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# Supporting Information

## A selective solvent-free self-condensation of carbonyl compounds utilizing microwave irradiation

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### General Methods

All microwave reactions were carried out in sealed tubes in Biotage Initiator™ Microwave Synthesizer. All commercial reagents were obtained from Sigma-Aldrich Chemical Co. or Acros Organics. Triethylamine and aldehydes were distilled under reduced pressure before using. Distillation was done using Kuglore distillator. Silica gel column chromatography was performed using #R12030B, SilicaFlash® P60, 40-63 μm obtained from SiliCycle Inc. TLC plates were visualized by exposure to ultraviolet light (254 nm) and/or by immersion in a staining solution of vanillin, followed by heating on a hot plate. $^{1}$H and $^{13}$C spectra were recorded on a Varian Inova 500 spectrometer at 500 and 125 MHz respectively (unless otherwise noted), using $CDCl_3$ or $CD_3OD$ as a solvent. The chemical shifts are reported in δ (ppm) values relative to $CHCl_3$ (δ 7.26 ppm for $^{1}$H NMR and δ 77.23 ppm for $^{13}$C NMR). Coupling constants are reported in hertz (Hz). Infrared spectra were recorded using either a Mattson Infinity Series FTIR or Mattson Galaxy Series FTIR 5000 spectrometer. The following abbreviations are used to designate the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet.

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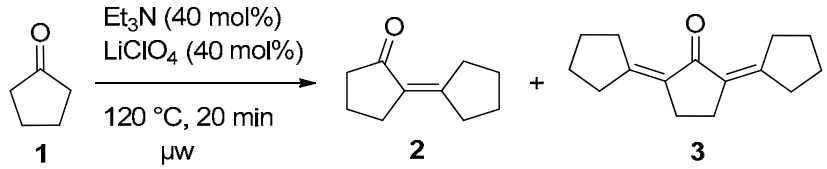
## Self-condensation of ketones:

### Reaction Procedure A

To a 0.2-0.5 ml microwave vial containing ketone (1 mmol) was added anhydrous $LiClO_4$ (0.043g, 40 mol %) and $Et_3N$ (0.056mL, 40 mol %). Vial was sealed and the reaction mixture was stirred for 20 min. at 120 °C (or as specified conditions) in the microwave reactor. After cooling, the microwave vessel was uncapped and 15mL of sat. $NH_4Cl$ was added. The product was extracted with (2x20mL) ethyl acetate. The organic layer was dried over $MgSO_4$, filtered, and evaporated to dryness under reduced pressure to obtain crude. All the liquid products were purified using distillation while the solid products were purified either by crystallization or by silica gel column.

### Self-condensation of cyclopentanone:




Reaction procedure A was followed to obation crude. The crude was distilled to obtain the enone **2** (80%) as colorless liquid, while the remaining solid was crystalized using hexane-ethyl acetate (3:1) to yield **3** in pure form.

**2-cyclopentylidenecyclopentan-1-one (2):** IR ($\nu$, $cm^{-1}$): 2955, 2870, 1706, 1636, 725; $^1H$ NMR (500 MHz, $CDCl_3$): *ä* 2.77 (m, 2H), 2.51 (m, 2H), 2.29 (m, 4H), 1.90 (m, 2H), 1.76-1.64 (m, 4H); $^{13}C$ NMR (125 MHz, $CDCl_3$): *ä* 207.57, 158.82, 128.11, 40.02, 34.51, 32.77, 27.17, 26.91, 25.45, 20.31.

**2,5-Dicyclopentylidenecyclopentaone (3):** White solid; mp=83-84 °C; IR ($\nu$, $cm^{-1}$): 2952, 2862, 1689, 1637, 1617, 1260, 1173, 767; $^1H$ NMR (500 MHz, $CDCl_3$): *ä* 2.87 (t, *J*=6.5 Hz, 4H), 2.52 (bs, 4H), 2.28 (t, *J*=6.5 Hz, 4H), 1.76-1.64 (m, 8H); $^{13}C$ NMR (125 MHz, $CDCl_3$): *ä* 196.06, 157.76, 131.37, 34.31, 32.45, 27.32, 26.16, 25.47.

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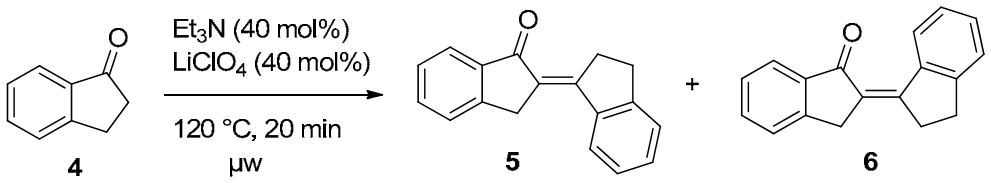
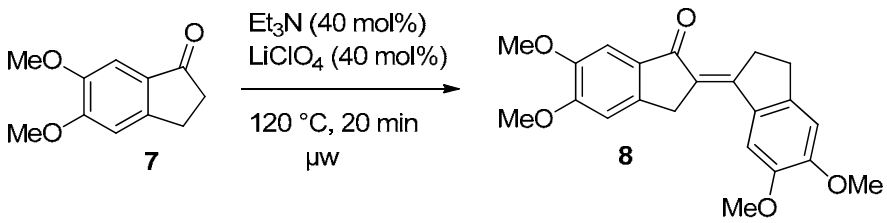
**Self-condensation of 1-indanone:**




Reaction procedure A was followed to obtain solid crude. $^{1}$H NMR of crude product showed the formation of very small amount of **6**. The crude was crystallized using hexane-ethyl acetate (3:1) to obtain **5** (73%) in pure form (compound **6** was not isolated).

***trans*-2-(1-indanylidene)indan-1-one (5):** White solid; mp=143-144 °C; IR ($\nu$, cm$^{-1}$): 3064, 2918, 1673, 1597, 1325, 733; $^{1}$H NMR (500 MHz, $CDCl_3$): *ä* 7.83 (d, *J*=7.5 Hz, 1H), 7.82 (d, *J*=7.5 Hz, 1H), 7.60-7.80 (m, 2H), 7.44-7.34 (m, 4H), 4.03 (s, 2H), 3.58 (t, *J*=6.5 Hz, 2H), 3.14 (t, *J*=6.5 Hz, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 195.51, 155.28, 151.97, 148.77, 141.13, 139.78, 133.85, 130.65, 127.52, 127.09, 126.52, 126.22, 126.20, 126.01, 123.85, 33.26, 31.79, 31.17.

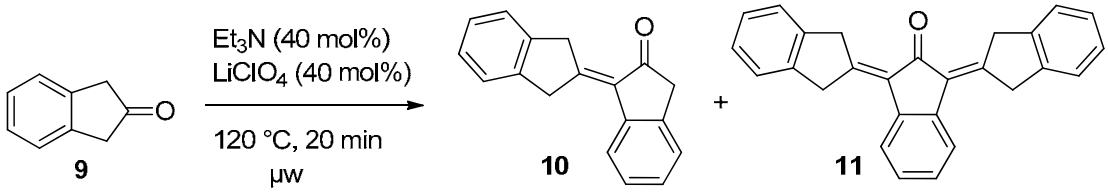
**Self-condensation of 5,6-dimethoxy-1-indanone:**




Reaction procedure A was followed to obtain solid. Purification of silica gel (50% EtOAc/hexane) afforded **8** in 70% yield.

**Dione 8:** Yellow solid; IR ($\nu$, cm$^{-1}$): 3064, 2918, 1673, 1597, 1325, 733; $^{1}$H NMR (500 MHz, $CDCl_3$): *ä* 7.29 (s, 1H), 7.27 (s, 1H), 7.18 (s, 1H), 7.00 (s, 1H), 4.00 (s, 3H), 3.97 (s, 3H), 3.95 (s, 6H), 3.91 (s, 2H), 3.57 (t, *J*=6.0 Hz, 2H), 2.68 (t, J=6.0 Hz, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 194.22, 154.51, 154.36, 151.99, 149.54, 148.73, 143.04, 133.37, 108.07, 107.82, 107.67, 107.29, 105.21, 104.74, 104.35, 56.44, 56.32, 56.30, 56.22, 32.55, 32.30, 31.15.

**Self-condensation of 2-indanone:**



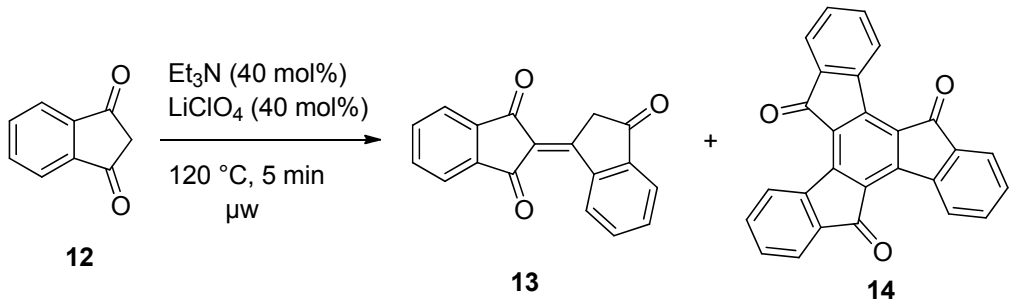

9 10 11

Reaction procedure A was followed to obtain solid crude. Purification of silica gel (3% EtOAc/hexane) afforded dione **10** in 71% yield and **11** in 8% yield.

**Dione (10):** Yellow solid; mp=160-162 °C, IR ($\nu$, $cm^{-1}$): 3027, 2906, 1707, 1625, 1393, 731; $^1H$ NMR (500 MHz, $CDCl_3$): *ä* 7.63 (d, *J*=5.0 Hz, 1H), 7.42-7.38 (m, 4H), 7.33 (d, *J*=10.0 Hz, 1H), 7.28-7.26 (m, 2H), 4.42 (s, 2H), 4.01 (s, 2H), 3.51 (s, 2H); $^{13}C$ NMR (125 MHz, $CDCl_3$): *ä* 204.29, 154.40, 141.37, 140.43, 139.49, 137.64, 129.89, 127.77, 127.51, 127.28, 126.92, 125.37, 124.86, 124.56, 123.75, 42.57, 41.45, 41.01.

**Compound (11)**: Green solid; mp=178-180 °C, IR ($\nu$, $cm^{-1}$): 3022, 2900, 1700, 1625, 1390, 722; $^1H$ NMR (500 MHz, $CDCl_3$): *ä* 7.69 (m, 2H), 7.41 (m, 6H), 7.27 (m, 4H), 4.58 (s, 4H), 4.25 (s, 4H).

**Self-condensation of 1,3-indandione:**




12 13 14

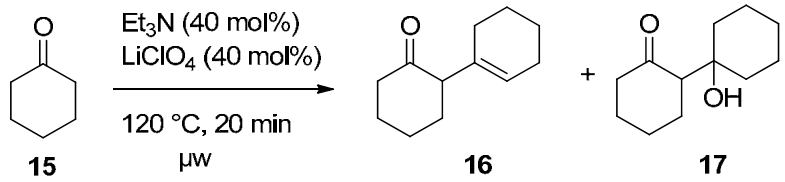
Reaction procedure A was followed to obtain solid crude and crude was crystallized using hexane-ethyl acetate (3:1) to obtain **13** (92%) in pure form. When the reaction was conducted for 20 min, truxenequinone **14** was obtained in 55% yield while compound **13** was obtained in 25% yield by column chromatography (5% Ethyl acetate/hexane).

**1-(indan-1,3-dione-2-ylidene)indan-3-one (13):** Yellow solid; IR ($\nu$, $cm^{-1}$): 3020, 2901, 1707, 1680, 1340, 931; $^1H$ NMR (500 MHz, $CDCl_3$): *ä* 9.64 (d, *J*=8.0 Hz, 1H), 8.00 (m, 1H), 7.96-7.90 (m, 2H), 7.88-7.74 (m, 3H), 7.72 (1.75, *J*=6.5Hz, 1H), 4.11 (s, 2H); $^{13}C$ NMR (125 MHz,

$CDCl_3$): *ä* 201.14, 191.19, 189.49, 155.55, 146.06, 141.83, 141.43, 140.57, 135.50, 134.34, 131.85, 126.04, 123.68, 123.57, 123.22, 43.61.

**Truxenequinone** (**14**)**:** Yellow solid; $^1$H NMR (500 MHz, $CDCl_3$): *ä* 9.30 (d, *J*= 10 Hz, 3H), 7.87 (d, *J*= 10 Hz, 3H), 7.72 (t, *J*= 10 Hz, 3H), 7.85 (t, *J*= 10 Hz, 3H).

**Self-condensation of cyclohexanone:**



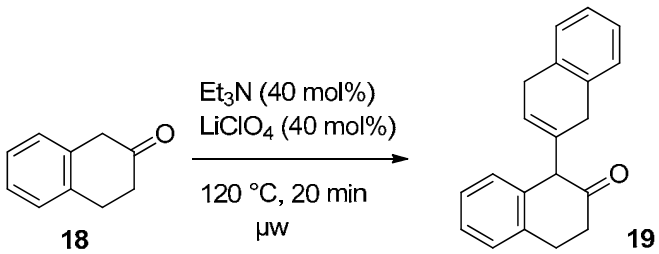

**15** **16** **17**

Reaction procedure A was followed to obtain crude as yellow oil. The crude was distilled to obtain **16** (50%) and **17** (2%) in pure form.

**[1,1'-bi(cyclohexylidene)]-2-one** (**16**): Colorless oil; IR (*v*, $cm^{-1}$): 2922, 2851, 1675, 1639, 1444, 729; $^1$H NMR (500 MHz, $CDCl_3$): *ä* 5.38 (t, J=10 Hz, 1H), 2.88 (dd, *J*=11.2 and 5.0Hz, 1H), 2.42-2.36 (m, 1H), 2.34-2.26 (m, 1H), 2.06-1.96 (m, 4H), 1.96-1.80 (m, 4H), 1.74-1.52 (m, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 211.82, 136.07, 123.88, 58.98, 42.33, 31.05, 27.88, 27.49, 25.50, 25.06, 23.06, 22.62.

**1'-hydroxy-[1,1'-bi(cyclohexan)]-2-one** (**17**): Colorless oil; IR (*v*, $cm^{-1}$): 3300, 1670, 1429; $^1$H NMR (500 MHz, $CDCl_3$): *ä* 3.64 (s, 1H), 2.39 (dd, *J*=12.0 and 5Hz, 1H), 2.36-2.28 (m, 2H), 2.22-2.16 (m, 1H), 2.10-2.04 (m, 1H), 1.96-1.90 (m, 1H), 1.74-1.54 (m, 8H), 1.46-1.38 (m, 3H), 1.30-1.12 (m, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 216.65, 72.18, 59.21, 44.11, 36.49, 33.50, 29.21, 28.51, 26.11, 25.75, 21.92, 21.63.

**Self-condensation of *β*-tetralone:**

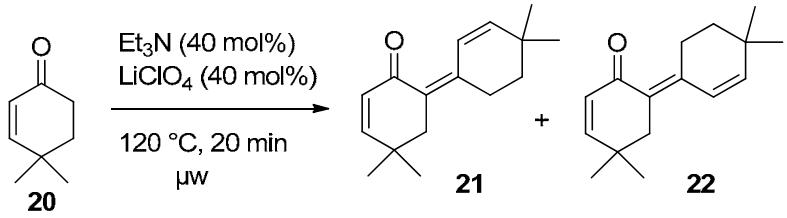



**18** **19**

Reaction procedure A was followed to obtain solid crude and crude was crystallized using hexane-ethyl acetate (3:1) to obtain **19** (61%) in pure form.

**1',3,4,4'-tetrahydro-[1,2'-binaphthalen]-2(1H)-one** (**19**): White solid; IR ($\nu$, $cm^{-1}$): 2918, 2842, 1678, 1629, 1451, 780; $^1H$ NMR (500 MHz, $CDCl_3$): *ä* 7.30-7.20 (m, 3 H), 7.15-7.05 (m, 4H), 6.97 (d, *J*=6 Hz, 1H), 6.27 (s, 1H), 3.68 (s, 2H), 3.36-3.26 (m, 2H), 3.13 (dd, *J*=14.0, 4.5 Hz, 1H), 2.90-2.68 (m, 2H), 2.36-2.18 (m, 2H); $^{13}C$ NMR (125 MHz, $CDCl_3$): *ä* 209.56, 138.25, 136.12, 134.97, 134.18, 133.11, 128.25, 127.92, 127.37, 127.16, 127.13, 127.01, 126.59, 126.11, 125.77, 55.36, 45.16, 33.77, 28.21, 26.15.

**Self-condensation of 3,3-dimethylcyclohexenone:**




Reaction procedure A was followed to obtain crude. Purification of silica gel (3% EtOAc/hexane) afforded a mixture of (**21**) and (**22**) as **c**olorless oil (40% yield); $^1H$ NMR (500 MHz, $CDCl_3$): *ä* 7.11 (d, *J*=10 Hz, 1H), 6.57 (d, *J*=2.5 Hz, 1H), 6.55 (d, *J*=2.5 Hz, 1H), 6.33 (d, *J*=10 Hz, 1H), 5.93 (d, *J*=10 Hz, 1H), 5.89 (d, *J*=1.5 Hz, 1H), 5.87 (d, *J*=1.5 Hz, 1H), 5.79 (d, *J*=10.5 Hz, 1H), 2.86 (t, *J*=6.5 Hz, 2 H), 2.60 (s, 2H), 2.57 (s, 2H), 2.44 (t, *J*=6.5 Hz, 2H), 1.62 (t, *J*=7.0 Hz, 2H), 1.52 (t, *J*=7.0Hz, 2H), 1.13 (s, 6H), 1.12 (s, 6H), 1.04 (s, 6H), 1.03 (s, 6H); $^{13}C$ NMR (125 MHz, $CDCl_3$): *ä* 192.2, 191.9, 157.3, 157.2, 147.5, 145.3, 143.0, 142.2, 129.8, 129.6, 127.3, 126.9, 123.9, 122.6, 42.3, 41.5, 36.9, 36.6, 36.2, 35.8, 32.4, 32.2, 28.6, 28.5, 27.9, 27.9, 25.0, 24.2.

**Self-condensation of 4-methylacetophenone (Table V, Entry 8):**


Reaction procedure A was followed to obtain crude. The condensation product was isolated by column chromatography on silica gel (3% EtOAc/hexane). $^1H$ NMR (500 MHz, $CDCl_3$): $\delta$ 8.01

(d, *J*=5.0 Hz, 2H), 7.59 (d, *J*=5.0 Hz, 2H), 7.37 (d, *J*=8.0 Hz, 2H), 7.33 (d, *J*=8.0 Hz, 2H), 2.69 (s, 3H), 2.52 (s, 3H), 2.50 (s, 3H); $^{13}$C NMR (75 MHz, $CDCl_3$): $\delta$ 191.6, 163.8, 154.5, 143.2, 139.9, 139.3, 136.9, 129.4, 129.3, 128.5, 126.5, 121.5, 21.9, 21.5, 19.0.

## Self-condensation of aldehydes:

### Reaction Procedure B

To a 0.2-0.5 ml microwave vial containing substrate (1mmol) was added anhydrous $LiClO_4$ (0.043g, 40 mol %) and $Et_3N$ (0.056ml, 40 mol %). Vial was sealed and the reaction mixture was stirred for 20 min. at 120 $^{\circ}$C in microwave reactor. After cooled to ambient temperature, saturated $NH_4Cl$ (10 ml) was added and extraction was done using ether. The organic layer was dried over $MgSO_4$, filtered, and evaporated to dryness under reduced pressure to obtain crude. The condensation product was purified by distillation.

**Self-condensation of heptanal (Table V, Entry 1):**

$^1$H NMR (500 MHz, $CDCl_3$): *ä* 9.35 (s, 1H), 6.43 (t, *J*=7.5 Hz, 1H), 2.36 (m, 2H), 2.22 (t, *J*=7.4 Hz, 2H), 1.36-1.22 (m, 10H), 0.92-0.84 (m, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 195.42, 155.41, 143.90, 31.89, 31.82, 29.10, 29.02, 28.71, 28.63, 24.04, 22.68, 22.40, 14.15, 14.08.

**Self-condensation of hexanal (Table V, Entry 2):**

$^1$H NMR (500 MHz, $CDCl_3$): *ä* 9.36 (s, 1H), 6.44 (t, *J*=7.5 Hz, 1H), 2.40-2.16 (m, 4H), 1.60-1.25 (m, 10 H), 0.92-0.88 (m, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 195.5, 155.5, 143.8, 31.7, 31.1, 29.0, 28.5, 23.8, 22.9, 22.5, 14.0, 13.8.

**Self-condensation of pentanal (Table V, Entry 3):**

$^1$H NMR (500 MHz, $CDCl_3$): *ä* 9.36 (s, 1H), 6.48 (t, *J*=7.5 Hz, 1H), 2.35 (m, 2H), 2.21 (t, *J*=7.5 Hz, 2H), 1.54-1.26 (m, 6H), 0.94-0.88 (m, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 195.45, 155.63, 143.71, 31.02, 28.82, 26.07, 22.59, 22.11, 14.21, 14.06.

**Self-condensation of butanal (Table V, Entry 4):**

$^1$H NMR (500 MHz, $CDCl_3$): *ä* 9.35 (s, 1H), 6.40 (t, *J*=7.5 Hz, 1H), 2.35 (t, *J*=7.5 Hz, 2H), 2.24 (q, *J*=7.5 Hz, 2H), 1.54 (m, 2H), 1.0-0.92 (m, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 195.13, 154.61, 145.42, 30.76, 22.01, 17.19, 13.92, 13.36.

**Self-condensation of isovaleraldehyde (Table V, Entry 5):**

$^{1}$H NMR (500 MHz, $CDCl_3$): *ä* 9.31 (s, 1H), 6.33 (t, *J*=7.5 Hz, 1H), 2.90-2.80 (m, 1H), 2.5 (t, *J*=7.5 Hz, 2H), 1.82-1.75 (m, 1H), 1.15 (d, *J*=7 Hz, 6H), 0.95 (d, *J*=7 Hz, 6H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 195.58, 152.90, 137.12, 46.35, 43.74, 41.80, 37.64, 33.46.

**Self-condensation of phenylacetaldehyde (Table V, Entry 6):**

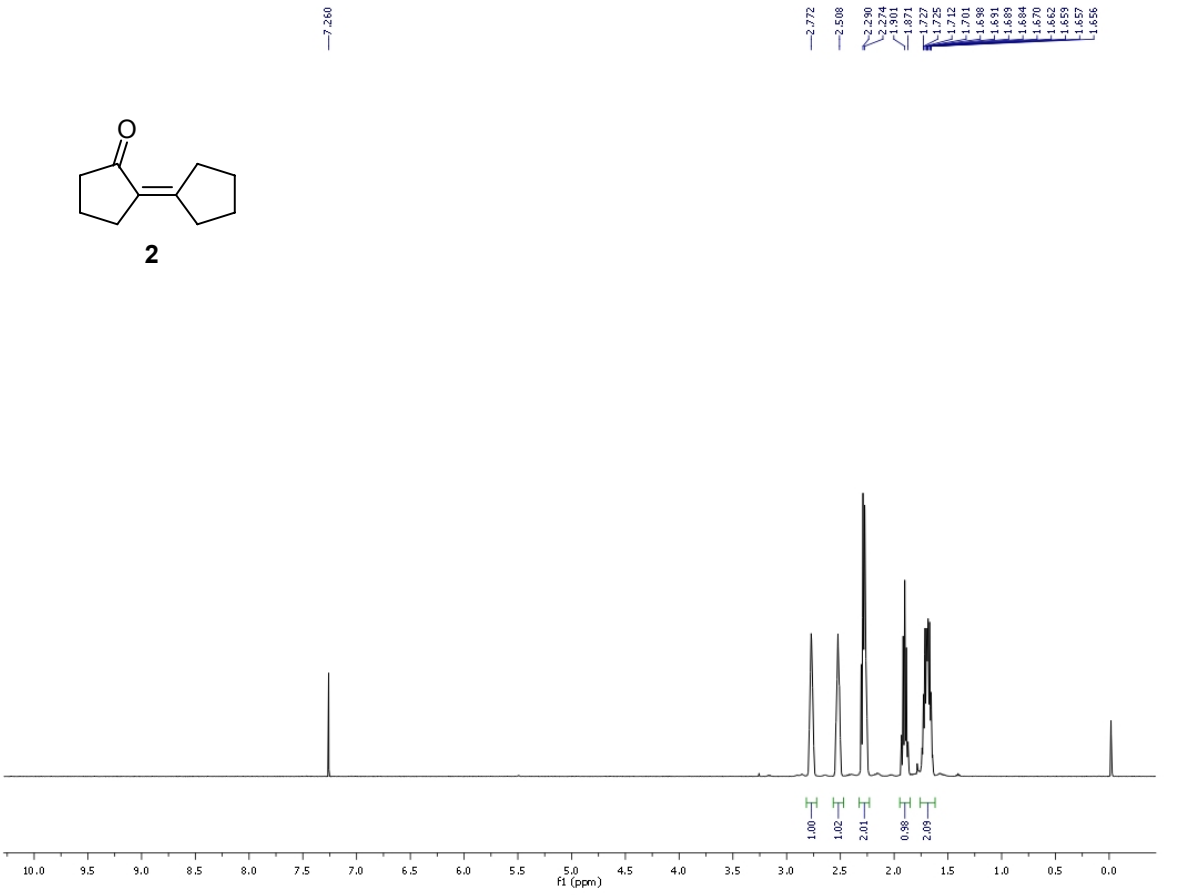
$^{1}$H NMR (500 MHz, $CDCl_3$): *ä* 9.45 (s, 1H), 7.30-7.10 (m, 10H), 6.65 (t, *J*=7.4, 1H), 3.42 (d, J=7 Hz, 2H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 195.07, 154.72, 142.66, 140.41, 128.88, 128.53, 128.40, 128.31, 128.25, 128.14, 126.32, 126.03, 35.01.

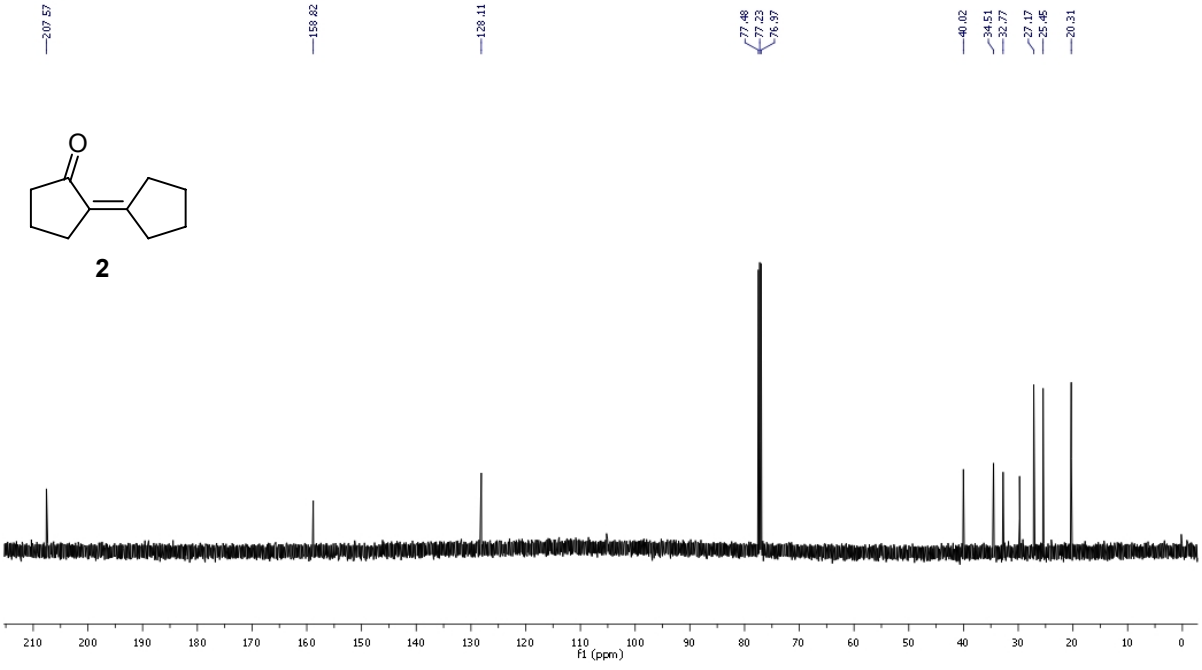
**Self-condensation of 3-phenyl propionaldehyde (Table V, Entry 7):**

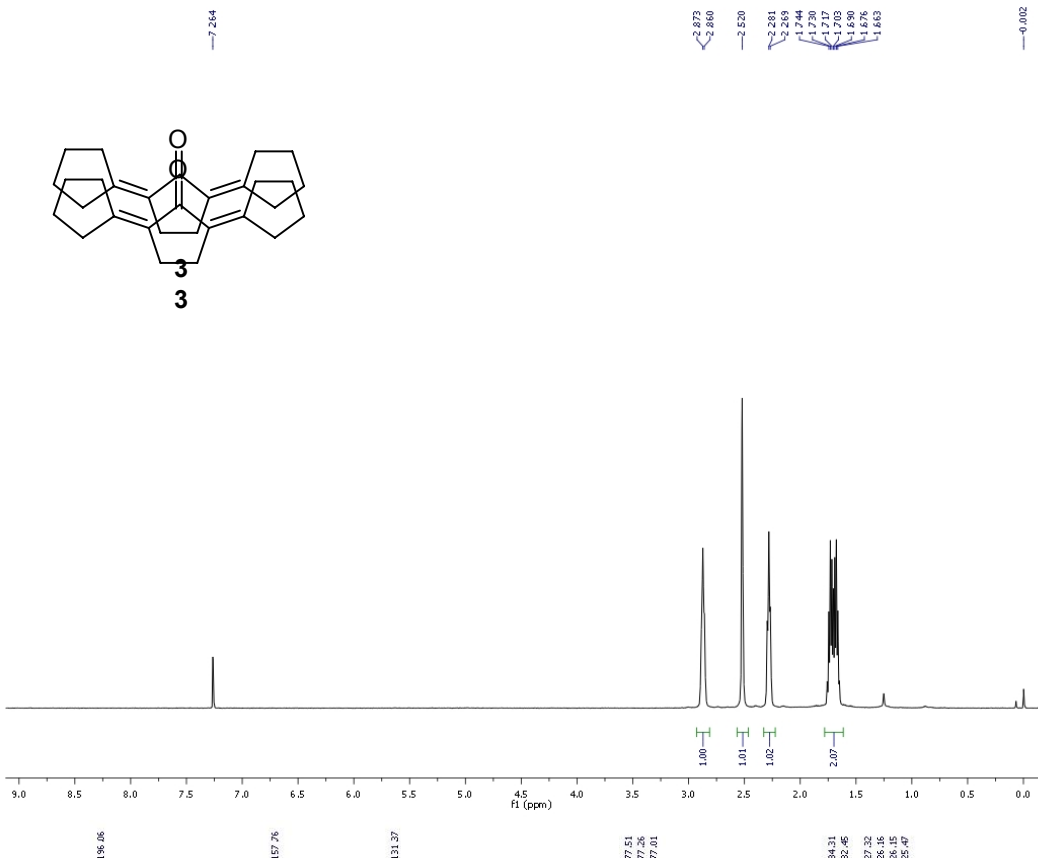
$^{1}$H NMR (500 MHz, $CDCl_3$): *ä* 9.45 (s, 1H), 7.32-7.10 (m, 10H), 6.65 (t, J=7.0, 1H), 3.58 (s, 2H), 2.80-2.70 (m, 4H); $^{13}$C NMR (125 MHz, $CDCl_3$): *ä* 194.80, 155.09, 142.69, 140.52, 139.03, 128.61, 128.55, 128.46, 128.30, 126.41, 126.24, 34.41, 31.10, 29.61.

**Note:** All the spectral data of self-condensation of aldehydes are consistent with the data given in *Green Chem.,* 2010, **12**, 384-386.

## Copies of $^{1}H$ and $^{13}C$ NMR spectra

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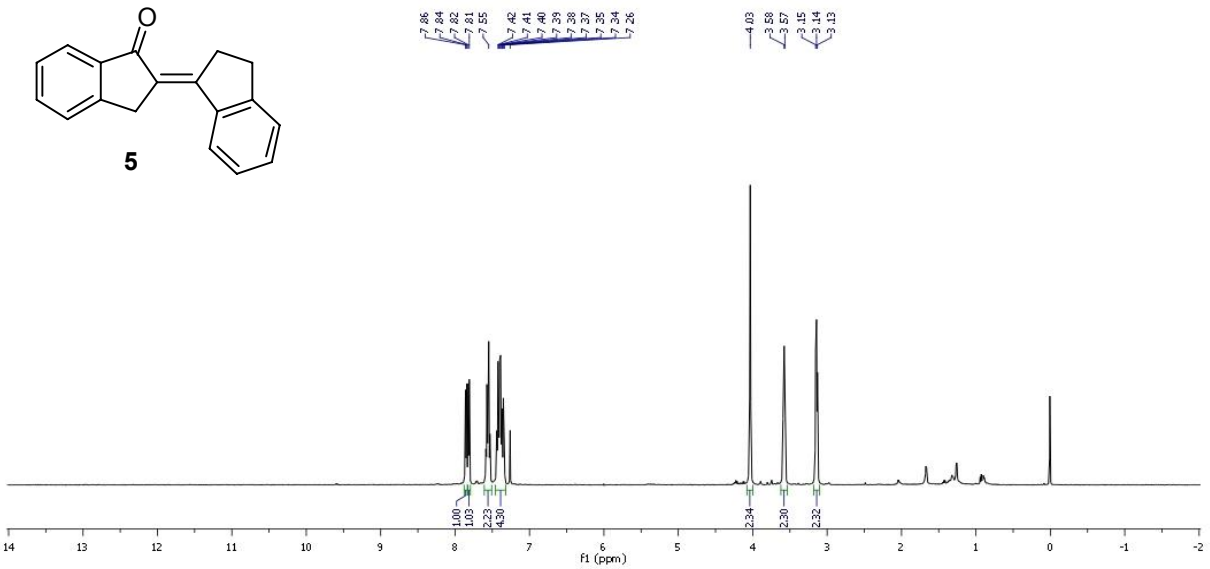
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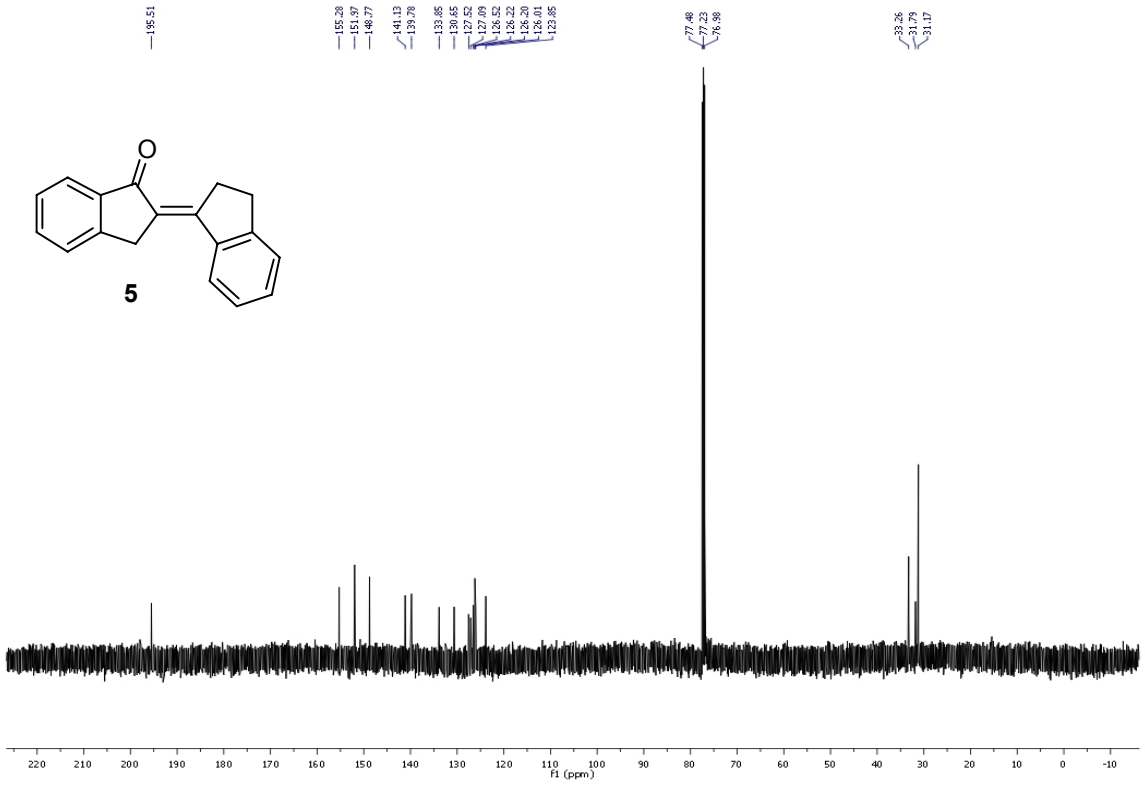
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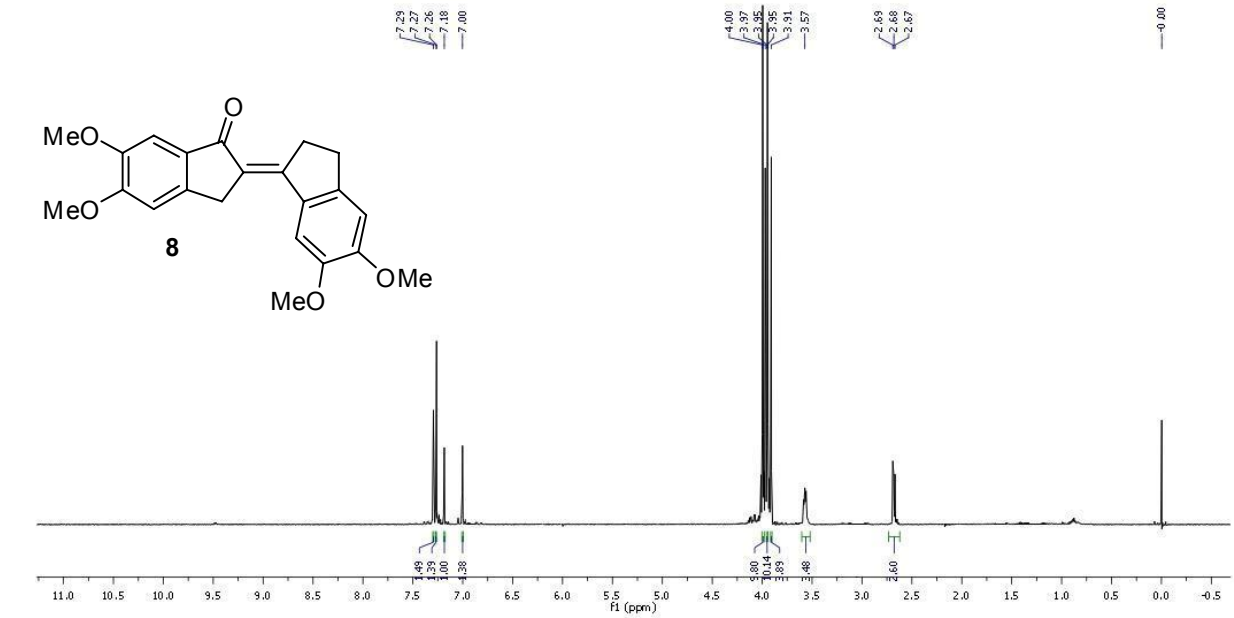
f1 (ppm)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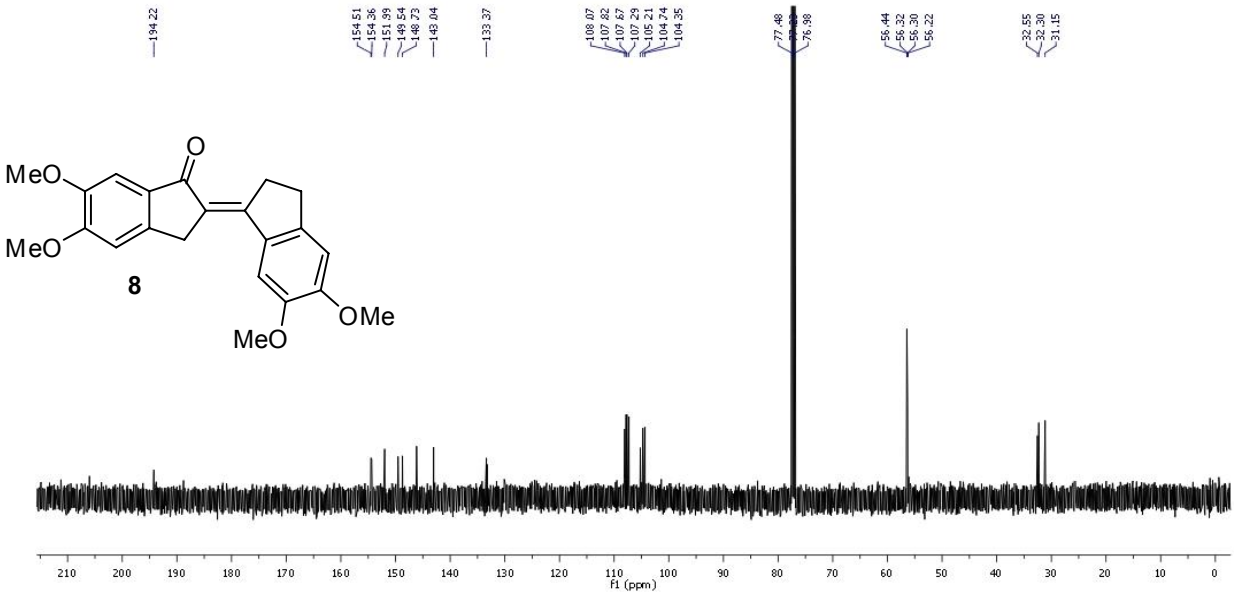
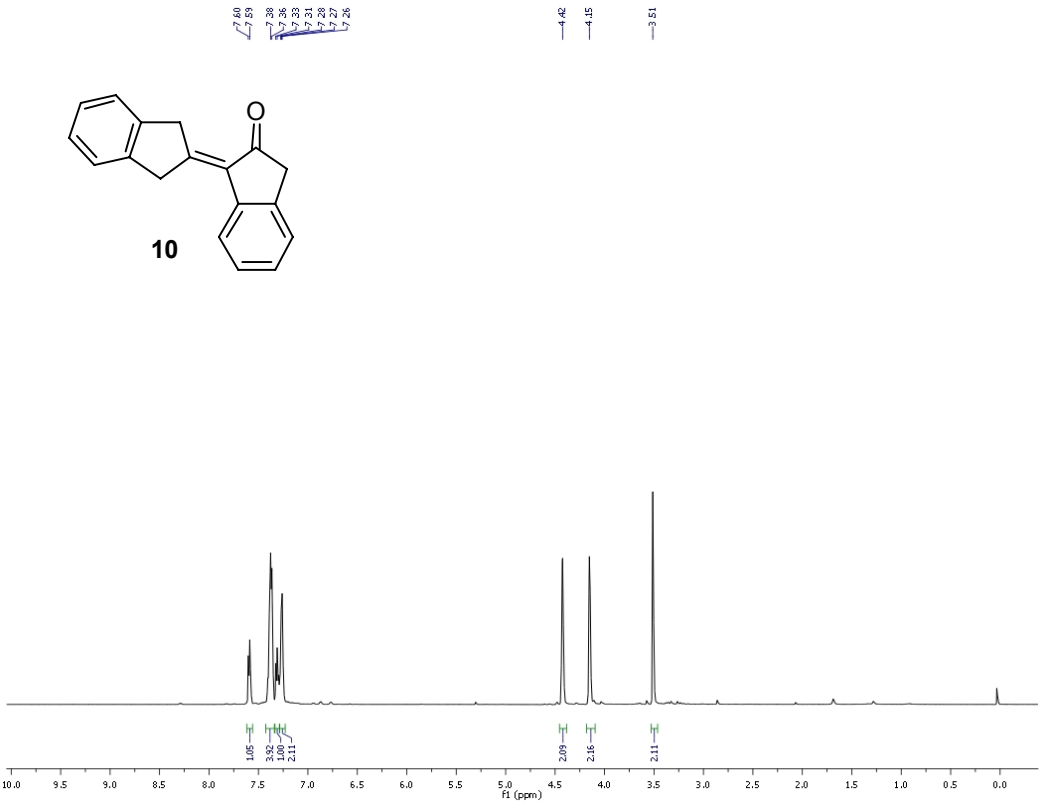
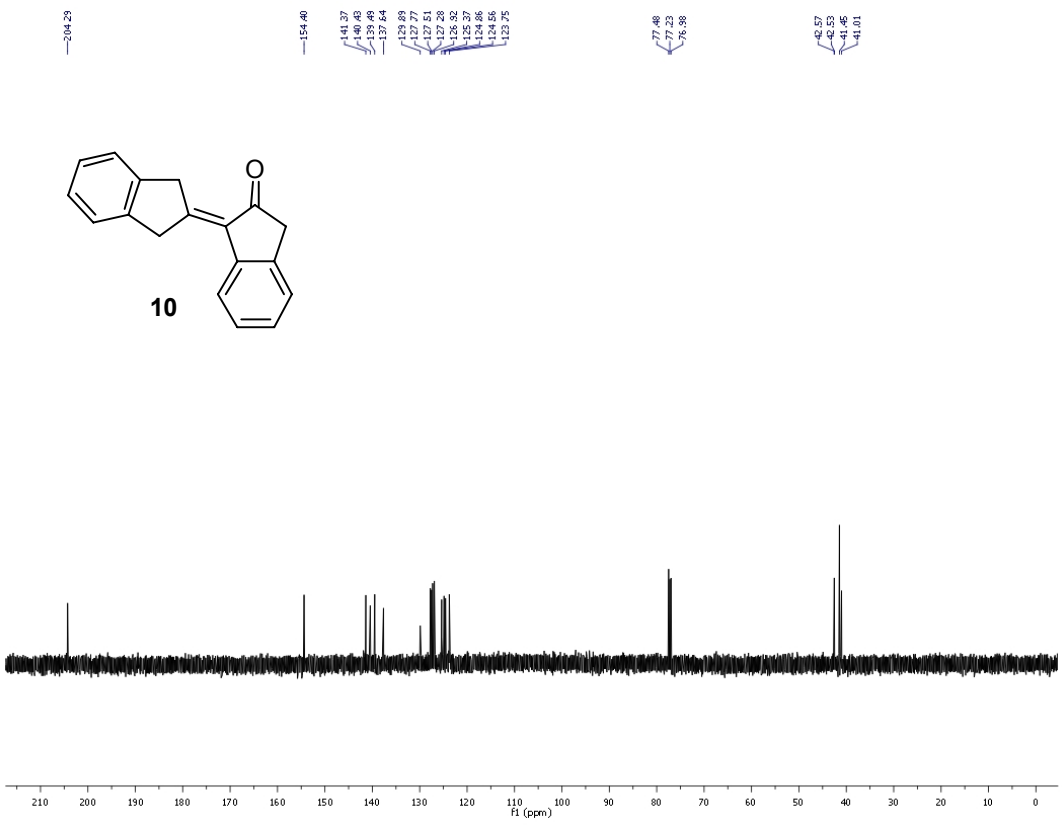
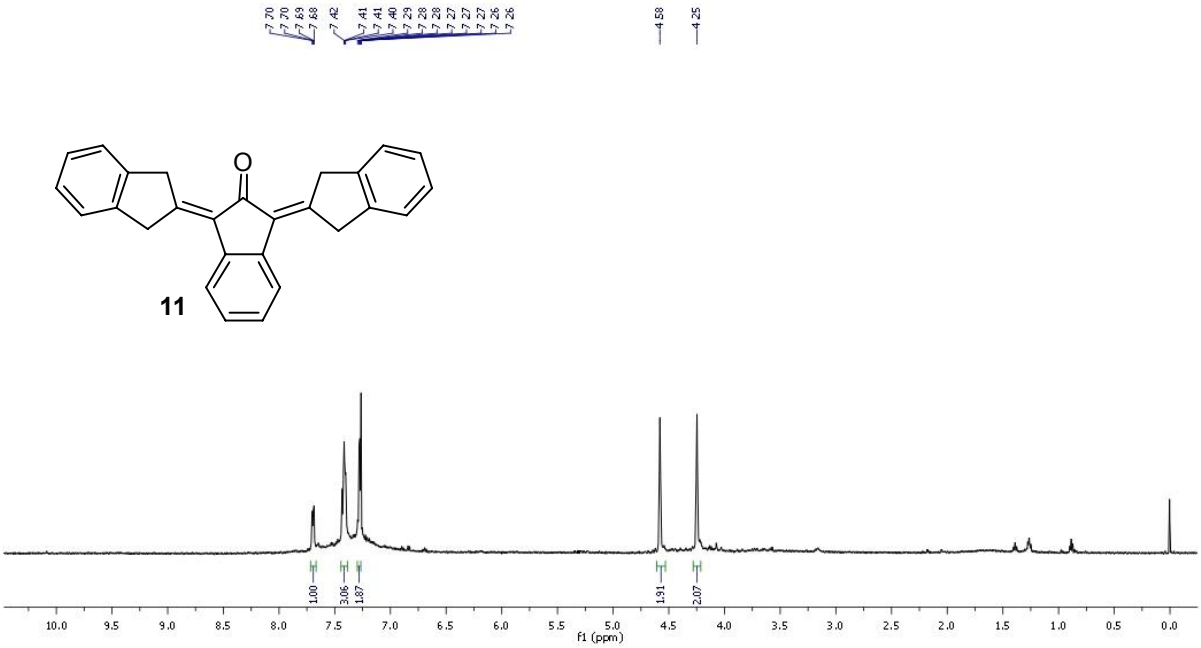
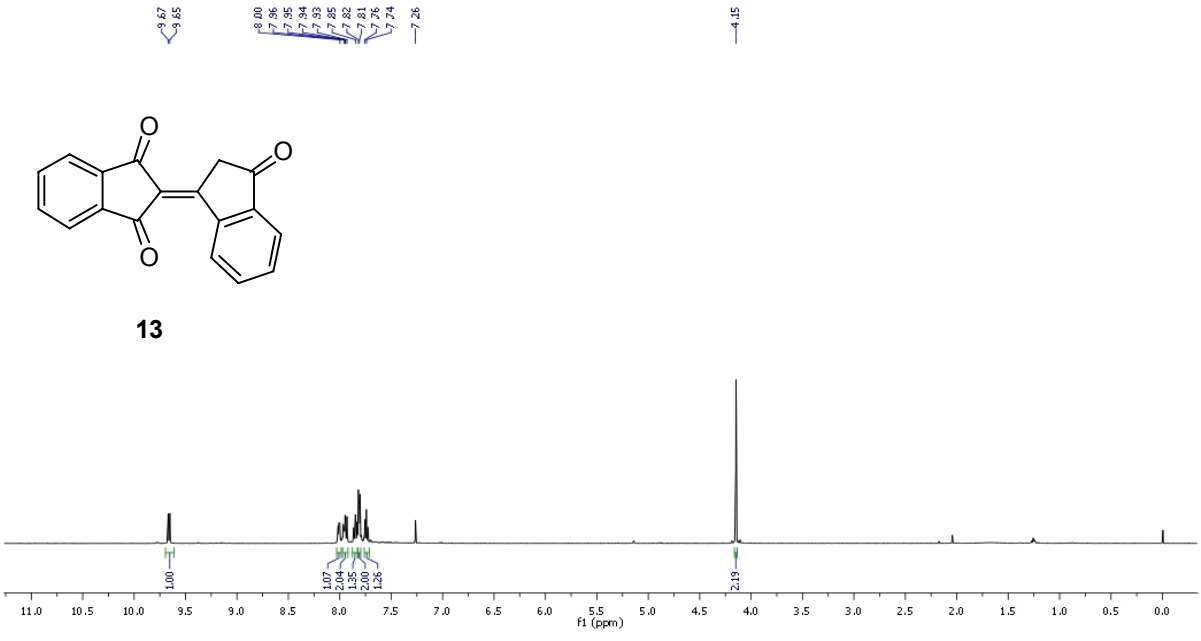
MeO
8

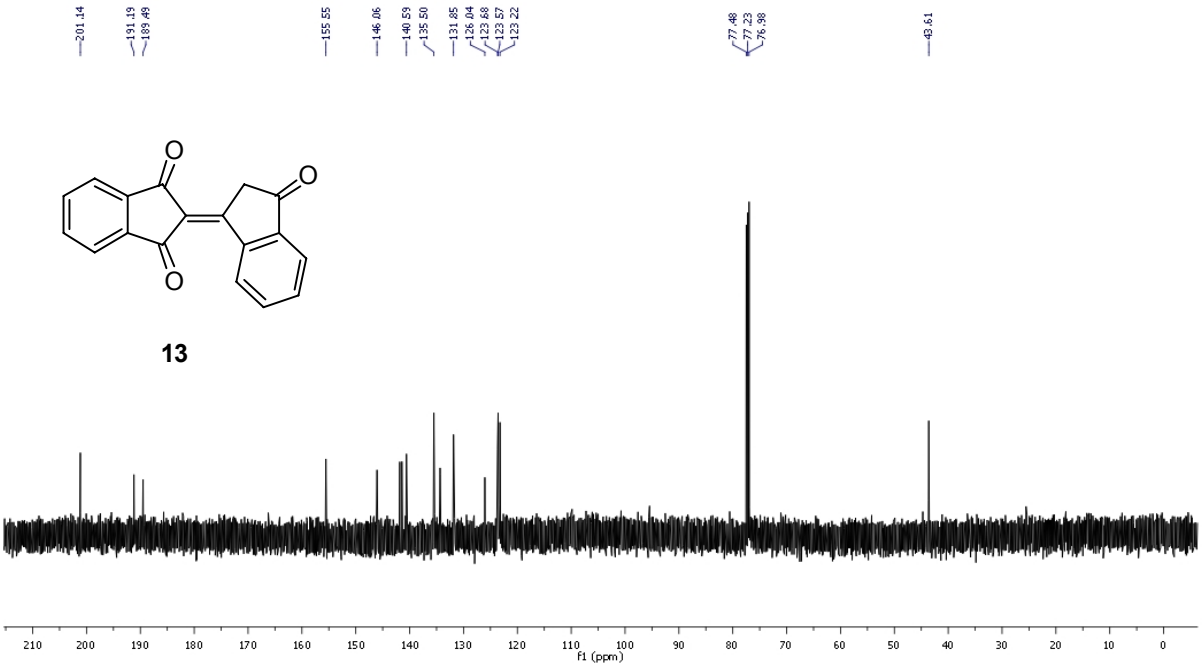

MeO
MeO
O
OMe
MeO
8

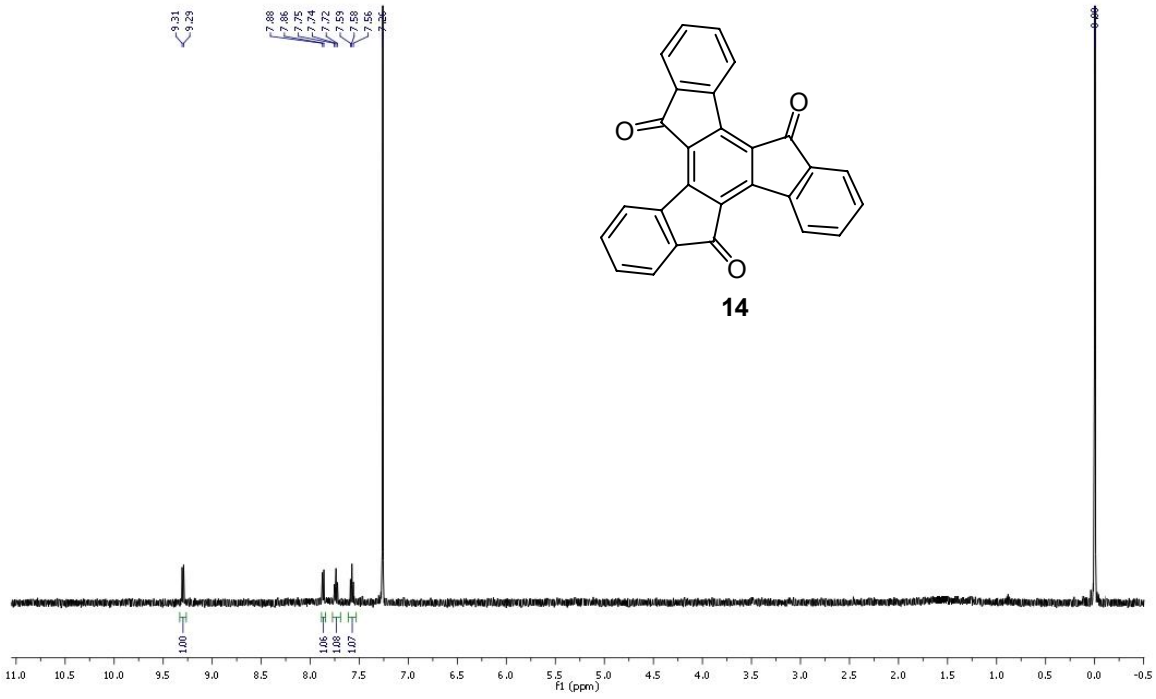

7.60
7.59
7.38
7.36
7.33
7.31
7.28
7.27
7.26
4.42
4.15
3.51
O
10
1.05
3.32
1.00
2.11
2.09
2.16
2.11
f1 (ppm)

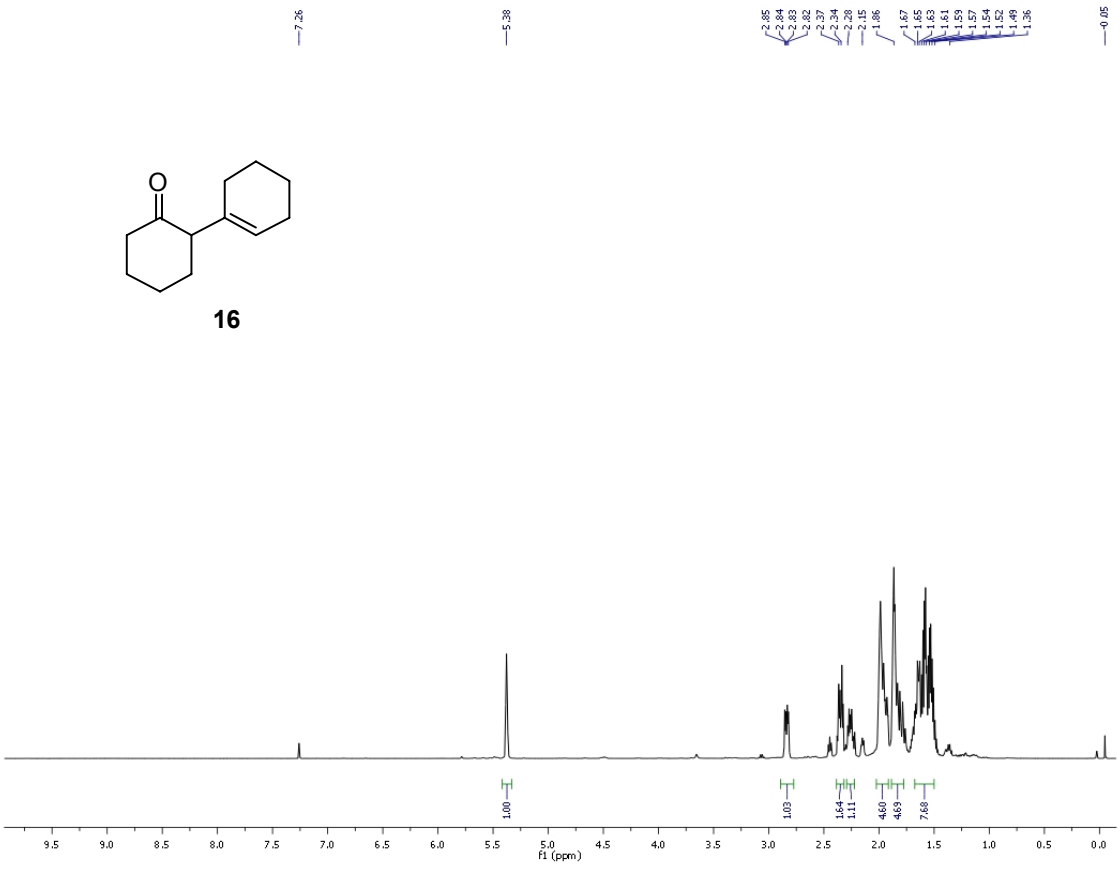

204.29
154.40
141.37
140.43
139.49
137.64
129.89
127.77
127.51
127.28
126.32
125.37
124.86
124.56
123.75
77.48
77.23
76.98
43.57
43.53
41.46
41.01
O
10
f1 (ppm)

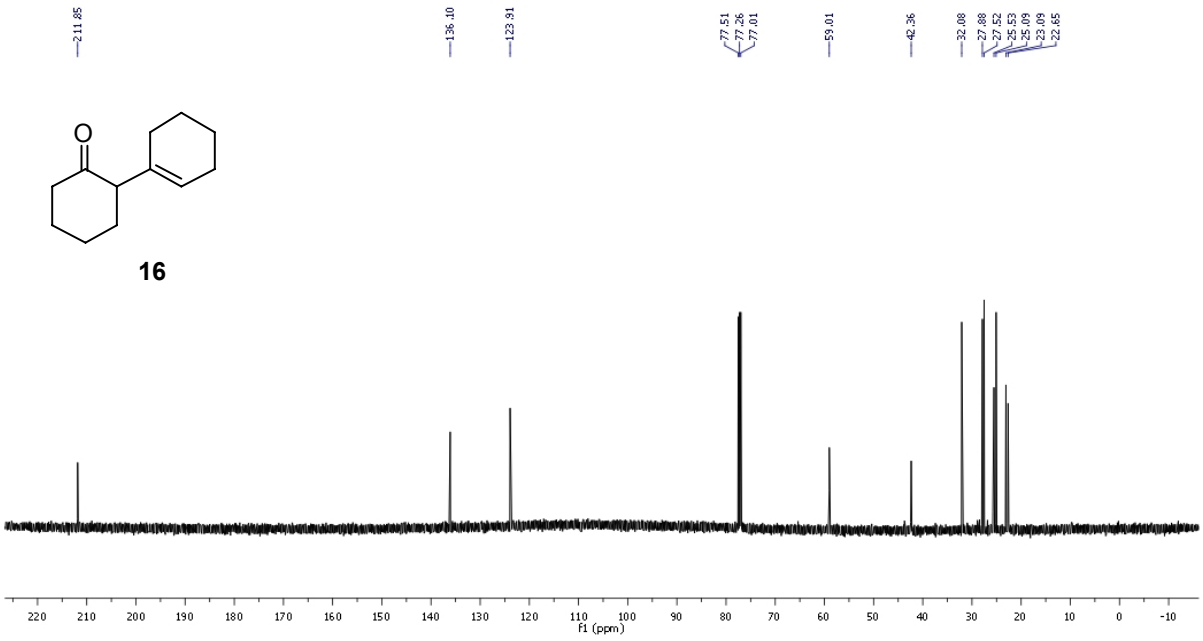

7.70
7.70
7.69
7.68
7.42
7.41
7.41
7.40
7.29
7.28
7.28
7.27
7.27
7.27
7.26
7.26
4.58
4.25
O
11
1.00
3.06
1.87
1.91
2.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

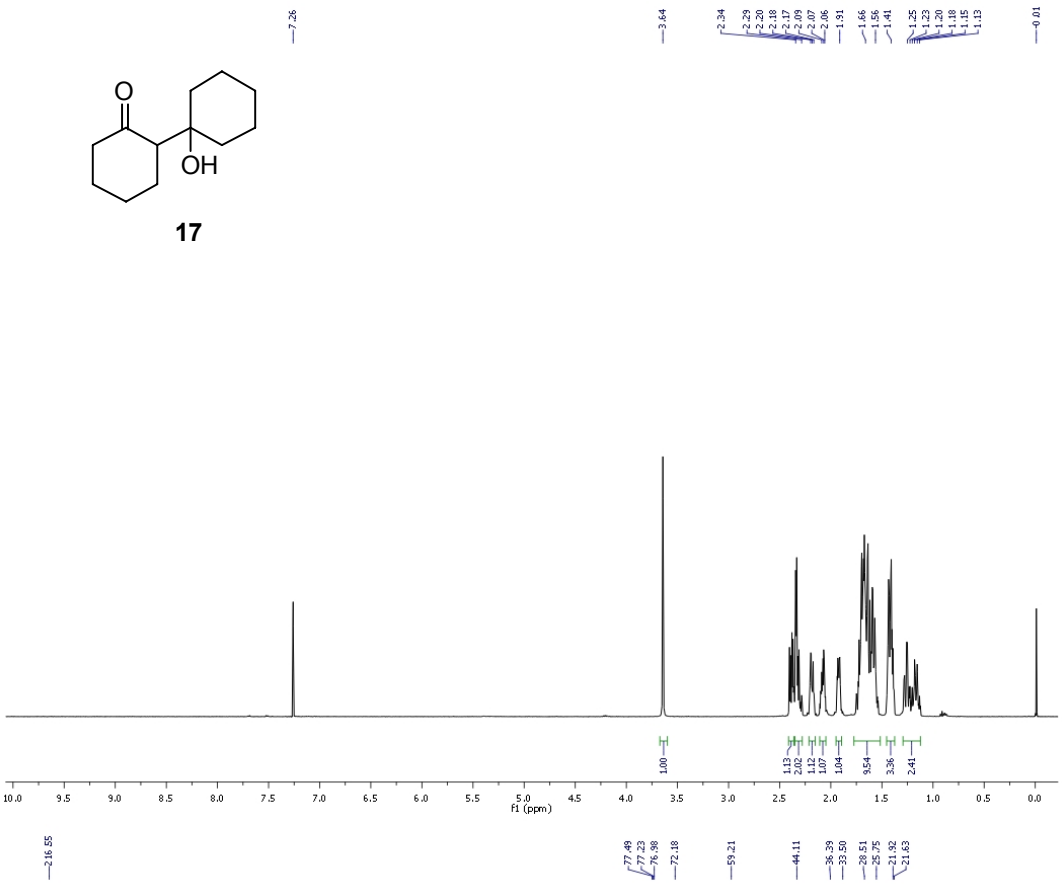

9.67
9.65
8.00
7.96
7.95
7.94
7.93
7.85
7.82
7.81
7.76
7.74
7.26
4.15
O
O
O
13
1.00
1.07
2.04
1.35
2.00
1.26
2.19
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


201.14
191.19
189.49
155.55
146.06
140.59
135.50
131.85
126.04
123.68
123.57
123.22
77.48
77.23
76.98
43.61
O
O
O
13
f1 (ppm)

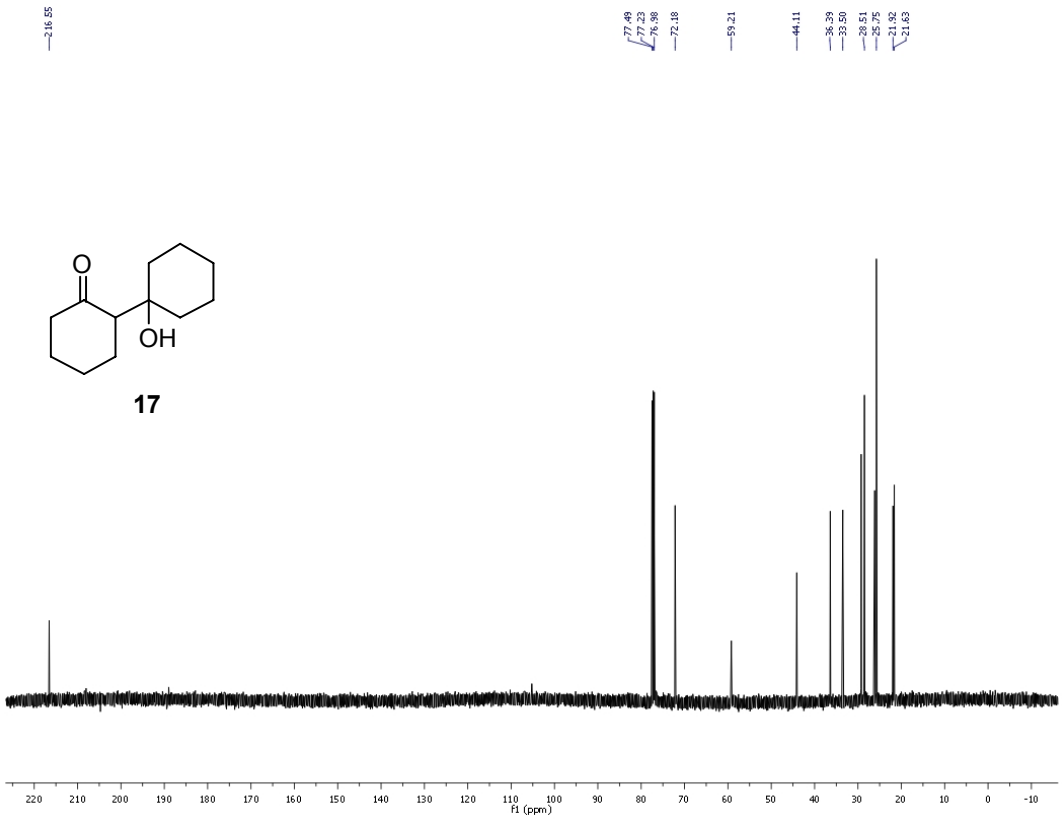

9.31
9.29
7.88
7.86
7.75
7.74
7.72
7.59
7.58
7.56
O
O
O
14
1.00
1.06
1.08
1.07
f1 (ppm)


7.26
5.38
2.85
2.84
2.83
2.82
2.37
2.34
2.28
2.15
1.86
1.67
1.65
1.63
1.61
1.59
1.57
1.54
1.52
1.49
1.36
0.05
O
16
1.00
1.03
1.64
1.11
4.60
4.63
7.68
f1 (ppm)

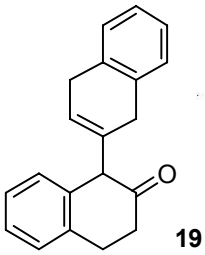

211.85
136.10
123.91
77.51
77.26
77.01
59.01
42.36
32.08
27.88
27.52
25.53
25.09
23.09
22.65
O
16
f1 (ppm)


7.26
3.64
2.34
2.29
2.20
2.18
2.17
2.09
2.07
2.06
1.91
1.66
1.56
1.41
1.25
1.23
1.20
1.18
1.15
1.13
0.01
O
OH
1.00
1.13
2.02
1.12
1.07
1.04
9.54
3.36
2.41
f1 (ppm)

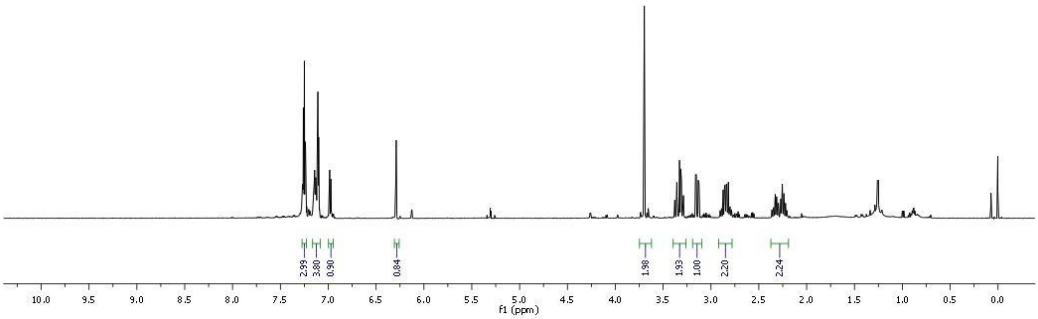
**17**

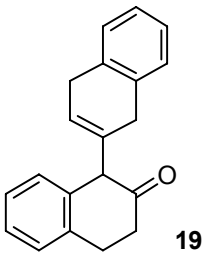

216.55
77.49
77.23
76.98
72.18
59.21
44.11
36.39
33.50
28.51
25.75
21.92
21.63
O
OH
f1 (ppm)

**17**

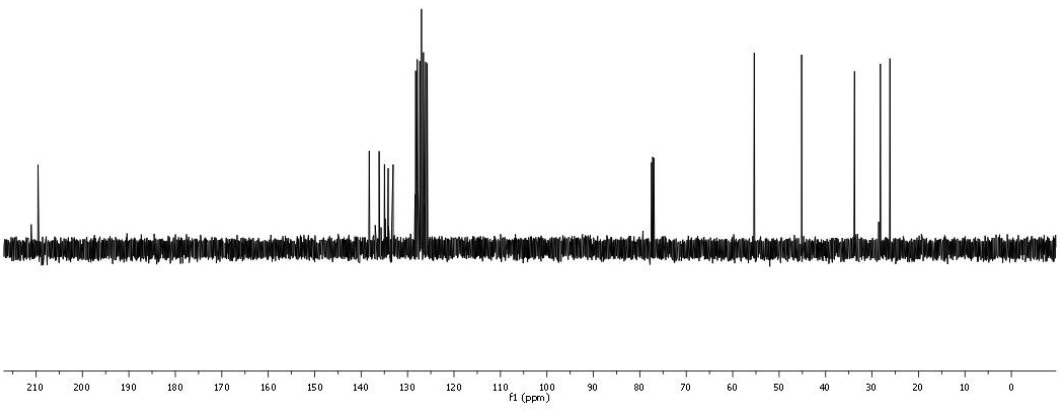


**19**





**19**



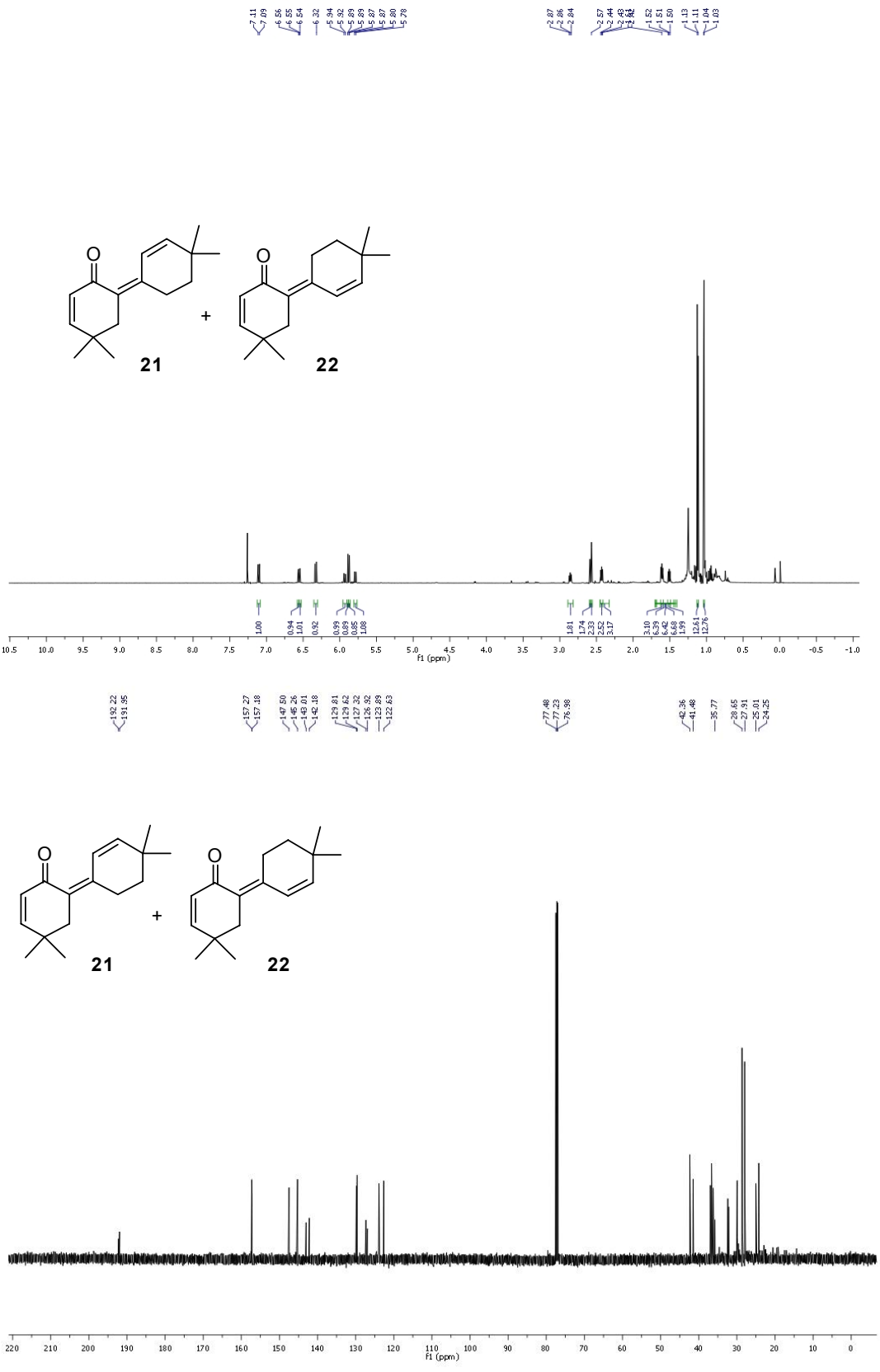

21
22
f1 (ppm)
f1 (ppm)

**Table V, entry 8**