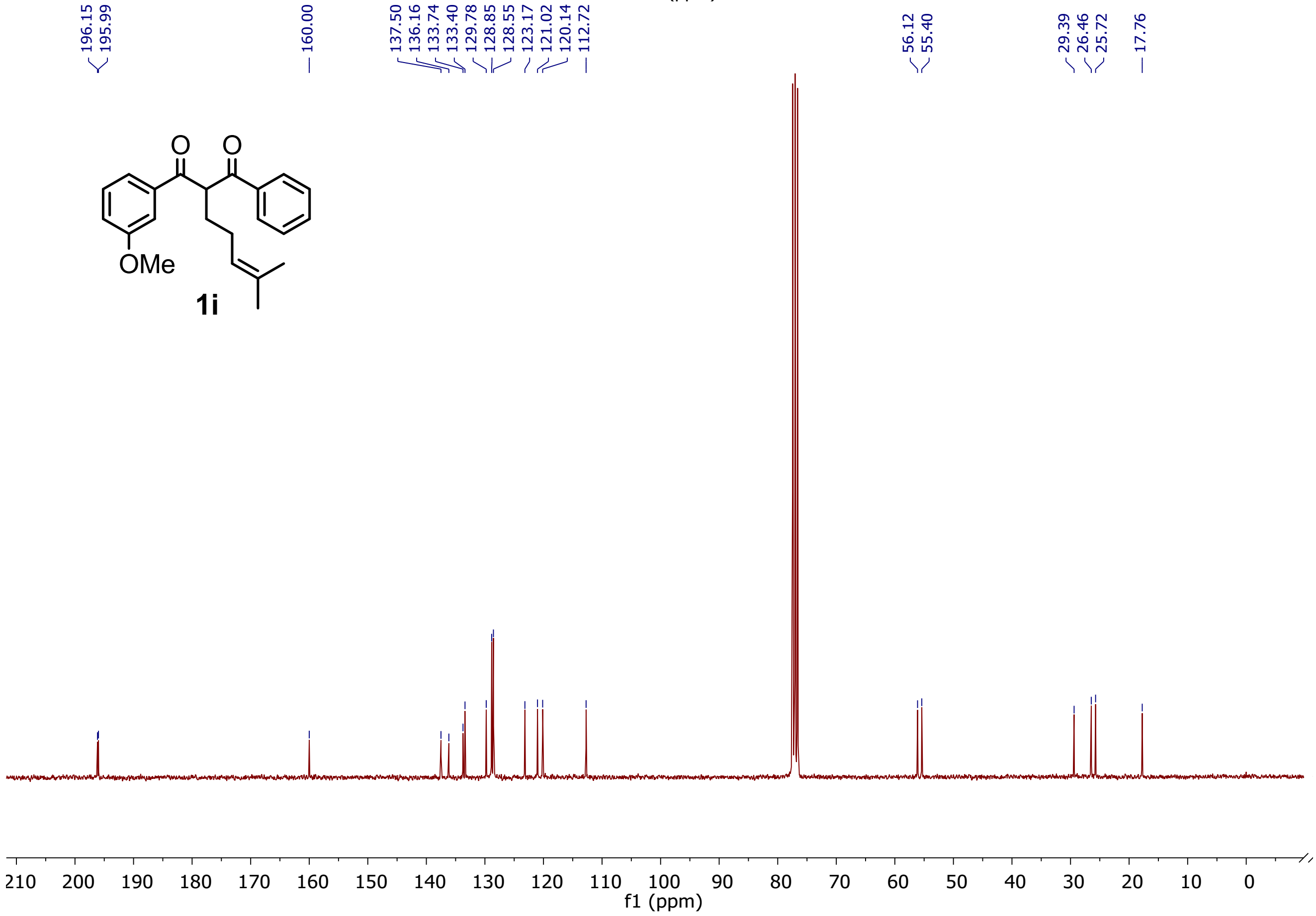
+ Traces of **9h (*)**

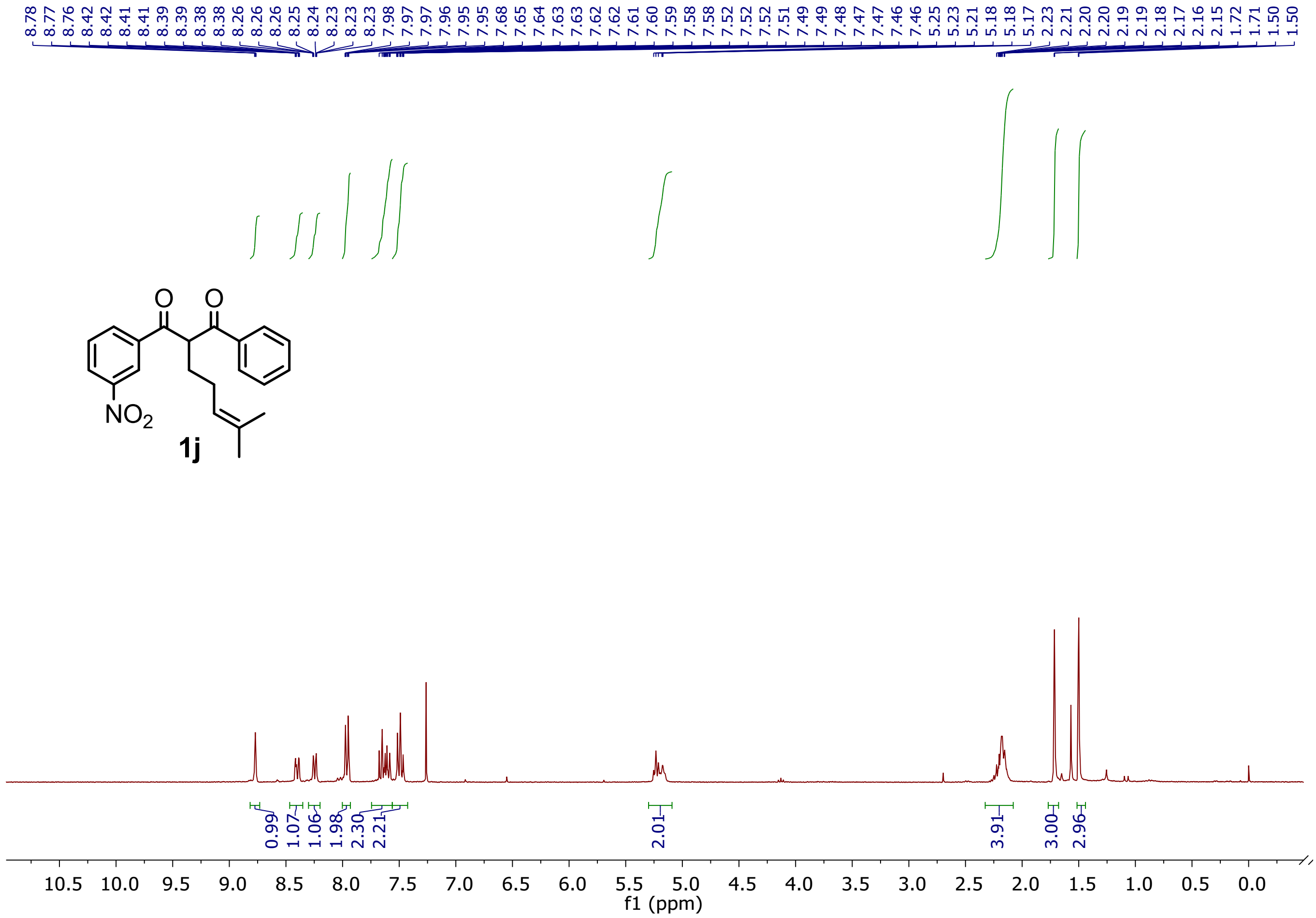


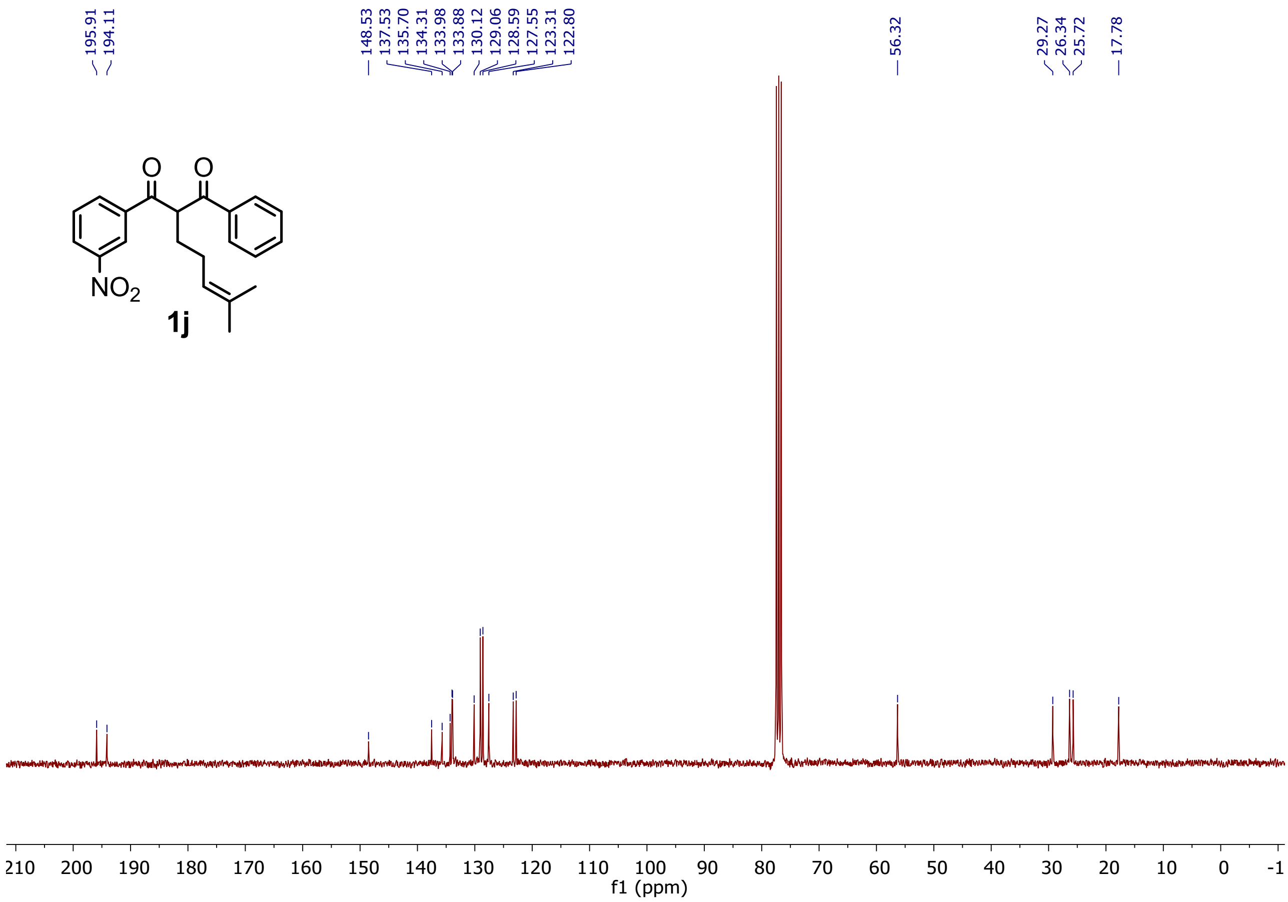


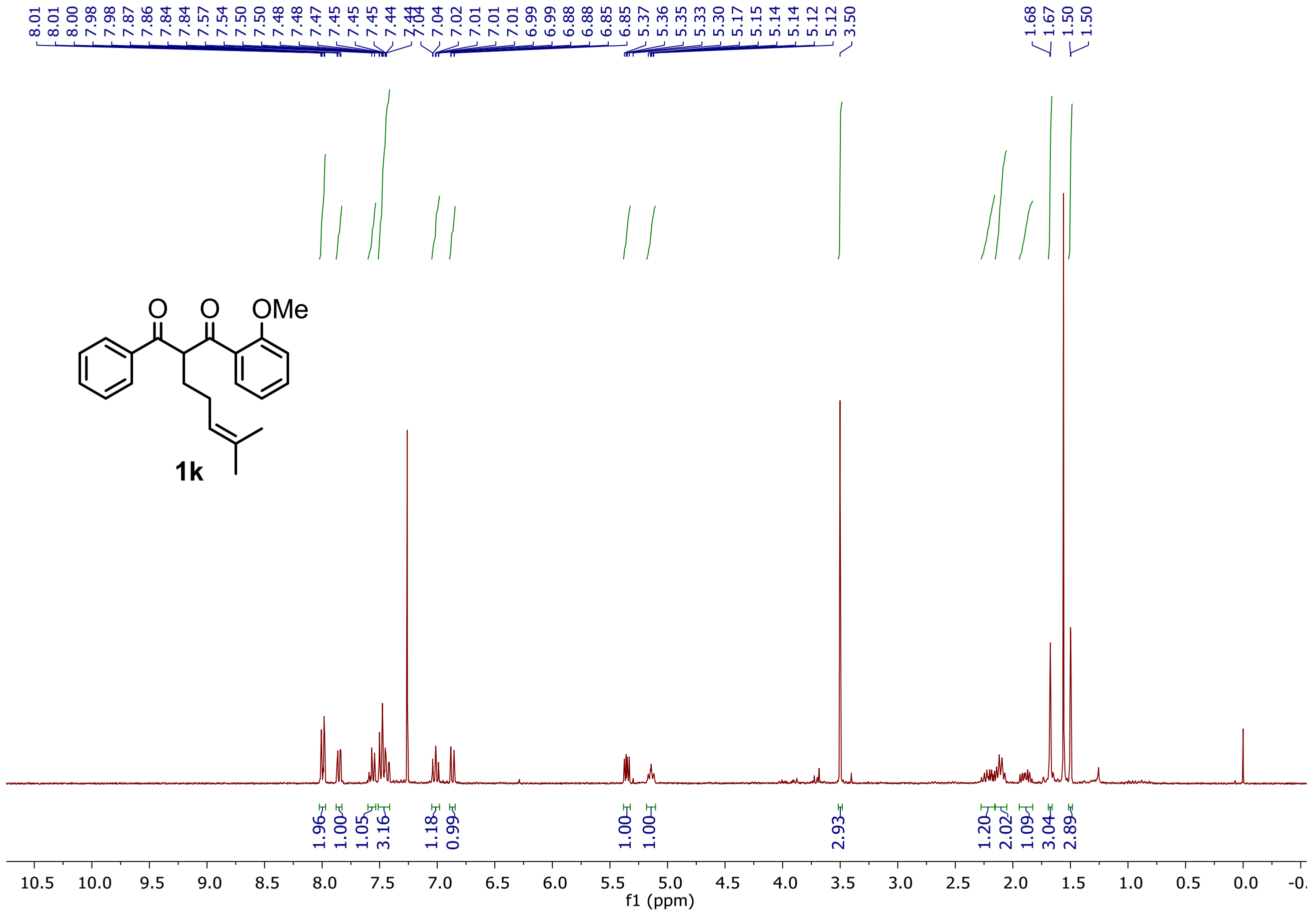
195.97
194.89
139.30
135.62
134.10
133.87
132.65
132.53
132.48
129.04
128.84
128.81
128.71
128.62
127.57
127.39
122.86
117.77
116.56
56.55
29.22
26.36
25.72
17.76
O
O
CN
1h
+ Traces of 9h (*)
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


7.97 7.97 7.96 7.95 7.94 7.94 7.58 7.55 7.54 7.54 7.54 7.53 7.53 7.53 7.52 7.51 7.51 7.50 7.50 7.49 7.49 7.48 7.47 7.46 7.44 7.44 7.42 7.42 7.41 7.36 7.34 7.31 7.26 7.11 7.11 7.11 7.10 7.09 7.08 7.08 7.07 5.24 5.23 5.22 5.19 5.19 5.18 5.17 5.17 5.16 5.16 5.16 5.15 5.15 5.14 3.79 2.18 2.17 2.16 2.15 2.14 2.13 1.70 1.70 1.68 1.50 1.50
O
O
OMe
1i
2.01
3.14
2.16
1.06
1.09
2.00
2.91
3.88
3.27
2.90
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

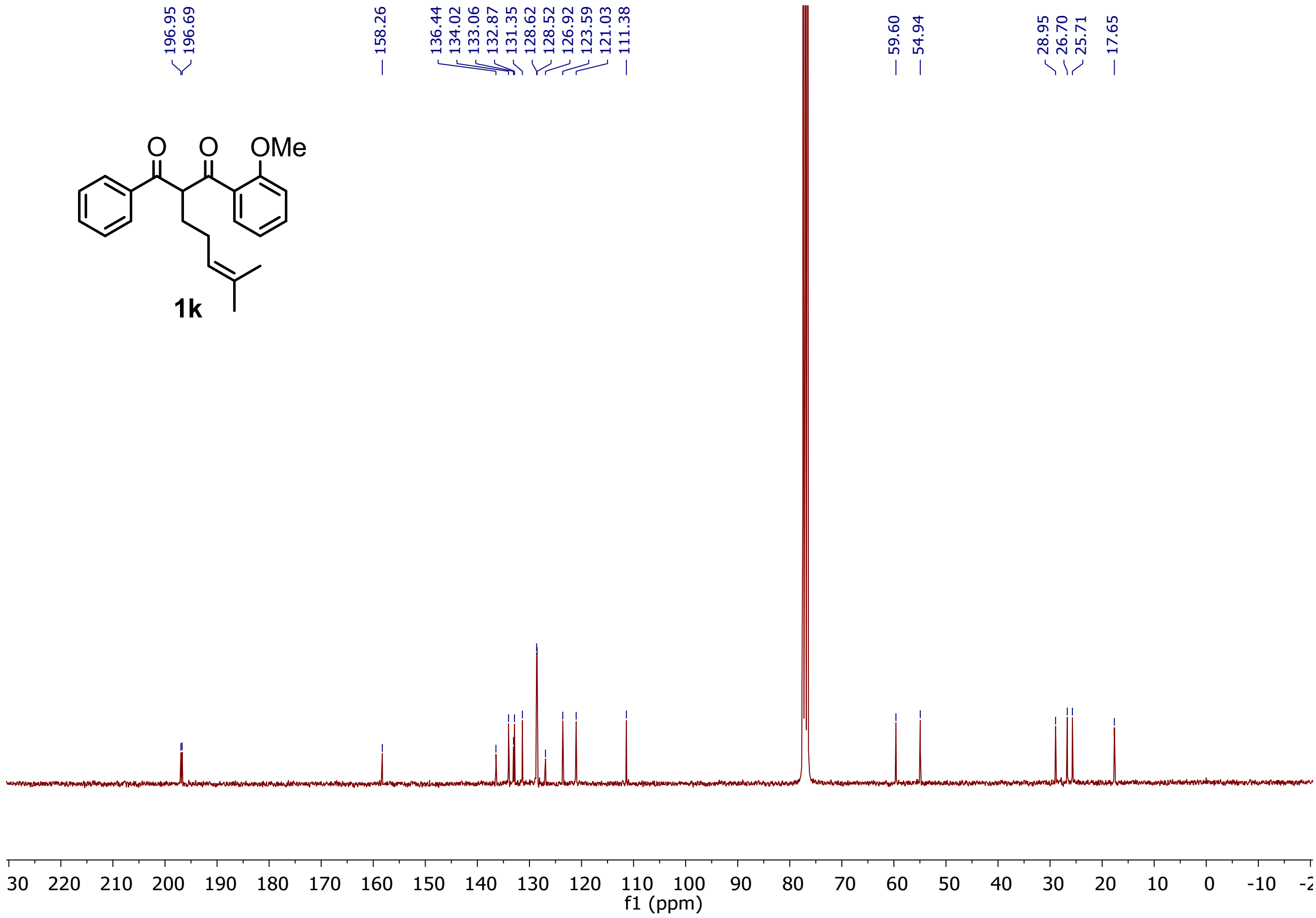

196.15 195.99
160.00
137.50 136.16 133.74 133.40 129.78 128.85 128.55 123.17 121.02 120.14 112.72
56.12 55.40
29.39 26.46 25.72 17.76
O
O
OMe
1i
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.78 8.77 8.76 8.42 8.42 8.41 8.41 8.39 8.39 8.38 8.38 8.26 8.26 8.25 8.24 8.23 8.23 8.23 7.98 7.97 7.97 7.96 7.95 7.95 7.68 7.65 7.64 7.63 7.63 7.62 7.62 7.61 7.60 7.59 7.58 7.58 7.52 7.52 7.51 7.49 7.49 7.48 7.47 7.47 7.46 7.46 5.25 5.23 5.21 5.18 5.18 5.17 2.23 2.21 2.20 2.20 2.19 2.19 2.18 2.17 2.16 2.15 1.72 1.71 1.50 1.50
NO2
1j
0.99 1.07 1.06 1.98 2.30 2.21 2.01 3.91 3.00 2.96
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)

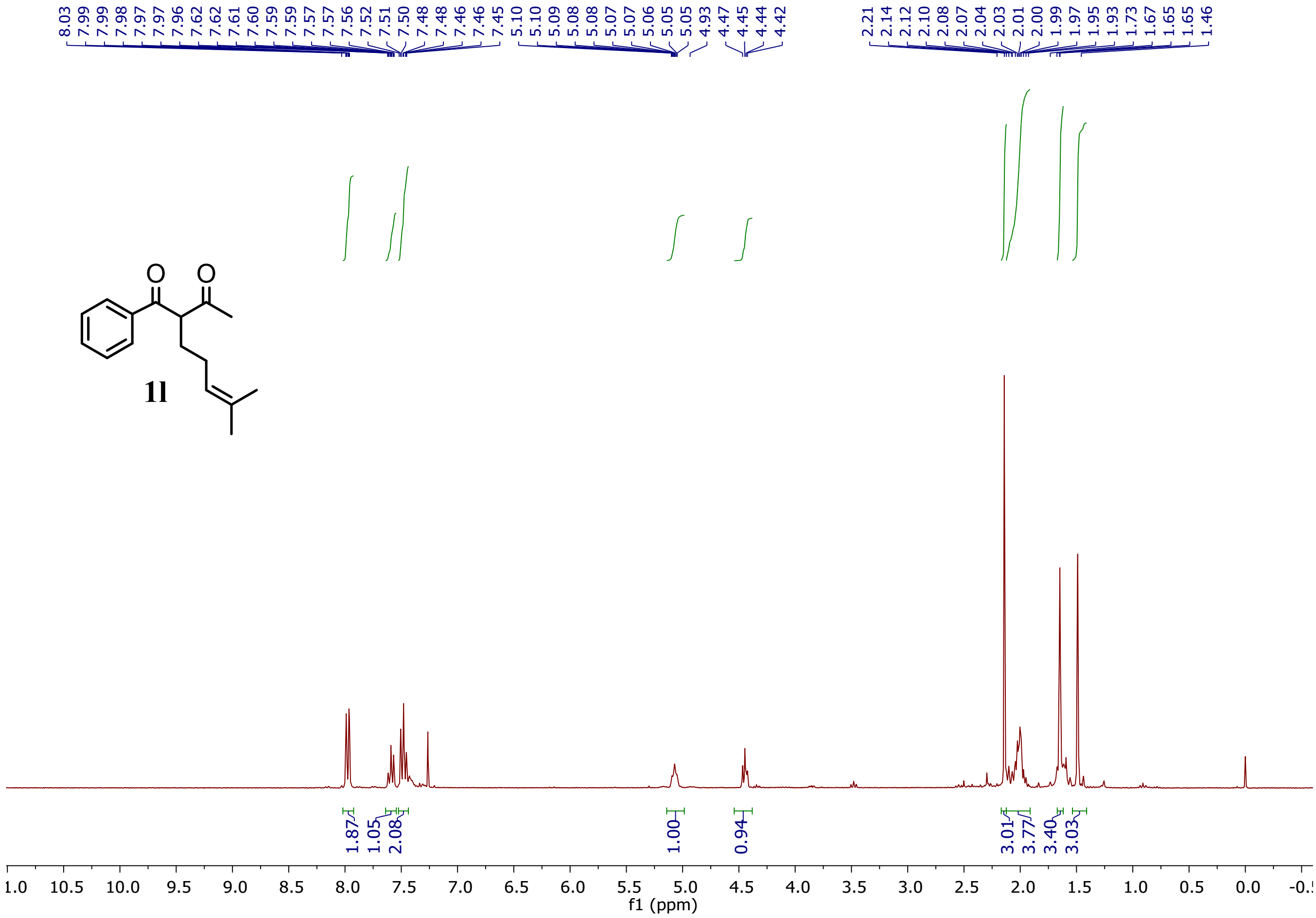

195.91 194.11
148.53 137.53 135.70 134.31 133.98 133.88 130.12 129.06 128.59 127.55 123.31 122.80
56.32
29.27 26.34 25.72
17.78
NO2
1j
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)



1k



1k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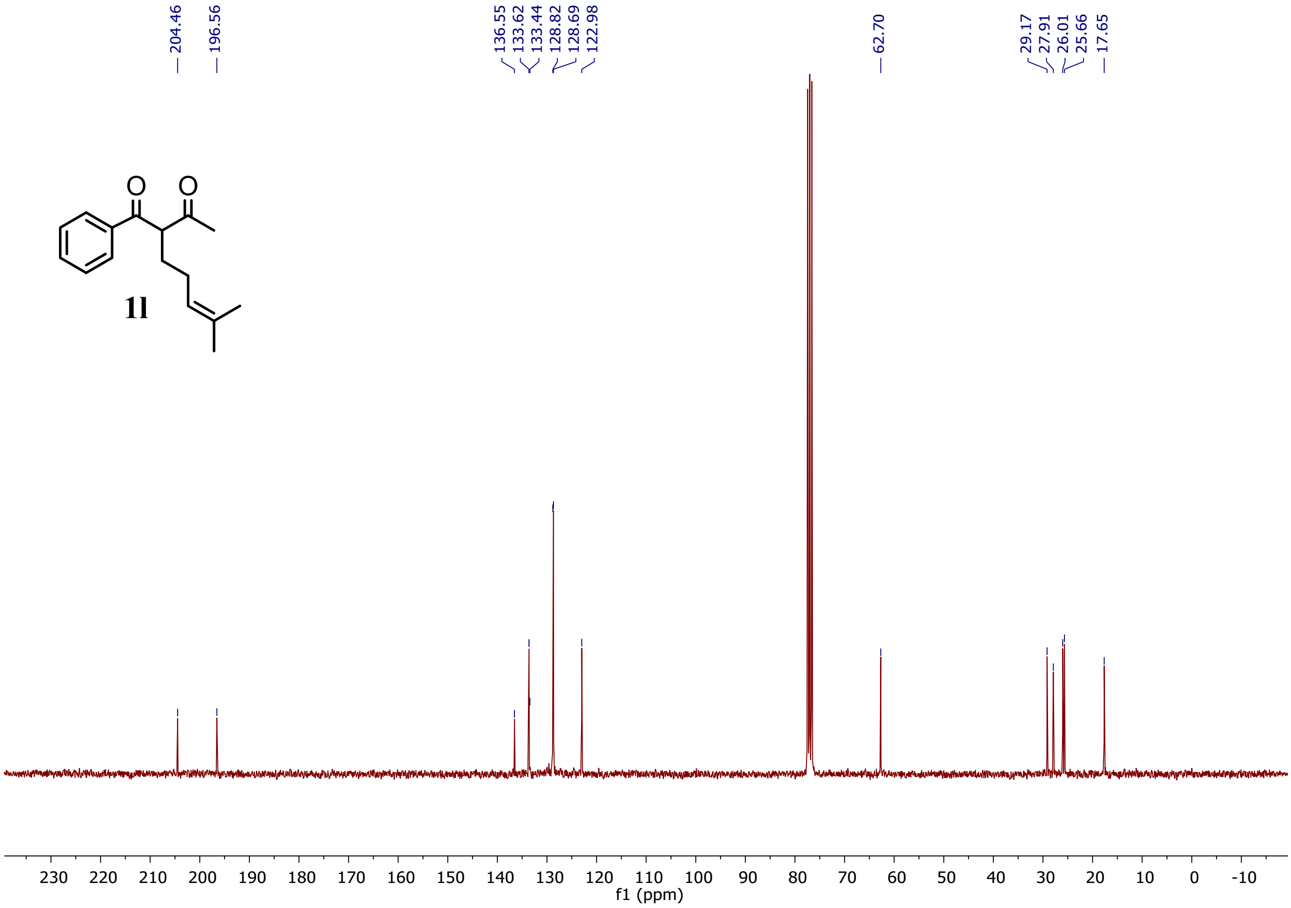
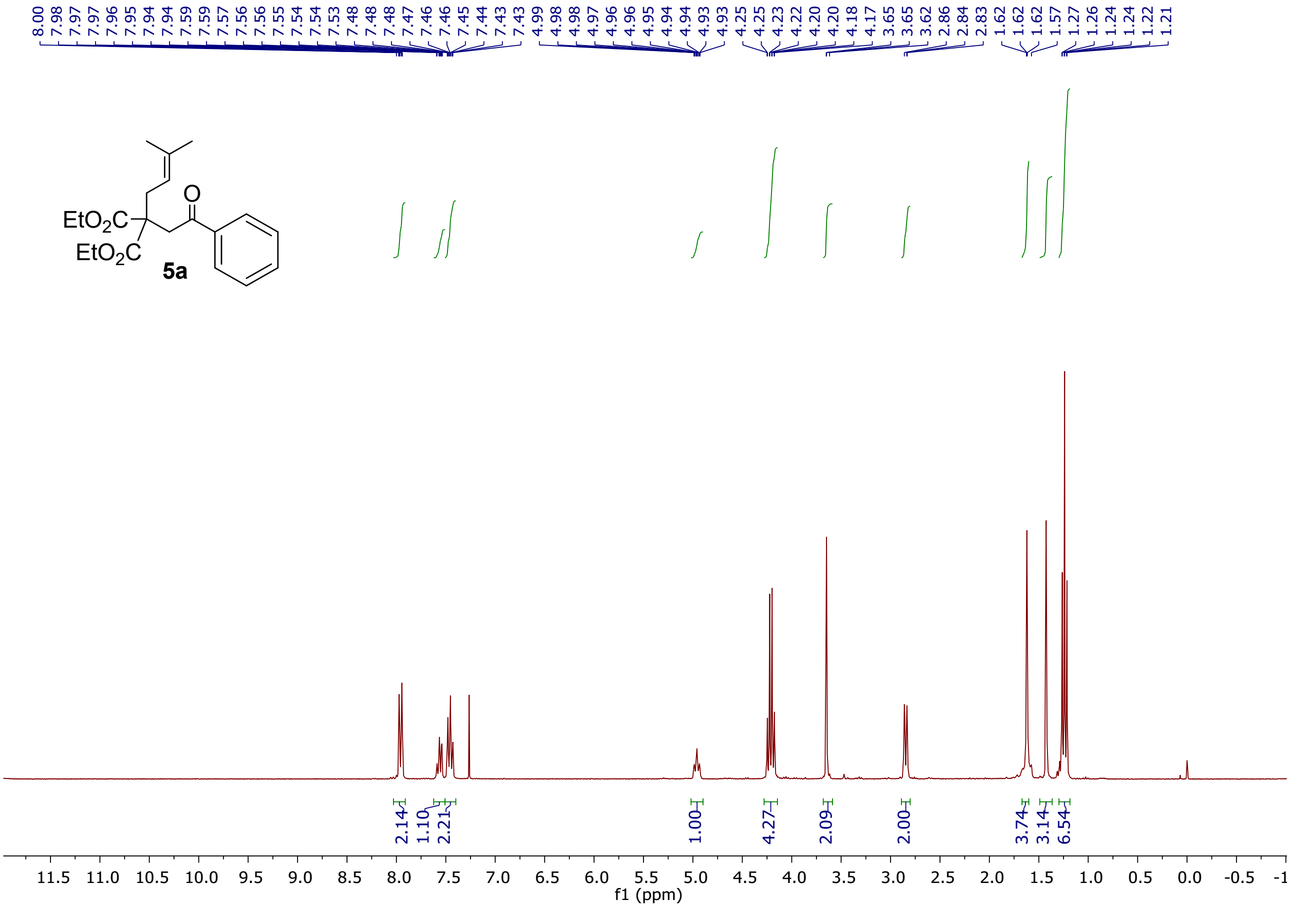
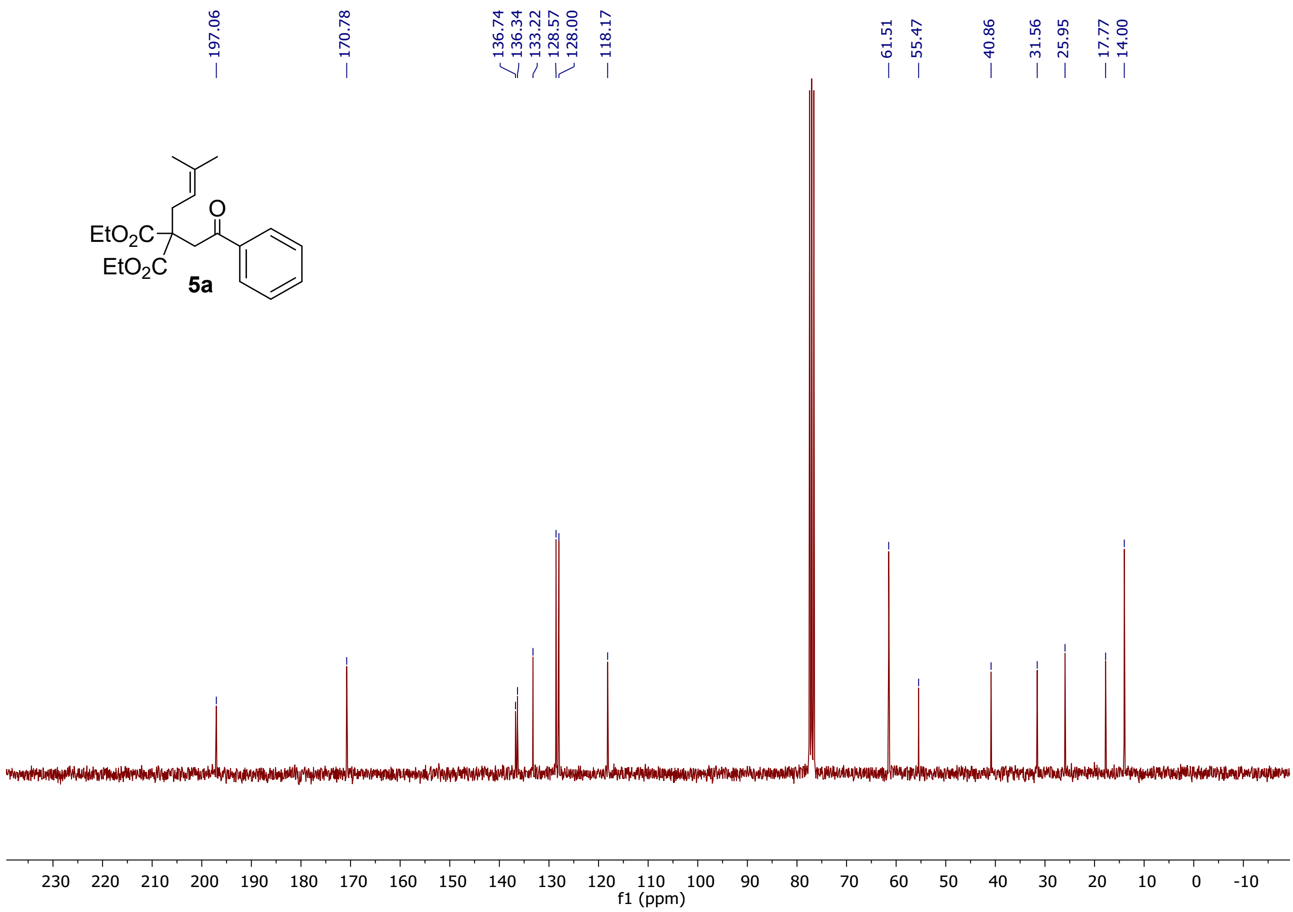
7.99
7.99
7.98
7.97
7.97
7.96
7.62
7.62
7.61
7.60
7.59
7.59
7.57
7.57
7.56
7.52
7.51
7.50
7.48
7.48
7.46
7.45
5.10
5.10
5.09
5.08
5.08
5.07
5.07
5.06
5.05
5.05
4.93
4.47
4.45
4.44
4.42
2.21
2.14
2.12
2.10
2.08
2.07
2.04
2.03
2.01
2.00
1.99
1.97
1.95
1.93
1.73
1.67
1.65
1.65
1.46
1l
1.87
1.05
2.08
1.00
0.94
3.01
3.77
3.40
3.03
f1 (ppm)



1l
204.46
196.56
136.55
133.62
133.44
128.82
128.69
122.98
62.70
29.17
27.91
26.01
25.66
17.65
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.00 7.98 7.97 7.97 7.96 7.95 7.94 7.94 7.59 7.59 7.57 7.56 7.56 7.55 7.54 7.54 7.53 7.48 7.48 7.48 7.47 7.46 7.46 7.45 7.44 7.43 7.43 4.99 4.98 4.98 4.97 4.96 4.96 4.95 4.94 4.94 4.93 4.93 4.93 4.25 4.25 4.23 4.22 4.20 4.20 4.18 4.17 3.65 3.65 3.62 2.86 2.84 2.83 1.62 1.62 1.62 1.57 1.27 1.26 1.24 1.24 1.22 1.21
EtO2C
EtO2C
O
5a
2.14
1.10
2.21
1.00
4.27
2.09
2.00
3.74
3.14
6.54
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


197.06
170.78
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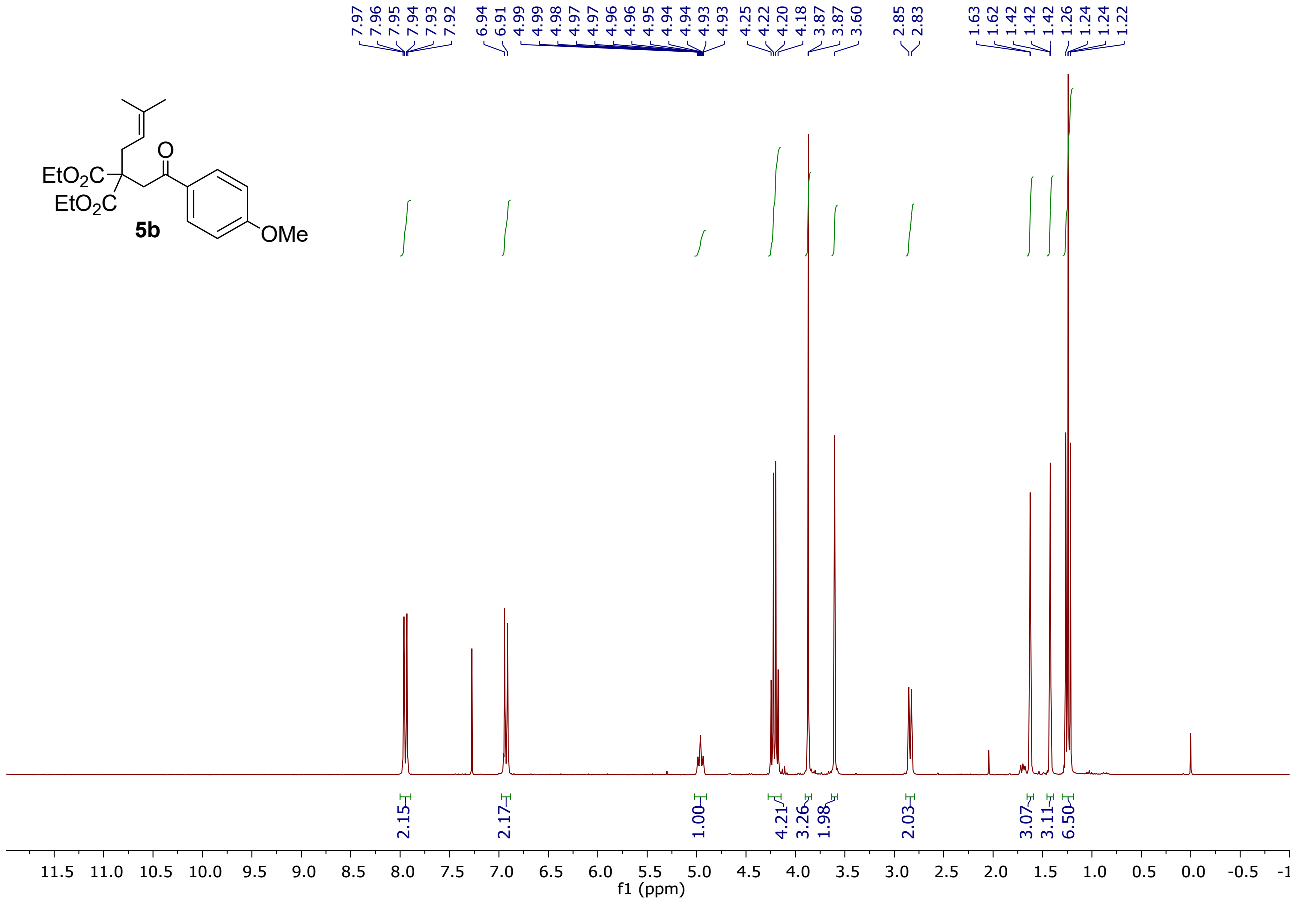
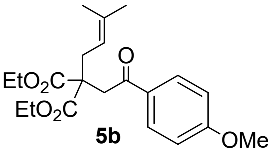
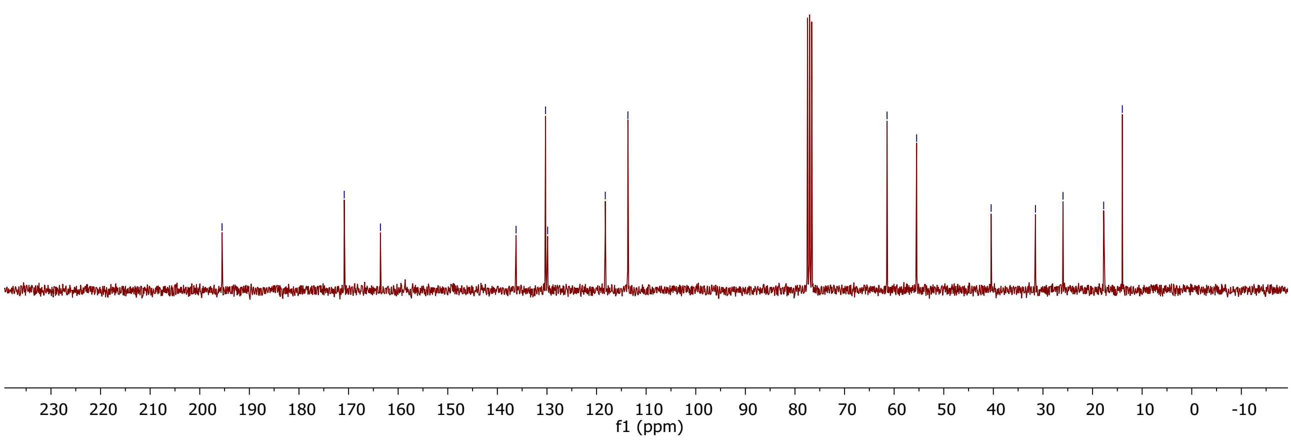
136.34
133.22
128.57
128.00
118.17
61.51
55.47
40.86
31.56
25.95
17.77
14.00
EtO2C
EtO2C
O
5a
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

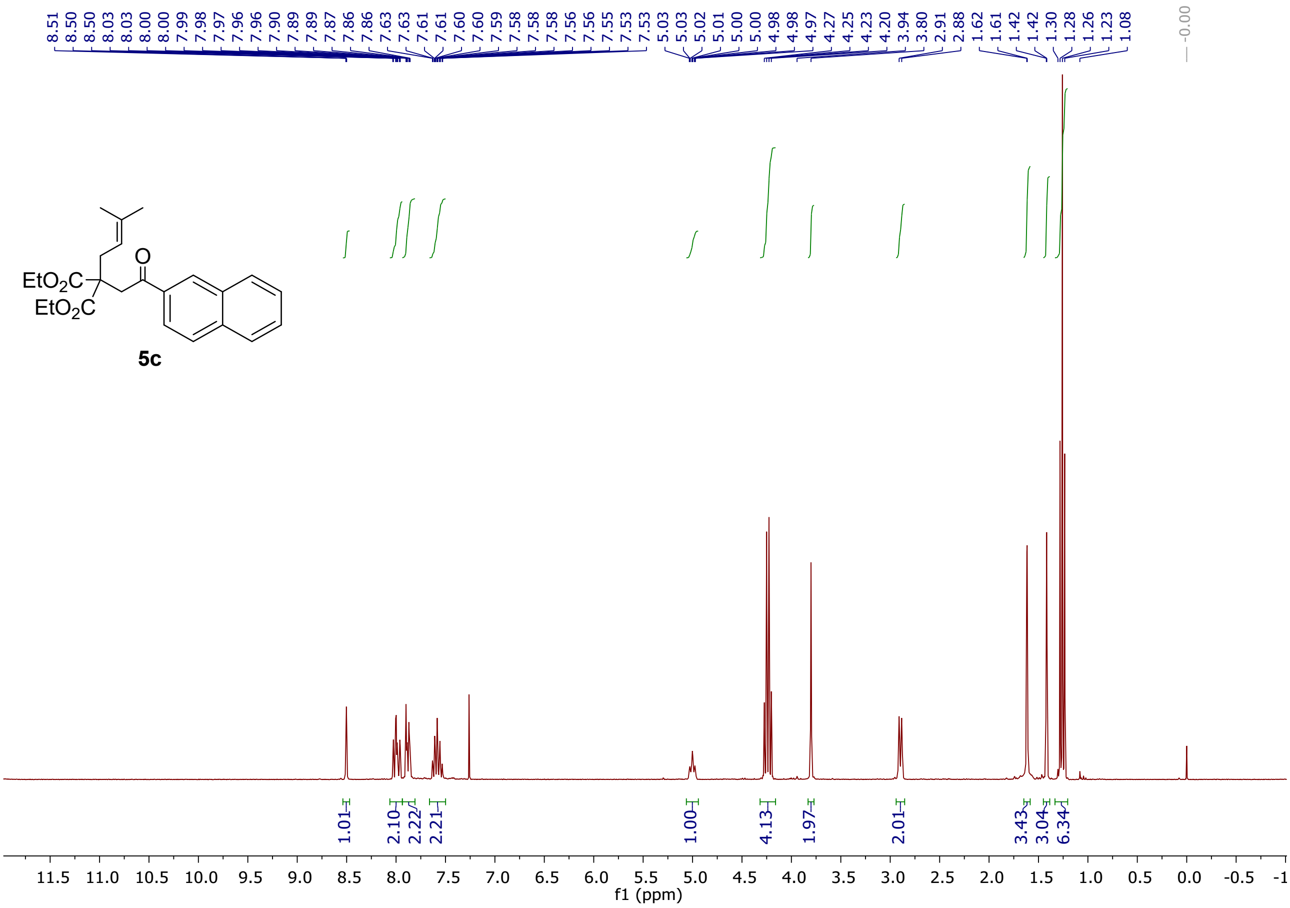


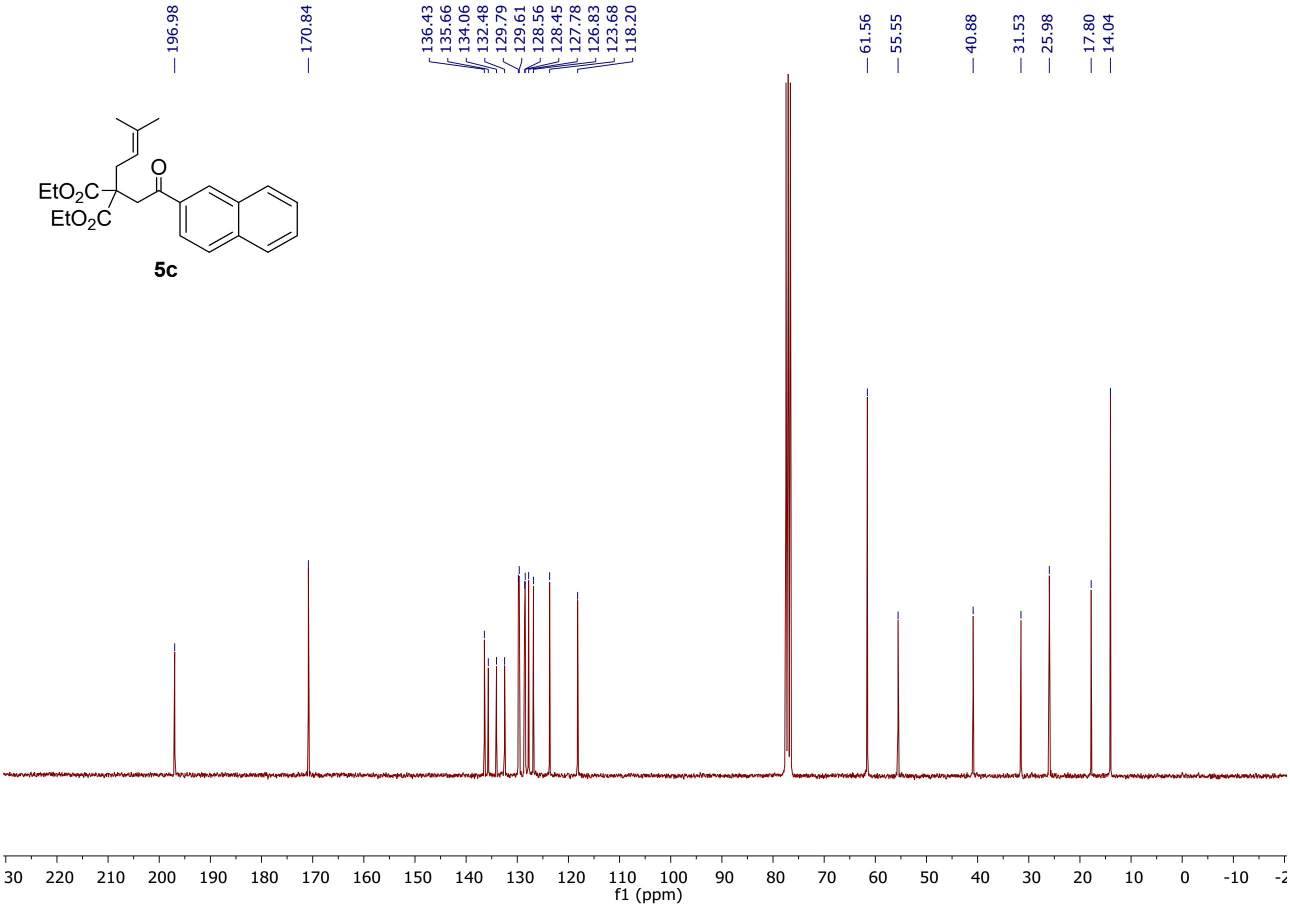
EtO2C
EtO2C
O
OMe
5b
7.97
7.96
7.95
7.94
7.93
7.92
6.94
6.91
4.99
4.98
4.97
4.97
4.96
4.96
4.95
4.94
4.94
4.93
4.93
4.25
4.22
4.20
4.18
3.87
3.87
3.60
2.85
2.83
1.63
1.62
1.42
1.42
1.42
1.26
1.24
1.24
1.22
2.15
2.17
1.00
4.21
3.26
1.98
2.03
3.07
3.11
6.50
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

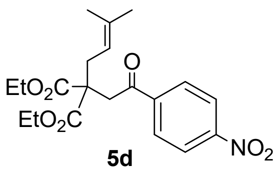

EtO2C
EtO2C
O
OMe

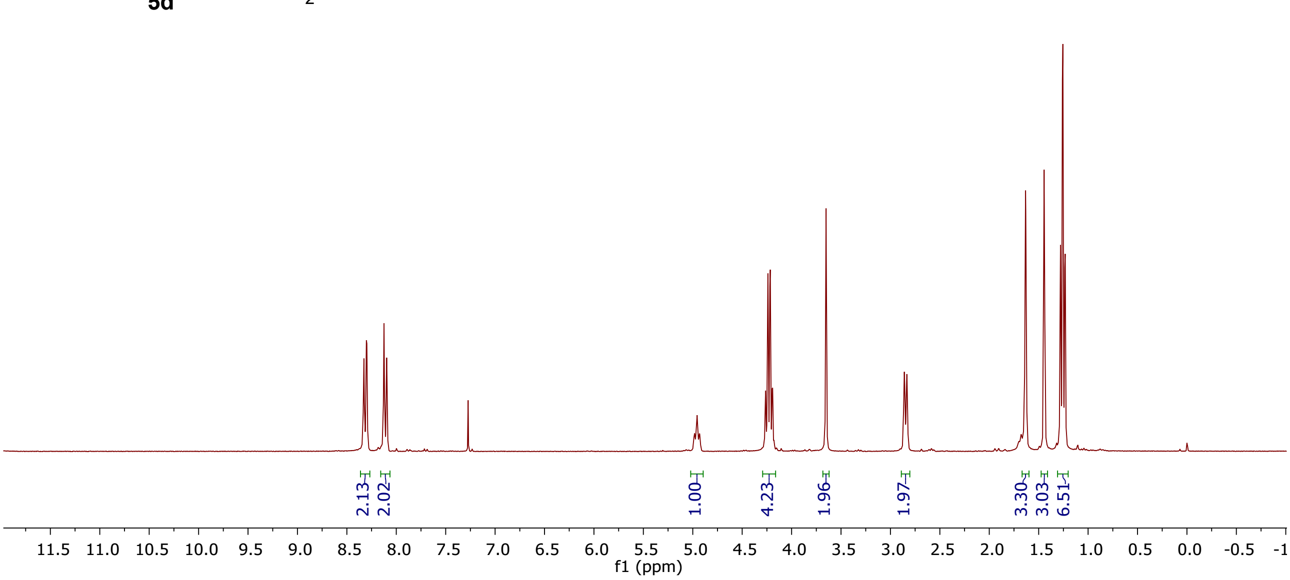
5b

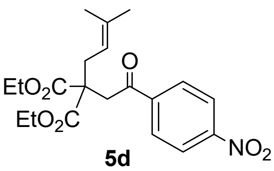

195.51
170.87
163.58
136.23
130.28
129.86
118.24
113.68
61.43
55.47
40.45
31.51
25.96
17.76
14.00
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


EtO2C
EtO2C
O
5c
f1 (ppm)

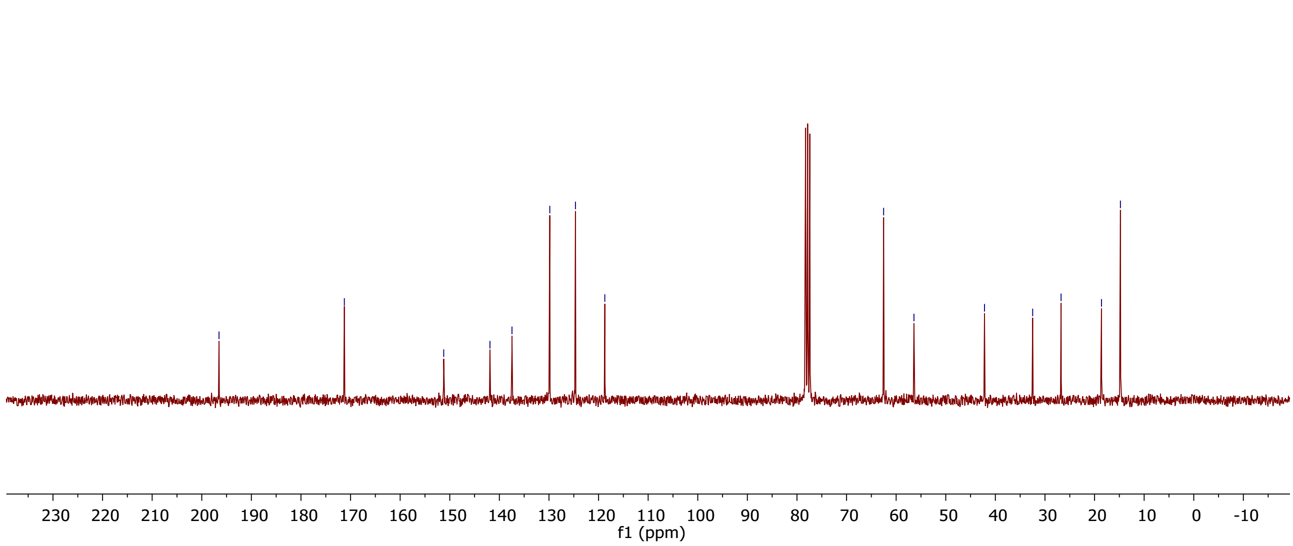

196.98
170.84
136.43
135.66
134.06
132.48
129.79
129.61
128.56
128.45
127.78
126.83
123.68
118.20
61.56
55.55
40.88
31.53
25.98
17.80
14.04
O
EtO2C
EtO2C
5c
f1 (ppm)


EtO2C
EtO2C
O
NO2
5d

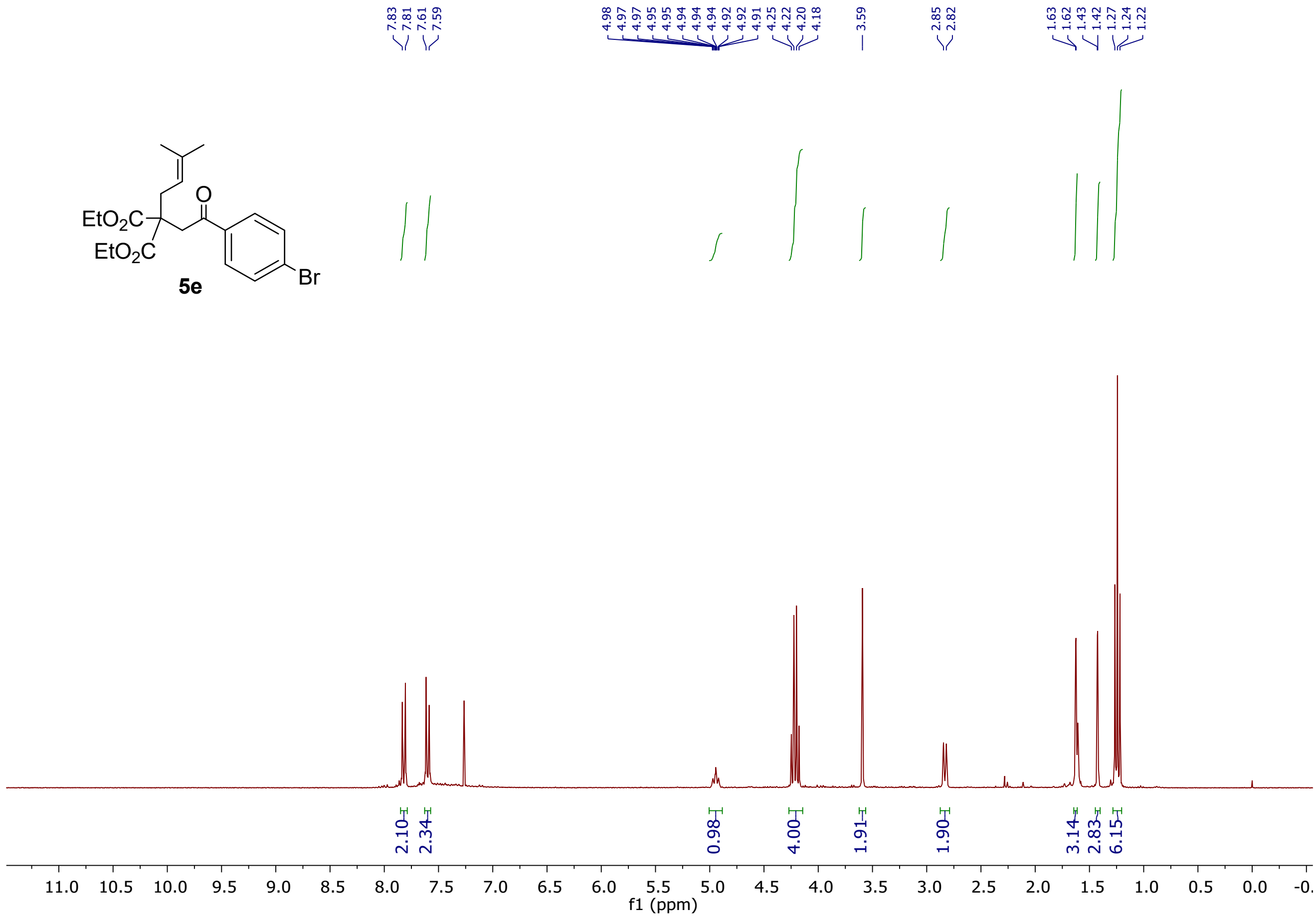

8.33
8.33
8.30
8.30
8.13
8.12
8.10
8.09
4.99
4.99
4.98
4.98
4.97
4.96
4.96
4.96
4.95
4.94
4.93
4.93
4.93
4.92
4.26
4.24
4.24
4.22
4.22
4.20
4.19
3.65
2.86
2.83
1.64
1.63
1.63
1.45
1.44
1.28
1.26
1.26
1.23
2.13
2.02
1.00
4.23
1.96
1.97
3.30
3.03
6.51
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

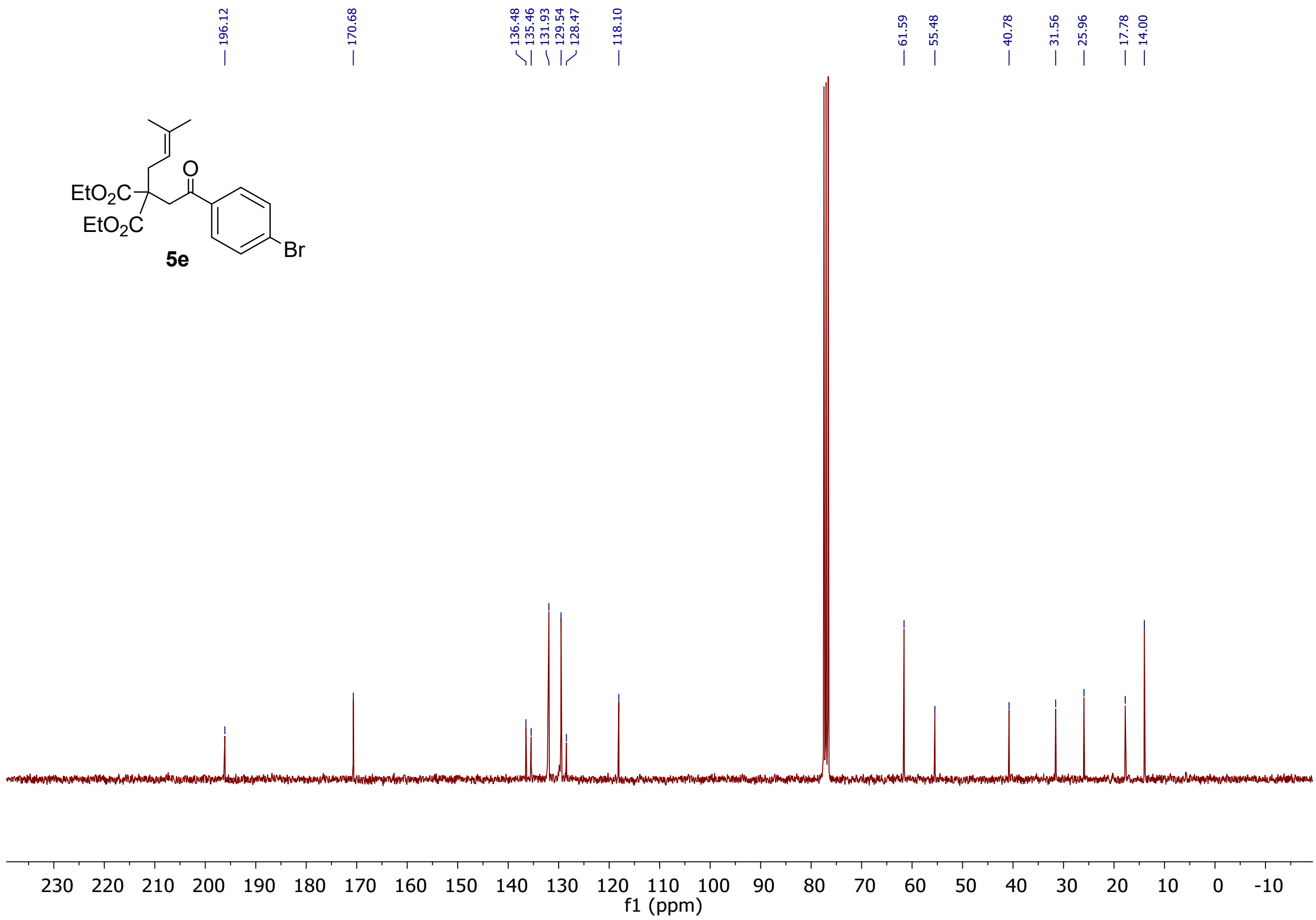


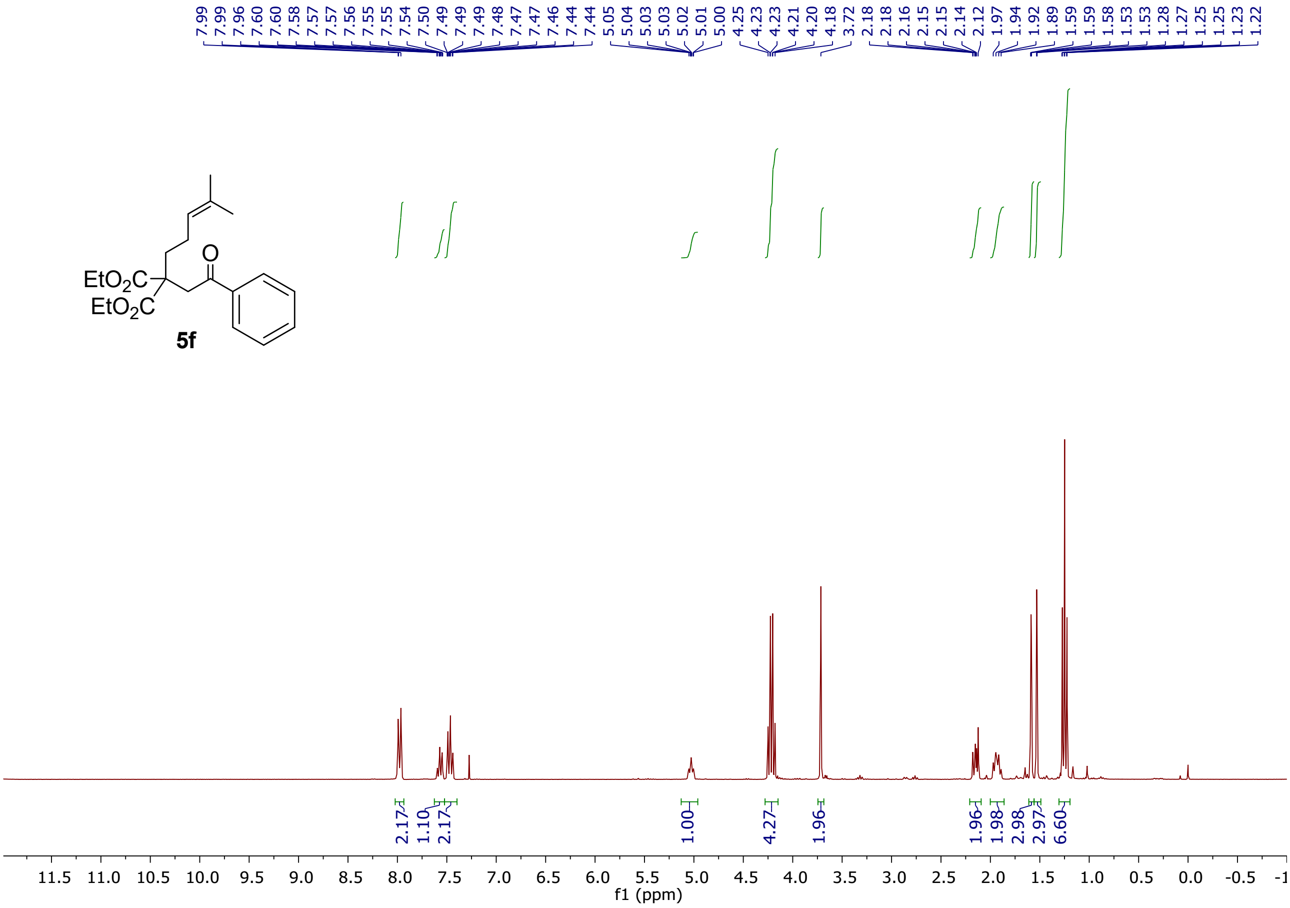
5d

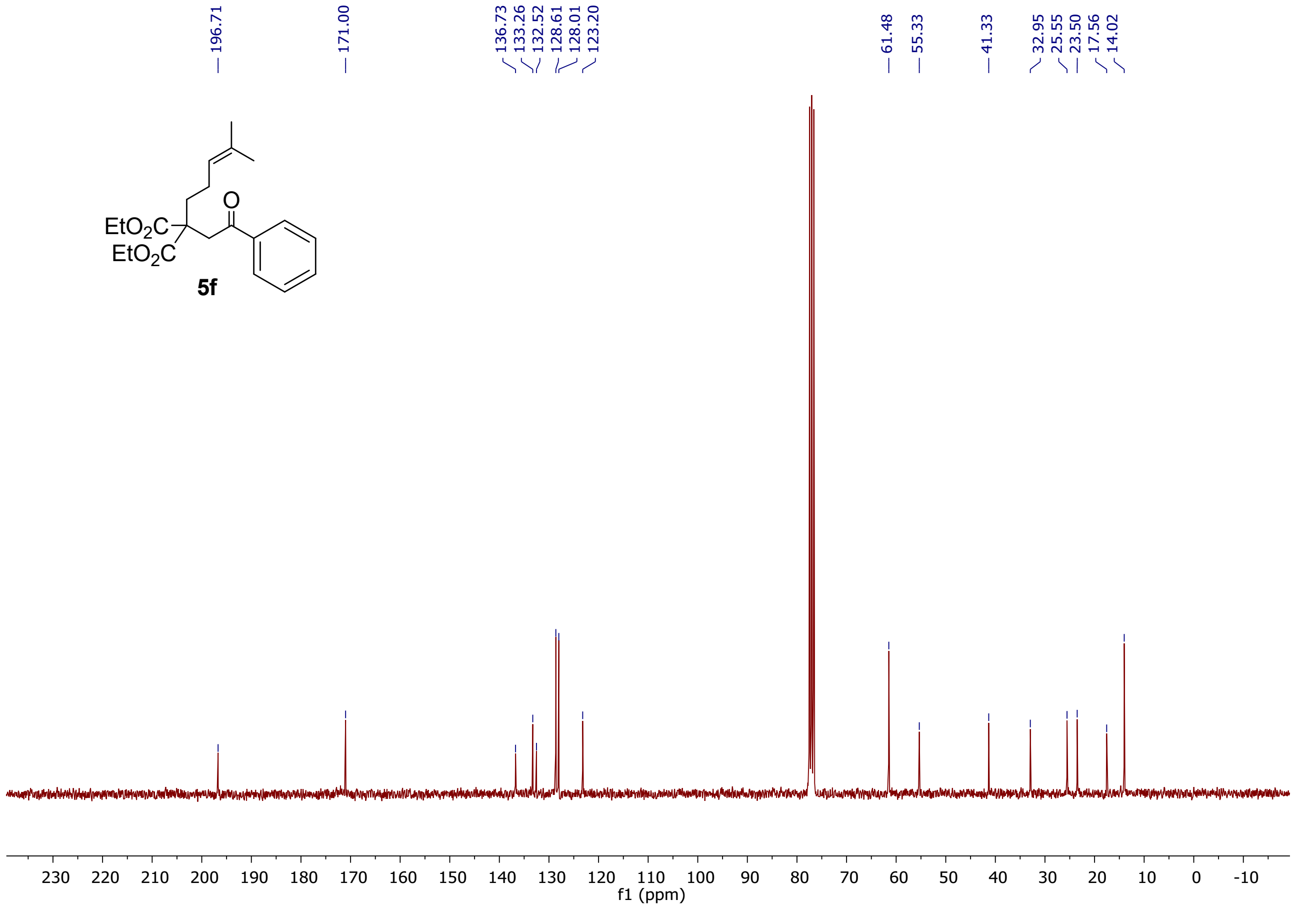


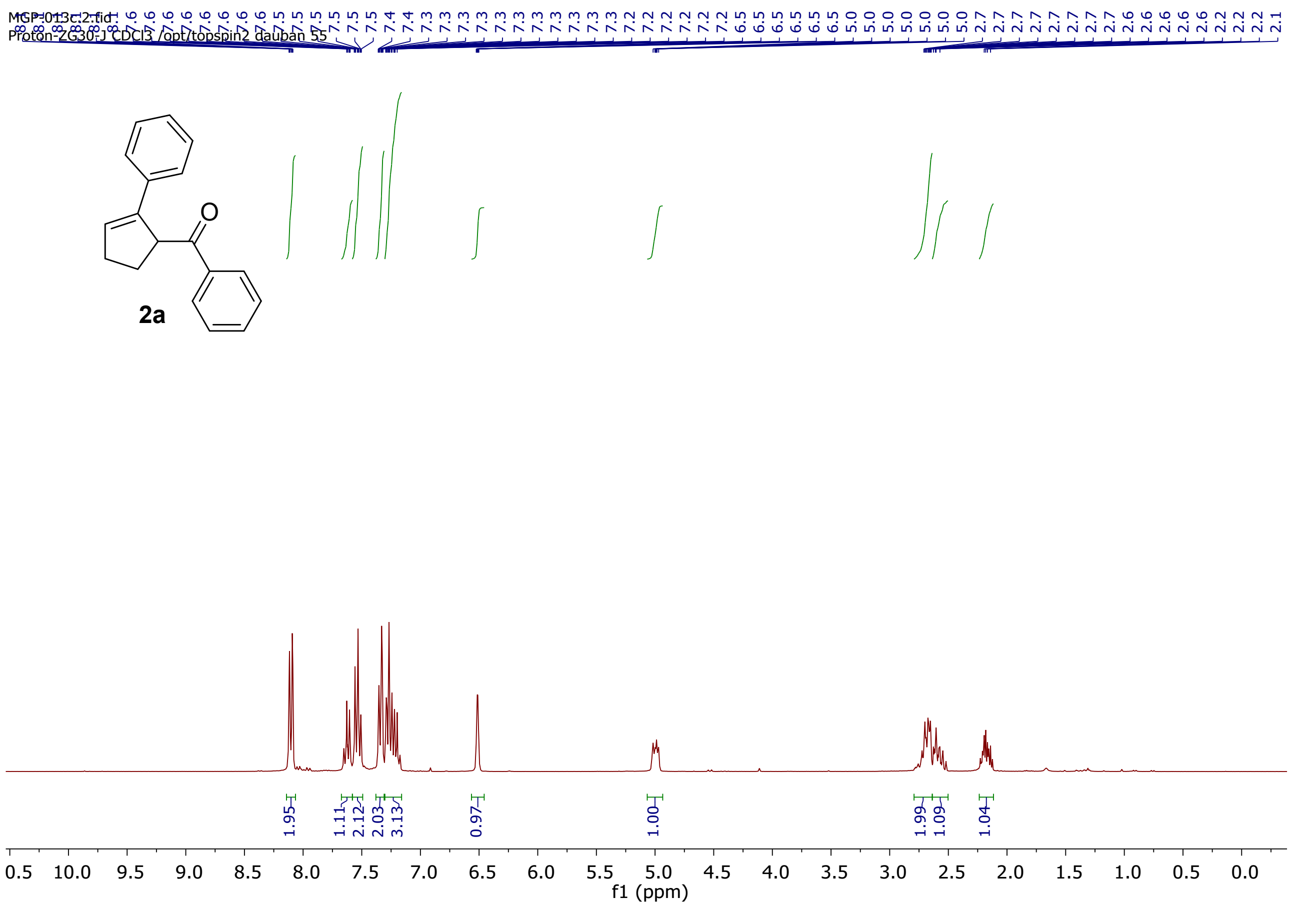
196.52
171.25
151.22
141.90
137.46
129.83
124.66
118.74
62.53
56.41
42.19
32.48
26.75
18.60
14.79
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

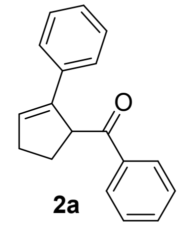

7.83
7.81
7.61
7.59
4.98
4.97
4.97
4.95
4.95
4.94
4.94
4.94
4.92
4.92
4.91
4.25
4.22
4.20
4.18
3.59
2.85
2.82
1.63
1.62
1.43
1.42
1.27
1.24
1.22
EtO2C
EtO2C
O
Br
5e
2.10
2.34
0.98
4.00
1.91
1.90
3.14
2.83
6.15
f1 (ppm)

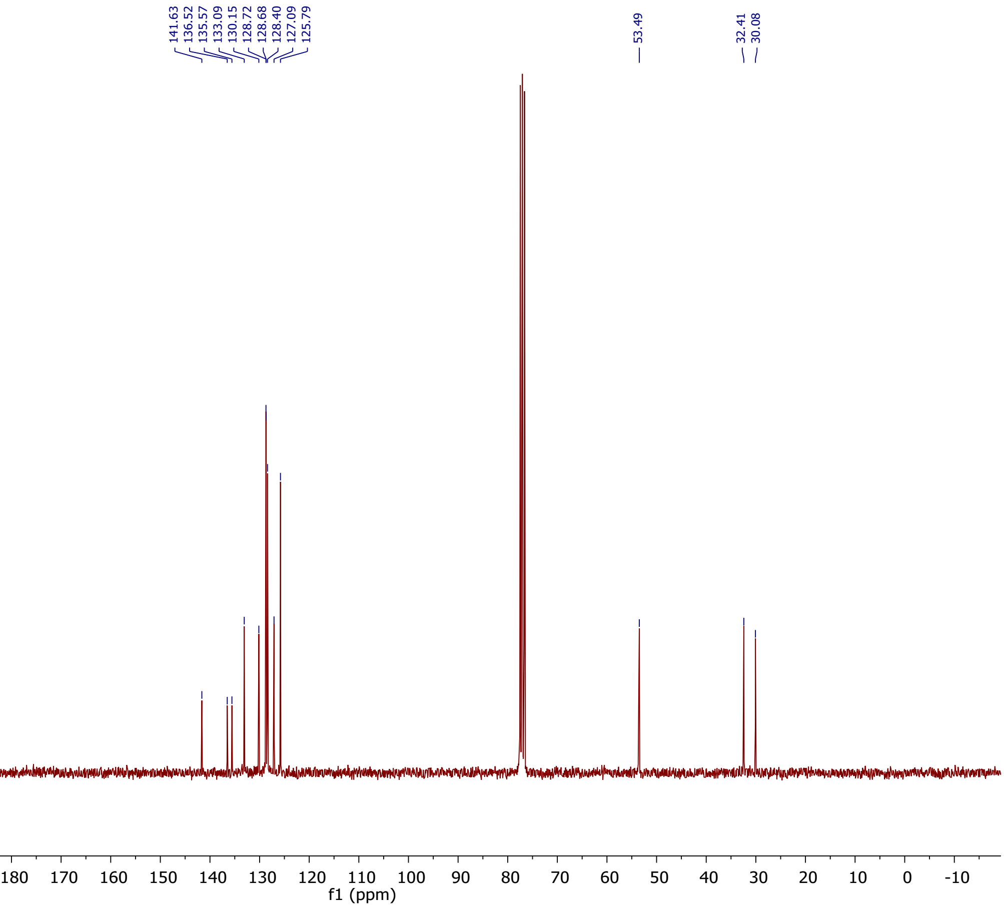

196.12
170.68
136.48
135.46
131.93
129.54
128.47
118.10
61.59
55.48
40.78
31.56
25.96
17.78
14.00
EtO2C
EtO2C
O
Br
5e
f1 (ppm)

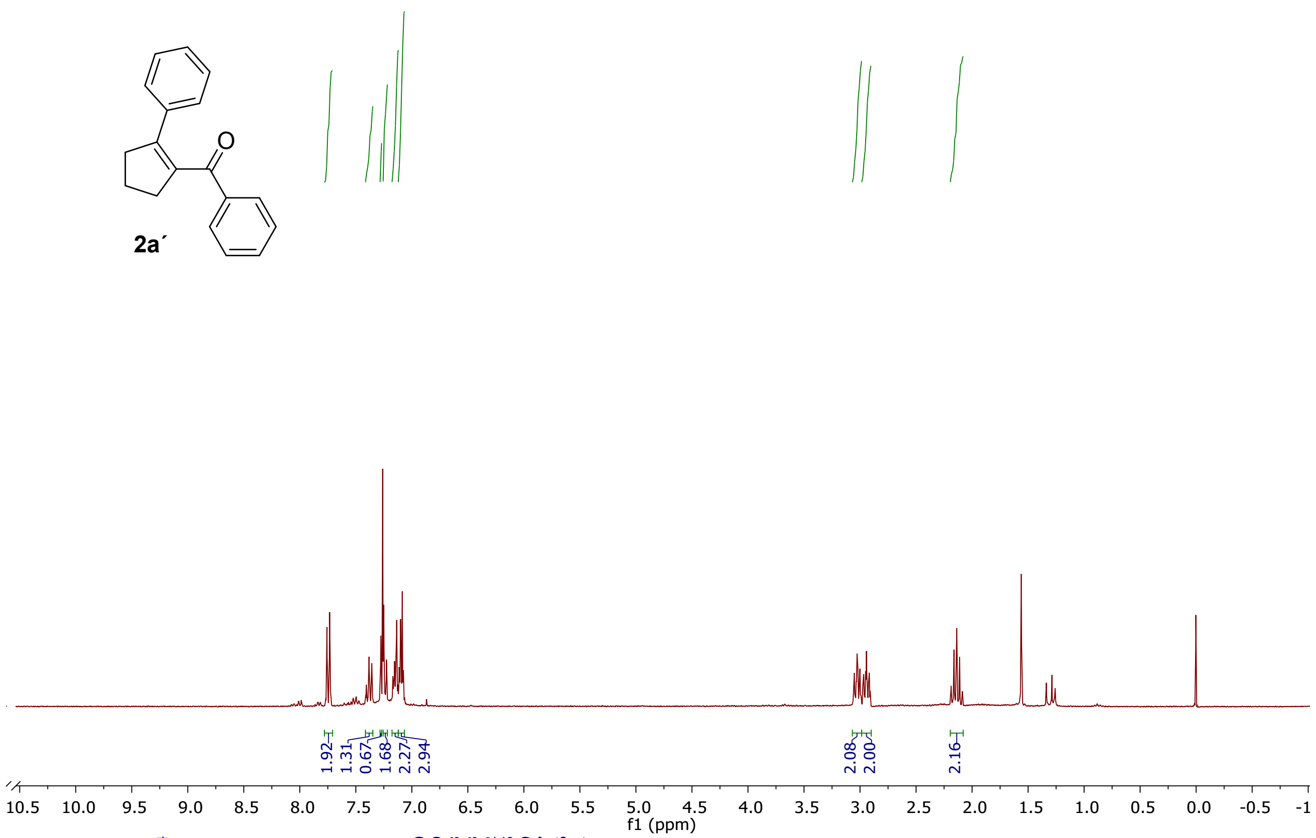

EtO2C
EtO2C
O
5f
7.99 7.99 7.96 7.60 7.60 7.58 7.57 7.57 7.56 7.55 7.55 7.54 7.50 7.49 7.49 7.49 7.48 7.47 7.47 7.46 7.44 7.44 5.05 5.04 5.03 5.03 5.02 5.01 5.00 4.25 4.23 4.23 4.21 4.20 4.18 3.72 2.18 2.18 2.16 2.15 2.15 2.14 2.12 1.97 1.94 1.92 1.89 1.59 1.59 1.58 1.53 1.53 1.28 1.27 1.25 1.25 1.23 1.22
2.17 1.10 2.17 1.00 4.27 1.96 1.96 1.98 2.98 2.97 6.60
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


196.71
171.00
136.73
133.26
132.52
128.61
128.01
123.20
61.48
55.33
41.33
32.95
25.55
23.50
17.56
14.02
EtO_2C
EtO_2C
O
5f
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

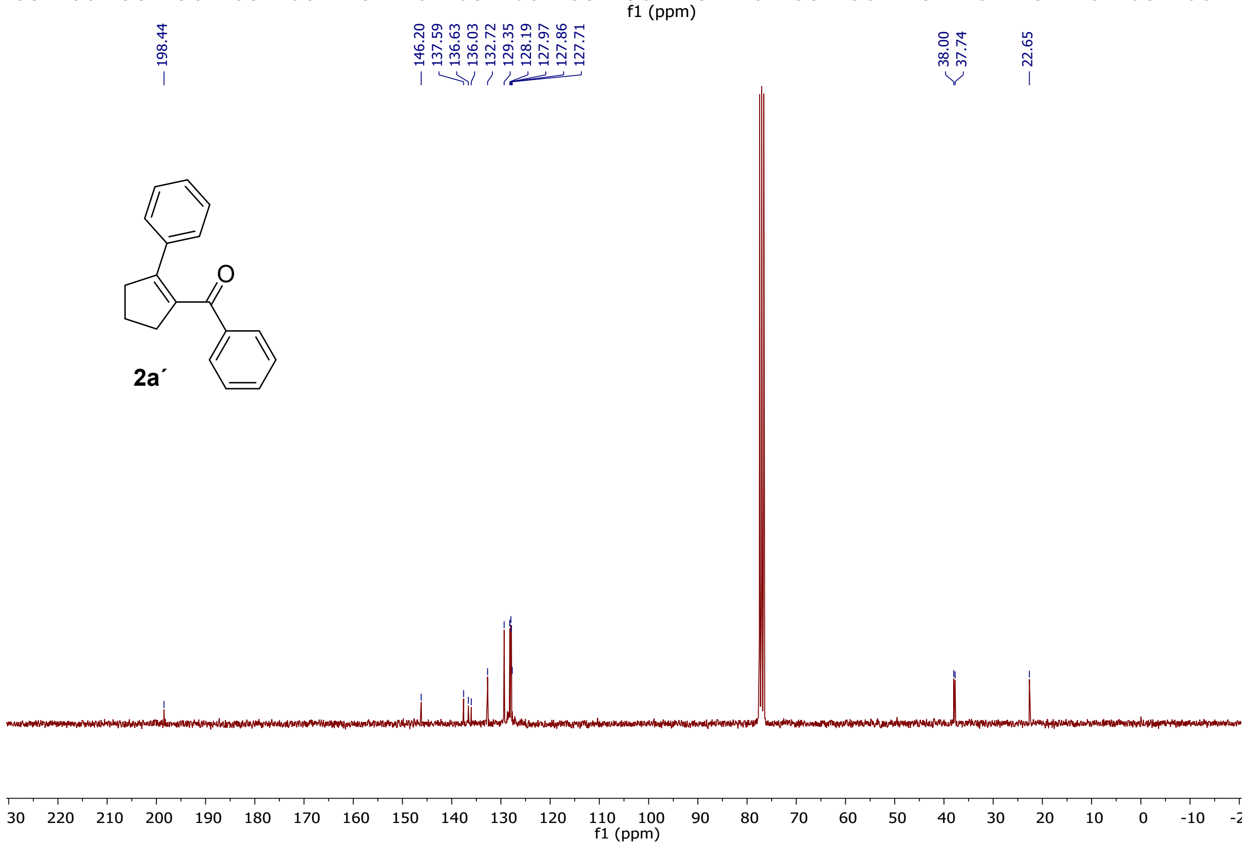

MGP-013c.2.fid
Proton-ZG30-J CDCl3 /opt/topspin2 dauban 55
O
2a
1.95
1.11
2.12
2.03
3.13
0.97
1.00
1.99
1.09
1.04
0.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


2a

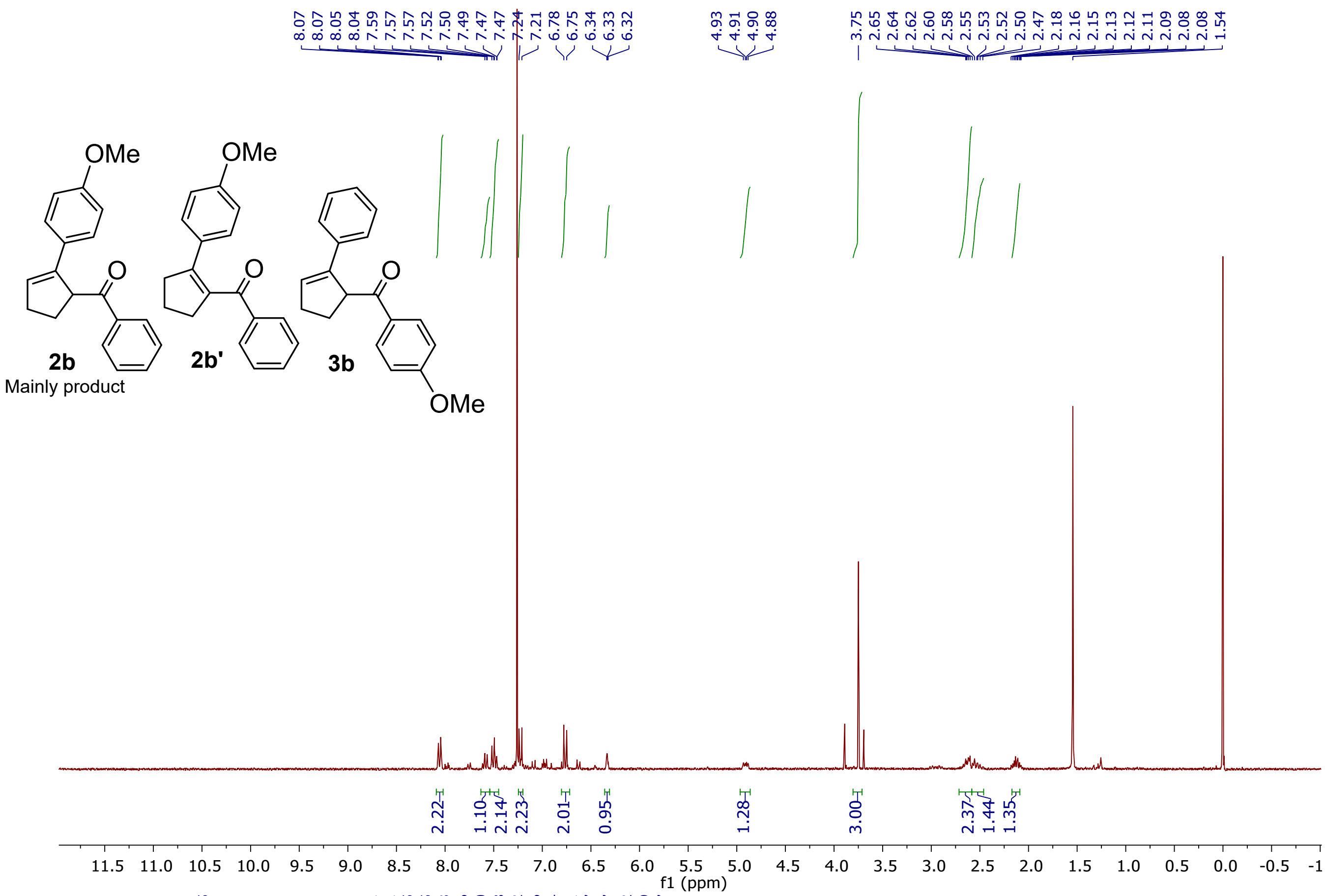

201.16
141.63
136.52
135.57
133.09
130.15
128.72
128.68
128.40
127.09
125.79
53.49
32.41
30.08
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

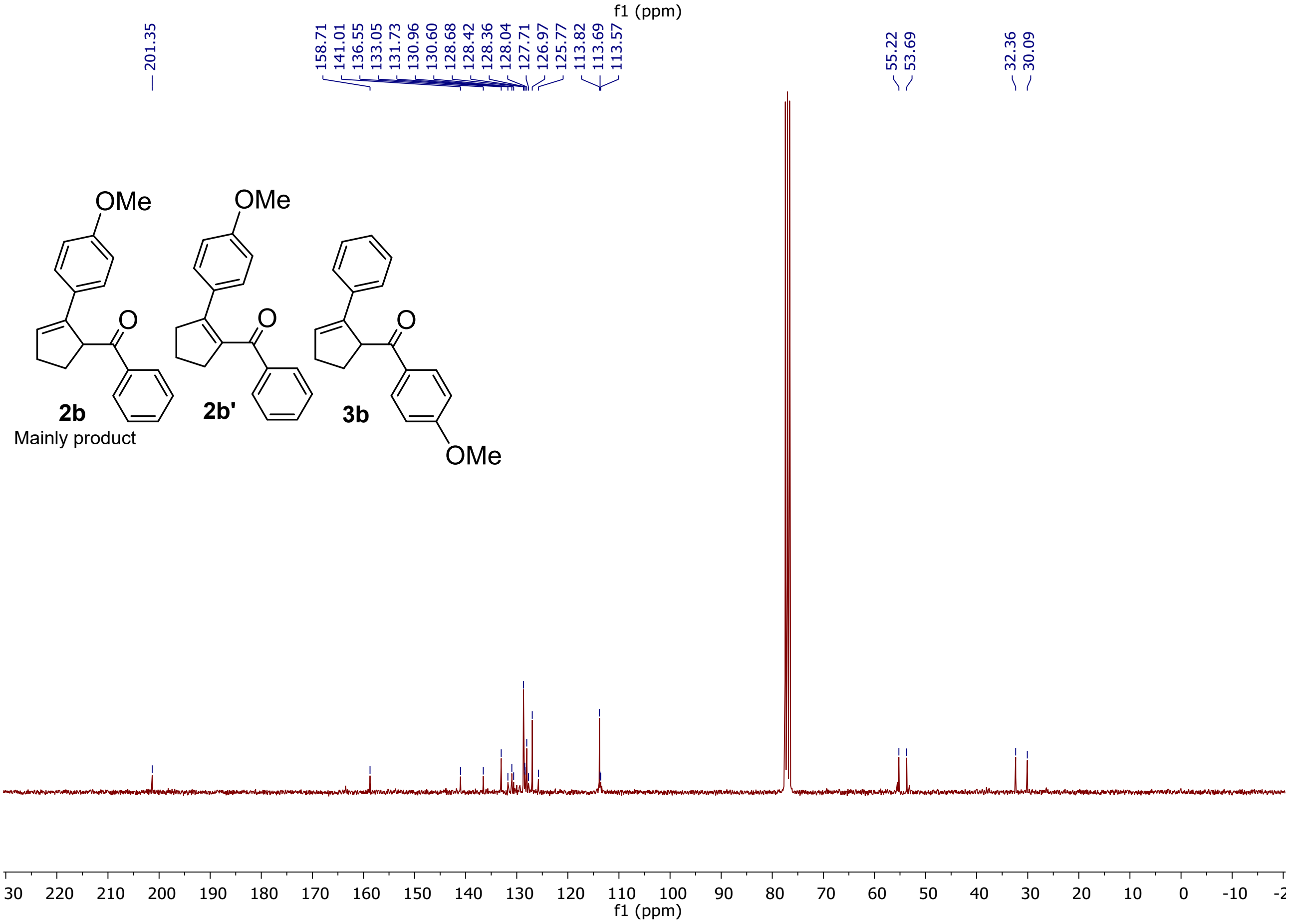


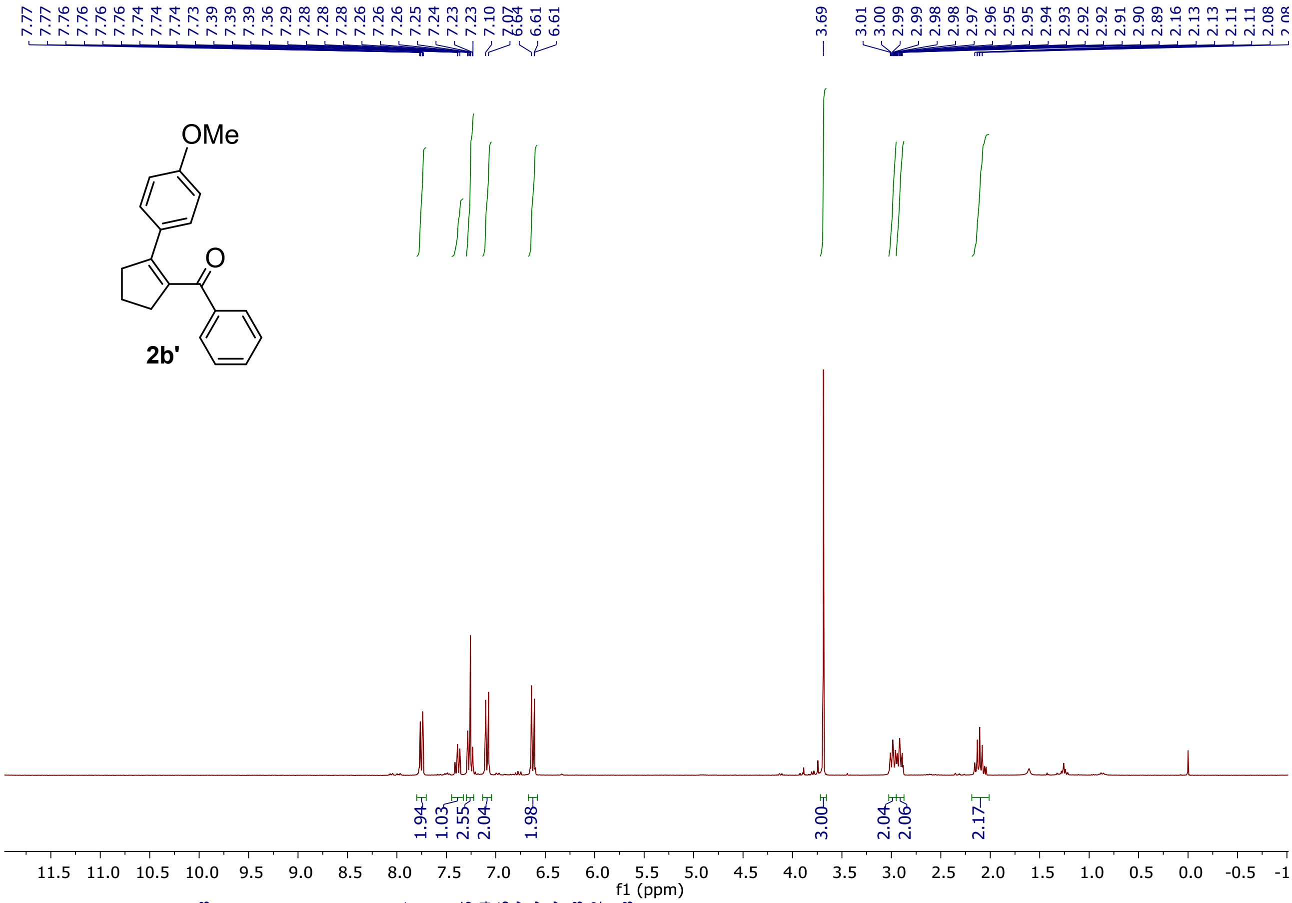
2a´
1.92
1.31
0.67
1.68
2.27
2.94
2.08
2.00
2.16
f1 (ppm)



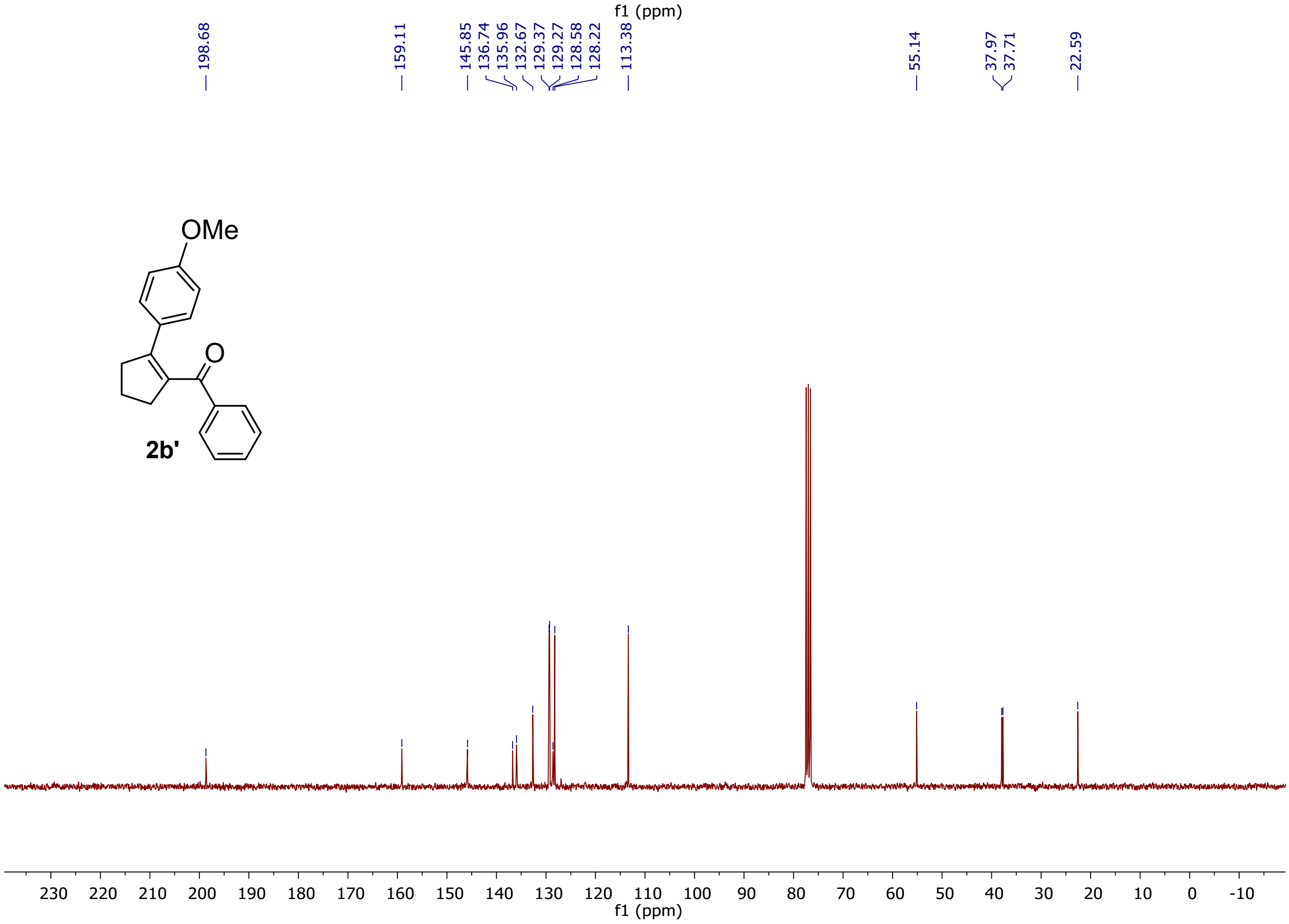
198.44
146.20
137.59
136.63
136.03
132.72
129.35
128.19
127.97
127.86
127.71
38.00
37.74
22.65
2a´
f1 (ppm)



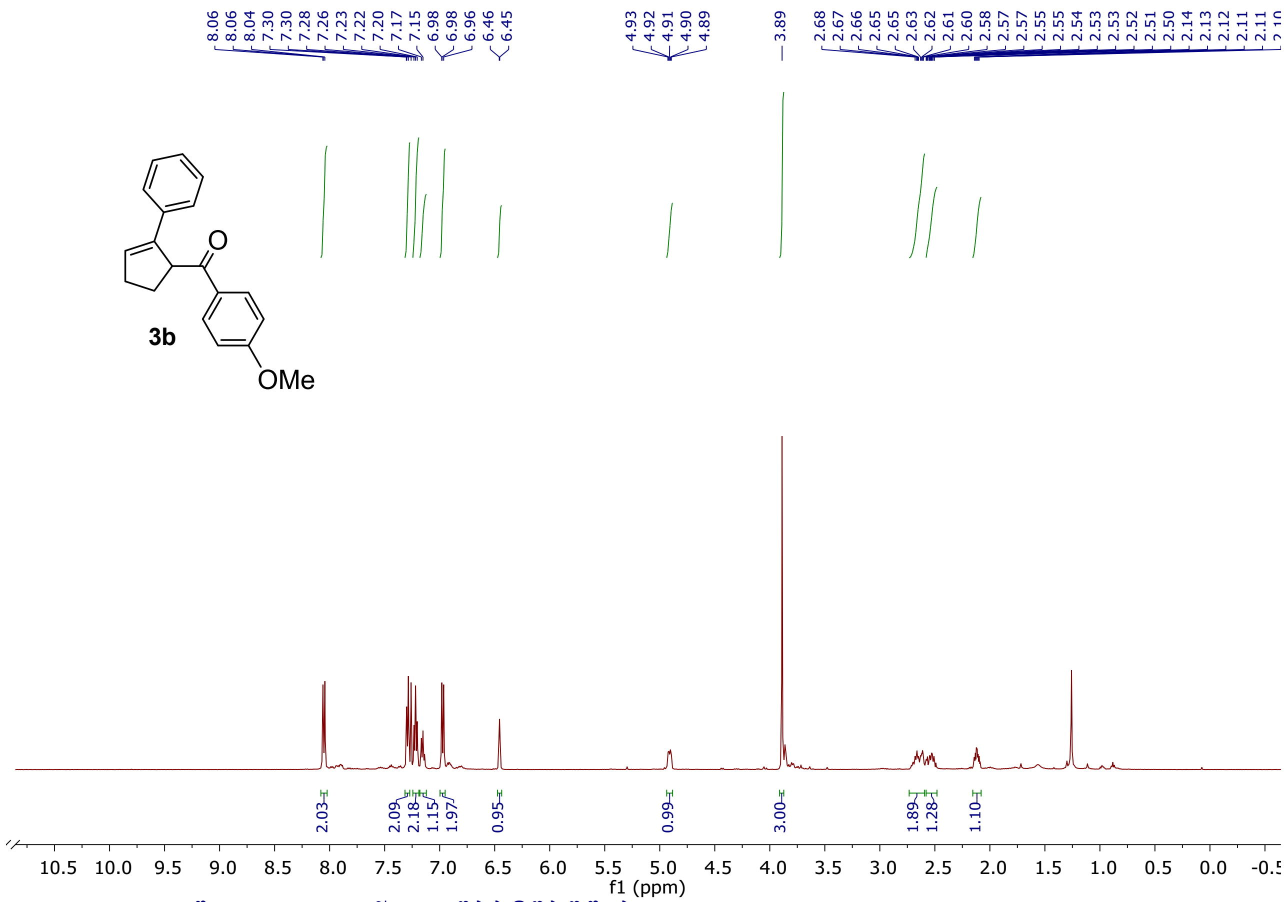


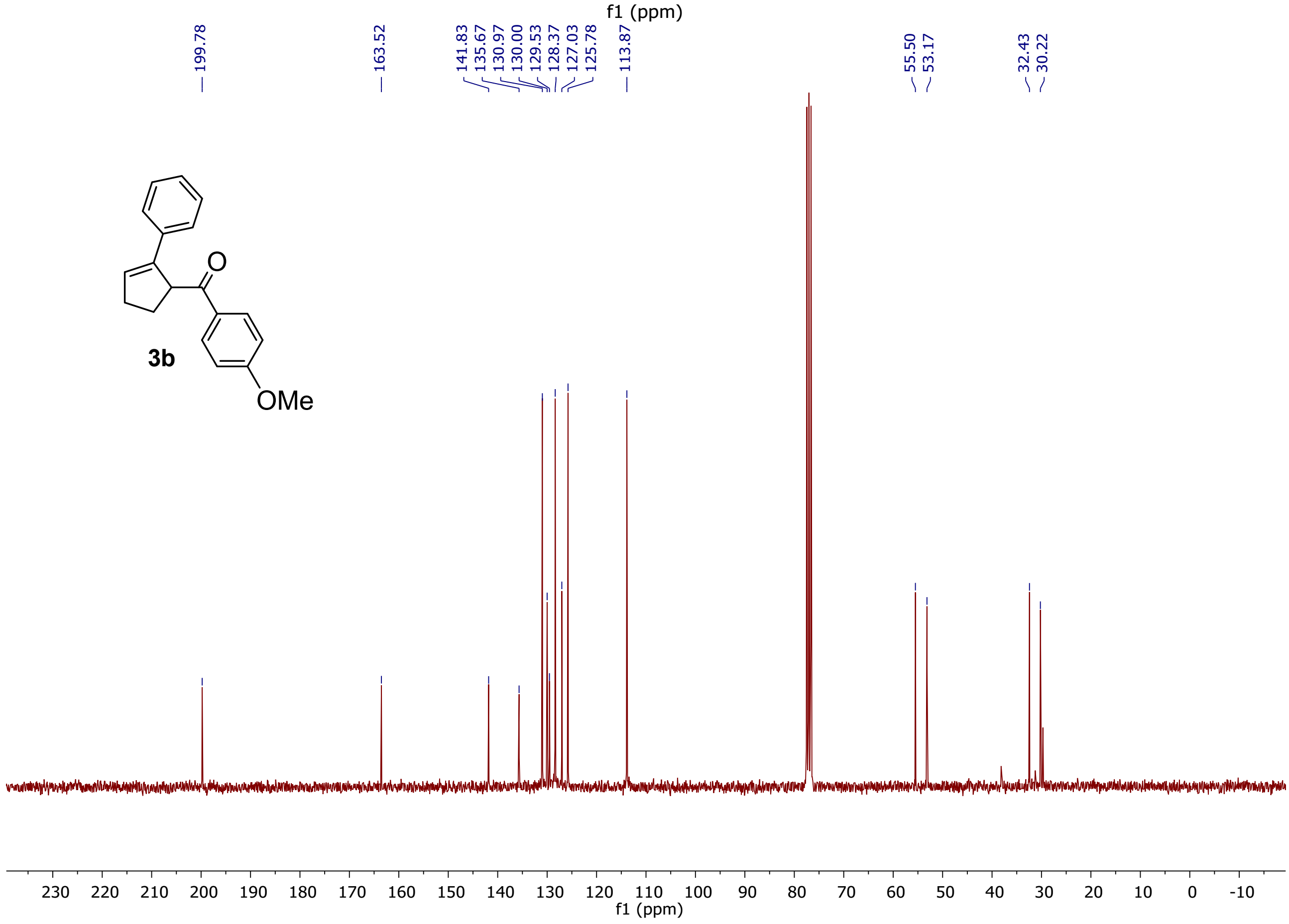


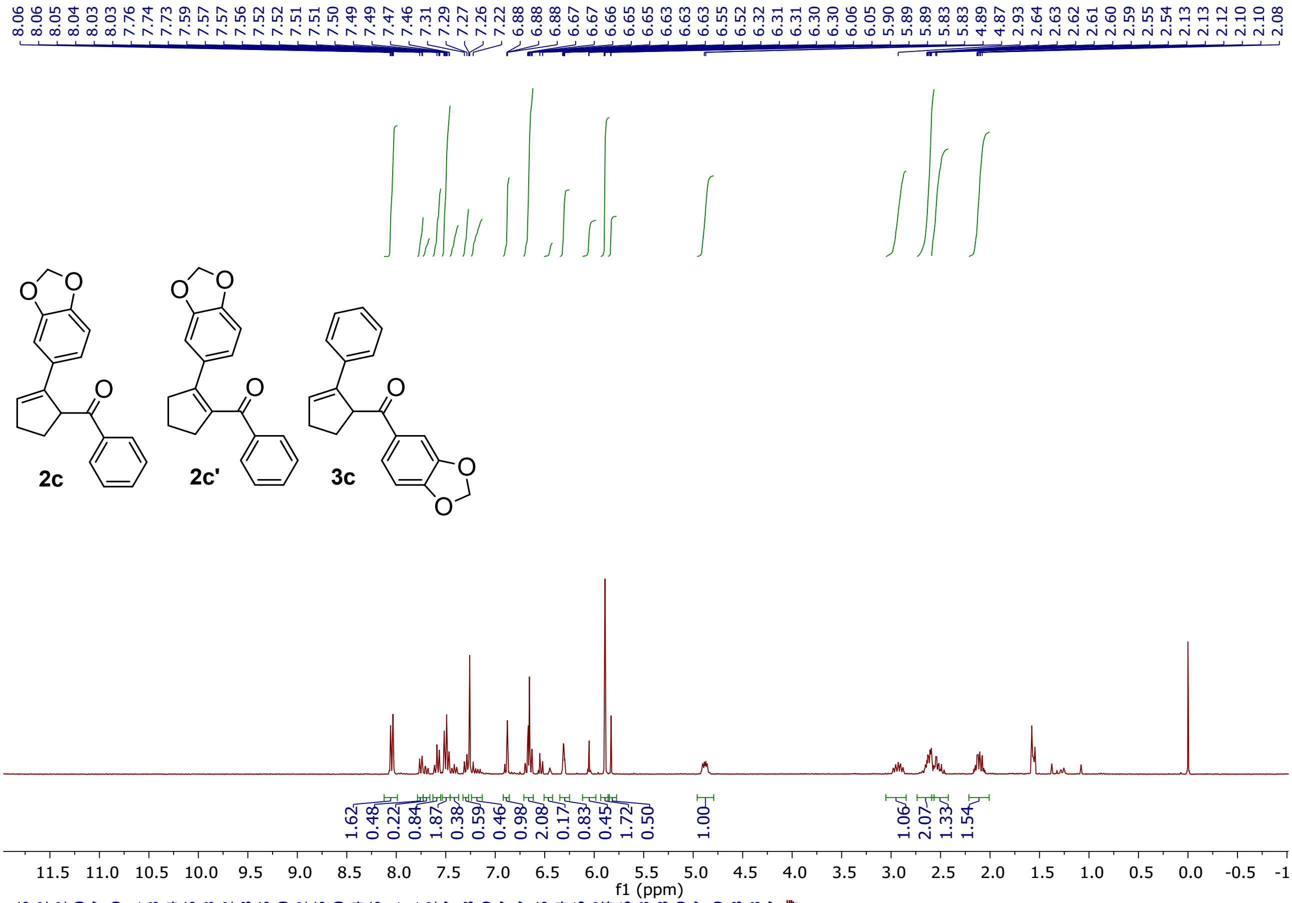
7.77 7.77 7.76 7.76 7.76 7.76 7.74 7.74 7.74 7.73 7.39 7.39 7.39 7.36 7.29 7.28 7.28 7.28 7.26 7.26 7.26 7.25 7.24 7.23 7.23 7.10 7.07 6.64 6.61 6.61
3.69
3.01 3.00 2.99 2.99 2.98 2.98 2.97 2.96 2.95 2.95 2.94 2.93 2.92 2.92 2.91 2.90 2.89 2.16 2.13 2.13 2.11 2.11 2.08
OMe
O
2b'
1.94 1.03 2.55 2.04 1.98 3.00 2.04 2.06 2.17
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

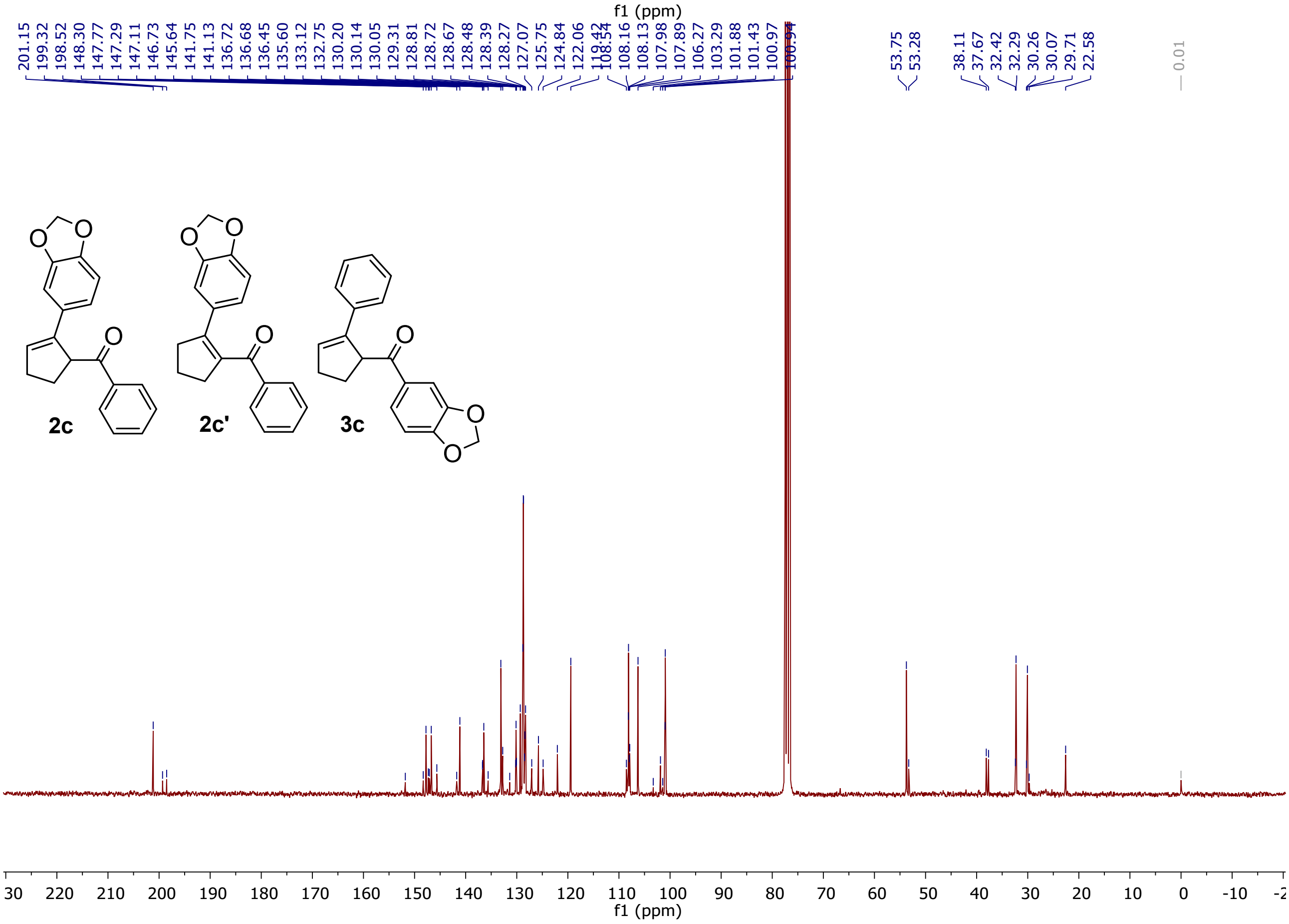


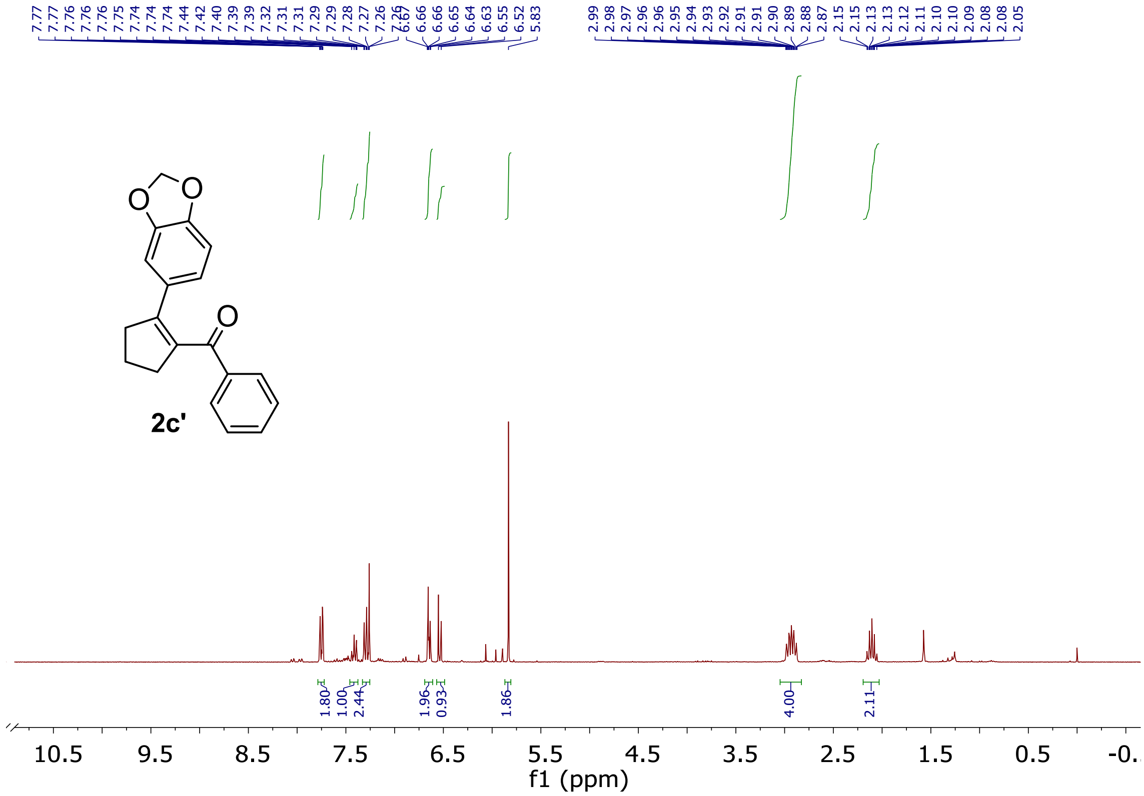
198.68
159.11
145.85 136.74 135.96 132.67 129.37 129.27 128.58 128.22
113.38
55.14
37.97 37.71
22.59
OMe
O
2b'
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

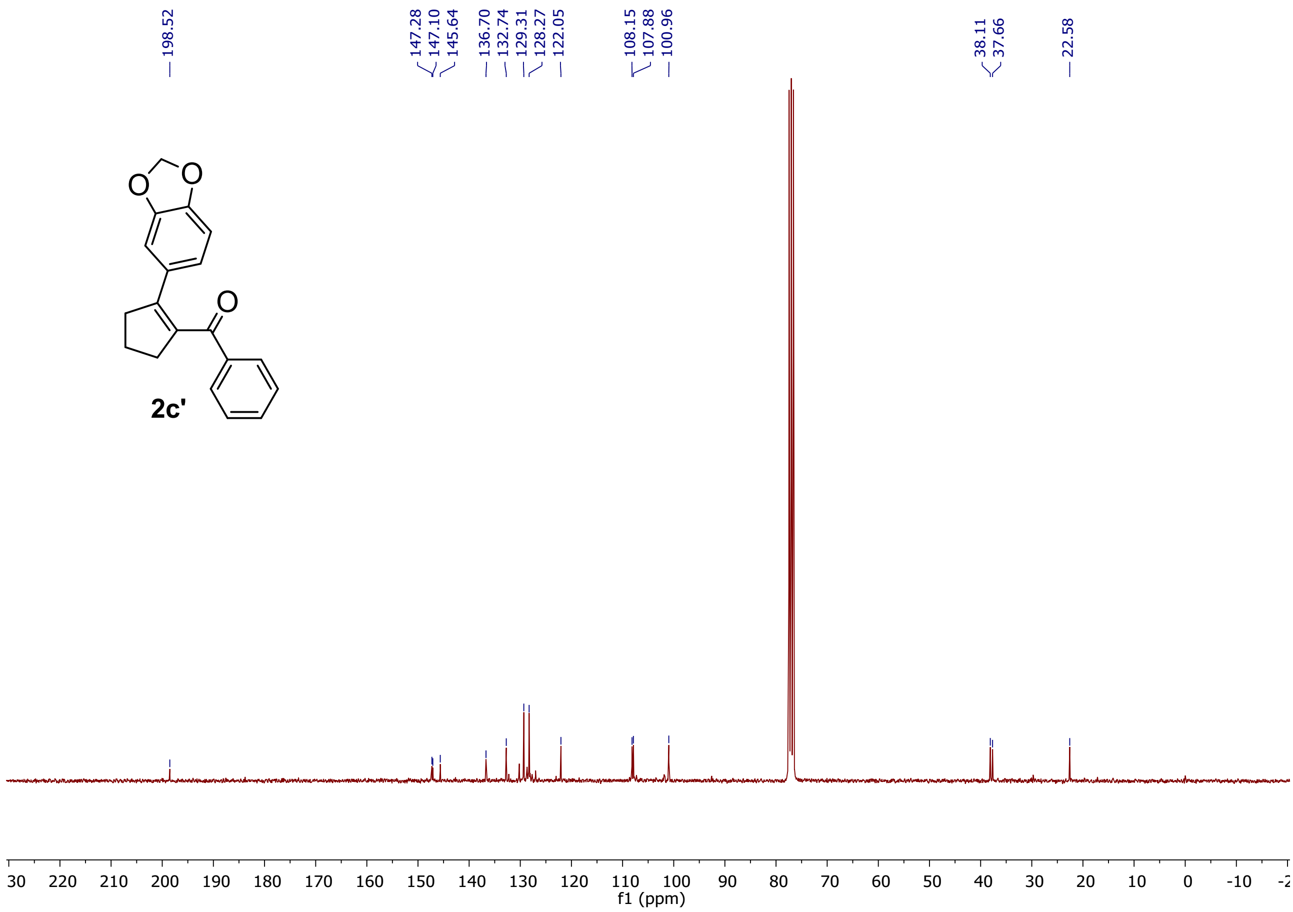

3b
OMe
f1 (ppm)


3b
OMe
f1 (ppm)


2c
2c'
3c
f1 (ppm)


2c
2c'
3c
f1 (ppm)


7.77
7.77
7.76
7.76
7.75
7.74
7.74
7.44
7.42
7.40
7.39
7.39
7.32
7.31
7.29
7.29
7.28
7.27
7.26
7.26
6.67
6.66
6.66
6.65
6.64
6.63
6.55
6.52
5.83
2.99
2.98
2.97
2.96
2.96
2.95
2.94
2.93
2.92
2.91
2.91
2.90
2.89
2.88
2.87
2.15
2.15
2.13
2.13
2.12
2.11
2.10
2.09
2.08
2.08
2.05
O
O
O
2c'
1.80
1.00
2.44
1.96
0.93
1.86
4.00
2.11
f1 (ppm)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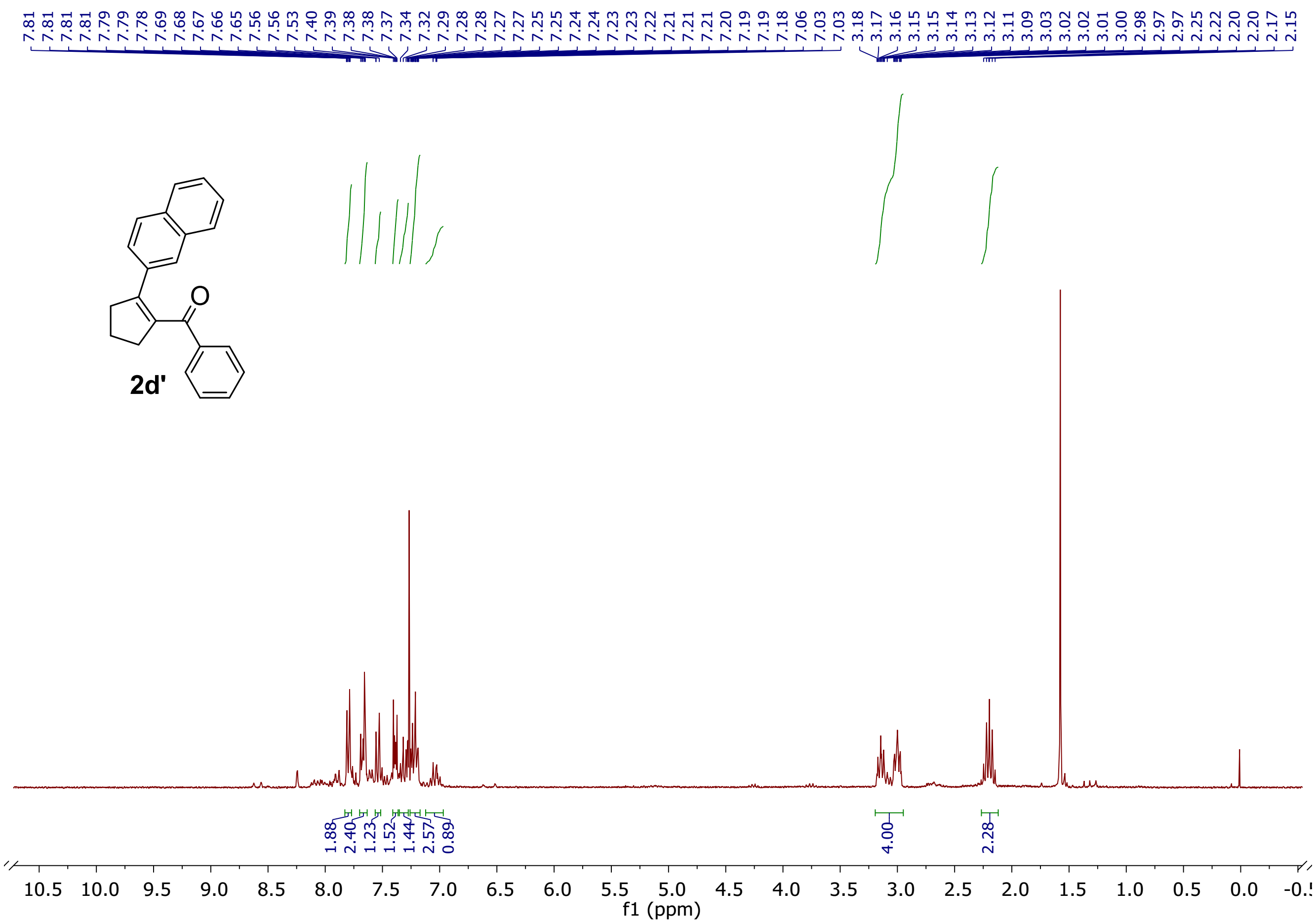
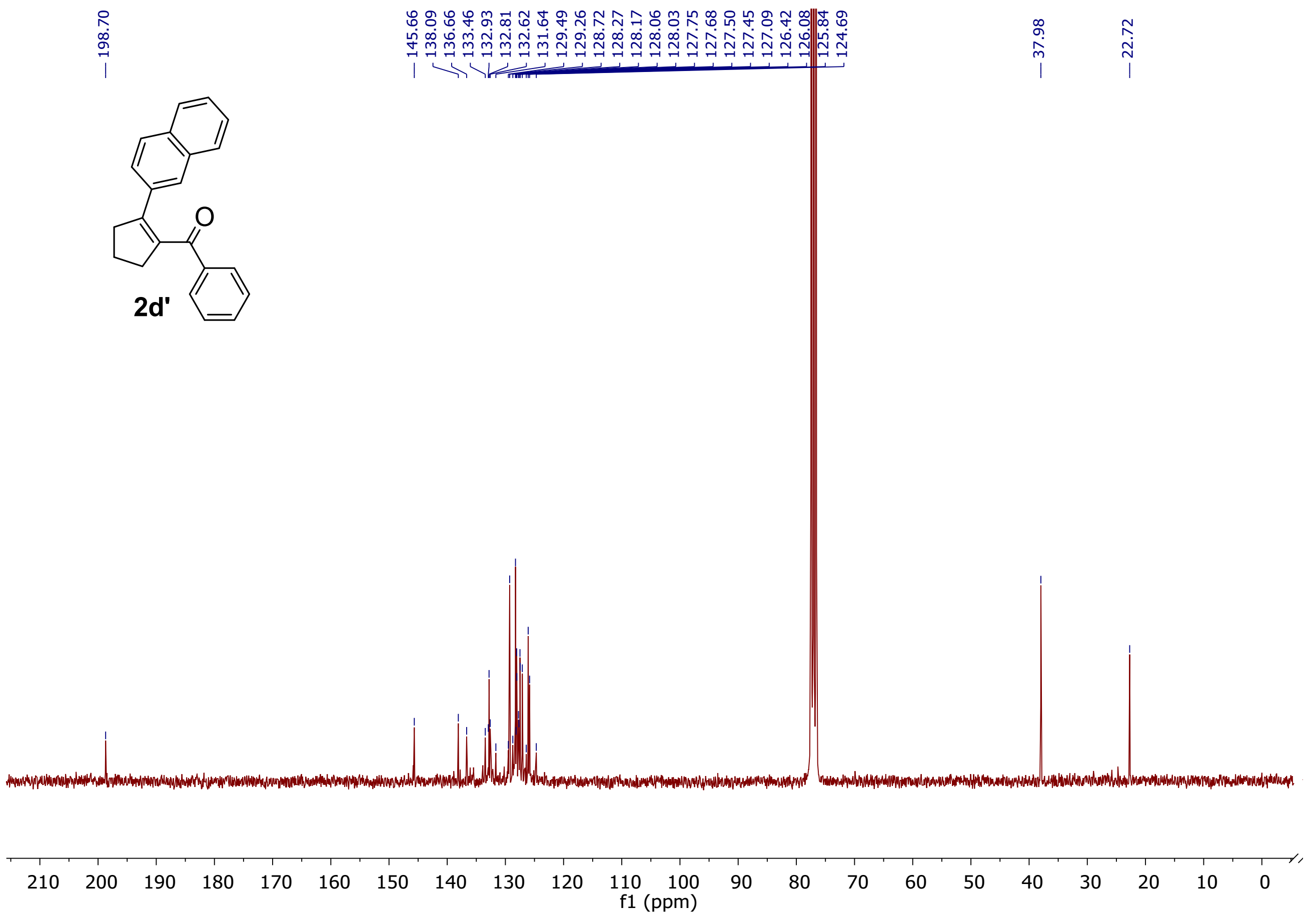
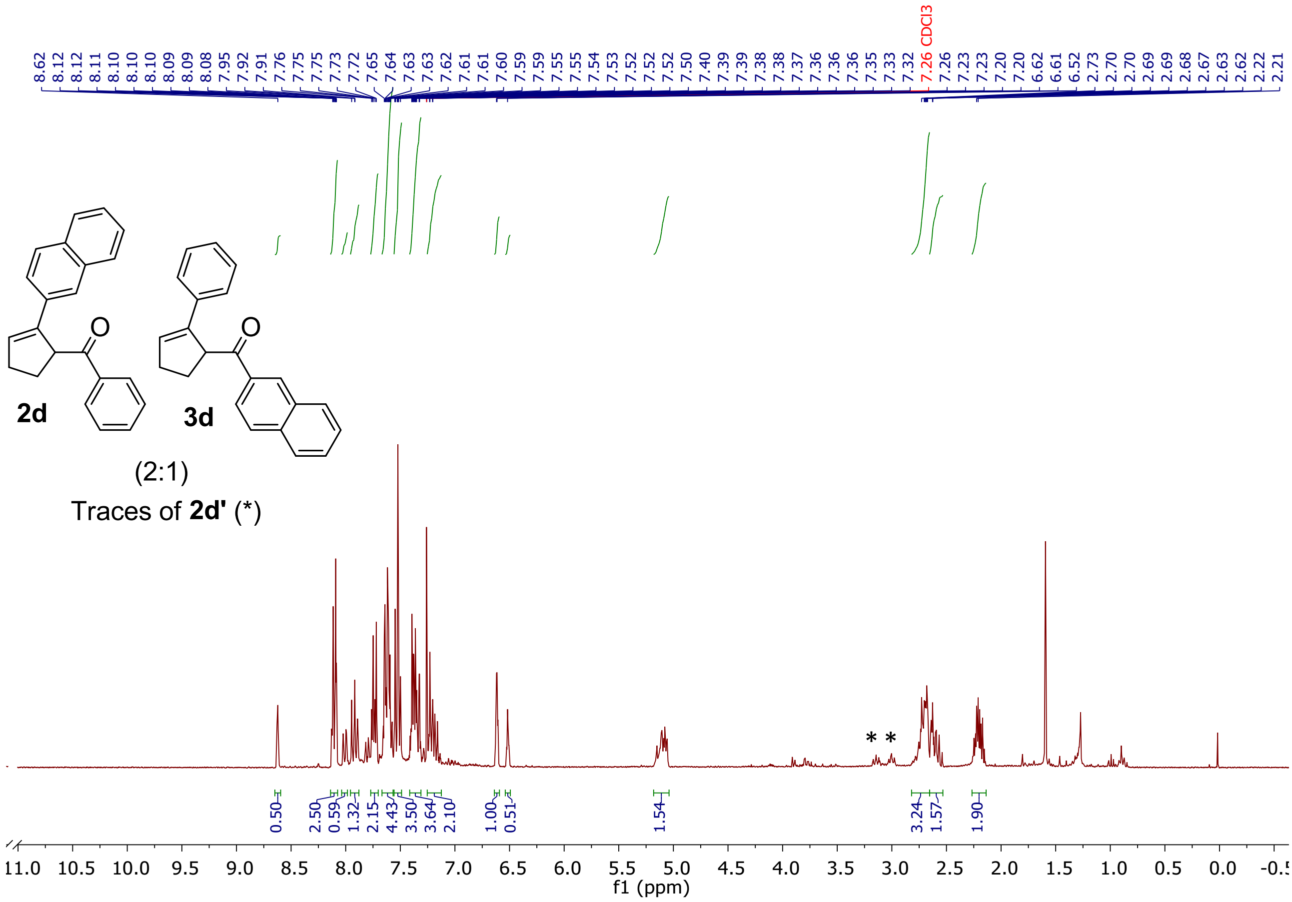
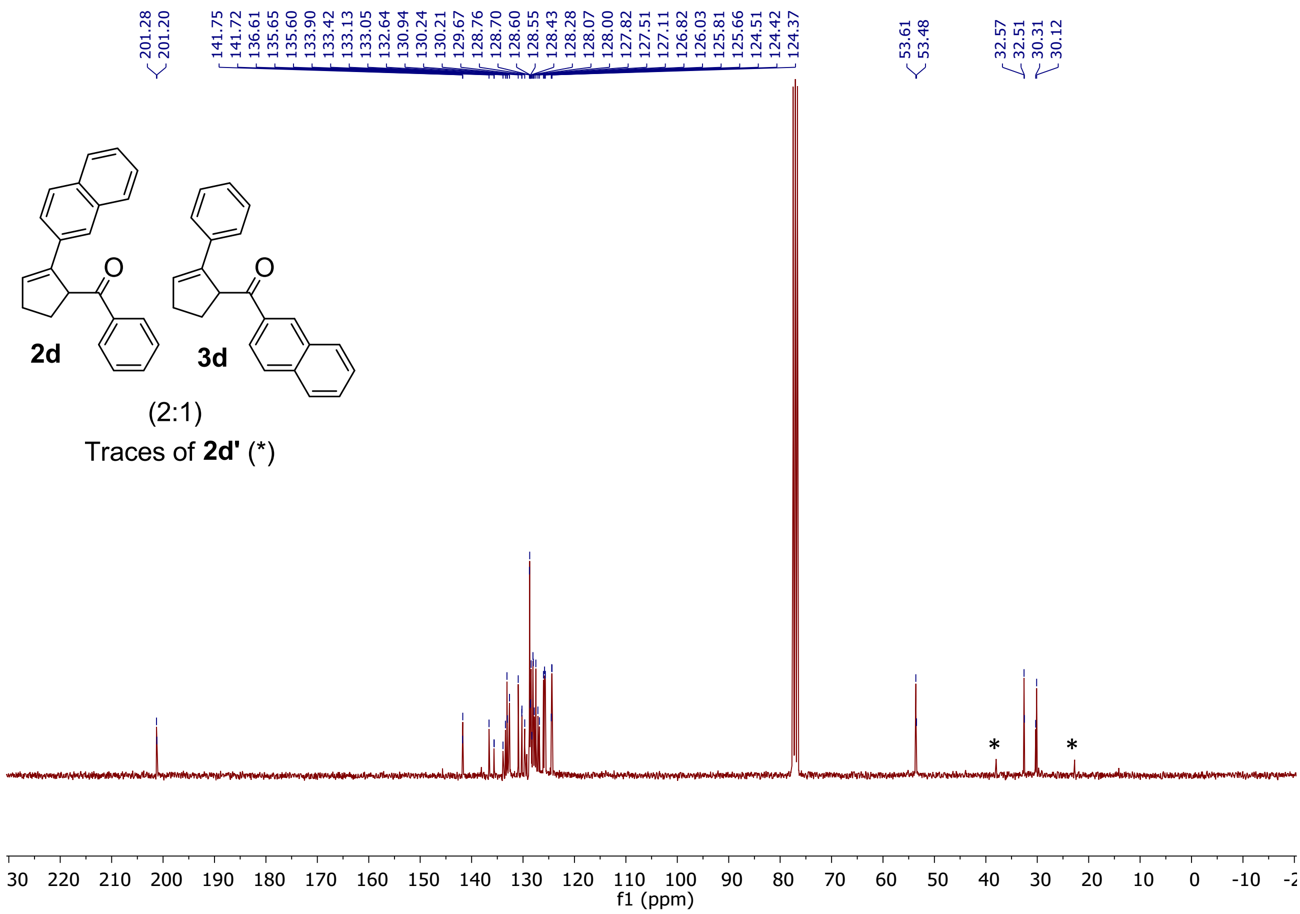
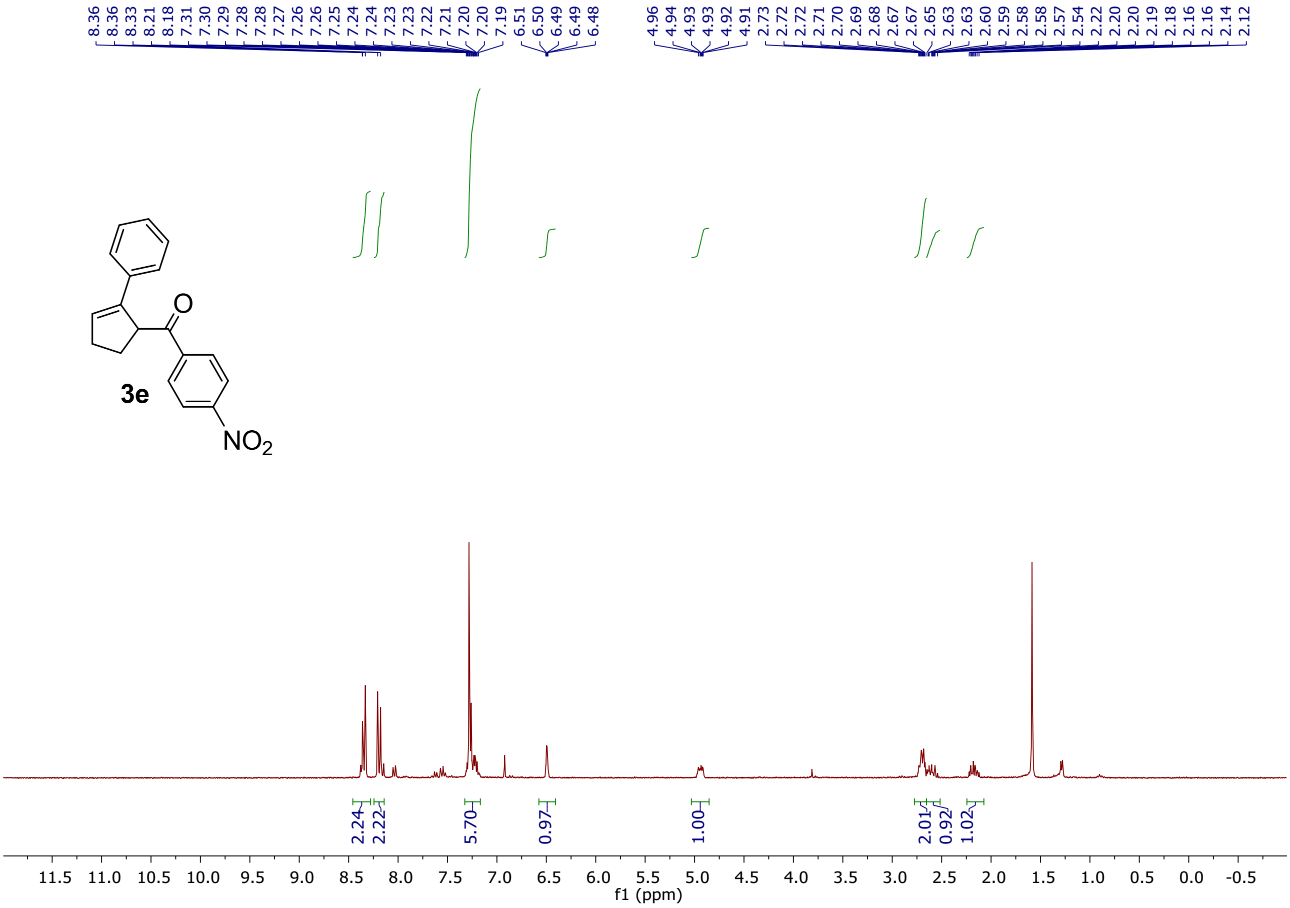
147.28
147.10
145.64
136.70
132.74
129.31
128.27
122.05
108.15
107.88
100.96
38.11
37.66
22.58
O
O
O
2c'
f1 (ppm)


7.81 7.81 7.81 7.81 7.79 7.79 7.78 7.69 7.68 7.67 7.66 7.65 7.56 7.56 7.53 7.40 7.39 7.38 7.38 7.37 7.34 7.32 7.29 7.28 7.28 7.27 7.27 7.25 7.25 7.24 7.24 7.23 7.23 7.22 7.21 7.21 7.21 7.20 7.19 7.19 7.18 7.06 7.03 7.03 3.18 3.17 3.16 3.15 3.14 3.13 3.12 3.11 3.09 3.03 3.02 3.02 3.01 3.00 2.98 2.97 2.25 2.22 2.20 2.20 2.17 2.15
2d'
1.88 2.40 1.23 1.52 1.44 2.57 0.89 4.00 2.28
f1 (ppm)


198.70
145.66 138.09 136.66 133.46 132.93 132.81 132.62 131.64 129.49 129.26 128.72 128.27 128.17 128.06 128.03 127.75 127.68 127.50 127.45 127.09 126.42 126.08 125.84 124.69
37.98
22.72
2d'
f1 (ppm)

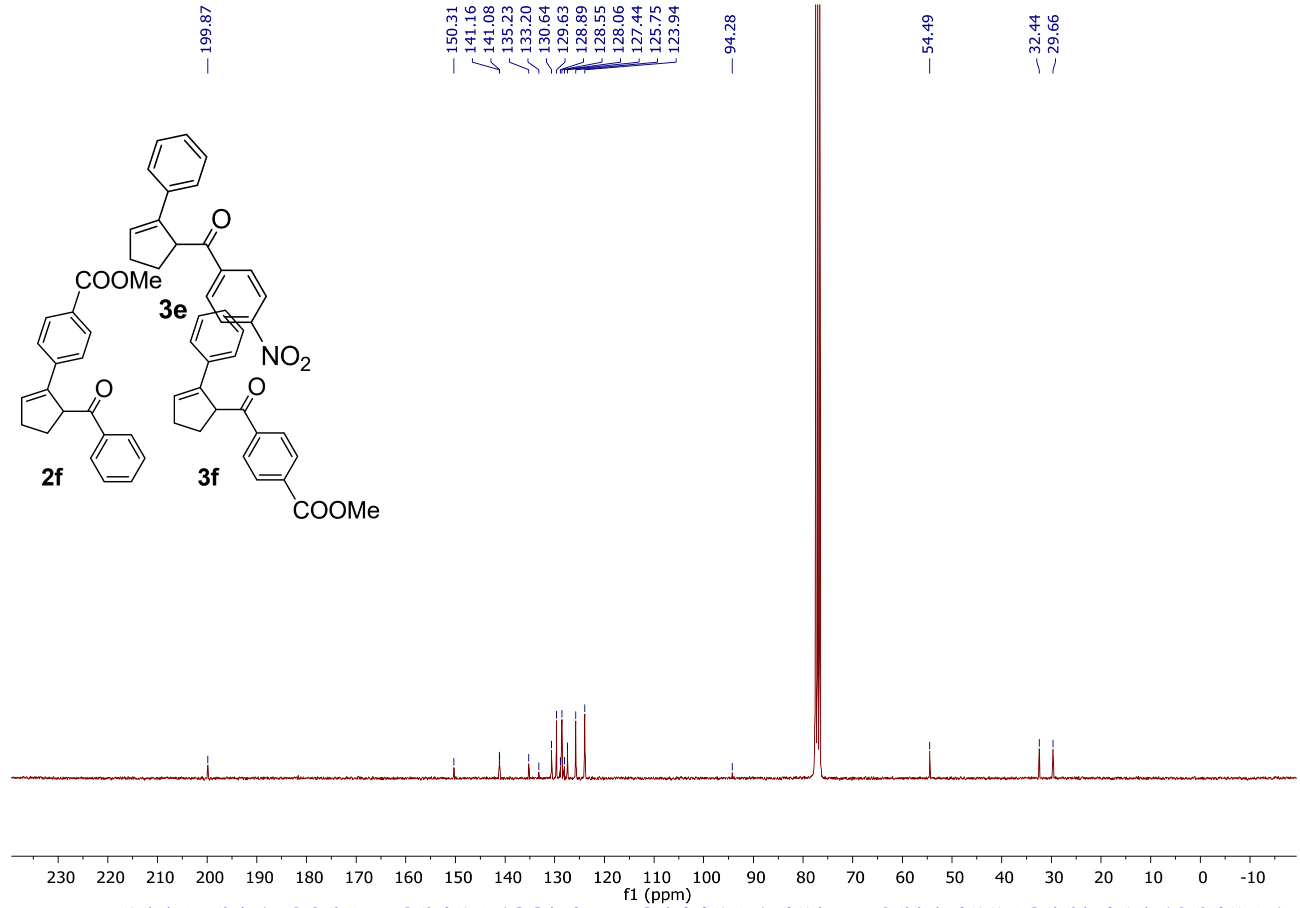

8.62 8.12 8.12 8.11 8.10 8.10 8.10 8.09 8.09 8.08 7.95 7.92 7.91 7.76 7.75 7.75 7.73 7.72 7.65 7.64 7.63 7.63 7.62 7.61 7.61 7.60 7.59 7.59 7.55 7.55 7.54 7.53 7.52 7.52 7.50 7.40 7.39 7.39 7.38 7.38 7.37 7.36 7.36 7.35 7.33 7.32 7.26 CDCl3 7.26 7.23 7.23 7.20 7.20 6.62 6.61 6.52 2.73 2.70 2.70 2.69 2.69 2.68 2.67 2.63 2.62 2.22 2.21
2d
3d
(2:1)
Traces of 2d' (*)
* *
0.50 2.50 0.59 1.32 2.15 4.43 3.50 3.64 2.10 1.00 0.51 1.54 3.24 1.57 1.90
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


201.28 201.20
141.75 141.72 136.61 135.65 135.60 133.90 133.42 133.13 133.05 132.64 130.94 130.24 130.21 129.67 128.76 128.70 128.60 128.55 128.43 128.28 128.07 128.00 127.82 127.51 127.11 126.82 126.03 125.81 125.66 124.51 124.42 124.37
53.61 53.48
32.57 32.51 30.31 30.12
2d
3d
(2:1)
Traces of 2d' (*)
* *
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)



8.36
8.36
8.33
8.21
8.18
7.31
7.30
7.29
7.28
7.28
7.27
7.26
7.26
7.25
7.24
7.24
7.23
7.23
7.22
7.21
7.20
7.20
7.19
6.51
6.50
6.49
6.49
6.48
4.96
4.94
4.93
4.93
4.92
4.91
2.73
2.72
2.72
2.71
2.70
2.69
2.68
2.67
2.67
2.65
2.63
2.63
2.60
2.59
2.58
2.58
2.57
2.54
2.22
2.20
2.20
2.19
2.18
2.16
2.16
2.14
2.12
2.24
2.22
5.70
0.97
1.00
2.01
0.92
1.02
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

3e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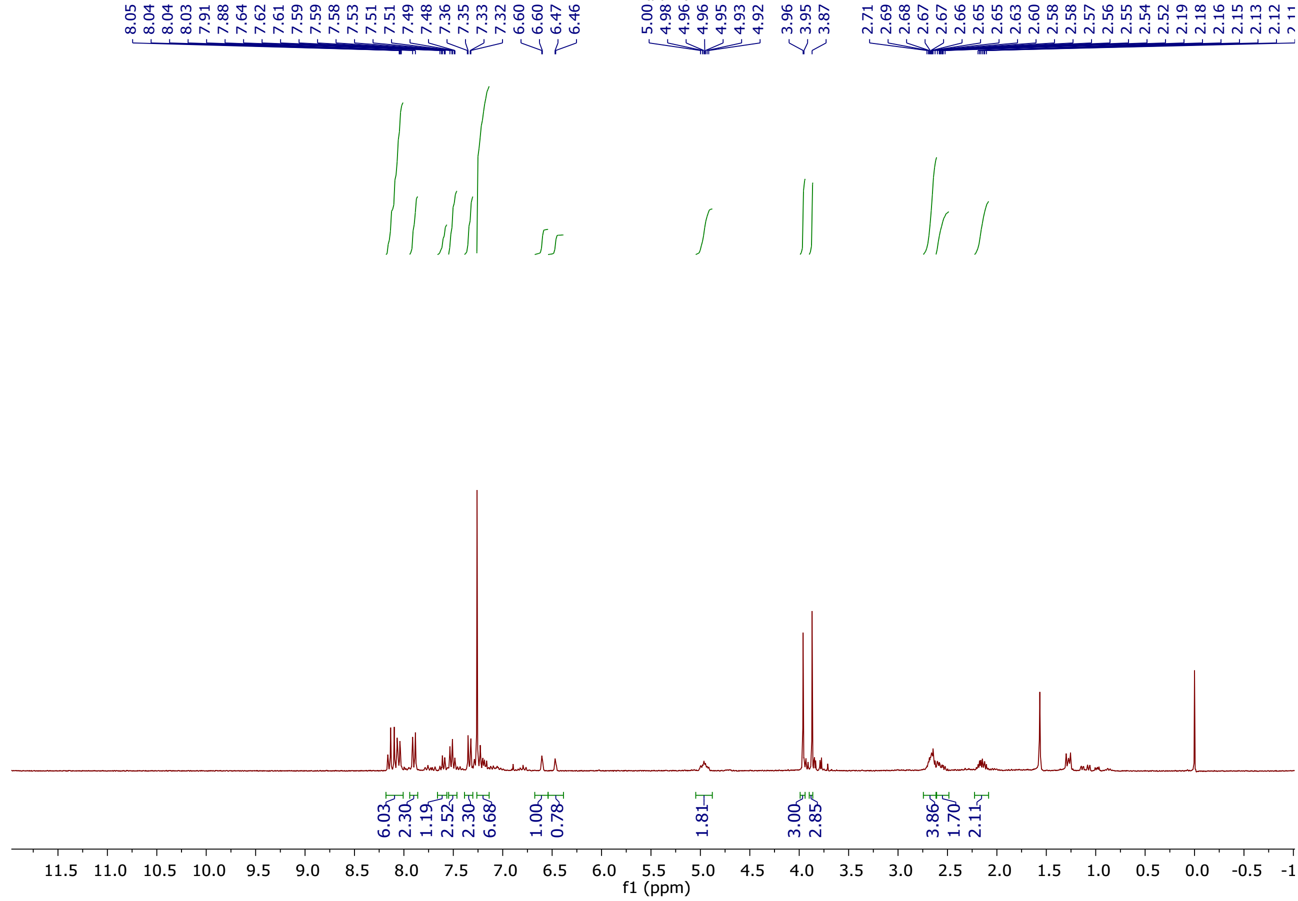
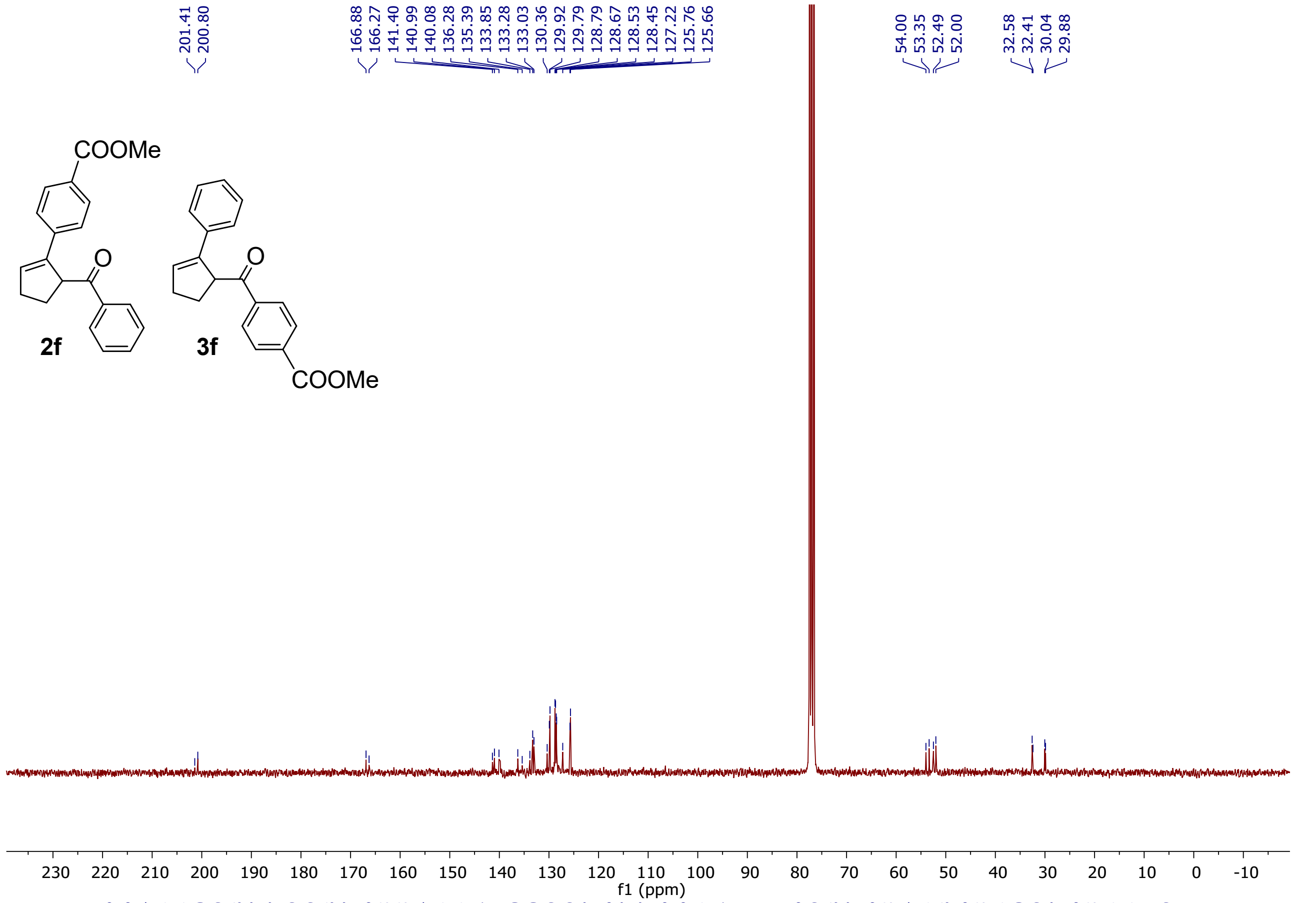
150.31
141.16
141.08
135.23
133.20
130.64
129.63
128.89
128.55
128.06
127.44
125.75
123.94
94.28
54.49
32.44
29.66
COOMe
3e
NO2
O
O
O
2f
3f
COOMe
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.05
8.04
8.04
8.03
7.91
7.88
7.64
7.62
7.61
7.59
7.59
7.58
7.53
7.51
7.51
7.49
7.48
7.36
7.35
7.33
7.32
6.60
6.60
6.47
6.46
5.00
4.98
4.96
4.96
4.95
4.93
4.92
3.96
3.95
3.87
2.71
2.69
2.68
2.67
2.67
2.66
2.65
2.65
2.63
2.60
2.58
2.58
2.57
2.56
2.55
2.54
2.52
2.19
2.18
2.16
2.15
2.13
2.12
6.03
2.30
1.19
2.52
2.30
6.68
1.00
0.78
1.81
3.00
2.85
3.86
1.70
2.11
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)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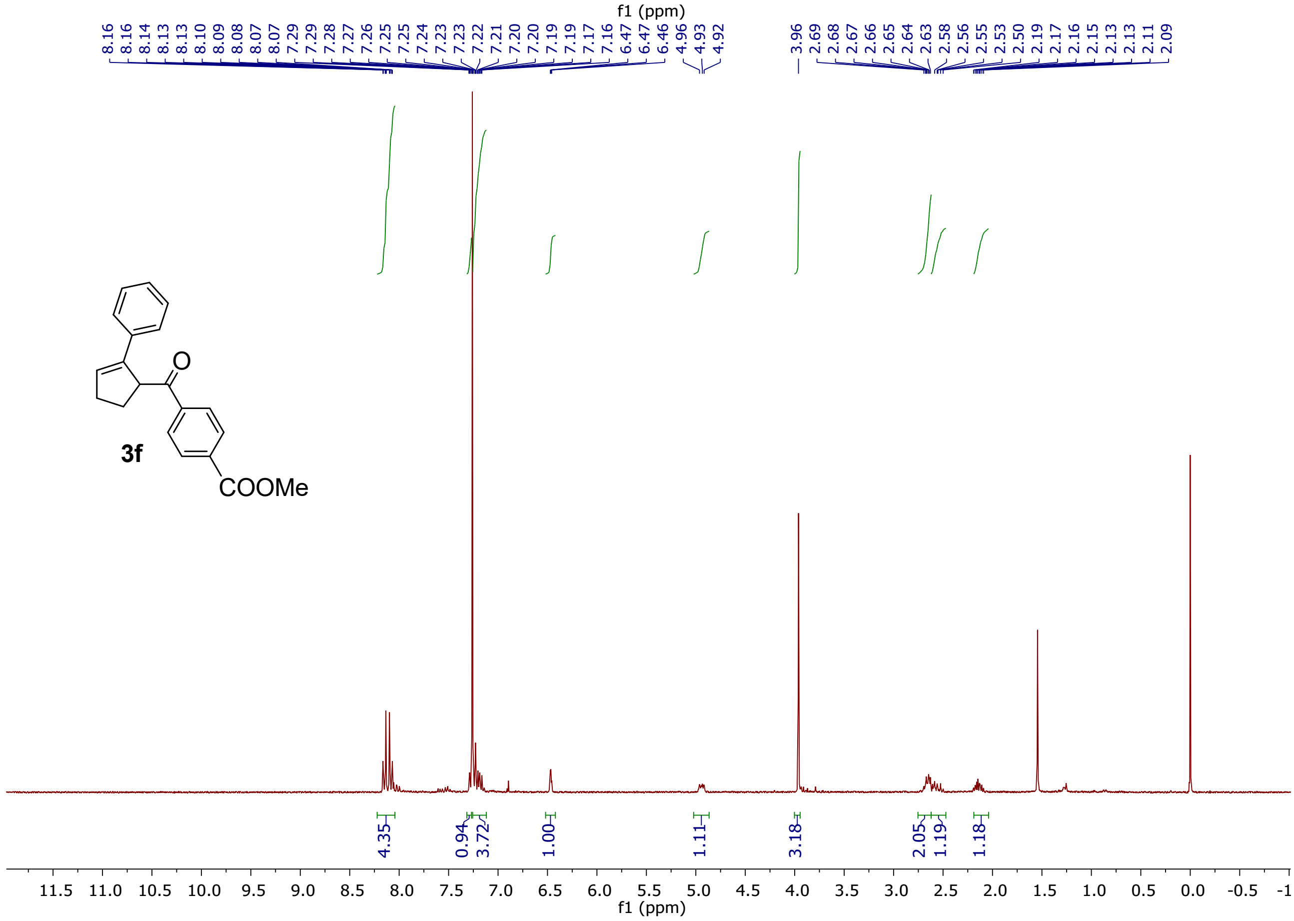
200.80
166.88
166.27
141.40
140.99
140.08
136.28
135.39
133.85
133.28
133.03
130.36
129.92
129.79
128.79
128.67
128.53
128.45
127.22
125.76
125.66
54.00
53.35
52.49
52.00
32.58
32.41
30.04
29.88
COOMe
2f
3f
COOMe
f1 (ppm)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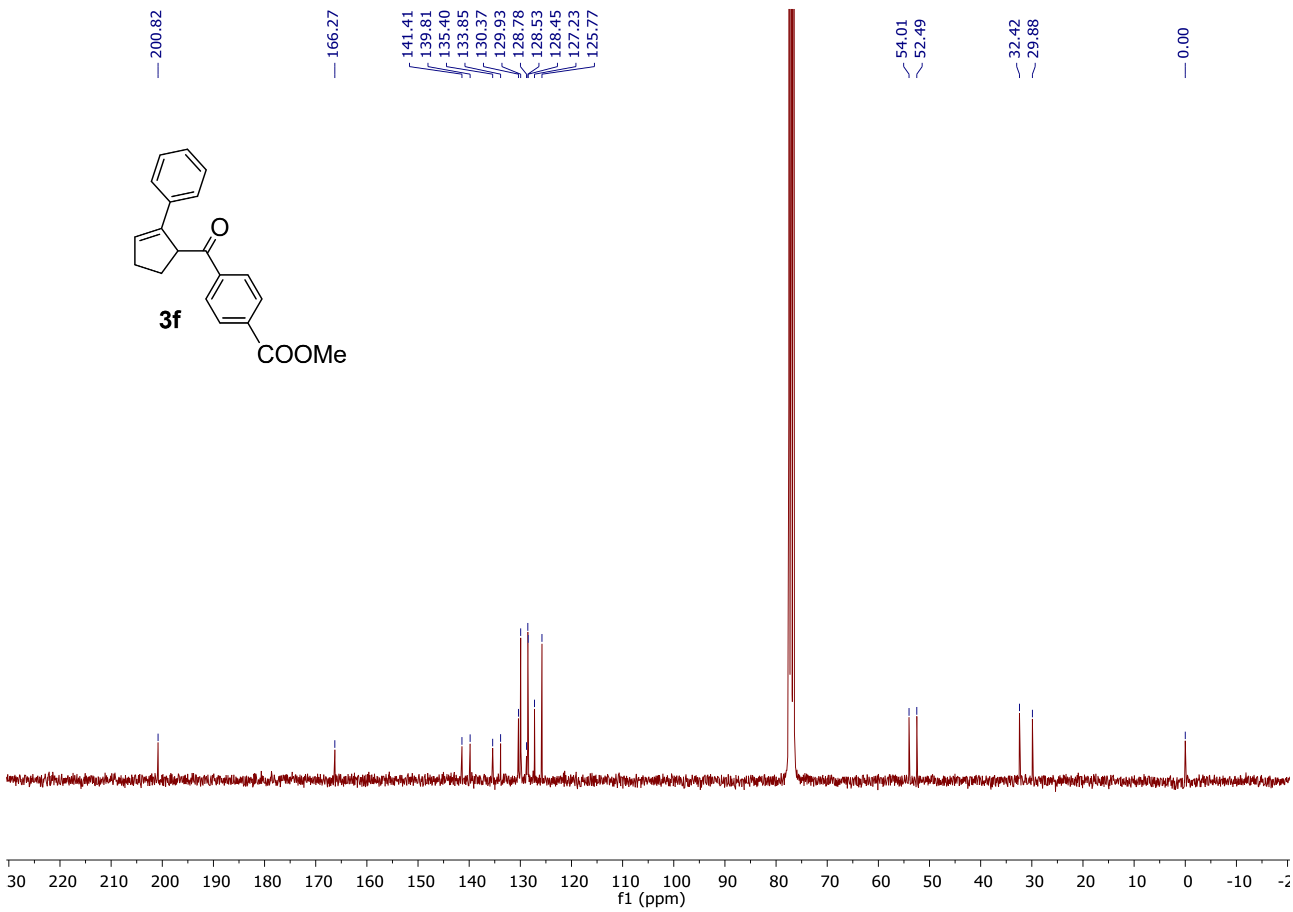
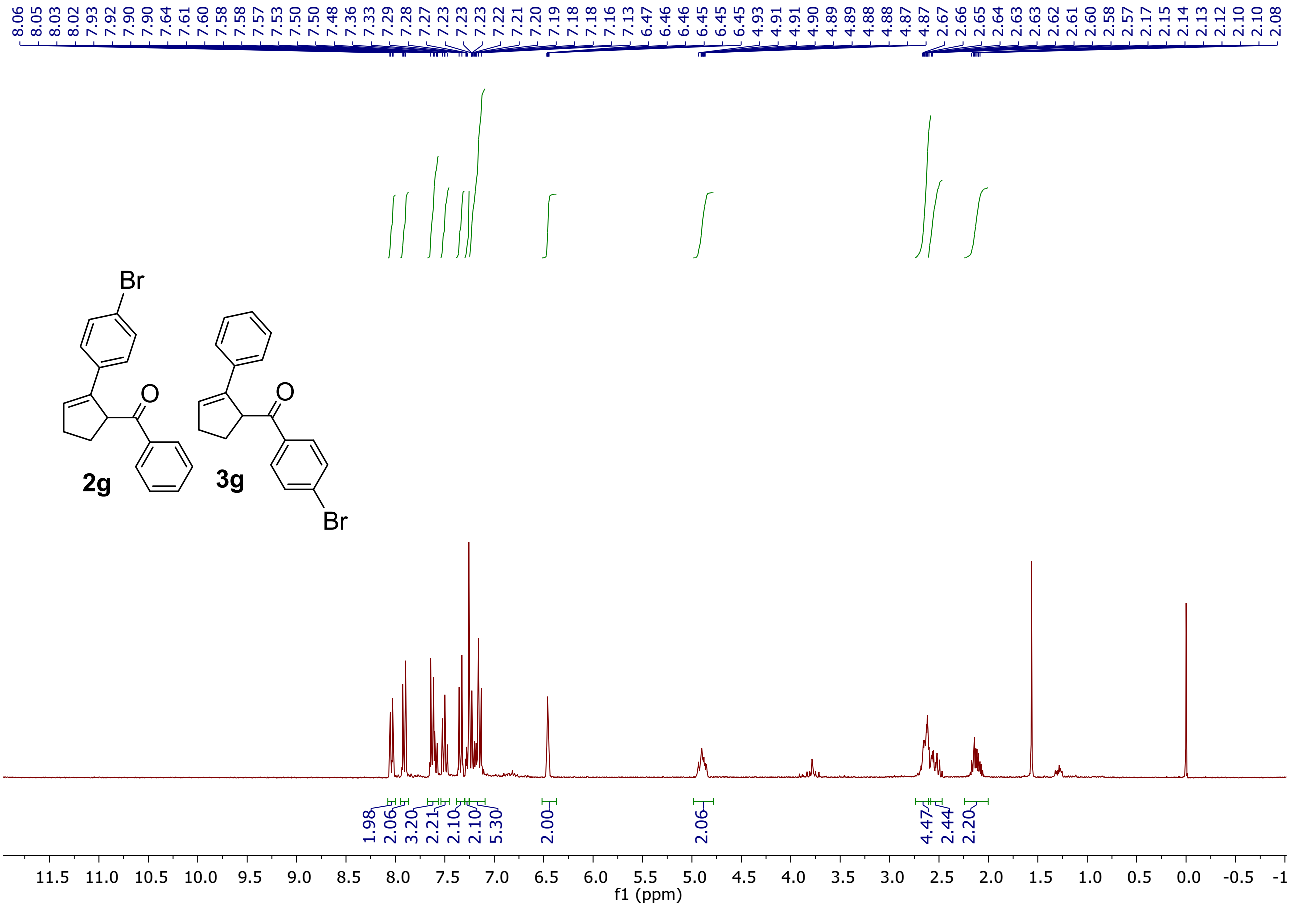
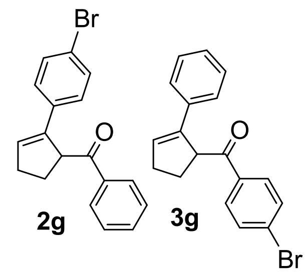
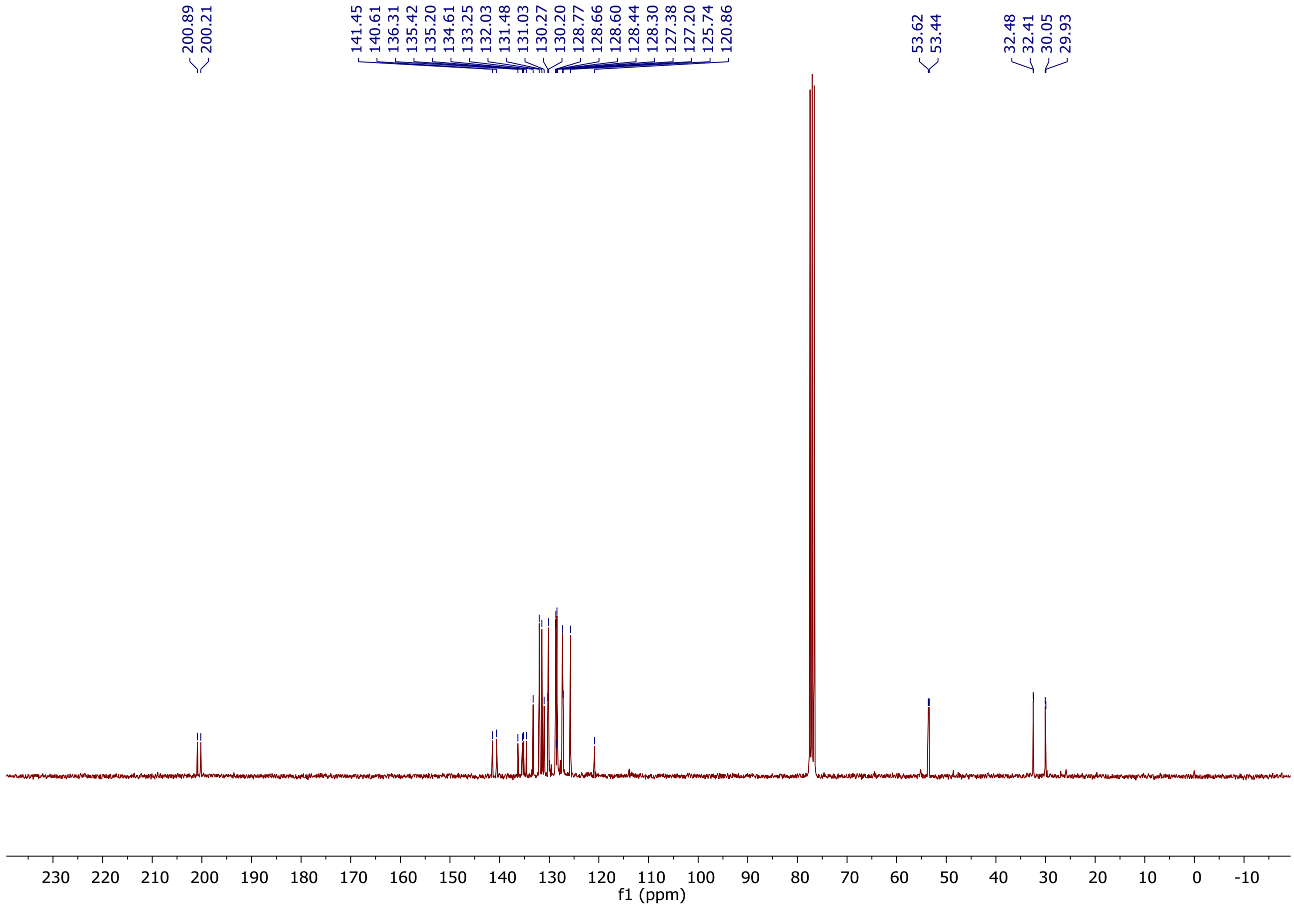
8.16
8.14
8.13
8.13
8.10
8.09
8.08
8.07
8.07
7.29
7.28
7.27
7.26
7.25
7.25
7.24
7.23
7.23
7.22
7.21
7.20
7.20
7.19
7.19
7.17
7.16
6.47
6.47
6.46
4.96
4.93
4.92
3.96
2.69
2.68
2.67
2.66
2.65
2.64
2.63
2.58
2.56
2.55
2.53
2.50
2.19
2.17
2.16
2.15
2.13
2.13
2.11
2.09
3f
COOMe
4.35
0.94
3.72
1.00
1.11
3.18
2.05
1.19
1.18
f1 (ppm)



200.82
166.27
141.41
139.81
135.40
133.85
130.37
129.93
128.78
128.53
128.45
127.23
125.77
54.01
52.49
32.42
29.88
0.00
O
3f
COOMe
230
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)


2g
3g
f1 (ppm)


2g
3g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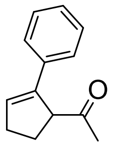
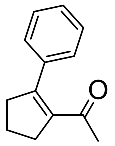
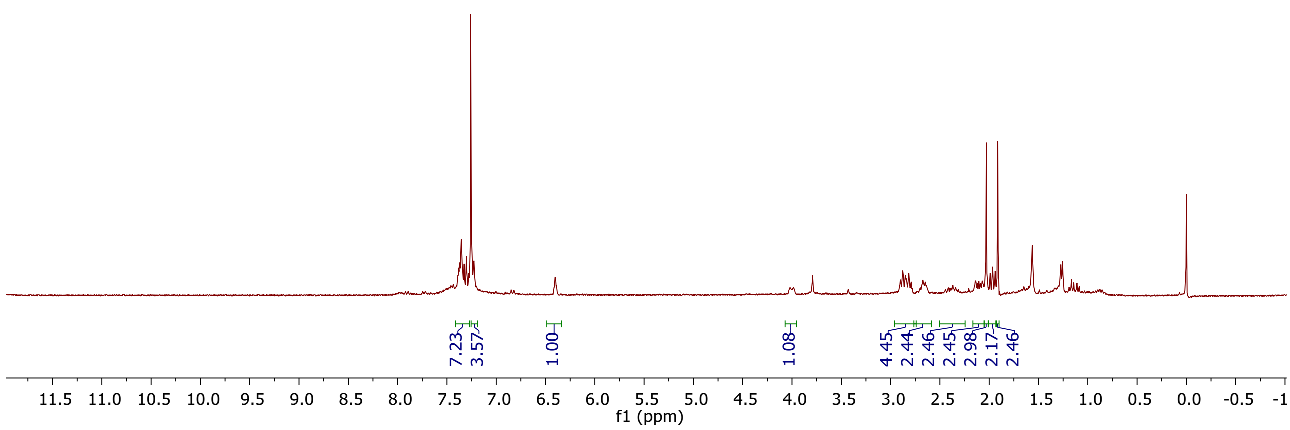
200.21
141.45
140.61
136.31
135.42
135.20
134.61
133.25
132.03
131.48
131.03
130.27
130.20
128.77
128.66
128.60
128.44
128.30
127.38
127.20
125.74
120.86
53.62
53.44
32.48
32.41
30.05
29.93
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

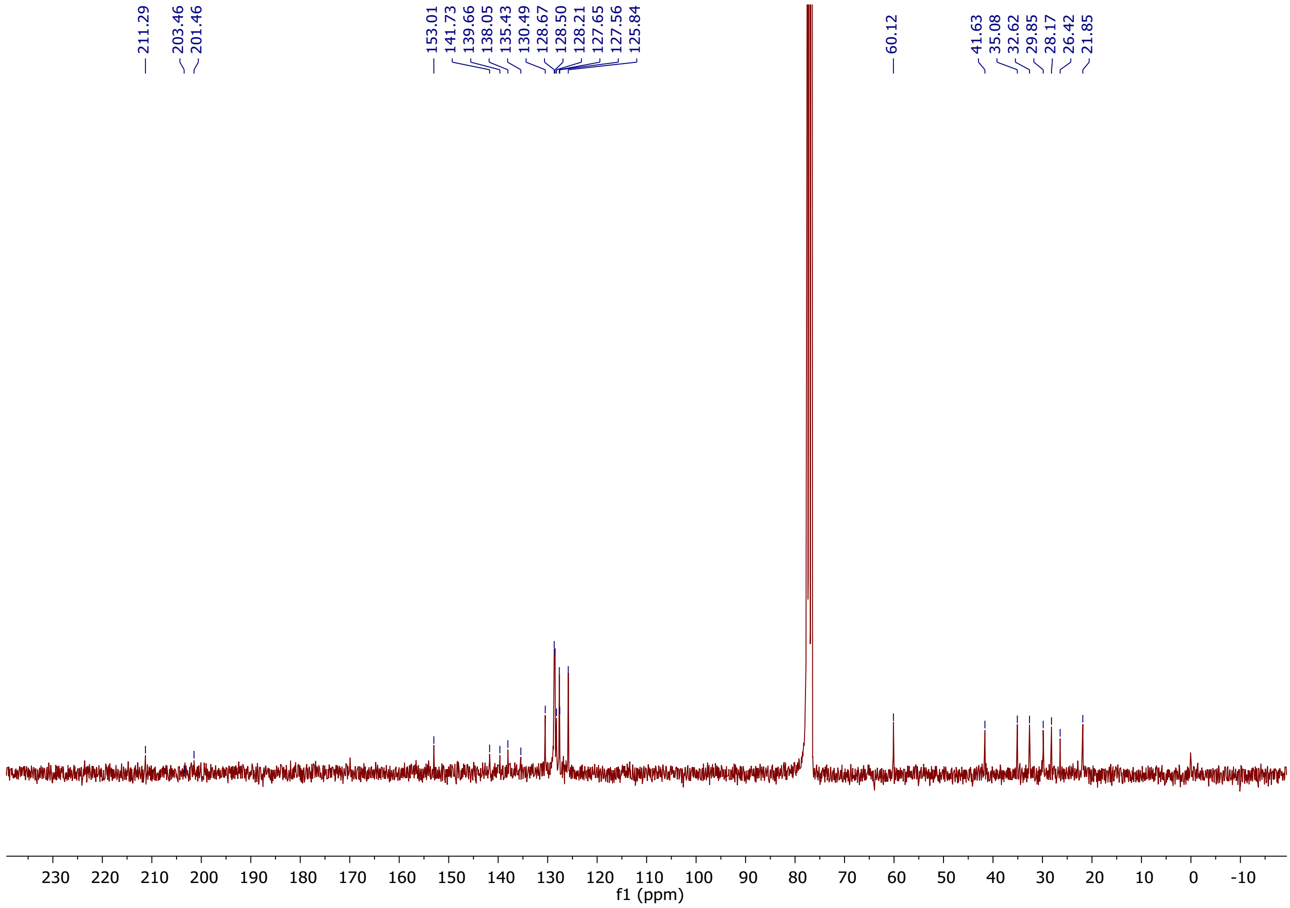


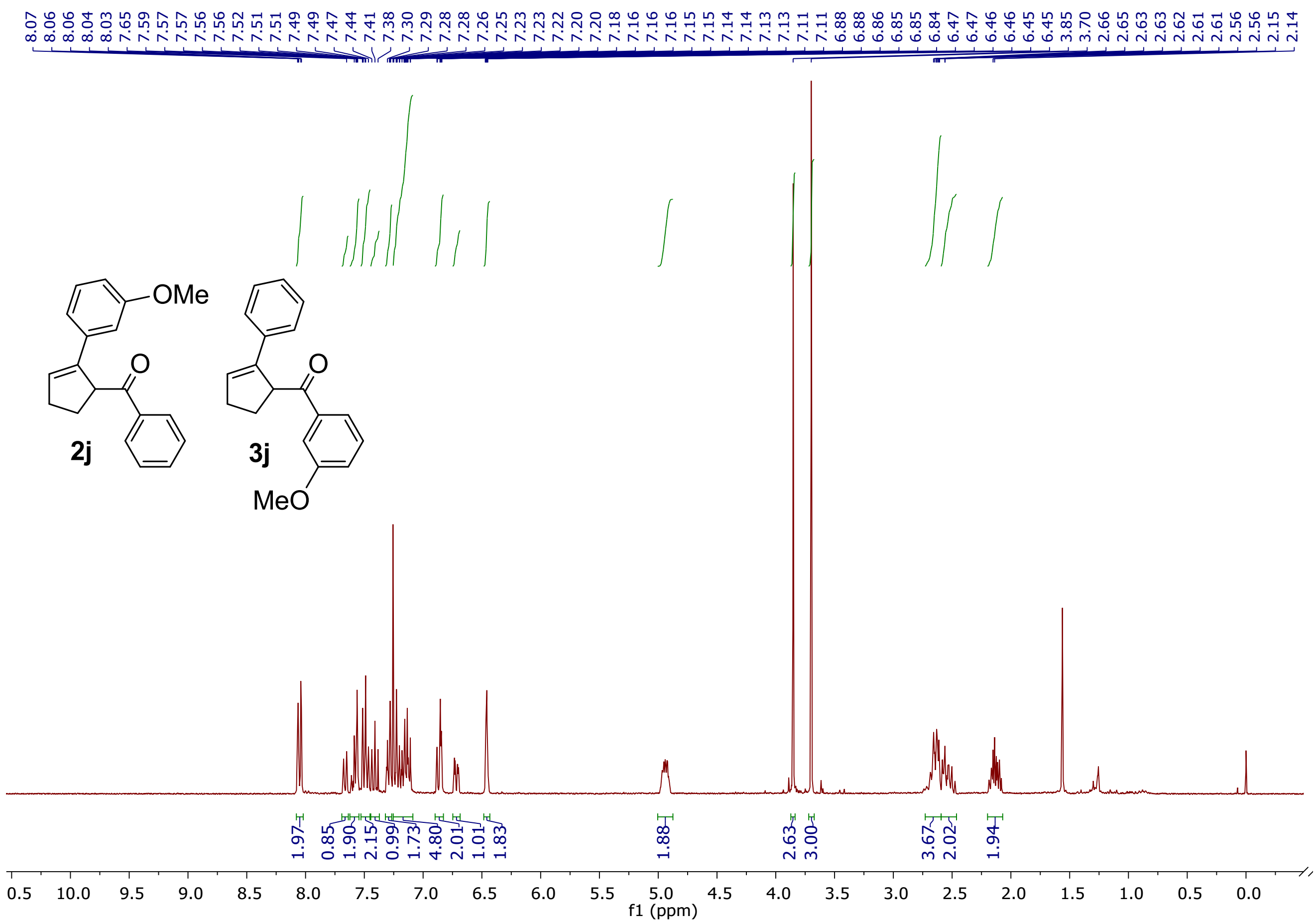
3i



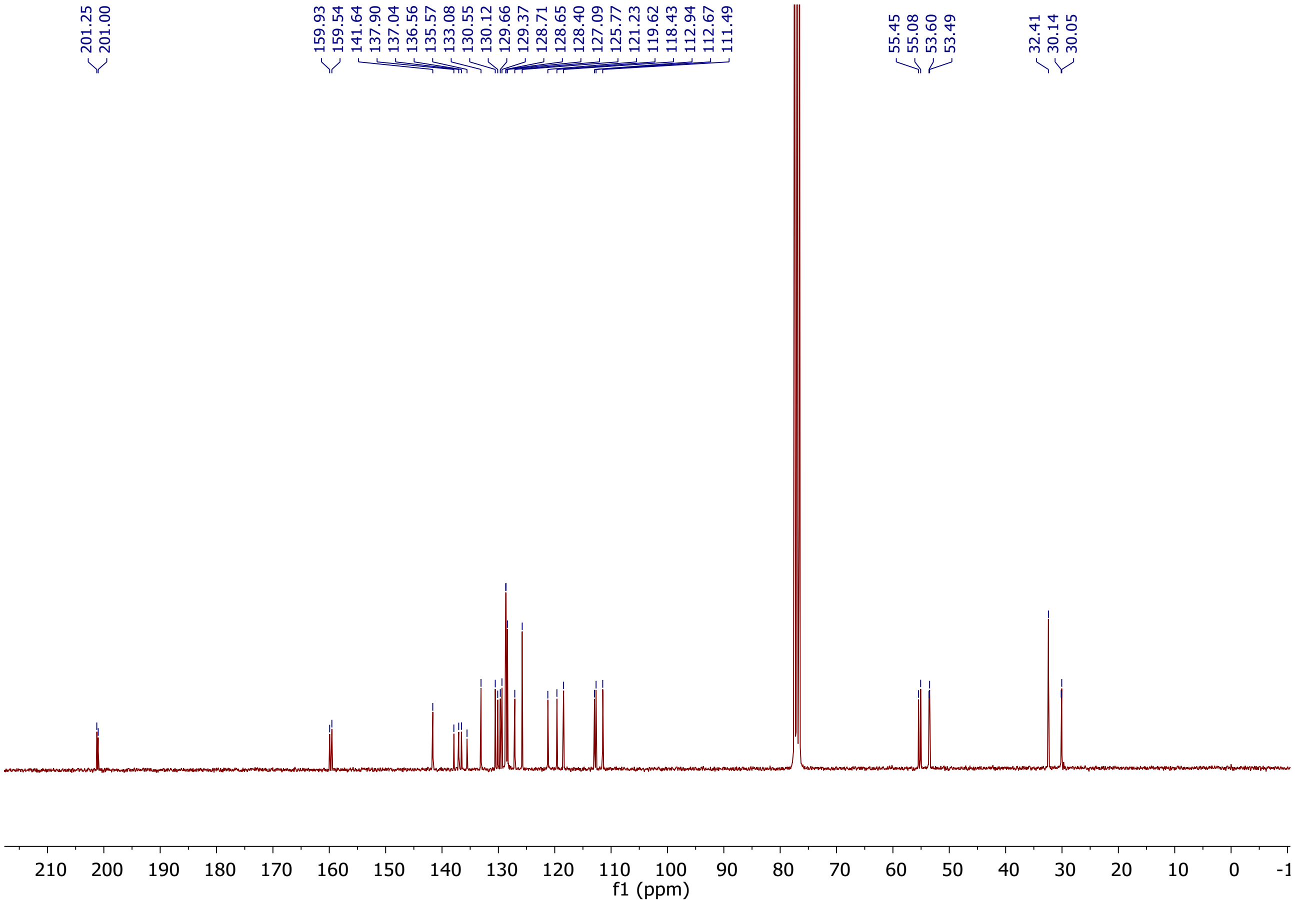
3i'

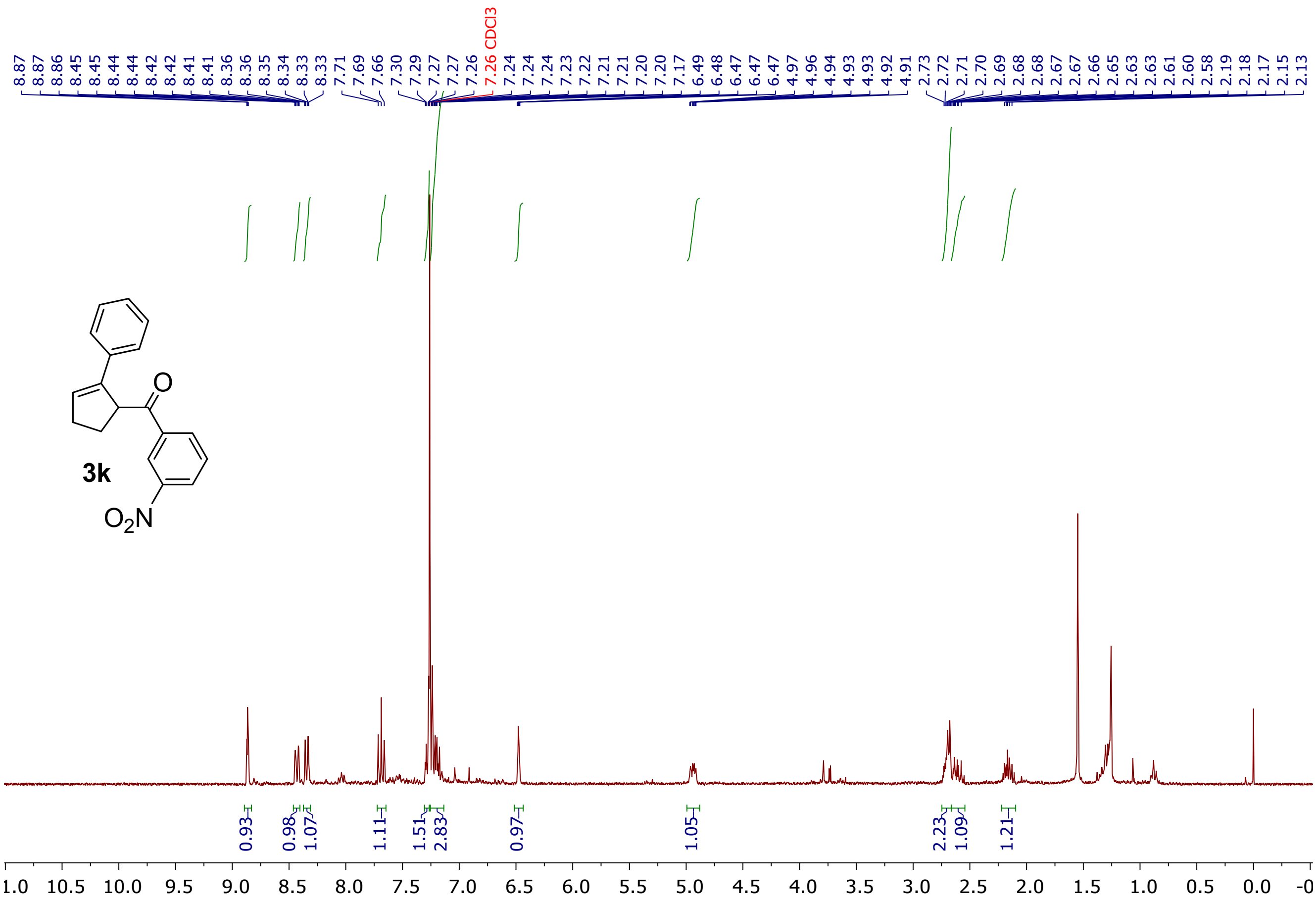

7.39
7.38
7.37
7.35
7.34
7.33
7.30
7.30
7.28
7.23
7.22
6.40
6.40
6.39
4.02
3.99
2.90
2.89
2.88
2.87
2.85
2.84
2.82
2.82
2.80
2.79
2.67
2.65
2.64
2.37
2.14
2.13
2.12
2.10
2.09
2.07
2.06
2.03
1.99
1.97
7.23
3.57
1.00
1.08
4.45
2.44
2.46
2.45
2.98
2.17
2.46
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

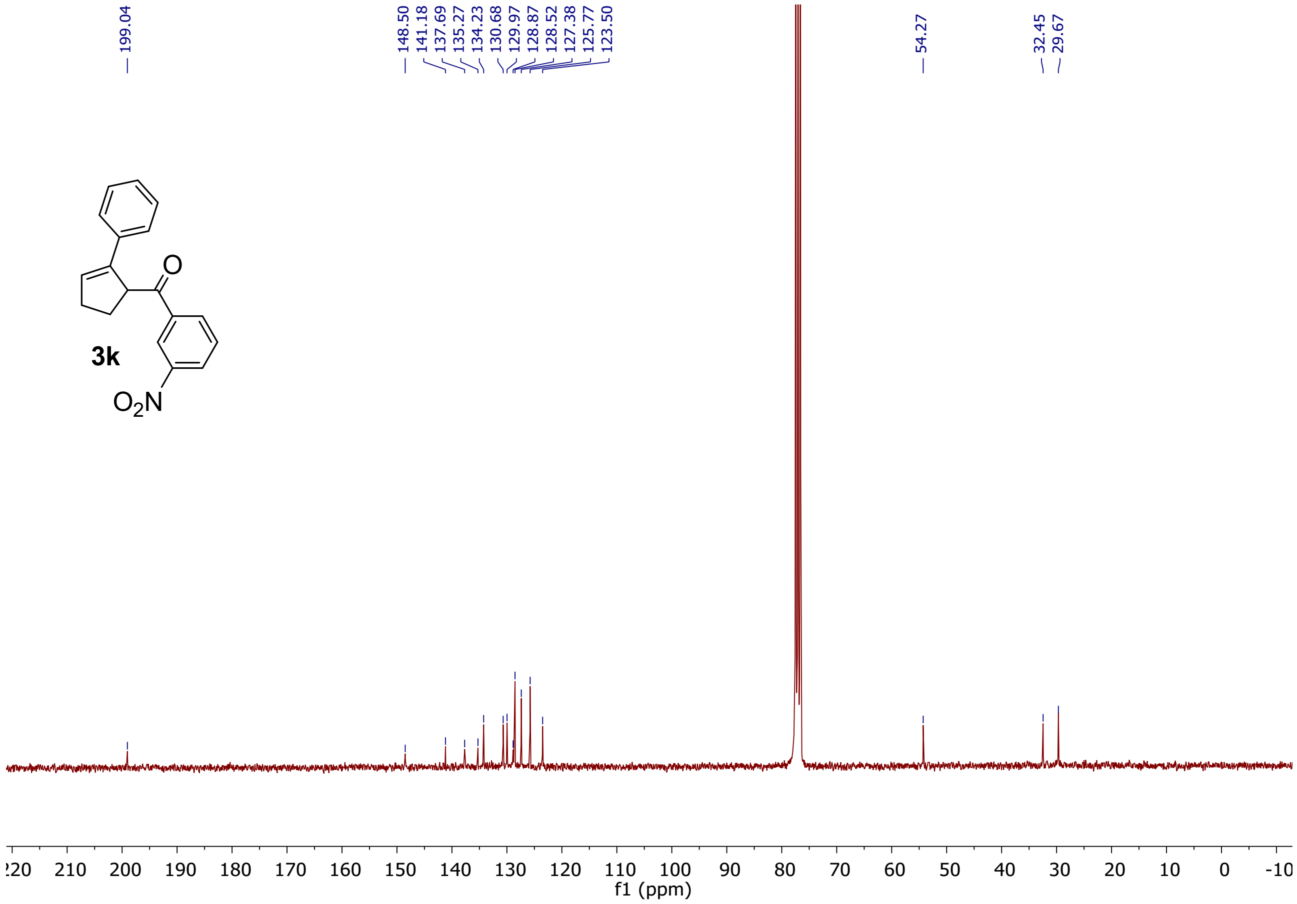

211.29
203.46
201.46
153.01
141.73
139.66
138.05
135.43
130.49
128.67
128.50
128.21
127.65
127.56
125.84
60.12
41.63
35.08
32.62
29.85
28.17
26.42
21.85
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.07
8.06
8.06
8.04
8.03
7.65
7.59
7.57
7.57
7.56
7.56
7.52
7.51
7.51
7.49
7.49
7.47
7.44
7.41
7.38
7.30
7.29
7.28
7.28
7.26
7.25
7.23
7.23
7.22
7.20
7.18
7.16
7.16
7.15
7.15
7.14
7.14
7.13
7.13
7.11
7.11
6.88
6.88
6.86
6.85
6.85
6.84
6.47
6.47
6.46
6.46
6.45
6.45
3.85
3.70
2.66
2.65
2.63
2.63
2.62
2.61
2.61
2.56
2.56
2.15
2.14
OMe
O
2j
O
3j
MeO
1.97
0.85
1.90
2.15
0.99
1.73
4.80
2.01
1.01
1.83
1.88
2.63
3.00
3.67
2.02
1.94
0.5 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)

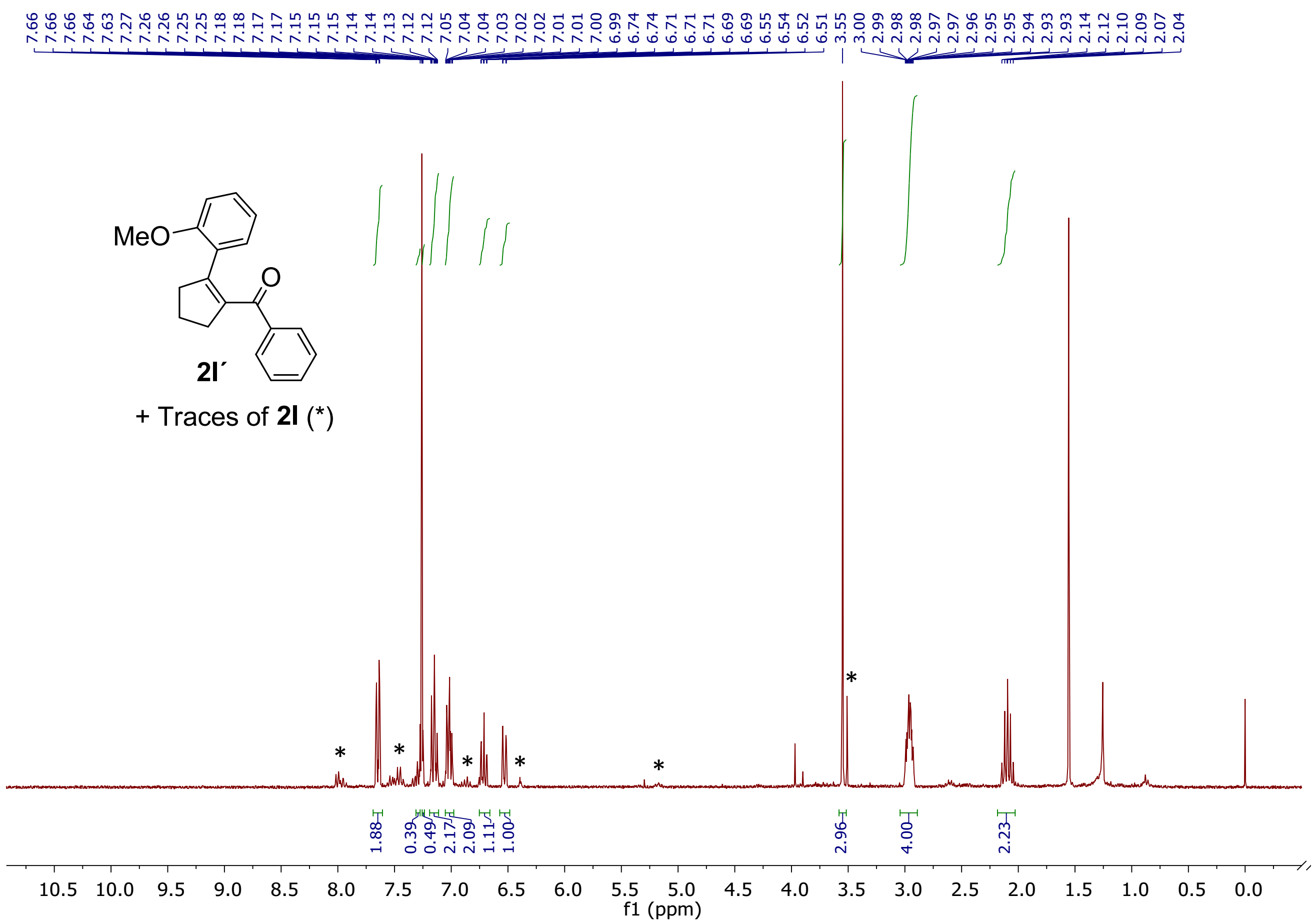

OMe


201.25
201.00
159.93
159.54
141.64
137.90
137.04
136.56
135.57
133.08
130.55
130.12
129.66
129.37
128.71
128.65
128.40
127.09
125.77
121.23
119.62
118.43
112.94
112.67
111.49
55.45
55.08
53.60
53.49
32.41
30.14
30.05
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -1
f1 (ppm)

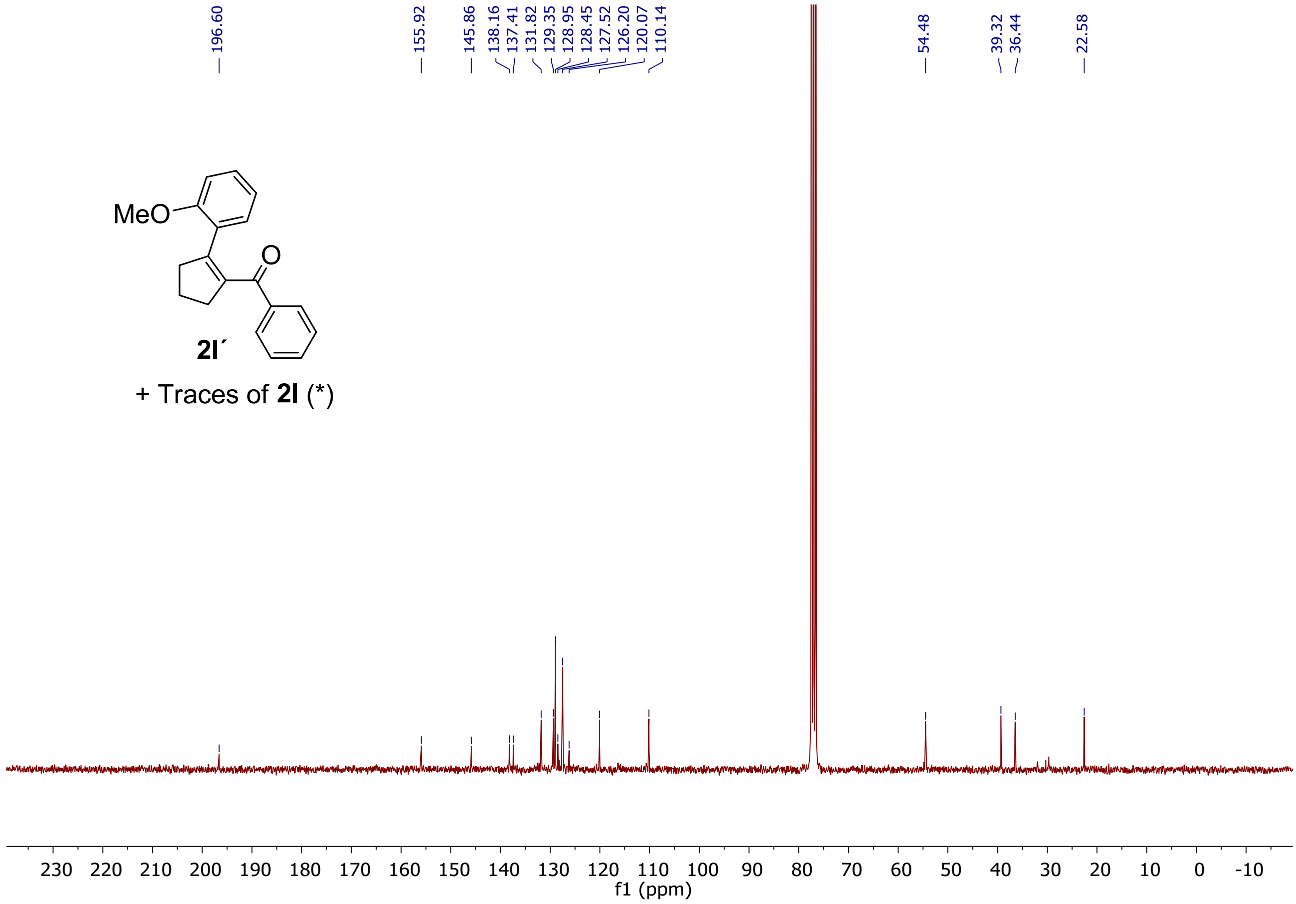

8.87 8.87 8.86 8.45 8.44 8.44 8.42 8.42 8.41 8.41 8.36 8.36 8.35 8.34 8.33 8.33 7.71 7.69 7.66 7.30 7.29 7.27 7.27 7.26 7.26 CDCl3 7.24 7.24 7.23 7.22 7.21 7.21 7.20 7.20 7.17 6.49 6.48 6.47 6.47 6.47 4.97 4.96 4.94 4.93 4.93 4.92 4.91 2.73 2.72 2.71 2.70 2.69 2.68 2.68 2.67 2.67 2.66 2.65 2.63 2.63 2.61 2.60 2.58 2.19 2.18 2.17 2.15 2.13
O
3k
O_2N
0.93
0.98
1.07
1.11
1.51
2.83
0.97
1.05
2.23
1.09
1.21
1.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

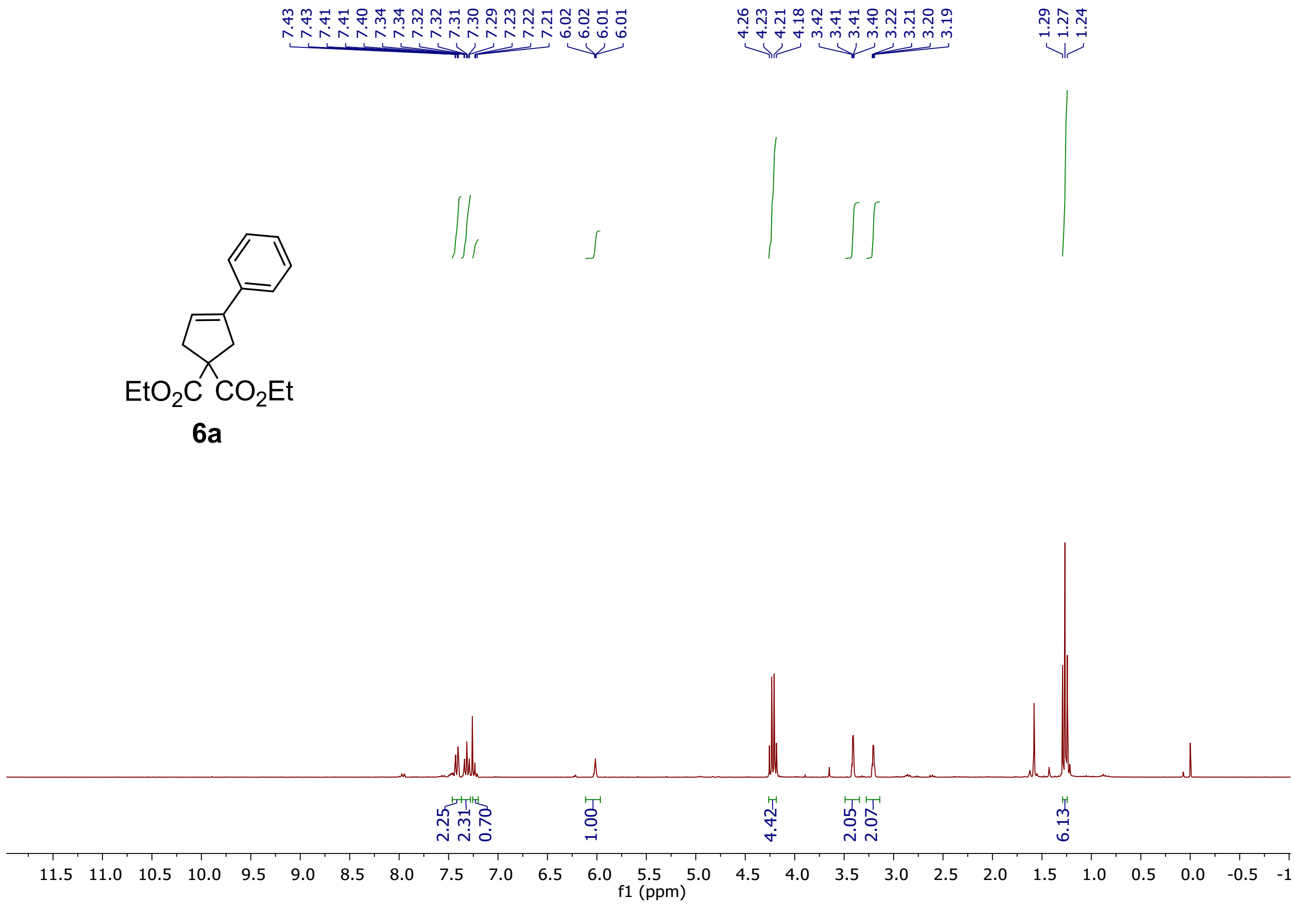


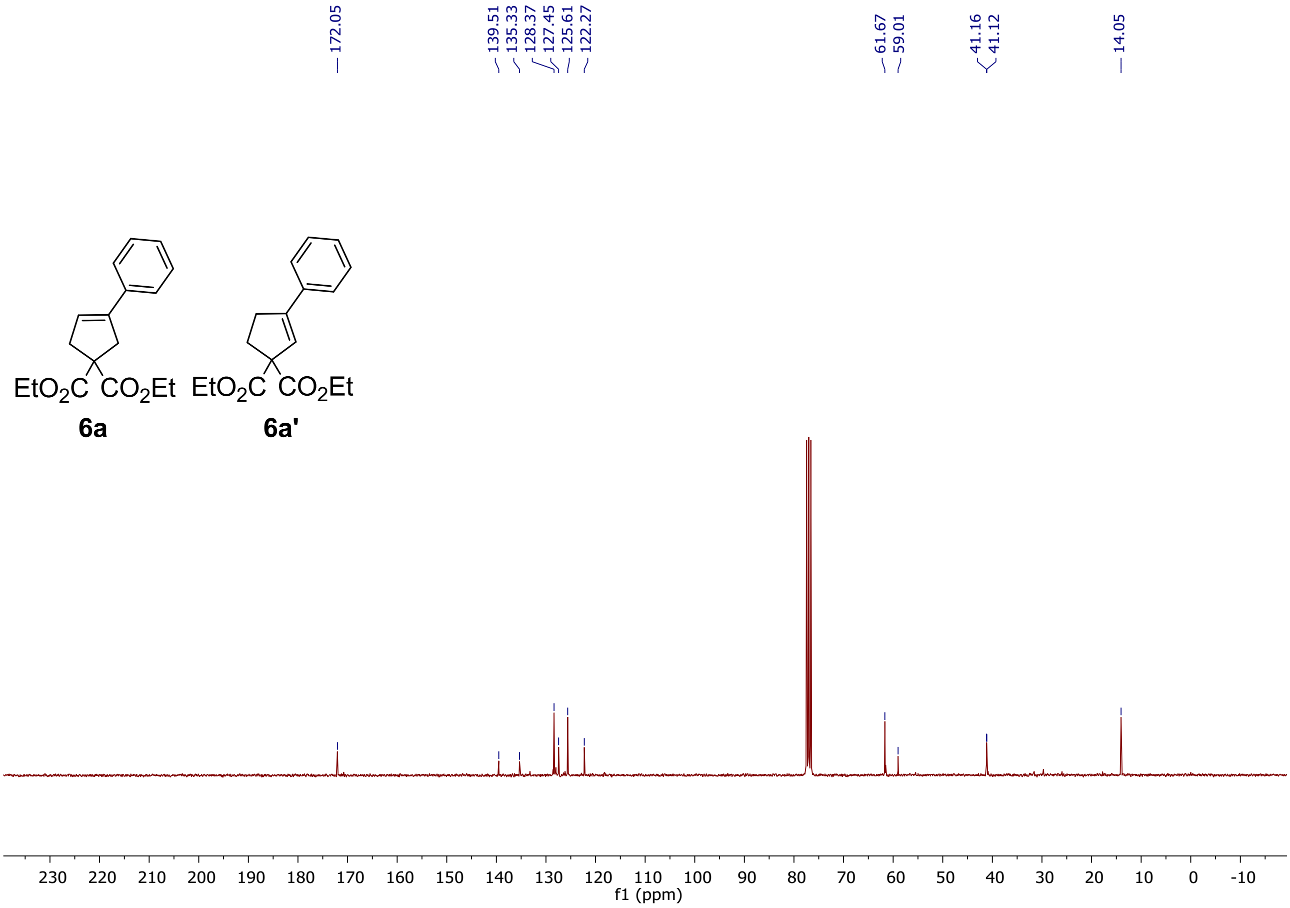
199.04
148.50
141.18
137.69
135.27
134.23
130.68
129.97
128.87
128.52
127.38
125.77
123.50
54.27
32.45
29.67
O
3k
O2N
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

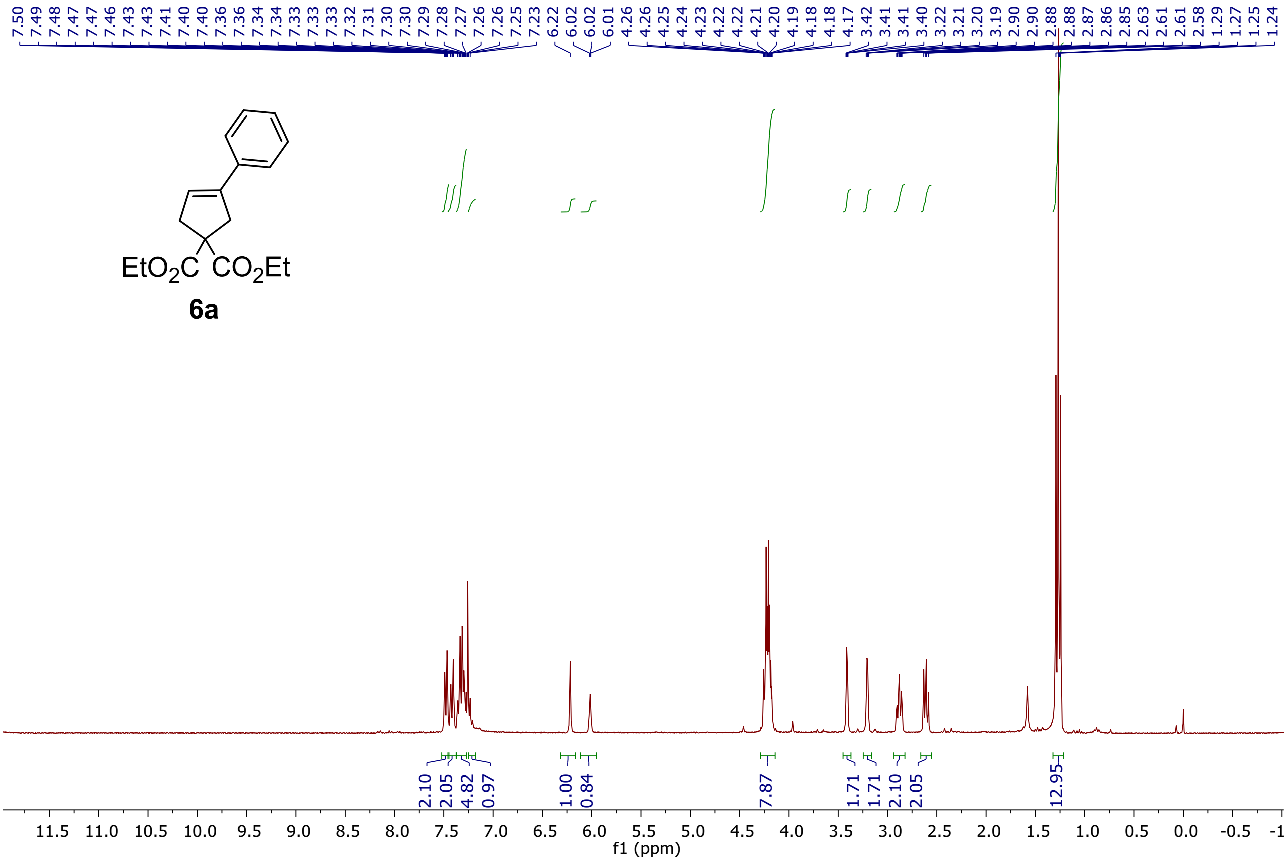


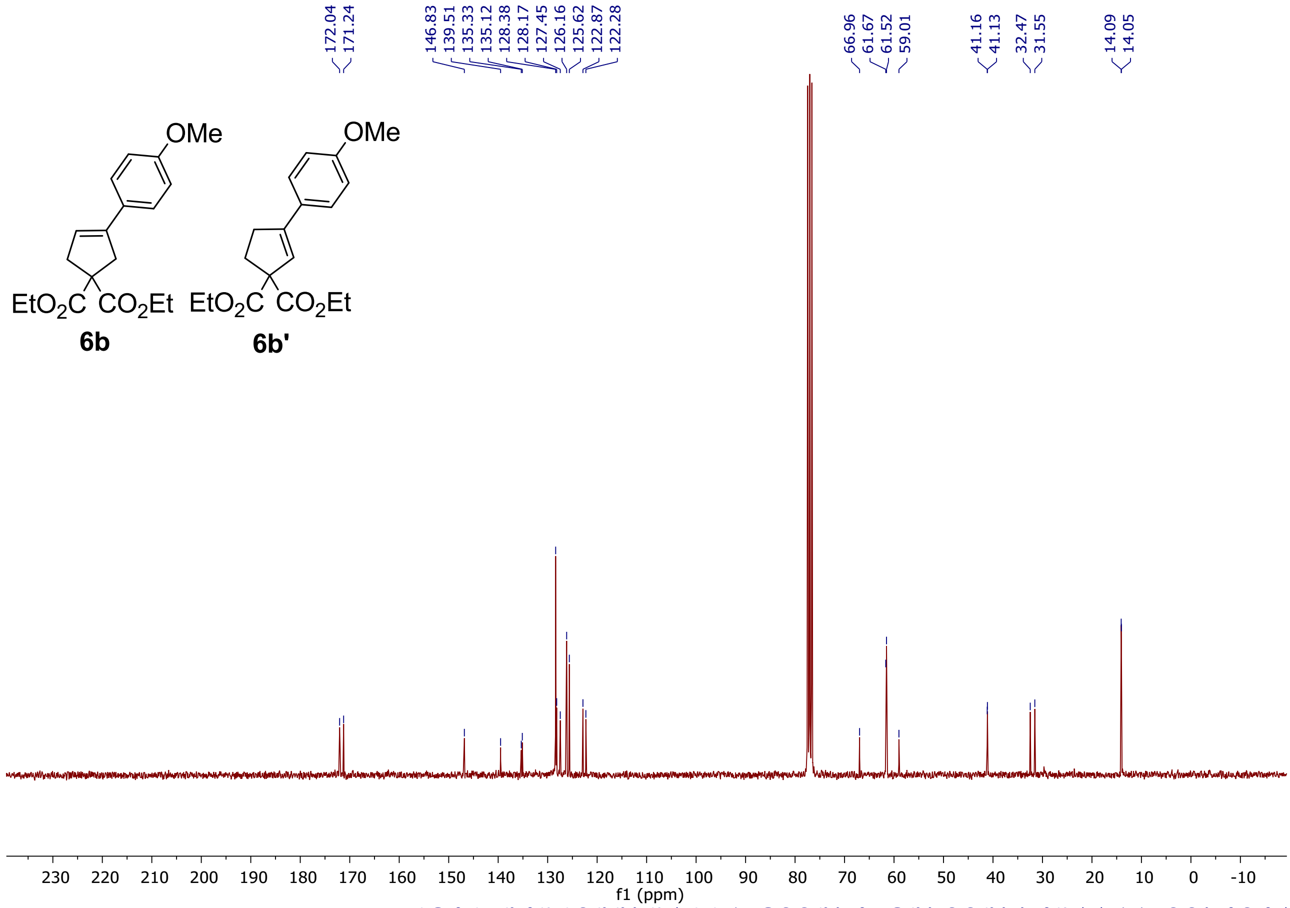
7.66 7.66 7.64 7.63 7.27 7.26 7.25 7.25 7.18 7.18 7.17 7.17 7.15 7.15 7.14 7.14 7.13 7.12 7.12 7.05 7.04 7.03 7.02 7.02 7.01 7.01 7.00 6.99 6.74 6.74 6.71 6.71 6.69 6.69 6.55 6.54 6.52 6.51
3.55
3.00 2.99 2.98 2.98 2.97 2.97 2.96 2.95 2.95 2.94 2.93 2.93 2.14 2.12 2.10 2.09 2.07 2.04
MeO
O
2l´
+ Traces of 2l (*)
*
1.88
0.39
0.49
2.17
2.09
1.11
1.00
2.96
4.00
2.23
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)


196.60
155.92
145.86
138.16
137.41
131.82
129.35
128.95
128.45
127.52
126.20
120.07
110.14
54.48
39.32
36.44
22.58
MeO
O
2l´
+ Traces of 2l (*)
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.43
7.43
7.41
7.41
7.40
7.34
7.34
7.32
7.32
7.31
7.30
7.29
7.23
7.22
7.21
6.02
6.02
6.01
6.01
4.26
4.23
4.21
4.18
3.42
3.41
3.41
3.40
3.22
3.21
3.20
3.19
1.29
1.27
1.24
EtO2C CO2Et
6a
2.25
2.31
0.70
1.00
4.42
2.05
2.07
6.13
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

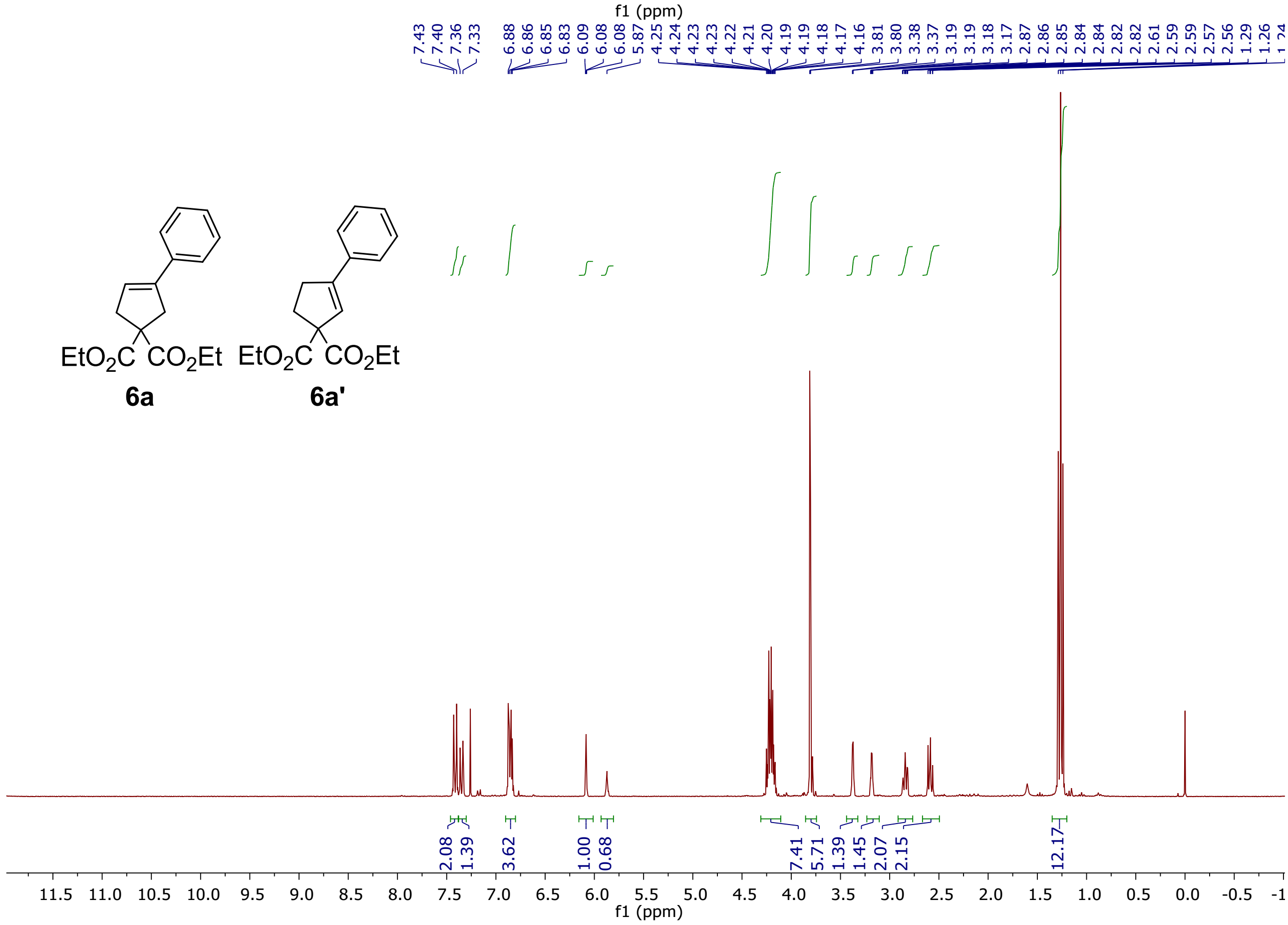

172.05
139.51
135.33
128.37
127.45
125.61
122.27
61.67
59.01
41.16
41.12
14.05
EtO2C CO2Et EtO2C CO2Et
6a
6a'
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.50 7.49 7.48 7.47 7.47 7.46 7.43 7.43 7.41 7.40 7.40 7.36 7.36 7.34 7.34 7.33 7.33 7.33 7.32 7.31 7.30 7.30 7.29 7.28 7.27 7.26 7.26 7.25 7.23 6.22 6.02 6.02 6.01 4.26 4.25 4.24 4.23 4.22 4.22 4.21 4.20 4.19 4.18 4.18 4.17 3.42 3.41 3.41 3.40 3.22 3.21 3.20 3.19 2.90 2.88 2.88 2.87 2.86 2.85 2.63 2.61 2.61 2.58 1.29 1.27 1.25 1.24
EtO2C CO2Et
6a
2.10
2.05
4.82
0.97
1.00
0.84
7.87
1.71
1.71
2.10
2.05
12.95
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)



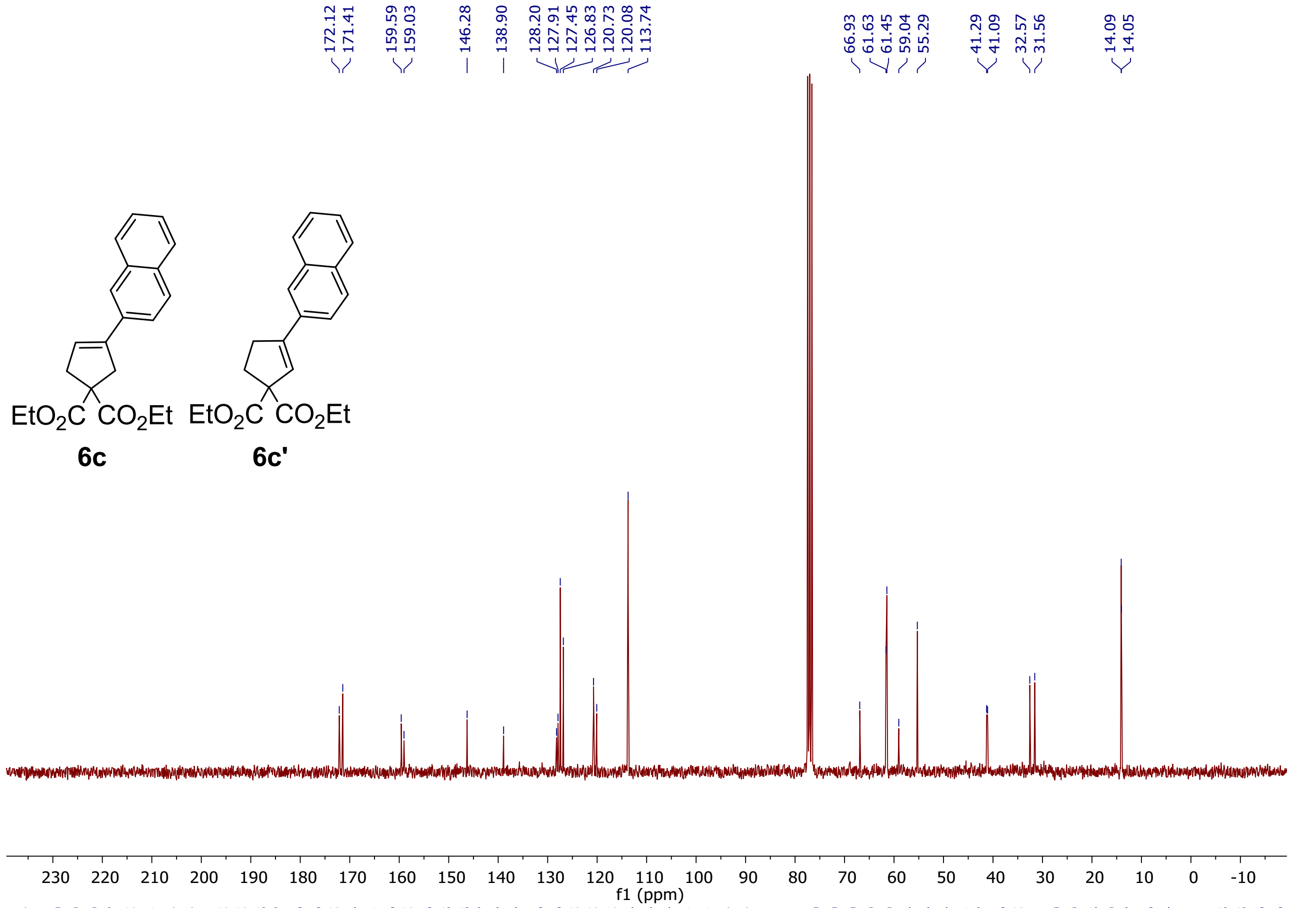
6b **6b'**

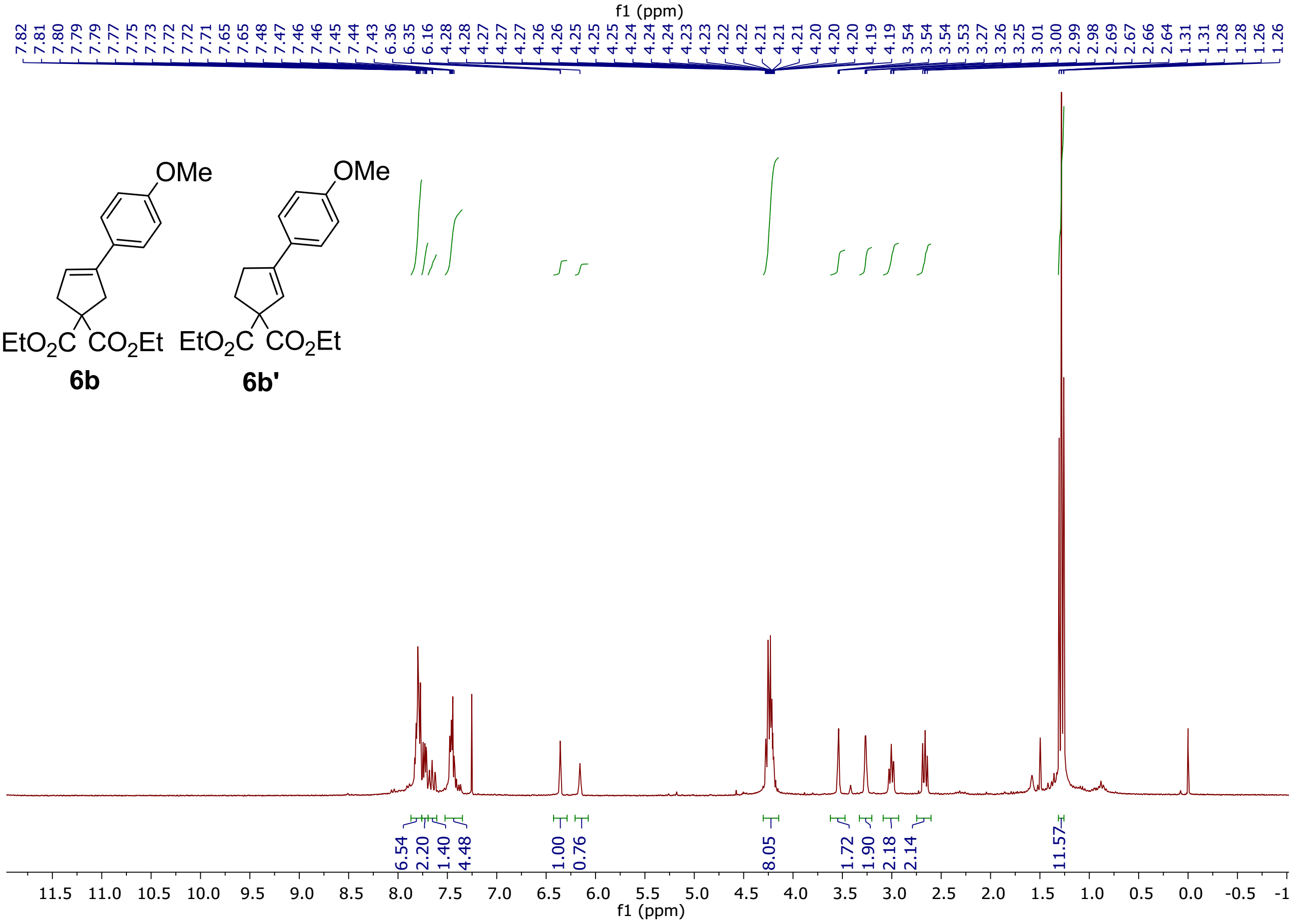
172.04
171.24
146.83
139.51
135.33
135.12
128.38
128.17
127.45
126.16
125.62
122.87
122.28
66.96
61.67
61.52
59.01
41.16
41.13
32.47
31.55
14.09
14.05
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

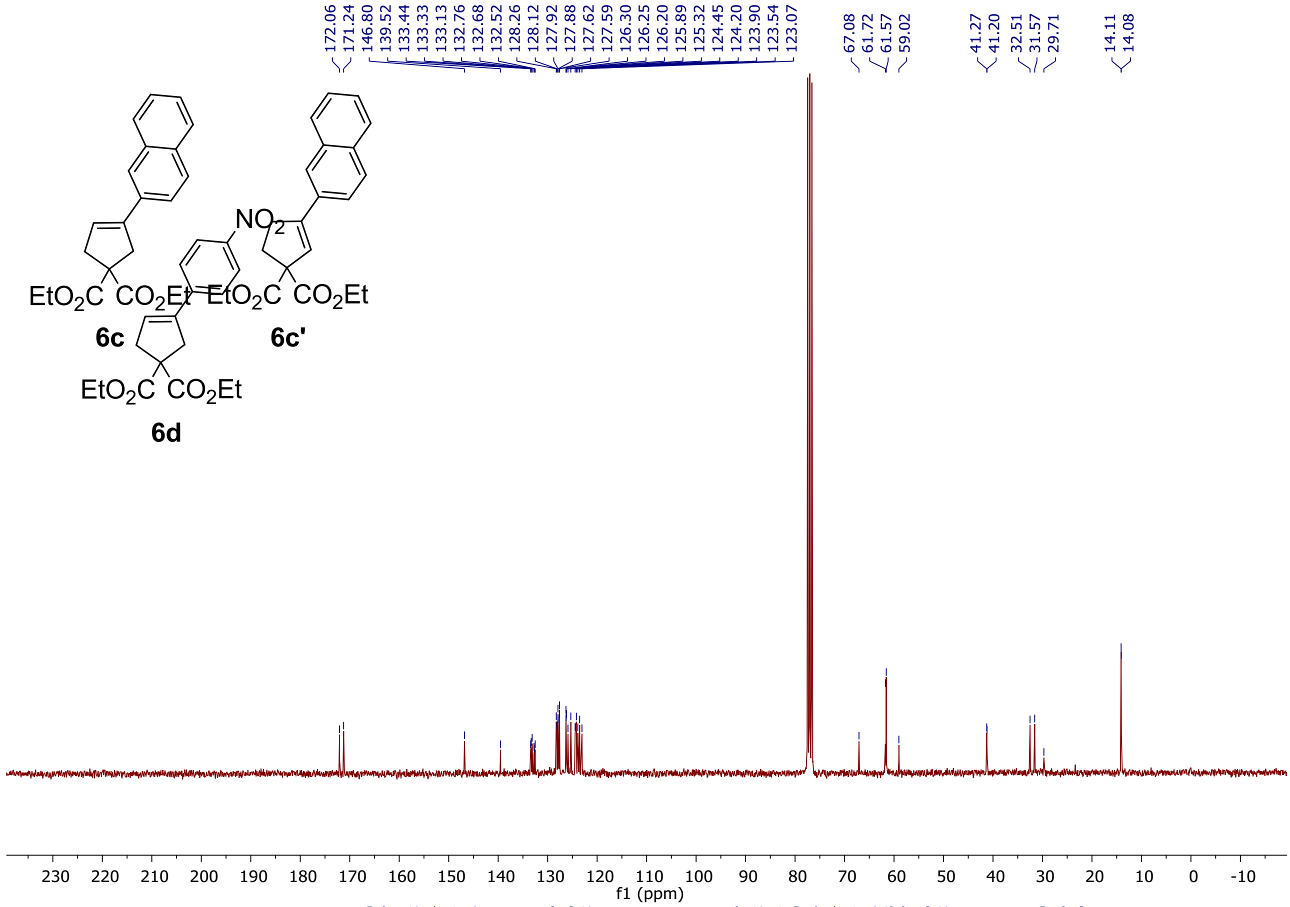


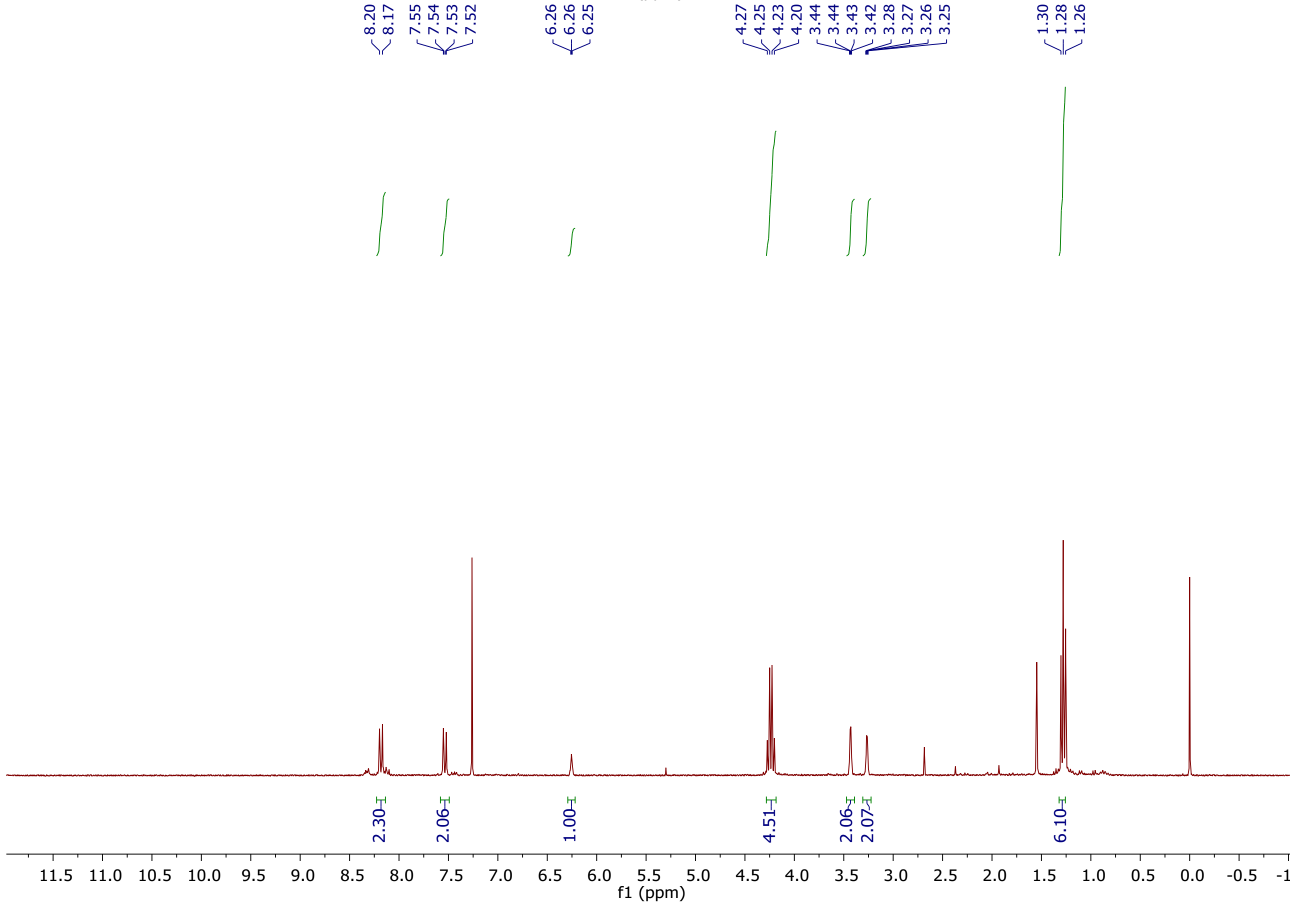
6a **6a'**

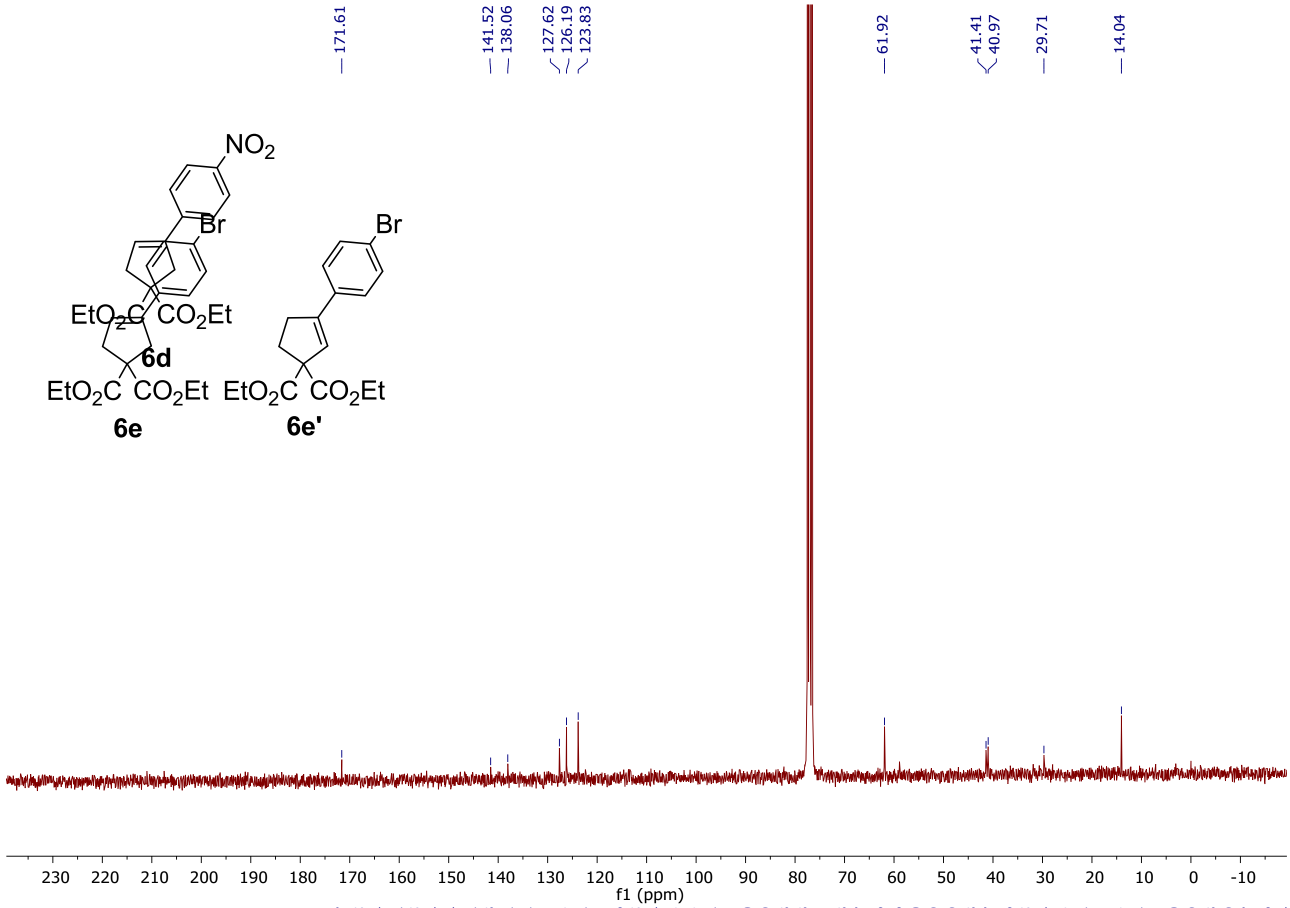
7.43
7.40
7.36
7.33
6.88
6.86
6.85
6.83
6.09
6.08
6.08
5.87
4.25
4.24
4.23
4.23
4.22
4.21
4.20
4.19
4.19
4.18
4.17
4.16
3.81
3.80
3.38
3.37
3.19
3.19
3.18
3.17
2.87
2.86
2.85
2.84
2.84
2.82
2.82
2.61
2.59
2.59
2.57
2.56
1.29
1.26
2.08
1.39
3.62
1.00
0.68
7.41
5.71
1.39
1.45
2.07
2.15
12.17
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

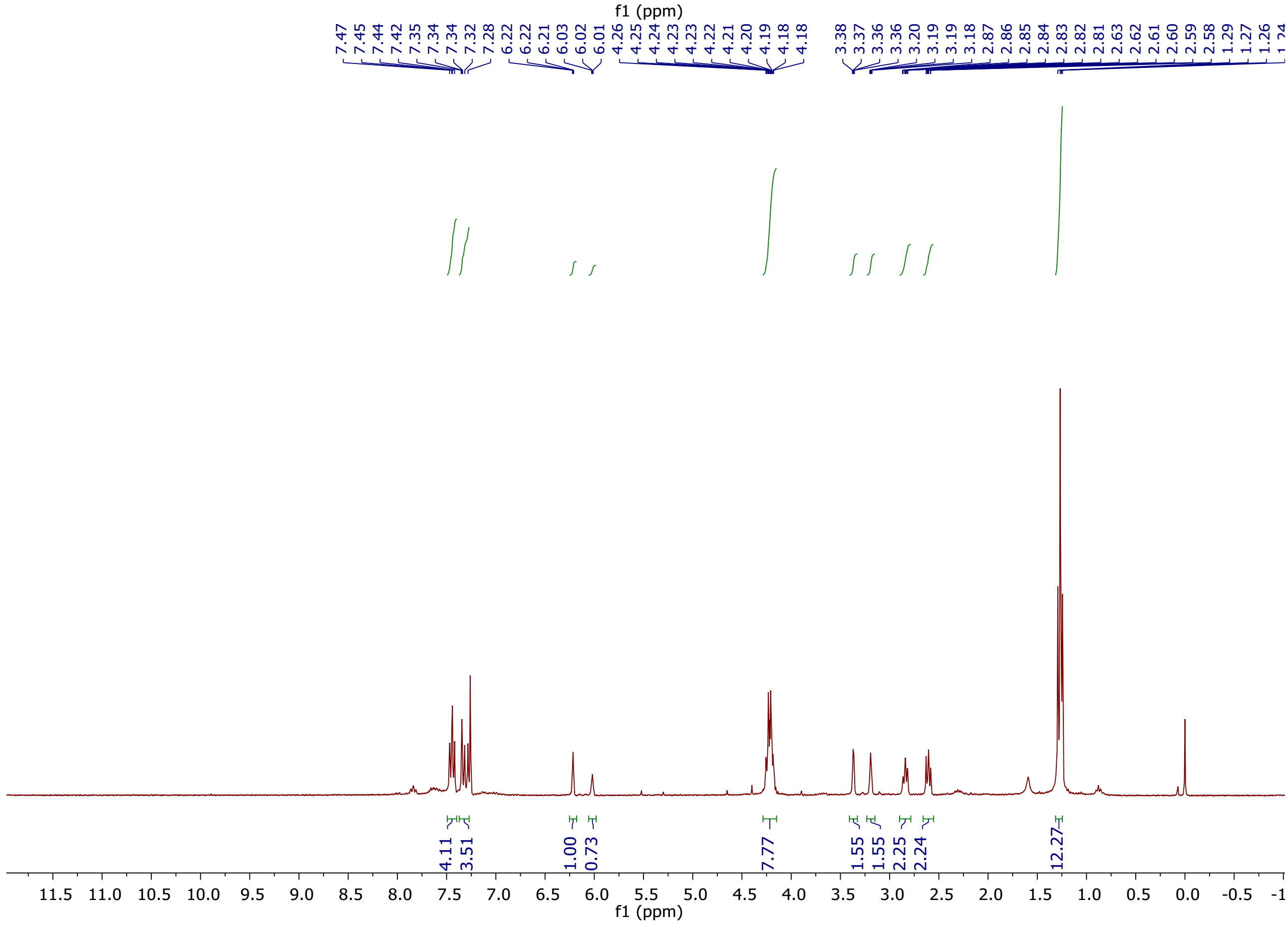

172.12
171.41
159.59
159.03
146.28
138.90
128.20
127.91
127.45
126.83
120.73
120.08
113.74
66.93
61.63
61.45
59.04
55.29
41.29
41.09
32.57
31.56
14.09
14.05
EtO2C CO2Et
6c
EtO2C CO2Et
6c'
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

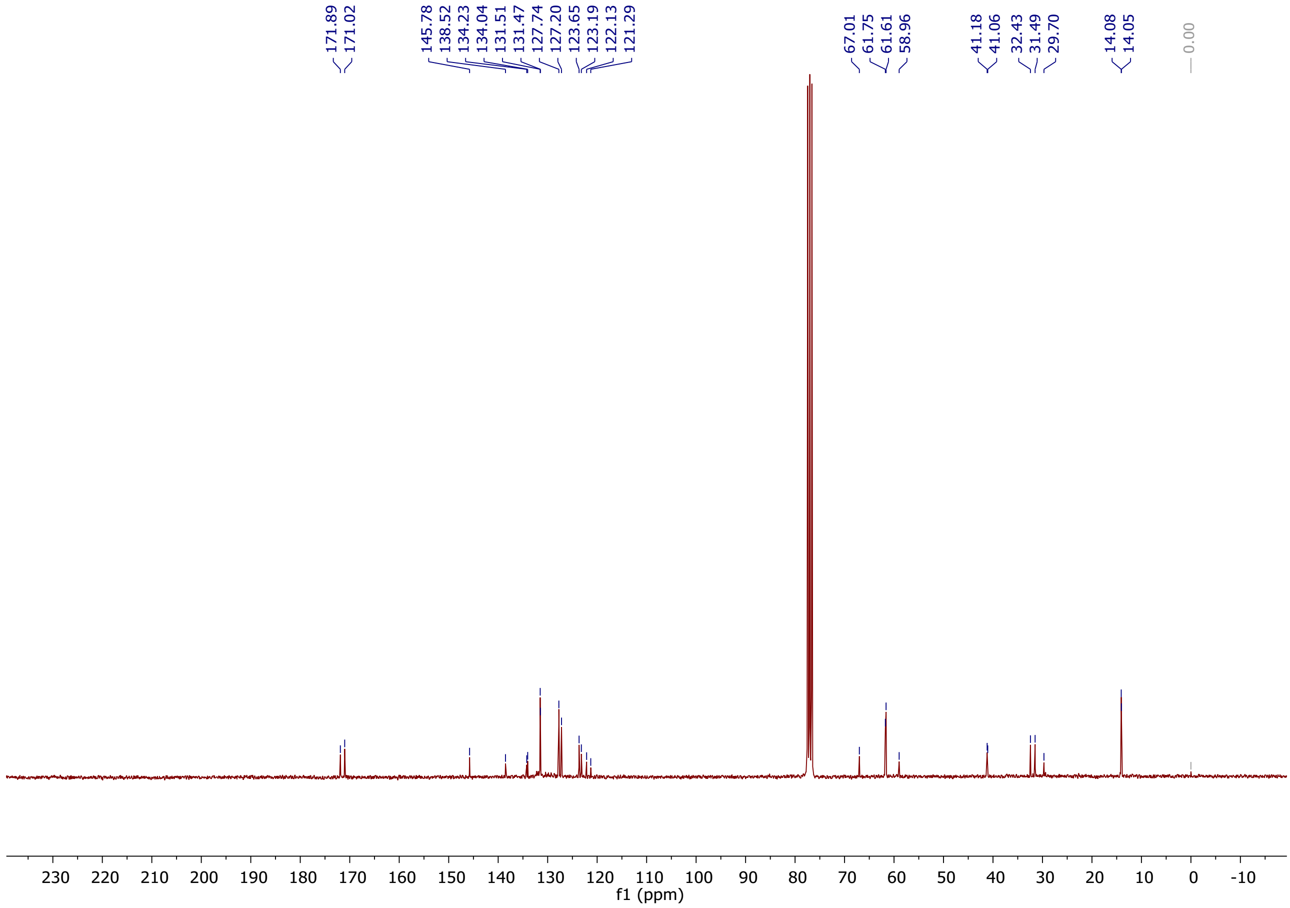

7.82 7.81 7.80 7.79 7.79 7.77 7.75 7.73 7.72 7.72 7.71 7.65 7.65 7.48 7.47 7.46 7.46 7.45 7.44 7.43 6.36 6.35 6.16 4.28 4.27 4.27 4.27 4.26 4.26 4.25 4.25 4.25 4.24 4.24 4.24 4.23 4.23 4.22 4.22 4.21 4.21 4.21 4.20 4.20 4.20 4.19 4.19 3.54 3.54 3.53 3.27 3.26 3.25 3.01 3.00 2.99 2.98 2.69 2.67 2.66 2.64 1.31 1.31 1.28 1.28 1.26 1.26
OMe
EtO2C CO2Et
6b
OMe
EtO2C CO2Et
6b'
6.54
2.20
1.40
4.48
1.00
0.76
8.05
1.72
1.90
2.18
2.14
11.57
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

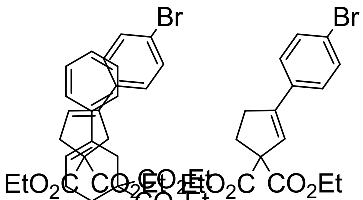

NO2
EtO2C CO2Et
EtO2C CO2Et
EtO2C CO2Et
6c
6c'
6d
172.06
171.24
146.80
139.52
133.44
133.33
133.13
132.76
132.68
132.52
128.26
128.12
127.92
127.88
127.62
127.59
126.30
126.25
126.20
125.89
125.32
124.45
124.20
123.90
123.54
123.07
67.08
61.72
61.57
59.02
41.27
41.20
32.51
31.57
29.71
14.11
14.08
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


8.20
8.17
7.55
7.54
7.53
7.52
6.26
6.26
6.25
4.27
4.25
4.23
4.20
3.44
3.43
3.42
3.28
3.27
3.26
3.25
1.30
1.28
1.26
2.30
2.06
1.00
4.51
2.06
2.07
6.10
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

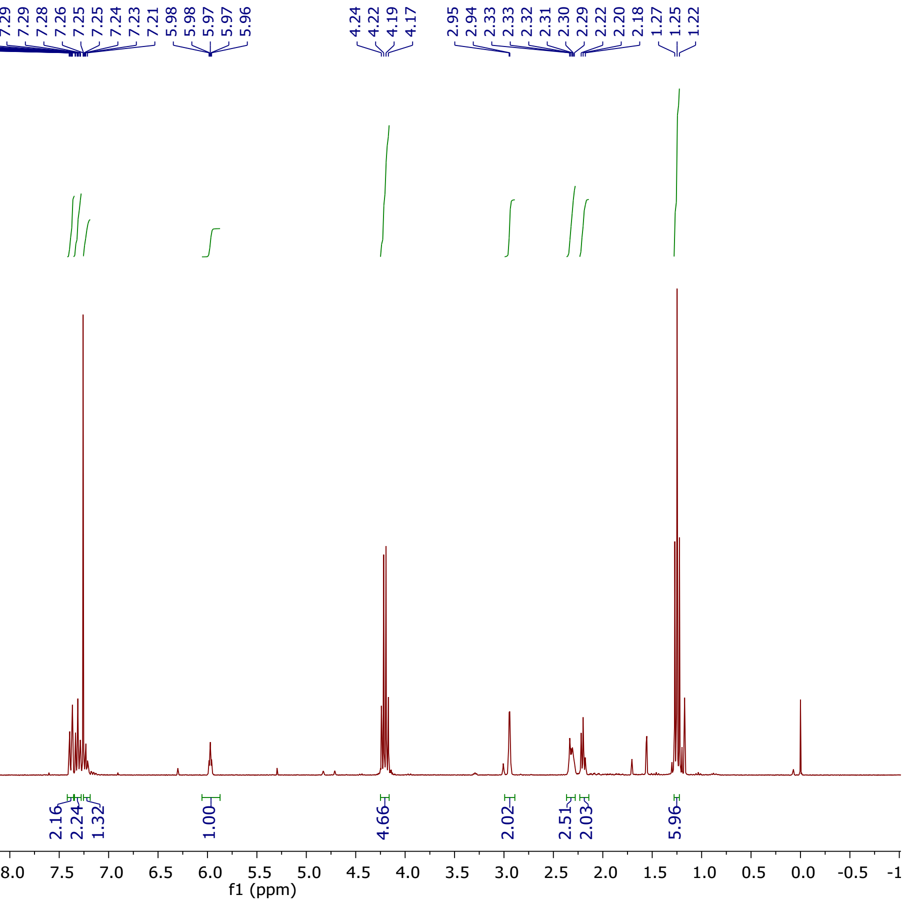

NO2
Br
EtO2C CO2Et
6d
EtO2C CO2Et
6e
Br
EtO2C CO2Et
6e'
171.61
141.52
138.06
127.62
126.19
123.83
61.92
41.41
40.97
29.71
14.04
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

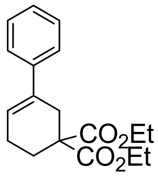

7.47 7.45 7.44 7.42 7.35 7.34 7.34 7.32 7.28 6.22 6.22 6.21 6.03 6.02 6.01 4.26 4.25 4.24 4.23 4.23 4.22 4.21 4.20 4.19 4.18 4.18 3.38 3.37 3.36 3.36 3.20 3.19 3.18 2.87 2.86 2.85 2.84 2.83 2.82 2.81 2.63 2.62 2.61 2.60 2.59 2.58 1.29 1.27 1.26 1.24
4.11
3.51
1.00
0.73
7.77
1.55
1.55
2.25
2.24
12.27
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


171.89
171.02
145.78
138.52
134.23
134.04
131.51
131.47
127.74
127.20
123.65
123.19
122.13
121.29
67.01
61.75
61.61
58.96
41.18
41.06
32.43
31.49
29.70
14.08
14.05
0.00
f1 (ppm)

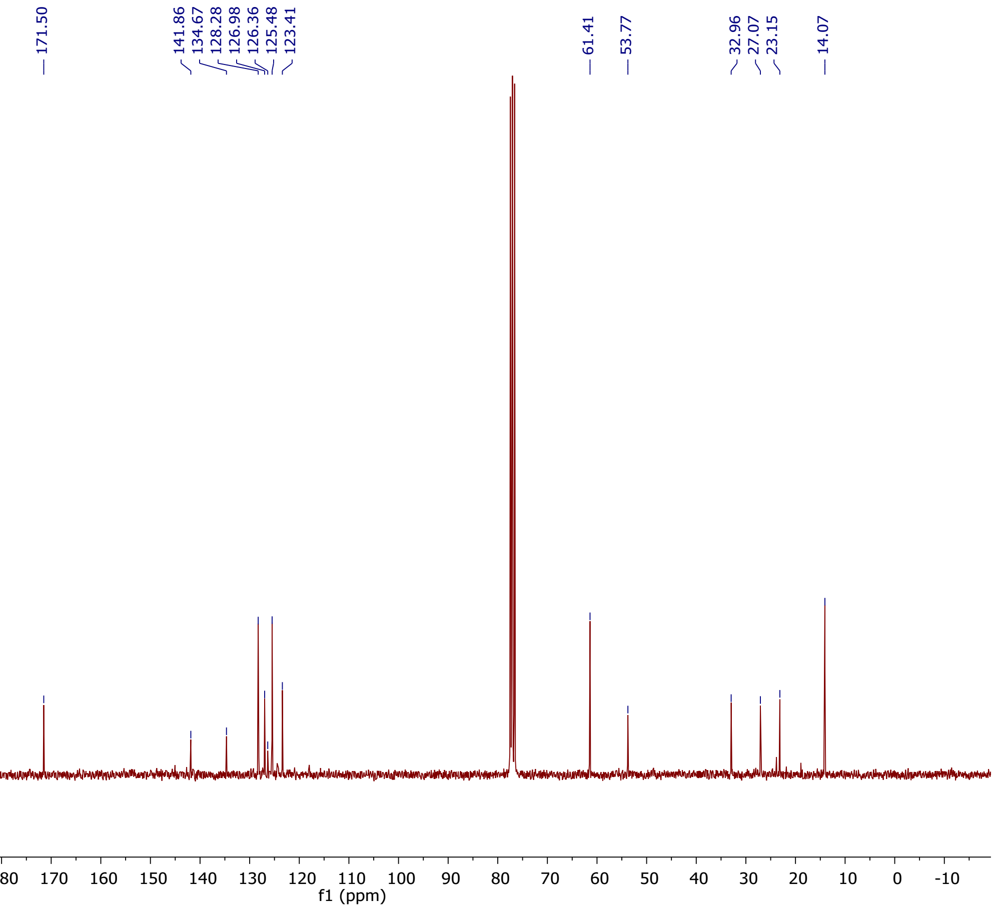

Br
Br
EtO_2C
CO_2Et
CO_2Et
EtO_2C
CO_2Et

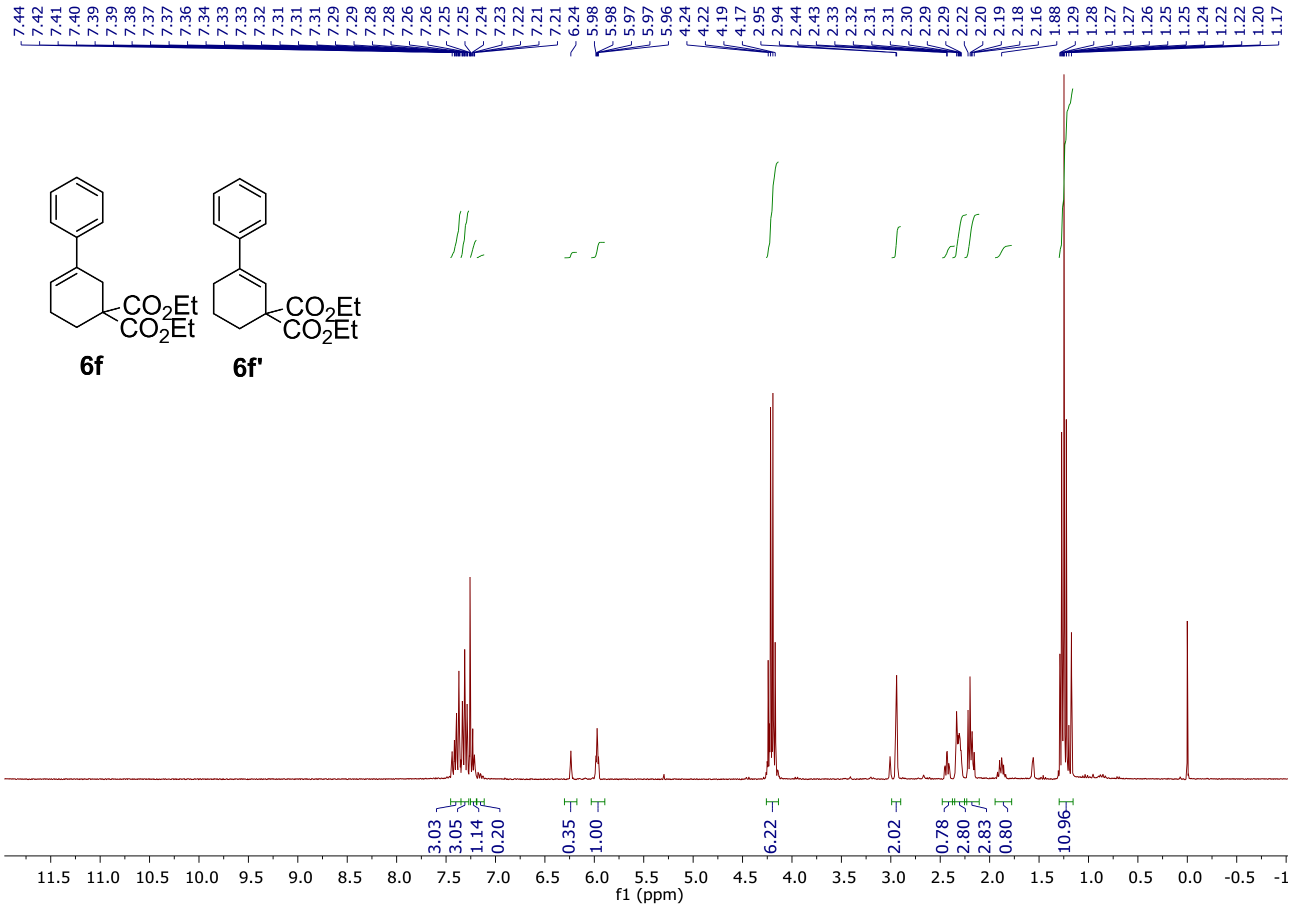
6e 6f 6e'


7.40
7.39
7.39
7.38
7.38
7.37
7.37
7.34
7.34
7.32
7.31
7.31
7.31
7.29
7.29
7.28
7.26
7.25
7.25
7.24
7.23
7.21
5.98
5.98
5.97
5.97
5.96
4.24
4.22
4.19
4.17
2.95
2.94
2.33
2.33
2.32
2.31
2.30
2.29
2.22
2.20
2.18
1.27
1.25
1.22
2.16
2.24
1.32
1.00
4.66
2.02
2.51
2.03
5.96
f1 (ppm)

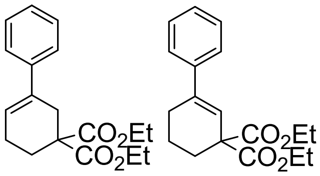

CO2Et
CO2Et

6f


171.50
141.86
134.67
128.28
126.98
126.36
125.48
123.41
61.41
53.77
32.96
27.07
23.15
14.07
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

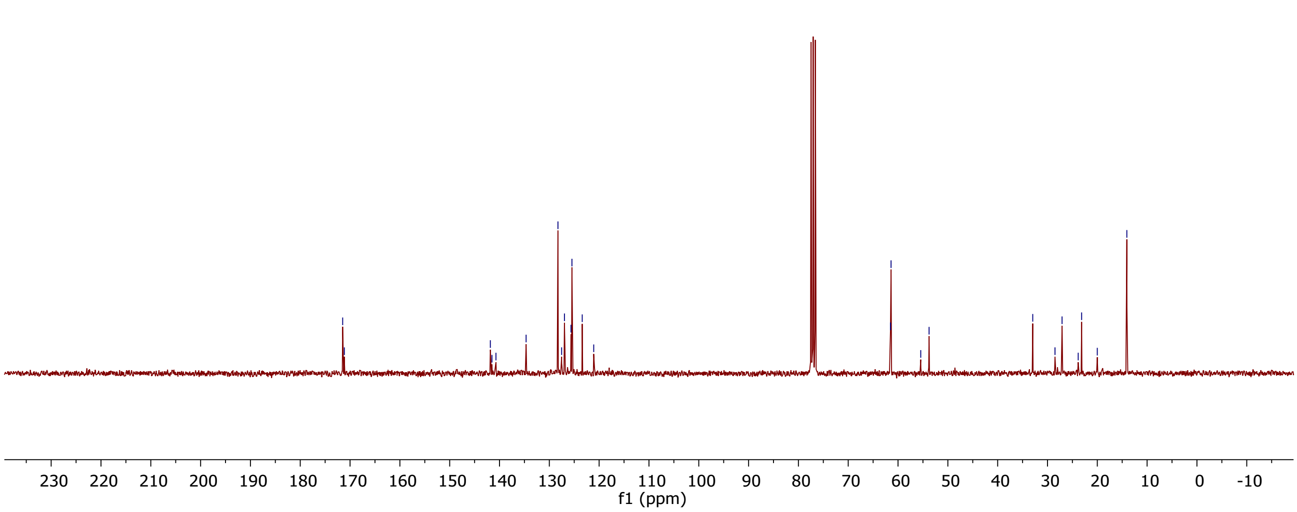


7.44 7.42 7.41 7.40 7.39 7.39 7.38 7.37 7.37 7.36 7.34 7.33 7.33 7.32 7.31 7.31 7.31 7.29 7.29 7.28 7.28 7.26 7.26 7.25 7.25 7.24 7.23 7.22 7.21 7.21 6.24 5.98 5.98 5.97 5.97 5.96 4.24 4.22 4.19 4.17 2.95 2.94 2.44 2.43 2.33 2.32 2.31 2.31 2.30 2.29 2.29 2.22 2.20 2.19 2.18 2.16 1.88 1.29 1.28 1.27 1.27 1.26 1.25 1.25 1.24 1.22 1.22 1.20 1.17
CO2Et
CO2Et
6f
CO2Et
CO2Et
6f'
3.03 3.05 1.14 0.20 0.35 1.00 6.22 2.02 0.78 2.80 2.83 0.80 10.96
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

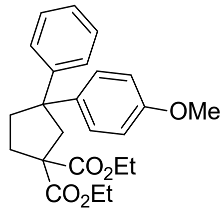


CO2Et
CO2Et
CO2Et
CO2Et

6f **6f'**

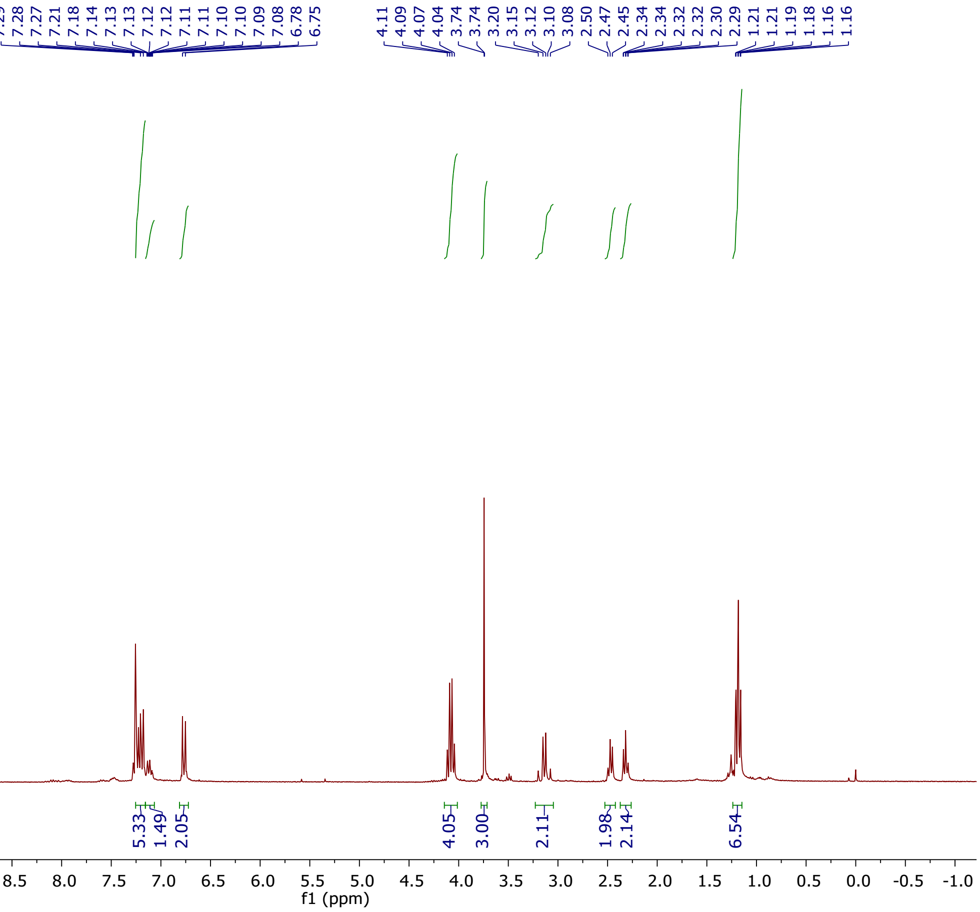


171.48
171.15
141.84
141.52
140.72
134.66
128.27
127.53
126.97
125.65
125.46
123.40
121.09
61.52
61.40
55.44
53.77
32.96
28.49
27.07
23.83
23.15
20.00
14.07
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

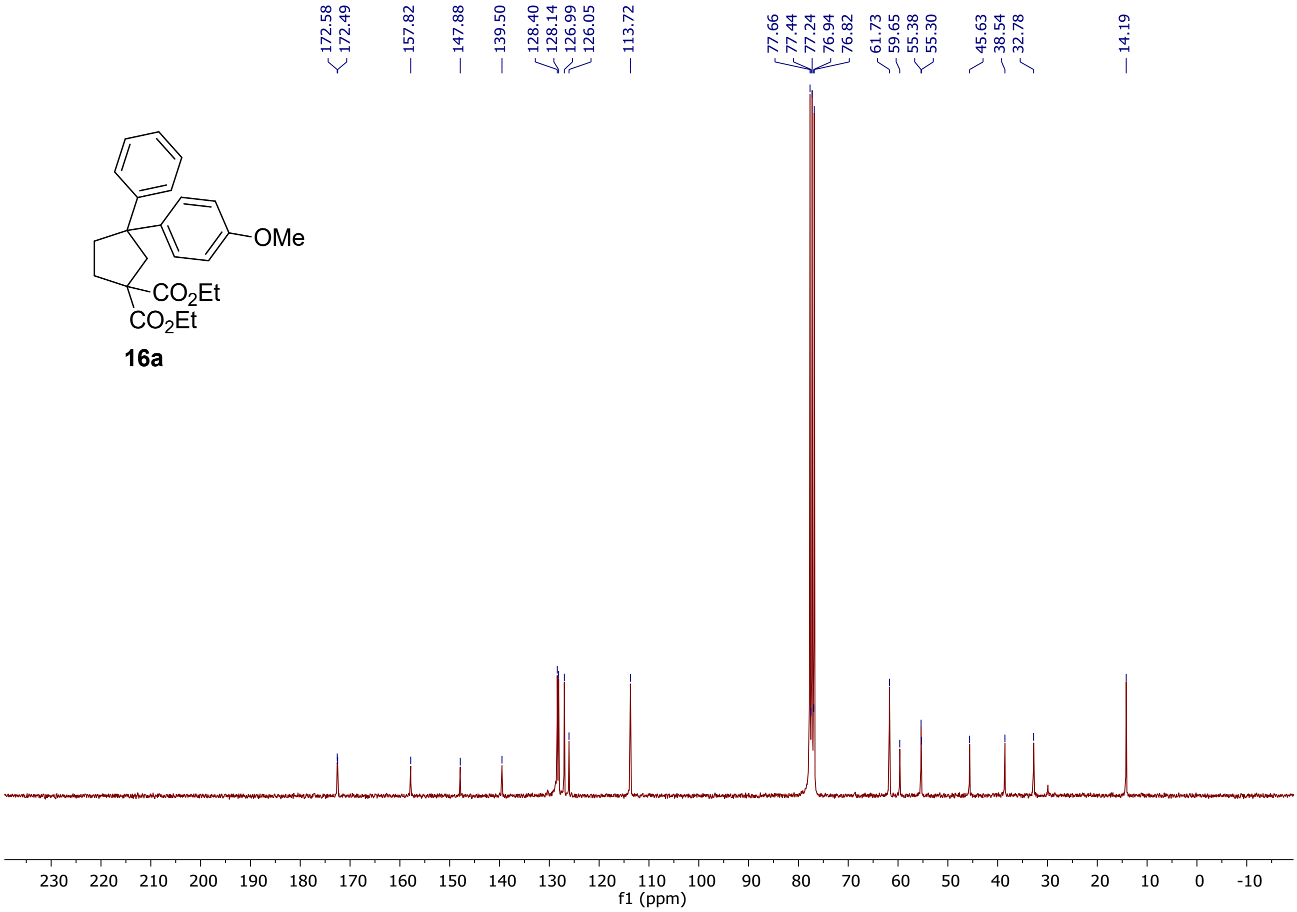


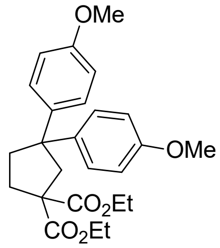
OMe
CO2Et
CO2Et

16a

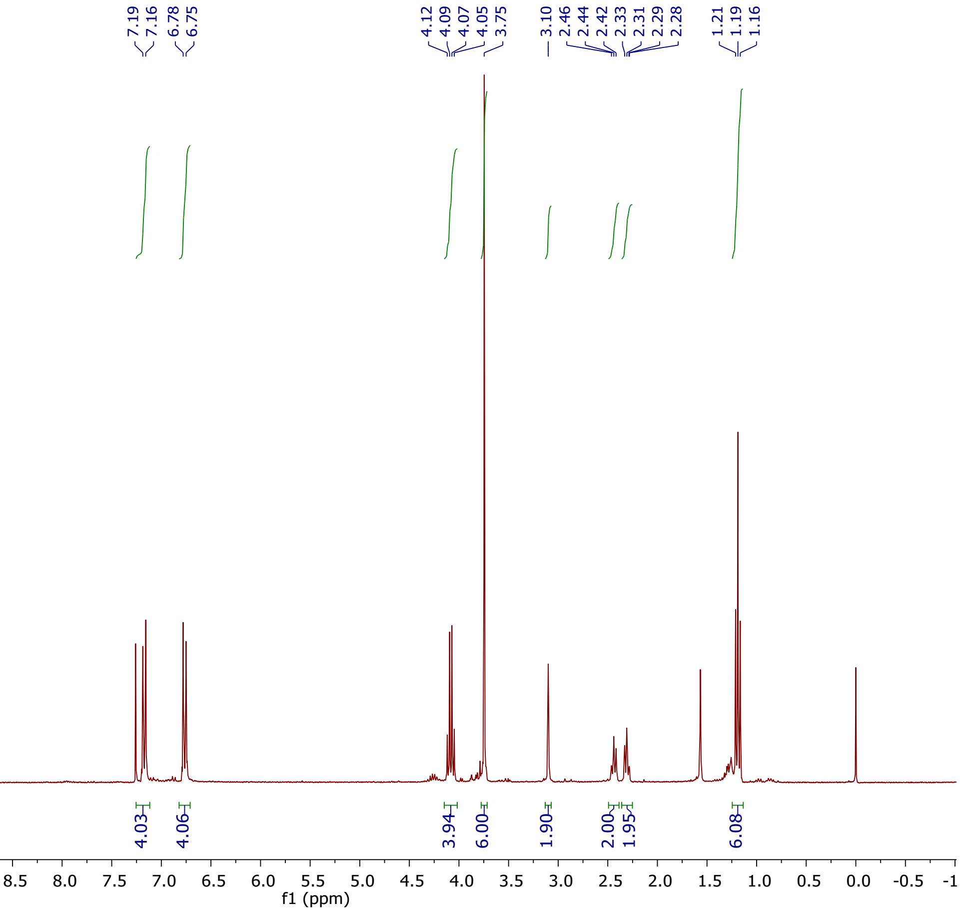


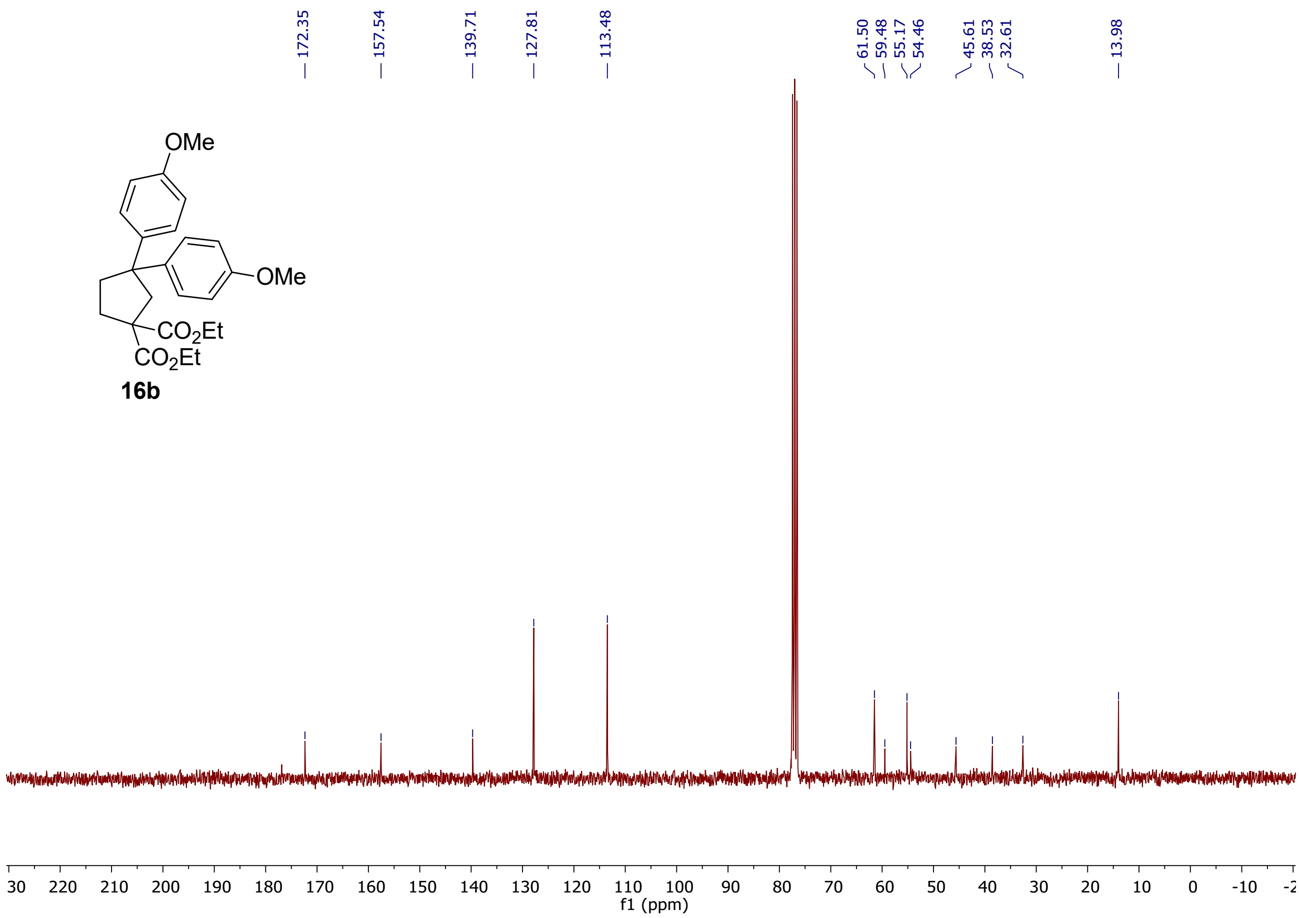
7.29
7.28
7.27
7.21
7.18
7.14
7.13
7.13
7.12
7.12
7.11
7.11
7.10
7.10
7.09
7.08
6.78
6.75
4.11
4.09
4.07
4.04
3.74
3.74
3.20
3.15
3.12
3.10
3.08
2.50
2.47
2.45
2.34
2.34
2.32
2.32
2.30
2.29
1.21
1.21
1.19
1.18
1.16
1.16
5.33
1.49
2.05
4.05
3.00
2.11
1.98
2.14
6.54
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)

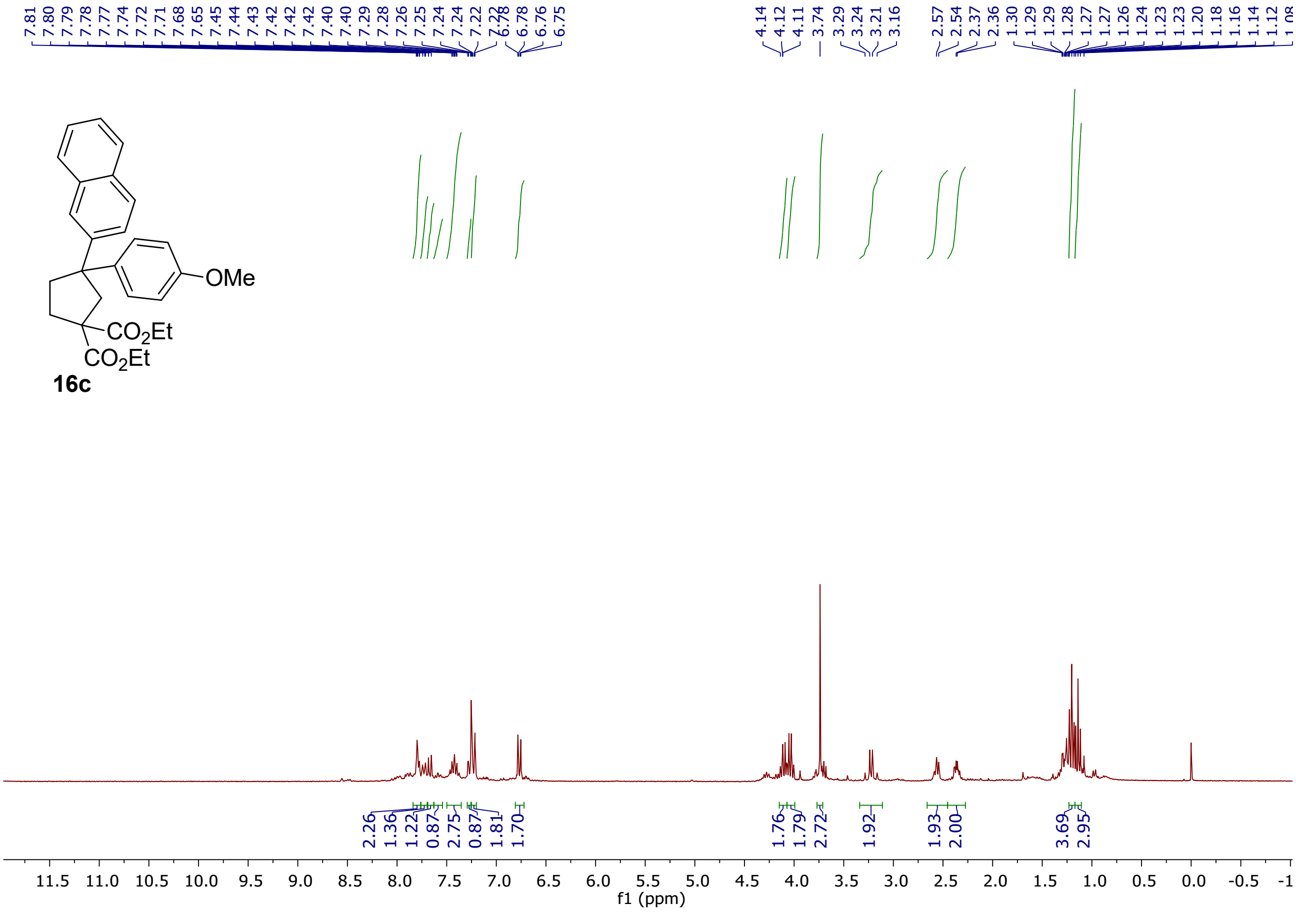

OMe
CO2Et
CO2Et
16a
172.58
172.49
157.82
147.88
139.50
128.40
128.14
126.99
126.05
113.72
77.66
77.44
77.24
76.94
76.82
61.73
59.65
55.38
55.30
45.63
38.54
32.78
14.19
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

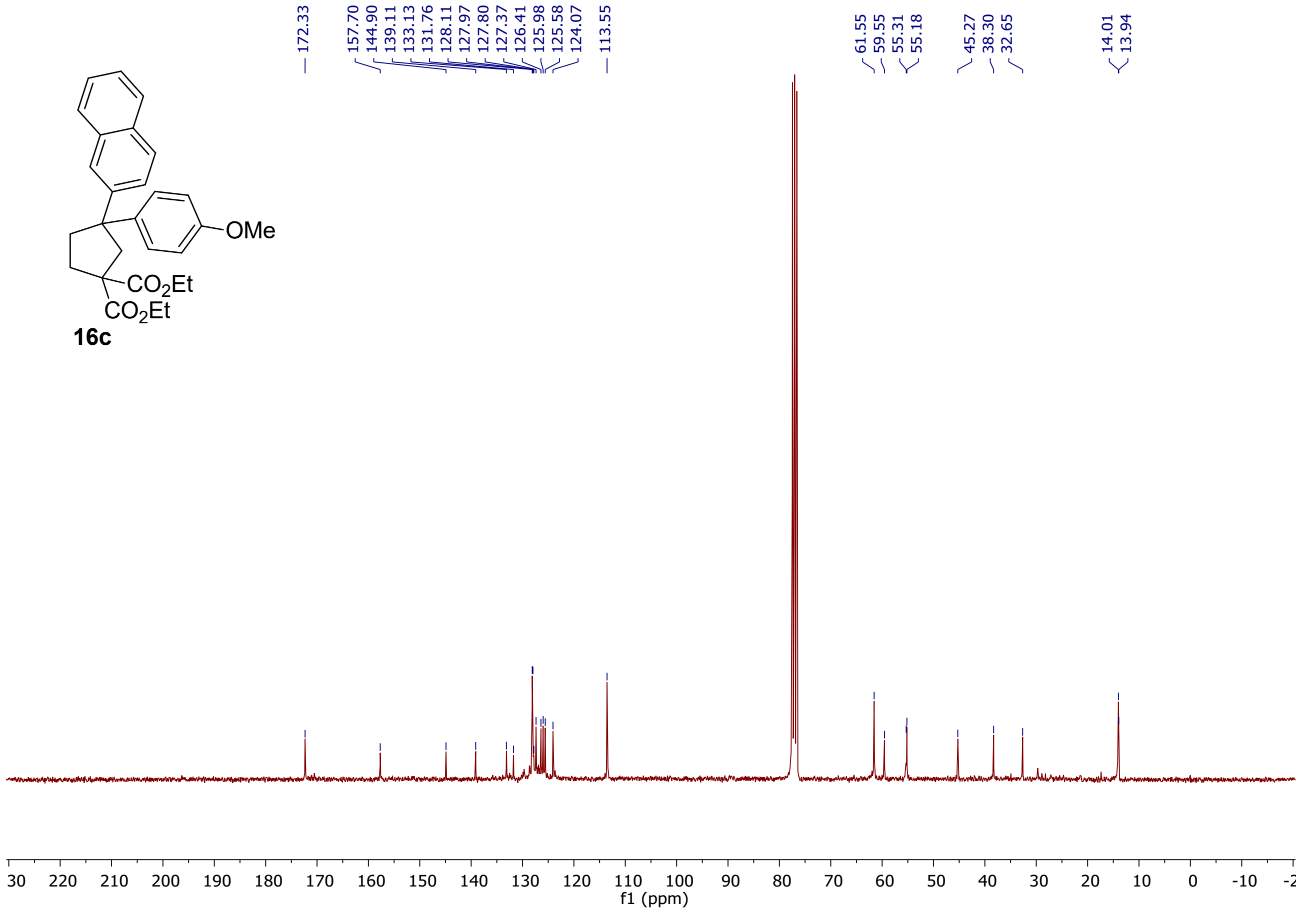

OMe
OMe
CO2Et
CO2Et

16b


7.19
7.16
6.78
6.75
4.12
4.09
4.07
4.05
3.75
3.10
2.46
2.44
2.42
2.33
2.31
2.29
2.28
1.21
1.19
1.16
4.03
4.06
3.94
6.00
1.90
2.00
1.95
6.08
11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


172.35
157.54
139.71
127.81
113.48
61.50
59.48
55.17
54.46
45.61
38.53
32.61
13.98
OMe
OMe
CO2Et
CO2Et
16b
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

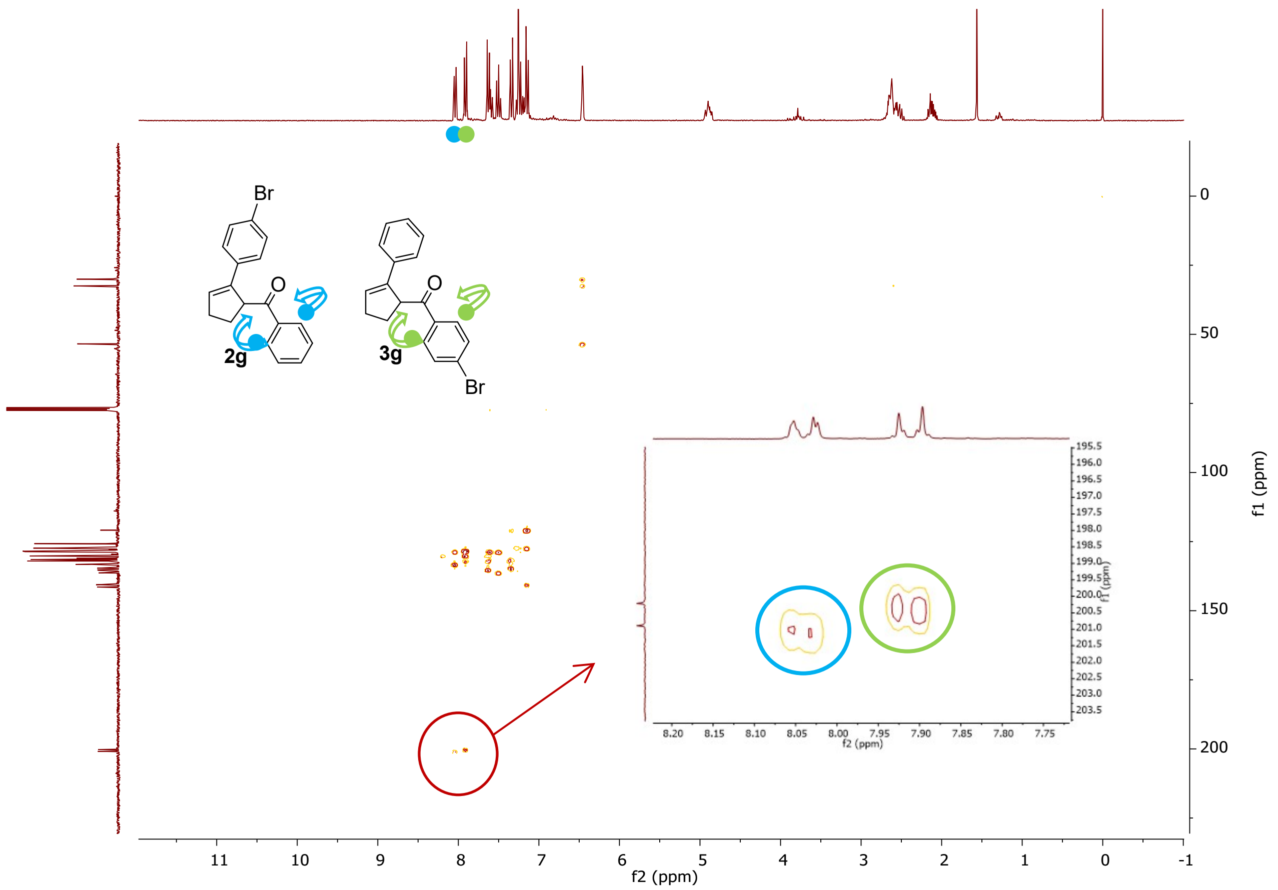




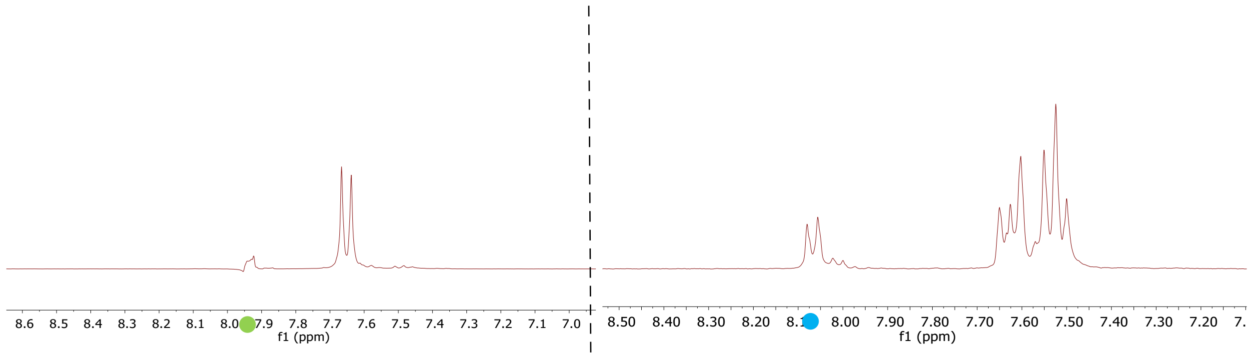
16c

7. Unambiguous assignment of isomers 2 and 3 (exemplified by 2g/3g)

HMBC (Heteronuclear Multiple Bond Correlation)



TOCSY (Total correlation espectroscopy).



In the TOCSY spectrum (right), the signal at 7.91 ppm was irradiated, belonging to the protons represented by the green circle, which, as can be seen in the HMBC spectrum, are related to one of the carbonyl groups. These protons are only related to the signal at 7.62 ppm, indicating that they are part of a *p*-substituted aromatic ring, then this ring is one at the α position to the carbonyl group (product **3g**). When the signal at 8.05 ppm was irradiated (light blue circle, left TOCSY experiment), it correlated with the signals corresponding to the protons at 7.64 ppm and 7.52 ppm, indicating that the signal belongs to an unsubstituted aromatic ring. This ring is then at the α position to the carbonyl group belonging to the other compound in the mixture (product **2g**).

8. References

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