Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Catalytic Applications of [IPr·GaX$_2$][SbF$_6$] and Related Species

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1. General Information

All reactions were performed in oven-dried flasks under argon. Unless otherwise stated, commercially available reagents were used as received without further purification. Gallium chloride, bromide and iodide were obtained from Alfa Aesar and used as received. 1,4-Cyclohexadiene was obtained from Sigma-Aldrich and used as received. Anisole was distilled prior to use. 1,2-Dichloroethane was distilled from calcium hydride and degassed by Freeze-Pump-Thaw technique. Wet DCE was prepared by shaking DCE with water in a separatory funnel followed by collection of the organic layer. Unless otherwise stated, products were purified by chromatography over silica gel. TLC plates were visualized by UV light (254 nm) and *p*-anisaldehyde staining. GC analysis was performed on a Varian 430-GC Instrument, equipped with an autoinjector (CP8410) using a Zebron ZB-1MS or ZB-1 capillary GC column (15 m x 0.25 mm x 0.25 µm). *dl* : *meso* ratio was determined by HPLC equipped with a Circular Dichroism detector (PU-2089 JASCO, CD-2095 JASCO) using a chiral column (chiralpak IC, 250 x 4.6 mm). NMR spectra were recorded on AM250, AV300 or AV360 MHz Bruker spectrometers. Chemical shifts are reported in parts per million (ppm). The spectra were referenced to the residual ^{1}H and ^{13}C signals of the solvents as follows: $CDCl_3$ (^{1}H, δ = 7.27 ppm; ^{13}C, δ = 77 ppm), CD_2Cl_2 (^{1}H, δ = 5.32 ppm). Data are given in the following order: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant (*J*) in Hz and integration. Infrared spectra were recorded on a FTIR spectrometer (Perkin-Elmer spectrum one, NaCl pellets or Bruker Vertex 70 ATR Pike Germanium) and are reported in cm^{-1}. HRMS were performed on MicrOTOFq Bruker spectrometer by electrospray ionization. MS were recorded on DSQ Thermo Fisher instrument by electronic impact. IPr·GaX_3 **1** (X = Cl, Br, I) and [IPr·$GaCl_2$(TFBN)][SbF_6] **3** were synthesized following a reported procedure.[1] The following compounds were previously described: **4**,[2] **6**,[2] **7**,[1b] **8**,[3] **9**,[1b] **12**,[4] **15**,[5] **17**,[5] **18**,[6] **22**,[7] **28**,[8] **30**,[8] **32**,[8] **46**,[2] **48,**[9] **49,**[9] **59**,[1b] **62**,[2] **65**,[2] **71**,[10] **72**,[11] **77**,[2] **86**.[2] NMR spectra of the new compounds **20**, **23**, **24**, **25**, **26**, **47**, **49**, **51**, **53**, **54**, **56**, **60**, **63**, **66**, **67**, **68**, **69**, **73**, **74**, **75**, **76**, **78**, **79**, **80**, **81**, **82**, **84**, **85**, **88** are shown in the appendix.

2. Synthesis of Substrates 23, 53, 68, 69, 73 and 75:

Dimethyl 2-benzyl-2-(4-hydroxy-4,4-diphenylbut-2-yn-1-yl)malonate 23:

To a solution of arenyne **4** (1 equiv, 1 g, 3.84 mmol) in THF (40 mL) was added *n*-butyllithium (1.05 equiv, 1.6 M in hexane, 2.52 mL, 4.03 mmol) dropwise at -78 °C. The mixture was stirred for half an hour and benzophenone (1.05 equiv, 0.735 g, 4.03 mmol) was added in one portion. The resulting mixture was allowed to warm up to 0 °C gradually and stirred for an additional hour. The reaction mixture was warmed to room temperature and stirred overnight. The reaction was then quenched with

[1] (a) N. Marion, E. C. Escudero-Adán, J. Benet-Buchholz, E. D. Stevens, L. Fensterbank, M. Malacria, S. P. Nolan, *Organometallics*, **2007**, *26*, 3256-3259. (b) S. Tang, J. Monot, A. El-Hellani, B. Michelet, R. Guillot, C. Bour, V. Gandon, V. *Chem. Eur. J*., **2012**, *18*, 10239-10243. (c) C. Bour, J. Monot, S. Tang, R. Guillot, J. Farjon, V. Gandon, *Organometallics*, **2014**, *33*, 594-599.
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[10] S. T. A. Shah, K. M. Khan, H. Hussain, M. U. Anwar, M. Fecker, W. Voelter, *Tetrahedron* **2005**, *61*, 6652-6656.
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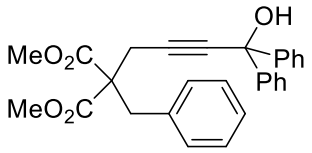
a satd aq. $NaHCO_3$ solution. The organic layer was separated and the aqueous layer was extracted with Et_2O. The combined organics were washed with brine and dried over $MgSO_4$. The solvent was removed under vacuum to give the crude product, which was further purified by silica gel chromatography to afford compound **23** (47%, 792 mg, 1.79 mmol).

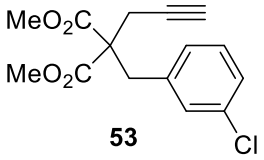


23

Sticky yellow oil. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.62 (d, J = 7.7 Hz, 4H), 7.39-7.24 (m, 9H), 7.22-7.05 (m, 2H), 3.73 (s, 6H), 3.42 (s, 2H), 2.89 (br s, 1H), 2.82 (s, 2H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 170.2, 145.0, 135.3, 129.8, 128.4, 128.2, 127.7, 127.2, 126.0, 87.1, 82.9, 74.5, 58.5, 52.8, 37.9, 22.8. FT-IR (film): ν 3479, 3030, 1737, 1450, 1210, 701 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{28}H_{26}O_5Na$ $[M+Na]^+$: 465.1672 found: 465.1691.

Dimethyl 2-(3-chlorobenzyl)-2-(prop-2-yn-1-yl)malonate 53:

Dimethyl propargyl malonate (1 equiv, 742 mg, 4.1 mmol) was added to a suspension of NaH (1.2 equiv, 60% dispersion in mineral oil, 199 mg, 5.0 mmol) in 10 mL THF at -20 °C. The resulting mixture was stirred at room temperature until the evolution of hydrogen gas subsided. 1-(Bromomethyl)-3-chlorobenzene (1.2 equiv, 1 g, 5.0 mmol) was then added at 0 °C. The resulting mixture was stirred at room temperature for 20 h and 20 mL of water were added. The two layers were separated, and the aqueous layer was extracted with DCM (3 × 50 mL). The combined organic extracts were washed with brine, dried over $MgSO_4$, filtered, and concentrated under vacuum. The residue was purified by column chromatography over silica gel (cyclohexane, EtOAc) to afford compound **53** (87%, 1.1 g, 3.6 mmol).



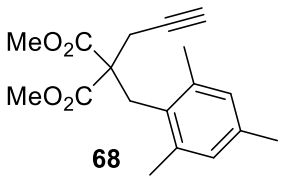
53

White solid. mp = 73 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.24-7.22 (m, 2H), 7.15 (m, 1H), 7.06 (dt, J = 6.4 Hz, J = 1.9 Hz, 1H), 3.77 (s, 6H), 3.39 (s, 2H), 2.70 (d, J = 2.8 Hz, 2H), 2.18 (t, J = 2.8 Hz, 1H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 169.8, 137.5, 134.3, 129.9, 129.7, 128.0, 127.5, 78.9, 72.5, 58.1, 52.9, 37.1, 22.2. FT-IR (film): ν 3288, 2363, 1734, 1432, 1208, 1195, 1179, 853 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{15}H_{15}O_5ClNa$ $[M+Na]^+$: 317.0551 found: 317.0545.

Dimethyl 2-(prop-2-yn-1-yl)-2-(2,4,6-trimethylbenzyl)malonate 68:

To a suspension of NaH (1.2 equiv, 60% dispersion in mineral oil, 316 mg, 7.9 mmol) in 30 mL THF, was added dimethyl propargylmalonate (1 equiv, 1.12 g, 6.6 mmol) dropwise at -78 °C. The resulting mixture was allowed to warm up to room temperature and stirred until the evolution of hydrogen gas subsided. 2-(Bromomethyl)-1,3,5-trimethylbenzene (1.2 equiv, 1.7 g, 7.9 mmol) was then added at -78 °C in one portion. The resulting mixture was stirred at room temperature for 20 h and water (20 mL) were added. The two layers were separated and the aqueous layer was extracted with Et_2O

(3 x 30 mL). The combined organic extracts were washed with brine, dried over anhydrous $MgSO_4$, filtered and concentrated. The residue was purified by chromatography over silica gel to afford compound **68** in quantitative yield (1.99 g, 6.6 mmol).

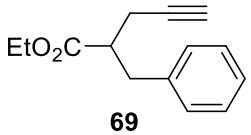


68

Colorless oil. ^{1}H NMR (360 MHz, $CDCl_3$) δ 6.81 (s, 2H), 3.62 (s, 6H), 3.57 (s, 2H), 2.83 (d, J = 2.5 Hz, 2H), 2.29 (s, 6H), 2.23 (s, 3H), 2.07 (t, J = 2.5 Hz, 1H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 170.9, 138.2, 136.1, 130.6, 129.1, 79.8, 71.4, 58.5, 52.5, 31.4, 25.2, 20.8, 20.7. FT-IR (film): ν 3283, 2953, 1736, 1435, 1199 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{18}H_{22}O_4Na$ $[M+Na]^+$: 325.1410 found: 325.1397.

Ethyl 2-benzylpent-4-ynoate 69:

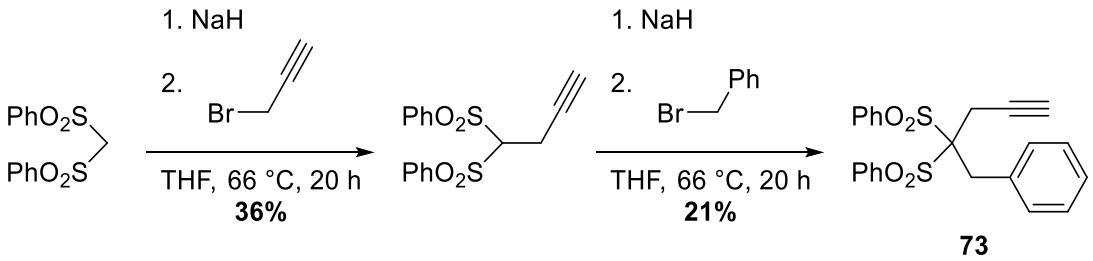
Diisopropylamine (1.1 equiv, 8.7 mL, 62.4 mmol) was added dropwise at -78 °C to *n*-butyllithium (1.05 equiv, 1.6 M in hexane, 37 mL, 59.5 mmol). Ethyl 3-phenylpropanoate (1 equiv, 10 g, 56.7 mmol) was added dropwise and the resulting mixture was stirred for 1 h at -78 °C. Propargyl bromide (1.05 equiv, 6.41 mL, 59.5 mmol) was then added and the mixture was stirred for 2 h at -78 °C. After allowing the solution to warm to room temperature, the reaction was quenched with a satd aq. NH_4Cl solution and the organic layer was extracted three times with EtOAc. The organic layer was washed with an aq. HCl 2M solution, then with a satd aq. $NaHCO_3$ solution, dried over $MgSO_4$ and concentrated under vacuum. The residue was purified by chromatography over silica gel (cyclohexane, EtOAc) to afford compound **69** (66%, 8.1 g, 37.4 mmol).



69

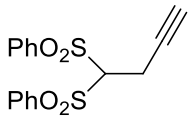
Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33-7.19 (m, 5H), 4.14 (q, J = 7.2 Hz, 2H), 3.09-2.93 (m, 2H), 2.90-2.81 (m, 1H), 2.47-2.38 (m, 2H), 2.06 (t, J = 2.5 Hz, 1H), 1.21 (t, J = 7.2 Hz, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 173.6, 138.4, 129.0, 128.4, 126.5, 81.2, 70.3, 60.6, 46.2, 36.9, 20.5, 14.1. HRMS (ESI) *m/z*: Calcd for $C_{14}H_{16}O_2Na$ $[M+Na]^+$: 239.1043 found: 239.1038.

1-Phenyl-2,2-bis(phenylsulfonyl)pent-4-yne 73:



73

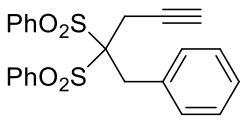
To a suspension of NaH (1.1 equiv, 60% dispersion in mineral oil, 0.52 g, 13 mmol) in 10 mL THF was slowly added a solution of bis(phenylsulfonyl)methane (3.5 g, 11.8 mmol) in THF (40 mL). The resulting mixture was stirred at room temperature for 5 min and at 50 °C for 15 min. Propargyl bromide (1.05 equiv, 1.84 g, 1.38 mL, 12.4 mmol) was then added dropwise and the mixture was stirred under reflux for 20 h. The reaction was diluted with Et_2O (20 mL) and quenched with a satd aq. NH_4Cl solution (20 mL). The two layers were separated and the aqueous phase was extracted three times with Et_2O. The combined organics were washed with an aq. HCl 5% solution, brine, dried over $MgSO_4$ and concentrated under vacuum. The crude product was filtered on a pad of silica gel (DCM) and concentrated in vacuo to obtain a pale yellow foam which was further purified by chromatography over silica gel (cyclohexane, EtOAc) and recrystallized from EtOH to afford 1,1-bis(phenylsulfonyl)but-3-yne (36%, 1.43 g, 4.26 mmol).



1,1-bis(phenylsulfonyl)but-3-yne

White solid. ^1H NMR (250 MHz, $CDCl_3$) δ 8.02 (d, J = 8.4 Hz, 4H), 7.70-7.58 (m, 6H), 4.60 (t, J = 6.1 Hz, 1H), 3.14 (dd, J = 6.1 Hz, J = 2.7 Hz, 2H), 1.95 (t, J = 2.7 Hz, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 137.6, 134.9, 129.8, 129.2, 82.0, 76.9, 72.2, 16.6. HRMS (ESI) *m/z*: Calcd for $C_{16}H_{14}O_4S_2Na$ $[M+Na]^+$: 357.0226 found: 357.0227. The data correspond to those previously reported in the literature.[12]

To a suspension of NaH (1.1 equiv, 60% dispersion in mineral oil, 92.2 mg, 2.31 mmol) in 10 mL THF was slowly added a solution of 1,1-bis(phenylsulfonyl)but-3-yne (1 equiv, 700 mg, 2.09 mmol) in THF (10 mL). The resulting mixture was stirred at room temperature for 5 min and at 50 °C for 15 min. Benzyl bromide (1.2 equiv, 429 mg, 0.3 mL, 2.51 mmol) was then added dropwise and the mixture was stirred under reflux for 20 h. The reaction was diluted with Et_2O (20 mL) and quenched with a satd aq. NH_4Cl solution (20 mL). The two layers were separated and the aqueous phase was extracted three times with Et_2O. The combined organics were washed with an aq. HCl 5% solution, brine, dried over $MgSO_4$ and concentrated under vacuum. The crude product was purified by chromatography over silica gel (pentane, Et_2O) to obtain a pale yellow foam which was triturated with boiling Et_2O and filtered while still warm to afford compound **73** (21%, 188 mg, 0.443 mmol).

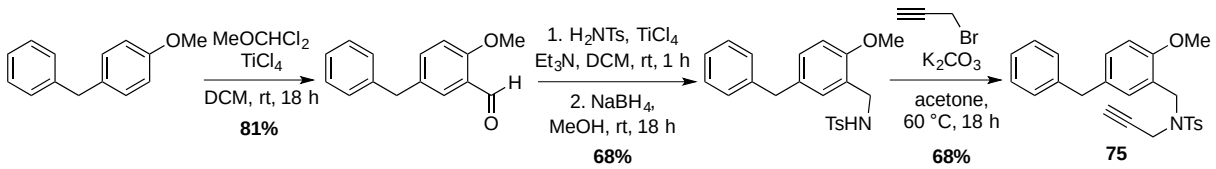


73

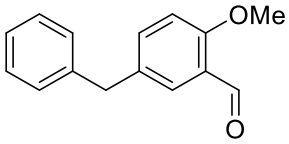
White solid. mp = 95-97 °C. ^1H NMR (250 MHz, $CDCl_3$) δ 7.94 (d, J = 8.2 Hz, 4H), 7.67 (tt, J = 7.4 Hz, J = 1.1 Hz, 2H), 7.53-7.46 (m, 6H), 7.30-7.26 (m, 3H), 3.77 (s, 6H), 3.80 (s, 2H), 3.22 (d, J = 2.8 Hz, 2H), 2.14 (t, J = 2.8 Hz, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 137.4, 134.6, 132.5, 131.5 (2C), 128.5, 128.3, 127.7, 90.7, 75.8, 35.1, 22.2 (one quaternary C is missing). FT-IR (film): ν 3273, 1447, 1334, 1311, 1145, 1076, 753, 733, 579 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{23}H_{21}O_4S_2$ $[M+H]^+$: 425.0876 found: 425.0875.

[12] J. R. Rodríguez, L. Castedo , J. L. Mascareñas, *J. Org. Chem.*, **2000**, *65*, 2528-2531.

***N*-(5-benzyl-2-methoxybenzyl)-4-methyl-N-(prop-2-yn-1-yl)benzenesulfonamide 75:**



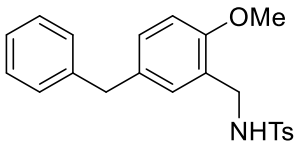
To a solution of 1-benzyl-4-methoxybenzene[5] (1 equiv, 1.98 g, 10.0 mmol) and α,α-dichloromethyl methyl ether (1.1 equiv, $MeOCHCl_2$, 1.26 g, 11.0 mmol) in DCM (30 mL), $TiCl_4$ (1.1 equiv, 1.2 mL, 11.0 mmol) in DCM (20 mL) was added dropwise over 20 minutes at 0 °C. The mixture was magnetically stirred at room temperature overnight, then 50 mL of DCM and 30 mL of water were added. The two layers were separated, and the aqueous layer was extracted with DCM (3×50 mL). The combined organic extracts were washed with brine, dried over anhydrous $MgSO_4$, filtered, and concentrated. The crude product was purified by silica gel column chromatography using cyclohexane/EtOAc (80/20) as eluent to afford 5-benzyl-2-methoxybenzaldehyde (81%, 1.84 g, 8.1 mmol).



5-benzyl-2-methoxybenzaldehyde

Yellow oil. ^{1}H NMR (250 MHz, $CDCl_3$) δ 10.48 (s, 1H), 7.72 (s, 1H), 7.40-7.18 (m, 6H), 6.93 (d, J = 8.7 Hz, 1H), 3.97 (s, 2H), 3.91 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 189.6, 160.2, 140.6, 136.3, 133.4, 129.9, 129.2, 128.6, 128.4, 128.3, 126.1, 124.4, 111.7, 55.5, 40.6. HRMS (ESI) *m/z*: Calcd for $C_{15}H_{14}O_2Na$ $[M+H]^+$: 249.0891, found: 226.0888.

5-Benzyl-2-methoxybenzaldehyde (1 equiv, 1.81 g, 8.0 mmol), tosylamide (2 equiv, 2.04 g, 16.0 mmol) and triethylamine (5 equiv, 4.05 g, 40.0 mmol) were dissolved in DCM (50 mL) and cooled to 0 °C. $TiCl_4$ (1 equiv, 0.9 mL, 8.0 mmol) in DCM (10 mL) was added dropwise over 10 minutes, then the ice-bath was removed and stirring was continued for 1 hour. The mixture was hydrolyzed with a satd aq. $NaHCO_3$ solution, the two phases were separated, the aqueous phase was extracted three times with DCM and the combined organic layers were washed with brine, dried over $MgSO_4$ and concentrated under reduced pressure. To a solution of the above crude product in MeOH (30 mL), $NaBH_4$ (0.61 g, 16.0 mmol) was added in small portions at room temperature, then the solution was magnetically stirred overnight. After hydrolysis with water (30 mL), phase separation, extraction with DCM (3×50 mL), drying of the organic phase over $MgSO_4$ and concentration under reduced pressure, the crude product was purified by silica gel column chromatography using cyclohexane/EtOAc (85/15) as eluent to afford *N*-(5-benzyl-2-methoxybenzyl)-4-methylbenzenesulfonamide (68%, 1.93 g, 5.1 mmol).

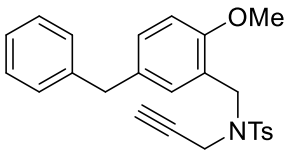


N-(5-benzyl-2-methoxybenzyl)-4-methylbenzenesulfonamide

Pale yellow oil. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.65 (d, J = 8.3 Hz, 2H), 7.33-7.14 (m, 7H), 7.00 (dd, J = 8.3, 2.3 Hz, 1H), 6.91 (d, J = 2.3 Hz, 1H), 6.65 (d, J = 8.3 Hz, 1H), 5.27 (t, J = 6.4 Hz, 1H), 4.12

(d, *J* = 6.4 Hz, 2H), 3.83 (s, 2H), 3.72 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 155.1, 142.5, 140.4, 136.6, 133.0, 129.7, 129.3, 128.5, 128.1, 127.2, 126.2, 124.3, 112.7, 56.4, 43.5, 41.0, 21.5. HRMS (ESI) *m/z*: Calcd for $C_{22}H_{23}O_3NSNa$ $[M+Na]^+$: 404.1296, found: 404.1298.

To a mixture of propargyl bromide (1.2 equiv, 80% in toluene, 0.97 g, 6.5 mmol) and K_2CO_3 (3.7 equiv, 2.76 g, 20.0 mmol) in 50 mL acetone was added *N*-(5-benzyl-2-methoxybenzyl)-4-methylbenzenesulfonamide (1 equiv, 1.93 g, 5.4 mmol). The reaction mixture was magnetically stirred at 60 °C for 12 hours, and then quenched with water. The aqueous layer was extracted with ether (3×20 mL). The combined organic layers were washed with brine, dried over $MgSO_4$, and solvents were evaporated under reduced pressure. The crude product was purified by silica gel column chromatography using cyclohexane/EtOAc (90/10) as eluent to give **75** (75%, 2.07 g, 4.9 mmol).



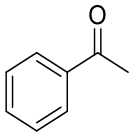
75

White solid. mp = 82-83°C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.32-7.17 (m, 8H), 7.07 (dd, *J* = 8.3, 2.3 Hz, 1H), 6.77 (d, *J* = 8.3 Hz, 1H), 4.43 (s, 2H), 4.01 (d, *J* = 2.3 Hz, 2H), 3.93 (s, 2H), 3.76 (s, 3H), 2.47 (s, 3H), 2.00 (t, *J* = 2.3 Hz, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 156.2, 143.3, 141.4, 136.5, 133.3, 130.5, 129.3, 128.7, 128.4, 127.8, 126.0, 123.3, 110.7, 77.2, 73.4, 55.4, 44.7, 41.0, 36.3, 21.5. HRMS (ESI) *m/z*: Calcd for $C_{25}H_{26}O_3NS$ $[M+H]^+$: 420.1628, found: 420.1622. Calcd for $C_{25}H_{25}O_3NSNa$ $[M+Na]^+$: 442.1447, found: 442.1440.

3. C-O Bond Formation from Alkynes and Alkenes (Scheme 3):

General procedure: IPr·GaX_3 (X = Cl, Br or I, 5 mol%, 0.0125 mmol) and $AgSbF_6$ (7 mol%, 6 mg, 0.0175 mmol) were mixed in a screw-cap vial under argon. Wet DCE (0.5 mL) was added and the mixture was stirred at room temperature for 5 min. A solution of phenylacetylene, **12**, or **18** (1 equiv, 0.25 mmol) diluted in wet DCE (0.5 mL) was added and the mixture was stirred at 80 °C for 20 h. The mixture was then filtered on a short pad of silica gel, which was rinsed with DCM (5 mL). Unless otherwise stated, solvents were removed under reduced pressure and the yield was determined by ^{1}H NMR analysis after addition of *p*-anisaldehyde (1 equiv, 30 µL) as internal standard.

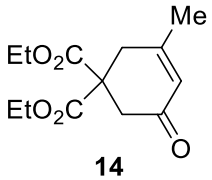
Acetophenone:



63%. ^{1}H NMR (250 MHz, $CDCl_3$) δ 8.01-7.97 (m, 2H), 7.63-7.46 (m, 3H), 2.64 (s, 3H).

Diethyl 3-methyl-5-oxocyclohex-3-ene-1,1-dicarboxylate 14:

Following the general procedure and using IPr·$GaBr_3$ as precatalyst. After the work-up, solvents were removed under reduced pressure and the crude product was purified by chromatography over silica gel (cyclohexane, EtOAc) to afford compound **14** (79%, 26 mg, 0.102 mmol).

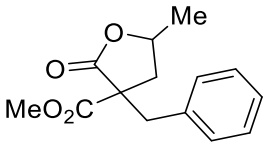


14

^{1}H NMR (360 MHz, $CDCl_3$) δ 5.89 (br s, 1H), 4.20 (q, J = 7.1 Hz, 4H), 2.88 (s, 2H), 2.86 (s, 2H), 2.01 (s, 3H), 1.24 (t, J = 7.1 Hz, 6H). The data correspond to those previously reported in the literature.[13]

Methyl 3-benzyl-5-methyl-2-oxotetrahydrofuran-3-carboxylate 20:

Following the general procedure and using IPr·$GaCl_3$ as precatalyst. After the work-up, solvents were removed under reduced pressure and the crude product was purified by chromatography over silica gel (cyclohexane, EtOAc) to afford compound **20** (64%, 40 mg, 0.16 mmol).



20

Isolated as a mixture of diastereoisomers, *d.r.* = 7:3 (determined by ^{1}H NMR). Colorless oil. Major isomer: ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.34-7.16 (m, 5H), 4.61 (m, 1H), 3.82 (s, 3H), 3.33 (d, J = 3.0 Hz, 2H), 2.68 (dd, J = 13.1 Hz, J = 6.1 Hz, 1H), 1.82 (dd, J = 13.1 Hz, J = 9.8 Hz, 1H), 1.21 (d, J = 6.1 Hz, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 173.9, 169.8, 135.6, 130.0, 128.6, 127.3, 75.1, 57.9, 53.2, 39.5, 38.3, 20.6. Minor isomer: ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.34-7.16 (m, 5H), 3.85 (s, 3H), 3.73 (m, 1H), 3.39 (d, J = 13.7 Hz, 1H), 3.24 (d, J = 13.7 Hz, 1H), 2.43 (dd, J = 7.5 Hz, J = 6.1 Hz, 2H), 1.31 (d, J = 6.1 Hz, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 173.9, 170.7, 135.1, 129.9, 128.8, 127.6, 74.6, 57.2, 53.2, 39.7, 37.8, 21.3. FT-IR (film): ν 2955, 2931, 2850, 1773, 1736, 1497, 1455, 1348, 1266, 1180, 1107, 1031, 997, 948, 703 cm^{-1}. GC-MS (CI) *m/z*: Calcd for $C_{14}H_{20}O_4N$ $[M+NH_4]^+$: 266.1 found: 266.0 (maj), 266.2 (min).

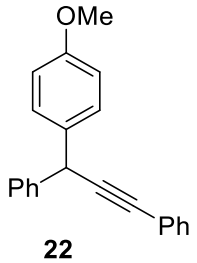
4. C-C Bond Formation from Alcohols (Scheme 4):

(3-(4-Methoxyphenyl)prop-1-yne-1,3-diyl)dibenzene 22:

A [IPr·$GaCl_2$][SbF_6] solution was prepared by adding IPr·$GaCl_3$ (5 mol%, 7 mg, 0.0125 mmol) and $AgSbF_6$ (7 mol%, 6 mg, 0.0175 mmol) to DCE (1 mL) in a screw-cap vial under argon. In a separated

[13] C. Zhang, D.-M. Cui, L.-Y. Yao, B.-S. Wang, Y.-Z. Hu, T. Hayashi, *J. Org. Chem.* **2008**, *73*, 7811-13.

tube, anisole (3 equiv, 81.1 mg, 0.0815 mL, 0.75 mmol) was added to a solution of **21** (1 equiv, 52.1 mg, 0.25 mmol) in DCE (0.9 mL). 0.1 mL of the [IPr·$GaCl_2$][SbF_6] solution previously prepared was then added and the mixture was stirred at room temperature for 1 h. The reaction was monitored by TLC. After filtration on a celite pad and evaporation of the volatiles, the crude product was purified by chromatography over silica gel (cyclohexane) to afford compound **22** (80%, 60 mg, 0.201 mmol).



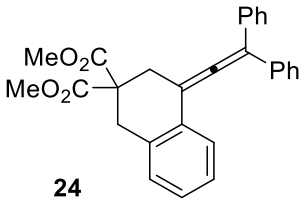
22

Pale yellow oil. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.48-7.20 (m, 12 H), 6.84 (d, J = 8.7 Hz, 2H), 5.15 (s, 1H), 3.75 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 158.5, 142.0, 133.9, 131.6, 128.9, 128.6, 128.2, 127.9, 127.8, 126.8, 123.5, 114.0, 90.5, 84.7, 55.2, 42.9. The data correspond to those previously reported in the literature.[14]

Cyclization of compound 23:

A [IPr·$GaCl_2$][SbF_6] solution was prepared by adding IPr·$GaCl_3$ (5 mol%, 7 mg, 0.0125 mmol) and $AgSbF_6$ (7 mol%, 6 mg, 0.0175 mmol) to DCE (1 mL) in a screw-cap vial under argon. In a separated tube, compound **23** (1 equiv, 111 mg, 0.25 mmol) was dissolved in DCE (0.9 mL). 0.1 mL of the [IPr-$GaCl_2$][SbF_6] solution previously prepared was then added and the mixture was stirred at the indicated temperature for 1-16 h. The mixture was then filtered on a short pad of silica gel, which was rinsed with DCM (5 mL). After evaporation, the crude product was purified by flash chromatography over silica gel (cyclohexane, EtOAc).

Dimethyl 4-(2,2-diphenylvinylidene)-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 24:

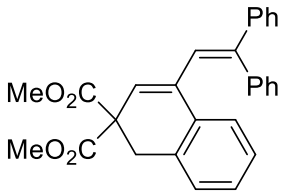


24

Sticky white paste. ^{1}H NMR (360 MHz, C_6D_6) δ 7.80 (d, J = 7.3 Hz, 1H), 7.66 (d, J = 7.3 Hz, 4H), 7.30-7.19 (m, 6H), 7.14-7.01 (m, 3H), 3.50 (s, 2H), 3.40 (s, 2H), 3.35 (s, 6H). ^{13}C NMR (90 MHz, C_6D_6) δ 206.6, 170.8, 137.3, 133.7, 130.2, 129.8, 129.1, 128.9, 127.9, 127.8, 127.2, 126.9, 114.3, 102.7, 54.2, 52.3, 35.8, 34.3. FT-IR (film): ν 3024, 2952, 2279, 1736, 1598, 1492, 1443, 1251, 1074, 769, 697 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{28}H_{24}O_4Na$ [M+Na]$^+$: 447.1567 found: 447.1554.

[14] Z.-P. Zhan, J.-L.Yu, H.-J. Liu, Y.-Y. Cui, R.-F. Yang, W.-Z. Yang, J.-P. Li, *J. Org. Chem.*, **2006**, *71*, 8298-8301.

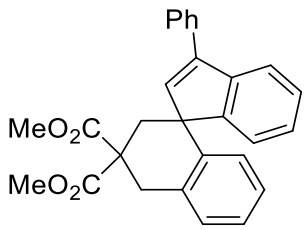
Dimethyl 4-(2,2-diphenylvinyl)naphthalene-2,2(1*H*)-dicarboxylate 25:



25

White solid. mp = 144 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.43-7.35 (m, 6H), 7.25-7.15 (m, 8H), 6.72 (d, J = 1.6 Hz, 1H), 5.80 (d, J = 1.6 Hz, 1H), 3.58 (s, 6H), 3.36 (s, 2H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 170.3, 146.0, 142.7, 139.9, 137.0, 132.7, 132.5, 129.9, 128.3, 128.2, 128.0, 127.9, 127.8, 127.7, 127.0, 126.8, 125.7, 124.8, 123.7, 54.6, 52.8, 34.2. FT-IR (film): ν 3056, 3023, 2953, 1737, 1445, 1434, 1271, 1227, 766, 732, 700 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{28}H_{24}O_4Na$ $[M+Na]^+$: 447.1567 found: 447,1579.

Dimethyl 3-phenyl-2'*H*-spiro[indene-1,1'-naphthalene]-3',3'(4'*H*)-dicarboxylate 26:



26

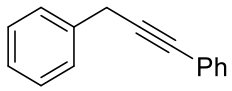
White solid. mp = 162 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.61-7.57 (m, 3H), 7.48-7.43 (m, 3H), 7.41-7.32 (m, 2H), 7.26-7.22 (m, 3H), 7.17 (td, J = 7.5 Hz, J = 1.3 Hz, 1H), 6.96 (t, J = 7.5 Hz, 1H), 6.50 (dd, J = 8.0 Hz, J = 1.0 Hz, 1H), 6.43 (s, 1H), 3.78 (s, 3H), 3.75 (s, 3H), 3.71 (dd, J = 16.3 Hz, J = 2.2 Hz, 1H), 3.33 (d, J = 16.3 Hz, 1H), 2.97 (d, J = 14.3 Hz, 1H), 2.60 (dd, J = 14.3 Hz, J = 2.2 Hz, 1H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 172.0, 171.7, 155.1, 142.7, 141.7, 141.6, 135.3, 135.3, 133.9, 129.0, 128.6, 127.8, 127.7, 127.1, 127.0, 126.9, 126.7, 126.3, 123.5, 120.8, 54.7, 53.3, 52.9, 52.6, 38.1, 35.3. FT-IR (film): ν 3062, 3025, 2952, 1736, 1491, 1445, 1273, 1244, 1213, 911, 754, 735, 700 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{28}H_{24}O_4Na$ $[M+Na]^+$: 447.1567 found: 447,1561.

5. C-H Bond Formation from Alcohols (Table 1):

General procedure A: a $[IPr{\cdot}GaCl_2][SbF_6]$ solution was prepared by adding $IPr{\cdot}GaCl_3$ (5 mol%, 7 mg, 0.0125 mmol) and $AgSbF_6$ (7 mol%, 6 mg, 0.0175 mmol) to DCE (1 mL) in a screw-cap vial under argon. In a separated tube, Et_3SiH or Ph_2SiHCl (3 equiv, 0.75 mmol) was added to a solution of alcohol **21**, **34**, **42** or **44** in DCE (0.9 mL). 0.1 mL of the $[IPr{\cdot}GaCl_2][SbF_6]$ solution was then added and the mixture was stirred at room temperature for 1 h. After filtration on a celite pad and evaporation of the volatiles, the crude product was purified by chromatography over silica gel (cyclohexane, EtOAc) to afford the corresponding deoxygenated product.

General procedure B: [IPr·$GaCl_2$(TFBN)][SbF_6] (5 mol%, 11.5 mg, 0.0125 mmol) was dissolved in DCE (1 mL) in a screw-cap vial under argon. In a separated tube, Et_3SiH or Ph_2SiHCl (3 equiv, 0.75 mmol) was added to a solution of alcohol **21**, **28**, **30**, **32**, **34**, **36**, **38**, **40** or **42** in DCE (0.9 mL). 0.1 mL of the [IPr·$GaCl_2$(TFBN)][SbF_6] solution was then added and the mixture was stirred at room temperature for 1 h. After filtration on a celite pad and evaporation of the volatiles, the crude product was purified by chromatography over silica gel (cyclohexane, EtOAc) to afford the corresponding deoxygenated product.

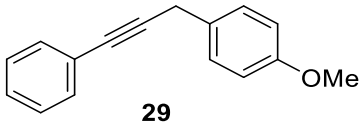
Prop-1-yne-1,3-diyldibenzene 27:



27

Following the general procedure **B**. 50%. Colorless oil. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.55-7.26 (m, 10H), 3.88 (s, 2H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 136.8, 131.6, 128.5, 128.2, 127.9, 127.8, 126.6, 123.7, 87.5, 82.7, 25.8. MS (EI) *m/z* (%I): 192.1 (82) $[M]^+$, 191.1 (100), 105.0 (27), 77.0 (21). The data correspond to those previously reported in the literature.[8]

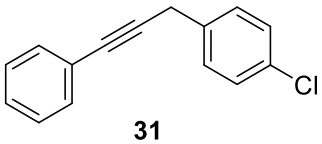
1-Methoxy-4-(3-phenylprop-2-yn-1-yl)benzene 29:



29

Following the general procedure **B**. 90%. Yellow oil. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.49-7.46 (m, 2H), 7.36-7.30 (m, 5H), 6.91 (d, J = 8.6 Hz, 2H), 3.81 (s, 3H), 3.79 (s, 2H). The data correspond to those previously reported in the literature.[8]

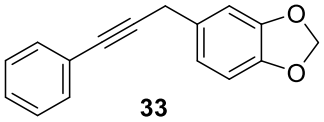
1-Chloro-4-(3-phenylprop-2-yn-1-yl)benzene 31:



31

Following the general procedure **B**. 53%. Yellow oil. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.49-7.46 (m, 2H), 7.39-7.27 (m, 7H), 3.82 (s, 2H). The data correspond to those previously reported in the literature.[8]

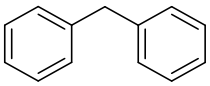
5-(3-Phenylprop-2-yn-1-yl)benzo[*d*][1,3]dioxole 33:



33

Following the general procedure **B**. 90%. Yellow oil. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.49-7.46 (m, 2H), 7.34-7.27 (m, 3H), 6.95 (s, 1H), 6.88 (d, J = 8.2 Hz, 1H), 6.80 (d, J = 8.2 Hz, 1H), 5.96 (s, 2H), 3.77 (s, 2H). The data correspond to those previously reported in the literature.[8]

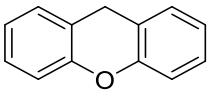
Diphenylmethane 35:



35

Following the general procedure **B**. 95%. Yellow oil. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.40-7.24 (m, 10H), 4.06 (s, 2H).

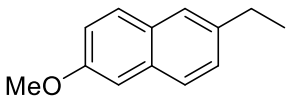
9*H*-Xanthene 37:



37

Following the general procedure **B**. 85%. White solid. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.30-7.21 (m, 4H), 7.13-7.05 (m, 4H), 4.11 (s, 2H). The data correspond to those previously reported in the literature.[15]

2-Ethyl-6-methoxynaphthalene 39:

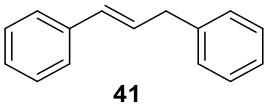


39

Following the general procedure **B**. 95%. White solid. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.75-7.71 (m, 2H), 7.61 (s, 1H), 7.37 (dd, J = 3.3 Hz, J = 1.6 Hz, 1H), 7.20-7.16 (m, 2H), 3.96 (s, 3H), 2.83 (q, J = 7.5 Hz, 2H), 1.37 (t, J = 7.5 Hz, 3H). The data correspond to those previously reported in the literature.[16]

[15] Z. Cong, T. Miki, O. Urakawa, H. Nishino, *J. Org. Chem.* **2009**, *74*, 3978-81.
[16] B.-T. Guan, S.-K. Xiang, B.-Q. Wang, Z.-P. Sun, Y. Wang, K.-Q. Zhao, Z.-J. Shi, *J. Am. Chem. Soc.* **2008**, *130*, 3268-3269.

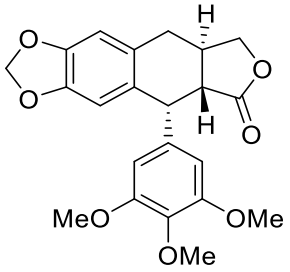
(*E*)-Prop-1-ene-1,3-diyldibenzene 41:



41

Following the general procedure **B**. 91%. Yellow oil. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.43-7.22 (m, 10H), 6.55-6.35 (m, 2H), 3.60 (d, J = 6.4 Hz, 2H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 140.2, 137.5, 131.1, 129.2, 128.6, 128.5 (2C), 127.1, 126.2, 126.1, 39.3. MS (EI) *m/z* (%I): 194.1 (100) $[M]^+$, 179.1 (47), 115.0 (75). The data correspond to those previously reported in the literature.[17]

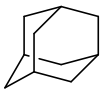
Deoxypodophyllotoxin 43:



43

Following the general procedure **B**. 62%. White solid. ^{1}H NMR (250 MHz, $CDCl_3$) δ 6.68 (s, 1H), 6.53 (s, 1H), 6.35 (s, 2H), 5.96 (s, 1H), 5.94 (s, 1H), 4.61 (brs, 1H), 4.49-4.43 (1H), 3.97-3.89 (m, 1H), 3.81 (s, 3H), 3.76 (s, 6H), 3.12-3.03 (m, 1H), 2.80-2.74 (m, 3H). The data correspond to those previously reported in the literature.[18]

Adamantane 45:



45

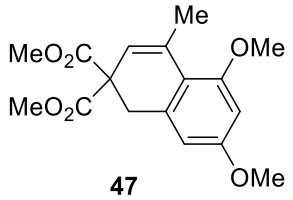
Following the general procedure **A** using 5 mol% of $[IPr{\cdot}GaCl_2][SbF_6]$ at 80 °C. 99% conversion determined by ^{1}H-NMR analysis of the crude product using *p*-anisaldehyde (1 equiv) as internal standard.

[17] P. Liu, Y.-m. Pan, K. Hu, X.-c. Huang, Y. Liang, H.-s. Wang, *Tetrahedron*, **2013**, *69*, 7925-7930.
[18] J. Wang, X. Zhi, X. Yu, H. Xu, *J. Agric. Food Chem.* **2013**, *61*, 6336-6343.

6. (Di)Hydroarylation of Arenynes (Schemes 5, 6, 7, 9, 13, 14, 15, 16 and 17):

General procedure: IPr·$GaCl_3$ (5 mol%, 7 mg, 0.0125 mmol) and $AgSbF_6$ (7 mol%, 6 mg, 0.0175 mmol) were mixed in a screw-cap vial under argon. DCE (0.5 mL) was added and the mixture was stirred at room temperature for 5 min. Arenyne **4**, **46**, **48**, **53**, **62**, **65**, **68**, **69-73**, **77** or **86** (1 equiv, 0.25 mmol) and the corresponding aromatic nucleophile (0 or 3 equiv, 0.75 mmol) diluted in DCE (0.5 mL) were added and the mixture was stirred at the indicated temperature until completion of the reaction. The mixture was then filtered on a short pad of silica gel, which was rinsed with DCM (5 mL). After evaporation, the crude product was purified by flash chromatography over silica gel (cyclohexane, EtOAc).

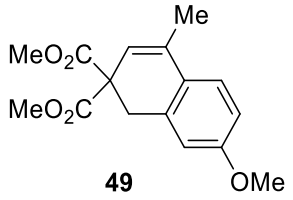
Dimethyl 5,7-dimethoxy-4-methylnaphthalene-2,2(1*H*)-dicarboxylate 47:



47

White solid. mp = 133-135 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 6.40 (d, J = 2.4 Hz, 1H), 6.32 (d, J = 2.4 Hz, 1H), 5.75 (q, J = 1.4 Hz, 1H), 3.81 (s, 3H), 3.76 (s, 3H), 3.71 (s, 6H), 3.25 (s, 2H), 2.24 (d, J = 1.4 Hz, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 171.0, 159.8, 158.1, 136.6, 135.3, 119.3, 115.9, 105.3, 97.8, 55.2, 55.2, 54.3, 52.8, 36.5, 23.5. FT-IR (film): ν 2955, 2840, 1736, 1604, 1573, 1457, 1432, 1332, 1260, 1230, 1199, 1162, 1112, 1069, 1050, 825 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{17}H_{20}O_6Na$ $[M+Na]^+$: 343.1152 found: 343.1153.

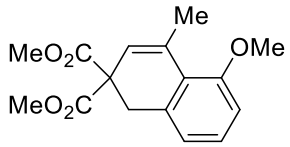
Dimethyl 7-methoxy-4-methylnaphthalene-2,2(1*H*)-dicarboxylate 49:



49

Colorless oil. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.19 (d, J = 8.2 Hz, 1H), 6.78-6.71 (m, 2H), 5.84 (s, 1H), 3.80 (s, 3H), 3.72 (s, 6H), 3.45 (s, 2H), 2.11 (d, J = 1.0 Hz, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 171.1, 159.3, 134.7, 134.5, 126.5, 124.7, 118.6, 113.8, 111.5, 55.2, 54.8, 52.9, 35.0, 19.4. FT-IR (film): ν 2954, 1736, 1609, 1571, 1502, 1433, 1257, 1228, 1140, 831 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{16}H_{18}O_5Na$ $[M+Na]^+$: 313.1046 found: 313.1056.

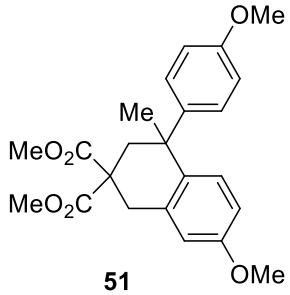
Dimethyl 5-methoxy-4-methylnaphthalene-2,2(1*H*)-dicarboxylate 50:



50

This regioisomer was observed in low proportion and could not have been fully characterized. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.14 (dd, J = 8.2 Hz, J = 7.1 Hz, 1H), 6.84 (d, J = 7.1 Hz, 1H), 6.78 (d, J = 8.2 Hz, 1H), 5.89 (q, J = 1.7 Hz, 1H), 3.79 (s, 3H), 3.70 (s, 6H), 3.29 (s, 2H), 2.28 (d, J = 1.7 Hz, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 170.9, 156.9, 135.6, 135.5, 128.6, 121.9, 120.8, 116.9, 110.9, 55.3, 55.2, 52.9, 35.9, 23.5.

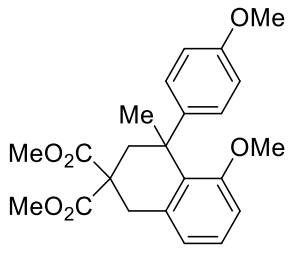
Dimethyl 7-methoxy-4-(4-methoxyphenyl)-4-methyl-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 51:



51

Colorless oil. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.07 (d, J = 8.8 Hz, 1H), 6.94 (d, J = 8.8 Hz, 2H), 6.80 (m, 1H), 6.78-6.73 (m, 3H), 3.83 (s, 3H), 3.75 (s, 3H), 3.71 (s, 3H), 3.36 (d, J = 16.2 Hz, 1H), 3.16 (s, 3H), 3.07 (d, J = 16.2 Hz, 1H), 2.87 (d, J = 14.5 Hz, 1H), 2.46 (d, J = 14.5 Hz, 1H), 1.66 (s, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 172.3, 170.8, 157.9, 157.5, 141.3, 135.1, 133.6, 129.5, 128.6, 113.0, 112.9, 112.8, 55.2, 55.1, 52.7, 52.2, 52.1, 43.6, 40.9, 35.4, 32.4. FT-IR (film): ν 2953, 1735, 1610, 1508, 1444, 1250, 1179, 1033 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{23}H_{26}O_6Na$ $[M+Na]^+$: 421.1622 found: 421.1629.

Dimethyl 5-methoxy-4-(4-methoxyphenyl)-4-methyl-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 52:

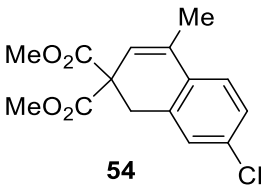


52

This regioisomer was observed in low proportion and could not have been fully characterized. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.21 (dd, J = 8.7 Hz, J = 7.7 Hz, 1H), 6.94 (d,

J = 8.7 Hz, 2H), 6.80 (d, *J* = 7.7 Hz, 1H), 6.75-6.72 (m, 3H), 3.76 (s, 3H), 3.71 (s, 3H), 3.45 (s, 3H), 3.34 (d, *J* = 10.3 Hz, 1H), 3.23 (s, 3H), 3.17 (d, *J* = 10.3 Hz, 1H), 2.65 (d, *J* = 14.1 Hz, 1H), 2.49 (d, *J* = 14.1 Hz, 1H), 1.75 (s, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 172.2, 170.1, 158.4, 157.0, 141.9, 135.6, 130.0, 127.5, 127.3, 121.7, 112.7, 110.2, 55.2, 52.8, 52.5, 52.2, 51.7, 46.6, 40.7, 35.9, 28.6.

Dimethyl 7-chloro-4-methylnaphthalene-2,2(1*H*)-dicarboxylate 54:

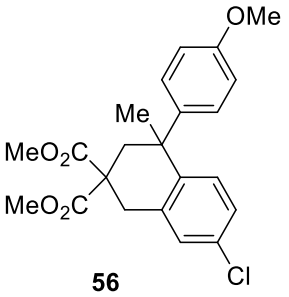


54

White solid. mp = 71 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.20-7.18 (m, 3H), 5.99 (q, *J* = 1.5 Hz, 1H), 3.73 (s, 6H), 3.35 (s, 2H), 2.12 (d, *J* = 1.5 Hz, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 170.6, 134.6, 134.2, 133.4, 131.9, 127.8, 127.0, 124.7, 121.5, 54.6, 53.0, 34.3, 19.4. FT-IR (film): ν 2953, 2923, 1736, 1434, 1270, 1230, 839 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{15}H_{15}O_4ClNa$ $[M+Na]^+$: 317.0551 found: 317.0545.

The regioisomer **55** was observed in very low proportion and could not have been isolated.

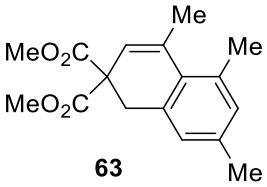
Dimethyl 7-loro-4-(4-methoxyphenyl)-4-methyl-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 56:



56

Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.23 (d, *J* = 2.3 Hz, 1H), 7.17 (dd, *J* = 8.5 Hz, *J* = 2.3 Hz, 1H), 7.08 (d, *J* = 8.5 Hz, 1H), 6.92 (d, *J* = 9.0 Hz, 2H), 6.75 (d, *J* = 9.0 Hz, 2H), 3.76 (s, 3H), 3.71 (s, 3H), 3.32 (d, *J* = 16.5 Hz, 1H), 3.21 (s, 3H), 3.08 (d, *J* = 16.5 Hz, 1H), 2.88 (d, *J* = 14.4 Hz, 1H), 2.45 (d, *J* = 14.4 Hz, 1H), 1.65 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 171.9, 170.6, 157.7, 140.5, 140.3, 135.9, 132.0, 129.8, 128.5, 128.4, 126.6, 113.1, 55.2, 52.7, 52.3, 52.2, 43.4, 41.4, 34.8, 32.0. FT-IR (film): ν 2953, 2838, 1736, 1608, 1509, 1486, 1435, 1250, 1179, 1097, 1035, 910, 830, 734 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{22}H_{23}O_5ClNa$ $[M+Na]^+$: 425.1126 found: 425.1114.

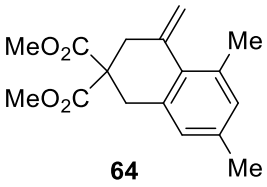
Dimethyl 4,5,7-trimethylnaphthalene-2,2(1*H*)-dicarboxylate 63:



63

White solid. mp = 85 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 6.90 (s, 1H), 6.83 (s, 1H), 5.97 (s, 1H), 3.70 (s, 6H), 3.25 (s, 2H), 2.44 (s, 3H), 2.27 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 170.9, 137.0, 136.6, 134.3, 132.2, 130.5, 126.9, 123.2, 54.4, 52.8, 36.7, 24.1, 23.4, 20.8. FT-IR (film): ν 2955, 1737, 1611, 1435, 1263, 1223 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{17}H_{20}O_4Na$ $[M+Na]^+$: 311.1254 found: 311.1248.

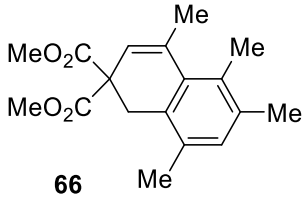
Dimethyl 5,7-dimethyl-4-methylene-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 64:



64

Obtained as a mixture of regioisomers (**63** : **64** = 4 : 1 ; determined by ^{1}H NMR). **64**: ^{1}H NMR (250 MHz, $CDCl_3$) δ 6.90 (s, 1H), 6.83 (s, 1H), 5.31 (s, 1H), 5.19 (s, 1H), 3.72 (s, 6H), 3.23 (s, 2H), 3.00 (s, 2H), 2.42 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 171.5, 139.0, 134.7, 134.6, 132.0, 130.5, 126.7, 116.0, 55.2, 52.7, 40.0, 35.7, 21.9, 20.9 (1 quaternary carbon is missing). GC-MS (EI) *m/z* (%I): 288.0 (15) $[M]^+$, 229.0 (41), 197.0 (86), 169.0 (100).

Dimethyl 4,5,6,8-tetramethylnaphthalene-2,2(1*H*)-dicarboxylate 66:



66

White solid. mp = 123-125 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 6.89 (s, 1H), 6.10 (s, 1H), 3.70 (s, 6H), 3.18 (s, 2H), 2.29 (s, 3H), 2.27 (s, 3H), 2.24 (s, 3H), 2.23 (s, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 171.0, 137.1, 135.5, 134.7, 132.0, 131.4, 130.7, 130.5, 124.1, 54.5, 52.8, 32.9, 23.6, 20.6, 19.7, 18.6. FT-IR (film): ν 2952, 1737, 1437, 1264, 1158 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{18}H_{22}O_4Na$ $[M+Na]^+$: 325.1410 found: 325.1424.

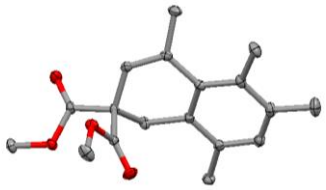
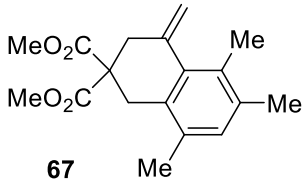


Figure S1. Crystal structure of **66** (thermal ellipsoids at 50% probability, hydrogen atoms omitted for clarity).

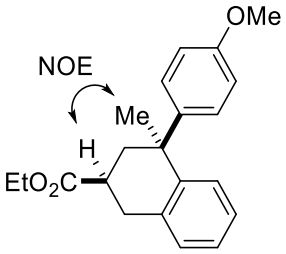
Dimethyl 5,6,8-trimethyl-4-methylene-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 67:



67

White solid. mp = 103-104 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 6.90 (s, 1H), 5.36 (s, 1H), 5.09 (s, 1H), 3.72 (s, 6H), 3.12 (s, 2H), 3.02 (s, 2H), 2.32 (s, 3H), 2.26 (s, 3H), 2.25 (s, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 171.8, 140.1, 136.4, 135.3, 132.3, 130.6, 130.4, 130.3, 116.7, 55.4, 52.7, 39.4, 32.2, 20.6. FT-IR (film): ν 2951, 1735, 1436, 1255, 1197, 1170, 1065, 908 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{18}H_{22}O_4Na$ $[M+Na]^+$: 325.1410 found: 325.1410.

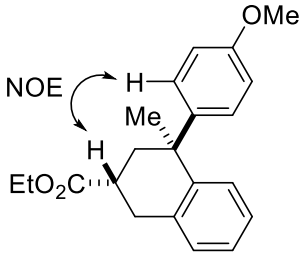
Ethyl 4-(4-methoxyphenyl)-4-methyl-1,2,3,4-tetrahydronaphthalene-2-carboxylate 74 *syn*:



74 *syn*

Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21-7.02 (m, 4H), 7.17 (d, J = 8.9 Hz, 2H), 6.82 (d, J = 8.9 Hz, 2H), 4.16 (q, J = 7.1 Hz, 2H), 3.80 (s, 3H), 3.15-3.10 (m, 2H), 3.02-2.95 (m, 1H), 2.16-2.13 (m, 2H), 1.70 (s, 3H), 1.27 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.3, 157.6, 144.8, 143.0, 134.5, 129.5, 128.8, 128.3, 126.2, 125.8, 113.3, 60.5, 55.2, 44.3, 43.2, 37.8, 32.7, 29.5, 14.2. FT-IR (film): ν 2929, 1731, 1510, 1250, 1180, 1034 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{21}H_{24}O_3Na$ $[M+Na]^+$: 347.1618 found: 347.1607. Relative stereochemistry determined by 1D selective NOE experiment.

Ethyl 4-(4-methoxyphenyl)-4-methyl-1,2,3,4-tetrahydronaphthalene-2-carboxylate 74 *anti*:

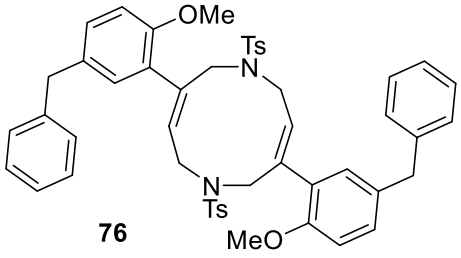


74 *anti*

Colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.23-7.19 (m, 4H), 6.90 (d, J = 8.9 Hz, 2H), 6.77 (d, J = 8.9 Hz, 2H), 4.12 (q, J = 7.1 Hz, 2H), 3.77 (s, 3H), 3.07-3.01 (m, 2H), 2.58-2.50 (m, 1H), 2.33 (dt, J = 12.9 Hz, J = 2.1 Hz, 1H), 2.00 (t, J = 12.9 Hz, 1H), 1.78 (s, 3H), 1.24 (t, J = 7.1 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.5, 157.5, 142.4, 142.2, 135.3, 129.0, 128.3, 128.2, 126.3, 126.3, 113.3, 60.4, 55.2, 42.8, 42.37, 36.2, 32.6, 30.7, 14.2. FT-IR (film): ν 2930, 1731, 1510, 1251, 1182, 1035 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{21}H_{24}O_3Na$ $[M+Na]^+$: 347.1618 found: 347.1600. Relative stereochemistry determined by 1D selective NOE experiment.

(3Z,8Z)-3,8-bis(5-benzyl-2-methoxyphenyl)-1,6-ditosyl-1,2,5,6,7,10-hexahydro-1,6-diazecine 76:

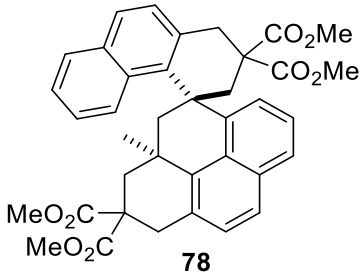
To a solution of arenyne **75** (1 equiv, 210 mg, 0.5 mmol) in DCE (2 mL) was added $GaCl_3$ (10 mol%, 8.8 mg, 0.05 mmol) in one portion. The mixture was stirred at room temperature for 20 h and the reaction was quenched with water. The two layers were separated and the aqueous phase was extracted with Et_2O (3 x 10 mL). The combined organic extracts were dried over $MgSO_4$, filtered and concentrated under reduced pressure. The crude product was purified by chromatography over silica gel (cyclohexane, EtOAc) and recrystallized in Et_2O to afford compound **76** (12%, 25 mg, 0.03 mmol).



76

Colorless crystals. mp = 99-101 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.36-6.67 (m, 24H), 5.63 (t, J = 8.3 Hz, 2H), 4,75 (d, J = 13.6 Hz, 2H), 4.25 (d, J = 13.6 Hz, 2H), 3.98 (d, J = 8.3 Hz, 4H), 3.91 (s, 4H), 3.69 (s, 6H), 2.33 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 155.1, 142.5, 141.2, 138.8, 133.1, 130.3, 130.1, 129.3, 129.0, 128.8, 128.5, 128.3, 126.9, 126.1, 111.0, 55.4, 42.5, 41.4, 40.9, 21.4. HRMS (ESI) *m/z*: Calcd for $C_{50}H_{50}O_6N_2S_2Na$ $[M+Na]^+$: 861.3008 found: 861.2996.

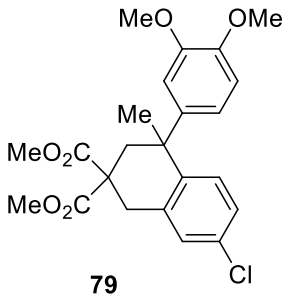
Tetramethyl 5a'-methyl-5a',6'-dihydro-1*H*,5'*H*-spiro[phenanthrene-4,4'-pyrene]-2,2,7',7'(3*H*,8'*H*)-tetracarboxylate 78:



78

White solid. mp > 275 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.82 (d, J = 8.3 Hz, 1H), 7.79 (d, J = 8.3 Hz, 1H), 7.72 (d, J = 8.2 Hz, 1H), 7.62 (d, J = 8.2 Hz, 2H), 7.40 (t, J = 8.0 Hz, 2H), 7.30 (t, J = 7.2 Hz, 1H), 7.12-7.04 (m, 2H), 6.64 (d, J = 7.2 Hz, 1H), 3.82 (s, 3H), 3.77 (d, J = 16.8 Hz, 1H), 3.72 (s, 3H), 3.65 (s, 3H), 3.61 (d, J = 16.8 Hz, 1H), 3.45 (s, 2H), 3.29 (s, 3H), 3.21 (d, J = 15.5 Hz, 1H), 3.15 (d, J = 14.4 Hz, 1H), 2.84 (d, J = 14.6 Hz, 1H), 2.55 (d, J = 14.4 Hz, 1H), 2.38 (d, J = 14.6 Hz, 1H), 2.20 (d, J = 15.5 Hz, 1H), 1.24 (s, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 173.2, 172.6, 172.0, 170.9, 142.2, 136.8, 135.0, 134.5, 134.2, 133.3, 130.8, 130.6, 129.8, 129.3, 128.4, 128.4, 127.8, 127.5, 126.1, 125.8, 125.1, 124.8, 124.4, 124.2, 54.5, 53.0, 52.9, 52.6, 52.5, 51.3, 45.3, 44.2, 43.2, 37.2, 35.0, 33.6, 32.5, 26.9. FT-IR (film): ν 2953, 1734, 1434, 1256, 1211, 736 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{38}H_{37}O_8$ $[M+H]^+$: 621.2483 found: 621.2466. Crystals suitable for X-ray diffraction were obtained by slow diffusion of a DCM solution of **78** in cyclohexane.

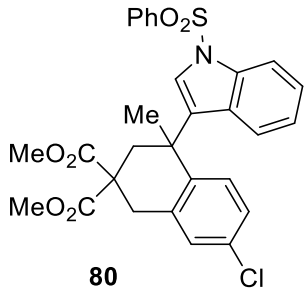
Dimethyl 7-chloro-4-(3,4-dimethoxyphenyl)-4-methyl-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 79:



79

Colorless oil. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.23 (d, J = 2.2 Hz, 1H), 7.18 (dd, J = 8.4 Hz, J = 2.2 Hz, 1H), 7.10 (d, J = 8.4 Hz, 1H), 6.69 (d, J = 8.5 Hz, 1H), 6.59 (d, J = 2.4 Hz, 1H), 6.45 (dd, J = 8.5 Hz, J = 2.4 Hz, 1H), 3.82 (s, 3H), 3.78 (s, 3H), 3.71 (s, 3H), 3.29 (d, J = 16.4 Hz, 1H), 3.23 (s, 3H), 3.07 (d, J = 16.4 Hz, 1H), 2.90 (d, J = 14.5 Hz, 1H), 2.43 (d, J = 14.5 Hz, 1H), 1.66 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 172.0, 170.7, 148.2, 147.2, 141.0, 140.3, 136.0, 132.1, 129.7, 128.5, 126.6, 119.7, 111.2, 110.4, 55.8, 52.8, 52.3, 52.2, 43.3, 41.8, 34.8, 32.0. FT-IR (film): ν 2953, 2850, 2255, 1736, 1595, 1512, 1447, 1262, 1027, 912, 733 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{23}H_{25}O_6ClNa$ $[M+Na]^+$: 455.1232 found: 455.1219.

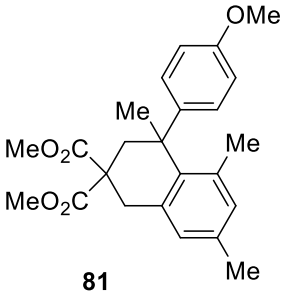
Dimethyl 7-chloro-4-methyl-4-(1-(phenylsulfonyl)-1*H*-indol-3-yl)-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 80:



80

White solid. mp = 175 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.97-7.89 (m, 3H), 7.57-7.42 (m, 4H), 7.26 (m, 1H), 7.15-7.07 (m, 3H), 7.01-6.97 (m, 2H), 3.72 (s, 3H), 3.32 (s, 2H), 3.05 (d, J = 14.5 Hz, 1H), 2.91 (s, 3H), 2.43 (d, J = 14.5 Hz, 1H), 1.70 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 171.8, 170.7, 138.9, 138.0, 135.7, 134.9, 133.8, 132.5, 129.9, 129.3, 129.2, 128.7, 128.5, 127.0, 126.9, 124.5, 124.4, 123.0, 121.3, 113.7, 52.7, 51.9, 51.8, 39.8, 37.8, 34.5, 29.9. FT-IR (film): ν 2933, 1736, 1595, 1448, 1365, 1268, 1177, 1136, 962, 903, 752, 728 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{29}H_{26}O_6NClSNa$ $[M+Na]^+$: 574.1062 found: 574.1048.

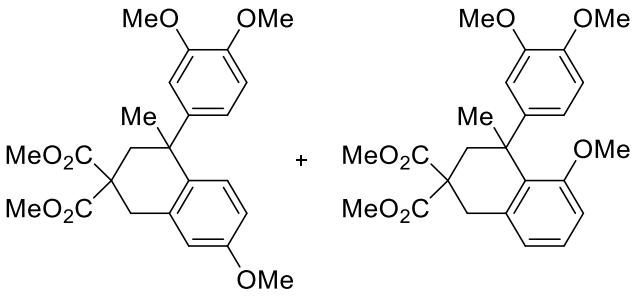
Dimethyl 4-(4-methoxyphenyl)-4,5,7-trimethyl-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 81:



81

Colorless oil. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.00 (d, J = 8.6 Hz, 2H), 6.92 (s, 1H), 6.81 (s, 1H), 6.77 (d, J = 8.6 Hz, 2H), 3.78 (s, 3H), 3.72 (s, 3H), 3.40 (s, 3H), 3.28 (s, 2H), 2.61 (d, J = 14.1 Hz, 1H), 2.51 (d, J = 14.1 Hz, 1H), 2.29 (s, 3H), 1.82 (s, 3H), 1.71 (s, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 172.1, 171.2, 157.3, 142.0, 137.3, 136.5, 135.7, 134.1, 132.0, 127.8, 127.7, 113.3, 55.2, 52.5, 52.3, 51.7, 47.9, 41.7, 36.6, 28.5, 22.5, 20.6. FT-IR (film): ν 2952, 1736, 1609, 1509, 1250, 1215, 1180, 1034 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{24}H_{28}O_5Na$ $[M+Na]^+$: 419.1829 found: 419.1813.

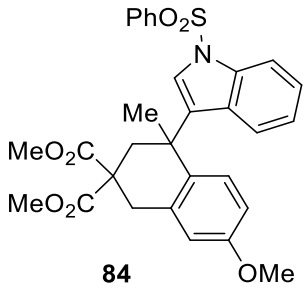
Dimethyl 4-(3,4-dimethoxyphenyl)-7-methoxy-4-methyl-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 82 and dimethyl 4-(3,4-dimethoxyphenyl)-5-methoxy-4-methyl-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 83:



82 : **83** = 9 : 1

Obtained as a mixture **82** : **83** = 9 : 1 (determined by GC). NMR of the major isomer **82**: ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.08 (d, J = 8.5 Hz, 1H), 6.79-6.73 (m, 2H), 6.68 (d, J = 8.1 Hz, 1H), 6.60 (d, J = 2.1 Hz, 1H), 6.48 (dd, J = 8.5 Hz, J = 2.1 Hz, 1H), 3.81 (s, 3H), 3.80 (s, 3H), 3.76 (s, 3H), 3.70 (s, 3H), 3.33 (d, J = 16.0 Hz, 1H), 3.17 (s, 3H), 3.06 (d, J = 16.0 Hz, 1H), 2.88 (d, J = 14.4 Hz, 1H), 2.44 (d, J = 14.4 Hz, 1H), 1.66 (s, 3H). ^{13}C NMR (90 MHz, $CDCl_3$) δ 172.2, 170.8, 157.9, 148.0, 146.9, 141.8, 135.2, 133.6, 129.4, 119.8, 112.8, 111.3, 110.2, 55.8, 55.7, 55.1, 52.7, 52.3, 52.1, 43.5, 43.4, 41.2, 35.3, 32.3. GC-MS (IE) *m/z*: Calcd for $C_{23}H_{26}O_6$ [M]: 428.47 found: **82**: 428.1, **83**: 428.2. Minor isomer **83** was obtained in very low proportion and could not have been fully characterized by NMR.

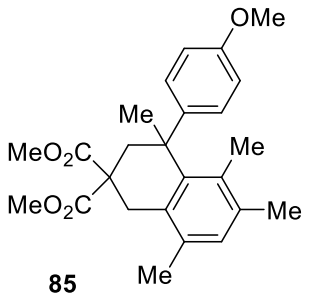
Dimethyl 7-methoxy-4-methyl-4-(1-(phenylsulfonyl)-1*H*-indol-3-yl)-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 84:



84

White solid. mp = 99 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.95-7.87 (m, 3H), 7.55-7.43 (m, 3H), 7.27-7.21 (m, 2H), 7.12 (dd, J = 7.1 Hz, J = 1.1 Hz, 1H), 7.00 (d, J = 8.5 Hz, 1H), 6.94 (s, 1H), 6.77 (d, J = 2.8 Hz, 1H), 6.72 (dd, J = 8.5 Hz, J = 2.8 Hz, 1H), 3.83 (s, 3H), 3.70 (s, 3H), 3.38 (d, J = 16.5 Hz, 1H), 3.26 (d, J = 16.5 Hz, 1H), 3.06 (d, J = 14.1 Hz, 1H), 2.80 (s, 3H), 2.43 (d, J = 14.1 Hz, 1H), 1.71 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 172.1, 170.9, 158.1, 145.5, 138.0, 135.7, 134.1, 133.7, 132.5, 130.7, 129.2, 128.9, 127.0, 124.6, 124.2, 122.8, 121.5, 113.6, 113.2, 113.1, 55.1, 52.6, 52.1, 51.5, 39.9, 37.4, 34.9, 30.1. FT-IR (film): ν 2954, 1735, 1610, 1502, 1448, 1370, 1259, 1175, 1134, 748, 727 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{30}H_{29}O_7NSNa$ $[M+Na]^+$: 570.1557 found: 570.1552.

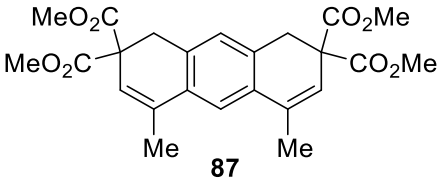
Dimethyl 4-(4-methoxyphenyl)-4,5,6,8-tetramethyl-3,4-dihydronaphthalene-2,2(1*H*)-dicarboxylate 85:



85

White solid. mp = 142-144 °C. ^{1}H NMR (250 MHz, $CDCl_3$) δ 7.07-6.97 (m, 3H), 6.77 (d, J = 8.5 Hz, 2H), 3.78 (s, 3H), 3.73 (s, 3H), 3.29 (s, 3H), 3.19 (d, J = 16.5 Hz, 1H), 3.08 (d, J = 16.5 Hz, 1H), 2.61 (d, J = 14.2 Hz, 1H), 2.49 (d, J = 14.2 Hz, 1H), 2.32 (s, 3H), 2.16 (s, 3H), 1.74 (s, 3H), 1.72 (s, 3H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 172.5, 171.3, 157.3, 142.4, 139.5, 136.0, 133.3, 133.2, 130.5, 130.4, 127.8, 113.3, 55.2, 52.5, 52.3, 51.4, 47.6, 42.3, 33.3, 29.4, 20.8, 20.4, 19.2. FT-IR (film): ν 2952, 1736, 1608, 1509, 1463, 1248, 1180, 1034, 912, 834, 733 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{25}H_{30}O_5Na$ $[M+Na]^+$: 433.1985 found: 433.1983.

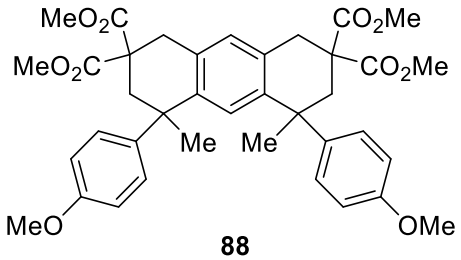
Tetramethyl 4,5-dimethylanthracene-2,2,7,7(1*H*,8*H*)-tetracarboxylate 87:



87

White solid. mp = 195 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.15 (s, 1H), 7.05 (s, 1H), 5.94 (s, 2H), 3.72 (s, 12H), 3.35 (s, 2H), 2.14 (d, J = 1.4 Hz, 6H). ^{13}C NMR (63 MHz, $CDCl_3$) δ 170.9, 134.8, 132.4, 132.0, 127.4, 120.6, 118.7, 54.7, 52.9, 34.3, 19.5. FT-IR (film): ν 2956, 2539, 1721, 1431, 1255, 1219, 1172, 1069, 1048, 905, 829, 817 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{24}H_{26}O_8Na$ $[M+Na]^+$: 465.1520 found: 465.1499. The data correspond to those previously reported in the literature.[2]

Tetramethyl 4,5-bis(4-methoxyphenyl)-4,5-dimethyl-3,4,5,6-tetrahydroanthracene-2,2,7,7(1*H*,8*H*)-tetracarboxylate 88:

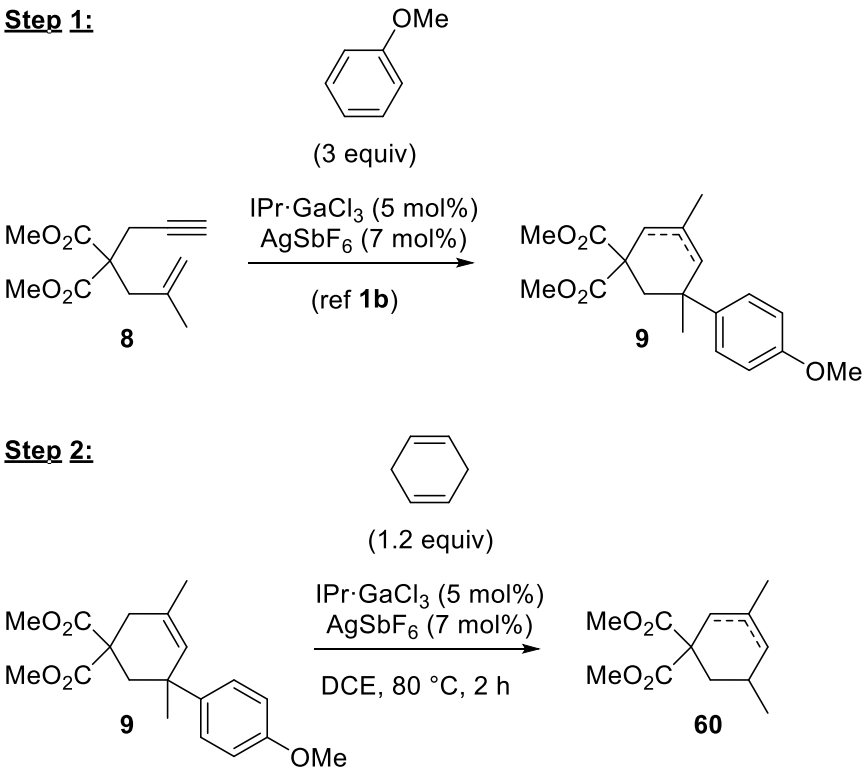


88

Obtained as a mixture *dl* : *meso* = 3 : 1 (determined by HPLC-Circular Dichroism). White solid. mp = 214 °C. ^{1}H NMR (360 MHz, $CDCl_3$) δ 7.09 (s, 1H, *dl*), 7.08 (s, 1H, *meso*), 6.95 (s, 1H, *dl*), 6.94 (s, 1H, *meso*), 6.91 (br d, J = 8.6 Hz, 4H), 6.70 (br d, J = 8.6 Hz, 4H), 3.74-3.72 (m, 12H), 3.42 (br d, J

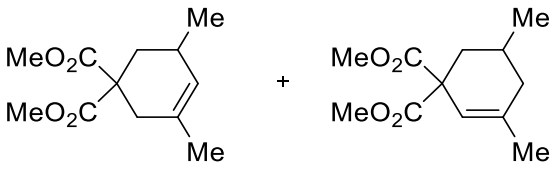
= 16.4 Hz, 2H), 3.15 (s, 6H, *dl*), 3.07 (s, 6H, *meso*), 3.07 (br d, *J* = 16.4 Hz, 2H), 2.85 (d, *J* = 14.2 Hz, 2H, *meso*), 2.84 (d, *J* = 14.2 Hz, 2H, *dl*), 2.47 (d, *J* = 14.2 Hz, 2H, *meso*), 2.46 (d, *J* = 14.2 Hz, 2H, *dl*), 1.60 (s, 6H, *dl*), 1.56 (s, 6H, *meso*). ^{13}C NMR (90 MHz, $CDCl_3$) δ 172.4, 170.8 (*dl*), 170.7 (*meso*), 157.4, 141.0, 139.6 (*dl*), 139.0 (*meso*), 132.2 (*dl*), 132.1 (*meso*), 129.1 (*meso*), 128.9 (*dl*), 128.7 (*dl*), 128.6 (*meso*), 112.9, 55.2, 52.7, 52.1 (*dl*), 52.0 (*meso*), 43.6 (*meso*), 43.5 (*dl*), 41.3, 34.7 (*meso*), 34.6 (*dl*), 32.8, 32.3. FT-IR (film): ν 2957, 2364, 1723, 1509, 1432, 1240, 1174, 1086, 1026, 802 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{38}H_{42}O_{10}Na$ $[M+Na]^+$: 681.2670 found: 681.2651.

7. Two-Step Formal Transfer Hydrogenative Cyclization of Enyne 8:



Dimethyl 3,5-dimethylcyclohex-3-ene-1,1-dicarboxylate and dimethyl 3,5-dimethylcyclohex-2-ene-1,1-dicarboxylate 60:

$IPr{\cdot}GaCl_3$ (5 mol%, 7 mg, 0.0125 mmol) and $AgSbF_6$ (7 mol%, 6 mg, 0.0175 mmol) were mixed in a screw-cap vial under argon. DCE (0.5 mL) was added and the mixture was stirred at room temperature for 5 min. A solution of Friedel-Crafts adduct **9** (1 equiv, 0.25 mmol) and CHD-1,4 (1.2 equiv, 29 µL, 0.30 mmol) in DCE (0.5 mL) was added and the mixture was stirred at 80 °C for 2 h. The crude mixture was then filtered through a pad of Celite and the volatiles were removed under reduced pressure. The crude product was purified by chromatography over silica gel (cyclohexane, EtOAc) to afford compound **60** as an equimolar mixture of regioisomers (74%, 42 mg, 0.19 mmol).



60 : **60'** = 1 : 1

Colorless oil. Isolated as an equimolar mixture of regioisomers **60** and **60'** (determined by ^{1}H NMR). ^{1}H NMR peaks attribution determined by 1D selective TOCSY experiments. ^{1}H NMR of **60**: (360 MHz, $CDCl_3$) δ 5.57 (s, 1H), 3.72 (s, 6H), 2.39-2.32 (m, 2H), 2.15 (m, 1H), 1.75 (s, 3H), 1.64-1.57 (m, 1H), 1.41 (dd, J = 12.5 Hz, J = 13.2 Hz, 1H), 0.98 (d, J = 1.8 Hz, 3H). ^{1}H NMR of **60'**: (360 MHz, $CDCl_3$) δ 5.21 (s, 1H), 3.72 (s, 6H), 2.61 (d, J = 16.8 Hz, 1H), 2.23 (d, J = 16.8 Hz, 1H), 1.96 (dd, J = 17.1 Hz, J = 5.0 Hz, 1H), 1.83 (m, 1H), 1.70 (s, 3H), 1.49 (dd, J = 13.0 Hz, J = 10.8 Hz, 1H), 1.00 (d, J = 1.2 Hz, 3H). ^{13}C NMR of **60** and **60'** (63 MHz, $CDCl_3$) δ 172.7, 172.4, 171.5, 171.5, 139.1, 130.4, 126.6, 117.7, 56.2, 54.2, 52.7, 52.6, 52.6, 52.5, 38.3, 36.7, 36.0, 35.1, 27.9, 26.2, 23.8, 23.2, 21.7, 21.6. FT-IR (film): ν 2954, 2927, 1736, 1434, 1250, 1151 cm^{-1}. HRMS (ESI) *m/z*: Calcd for $C_{21}H_{26}O_4Na$ $[M+Na]^+$: 365.1723 found: 365.1728. HRMS (ESI) *m/z*: Calcd for $C_{12}H_{18}O_4Na$ $[M+Na]^+$: 249.1097 found: 249.1093.

8. Single-crystal X-ray structure analyses of compounds 66, 76:

X-ray diffraction data for compounds **76** was collected by using a Kappa X8 APPEX II Bruker diffractometer with graphite-monochromated $Mo_{K\alpha}$ radiation. X-ray diffraction data for compound **66** was collected by using a VENTURE PHOTON100 CMOS Bruker diffractometer with Micro-focus IuS source Mo $_{K\alpha}$ radiation. Crystal was mounted on a CryoLoop (Hampton Research) with Paratone-N (Hampton Research) as cryoprotectant and then flashfrozen in a nitrogen-gas stream at 100 K. The temperature of the crystal was maintained at the selected value (100K) by means of a 700 series Cryostream cooling device to within an accuracy of ±1 K. The data were corrected for Lorentz polarization, and absorption effects. The structures were solved by direct methods using SHELXS-97[19] and refined against F^2 by full-matrix least-squares techniques using SHELXL-2014[20] with anisotropic displacement parameters for all non-hydrogen atoms. Hydrogen atoms were located on a difference Fourier map and introduced into the calculations as a riding model with isotropic thermal parameters. All calculations were performed by using the Crystal Structure crystallographic software package WINGX.[21]

The crystal data collection and refinement parameters are given in Table S1.

CCDC 1483915-1483916 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via http://www.ccdc.cam.ac.uk/Community/Requestastructure.

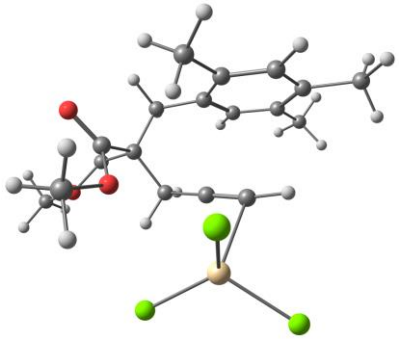
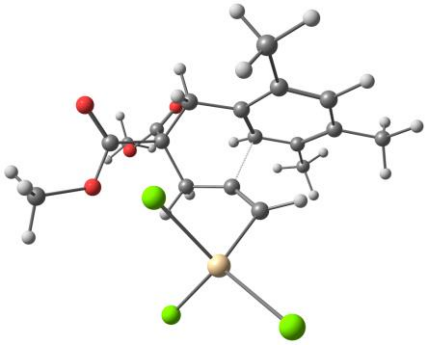
[19] Sheldrick, G. M. SHELXS-97, Program for Crystal Structure Solution, University of Göttingen, Göttingen, Germany, **1997**.
[20] G. M. Sheldrick, Acta Crystallogr., Sect. A: Found. Crystallogr., **2008**, 64, 112-122
[21] Farrugia, L. J. *J. Appl. Cryst*., **1999**, *32*, 837.

Table S1. Crystallographic data and structure refinement details for compounds **66** and **76**.

Compound	**66**	**76**
Empirical Formula	$C_{18}H_{22}O_4$	$C_{50}H_{50}N_2O_6S_2$
M_r	302.35	839.04
Crystal size, mm^3	0,11 x 0.10 x 0.03	0.21 x 0.17 x0.09
Crystal system	orthorhombic	monoclinic
Space group	*P b c a*	*P* $2_1/c$
a, Å	7.6825(3)	12.0255(7)
b, Å	17.5861(8)	18.0910(12)
c, Å	22.9639(11)	10.1121(7)
α, °	90	90
β, °	90	105.935(2)
γ, °	90	90
Cell volume, $Å^3$	3102.5(2)	2115.4(2)
Z ; Z’	8 ; 1	2 ; 1/2
T, K	100(1)	100(1)
Radiation type ; wavelength Å	MoKα ; 0.71073	MoKα ; 0.71073
F_{000}	1296	888
μ, mm^{-1}	0.090	0.180
θ range, °	2.918 - 33.765	1.761 - 30.561
Reflection collected	33 166	25 809
Reflections unique	5 651	6 061
R_{int}	0.0423	0.0506
GOF	1.041	1.023
Refl. obs. (I>2σ(I))	4 920	4 268
Parameters	205	273
wR_2 (all data)	0.1604	0.1223
R value (I>2σ(I))	0.0581	0.0468
Largest diff. peak and hole (e-.$Å^{-3}$)	-0.324 ; 0.735	-0.417 ; 0.465

9. Calculations:

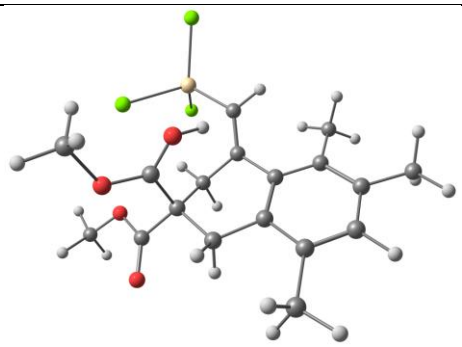
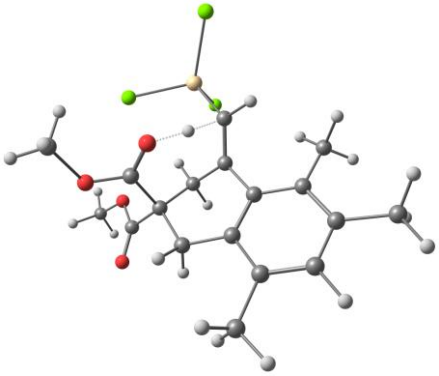
Table S2. Coordinates (x,y,z) and energy (Hartree) of the computed species.

K E(RM062X) = -4305.49913421 				**TS_{KL}** E(RM062X) = -4305.47048622 Frequency -215.5918 			
C	-2.286685000	2.358003000	-0.811673000	O	-3.521889000	1.942653000	-0.158076000
C	-0.303268000	-0.113726000	-0.856046000	H	-1.262924000	2.366827000	-0.993473000
C	-1.201926000	-0.890686000	-0.619103000	C	-0.358049000	2.457850000	-0.404920000
Ga	0.313580000	-2.611582000	-0.266766000	C	0.286021000	0.576159000	-0.714069000
Cl	2.325193000	-2.361295000	-1.042950000	C	-0.359143000	1.955122000	0.923016000
Cl	0.044898000	-2.721039000	1.890337000	C	0.684571000	2.338535000	1.790323000
Cl	-0.877723000	-4.046675000	-1.385088000	C	1.660371000	3.181897000	1.292572000
H	-2.126827000	-1.385200000	-0.407764000	C	1.539675000	0.314509000	-0.627552000
C	0.748077000	0.830516000	-1.216446000	C	1.666939000	3.699502000	-0.022362000
H	1.646182000	0.256982000	-1.463536000	H	2.482633000	3.456782000	1.947927000
H	0.411851000	1.339531000	-2.127017000	C	0.627676000	3.367499000	-0.868356000
C	1.097648000	1.901833000	-0.153280000	C	-1.384939000	0.957893000	1.381890000
C	-0.060049000	2.876778000	0.179607000	H	-0.910406000	0.277197000	2.089469000
C	-1.433811000	2.257056000	0.292124000	H	-2.187970000	1.470505000	1.918736000
C	1.715044000	1.316836000	1.120948000	C	-1.999517000	0.101757000	0.251633000
O	2.082739000	2.012393000	2.027330000	H	2.305631000	1.038827000	-0.360959000
O	1.844751000	-0.004992000	1.084646000	C	-1.008483000	-0.107275000	-0.931885000
C	2.579461000	-0.581412000	2.177223000	H	-0.789590000	-1.171118000	-1.050243000
H	3.514319000	-0.038410000	2.310088000	H	-1.443566000	0.220649000	-1.879152000
H	2.758208000	-1.614912000	1.896436000	Ga	1.949670000	-1.687681000	-0.366310000
H	1.983820000	-0.529817000	3.088793000	Cl	0.748737000	-2.060730000	1.496532000
C	2.246247000	2.717009000	-0.788073000	Cl	1.131970000	-2.916743000	-1.994660000
O	2.143618000	3.819551000	-1.242023000	Cl	4.097217000	-1.897398000	-0.017636000
O	3.371256000	1.999376000	-0.807341000	C	-2.445303000	-1.231256000	0.884701000
C	4.517298000	2.650006000	-1.370822000	O	-2.929283000	-1.276150000	1.982621000
H	4.325879000	2.909179000	-2.411989000	O	-2.257414000	-2.273890000	0.094312000
H	4.744350000	3.554064000	-0.806325000	C	-2.536553000	-3.554662000	0.673587000
H	5.327923000	1.931350000	-1.293702000	H	-2.314680000	-4.277969000	-0.105610000
H	-0.079564000	3.619411000	-0.618859000	H	-1.887304000	-3.707012000	1.535892000
H	0.223636000	3.408782000	1.090456000	H	-3.581952000	-3.607645000	0.977190000

C	-1.879304000	1.565100000	1.425334000	C	-3.257247000	0.779096000	-0.297343000
C	-3.150549000	0.991036000	1.390704000	O	-3.999429000	-0.075752000	-0.997439000
H	-1.947376000	2.916239000	-1.681064000	C	-5.184807000	0.466839000	-1.592482000
C	-3.547320000	1.773026000	-0.849249000	H	-4.923107000	1.260263000	-2.292708000
C	-3.988181000	1.067383000	0.280513000	H	-5.839709000	0.868062000	-0.819554000
H	-3.496376000	0.450994000	2.268047000	H	-5.658413000	-0.363050000	-2.108629000
C	-4.423457000	1.901638000	-2.067067000	C	0.565044000	3.872272000	-2.280301000
H	-3.925677000	2.476378000	-2.848386000	H	1.348209000	3.402248000	-2.885050000
H	-4.678709000	0.920585000	-2.478041000	H	-0.396730000	3.645758000	-2.740167000
H	-5.365386000	2.402153000	-1.825532000	H	0.724063000	4.951919000	-2.325928000
C	-5.349452000	0.423580000	0.297740000	C	2.778231000	4.608335000	-0.474363000
H	-6.137999000	1.169800000	0.164516000	H	3.565228000	4.673227000	0.276551000
H	-5.457874000	-0.301657000	-0.513870000	H	3.222475000	4.251183000	-1.406780000
H	-5.527181000	-0.092240000	1.241420000	H	2.403590000	5.619117000	-0.659402000
C	-1.018256000	1.345598000	2.641932000	C	0.779553000	1.780670000	3.184153000
H	-1.640225000	1.169484000	3.520603000	H	-0.156734000	1.904945000	3.732097000
H	-0.393707000	0.453576000	2.508165000	H	1.004285000	0.709043000	3.150122000
H	-0.358503000	2.187858000	2.851155000	H	1.572352000	2.277822000	3.742487000
L E(RM062X) = -4305.46292359				**TS_{LM}** E(RM062X) = -4305.45966732 Frequency -600.4684			
H	-1.891285000	-0.853722000	1.281617000	H	-2.097160000	-0.543993000	0.976488000
C	-1.865511000	-0.908987000	0.148181000	C	-1.840362000	-0.947484000	-0.140610000
C	0.607822000	-1.252933000	0.415379000	C	0.586877000	-1.322671000	0.252495000
O	-1.070812000	1.225883000	2.232865000	O	-1.152433000	1.097823000	2.099465000
C	-0.426308000	1.758021000	1.361567000	C	-0.504871000	1.724541000	1.292012000
O	0.766065000	2.288603000	1.511810000	O	0.612336000	2.361146000	1.548524000
C	1.393900000	2.102129000	2.791246000	C	1.153968000	2.201372000	2.871902000
H	1.512137000	1.035901000	2.981071000	H	1.323771000	1.144218000	3.068025000
H	0.786272000	2.564019000	3.569344000	H	0.461011000	2.621071000	3.601046000
H	2.367292000	2.573711000	2.704466000	H	2.099018000	2.734607000	2.860320000
C	-0.910585000	1.836910000	-0.092939000	C	-0.907499000	1.819529000	-0.184621000
C	-0.206241000	0.713795000	-0.895048000	C	-0.137781000	0.733743000	-0.974729000
C	-0.398415000	-0.569048000	-0.133407000	C	-0.384506000	-0.594062000	-0.307785000
Ga	2.547066000	-1.136969000	-0.111173000	Ga	2.567537000	-1.136067000	-0.065462000
Cl	3.526386000	-2.908734000	0.787879000	Cl	3.512058000	-2.934586000	0.810218000
Cl	2.573557000	-1.226782000	-2.339119000	Cl	2.835675000	-1.048469000	-2.273469000

H	0.348541000	-2.063773000	1.095317000	H	0.281417000	-2.184847000	0.843277000
Cl	3.522599000	0.752494000	0.535745000	Cl	3.386397000	0.730387000	0.828113000
H	0.852048000	0.943157000	-1.007768000	H	0.925352000	0.968208000	-0.986815000
H	-0.655799000	0.672355000	-1.895148000	H	-0.496754000	0.745681000	-2.010497000
C	-2.419281000	1.606266000	-0.109099000	C	-2.410978000	1.564756000	-0.276164000
C	-0.621836000	3.239425000	-0.626959000	C	-0.625039000	3.239585000	-0.675481000
O	0.535043000	3.314504000	-1.261136000	O	0.554097000	3.348614000	-1.261670000
C	0.932181000	4.620604000	-1.693479000	C	0.943662000	4.671204000	-1.649584000
H	0.993469000	5.290098000	-0.835725000	H	0.977161000	5.316797000	-0.772163000
H	1.907559000	4.488877000	-2.152284000	H	1.930619000	4.564285000	-2.089593000
H	0.211433000	5.013547000	-2.410605000	H	0.233750000	5.074520000	-2.371581000
O	-1.378921000	4.161685000	-0.466371000	O	-1.405324000	4.143807000	-0.525378000
H	-2.909406000	2.193162000	0.673010000	H	-2.944713000	2.184537000	0.445170000
H	-2.822754000	1.991016000	-1.055188000	H	-2.761498000	1.880150000	-1.267521000
C	-2.851370000	0.176808000	-0.021553000	C	-2.828346000	0.127181000	-0.144112000
C	-2.344597000	-2.301585000	-0.043769000	C	-2.317492000	-2.322847000	-0.200790000
C	-1.390023000	-3.440483000	-0.193650000	C	-1.394594000	-3.467443000	-0.507040000
H	-0.499002000	-3.135994000	-0.743554000	H	-0.524515000	-3.139894000	-1.072915000
H	-1.053698000	-3.810321000	0.780803000	H	-1.030009000	-3.947915000	0.406315000
C	-3.709944000	-2.545372000	-0.045297000	C	-3.668037000	-2.572165000	-0.021102000
C	-4.274616000	-3.942930000	-0.109482000	C	-4.209330000	-3.978164000	0.004993000
H	-1.874738000	-4.269860000	-0.705956000	H	-1.930124000	-4.224765000	-1.079536000
H	-3.812054000	-4.593195000	0.634579000	H	-3.607445000	-4.623430000	0.646532000
H	-4.108643000	-4.391972000	-1.092119000	H	-4.206379000	-4.415353000	-0.997490000
H	-5.348895000	-3.929387000	0.072645000	H	-5.235418000	-3.988381000	0.371209000
C	-4.589033000	-1.454433000	-0.033008000	C	-4.570468000	-1.497044000	0.089476000
C	-4.207950000	-0.112848000	-0.056910000	C	-4.202330000	-0.172425000	-0.000919000
H	-5.654748000	-1.671762000	-0.037278000	H	-5.622562000	-1.728377000	0.229642000
C	-5.245143000	0.975276000	-0.132850000	C	-5.224691000	0.928801000	0.057678000
H	-5.193097000	1.630394000	0.740213000	H	-5.083386000	1.546877000	0.948245000
H	-5.098672000	1.600864000	-1.016704000	H	-5.153928000	1.587793000	-0.810723000
H	-6.247496000	0.551198000	-0.181827000	H	-6.230591000	0.512075000	0.087983000
M E(RM062X) = -4305.48291616				**TS_{MN}** E(RM062X) = -4305.47588290 Frequency -848.9633			
H	-2.305205000	-0.024540000	1.429238000	H	-2.142029000	0.266835000	1.071112000
C	-1.695721000	-1.172614000	-0.142360000	C	-1.795654000	-1.030773000	-0.430079000
C	0.699947000	-1.472571000	0.181628000	C	0.580264000	-1.520619000	-0.044173000

O	-1.114319000	1.498729000	2.175227000	O	-1.220823000	0.974064000	1.883968000
C	-0.590575000	1.981437000	1.200430000	C	-0.606619000	1.737601000	1.135164000
O	0.443990000	2.795626000	1.232177000	O	0.287887000	2.571157000	1.556820000
C	1.014828000	3.055425000	2.525869000	C	0.646658000	2.512664000	2.956162000
H	1.257163000	2.114076000	3.014551000	H	0.940721000	1.495995000	3.206569000
H	0.307013000	3.629348000	3.124437000	H	-0.203933000	2.838169000	3.554040000
H	1.919825000	3.622311000	2.330379000	H	1.488546000	3.189575000	3.056779000
C	-1.043696000	1.712394000	-0.241635000	C	-0.862764000	1.768960000	-0.367086000
C	-0.112054000	0.666258000	-0.880059000	C	-0.008286000	0.682901000	-1.060583000
C	-0.313314000	-0.713558000	-0.282311000	C	-0.358027000	-0.700109000	-0.550182000
Ga	2.668602000	-1.041195000	0.073085000	Ga	2.560956000	-1.175207000	0.040906000
Cl	3.796850000	-2.766011000	0.856676000	Cl	3.571525000	-2.953767000	0.861220000
Cl	3.078929000	-0.684252000	-2.085187000	Cl	3.294311000	-0.637249000	-1.985089000
H	0.423660000	-2.434592000	0.614055000	H	0.230452000	-2.461036000	0.377700000
Cl	3.102657000	0.816779000	1.219879000	Cl	2.870280000	0.601718000	1.378856000
H	0.925367000	0.983804000	-0.777586000	H	1.049698000	0.894039000	-0.916357000
H	-0.323804000	0.631926000	-1.954284000	H	-0.205189000	0.763422000	-2.135042000
C	-2.497324000	1.229414000	-0.253215000	C	-2.344550000	1.458698000	-0.595600000
C	-1.003260000	3.062007000	-0.965697000	C	-0.563095000	3.184762000	-0.866396000
O	0.042951000	3.185222000	-1.767249000	O	0.629444000	3.280225000	-1.427336000
C	0.197875000	4.461254000	-2.398638000	C	1.018789000	4.590649000	-1.857058000
H	0.308881000	5.235441000	-1.639473000	H	2.008022000	4.471235000	-2.288523000
H	1.097253000	4.379873000	-3.001760000	H	0.311241000	4.967783000	-2.595208000
H	-0.670867000	4.682822000	-3.018373000	H	1.046086000	5.264961000	-1.001359000
O	-1.844359000	3.907439000	-0.804406000	O	-1.343647000	4.091716000	-0.746318000
H	-3.115849000	1.949533000	0.280632000	H	-2.954479000	2.219235000	-0.109007000
H	-2.850860000	1.189681000	-1.288134000	H	-2.557247000	1.504446000	-1.667184000
C	-2.660938000	-0.172510000	0.382037000	C	-2.685502000	0.058525000	-0.060786000
C	-2.106745000	-2.476235000	-0.437071000	C	-2.299992000	-2.336795000	-0.527619000
C	-1.199738000	-3.500054000	-1.075735000	C	-1.497169000	-3.488149000	-1.083332000
H	-0.348679000	-3.025213000	-1.559231000	H	-0.634190000	-3.137218000	-1.644272000
H	-0.806685000	-4.206972000	-0.339381000	H	-1.132431000	-4.151445000	-0.293570000
C	-3.443724000	-2.823958000	-0.169741000	C	-3.627751000	-2.573603000	-0.131847000
C	-3.917834000	-4.217373000	-0.440558000	C	-4.185931000	-3.967409000	-0.167078000
H	-1.744323000	-4.076335000	-1.824948000	H	-2.121414000	-4.088787000	-1.747251000
H	-3.217586000	-4.953883000	-0.041510000	H	-3.501308000	-4.678469000	0.299636000
H	-3.969033000	-4.385019000	-1.521908000	H	-4.327012000	-4.292808000	-1.202387000
H	-4.906347000	-4.391914000	-0.019645000	H	-5.148362000	-4.018537000	0.339706000
C	-4.391987000	-1.893465000	0.332693000	C	-4.465414000	-1.531611000	0.300030000
C	-4.064073000	-0.593558000	0.553933000	C	-4.054239000	-0.221549000	0.273713000
H	-5.405038000	-2.236721000	0.511466000	H	-5.477141000	-1.769222000	0.610320000
C	-5.070057000	0.407696000	1.022436000	C	-5.001254000	0.890474000	0.616960000
H	-4.673353000	0.996033000	1.853915000	H	-4.571137000	1.559492000	1.366733000
H	-5.304686000	1.110707000	0.216790000	H	-5.223847000	1.494845000	-0.267287000
H	-5.992686000	-0.080153000	1.333860000	H	-5.938324000	0.491952000	1.003653000
N E(RM062X) = -4305.50925847				**TS_{NO}** E(RM062X) = -4305.50214629			

				Frequency -932.0186 			
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C	-2.077780000	-0.786412000	-0.280639000	C	-2.062782000	-0.785754000	-0.230751000
C	0.269585000	-1.602487000	0.134755000	C	0.295691000	-1.456586000	0.318657000
O	-0.026533000	0.701637000	1.871143000	O	0.162810000	0.753170000	1.842314000
C	0.080424000	1.707367000	1.102911000	C	0.122275000	1.760347000	1.131578000
O	0.543505000	2.793824000	1.584013000	O	0.597483000	2.898462000	1.536013000
C	1.130397000	2.767146000	2.914838000	C	1.315978000	2.895598000	2.791823000
H	1.907697000	2.004139000	2.926600000	H	2.138287000	2.184974000	2.719587000
H	0.351140000	2.551784000	3.643459000	H	0.638490000	2.618509000	3.597850000
H	1.539429000	3.762093000	3.051922000	H	1.675721000	3.912328000	2.910851000
C	-0.496068000	1.748046000	-0.288174000	C	-0.562634000	1.795263000	-0.228401000
C	-0.105109000	0.508782000	-1.132915000	C	-0.138695000	0.568675000	-1.075860000
C	-0.596263000	-0.737820000	-0.436476000	C	-0.598354000	-0.674318000	-0.362629000
Ga	2.281170000	-1.501131000	0.002589000	Ga	2.316922000	-1.469489000	0.011323000
Cl	3.220784000	-2.994818000	1.308094000	Cl	3.211274000	-2.997177000	1.300587000
Cl	2.913788000	-1.612626000	-2.110532000	Cl	2.606430000	-1.812530000	-2.152302000
H	-0.170877000	-2.435500000	0.683217000	H	-0.143027000	-2.271948000	0.892790000
Cl	2.882357000	0.585768000	0.714948000	Cl	3.098174000	0.582882000	0.495826000
H	0.967022000	0.499277000	-1.314722000	H	0.933596000	0.582639000	-1.257160000
H	-0.614362000	0.623389000	-2.095330000	H	-0.654781000	0.640282000	-2.037793000
C	-2.036302000	1.781595000	-0.126315000	C	-2.093675000	1.776993000	-0.017156000
C	-0.005611000	3.030710000	-0.979464000	C	-0.143747000	3.087318000	-0.945047000
O	1.291259000	2.953698000	-1.225469000	O	1.125090000	3.019996000	-1.320792000
C	1.886684000	4.090936000	-1.862478000	C	1.662642000	4.190978000	-1.946458000
H	2.943049000	3.853658000	-1.944871000	H	2.696603000	3.948387000	-2.173273000
H	1.442299000	4.239959000	-2.846359000	H	1.105973000	4.418797000	-2.855230000
H	1.730357000	4.981583000	-1.253714000	H	1.601755000	5.036302000	-1.260864000
O	-0.713299000	3.954128000	-1.270520000	O	-0.872681000	4.018715000	-1.142930000
H	-2.308865000	2.410928000	0.727315000	H	-2.350619000	2.340914000	0.885150000
H	-2.409397000	2.321753000	-1.001712000	H	-2.524691000	2.354844000	-0.840251000
C	-2.735143000	0.436605000	-0.043591000	C	-2.758380000	0.414077000	0.011161000
C	-2.800858000	-1.994074000	-0.332978000	C	-2.722860000	-2.027784000	-0.283987000
C	-2.163468000	-3.305077000	-0.726980000	C	-2.013300000	-3.307607000	-0.654961000
H	-1.231383000	-3.159555000	-1.269148000	H	-1.058489000	-3.129969000	-1.146531000
H	-1.947388000	-3.929032000	0.146371000	H	-1.826686000	-3.929336000	0.226715000
C	-4.175330000	-1.970057000	-0.060730000	C	-4.099827000	-2.060401000	-0.034781000

C	-4.992572000	-3.236318000	-0.089134000	C	-4.864153000	-3.358141000	-0.078382000
H	-2.841683000	-3.873909000	-1.364616000	H	-2.634040000	-3.895459000	-1.332928000
H	-4.525745000	-4.026967000	0.502624000	H	-4.379870000	-4.127437000	0.527276000
H	-5.098827000	-3.615979000	-1.109487000	H	-4.930100000	-3.743792000	-1.099867000
H	-5.992336000	-3.057985000	0.307009000	H	-5.879290000	-3.220133000	0.293679000
C	-4.796100000	-0.758421000	0.228192000	C	-4.768090000	-0.871920000	0.250249000
C	-4.109602000	0.449690000	0.224115000	C	-4.133126000	0.365155000	0.269143000
H	-5.860327000	-0.753772000	0.444243000	H	-5.834380000	-0.910400000	0.452807000
C	-4.843485000	1.737657000	0.498115000	C	-4.917393000	1.617998000	0.561182000
H	-4.490612000	2.212475000	1.418654000	H	-4.580411000	2.092336000	1.487556000
H	-4.708603000	2.460664000	-0.310899000	H	-4.809046000	2.356650000	-0.237497000
H	-5.911717000	1.552920000	0.608728000	H	-5.977714000	1.391061000	0.668872000
O E(RM062X) = -4305.55120165				**P** E(RM062X) = -4305.49678873			
H	-0.951248000	-1.417215000	1.833030000	C	1.951891000	2.737935000	-0.867886000
C	-0.028392000	1.465517000	0.115241000	C	-0.193655000	0.324547000	-0.865565000
C	-1.112138000	-0.409999000	1.458096000	C	-1.131126000	1.078164000	-0.720204000
O	2.013754000	-0.522546000	2.243050000	Ga	-2.567897000	-0.705104000	-0.333553000
C	2.645967000	-0.369475000	1.236220000	Cl	-1.935528000	-2.669186000	-1.010654000
O	3.933084000	-0.009827000	1.208112000	Cl	-2.792603000	-0.377870000	1.806654000
C	4.552675000	0.161436000	2.487460000	Cl	-4.159921000	0.147188000	-1.543234000
H	4.499505000	-0.767391000	3.055317000	H	-1.788194000	1.913232000	-0.593558000
H	4.050575000	0.953353000	3.043177000	C	0.929078000	-0.566457000	-1.131499000
H	5.585156000	0.429144000	2.280860000	H	0.523402000	-1.563733000	-1.327910000
C	2.105453000	-0.552106000	-0.181924000	H	1.396989000	-0.213361000	-2.055890000
C	0.643487000	-0.987641000	-0.136437000	C	2.010844000	-0.667724000	-0.024517000
C	-0.226545000	0.057450000	0.523662000	C	2.745048000	0.659816000	0.313943000
Ga	-2.620628000	-1.204917000	-0.097685000	C	1.901354000	1.915012000	0.273927000
Cl	-4.436745000	-0.954655000	1.073732000	C	1.497012000	-1.347332000	1.249357000
Cl	-2.504145000	-0.014936000	-1.923874000	O	2.203794000	-1.543739000	2.199037000
H	-1.711259000	0.236618000	2.078115000	O	0.226445000	-1.726874000	1.164567000
Cl	-1.960610000	-3.267219000	-0.359545000	C	-0.257944000	-2.507436000	2.269625000
H	0.539490000	-1.941839000	0.376554000	H	0.427107000	-3.333977000	2.454407000
H	0.302822000	-1.114786000	-1.173332000	H	-1.238040000	-2.863848000	1.968083000
C	2.192731000	0.737065000	-0.982784000	H	-0.332695000	-1.879874000	3.157953000
C	2.929780000	-1.646554000	-0.861217000	C	3.041951000	-1.659833000	-0.606674000
O	3.041650000	-2.711197000	-0.063602000	O	4.091045000	-1.355886000	-1.096932000
C	3.760765000	-3.823778000	-0.608652000	O	2.573678000	-2.907527000	-0.551791000

H	3.745766000	-4.588261000	0.162937000	C	3.436180000	-3.923509000	-1.079499000
H	3.268775000	-4.178683000	-1.514040000	H	3.647243000	-3.726578000	-2.130364000
H	4.783163000	-3.528261000	-0.844171000	H	4.370023000	-3.942782000	-0.518183000
O	3.388286000	-1.577818000	-1.965632000	H	2.894662000	-4.857480000	-0.961342000
H	3.202958000	1.138717000	-0.907308000	H	3.566981000	0.749272000	-0.392595000
H	2.041958000	0.484104000	-2.038391000	H	3.203267000	0.520503000	1.295109000
C	1.175942000	1.776886000	-0.569418000	C	1.053141000	2.265525000	1.337466000
C	-0.957715000	2.503345000	0.409878000	C	0.252530000	3.400671000	1.228312000
C	-2.317985000	2.276151000	1.020038000	C	1.125028000	3.857067000	-0.945066000
H	-2.803081000	1.379221000	0.647249000	H	1.160253000	4.478255000	-1.835252000
H	-2.273834000	2.213126000	2.112456000	C	0.261838000	4.203533000	0.090835000
C	-0.629352000	3.825433000	0.081561000	H	-0.406568000	3.656490000	2.053224000
C	-1.544978000	4.982055000	0.404049000	C	2.899075000	2.458855000	-2.012410000
H	-2.982991000	3.100111000	0.775051000	H	2.789118000	1.452360000	-2.422580000
H	-1.854816000	4.974261000	1.451147000	H	2.733807000	3.169683000	-2.821894000
H	-2.450657000	4.960731000	-0.208285000	H	3.939997000	2.553984000	-1.690829000
H	-1.037521000	5.927009000	0.210616000	C	0.905338000	1.411608000	2.570980000
C	0.567175000	4.094533000	-0.572215000	H	0.519353000	2.008343000	3.398145000
C	1.464955000	3.098578000	-0.924221000	H	0.179486000	0.609286000	2.391901000
H	0.801112000	5.123426000	-0.829596000	H	1.841311000	0.952119000	2.888799000
C	2.720197000	3.460277000	-1.677748000	C	-0.599617000	5.436700000	0.003946000
H	3.616222000	3.291011000	-1.073866000	H	-0.087398000	6.293173000	0.451150000
H	2.824841000	2.867100000	-2.589285000	H	-0.824681000	5.689302000	-1.033433000
H	2.701724000	4.512771000	-1.960289000	H	-1.541211000	5.300987000	0.538716000
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C	-1.789089000	-1.017959000	-0.521370000	C	-1.812712000	-0.877178000	-0.291476000
C	-0.366013000	-0.554503000	-0.621033000	C	-0.427176000	-0.493185000	-0.508474000
C	0.643997000	-1.294718000	-0.148450000	C	0.601297000	-1.277006000	-0.103317000
Ga	2.637810000	-0.998071000	-0.064321000	Ga	2.612204000	-1.054189000	-0.085970000
Cl	3.345395000	1.058081000	-0.508528000	Cl	3.404013000	0.952810000	-0.564186000
Cl	3.214289000	-1.532752000	2.016885000	Cl	3.170571000	-1.602085000	1.995039000
Cl	3.469824000	-2.449166000	-1.523874000	Cl	3.284670000	-2.580505000	-1.546057000
H	0.378991000	-2.263229000	0.281244000	H	0.334130000	-2.237305000	0.342655000
C	-0.223586000	0.863090000	-1.111782000	C	-0.217228000	0.896880000	-1.061788000
H	0.820529000	1.166627000	-1.090259000	H	0.839707000	1.149678000	-1.067975000

H	-0.583209000	0.987751000	-2.141722000	H	-0.594788000	0.964040000	-2.088173000
C	-1.063192000	1.771439000	-0.194563000	C	-1.003446000	1.882849000	-0.185180000
C	-2.546165000	1.411280000	-0.287002000	C	-2.495435000	1.580534000	-0.277544000
C	-2.816410000	-0.061412000	-0.132526000	C	-2.805603000	0.101672000	-0.187462000
C	-0.593441000	1.540440000	1.252606000	C	-0.535586000	1.683901000	1.268004000
O	-1.298979000	1.098087000	2.120361000	O	-1.261251000	1.353607000	2.168244000
O	0.683323000	1.846301000	1.375111000	O	0.768749000	1.869673000	1.361464000
C	1.317296000	1.518609000	2.623860000	C	1.385216000	1.545282000	2.618239000
H	0.953129000	2.186295000	3.405017000	H	1.045706000	2.240417000	3.386357000
H	2.380974000	1.649861000	2.444964000	H	2.453874000	1.630879000	2.441037000
H	1.105017000	0.481915000	2.882505000	H	1.133233000	0.522409000	2.897334000
C	-0.899694000	3.260891000	-0.493115000	C	-0.768757000	3.346504000	-0.554988000
O	-1.674862000	4.092039000	-0.098220000	O	-1.554637000	4.220370000	-0.297363000
O	0.181371000	3.522499000	-1.213083000	O	0.387860000	3.534324000	-1.173200000
C	0.467457000	4.908618000	-1.430842000	C	0.728053000	4.892500000	-1.470223000
H	-0.353170000	5.382672000	-1.969395000	H	-0.003591000	5.320957000	-2.155523000
H	0.610415000	5.409868000	-0.473742000	H	0.751162000	5.479302000	-0.552176000
H	1.382360000	4.927288000	-2.015537000	H	1.712463000	4.850359000	-1.927061000
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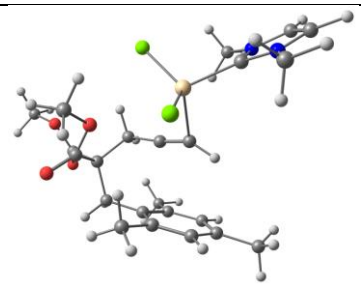
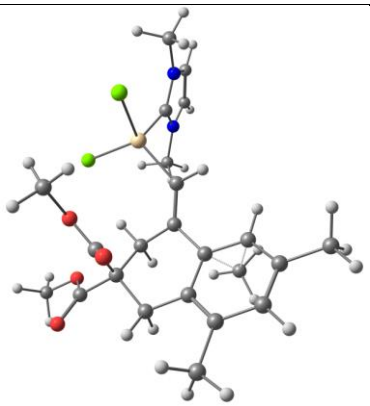
H	-3.101526000	1.980767000	0.456441000	H	-3.013646000	2.119649000	0.515822000
C	-4.020145000	-0.523970000	0.343238000	C	-4.123087000	-0.295126000	0.078149000
C	-4.256449000	-1.925682000	0.435481000	C	-4.483751000	-1.662352000	0.251670000
C	-2.098420000	-2.403739000	-0.433747000	C	-2.171571000	-2.325878000	-0.236746000
H	-1.297786000	-3.110404000	-0.622636000	H	-1.503075000	-2.833003000	0.468119000
C	-3.346051000	-2.873701000	0.049657000	C	-3.569092000	-2.654609000	0.139124000
H	-5.214453000	-2.252890000	0.829452000	H	-5.513943000	-1.894701000	0.499410000
C	-2.295254000	-1.568964000	-2.199650000	C	-1.877977000	-2.959514000	-1.637274000
H	-1.898245000	-0.647952000	-2.625112000	H	-0.842213000	-2.760385000	-1.909643000
H	-1.759223000	-2.407337000	-2.636434000	H	-2.035219000	-4.036709000	-1.598532000
H	-3.374638000	-1.627605000	-2.290810000	H	-2.541707000	-2.526751000	-2.388454000
C	-5.088400000	0.427976000	0.811282000	C	-5.191066000	0.735775000	0.250447000
H	-5.999661000	-0.106351000	1.077348000	H	-6.183849000	0.289646000	0.249548000
H	-4.740913000	0.975730000	1.691737000	H	-5.040228000	1.245686000	1.209230000
H	-5.331997000	1.163067000	0.041485000	H	-5.132597000	1.502809000	-0.524084000
C	-3.603046000	-4.351879000	0.123676000	C	-3.934799000	-4.093424000	0.325110000
H	-3.646240000	-4.788112000	-0.878405000	H	-4.085288000	-4.572792000	-0.647472000
H	-2.804397000	-4.859345000	0.669113000	H	-3.140275000	-4.639623000	0.837910000
H	-4.547250000	-4.559310000	0.626148000	H	-4.859851000	-4.190622000	0.892534000
P' E(RM062X) = -4149.84176093				**$TS_{P'Q'}$** E(RM062X) = -4149.81460050 Frequency -419.6708			

							
C	2.074920000	2.842247000	-1.106692000	C	1.941640000	1.500018000	-0.554979000
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C	-0.616890000	0.856279000	-0.469937000	C	-0.400027000	0.940005000	0.046591000
Ga	-1.771869000	-0.822384000	0.279737000	Ga	-2.045636000	-0.117656000	0.513407000
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H	-1.098363000	1.798665000	-0.256675000	H	-0.427066000	1.938887000	0.486511000
C	1.579853000	-0.497473000	-1.153499000	C	1.033465000	-0.796018000	-1.079798000
H	1.221997000	-1.533215000	-1.232160000	H	0.163407000	-1.439983000	-0.973024000
H	1.879964000	-0.178160000	-2.156978000	H	1.304487000	-0.780304000	-2.143270000
C	2.796821000	-0.439053000	-0.197733000	C	2.219686000	-1.381005000	-0.295413000
C	3.370927000	0.990529000	0.008837000	C	3.476189000	-0.537893000	-0.515810000
C	2.338746000	2.093663000	0.062035000	C	3.251153000	0.931727000	-0.285269000
C	2.525421000	-1.117000000	1.148595000	C	1.884934000	-1.367533000	1.204801000
O	3.354575000	-1.182445000	2.008503000	O	2.504036000	-0.744870000	2.023519000
O	1.301342000	-1.643928000	1.238474000	O	0.816087000	-2.108535000	1.446252000
C	1.068844000	-2.432165000	2.420912000	C	0.394992000	-2.201752000	2.820396000
H	1.855235000	-3.179420000	2.516749000	H	1.141398000	-2.755650000	3.389495000
H	0.098866000	-2.899584000	2.277227000	H	-0.553828000	-2.730250000	2.793504000
H	1.062196000	-1.786697000	3.299113000	H	0.267282000	-1.204586000	3.237814000
C	3.862864000	-1.307667000	-0.904196000	C	2.538912000	-2.831968000	-0.662006000
O	4.724735000	-0.871492000	-1.609793000	O	3.513342000	-3.395076000	-0.245659000
O	3.638273000	-2.600121000	-0.688467000	O	1.638147000	-3.372508000	-1.472217000
C	4.563343000	-3.508641000	-1.312181000	C	1.847006000	-4.758136000	-1.791390000
H	4.523763000	-3.393462000	-2.394859000	H	2.800427000	-4.883561000	-2.303678000
H	5.572796000	-3.303226000	-0.958424000	H	1.845133000	-5.350384000	-0.877193000
H	4.242212000	-4.501622000	-1.013375000	H	1.017645000	-5.037281000	-2.434089000
H	4.066985000	1.172059000	-0.807223000	H	3.812908000	-0.676778000	-1.553880000
H	3.969579000	0.958731000	0.920629000	H	4.272374000	-0.910499000	0.126164000
C	1.636257000	2.390601000	1.245630000	C	4.264697000	1.756461000	0.146758000
C	0.667741000	3.391574000	1.229519000	C	4.035278000	3.156725000	0.276417000
C	1.085886000	3.823651000	-1.083798000	C	1.785209000	2.910455000	-0.446704000
H	0.888968000	4.395053000	-1.986002000	H	0.785735000	3.319937000	-0.540726000
C	0.368028000	4.113928000	0.074307000	C	2.843905000	3.759903000	-0.029560000
H	0.135034000	3.618528000	2.148712000	H	4.857452000	3.773507000	0.626957000
C	2.877439000	2.655050000	-2.373081000	C	2.109401000	2.245673000	-2.244967000

H	2.943279000	1.615074000	-2.699063000	H	1.939878000	1.264474000	-2.687983000
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H	3.905819000	2.997883000	-2.227479000	H	3.126844000	2.589697000	-2.394783000
C	1.844976000	1.622949000	2.526142000	C	5.613590000	1.202567000	0.515848000
H	1.503398000	2.211918000	3.377571000	H	6.297458000	1.997893000	0.807984000
H	1.257560000	0.697504000	2.520719000	H	5.513733000	0.508799000	1.355110000
H	2.886754000	1.352038000	2.696311000	H	6.060764000	0.653630000	-0.315734000
C	-0.648229000	5.225459000	0.095310000	C	2.614754000	5.240735000	0.065644000
H	-0.159090000	6.177320000	0.319278000	H	2.461028000	5.673190000	-0.927405000
H	-1.142460000	5.332407000	-0.871757000	H	1.728674000	5.463016000	0.664260000
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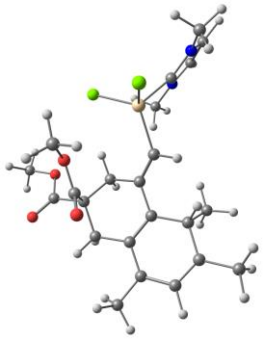
C	-3.617603000	-0.416153000	-0.495663000	C	-3.727166000	0.629192000	-0.443392000
N	-3.932865000	-0.515989000	-1.802012000	N	-3.935107000	0.496386000	-1.769632000
H	-3.406946000	-0.535915000	-3.815456000	H	-3.166940000	0.305011000	-3.695542000
C	-3.012800000	-0.908404000	-2.872267000	C	-2.999138000	-0.120518000	-2.707593000
H	-2.919360000	-1.993056000	-2.902574000	H	-3.147614000	-1.199608000	-2.725904000
H	-2.036120000	-0.460625000	-2.693238000	H	-1.979137000	0.096790000	-2.390811000
C	-5.268397000	-0.257434000	-1.993912000	C	-5.188788000	0.946112000	-2.114912000
H	-5.726579000	-0.288698000	-2.967869000	H	-5.552049000	0.922944000	-3.128120000
H	-6.793435000	0.271623000	-0.474533000	H	-6.740631000	1.809263000	-0.790785000
C	-5.790859000	0.015100000	-0.771878000	C	-5.770388000	1.378301000	-0.969971000
N	-4.761691000	-0.086299000	0.133732000	N	-4.857436000	1.178849000	0.041105000
H	-4.641331000	-0.770938000	2.119838000	H	-4.298092000	2.054403000	1.867877000
C	-4.920303000	0.129735000	1.577033000	C	-5.126259000	1.488659000	1.448867000
H	-5.965554000	0.362369000	1.766581000	H	-5.250324000	0.566709000	2.014149000
H	-4.294795000	0.959265000	1.900431000	H	-6.038547000	2.079700000	1.492714000

Q'

E(RM062X) = -4149.85590017

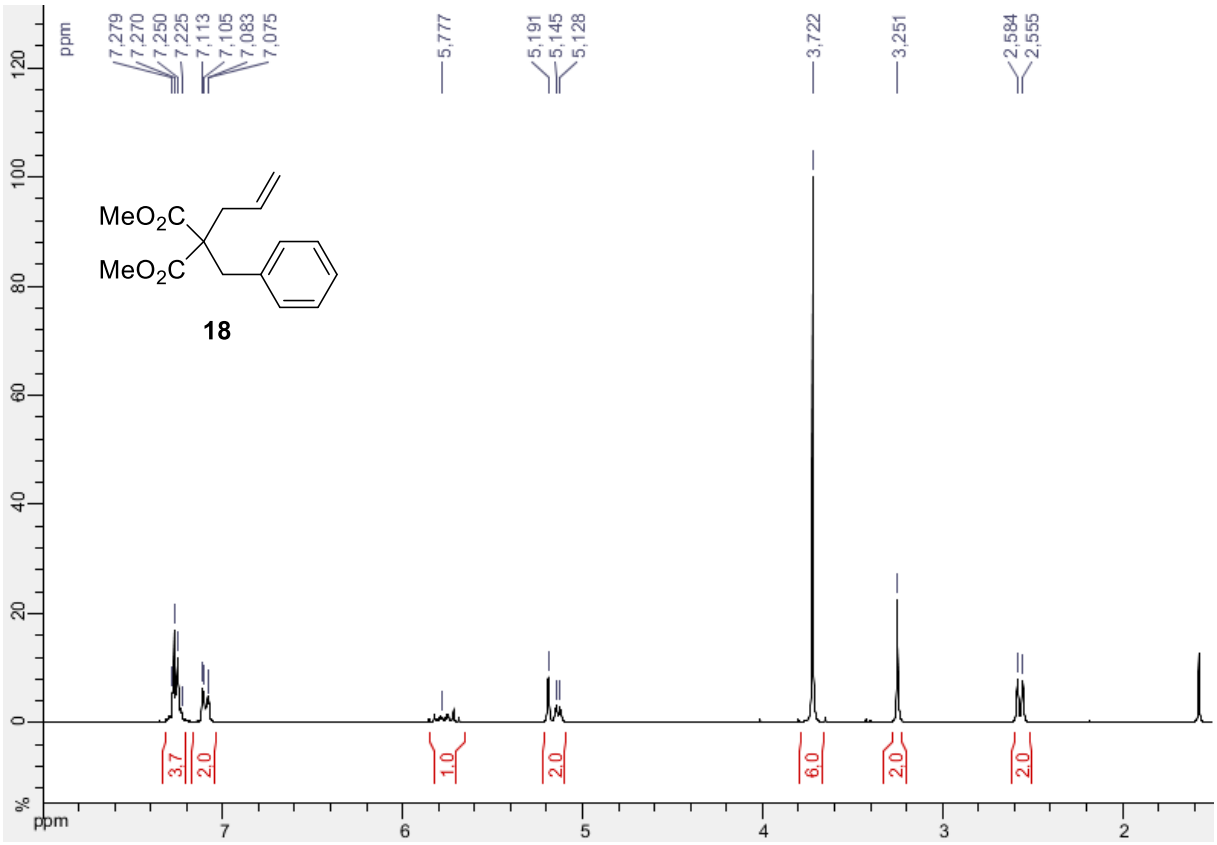


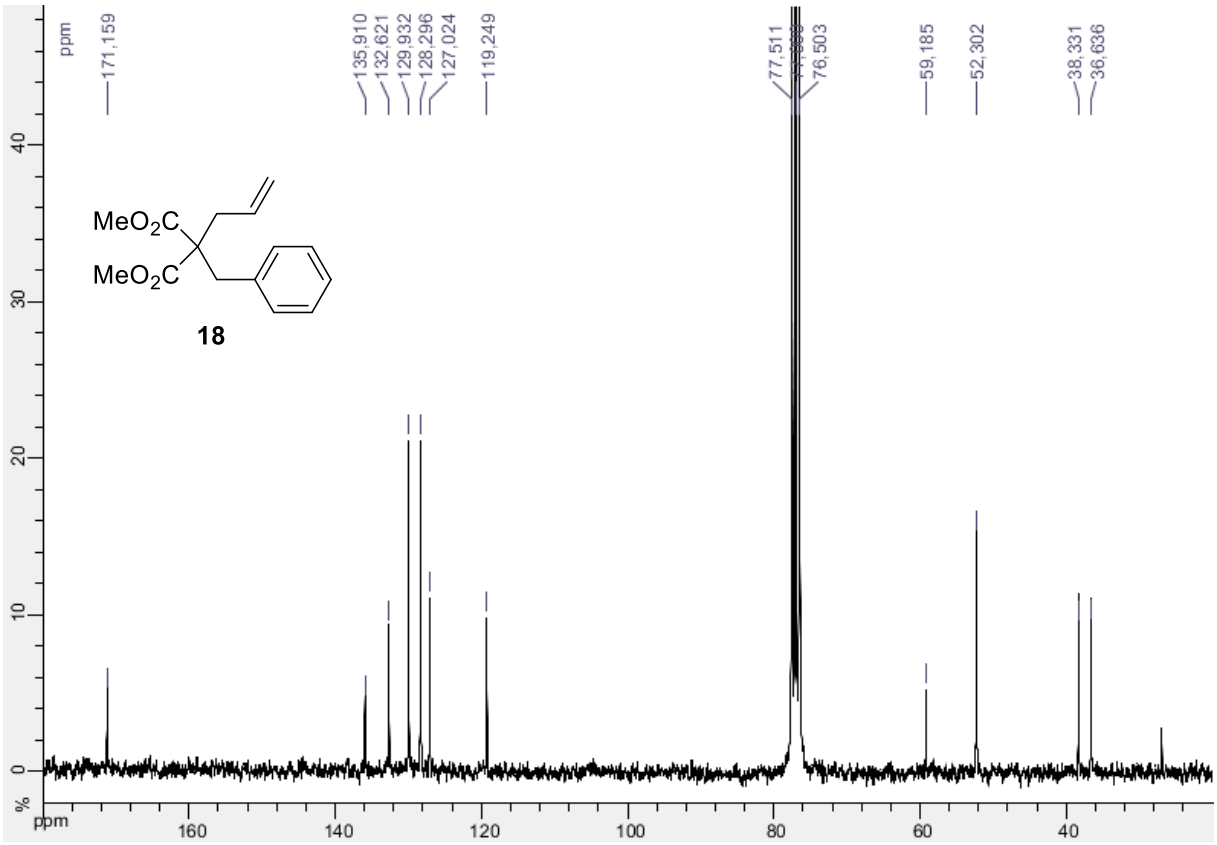
C	1.996490000	1.401795000	-0.315597000
C	0.796234000	0.552484000	-0.407605000
C	-0.380460000	0.909262000	0.150735000
Ga	-2.060737000	-0.133684000	0.533938000
Cl	-2.176159000	-2.264686000	-0.052992000
Cl	-2.410433000	0.148935000	2.702103000
H	-0.418709000	1.892520000	0.623306000
C	1.024426000	-0.809648000	-1.018824000
H	0.138540000	-1.432775000	-0.925108000
H	1.269921000	-0.718343000	-2.082985000

C	2.212287000	-1.464047000	-0.302320000
C	3.477233000	-0.652306000	-0.558617000
C	3.258968000	0.832853000	-0.375420000
C	1.925048000	-1.472249000	1.208328000
O	2.600038000	-0.909190000	2.026075000
O	0.815024000	-2.147581000	1.461707000
C	0.400023000	-2.209740000	2.838170000
H	1.140113000	-2.760220000	3.418472000
H	-0.556282000	-2.725273000	2.825670000
H	0.286425000	-1.202072000	3.236088000
C	2.466839000	-2.913743000	-0.716375000
O	3.469275000	-3.499147000	-0.409936000
O	1.476625000	-3.429332000	-1.431942000
C	1.624333000	-4.814680000	-1.782473000
H	2.527322000	-4.955499000	-2.375769000
H	1.685985000	-5.418199000	-0.877550000
H	0.736806000	-5.067000000	-2.354769000
H	3.823685000	-0.842563000	-1.581485000
H	4.258871000	-1.005058000	0.113914000
C	4.393174000	1.661927000	-0.196275000
C	4.277868000	3.052054000	0.049298000
C	1.836852000	2.878668000	-0.180640000
H	1.128984000	3.088968000	0.629700000
C	3.065315000	3.664471000	0.087364000
H	5.183231000	3.623095000	0.222457000
C	1.185938000	3.437609000	-1.489058000
H	0.261654000	2.897391000	-1.687408000
H	0.963468000	4.497603000	-1.373379000
H	1.869237000	3.305555000	-2.329882000
C	5.757945000	1.063196000	-0.201282000
H	6.532898000	1.825592000	-0.246167000
H	5.889965000	0.487588000	0.723801000
H	5.884833000	0.359074000	-1.025927000
C	2.934378000	5.132544000	0.332474000
H	2.892796000	5.666496000	-0.623250000
H	2.020605000	5.368383000	0.880672000
H	3.793244000	5.513054000	0.884611000
C	-3.673440000	0.644105000	-0.504359000
N	-3.798866000	0.537236000	-1.842940000
H	-2.935988000	0.331882000	-3.727156000
C	-2.814176000	-0.082893000	-2.728202000
H	-2.955827000	-1.163060000	-2.743163000
H	-1.811507000	0.144304000	-2.365485000
C	-5.020859000	1.014628000	-2.257606000
H	-5.320241000	1.014934000	-3.291904000
H	-6.639700000	1.880073000	-1.016632000

C	-5.666598000	1.436929000	-1.143304000	
N	-4.822539000	1.203750000	-0.080853000	
H	-4.369048000	2.050734000	1.788484000	
C	-5.170457000	1.489479000	1.314595000	
H	-5.321896000	0.557525000	1.856501000	
H	-6.086507000	2.076175000	1.318628000	

10. Copies of ^{1}H and ^{13}C NMR Spectra:

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129,932
128,296
127,024
119,249
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76,503
59,185
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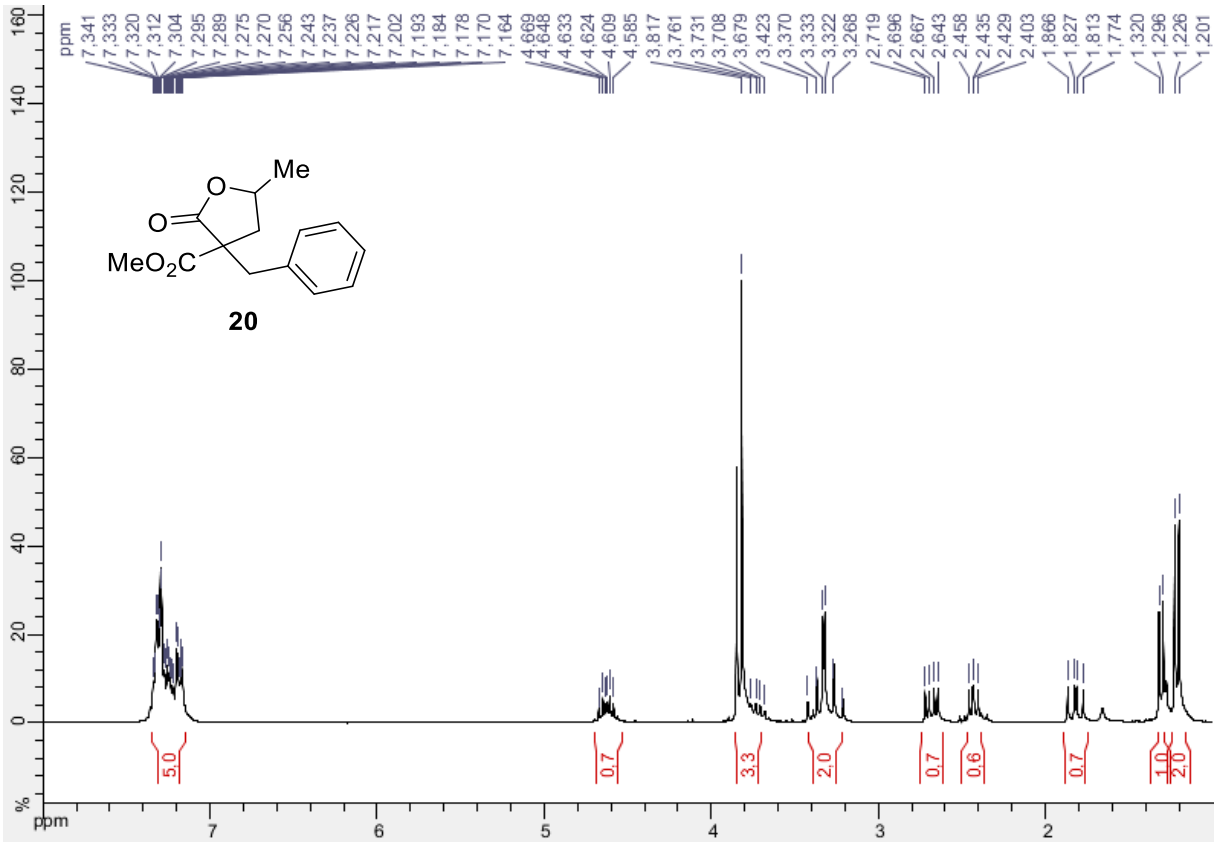
36,636
MeO2C
MeO2C
18
%
ppm
160
140
120
100
80
60
40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7,295
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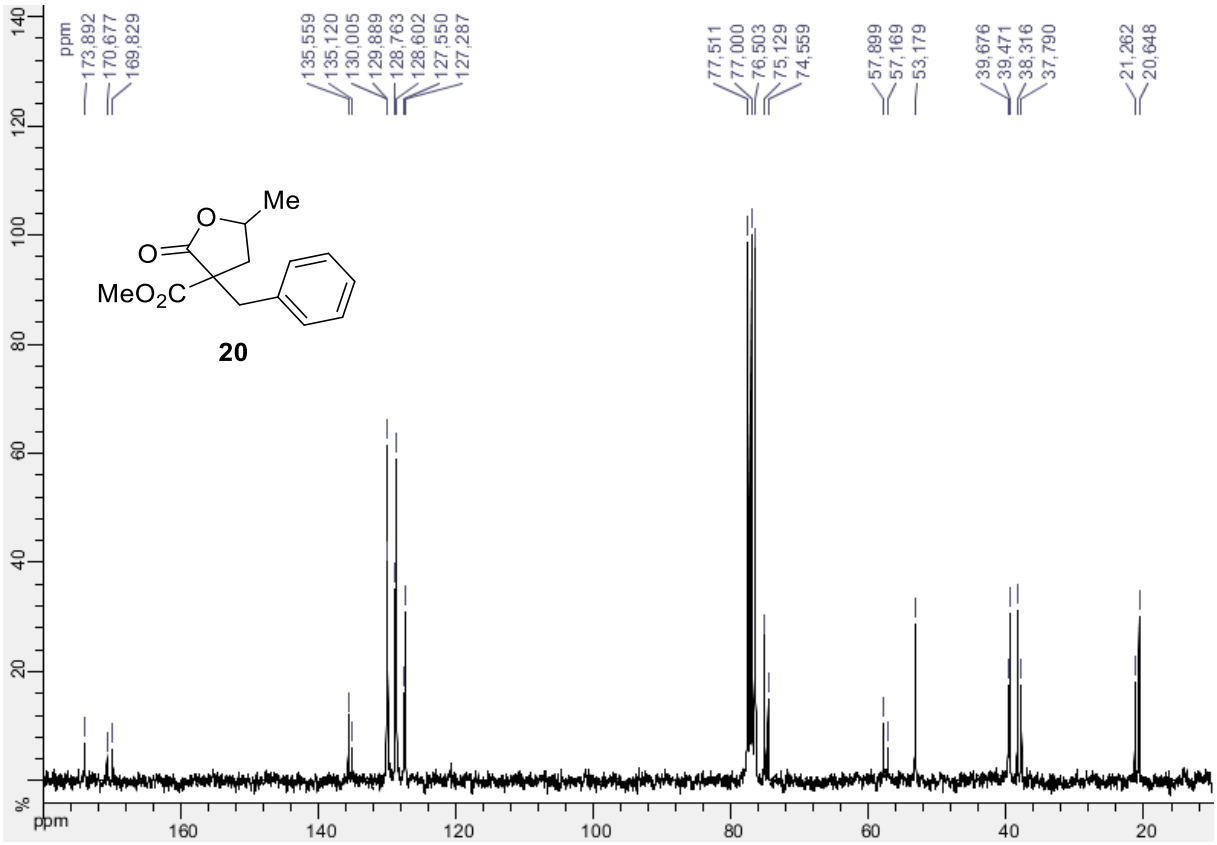
7,275
7,270
7,256
7,243
7,237
7,226
7,217
7,202
7,193
7,184
7,178
7,170
7,164
4,669
4,648
4,633
4,624
4,609
4,585
3,817
3,761
3,731
3,708
3,679
3,423
3,370
3,333
3,322
3,268
2,719
2,696
2,667
2,643
2,458
2,435
2,429
2,403
1,866
1,827
1,813
1,774
1,320
1,296
1,226
1,201
O
Me
O
MeO2C
20
5,0
0,7
3,3
2,0
0,7
0,6
0,7
1,0
2,0
%
ppm
7
6
5
4
3
2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169,829
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128,602
127,550
127,287
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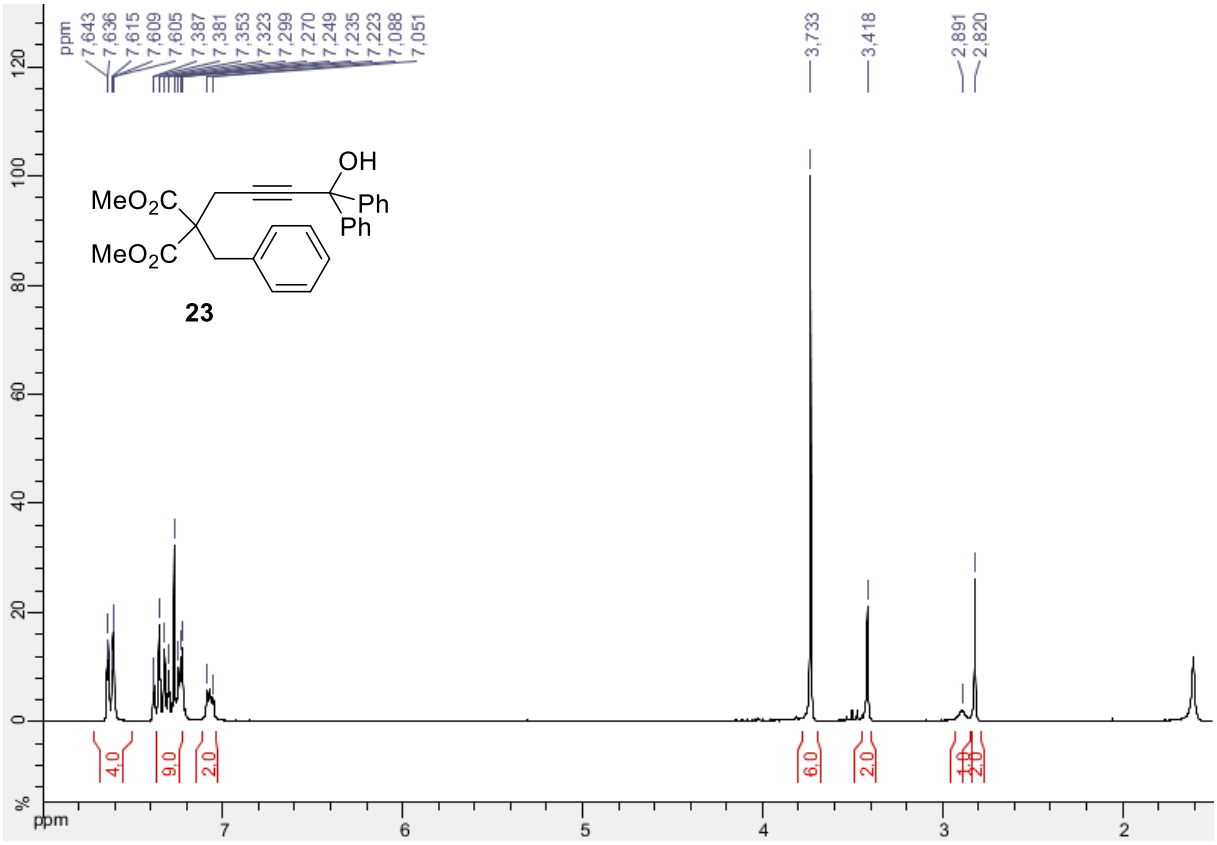
76,503
75,129
74,559
57,899
57,169
53,179
39,676
39,471
38,316
37,790
21,262
20,648
Me
O
O
MeO2C
20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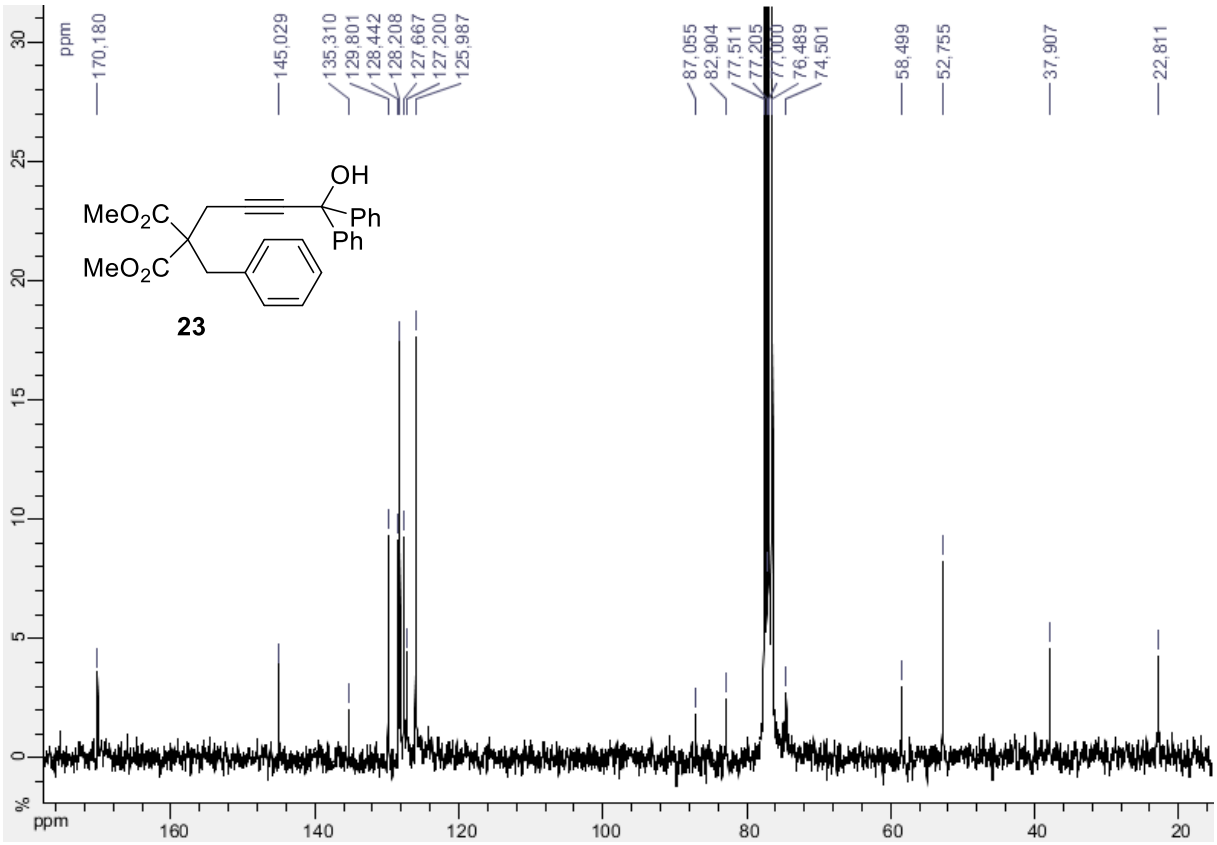
7,615
7,609
7,605
7,387
7,381
7,353
7,323
7,299
7,270
7,249
7,235
7,223
7,088
7,051
3,733
3,418
2,891
2,820
OH
Ph
Ph
MeO2C
MeO2C
23
4.0
9.0
2.0
6.0
2.0
1.0
2.0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127,200
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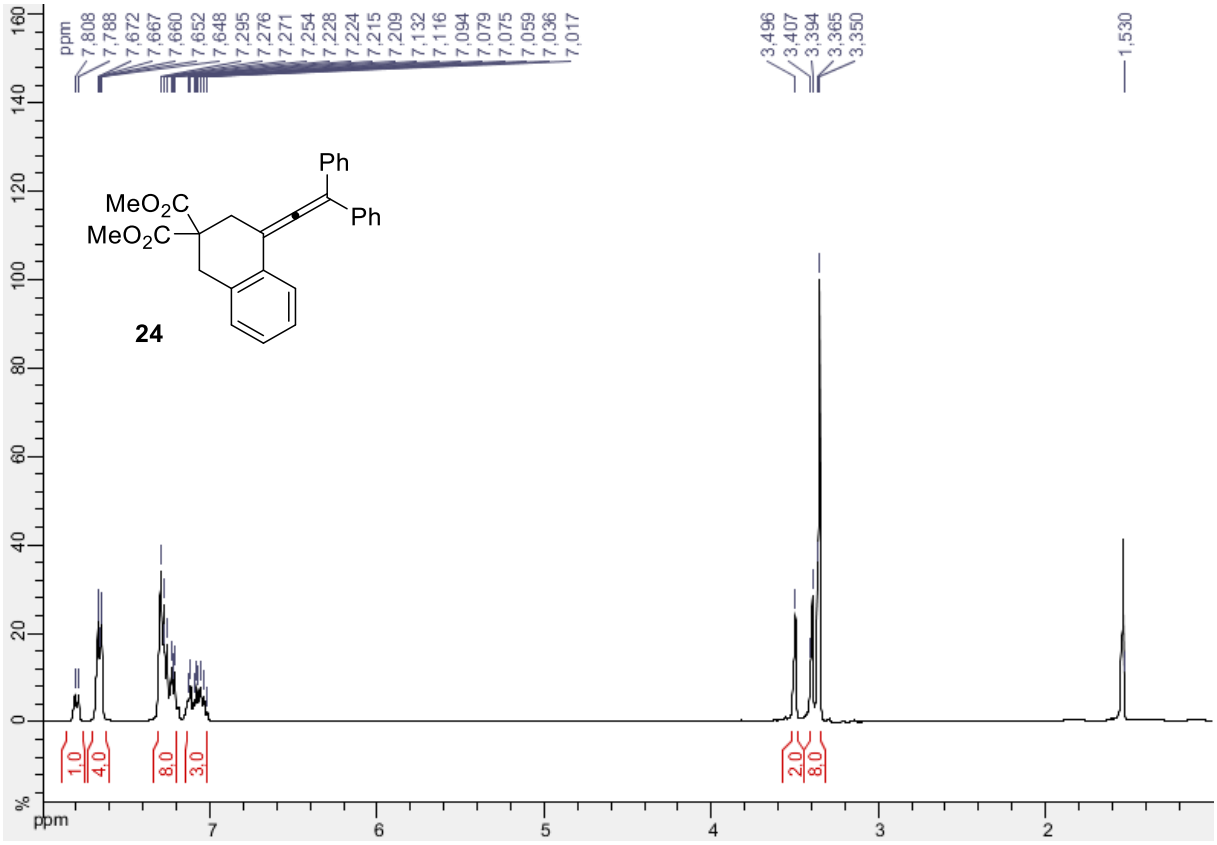
87,055
82,904
77,511
77,205
77,000
76,489
74,501
58,499
52,755
37,907
22,811
OH
Ph
Ph
MeO2C
MeO2C
23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7,660
7,652
7,648
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7,276
7,271
7,254
7,228
7,224
7,215
7,209
7,132
7,116
7,094
7,079
7,075
7,059
7,036
7,017
3,496
3,407
3,394
3,365
3,350
1,530
Ph
Ph
MeO2C
MeO2C
24
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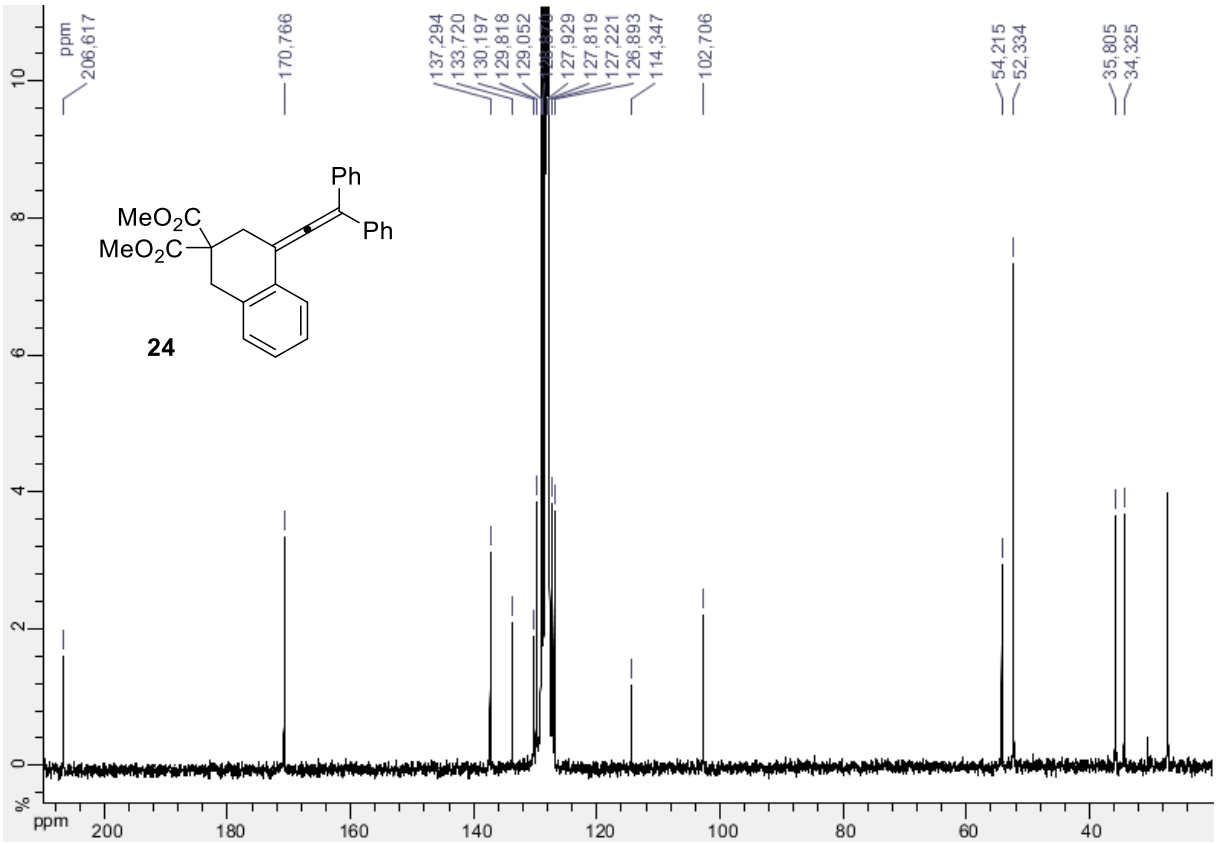
4,0
8,0
3,0
2,0
8,0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133,720
130,197
129,818
129,052
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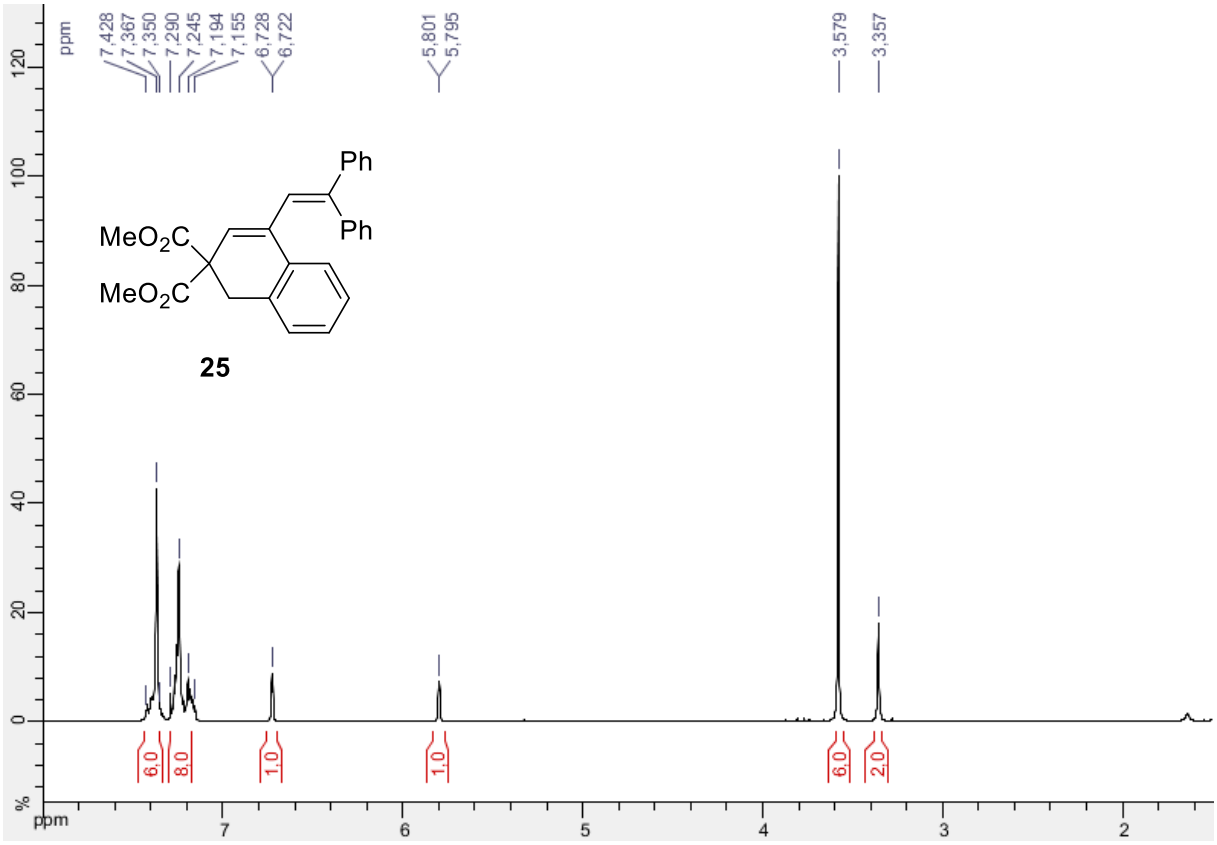
127,819
127,221
126,893
114,347
102,706
54,215
52,334
35,805
34,325
Ph
MeO2C
MeO2C
Ph
24
ppm
200
180
160
140
120
100
80
60
40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7,245
7,194
7,155
6,728
6,722
5,801
5,795
3,579
3,357
Ph
MeO2C
MeO2C
Ph
25
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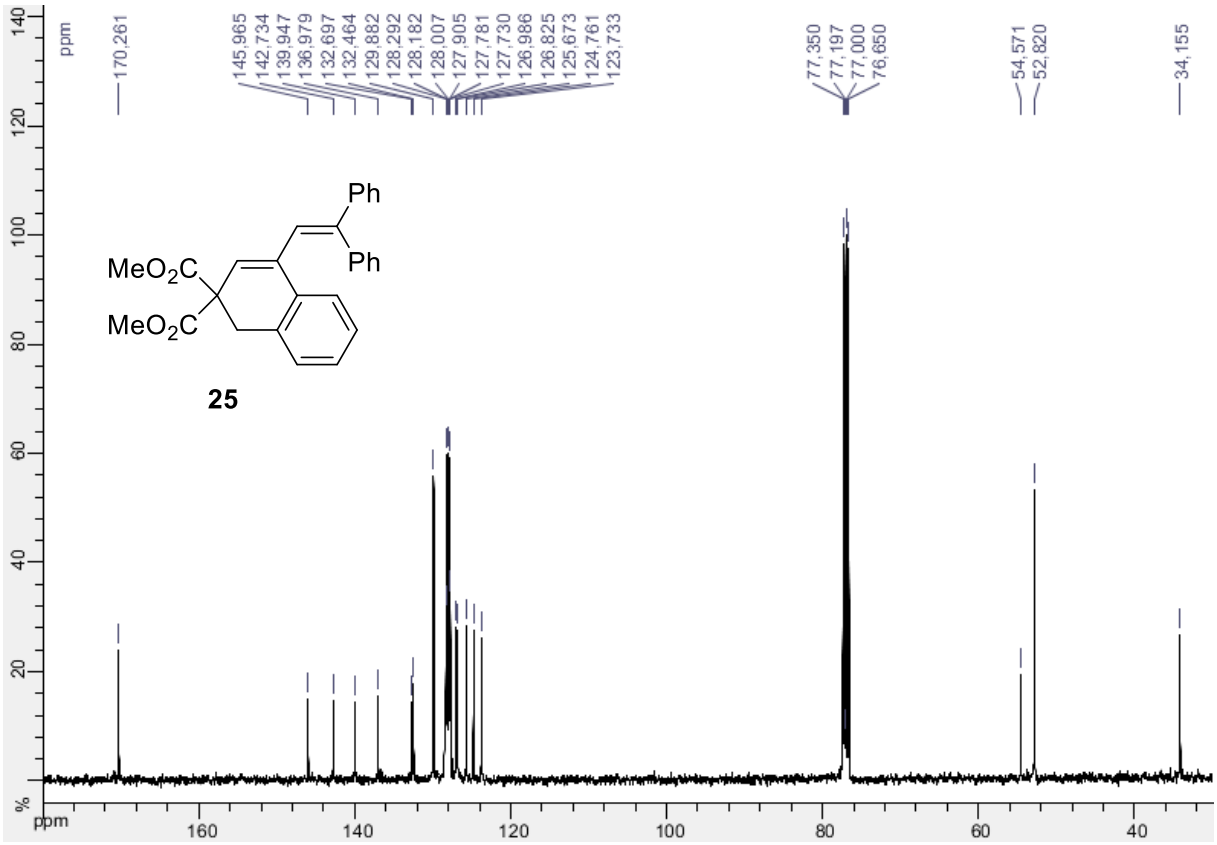
8,0
1,0
1,0
6,0
2,0
ppm
7
6
5
4
3
2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136,979
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132,464
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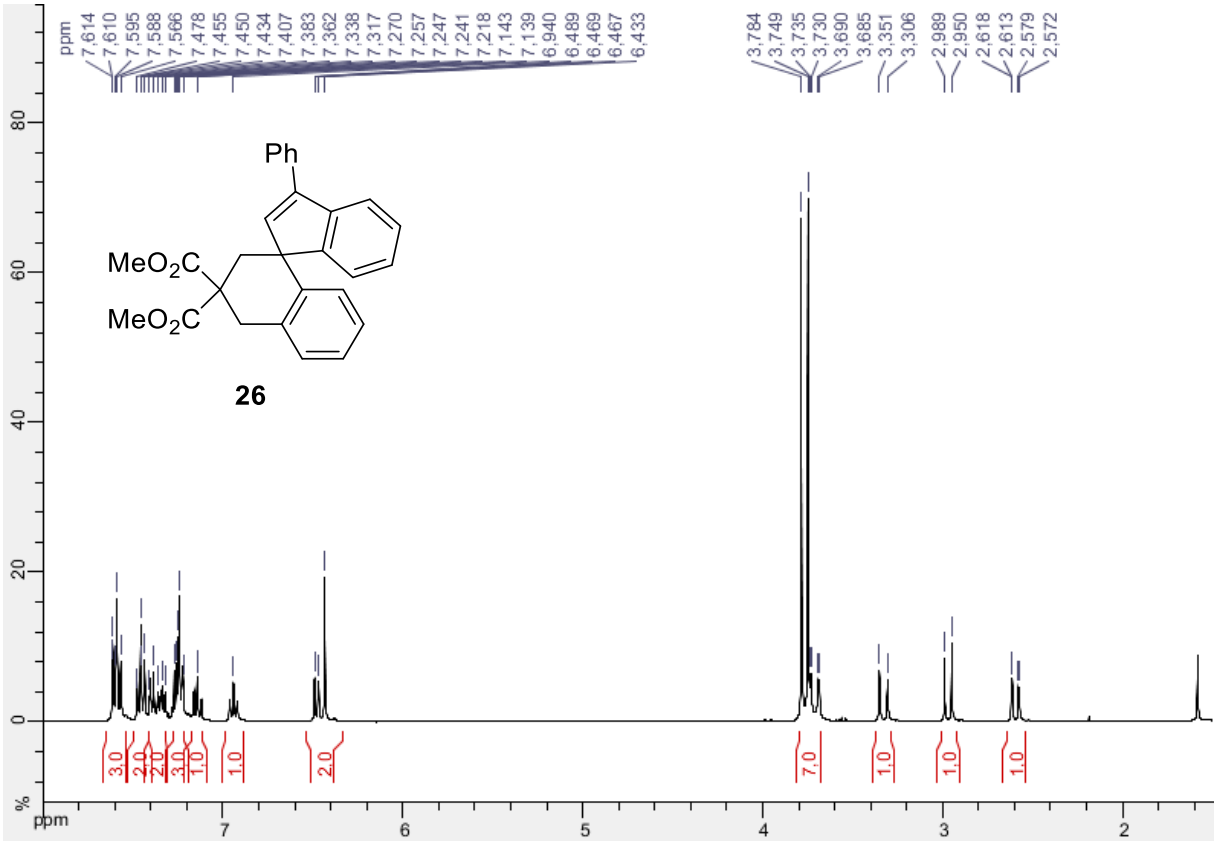
128,292
128,182
128,007
127,905
127,781
127,730
126,986
126,825
125,673
124,761
123,733
77,350
77,197
77,000
76,650
54,571
52,820
34,155
Ph
Ph
MeO2C
MeO2C
25


ppm
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7,566
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7,455
7,450
7,434
7,407
7,383
7,362
7,338
7,317
7,270
7,257
7,247
7,241
7,218
7,143
7,139
6,940
6,489
6,469
6,467
6,433
3,784
3,749
3,735
3,730
3,690
3,685
3,351
3,306
2,989
2,950
2,618
2,613
2,579
2,572
Ph
MeO2C
MeO2C
26
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2,0
3,0
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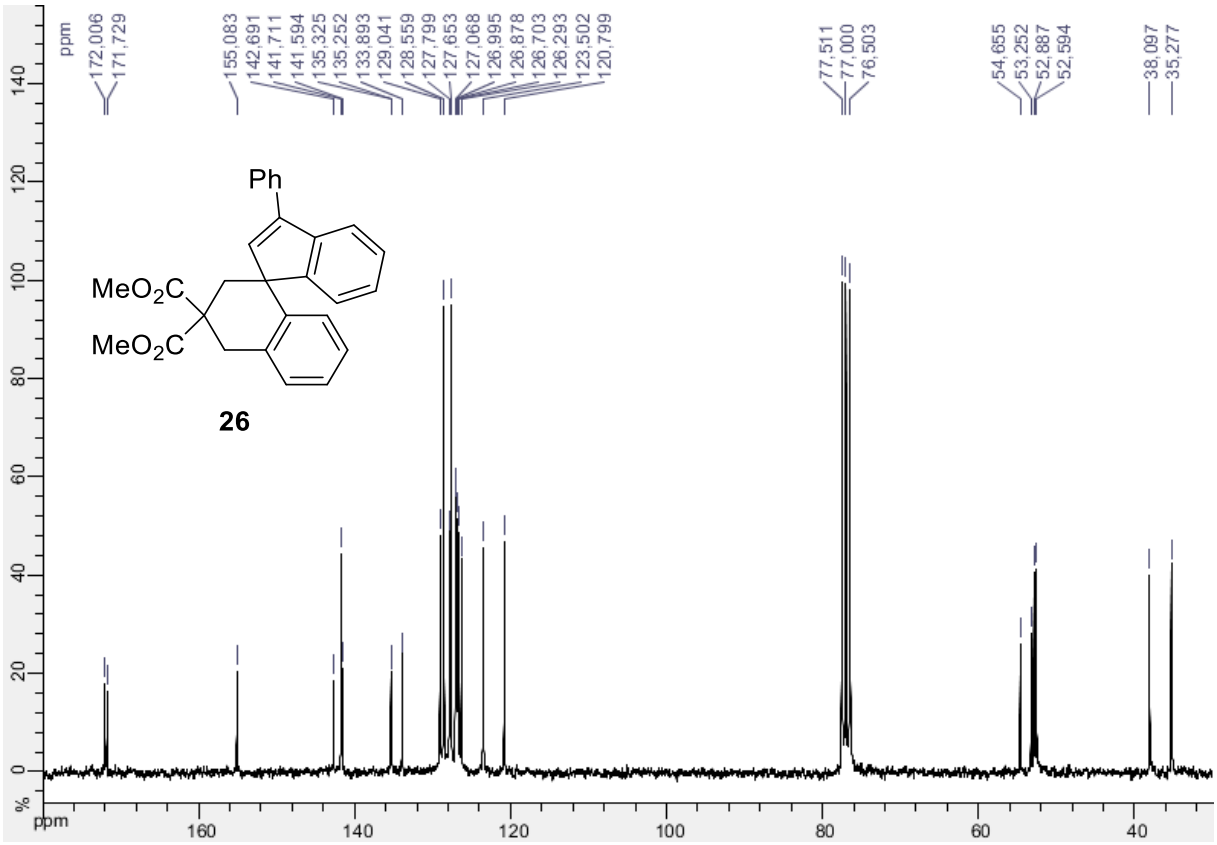
1,0
2,0
7,0
1,0
1,0
1,0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129,041
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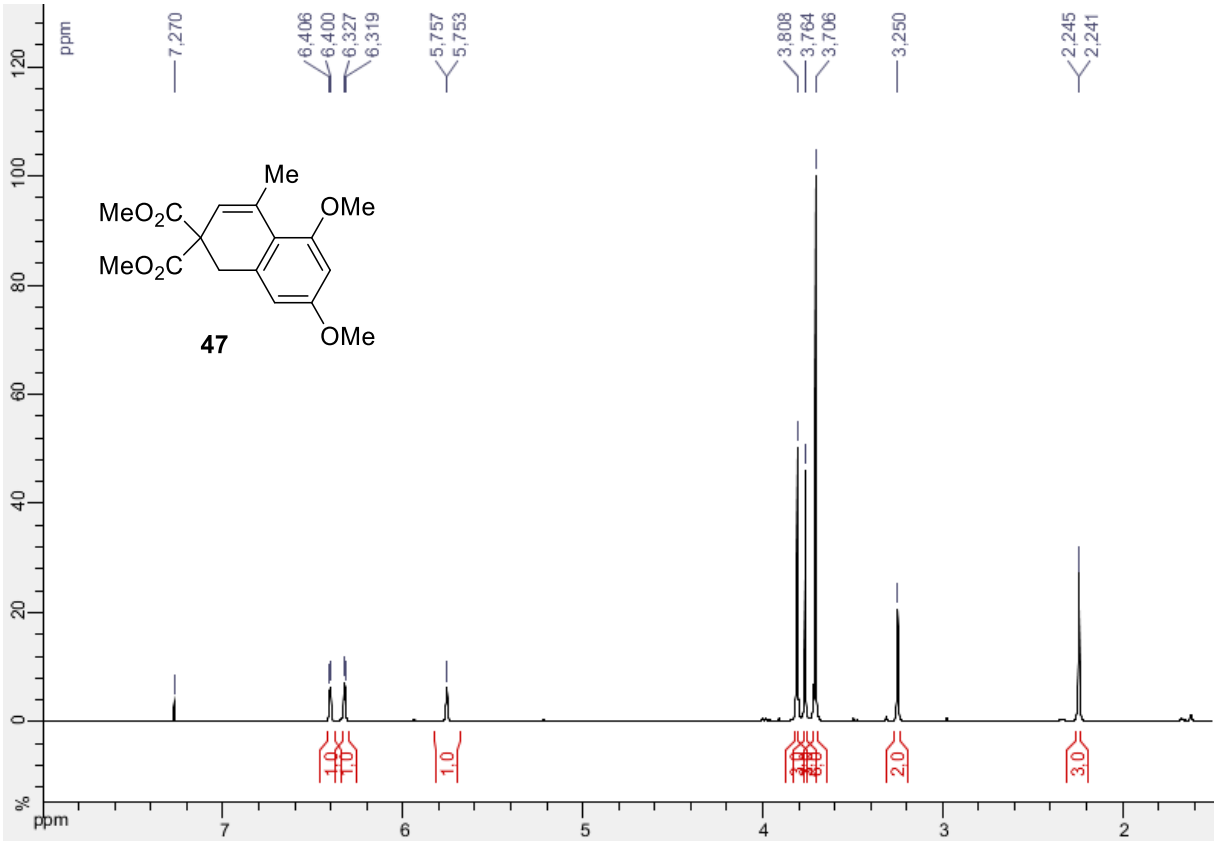
127,799
127,653
127,068
126,995
126,878
126,703
126,293
123,502
120,799
77,511
77,000
76,503
54,655
53,252
52,887
52,594
38,097
35,277
Ph
MeO2C
MeO2C
26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5,753
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3,764
3,706
3,250
2,245
2,241
Me
MeO2C
MeO2C
OMe
OMe
47
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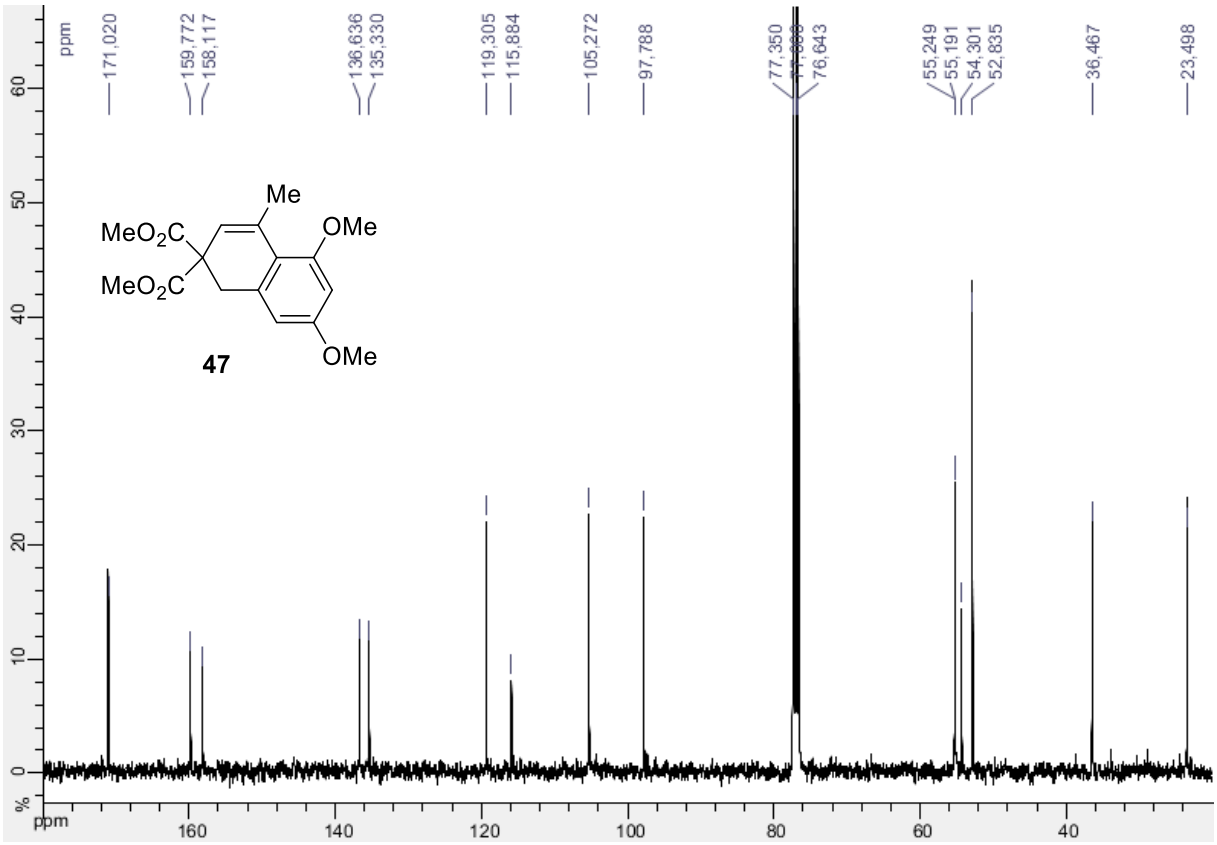
1.0
1.0
2.0
3.0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135,330
119,305
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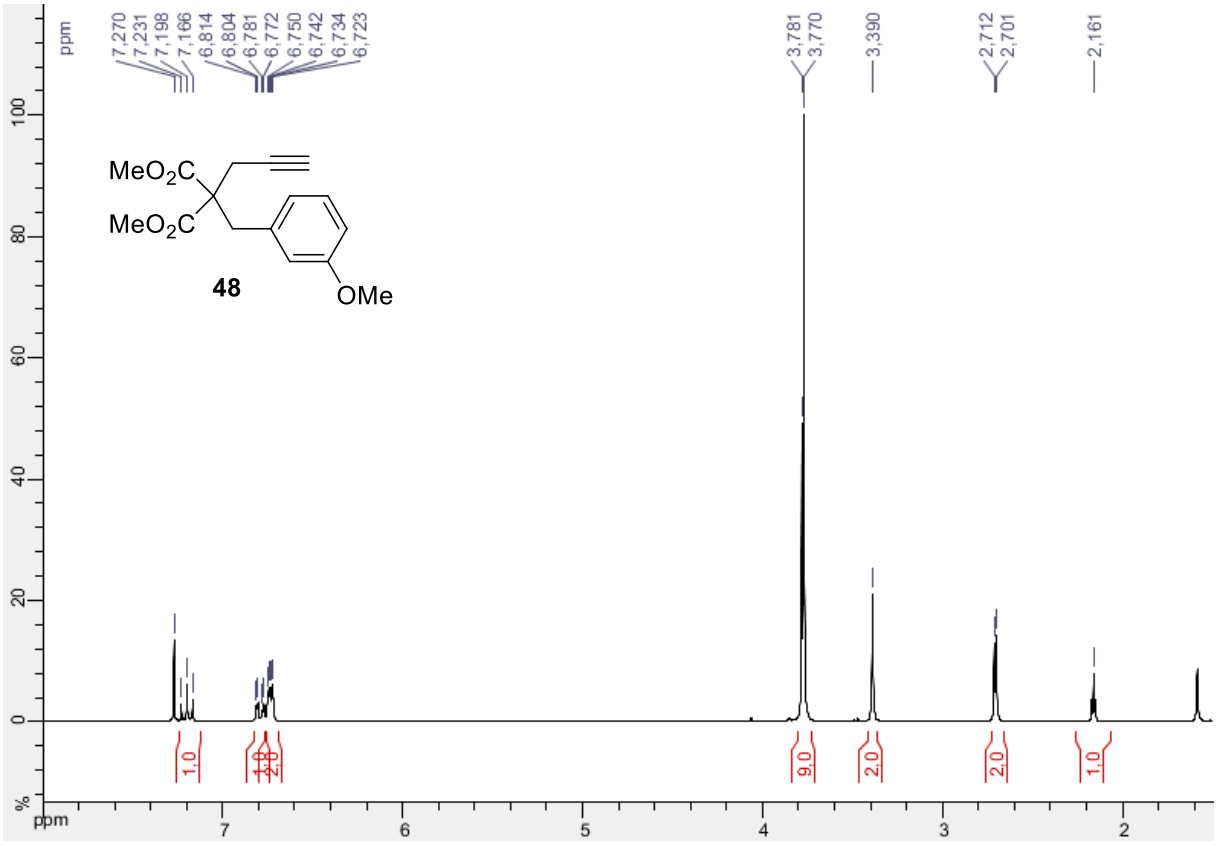
105,272
97,788
77,350
76,643
55,249
55,191
54,301
52,835
36,467
23,498
Me
MeO2C
MeO2C
OMe
OMe
47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7,166
6,814
6,804
6,781
6,772
6,750
6,742
6,734
6,723
3,781
3,770
3,390
2,712
2,701
2,161
MeO2C
MeO2C
OMe
48
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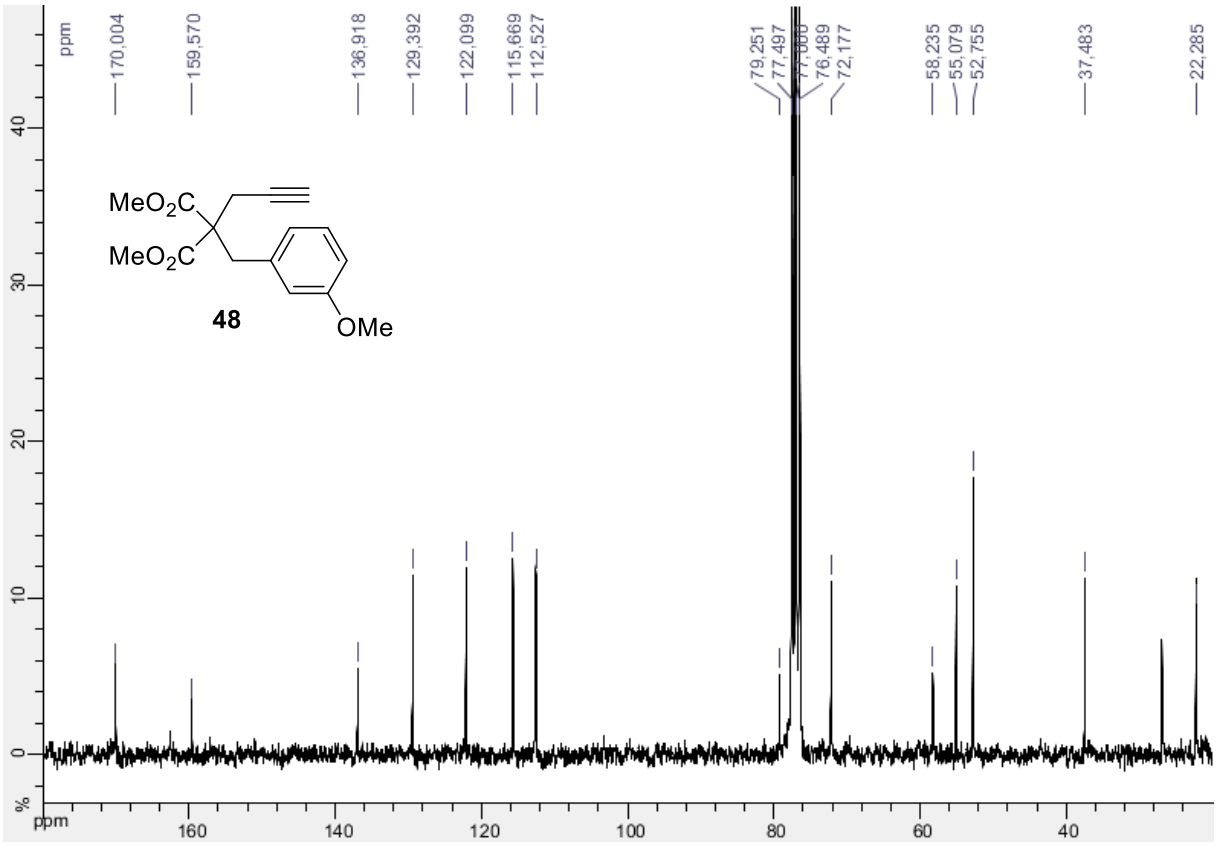
1,0
2,0
9,0
2,0
2,0
1,0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79,251
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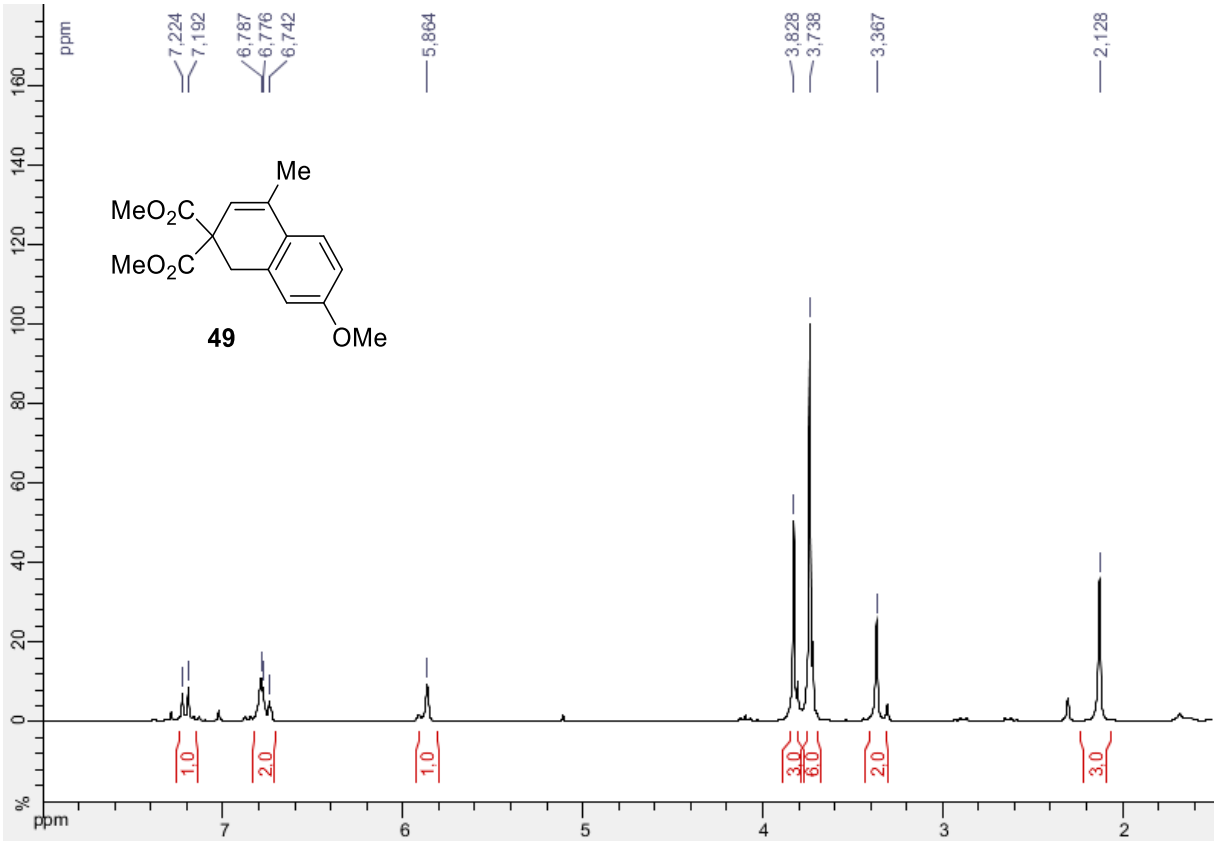
77,080
76,489
72,177
58,235
55,079
52,755
37,483
22,285
MeO2C
MeO2C
OMe
48
%
ppm
160
140
120
100
80
60
40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6,742
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3,367
2,128
Me
MeO2C
MeO2C
OMe
49
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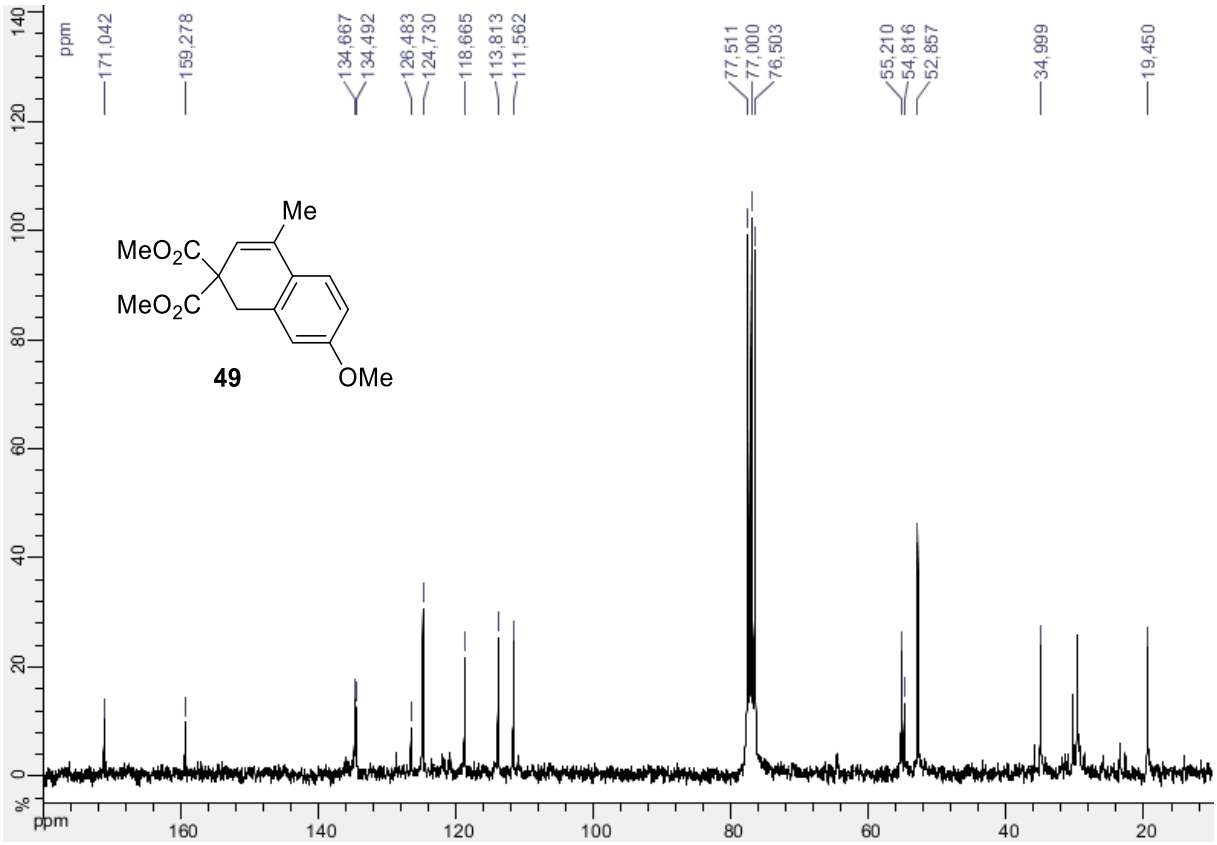
2,0
1,0
3,0
6,0
2,0
3,0
%
ppm
7
6
5
4
3
2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111,562
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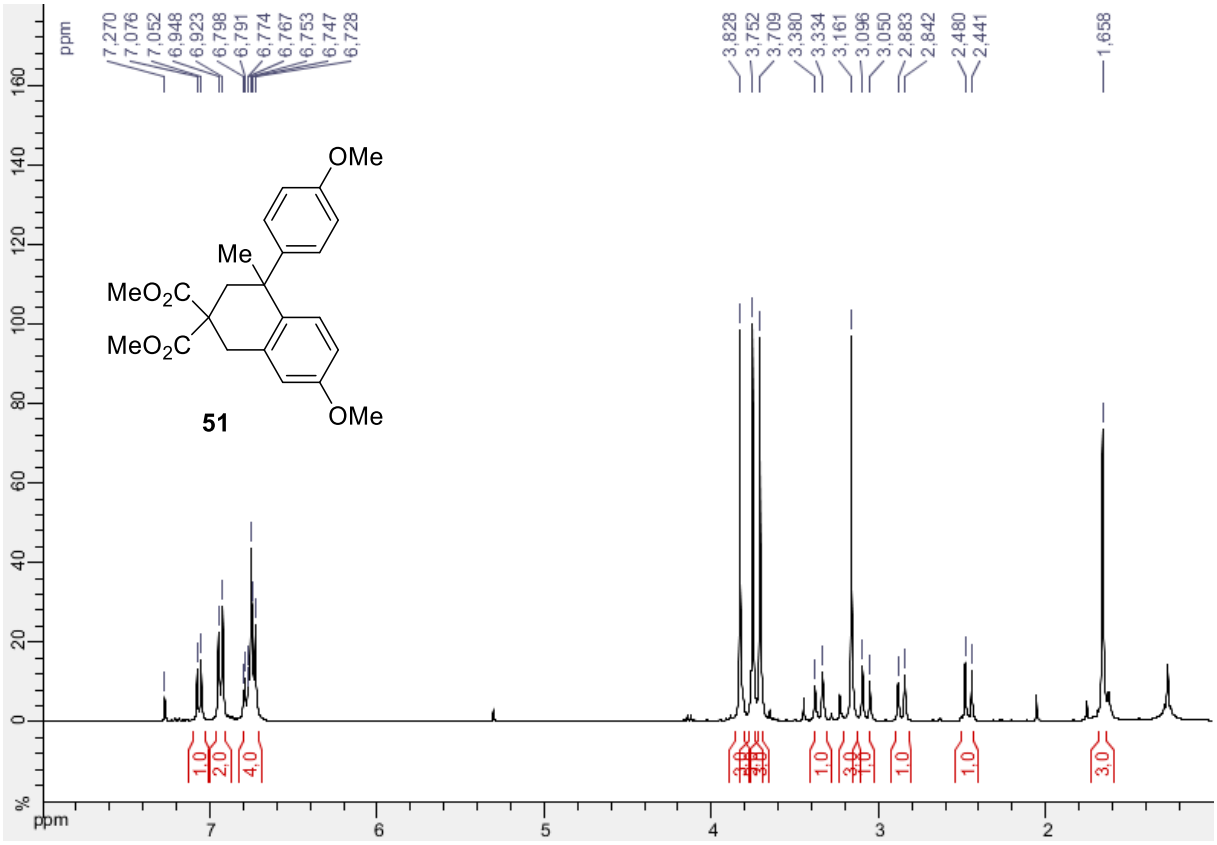
77,000
76,503
55,210
54,816
52,857
34,999
19,450
Me
MeO2C
MeO2C
OMe
49
%
ppm
160
140
120
100
80
60
40
20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6,747
6,728
3,828
3,752
3,709
3,380
3,334
3,161
3,096
3,050
2,883
2,842
2,480
2,441
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Me
MeO2C
MeO2C
OMe
51
1,0
2,0
4,0
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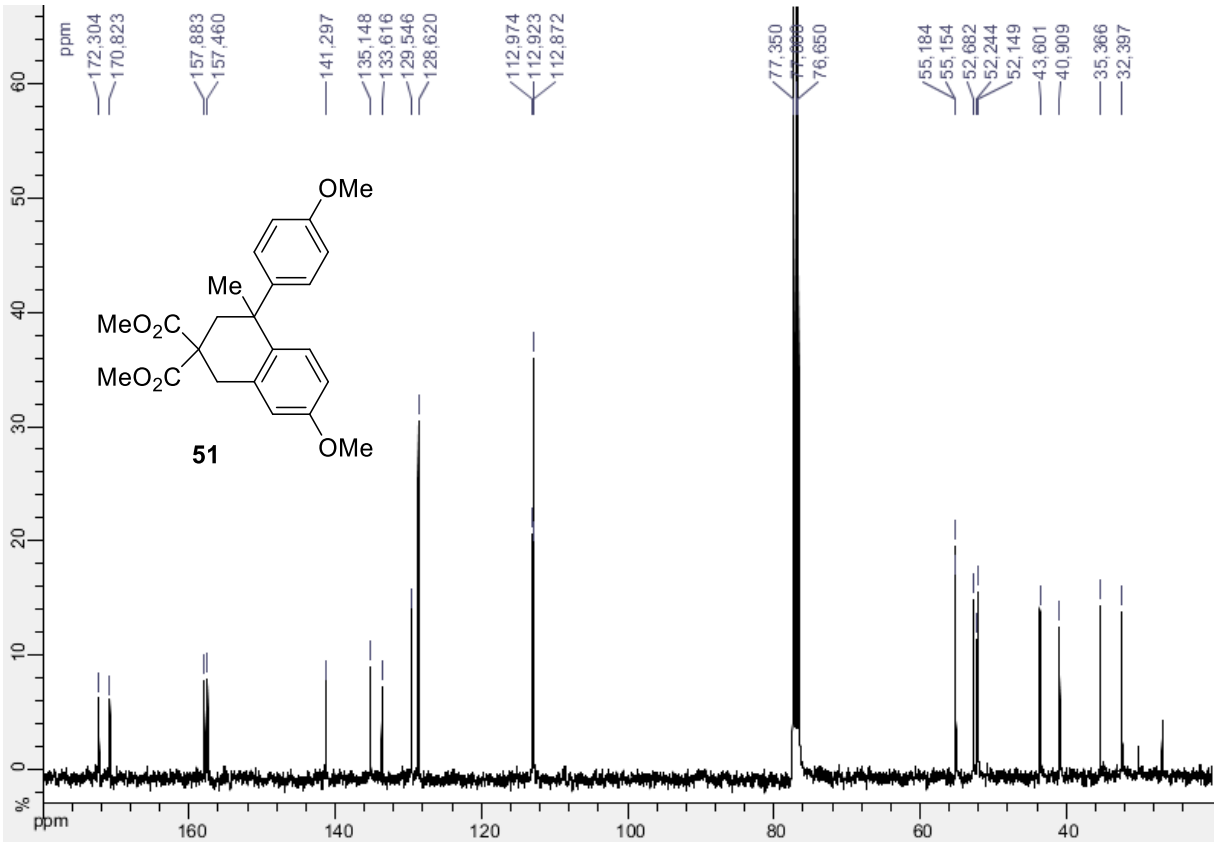
3,0
1,0
1,0
1,0
3,0
%
ppm
7
6
5
4
3
2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112,923
112,872
77,350
76,650
55,184
55,154
52,682
52,244
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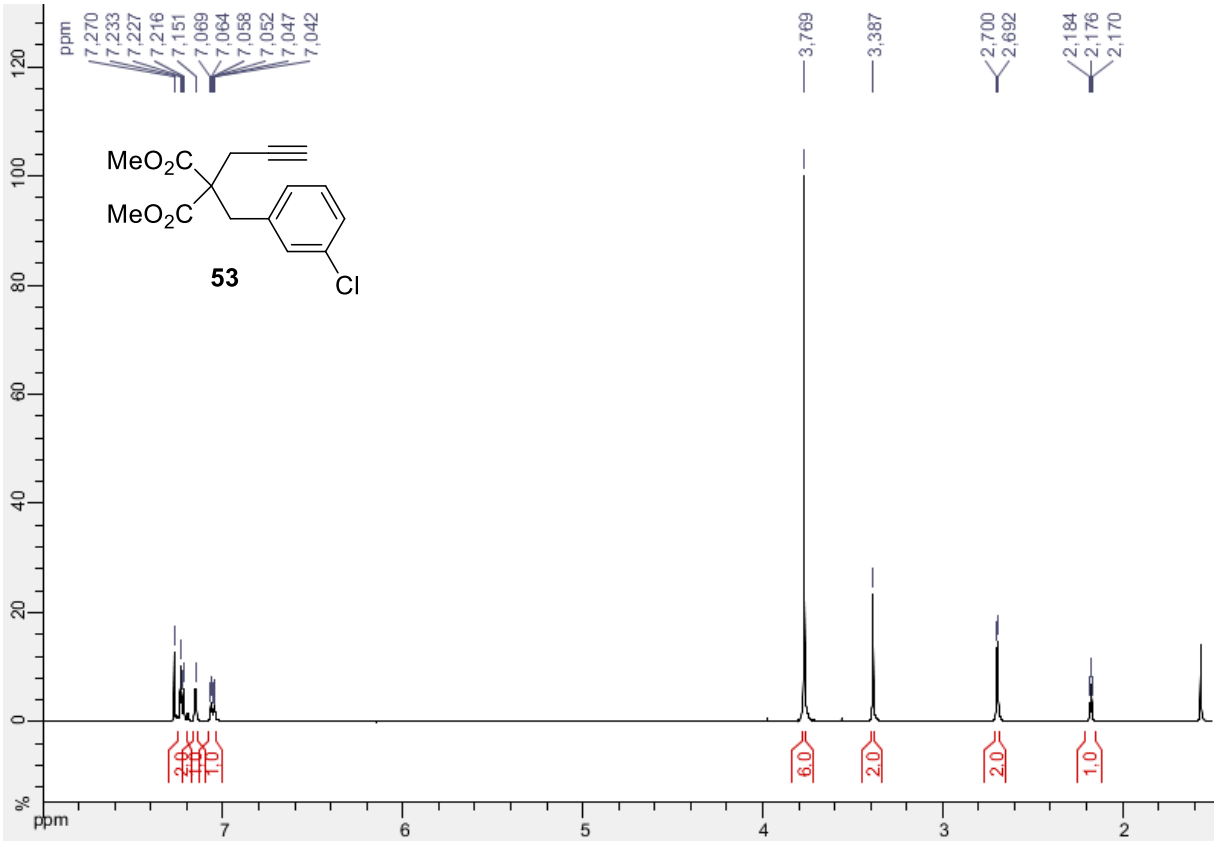
43,601
40,909
35,366
32,397
OMe
Me
MeO2C
MeO2C
OMe
51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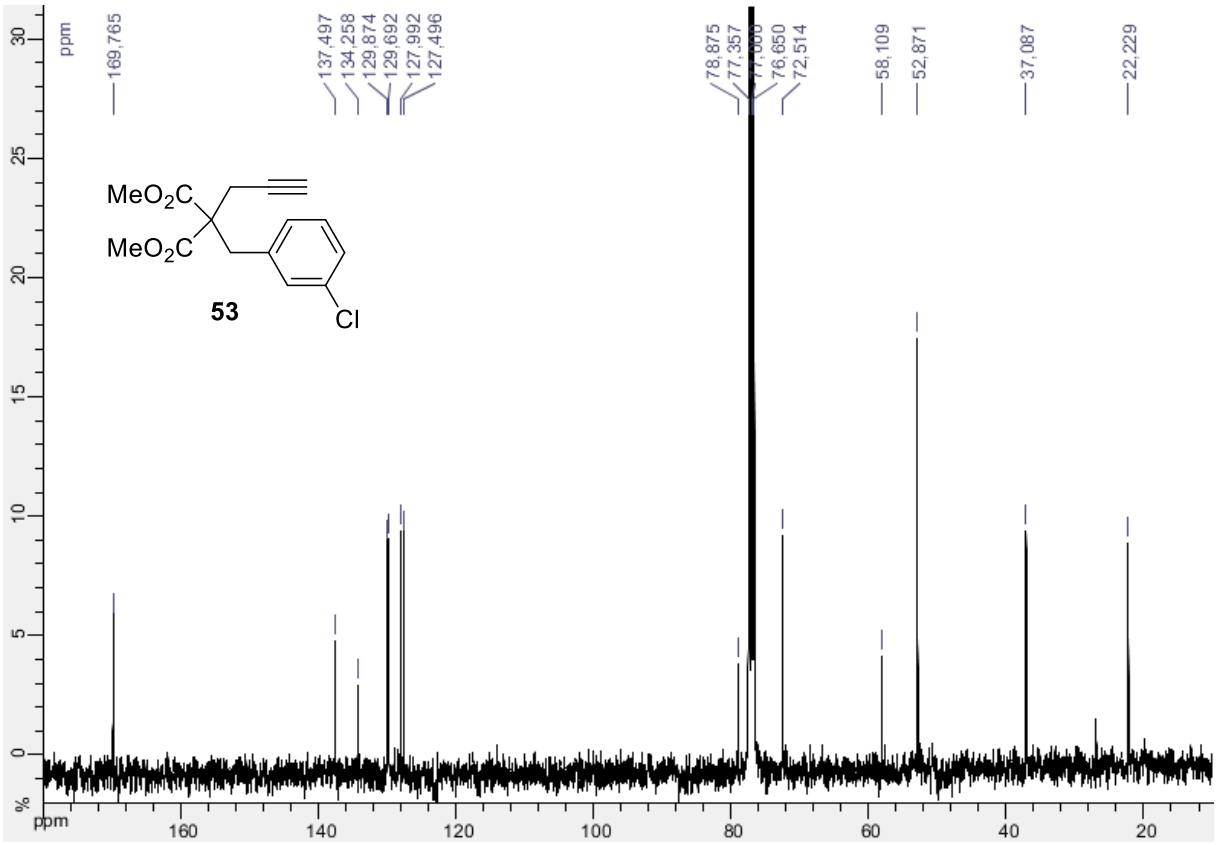
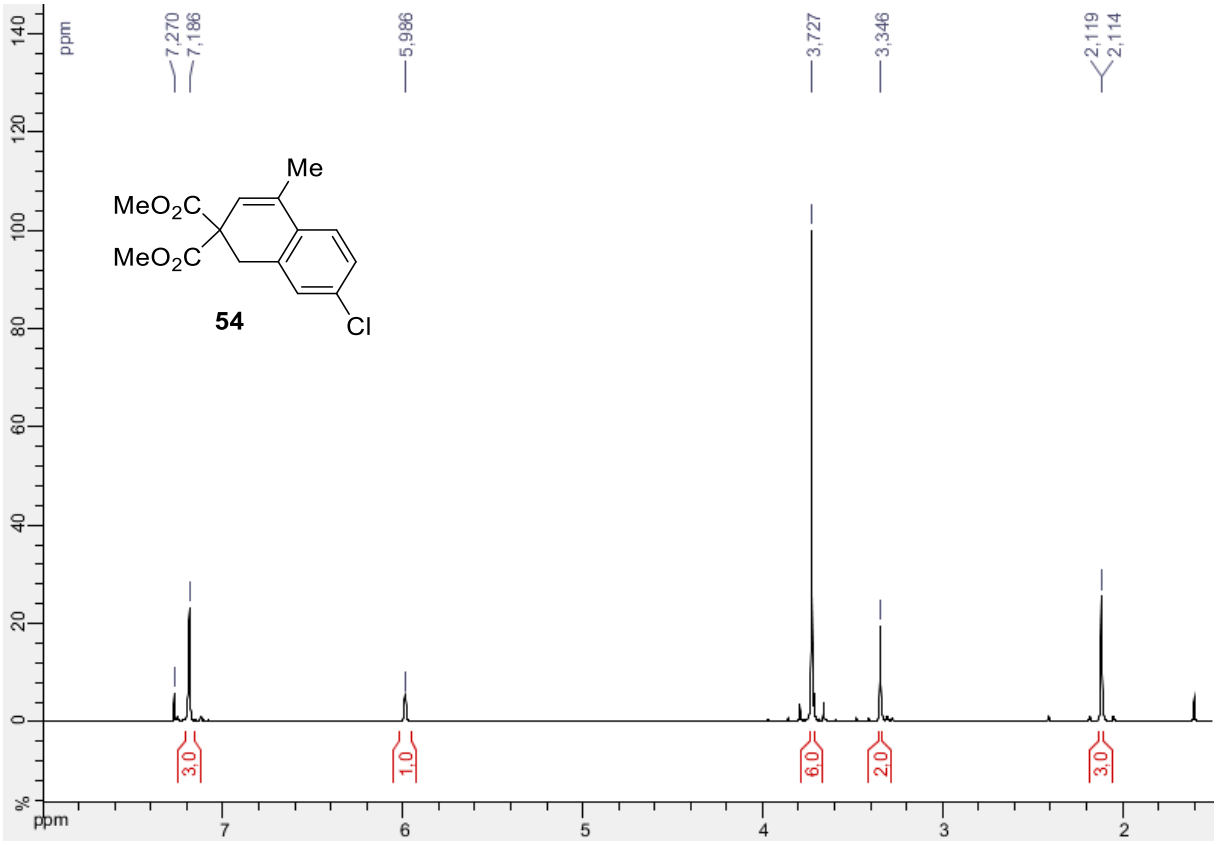
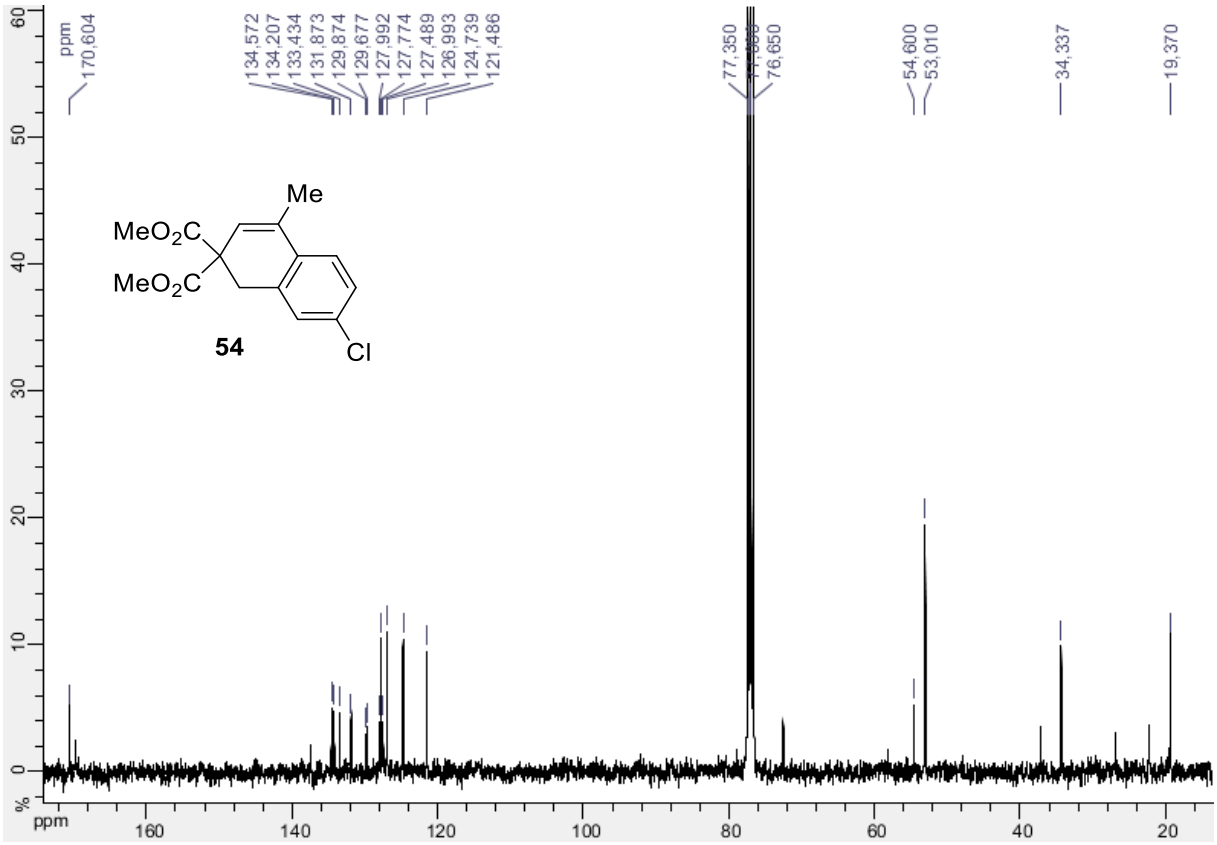
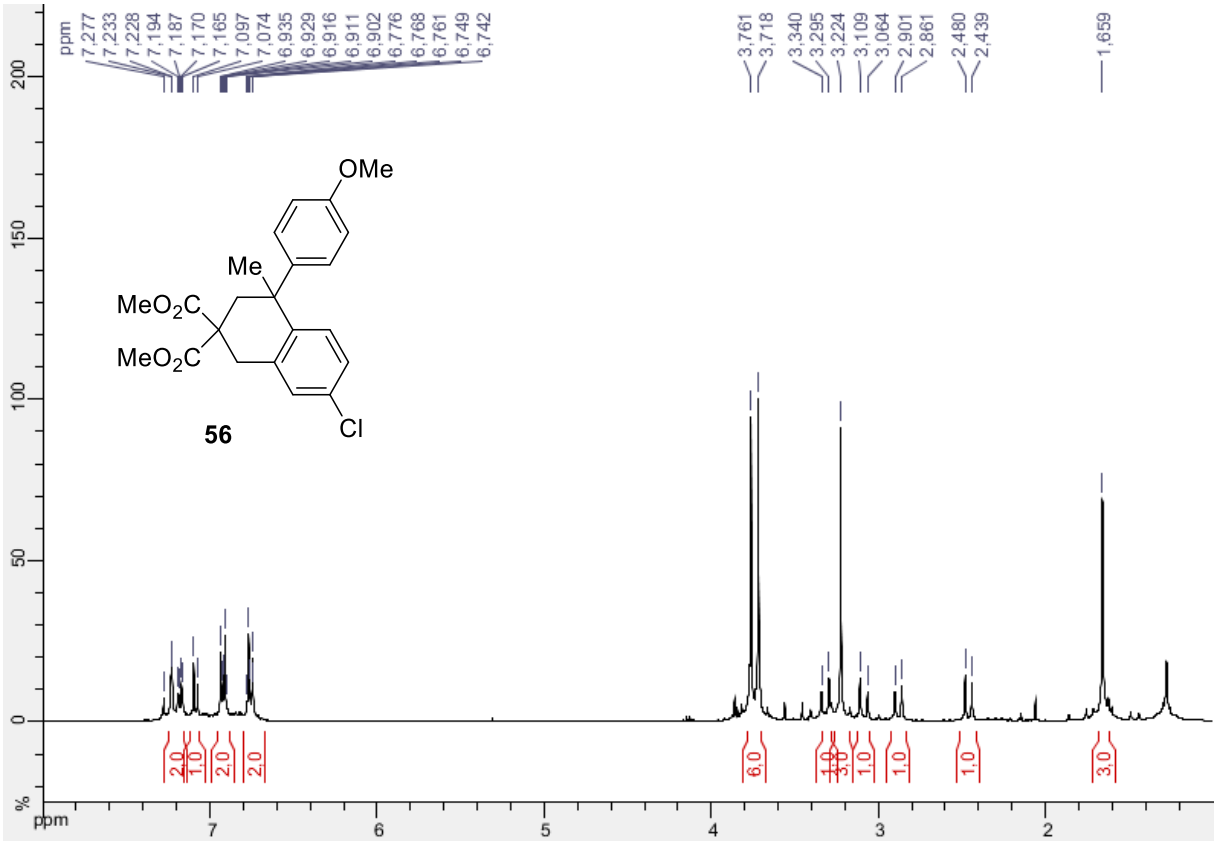
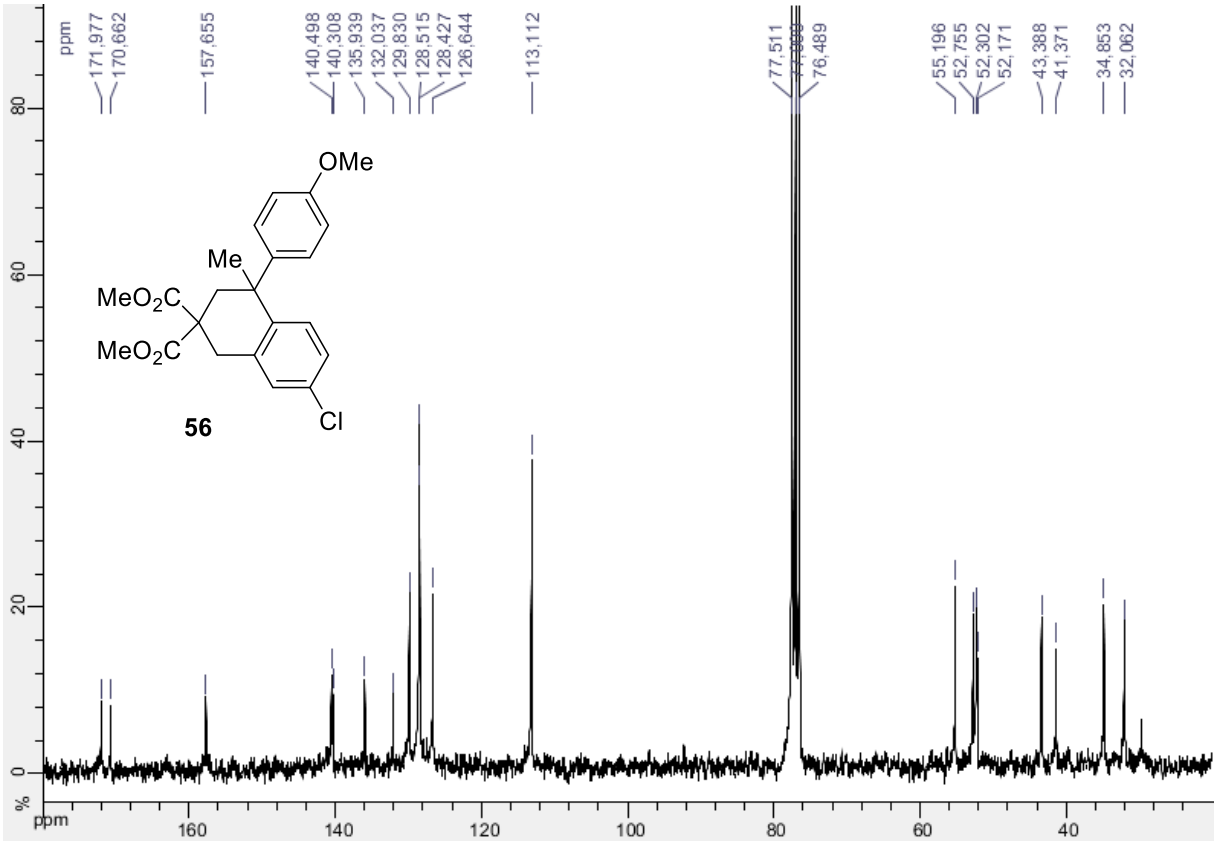
7,042
3,769
3,387
2,700
2,692
2,184
2,176
2,170
MeO2C
MeO2C
Cl
53
6.0
2.0
2.0
1.0

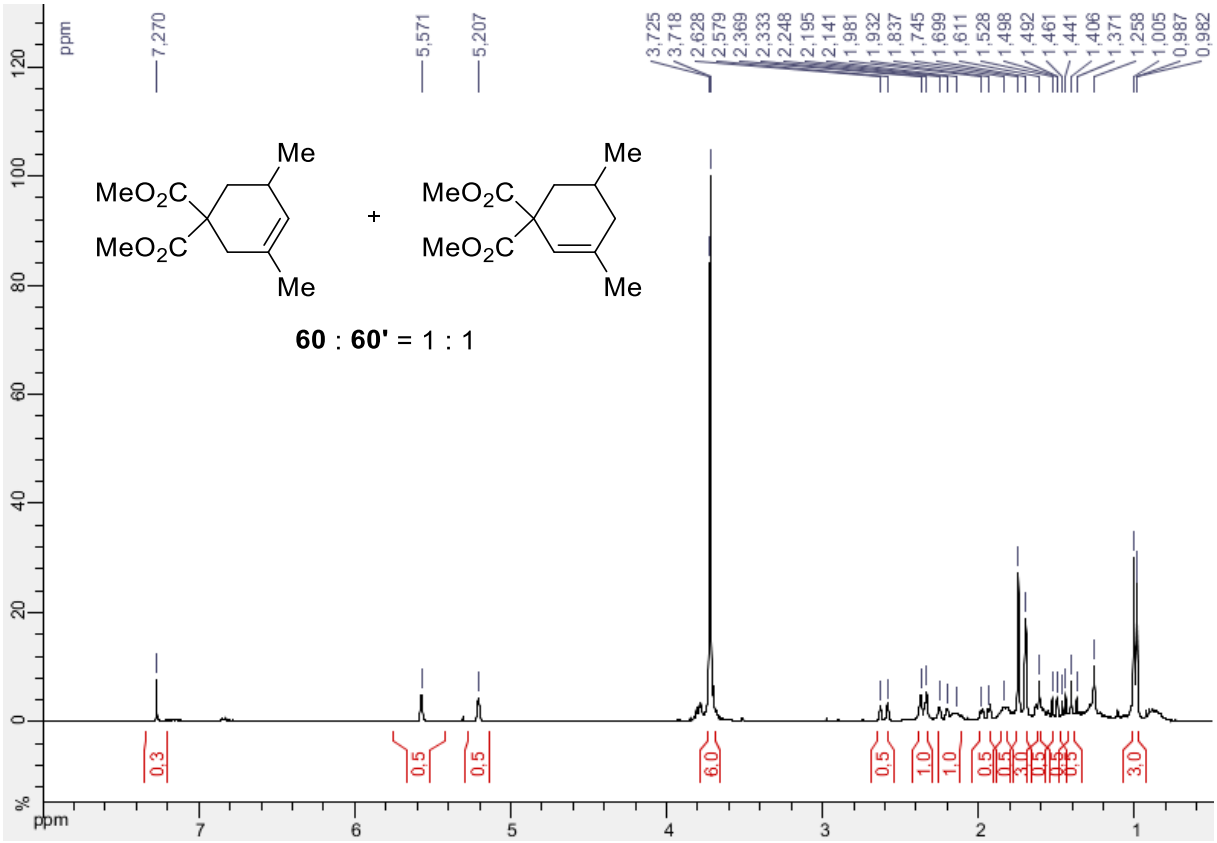

ppm
169,765
137,497
134,258
129,874
129,692
127,992
127,496
78,875
77,357
76,650
72,514
58,109
52,871
37,087
22,229
MeO2C
MeO2C
Cl
53
%
ppm
160
140
120
100
80
60
40
20

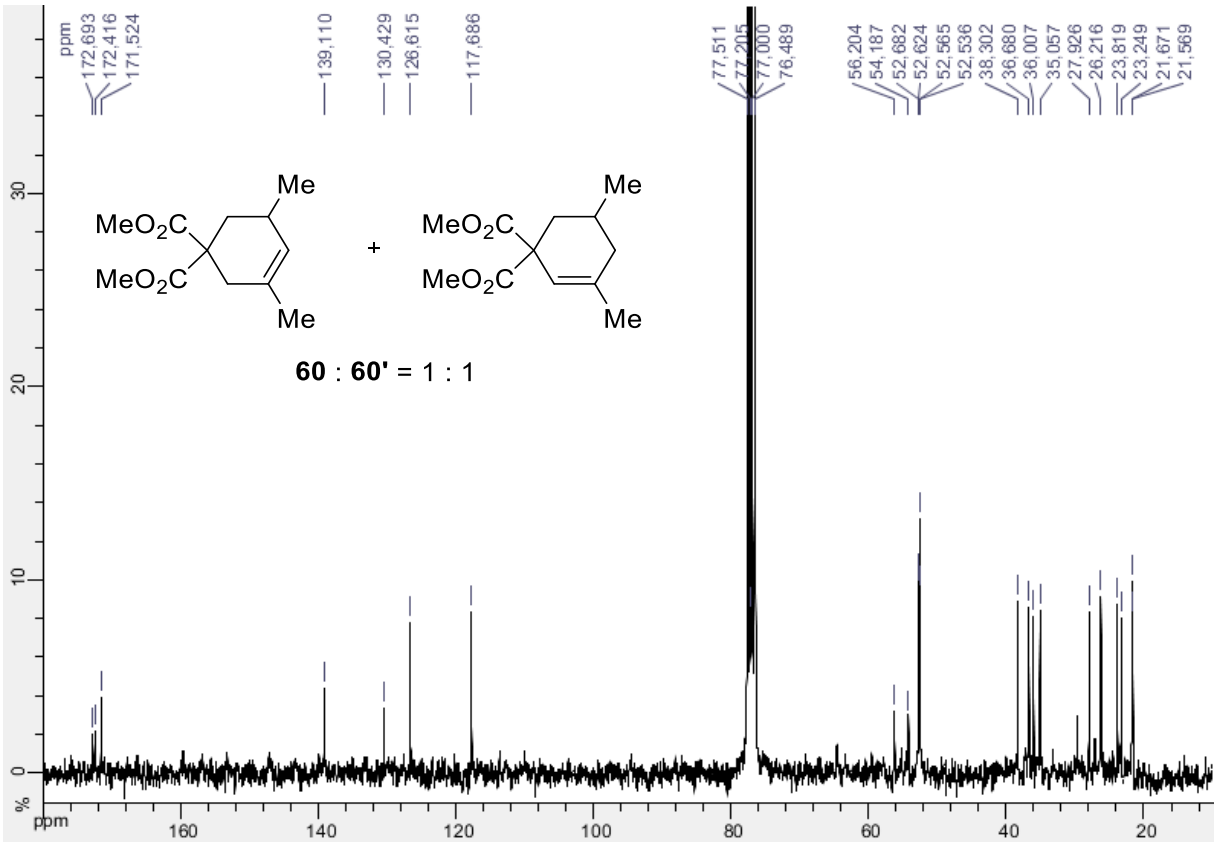

ppm
7,270
7,186
5,986
3,727
3,346
2,119
2,114
Me
MeO2C
MeO2C
Cl
54
3,0
1,0
6,0
2,0
3,0
%
ppm
7
6
5
4
3
2

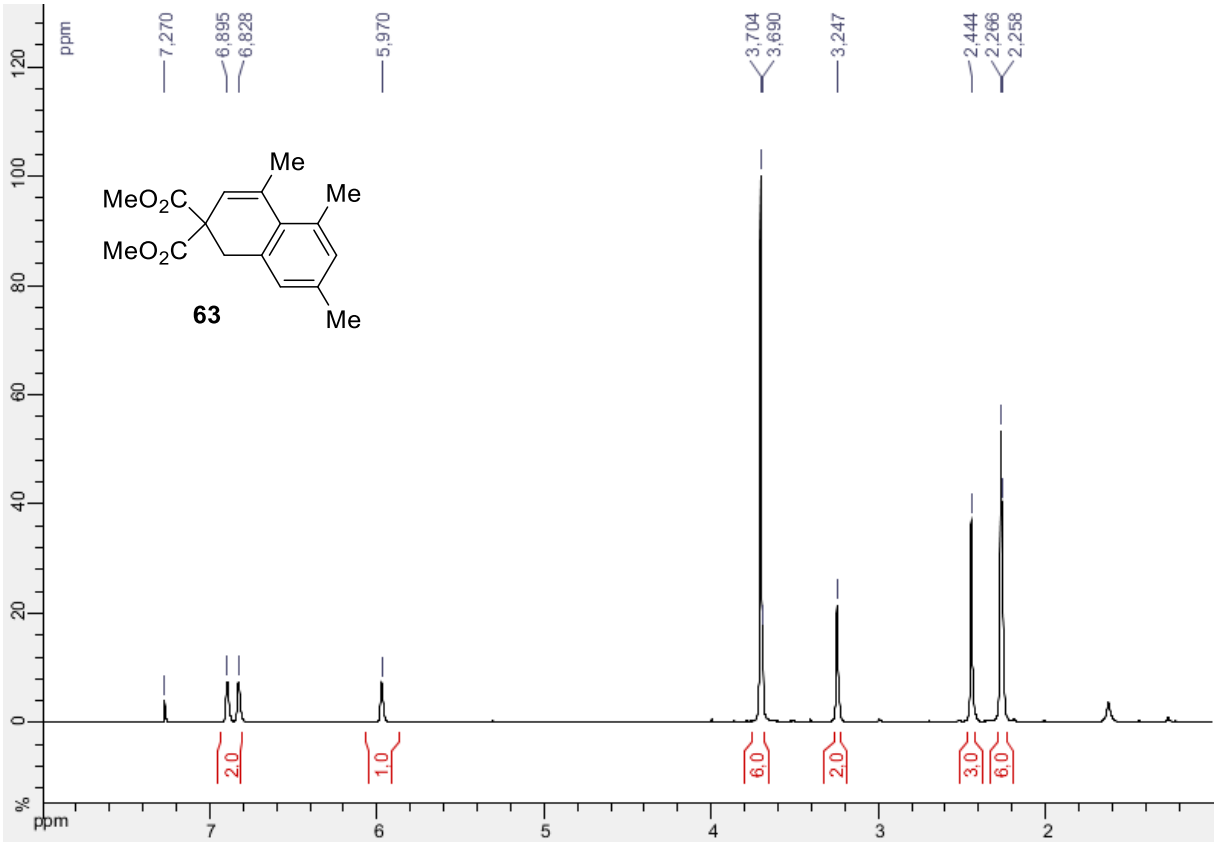

ppm
170,604
134,572
134,207
133,434
131,873
129,874
129,677
127,992
127,774
127,489
126,993
124,739
121,486
77,350
76,650
54,600
53,010
34,337
19,370
Me
MeO2C
MeO2C
Cl
54
%
ppm
160
140
120
100
80
60
40
20

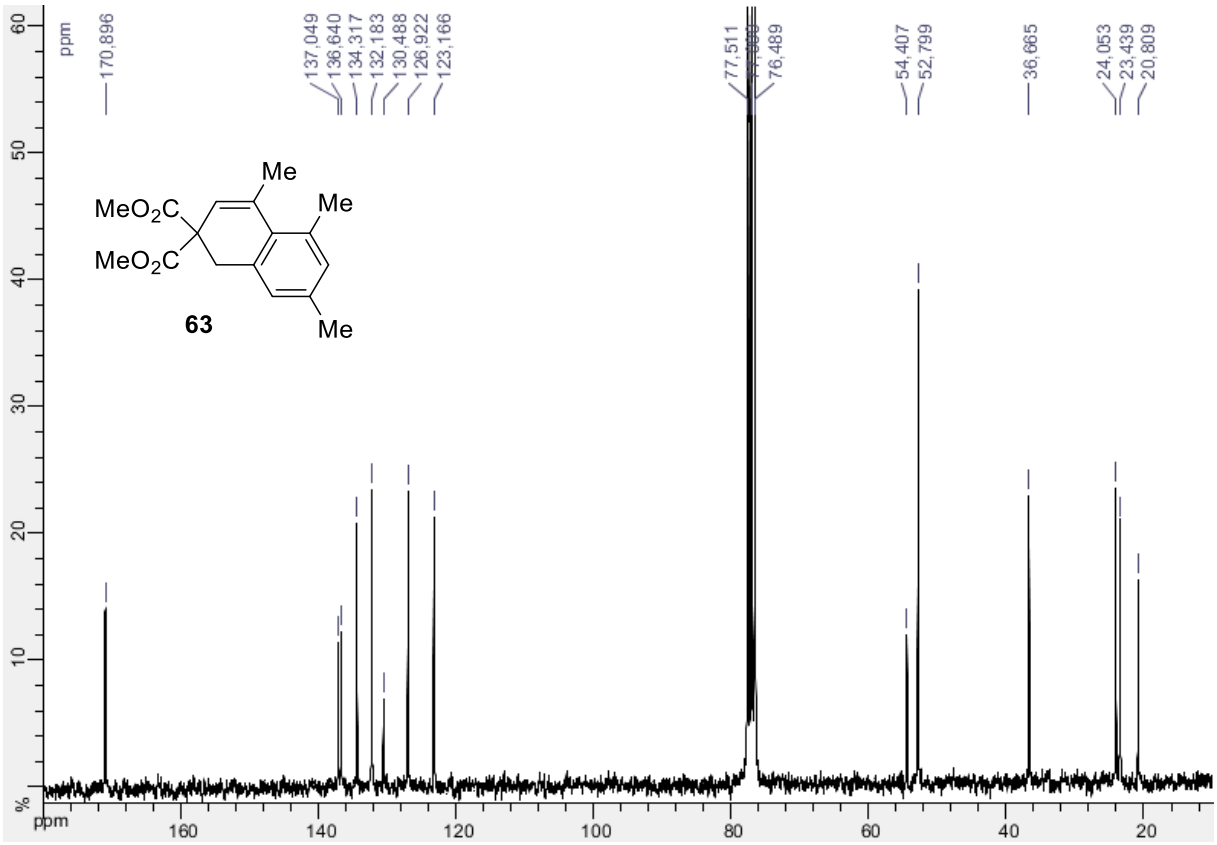

ppm
7,277
7,233
7,228
7,194
7,187
7,170
7,165
7,097
7,074
6,935
6,929
6,916
6,911
6,902
6,776
6,768
6,761
6,749
6,742
3,761
3,718
3,340
3,295
3,224
3,109
3,064
2,901
2,861
2,480
2,439
1,659
OMe
Me
MeO2C
MeO2C
Cl
56
2,0
1,0
2,0
2,0
6,0
1,0
3,0
1,0
1,0
1,0
3,0
%
ppm
7
6
5
4
3
2

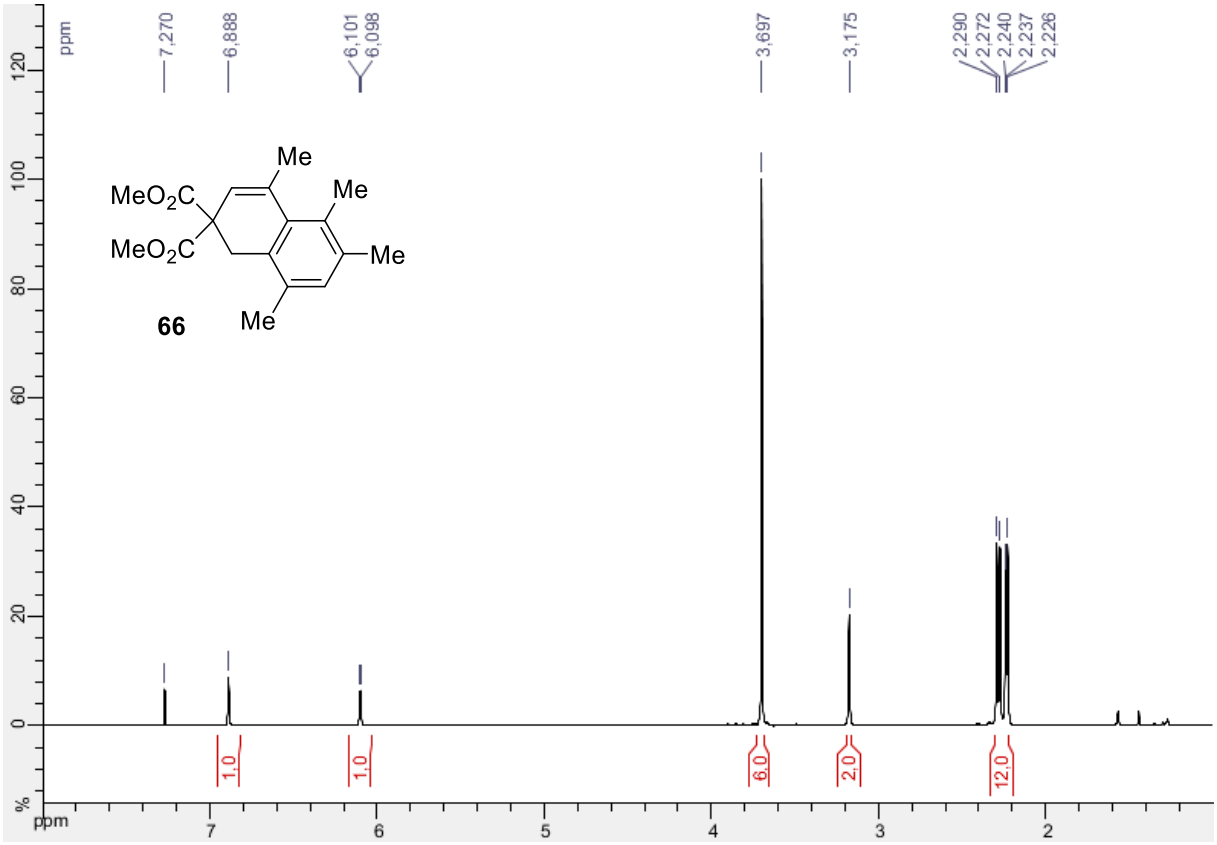

ppm
171,977
170,662
157,655
140,498
140,308
135,939
132,037
129,830
128,515
128,427
126,644
113,112
77,511
76,489
55,196
52,755
52,302
52,171
43,388
41,371
34,853
32,062
OMe
Me
MeO2C
MeO2C
Cl
56
%
ppm
160
140
120
100
80
60
40

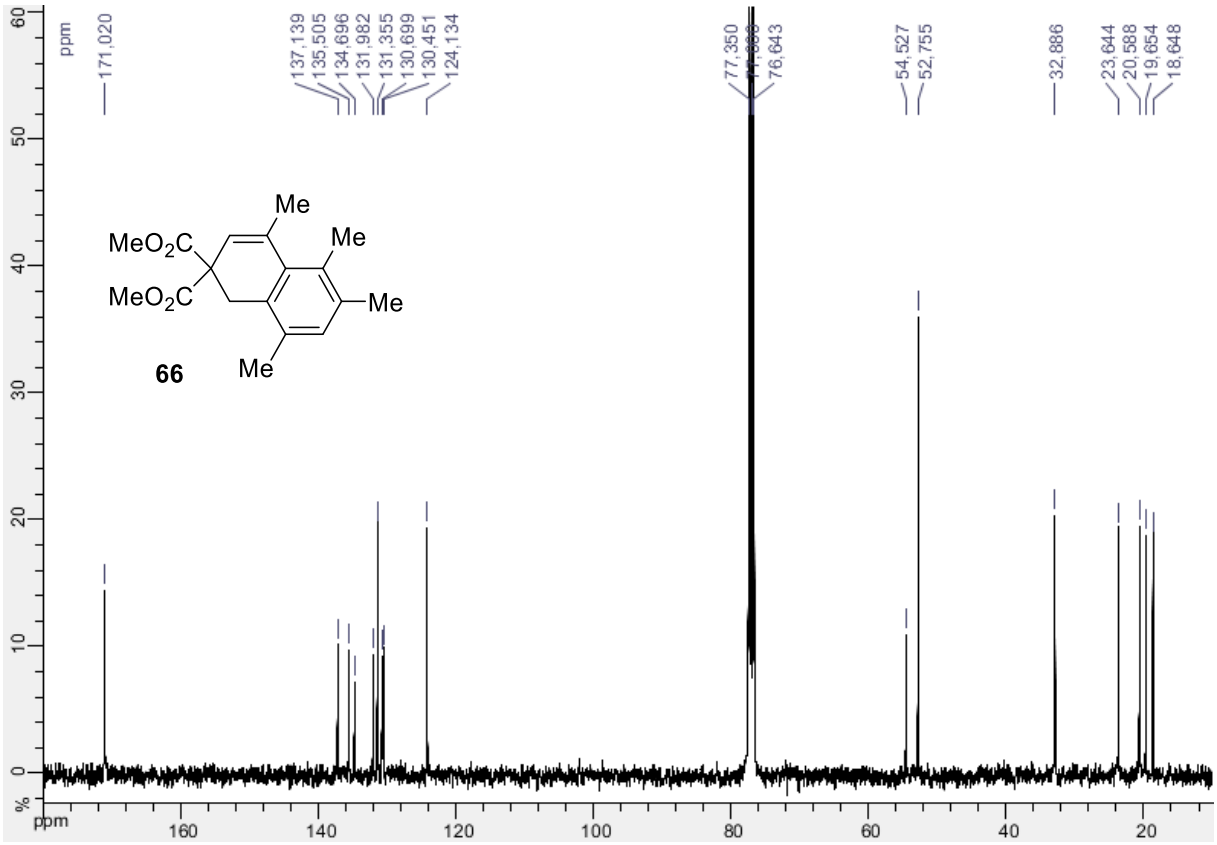

ppm
7,270
5,571
5,207
3,725
3,718
2,628
2,579
2,369
2,333
2,248
2,195
2,141
1,981
1,932
1,837
1,745
1,699
1,611
1,528
1,498
1,492
1,461
1,441
1,406
1,371
1,258
1,005
0,987
0,982
Me
MeO2C
MeO2C
Me
+
Me
MeO2C
MeO2C
Me
60 : 60' = 1 : 1
0,3
0,5
0,5
6,0
0,5
1,0
1,0
0,5
3,0
3,0
3,0
3,0
%
ppm
7
6
5
4
3
2
1

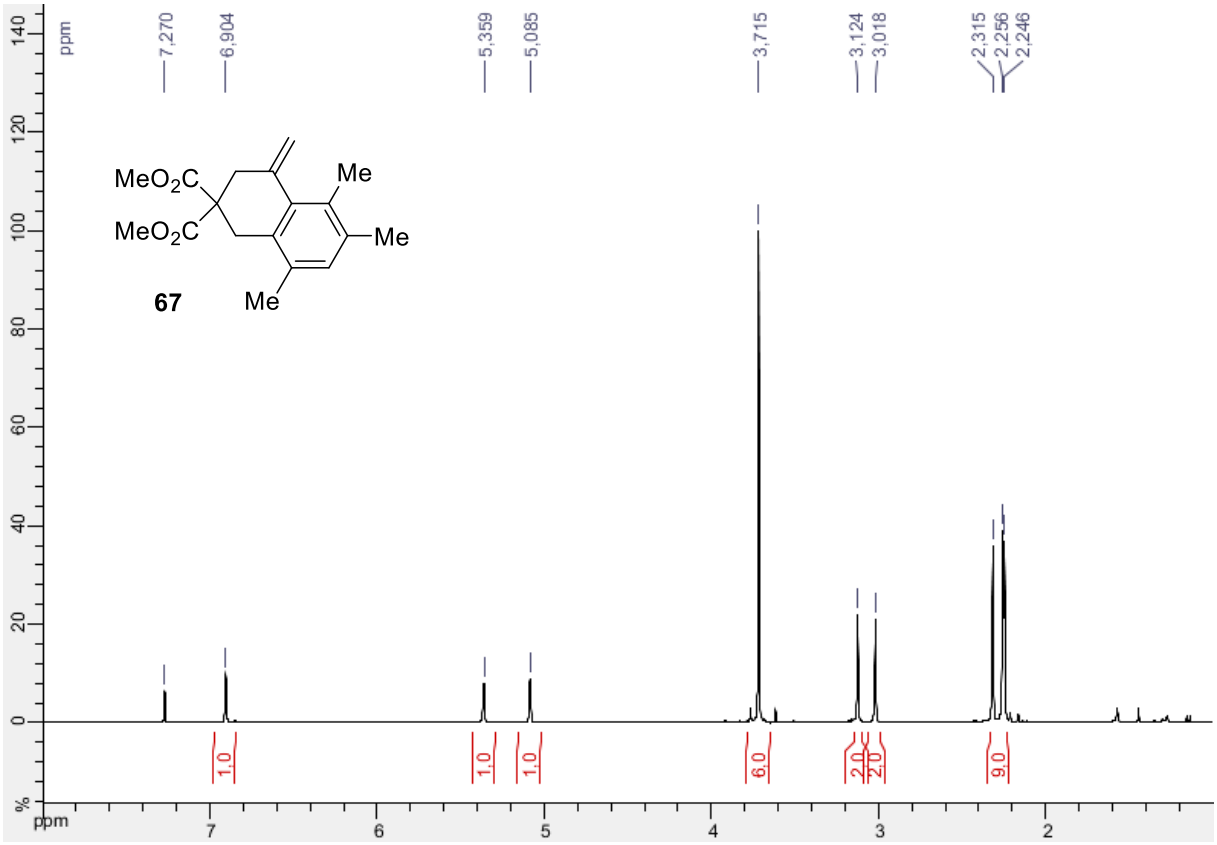

ppm
172,693
172,416
171,524
139,110
130,429
126,615
117,686
77,511
77,205
77,000
76,489
56,204
54,187
52,682
52,624
52,565
52,536
38,302
36,680
36,007
35,057
27,926
26,216
23,819
23,249
21,671
21,569
Me
MeO2C
MeO2C
Me
+
Me
MeO2C
MeO2C
Me
60 : 60' = 1 : 1
%
ppm

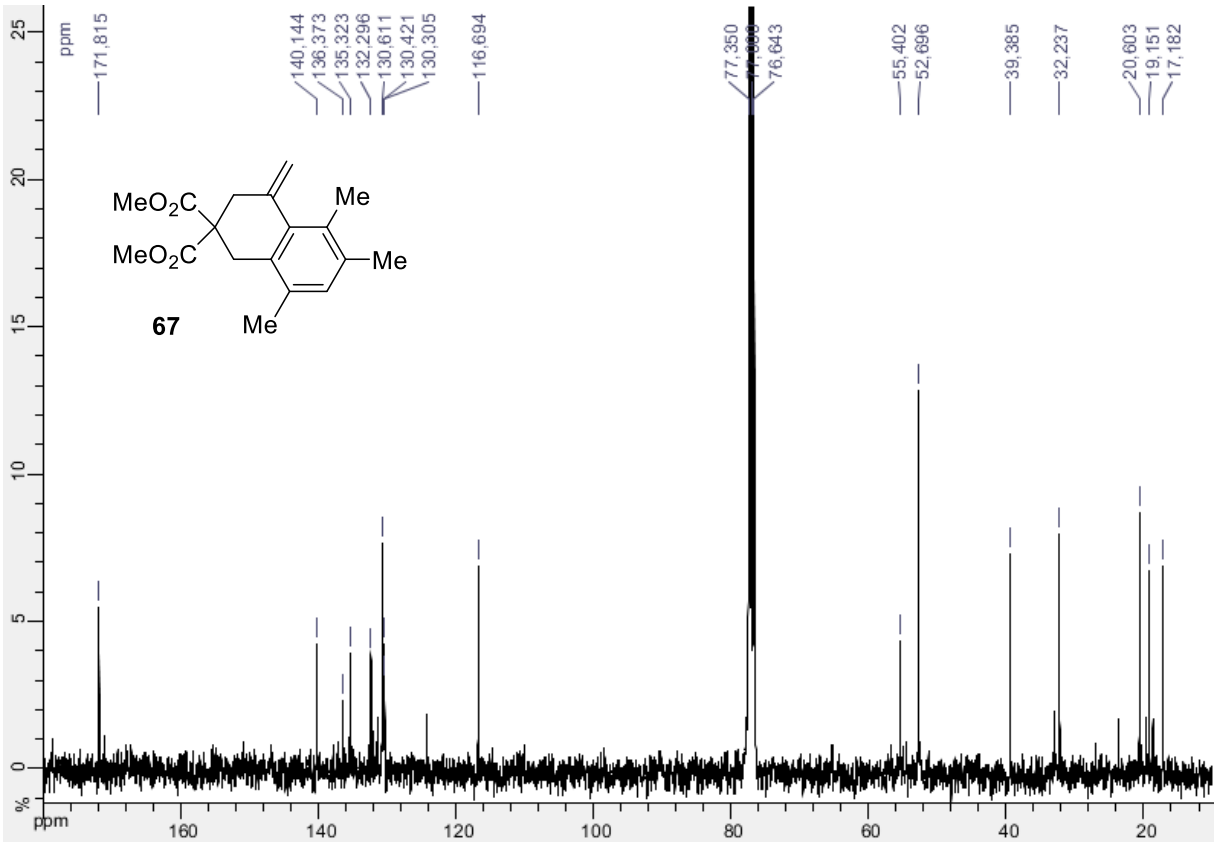

ppm
7,270
6,895
6,828
5,970
3,704
3,690
3,247
2,444
2,266
2,258
Me
MeO2C
MeO2C
Me
Me
63
2,0
1,0
6,0
2,0
3,0
6,0
%
ppm

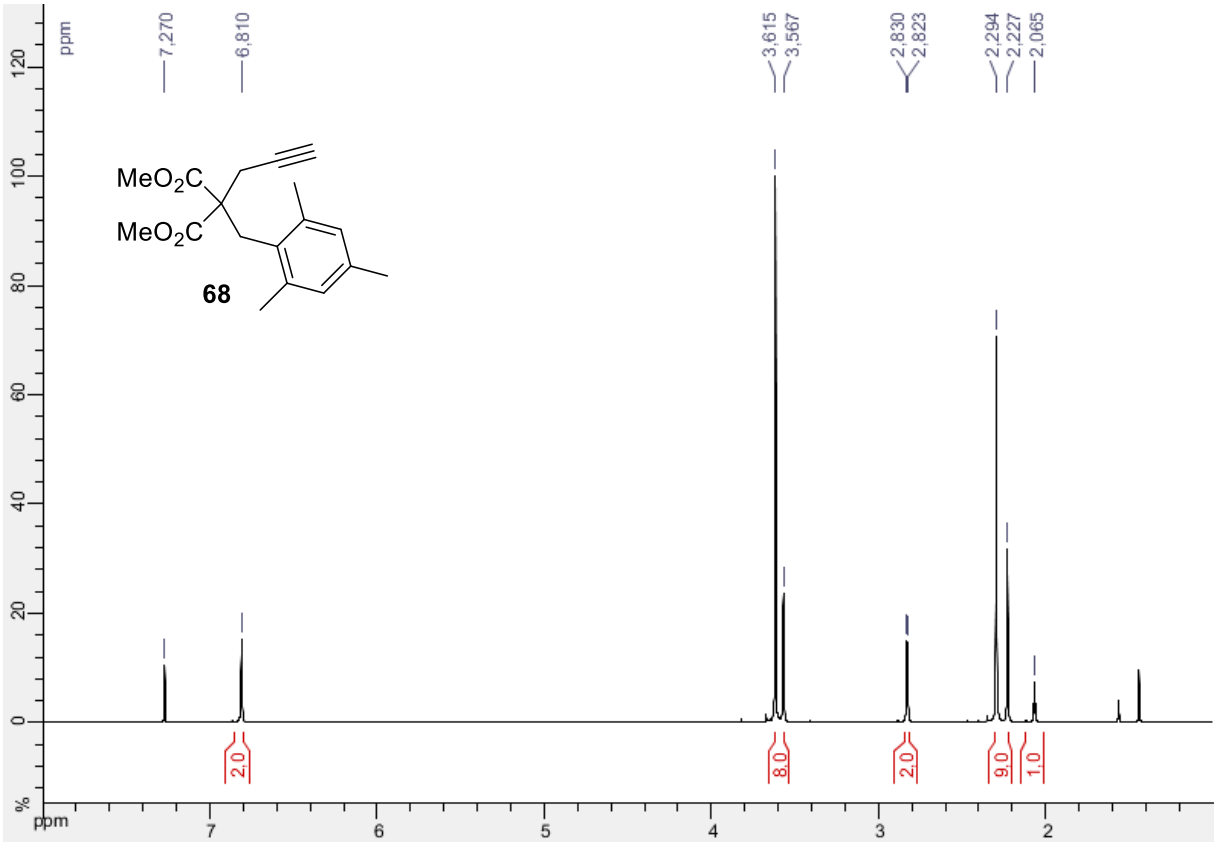

ppm
170,896
137,049
136,640
134,317
132,183
130,488
126,922
123,166
77,511
76,489
54,407
52,799
36,665
24,053
23,439
20,809
Me
MeO2C
MeO2C
Me
Me
63
%
ppm
160
140
120
100
80
60
40
20

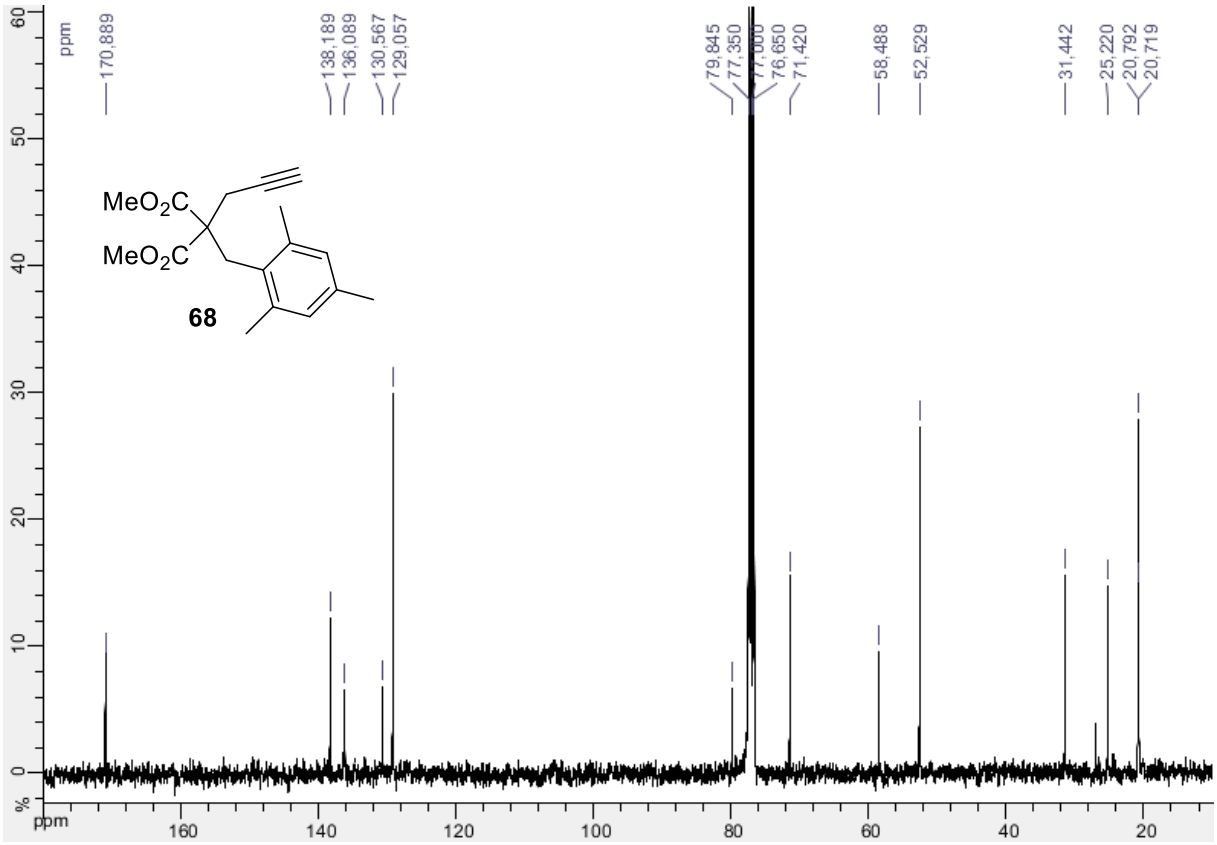

ppm
7,270
6,888
6,101
6,098
3,697
3,175
2,290
2,272
2,240
2,237
2,226
Me
MeO2C
MeO2C
Me
Me
Me
66
1,0
1,0
6,0
2,0
12,0
%
ppm
7
6
5
4
3
2

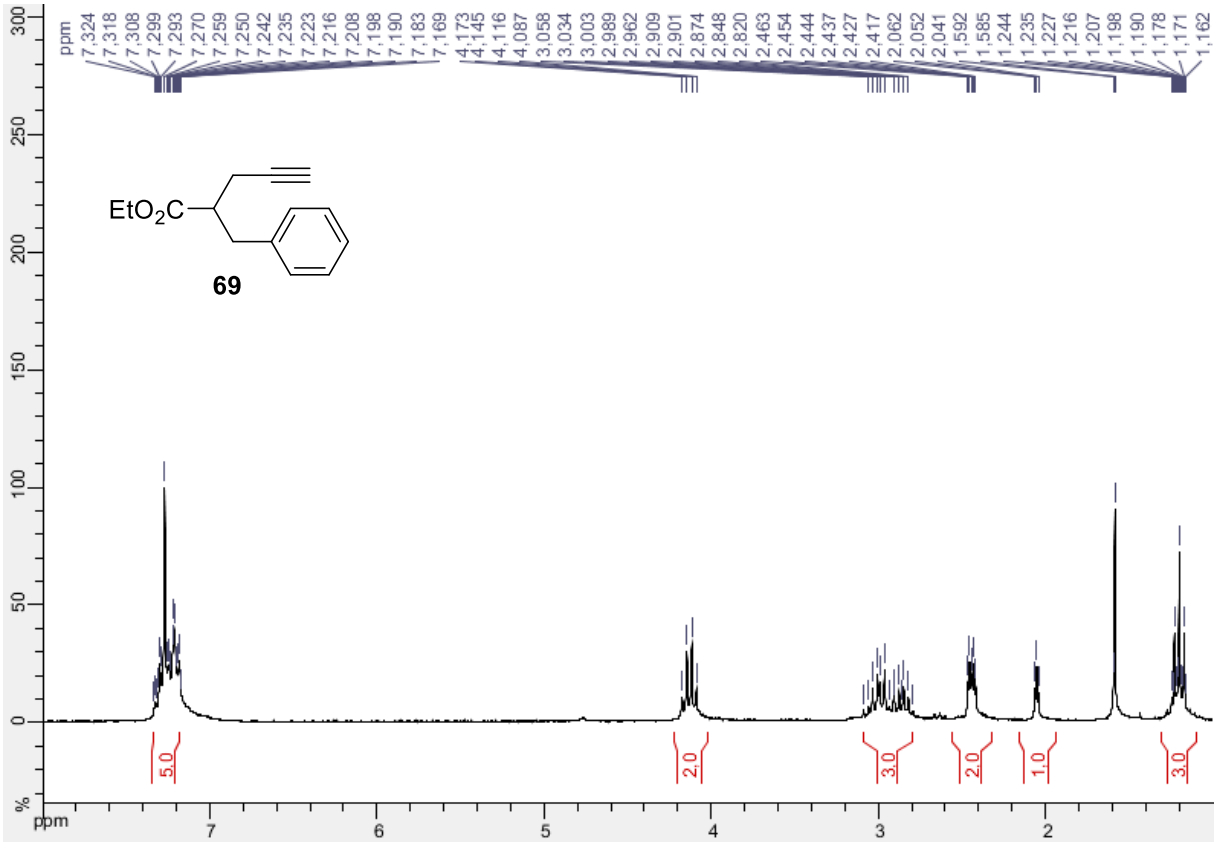

ppm
171,020
137,139
135,505
134,696
131,982
131,355
130,699
130,451
124,134
77,350
76,643
54,527
52,755
32,886
23,644
20,588
19,654
18,648
MeO2C
MeO2C
Me
Me
Me
Me
66

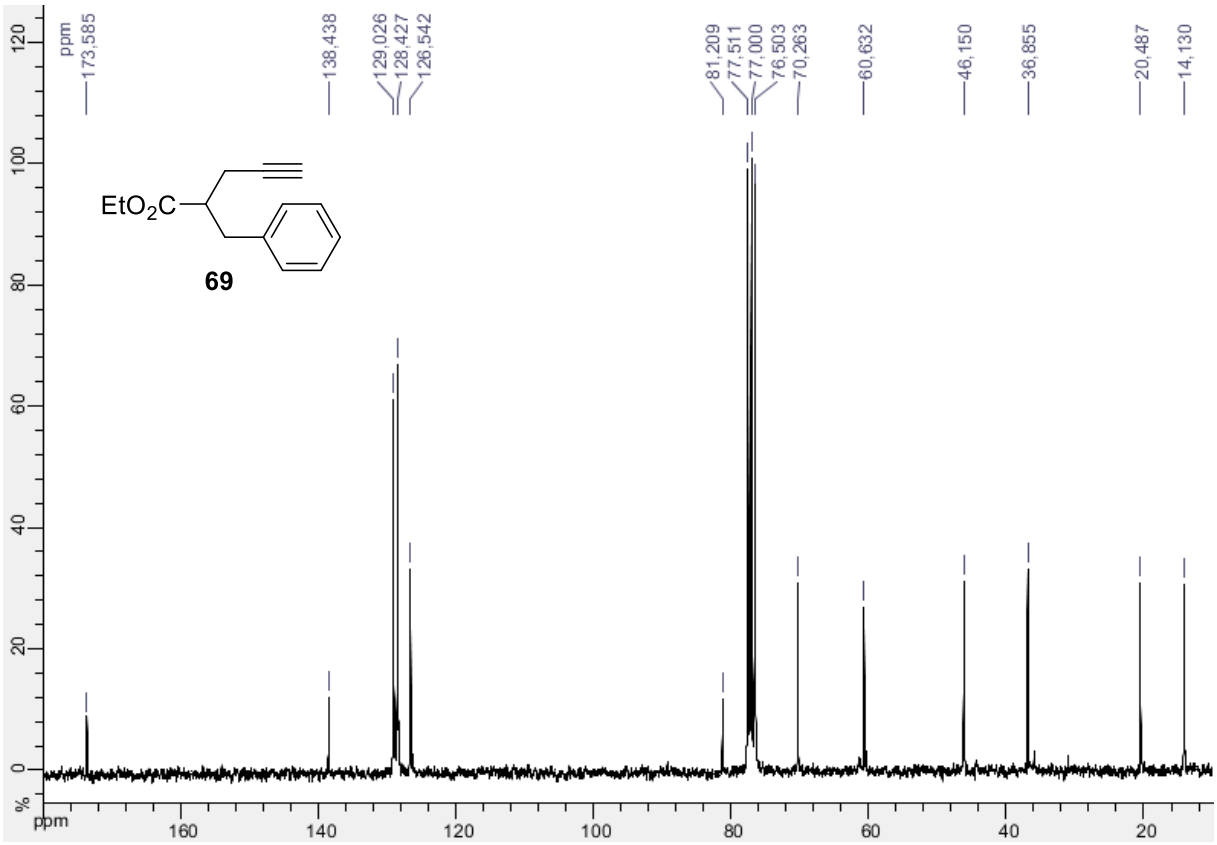

ppm
7,270
6,904
5,359
5,085
3,715
3,124
3,018
2,315
2,256
2,246
MeO2C
MeO2C
Me
Me
Me
67
1,0
1,0
1,0
6,0
2,0
2,0
9,0

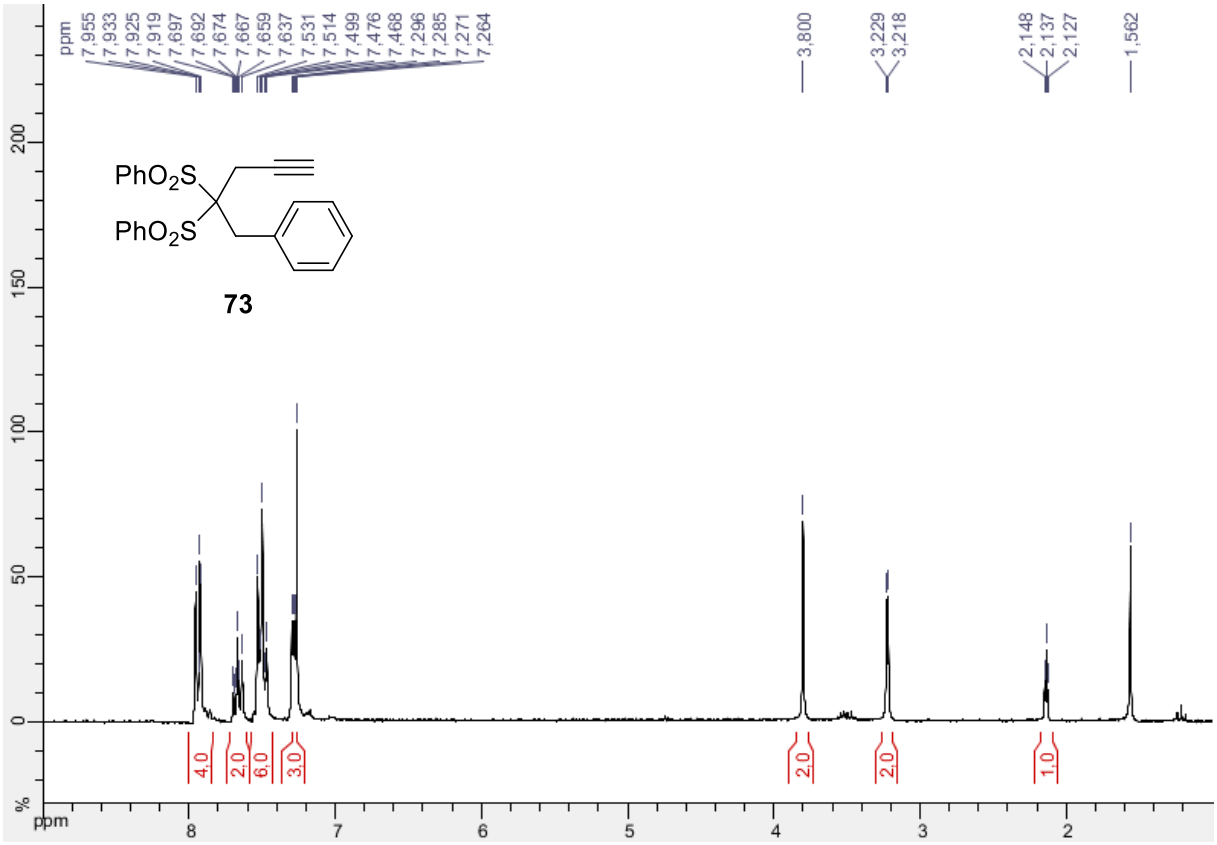

ppm
171,815
140,144
136,373
135,323
132,296
130,611
130,421
130,305
116,694
77,350
76,643
55,402
52,696
39,385
32,237
20,603
19,151
17,182
MeO2C
MeO2C
Me
Me
Me
67
%
ppm
160
140
120
100
80
60
40
20

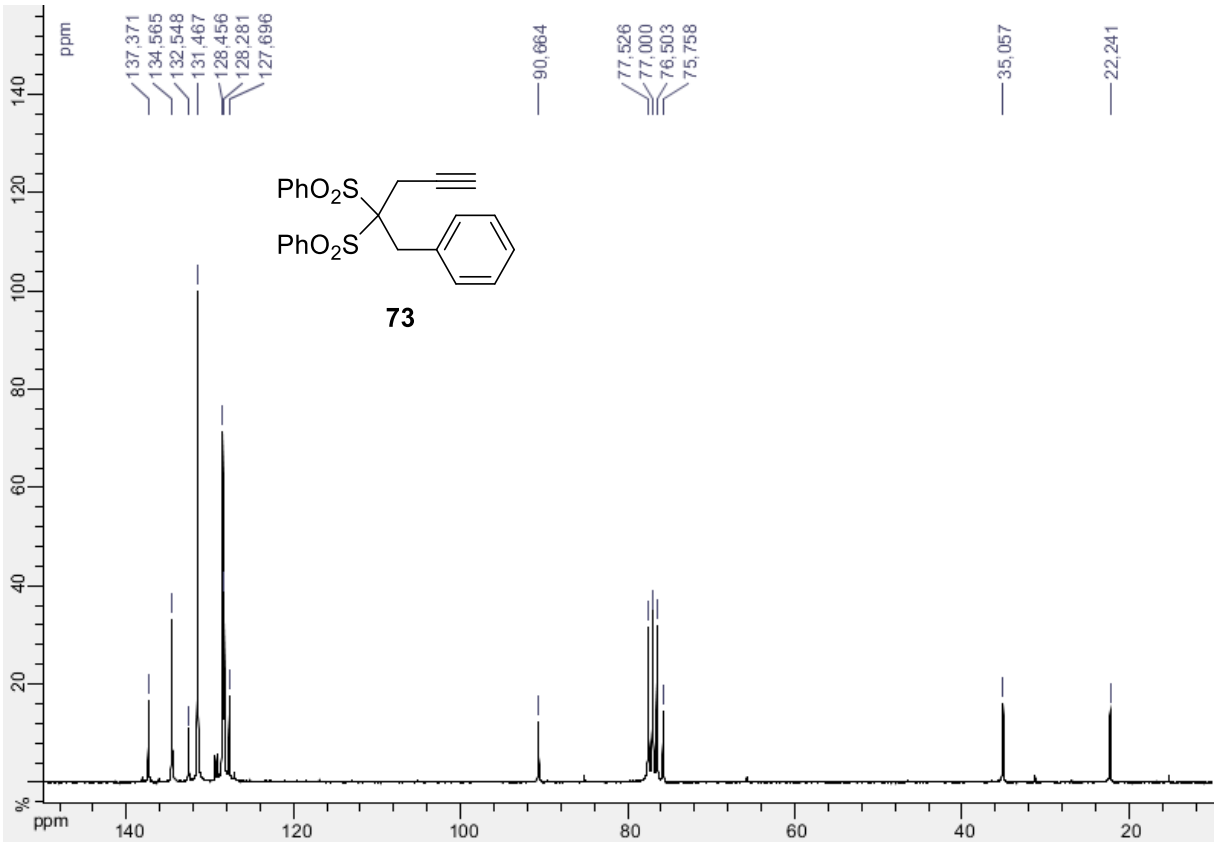

ppm
7,270
6,810
3,615
3,567
2,830
2,823
2,294
2,227
2,065
MeO2C
MeO2C
68
2,0
8,0
2,0
9,0
1,0
%
ppm
7
6
5
4
3
2

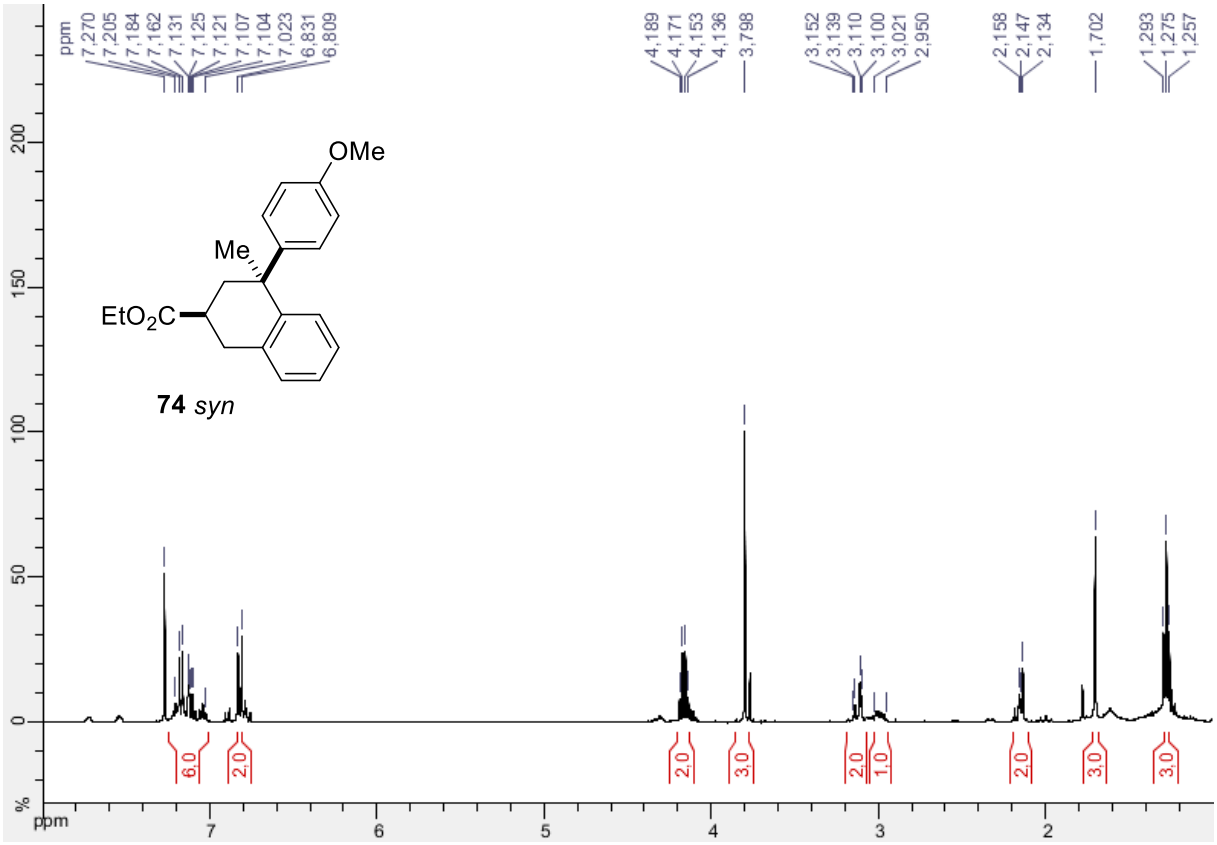

ppm
170,889
138,189
136,089
130,567
129,057
79,845
77,350
77,000
76,650
71,420
58,488
52,529
31,442
25,220
20,792
20,719
MeO2C
MeO2C
68
%
ppm
160
140
120
100
80
60
40
20

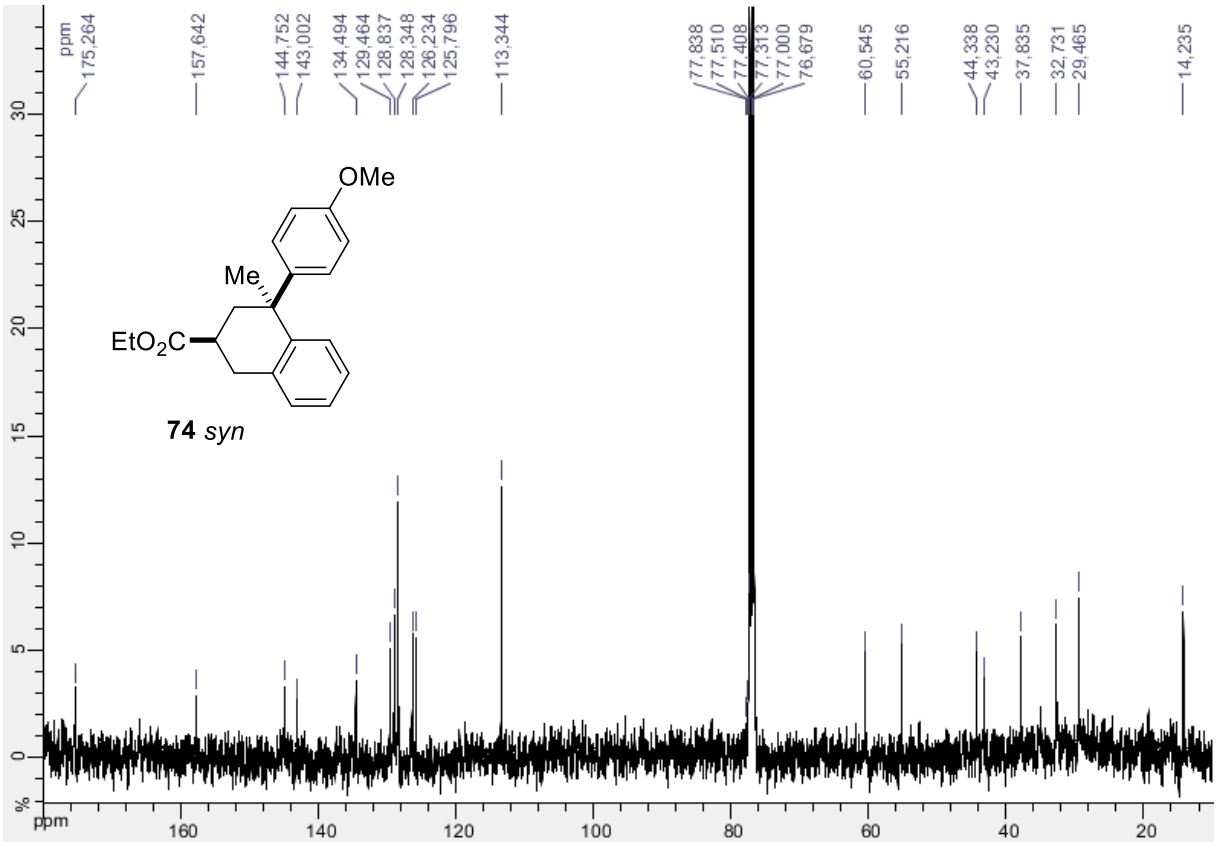

ppm
7,324
7,318
7,308
7,299
7,293
7,270
7,259
7,250
7,242
7,235
7,223
7,216
7,208
7,198
7,190
7,183
7,169
4,173
4,145
4,116
4,087
4,058
3,034
3,003
2,989
2,962
2,909
2,901
2,874
2,848
2,820
2,463
2,454
2,444
2,437
2,427
2,417
2,062
2,052
2,041
1,592
1,585
1,244
1,235
1,227
1,216
1,207
1,198
1,190
1,178
1,171
1,162
EtO2C
69
5,0
2,0
3,0
2,0
1,0
3,0
%
ppm
7
6
5
4
3
2

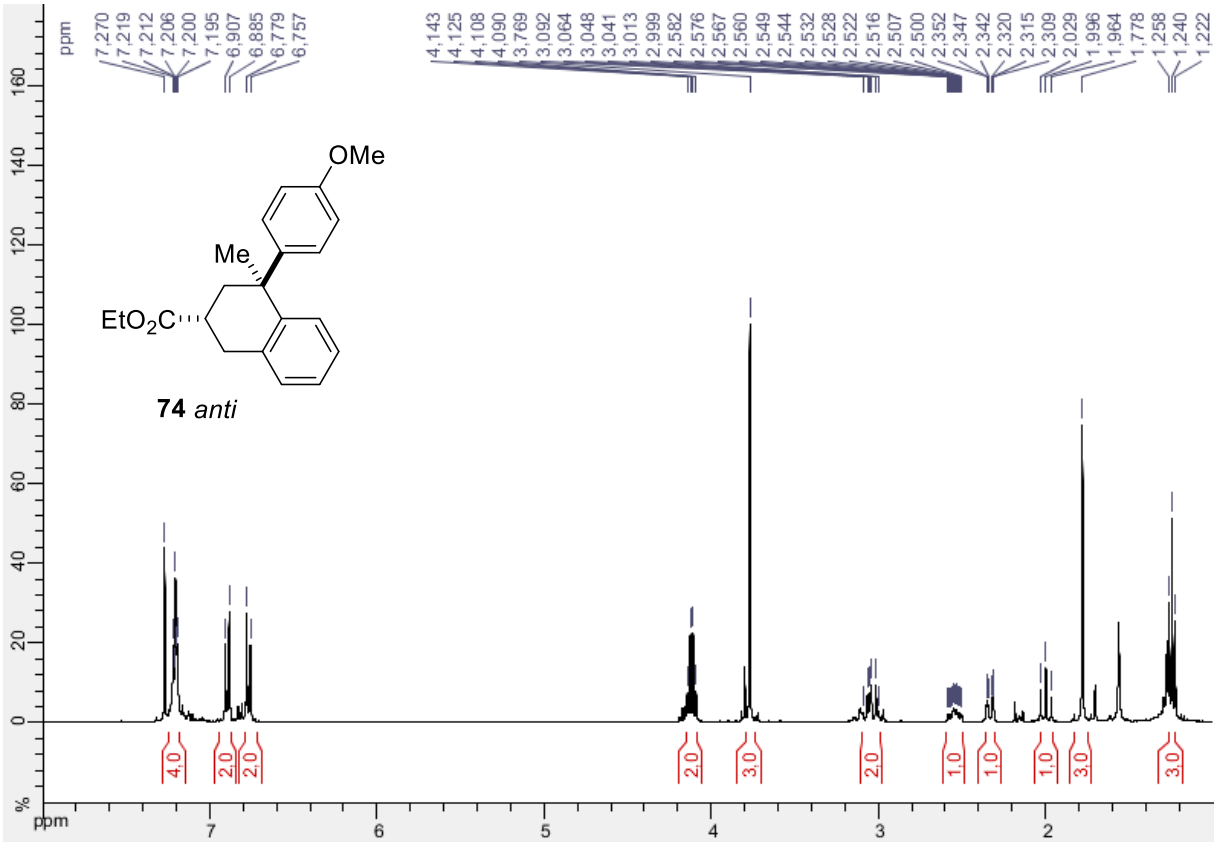

ppm
173,585
138,438
129,026
128,427
126,542
81,209
77,511
77,000
76,503
70,263
60,632
46,150
36,855
20,487
14,130
EtO2C
69
%
ppm
160
140
120
100
80
60
40
20

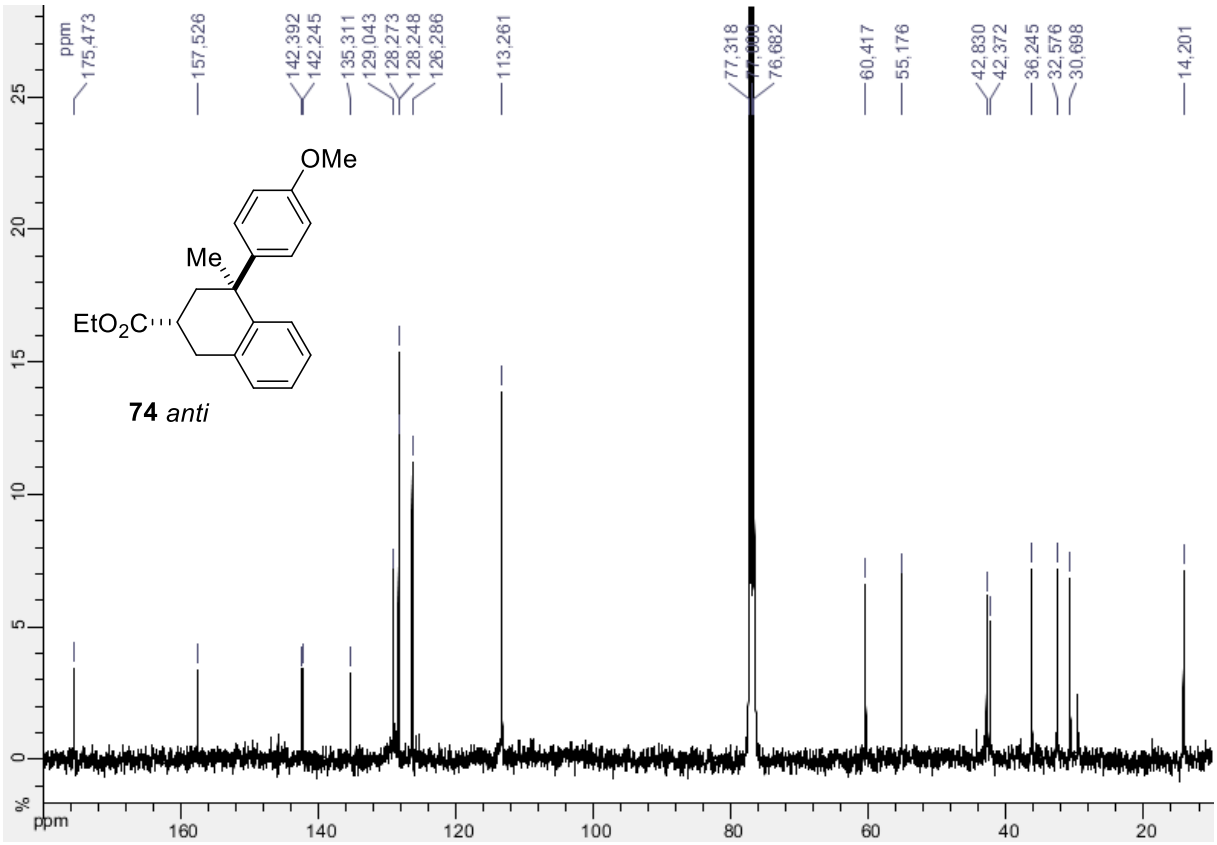

ppm
7,955
7,933
7,925
7,919
7,697
7,692
7,674
7,667
7,659
7,637
7,531
7,514
7,499
7,476
7,468
7,296
7,285
7,271
7,264
3,800
3,229
3,218
2,148
2,137
2,127
1,562
PhO2S
PhO2S
73
4,0
2,0
6,0
3,0
2,0
2,0
1,0
%
ppm
8
7
6
5
4
3
2

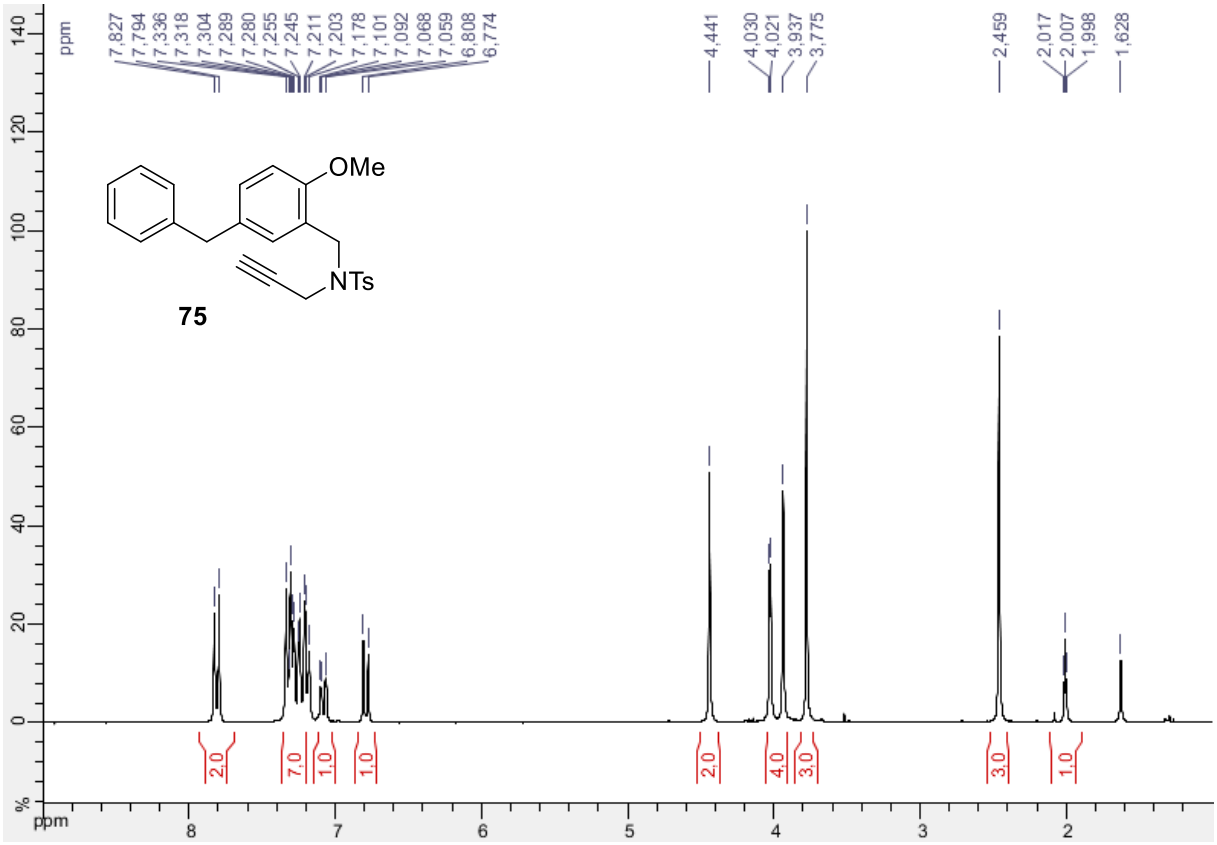

ppm
137,371
134,565
132,548
131,467
128,456
128,281
127,696
90,664
77,526
77,000
76,503
75,758
35,057
22,241
PhO2S
PhO2S
73

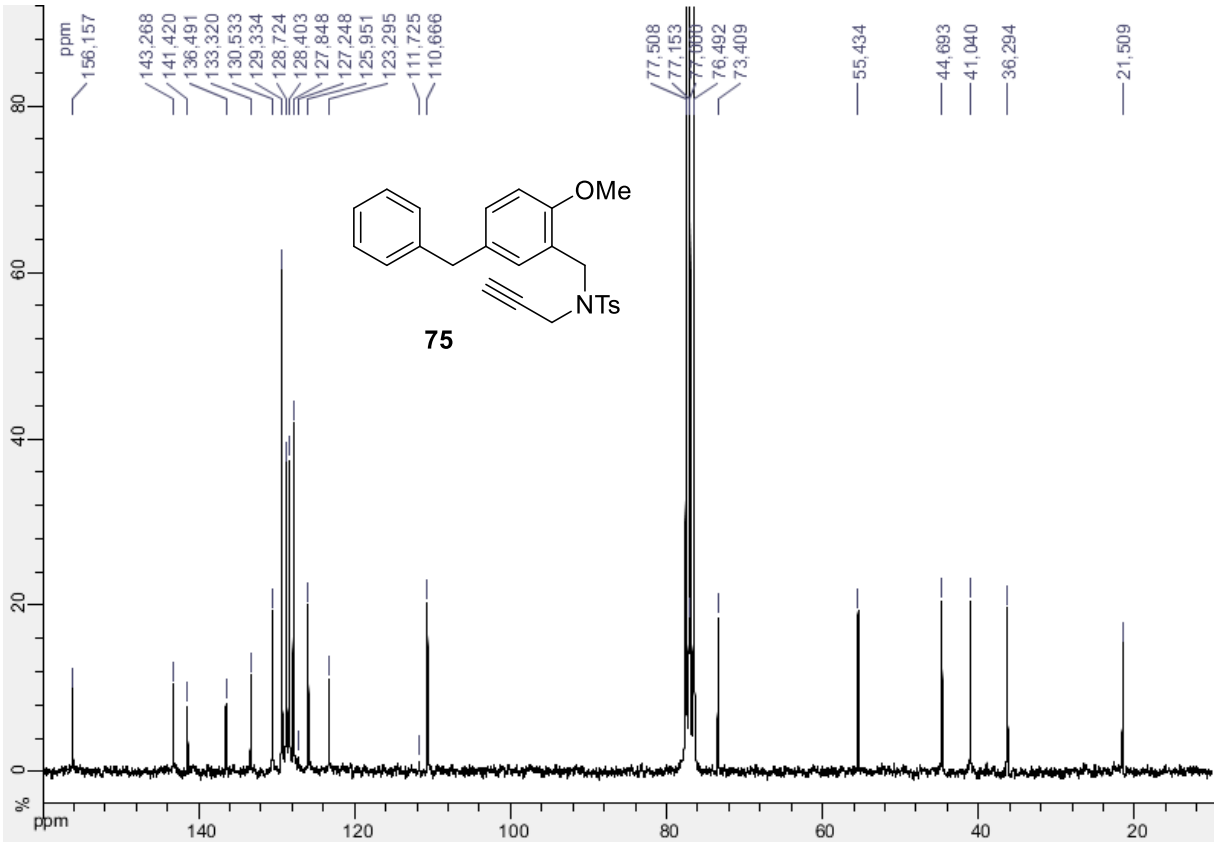

ppm
7,270
7,205
7,184
7,162
7,131
7,125
7,121
7,107
7,104
7,023
6,831
6,809
4,189
4,171
4,153
4,136
3,798
3,152
3,139
3,110
3,100
3,021
2,950
2,158
2,147
2,134
1,702
1,293
1,275
1,257
OMe
Me
EtO2C
74 syn
6,0
2,0
2,0
3,0
2,0
1,0
2,0
3,0
3,0

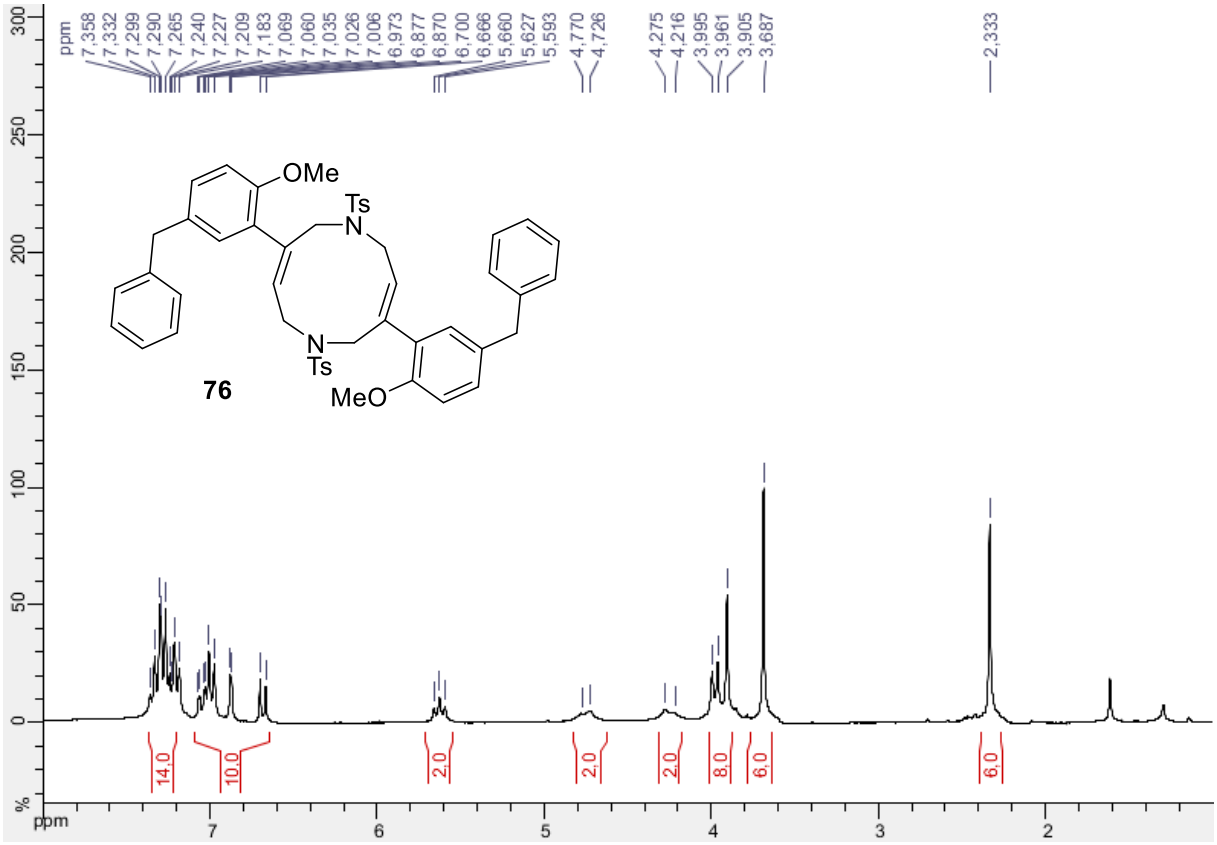

ppm
175,264
157,642
144,752
143,002
134,494
129,464
128,837
128,348
126,234
125,796
113,344
77,838
77,510
77,408
77,313
77,000
76,679
60,545
55,216
44,338
43,230
37,835
32,731
29,465
14,235
OMe
Me
EtO2C
74 syn

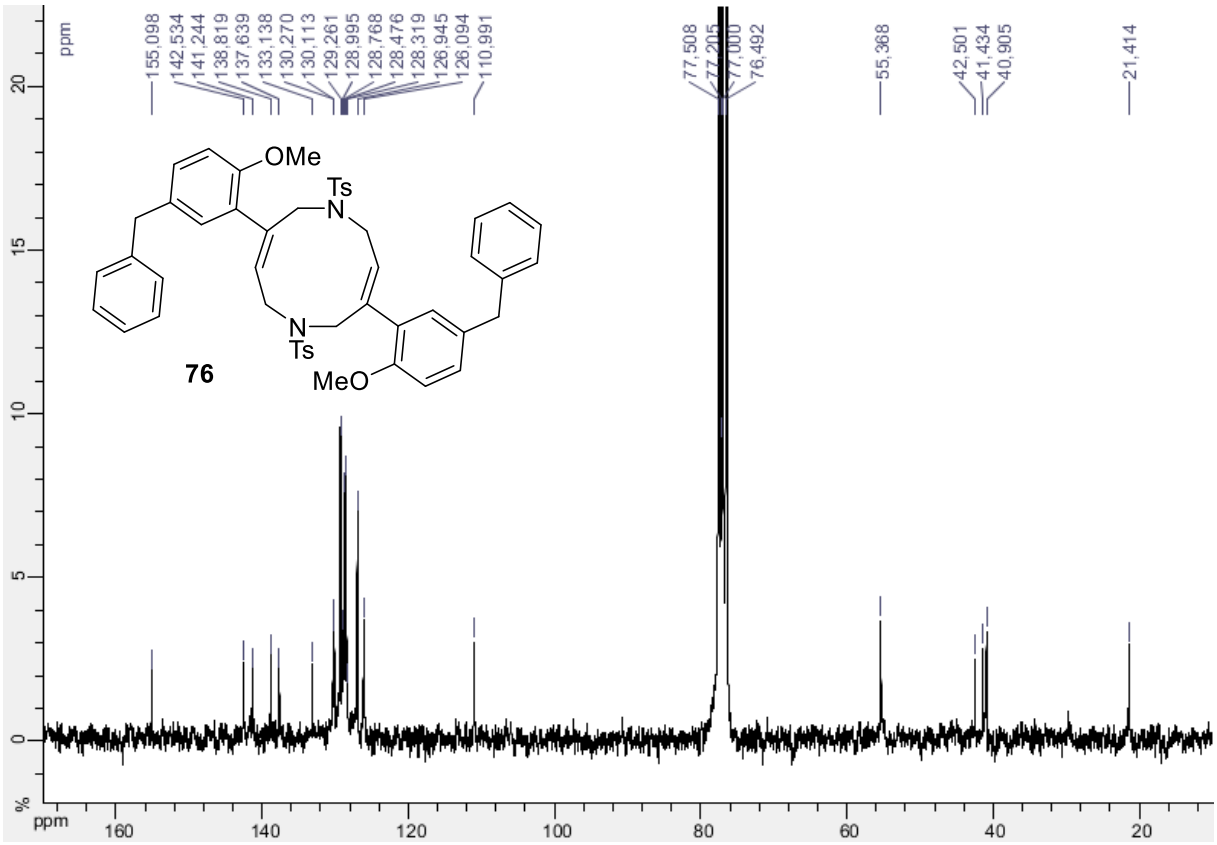

ppm
7,270
7,219
7,212
7,206
7,200
7,195
6,907
6,885
6,779
6,757
4,143
4,125
4,108
4,090
3,769
3,092
3,064
3,048
3,041
3,013
2,999
2,582
2,576
2,567
2,560
2,549
2,544
2,532
2,528
2,522
2,516
2,507
2,500
2,352
2,347
2,342
2,320
2,315
2,309
2,029
1,996
1,964
1,778
1,258
1,240
1,222
OMe
Me
EtO2C
74 anti
4,0
2,0
2,0
2,0
3,0
2,0
1,0
1,0
1,0
3,0
3,0

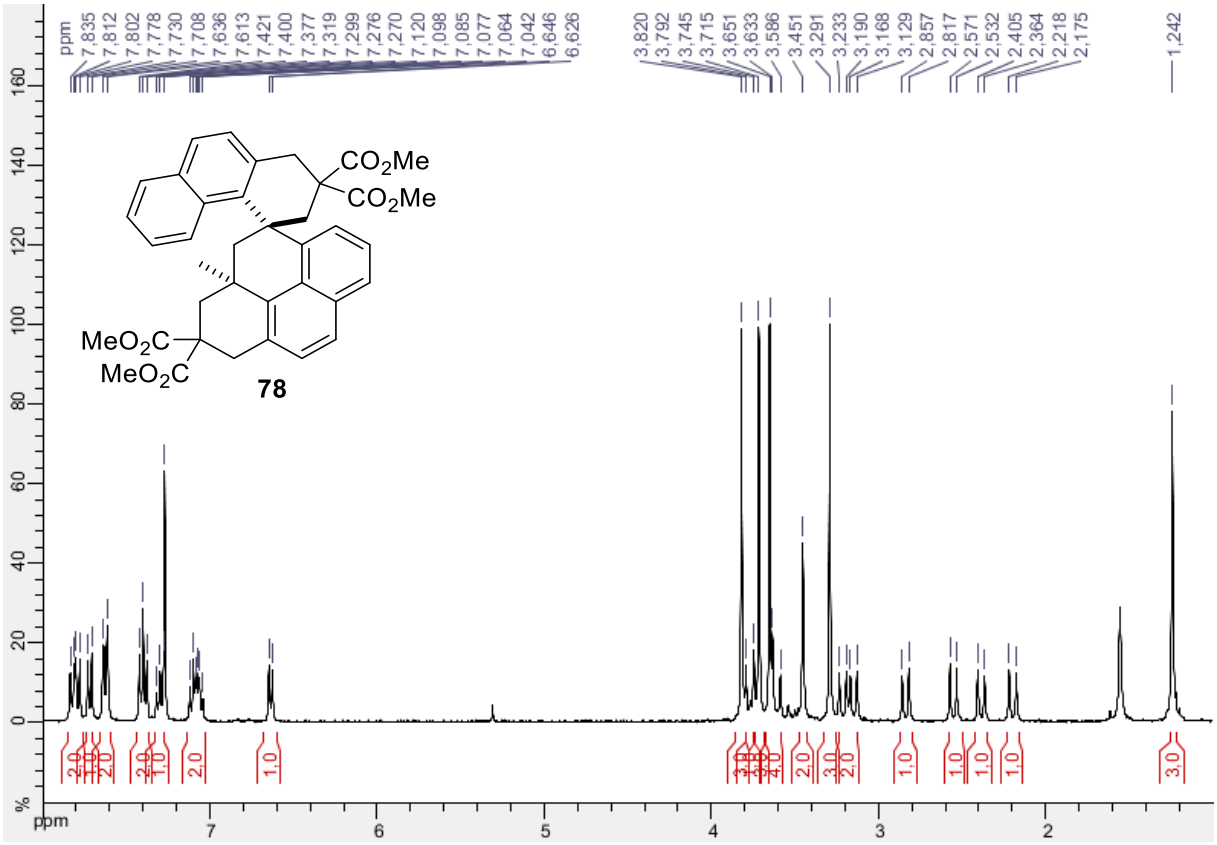

ppm
175,473
157,526
142,392
142,245
135,311
129,043
128,273
128,248
126,286
113,261
77,318
76,682
60,417
55,176
42,830
42,372
36,245
32,576
30,698
14,201
OMe
Me
EtO2C
74 anti

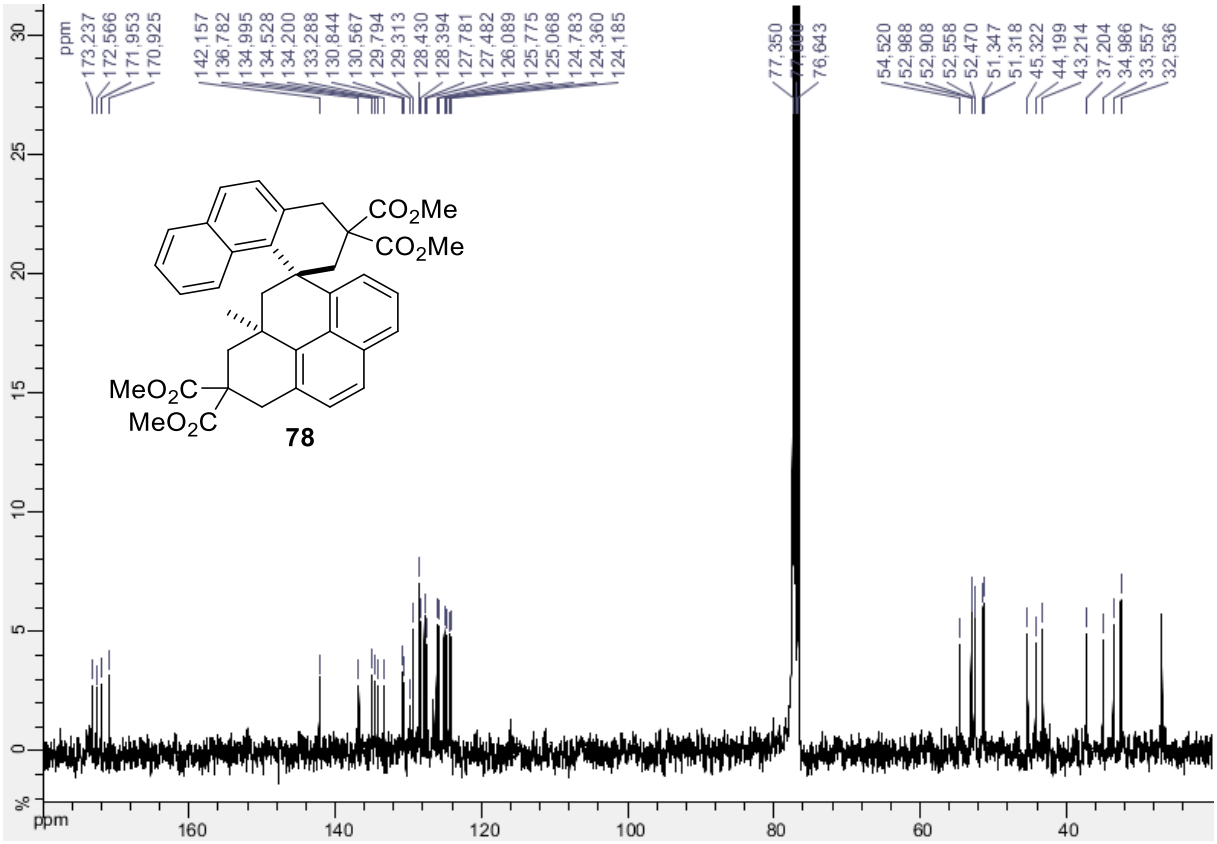

ppm
7,827
7,794
7,336
7,318
7,304
7,289
7,280
7,255
7,245
7,211
7,203
7,178
7,101
7,092
7,068
7,059
6,808
6,774
4,441
4,030
4,021
3,937
3,775
2,459
2,017
2,007
1,998
1,628
OMe
NTs
75
2,0
7,0
1,0
1,0
2,0
4,0
3,0
3,0
1,0

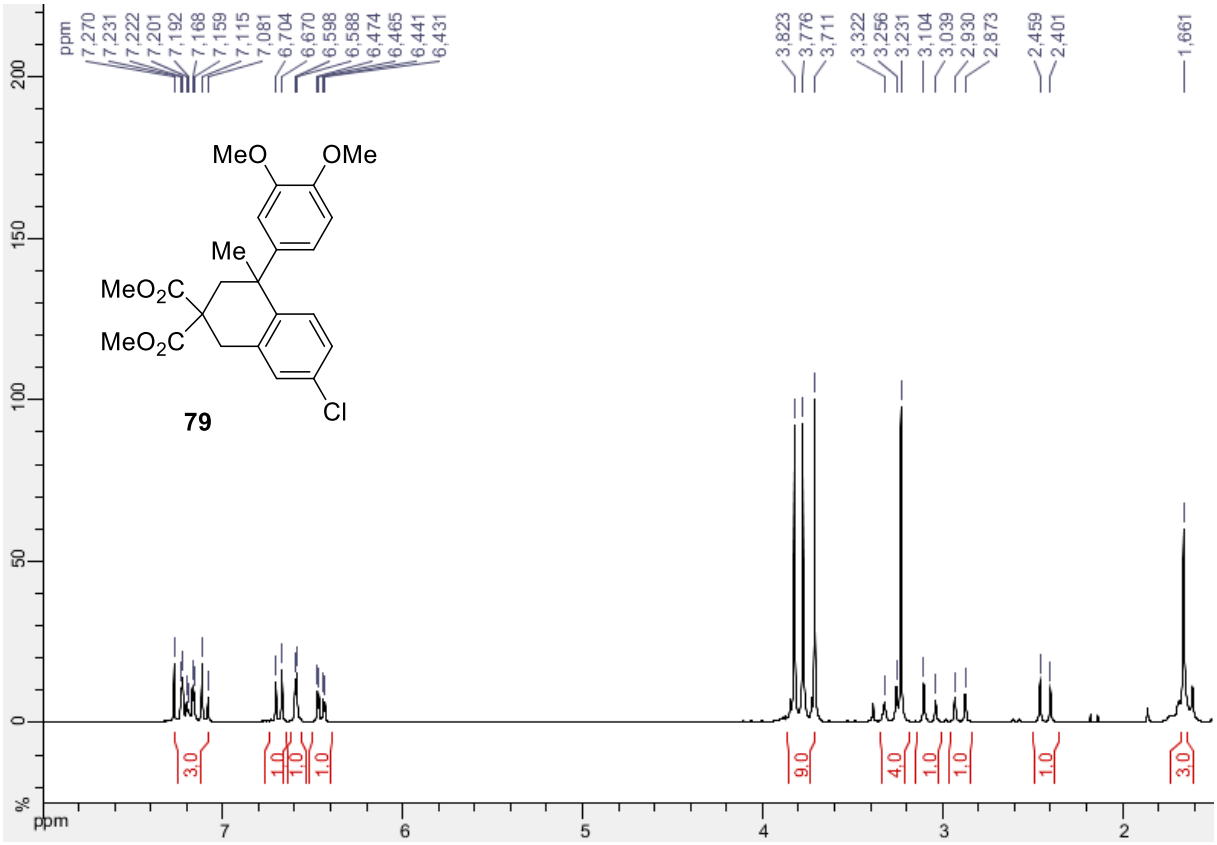

ppm
156,157
143,268
141,420
136,491
133,320
130,533
129,334
128,724
128,403
127,848
127,248
125,951
123,295
111,725
110,666
77,508
77,153
77,000
76,492
73,409
55,434
44,693
41,040
36,294
21,509
OMe
NTs
75
%
ppm
140
120
100
80
60
40
20

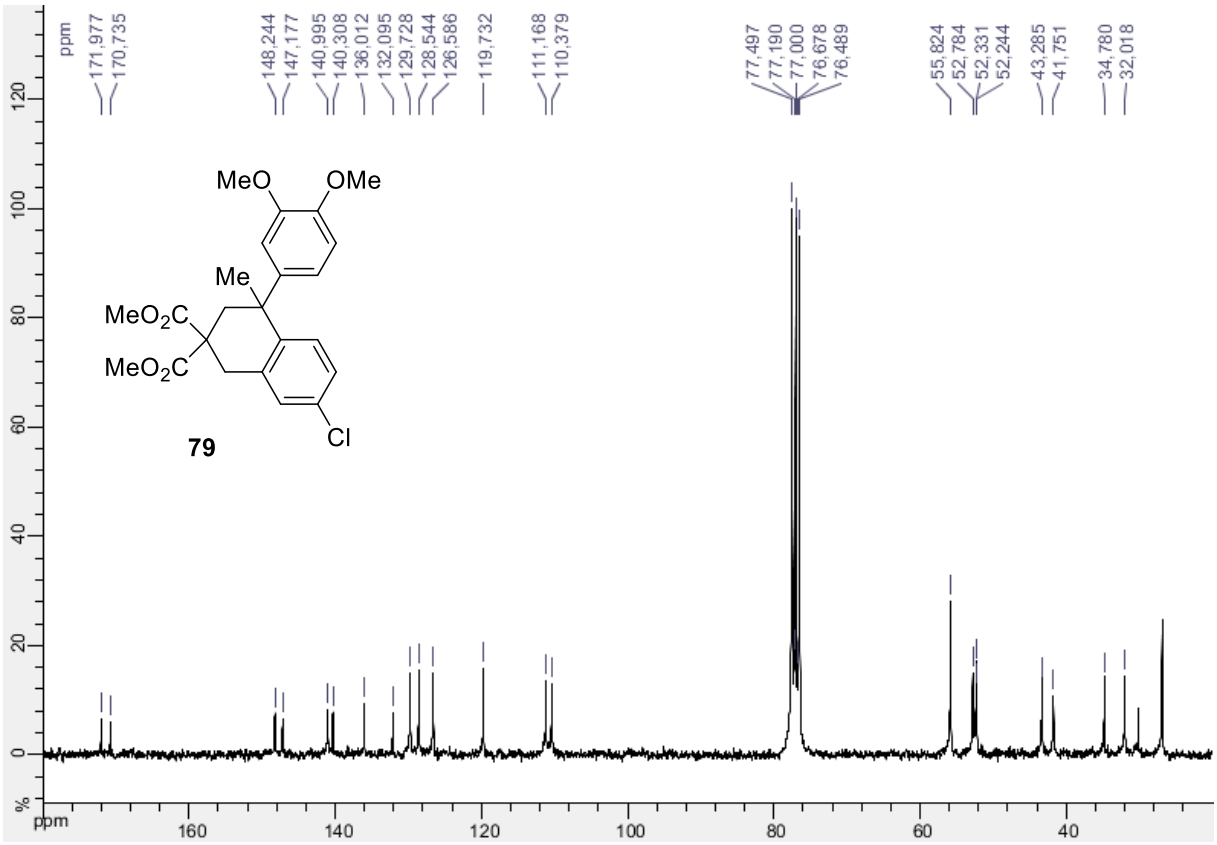

ppm
7,358
7,332
7,299
7,290
7,265
7,240
7,227
7,209
7,183
7,069
7,060
7,035
7,026
7,006
6,973
6,877
6,870
6,700
6,666
5,660
5,627
5,593
4,770
4,726
4,275
4,216
3,995
3,961
3,905
3,687
2,333
OMe
Ts
N
N
Ts
MeO
76
14,0
10,0
2,0
2,0
2,0
8,0
6,0
6,0
%
ppm
7
6
5
4
3
2

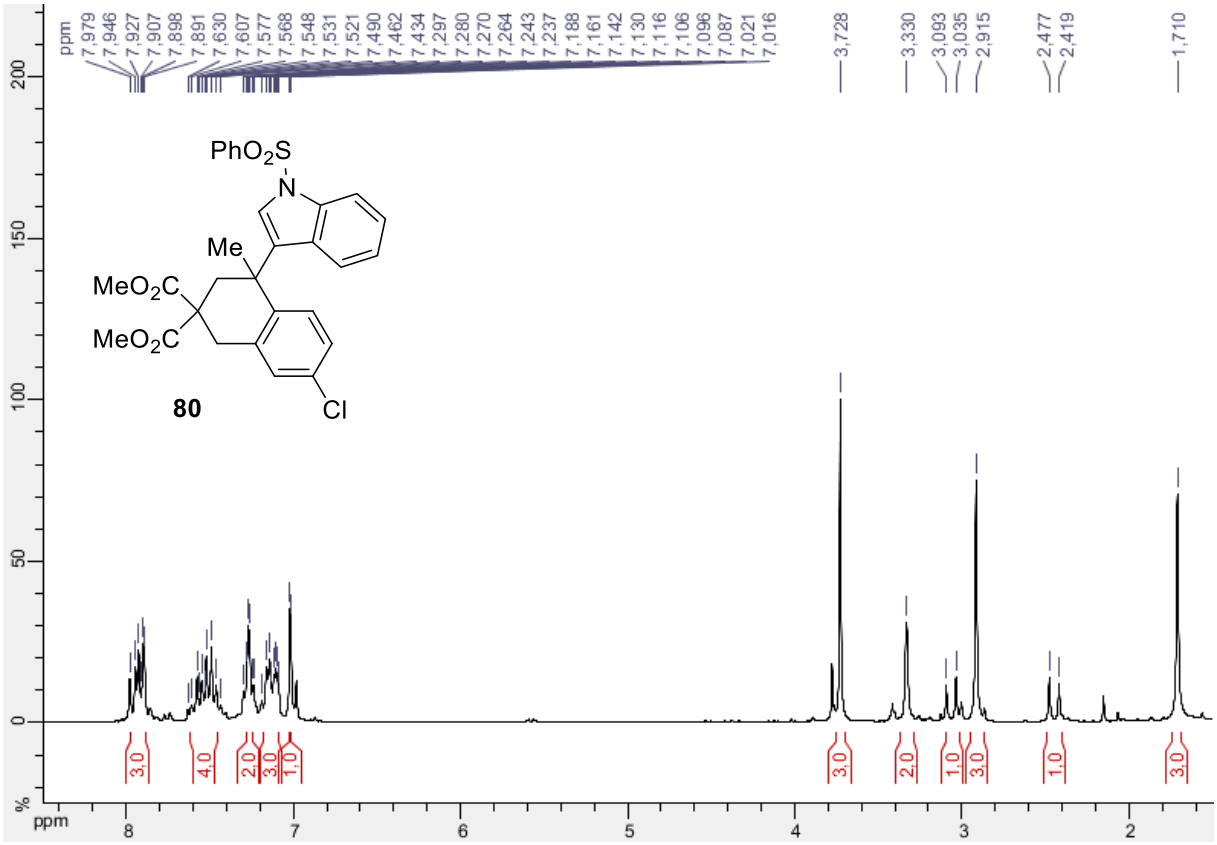

ppm
155,098
142,534
141,244
138,819
137,639
133,138
130,270
130,113
129,261
128,995
128,768
128,476
128,319
126,945
126,094
110,991
77,508
77,205
77,000
76,492
55,368
42,501
41,434
40,905
21,414
OMe
Ts
N
N
Ts
MeO
76
%
ppm
160
140
120
100
80
60
40
20

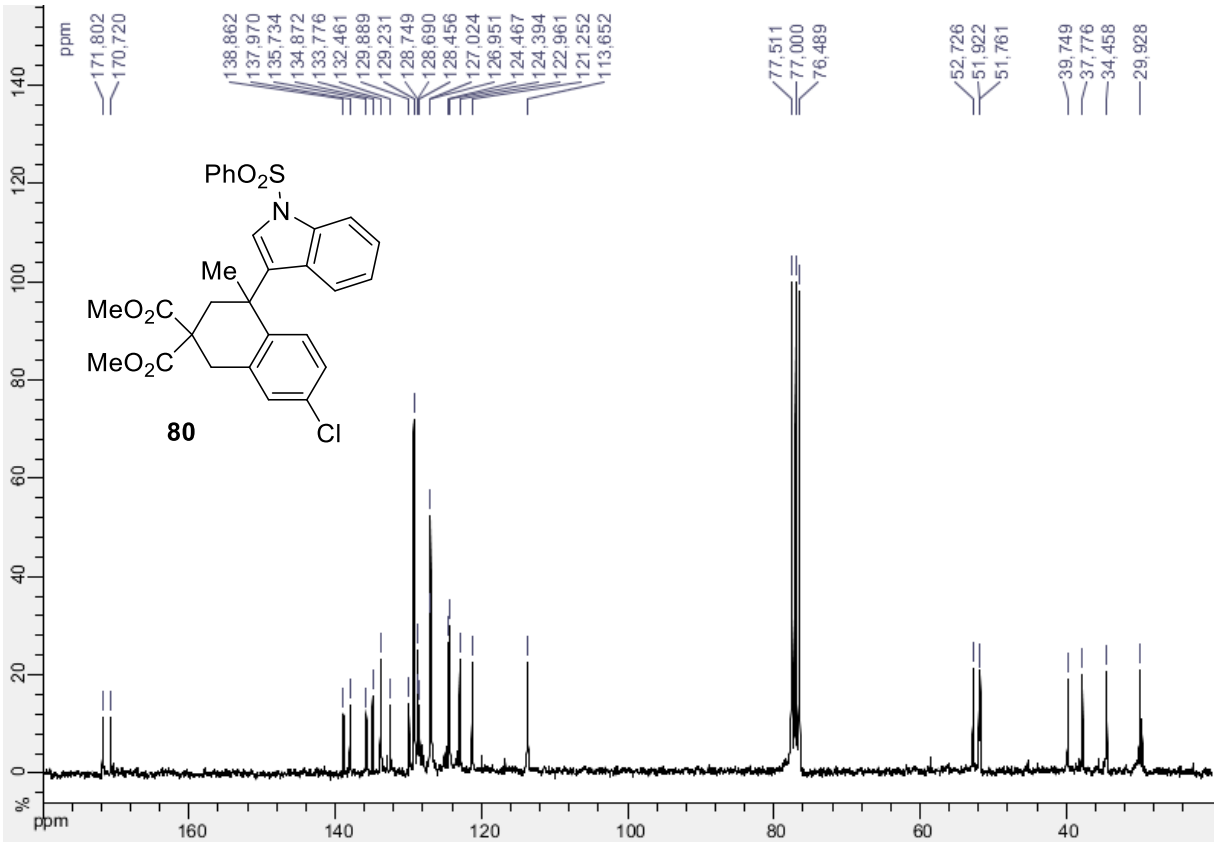

ppm
7,835
7,812
7,802
7,778
7,730
7,708
7,636
7,613
7,421
7,400
7,377
7,319
7,299
7,276
7,270
7,120
7,098
7,085
7,077
7,064
7,042
6,646
6,626
3,820
3,792
3,745
3,715
3,651
3,633
3,586
3,451
3,291
3,233
3,190
3,168
3,129
2,857
2,817
2,571
2,532
2,405
2,364
2,218
2,175
1,242
CO2Me
CO2Me
MeO2C
MeO2C
78
%
ppm
7
6
5
4
3
2

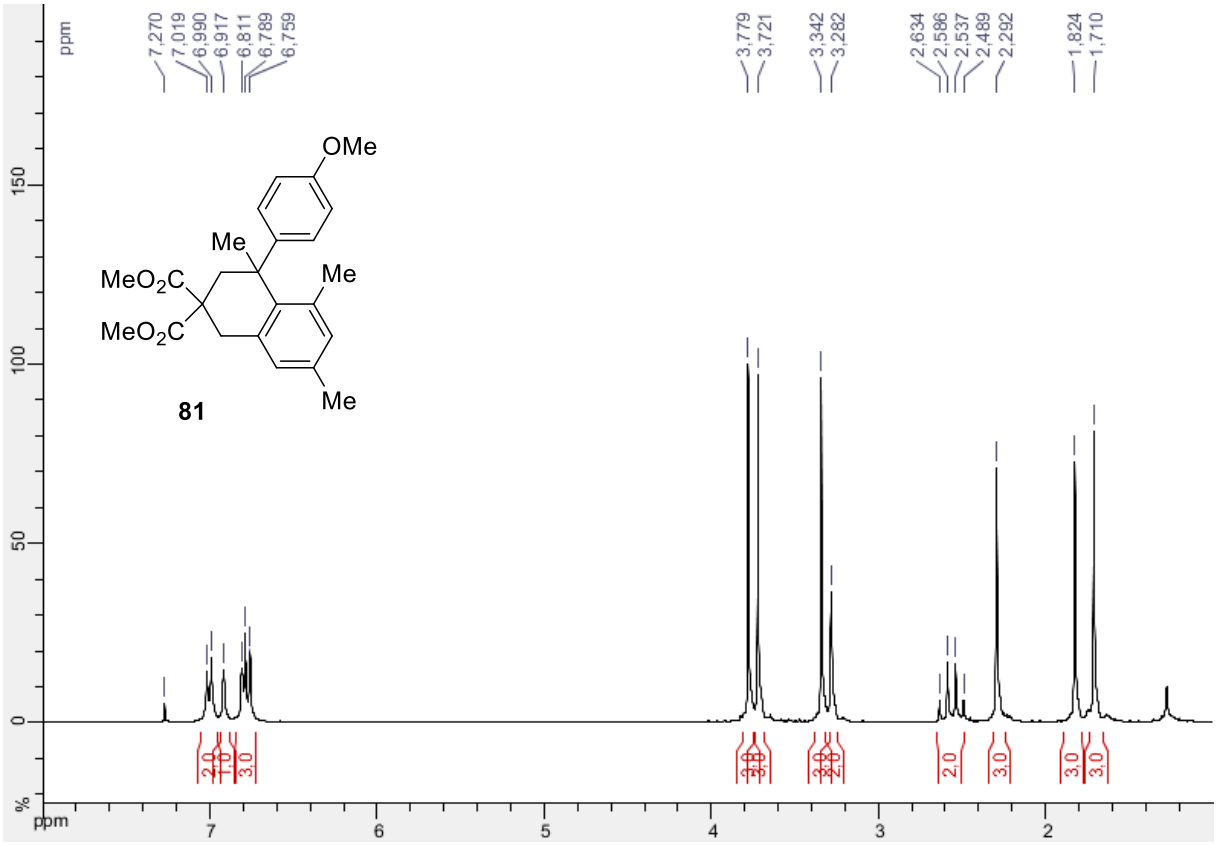

ppm
173,237
172,566
171,953
170,925
142,157
136,782
134,995
134,528
134,200
133,288
130,844
130,567
129,794
129,313
128,430
128,394
127,781
127,482
126,089
125,775
125,068
124,783
124,360
124,185
77,350
76,643
54,520
52,988
52,908
52,558
52,470
51,347
51,318
45,322
44,199
43,214
37,204
34,986
33,557
32,536
CO2Me
CO2Me
MeO2C
MeO2C
78
%
ppm
160
140
120
100
80
60
40

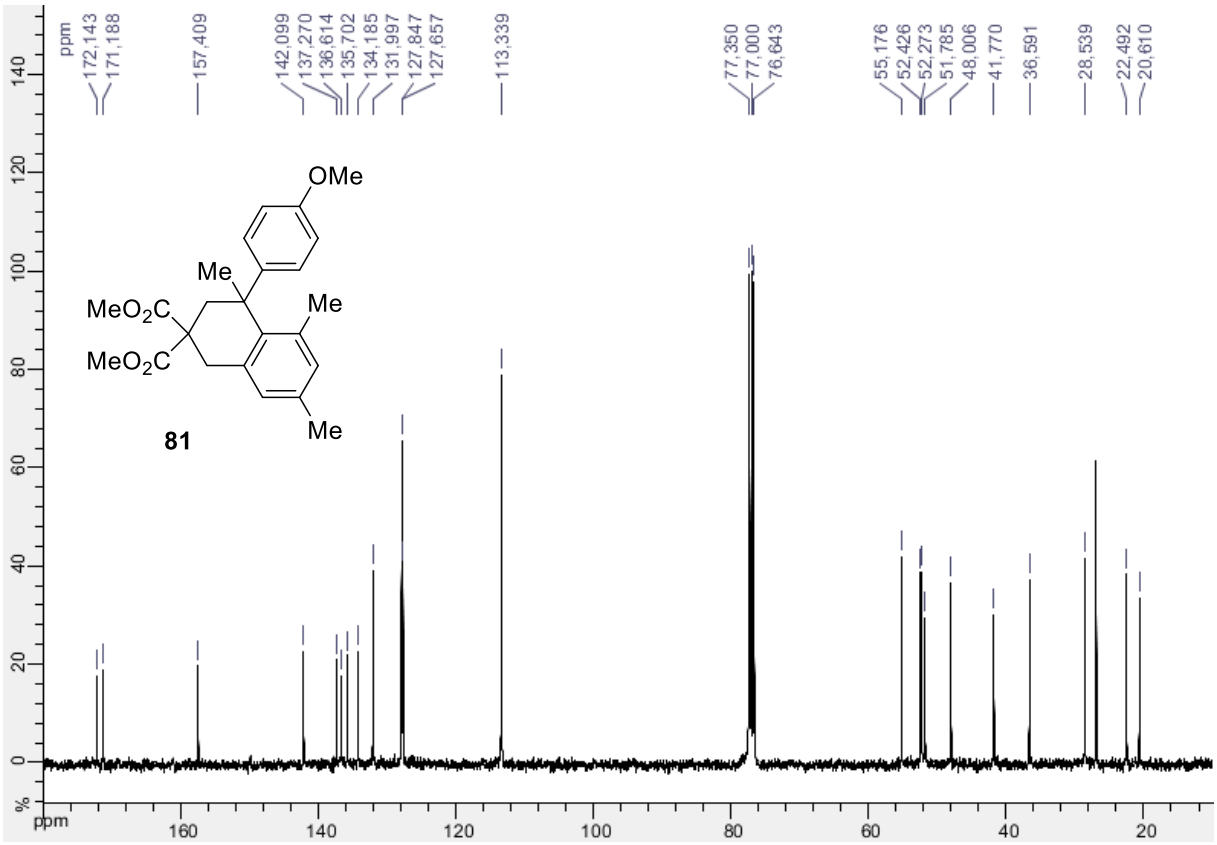

ppm
7,270
7,231
7,222
7,201
7,192
7,168
7,159
7,115
7,081
6,704
6,670
6,598
6,588
6,474
6,465
6,441
6,431
3,823
3,776
3,711
3,322
3,256
3,231
3,104
3,039
2,930
2,873
2,459
2,401
1,661
MeO
OMe
Me
MeO2C
MeO2C
Cl
79
3,0
1,0
1,0
1,0
9,0
4,0
1,0
1,0
1,0
3,0
%
ppm
7
6
5
4
3
2

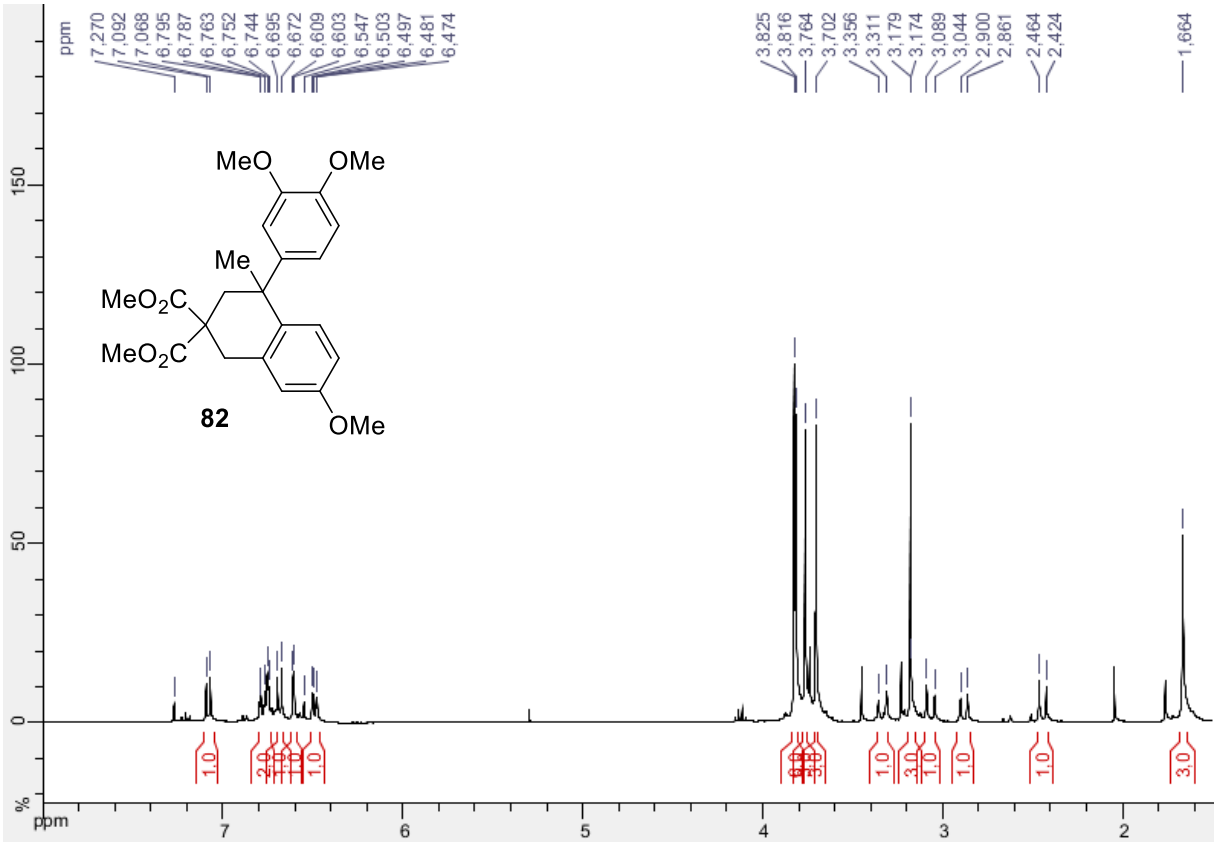

ppm
171,977
170,735
148,244
147,177
140,995
140,308
136,012
132,095
129,728
128,544
126,586
119,732
111,168
110,379
77,497
77,190
77,000
76,678
76,489
55,824
52,784
52,331
52,244
43,285
41,751
34,780
32,018
MeO
OMe
Me
MeO2C
MeO2C
Cl
79
%
ppm
160
140
120
100
80
60
40

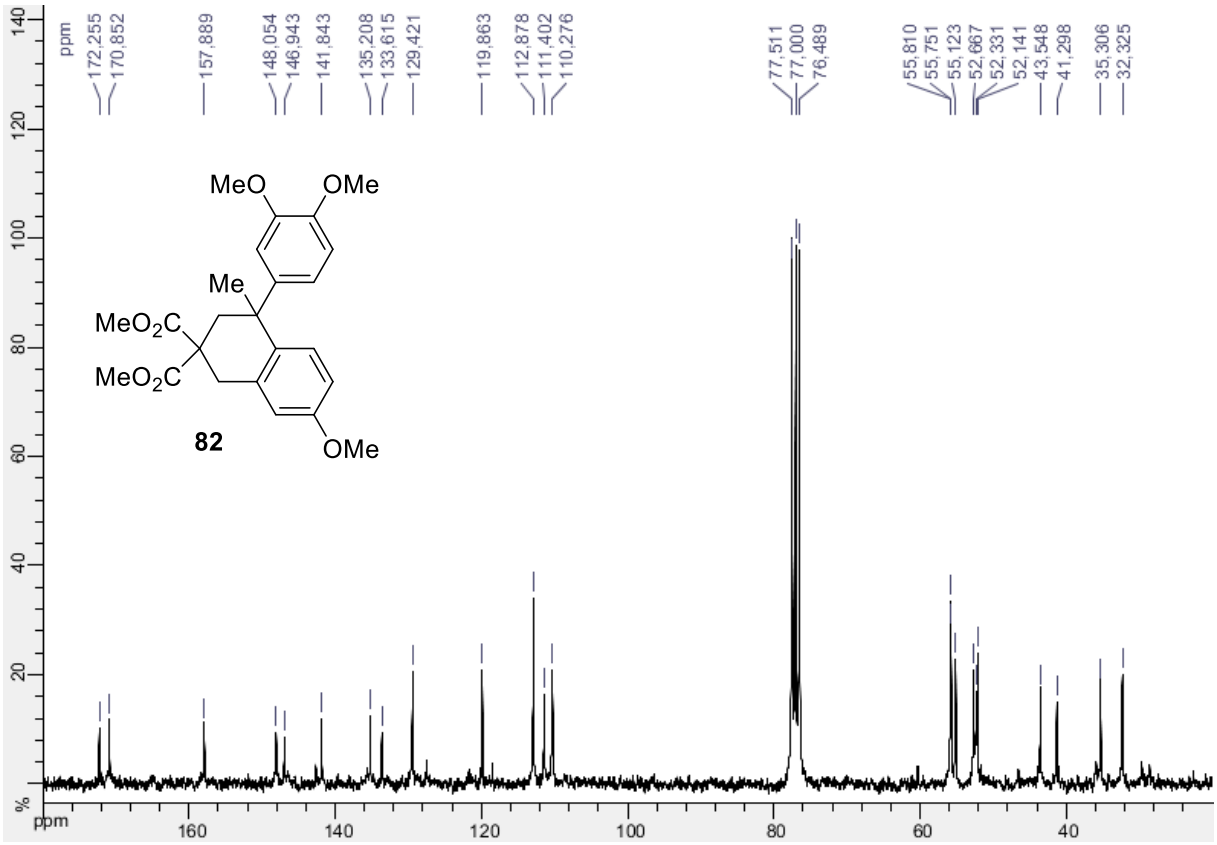

ppm
7,979
7,946
7,927
7,907
7,898
7,891
7,630
7,607
7,577
7,568
7,548
7,531
7,521
7,490
7,462
7,434
7,297
7,280
7,270
7,264
7,243
7,237
7,188
7,161
7,142
7,130
7,116
7,106
7,096
7,087
7,021
7,016
3,728
3,330
3,093
3,035
2,915
2,477
2,419
1,710
PhO2S
N
Me
MeO2C
MeO2C
Cl
80
3,0
4,0
2,0
3,0
1,0
3,0
2,0
1,0
3,0
1,0
3,0
%
ppm
8
7
6
5
4
3
2

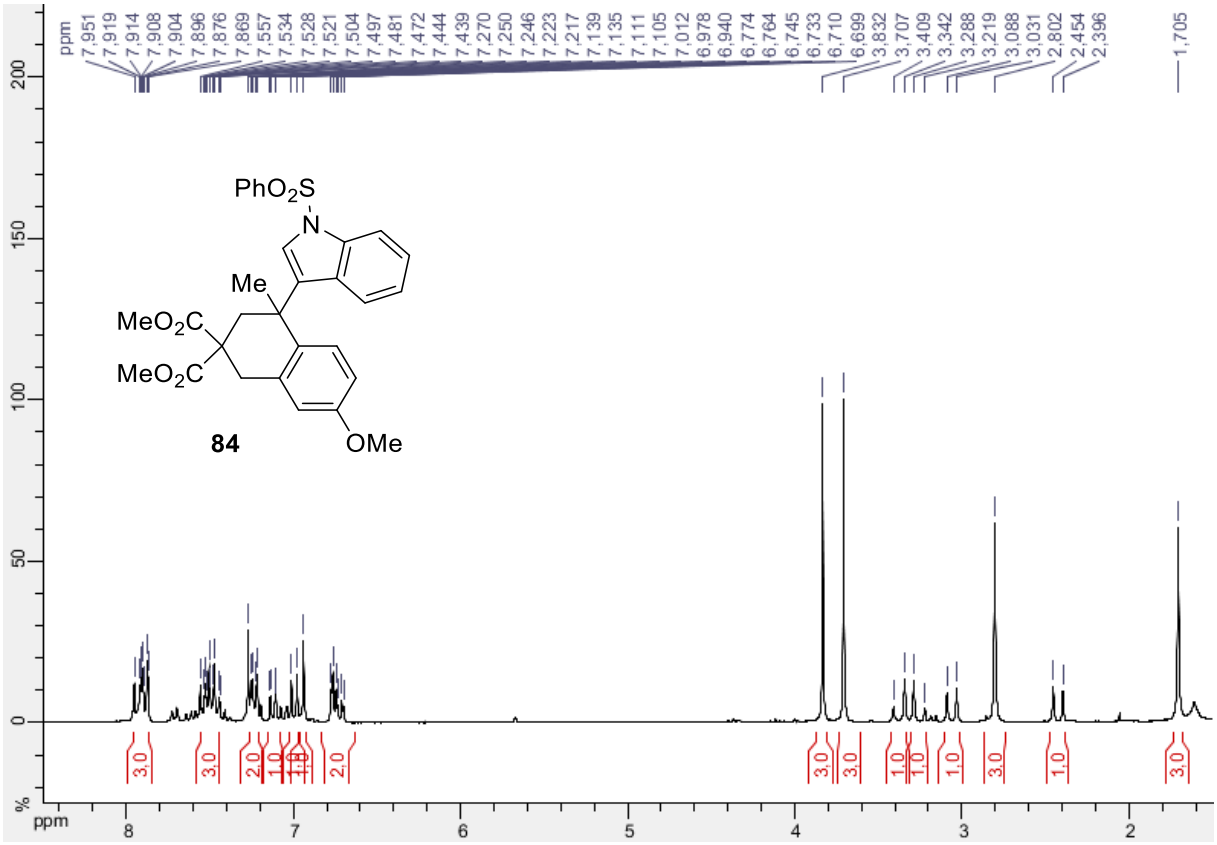

ppm
171,802
170,720
138,862
137,970
135,734
134,872
133,776
132,461
129,889
129,231
128,749
128,690
128,456
127,024
126,951
124,467
124,394
122,961
121,252
113,652
77,511
77,000
76,489
52,726
51,922
51,761
39,749
37,776
34,458
29,928
PhO2S
N
Me
MeO2C
MeO2C
Cl
80
%
ppm
160
140
120
100
80
60
40

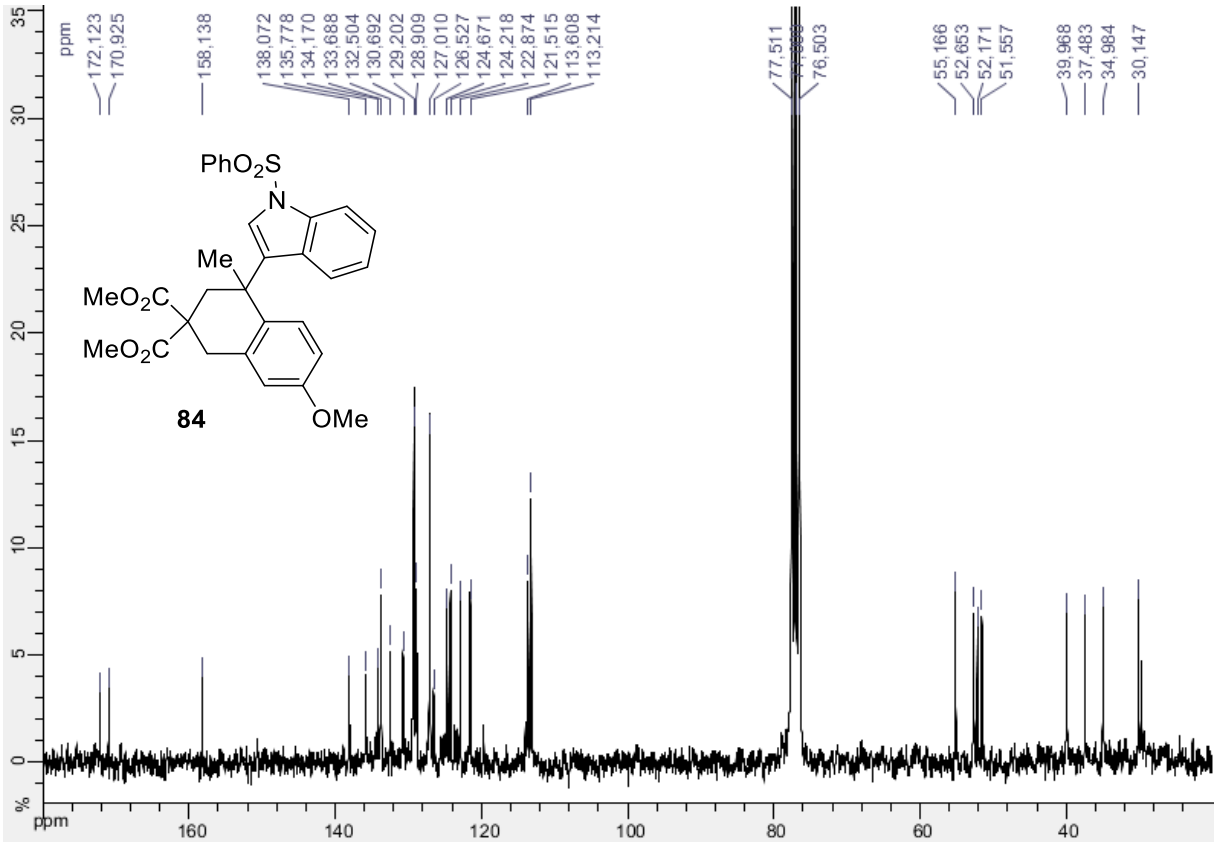

ppm
7,270
7,019
6,990
6,917
6,811
6,789
6,759
3,779
3,721
3,342
3,282
2,634
2,586
2,537
2,489
2,292
1,824
1,710
OMe
Me
MeO2C
MeO2C
Me
Me
81
2,0
1,0
3,0
3,0
2,0
3,0
2,0
3,0
3,0
%
ppm
7
6
5
4
3
2

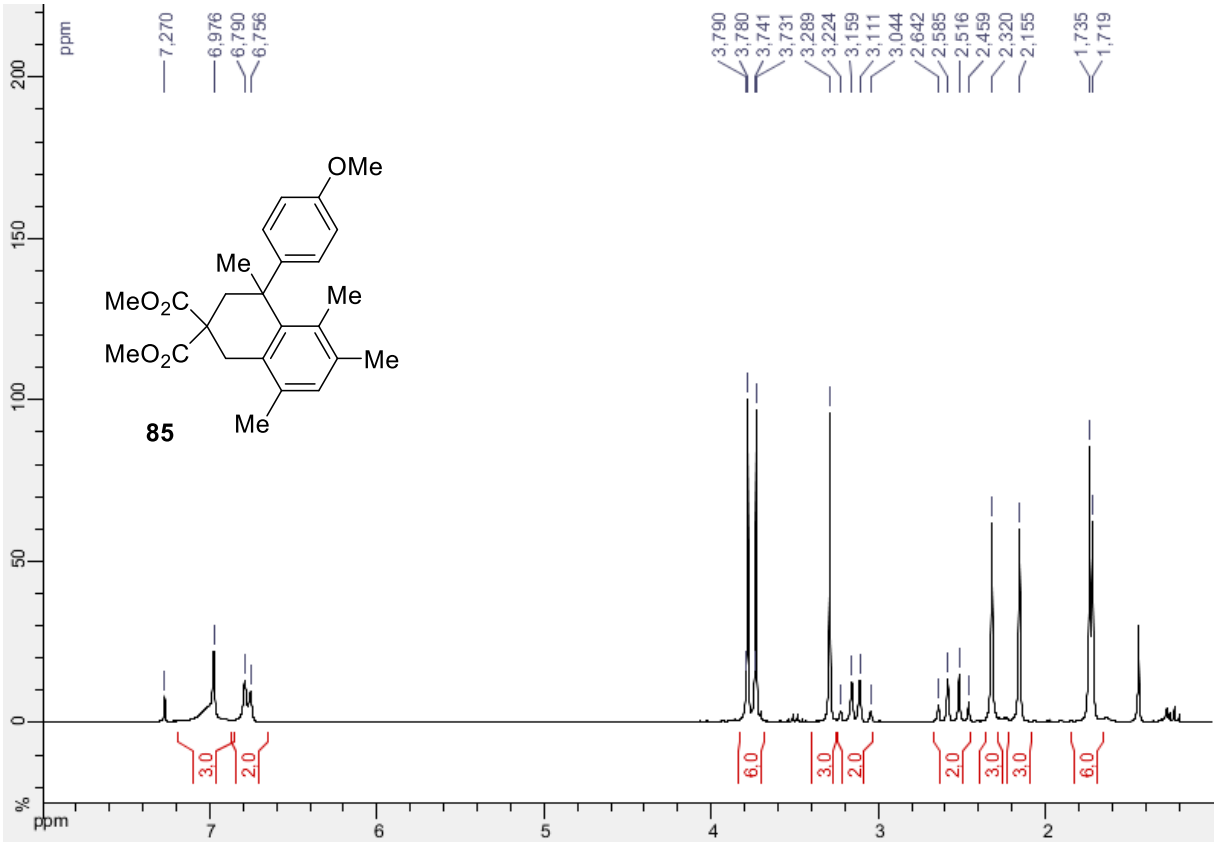

ppm
172,143
171,188
157,409
142,099
137,270
136,614
135,702
134,185
131,997
127,847
127,657
113,339
77,350
77,000
76,643
55,176
52,426
52,273
51,785
48,006
41,770
36,591
28,539
22,492
20,610
OMe
Me
MeO2C
MeO2C
Me
Me
81

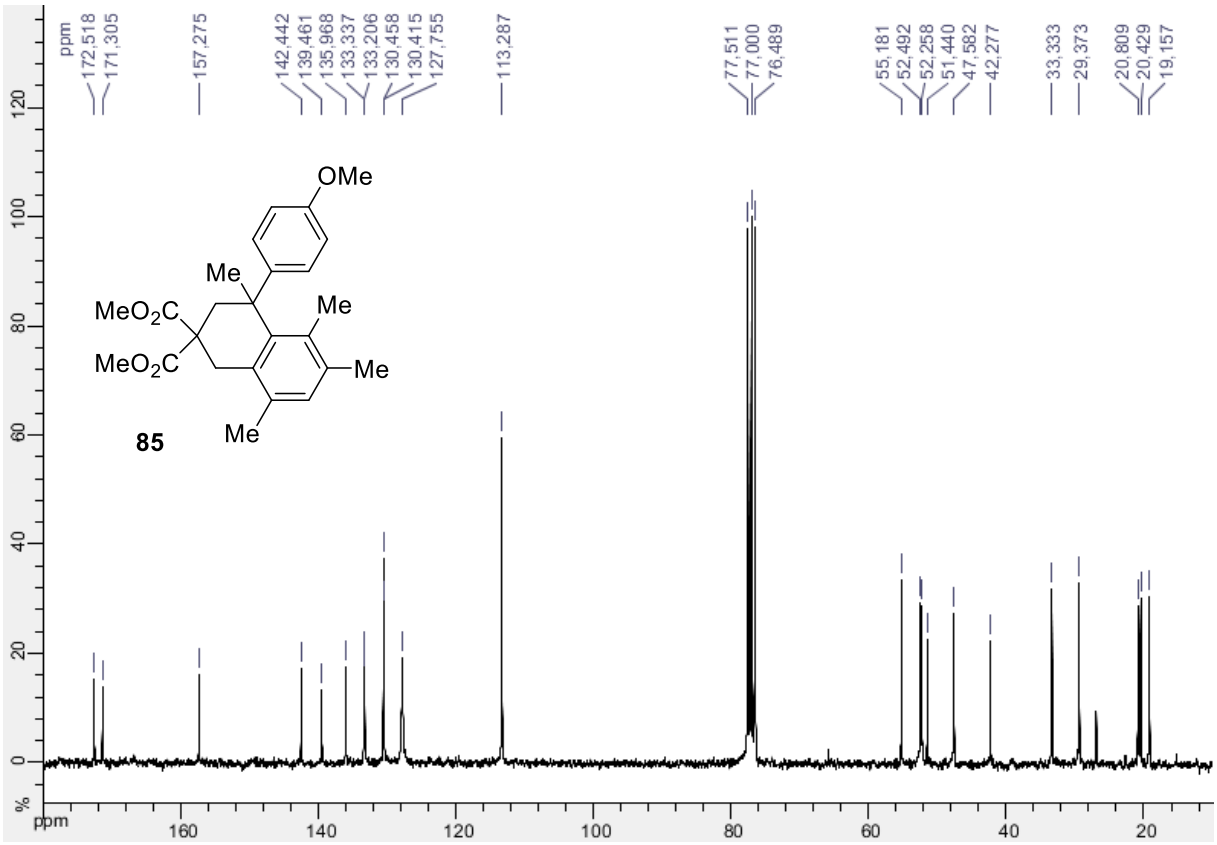

ppm
7,270
7,092
7,088
6,795
6,787
6,763
6,752
6,744
6,695
6,672
6,609
6,603
6,547
6,503
6,497
6,481
6,474
3,825
3,816
3,764
3,702
3,356
3,311
3,179
3,174
3,089
3,044
2,900
2,861
2,464
2,424
1,664
MeO
OMe
Me
MeO2C
MeO2C
82
OMe

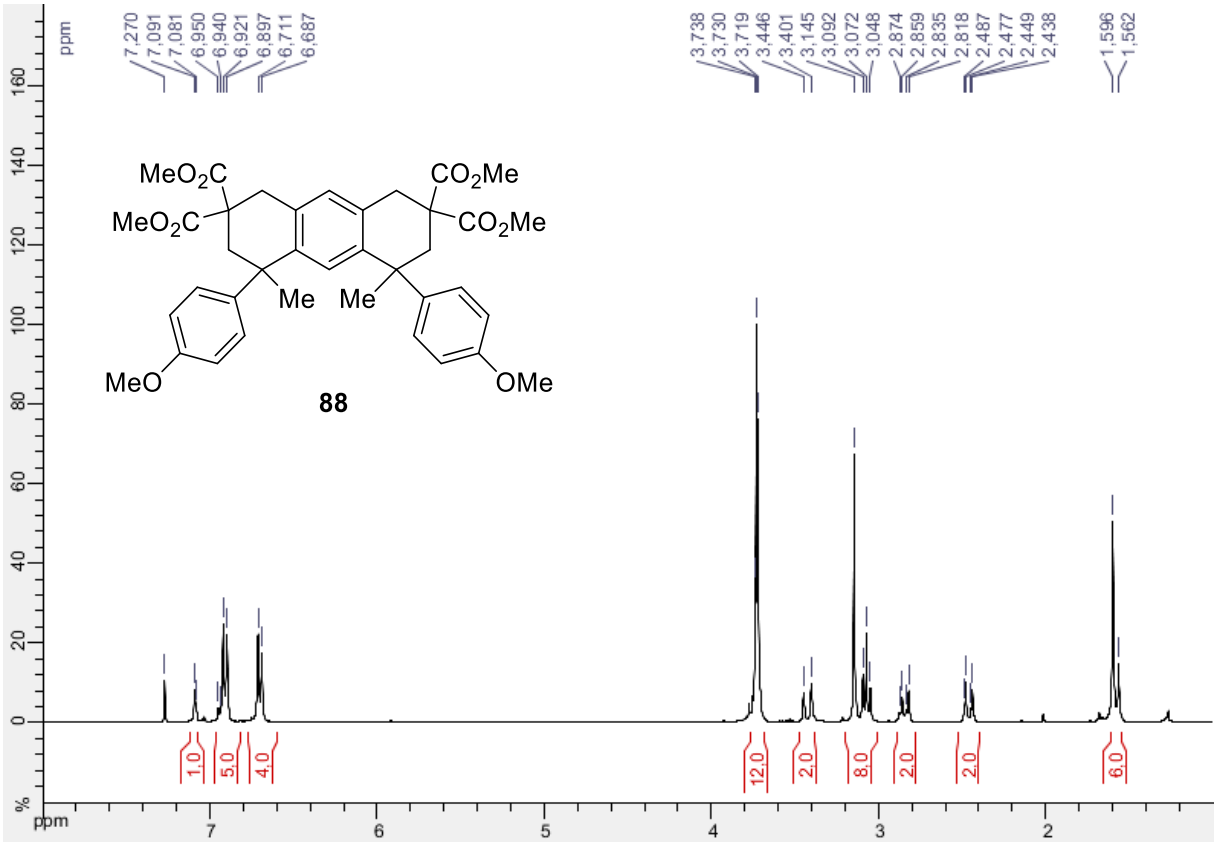

ppm
172,255
170,852
157,889
148,054
146,943
141,843
135,208
133,615
129,421
119,863
112,878
111,402
110,276
77,511
77,000
76,489
55,810
55,751
55,123
52,667
52,331
52,141
43,548
41,298
35,306
32,325
MeO
OMe
Me
MeO2C
MeO2C
OMe
82
%
ppm
160
140
120
100
80
60
40

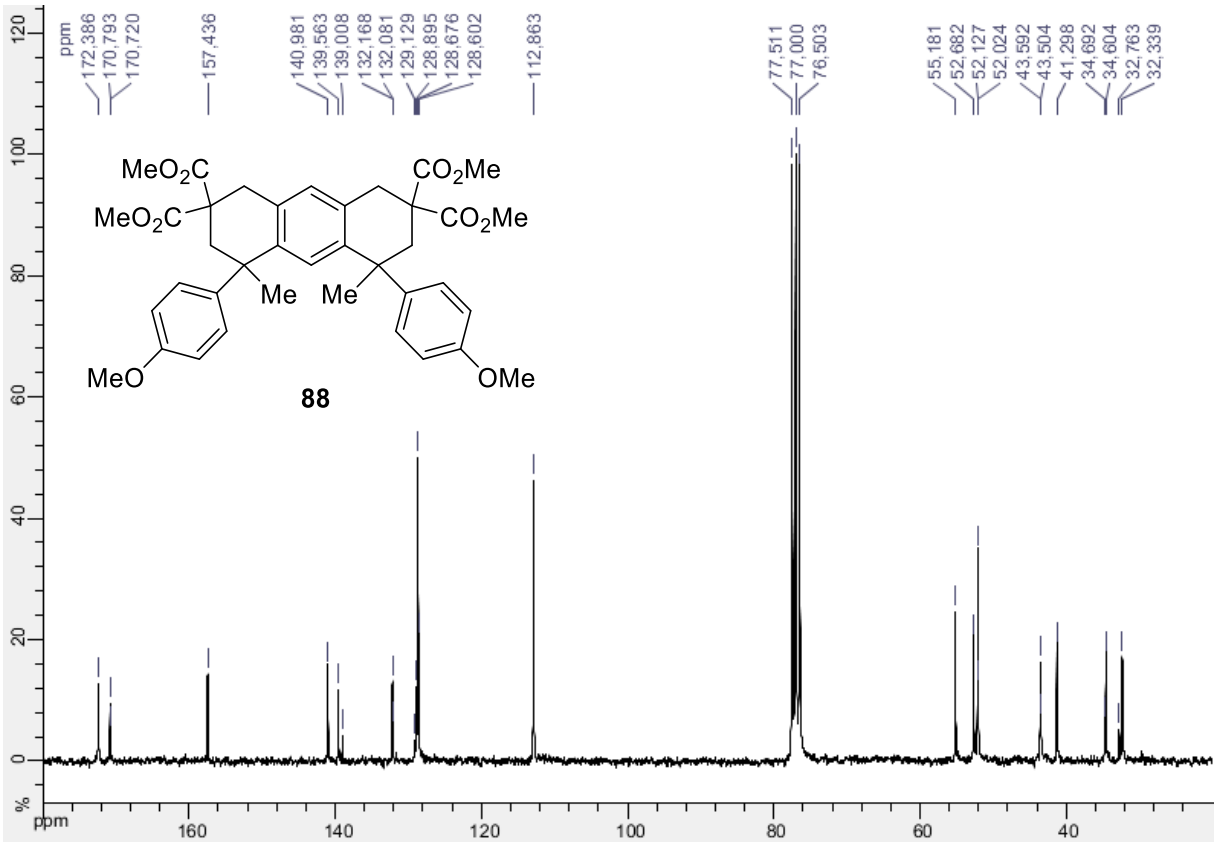

ppm
7,951
7,919
7,914
7,908
7,904
7,896
7,876
7,869
7,557
7,534
7,528
7,521
7,504
7,497
7,481
7,472
7,444
7,439
7,270
7,250
7,246
7,223
7,217
7,139
7,135
7,111
7,105
7,012
6,978
6,940
6,774
6,764
6,745
6,733
6,710
6,699
3,832
3,707
3,409
3,342
3,288
3,219
3,088
3,031
2,802
2,454
2,396
1,705
PhO2S
N
Me
MeO2C
MeO2C
OMe
84
3,0
3,0
2,0
1,0
1,0
2,0
3,0
3,0
1,0
1,0
1,0
3,0
1,0
3,0
%
ppm
8
7
6
5
4
3
2


ppm
172,123
170,925
158,138
138,072
135,778
134,170
133,688
132,504
130,692
129,202
128,909
127,010
126,527
124,671
124,218
122,874
121,515
113,608
113,214
77,511
76,503
55,166
52,653
52,171
51,557
39,968
37,483
34,984
30,147
PhO2S
N
Me
MeO2C
MeO2C
OMe
84


ppm
7,270
6,976
6,790
6,756
3,790
3,780
3,741
3,731
3,289
3,224
3,159
3,111
3,044
2,642
2,585
2,516
2,459
2,320
2,155
1,735
1,719
OMe
Me
MeO2C
MeO2C
Me
Me
Me
85
3,0
2,0
6,0
3,0
2,0
2,0
3,0
3,0
6,0


ppm
172,518
171,305
157,275
142,442
139,461
135,968
133,337
133,206
130,458
130,415
127,755
113,287
77,511
77,000
76,489
55,181
52,492
52,258
51,440
47,582
42,277
33,333
29,373
20,809
20,429
19,157
OMe
Me
MeO2C
Me
MeO2C
Me
Me
85


ppm
7,270
7,091
7,081
6,950
6,940
6,921
6,897
6,711
6,687
3,738
3,730
3,719
3,446
3,401
3,145
3,092
3,072
3,048
2,874
2,859
2,835
2,818
2,487
2,477
2,449
2,438
1,596
1,562
MeO2C
CO2Me
MeO2C
CO2Me
Me
Me
MeO
OMe
88
1,0
5,0
4,0
12,0
2,0
8,0
2,0
2,0
6,0


ppm
172,386
170,793
170,720
157,436
140,981
139,563
139,008
132,168
132,081
129,129
128,895
128,676
128,602
112,863
77,511
77,000
76,503
55,181
52,682
52,127
52,024
43,592
43,504
41,298
34,692
34,604
32,763
32,339
MeO2C
MeO2C
CO2Me
CO2Me
Me
Me
MeO
OMe
88
%
ppm
160
140
120
100
80
60
40