Electronic Supplementary Information

Rhodium(II)-catalysed generation of cycloprop-1-en-1-yl ketones and their rearrangement to 5-aryl-2-siloxyfurans

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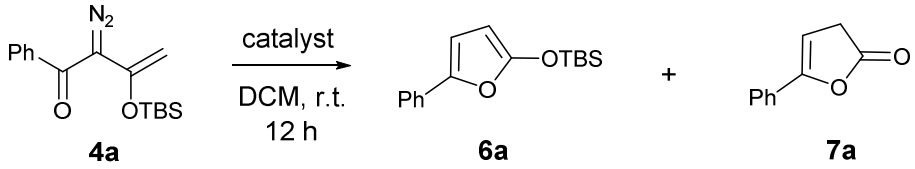
General information

All reactions, unless otherwise noted, were carried out in oven-dried (120 °C) glassware with magnetic stirring under an inert atmosphere of dry nitrogen. Tetrahydrofuran, dichloromethane, chloroform, and toluene were purified using a JC-Meyer solvent purification system. All other solvents were purified and dried using standard methods. Thin layer chromatography (TLC) was carried out using Dynamic Adsorbents precoated (0.25 mm, F254) silica gel plates. Column chromatography was performed on CombiFlash® Rf200 and Rf+ purification systems using normal phase disposable columns. Melting points were measured uncorrected from an Electro Thermo Mel-Temp DLX 104 device. High-resolution mass spectra (HRMS) were performed on a Bruker MicroTOF-ESI mass spectrometer with an ESI resource using CsI or LTQ ESI Positive Ion Calibration Solution as standard. Accurate masses were reported for the molecular ions $[M+H]^+$. ^{1}H NMR spectra were recorded in $CDCl_3$ (and CD_2Cl_2 for kinetic experiments) on a Bruker spectrometer (300 or 500 MHz) with residual $CHCl_3$ (δ 7.26 ppm), CH_2Cl_2 (δ 5.30 ppm), and H_2O (δ 1.56 ppm), as well as CD_3OD (δ CH_3OH 3.31 ppm). Chemical shifts (δ values) were reported in ppm downfield from the internal standard tetramethylsilane (TMS). Multiplicities are reported as: s (singlet); br (broad singlet); d (doublet); t (triplet); q (quartet); sep (septet); dd (doublet of doublets); ddd (doublet of doublet of doublets); dt and td (doublet of triplets or triplet of doublets); m (multiplet); comp (composite of magnetically nonequivalent protons). The number of protons (n) for a given resonance is reported as nH. Coupling constants (*J*) are given in Hertz (Hz). ^{13}C NMR spectra were recorded in $CDCl_3$ on a Bruker spectrometer at 75 or 126 MHz with the central resonance of $CDCl_3$ δ 77.16 or CD_3OD 49.00 ppm.

Materials

1-Arylbutane-1,3-diones – precursors for diazo compounds **1** were prepared according to the literature procedure.[1] 1-Phenylbutane-1,3-dione (benzoylacetone) – precursor for diazo compound **1a** was purchased from Sigma-Aldrich. All metal catalysts were purchased from Sigma-Aldrich or Strem and used without further purification. All the other chemicals were obtained from commercial sources and used as received.

Catalyst screening in transformation of 4a to 6a

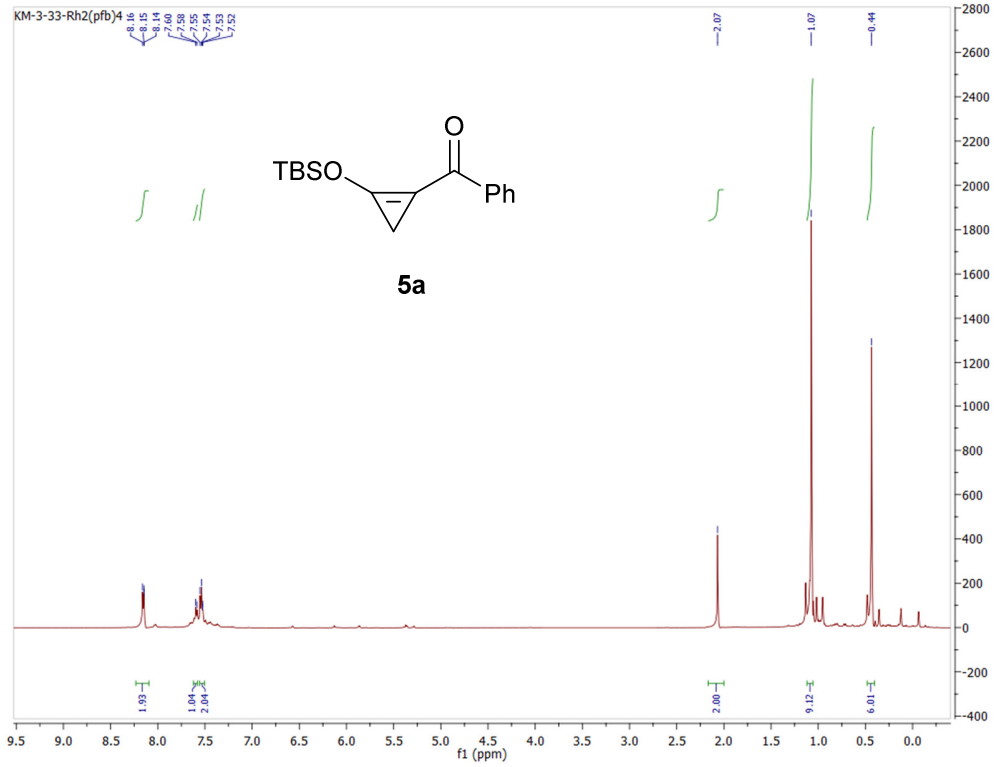


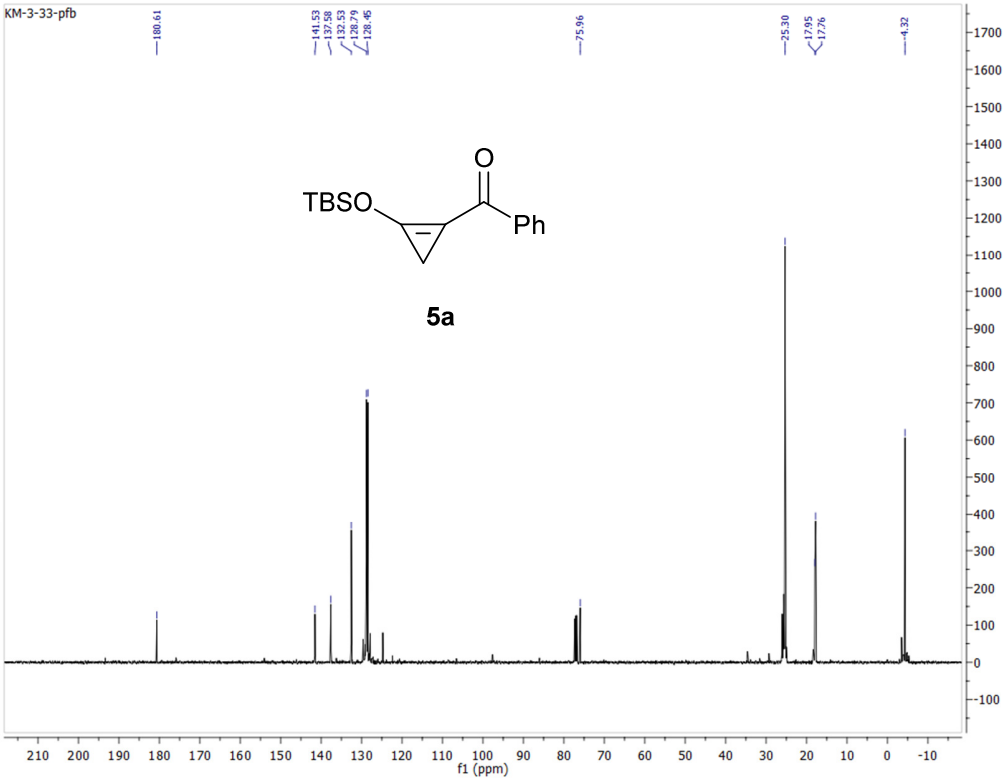
4a **6a** **7a**

Entry[a]	Catalyst	Conversion of **2a**, %	Yield **3a**, %	Yield **4**, %
1	1% $Rh_2(OAc)_4$	100	88	<5
2	1% $Rh_2(esp)_2$	100	90	<5
3	1% $Rh_2(oct)_4$	100	90	<5
4	0.5% $Rh_2(oct)_4$	100	91	<5
5	2% $Rh_2(oct)_4$	100	83	<5
6	1% $Rh_2(pfb)_4$	100	<5	<5
7	1% $Rh_2(tpa)_4$	100	<5	<5
8	2% $Rh_2(cap)_4$	35	12	<5
9	5% $Cu(MeCN)_4BF_4$	100	<5	<5
10	5% $Pd(PhCN)_2Cl_2$	73	34	22
11	5% [Ru(p-cymene)Cl_2]	55	26	<5
12	5% Au(JohnPhos)(MeCN)SbF_6	100	<5	<5
13	5% $AgBF_4$	100	<5	36
14	1% $Rh_2(pfb)_4$ then 5% $Sc(OTf)_3$	100	<5	58

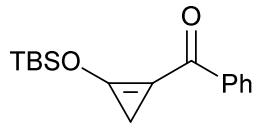
[a] Reactions were carried out on 0.1 mmol scale; conversion of **2a** and yield of **3a** were determined by ^{1}H NMR spectroscopy using 1,3,5-trimethoxybenzene as the internal standard.

Confirmation of cyclopropene 5a structure by NMR





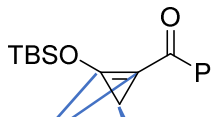
HSQC


O
TBSO
Ph

5a

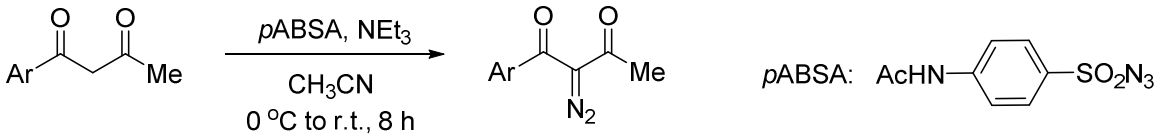
KM-3-33-pfb
f2 (ppm)
f1 (ppm)

HMBC


O
TBSO
Ph

KM-3-33-pfb
f2 (ppm)
f1 (ppm)

General procedure for the preparation of 1-aryl-2-diazobutane-1,3-diones 3

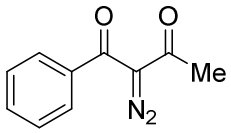


3

To an oven-dried round-bottom flask equipped with a magnetic stirring bar 1-arylbutane-1,3-dione (10 mmol) and *p*ABSA (2.9 g, 12 mmol) were added, and the system was filled with nitrogen. Acetonitrile (50 mL) was then added, and the reaction mixture was cooled to 0 °C using an ice-bath. Triethylamine (2.8 mL, 20 mmol) was added dropwise within 2 min; the reaction mixture was slowly warmed to room temperature, and allowed to stir for 8 h. A white precipitate of *N*-(4-sulfamoylphenyl)acetamide was filtered and washed with dicloromethane (2 x 10 mL). Solvents were evaporated, and diazo compound **3** was purified by column chromatography on silica gel with a 9:1 to 4:1 (v/v) gradient of hexane:ethyl acetate as eluents.

Characterization of 1-aryl-2-diazobutane-1,3-diones 3

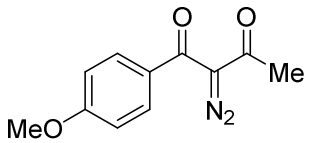
2-Diazo-1-phenylbutane-1,3-dione (3a)



3a

Known compound.[2] 1.65 g, 88% yield. Light yellow solid, mp 63.5–64.5 °C (62–63 °C lit.[2]). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (dd, *J* = 7.6, 1.3 Hz, 2H, *ortho*-Bz), 7.59 (t, *J* = 7.6 Hz, 1H, *para*-Bz), 7.50 (t, *J* = 7.6 Hz, 2H, *meta*-Bz), 2.58 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.8, 185.1, 137.3, 132.7, 128.9, 127.3, 83.7, 29.2. HRMS (ESI) *m/z* calcd for $C_{10}H_9N_2O_2$ $[M+H]^+$ 189.0659, found: 189.0659.

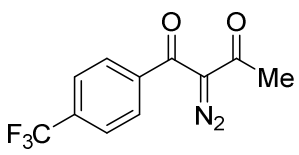
2-Diazo-1-(4-methoxyphenyl)butane-1,3-dione (3d)



3d

Known compound.[2] 1.81 g, 83% yield. Light yellow solid, mp 63–64 °C (63–64 °C lit.[2]). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.8 Hz, 2H, Ar), 6.97 (d, *J* = 8.8 Hz, 2H, Ar), 3.88 (s, 3H, OMe), 2.56 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.1, 183.8, 163.3, 129.8, 129.7, 114.1, 82.8, 55.5, 29.0. HRMS (ESI) *m/z* calcd for $C_{11}H_{11}N_2O_3$ $[M+H]^+$ 219.0764, found: 219.0761.

2-Diazo-1-[4-(trifluoromethyl)phenyl]butane-1,3-dione (3e)

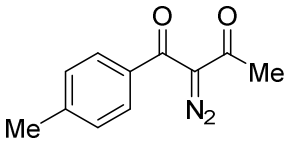


3e

1.95 g, 76% yield. Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.81 – 7.73 (comp, 4H, Ar), 2.59 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 189.8, 183.9, 140.4, 134.1 (q, *J* = 32.9 Hz, C-CF_3), 127.8, 126.0 (dd, *J* = 6.9, 3.4

Hz), 123.4 (q, *J* = 272.8 Hz, CF_3), 84.1, 29.2. HRMS (ESI) *m/z* calcd for $C_{11}H_8F_3N_2O_2$ $[M+H]^+$ 257.0532, found: 257.0534.

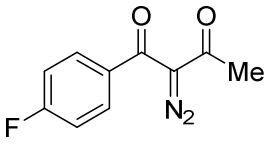
2-Diazo-1-(*p*-tolyl)butane-1,3-dione (3f)



3f

Known compound.[2] 1.82 g, 90% yield. Light yellow solid, mp 74–75 °C (75–76 °C lit.[2]). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 8.1 Hz, 2H, Ar), 7.30 (d, *J* = 8.1 Hz, 2H, Ar), 2.58 (s, 3H, Me-CO), 2.44 (s, 3H, Me-Ar). ^{13}C NMR (126 MHz, $CDCl_3$) δ 191.0, 184.8, 143.6, 134.6, 129.5, 127.5, 83.4, 29.2, 21.6. HRMS (ESI) *m/z* calcd for $C_{11}H_{11}N_2O_2$ $[M+H]^+$ 203.0815, found: 203.0812.

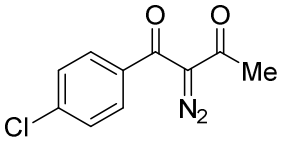
2-Diazo-1-(4-fluorophenyl)butane-1,3-dione (3g)



3g

1.69 g, 82% yield. Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 (dd, *J* = 8.8, 5.2 Hz, 2H, *ortho*-Bz), 7.19 (t, *J* = 8.8 Hz, 2H, H-C-C-F), 2.57 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.4, 183.7, 165.2 (d, *J* = 254.6 Hz, C-F), 133.5 (d, *J* = 3.0 Hz), 130.0 (d, *J* = 9.2 Hz), 116.2 (d, *J* = 22.1 Hz), 83.4, 29.1. HRMS (ESI) *m/z* calcd for $C_{10}H_8FN_2O_2$ $[M+H]^+$ 207.0564, found: 207.0566.

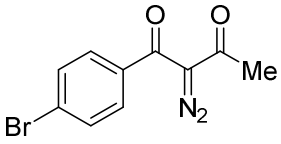
1-(4-Chlorophenyl)-2-diazobutane-1,3-dione (3h)



3h

1.91 g, 86% yield. Light yellow solid, mp 59–60 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.6 Hz, 2H, Ar), 7.50 (d, *J* = 8.6 Hz, 2H, Ar), 2.59 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.3, 183.8, 139.1, 135.6, 129.3, 128.9, 83.6, 29.2. HRMS (ESI) *m/z* calcd for $C_{10}H_8ClN_2O_2$ $[M+H]^+$ 223.0269, found: 223.0267.

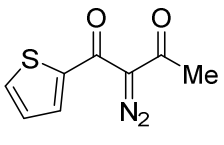
1-(4-Bromophenyl)-2-diazobutane-1,3-dione (3i)



3i

Known compound.[2] 2.37 g, 89% yield. Light yellow solid, mp 77–78 °C (76–77 °C lit.[2]). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 2H, Ar), 7.52 (d, *J* = 8.4 Hz, 2H, Ar), 2.56 (s, 3H, Me). ^{13}C NMR (75 MHz, $CDCl_3$) δ 190.2, 183.9, 136.0, 132.2, 129.0, 127.5, 83.8, 29.2. HRMS (ESI) *m/z* calcd for $C_{10}H_8BrN_2O_2$ $[M+H]^+$ 266.9764, found: 266.9763.

2-Diazo-1-(thiophen-2-yl)butane-1,3-dione (3j)

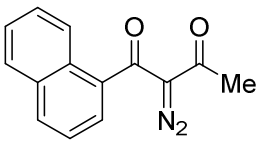


3j

1.51 g, 78% yield. Light yellow solid, mp 56–57.5 °C. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.71 (dd, *J* = 5.0, 1.0 Hz, 1H, Ar), 7.62 (dd, *J* = 3.8, 1.0 Hz, 1H, Ar), 7.17 (dd, *J* = 5.0, 3.8 Hz, 1H, Ar), 2.62 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$)

δ 190.8, 175.1, 141.9, 133.5, 130.5, 127.9, 81.7, 29.3. HRMS (ESI) *m/z* calcd for $C_8H_7N_2O_2S$ $[M+H]^+$ 195.0223, found: 195.0222.

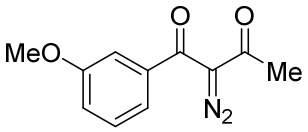
2-Diazo-1-(naphthalen-1-yl)butane-1,3-dione (3k)



3k

2.02 g, 85% yield. Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.08 (d, *J* = 8.2 Hz, 1H, Ar), 8.02 (d, *J* = 8.2 Hz, 1H, Ar), 7.97 – 7.92 (m, 1H, Ar), 7.64 – 7.57 (comp, 3H, Ar), 7.57 – 7.52 (m, 1H, Ar), 2.62 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.3, 186.0, 135.3, 133.8, 131.8, 129.5, 128.7, 127.9, 127.0, 125.0, 124.7, 124.3, 87.5, 29.4. HRMS (ESI) *m/z* calcd for $C_{14}H_{11}N_2O_2$ $[M+H]^+$ 239.0815, found: 239.0815.

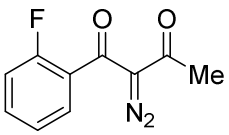
2-Diazo-1-(3-methoxyphenyl)butane-1,3-dione (3l)



3l

1.92 g, 88% yield. Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.43 – 7.36 (m, 1H, Ar), 7.24 – 7.19 (m, 1H, Ar), 7.17 – 7.15 (m, 1H, Ar), 7.12 (d, *J* = 8.3 Hz, 1H), 3.86 (s, 3H, OMe), 2.58 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.8, 184.8, 160.0, 138.6, 129.9, 119.4, 118.8, 112.3, 83.8, 55.5, 29.2. HRMS (ESI) *m/z* calcd for $C_{11}H_{11}N_2O_3$ $[M+H]^+$ 219.0764, found: 219.0764.

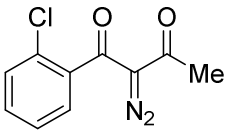
2-Diazo-1-(2-fluorophenyl)butane-1,3-dione (3m)



3m

1.52 g, 74% yield. Yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.59 – 7.52 (comp, 2H, Ar), 7.30 (td, *J* = 7.6, 0.7 Hz, 1H, Ar), 7.21 – 7.15 (m, 1H, Ar), 2.59 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 189.8, 180.9, 158.9 (d, *J* = 250.4 Hz, C-F), 133.9 (d, *J* = 8.6 Hz), 130.0 (d, *J* = 2.3 Hz), 125.9 (d, *J* = 15.3 Hz), 125.2 (d, *J* = 3.3 Hz), 116.3 (d, *J* = 22.0 Hz), 86.8, 29.3. HRMS (ESI) *m/z* calcd for $C_{10}H_8FN_2O_2$ $[M+H]^+$ 207.0564, found: 207.0566.

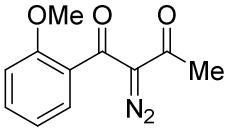
1-(2-Chlorophenyl)-2-diazobutane-1,3-dione (3n)



3n

1.82 g, 82% yield. Light yellow solid, mp 64–65 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 – 7.44 (comp, 2H, Ar), 7.42 – 7.37 (comp, 2H, Ar), 2.53 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 189.5, 183.4, 137.3, 132.1, 130.2, 128.3, 127.5, 87.4, 29.1. HRMS (ESI) *m/z* calcd for $C_{10}H_8ClN_2O_2$ $[M+H]^+$ 223.0269, found: 223.0264.

2-Diazo-1-(2-methoxyphenyl)butane-1,3-dione (3o)

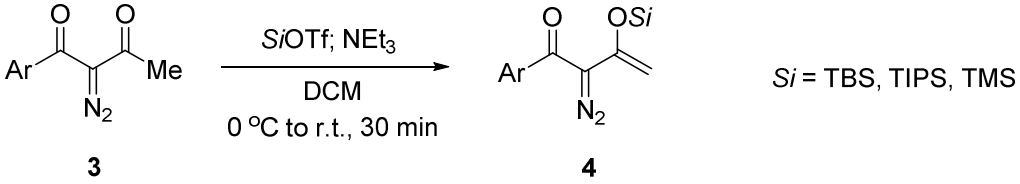


3o

1.85 g, 85% yield. Light yellow solid, mp 65.5–67 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (td, *J* = 7.5, 1.7 Hz, 1H, Ar), 7.44 (dd, *J* = 7.5, 1.7 Hz, 1H, Ar),

7.08 (td, *J* = 7.5, 1.7 Hz, 1H, Ar), 6.98 (dd, *J* = 7.5, 1.7 Hz, 1H, Ar), 3.90 (s, 3H, OMe), 2.59 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 190.8, 184.0, 156.1, 133.1, 129.6, 127.5, 121.4, 111.2, 87.2, 55.8, 29.3. HRMS (ESI) *m/z* calcd for $C_{11}H_{11}N_2O_3$ $[M+H]^+$ 219.0764, found: 219.0765.

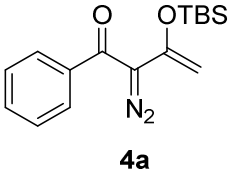
General procedure for the synthesis of enoldiazoketones 4



An oven-dried round-bottom flask equipped with a magnetic stirring bar was loaded with diazo compound **3** (3.0 mmol), and the system was filled with nitrogen. Dichloromethane (15 mL) was then added, and the reaction mixture was cooled to 0 °C using an ice-bath. Triethylamine (0.7 mL, 5.1 mmol) was added in one portion followed by a dropwise addition of trialkylsilyl trifluoromethanesulfonate (3.6 mmol). The ice-bath was removed, and the reaction mixture was allowed to stir for 30 min. Dichloromethane was evaporated, the residue was dissolved in hexane (15 mL), and loaded to a silica gel column treated with a 3% (v/v) solution of triethylamine in hexane (a column was purged with 300 mL of the solution). Enoldiazo compound **4** was eluted with a 19:1 to 9:1 (v/v) gradient of hexane:ethyl acetate, and isolated as an orange to red colored oil (unless otherwise noted). Products are hydrolytically unstable, and must be stored below 0 °C.

Characterization of enoldiazoketones 4

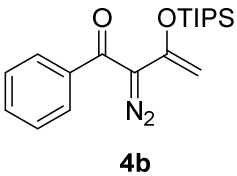
3-[(*tert*-Butyldimethylsilyl)oxy]-2-diazo-1-phenylbut-3-en-1-one (4a)



4a

788 mg, 87% yield. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.64 (dd, *J* = 8.3, 1.3 Hz, 2H, *ortho*-Bz), 7.58 – 7.53 (m, 1H, *para*-Bz), 7.51 – 7.46 (m, 2H, *meta*-Bz), 5.21 (d, *J* = 2.0 Hz, 1H, $=CH_2$), 4.49 (d, *J* = 2.0 Hz, 1H, $=CH_2$), 0.96 (s, 9H, *t*-Bu), 0.30 (s, 6H, Me). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 187.3, 141.5, 138.2, 131.5, 128.5, 127.3, 92.9, 25.3, 18.0, -5.1. HRMS (ESI) *m/z* calcd for $C_{16}H_{23}N_2O_2Si$ $[M+H]^+$ 303.1523, found: 303.1520.

2-Diazo-1-phenyl-3-[(triisopropylsilyl)oxy]but-3-en-1-one (4b)

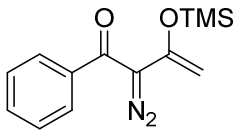


4b

929 mg, 90% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 7.4 Hz, 2H, *ortho*-Bz), 7.51 (t, *J* = 7.4 Hz, 1H, *para*-Bz), 7.44 (t, *J* = 7.4 Hz, 2H, *meta*-Bz), 5.22 (d, *J* = 2.1 Hz, 1H, $=CH_2$), 4.48 (d, *J* = 2.1 Hz, 1H, $=CH_2$), 1.27 (sep, *J* = 7.5 Hz, 3H, C<u>H</u>-Me), 1.13 (d, *J* = 7.5 Hz, 18H, <u>Me</u>-CH). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.7, 141.37, 138.2, 131.6, 128.5, 127.4, 92.7, 18.0, 12.7. HRMS

(ESI) *m/z* calcd for $C_{19}H_{29}N_2O_2Si$ $[M+H]^+$ 345.1993, found: 345.1990.

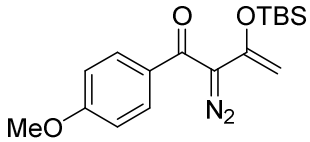
2-Diazo-1-phenyl-3-[(trimethylsilyl)oxy]but-3-en-1-one (4c)



4c

530 mg, 68% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.61 (d, *J* = 7.5 Hz, 2H, *ortho*-Bz), 7.51 (t, *J* = 7.5 Hz, 1H, *para*-Bz), 7.44 (t, *J* = 7.5 Hz, 2H, *meta*-Bz), 5.21 (d, *J* = 2.0 Hz, 1H, =CH_2), 4.47 (d, *J* = 2.0 Hz, 1H, =CH_2), 0.27 (s, 9H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.6, 141.2, 138.2, 131.6, 128.5, 127.3, 93.4, -0.2. HRMS (ESI) *m/z* calcd for $C_{13}H_{17}N_2O_2Si$ $[M+H]^+$ 261.1059, found: 261.1057.

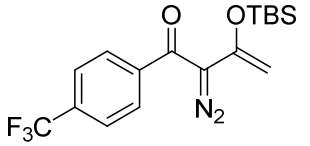
3-[(*tert*-Butyldimethylsilyl)oxy]-2-diazo-1-(4-methoxyphenyl)but-3-en-1-one (4d)



4d

897 mg, 90% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.64 (d, *J* = 8.8 Hz, 2H, Ar), 6.93 (d, *J* = 8.8 Hz, 2H, Ar), 5.16 (d, *J* = 2.0 Hz, 1H, =CH_2), 4.45 (d, *J* = 2.0 Hz, 1H, =CH_2), 3.87 (s, 3H, OMe), 0.93 (s, 9H, *t*-Bu), 0.26 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.6, 162.4, 141.7, 130.6, 129.6, 113.7, 93.2, 55.4, 25.6, 18.1, -4.8. HRMS (ESI) *m/z* calcd for $C_{17}H_{25}N_2O_3Si$ $[M+H]^+$ 333.1629, found: 333.1623.

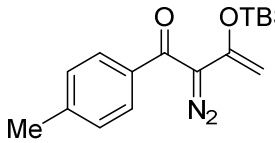
3-[(*tert*-Butyldimethylsilyl)oxy]-2-diazo-1-[4-(trifluoromethyl)phenyl]but-3-en-1-one (4e)



4e

955 mg, 86% yield. Light orange solid, mp 56.5–58 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.76 – 7.71 (comp, 4H, Ar), 5.13 (br, 1H, =CH_2), 4.48 (d, *J* = 2.2 Hz, 1H, =CH_2), 0.91 (s, 9H, *t*-Bu), 0.26 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.2, 141.16, 141.11, 133.2 (q, *J* = 32.8 Hz), 127.8, 125.6 (q, *J* = 3.6 Hz), 123.6 (q, *J* = 272.6 Hz, C-F), 93.7, 25.5, 18.1, -4.8. HRMS (ESI) *m/z* calcd for $C_{17}H_{22}F_3N_2O_2Si$ $[M+H]^+$ 371.1397, found: 371.1388.

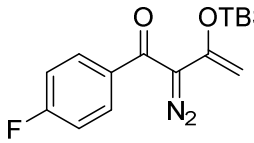
3-[(*tert*-Butyldimethylsilyl)oxy]-2-diazo-1-(*p*-tolyl)but-3-en-1-one (4f)



4f

872 mg, 92% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 8.1 Hz, 2H, Ar), 7.24 (d, *J* = 8.1 Hz, 2H, Ar), 5.22 (d, *J* = 1.9 Hz, 1H, =CH_2), 4.45 (d, *J* = 1.9 Hz, 1H, =CH_2), 2.41 (s, 3H, Me-Ar), 0.93 (s, 9H, *t*-Bu), 0.27 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.5, 142.2, 141.4, 135.4, 129.1, 127.5, 93.1, 25.6, 21.6, 18.1, -4.8. HRMS (ESI) *m/z* calcd for $C_{17}H_{25}N_2O_2Si$ $[M+H]^+$ 317.1685, found: 317.1683.

3-[(*tert*-Butyldimethylsilyl)oxy]-2-diazo-1-(4-fluorophenyl)but-3-en-1-one (4g)

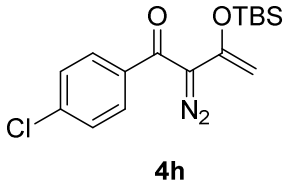


4g

884 mg, 92% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (dd, *J* = 8.7, 5.3 Hz, 2H, *ortho*-Bz), 7.13 (t, *J* = 8.7 Hz, 2H, H-C-C-F), 5.13 (d, *J* = 2.0 Hz, 1H,

=CH_2), 4.46 (d, *J* = 2.0 Hz, 1H, =CH_2), 0.92 (s, 9H, *t*-Bu), 0.26 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.2, 164.6 (d, *J* = 252.7 Hz, C-F), 141.4, 134.2 (d, *J* = 3.2 Hz), 129.9 (d, *J* = 9.0 Hz), 115.6 (d, *J* = 22.0 Hz), 93.5, 25.54, 18.07, -4.8. HRMS (ESI) *m/z* calcd for $C_{16}H_{22}FN_2O_2Si$ $[M+H]^+$ 321.1429, found: 321.1425.

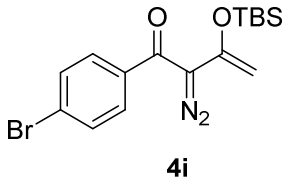
3-[(*tert*-Butyldimethylsilyl)oxy]-1-(4-chlorophenyl)-2-diazobut-3-en-1-one (4h)



4h

877 mg, 87% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.5 Hz, 2H, Ar), 7.43 (d, *J* = 8.5 Hz, 2H, Ar), 5.13 (d, *J* = 2.1 Hz, 1H, =CH_2), 4.46 (d, *J* = 2.1 Hz, 1H, =CH_2), 0.92 (s, 9H, *t*-Bu), 0.26 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 186.3, 141.3, 137.9, 136.4, 128.9, 128.8, 93.5, 25.6, 18.1, -4.8. HRMS (ESI) *m/z* calcd for $C_{16}H_{22}ClN_2O_2Si$ $[M+H]^+$ 337.1134, found: 337.1130.

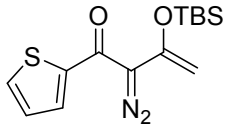
1-(4-Bromophenyl)-3-[(*tert*-butyldimethylsilyl)oxy]-2-diazobut-3-en-1-one (4i)



4i

958 mg, 84% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.6 Hz, 2H, Ar), 7.51 (d, *J* = 8.6 Hz, 2H, Ar), 5.13 (d, *J* = 2.1 Hz, 1H, =CH_2), 4.46 (d, *J* = 2.1 Hz, 1H, =CH_2), 0.92 (s, 9H, *t*-Bu), 0.26 (s, 6H, Me). ^{13}C NMR (75 MHz, $CDCl_3$) δ 186.3, 141.3, 136.8, 131.8, 129.0, 126.3, 93.6, 25.6, 18.1, -4.8. HRMS (ESI) *m/z* calcd for $C_{16}H_{22}BrN_2O_2Si$ $[M+H]^+$ 381.0628, found: 381.0629.

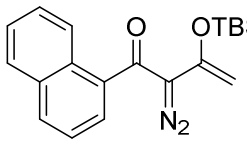
3-[(*tert*-Butyldimethylsilyl)oxy]-2-diazo-1-(thiophen-2-yl)but-3-en-1-one (4j)



4j

795 mg, 86% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60 (d, *J* = 5.0 Hz, 1H, Ar), 7.53 (d, *J* = 3.8 Hz, 1H, Ar), 7.10 (dd, *J* = 5.0, 3.8 Hz, 1H, Ar), 5.27 (d, *J* = 1.9 Hz, 1H, =CH_2), 4.52 (d, *J* = 1.9 Hz, 1H, =CH_2), 0.94 (s, 9H, *t*-Bu), 0.26 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 177.7, 142.5, 141.0, 131.9, 129.9, 127.4, 94.4, 25.6, 18.1, -4.8. HRMS (ESI) *m/z* calcd for $C_{14}H_{21}N_2O_2SSi$ $[M+H]^+$ 309.1093, found: 309.1095.

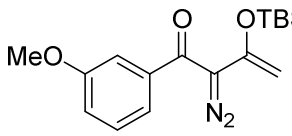
3-[(*tert*-Butyldimethylsilyl)oxy]-2-diazo-1-(naphthalen-1-yl)but-3-en-1-one (4k)



4k

919 mg, 87% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.09 (d, *J* = 8.0 Hz, 1H, Ar), 7.96 (d, *J* = 8.0 Hz, 1H, Ar), 7.91 (d, *J* = 7.4 Hz, 1H, Ar), 7.62 – 7.53 (comp, 3H, Ar), 7.51 (dd, *J* = 8.0, 7.4 Hz, 1H, Ar), 5.39 (br, 1H, =CH_2), 4.50 (d, *J* = 1.9 Hz, 1H, =CH_2), 0.93 (s, 9H, *t*-Bu), 0.29 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 188.4, 140.6, 136.0, 133.7, 130.9, 129.8, 128.5, 127.5, 126.6, 124.8, 124.73, 124.70, 93.1, 25.6, 18.1, -4.7. HRMS (ESI) *m/z* calcd for $C_{20}H_{25}N_2O_2Si$ $[M+H]^+$ 353.1685, found: 353.1686.

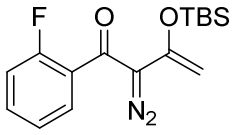
3-[(*tert*-Butyldimethylsilyl)oxy]-2-diazo-1-(3-methoxyphenyl)but-3-en-1-one (4l)



4l

897 mg, 90% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (t, *J* = 7.9 Hz, 1H, Ar), 7.20 (d, *J* = 7.9 Hz, 1H, Ar), 7.16 – 7.13 (m, 1H, Ar), 7.05 (dd, *J* = 7.9, 2.3 Hz, 1H, Ar), 5.23 (d, *J* = 2.0 Hz, 1H, $=CH_2$), 4.46 (d, *J* = 2.0 Hz, 1H, $=CH_2$), 3.85 (s, 3H, OMe), 0.93 (s, 9H, *t*-Bu), 0.27 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.4, 159.7, 141.2, 139.3, 129.5, 119.5, 117.9, 112.3, 93.2, 55.4, 25.6, 18.1, -4.8. HRMS (ESI) *m/z* calcd for $C_{17}H_{25}N_2O_3Si$ $[M+H]^+$ 333.1629, found: 333.1627.

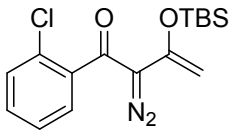
3-[(*tert*-Butyldimethylsilyl)oxy]-2-diazo-1-(2-fluorophenyl)but-3-en-1-one (4m)



4m

845 mg, 88% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (td, *J* = 7.5, 1.7 Hz, 1H, *ortho*-Bz), 7.48 (ddd, *J* = 15.4, 7.5, 1.7 Hz, 1H, H-C-C-F), 7.25 (t, *J* = 7.5 Hz, 1H, Ar), 7.16 – 7.10 (m, 1H, Ar), 5.28 (br, 1H, $=CH_2$), 4.46 (d, *J* = 2.0 Hz, 1H, $=CH_2$), 0.94 (s, 9H, *t*-Bu), 0.27 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 183.1, 158.7 (d, *J* = 250.0 Hz, C-F), 140.4, 132.8 (d, *J* = 8.3 Hz), 129.9 (d, *J* = 3.0 Hz), 126.6 (d, *J* = 16.2 Hz), 124.8 (d, *J* = 3.2 Hz), 116.1 (d, *J* = 22.1 Hz), 93.1, 25.6, 18.1, -4.8. HRMS (ESI) *m/z* calcd for $C_{16}H_{22}FN_2O_2Si$ $[M+H]^+$ 321.1429, found: 321.1424.

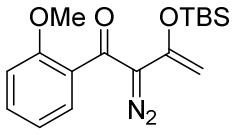
3-[(*tert*-Butyldimethylsilyl)oxy]-1-(2-chlorophenyl)-2-diazobut-3-en-1-one (4n)



4n

907 mg, 90% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 – 7.31 (comp, 4H, Ar), 5.25 (br, 1H, $=CH_2$), 4.45 (s, 1H, $=CH_2$), 0.94 (s, 9H, *t*-Bu), 0.27 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 185.6, 148.6, 137.9, 131.3, 130.5, 130.0, 128.4, 127.3, 93.2, 25.6, 18.1, -4.8. HRMS (ESI) *m/z* calcd for $C_{16}H_{22}ClN_2O_2Si$ $[M+H]^+$ 337.1134, found: 337.1132.

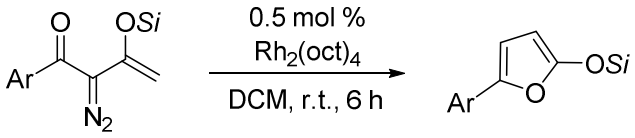
3-[(*tert*-Butyldimethylsilyl)oxy]-2-diazo-1-(2-methoxyphenyl)but-3-en-1-one (4o)



4o

827 mg, 83% yield. Dark orange solid, mp 58–59.5 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.34 (t, *J* = 7.9 Hz, 1H, Ar), 7.20 (d, *J* = 7.9 Hz, 1H, Ar), 7.16 – 7.13 (m, 1H, Ar), 7.05 (dd, *J* = 7.9, 2.3 Hz, 1H, Ar), 5.23 (d, *J* = 2.0 Hz, 1H, $=CH_2$), 4.46 (d, *J* = 2.0 Hz, 1H, $=CH_2$), 3.85 (s, 3H, OMe), 0.93 (s, 9H, *t*-Bu), 0.27 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 187.4, 159.7, 141.2, 139.3, 129.5, 119.5, 117.9, 112.3, 93.2, 55.4, 25.6, 18.1, -4.8. HRMS (ESI) *m/z* calcd for $C_{17}H_{25}N_2O_3Si$ $[M+H]^+$ 333.1629, found: 333.1625.

Procedure for the preparative synthesis of 5-aryl-2-siloxyfurans 6

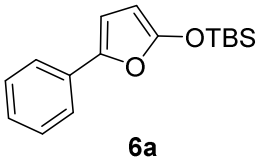


4 **6**

An oven-dried round-bottom flask equipped with a magnetic stirring bar was loaded with enoldiazo ketone **4** (1.0 mmol), dirhodium tetraoctanoate ($Rh_2(oct)_4$, 3.9 mg, 0.005 mmol), and the system was filled with nitrogen. Dichloromethane (6.0 mL) was then added in one portion (dinitrogen extrusion occurred rapidly), and the reaction mixture was stirred at 22 °C for 6 h. After completion of the reaction (monitoring by TLC), 1,3,5-trimethoxybenzene (168.2 mg, 1.0 mmol) was added as the internal standard for determination of NMR yield for the product, and dichloromethane evaporated. Pure 5-aryl-2-siloxyfurans **6** were obtained after column chromatography on silica gel with a 50:1 to 20:1 (v/v) gradient of hexane:ethyl acetate (isolated yield).

Characterization of 5-aryl-2-siloxyfurans 6

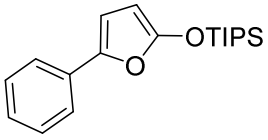
***tert*-Butyldimethyl[(5-phenylfuran-2-yl)oxy]silane (6a)**



6a

233 mg, 85% isolated yield; from 1.5 g (5.0 mmol) **4a** – 1.2 g, 88% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.52 (dd, *J* = 7.5, 1.1 Hz, 2H, Ar), 7.32 (t, *J* = 7.5 Hz, 2H, Ar), 7.16 (t, *J* = 7.5 Hz, 1H, Ar), 6.49 (d, *J* = 3.3 Hz, 1H, C^4-H), 5.22 (d, *J* = 3.3 Hz, 1H, C^3-H), 1.00 (s, 9H, *t*-Bu), 0.30 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.7, 143.5, 131.2, 128.6, 126.0, 122.4, 106.5, 86.0, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{16}H_{23}O_2Si$ $[M+H]^+$ 275.1462, found: 275.1460.

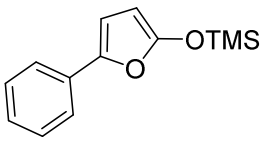
Triisopropyl[(5-phenylfuran-2-yl)oxy]silane (6b)



6b

281 mg, 89% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.4 Hz, 2H, Ar), 7.36 (t, *J* = 7.4 Hz, 2H, Ar), 7.19 (t, *J* = 7.4 Hz, 1H, Ar), 6.53 (d, *J* = 3.3 Hz, 1H, C^4-H), 5.28 (d, *J* = 3.3 Hz, 1H, C^3-H), 1.35 (sep, *J* = 7.5 Hz, 3H, CH-Me), 1.17 (d, *J* = 7.5 Hz, 18H, Me-CH). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.8, 143.2, 131.3, 128.6, 125.9, 122.3, 106.7, 86.1, 17.6, 12.3. HRMS (ESI) *m/z* calcd for $C_{19}H_{29}O_2Si$ $[M+H]^+$ 317.1931, found: 317.1931.

Trimethyl[(5-phenylfuran-2-yl)oxy]silane (6c)

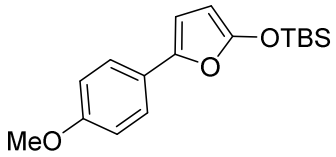


6c

150 mg, 65% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 7.5, 1.2 Hz, 2H, Ar), 7.36 (t, *J* = 7.5 Hz, 2H, Ar), 7.20 (t, *J* = 7.5

Hz, 1H, Ar), 6.54 (d, *J* = 3.3 Hz, 1H, C^4-H), 5.26 (d, *J* = 3.3 Hz, 1H, C^3-H), 0.40 (s, 9H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.4, 143.7, 131.1, 128.6, 126.1, 122.4, 106.5, 85.8, -0.1. HRMS (ESI) *m/z* calcd for $C_{13}H_{17}O_2Si$ $[M+H]^+$ 233.0992, found: 233.0991.

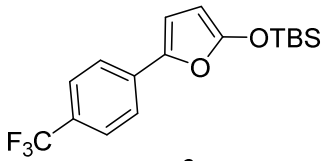
tert-Butyl[(5-(4-methoxyphenyl)furan-2-yl)oxy]dimethylsilane (6d)



6d

237 mg, 78% isolated yield. Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.8 Hz, 2H, Ar), 6.90 (d, *J* = 8.8 Hz, 2H, Ar), 6.37 (d, *J* = 3.2 Hz, 1H, C^4-H), 5.21 (d, *J* = 3.2 Hz, 1H, C^3-H), 3.83 (s, 3H, Me), 1.03 (s, 9H, *t*-Bu), 0.32 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.1, 156.1, 143.6, 131.5, 123.8, 114.1, 104.7, 85.7, 55.3, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{17}H_{25}O_3Si$ $[M+H]^+$ 305.1567, found: 305.1569.

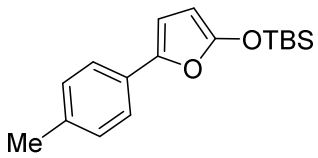
tert-Butyldimethyl[(5-[4-(trifluoromethyl)phenyl]furan-2-yl)oxy]silane (6e)



6e

291 mg, 85% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.63 – 7.57 (comp, 4H, Ar), 6.65 (d, *J* = 3.3 Hz, 1H, C^4-H), 5.30 (d, *J* = 3.3 Hz, 1H, C^3-H), 1.04 (s, 9H, *t*-Bu), 0.34 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.5, 142.0, 134.2, 127.5 (q, *J* = 32.5 Hz), 125.6 (dd, *J* = 7.1, 3.4 Hz), 124.3 (q, *J* = 271.6 Hz, C-F), 122.1, 109.0, 86.6, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{17}H_{22}F_3O_2Si$ $[M+H]^+$ 343.1336, found: 343.1341.

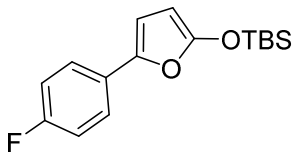
tert-Butyldimethyl[(5-(*p*-tolyl)furan-2-yl)oxy]silane (6f)



6f

242 mg, 84% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.44 (d, *J* = 8.7 Hz, 2H, Ar), 7.16 (d, *J* = 8.7 Hz, 2H, Ar), 6.45 (d, *J* = 3.2 Hz, 1H, C^4-H), 5.22 (d, *J* = 3.2 Hz, 1H, C^3-H), 2.36 (s, 3H, Me-Ar), 1.02 (s, 9H, *t*-Bu), 0.32 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.3, 143.7, 135.7, 129.2, 128.5, 122.4, 105.6, 85.8, 29.7, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{17}H_{25}O_2Si$ $[M+H]^+$ 289.1618, found: 289.1618.

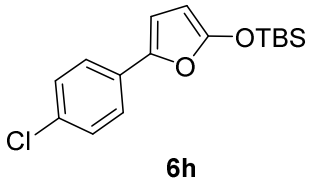
tert-Butyl[(5-(4-fluorophenyl)furan-2-yl)oxy]dimethylsilane (6g)



6g

245 mg, 84% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (dd, *J* = 8.8, 5.3 Hz, 2H, Ar), 7.05 (t, *J* = 8.8 Hz, 2H, Ar), 6.44 (d, *J* = 3.3 Hz, 1H, C^4-H), 5.23 (d, *J* = 3.3 Hz, 1H, C^3-H), 1.03 (s, 9H, *t*-Bu), 0.33 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 161.3 (d, *J* = 245.3 Hz, C-F), 156.6, 142.7, 127.6 (d, *J* = 3.0 Hz), 124.0 (d, *J* = 7.7 Hz), 115.5 (d, *J* = 21.9 Hz), 106.1, 86.0, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{16}H_{22}FO_2Si$ $[M+H]^+$ 293.1368, found: 293.1369.

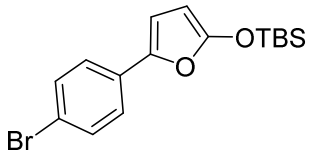
***tert*-Butyl[(5-(4-chlorophenyl)furan-2-yl)oxy]dimethylsilane (6h)**



6h

256 mg, 83% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.6 Hz, 2H, Ar), 7.31 (d, *J* = 8.6 Hz, 2H, Ar), 6.51 (d, *J* = 3.2 Hz, 1H, C^4-H), 5.25 (d, *J* = 3.2 Hz, 1H, C^3-H), 1.03 (s, 9H, *t*-Bu), 0.33 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.8, 142.5, 131.4, 129.7, 128.7, 123.6, 107.1, 86.2, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{16}H_{22}ClO_2Si$ $[M+H]^+$ 309.1072, found: 309.1073.

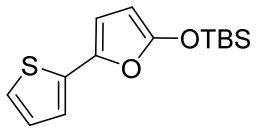
[(5-(4-Bromophenyl)furan-2-yl)oxy](*tert*-butyl)dimethylsilane (6i)



6i

274 mg, 78% isolated yield. White solid, mp 127–129 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.6 Hz, 2H, Ar), 7.40 (d, *J* = 8.6 Hz, 2H, Ar), 6.52 (d, *J* = 3.3 Hz, 1H, C^4-H), 5.25 (d, *J* = 3.3 Hz, 1H, C^3-H), 1.03 (s, 9H, *t*-Bu), 0.33 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.9, 142.4, 131.7, 130.1, 123.9, 119.4, 107.3, 86.3, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{16}H_{22}BrO_2Si$ $[M+H]^+$ 353.0567, found: 353.0565.

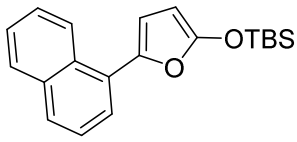
***tert*-Butyldimethyl[(5-(thiophen-2-yl)furan-2-yl)oxy]silane (6j)**



6j

210 mg, 75% isolated yield. Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.12 (dd, *J* = 5.0, 0.8 Hz, 1H, Ar), 7.10 (dd, *J* = 3.7, 0.8 Hz, 1H, Ar), 7.00 (dd, *J* = 5.0, 3.7 Hz, 1H, Ar), 6.35 (d, *J* = 3.2 Hz, 1H, C^4-H), 5.21 (d, *J* = 3.2 Hz, 1H, C^3-H), 1.02 (s, 9H, *t*-Bu), 0.32 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.2, 139.3, 134.4, 127.4, 122.3, 120.5, 106.6, 85.8, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{14}H_{21}O_2SSi$ $[M+H]^+$ 281.1026, found: 281.1025.

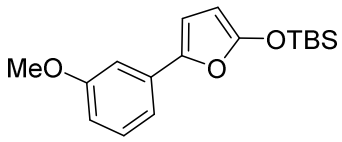
***tert*-Butyldimethyl[(5-(naphthalen-1-yl)furan-2-yl)oxy]silane (6k)**



6k

233 mg, 72% isolated yield. Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 8.50 (d, *J* = 8.0 Hz, 1H, Ar), 7.91 – 7.87 (m, 1H, Ar), 7.79 (d, *J* = 8.0 Hz, 1H, Ar), 7.69 (dd, *J* = 7.2, 0.9 Hz, 1H, Ar), 7.57 – 7.49 (comp, 3H, Ar), 6.63 (d, *J* = 3.2 Hz, 1H, C^4-H), 5.38 (d, *J* = 3.2 Hz, 1H, C^3-H), 1.06 (s, 9H, *t*-Bu), 0.37 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 157.0, 142.8, 134.0, 129.9, 128.8, 128.5, 127.3, 126.2, 125.8, 125.6, 125.4, 124.8, 111.1, 85.9, 25.6, 18.2, -4.6. HRMS (ESI) *m/z* calcd for $C_{20}H_{25}O_2Si$ $[M+H]^+$ 325.1618, found: 325.1624.

***tert*-Butyl[(5-(3-methoxyphenyl)furan-2-yl)oxy]dimethylsilane (6l)**

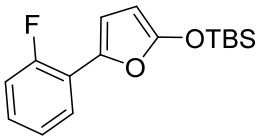


6l

249 mg, 82% isolated yield. Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.26 (t, *J* = 8.0 Hz, 1H, Ar), 7.17 – 7.12 (m, 1H, Ar), 7.11 – 7.08 (m, 1H, Ar), 6.75 (ddd, *J* = 8.0, 2.5, 0.7 Hz, 1H, Ar), 6.52 (d, *J* =

3.3 Hz, 1H, C^4-H), 5.25 (d, *J* = 3.3 Hz, 1H, C^3-H), 3.86 (s, 3H, OMe), 1.03 (s, 9H, *t*-Bu), 0.33 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 159.9, 156.6, 143.3, 132.5, 129.6, 115.1, 111.7, 107.9, 107.0, 86.1, 55.2, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{17}H_{25}O_3Si$ $[M+H]^+$ 305.1567, found: 305.1568.

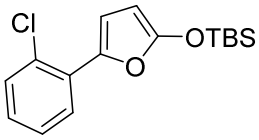
tert-Butyl[(5-(2-fluorophenyl)furan-2-yl)oxy]dimethylsilane (6m)



6m

268 mg, 92% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.69 – 7.64 (m, 1H, Ar), 7.19 – 7.06 (comp, 3H, Ar), 6.73 (t, *J* = 3.5 Hz, 1H, C^4-H), 5.30 (d, *J* = 3.3 Hz, 1H, C^3-H), 1.04 (s, 9H, *t*-Bu), 0.34 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 158.2 (d, *J* = 249.3 Hz, C-F), 156.7, 137.9 (d, *J* = 2.5 Hz), 126.6 (d, *J* = 8.2 Hz), 124.7 (d, *J* = 3.4 Hz), 124.2 (d, *J* = 3.2 Hz), 119.4 (d, *J* = 11.9 Hz), 115.7 (d, *J* = 21.3 Hz), 112.3 (d, *J* = 12.3 Hz), 86.4, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{16}H_{22}FO_2Si$ $[M+H]^+$ 293.1368, found: 293.1368.

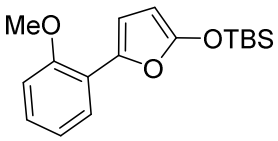
tert-Butyl[(5-(2-chlorophenyl)furan-2-yl)oxy]dimethylsilane (6n)



6n

210 mg, 68% isolated yield. Colorless oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.75 (dd, *J* = 8.0, 1.5 Hz, 1H, Ar), 7.32 – 7.26 (comp, 2H, Ar), 7.12 (td, *J* = 8.0, 1.5 Hz, 1H, Ar), 7.08 (d, *J* = 3.4 Hz, 1H, C^4-H), 5.32 (d, *J* = 3.4 Hz, 1H, C^3-H), 1.04 (s, 9H, *t*-Bu), 0.35 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.7, 139.9, 130.7, 130.3, 128.8, 126.8, 126.5, 126.4, 113.4, 86.3, 25.5, 18.2, -4.7. HRMS (ESI) *m/z* calcd for $C_{16}H_{22}ClO_2Si$ $[M+H]^+$ 309.1072, found: 309.1075.

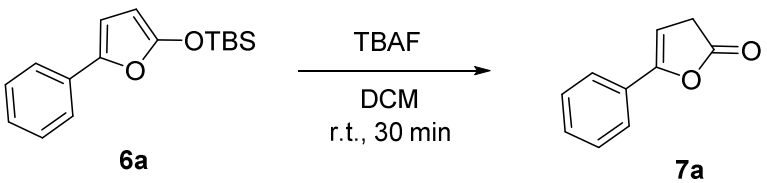
tert-Butyl[(5-(2-methoxyphenyl)furan-2-yl)oxy]dimethylsilane (6o)



6o

213 mg, 70% isolated yield. Pale yellow oil. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 (dd, *J* = 7.5, 1.7 Hz, 1H, Ar), 7.17 (ddd, *J* = 8.2, 7.5, 1.7 Hz, 1H, Ar), 7.01 (td, *J* = 7.5, 1.7 Hz, 1H, Ar), 6.94 (d, *J* = 8.2 Hz, 1H, Ar), 6.83 (d, *J* = 3.3 Hz, 1H, C^4-H), 5.27 (d, *J* = 3.3 Hz, 1H, C^3-H), 3.95 (s, 3H, OMe), 1.03 (s, 9H, *t*-Bu), 0.33 (s, 6H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 156.1, 154.9, 140.2, 126.4, 124.6, 120.7, 120.1, 112.0, 110.8, 86.0, 55.3, 25.6, 18.3, -4.7. HRMS (ESI) *m/z* calcd for $C_{17}H_{25}O_3Si$ $[M+H]^+$ 305.1567, found: 305.1564.

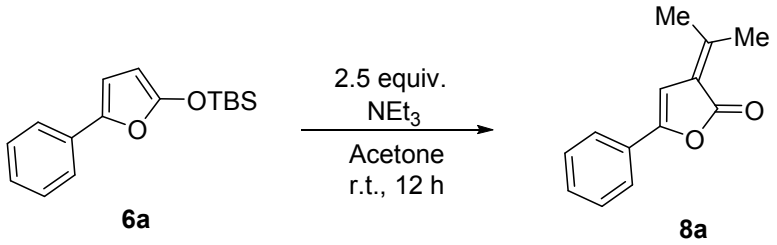
Procedure for desilylation of _tert_-butyldimethyl[(5-phenylfuran-2-yl)oxy]silane (6a)



6a **7a**

A round-bottom flask equipped with a magnetic stirring bar was loaded with *tert*-butyldimethyl[(5-phenylfuran-2-yl)oxy]silane (**6a**) (548 mg, 2.0 mmol) dissolved in dichloromethane (10 mL). A 1*M* solution of TBAF (3 mL, 1.5 equiv.) was then added dropwise at 0 °C. The reaction mixture was capped and stirred at rt for 30 min. Solvent was evaporated, and the residue was purified by column chromatography on silica gel with a 4:1 (v/v) mixture of hexane:ethyl acetate as the eluent to afford 5-phenylfuran-2(3*H*)-one (**7a**) as an off-white solid, mp 83.5–84.5 °C (82–83 °C lit.[3]). 314 mg, 98% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.65 – 7.60 (comp, 2H, Ar), 7.46 – 7.37 (comp, 3H, Ar), 5.80 (t, *J* = 2.5 Hz, 1H, C–H), 3.43 (d, *J* = 2.5 Hz, 2H, CH_2). ^{13}C NMR (126 MHz, $CDCl_3$) δ 175.9, 154.0, 129.6, 128.7, 128.4, 124.7, 97.7, 34.7. HRMS (ESI) *m/z* calcd for $C_{10}H_9O_2$ $[M+H]^+$ 161.0597, found: 161.0599.

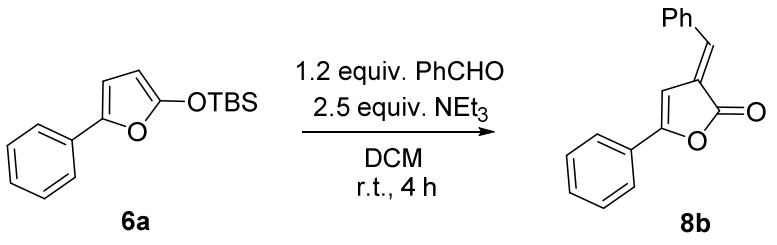
Procedure for the reaction of 6a with acetone



6a **8a**

A round-bottom flask equipped with a magnetic stirring bar was loaded with *tert*-butyldimethyl[(5-phenylfuran-2-yl)oxy]silane (**6a**) (274 mg, 1.0 mmol) dissolved in acetone (6 mL). Triethylamine (0.35 mL, 2.5 mmol) was added in one portion, and then the reaction mixture was capped and stirred at rt for 12 h. Acetone was evaporated, and the residue purified by column chromatography on silica gel with a 5:1 (v/v) mixture of hexane:ethyl acetate as the eluent to afford 5-phenyl-3-(propan-2-ylidene)furan-2(3*H*)-one (**8a**) as a white solid, mp 106–108 °C (104–108 °C lit.[4]). 180 mg, 90% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.70 – 7.67 (comp, 2H, Ar), 7.46 – 7.35 (comp, 3H, Ar), 6.48 (s, 1H, C–H), 2.44 (s, 3H, Me), 2.16 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.2, 153.5, 151.4, 129.4, 128.7, 124.7, 123.5, 100.3, 24.5, 21.0. HRMS (ESI) *m/z* calcd for $C_{13}H_{13}O_2$ $[M+H]^+$ 201.0910, found: 201.0912.

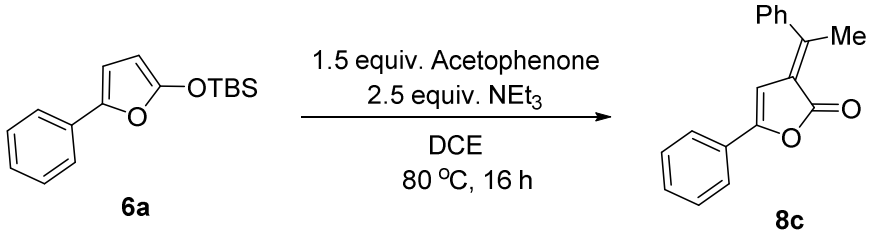
Procedure for the reaction of 6a with benzaldehyde



6a **8b**

A round-bottom flask equipped with a magnetic stirring bar was loaded with *tert*-butyldimethyl[(5-phenylfuran-2-yl)oxy]silane (**6a**) (274 mg, 1.0 mmol) dissolved in dichloromethane (5 mL). Benzaldehyde (127 mg, 1.2 mmol) in 1.0 mL DCM followed by triethylamine (0.35 mL, 2.5 equiv.) were added dropwise, and then the reaction mixture was capped and stirred at rt for 4 h. DCM was evaporated, and the residue purified by column chromatography on silica gel with a 5:1 (v/v) mixture of hexane:ethyl acetate as the eluent to afford (*E*)-3-benzylidene-5-phenylfuran-2(3*H*)-one (**8b**) as a yellow solid, mp 155−156 °C (156.8−157.6 °C lit.[5]). 233 mg, 94% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.80 (dd, *J* = 7.7, 1.4 Hz, 2H, Ar), 7.67 (d, *J* = 7.4 Hz, 2H, Ar), 7.54 – 7.42 (comp, 7H, Ar + Ar-CH), 6.97 (s, 1H, C−H). ^{13}C NMR (126 MHz, $CDCl_3$) δ 169.4, 157.0, 135.5, 135.2, 130.5, 130.3, 130.1, 129.1, 128.9, 128.1, 125.5, 125.4, 99.8. HRMS (ESI) *m/z* calcd for $C_{17}H_{13}O_2$ $[M+H]^+$ 249.0916, found: 249.0915.

Procedure for the reaction of 6a with acetophenone



6a **8c**

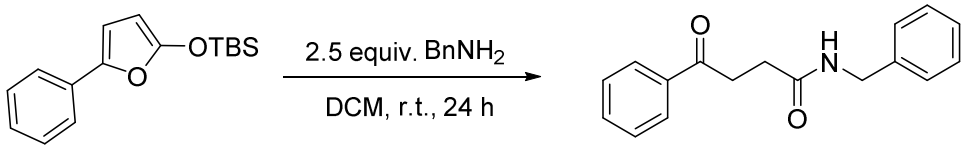
A round-bottom flask equipped with a magnetic stirring bar and a reflux condenser was loaded with *tert*-butyldimethyl[(5-phenylfuran-2-yl)oxy]silane (**6a**) (274 mg, 1.0 mmol) dissolved in 1,2-dichloroethane (7 mL). Acetophenone (180 mg, 1.5 mmol) in 1 mL DCE, and triethylamine (0.35 mL, 2.5 equiv.) were added sequentially in one portion, and then the reaction mixture was heated to reflux and stirred at 80 °C for 16 h. DCE was evaporated, and the residue purified by column chromatography on silica gel with a 5:1 (v/v) mixture of hexane:ethyl acetate as the eluent to afford (*E*)-5-phenyl-3-(1-phenylethylidene)furan-2(3*H*)-one (**8c**) as a yellow solid, mp 183−184 °C. 215 mg, 82% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.66 (d, *J* = 7.1 Hz, 2H, Ar), 7.52 – 7.44 (comp, 5H, Ar), 7.42 – 7.35 (comp, 3H, Ar), 6.47 (s, 1H, C−H), 2.77 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 167.7, 152.7, 133.3, 129.8, 129.7, 129.1, 128.7, 128.6, 128.5, 128.0, 124.8, 124.3, 101.7, 20.5. HRMS (ESI) *m/z* calcd for $C_{18}H_{15}O_2$ $[M+H]^+$ 263.1072, found: 263.1072.

Procedure for the synthesis of 3-benzyl-5-phenylfuran-2(3*H*)-one (9)

6a **9**

An oven-dried round-bottom flask equipped with a magnetic stirring bar was loaded with *tert*-butyldimethyl[(5-phenylfuran-2-yl)oxy]silane (**6a**) (274 mg, 1.0 mmol), and the system was filled with nitrogen. Dichloromethane (6 mL) was then added, and the reaction mixture was cooled to 0 °C using an ice-bath. Benzaldehyde (127 mg, 1.2 mmol) in 1 mL of DCM followed by triethylsilane (174 mg, 1.5 mmol) in 1.0 mL DCM were added in one portion. Anhydrous scandium triflate (25 mg, 0.05 mmol) was added under nitrogen atmosphere, and the reaction mixture was stirred at rt for 2 h. DCM was evaporated, and the residue purified by column chromatography on silica gel with a 5:1 (v/v) mixture of hexane:ethyl acetate as the eluent to afford 3-benzyl-5-phenylfuran-2(3*H*)-one (**9**) as a white solid, mp 93−94 °C. 200 mg, 80% yield. ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.81 (d, *J* = 7.5 Hz, 2H, Ar), 7.61 (t, *J* = 7.5 Hz, 1H, Ar), 7.51 – 7.42 (comp, 2H, Ar), 7.40 – 7.31 (comp, 5H, Ar), 5.84 (d, *J* = 7.4 Hz, 1H, =C−H), 4.31 (td, *J* = 9.3, 7.4 Hz, 1H, C<u>H</u>−Bn), 3.05 (d, *J* = 9.3 Hz, 2H, CH_2). ^{13}C NMR (126 MHz, $CDCl_3$) δ 174.2, 156.6, 138.3, 135.3, 134.2, 133.8, 129.0, 128.9, 128.6, 125.6, 82.4, 51.0, 33.6. HRMS (ESI) *m/z* calcd for $C_{17}H_{15}O_2$ $[M+H]^+$ 251.1072, found: 251.1068.

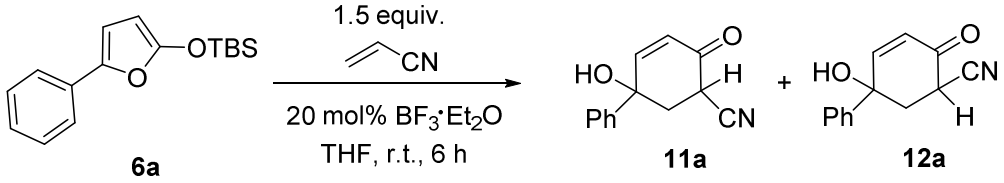
Procedure for the synthesis of *N*-benzyl-4-oxo-4-phenylbutanamide (10)



6a **10**

A round-bottom flask equipped with a magnetic stirring bar was loaded with *tert*-butyldimethyl[(5-phenylfuran-2-yl)oxy]silane (**6a**) (548 mg, 2.0 mmol) dissolved in dichloromethane (10 mL). Benzylamine (0.55 mL, 5.0 mmol) was added in one portion at r.t. The reaction mixture was capped and stirred at rt for 24 h. DCM was evaporated, and the residue purified by column chromatography on silica gel with a 4:1 (v/v) mixture of hexane:ethyl acetate as the eluent to afford *N*-benzyl-4-oxo-4-phenylbutanamide (**10**) as a white solid, mp 115−116 °C (113−114 °C lit.[6]). 513 mg, 96% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 7.7, 2H, *ortho*-Bz), 7.58 (t, *J* = 7.7 Hz, 1H, *para*-Bz), 7.47 (t, *J* = 7.7 Hz, 2H, *meta*-Bz), 7.40 – 7.24 (comp, 5H, Ar), 6.34 (br, 1H, NH), 4.45 (d, *J* = 5.8 Hz, 2H, <u>CH_2</u>Ph), 3.39 (t, *J* = 6.6 Hz, 2H, <u>CH_2</u>COPh), 2.67 (t, *J* = 6.6 Hz, 2H, <u>CH_2</u>CONH). ^{13}C NMR (126 MHz, $CDCl_3$) δ 199.2, 172.0, 138.3, 136.5, 133.3, 128.7, 128.6, 128.1, 127.7, 127.4, 43.7, 34.1, 30.2. HRMS (ESI) *m/z* calcd for $C_{17}H_{18}NO_2$ $[M+H]^+$ 268.1332, found: 268.1341.

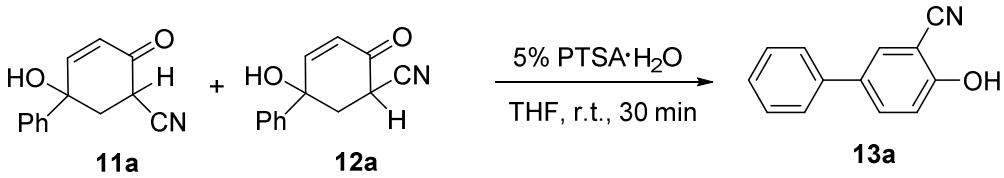
Procedure for the synthesis of *cis*- and *trans*-1-hydroxy-4-oxo-1,2,3,4-tetrahydro-[1,1'-biphenyl]-3-carbonitriles (11a and 12a)



6a **11a** **12a**

An oven-dried round-bottom flask equipped with a magnetic stirring bar was loaded with *tert*-butyldimethyl[(5-phenylfuran-2-yl)oxy]silane (**6a**) (274 mg, 1.0 mmol), and the system was filled with nitrogen. THF (8 mL) was then added, and the reaction mixture was cooled to 0 °C using an ice-bath. Acrylonitrile (80 mg, 1.5 mmol) in 1.0 mL THF followed by freshly distilled $BF_3{\cdot}Et_2O$ (30 mg, 0.2 mmol) in 0.5 mL THF were added in one portion at 0 °C. The reaction mixture was allowed to stir at r.t. for 6 h. Solvent was evaporated, and the residue was purified by column chromatography on silica gel with a 9:1 (v/v) mixture of hexane:ethyl acetate as the eluent to afford *cis*- and *trans*- 1-hydroxy-4-oxo-1,2,3,4-tetrahydro-[1,1'-biphenyl]-3-carbonitriles (**11a**:**12a** = 3:2) as a colorless oil (150 mg, 70% yield). ^{13}C NMR (126 MHz, $CDCl_3$) δ 188.7, 188.1, 154.3, 151.1, 144.3, 140.2, 129.3, 129.3, 129.1, 128.6, 127.9, 127.5, 125.6, 124.5, 116.3, 115.9, 72.8, 70.3, 42.4, 42.1, 37.6, 37.1. HRMS (ESI) *m/z* calcd for $C_{13}H_{12}NO_2$ $[M+H]^+$ 214.0868, found: 214.0863.

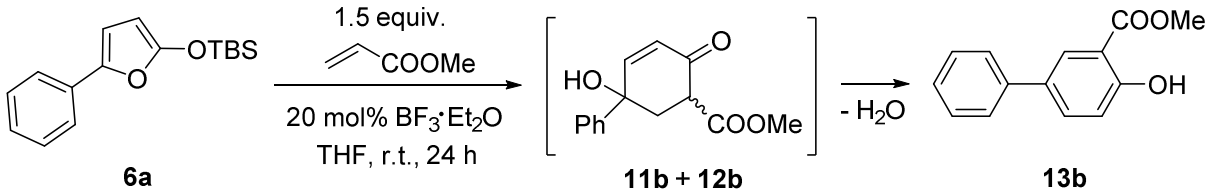
Procedure for the synthesis of 4-hydroxy-[1,1'-biphenyl]-3-carbonitrile (13a)



11a **12a** **13a**

A screw-capped vial (8 mL) equipped with a magnetic stirring bar was loaded with a mixture **11a** + **12a** (120 mg, 0.563 mmol) dissolved in THF (4 mL). *p*-Toluenesulfonic acid monohydrate (6 mg, 5 mol%) was added at rt, the reaction mixture was capped and stirred at r.t. for 30 min. THF was evaporated, and the residue purified by column chromatography on silica gel with a 2:1 (v/v) mixture of hexane:ethyl acetate as the eluent to afford 4-hydroxy-[1,1'-biphenyl]-3-carbonitrile (**13a**) as a white solid, mp 195–196 °C (193–194 °C lit.[7]). 105 mg, 96% yield. ^{1}H NMR (500 MHz, MeOD) δ 7.76 – 7.68 (comp, 2H, Ar), 7.53 (d, *J* = 7.7 Hz, 2H, Ar), 7.41 (t, *J* = 7.7 Hz, 2H, Ar), 7.32 (t, *J* = 7.3 Hz, 1H, Ar), 7.03 (d, *J* = 8.6 Hz, 1H, Ar). ^{13}C NMR (126 MHz, MeOD) δ 159.6, 138.9, 133.0, 132.8, 130.9, 128.6, 127.0, 126.1, 116.4, 116.1, 99.7. HRMS (ESI) *m/z* calcd for $C_{13}H_{10}NO$ $[M+H]^+$ 196.0757, found: 196.0750.

Procedure for the synthesis of methyl 4-hydroxy-[1,1'-biphenyl]-3-carboxylate (13b)



6a **11b + 12b** **13b**

Synthetic procedure is identical to **11a** and **12a**. However, the formed non-aromatic carbocycle was not stable, and underwent complete aromatization to form methyl 4-hydroxy-[1,1'-biphenyl]-3-carboxylate (**10**). Product was purified by column chromatography on silica gel with a 19:1 (v/v) mixture of hexane:ethyl acetate as the eluent and isolated as a white solid, mp 94–95 °C (94–95 °C lit.[8]). 144 mg, 63% yield. ^{1}H NMR (500 MHz, $CDCl_3$) δ 10.8 (s, 1H, OH), 8.11 (d, *J* = 2.4 Hz, 1H, Ar), 7.74 (dd, *J* = 8.6, 2.4 Hz, 1H, Ar), 7.58 (d, *J* = 8.6, 2H, Ar), 7.46 (t, *J* = 7.7 Hz, 2H, Ar), 7.40 – 7.33 (m, 1H, Ar), 7.10 (d, *J* = 8.6 Hz, 1H, Ar), 4.01 (s, 3H, Me). ^{13}C NMR (126 MHz, $CDCl_3$) δ 170.6, 161.0, 139.9, 134.4, 132.5, 128.9, 128.2, 127.1, 126.6, 118.1, 112.5, 52.4. HRMS (ESI) *m/z* calcd for $C_{14}H_{13}O_3$ $[M+H]^+$ 229.0859, found: 229.0864.

Computational methods

DFT calculations were performed with Gaussian 09.[9] Pruned integration grids with 99 radial shells and 590 angular points per shell were used. Geometry optimisations of the stationary points were carried out at the B3LYP/def2-SVP level without any constrains.[10] Unscaled harmonic frequency calculations at the same level were performed to validate each structure as either a minimum or a transition state and to evaluate its zero-point energy and thermal corrections at 298 K. Quasiharmonic corrections were applied during the entropy calculations by setting all positive frequencies that are less than 100 cm^{-1} to 100 cm^{-1}.[11] All discussed energy differences were based on Gibbs energies in the gas phase at 298 K. Standard states for gases are the hypothetical states at 1 atm.

DFT study on the substituent effect

To understand the notable substituent effect of both the donor and the acceptor, we performed DFT calculations on the Gibbs energy profiles for the reaction of two model substrates **4p** (a substrate without the donor substituent) and **4q** (a substrate with an acyl acceptor) under the catalysis of rhodium(II) formate (Figure S1). Although the catalytic reaction of these two substrates follows the same reaction mechanism as that of **4c**, the overall Gibbs energies of activation for the reaction of **4p** (38.8 kcal mol^{-1}, from **B** to **TS3**) and **4q** (26.4 kcal mol^{-1}, from **C** to **TS4**) are higher than that for the reaction of **4c** (24.3 kcal mol^{-1}, from **C** to **TS3**). We reasoned that both the electron-donating siloxy and aryl groups are important to the stabilisation of the cationic centers of intermediates **D** and **E** (as well as the transition states

TS2–**4**), which facilitates the reaction to occur. These computational results may help chemists to understand the substituent effect and to design new reactions of donor–acceptor cyclopropenes.

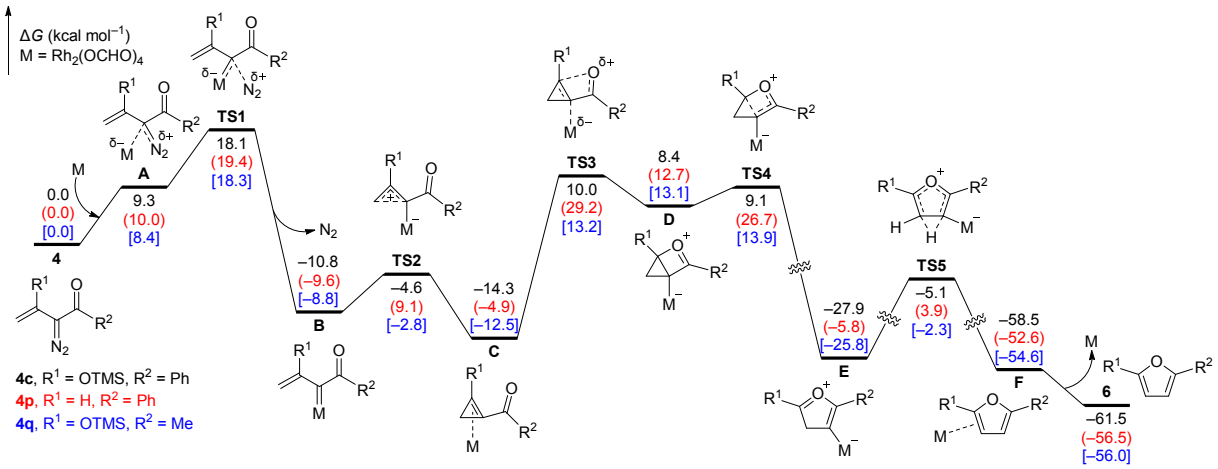


Fig. S1 Gibbs energy profiles for the reaction of substrates **4c**, **4p** and **4q** under the catalysis of rhodium(II) formate. Computed at the B3LYP/def2-SVP level.

Computed energies for the stationary points

Table S1 Thermal corrections to Gibbs energies (TCGs) and single-point energies (SPEs)

	TCG [a.u.]	SPE [a.u.]
$Rh_2(OCHO)_4$	0.061835	−977.421177
N_2	−0.012766	−109.439221
4c (R^1 = OTMS, R^2 = Ph)	0.217265	−1053.839024
6c (R^1 = OTMS, R^2 = Ph)	0.213367	−944.481188
A (R^1 = OTMS, R^2 = Ph)	0.304182	−2031.270463
B (R^1 = OTMS, R^2 = Ph)	0.296581	−1921.842893
C (R^1 = OTMS, R^2 = Ph)	0.298122	−1921.850037
D (R^1 = OTMS, R^2 = Ph)	0.298676	−1921.814424
E (R^1 = OTMS, R^2 = Ph)	0.298435	−1921.871980
F (R^1 = OTMS, R^2 = Ph)	0.300492	−1921.922754
TS1 (R^1 = OTMS, R^2 = Ph)	0.301339	−2031.253670
TS2 (R^1 = OTMS, R^2 = Ph)	0.295939	−1921.832331
TS3 (R^1 = OTMS, R^2 = Ph)	0.297752	−1921.810855
TS4 (R^1 = OTMS, R^2 = Ph)	0.298459	−1921.813089
TS5 (R^1 = OTMS, R^2 = Ph)	0.295092	−1921.832257

4p (R^1 = OTMS, R^2 = Ph)	0.121248	−570.121871
6p (R^1 = OTMS, R^2 = Ph)	0.118158	−460.756813
A (R^1 = H, R^2 = Ph)	0.207246	−1547.551200
B (R^1 = H, R^2 = Ph)	0.199512	−1438.122741
C (R^1 = H, R^2 = Ph)	0.200568	−1438.116412
D (R^1 = H, R^2 = Ph)	0.201729	−1438.089454
E (R^1 = H, R^2 = Ph)	0.201053	−1438.118275
F (R^1 = H, R^2 = Ph)	0.204071	−1438.195871
TS1 (R^1 = H, R^2 = Ph)	0.204755	−1547.533843
TS2 (R^1 = H, R^2 = Ph)	0.198482	−1438.092014
TS3 (R^1 = H, R^2 = Ph)	0.199039	−1438.060486
TS4 (R^1 = H, R^2 = Ph)	0.200108	−1438.065606
TS5 (R^1 = H, R^2 = Ph)	0.199255	−1438.101053
4q (R^1 = OTMS, R^2 = Me)	0.166396	−862.239552
6q (R^1 = OTMS, R^2 = Me)	0.163247	−752.873647
A (R^1 = OTMS, R^2 = Me)	0.253105	−1839.672161
B (R^1 = OTMS, R^2 = Me)	0.245132	−1730.239723
C (R^1 = OTMS, R^2 = Me)	0.246412	−1730.246912
D (R^1 = OTMS, R^2 = Me)	0.246957	−1730.206663
E (R^1 = OTMS, R^2 = Me)	0.247283	−1730.268972
F (R^1 = OTMS, R^2 = Me)	0.249571	−1730.317071
TS1 (R^1 = OTMS, R^2 = Me)	0.249279	−1839.652584
TS2 (R^1 = OTMS, R^2 = Me)	0.244885	−1730.229870
TS3 (R^1 = OTMS, R^2 = Me)	0.246581	−1730.206053
TS4 (R^1 = OTMS, R^2 = Me)	0.247058	−1730.205345
TS5 (R^1 = OTMS, R^2 = Me)	0.244279	−1730.228499

Computed at the B3LYP/def2-SVP level. Standard states at 1 atm and 298 K were used.

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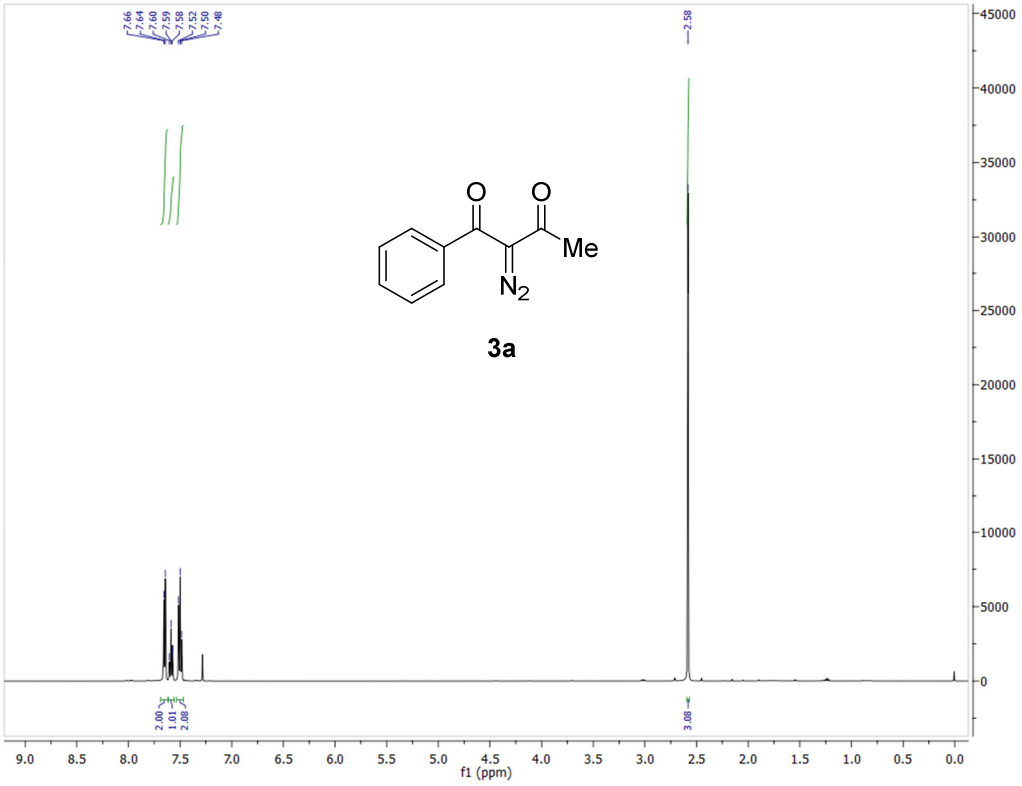
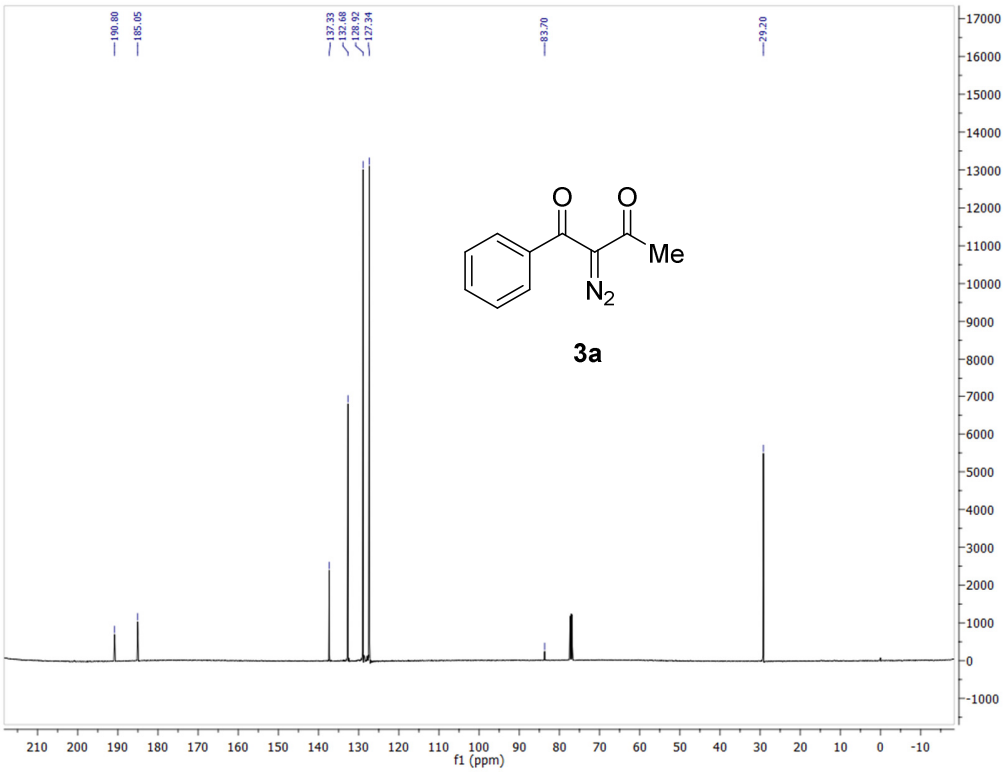
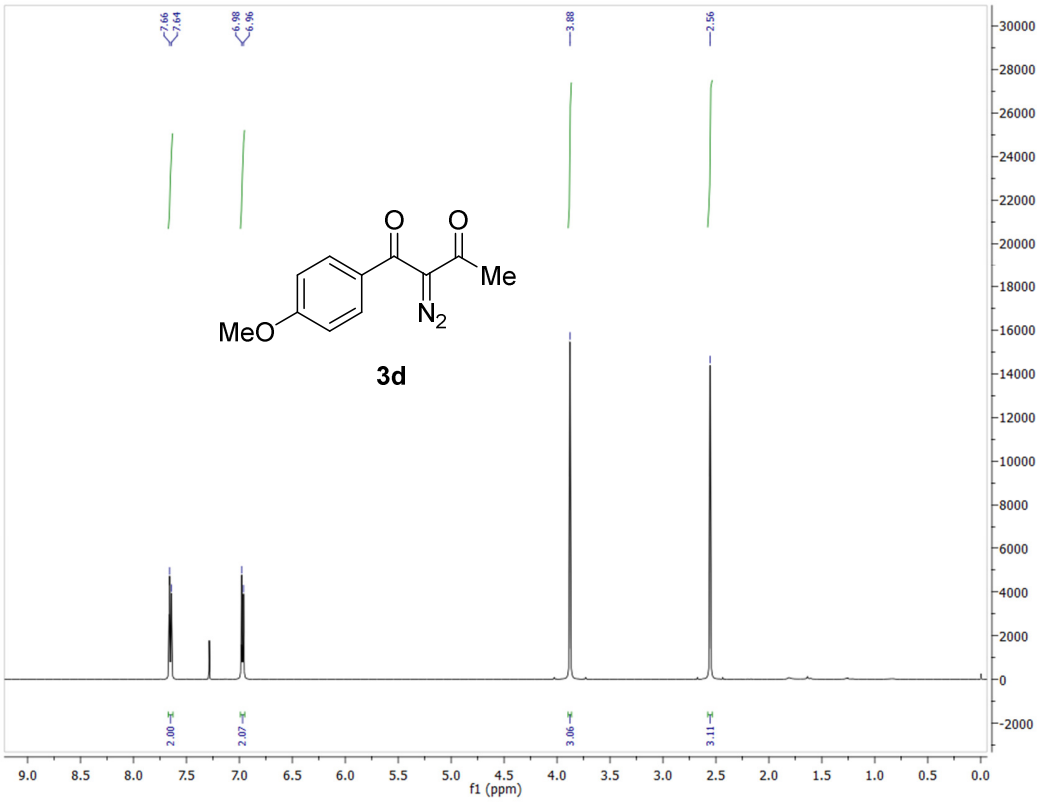
NMR spectra of compounds



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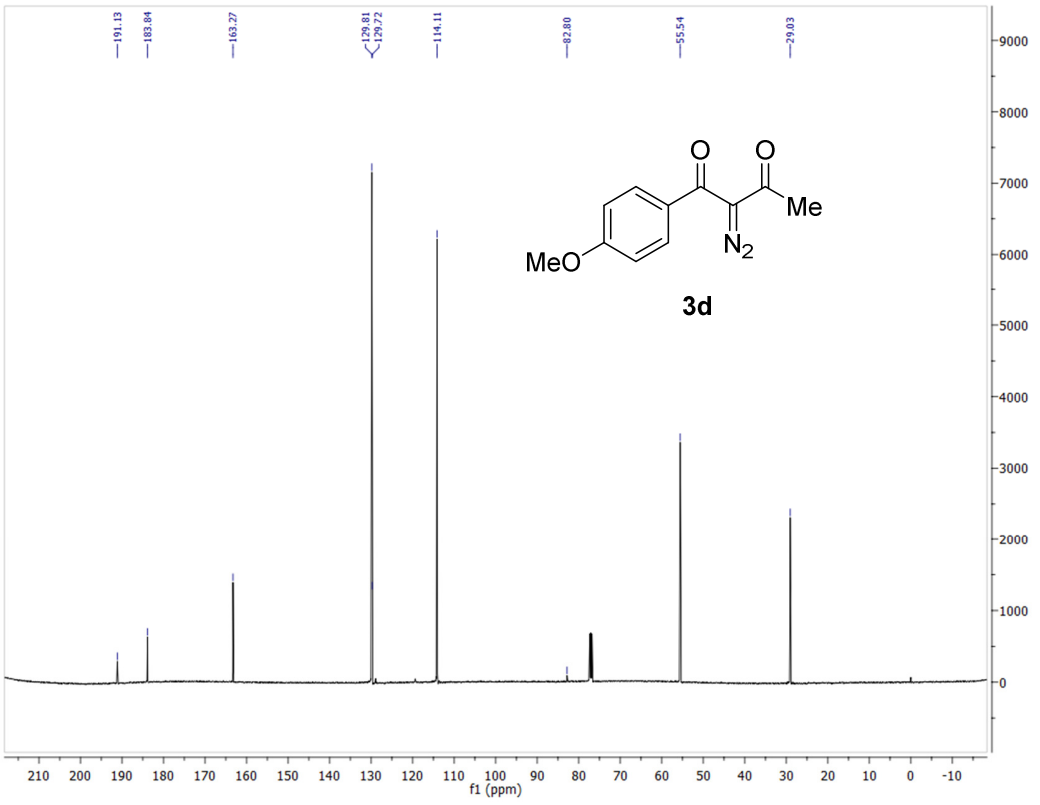
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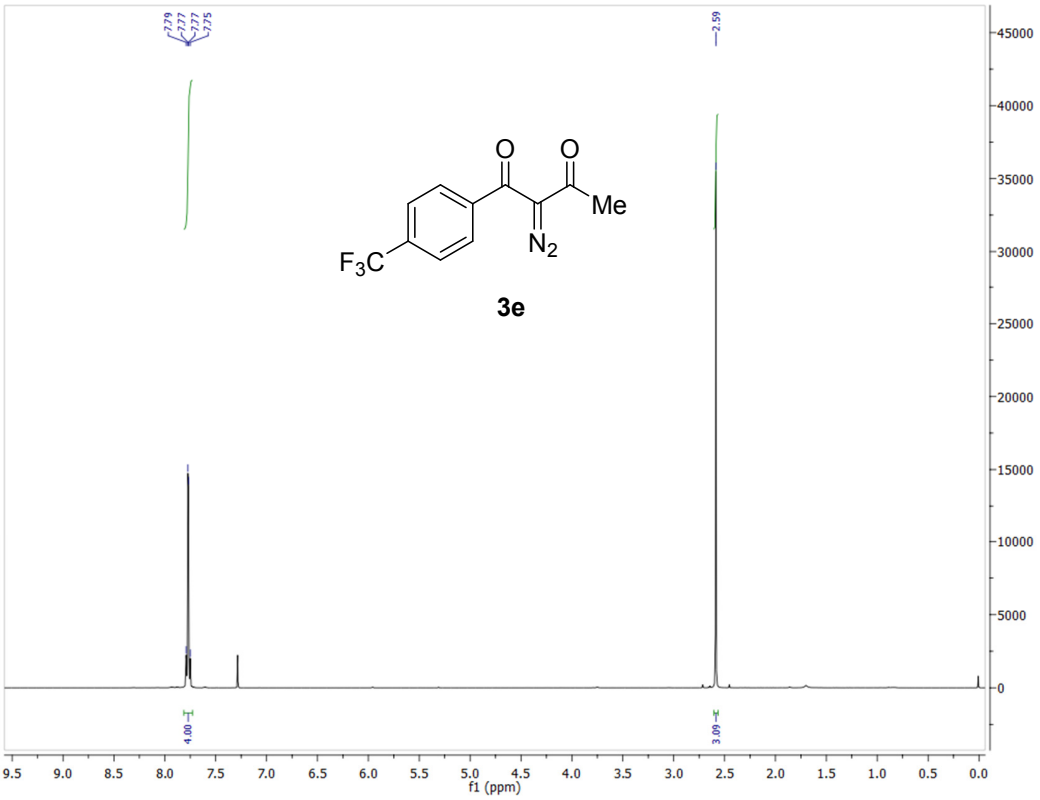
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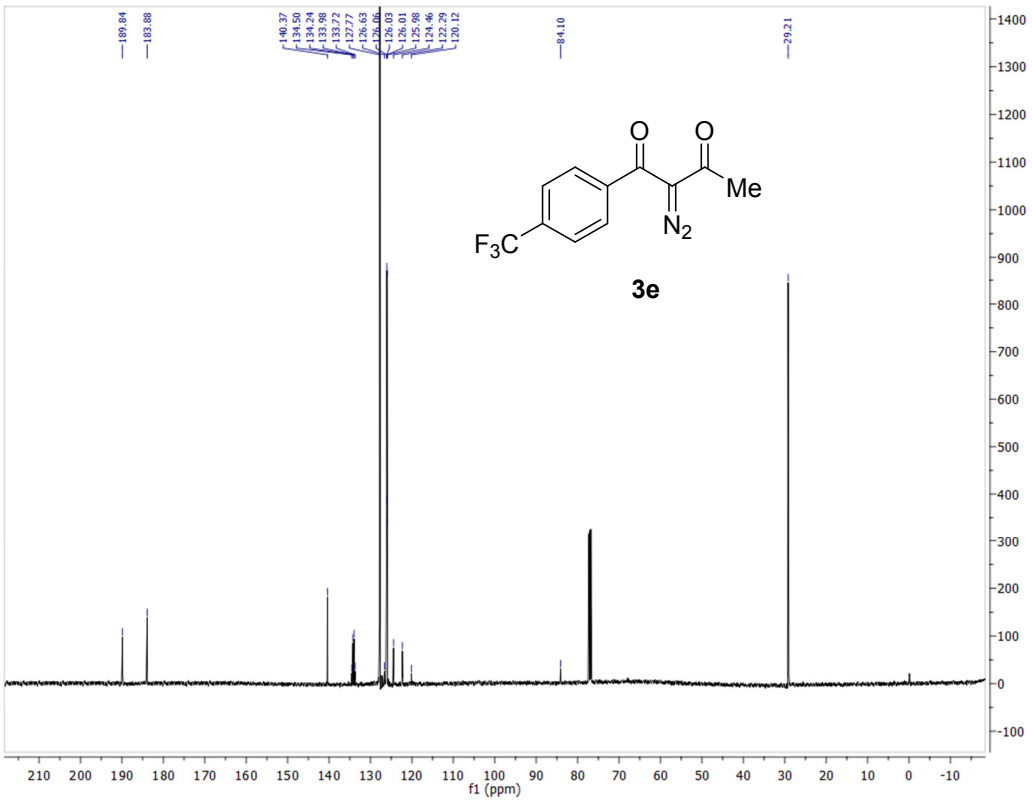
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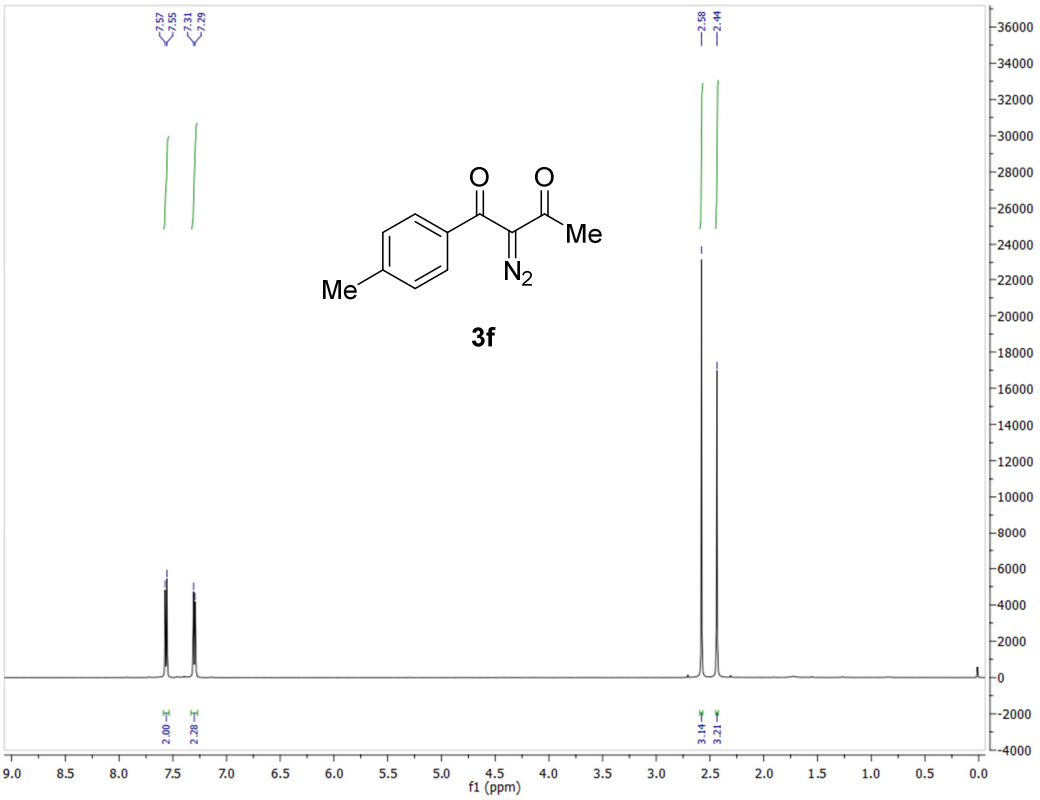
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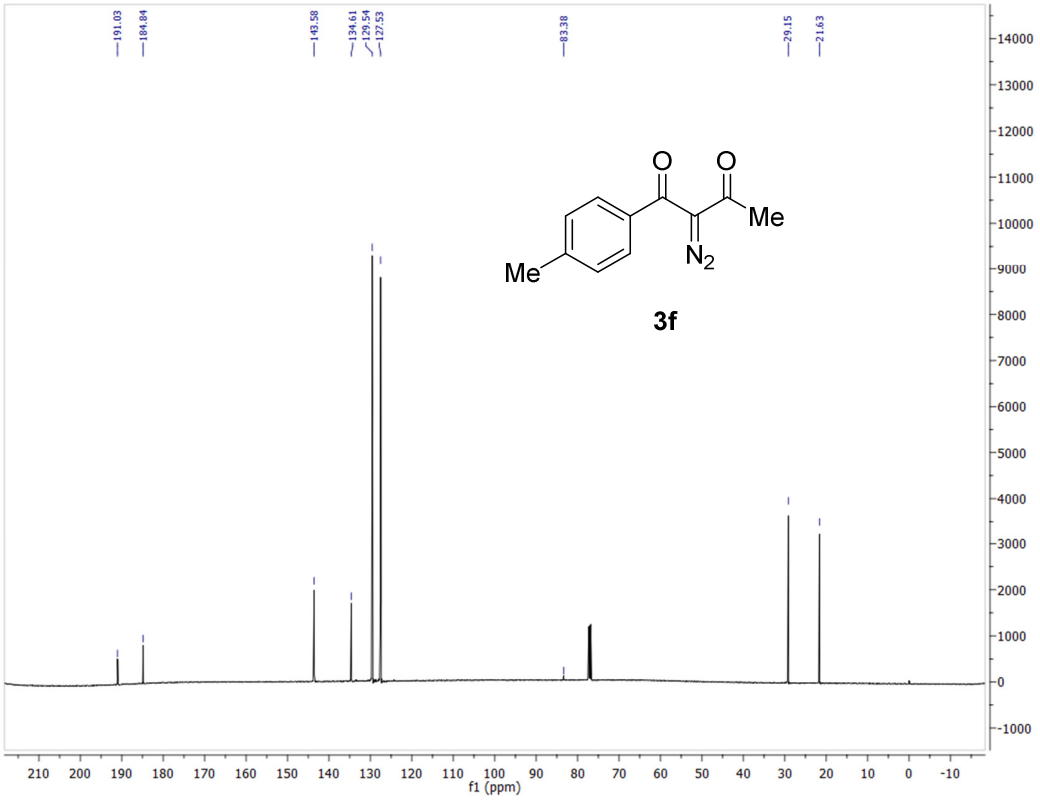
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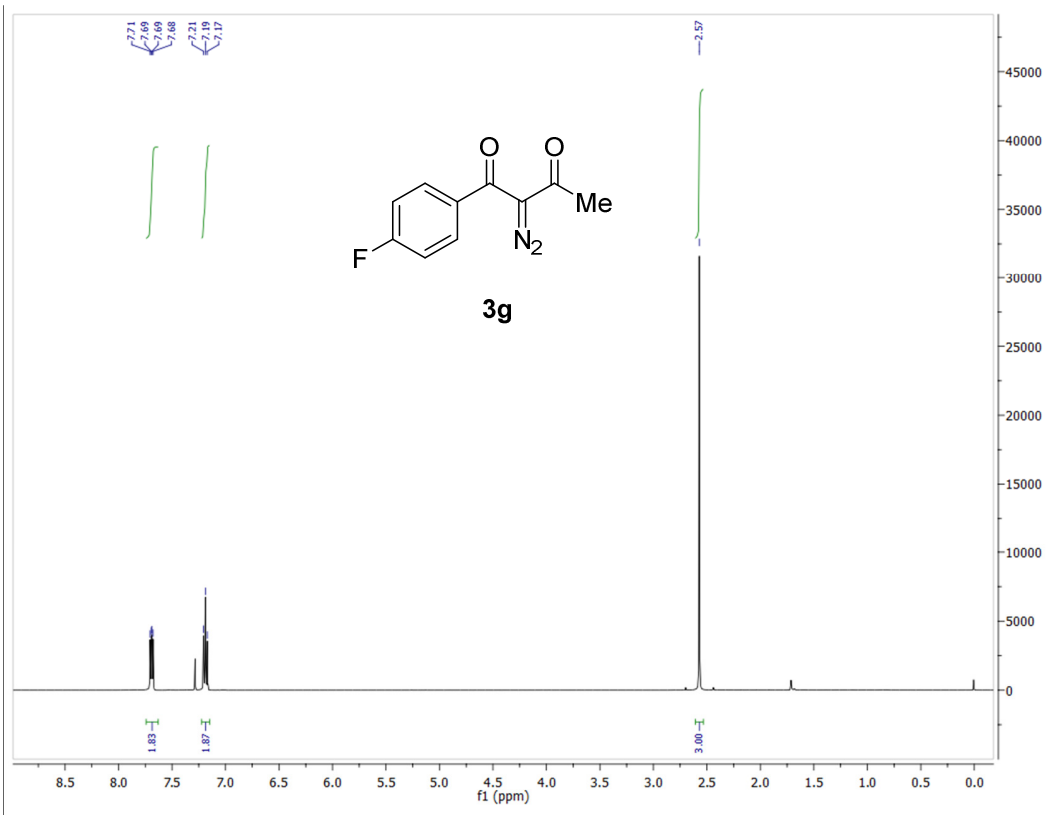
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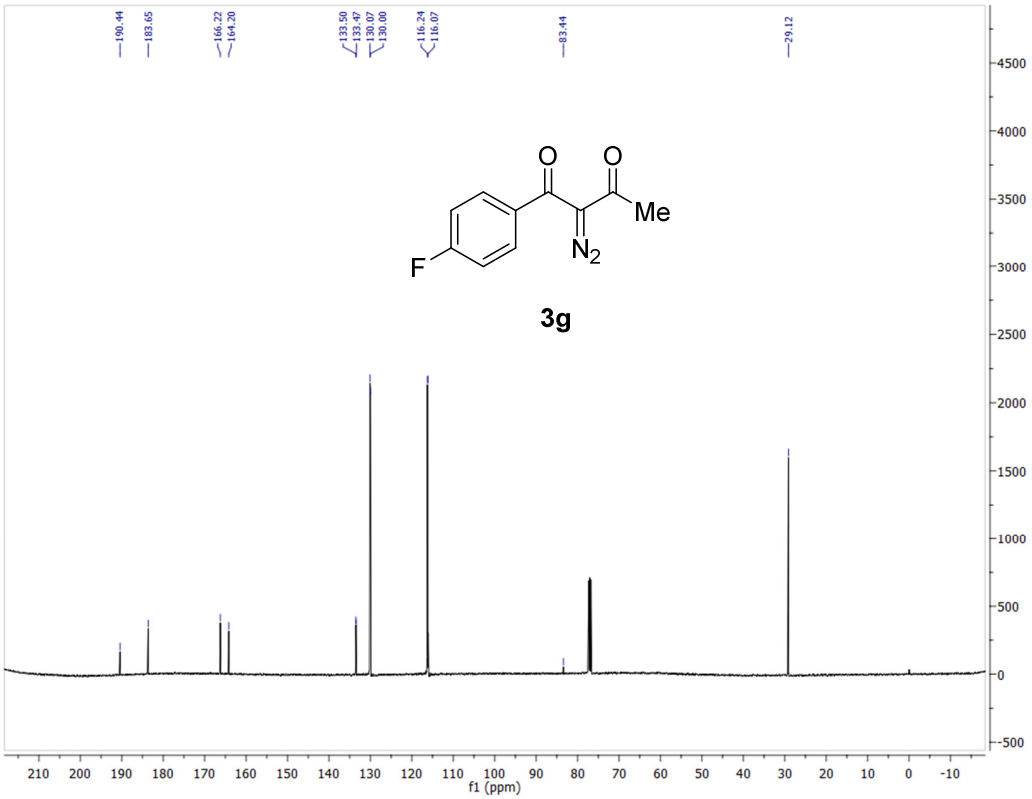
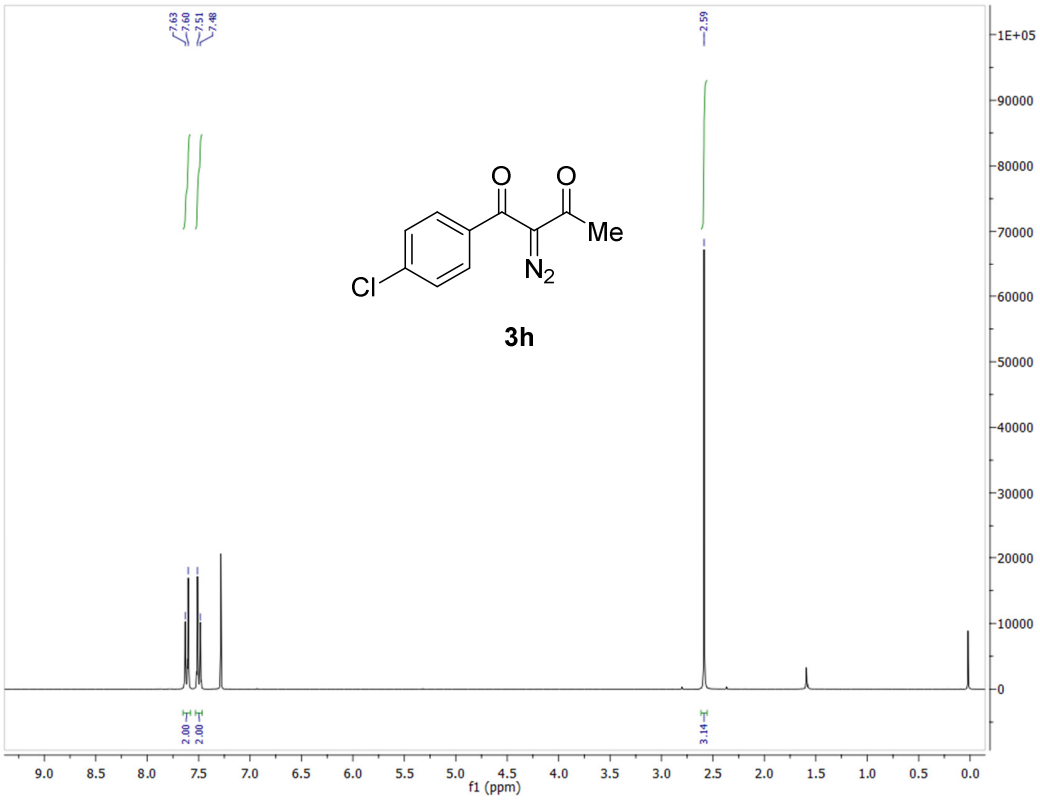
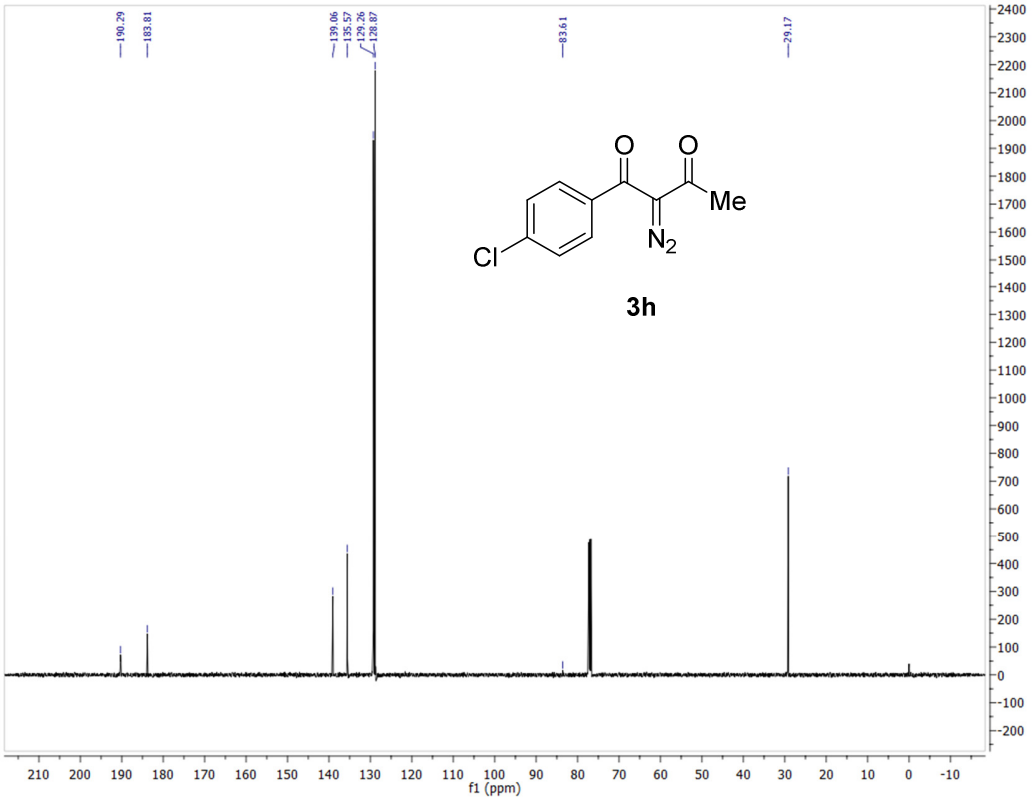
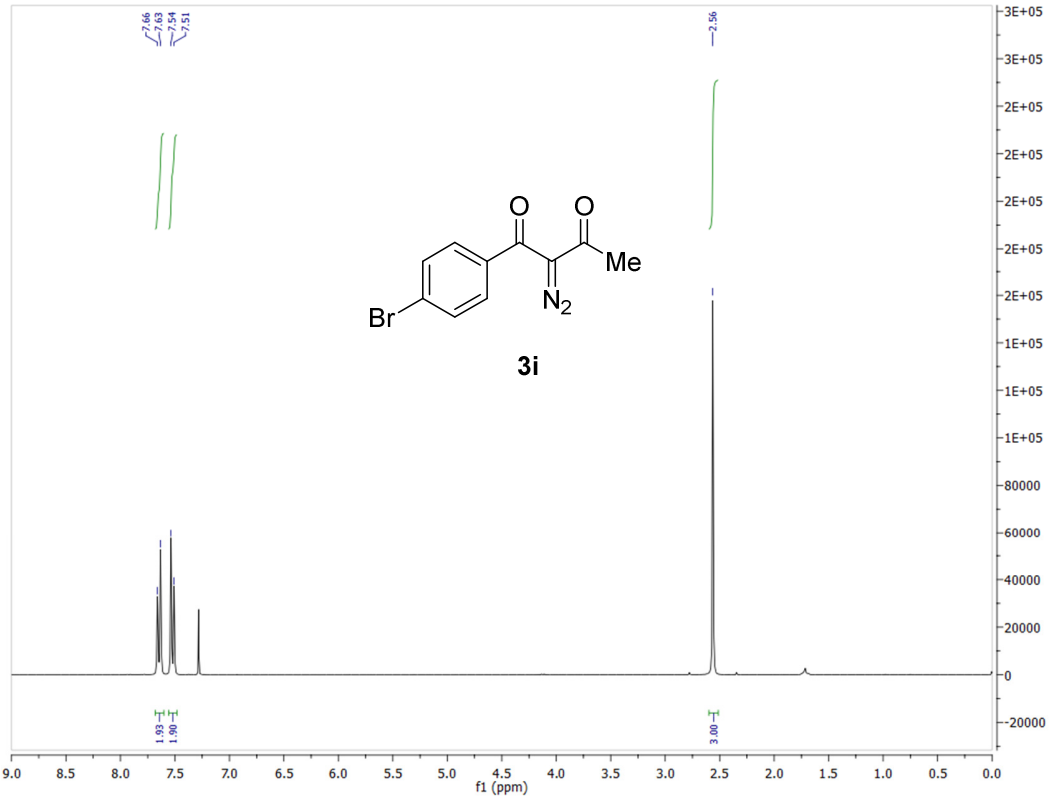
N2
F
3g
1.83
1.87
3.00
f1 (ppm)

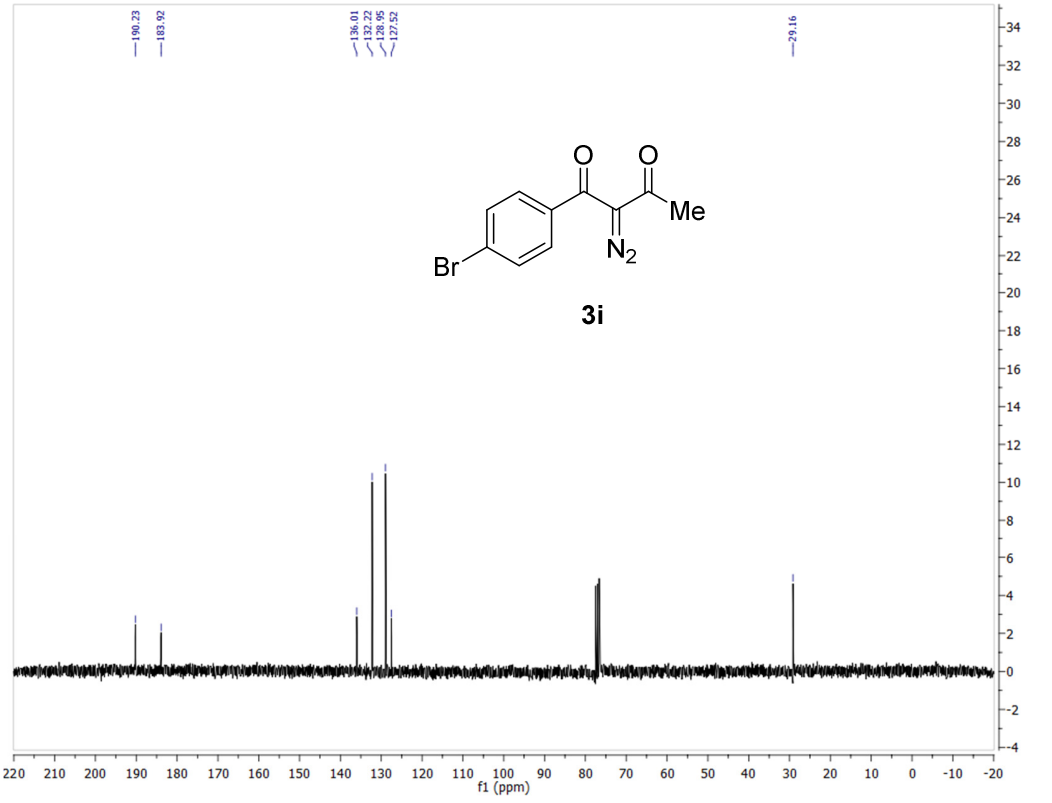

190.44
183.65
166.22
164.20
133.50
133.47
130.07
130.00
116.24
116.07
83.44
29.12
O
O
Me
N2
F
3g
f1 (ppm)


7.63
7.60
7.51
7.48
2.59
2.00
2.00
3.14
O
O
Me
N2
Cl
3h
f1 (ppm)

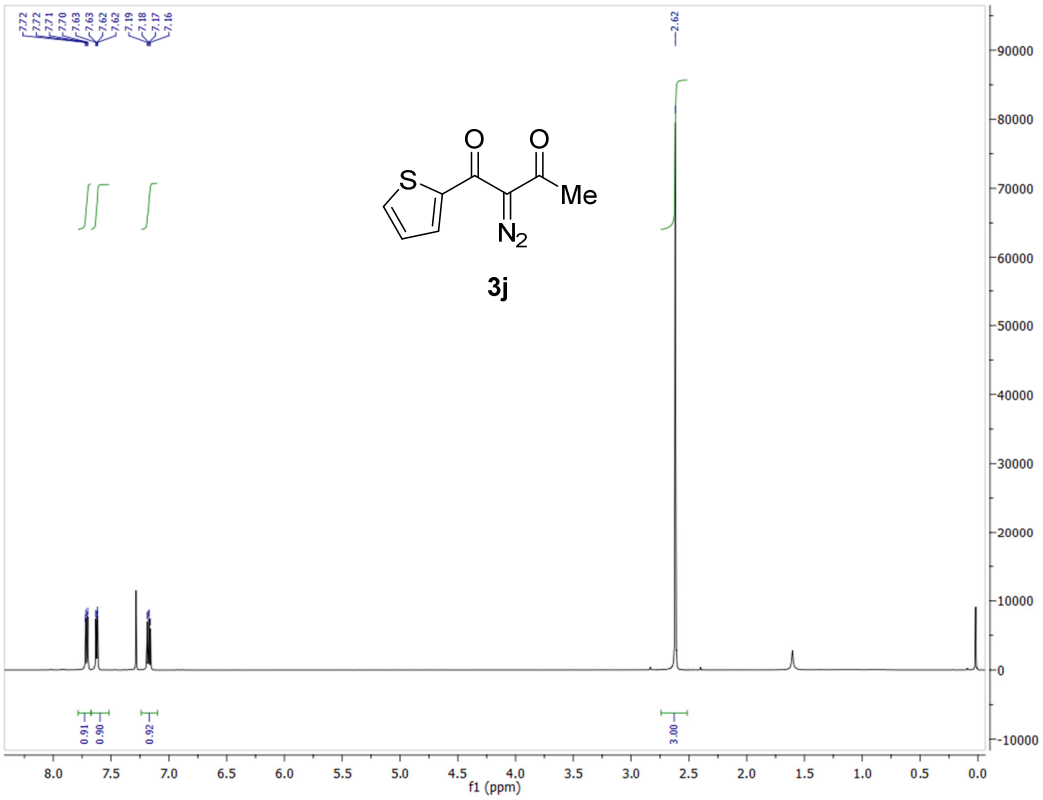

190.29
183.81
139.06
135.57
129.26
128.87
83.61
29.17
O
O
Me
N2
Cl
3h
f1 (ppm)

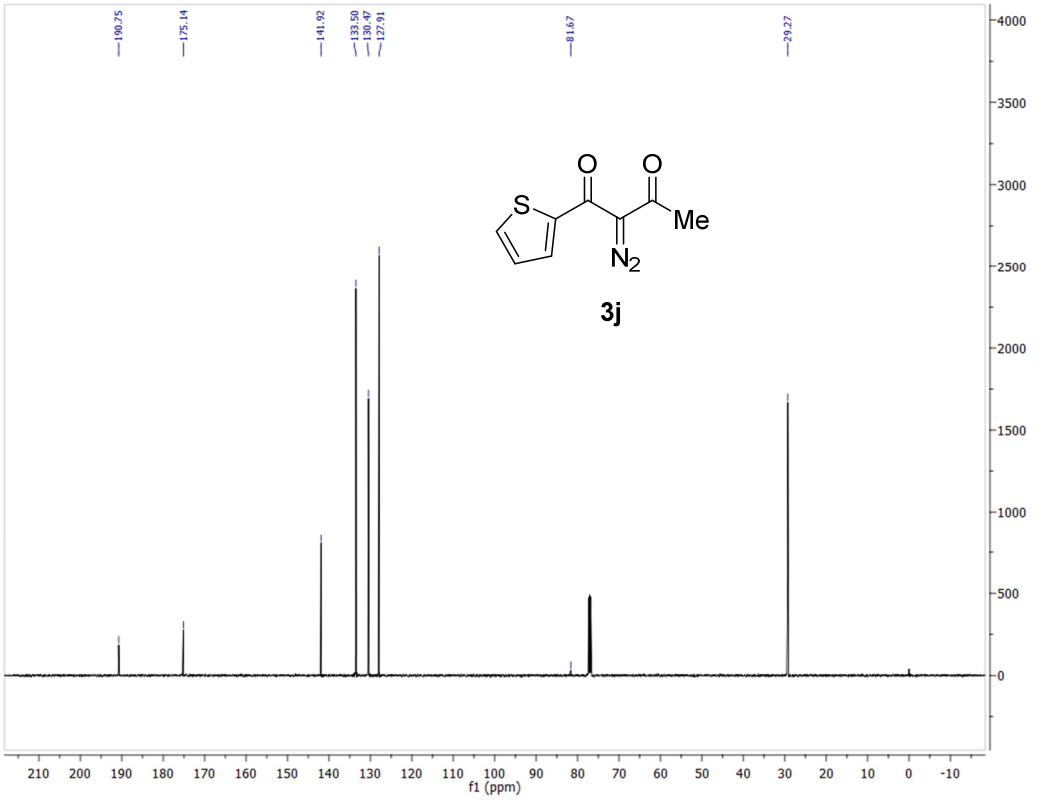

7.66
7.63
7.54
7.51
2.56
O
O
Me
N2
Br
1.93
1.90
3.00
f1 (ppm)

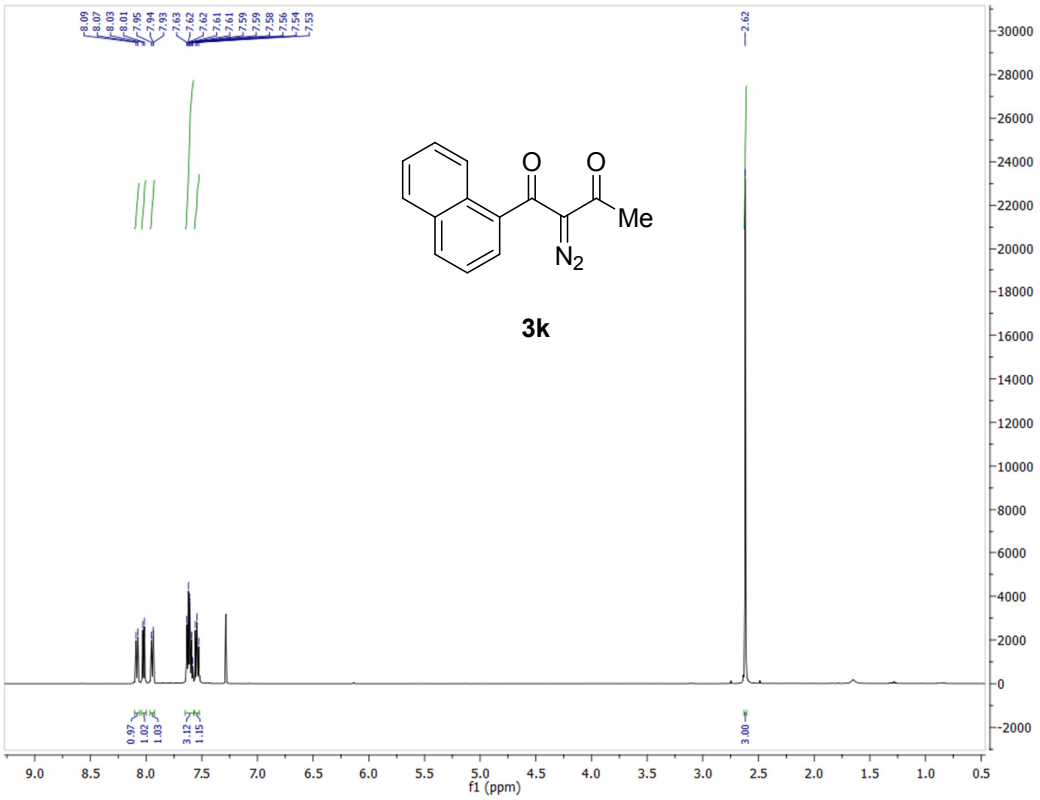
3i

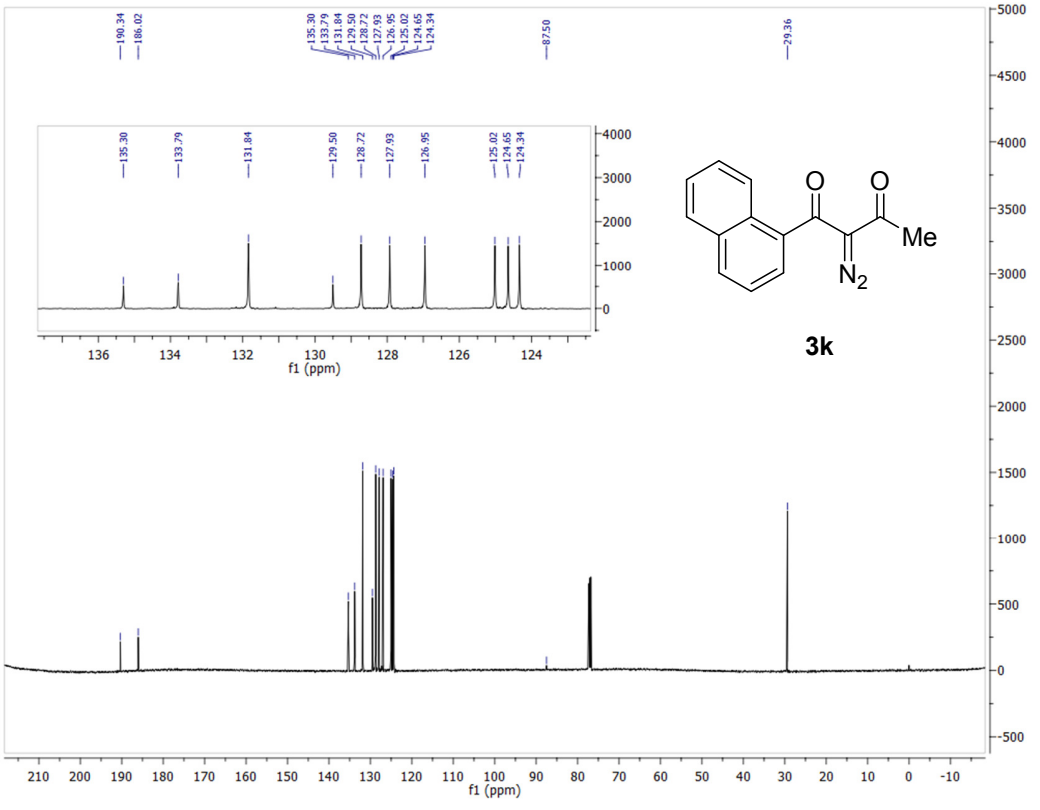

190.23
183.92
136.01
132.22
128.95
127.52
29.16
O
O
Me
N2
Br
f1 (ppm)

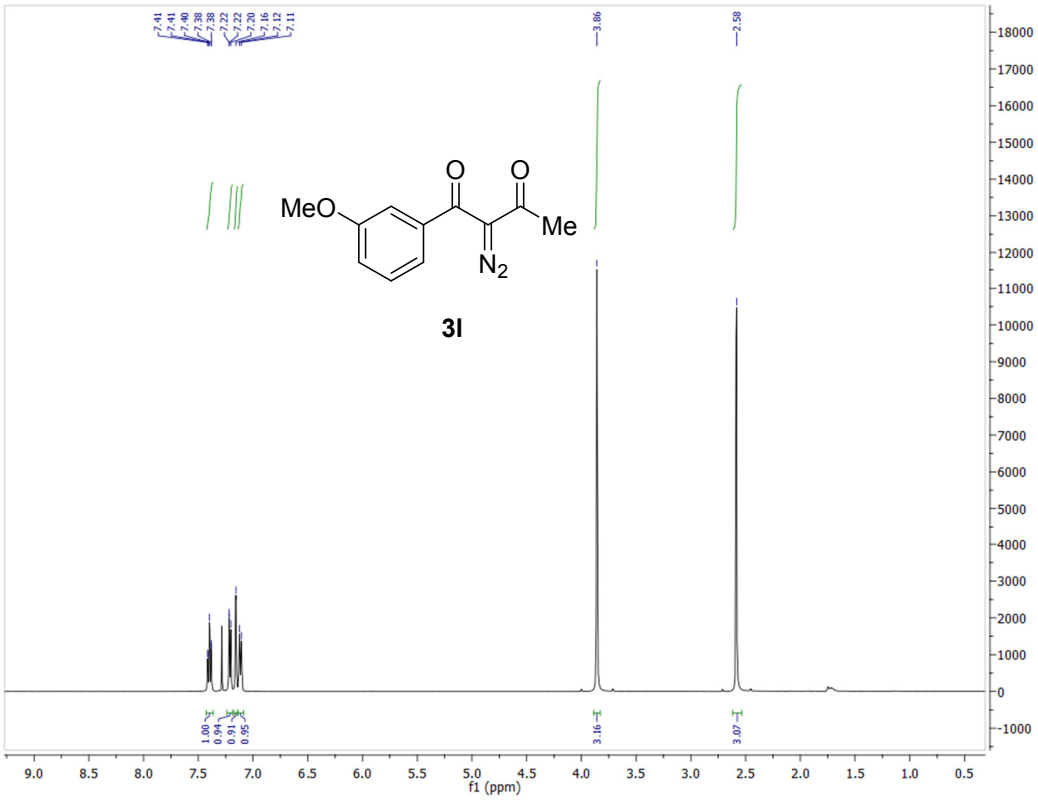
3i

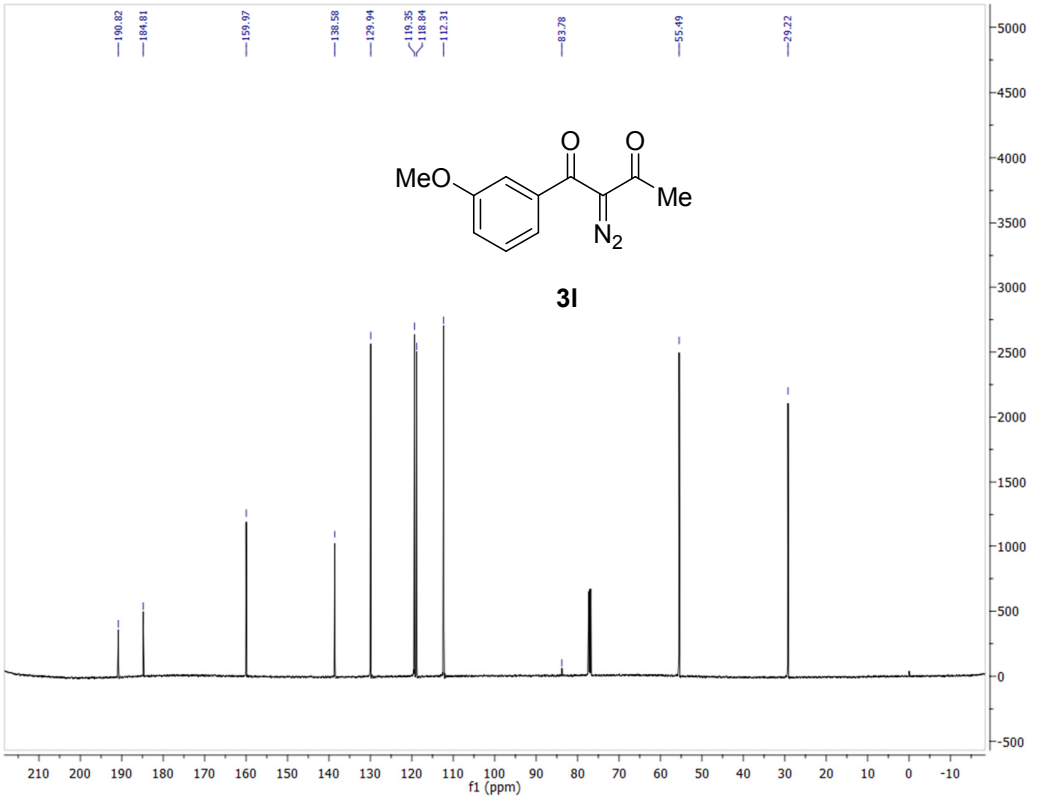

7.72
7.72
7.71
7.70
7.63
7.63
7.62
7.62
7.18
7.18
7.17
7.16
2.62
O
O
S
Me
N2
3j
0.91
0.90
0.92
3.00
f1 (ppm)

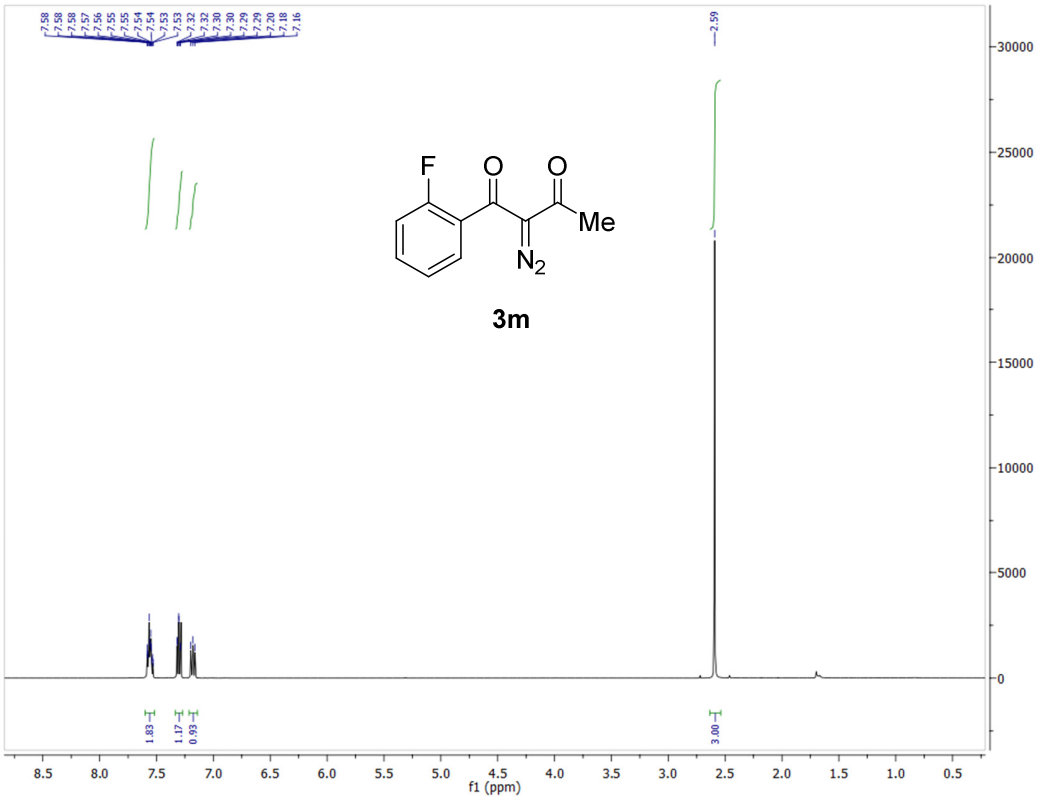

190.75
175.14
141.92
133.59
130.47
127.91
81.67
29.27
O
O
S
Me
N2
3j
f1 (ppm)

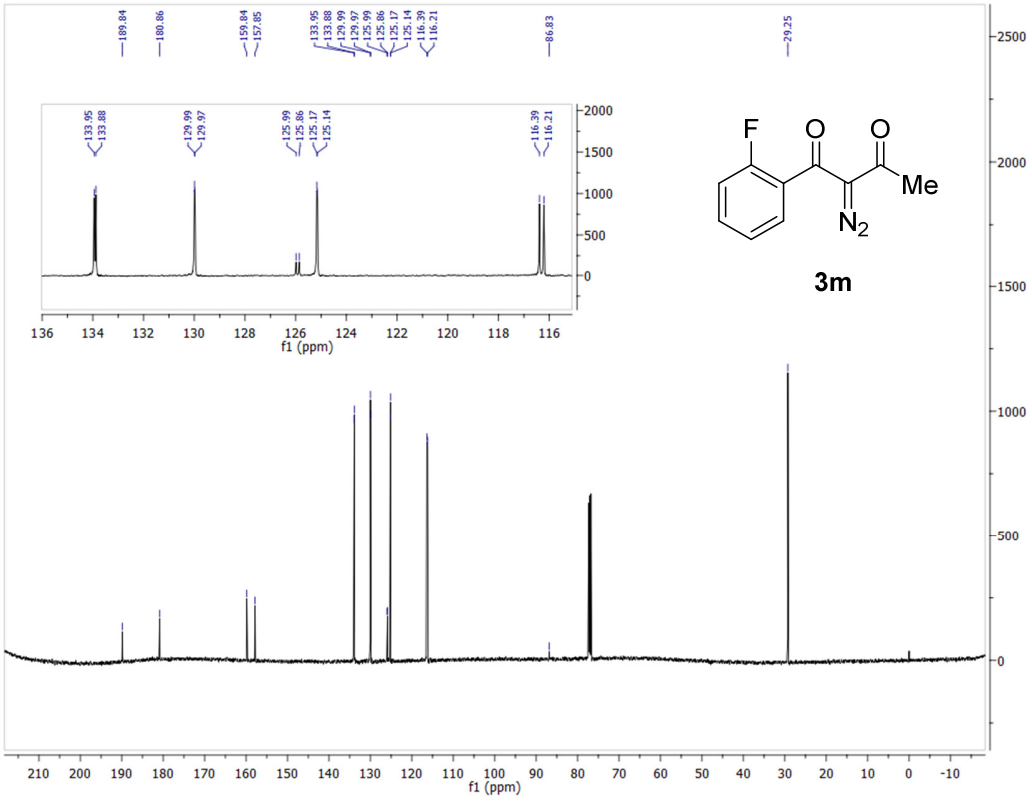

8.09
8.07
8.03
8.01
7.95
7.94
7.93
7.63
7.62
7.62
7.61
7.61
7.59
7.59
7.58
7.56
7.54
7.53
2.62
O
O
Me
N2
3k
0.97
1.02
1.03
3.12
1.15
3.00
f1 (ppm)

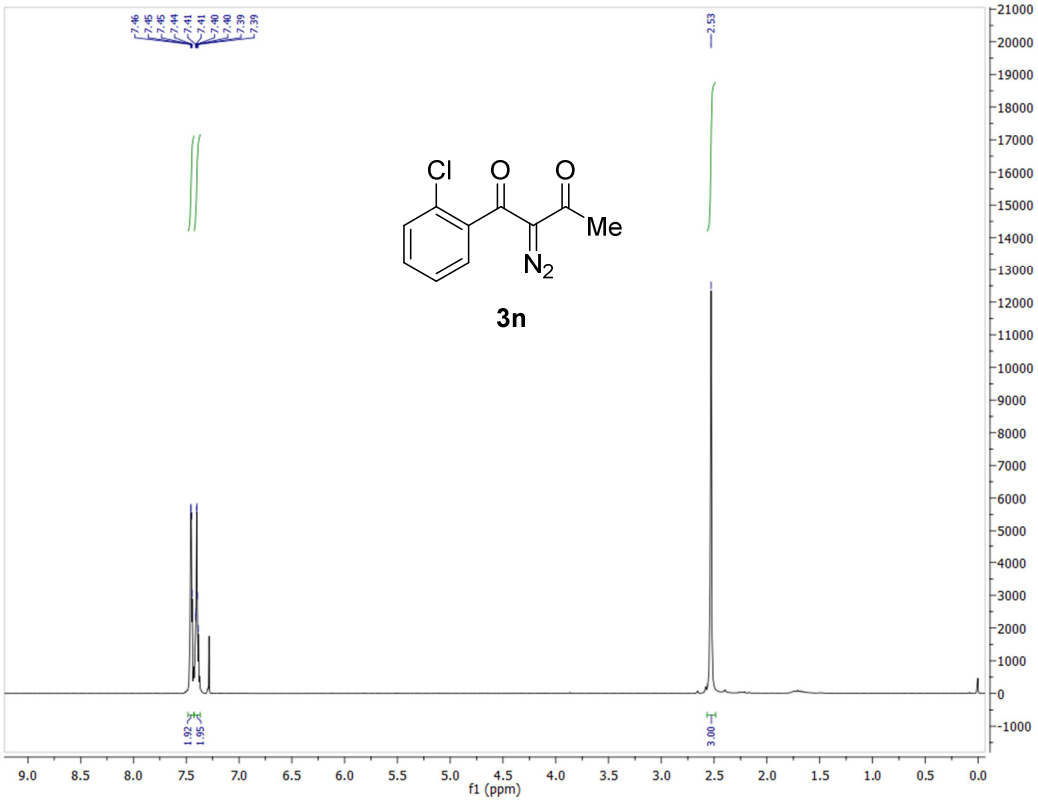

190.34
186.02
135.30
133.79
131.84
129.50
128.72
127.93
126.95
125.02
124.65
124.34
87.50
29.36
f1 (ppm)
O
O
Me
N2
3k

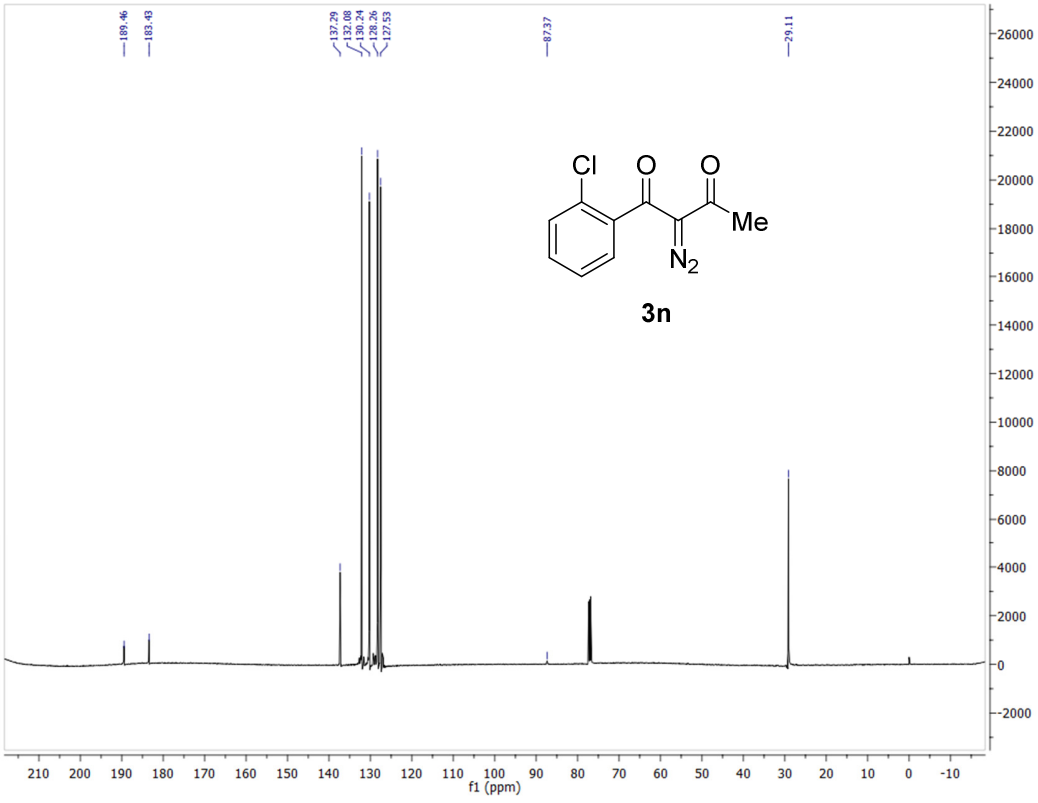

7.41
7.41
7.40
7.38
7.38
7.22
7.20
7.16
7.12
7.11
3.86
2.58
MeO
O
O
Me
N2
3l
1.00
0.94
0.91
0.95
3.16
3.07
f1 (ppm)

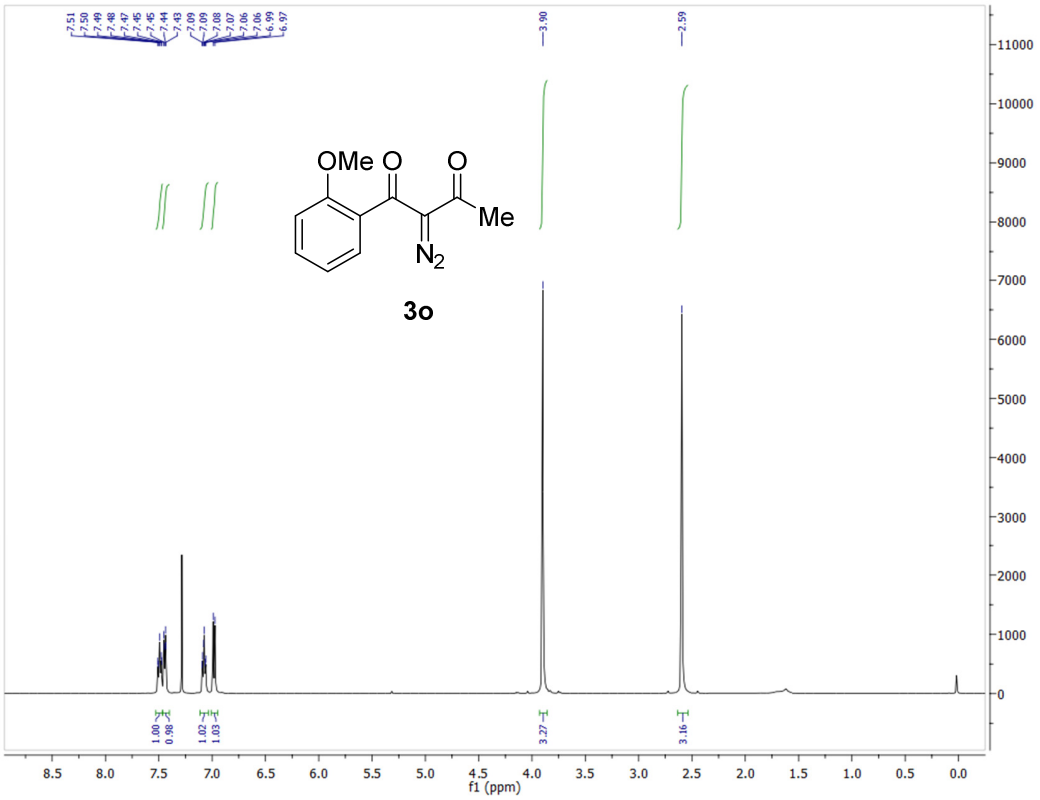

190.82
184.81
159.97
138.58
129.94
119.35
118.84
112.31
83.78
55.49
29.22
MeO
O
O
Me
N2
3l
f1 (ppm)

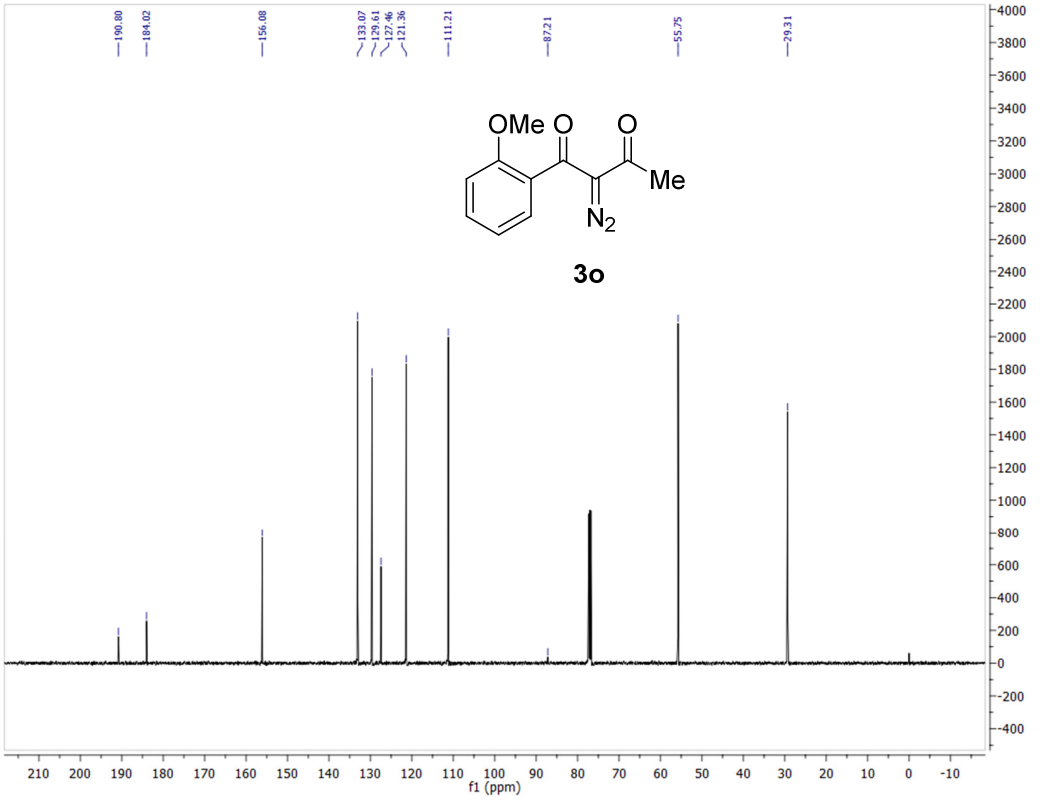

F
O
O
Me
N2
3m
f1 (ppm)

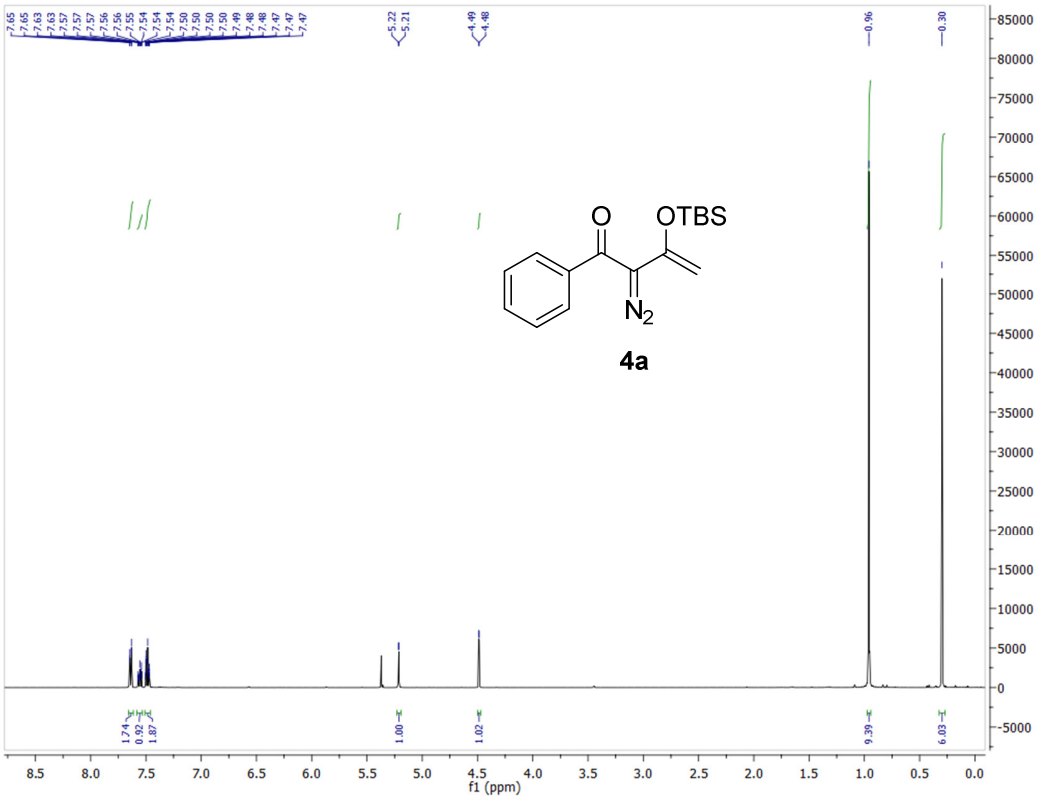

F
O
O
Me
N2
3m
f1 (ppm)

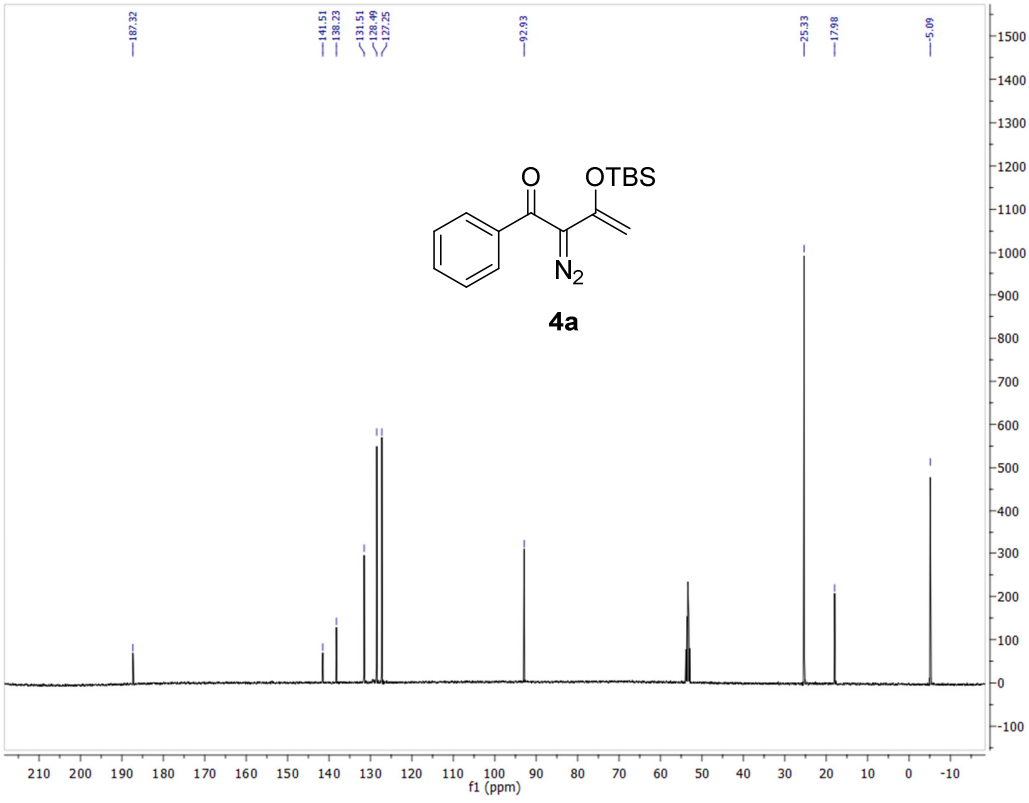

7.46
7.45
7.45
7.44
7.41
7.40
7.40
7.39
7.39
2.53
Cl
O
O
Me
N2
3n
1.92
1.95
3.00
f1 (ppm)

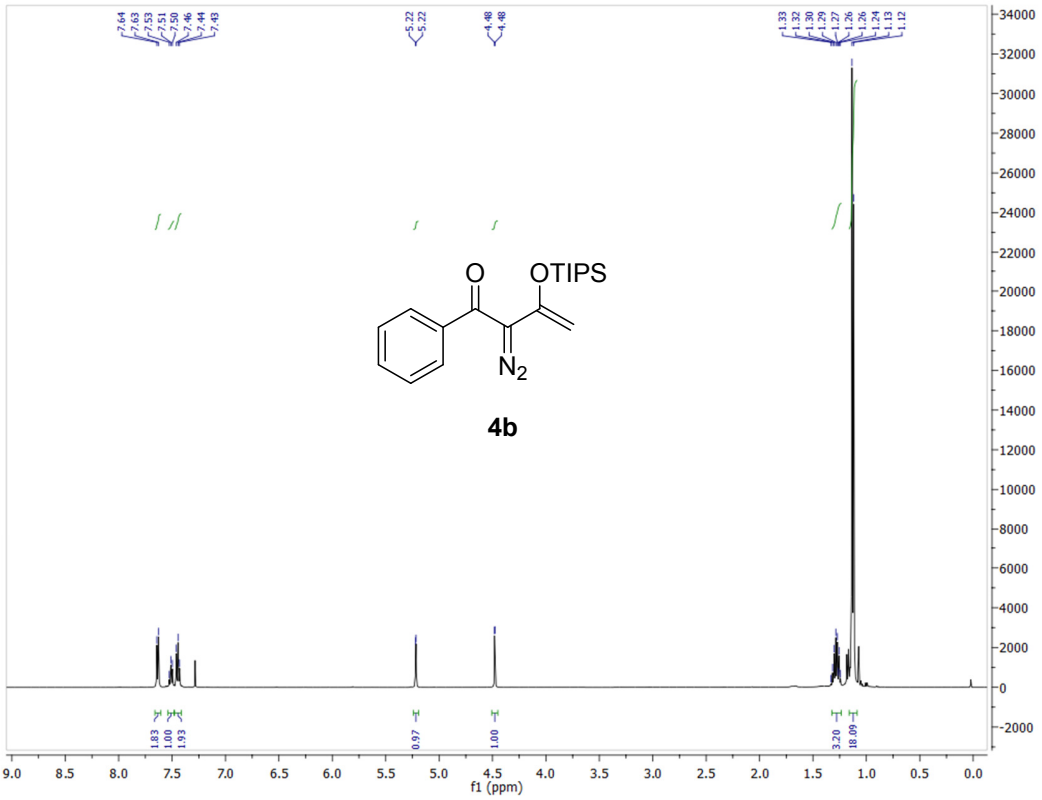

189.46
183.43
137.29
132.08
130.24
128.26
127.53
87.37
29.11
Cl
O
O
Me
N2
3n
f1 (ppm)

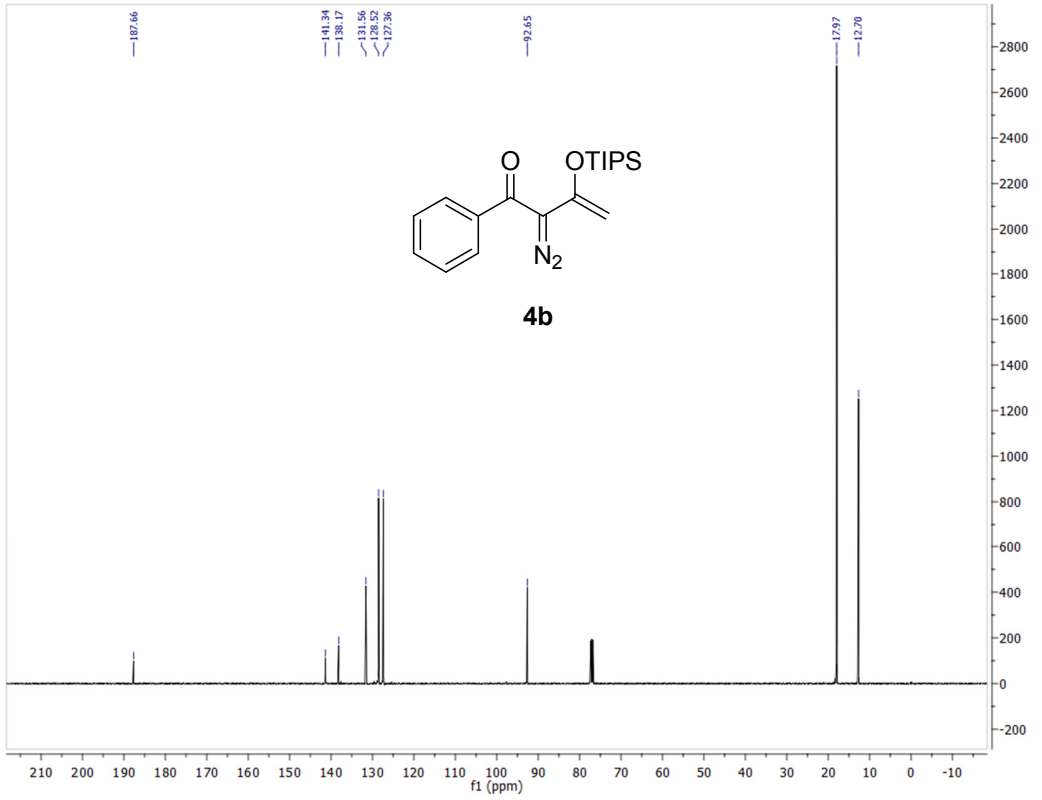

OMe O O
Me
N2
3o
f1 (ppm)


OMe O O
Me
N2
3o
f1 (ppm)


O
OTBS
N2
4a
f1 (ppm)


O
OTBS
N2
4a
f1 (ppm)


7.64
7.63
7.53
7.51
7.50
7.46
7.44
7.43
5.22
5.22
4.48
4.48
1.33
1.32
1.30
1.29
1.27
1.26
1.26
1.24
1.13
1.12
O
OTIPS
N2
4b
1.83
1.00
1.93
0.97
1.00
3.20
18.09
f1 (ppm)


187.66
141.34
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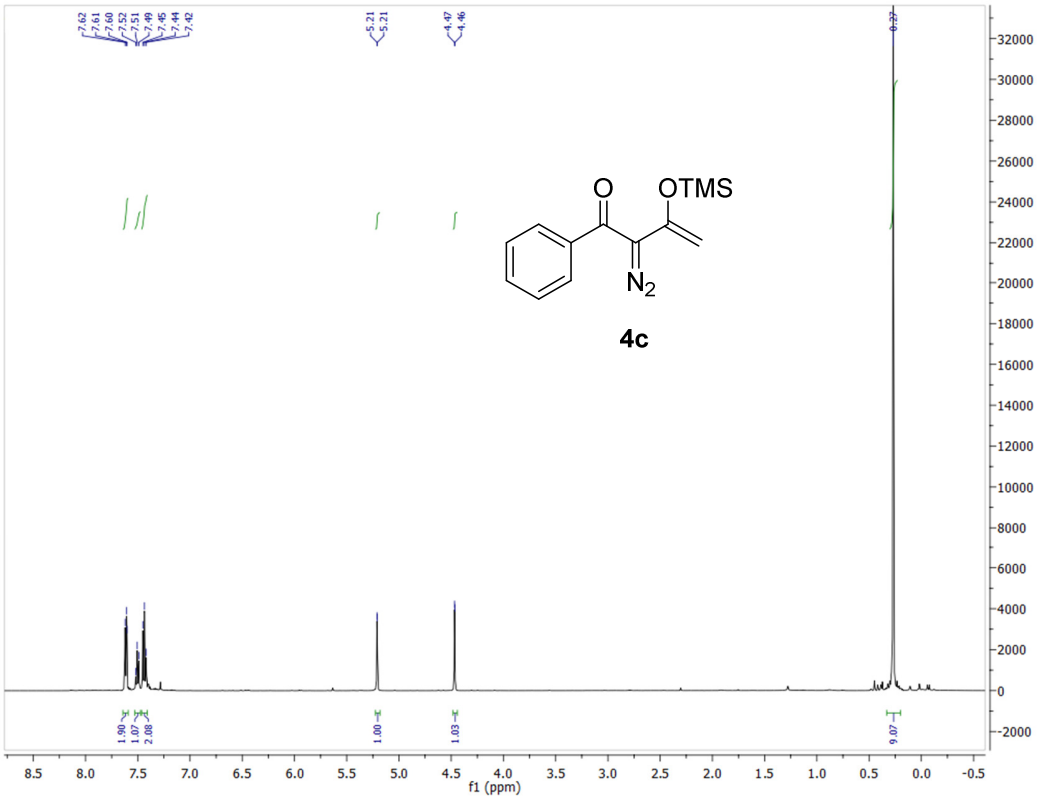
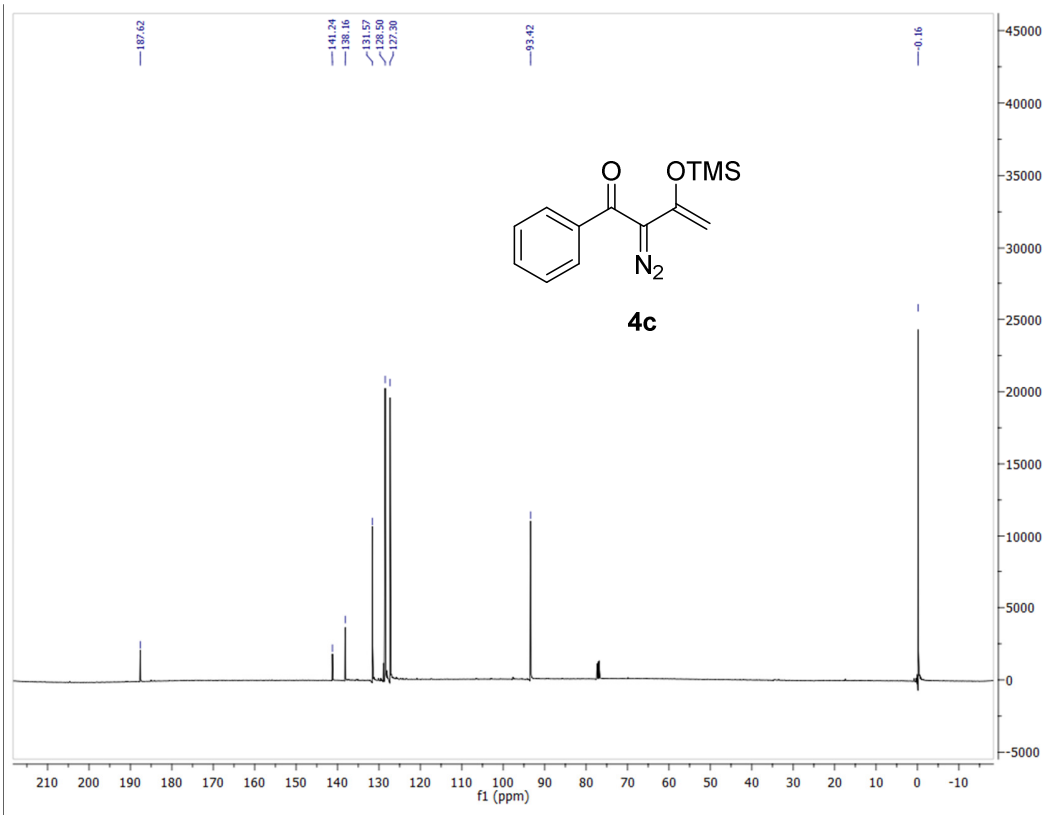
128.52
127.36
92.65
17.97
12.70
O
OTIPS
N2
4b
f1 (ppm)


7.62
7.61
7.60
7.52
7.51
7.49
7.45
7.44
7.42
5.21
5.21
4.47
4.46
0.27
O
OTMS
N2
4c
1.90
1.07
2.08
1.00
1.03
9.07
f1 (ppm)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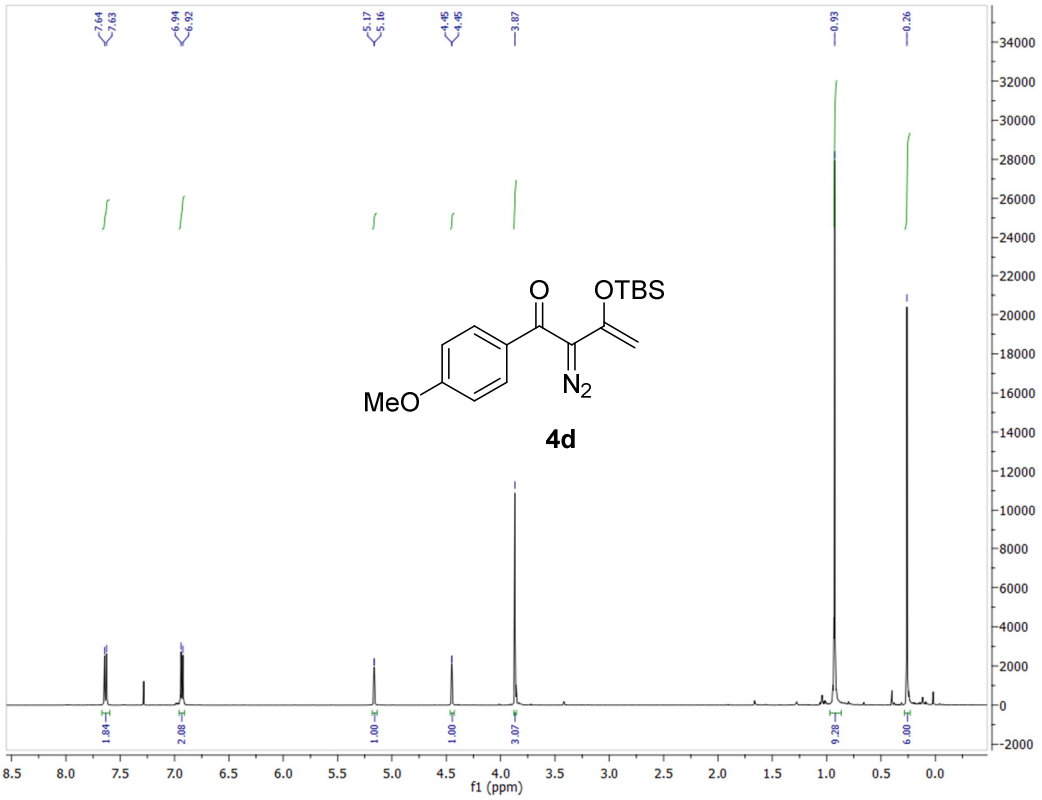
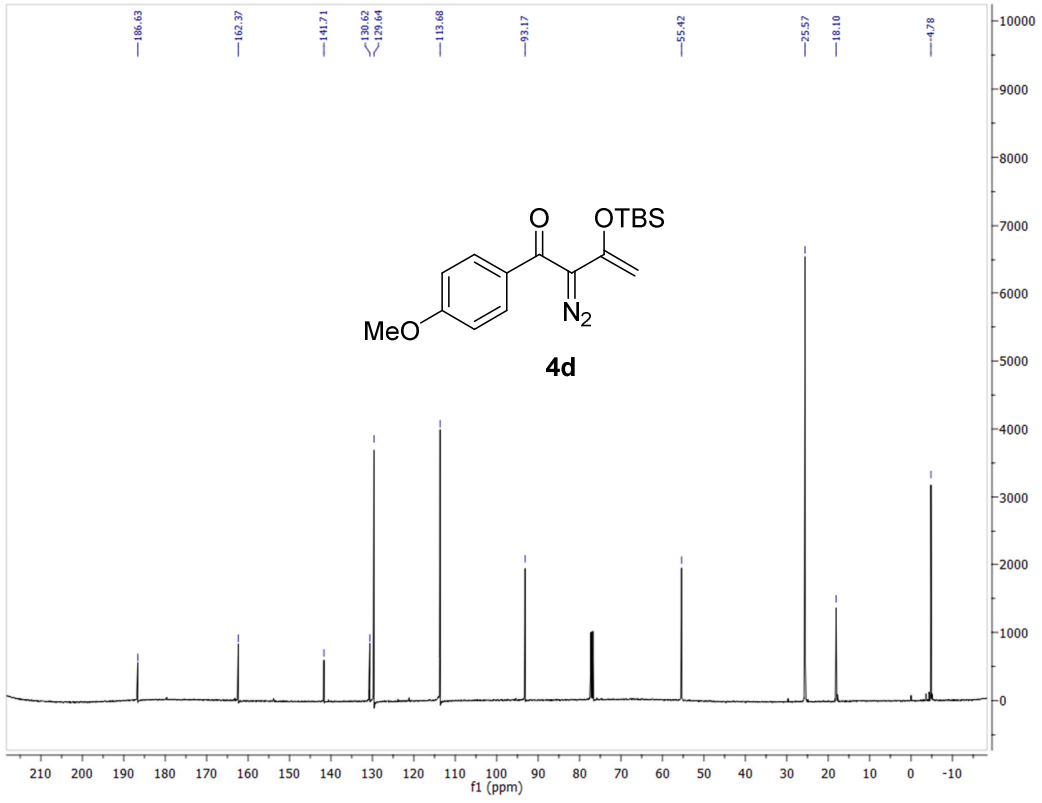
141.24
138.16
131.57
128.50
127.30
93.42
0.16
O
OTMS
N2
4c
f1 (ppm)


7.64
7.63
6.94
6.92
5.17
5.16
4.45
4.45
3.87
0.93
0.26
O
OTBS
N2
MeO
4d
1.84
2.08
1.00
1.00
3.07
9.28
6.00
f1 (ppm)


186.63
162.37
141.71
130.62
129.64
113.68
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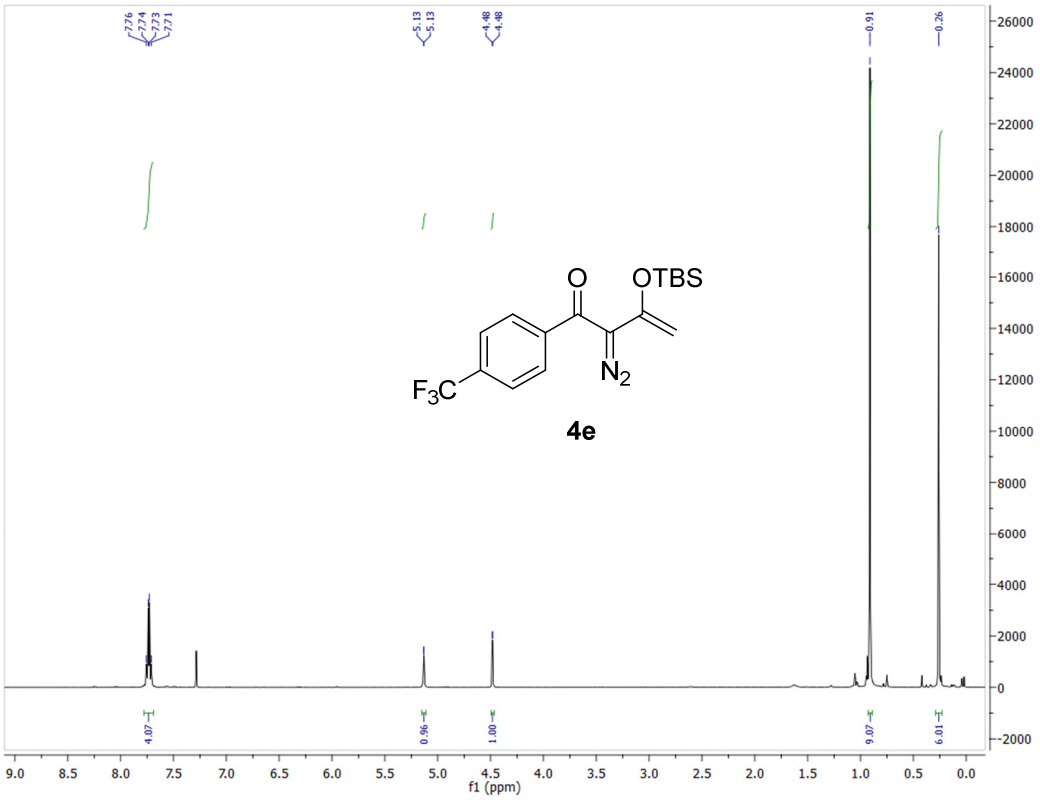
55.42
25.57
18.10
-4.78
O
OTBS
N2
MeO
4d
f1 (ppm)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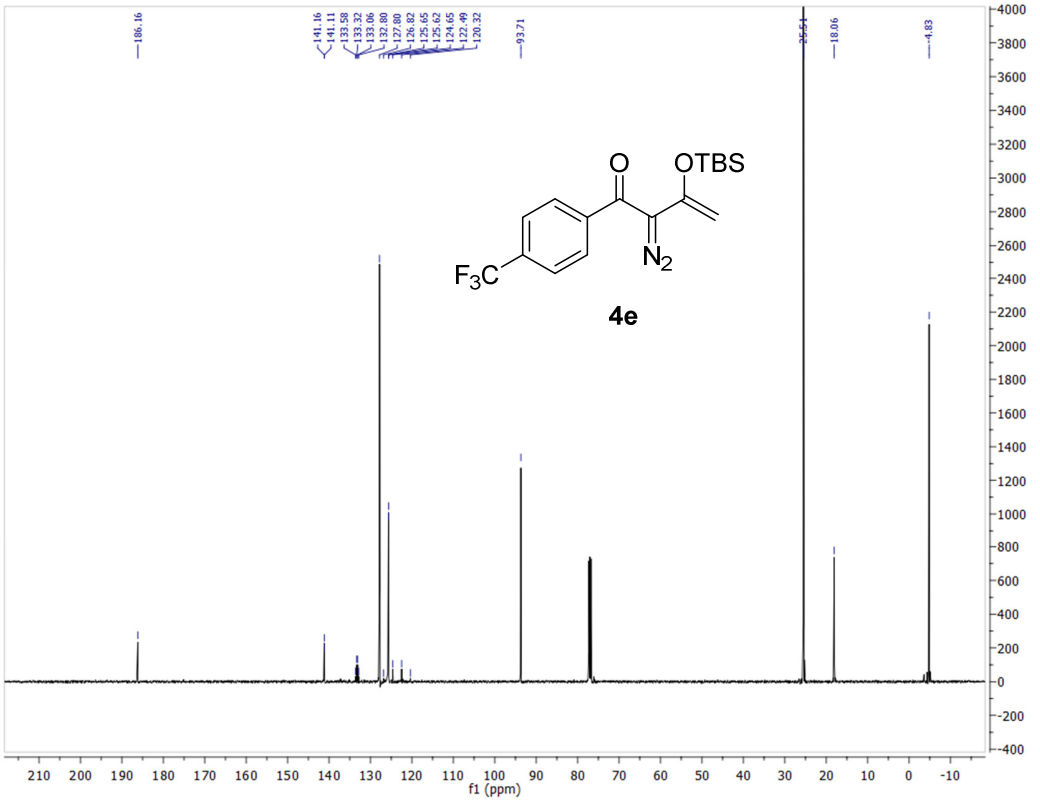
7.74
7.73
7.71
5.13
5.13
4.48
4.48
0.91
0.26
O
OTBS
N2
F3C
4e
4.07
0.96
1.00
9.07
6.01
f1 (ppm)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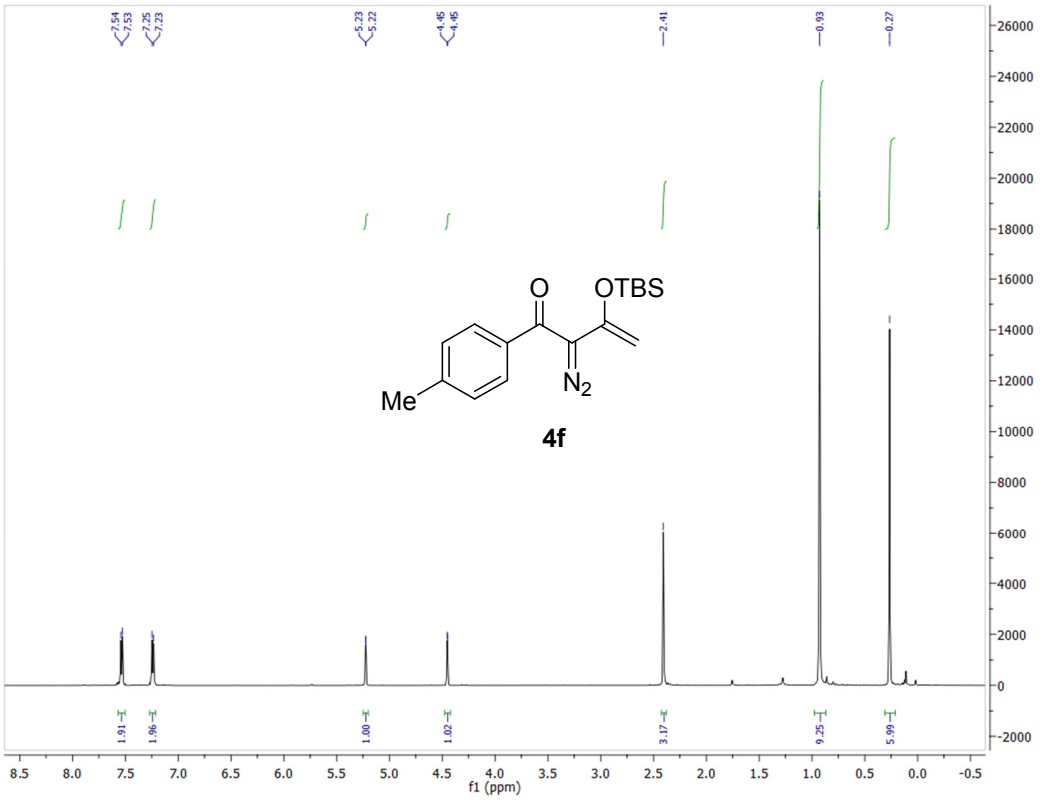
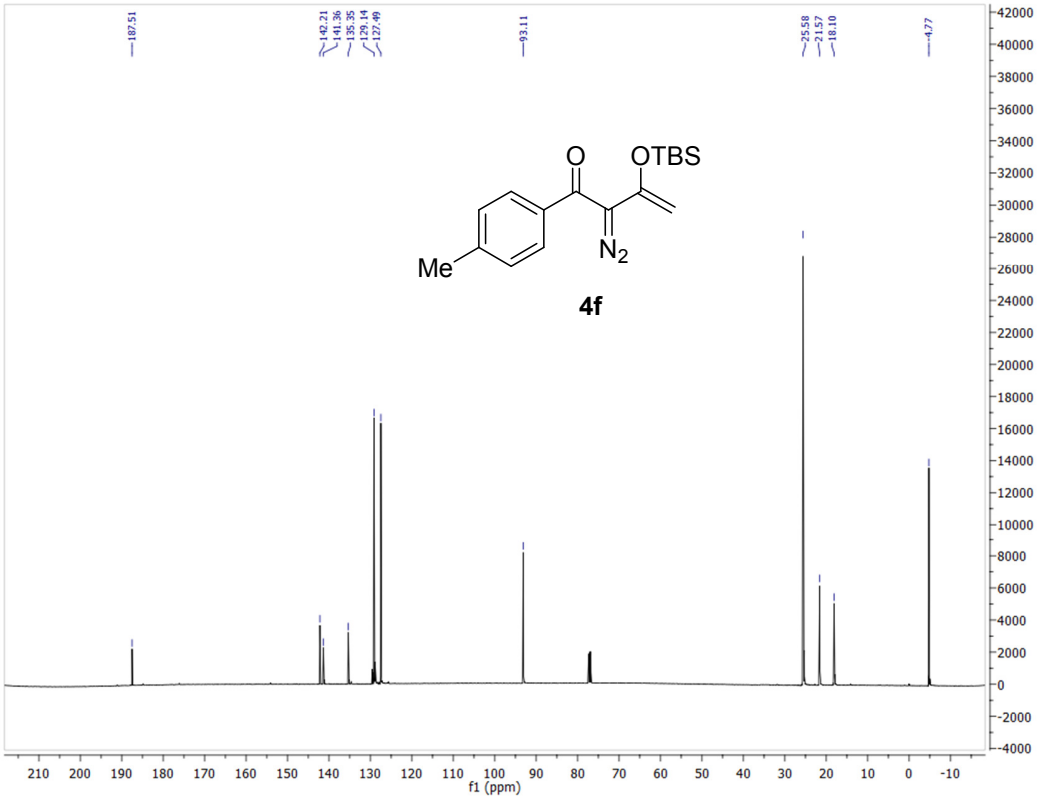
141.16
141.11
133.58
133.32
133.06
132.80
127.80
126.62
125.65
125.62
124.65
122.49
120.32
93.71
25.54
18.06
4.83
O
OTBS
N2
F3C
4e
f1 (ppm)


7.54
7.53
7.25
7.23
5.23
5.22
4.45
4.45
2.41
0.93
0.27
O
OTBS
N2
Me
4f
1.91
1.96
1.00
1.02
3.17
9.25
5.99
f1 (ppm)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135.35
129.14
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93.11
25.58
21.57
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4.77
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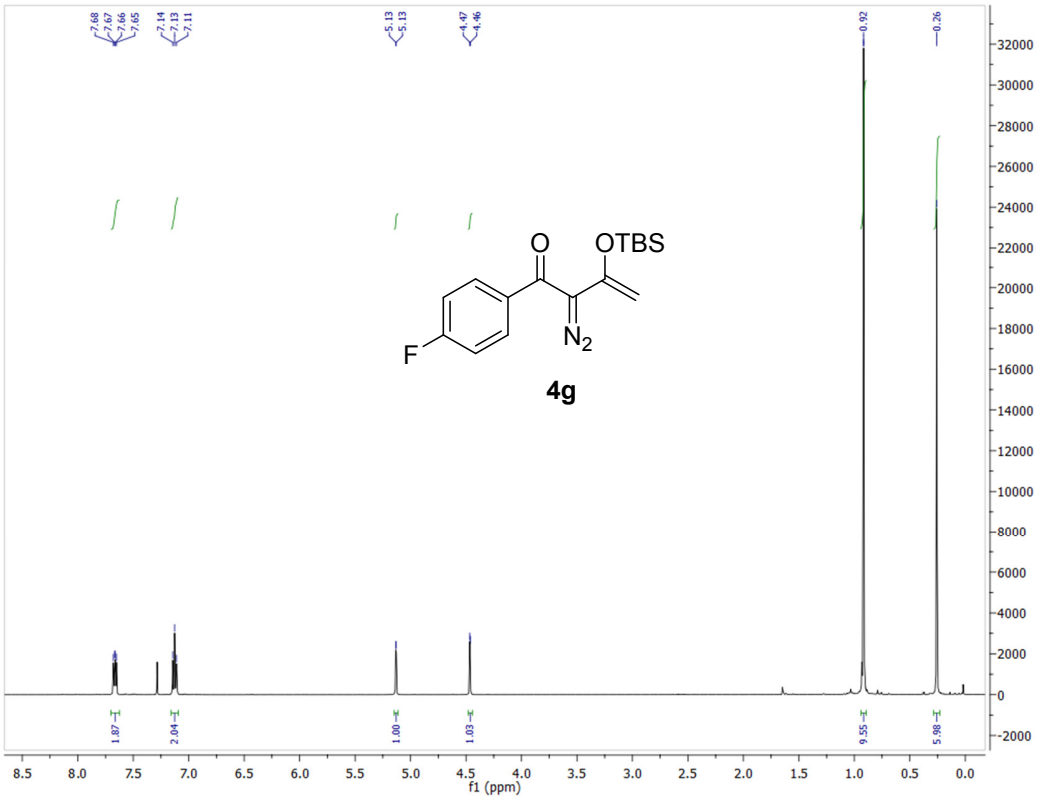
OTBS
N2
Me
4f
f1 (ppm)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7.67
7.66
7.65
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7.13
7.11
5.13
5.13
4.47
4.46
0.92
0.26
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N2
F
4g
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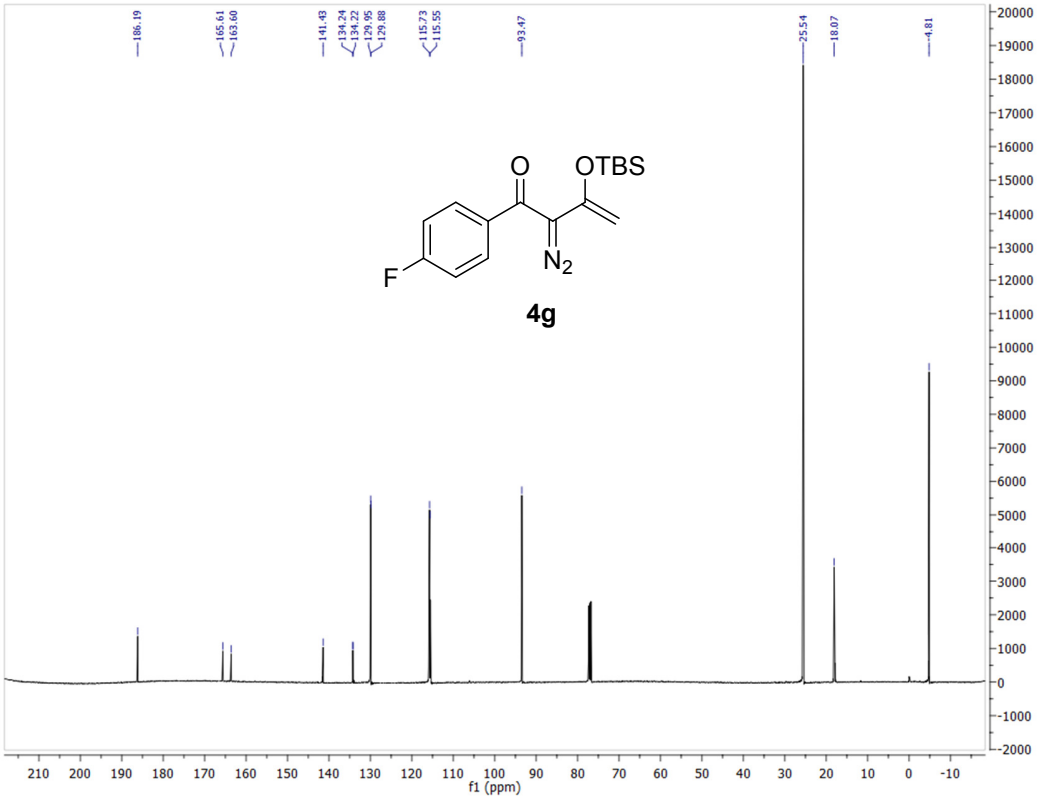
2.04
1.00
1.03
9.55
5.98
f1 (ppm)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134.22
129.95
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93.47
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18.07
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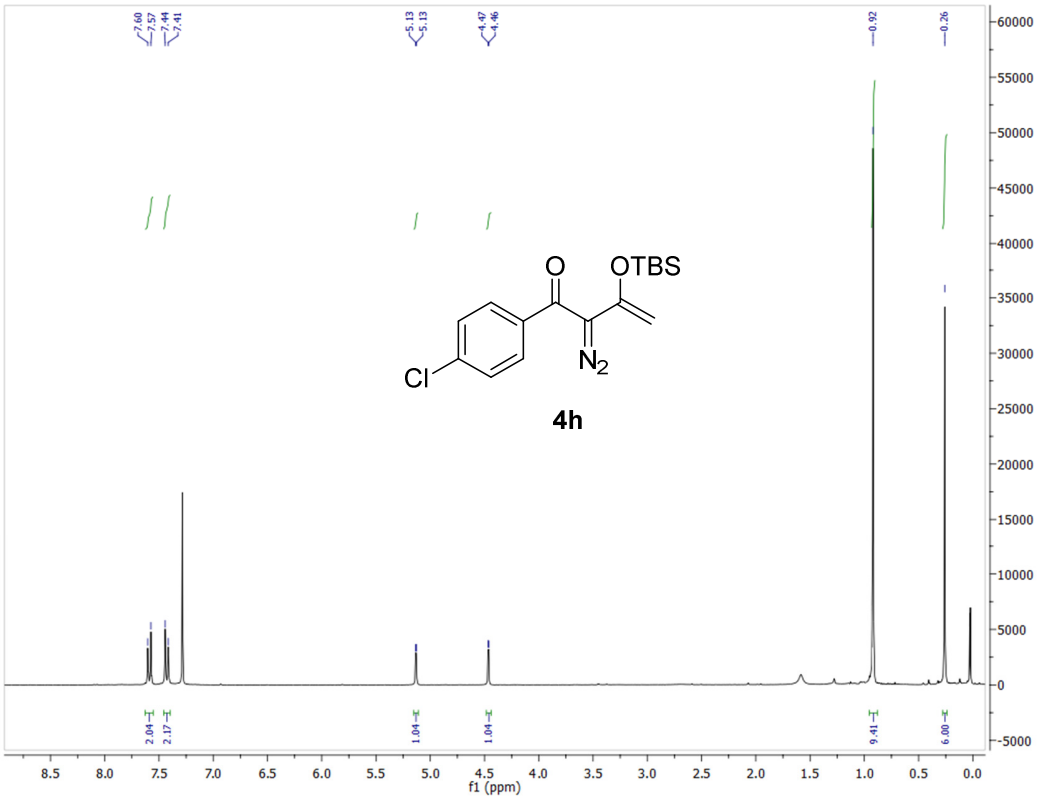
OTBS
N2
F
4g
f1 (ppm)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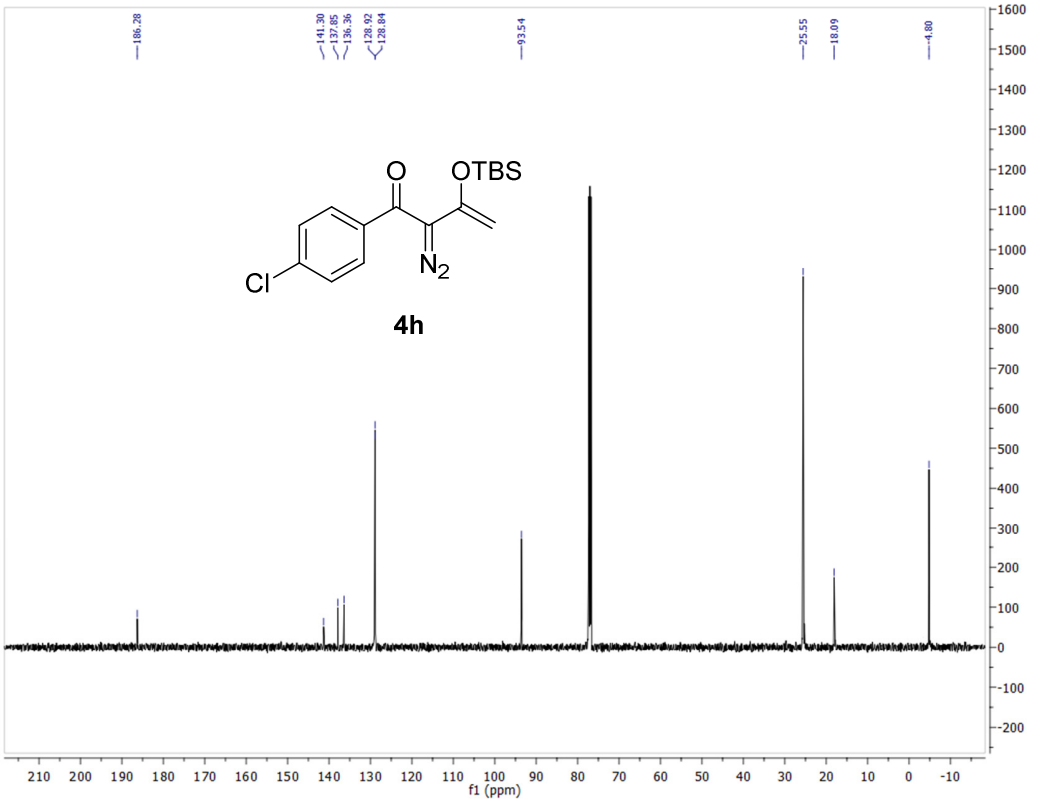
7.57
7.44
7.41
5.13
5.13
4.47
4.46
0.92
0.26
O
OTBS
N2
Cl
4h
2.04
2.17
1.04
1.04
9.41
6.00
f1 (ppm)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137.85
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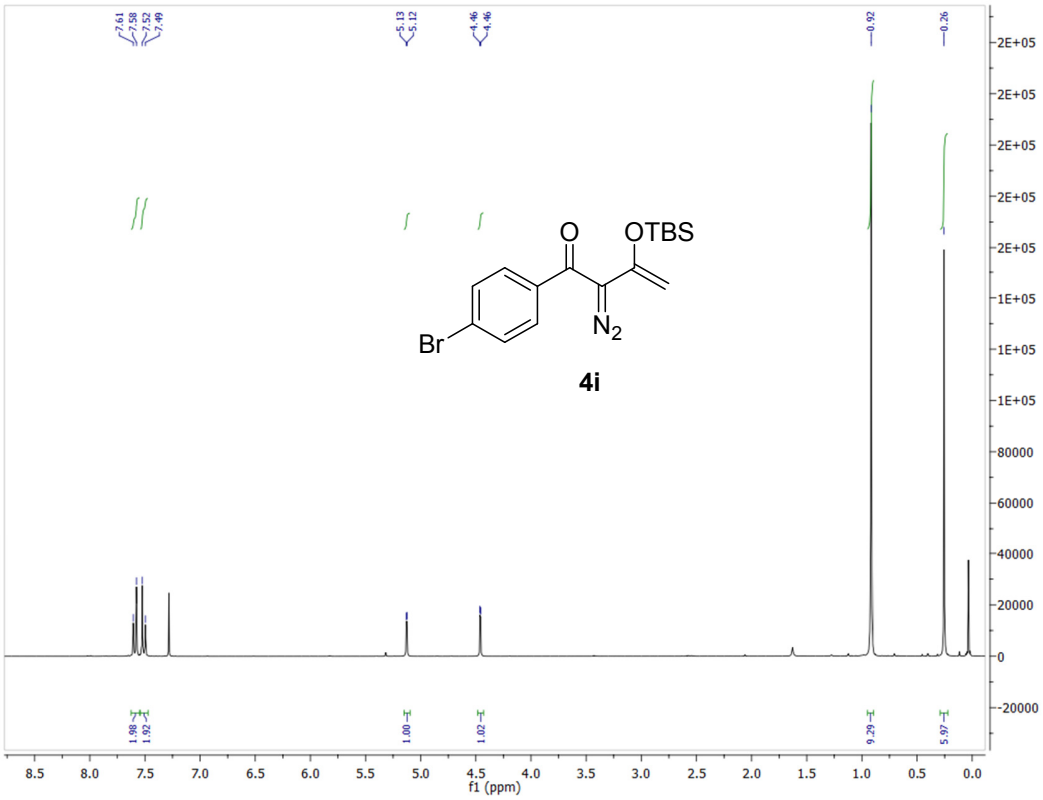
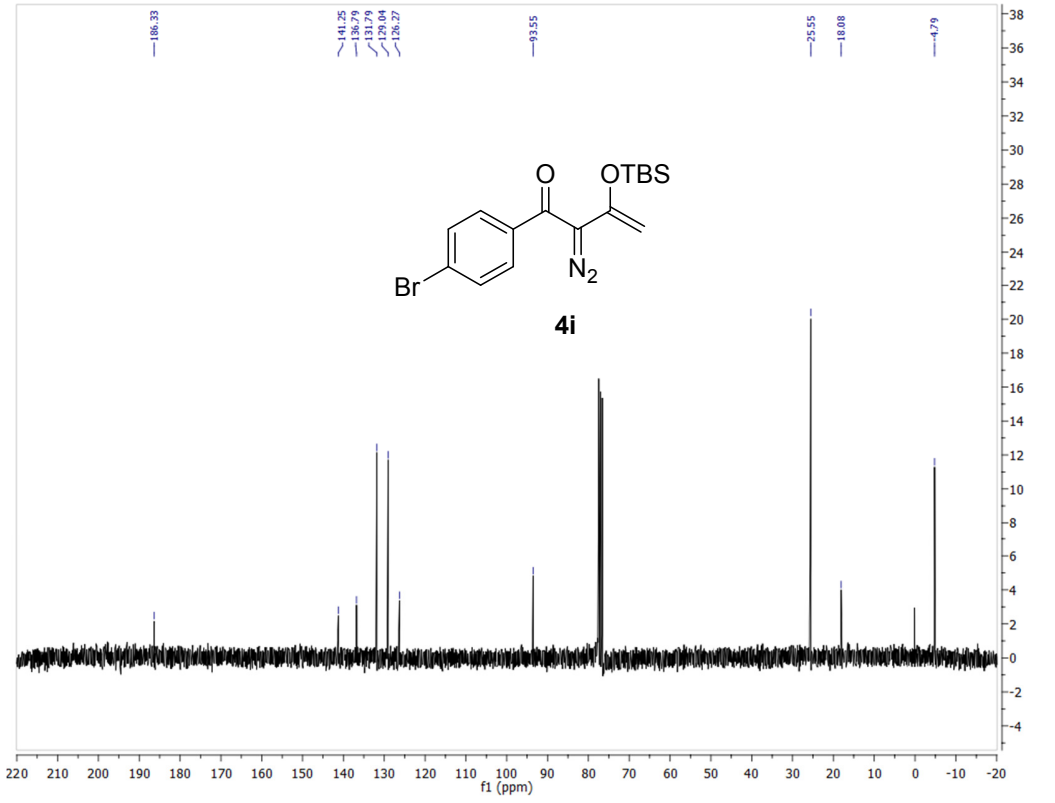
128.64
93.54
25.55
18.09
4.80
O
OTBS
N2
Cl
4h
f1 (ppm)


7.61
7.58
7.52
7.49
5.13
5.12
4.46
4.46
0.92
0.26
O
OTBS
N2
Br
4i
1.98
1.92
1.00
1.02
9.29
5.97
f1 (ppm)


186.33
141.25
136.79
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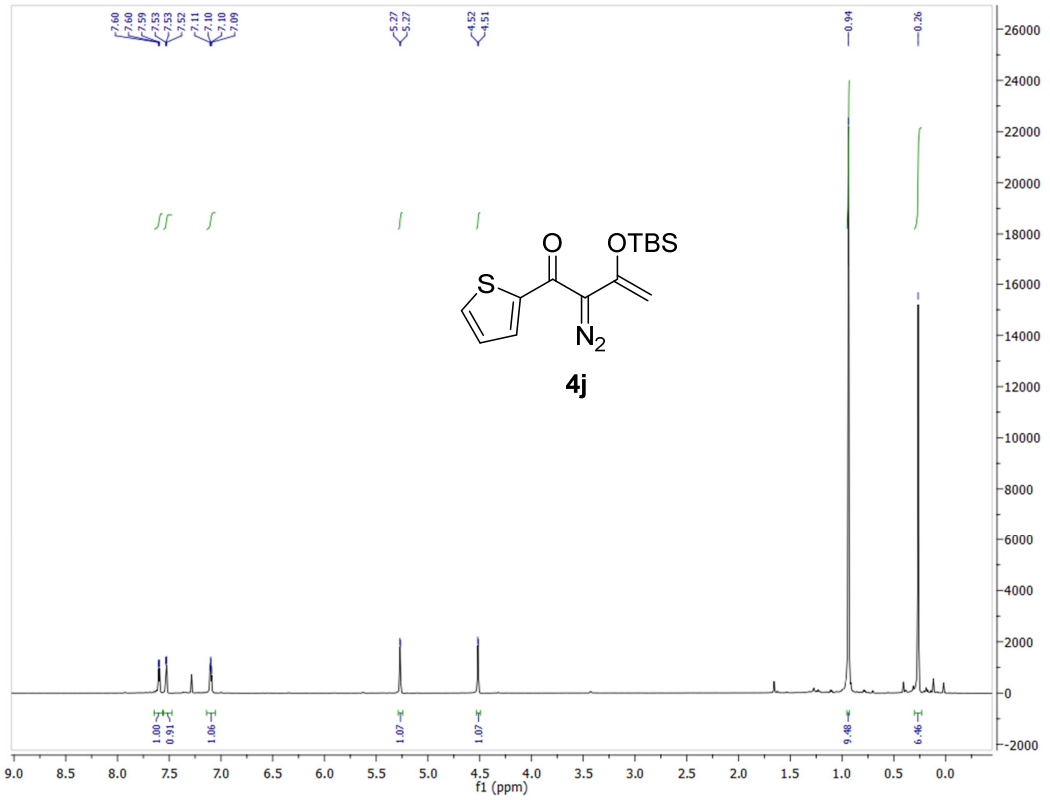
129.04
126.27
93.55
25.55
18.08
-4.79
O
OTBS
N2
Br
4i
f1 (ppm)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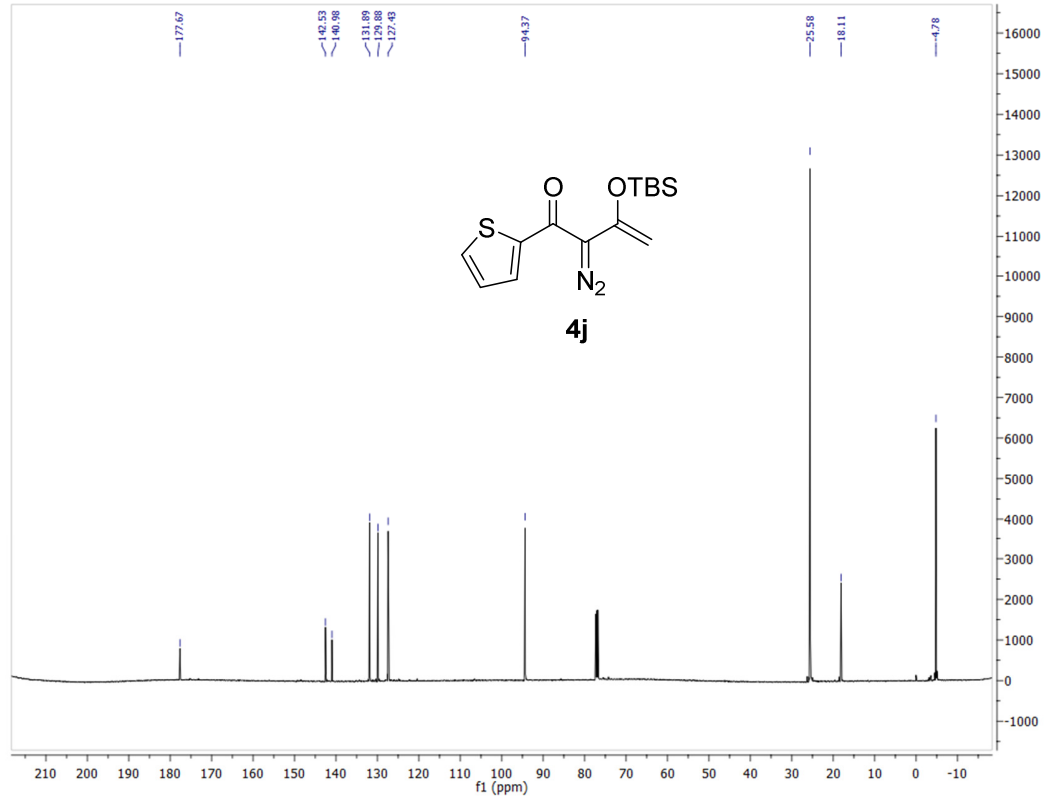
7.60
7.59
7.53
7.53
7.52
7.11
7.10
7.10
7.09
5.27
5.27
4.52
4.51
0.94
0.26
O
OTBS
S
N2
4j
1.00
0.91
1.06
1.07
1.07
9.48
6.46
f1 (ppm)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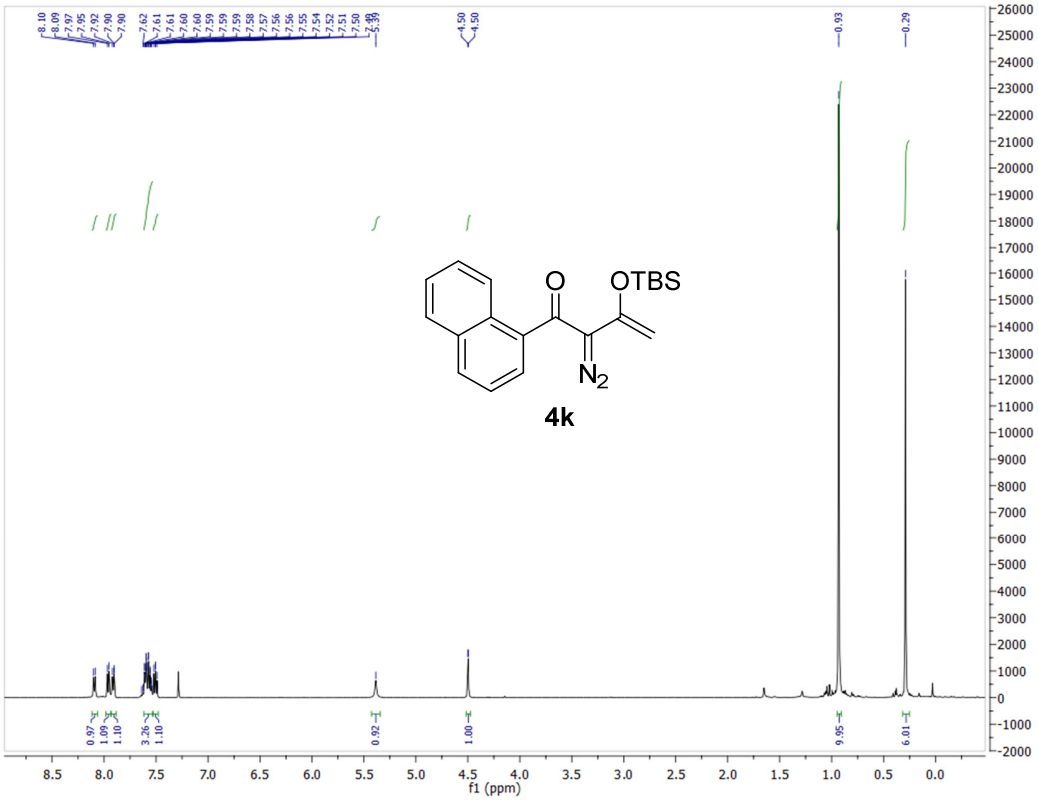
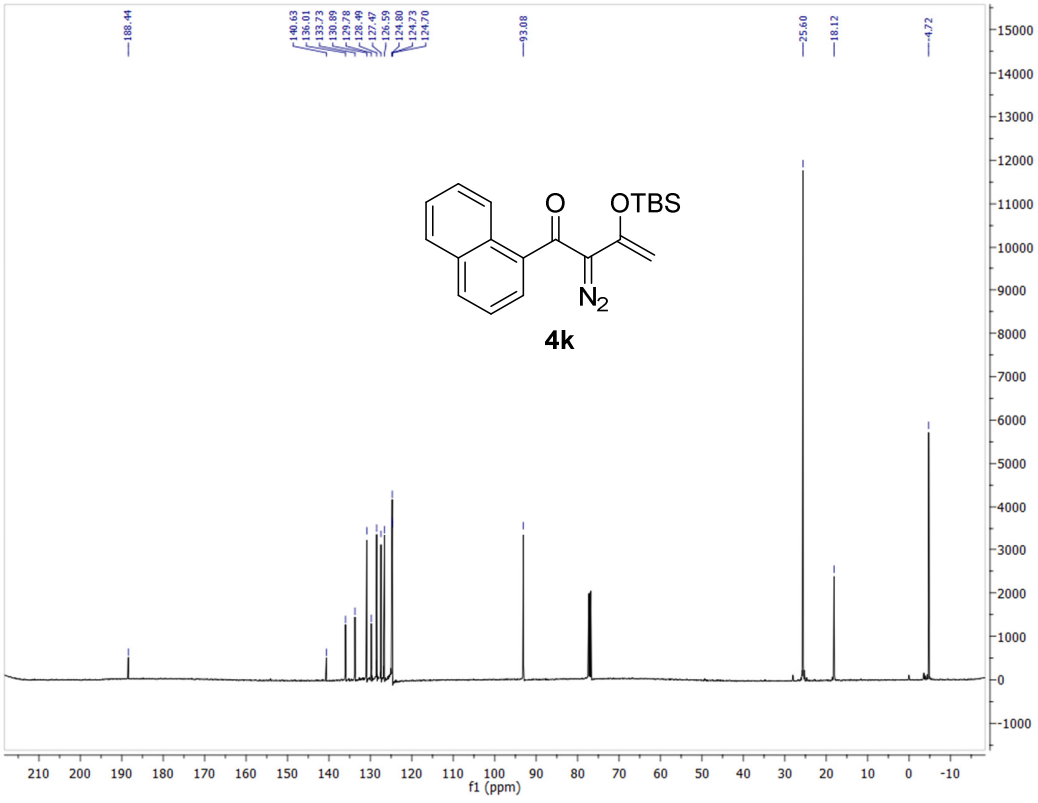
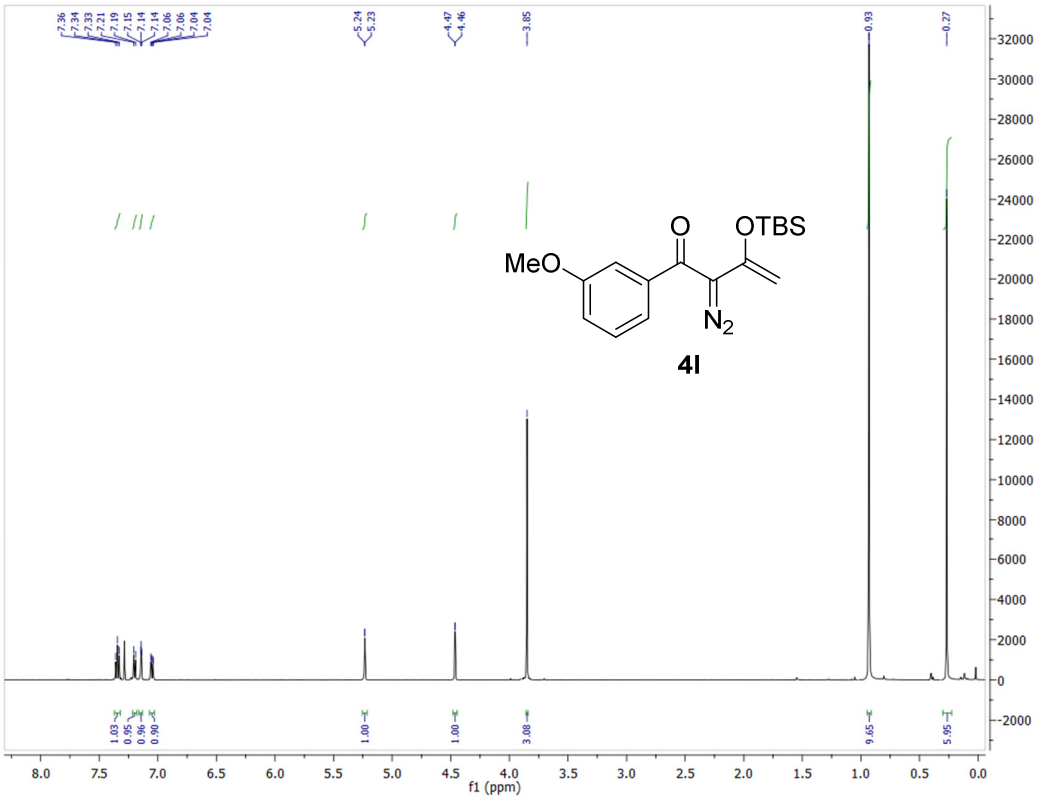
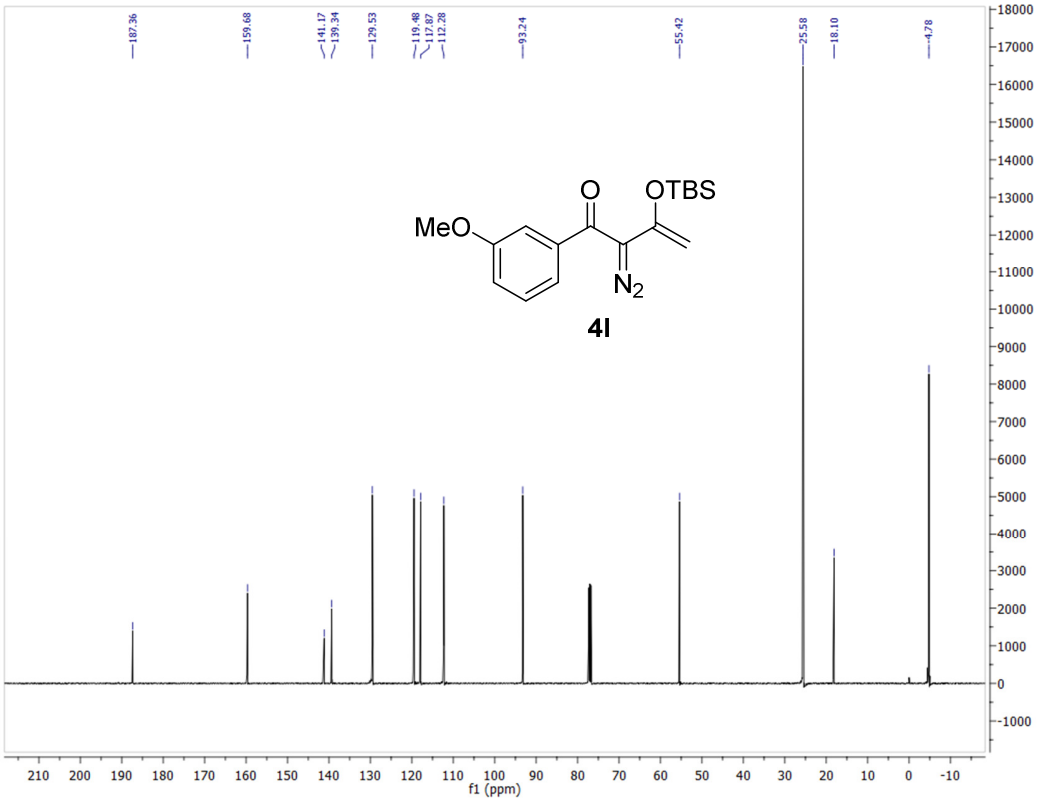
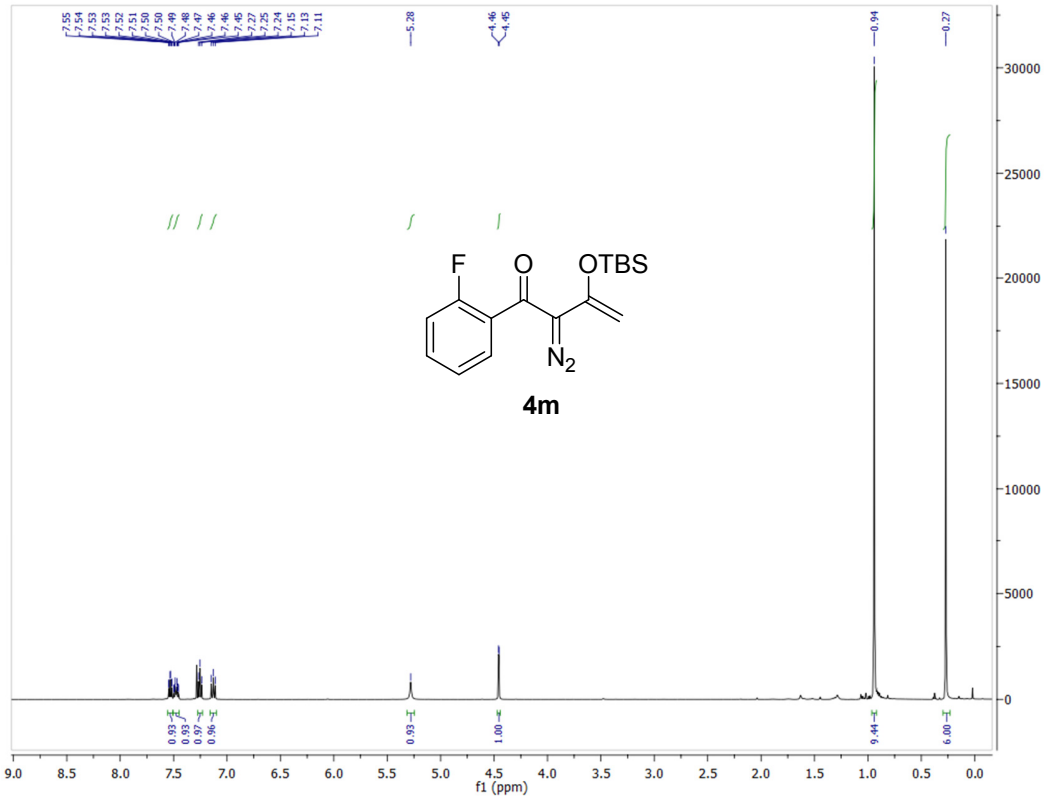
142.53
140.98
131.89
129.88
127.43
94.37
25.58
18.11
4.78
O
OTBS
S
N2
4j
f1 (ppm)

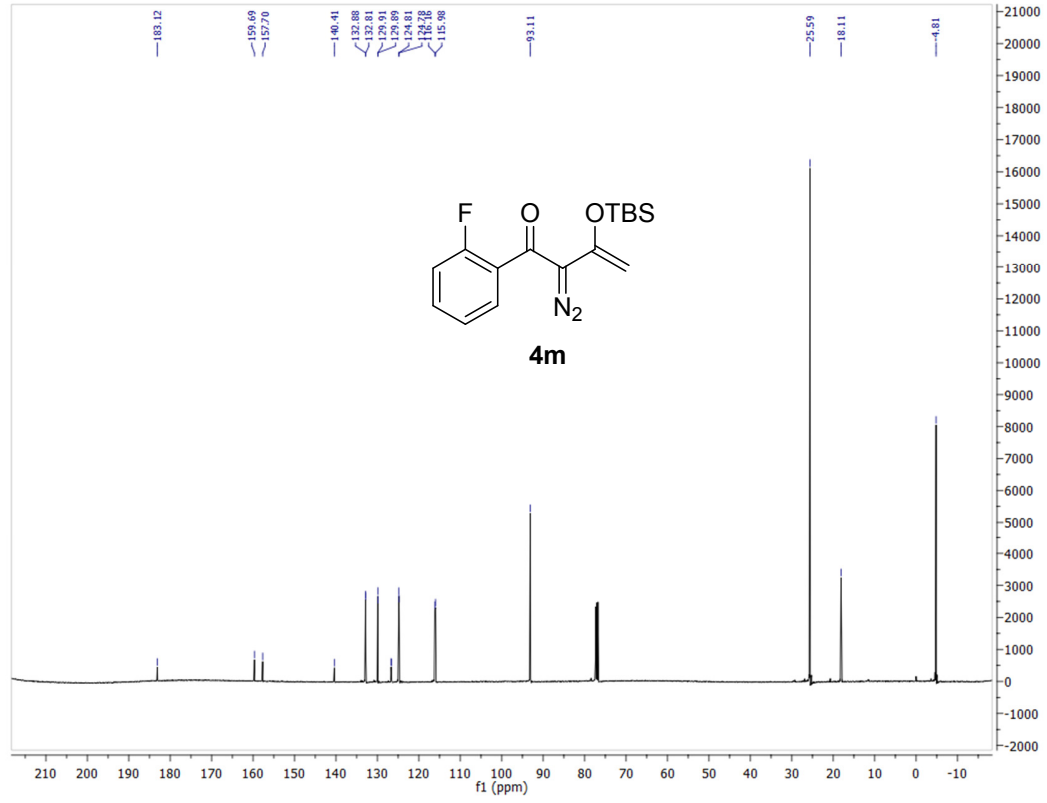

O
OTBS
N2
4k
f1 (ppm)

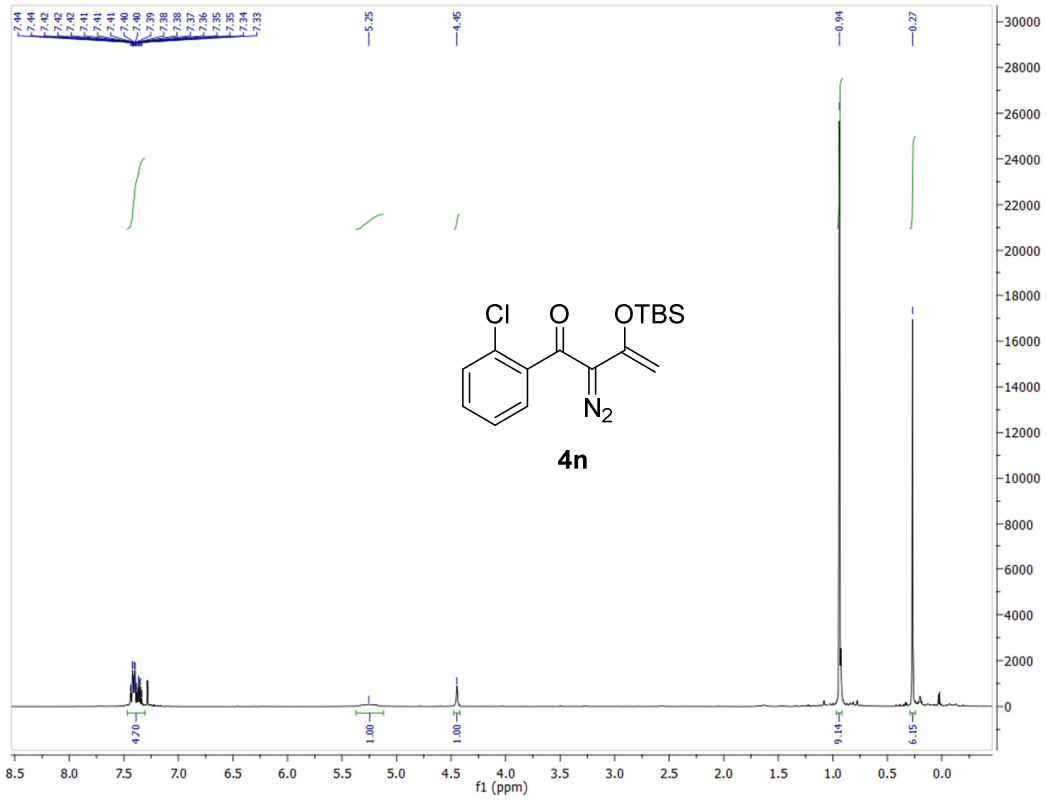

O
OTBS
N2
4k
f1 (ppm)

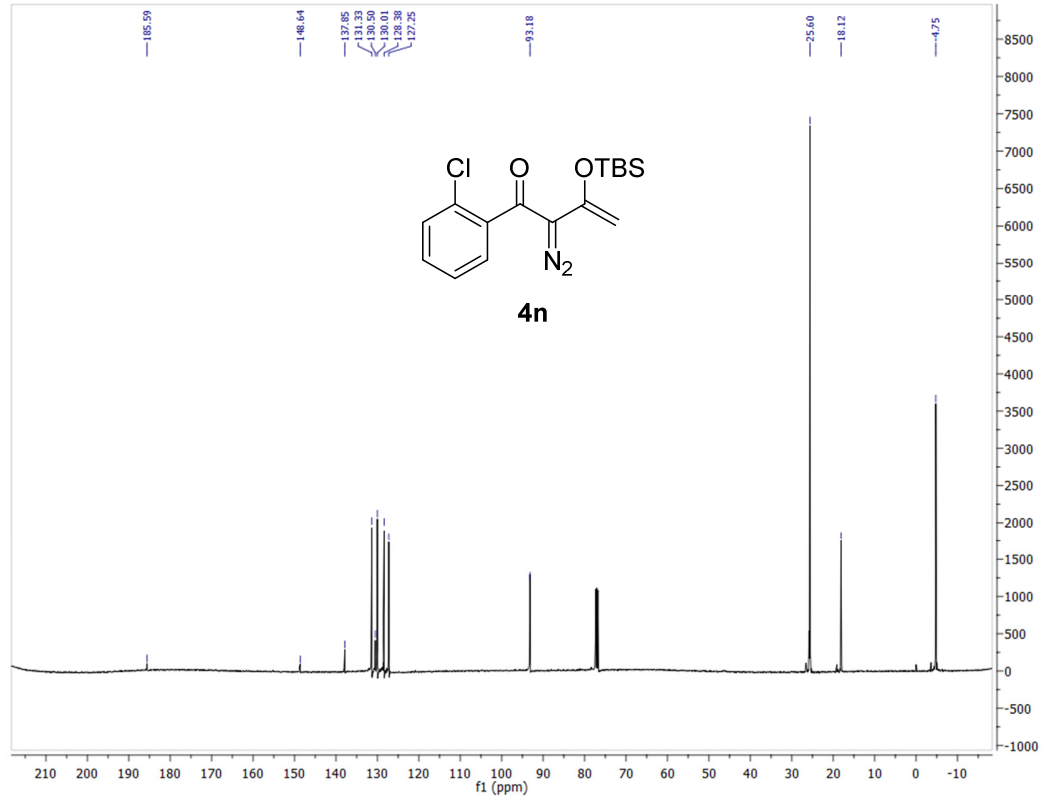

MeO
O
OTBS
N2
4l
f1 (ppm)

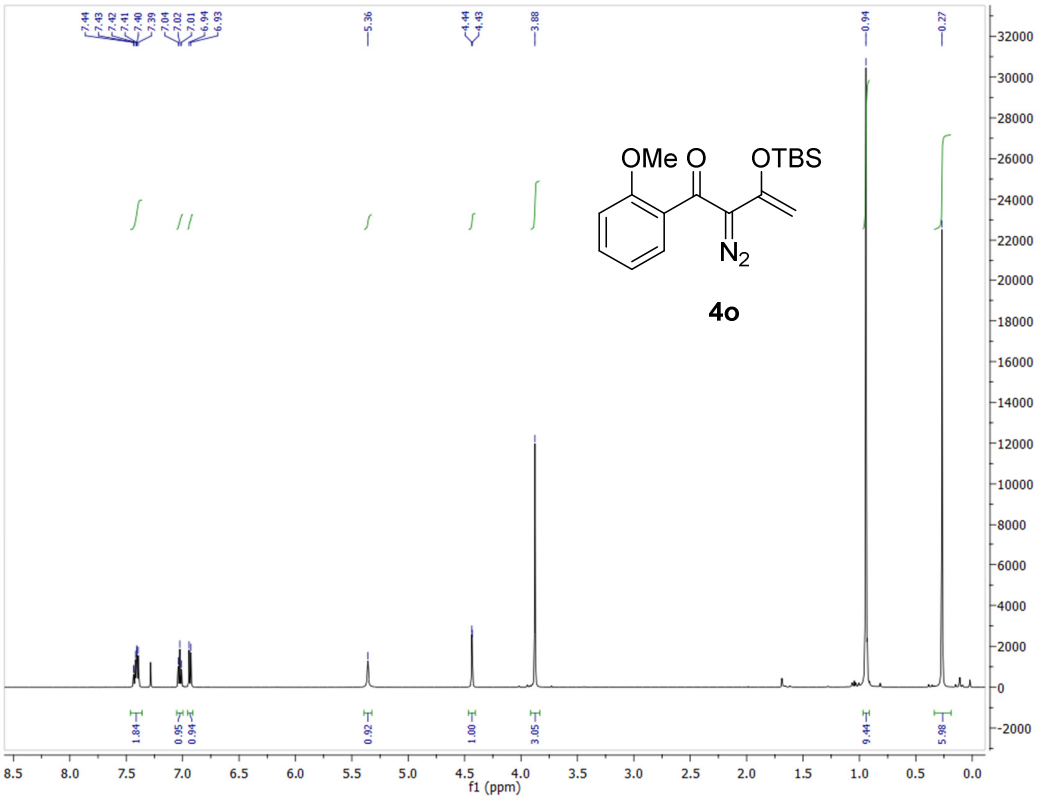

MeO
O
OTBS
N2
4l
f1 (ppm)

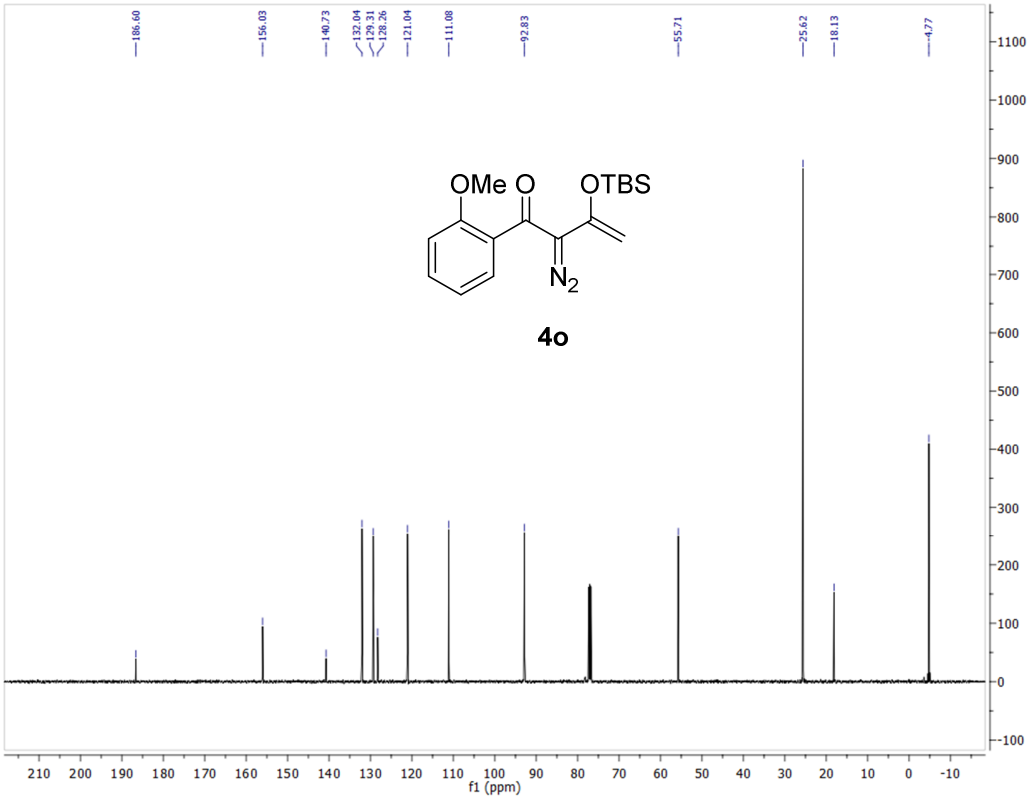

F
O
OTBS
N2
4m
f1 (ppm)

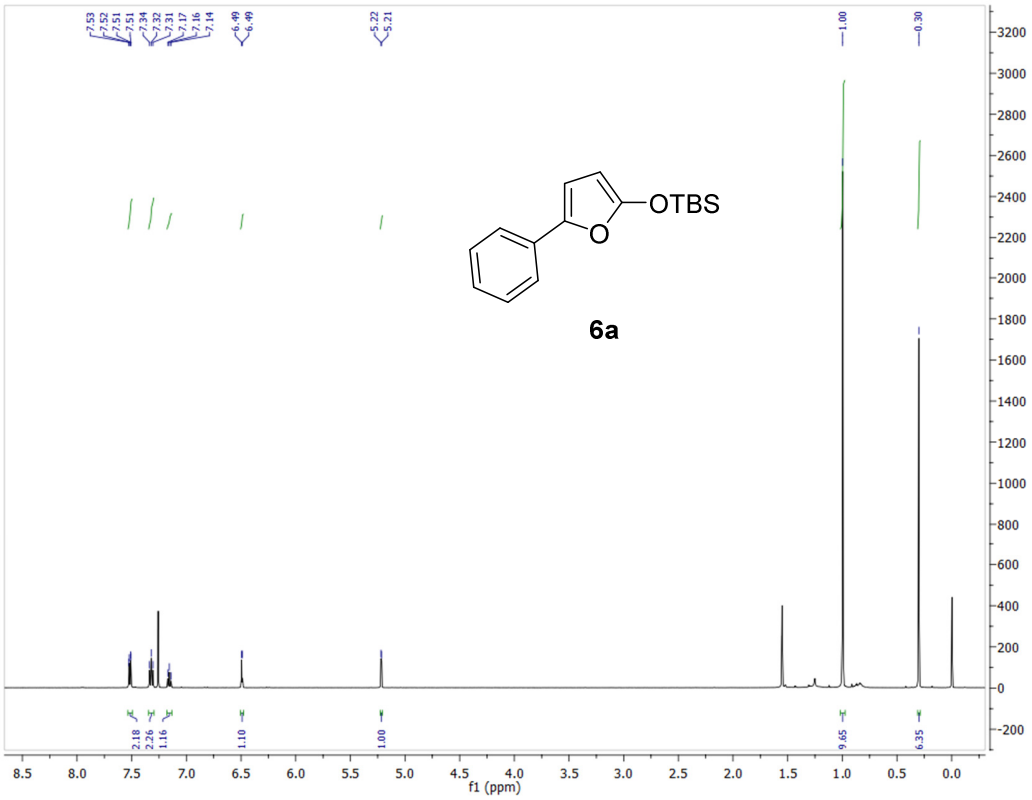

F
O
OTBS
N2
4m
f1 (ppm)

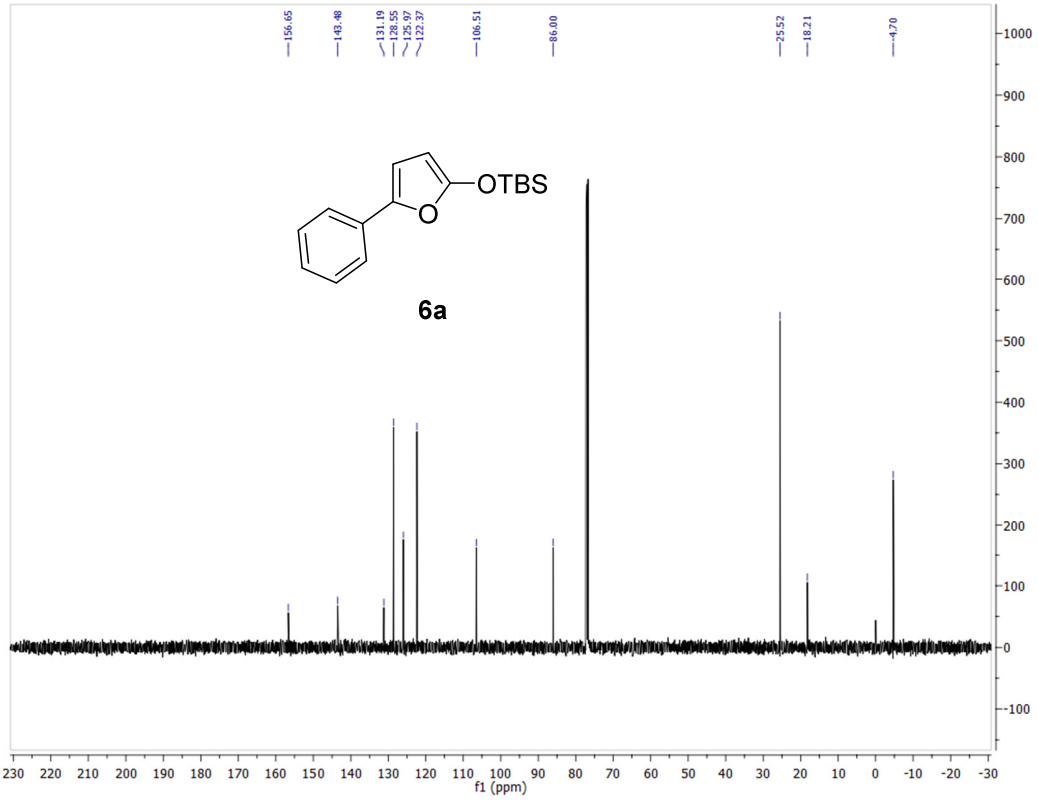

Cl
O
OTBS
N2
4n
f1 (ppm)

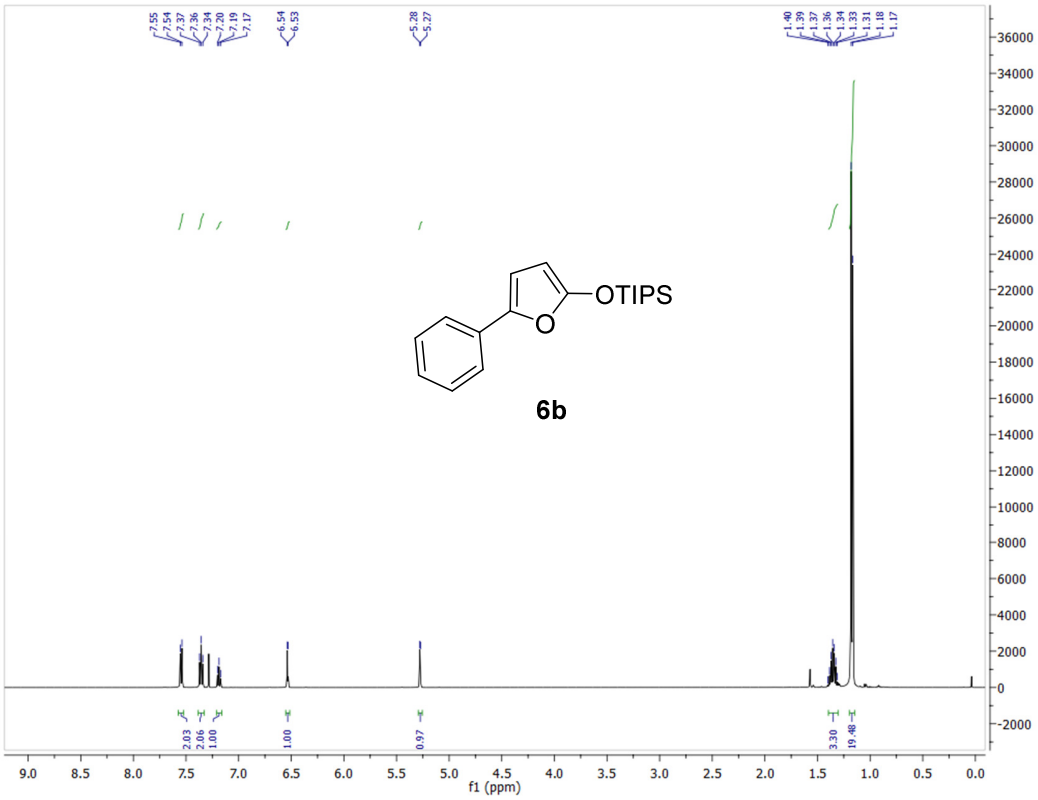

Cl
O
OTBS
N2
4n
f1 (ppm)

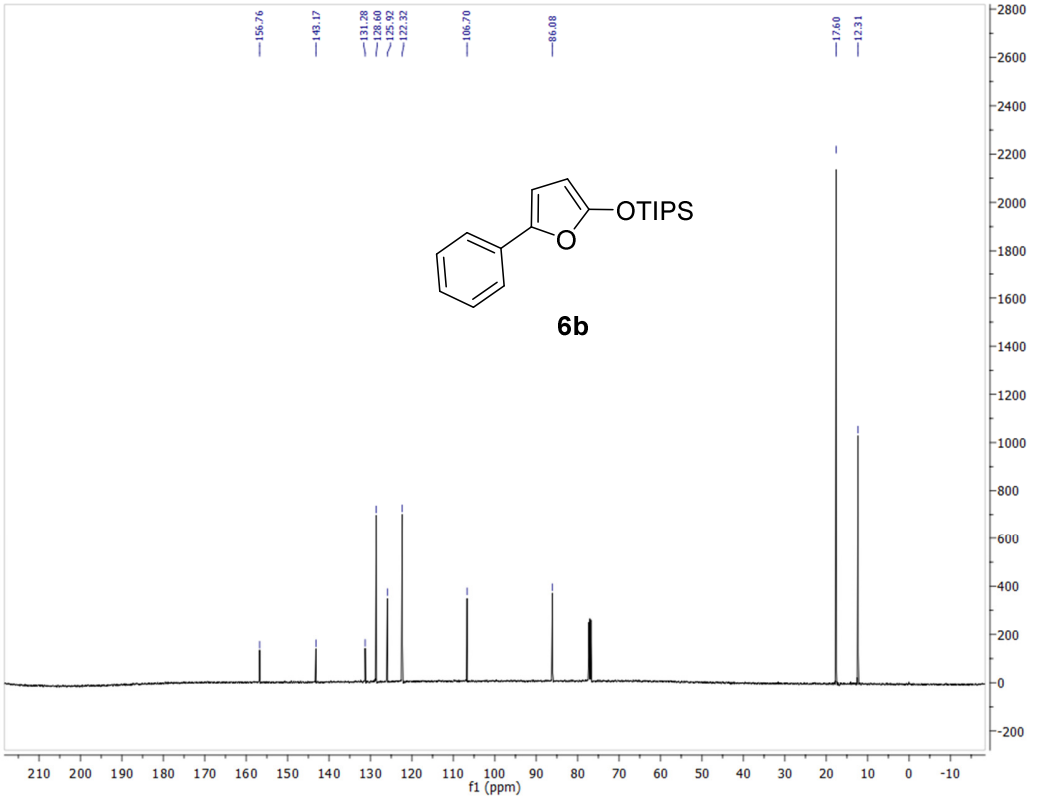

OMe O
OTBS
N2
4o
f1 (ppm)

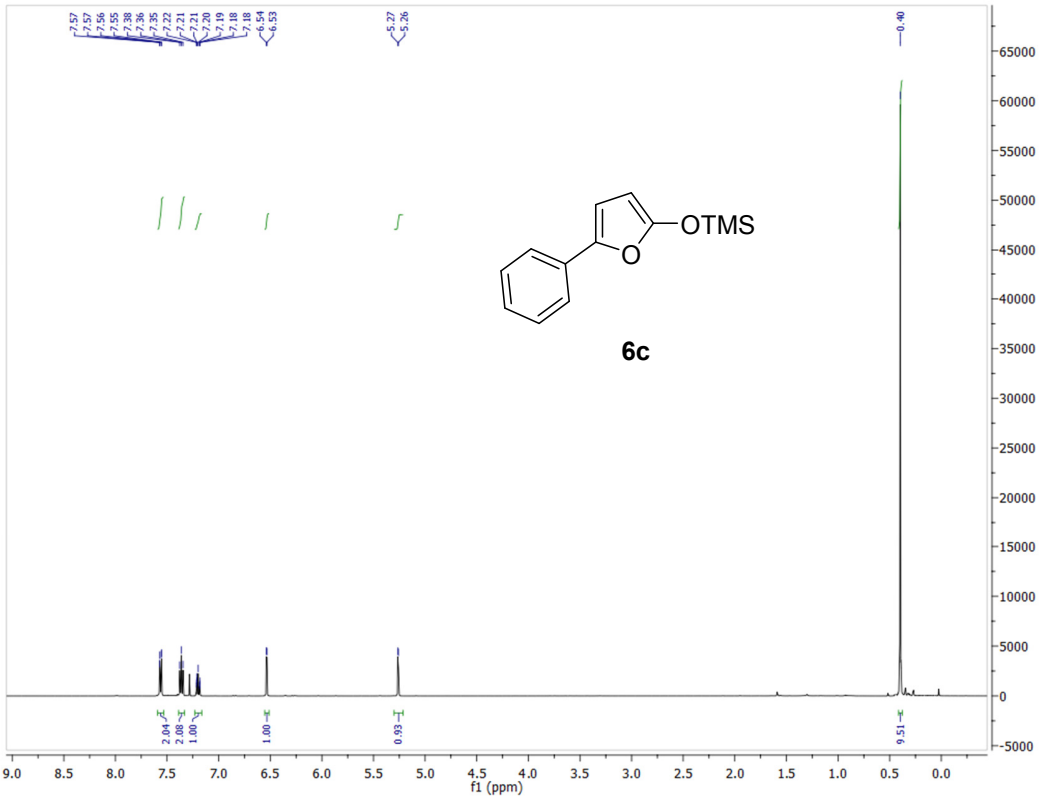

OMe O
OTBS
N2
4o
f1 (ppm)

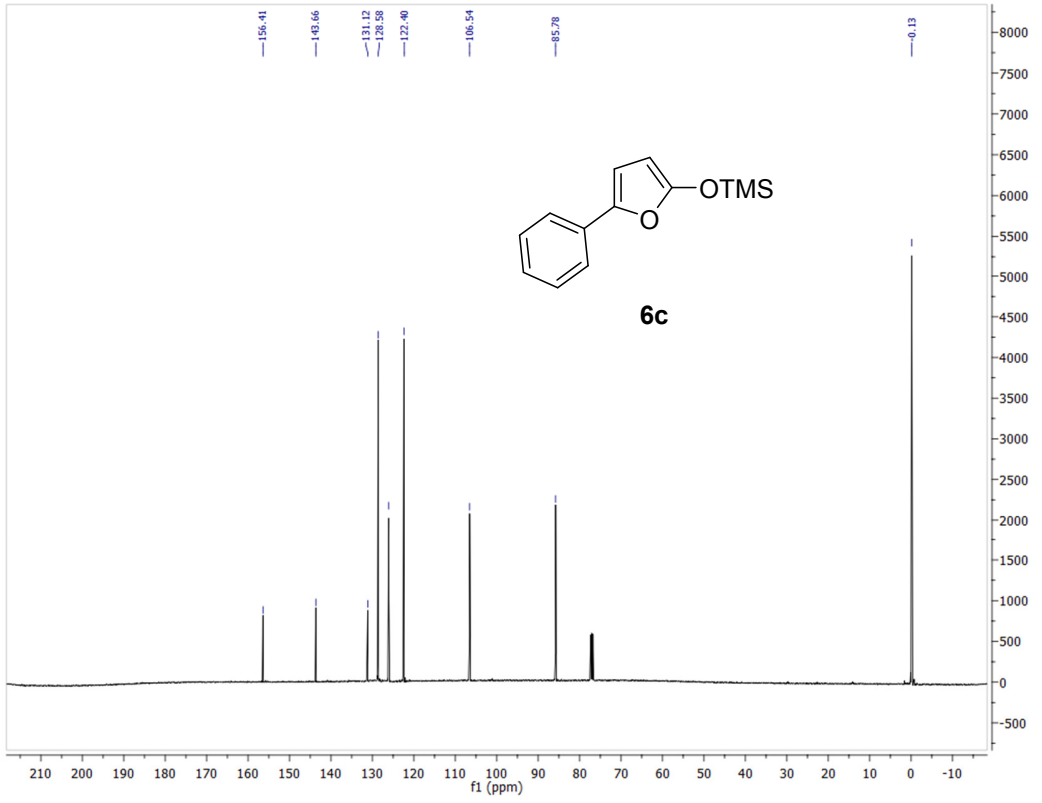

7.53
7.52
7.51
7.51
7.34
7.32
7.31
7.17
7.16
7.14
6.49
6.49
5.22
5.21
1.00
0.30
OTBS
O
6a
2.18
2.26
1.16
1.10
1.00
9.65
6.35
f1 (ppm)


156.65
143.48
131.19
128.55
125.97
122.37
106.51
86.00
25.52
18.21
4.70
OTBS
O
6a
f1 (ppm)


OTIPS
O
6b
f1 (ppm)


OTIPS
O
6b
f1 (ppm)


7.57
7.57
7.56
7.55
7.38
7.36
7.35
7.22
7.21
7.21
7.20
7.19
7.18
7.18
6.54
6.53
5.27
5.26
0.40
OTMS
O
6c
2.04
2.08
1.00
1.00
0.93
9.51
f1 (ppm)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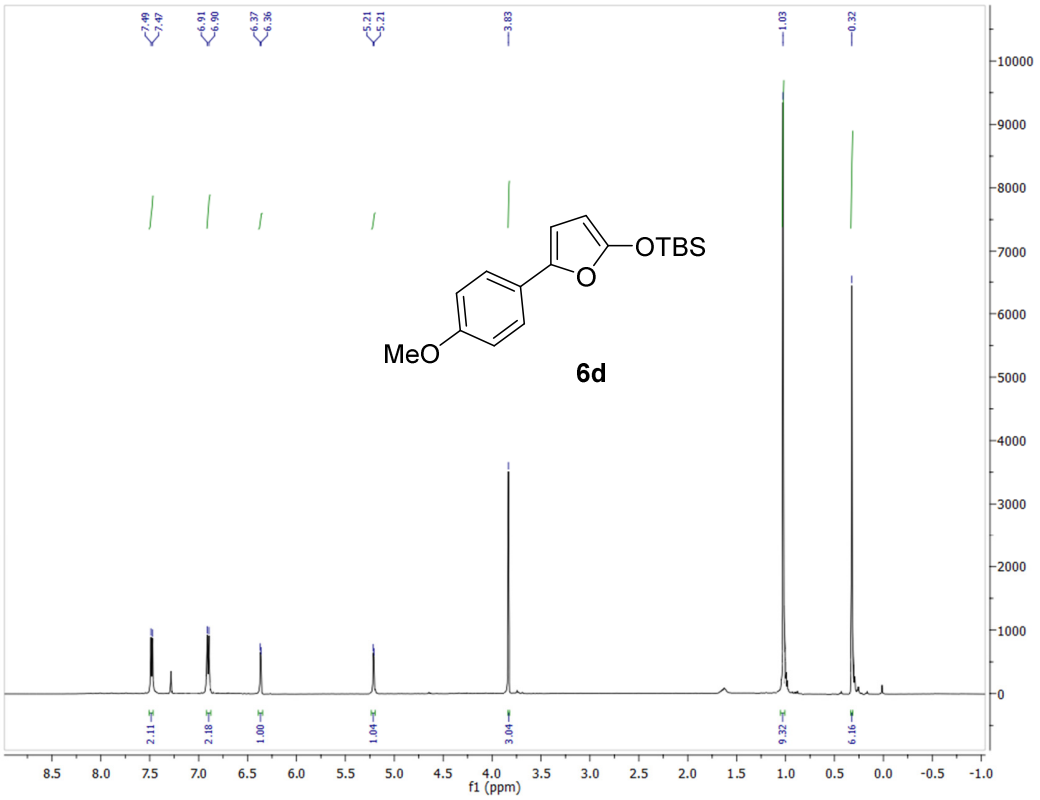
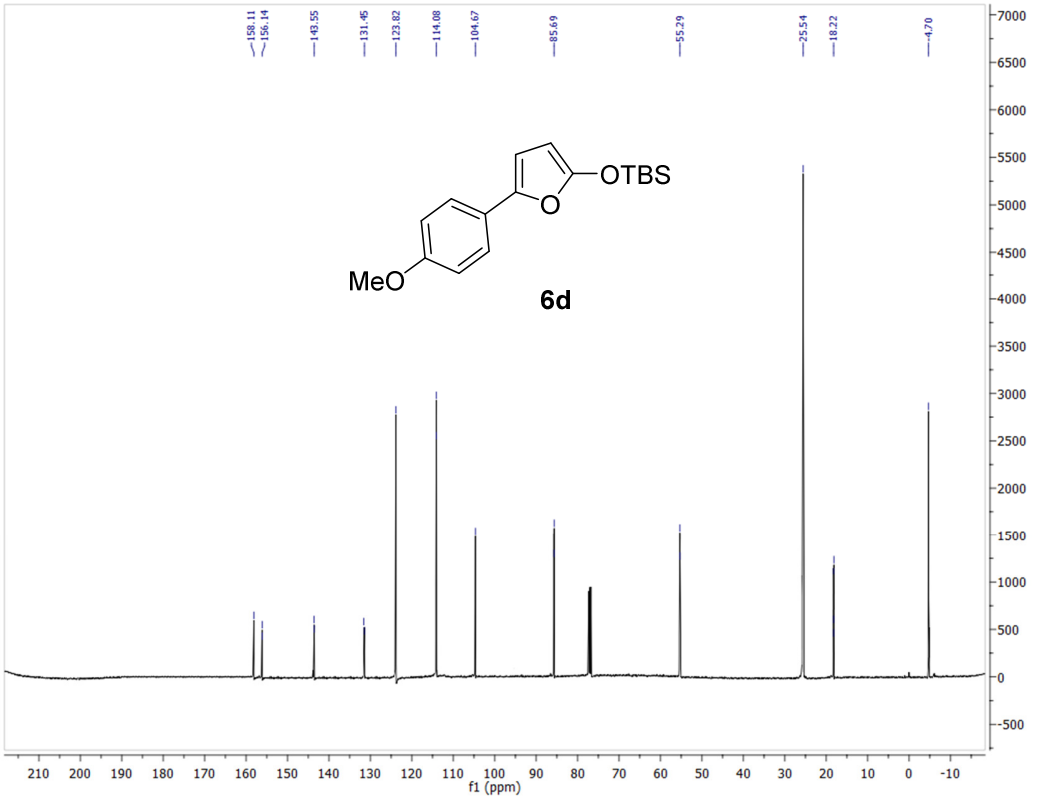
143.66
131.12
128.58
122.40
106.54
85.78
0.13
OTMS
O
6c
f1 (ppm)


7.49
7.47
6.91
6.90
6.37
6.36
5.21
5.21
3.83
1.03
0.32
OTBS
O
MeO
6d
2.11
2.18
1.00
1.04
3.04
9.32
6.16
f1 (ppm)


158.11
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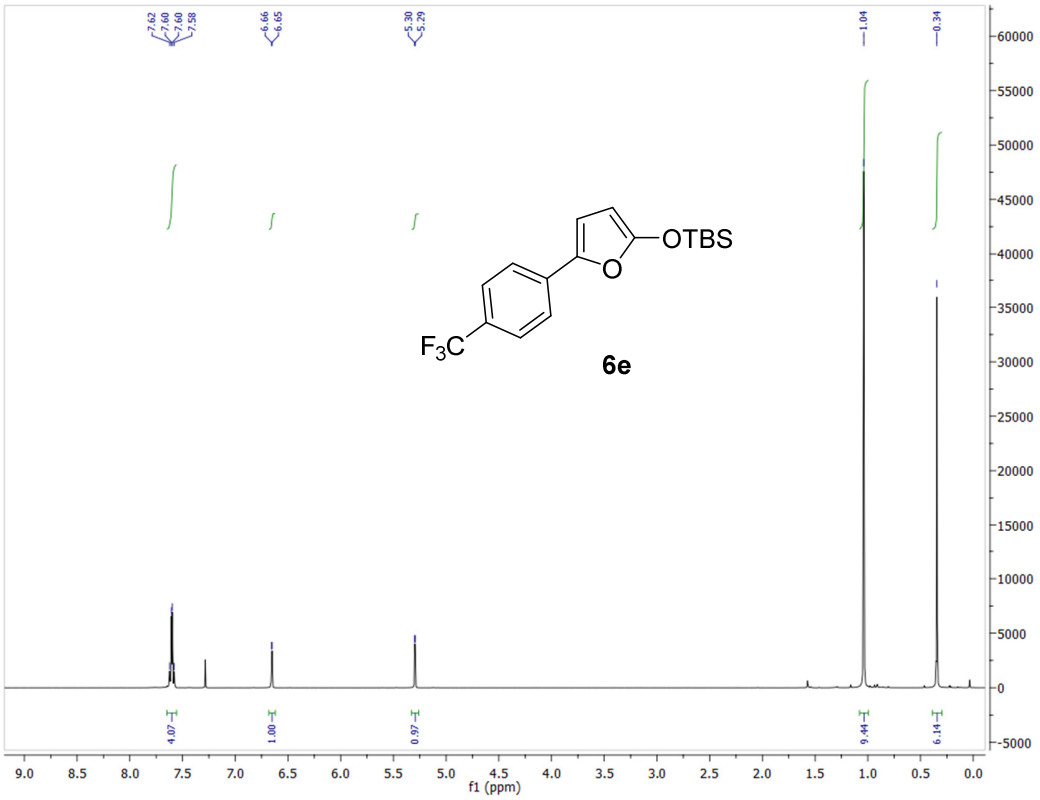
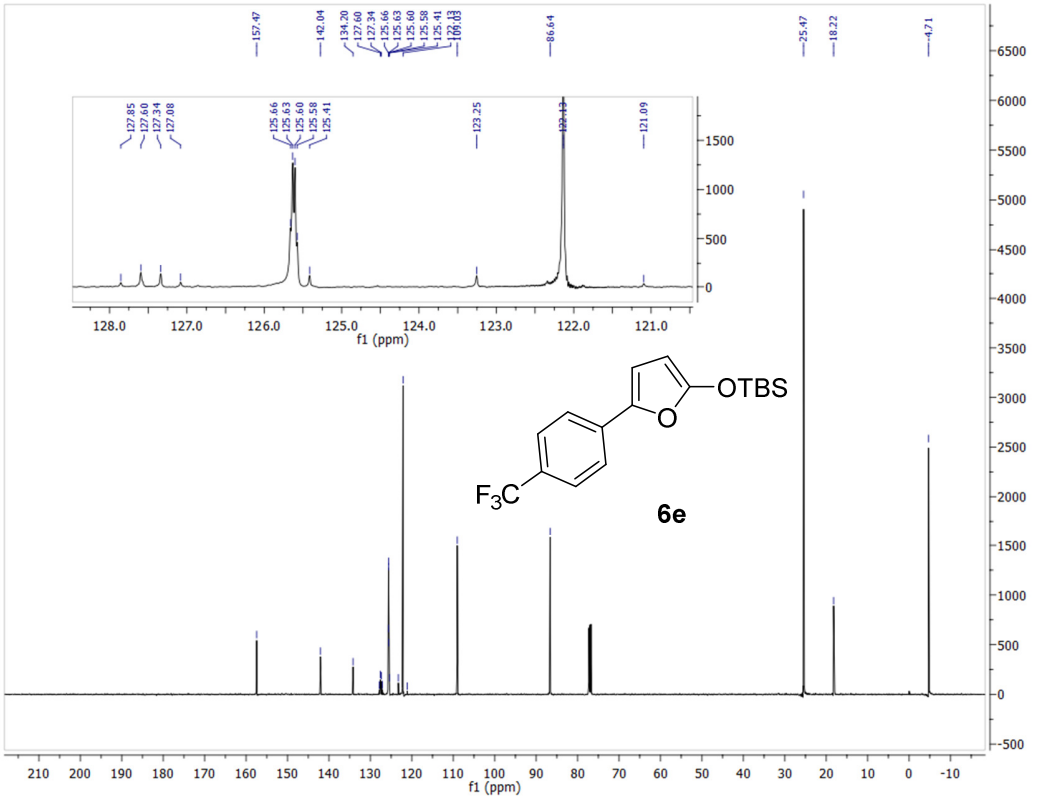
149.55
131.45
123.82
114.08
104.67
85.69
55.29
25.54
18.22
-4.70
OTBS
O
MeO
6d
f1 (ppm)


7.62
7.60
7.60
7.58
6.66
6.65
5.30
5.29
1.04
0.34
OTBS
O
F3C
6e
4.07
1.00
0.97
9.44
6.14
f1 (ppm)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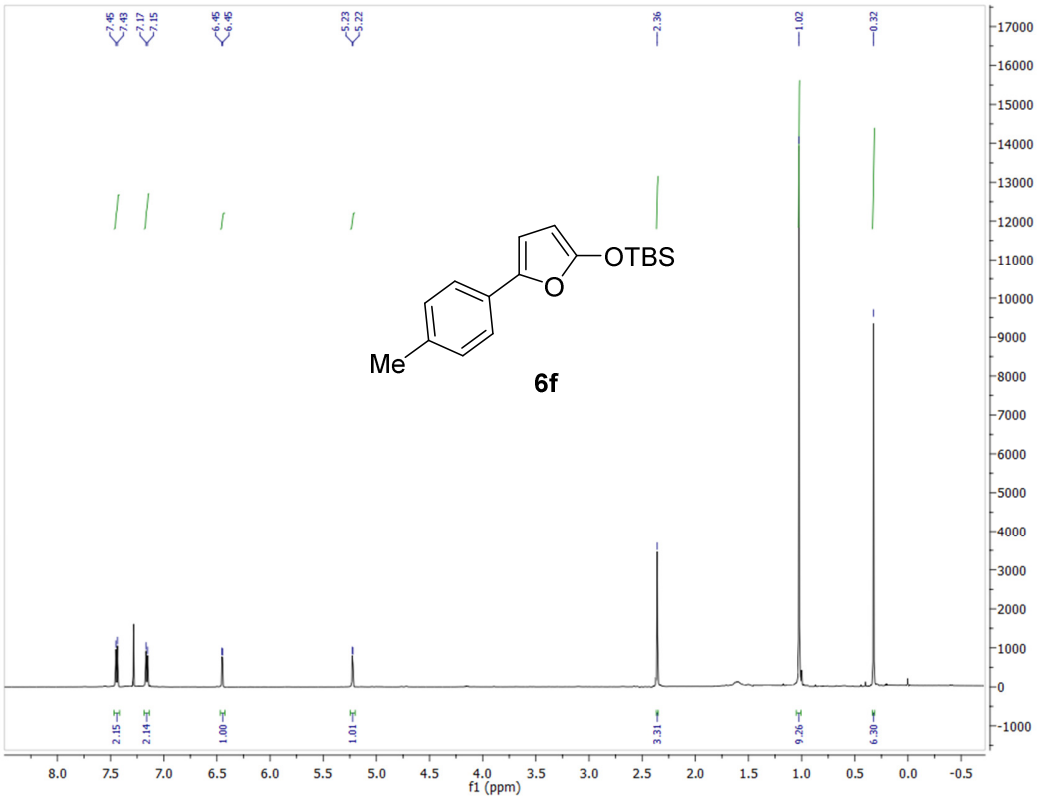
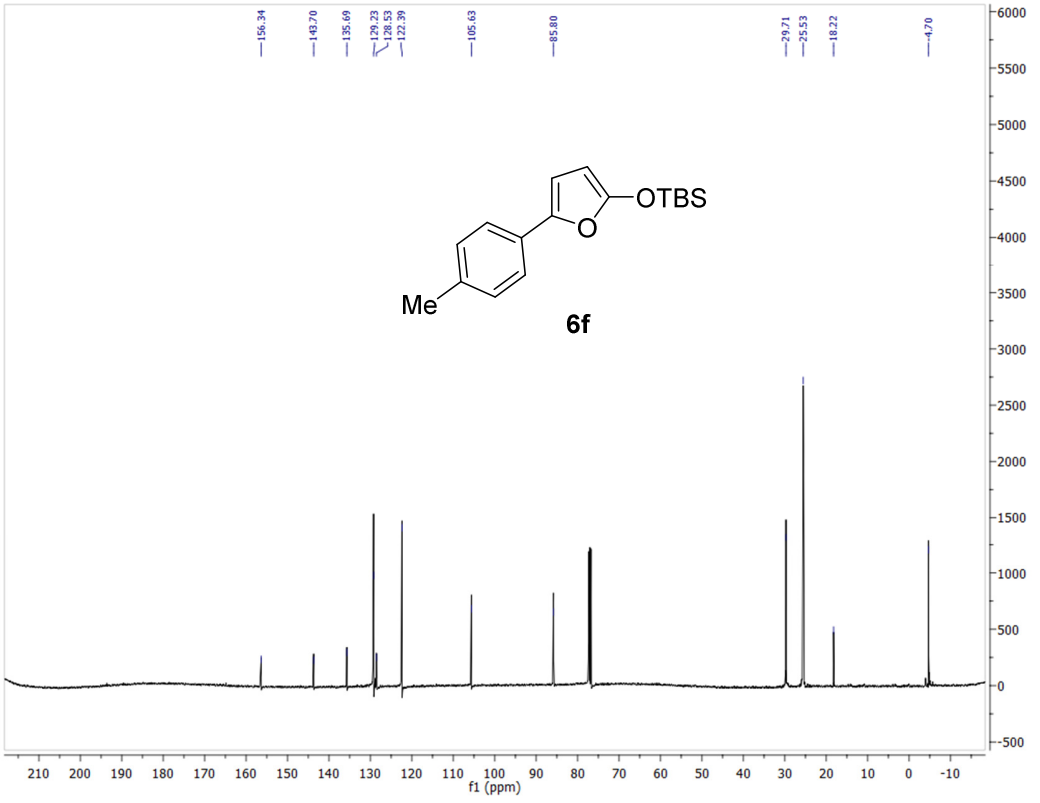
134.20
127.60
127.34
125.66
125.63
125.60
125.58
125.41
86.64
25.47
18.22
4.71
127.85
127.60
127.34
127.08
125.66
125.63
125.60
125.58
125.41
123.25
121.09
OTBS
O
F3C
6e
f1 (ppm)


7.45
7.43
7.17
7.15
6.45
6.45
5.23
5.22
2.36
1.02
0.32
OTBS
O
Me
6f
2.15
2.14
1.00
1.01
3.31
9.26
6.30
f1 (ppm)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129.23
128.53
122.39
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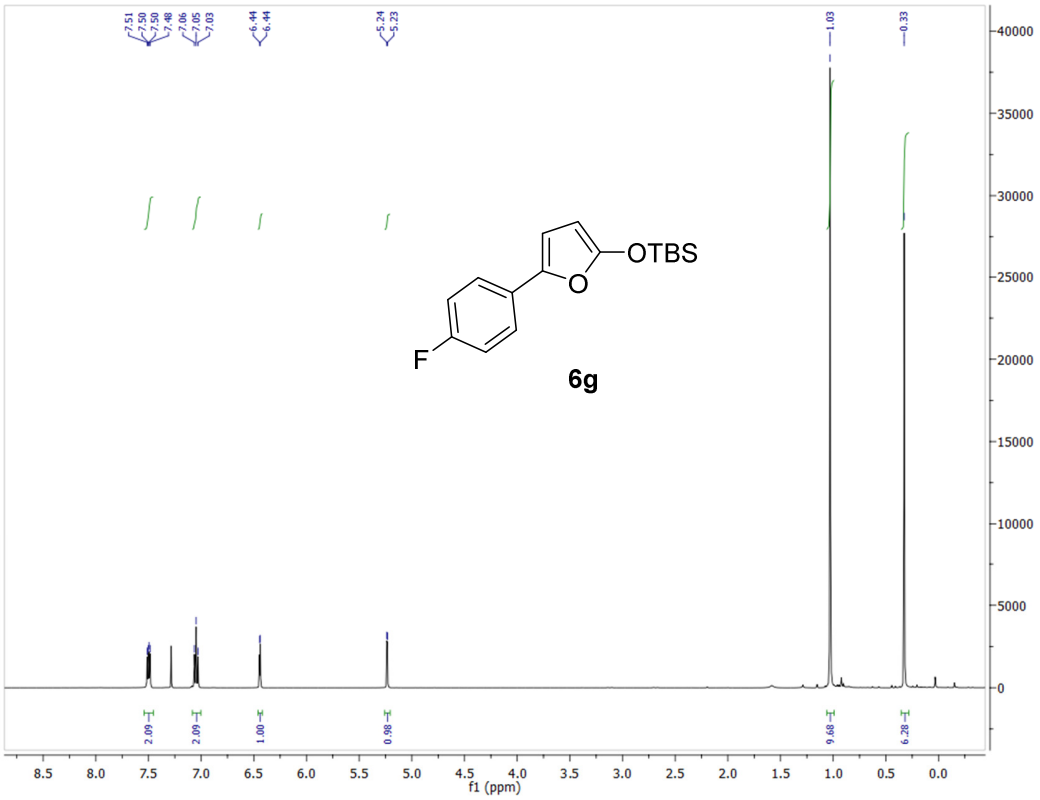
85.80
29.71
25.53
18.22
-4.70
OTBS
O
Me
6f
f1 (ppm)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7.50
7.48
7.06
7.05
7.03
6.44
6.44
5.24
5.23
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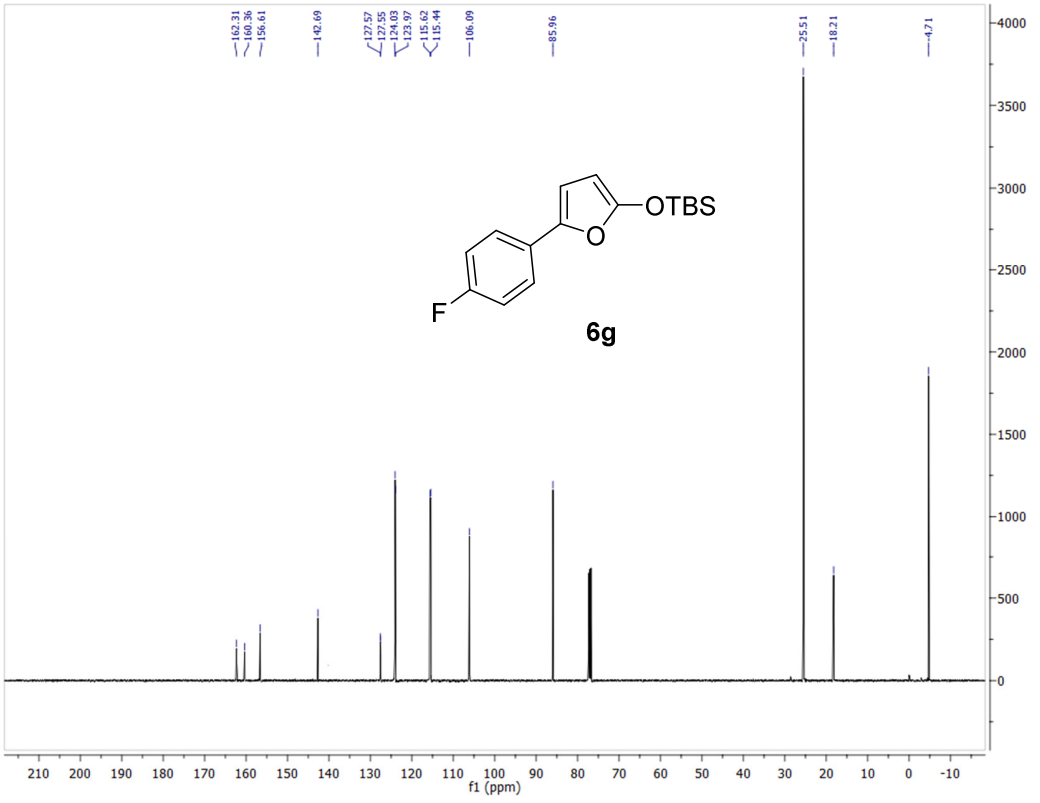
0.33
OTBS
O
F
6g
2.09
2.09
1.00
0.98
9.68
6.28
f1 (ppm)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160.36
156.61
142.69
127.67
127.55
124.03
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115.62
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106.09
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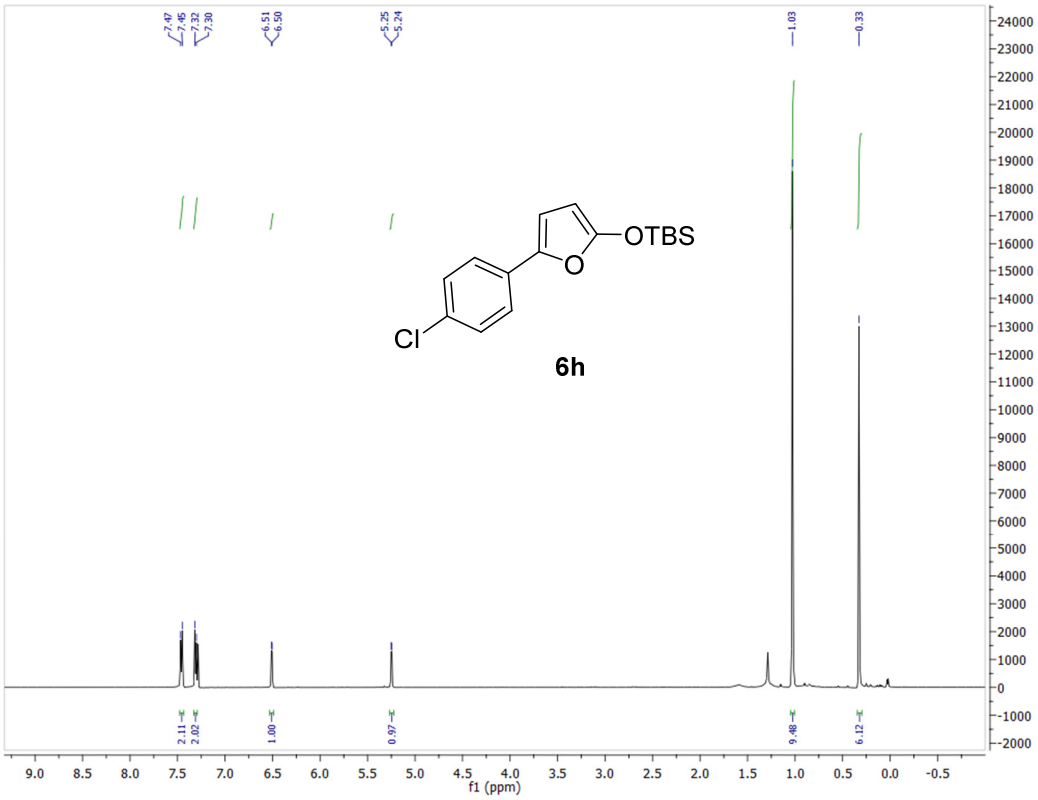
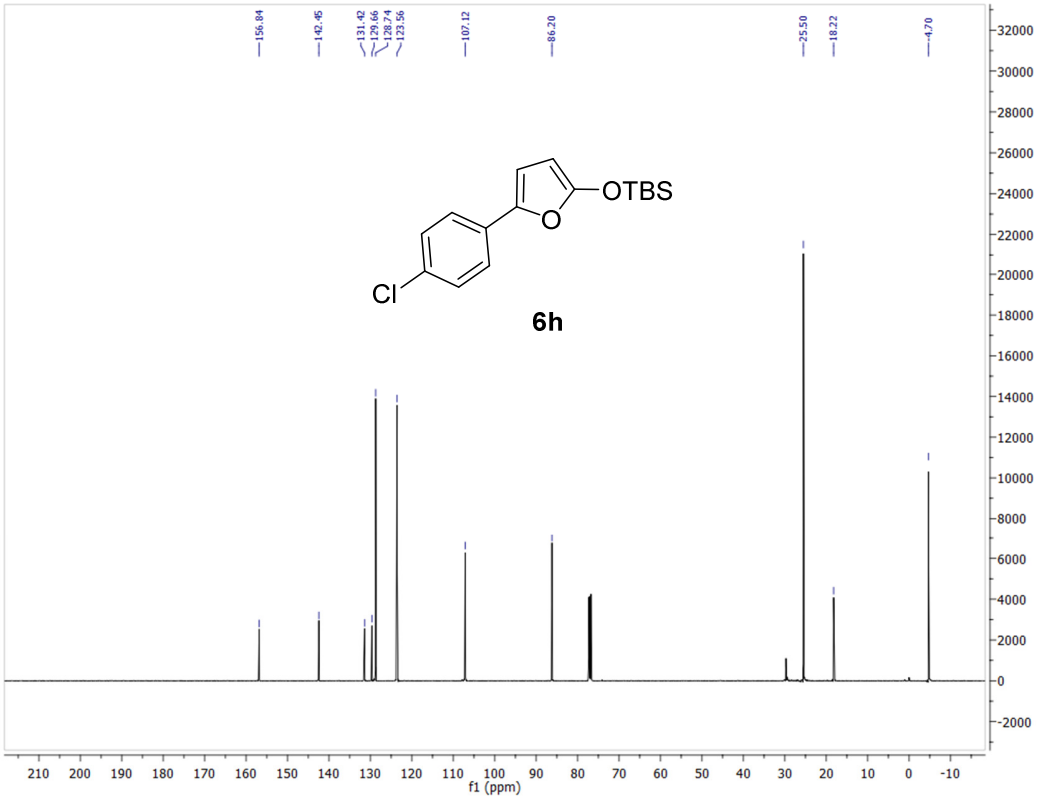
25.51
18.21
-4.71
OTBS
O
F
6g
f1 (ppm)


7.47
7.45
7.32
7.30
6.51
6.50
5.25
5.24
1.03
0.33
OTBS
O
Cl
6h
2.11
2.02
1.00
0.97
9.48
6.12
f1 (ppm)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107.12
86.20
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18.22
-4.70
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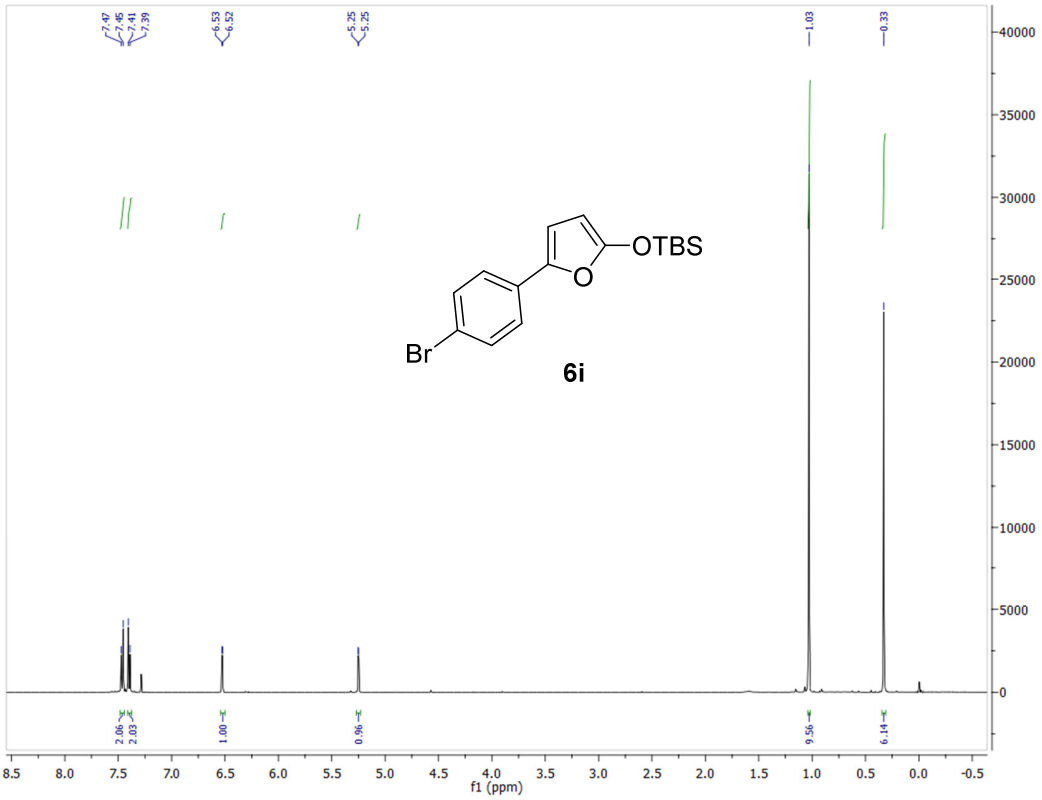
Cl
6h
f1 (ppm)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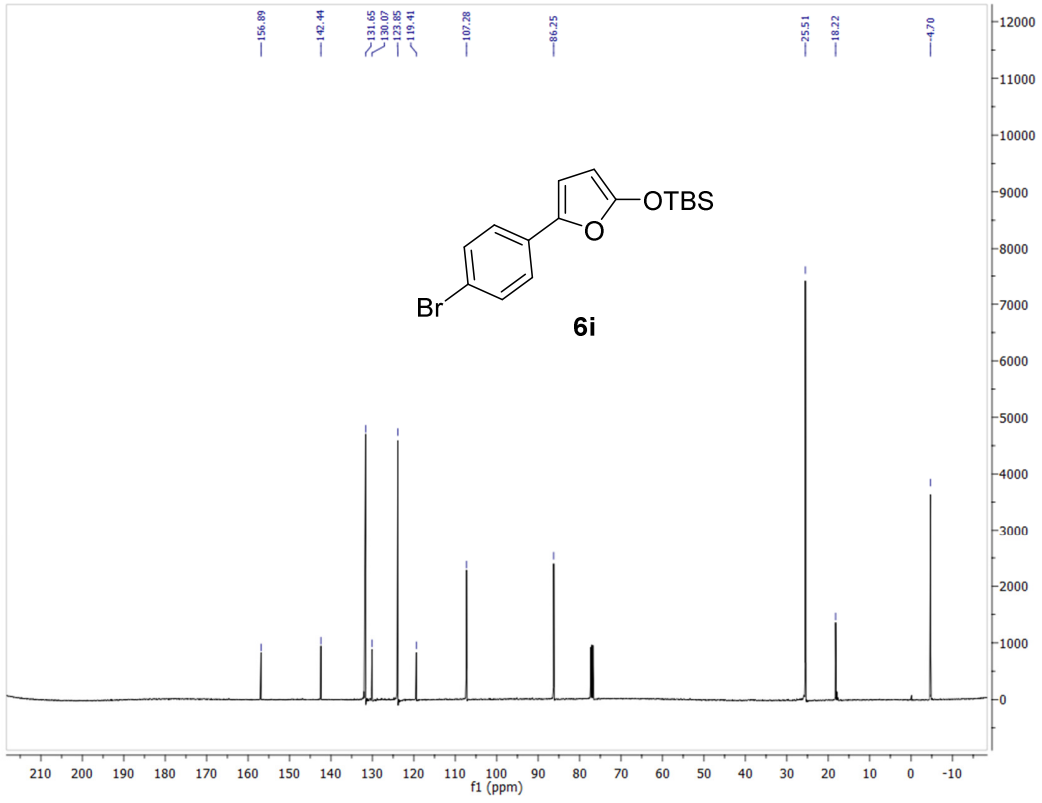
7.45
7.41
7.39
6.53
6.52
5.25
5.25
1.03
0.33
OTBS
O
Br
6i
2.06
2.03
1.00
0.96
9.56
6.14
f1 (ppm)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86.25
25.51
18.22
-4.70
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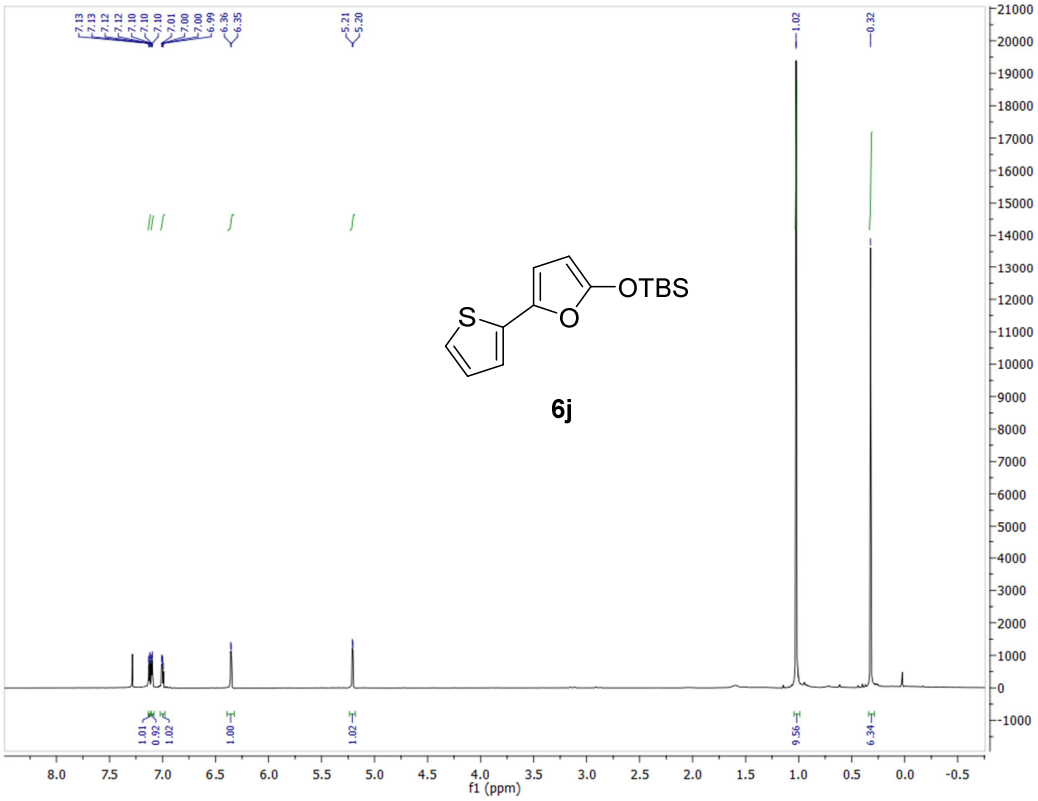
O
Br
6i
f1 (ppm)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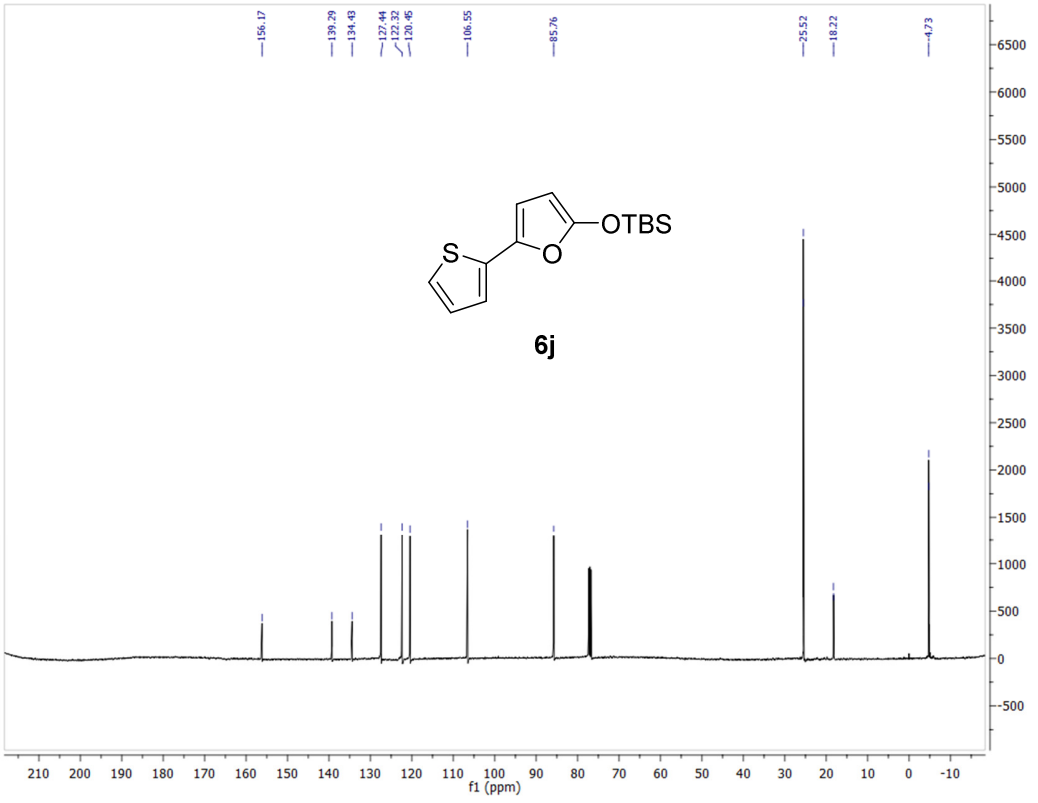
7.12
7.10
7.10
7.10
7.01
7.00
6.99
6.36
6.35
5.21
5.20
1.02
0.32
OTBS
S
O
6j
1.01
0.92
1.02
1.00
1.02
9.56
6.34
f1 (ppm)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122.32
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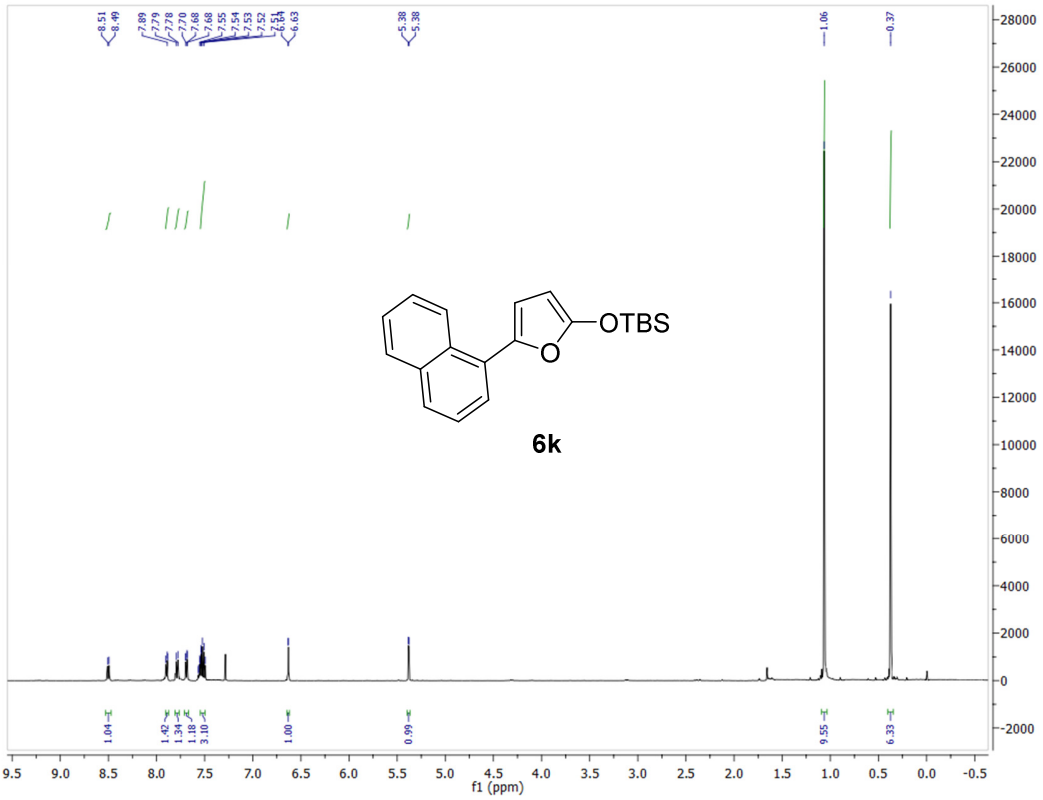
85.76
25.52
18.22
-4.73
OTBS
S
O
6j
f1 (ppm)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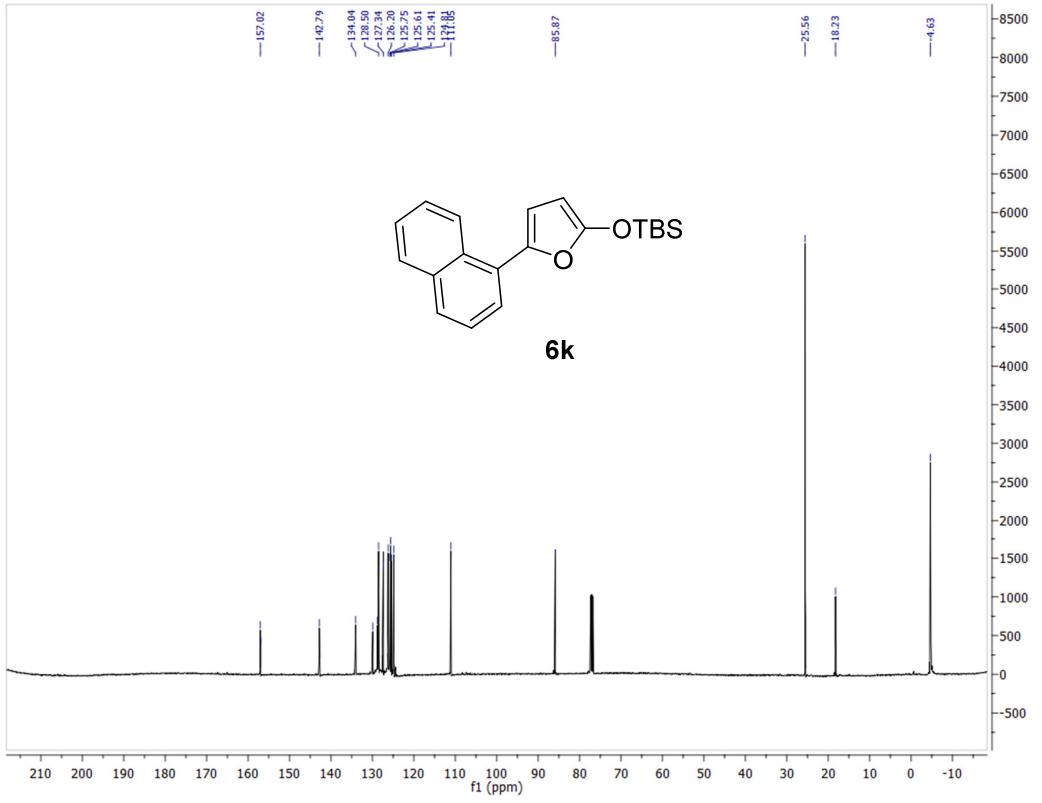
7.68
7.68
7.55
7.54
7.53
7.52
6.64
6.63
5.38
5.38
1.06
0.37
OTBS
O
6k
1.04
1.42
1.34
1.18
3.10
1.00
0.99
9.55
6.33
f1 (ppm)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128.50
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125.61
125.41
85.87
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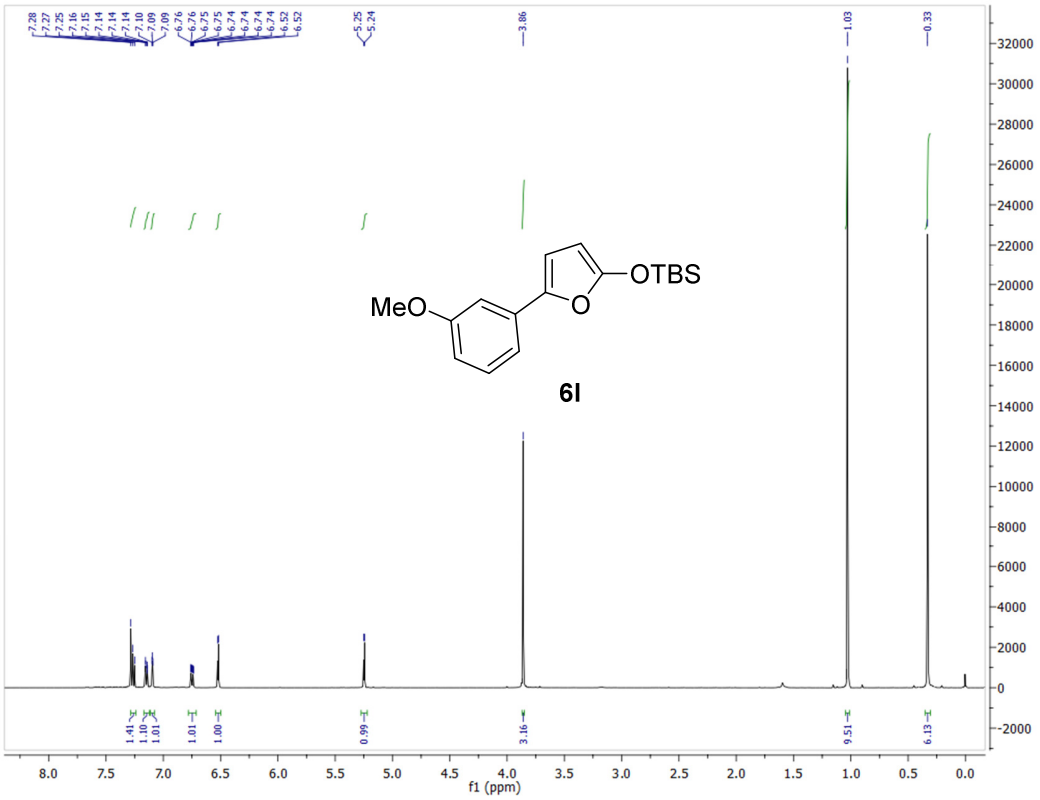
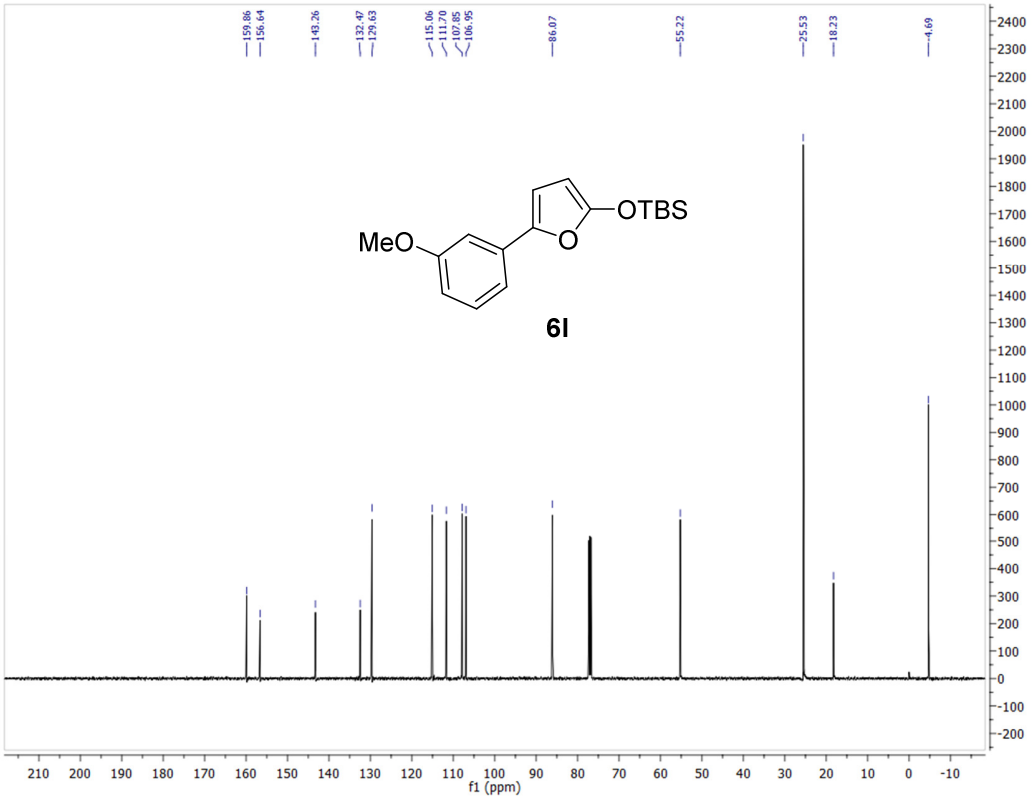
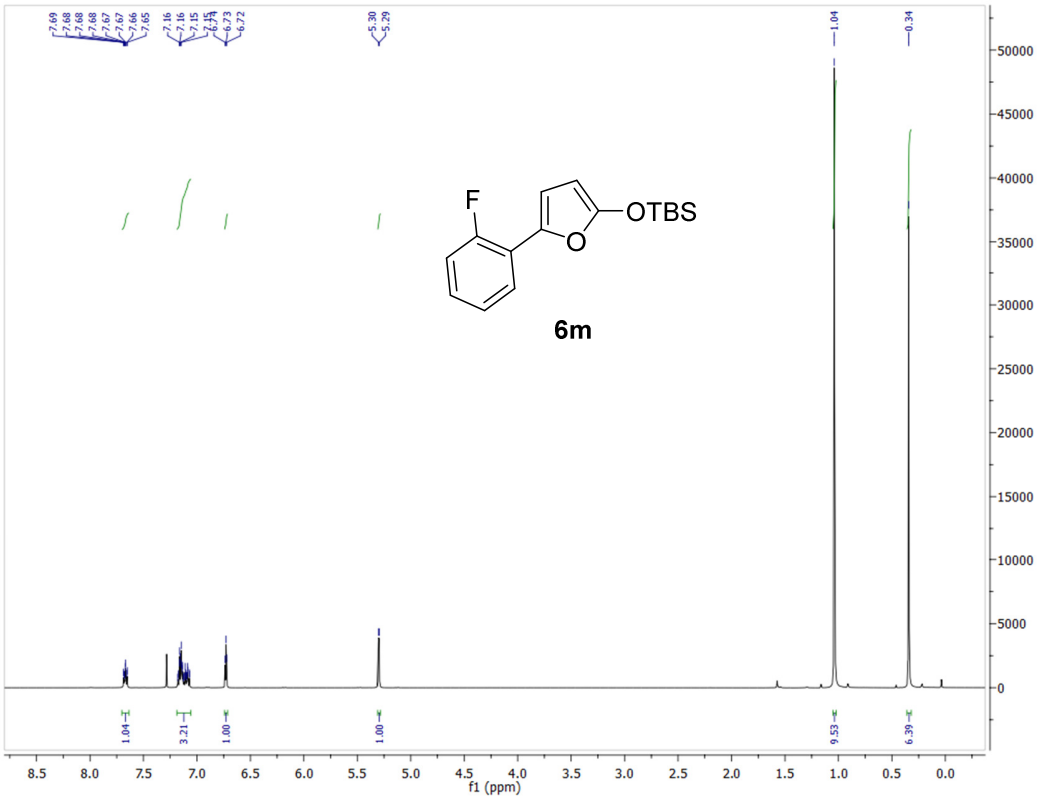
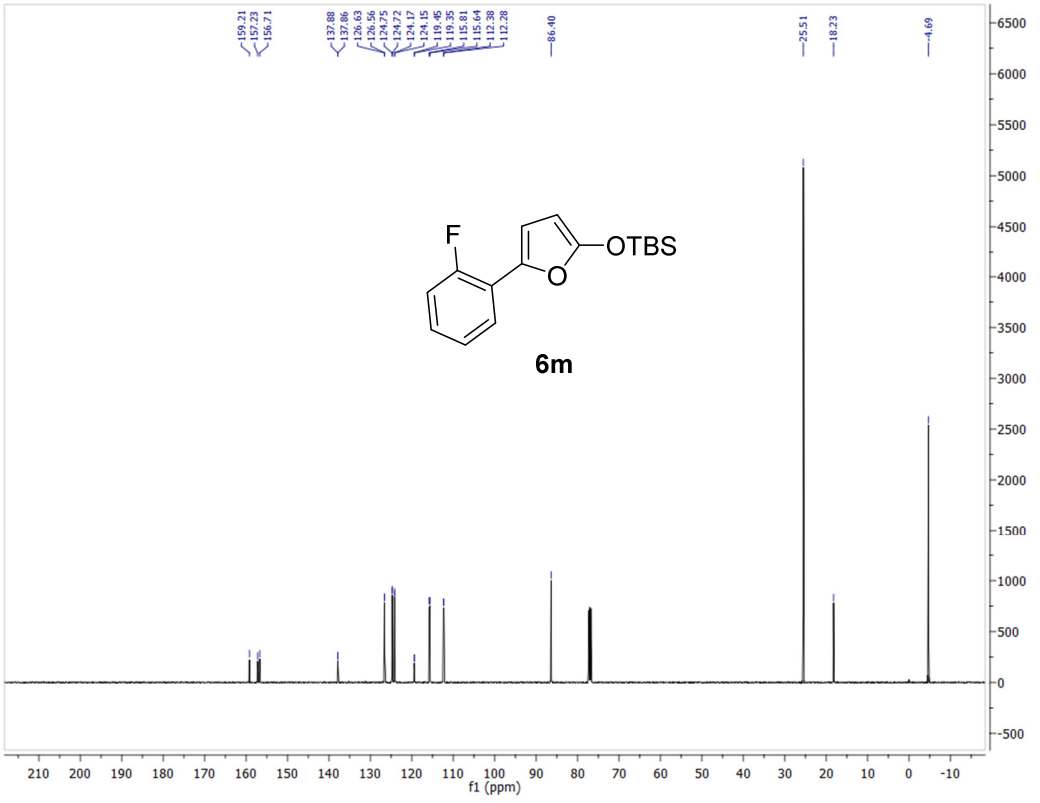
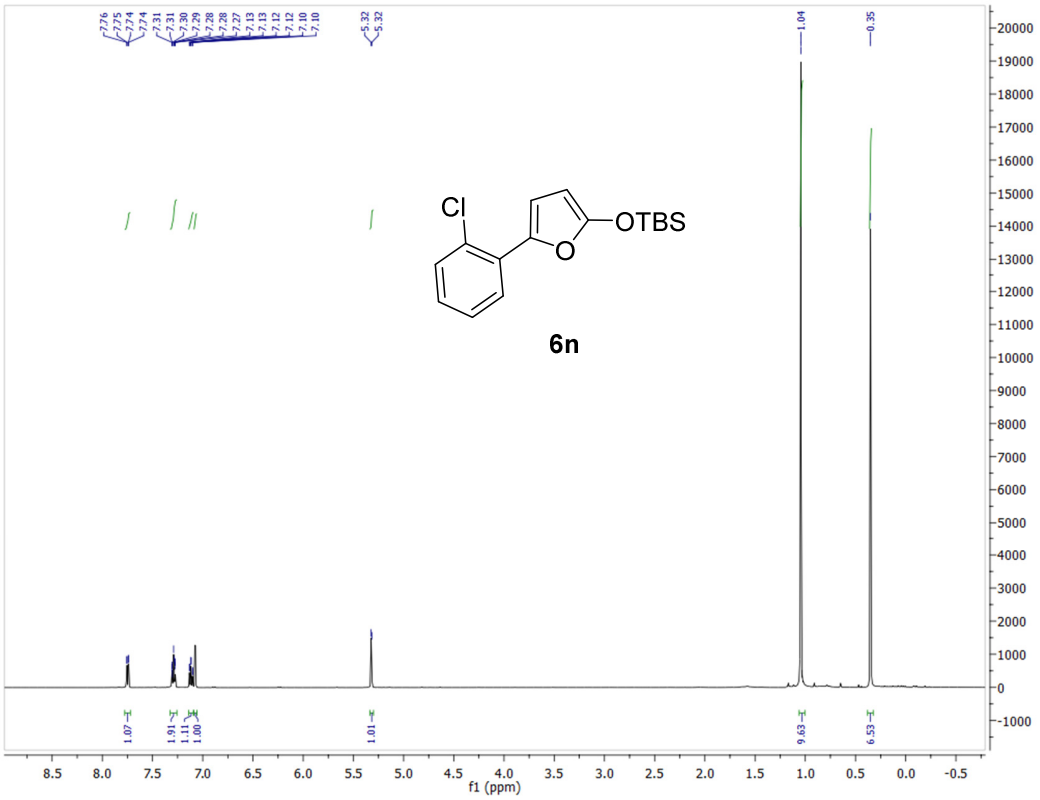
4.63
OTBS
O
6k
f1 (ppm)


OTBS
MeO
O
6l
f1 (ppm)


OTBS
MeO
O
6l
f1 (ppm)


F
OTBS
O
6m
f1 (ppm)


F
OTBS
O
6m
f1 (ppm)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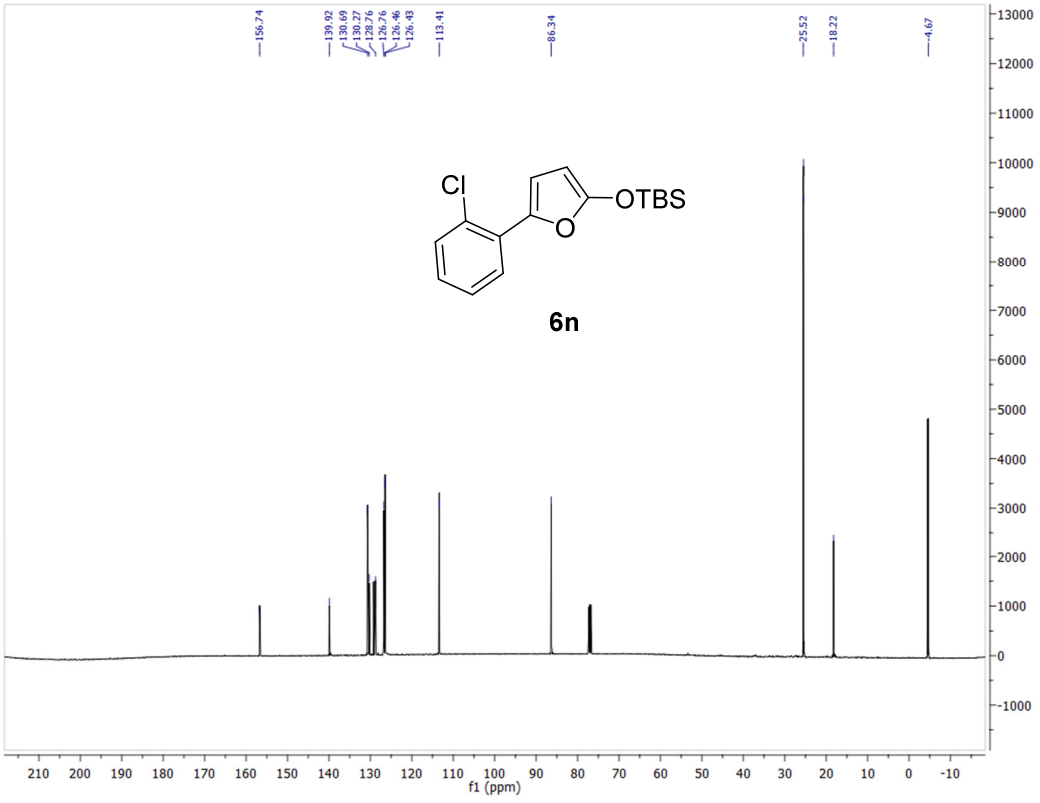
7.28
7.28
7.27
7.13
7.12
7.12
7.10
7.10
5.32
5.32
1.04
0.35
Cl
O
OTBS
6n
1.07
1.91
1.11
1.00
1.01
9.63
6.53
f1 (ppm)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86.34
25.52
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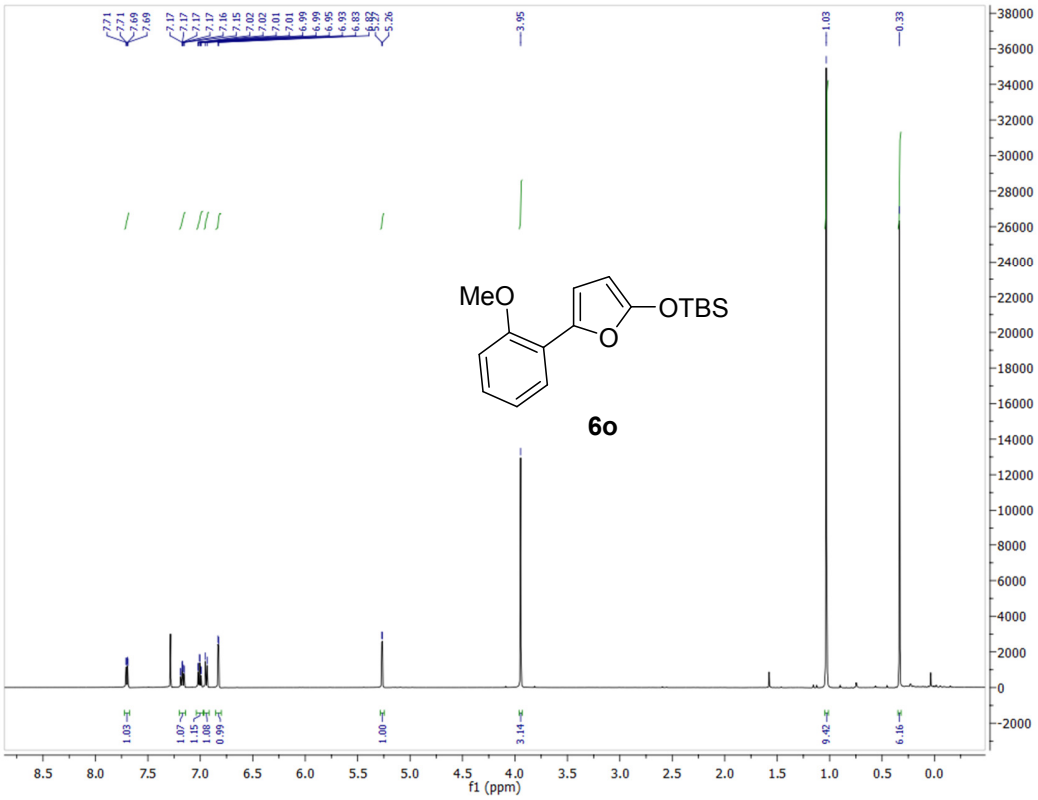
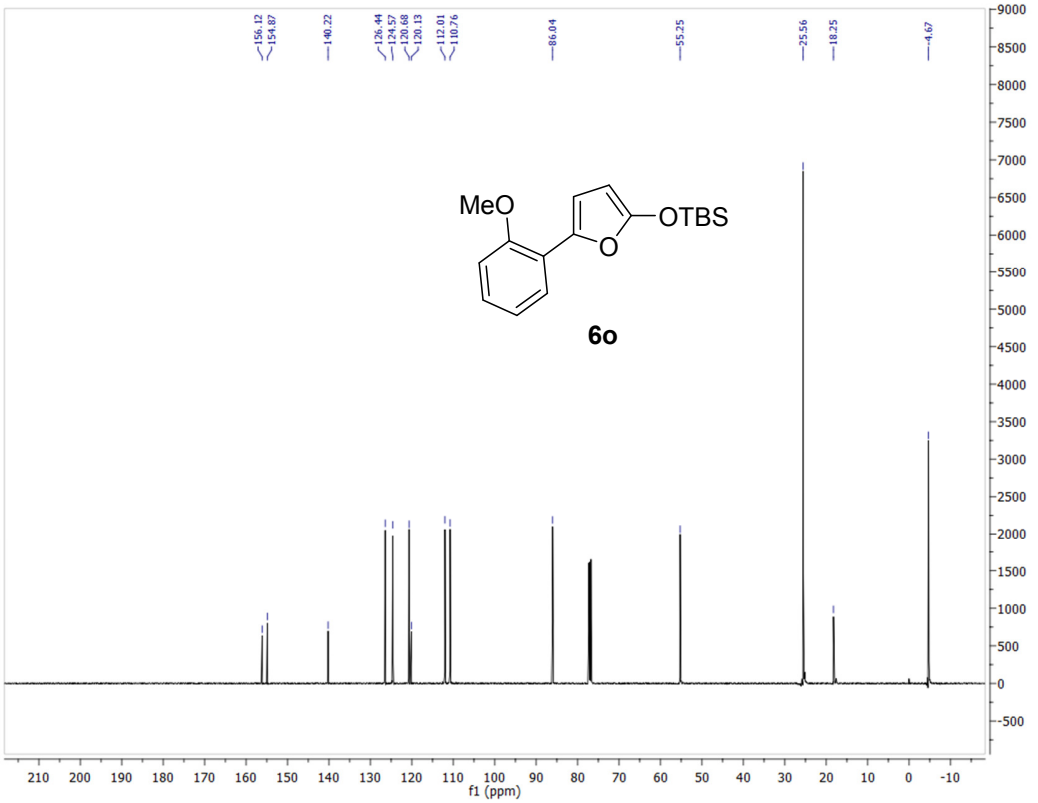
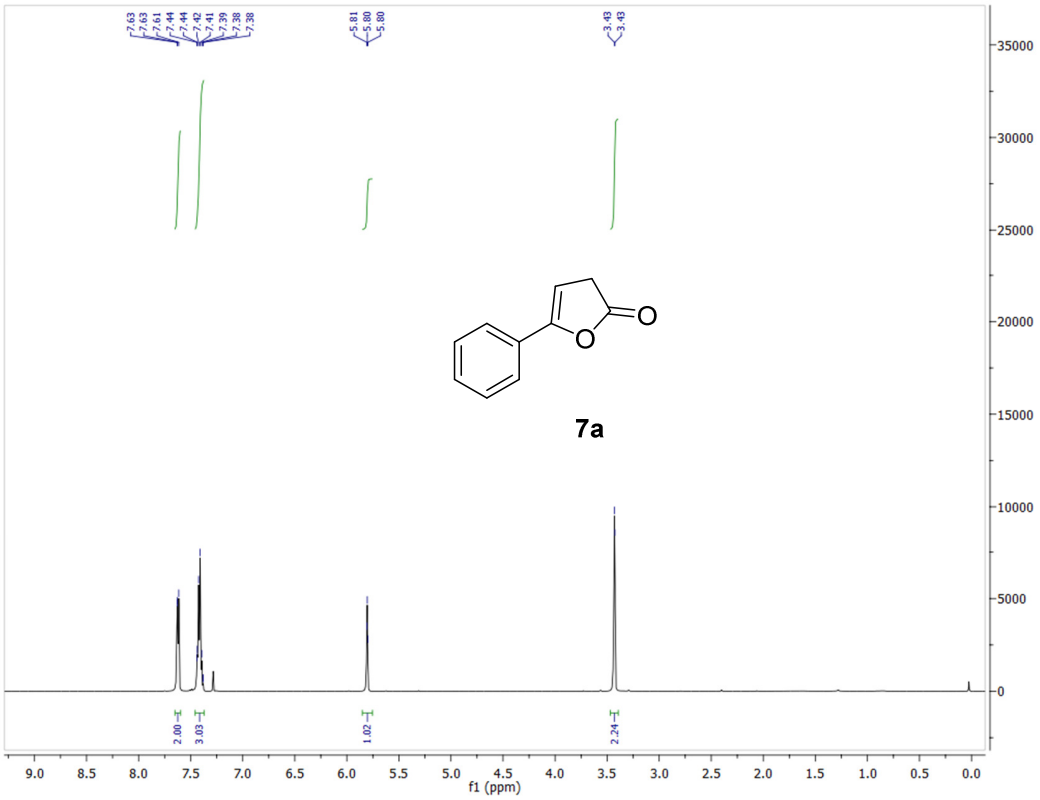
Cl
O
OTBS
6n
f1 (ppm)


MeO
OTBS
O
6o
f1 (ppm)


MeO
OTBS
O
6o
f1 (ppm)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7.63
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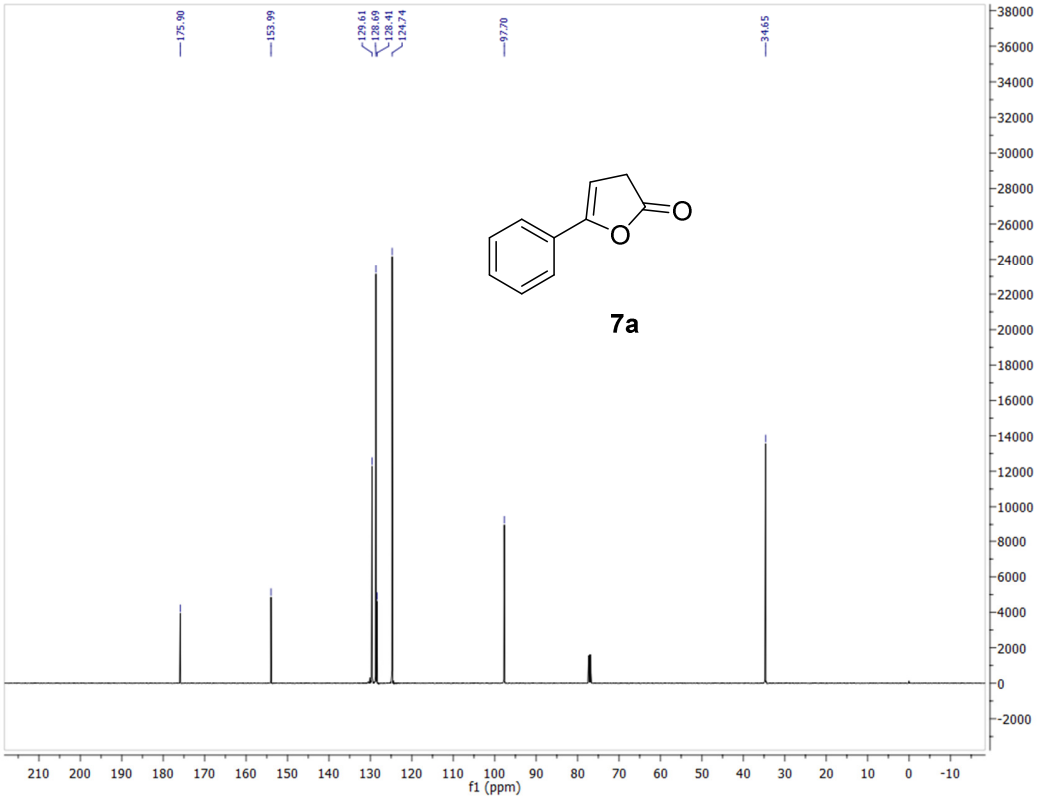
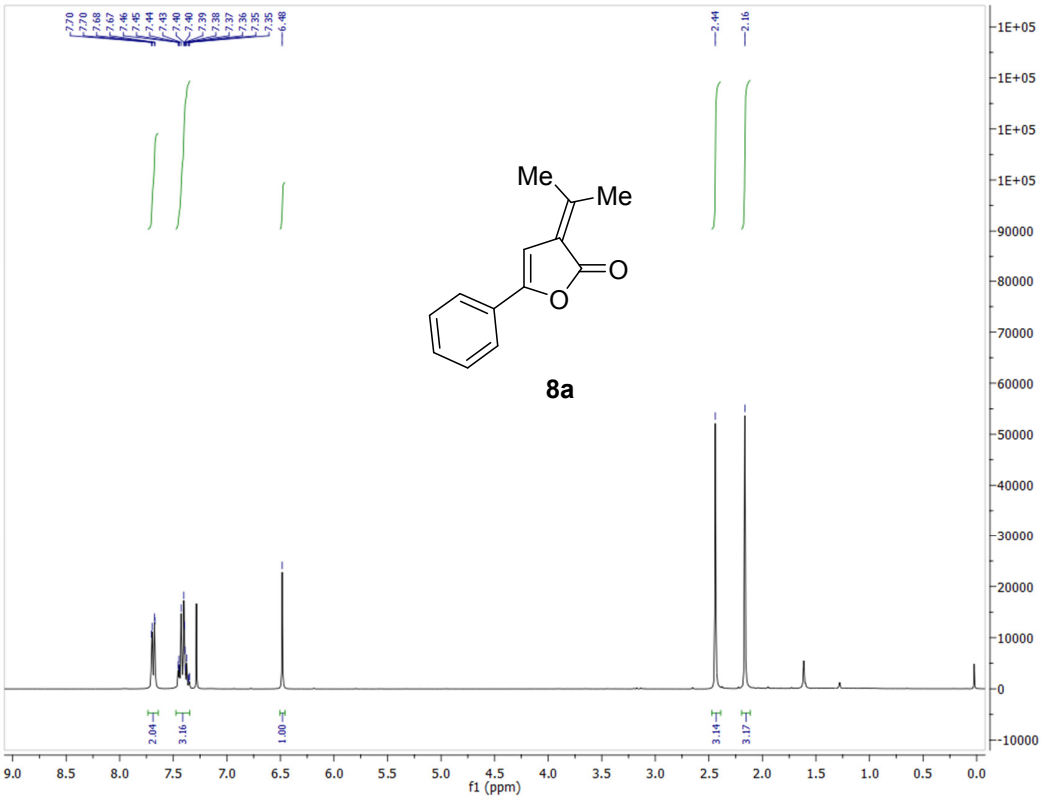
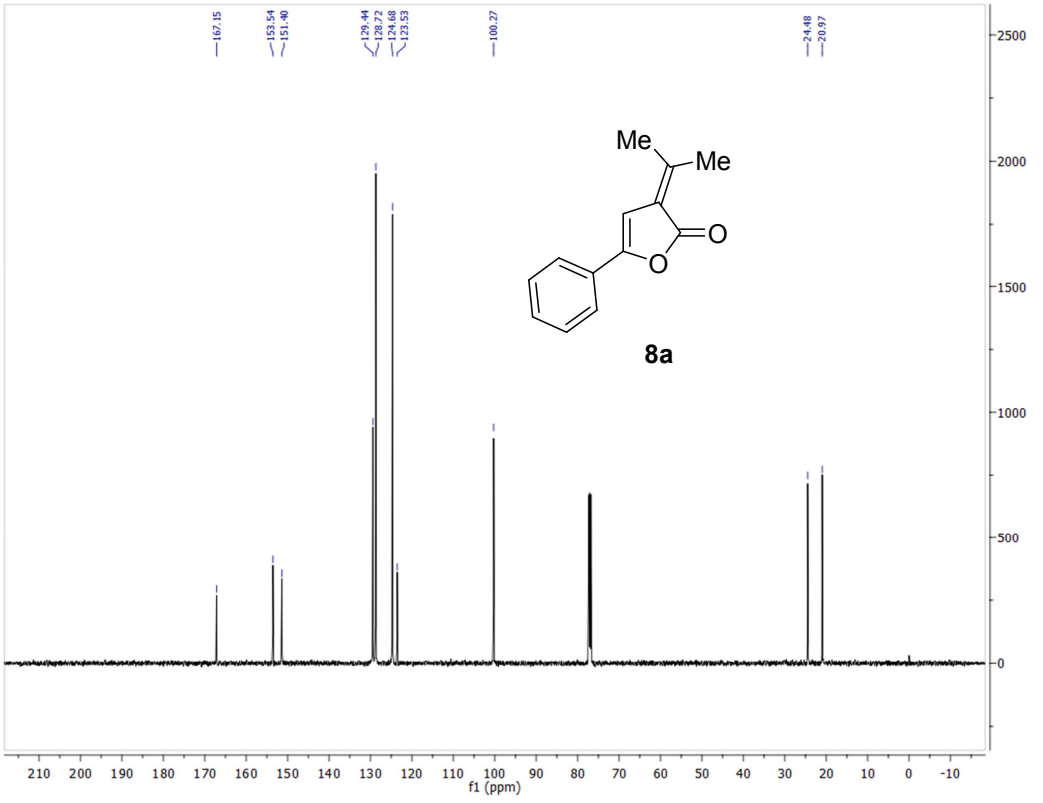
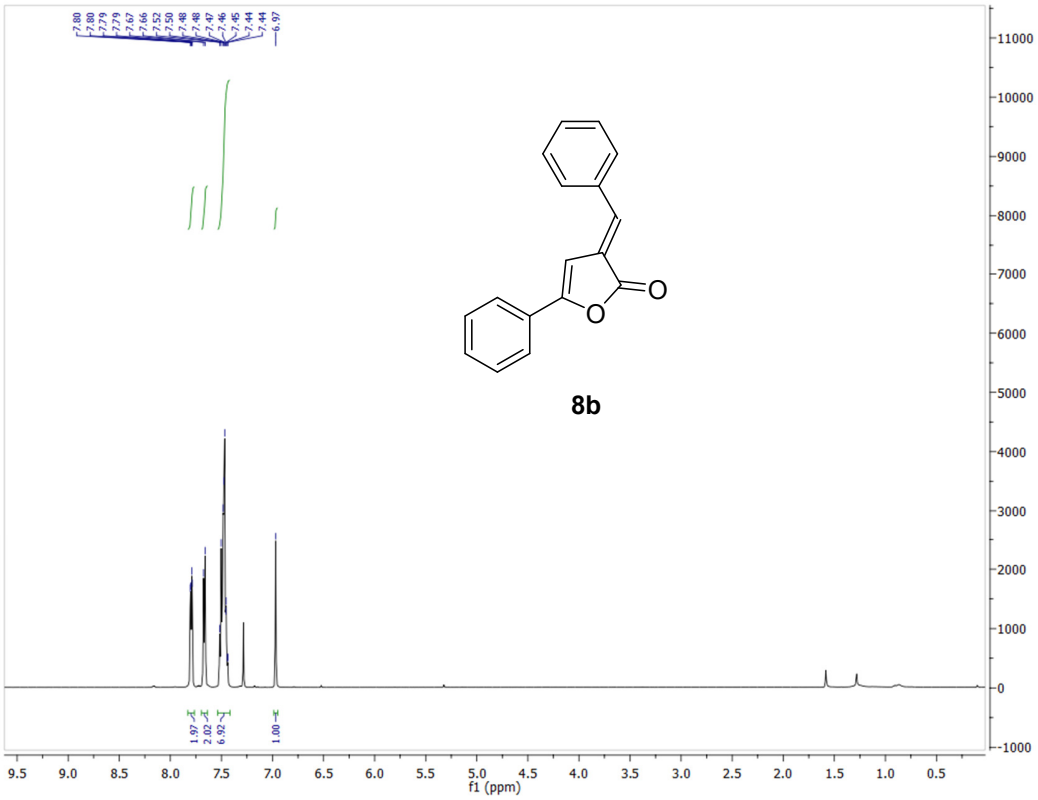
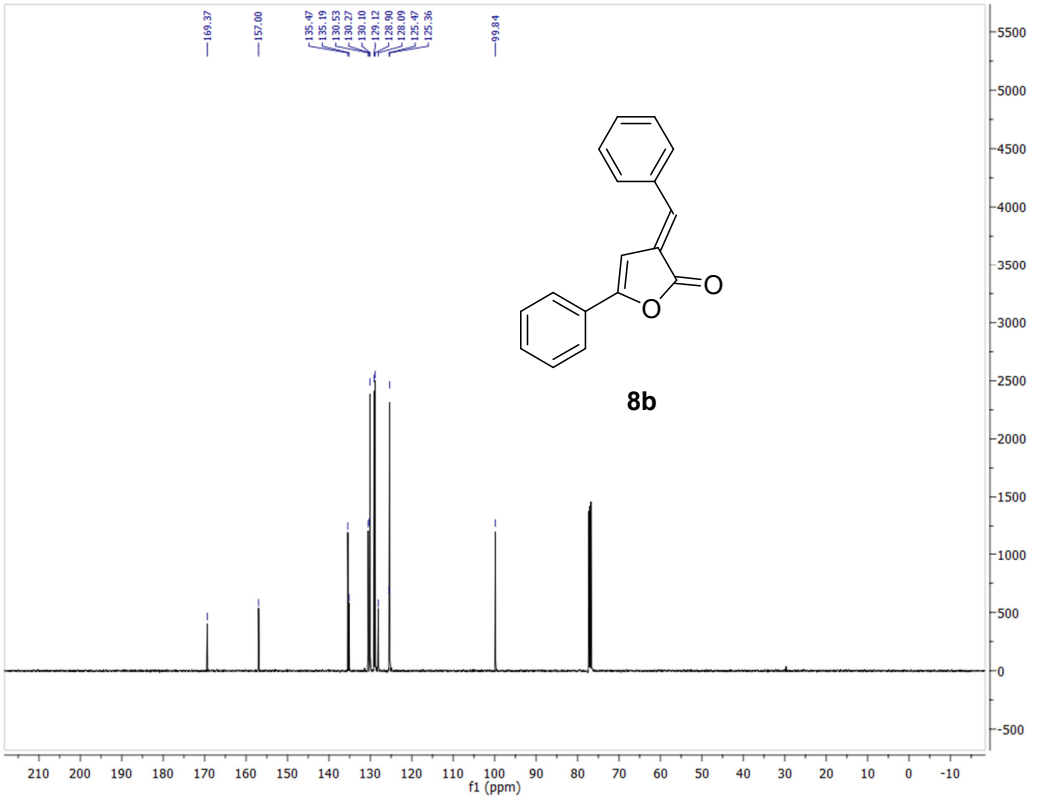
7.41
7.39
7.38
7.38
5.81
5.80
5.80
3.43
3.43
O
O
7a
2.00
3.03
1.02
2.24
f1 (ppm)

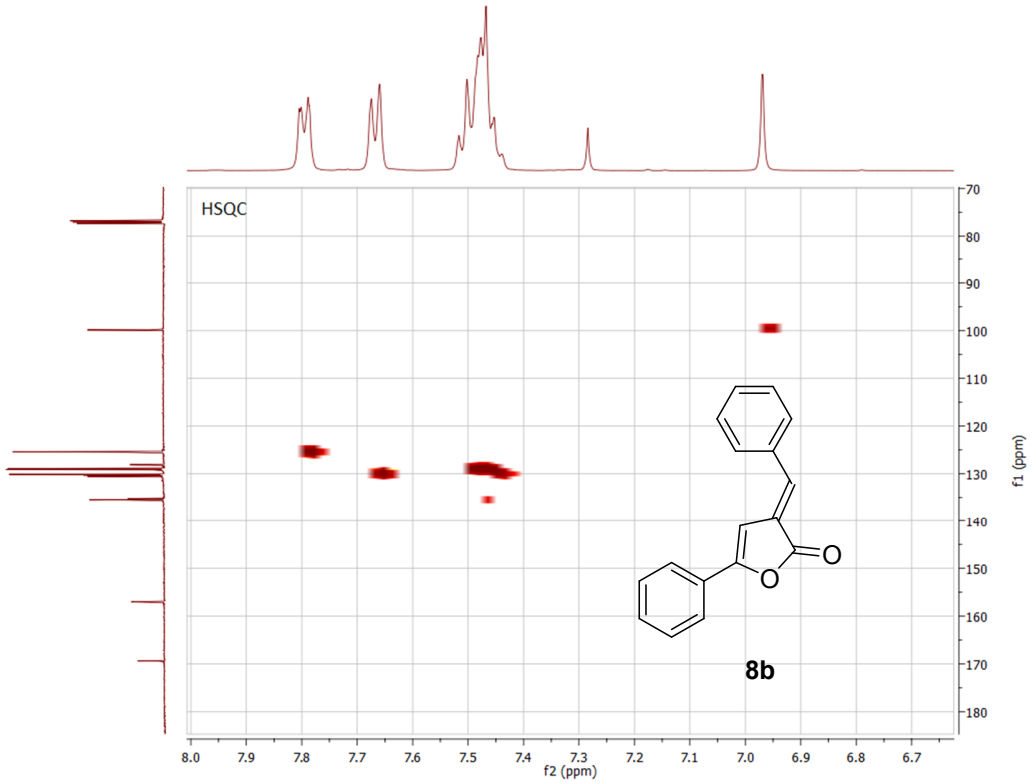

175.90
153.99
129.61
128.69
128.41
124.74
97.70
34.65
O
O
7a
f1 (ppm)

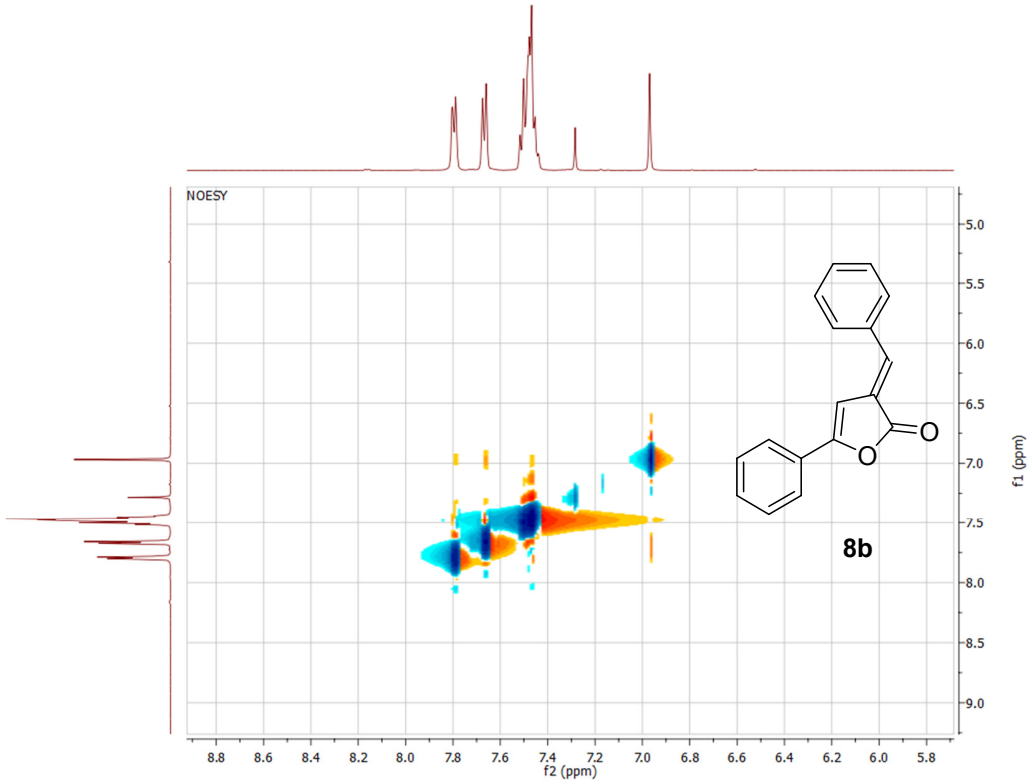

Me
Me
O
O
8a
f1 (ppm)

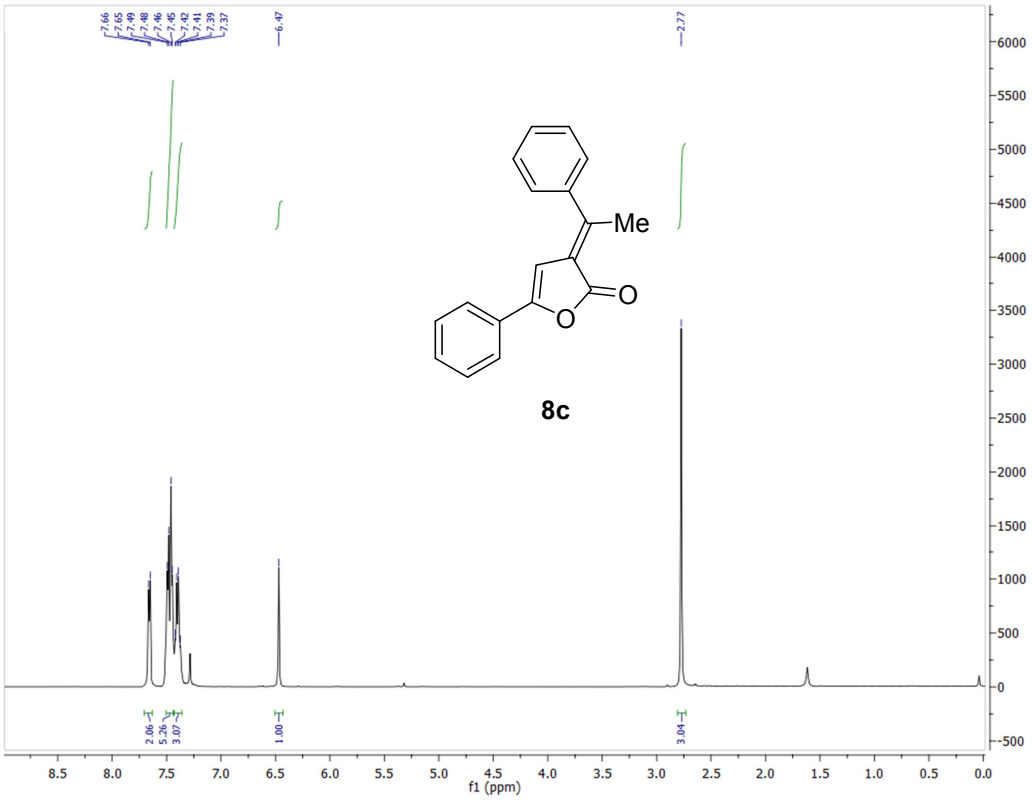

Me
Me
O
O
8a
f1 (ppm)

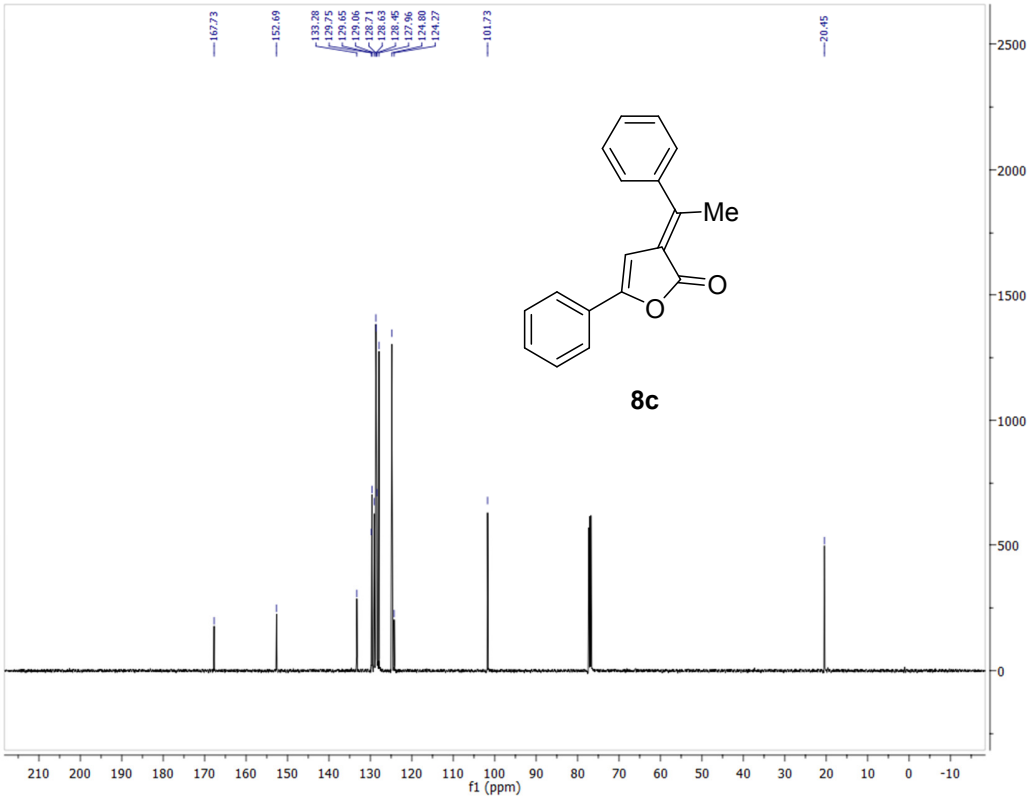

7.80
7.80
7.79
7.79
7.67
7.66
7.52
7.50
7.48
7.48
7.47
7.46
7.45
7.44
7.44
6.97
O
O
8b
1.97
2.02
6.92
1.00
f1 (ppm)

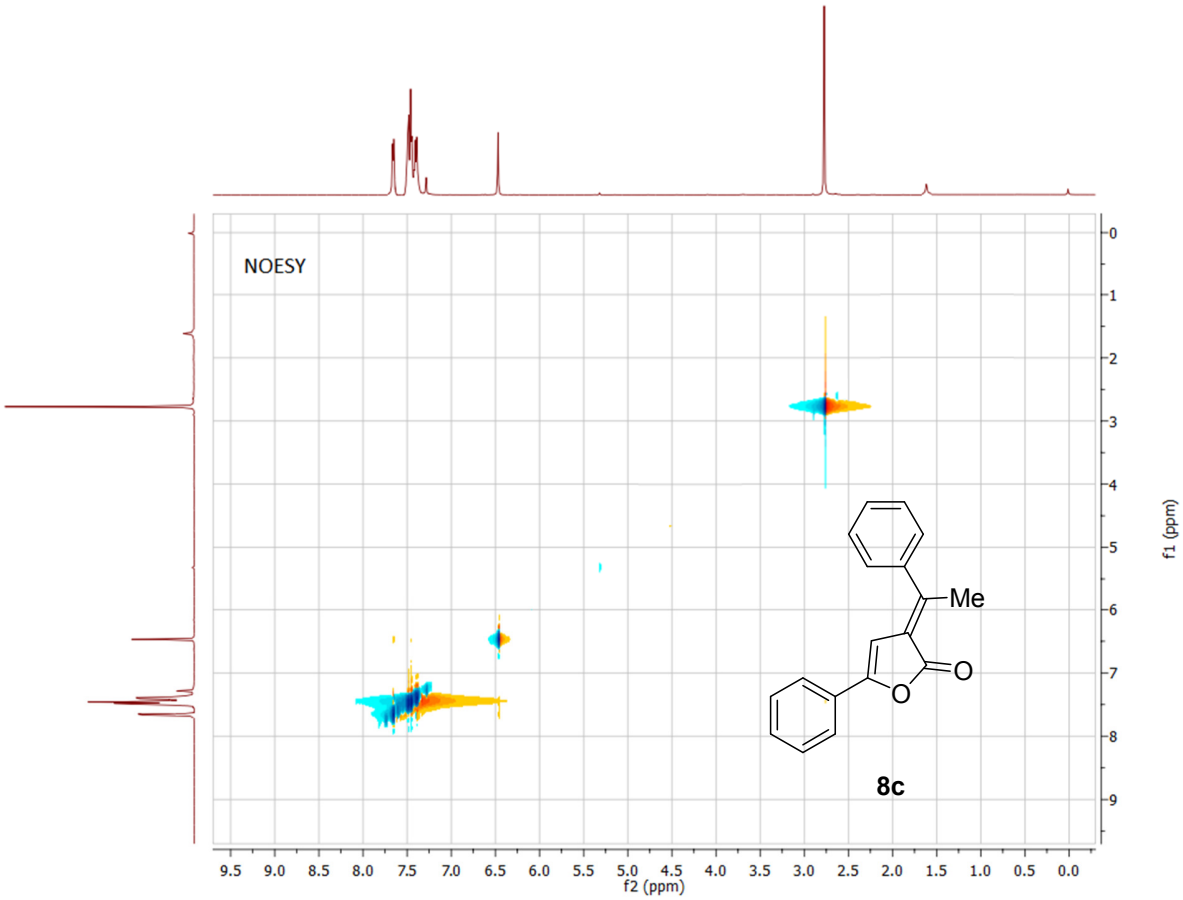

169.37
157.00
135.47
135.19
130.53
130.27
130.10
129.12
128.90
128.09
125.47
125.36
99.84
O
O
8b
f1 (ppm)

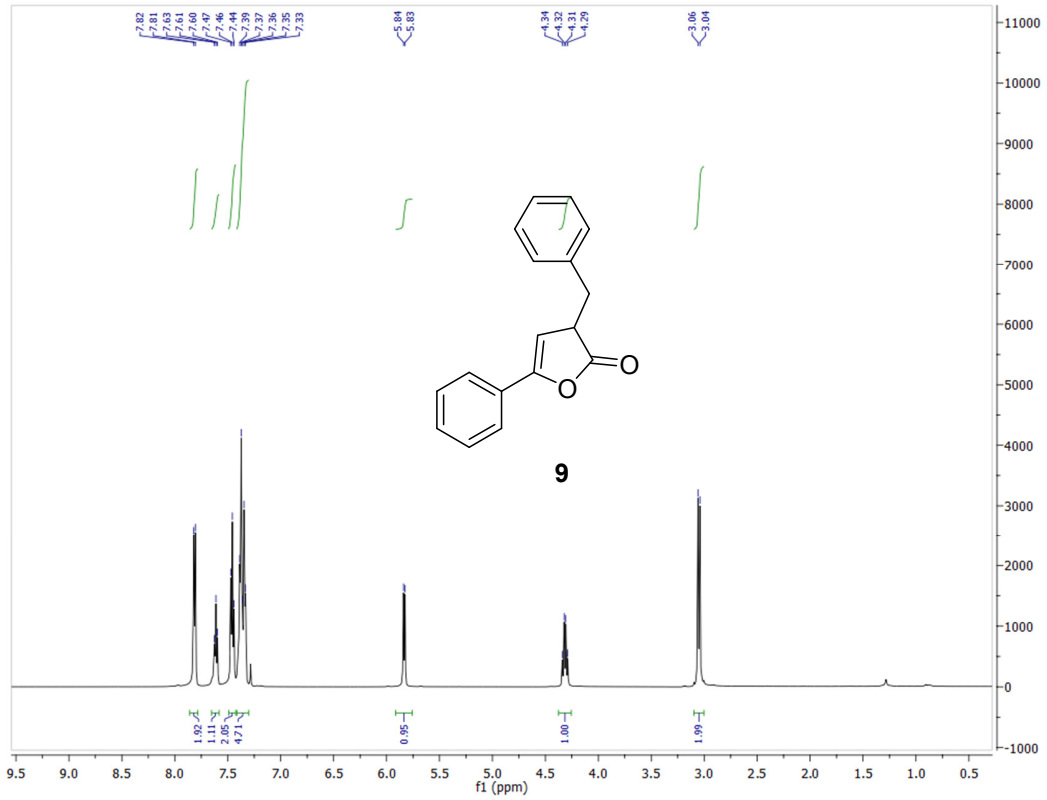

HSQC
f1 (ppm)
f2 (ppm)
O
O
8b

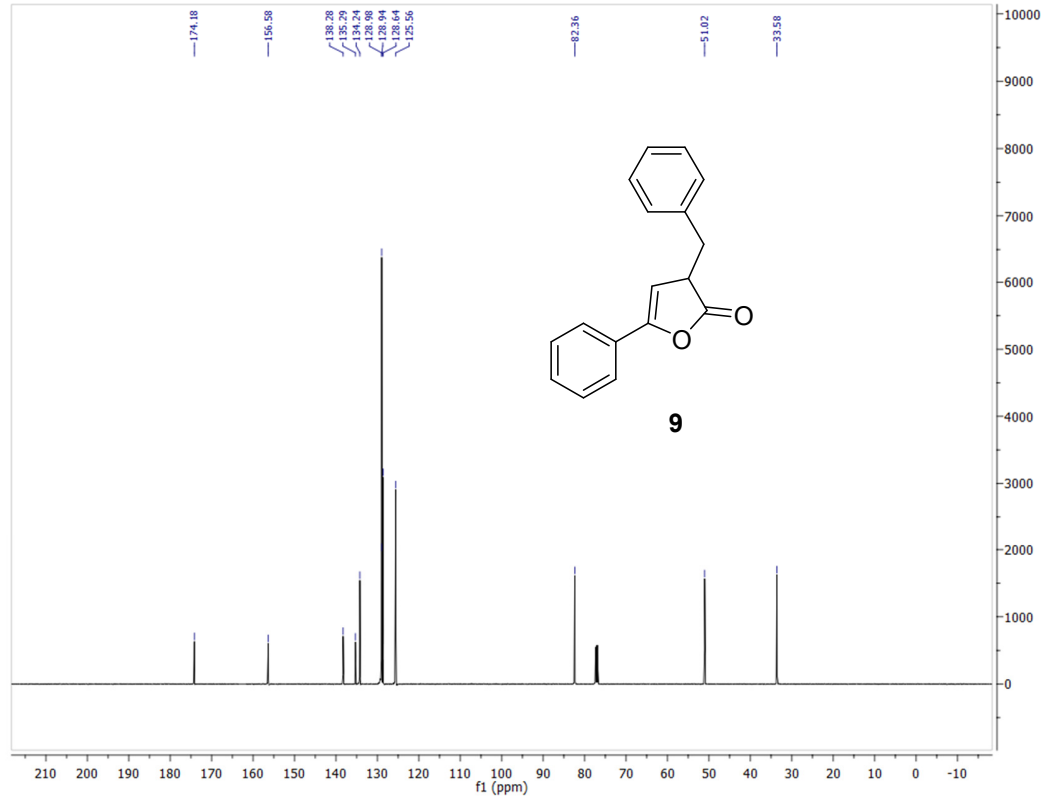

NOESY
f1 (ppm)
f2 (ppm)
O
O
8b

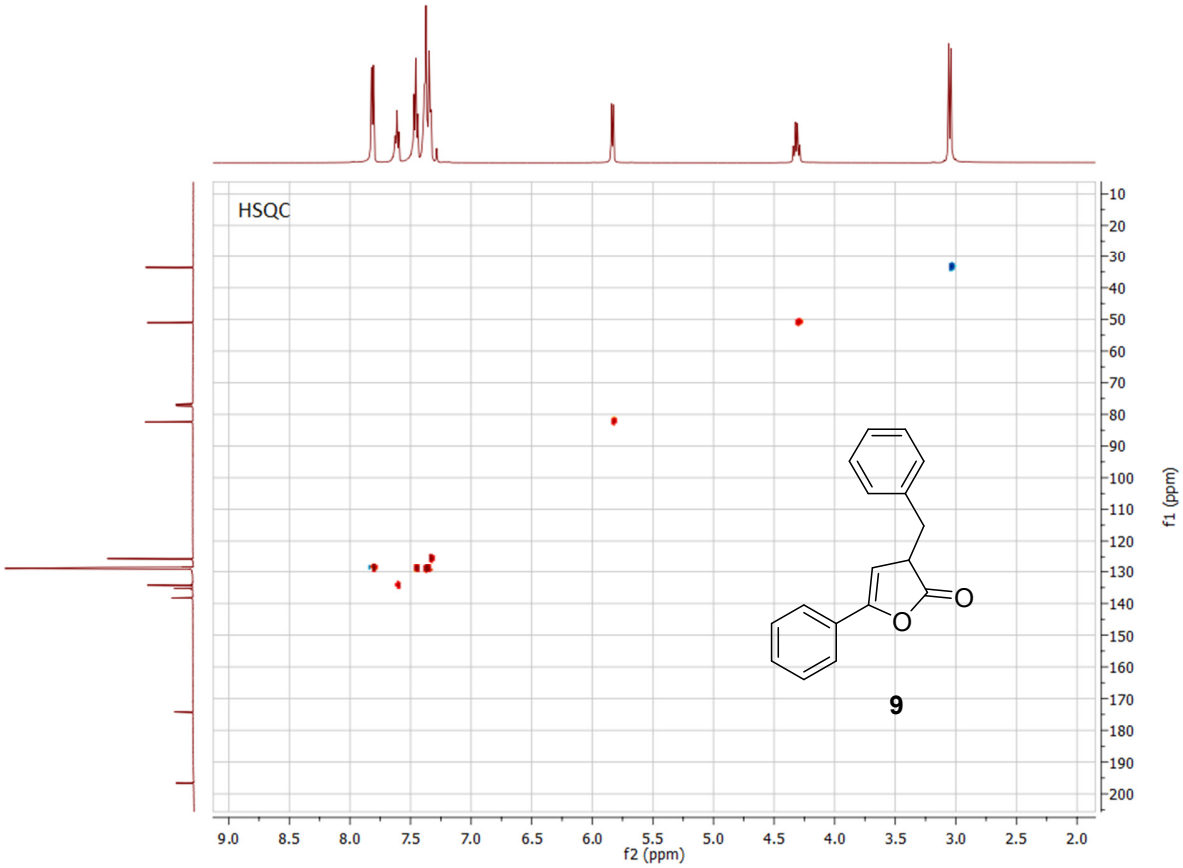

7.66
7.65
7.49
7.48
7.46
7.45
7.42
7.41
7.39
7.37
6.47
2.77
Me
O
O
8c
2.06
5.26
3.07
1.00
3.04
f1 (ppm)

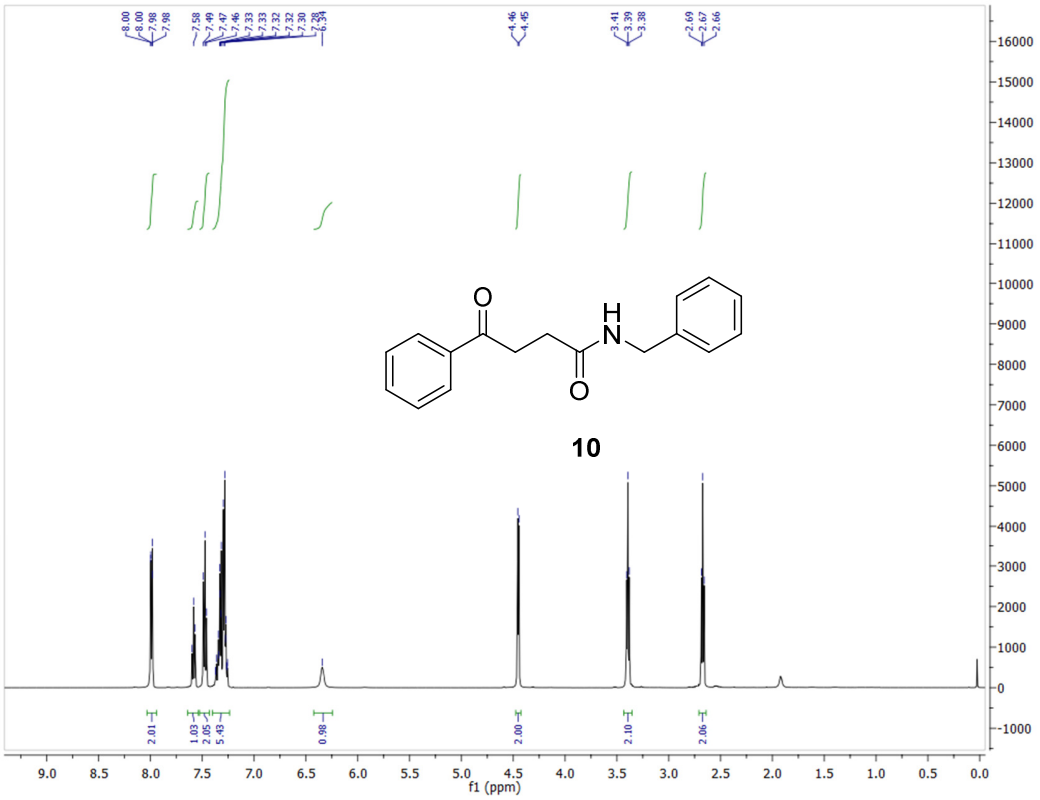

167.73
152.69
133.28
129.75
129.65
129.06
128.71
128.63
128.45
127.96
124.80
124.27
101.73
20.45
Me
O
O
8c
f1 (ppm)

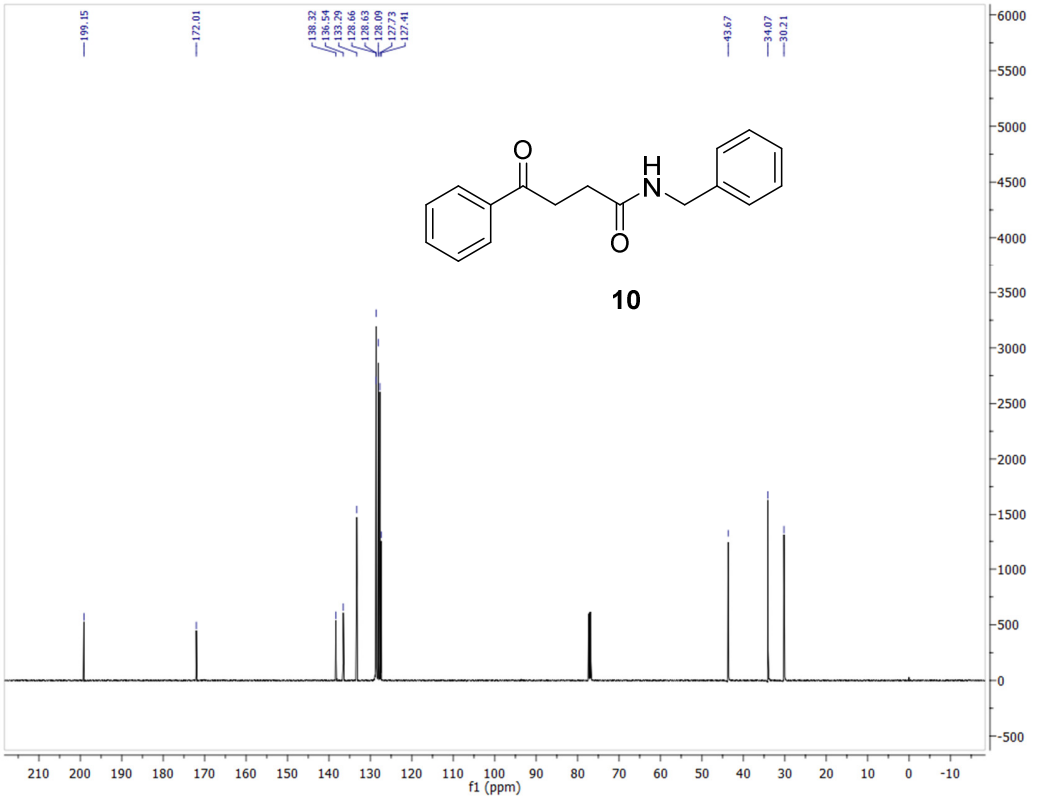

NOESY
Me
O
O
8c
f2 (ppm)
f1 (ppm)

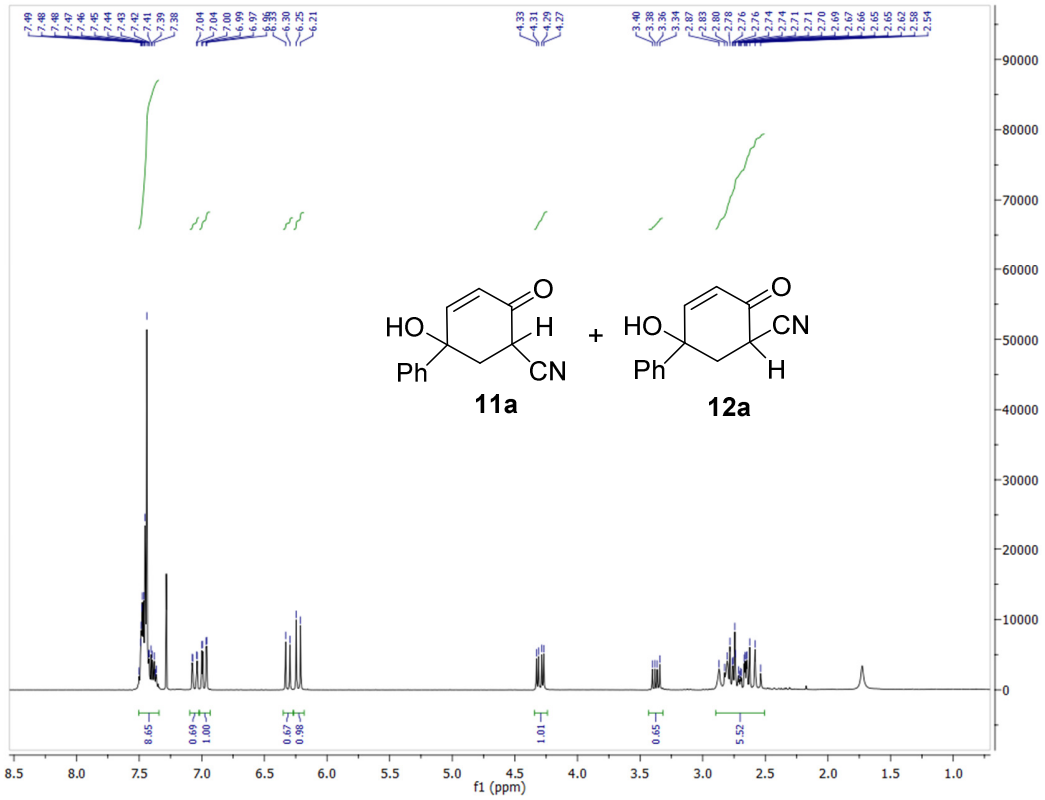

7.82
7.81
7.63
7.61
7.60
7.47
7.46
7.44
7.39
7.37
7.36
7.35
7.33
5.84
5.83
4.34
4.32
4.31
4.29
3.06
3.04
O
O
9
1.92
1.11
2.05
4.71
0.95
1.00
1.99
f1 (ppm)

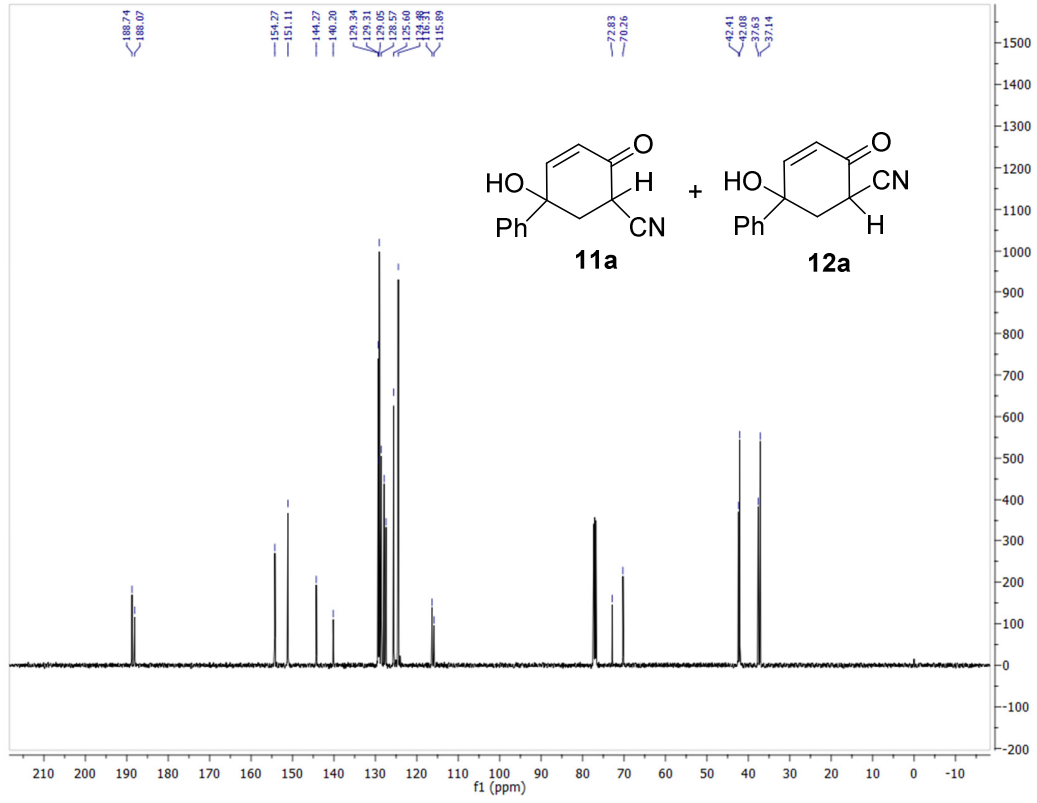

174.18
156.58
138.28
135.29
134.24
128.98
128.94
128.64
125.56
82.36
51.02
33.58
O
O
9
f1 (ppm)

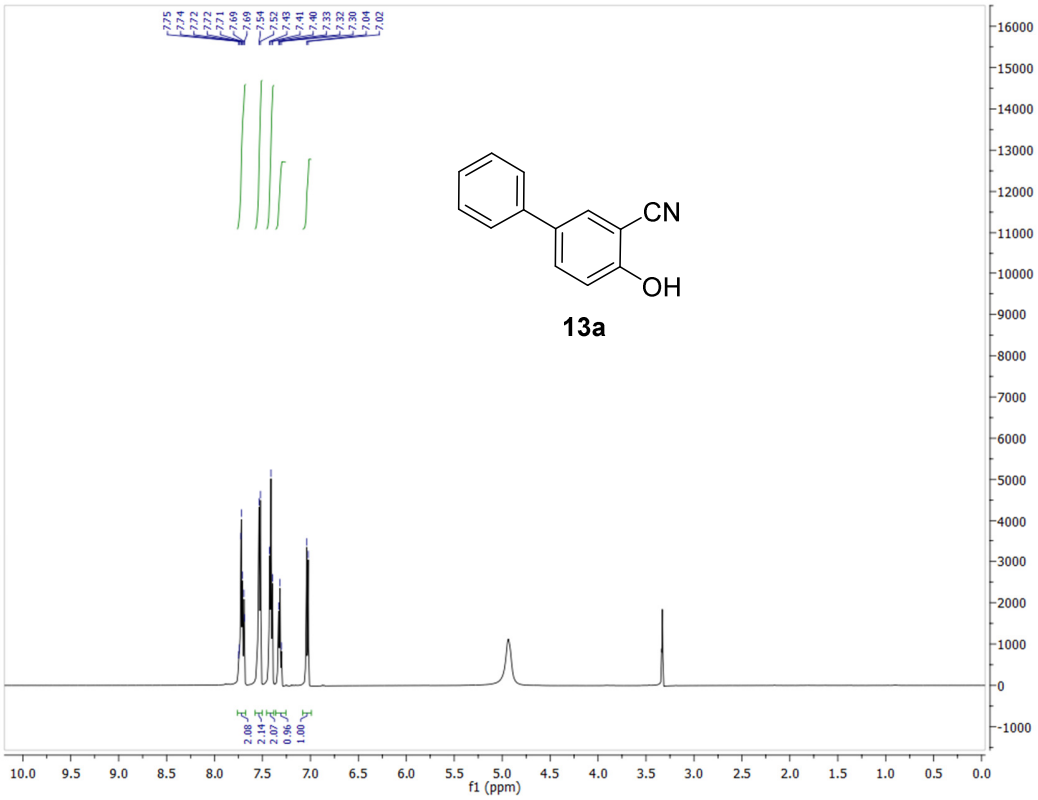

HSQC
f2 (ppm)
f1 (ppm)
O
O
9

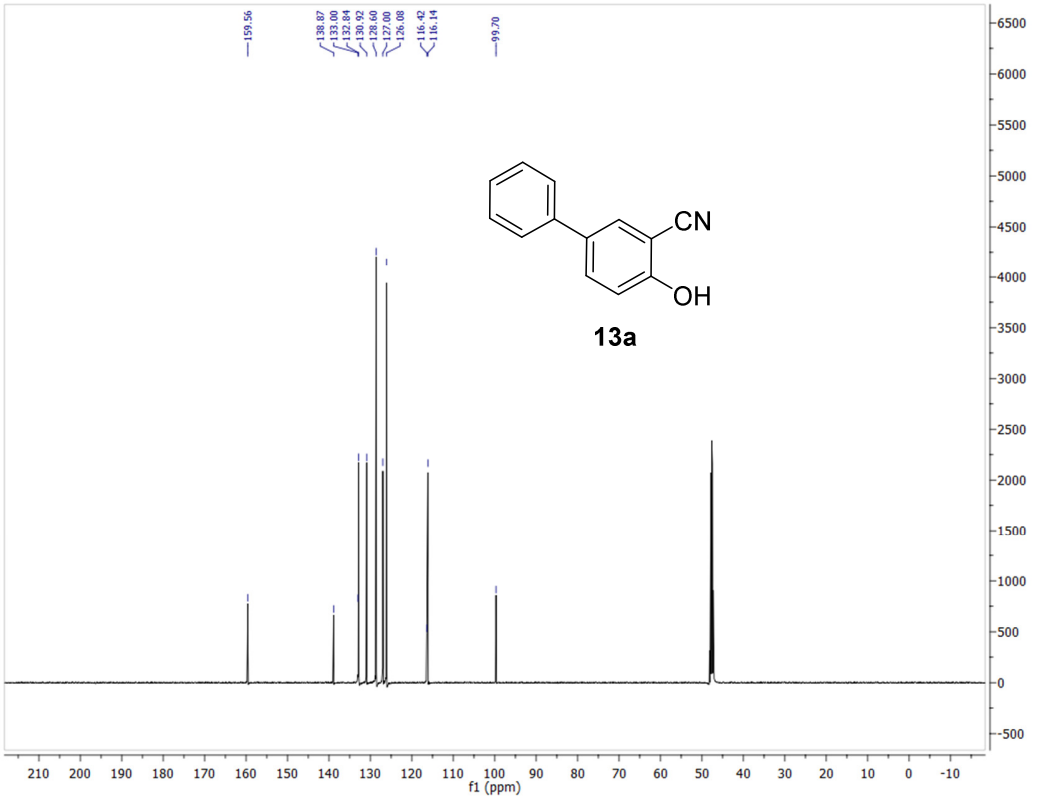

8.00
8.00
7.98
7.98
7.58
7.49
7.47
7.46
7.33
7.33
7.32
7.32
7.30
7.28
6.94
4.46
4.45
3.41
3.39
3.38
2.69
2.67
2.66
O
H
N
O
10
2.01
1.03
2.05
5.43
0.98
2.00
2.10
2.06
f1 (ppm)

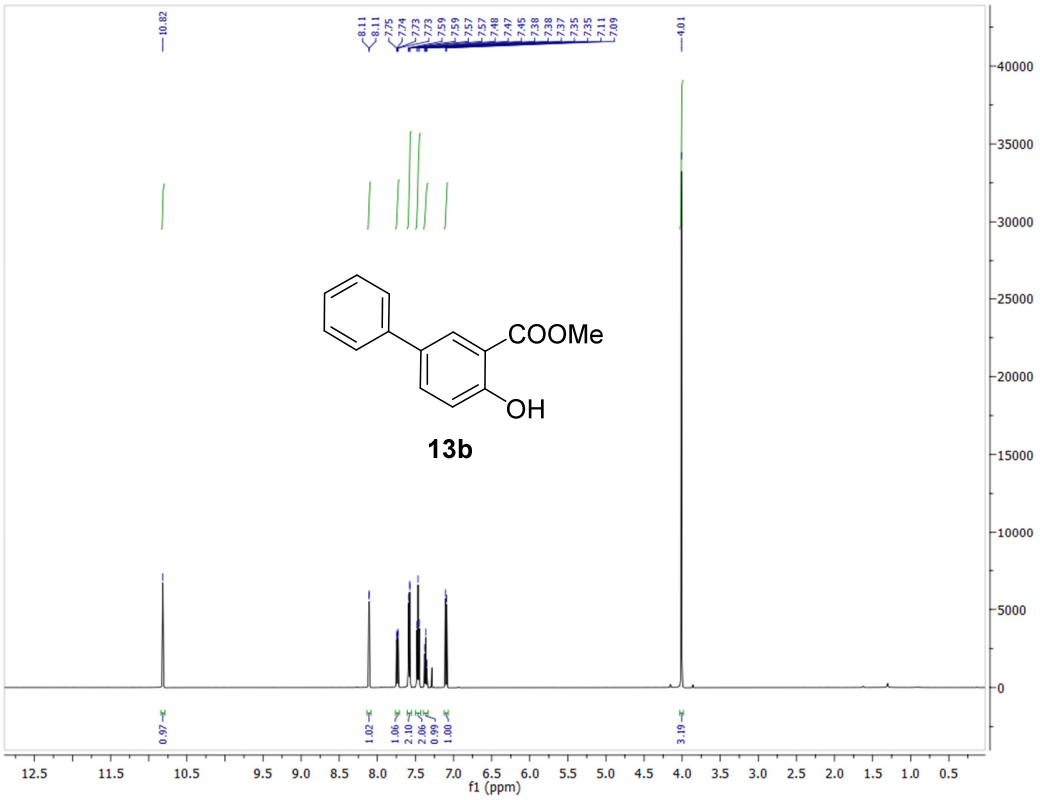

199.15
172.01
138.32
136.54
133.29
128.66
128.63
128.09
127.73
127.41
43.67
34.07
30.21
O
H
N
O
10
f1 (ppm)

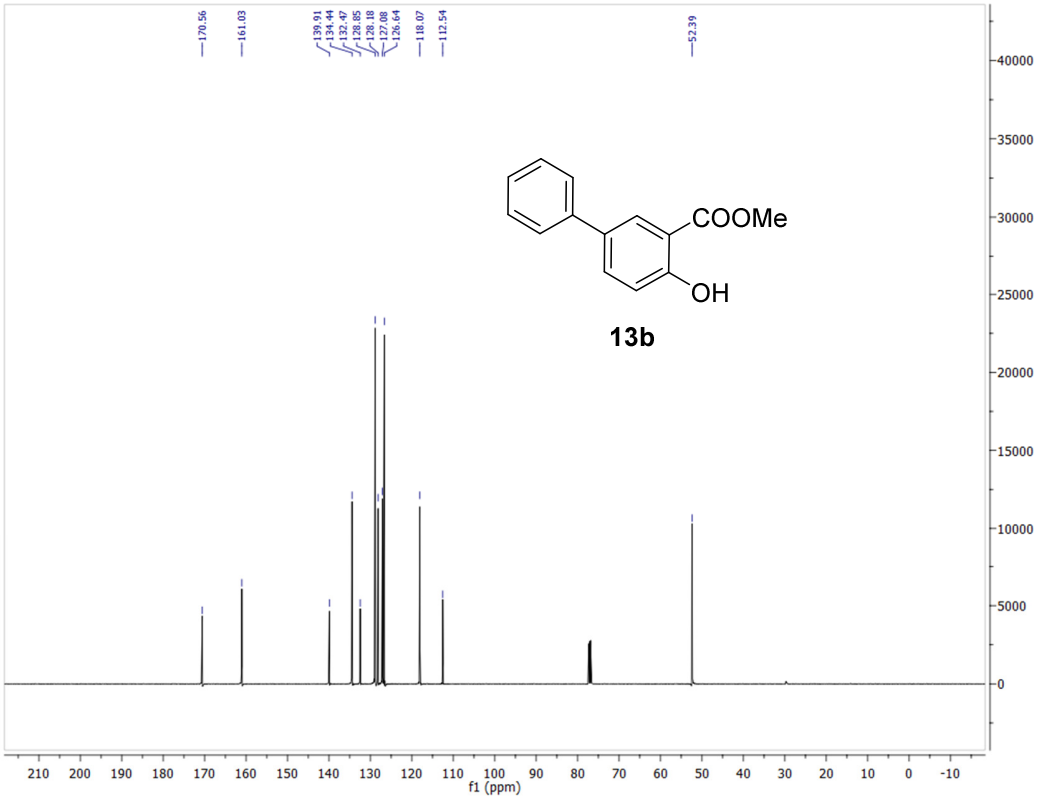

HO
Ph
O
H
CN
11a
+
HO
Ph
O
CN
H
12a
f1 (ppm)


HO
Ph
O
H
CN
11a
+
HO
Ph
O
CN
H
12a
f1 (ppm)


7.75
7.74
7.72
7.72
7.71
7.69
7.69
7.54
7.52
7.43
7.41
7.40
7.33
7.33
7.30
7.04
7.02
CN
OH
13a
2.08
2.14
2.07
0.96
1.00
f1 (ppm)


159.56
138.87
133.00
132.84
130.92
128.60
127.00
126.08
116.42
116.14
99.70
CN
OH
13a
f1 (ppm)


10.82
8.11
8.11
7.75
7.74
7.73
7.73
7.59
7.59
7.57
7.57
7.48
7.47
7.45
7.38
7.38
7.37
7.35
7.35
7.11
7.09
4.01
COOMe
OH
13b
0.97
1.02
1.06
2.10
2.06
0.99
1.00
3.19
f1 (ppm)


170.56
161.03
139.91
134.44
132.47
128.85
128.18
127.08
126.64
118.07
112.54
52.39
COOMe
OH
13b
f1 (ppm)

Cartesian coordinates for the stationary points

$Rh_2(OCHO)_4$

Rh	-0.000009	0.000024	-1.194426
Rh	0.000009	-0.000024	1.194426
O	-1.496963	1.403149	-1.130170
O	-1.403135	-1.496931	-1.130229
O	1.496945	-1.403103	-1.130250
O	1.403117	1.496977	-1.130191
O	-1.496958	1.403089	1.130250
O	-1.403103	-1.496990	1.130191
O	1.496976	-1.403135	1.130170
O	1.403121	1.496944	1.130229
C	-1.906299	1.786796	0.000051
C	-1.786796	-1.906299	-0.000024
C	1.906299	-1.786796	-0.000051
C	1.786796	1.906299	0.000024
H	-2.714750	2.544562	0.000072
H	-2.544562	-2.714750	-0.000035
H	2.714750	-2.544562	-0.000073
H	2.544562	2.714750	0.000034

N_2

N	0.000000	0.000000	0.550174
N	0.000000	0.000000	-0.550174

4c (R^1 = OTMS, R^2 = Ph)

Si	3.693938	-0.273050	-0.003842
O	1.988300	-0.225866	0.022386
O	-1.528990	2.262366	0.113526
N	-0.370312	-1.001574	-0.428617
N	-0.402541	-2.083723	-0.762127
C	4.336027	0.785586	-1.419628
C	4.062410	-2.088630	-0.299416
C	4.376715	0.280599	1.659752
C	1.081749	0.781850	0.131338
C	1.375657	2.070303	0.384163
C	-0.297780	0.262748	-0.057814
C	-1.551580	1.042788	0.048462
C	-2.874799	0.322473	0.059588
C	-3.094114	-0.875991	0.758160
C	-4.366281	-1.454024	0.785611
C	-5.428125	-0.845584	0.110663
C	-5.220300	0.355761	-0.576872
C	-3.955560	0.942698	-0.590781
H	3.905416	0.454712	-2.378846
H	5.433145	0.699170	-1.495683
H	4.090099	1.850834	-1.290958
H	3.649351	-2.713450	0.508892
H	5.149667	-2.267179	-0.343335
H	3.623801	-2.432864	-1.249889
H	4.174223	1.342361	1.868673
H	5.469838	0.135070	1.690980
H	3.935606	-0.312840	2.477267
H	0.580974	2.809661	0.432742
H	2.408729	2.382008	0.541338
H	-2.280553	-1.351780	1.310228
H	-4.528681	-2.380381	1.342183
H	-6.420743	-1.302924	0.127359
H	-6.050621	0.839171	-1.097829
H	-3.784020	1.892728	-1.100794

6c (R^1 = OTMS, R^2 = Ph)

Si	-3.005583	-0.575160	-0.000001
O	-2.305315	0.996386	0.000007
O	-0.082143	0.427203	0.000004
C	-2.473671	-1.477079	-1.558943
C	-4.843474	-0.210805	0.000003
C	-2.473667	-1.477096	1.558928
C	-1.042977	1.384678	0.000004
C	-0.477932	2.634610	0.000002
C	0.936169	2.416115	0.000000
C	1.148584	1.058802	0.000001
C	2.338109	0.219533	0.000000
C	3.625444	0.798330	-0.000003
C	4.767681	0.000433	-0.000003
C	4.659722	-1.395478	-0.000001
C	3.390544	-1.981257	0.000002
C	2.242573	-1.187378	0.000003
H	-2.763377	-0.910949	-2.459139
H	-2.951596	-2.469581	-1.616342
H	-1.382511	-1.621923	-1.584443
H	-5.132052	0.369672	0.890971
H	-5.427926	-1.145852	-0.000001
H	-5.132054	0.369681	-0.890957
H	-1.382508	-1.621943	1.584424
H	-2.951594	-2.469599	1.616318
H	-2.763369	-0.910976	2.459132
H	-1.015514	3.578478	0.000002
H	1.707909	3.182696	-0.000002
H	3.730711	1.885548	-0.000004
H	5.753648	0.472732	-0.000006
H	5.557130	-2.018920	-0.000002
H	3.291064	-3.070070	0.000004
H	1.257227	-1.655912	0.000006

A (R^1 = OTMS, R^2 = Ph)

Rh	-1.132684	-0.229430	0.180020
Rh	-3.428708	0.116052	-0.535982
Si	4.902804	-1.321427	-0.474358
O	-0.593120	-0.033017	-1.809458
O	-1.450150	-2.255657	-0.089070
O	-1.854041	-0.399554	2.098038
O	-1.012626	1.813065	0.415127
O	-2.736962	0.270151	-2.467032
O	-3.586205	-1.926921	-0.756600
O	-3.988542	-0.052976	1.435806
O	-3.143626	2.131670	-0.272805
O	3.395056	-0.993510	0.268671
O	1.372559	0.935871	2.736087
N	0.806720	-1.457126	1.949365
N	0.468032	-2.126855	2.778239
C	-1.499759	0.169436	-2.666786
C	-2.588285	-2.640548	-0.487932

C	-3.095835	-0.268024	2.295330
C	-2.021339	2.521914	0.143507
C	5.280437	-3.158538	-0.317976
C	6.105148	-0.297966	0.533440
C	4.859166	-0.765467	-2.270008
C	2.111500	-1.312422	-0.013884
C	1.703574	-2.188814	-0.944479
C	1.162837	-0.610900	0.945985
C	1.541977	0.740203	1.548370
C	2.130054	1.789050	0.656538
C	2.044610	1.765557	-0.744793
C	2.608409	2.799462	-1.496252
C	3.266284	3.858074	-0.860861
C	3.349988	3.888081	0.535784
C	2.779106	2.862922	1.289497
H	-1.160171	0.267635	-3.718248
H	-2.712646	-3.735487	-0.613632
H	-3.430142	-0.354754	3.348775
H	-1.899437	3.614195	0.289079
H	5.239382	-3.477558	0.736328
H	6.295893	-3.371619	-0.692833
H	4.577253	-3.785931	-0.887848
H	5.845653	0.771524	0.483518
H	7.135859	-0.419006	0.160896
H	6.088839	-0.600888	1.592733
H	4.129117	-1.331467	-2.869126
H	5.851026	-0.901516	-2.733288
H	4.597477	0.302777	-2.336087
H	0.643756	-2.377879	-1.096807
H	2.422606	-2.728923	-1.562838
H	1.514504	0.960788	-1.254827
H	2.527062	2.781515	-2.586154
H	3.708944	4.662773	-1.453971
H	3.857977	4.715700	1.037409
H	2.821210	2.872886	2.380010

B (R^1 = OTMS, R^2 = Ph)

Rh	0.797217	-0.130346	0.088425
Rh	3.253204	-0.225357	-0.207984
Si	-4.158884	-2.175118	-0.128745
O	1.185329	0.305787	2.077405
O	0.887539	-2.150110	0.522324
O	0.673059	-0.577646	-1.916310
O	0.935094	1.872356	-0.385950
O	3.431422	0.226526	1.800472
O	3.135918	-2.234535	0.252789
O	2.919981	-0.666669	-2.189513
O	3.183098	1.788114	-0.654417
O	-3.337662	-1.025189	0.854209
O	-2.317585	0.376710	-1.651292
C	2.389461	0.385546	2.474181
C	2.013931	-2.733075	0.502228
C	1.733032	-0.739707	-2.589627
C	2.071414	2.367442	-0.650913
C	-5.435455	-1.188600	-1.079515
C	-4.981260	-3.389245	1.051004
C	-2.908670	-3.025022	-1.238763
C	-2.017725	-0.910389	1.132977
C	-1.486689	-1.441303	2.272425
C	-1.205838	-0.052786	0.305379
C	-1.953076	0.870847	-0.591707
C	-2.223194	2.274715	-0.197117
C	-1.786741	2.788048	1.035308
C	-2.091609	4.103184	1.389676
C	-2.825504	4.910808	0.514159
C	-3.257615	4.404245	-0.718468
C	-2.959077	3.090206	-1.073186
H	2.517666	0.624902	3.550181
H	1.989927	-3.817330	0.737651
H	1.578754	-0.974856	-3.662576
H	2.067880	3.446880	-0.907132
H	-6.080377	-0.615149	-0.393962
H	-6.081871	-1.851715	-1.678249
H	-4.938085	-0.480329	-1.760086
H	-4.234608	-3.944057	1.642888
H	-5.584288	-4.128739	0.497435
H	-5.651306	-2.866598	1.753097
H	-2.393314	-2.282278	-1.867608
H	-3.410796	-3.753391	-1.897333
H	-2.147218	-3.566799	-0.654497
H	-0.425632	-1.344590	2.487987
H	-2.146718	-1.915255	3.003944
H	-1.198398	2.162573	1.711066
H	-1.752089	4.502260	2.348497
H	-3.061340	5.941346	0.792585
H	-3.828931	5.038897	-1.400471
H	-3.285693	2.670302	-2.026819

C (R^1 = OTMS, R^2 = Ph)

Rh	0.647542	0.052626	0.218158
Rh	3.009126	0.221543	-0.360059
Si	-2.604024	-3.428347	-0.126195
O	1.216620	0.371311	2.182219
O	0.957096	-1.984282	0.467705
O	0.279568	-0.241417	-1.786970
O	0.548632	2.092399	-0.073056
O	3.404853	0.544609	1.635653
O	3.153795	-1.809226	-0.048892
O	2.476053	-0.108807	-2.317792
O	2.735629	2.238960	-0.634742
O	-2.112043	-2.411633	1.245694
O	-2.854736	0.070592	-1.284354
C	2.442330	0.545265	2.442997
C	2.122723	-2.442024	0.289533
C	1.255470	-0.256057	-2.588100
C	1.587892	2.713272	-0.432978
C	-4.397113	-2.985032	-0.429692
C	-2.388699	-5.135132	0.611694
C	-1.513707	-3.107656	-1.600654
C	-1.828319	-1.168885	1.326501
C	-1.784584	-0.075052	2.300187
C	-1.671317	0.047009	0.744624
C	-2.466845	0.714679	-0.318358
C	-2.836649	2.155213	-0.149898
C	-2.320973	2.964633	0.876608
C	-2.718324	4.299446	0.984149

C	-3.630493	4.837547	0.071306
C	-4.144683	4.038556	-0.957674
C	-3.749181	2.707083	-1.067556
H	2.690642	0.718136	3.510280
H	2.244199	-3.533236	0.450416
H	1.002257	-0.419821	-3.655455
H	1.469651	3.805352	-0.586611
H	-4.998046	-3.054330	0.491194
H	-4.837584	-3.670456	-1.173453
H	-4.465095	-1.960403	-0.827999
H	-1.335160	-5.321919	0.874314
H	-2.699805	-5.908612	-0.110132
H	-2.995277	-5.257595	1.523109
H	-1.579934	-2.051563	-1.902317
H	-1.849478	-3.738356	-2.441674
H	-0.462573	-3.341861	-1.380315
H	-0.891978	0.127672	2.903038
H	-2.741037	0.162947	2.794374
H	-1.595177	2.555952	1.578185
H	-2.310658	4.924167	1.782945
H	-3.940508	5.882263	0.159653
H	-4.854807	4.458892	-1.674445
H	-4.132244	2.064751	-1.862677

D (R^1 = OTMS, R^2 = Ph)

Rh	0.716656	0.039176	0.312516
Rh	3.075003	-0.082253	-0.429346
Si	-3.027448	-2.958802	-0.459152
O	1.319720	-0.945882	2.032149
O	0.449969	-1.796101	-0.624522
O	0.305596	1.003650	-1.474690
O	1.196814	1.860365	1.180246
O	3.476677	-1.065002	1.344218
O	2.606804	-1.884394	-1.319810
O	2.470523	0.908114	-2.144256
O	3.362317	1.731261	0.523700
O	-2.642588	-2.157486	1.031618
O	-3.443523	0.143300	0.856561
C	2.538759	-1.269292	2.151867
C	1.437399	-2.323706	-1.218379
C	1.261181	1.210920	-2.280688
C	2.392086	2.277291	1.097501
C	-4.850484	-3.383535	-0.302721
C	-1.959388	-4.495082	-0.450914
C	-2.700611	-1.827424	-1.916299
C	-2.375119	-0.901120	1.302020
C	-1.682707	-0.326794	2.456733
C	-1.299076	0.134232	0.970390
C	-2.435387	0.961802	0.620066
C	-2.657637	2.311781	0.168351
C	-1.572785	3.205282	0.042096
C	-1.810182	4.514111	-0.374241
C	-3.111708	4.933569	-0.672462
C	-4.192862	4.048241	-0.549992
C	-3.971285	2.741973	-0.129358
H	2.801254	-1.799029	3.091847
H	1.233541	-3.299787	-1.708051
H	0.984144	1.727961	-3.223991
H	2.592990	3.248742	1.597140
H	-5.039027	-3.995623	0.594038
H	-5.198047	-3.953562	-1.180773
H	-5.464681	-2.471607	-0.226591
H	-0.896070	-4.211754	-0.456247
H	-2.160325	-5.124559	-1.333604
H	-2.150234	-5.100686	0.449560
H	-3.366887	-0.950354	-1.906674
H	-2.881662	-2.373077	-2.858013
H	-1.656301	-1.480936	-1.911629
H	-0.905427	-0.953818	2.901009
H	-2.178329	0.381485	3.128750
H	-0.565188	2.865531	0.284626
H	-0.975993	5.212825	-0.469398
H	-3.288552	5.960439	-1.003284
H	-5.205508	4.384643	-0.783659
H	-4.799721	2.038757	-0.025116

E (R^1 = OTMS, R^2 = Ph)

Rh	1.182828	-0.200660	0.045798
Rh	3.638316	-0.514027	-0.084076
Si	-5.778073	-1.554808	0.012581
O	1.153450	-1.764524	1.412041
O	1.026754	-1.591113	-1.487371
O	1.409959	1.316088	-1.338097
O	1.549245	1.142326	1.579594
O	3.401329	-2.042945	1.297726
O	3.275047	-1.850316	-1.626067
O	3.659432	1.039008	-1.447991
O	3.794998	0.846775	1.464692
O	-4.022136	-1.874150	0.057810
O	-3.208038	0.201521	0.024230
C	2.253469	-2.314593	1.719950
C	2.092557	-2.083181	-1.966906
C	2.572284	1.584409	-1.759782
C	2.747757	1.352936	1.932573
C	-6.168595	-0.504538	1.508221
C	-6.466992	-3.285777	0.113419
C	-6.114478	-0.713802	-1.622669
C	-3.033047	-1.064090	0.061132
C	-1.593494	-1.419901	0.108202
C	-0.891329	-0.086723	0.107967
C	-1.840864	0.864927	0.061522
C	-1.951637	2.320115	0.036272
C	-0.839372	3.108709	0.395503
C	-0.924244	4.499642	0.359642
C	-2.110794	5.136079	-0.022415
C	-3.220409	4.362429	-0.370811
C	-3.144160	2.968344	-0.343075
H	2.179998	-3.142154	2.457948
H	1.948559	-2.812846	-2.792456
H	2.628559	2.410100	-2.500702
H	2.876788	2.079881	2.762583
H	-5.861105	-1.005623	2.440135
H	-7.255959	-0.328540	1.567054
H	-5.668596	0.474751	1.458439
H	-6.125994	-3.901243	-0.734122
H	-7.569128	-3.260793	0.091748

H	-6.158635	-3.784421	1.046000
H	-5.620434	0.267851	-1.685911
H	-7.199059	-0.554326	-1.744944
H	-5.770395	-1.331354	-2.467767
H	-1.313073	-2.042051	-0.762840
H	-1.357437	-2.039466	0.992877
H	0.080987	2.620449	0.713597
H	-0.052069	5.095152	0.641905
H	-2.170195	6.227184	-0.044655
H	-4.154275	4.845384	-0.670655
H	-4.017231	2.379034	-0.626871

F (R^1 = OTMS, R^2 = Ph)

Rh	-0.973603	0.141560	-0.480266
Rh	-3.025335	0.648941	0.718359
Si	2.072169	-3.528969	0.166881
O	-2.152199	-0.427503	-2.077682
O	-1.112021	-1.772358	0.307671
O	0.061090	0.736504	1.200414
O	-1.020650	2.093009	-1.168911
O	-4.060692	0.058014	-0.961612
O	-3.036916	-1.292235	1.397812
O	-1.851448	1.206316	2.317348
O	-2.915536	2.560519	-0.024743
O	1.507899	-2.400512	-1.030407
O	2.684034	-0.530901	-0.500693
C	-3.407194	-0.339448	-1.961006
C	-2.099706	-2.051583	1.046150
C	-0.600299	1.130082	2.202638
C	-1.959693	2.847742	-0.790807
C	3.845848	-3.950238	-0.280084
C	0.923428	-4.985465	-0.073559
C	1.926369	-2.746135	1.862732
C	1.674028	-1.119422	-1.162558
C	0.992032	-0.187881	-1.948236
C	1.742807	1.037575	-1.795135
C	2.736381	0.807934	-0.889783
C	3.766478	1.637085	-0.278439
C	3.844764	3.012908	-0.578962
C	4.834688	3.810411	-0.008759
C	5.768159	3.258019	0.876553
C	5.698303	1.896491	1.184059
C	4.710122	1.091806	0.614297
H	-4.000024	-0.650384	-2.845597
H	-2.139310	-3.092032	1.430291
H	-0.003980	1.444064	3.083669
H	-1.936722	3.885762	-1.181690
H	3.912110	-4.360969	-1.300508
H	4.251802	-4.705109	0.414347
H	4.492253	-3.059886	-0.227018
H	-0.120030	-4.684179	0.106695
H	1.174861	-5.805970	0.618595
H	0.991190	-5.374594	-1.102066
H	2.668042	-1.945500	2.004094
H	2.080219	-3.502888	2.650153
H	0.926002	-2.305615	1.988202
H	0.302919	-0.446845	-2.748485
H	1.509778	1.986004	-2.269805
H	3.120167	3.460661	-1.262385
H	4.877232	4.874522	-0.254988
H	6.542627	3.886118	1.323450
H	6.420833	1.453950	1.874790
H	4.664294	0.029820	0.859523

TS1 (R^1 = OTMS, R^2 = Ph)

Rh	-1.057266	-0.214678	0.111534
Rh	-3.461468	0.027744	-0.367413
Si	4.845314	-1.467804	-0.431034
O	-0.744841	0.300844	-1.876628
O	-1.254245	-2.206519	-0.415000
O	-1.612269	-0.699420	2.036922
O	-1.079144	1.783630	0.624829
O	-2.957646	0.504166	-2.309143
O	-3.463850	-1.979127	-0.860752
O	-3.819738	-0.453512	1.601785
O	-3.285081	2.009732	0.164692
O	3.291119	-1.062850	0.163810
O	1.638546	0.715097	2.559546
N	1.007933	-1.598210	1.888772
N	0.714247	-2.465852	2.502343
C	-1.744443	0.539766	-2.619119
C	-2.395404	-2.628830	-0.771693
C	-2.840611	-0.701232	2.345541
C	-2.163063	2.430719	0.540514
C	4.936221	-3.325446	-0.718962
C	5.984902	-0.942925	0.959251
C	5.183758	-0.496211	-2.005297
C	2.035971	-1.078784	-0.351600
C	1.686865	-1.629934	-1.530168
C	1.047313	-0.404699	0.537307
C	1.596959	0.753936	1.343124
C	2.077660	1.956896	0.585955
C	1.873371	2.153127	-0.790761
C	2.373511	3.299420	-1.414178
C	3.077997	4.255330	-0.675825
C	3.277296	4.068118	0.697092
C	2.776756	2.928387	1.324056
H	-1.505906	0.810488	-3.668719
H	-2.443964	-3.705645	-1.036242
H	-3.066564	-0.955542	3.401395
H	-2.104970	3.498723	0.834778
H	4.672568	-3.877169	0.198153
H	5.962243	-3.616807	-1.000790
H	4.263137	-3.664947	-1.521902
H	5.895313	0.137998	1.152339
H	7.036983	-1.160318	0.711110
H	5.738787	-1.473852	1.892821
H	4.524265	-0.790532	-2.836676
H	6.224505	-0.657675	-2.333492
H	5.047346	0.583546	-1.832212
H	0.650497	-1.618532	-1.853975
H	2.434670	-2.074195	-2.190390
H	1.302581	1.432883	-1.377560
H	2.204237	3.449832	-2.483410
H	3.467835	5.149726	-1.169104
H	3.822685	4.815510	1.279001

H	2.913933	2.764100	2.394216

TS2 (R^1 = OTMS, R^2 = Ph)

Rh	0.761999	-0.038442	0.166106
Rh	3.156906	-0.309527	-0.307959
Si	-3.774964	-2.535760	-0.112627
O	1.319252	0.675861	2.028933
O	0.792787	-1.971309	0.912263
O	0.421303	-0.780528	-1.728973
O	0.929215	1.862424	-0.619954
O	3.525234	0.434769	1.585468
O	3.002194	-2.214272	0.473864
O	2.630722	-1.031422	-2.161130
O	3.136950	1.609467	-1.059137
O	-3.163801	-1.490954	1.158432
O	-2.585406	0.342132	-1.449068
C	2.554493	0.749012	2.311564
C	1.887201	-2.608348	0.893931
C	1.409809	-1.101535	-2.449461
C	2.054701	2.247086	-1.051313
C	-5.166847	-1.625085	-0.969039
C	-4.431618	-3.989003	0.877123
C	-2.351735	-3.017263	-1.222459
C	-2.059679	-0.815478	1.315399
C	-1.615735	-0.197606	2.481704
C	-1.348548	0.079118	0.516977
C	-2.125457	0.899161	-0.461955
C	-2.317489	2.356455	-0.204907
C	-1.654792	3.041218	0.828647
C	-1.896489	4.401349	1.031894
C	-2.794005	5.087077	0.207237
C	-3.450015	4.412250	-0.829845
C	-3.211601	3.054985	-1.036047
H	2.791700	1.138484	3.323239
H	1.847944	-3.639940	1.301843
H	1.159555	-1.492476	-3.457147
H	2.080582	3.274228	-1.470155
H	-5.898479	-1.243614	-0.238319
H	-5.699643	-2.308983	-1.651351
H	-4.776942	-0.780627	-1.555448
H	-3.624772	-4.490442	1.435379
H	-4.894136	-4.734325	0.208374
H	-5.196805	-3.665275	1.601042
H	-1.928607	-2.135220	-1.725481
H	-2.702448	-3.728168	-1.989763
H	-1.548493	-3.503700	-0.646119
H	-0.560401	-0.045860	2.706088
H	-2.365867	0.127494	3.215105
H	-0.934278	2.516170	1.456314
H	-1.375473	4.931145	1.833186
H	-2.980292	6.152015	0.369702
H	-4.147296	4.949275	-1.477802
H	-3.707798	2.509332	-1.840852

TS3 (R^1 = OTMS, R^2 = Ph)

Rh	-0.680255	-0.046707	0.294442
Rh	-3.051438	0.069554	-0.411301
Si	2.938345	3.034026	-0.462595
O	-1.252547	0.974225	2.006045
O	-0.420618	1.773585	-0.679063
O	-0.301958	-1.039416	-1.481605
O	-1.164229	-1.839749	1.214081
O	-3.419384	1.090518	1.350081
O	-2.586469	1.851770	-1.346667
O	-2.478987	-0.959321	-2.113351
O	-3.336843	-1.720349	0.580504
O	2.516120	2.223611	1.049689
O	3.551532	-0.195065	0.731385
C	-2.469182	1.304688	2.139402
C	-1.416211	2.290376	-1.271177
C	-1.271770	-1.265080	-2.264848
C	-2.361037	-2.255484	1.155440
C	4.742541	3.464943	-0.195273
C	1.839703	4.545463	-0.468633
C	2.687428	1.880271	-1.909835
C	2.219430	1.007146	1.306871
C	1.694403	0.288523	2.454632
C	1.351446	-0.140082	0.940681
C	2.526557	-0.940096	0.564751
C	2.669136	-2.329256	0.142305
C	1.562041	-3.198077	0.103946
C	1.743338	-4.527353	-0.280646
C	3.013714	-4.991762	-0.636014
C	4.119133	-4.129919	-0.600540
C	3.950745	-2.805906	-0.208837
H	-2.714396	1.851524	3.074281
H	-1.217542	3.255513	-1.784632
H	-1.011377	-1.802722	-3.201184
H	-2.558088	-3.213950	1.680687
H	4.876176	4.086366	0.704505
H	5.138922	4.026220	-1.058079
H	5.348859	2.552771	-0.075978
H	0.782249	4.244422	-0.502278
H	2.052193	5.179210	-1.345557
H	1.999563	5.152597	0.436546
H	3.373566	1.021100	-1.857667
H	2.893310	2.421374	-2.849161
H	1.651833	1.510995	-1.939452
H	0.855193	0.773113	2.965390
H	2.339740	-0.344861	3.070625
H	0.575407	-2.831409	0.386961
H	0.886988	-5.205320	-0.305870
H	3.146852	-6.032899	-0.942040
H	5.109995	-4.497866	-0.877223
H	4.798480	-2.119492	-0.167025

TS4 (R^1 = OTMS, R^2 = Ph)

Rh	0.771292	0.045712	0.390138
Rh	3.060319	-0.102094	-0.541778
Si	-3.154084	-2.679470	-0.561654
O	1.529367	-0.842648	2.101124
O	0.445854	-1.841516	-0.421895
O	0.202411	0.903785	-1.407639
O	1.303316	1.913159	1.113841
O	3.624788	-0.972172	1.245564
O	2.543024	-1.960464	-1.277519

O	2.301742	0.775886	-2.256218
O	3.403164	1.768009	0.272981
O	-2.568861	-2.166089	0.993502
O	-3.366146	0.077248	1.262953
C	2.759531	-1.143329	2.137401
C	1.390482	-2.399842	-1.055813
C	1.082904	1.066328	-2.304541
C	2.479834	2.336453	0.900297
C	-5.014891	-2.839414	-0.364402
C	-2.333558	-4.344107	-0.792918
C	-2.691117	-1.436465	-1.882808
C	-2.336195	-0.983065	1.499082
C	-1.481180	-0.600319	2.588490
C	-1.182816	0.131281	1.201756
C	-2.345595	0.887523	0.906085
C	-2.627939	2.164315	0.294723
C	-1.590960	3.099052	0.089866
C	-1.891097	4.346857	-0.452579
C	-3.209604	4.668412	-0.796914
C	-4.243106	3.743537	-0.594535
C	-3.957465	2.495244	-0.050352
H	3.106689	-1.617155	3.079814
H	1.160158	-3.406568	-1.465518
H	0.720541	1.525768	-3.248690
H	2.709614	3.336951	1.324290
H	-5.269988	-3.545596	0.442144
H	-5.476427	-3.208599	-1.295761
H	-5.471935	-1.866568	-0.122082
H	-1.239824	-4.224989	-0.827050
H	-2.662548	-4.821956	-1.730424
H	-2.578446	-5.022734	0.039749
H	-3.242623	-0.489590	-1.772476
H	-2.936804	-1.849526	-2.876098
H	-1.613902	-1.214922	-1.854227
H	-0.688286	-1.302780	2.851818
H	-1.855274	0.032067	3.401013
H	-0.570014	2.839861	0.373139
H	-1.092901	5.076109	-0.608858
H	-3.435680	5.648441	-1.225368
H	-5.269909	4.001507	-0.863790
H	-4.750379	1.763677	0.114756

TS5 (R^1 = OTMS, R^2 = Ph)

Rh	-1.192354	-0.215019	-0.092143
Rh	-3.625960	-0.514207	0.163002
Si	5.775705	-1.525941	0.054636
O	-1.227481	-1.776317	-1.451987
O	-0.967222	-1.592195	1.436235
O	-1.340078	1.307064	1.297907
O	-1.622605	1.124715	-1.614855
O	-3.465370	-2.049216	-1.221552
O	-3.206304	-1.844484	1.685873
O	-3.580938	1.038930	1.520888
O	-3.858923	0.842055	-1.380392
O	4.081463	-1.873842	-0.170561
O	3.173160	0.221915	-0.127461
C	-2.342279	-2.326908	-1.702476
C	-2.006626	-2.078241	1.970525
C	-2.477418	1.580605	1.779163
C	-2.836674	1.341444	-1.907033
C	6.329336	-0.430478	-1.361731
C	6.542605	-3.229066	-0.008770
C	5.972689	-0.708854	1.729823
C	3.029351	-1.106436	-0.214204
C	1.678029	-1.414047	-0.341139
C	0.915460	-0.113385	-0.277247
C	1.935539	0.842255	-0.182290
C	1.958152	2.295985	-0.089335
C	0.814500	3.049612	-0.424020
C	0.845417	4.441061	-0.342243
C	2.004503	5.107244	0.070147
C	3.144304	4.367375	0.401377
C	3.124270	2.975599	0.323218
H	-2.308338	-3.156746	-2.439846
H	-1.825733	-2.802835	2.792603
H	-2.494253	2.405501	2.522308
H	-3.006517	2.064392	-2.732743
H	6.139534	-0.912830	-2.334235
H	7.412506	-0.234471	-1.290809
H	5.809424	0.540073	-1.351597
H	6.142191	-3.874690	0.789013
H	7.635641	-3.166644	0.121843
H	6.344339	-3.718647	-0.975548
H	5.461028	0.265206	1.772594
H	7.040598	-0.537929	1.946684
H	5.565293	-1.345637	2.531584
H	1.224065	-2.400818	-0.359880
H	1.196572	-0.732371	-1.363919
H	-0.087440	2.540062	-0.760659
H	-0.047493	5.012524	-0.607968
H	2.020261	6.198285	0.132429
H	4.054415	4.877617	0.726912
H	4.015620	2.406716	0.592286

4p (R^1 = H, R^2 = Ph)

O	-0.649538	2.155592	-0.247468
N	-1.529793	-1.185033	0.375054
N	-1.495648	-2.266286	0.719627
C	-3.010190	0.598123	-0.199399
C	-4.171506	-0.063217	-0.085913
C	-1.658032	0.065481	-0.009786
C	-0.474422	0.953123	-0.131190
C	0.914525	0.383192	-0.087959
C	1.260200	-0.853721	-0.657026
C	2.585011	-1.297840	-0.627197
C	3.573806	-0.515496	-0.024449
C	3.239435	0.724464	0.532528
C	1.921423	1.176564	0.489587
H	-2.984176	1.660776	-0.456039
H	-4.223762	-1.124930	0.175663
H	-5.119950	0.450290	-0.255231
H	0.507030	-1.465612	-1.157532
H	2.845634	-2.255979	-1.083470
H	4.608072	-0.867863	0.003748
H	4.012294	1.342751	0.995993
H	1.647741	2.151033	0.898677

6p (R^1 = H, R^2 = Ph)

O	1.707980	-1.047034	0.000265
C	3.032636	-0.762663	0.000073
C	3.226921	0.589768	-0.000174
C	1.921452	1.174586	-0.000182
C	1.021315	0.132913	0.000080
C	-0.438211	0.063653	0.000026
C	-1.214433	1.239829	0.000172
C	-2.606986	1.173488	0.000084
C	-3.256383	-0.066204	-0.000083
C	-2.495961	-1.239499	-0.000142
C	-1.101804	-1.178928	-0.000064
H	3.706460	-1.615416	-0.000054
H	4.183317	1.108337	-0.000429
H	1.682032	2.235168	-0.000241
H	-0.722953	2.215258	0.000300
H	-3.190978	2.097496	0.000137
H	-4.348045	-0.116069	-0.000141
H	-2.992816	-2.213235	-0.000287
H	-0.512145	-2.096923	-0.000139

A (R^1 = H, R^2 = Ph)

Rh	-0.441337	0.339384	0.054251
Rh	-2.519383	-0.900488	-0.122575
O	-0.030138	-0.790964	1.741186
O	-1.445282	1.709849	1.228775
O	-1.018542	1.371225	-1.627443
O	0.409120	-1.104632	-1.140610
O	-1.971295	-1.939089	1.566581
O	-3.383120	0.554850	1.057917
O	-2.946983	0.203736	-1.804190
O	-1.525002	-2.269696	-1.287121
O	2.712842	1.677234	-1.761804
N	1.026218	2.790417	-0.217703
N	0.539841	3.685240	-0.679254
C	-0.872346	-1.660323	2.108578
C	-2.674232	1.510083	1.460886
C	-2.118928	1.074148	-2.175393
C	-0.307784	-2.066052	-1.536642
C	1.775228	1.821503	1.795346
C	2.922071	1.677164	2.468569
C	1.592938	1.671732	0.317148
C	2.600151	1.121408	-0.683623
C	3.438043	-0.071332	-0.342376
C	3.106814	-1.022056	0.638115
C	3.939316	-2.122939	0.850652
C	5.108515	-2.282835	0.100041
C	5.441520	-1.341646	-0.880308
C	4.606992	-0.247951	-1.105545
H	-0.606813	-2.240910	3.015587
H	-3.177187	2.269387	2.093693
H	-2.377855	1.651671	-3.085512
H	0.198247	-2.816047	-2.177371
H	0.857826	2.083186	2.331136
H	3.867759	1.424616	1.985022
H	2.932016	1.788441	3.555908
H	2.193347	-0.921332	1.222670
H	3.670336	-2.863838	1.607755
H	5.758865	-3.143725	0.276423
H	6.351280	-1.464210	-1.473324
H	4.839589	0.487283	-1.877756

B (R^1 = H, R^2 = Ph)

Rh	0.344610	0.449993	-0.044984
Rh	2.466144	-0.818754	0.092237
O	-0.058047	-0.687480	-1.731672
O	1.361095	1.808140	-1.230733
O	0.991582	1.445379	1.634132
O	-0.495920	-1.007203	1.142494
O	1.883047	-1.844855	-1.600151
O	3.305620	0.651994	-1.095019
O	2.925487	0.275744	1.773903
O	1.441074	-2.177265	1.266413
O	-2.596883	1.649204	1.756046
C	0.781451	-1.557448	-2.118808
C	2.589373	1.604453	-1.479019
C	2.104378	1.141818	2.158152
C	0.231419	-1.973338	1.524086
C	-1.463638	2.656793	-0.957938
C	-2.568370	3.443191	-0.998302
C	-1.360624	1.464437	-0.160210
C	-2.510583	1.052134	0.691513
C	-3.466709	0.001923	0.257566
C	-3.309200	-0.686939	-0.956533
C	-4.251973	-1.643928	-1.338707
C	-5.349221	-1.915679	-0.514773
C	-5.506222	-1.232838	0.698644
C	-4.568225	-0.277789	1.084691
H	0.490019	-2.122564	-3.028158
H	3.075818	2.371852	-2.116111
H	2.370906	1.721806	3.065192
H	-0.278924	-2.723267	2.162676
H	-0.579000	2.931781	-1.538940
H	-3.462165	3.222139	-0.408199
H	-2.589266	4.350800	-1.609123
H	-2.438158	-0.497351	-1.588535
H	-4.128298	-2.183670	-2.280754
H	-6.085351	-2.665127	-0.817403
H	-6.362651	-1.450263	1.341783
H	-4.664427	0.268058	2.025711

C (R^1 = H, R^2 = Ph)

Rh	0.491709	0.578359	-0.162710
Rh	2.303431	-0.984881	0.280130
O	1.788652	1.491347	-1.504069
O	1.246853	1.733092	1.366785
O	-0.600920	-0.506780	1.215822
O	-0.111690	-0.703443	-1.669756
O	3.466463	0.042506	-1.061306
O	2.918255	0.267299	1.788490
O	1.082345	-1.961417	1.606077
O	1.577594	-2.149446	-1.253422
O	-2.703154	1.913701	1.623102
C	2.956605	1.030938	-1.646704
C	2.265641	1.323224	1.992870
C	-0.077410	-1.507773	1.780464

C	0.556898	-1.758770	-1.872649
C	-0.684726	2.573418	-0.704486
C	-1.465660	2.124848	-1.905860
C	-1.662986	1.703119	-0.465370
C	-2.687688	1.325244	0.559401
C	-3.693212	0.282025	0.205370
C	-3.567450	-0.526027	-0.937382
C	-4.529543	-1.500938	-1.212664
C	-5.623459	-1.669255	-0.358092
C	-5.752799	-0.867060	0.783302
C	-4.790692	0.099926	1.065949
H	3.601347	1.564655	-2.374151
H	2.621259	1.975544	2.815685
H	-0.718867	-2.041961	2.509592
H	0.194828	-2.409929	-2.693983
H	-0.060490	3.366870	-0.301249
H	-1.019795	1.436478	-2.633612
H	-2.195983	2.828063	-2.334927
H	-2.706106	-0.408823	-1.596349
H	-4.425673	-2.132381	-2.098615
H	-6.377810	-2.428781	-0.580051
H	-6.606758	-1.000995	1.452117
H	-4.863579	0.732331	1.952971

D (R^1 = H, R^2 = Ph)

Rh	-0.369371	0.400976	0.134199
Rh	-2.500288	-0.793920	-0.217674
O	-1.374779	1.586508	1.502964
O	-0.959688	1.693350	-1.370854
O	0.466823	-0.869243	-1.270050
O	0.055975	-0.990142	1.613140
O	-3.330396	0.487098	1.177465
O	-2.903922	0.577328	-1.711047
O	-1.489123	-1.972405	-1.585141
O	-1.917125	-2.064232	1.309094
O	3.169459	2.406704	-0.477678
C	-2.604939	1.362797	1.707112
C	-2.071224	1.486393	-1.942610
C	-0.273672	-1.748750	-1.801387
C	-0.807028	-1.885468	1.862421
C	1.775826	2.864067	-0.252525
C	1.478479	2.840390	1.178918
C	1.418872	1.504093	0.349142
C	2.789368	1.220737	-0.002737
C	3.662919	0.081509	0.004292
C	3.219786	-1.132551	0.573537
C	4.084613	-2.224367	0.606276
C	5.374014	-2.118192	0.070810
C	5.814381	-0.915265	-0.501033
C	4.964997	0.184589	-0.536414
H	-3.094476	2.029024	2.448524
H	-2.333875	2.204165	-2.748320
H	0.223380	-2.400672	-2.550719
H	-0.536851	-2.595833	2.672371
H	1.297287	3.381948	-1.083786
H	0.485010	3.179986	1.484007
H	2.282495	2.988525	1.908207
H	2.209208	-1.201219	0.981879
H	3.752368	-3.166835	1.047166
H	6.044307	-2.981406	0.096107
H	6.821327	-0.843718	-0.918248
H	5.288351	1.128891	-0.978762

E (R^1 = H, R^2 = Ph)

Rh	0.352222	0.348912	-0.047553
Rh	2.588112	-0.701655	0.087489
O	1.156472	1.659905	-1.439783
O	0.976192	1.639968	1.450433
O	-0.263252	-1.024320	1.365403
O	-0.070789	-1.009967	-1.548262
O	3.199785	0.685033	-1.327696
O	3.010181	0.652177	1.598073
O	1.784125	-1.993864	1.483532
O	1.981662	-1.965824	-1.428956
O	-3.501789	2.382869	-0.060509
C	2.377855	1.525834	-1.758102
C	2.143894	1.493467	1.927003
C	0.576315	-1.866143	1.800536
C	0.823400	-1.840409	-1.891590
C	-2.685318	3.357578	-0.089612
C	-1.308571	2.865613	-0.123807
C	-1.441469	1.368968	-0.118996
C	-2.779540	1.113718	-0.079383
C	-3.663848	-0.050243	-0.044533
C	-3.151667	-1.325225	-0.354495
C	-3.984608	-2.443006	-0.311587
C	-5.334622	-2.315375	0.031815
C	-5.850978	-1.052020	0.333280
C	-5.025482	0.072463	0.297034
H	2.754257	2.249664	-2.511781
H	2.420123	2.205263	2.733502
H	0.184986	-2.577260	2.558175
H	0.534383	-2.539372	-2.704475
H	-3.103068	4.367773	-0.081164
H	-0.720874	3.220829	0.750824
H	-0.731270	3.244601	-0.992629
H	-2.105969	-1.428539	-0.641226
H	-3.573608	-3.425883	-0.555830
H	-5.981665	-3.195646	0.061764
H	-6.904323	-0.938912	0.602243
H	-5.440887	1.051794	0.540192

F (R^1 = H, R^2 = Ph)

Rh	0.665736	0.543759	0.118569
Rh	2.569044	-0.923384	-0.190035
O	1.972750	2.137580	0.012540
O	1.030721	0.405437	2.153507
O	-0.511218	-1.141600	0.198743
O	0.482968	0.559321	-1.944918
O	3.748621	0.764769	-0.275796
O	2.795170	-0.974800	1.851351
O	1.267255	-2.511860	-0.085798
O	2.261352	-0.811128	-2.215964
O	-2.394929	1.121509	1.245500
C	3.200963	1.891193	-0.158845
C	1.992257	-0.309114	2.554023

C	0.042358	-2.270370	0.080440
C	1.303847	-0.108730	-2.632660
C	-1.288467	1.887711	1.081104
C	-1.228286	2.347644	-0.221900
C	-2.369013	1.797743	-0.886268
C	-3.046846	1.051300	0.048355
C	-4.260823	0.240970	-0.008331
C	-4.984786	0.119563	-1.210699
C	-6.147839	-0.646885	-1.263474
C	-6.610737	-1.306965	-0.119451
C	-5.898442	-1.193524	1.078444
C	-4.733650	-0.427682	1.137232
H	3.870381	2.773926	-0.211452
H	2.142716	-0.351406	3.652015
H	-0.632110	-3.149155	0.129324
H	1.163027	-0.070083	-3.732220
H	-0.734971	2.130769	1.983081
H	-0.503101	3.051137	-0.623004
H	-2.631783	1.926515	-1.932250
H	-4.633877	0.627750	-2.111336
H	-6.697330	-0.730859	-2.204437
H	-7.522651	-1.907591	-0.162954
H	-6.252478	-1.706695	1.976167
H	-4.177673	-0.342108	2.071879

TS1 (R^1 = H, R^2 = Ph)

Rh	-0.394024	0.330256	0.078683
Rh	-2.491766	-0.934846	-0.151411
O	-0.042134	-0.796990	1.785580
O	-1.451461	1.699841	1.211933
O	-0.945722	1.337161	-1.633387
O	0.481342	-1.125129	-1.090941
O	-1.977640	-1.951617	1.568073
O	-3.383702	0.538508	0.994000
O	-2.864790	0.157592	-1.858206
O	-1.443104	-2.305333	-1.276788
O	2.779964	1.847798	-1.524339
N	0.921506	3.015820	-0.393430
N	0.296630	3.864993	-0.717185
C	-0.897597	-1.665214	2.135162
C	-2.688594	1.495179	1.407748
C	-2.030128	1.024989	-2.209957
C	-0.225128	-2.093457	-1.497148
C	1.620038	1.852079	1.767100
C	2.801047	1.851601	2.409065
C	1.412130	1.438747	0.369551
C	2.556699	1.132871	-0.559791
C	3.392937	-0.085675	-0.299328
C	3.102548	-1.050805	0.681637
C	3.948992	-2.148284	0.851601
C	5.087153	-2.294706	0.052270
C	5.378357	-1.340163	-0.928940
C	4.534605	-0.245239	-1.106063
H	-0.651898	-2.233858	3.055965
H	-3.207422	2.261532	2.020068
H	-2.259791	1.594422	-3.133797
H	0.305145	-2.841379	-2.121657
H	0.705022	2.109539	2.309765
H	3.740309	1.588991	1.916662
H	2.848308	2.078781	3.477853
H	2.209833	-0.965398	1.301547
H	3.714087	-2.897980	1.611269
H	5.746841	-3.155171	0.192088
H	6.265021	-1.452200	-1.557929
H	4.737736	0.507390	-1.869613

TS2 (R^1 = H, R^2 = Ph)

Rh	-0.373357	0.486725	-0.092923
Rh	-2.335834	-0.948005	0.178937
O	-0.973601	1.471692	1.612147
O	-1.585938	1.742931	-1.210199
O	0.053725	-0.611647	-1.802215
O	0.651787	-0.880122	1.060540
O	-2.770799	0.120635	1.883488
O	-3.397317	0.414784	-0.948553
O	-1.770754	-1.926959	-1.544645
O	-1.159005	-2.217622	1.289630
O	2.658968	1.942019	1.555661
C	-2.011682	1.068988	2.210263
C	-2.803207	1.431436	-1.378591
C	-0.728438	-1.549622	-2.134252
C	0.042342	-1.903348	1.484168
C	1.834130	2.547925	-1.389461
C	0.888730	3.387683	-0.794709
C	1.464438	1.658577	-0.421398
C	2.559538	1.273277	0.546827
C	3.488518	0.163343	0.193940
C	3.312703	-0.627444	-0.953848
C	4.235778	-1.632427	-1.252334
C	5.331470	-1.853211	-0.411496
C	5.506059	-1.069662	0.736248
C	4.588186	-0.065749	1.038804
H	-2.281219	1.623994	3.132095
H	-3.404926	2.145790	-1.977130
H	-0.455679	-2.100346	-3.058256
H	0.645603	-2.602456	2.098425
H	2.817088	2.787257	-1.810237
H	-0.181550	3.182614	-0.814401
H	1.215377	4.355242	-0.386133
H	2.442039	-0.480776	-1.596626
H	4.096376	-2.250673	-2.142612
H	6.051396	-2.640847	-0.649166
H	6.360724	-1.245406	1.394352
H	4.700455	0.558890	1.927265

TS3 (R^1 = H, R^2 = Ph)

Rh	0.373053	0.436053	-0.107438
Rh	2.452469	-0.840573	0.200332
O	1.419649	1.639145	-1.425972
O	0.985881	1.639798	1.466567
O	-0.503136	-0.858376	1.242933
O	-0.062803	-0.865509	-1.660713
O	3.336757	0.470379	-1.132363
O	2.888712	0.445385	1.757136
O	1.407321	-2.049126	1.505879
O	1.860876	-2.029063	-1.379373

O	-3.337925	2.421842	0.541444
C	2.644592	1.386706	-1.635465
C	2.086440	1.369427	2.032947
C	0.199857	-1.788826	1.734129
C	0.767000	-1.781079	-1.941123
C	-1.363586	2.889807	0.172315
C	-1.375900	2.830725	-1.268384
C	-1.465440	1.566735	-0.335553
C	-2.862819	1.339337	0.089725
C	-3.666436	0.118686	0.023448
C	-3.181232	-1.038575	-0.613551
C	-3.990905	-2.172996	-0.690661
C	-5.270871	-2.164293	-0.127272
C	-5.756109	-1.014570	0.511934
C	-4.961154	0.124913	0.583186
H	3.157396	2.062943	-2.350629
H	2.368639	2.035651	2.874865
H	-0.321884	-2.453585	2.453712
H	0.484452	-2.440653	-2.788151
H	-1.176972	3.469362	1.075428
H	-0.419283	2.915296	-1.800495
H	-2.250783	3.253476	-1.781113
H	-2.180277	-1.042825	-1.046939
H	-3.619263	-3.071362	-1.189174
H	-5.897393	-3.058377	-0.185538
H	-6.756832	-1.012719	0.950505
H	-5.319548	1.034424	1.068972

TS4 (R^1 = H, R^2 = Ph)

Rh	-0.362716	0.400829	-0.015121
Rh	-2.545622	-0.754904	0.043870
O	-1.015935	1.512369	1.601495
O	-1.238338	1.783226	-1.285311
O	0.099312	-0.799833	-1.639337
O	0.313440	-1.069553	1.271283
O	-3.009408	0.436313	1.668854
O	-3.237777	0.718364	-1.232705
O	-1.907906	-1.852424	-1.585496
O	-1.687499	-2.135154	1.313841
O	3.544092	2.424082	-0.032304
C	-2.169186	1.275625	2.071007
C	-2.456863	1.627292	-1.599778
C	-0.763457	-1.633251	-2.048750
C	-0.484186	-1.981813	1.636954
C	2.513751	3.136664	-0.489856
C	1.264109	2.967573	0.182966
C	1.445958	1.403457	0.007148
C	2.788445	1.153469	0.023188
C	3.636963	-0.020514	-0.009278
C	3.122194	-1.281192	-0.382589
C	3.948770	-2.401828	-0.361181
C	5.293408	-2.288476	0.013827
C	5.815321	-1.039354	0.366508
C	4.997754	0.089127	0.353048
H	-2.463247	1.893623	2.945164
H	-2.874414	2.395625	-2.283881
H	-0.458817	-2.240886	-2.926622
H	-0.056852	-2.736818	2.329537
H	2.667229	3.663032	-1.444415
H	0.399956	3.383477	-0.345088
H	1.229524	3.185734	1.263126
H	2.083047	-1.363856	-0.696869
H	3.543383	-3.374533	-0.650544
H	5.936483	-3.172263	0.021234
H	6.866054	-0.944195	0.651140
H	5.405136	1.064610	0.621686

TS5 (R^1 = H, R^2 = Ph)

Rh	-0.358270	0.356415	0.030891
Rh	-2.585540	-0.693638	-0.074979
O	-1.148992	1.702519	1.390565
O	-0.980094	1.596935	-1.504345
O	0.259049	-1.056979	-1.343353
O	0.066904	-0.954098	1.578576
O	-3.195677	0.735129	1.298976
O	-3.016213	0.607847	-1.619985
O	-1.789004	-2.026555	-1.433189
O	-1.982511	-1.915777	1.478697
O	3.541052	2.348166	0.024840
C	-2.371493	1.582427	1.711563
C	-2.145109	1.436935	-1.975793
C	-0.581248	-1.908612	-1.756105
C	-0.827167	-1.775538	1.943924
C	2.711337	3.378540	0.026840
C	1.399473	2.904098	0.120025
C	1.464767	1.398404	0.101260
C	2.848920	1.161688	0.087503
C	3.667678	-0.046853	0.047278
C	3.108187	-1.299859	0.364868
C	3.900198	-2.447332	0.324520
C	5.251210	-2.368840	-0.027889
C	5.814083	-1.126804	-0.341172
C	5.031770	0.025918	-0.305674
H	-2.745134	2.324958	2.447813
H	-2.421230	2.121162	-2.805675
H	-0.193212	-2.640048	-2.495665
H	-0.542307	-2.449150	2.779333
H	3.148069	4.372653	-0.034487
H	0.479626	3.477024	0.016159
H	1.347408	2.303941	1.185810
H	2.061192	-1.365895	0.656824
H	3.456084	-3.413802	0.575330
H	5.865206	-3.272522	-0.057954
H	6.868698	-1.056239	-0.618819
H	5.475293	0.990451	-0.557850

4q (R^1 = OTMS, R^2 = Me)

Si	2.361868	0.046987	0.000097
O	0.666532	0.243147	0.000034
O	-3.206578	-1.685304	0.000011
N	-1.580443	1.416176	-0.000104
N	-1.524738	2.548777	-0.000147
C	2.899421	-0.855463	1.560658
C	2.991899	1.814025	-0.000112
C	2.899945	-0.855563	-1.560233
C	-0.375772	-0.630175	-0.000126

C	-0.274963	-1.971778	-0.000394
C	-1.665952	0.100719	-0.000054
C	-3.028010	-0.481050	0.000031
C	-4.201706	0.488090	0.000156
H	2.534461	-0.330104	2.458345
H	4.000309	-0.895804	1.619039
H	2.522902	-1.889145	1.600520
H	2.640837	2.360013	-0.890613
H	4.094323	1.838386	-0.000717
H	2.641792	2.360077	0.890720
H	2.523641	-1.889308	-1.600292
H	4.000880	-0.895704	-1.618021
H	2.535414	-0.330246	-2.458119
H	-1.175154	-2.580958	-0.000464
H	0.701588	-2.456803	-0.000457
H	-4.185404	1.140044	0.888963
H	-5.128675	-0.098431	0.000338
H	-4.185601	1.139900	-0.888755

6q (R^1 = OTMS, R^2 = Me)

Si	-1.861089	-0.138097	0.000000
O	-0.614168	1.039392	-0.000006
O	1.206381	-0.365586	-0.000003
C	-1.722105	-1.181867	-1.556266
C	-3.421083	0.901500	-0.000004
C	-1.722103	-1.181850	1.556278
C	0.704346	0.900014	-0.000003
C	1.716845	1.818333	-0.000001
C	2.933702	1.047639	0.000001
C	2.584370	-0.271073	0.000000
C	3.346272	-1.547450	0.000001
H	-1.765377	-0.551101	-2.459108
H	-2.547926	-1.910957	-1.613391
H	-0.772341	-1.738542	-1.573531
H	-3.465138	1.548587	0.890777
H	-4.319315	0.261863	-0.000003
H	-3.465137	1.548581	-0.890790
H	-0.772342	-1.738529	1.573547
H	-2.547927	-1.910937	1.613413
H	-1.765370	-0.551074	2.459113
H	1.600897	2.898441	-0.000001
H	3.951444	1.434104	0.000003
H	4.424709	-1.334673	0.000003
H	3.119950	-2.162164	-0.888816
H	3.119947	-2.162164	0.888817

A (R^1 = OTMS, R^2 = Me)

Rh	-0.678032	0.268888	0.054471
Rh	-2.772775	-0.955731	-0.074118
Si	4.629407	-0.990389	-0.009177
O	-0.737726	0.373371	-2.015608
O	0.289232	-1.559194	-0.015644
O	-0.807262	0.085517	2.098426
O	-1.803529	1.992303	0.123725
O	-2.676202	-0.787391	-2.121536
O	-1.667025	-2.688721	-0.164572
O	-2.758218	-1.051198	1.980298
O	-3.753227	0.849247	0.024208
O	3.456269	0.245056	0.180628
O	0.767621	3.644317	0.853257
N	1.659098	1.333604	1.514703
N	1.761816	1.279371	2.625283
C	-1.705344	-0.168434	-2.624294
C	-0.413059	-2.605550	-0.111855
C	-1.801437	-0.517757	2.596288
C	-3.063148	1.899008	0.098735
C	3.801935	-2.547571	-0.655058
C	5.275778	-1.224195	1.735555
C	5.998003	-0.380898	-1.146989
C	2.474297	0.719541	-0.624123
C	2.435178	0.572715	-1.958659
C	1.443001	1.470646	0.178850
C	0.997083	2.912111	-0.083202
C	0.851081	3.352061	-1.517486
H	-1.691057	-0.085318	-3.730255
H	0.146019	-3.562747	-0.155179
H	-1.824330	-0.580482	3.702992
H	-3.620576	2.856263	0.147757
H	2.925730	-2.792135	-0.034194
H	4.504002	-3.397471	-0.620016
H	3.453566	-2.435730	-1.692983
H	5.688087	-0.283295	2.134412
H	6.077515	-1.980873	1.758696
H	4.475313	-1.558419	2.415033
H	5.652155	-0.229779	-2.181597
H	6.823830	-1.111827	-1.175718
H	6.409514	0.575630	-0.785457
H	1.572569	0.893816	-2.534897
H	3.250698	0.075843	-2.484789
H	1.820306	3.310422	-2.037125
H	0.470717	4.381227	-1.513244
H	0.154483	2.690907	-2.052762

B (R^1 = OTMS, R^2 = Me)

Rh	0.577034	0.126746	0.176295
Rh	2.963408	-0.328768	-0.306353
Si	-4.850826	-0.448256	-0.289099
O	0.952172	-0.639308	2.064974
O	0.194672	-1.783413	-0.503098
O	0.460078	0.842524	-1.749231
O	1.193984	1.997795	0.815099
O	3.136375	-1.042169	1.623461
O	2.377020	-2.200753	-0.947231
O	2.638567	0.414162	-2.198111
O	3.374073	1.577893	0.366008
O	-3.678129	-0.072715	0.913463
O	-2.359368	1.925421	-0.978059
C	2.121721	-1.038972	2.356087
C	1.161422	-2.499787	-0.905960
C	1.489373	0.826326	-2.486853
C	2.426739	2.294637	0.761315
C	-5.793435	1.146207	-0.566620
C	-5.964543	-1.777261	0.442242
C	-3.964292	-1.049997	-1.828320
C	-2.372465	-0.432465	1.005887
C	-2.000106	-1.571166	1.659252

C	-1.375229	0.494931	0.531586
C	-1.896249	1.835640	0.146014
C	-1.812499	2.968636	1.126947
H	2.244847	-1.430525	3.387048
H	0.882301	-3.513265	-1.261192
H	1.342444	1.228553	-3.510040
H	2.683101	3.315766	1.111551
H	-6.218256	1.523856	0.377747
H	-6.625239	0.995343	-1.274687
H	-5.123226	1.916936	-0.978201
H	-5.408517	-2.709202	0.637122
H	-6.790227	-2.020639	-0.247632
H	-6.409136	-1.441539	1.393385
H	-3.275526	-0.271979	-2.193228
H	-4.689717	-1.277332	-2.627268
H	-3.379372	-1.963617	-1.634058
H	-0.951695	-1.845679	1.741090
H	-2.759580	-2.187214	2.148281
H	-2.361759	2.701794	2.045498
H	-2.247789	3.872679	0.678404
H	-0.759183	3.136751	1.398544

C (R^1 = OTMS, R^2 = Me)

Rh	0.475836	0.313985	0.209130
Rh	2.617732	-0.744288	-0.279973
Si	-4.133023	-1.034770	-0.166457
O	1.068365	0.341457	2.191911
O	-0.291127	-1.591973	0.480755
O	0.069259	0.199695	-1.807083
O	1.432430	2.125347	-0.091847
O	3.061164	-0.623069	1.727214
O	1.705809	-2.562296	0.040287
O	2.048564	-0.802910	-2.255888
O	3.409290	1.131147	-0.564662
O	-3.233264	-0.368921	1.216979
O	-2.487107	2.072472	-1.435921
C	2.205523	-0.120188	2.498008
C	0.487589	-2.579840	0.345738
C	0.928044	-0.324074	-2.570842
C	2.656937	2.125336	-0.407356
C	-5.424633	0.261835	-0.558865
C	-4.854971	-2.583030	0.597610
C	-2.978027	-1.362938	-1.589074
C	-2.337192	0.540335	1.265560
C	-1.734297	1.502058	2.193724
C	-1.549581	1.451349	0.640641
C	-1.845853	2.413035	-0.458114
C	-1.331352	3.819422	-0.267078
H	2.473869	-0.073331	3.573346
H	0.035717	-3.578823	0.516360
H	0.657572	-0.365047	-3.645736
H	3.117010	3.122775	-0.562359
H	-6.007025	0.545176	0.332439
H	-6.129672	-0.121027	-1.316056
H	-4.937378	1.159187	-0.972182
H	-4.059290	-3.278806	0.908374
H	-5.497759	-3.107000	-0.129244
H	-5.466787	-2.345539	1.482424
H	-2.503581	-0.426279	-1.918906
H	-3.553113	-1.783440	-2.431822
H	-2.187431	-2.073383	-1.309249
H	-0.879197	1.237625	2.826131
H	-2.428574	2.234553	2.638902
H	-1.682135	4.233734	0.692367
H	-1.669273	4.453253	-1.097329
H	-0.231405	3.789413	-0.222801

D (R^1 = OTMS, R^2 = Me)

Rh	-0.501162	0.336046	-0.185720
Rh	-2.694601	-0.726523	0.222881
Si	4.108237	-1.113855	0.200683
O	-0.775443	-0.090093	-2.189003
O	0.339833	-1.545162	0.084141
O	-0.392494	0.685157	1.862250
O	-1.513054	2.128383	-0.410458
O	-2.790149	-1.061676	-1.814627
O	-1.677212	-2.509443	0.466201
O	-2.400444	-0.302063	2.230693
O	-3.526798	1.148323	-0.054807
O	3.622028	0.054362	-1.002340
O	3.175864	2.284310	-0.009906
C	-1.840039	-0.681022	-2.539961
C	-0.430074	-2.518352	0.345400
C	-1.354151	0.285562	2.588159
C	-2.776232	2.121539	-0.300802
C	5.970113	-0.905373	0.283559
C	3.611288	-2.768669	-0.512777
C	3.275627	-0.725022	1.832568
C	2.771384	1.041889	-0.960121
C	1.913167	1.614623	-1.996126
C	1.329183	1.312614	-0.540281
C	1.904177	2.378913	0.240447
C	1.330748	3.373449	1.155976
H	-1.935493	-0.883251	-3.627674
H	0.072218	-3.499786	0.481811
H	-1.245873	0.487648	3.675170
H	-3.271067	3.106087	-0.440575
H	6.428304	-1.049306	-0.708176
H	6.415051	-1.643715	0.971546
H	6.244199	0.099891	0.642286
H	2.516433	-2.805912	-0.620900
H	3.928074	-3.595026	0.145073
H	4.068418	-2.926724	-1.502682
H	3.565714	0.269064	2.208734
H	3.582768	-1.468254	2.587983
H	2.179815	-0.767064	1.737928
H	1.542140	0.904509	-2.740648
H	2.025863	2.649538	-2.335443
H	0.470478	3.856360	0.665767
H	2.075532	4.102646	1.499142
H	0.903248	2.811065	2.005468

E (R^1 = OTMS, R^2 = Me)

Rh	-0.957116	0.084332	0.003015
Rh	-3.407383	-0.291537	-0.003969
Si	6.149963	-0.314260	-0.005176

O	-0.791634	-1.576332	-1.228168
O	-0.862277	-1.175163	1.647193
O	-1.309936	1.713869	1.230327
O	-1.240624	1.303809	-1.645205
O	-3.035240	-1.911993	-1.245815
O	-3.107881	-1.499559	1.655855
O	-3.552118	1.363315	1.232841
O	-3.482526	0.949389	-1.659677
O	4.473674	-0.922998	0.003842
O	3.329736	0.993530	0.003118
C	-1.853905	-2.180329	-1.565559
C	-1.943672	-1.665680	2.089603
C	-2.505662	1.973863	1.556957
C	-2.416203	1.451244	-2.090658
C	6.344646	0.676965	-1.577989
C	7.120315	-1.907984	-0.001926
C	6.357551	0.690671	1.557306
C	3.364848	-0.283800	0.006338
C	2.000508	-0.881678	0.016577
C	1.091939	0.318240	0.011788
C	1.855882	1.411170	0.009739
C	1.686843	2.879519	0.011831
H	-1.708411	-3.059525	-2.229800
H	-1.835980	-2.327527	2.976035
H	-2.634722	2.858971	2.216490
H	-2.506768	2.112801	-2.979088
H	6.115855	0.067142	-2.466683
H	7.385658	1.029037	-1.672958
H	5.686773	1.559409	-1.581913
H	6.897347	-2.509093	0.893844
H	8.202666	-1.697548	-0.007392
H	6.889900	-2.517300	-0.890229
H	5.700817	1.573949	1.558392
H	7.399691	1.042240	1.641167
H	6.134904	0.089072	2.453140
H	1.865389	-1.524397	0.906302
H	1.850548	-1.548947	-0.851643
H	0.610011	3.080215	0.091074
H	2.069604	3.347267	-0.911353
H	2.191730	3.351928	0.871497

F (R^1 = OTMS, R^2 = Me)

Rh	-0.540051	0.282608	-0.391769
Rh	-2.611120	-0.641036	0.490187
Si	3.983398	-1.316714	0.085884
O	-1.078746	-0.499585	-2.224726
O	0.354041	-1.519277	0.120500
O	-0.142995	0.991581	1.507062
O	-1.618768	1.994091	-0.830197
O	-3.012206	-1.344102	-1.403815
O	-1.587647	-2.374987	0.909511
O	-2.068230	0.123907	2.325810
O	-3.531283	1.135240	0.020674
O	2.922819	-0.409460	-0.947835
O	2.869534	1.595417	0.122934
C	-2.174538	-1.121710	-2.316302
C	-0.362441	-2.424573	0.635725
C	-0.983279	0.753790	2.420557
C	-2.844224	2.034361	-0.529094
C	5.709389	-0.623216	-0.169594
C	3.817933	-3.055380	-0.584905
C	3.409803	-1.155632	1.862495
C	2.374173	0.761631	-0.809146
C	1.343877	1.375989	-1.521462
C	1.312747	2.737323	-1.013025
C	2.214963	2.821426	-0.006034
C	2.592966	3.872474	0.971111
H	-2.424525	-1.517884	-3.321976
H	0.156980	-3.375482	0.876413
H	-0.730642	1.149247	3.426127
H	-3.375271	2.975747	-0.779952
H	6.009434	-0.680976	-1.228371
H	6.448086	-1.189698	0.422216
H	5.761261	0.431282	0.144821
H	2.776277	-3.401457	-0.498554
H	4.465521	-3.756329	-0.032784
H	4.101209	-3.095538	-1.648865
H	3.588124	-0.141090	2.249662
H	3.946130	-1.872179	2.506979
H	2.330766	-1.360171	1.929769
H	0.963270	1.016197	-2.474490
H	0.632539	3.522818	-1.330866
H	2.057793	4.803422	0.738106
H	3.676325	4.079152	0.948410
H	2.331497	3.574689	2.000856

TS1 (R^1 = OTMS, R^2 = Me)

Rh	-0.764233	0.103503	0.020933
Rh	-3.170691	-0.419138	-0.049371
Si	5.242115	-0.515902	-0.016930
O	-0.646467	-0.775457	-1.853729
O	-0.501446	-1.731887	0.940942
O	-1.124990	0.936586	1.873383
O	-1.243681	1.897981	-0.883694
O	-2.855891	-1.269817	-1.901317
O	-2.713153	-2.216201	0.857714
O	-3.338122	0.469171	1.800489
O	-3.455557	1.416644	-0.942566
O	3.660860	0.139855	-0.091851
O	1.698859	2.946530	0.141761
N	1.666495	0.969838	1.745609
N	1.566476	0.979218	2.843500
C	-1.697606	-1.250788	-2.379311
C	-1.517978	-2.459793	1.148807
C	-2.305035	0.938035	2.334522
C	-2.455796	2.146537	-1.150437
C	5.279887	-1.893086	1.263359
C	6.288539	0.944521	0.512238
C	5.753128	-1.129226	-1.721112
C	2.423129	-0.397945	-0.258962
C	2.172436	-1.646355	-0.695460
C	1.335132	0.580859	0.011943
C	1.580717	1.958777	-0.548977
C	1.638139	1.992415	-2.063011
H	-1.565595	-1.703829	-3.383838
H	-1.315881	-3.429851	1.648874

H	-2.427441	1.411248	3.330340
H	-2.647872	3.130243	-1.626255
H	4.952260	-1.522873	2.248485
H	6.307388	-2.278295	1.375890
H	4.633825	-2.741884	0.990283
H	6.215932	1.767543	-0.216694
H	7.349924	0.658088	0.596904
H	5.961593	1.332279	1.490287
H	5.158118	-1.991185	-2.061658
H	6.811231	-1.441251	-1.709702
H	5.649707	-0.329449	-2.472581
H	1.150860	-2.006361	-0.768280
H	2.982827	-2.306971	-1.010805
H	2.675950	1.779756	-2.369613
H	1.366766	3.002137	-2.397111
H	0.980133	1.242519	-2.522258

TS2 (R^1 = OTMS, R^2 = Me)

Rh	0.555808	0.282481	0.203345
Rh	2.785990	-0.621635	-0.300342
Si	-4.502840	-0.789033	-0.210816
O	1.191140	0.437351	2.169002
O	-0.040124	-1.665583	0.568317
O	0.130504	0.037479	-1.800959
O	1.344404	2.155338	-0.196538
O	3.244645	-0.387684	1.699894
O	2.015515	-2.493453	0.097157
O	2.184819	-0.798191	-2.260489
O	3.395230	1.315207	-0.662354
O	-3.653654	-0.022228	1.120761
O	-2.524269	1.693996	-1.410779
C	2.368980	0.072975	2.468115
C	0.810655	-2.594014	0.433306
C	1.020255	-0.438042	-2.563940
C	2.562351	2.244257	-0.534473
C	-5.572166	0.520535	-1.012492
C	-5.551210	-2.059884	0.688077
C	-3.247969	-1.578373	-1.348050
C	-2.402449	0.294302	1.317645
C	-1.828166	0.730526	2.508042
C	-1.445955	0.953289	0.545779
C	-1.932639	2.011530	-0.395858
C	-1.602070	3.437350	-0.034561
H	2.646409	0.179428	3.537127
H	0.437572	-3.618713	0.639775
H	0.727932	-0.546461	-3.628647
H	2.928392	3.271566	-0.739409
H	-6.198911	1.032932	-0.264509
H	-6.246021	0.055478	-1.751936
H	-4.951956	1.267416	-1.529157
H	-4.923711	-2.798564	1.212196
H	-6.192272	-2.605508	-0.024627
H	-6.207256	-1.580474	1.432463
H	-2.625717	-0.813410	-1.835446
H	-3.767942	-2.160864	-2.127421
H	-2.583442	-2.259839	-0.793470
H	-0.778169	0.563508	2.751000
H	-2.471197	1.234449	3.242402
H	-1.907626	3.662927	0.999693
H	-2.101847	4.116599	-0.738266
H	-0.508769	3.563321	-0.087120

TS3 (R^1 = OTMS, R^2 = Me)

Rh	-0.492049	0.340028	-0.178340
Rh	-2.683230	-0.736334	0.217367
Si	4.091869	-1.127964	0.212016
O	-0.756743	-0.080181	-2.185289
O	0.360266	-1.538873	0.085430
O	-0.391776	0.677484	1.870218
O	-1.515124	2.125375	-0.402693
O	-2.768329	-1.062784	-1.823139
O	-1.653579	-2.514450	0.456775
O	-2.398306	-0.317364	2.227536
O	-3.525060	1.134201	-0.055526
O	3.567132	0.008225	-1.030289
O	3.176982	2.349714	0.052170
C	-1.817714	-0.674514	-2.543034
C	-0.406698	-2.516958	0.340132
C	-1.355189	0.272725	2.590708
C	-2.778516	2.111751	-0.296552
C	5.944358	-0.853717	0.263440
C	3.628428	-2.799249	-0.481570
C	3.254570	-0.714889	1.831446
C	2.709869	0.965032	-0.997649
C	1.890467	1.630424	-2.001749
C	1.332701	1.326916	-0.530731
C	1.916469	2.408009	0.247468
C	1.272050	3.411638	1.114264
H	-1.907842	-0.872026	-3.632123
H	0.099793	-3.496766	0.474179
H	-1.251648	0.471919	3.678708
H	-3.277615	3.094292	-0.435079
H	6.396792	-1.012397	-0.728498
H	6.420245	-1.555488	0.968760
H	6.186107	0.170514	0.589881
H	2.534761	-2.860312	-0.589460
H	3.961278	-3.608732	0.189149
H	4.090172	-2.962511	-1.468315
H	3.524467	0.295196	2.177702
H	3.580663	-1.431659	2.604347
H	2.159997	-0.782169	1.739762
H	1.457186	0.969933	-2.760297
H	2.086045	2.659850	-2.317516
H	0.418986	3.856965	0.578598
H	1.983628	4.171228	1.462331
H	0.829923	2.863681	1.964857

TS4 (R^1 = OTMS, R^2 = Me)

Rh	-0.530772	0.385887	-0.201799
Rh	-2.692579	-0.727996	0.241165
Si	4.089135	-1.094678	0.199152
O	-0.950730	0.186783	-2.214197
O	0.324007	-1.511754	-0.205199
O	-0.273899	0.488691	1.861259
O	-1.550446	2.183548	-0.146602
O	-2.939935	-0.823445	-1.808327

O	-1.666202	-2.522560	0.198853
O	-2.253444	-0.542872	2.257956
O	-3.536222	1.160829	0.246162
O	3.516859	-0.042120	-1.066998
O	3.262987	2.184703	-0.178106
C	-2.041957	-0.361565	-2.552391
C	-0.430382	-2.511590	-0.008399
C	-1.181531	0.002944	2.604367
C	-2.801229	2.159014	0.056431
C	5.927293	-0.737982	0.310840
C	3.732584	-2.807317	-0.458040
C	3.201057	-0.718216	1.804638
C	2.796059	1.044985	-1.073341
C	1.878845	1.554517	-2.058802
C	1.284175	1.371058	-0.597887
C	1.996860	2.260361	0.234794
C	1.619666	3.035928	1.426575
H	-2.216505	-0.438684	-3.646317
H	0.075883	-3.500511	-0.022397
H	-0.992370	0.076243	3.696561
H	-3.300513	3.151066	0.067429
H	6.423352	-0.903621	-0.659012
H	6.408531	-1.396542	1.053327
H	6.111469	0.305389	0.613938
H	2.646551	-2.929840	-0.590129
H	4.093193	-3.583934	0.236465
H	4.221150	-2.966983	-1.432498
H	3.471496	0.275475	2.195977
H	3.496489	-1.462099	2.564259
H	2.108039	-0.767058	1.685082
H	1.472584	0.818098	-2.755602
H	1.961492	2.579159	-2.437078
H	0.754135	3.671959	1.181595
H	2.460437	3.625360	1.814092
H	1.255070	2.319674	2.183595

TS5 (R^1 = OTMS, R^2 = Me)

Rh	-0.973025	0.082458	-0.045987
Rh	-3.408888	-0.285832	0.077439
Si	6.143199	-0.327207	0.058058
O	-0.749383	-1.963402	0.184809
O	-1.006963	0.325334	2.008737
O	-1.398300	2.099990	-0.281906
O	-1.123912	-0.198296	-2.092211
O	-2.986992	-2.297734	0.316163
O	-3.246717	-0.015562	2.119476
O	-3.635397	1.753072	-0.173407
O	-3.364318	-0.526229	-1.980003
O	4.525642	-0.950458	-0.112981
O	3.299929	0.980969	-0.072633
C	-1.791316	-2.673255	0.313411
C	-2.115069	0.221283	2.609916
C	-2.611155	2.465940	-0.292422
C	-2.268178	-0.434023	-2.582350
C	6.485389	0.788895	-1.408879
C	7.176037	-1.884923	0.033052
C	6.240783	0.579786	1.695360
C	3.361859	-0.360521	-0.133302
C	2.074098	-0.876673	-0.206301
C	1.124757	0.300507	-0.147492
C	1.984280	1.393348	-0.097309
C	1.748629	2.853934	-0.001775
H	-1.612736	-3.762353	0.438438
H	-2.074177	0.358540	3.711431
H	-2.778882	3.555936	-0.424026
H	-2.294480	-0.575192	-3.683794
H	6.353179	0.247846	-2.359788
H	7.524324	1.157774	-1.374461
H	5.816884	1.663851	-1.413742
H	6.903149	-2.555471	0.863444
H	8.247035	-1.641927	0.131044
H	7.038808	-2.437287	-0.910217
H	5.577965	1.458874	1.710711
H	7.270843	0.930390	1.876239
H	5.958837	-0.079279	2.532308
H	1.767529	-1.919103	-0.193329
H	1.459500	-0.267981	-1.228810
H	0.672031	3.040734	-0.099808
H	2.289169	3.400158	-0.793115
H	2.092911	3.249957	0.969512