Electronic Supplementary Material (ESI) for ChemComm.
This journal is © The Royal Society of Chemistry 2015

Copper-Catalyzed Silylation of *p*-Quinone Methides: New Entry to Dibenzylic Silanes

Aurora López, Alejandro Parra, Carlos Jarava-Barrera and Mariola Tortosa*.

Departamento de Química Orgánica (Modulo 01), Facultad de Ciencias, Universidad Autónoma de Madrid. 28149-Madrid, Spain.

Supplementary Information

Table of contents

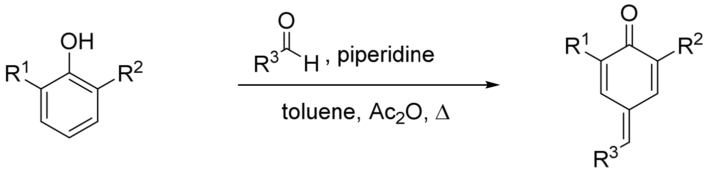
1. General experimental details

Tetrahydrofuran, toluene and dichloromethane were purified by passing through a Pure Solv™ column drying system from Innovative Technology, Inc. Additionally, THF and methanol were degassed through three consecutive freeze-pump-thaw cycles. Diethyl ether and chloroform were dried using activated 4Å molecular sieves and stored under argon. Dry-DMF was acquired from commercial sources. Unless indicated otherwise, all reactions were conducted under an argon atmosphere using flame-dried glassware with standard vacuum-line techniques. NMR spectra were acquired on a Bruker 300 spectrometer, running at 300, and 75 MHz for ^{1}H and ^{13}C, respectively. Chemical shifts (δ) are reported in ppm relative to residual solvent signals ($CDCl_3$, 7.26 ppm for ^{1}H NMR and 77.2 ppm for ^{13}C NMR respectively). ^{13}C NMR spectra were acquired on a broad band decoupled mode. The following abbreviations are used to describe peak patterns when appropriate: s (singlet), d (doublet), t (triplet), q (quartet), quint (quintet), sept (septuplet), m (multiplet), bs (broad singlet). Analytical thin layer chromatography (TLC) was performed using pre-coated aluminium-backed plates (Merck Kieselgel 60 F254) and visualized by ultraviolet irradiation or phosphomolybdic acid dip or vainilline dip. Purification of reaction mixtures was carried out by flash chromatography (FC) using silica gel Merck-60 or Florisil® 100-200 mesh from Aldrich. Mass Spectrometry (MS) and High Resolution Mass Spectrometry (HRMS) were registered in a spectrometer GCT Agilent Technologies 6890N using Electronic Impact (E.I.) techniques at 70 eV, electrospray (ESI+). Melting points were determined in a Büchi Melting Point B-540 apparatus in open capillary tubes. Infrared spectrometry (IR) was registered in a spectrometer *Bruker Vecter 22*, the band characteristic indicated in cm^{-1}.

All ligands, $[Cu(CH_3CN)_4]PF_6$, 2,6-disubstituted phenols, aldehydes, acid chlorides, piperidine, triethylamine, palladium on activated carbon, sodium borohydride, manganese (IV) oxide, hexamethylentetramine, bromobenzene, magnesium turnings and NaO*t*-Bu (2.0 M solution in THF) were acquired from commercial sources and were used without further purification.

2. Synthesis of Starting Materials

2.1. General procedure for the synthesis of 2,6-di-*tert*-butyl *p*-quinone methides, 1a-1j, 1o[1]



$R^1 = R^2 = {}^tBu$	$R^3 = C_6H_5$	**1a**
$R^1 = R^2 = {}^tBu$	$R^3 =$ *p*-OMe-C_6H_4	**1b**
$R^1 = R^2 = {}^tBu$	$R^3 =$ *p*-Me-C_6H_4	**1c**
$R^1 = R^2 = {}^tBu$	$R^3 =$ 2-thiophenyl	**1d**
$R^1 = R^2 = {}^tBu$	$R^3 =$ 2-naphthyl	**1e**
$R^1 = R^2 = {}^tBu$	$R^3 =$ *p*-Br-C_6H_4	**1f**
$R^1 = R^2 = {}^tBu$	$R^3 =$ *o*-Br-C_6H_4	**1g**
$R^1 = R^2 = {}^tBu$	$R^3 =$ *m*-CF_3-C_6H_4	**1h**
$R^1 = R^2 = {}^tBu$	$R^3 =$ *p*-$MeCO_2$-C_6H_4	**1i**
$R^1 = R^2 = {}^tBu$	$R^3 =$ p-CN-C_6H_4	**1j**
$R^1 =$ Me, $R^2 = {}^tBu$	$R^3 = C_6H_5$	**1o**

2,6-ditertbutyl *p*-quinone methides **1a**,[1] **1c**,[2] **1b**,[3] **1f**,[3] **1g**[3] and **1o**[3] were previously described in the literature.

In a Dean–Stark apparatus, a solution of 2,6-di-*tert*-butylphenol and the corresponding benzaldehyde in toluene was heated to reflux (140 ^{o}C). Piperidine was added within 1 h and heating was continued for 12 h. After cooling just below the boiling point of the reaction mixture, acetic anhydride was added and stirring was continued for 15 min. Then the reaction mixture was poured on ice-water and extracted with CH_2Cl_2 (x3). The combined organic phases were dried over Mg_2SO_4, and the solvent was removed under reduced pressure. The crude products were purified by column chromatography (cyclohexane) and recrystallized from *n*-hexane.

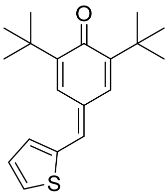
---

[1] Koutek, B.; Pavlickova, L.; Soucek, M. *Synthetic Commun*. **1976**, *6*, 305.

[2] Roos, E.; Hugl. E *DE* 2734239 A, **1979.**

[3] Chu, W.; Zhang, L.; Bao. X.; Zhao, X.; Zeng, C.; Du, J.; Zhang, G.; Wang, F.; Ma, X.; Fan, C. *Angew. Chem. Int. Ed*. **2013**, *52*, 9229.

2,6-di-*tert*-Butyl-4-(thiophen-2-ylmethylene)cyclohexa-2,5-dien-1-one, 1d

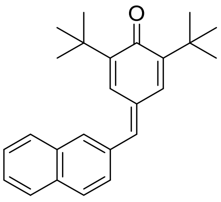


1d

From 2,6-di-*tert*-butylphenol (5.0 g, 24.3 mmol, 1.0 equiv) and thiophene-2-carbaldehyde (2.7 g, 24.3 mmol, 1.0 equiv), following the general procedure described above, compound **1d** was obtained in 58% yield as an orange solid. **R*f*** = 0.52 (100% hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.87 (s, 1H), 7.57 (d, *J* = 5.0 Hz, 1H), 7.33 (d, *J* = 3.6 Hz, 1H), 7.19 (s, 1H), 7.13 (dd, *J* = 5.0, 3.8 Hz, 1H), 6.96 (s, 1H), 1.37 (s, 9H), 1.32 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 186.2, 149.4, 147.5, 139.4, 135.2, 134.0, 133.8, 131.1, 129.2, 127.9, 127.0, 35.7, 35.0, 29.6, 29.5. **HRMS (EI$^+$)** calculated for $C_{19}H_{24}SO$ [M$^+$]: 300.1548, found: 300.1537. **mp** = 74-76 °C.

2,6-di-*tert*-Butyl-4-(naphthalen-2-ylmethylene)cyclohexa-2,5-dienone, 1e

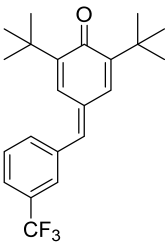


1e

From 2,6-di-*tert*-butylphenol (5.0 g, 24.3 mmol, 1.0 equiv) and 2-naphthaldehyde (3.8 g, 24.3 mmol, 1.0 equiv.), following the general procedure described above, compound **1e** was obtained in 65% yield as a yellow solid. **R*f*** = 0.24 (100% hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.97-7.83 (m, 4H), 7.65 (d, *J* = 2.3 Hz, 1H), 7.62-7.50 (m, 3H), 7.34 (s, 1H), 7.08 (d, *J* = 2.4 Hz, 1H), 1.36 (s, 9H), 1.32 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 185.2, 148.2, 146.6, 141.1, 133.8, 132.2, 132.0, 131.0, 129.3, 127.2, 127.1, 126.6, 126.4, 126.0, 125.9, 125.5, 34.2, 33.7, 28.3, 28.2. **HRMS (EI$^+$)** calculated for $C_{25}H_{28}O$ [M$^+$]: 344.21240, found: 344.2133. **mp** = 113-115 °C.

2,6-di-*tert*-Butyl-4-[3-(trifluoromethyl)benzylidene]cyclohexa-2,5-dien-1-one, 1h

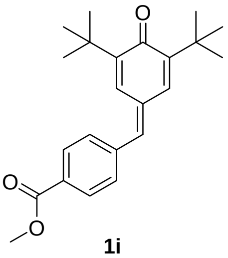


1h

From 2,6-di-*tert*-butylphenol (5.0 g, 24.3 mmol, 1.0 equiv) and 3-(trifluoromethyl)benzaldehyde (4.2 g, 24.3 mmol, 1.0 equiv), following the general procedure described above, compound **1h** was obtained in 70% yield as an orange solid. **R*f*** = 0.33 (100% hexanes).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.71 (s, 1H), 7.67-7.54 (m, 3H), 7.42 (s, 1H), 7.17 (s, 1H), 7.02 (s, 1H), 1.3H (s, 9H), 1.29 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 186.6, 150.3, 148.7, 139.8, 136.8, 134.7, 133.4, 133.37, 133.36, 131.5 (q, J_{C-F} = 32.0 Hz), 129.5, 127.2, 127.1 (q, J_{C-F} = 3.8 Hz), 125.5 (*q*, J_{C-F} = 3.8 Hz), 124.0 (q, J_{C-F} = 270.75 Hz), 35.7, 35.2, 29.7, 29.6. **^{19}F NMR** (282 MHz, $CDCl_3$) δ –62.95 (s). **HRMS (EI$^+$)** calculated for $C_{22}H_{25}OF_3$ [M$^+$]: 362.1858, found: 362.1866. **mp** = 54-56 °C.

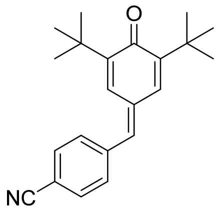
Methyl 4-[(3,5-di-*tert*-butyl-4-oxocyclohexa-2,5-dien-1-ylidene)methyl]benzoate, 1i


1i

From 2,6-di-*tert*-butylphenol (3.0 g, 14.5 mmol, 1.0 equiv) and methyl 4-formylbenzoate (2.4 g, 14.5 mmol, 1.0 equiv), following the general procedure described above, compound **1i** was obtained in 60% as an orange solid. **R*f*** = 0.5 (100% hexanes).

^{1}H NMR (300 MHz, CDCl$_3$): δ 8.11 (d, *J* = 8.3 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.45 (s, 1H), 7.17 (s, 1H), 7.01 (s, 1H), 3.95 (s, 3H), 1.33 (s, 9H), 1.29 (s, 9H). **^{13}C NMR** (75 MHz, CDCl$_3$): δ 186.5, 166.5, 150.0, 148.5, 140.4, 140.3, 134.7, 133.4, 130.1, 129.9, 127.3, 126.0, 52.3, 35.5, 35.1, 30.3, 29.5. **HRMS (EI+)** calculated for $C_{19}H_{19}O_3$ [M^+-C_4H_9]: 295.1334, found: 295.1388. **mp** = 99-101 °C.

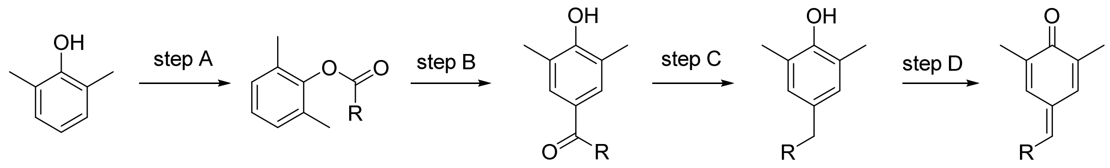
4-[(3,5-di-*tert*-Butyl-4-oxocyclohexa-2,5-dien-1-ylidene)methyl]benzonitrile, 1j


1j

From 2,6-di-*tert*-butylphenol (5.0 g, 24.3 mmol, 1.0 equiv) and 4-formylbenzonitrile (3.2 g, 24.3 mmol, 1.0 equiv), following the general procedure described above, compound **1j** was obtained in 70% yield as a yellow solid. **R*f*** = 0.29 (100% hexanes).

^{1}H NMR (300 MHz, CDCl$_3$): δ 7.73 (d, *J* = 8.3 Hz, 2H), 7.53 (d, *J* = 8.1 Hz, 2H), 7.36 (s, 1H), 7.11 (s, 1H), 7.00 (s, 1H), 1.33 (s, 9H), 1.29 (s, 9H). **^{13}C NMR** (75 MHz, CDCl$_3$): δ 186.4, 150.6, 149.0, 140.4, 138.8, 134.4, 134.0, 132.4, 130.6, 126.7, 112.2, 35.6, 35.2, 29.5, 29.5. **HRMS (EI$^+$)** calculated for $C_{22}H_{25}NO$ [M^+]: 319.1936, found: 319.1951. **mp** = 174-176 °C.

2.2. Synthesis of 2,6-dimethyl *p*-quinone methides, 1l-1m



SI-14, R = C_6H_5 **SI-16** **SI-18** **1l**
SI-15, R = *o*-Me-C_6H_4 **SI-17** **SI-19** **1m**

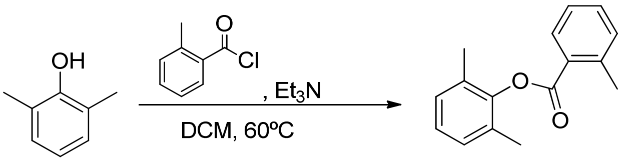
Compounds **SI-14**[4], **SI-16**[5], **SI-18**[5] and **1l**[5] were previously described in the literature.

---

[4] Pews, R. Garth *US 20050090673*, **2005.**

[5] Olah, M. G.; Robins, J. S.; Baker, M. S.; Phillips, S. T. *Macromolecules* **2013**, *46*, 5924.

2.2.1. Synthesis of 2,6-dimethylphenyl 2-methylbenzoate, SI-15, step A[4]

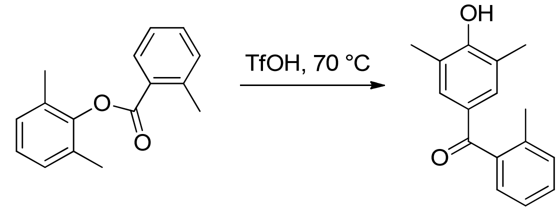


SI-15

A round bottom flask was charged with 2,6-dimethylphenol (2.5 g, 20.5 mmol, 1.0 equiv), triethylamine (1.4 equiv) and dissolved in DCM (2.0 mL/mmol phenol). A solution of 2-methylbenzoyl chloride (2.7 mL, 20.5 mmol, 1.0 equiv) in DCM (0.6 mL/mmol phenol) was added and the mixture was stirred at 60 °C until starting material disappearance was observed by TLC. The mixture was allowed to cool to room temperature and then was washed with water (x3). The organic layer was dried over Na_2SO_4, filtered and the solvent was removed under reduce pressure. The product was obtained in 99% yield as a colorless oil and was used in the next step without further purification. **R$_f$** = 0.55 (88% hexanes:AcOEt).

^{1}H NMR (300 MHz, $CDCl_3$): δ 8.30 (d, *J* = 7.6 Hz, 1H), 7.56 (t, *J* = 7.2 Hz, 1H), 7.46-7.35 (m, 2H), 7.22-7.14 (m, 3H), 2.76 (s, 3H), 2.29 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 165.1, 148.5, 141.3, 132.7, 132.1, 131.1, 130.4, 128.7, 128.7, 126.1, 125.9, 22.0, 16.6. **HRMS (EI$^+$)** calculated for $C_{16}H_{16}O_2$ [M$^+$]: 240.1150, found: 240.1152.

2.2.2. Synthesis of (4-hydroxy-3,5-dimethylphenyl)(*o*-tolyl)methanone, SI-17, step B[5]

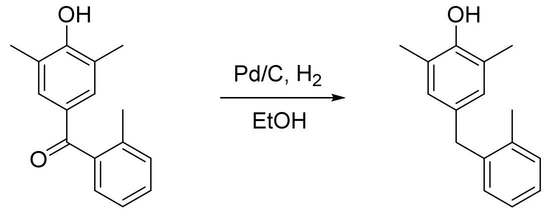


SI-15 **SI-17**

Triflic acid (0.3 mL/mmol **SI-15**) was added to **SI-15** (4.7 g, 19.5 g, 1.0 equiv) at 0 °C and the mixture was heated at 70 °C. The reaction mixture was stirred until starting material disappearance (TLC), then cooled to room temperature and poured into an ice-water bath. The layers were separated and the aqueous phase was extracted with AcOEt (x3). The aqueous layer was neutralized with saturated aqueous sodium bicarbonate and extracted with AcOEt (x2). The combined organic layers were dried over Na_2SO_4, filtered and concentrated. The crude product was purified by flash column chromatography (90% hexanes: AcOEt) to obtain **SI-17** in 81% yield as a brown solid. **R$_f$** = 0.12 (90% hexanes:AcOEt).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.41 (s, 2H), 7.33-7.25 (m, 1H), 7.21 (s, 1H), 7.18 (s, 2H), 2.22 (s, 3H), 2.18 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 197.9, 157.0, 139.4, 136.1, 131.4, 130.8, 130.0, 129.6, 127.9, 125.1, 123.0, 19.8, 15.8. **HRMS (EI$^+$)** calculated for $C_{16}H_{16}O_2$ [M$^+$]: 240.1150, found: 240.1142. **mp** = 173-175 °C.

2.2.3. Synthesis of 2,6-dimethyl-4-(2-methylbenzyl)phenol, SI-19, step C[5]

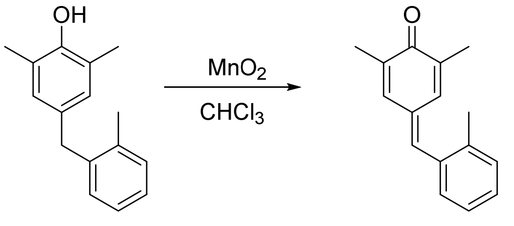


SI-17 **SI-19**

Palladium (10% by weight on carbon powder) (0.05 equiv) was added to a solution of **SI-17** (1.0 g, 4.2 mmol, 1.0 equiv) in ethanol (3.1 mL/ 1.0 mmol **SI-17**) under argon atmosphere. The flask was evacuated and purged with H_2 gas (ballon). The reaction mixture was stirred vigorously at room temperature until starting material disappearance (by TLC). The reaction mixture was filtered through a pad of celite and concentrated. The crude of product was purified by flash column chromatography (66 %, Cy/AcOEt) to obtain **SI-19** in 98% yield as a white solid. **R$_f$** = 0.66 (66% hexanes:AcOEt).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.18-7.06 (m, 4H), 6.75 (s, 2H), 4.46 (s, 1H), 3.86 (s, 2H), 2.27 (s, 3H), 2.21 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 150.4, 139.6, 136.5, 131.91, 130.2, 129.8, 128.9, 126.2, 125.9, 122.9, 38.6, 19.7, 15.9. **HRMS (EI$^+$)** calculated for $C_{16}H_{18}O$ [M$^+$]: 226.1358, found: 226.1362. **mp** = 75-77 °C.

2.2.4. Synthesis of 2,6-dimethyl-4-(2-methylbenzylidene)cyclohexa-2,5-dien-1-one, step D[6]



SI-19 **1m**

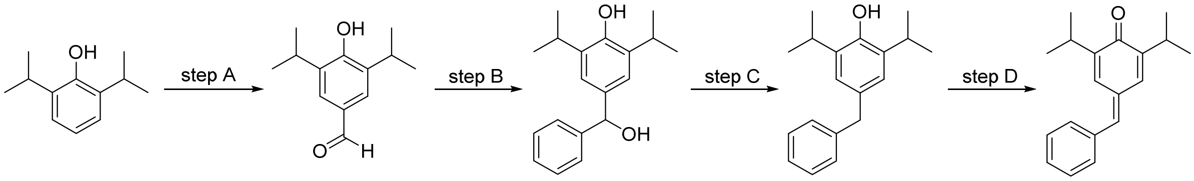
Manganese (IV) oxide (4.4 g, 50.4 mmol, 48.5 equiv) was added to a solution of **SI-19** in $CHCl_3$ (95 mL) and the reaction mixture was stirred at room temperature until starting disappearance (by TLC). The reaction mixture was filtered through a pad of celite and concentrated. The product was obtained in 99% as a yellow solid and was used in the next step without further purification. **R$_f$** = 0.58 (83% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.41-7.25 (m, 6H), 7.15 (s, 1H), 2.38 (s, 3H), 2.11 (s, 3H), 2.06 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 187.4, 141.8, 138.5, 137.7, 137.5, 135.8, 134.7, 132.0, 131.9, 130.9, 130.4, 129.3, 125.9, 20.1, 16.7, 16.2. **HRMS (EI$^+$)** calculated for $C_{16}H_{16}O$ [M$^+$]: 224.1201, found: 224.1207. **mp** = 80-82 °C.

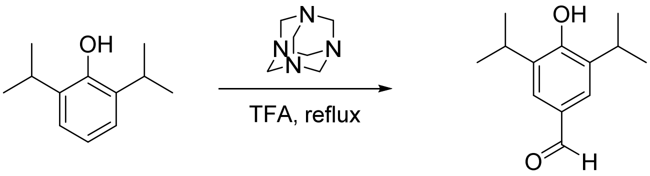
---

[6] Nakagawa, R.; Uno, T.; Kubo, M.; Itoh, T. *Polym. Bull.* **2012**, *68*, 1831.

2.3. Synthesis of 2,6-diisopropyl *p*-quinone methide, 1n



2.3.1. Synthesis of 4-hydroxy-3,5-diisopropylbenzaldehyde, SI-20, step A[7]



SI-20

2,6-diisopropylphenol (8.0 g, 44.8 mmol, 1.0 equiv), hexamethylenetetramine (12.6 g, 89.6 mmol, 2.0 equiv) and trifluoroacetic acid (44 mL) were mixed in a round bottom flask and the solution was heated under reflux (90 °C) for 12 hours. The reaction mixture was cooled at room temperature and neutralized with $NaHCO_3$. The aqueous layer was extracted with EtOAc (x3) and the combined organic layers were concentrated. A solution of HCl 3.0 M was added to the crude product and the mixture was stirred under reflux (80 °C) for 3 hours. The precipitated was filtered, washed with water and purified by recrystallization from EtOH. Compound **SI-20** was obtained in 98% yield as a white solid. $\mathbf{R}_f$ = 0.66 (80% hexanes/EtOAc). The spectroscopic data were in agreement with those reported in the literature.[8]

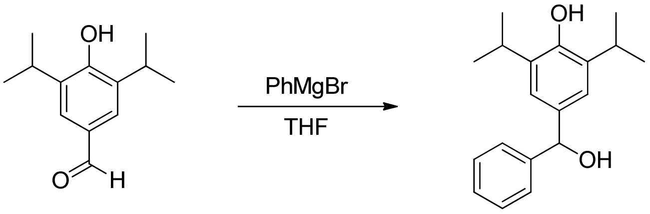
^{1}H NMR (300 MHz, $CDCl_3$): δ 9.86 (s, 1H), 7.62 (s, 2H), 5.43 (s, 1H), 3.18 (sept, *J* = 6.9 Hz, 2H), 1.31 (d, *J* = 6.8 Hz, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 192.1, 156.4, 134.7, 129.7, 126.4, 27.2, 22.7.

---

[7] Kurlovich, A. L.; Terasevich, V. A.; Kozlov, N. G. *Russ. J. Org. Chem.* **2009**, *45*, 1503.

[8] Geurink, P. P.; Florea, B. I.; Li, N.; Witte, M. D.; Verasdonk, J.; Kuo, C.; Van der Marel, G. A.; Overkleeft, H. S. *Angew. Chem. Int. Ed.* **2010**, *49*, 6802.

2.3.2. Synthesis of 4-(hydroxy(phenyl)methyl)-2,6-diisopropylphenol, SI-21, step B[9]

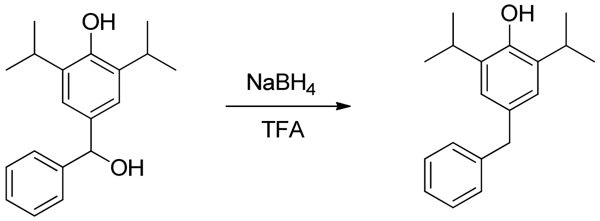


SI-20 **SI-21**

A solution of bromobenzene (1.23 mL, 11.7 mmol, 2.4 equiv) in dry THF (10 mL) was added dropwise to a suspension of magnesium turnings (302 mg, 12.6 mmol, 2.6 equiv) in dry THF (2 mL), under argon atmosphere. After 2 hours at reflux, the mixture was cooled at room temperature and a solution of **SI-20** (1.0 g, 4.8 mmol, 1.0 equiv) in dry THF (10 mL) was added dropwise and stirred for 12 hours. Then, the reaction mixture was hydrolyzed with saturated aqueous NH_4Cl solution. The aqueous layer was extracted with Et_2O (x3) and the combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated. Compound **SI-21** was obtained in 99% yield as white solid and was used in the next step without further purification. **R*f*** = 0.48 (80% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.42-7.19 (m, 5H), 7.04 (s, 2H), 5.77 (s, 1H), 4.83 (s, 1H), 3.11 (sept, *J* = 6.9 Hz, 2H), 1.22 (d, *J* = 6.8 Hz, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 149.6, 144.2, 135.9, 133.8, 128.4, 127.3, 126.5, 122.1, 76.6, 27.4, 22.7. **HRMS (EI$^+$)** calculated for $C_{19}H_{24}O_2$ [M$^+$]: 284.1776, found: 284.1773. **mp** = 94-96 °C.

2.3.3. Synthesis of 4-benzyl-2,6-diisopropylphenol, SI-22, step C[10]



SI-21 **SI-22**

Sodium borohydride (680.4 mg, 18.0 mmol, 4.0 equiv) was added to trifluoroacetic acid (39 mL) at 0 °C in small portions (*this addition must be done carefully: large amount of hydrogen gas is released in the process*). Then alcohol **SI-21** (1.3 g, 4.5 mmol, 1.0 equiv) was added and the reaction mixture was stirred 15 min at room temperature. Water was added and the aqueous phase was neutralized with $NaHCO_3$ and extracted with Et_2O (x3). The combined organic layers were washed with brine, dried over Na_2SO_4, filtered and concentrated. Compound **SI-22** was obtained in 85% yield as an orange solid and was used in the next step without further purification. **R*f*** = 0.63 (80% hexanes/EtOAc).

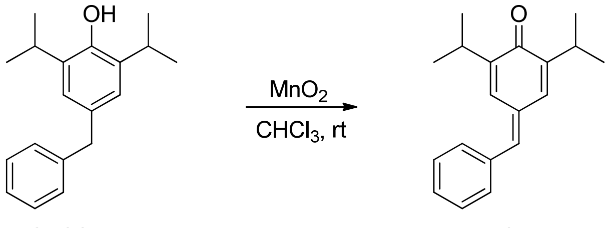
---

[9] Richter, D.; Hampel, N.; Singer, T.; Ofial, A. R.; Mayr, H. *Eur. J. Org. Chem*. **2009**, 3203.

[10] Bringman, G.; Pabst, T.; Henschel, P.; Michel, M. *Tetrahedron* **2001**, *57*, 1269.

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.41-7.16 (m, 5H), 6.94 (s, 2H), 4.75 (bs, 1H), 3.98 (s, 2H), 3.18 (sept, *J* = 6.9 Hz, 2H), 1.30 (d, *J* = 6.8 Hz, 12H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 148.4, 142.0, 133.8, 132.9, 128.9, 128.4, 125.9, 124.2, 41.8, 27.4, 22.9. **HRMS (EI$^+$)** calculated for $C_{19}H_{24}O$ [M$^+$]: 268.1827, found: 268.1836. **mp** = 34-36 °C.

2.3.4. Synthesis for 4-benzylidene-2,6-diisopropylcyclohexa-2,5-dienone, 2n, step D[6]



SI-22 **2n**

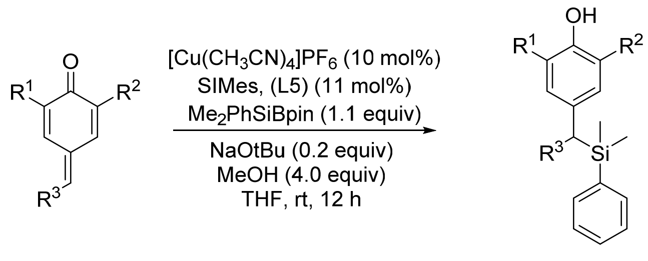
MnO_2 (13.4 g, 154.1 mmol, 48.5 equiv) was added to a solution of **SI-22** (852.9 mg, 3.2 mmol, 1.0 equiv) in $CHCl_3$ (288 mL) and the reaction mixture was stirred at room temperature for 15 min. The reaction mixture was filtered through a pad of celite and concentrated. Compound **2n** was obtained in 98% yield as an orange-red solid and was used in the next step without further purification. **R$_f$** = 0.64 (80% hexanes/EtOAc). The spectroscopic data were in agreement with those reported in the literature.[11]

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.51-7.45 (m, 5H), 7.26 (s, 1H), 7.23 (s, 1H), 6.99 (s, 1H), 3.28-3.11 (sept, *J* = 6.9 Hz, 2H), 1.17 (d, *J* = 6.9 Hz, 6H), 1.13 (d, *J* = 6.9 Hz, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 185.3, 147.5, 145.9, 142.7, 135.9, 134.9, 132.1, 130.5, 129.2, 128.8, 127.5, 27.0, 26.6, 22.1. **HRMS (EI$^+$)** calculated for $C_{19}H_{22}O$ [M$^+$]: 266.1671, found: 266.1668.

---

[11] Koutek, B.; Pavlickova, L.; Velek, J.; Beranek, V.; Soucek, M. *Chem. Comm.* **1976**, *41*, 2607.

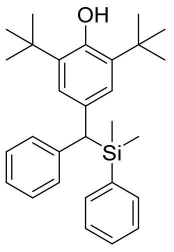
3. General procedure for synthesis of 2,6-disubtituted-4-[(dimethyl(phenyl)silyl)(aryl)methyl]phenols



1 **2**

An oven-dried vial was charged with $[Cu(CH_3CN)_4]PF_6$ (7.5 mg, 0.02 mmol, 10 mol%) and 1,3-bis(2,4,6-trimethylphenyl)imidazolinium chloride (SIMes) (7.5 mg, 0.022 mmol, 11 mol%) and sealed with a septum. The vial was connected to an argon-vacuum line, evacuated and backfilled with argon (x3). THF (1.0 mL/0.2 mmol of **1**) was added and the mixture was stirred for 5 min. 2-(dimethylphenylsilyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (60 µL, 0.22 mmol, 1.1 equiv) was added followed by NaO*t*Bu (2M solution in THF, 20 µL, 0.04 mmol, 0.2 equiv). The dark brown solution was stirred for 15 min at room temperature and a solution of **1** (1.0 equiv) in THF (1 mL) was added followed by methanol (32 µL, 0.8 mmol, 4.0 equiv). Then, the reaction mixture was stirred overnight at room temperature. Et_2O and water were added and the layers were separated. The aqueous phase was extracted with Et_2O (x3) and the combined organic layers were washed with saturated NaCl solution, dried over Na_2SO_4, filtered and concentrated. The crude product was purified by flash column chromatography (10% AcOEt/hexanes).

2,6-di-*tert*-Butyl-4-[(dimethyl(phenyl)silyl)(phenyl)methyl]phenol, 2a

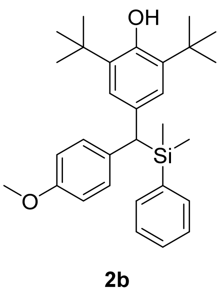


2a

From **1a** (58.9 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2a** was obtained in 86% yield as a yellow oil. **R*f*** = 0.65 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.38-7.29 (m, 2H), 7.29-7.19 (m, 5H), 7.18-7.10 (m, 3H), 6.88 (s, 2H), 4.94 (s, 1H), 3.64 (s, 1H), 1.35 (s, 18H), 0.29 (s, 3H), 0.26 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 151.6, 143.4, 138.3, 135.6, 134.8, 132.6, 130.7, 129.2, 128.4, 127.8, 125.7, 125.3, 45.8, 34.6, 30.6, -2.8, -3.1. **HRMS (EI$^+$)** calculated for $C_{29}H_{38}OSi$ [M$^+$]: 430.2692, found: 430.2696. **IR (thin film NaCl, cm^{-1})**: 3640.0, 2963.8, 1601.6, 1436.21, 832.9.

2,6-di-*tert*-Butyl-4-[(dimethyl(phenyl)silyl)(4-methoxyphenyl)methyl]phenol, 2b

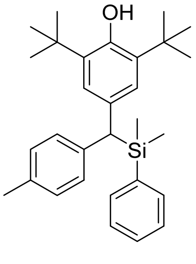


2b

From **1b** (65.3 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2b** was obtained in 80% yield as a yellow oil. **R*f*** = 0.70 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.28-7.14 (m, 5H), 6.98 (d, *J* = 8.6 Hz, 2H), 6.75 (s, 2H), 6.69 (d, *J* = 8.6 Hz, 2H), 4.83 (s, 1H), 3.67 (s, 3H), 3.48 (s, 1H), 1.24 (s, 18H), 0.18 (s, 3H), 0.16 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 157.3, 151.4, 138.2, 135.4, 135.3, 134.6, 132.8, 130.0, 129.0, 127.6, 125.3, 113.7, 55.3, 44.4, 34.4, 30.5, -2.9, -3.3. **HRMS (EI$^+$)** calculated for $C_{30}H_{40}O_2Si$ [M$^+$]: 460.2798, found: 460.2817. **IR (neat)**: 3640.0, 2958.9, 1514.1, 1441.1, 837.8 cm^{-1}.

2,6-di-*tert*-Butyl-4-[(dimethyl(phenyl)silyl)(*p*-tolyl)methyl]phenol, 2c

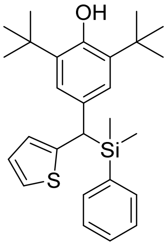


2c

From **1c** (61.7 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2c** was obtained in 82% yield as a yellow oil. **R*f*** = 0.66 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, CDCl$_3$): δ 7.22-7.19 (m, 4H), 6.98 (s, 5H), 6.79 (s, 2H), 4.85 (s, 1H), 3.52 (s, 1H), 2.24 (s, 3H), 1.28 (s, 18H), 0.21 (s, 3H), 0.19 (s, 3H). **^{13}C NMR** (75 MHz, CDCl$_3$): δ 151.4, 140.1, 138.3, 135.4, 134.6, 134.4, 132.7, 129.7, 129.0, 128.9, 127.6, 125.5, 45.1, 34.4, 30.5, 21.1, -2.9, -3.3. **HRMS (EI$^+$)** calculated for $C_{30}H_{40}OSi$ [M$^+$]: 444.2848, found: 444.2869. **IR (neat)**: 3644.4, 2962.3, 1437.2, 1256.4, 842.7 cm^{-1}.

2,6-di-*tert*-Butyl-4-[(dimethyl(phenyl)silyl)(thiophen-2-yl)methyl]phenol, 2d

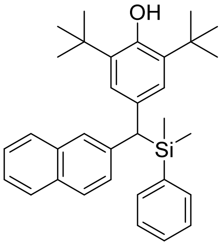


2d

From **1d** (60.1 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2d** was obtained in 89% yield as a yellow oil. **R*f*** = 0.72 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, CDCl$_3$): δ 7.40-7.22 (m, 5H), 7.04 (d, *J* = 5.0 Hz, 1H), 6.90 (m, 1H), 6.86 (s, 2H), 6.76-6.74 (m, 1H), 4.96 (s, 1H), 3.90 (s, 1H), 1.35 (s, 18H), 0.31 (s, 3H), 0.31 (s, 3H). **^{13}C NMR** (75 MHz, CDCl$_3$): δ 151.6, 146.2, 137.2, 135.4, 134.6, 131.7, 129.2, 127.6, 126.7, 125.0, 124.2, 122.2, 40.4, 34.4, 30.4, -3.5, -3.9. **HRMS (EI$^+$)** calculated for $C_{27}H_{36}OSiS$ [M$^+$]: 436.2256, found: 436.2252. **IR (neat)**: 3644.9, 2958.9, 1436.2, 1256.2, 832.9 cm^{-1}.

2,6-di-*tert*-Butyl-4-[(dimethyl(phenyl)silyl)(naphthalen-2-yl)methyl]phenol, 2e

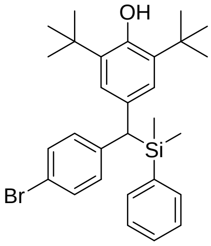


2e

From **1e** (68.9 mg, 0.2 mmol, 1.0 equiv.), following the general procedure described above, compound **2e** was obtained in 76% yield as yellow oil. **R*f*** = 0.63 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, CDCl$_3$): δ 7.77-7.61 (m, 3H), 7.57 (s, 1H), 7.42-7.28 (m, 5H), 7.25-7.18 (m, 3H), 6.92 (s, 2H), 4.92 (s, 1H), 3.79 (s, 1H), 1.32 (s, 18H), 0.29 (s, 3H), 0.27 (s, 3H). **^{13}C NMR** (75 MHz, CDCl$_3$): δ 151.5, 140.9, 138.1, 135.5, 134.7, 133.8, 132.4, 131.7, 129.1, 128.4, 127.7, 127.6 (2C), 127.5, 126.9, 125.8, 125.7, 124.9, 45.7, 34.5, 30.5, -2.8, -3.2. **HRMS (EI$^+$)** calculated for $C_{33}H_{40}OSi$ [M$^+$]: 480.2848, found: 480.2859. **IR (neat)**: 3640.0, 2958.9, 1441.1, 1256.2, 837.8 cm^{-1}.

4-[(4-Bromophenyl)(dimethyl(phenyl)silyl)methyl]-2,6-di-*tert*-butylphenol, 2f

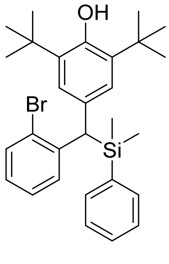


2f

From **1f** (74.4 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2f** was obtained in 75% yield as a yellow oil. **R*f*** = 0.73 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.35-7.31 (m, 5H), 7.27 (d, *J* = 8.4 Hz, 2H), 6.99 (d, *J* = 8.4 Hz, 2H), 6.82 (s, 2H), 4.94 (s, 1H), 3.56 (s, 1H), 1.32 (s, 18H), 0.27 (s, 3H), 0.26 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 151.6, 142.4, 137.6, 135.6, 134.6, 131.9, 131.3, 130.7, 129.3, 127.7, 125.5, 118.8, 45.1, 34.5, 30.5, -3.1, -3.3. **HRMS (EI$^+$)** calculated for $C_{29}H_{37}BrOSi$ [M$^+$]: 508.1797, found: 508.1784.

4-[(2-Bromophenyl)(dimethyl(phenyl)silyl)methyl]-2,6-di-*tert*-butylphenol, 2g

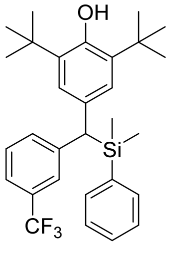


2g

From **1g** (74.7 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2g** was obtained in 77% yield as a pale yellow solid. **R$_f$** = 0.76 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.49 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.33-7.18 (m, 6H), 7.13 (dt, *J* = 7.7, 1.2 Hz, 1H), 6.92 (dt, *J* = 7.7, 1.7 Hz, 1H), 6.83 (s, 2H), 4.89 (s, 1H), 4.31 (s, 1H), 1.28 (s, 18H), 0.28 (s, 3H), 0.22 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 151.6, 142.8, 137.8, 135.4, 134.7, 133.2, 131.5, 130.6, 129.2, 127.7, 127.1, 126.7, 126.2, 125.8, 43.2, 34.4, 30.4, -2.5, -3.6. **HRMS (EI$^+$)** calculated for $C_{29}H_{37}BrOSi$ [M$^+$]: 508.1797, found: 508.1812. **mp** = 126-128 °C.

2,6-di-*tert*-Butyl-4-[(dimethyl(phenyl)silyl)(3-(trifluoromethyl)phenyl)methyl]phenol, 2h

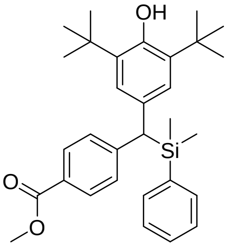


2h

From **1h** (72.5 mg, 0.2 mmol, 1.0 equiv), following the general procedure describe above, compound **2h** was obtained in 70% yield as a yellow oil. **R$_f$** = 0.50 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.40-7.30 (m, 6H), 7.28 (s, 1H), 7.24-7.19 (m, 2H), 6.86 (s, 2H), 4.99 (s, 1H), 3.67 (s, 1H), 1.34 (s, 18H), 0.27 (s, 3H), 0.26 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 151.8, 144.2, 137.2, 135.8, 134.6, 132.2, 132.1, 131.5, 130.4 (q, $J_{C\text{-}F}$ = 31.5 Hz), 129.4, 128.6, 127.8, 125.6 (q, $J_{C\text{-}F}$ = 3.8 Hz), 124.5 (q, *J* = 267.8 Hz), 121.9 (q, $J_{C\text{-}F}$ = 3.8 Hz), 45.8, 34.5, 30.5, -3.3, -3.4. **^{19}F NMR** (282 MHz, $CDCl_3$): δ -62.7. **HRMS (EI$^+$)** calculated for $C_{30}H_{37}F_3OSi$ [M$^+$]: 498.2566, found: 498.2543. **IR (neat)**: 3644.9, 2958.9, 1441.1, 1334.1, 1124.9, 837.8, 706.5 cm^{-1}.

Methyl 4-[(3,5-di-*tert*-butyl-4-hydroxyphenyl)(dimethyl(phenyl)silyl)methyl]benzoate, 2i

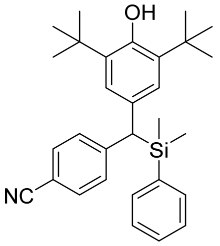


2i

From **1i** (50.5 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2i** was obtained in 70% yield as a yellow oil. **R$_f$** = 0.80 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.85 (d, *J* = 8.4 Hz, 2H), 7.35-7.19 (m, 5H), 7.15 (d, *J* = 8.2 Hz, 2H), 6.84 (s, 2H), 4.93 (s, 1H), 3.85 (s, 3H), 3.68 (s, 1H), 1.31 (s, 18H), 0.21 (s, 3H), 0.20 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 156.0, 151.5, 143.2, 138.1, 135.4, 134.6, 132.4, 130.5, 129.0, 128.3, 127.6, 125.6, 125.1, 45.7, 34.4, 30.5, 29.7, -2.9, -3.5. **HRMS (EI$^+$)** calculated for $C_{31}H_{40}O_3Si$ [M$^+$]: 488.2747, found: 488.2734. **IR (neat)**: 3635.1, 2958.9, 1728.1, 1441.1, 1285.4, 837.8 cm^{-1}.

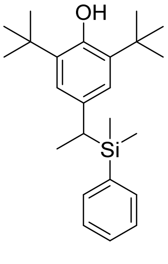
4-[(3,5-di-*tert*-Butyl-4-hydroxyphenyl)(dimethyl(phenyl)silyl)methyl]benzonitrile, 2j


2j

From **1j** (63.9 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2j** was obtained in 48% yield (purification carried out by preparative TLC) as a yellow oil. **R*f*** = 0.41 (92% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.45 (d, *J* = 8.3 Hz, 2H), 7.35-7.17 (m, 5H), 7.14 (d, *J* = 8.4 Hz, 2H), 6.84 (s, 2H), 4.99 (s, 1H), 3.68 (s, 1H), 1.33 (s, 18H), 0.27 (s, 3H), 0.26 (s, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 151.9, 149.4, 136.9, 135.9, 134.5, 132.0, 131.0, 129.5, 129.3, 127.8, 125.8, 119.5, 108.6, 46.5, 34.5, 30.4, -3.1, -3.3. **HRMS (EI$^+$)** calculated for $C_{30}H_{37}NOSi$ [M$^+$]: 455.2644, found: 455.2666**.** **IR (neat)**: 3640.0, 2958.9, 2229.2, 1441.1, 1256.2, 837.8 cm^{-1}.

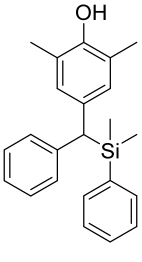
2,6-di-*tert*-Butyl-4-[1-(dimethyl(phenyl)silyl)ethyl]phenol, 2k


2k

From **1k**[12] (46.4 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2l** was obtained in 70% yield as yellow oil. **R*f*** = 0.76 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.31 (s, 5H), 6.66 (s, 2H), 4.90 (s, 1H), 2.29 (q, *J* = 7.4 Hz, 1H), 1.46 (d, *J* = 3.3 Hz, 3H), 1.37 (s, 18H), 0.22 (s, 3H), 0.19 (s, 3H).**^{13}C NMR** (75 MHz, $CDCl_3$): δ 150.9, 138.0, 135.2, 135.0, 134.4, 128.9, 127.6, 123.8, 34.4, 30.5, 29.1, 15.1, -4.7, -4.9. **HRMS (EI$^+$)** calculated for $C_{24}H_{36}OSi$ [M$^+$]: 368.2535, found: 368.2548. **IR (neat)**: 3649.7, 2958.9, 1436.2, 1236.7, 832.9 cm^{-1}.

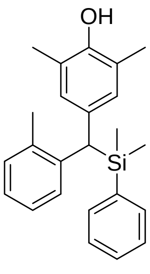
4-[(Dimethyl(phenyl)silyl)(phenyl)methyl]-2,6-dimethylphenol, 2l


2l

From **1l** (42.0 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2l** was obtained in 65% yield as yellow oil. **R*f*** = 0.45 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.30-7.16 (m, 5H), 7.14-7.07 (m, 2H), 7.02-6.98 (m, 3H), 6.64 (s, 2H), 4.29 (s, 1H), 3.50 (s, 1H), 2.06 (s, 6H), 0.20 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 150.0, 143.1, 138.0, 134.6, 133.9, 129.5, 129.2, 128.8, 128.2, 127.6, 125.1, 122.7, 44.7, 16.1, -2.9, -3.1. **HRMS (EI$^+$)** calculated for $C_{23}H_{26}OSi$ [M$^+$]: 346.1753, found: 346.1754. **IR (neat)**: 3576.8, 2958.9, 1489.7, 1256.2, 832.9 cm^{-1}.

4-[(Dimethyl(phenyl)silyl)(*o*-tolyl)methyl]-2,6-dimethylphenol, 2m


2m

From **1m** (44.0 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2m** was obtained in 60% yield as a yellow oil. **R*f*** = 0.40 (90% hexanes/EtOAc).

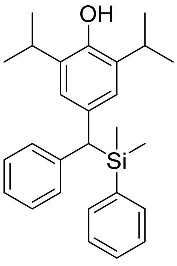
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.36-7.19 (m, 5H), 7.09-6.97 (m, 4H), 6.59 (s, 2H), 4.35 (s, 1H), 3.75 (s, 1H), 2.15 (s, 3H), 2.08 (s, 6H), 0.29 (s, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 149.9, 141.5, 138.5, 136.8, 134.7, 133.7, 130.8, 129.8, 129.3,

---

[12] Bacha, J. D.; Matthews, J. S. *US 4032547*, **1977.**

129.2, 127.6, 125.8, 125.5, 122.7, 39.7, 20.6, 16.2, -2.4, -3.0. **HRMS (EI$^+$)** calculated for C24H_{28}OSi [M$^+$]: 360.1909, found: 360.1907. **IR (neat)**: 3576.8, 2949.2, 1436.2, 1202.7, 829.1 cm^{-1}.

4-[(Dimethyl(phenyl)silyl)(phenyl)methyl]-2,6-diisopropylphenol, 2n

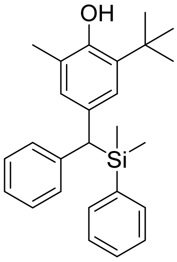


2n

From **1n** (53.3 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2n** was obtained in 86% yield as an orange oil. **R*f*** = 0.69 (80% hexanes/EtOAc).

^{1}H NMR (300 MHz, CDCl$_3$): δ 7.36-7.23 (m, 5H), 7.23-7.05 (m, 5H), 6.77 (s, 2H), 4.55 (s, 1H), 3.65 (s, 1H), 2.98-2.82 (m, 2H), 1.20-1.10 (m, 12H), 0.27 (s, 3H), 0.24 (s, 3H). **^{13}C NMR** (75 MHz, CDCl$_3$): δ 147.6, 143.1, 138.1, 134.6, 133.9, 133.4, 129.1, 128.8, 128.2, 127.6, 125.0, 124.3, 45.4, 27.3, 22.9, 22.8, -3.0, -3.1. **HRMS (EI$^+$)** calculated for $C_{27}H_{34}$OSi [M$^+$]: 402.2379, found: 402.2365. **IR (neat)**: 3562.2, 2963.8, 1475.1, 1256.2, 832.9 cm^{-1}.

2-(*tert*-Butyl)-4-[(dimethyl(phenyl)silyl)(phenyl)methyl]-6-methylphenol, 2o

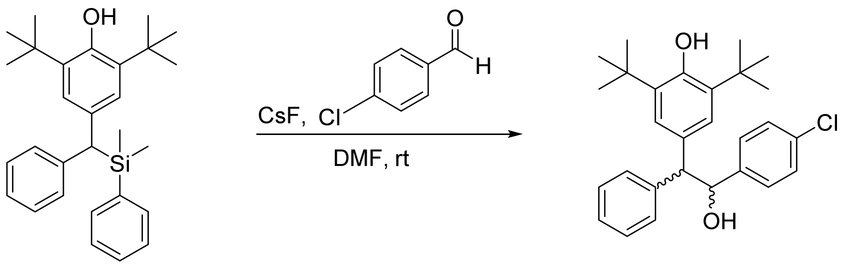


2o

From **1o** (50.5 mg, 0.2 mmol, 1.0 equiv), following the general procedure described above, compound **2o** was obtained in 86% yield as a yellow oil. **R*f*** = 0.60 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, CDCl$_3$): δ 7.26-7.24 (m, 5H), 7.21-7.14 (m, 2H), 7.09 (d, *J* = 7.3 Hz, 3H), 6.82 (s, 1H), 6.72 (s, 1H), 4.50 (s, 1H), 3.59 (s, 1H), 2.11 (s, 3H), 1.27 (s, 9H), 0.26 (s, 3H), 0.24 (s, 3H). **^{13}C NMR** (75 MHz, CDCl$_3$): δ 150.4, 143.2, 138.1, 135.1, 134.6, 133.3, 129.1, 129.0, 128.9, 128.3, 127.6, 126.1, 125.1, 122.8, 45.1, 34.6, 29.9, 16.2, -3.0, -3.1. **HRMS (EI$^+$)** calculated for $C_{26}H_{31}$OSi [M$^+$]: 387.2144, found: 387.2157. **IR (neat)**: 3576.8, 2954.1, 1484.9, 1256.1, 832.9 cm^{-1}.

4. Synthesis of 2,6-di-*tert*-butyl-4-(2-(4-chlorophenyl)-2-hydroxy-1-phenylethyl)phenol, 3[13]



1a **3** (dr = 1:1)

An oven-dried vial was charged with **1a** (43.0 mg, 0.1 mmol, 1.0 equiv), CsF (30.4 mg, 0.2 mmol, 2.0 equiv) and the 4-chlorobenzaldehyde (56.2 mg, 0.2 mmol, 2.0 equiv) and sealed with a septum. The vial was connected to an argon-vacuum line, evacuated and backfilled with argon (x3). Dry DMF (0.3 mL) was added and the mixture was stirred at room temperature

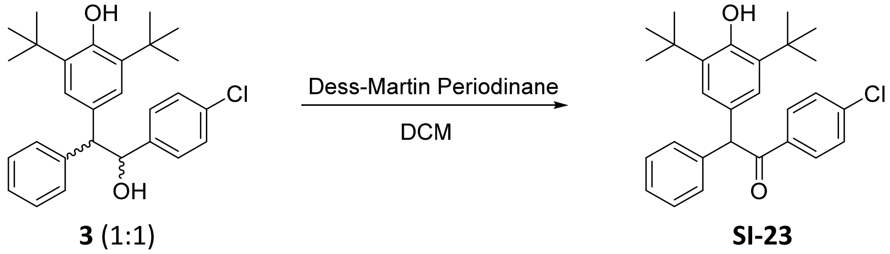
---

[13] Huang, C.; Ghavtadze, N.; Godoi, B.; Gevorgyan, V. *Chem. Eur. J.* **2012**, *18*, 9789.

until starting material dissaperance (by TLC). EtOAc was added and the mixture was filtered through a short pad of silica gel and concentrated. The crude product was purified by flash column chromatography (90% hexanes/EtOAc). Compound **3** was obtained in 60% yield as a 1:1 mixture of diastereomers (white solid). **R*f*** = 0.40 (90% hexanes/EtOAc).

Diastereomer A: **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.36-7.19 (m, 5H), 7.09-6.97 (m, 4H), 6.59 (s, 2H), 5.28 (dd, *J* = 8.6, 1.9 Hz, 1H), 5.13 (s, 1H), 4.05 (d, *J* = 3.0 Hz, 1H), 2.18 (d, *J* = 2.5 Hz, 1H), 1.42 (s, 18H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 153.4, 142.0, 141.2, 136.6, 133.3, 130.7, 129.2, 128.7, 128.6, 128.4, 127.3, 125.7, 77.6, 61.3, 34.8, 30.6. **Diastereomer B:** **^{1}H NMR** (300 MHz, $CDCl_3$): δ 7.36-7.19 (m, 5H), 7.09-6.97 (m, 4H), 6.59 (s, 2H), 5.22 (dd, *J* = 8.8, 1.3 Hz, 1H), 4.98 (s, 1H), 4.02 (d, *J* = 3.1 Hz, 1H), 2.12 (d, *J* = 2.2, 1H), 1.29 (s, 18H). **^{13}C NMR** (75 MHz, $CDCl_3$): 152.6, 141.4, 141.1, 135.8, 131.5, 129.3, 128.8, 128.7, 128.6, 128.2, 126.8, 125.6, 76.8, 61.2, 34.6, 30.5. **HRMS (ESI$^+$)** calculated for $C_{28}H_{33}ClO_2$ [M+Na]: 459.2061, found: 459.2058. **IR (neat)**: 3640.0, 3387.0, 2915.1, 1441.1, 1241.6 cm^{-1}.

5. Synthesis of 1-(4-chlorophenyl)-2-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-2-phenylethanone, SI-23[14]



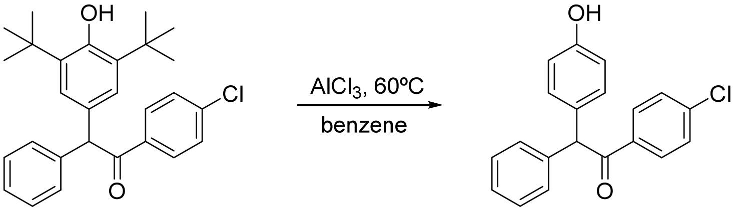
Dess-Martin periodinane (32.3 mg, 0.08 mmol, 1.2 equiv) was added to a solution of **3** (27.7 mg, 0.06 mmol, 1.0 equiv.) in DCM (1.5 mL). The reaction mixture was stirred at room temperature for 30 min and then quenched by addition of saturated aqueous Na_2CO_3. The layers were separated. The aqueous phase was extracted with EtOAc (x3) and the combined organic layers were washed with saturated NaCl solution, dried over Na_2SO_4, filtered and concentrated. The crude product was purified by flash column chromatography (90% hexanes/AcOEt). Compound **SI-23** was obtained in 89% yield as a white solid. **R*f*** = 0.42 (90% hexanes/EtOAc).

^{1}H NMR (300 MHz, $CDCl_3$): δ 7.93 (d, *J* = 8.6 Hz, 2H), 7.37 (d, *J* = 8.6 Hz, 2H), 7.33-7.19 (m, 5H), 7.04 (s, 2H), 5.86 (s, 1H), 5.14 (s, 1H), 1.38 (s, 18H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 197.6, 152.3, 139.4, 139.2, 136.0, 135.5, 130.3, 129.1, 129.0, 128.9, 128.7, 127.1, 125.8, 59.4, 34.4, 30.3. **HRMS (ESI$^+$)** calculated for $C_{28}H_{31}ClO_2$ [M+Na]: 457.1904, found: 457.1897. **mp** = 132-134 °C. **IR (neat)**: 3440.5, 2915.1, 1606.5, 1441.1, 1389.6 cm^{-1}.

---

[14] Wright, N. E; Snyder, S. *Angew. Chem. Int. Ed.* **2014**, *53*, 3409.

6. Synthesis of 1-(4-chlorophenyl)-2-(4-hydroxyphenyl)-2-phenylethanone, 4[3]



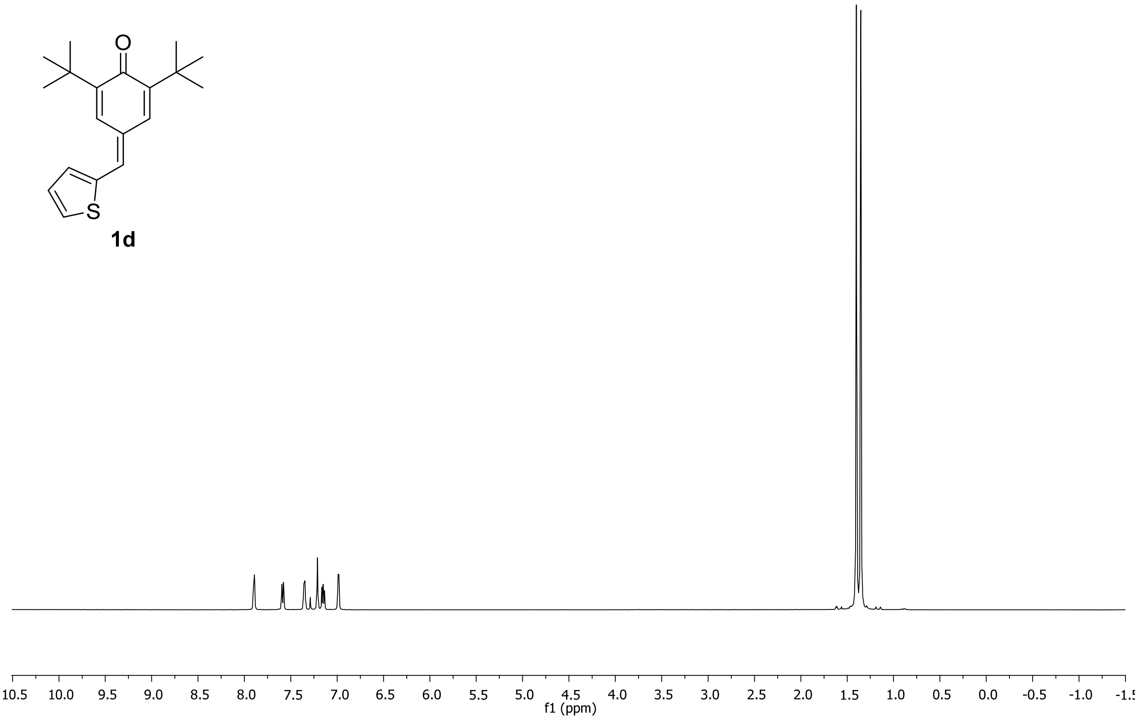
SI-23

4

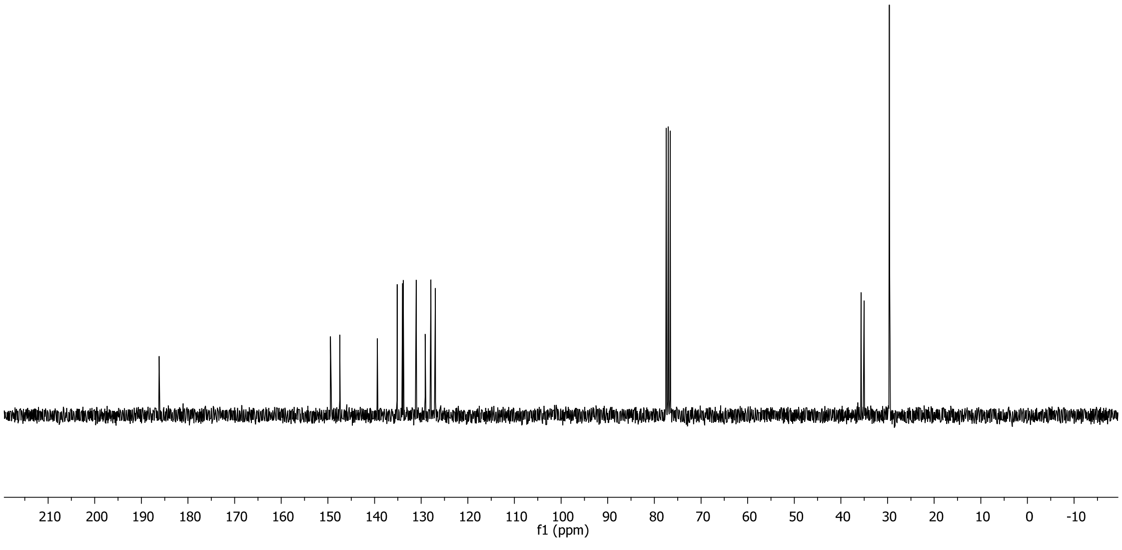
An oven-dried vial was charged with **SI-23** (24.5 mg, 0.06 mmol, 1 equiv.) and $AlCl_3$ (45.1 mg, 0.3 mmol, 6.0 equiv.) and sealed with a septum. The vial was connected to an argon-vacuum line, evacuated and backfilled with argon (x3). Benzene (2.6 mLo **SI-23**) was added and the reaction mixture was heated to 60 °C for 1 hour. EtOAc and water were added and the layers were separated. The aqueous phase was extracted with EtOAc (x3) and the combined organic layers were washed with saturated NaCl solution, dried over Na_2SO_4, filtered and concentrated. The crude product was purified by flash column chromatography (20-100 % EtOAc/hexanes). Compound **4** was obtained in 54% yield as a white solid. **R*f*** = 0.30 (80% hexanes/EtOAc).

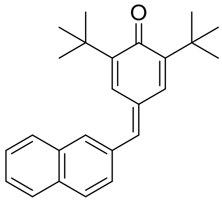
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.86 (d, *J* = 8.6 Hz, 2H), 7.31 (d, *J* = 8.6 Hz, 2H), 7.2-7.13 (m, 5H), 7.04 (d, *J* = 8.5 Hz, 2H), 6.71 (d, *J* = 6.9, 2H), 5.84 (s, 1H), 4.85 (s, 1H). **^{13}C NMR** (75 MHz, $CDCl_3$): δ 197.7, 155.0, 139.7, 139.2, 135.3, 131.1, 130.6, 130.5, 129.2, 129.1, 129.0, 127.4, 115.9, 58.9. **HRMS (EI$^+$)** calculated for $C_{20}H_{15}ClO_2$ [M+Na]: 345.0652, found: 345.0654. **mp** = 152-153 °C. **IR (neat)**: 3416.2, 2924.9, 1684.3, 1441.1, 1212.4 cm^{-1}.

7. NMR spectra

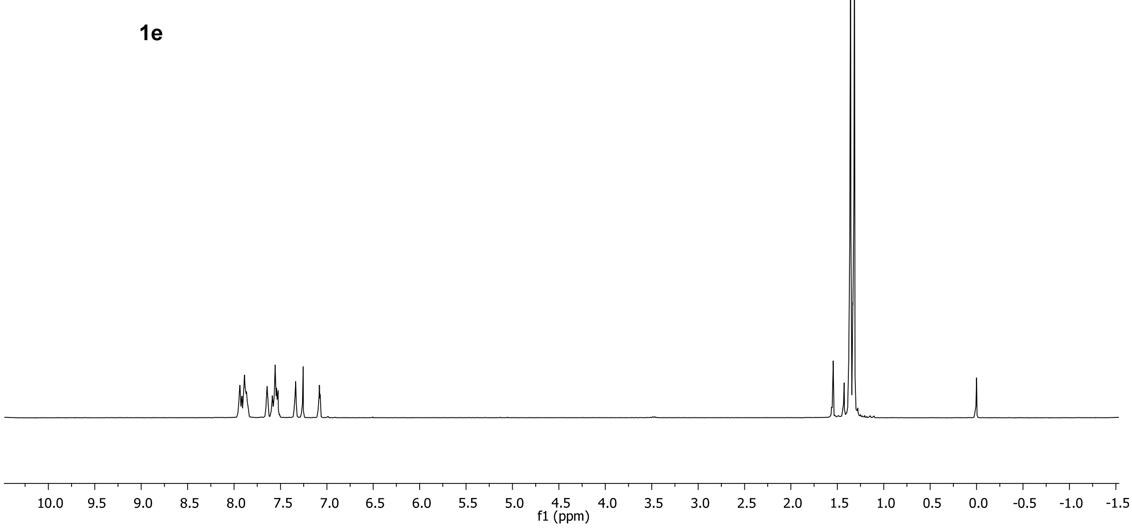


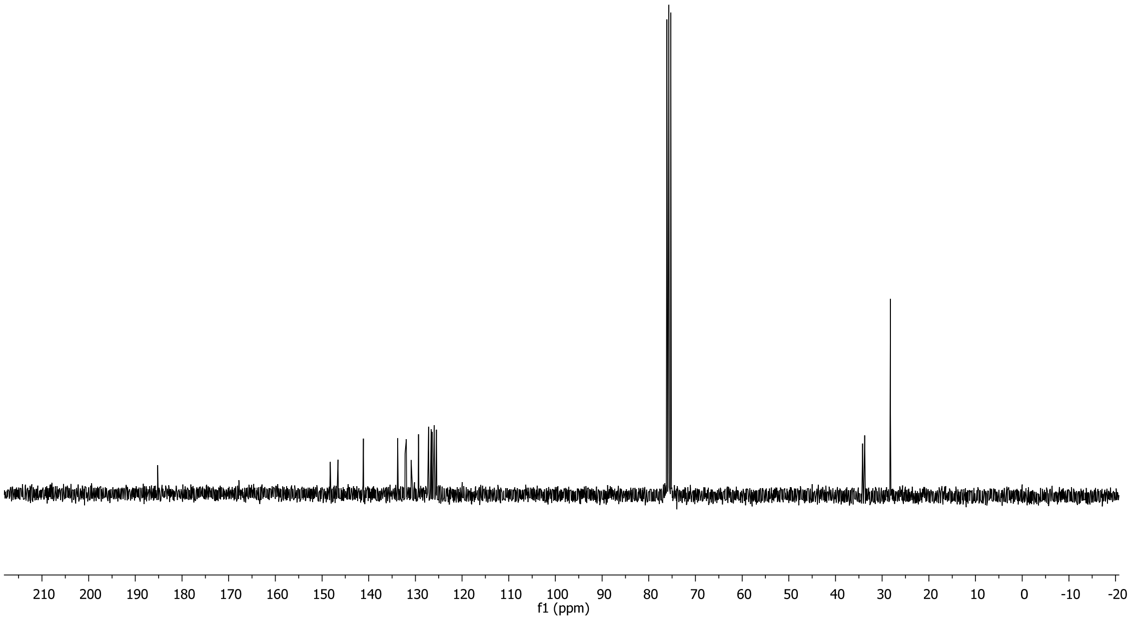
1d

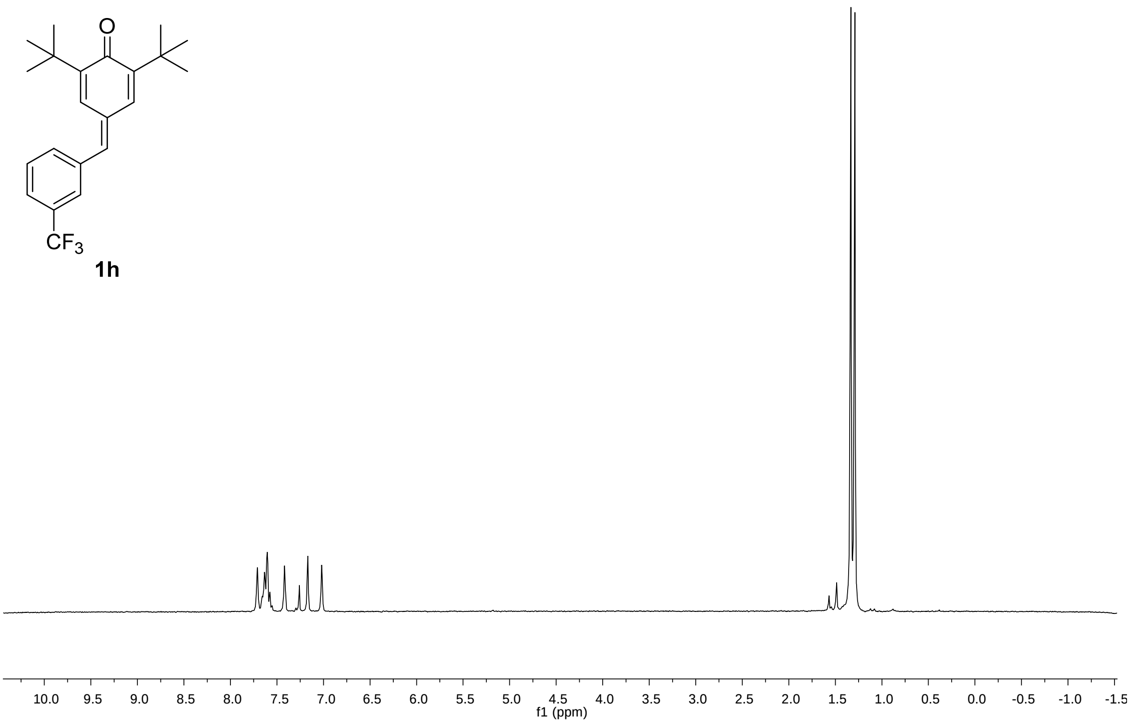




1e

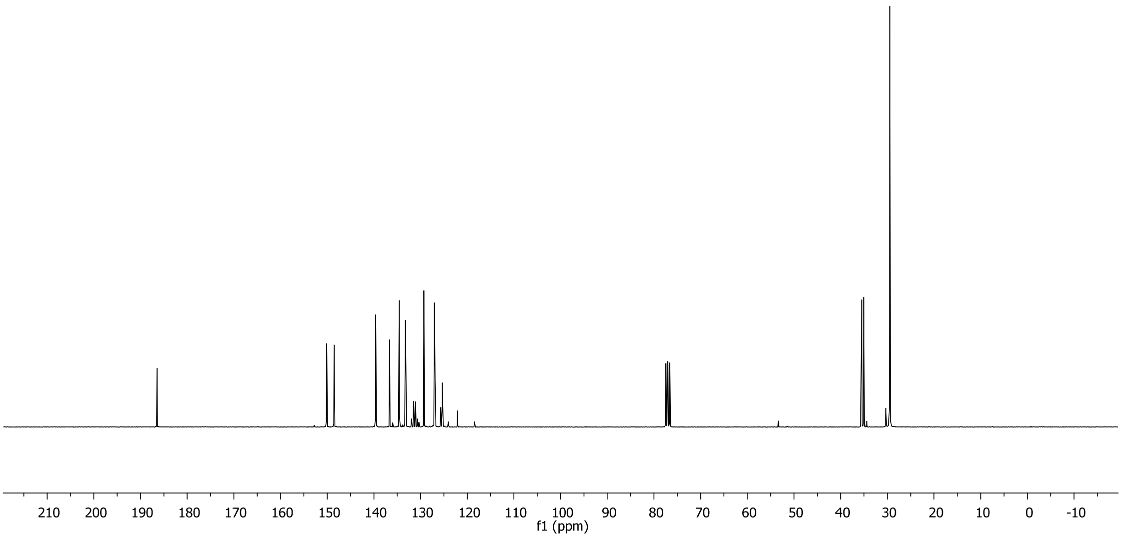

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)


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

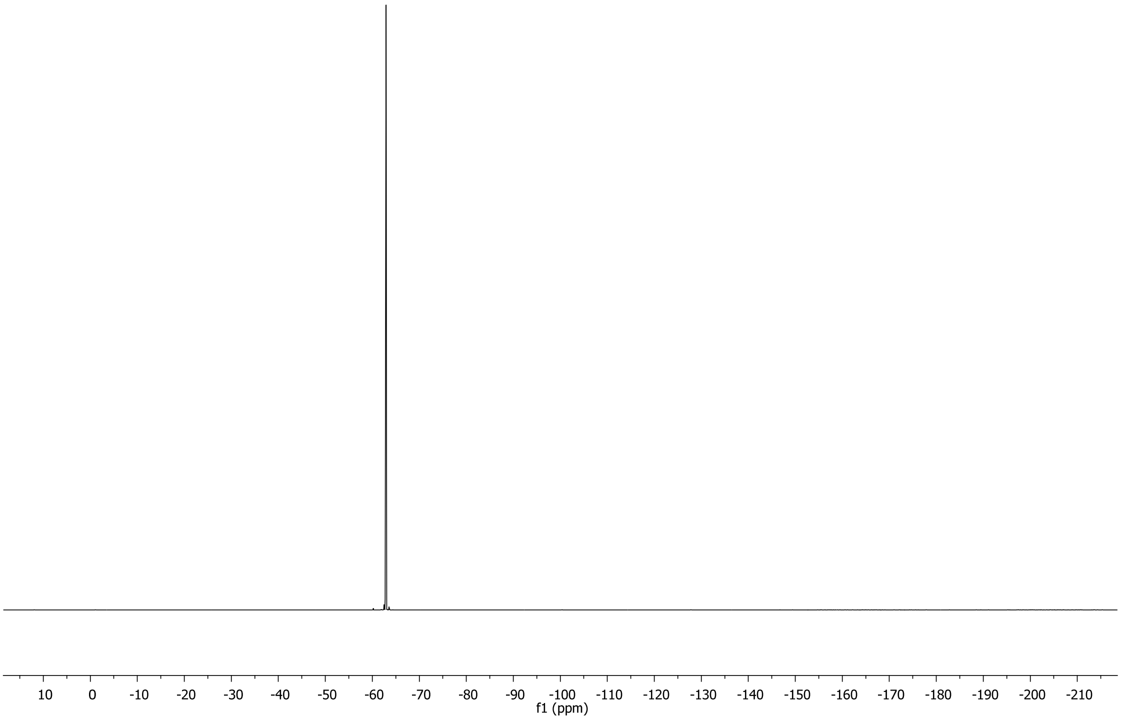


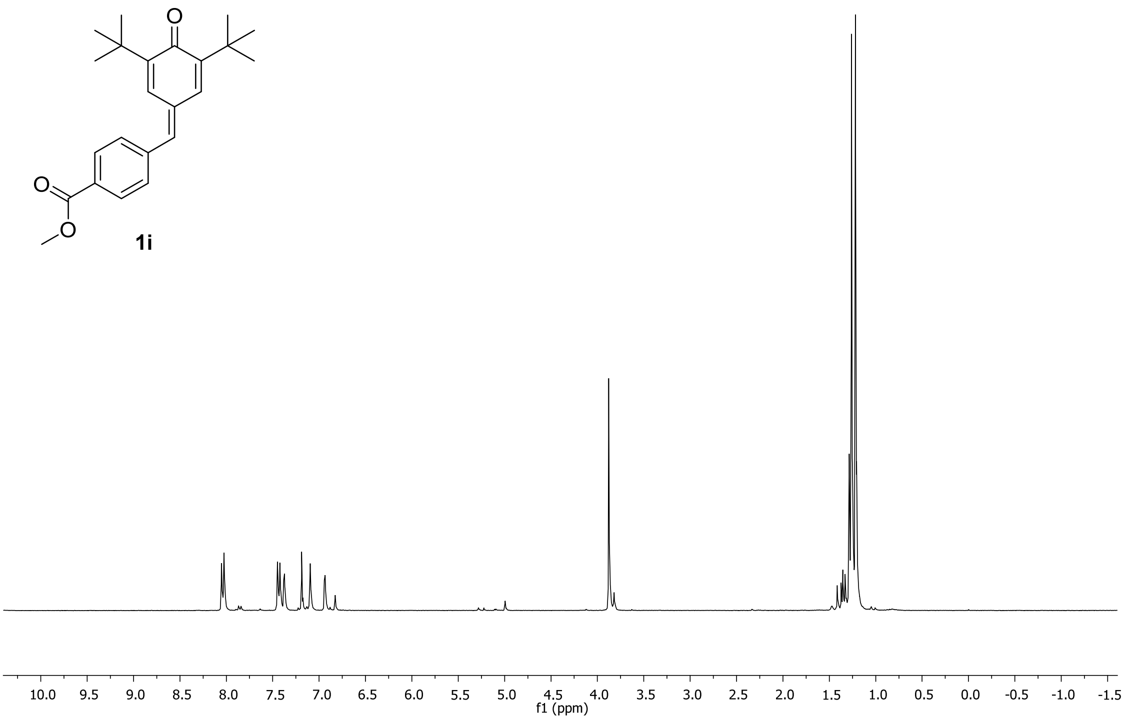
1h

O
CF3
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)



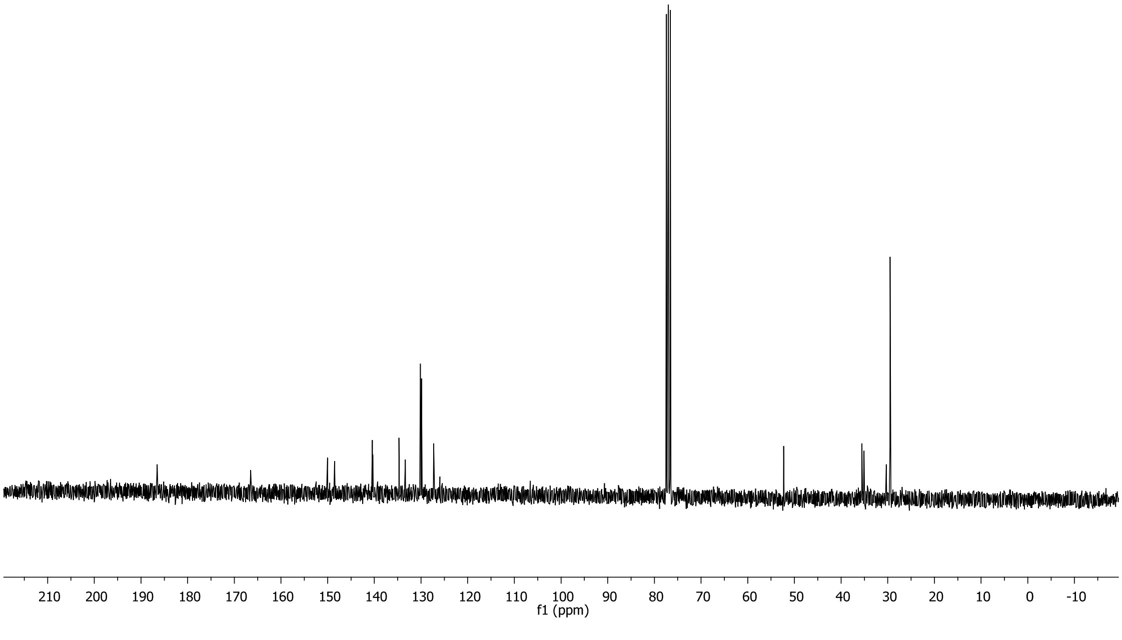
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


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

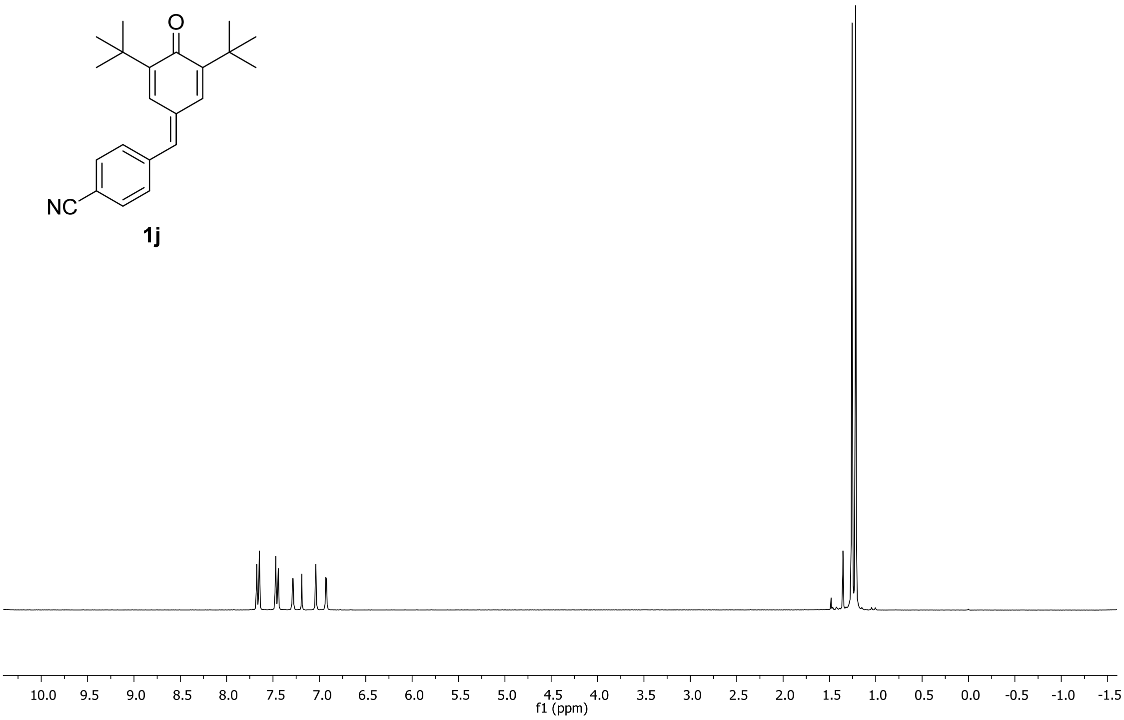


1i

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

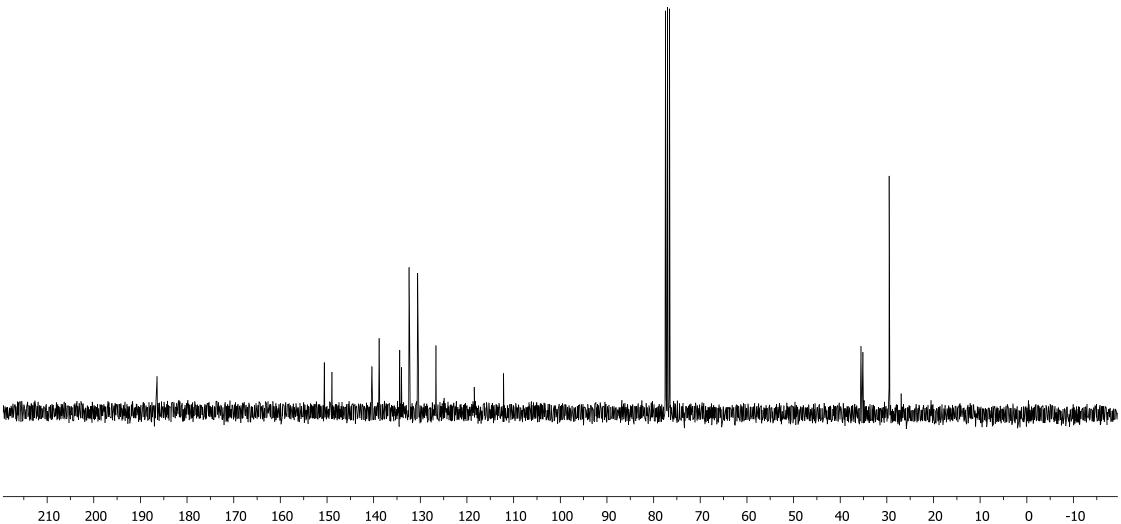


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

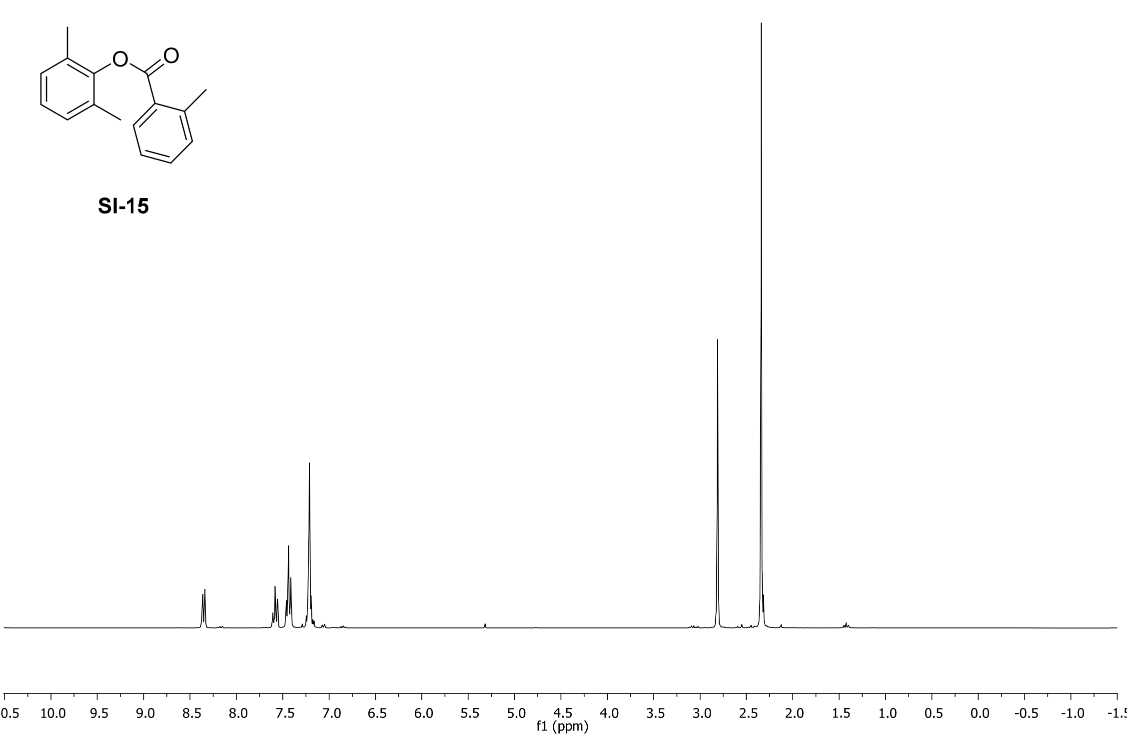


1j

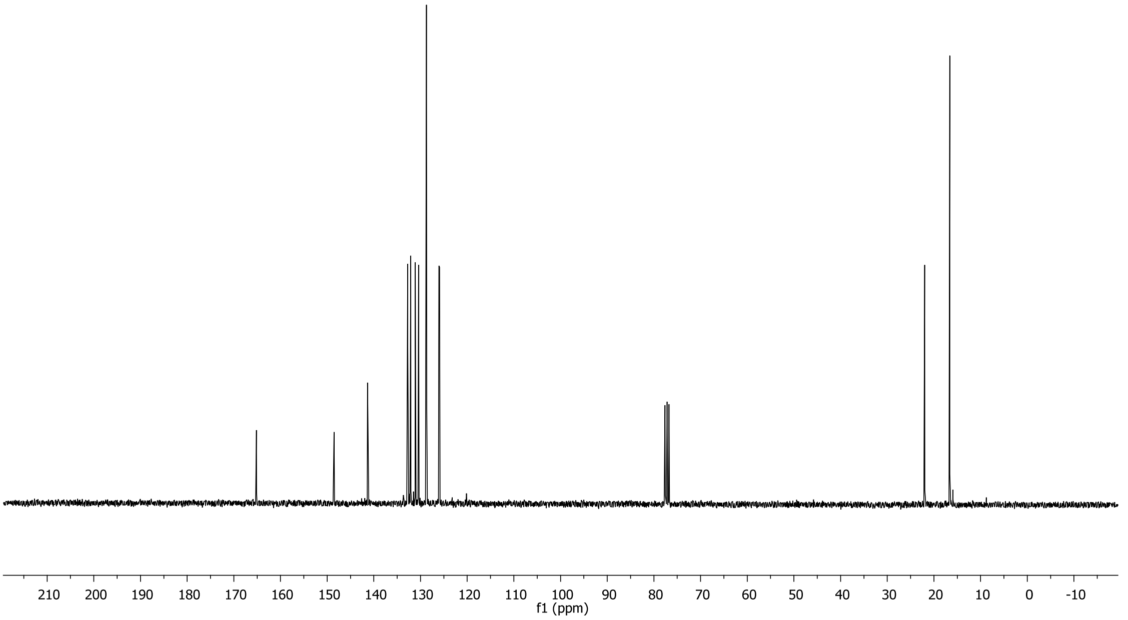
O
NC
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

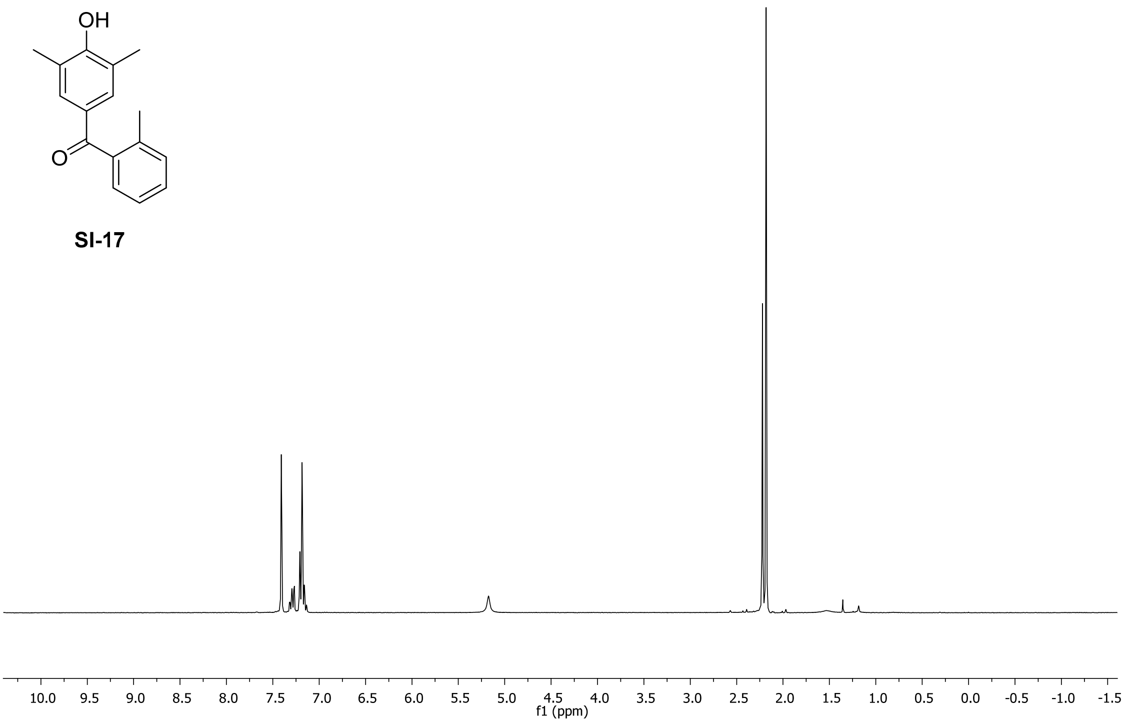


210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.!
f1 (ppm)

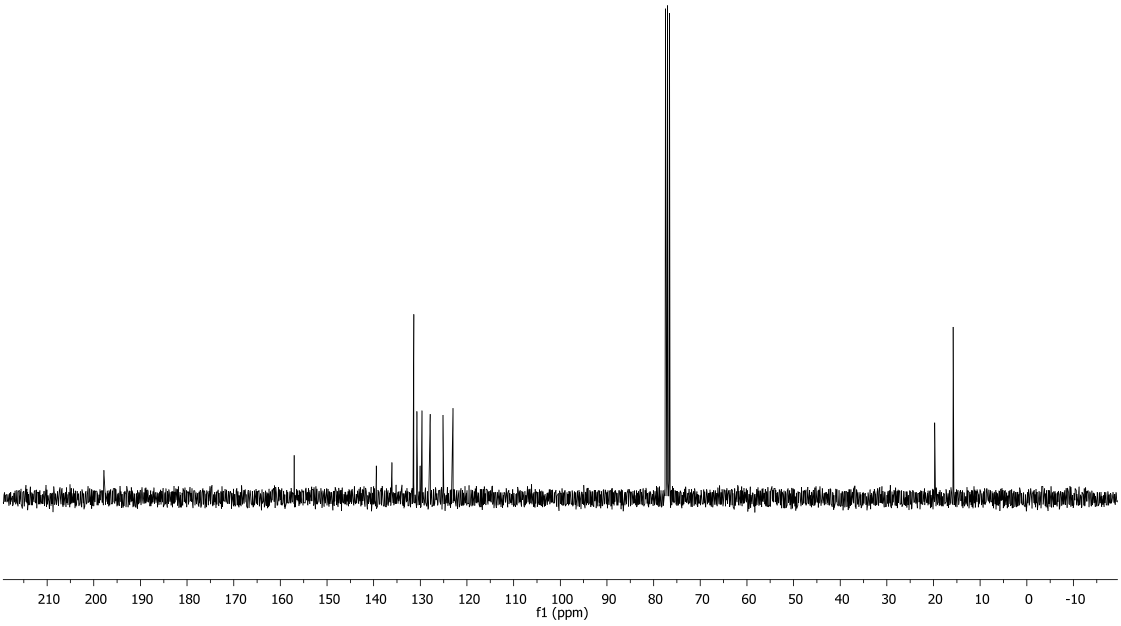
SI-15


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

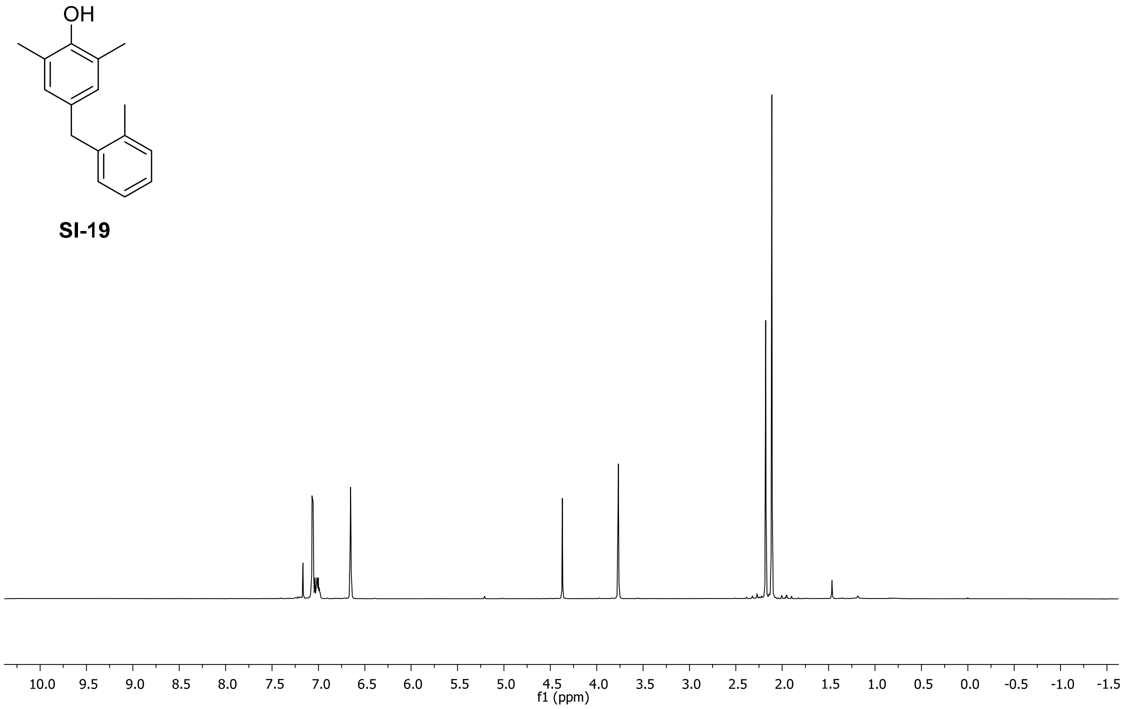


SI-17

OH
O
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

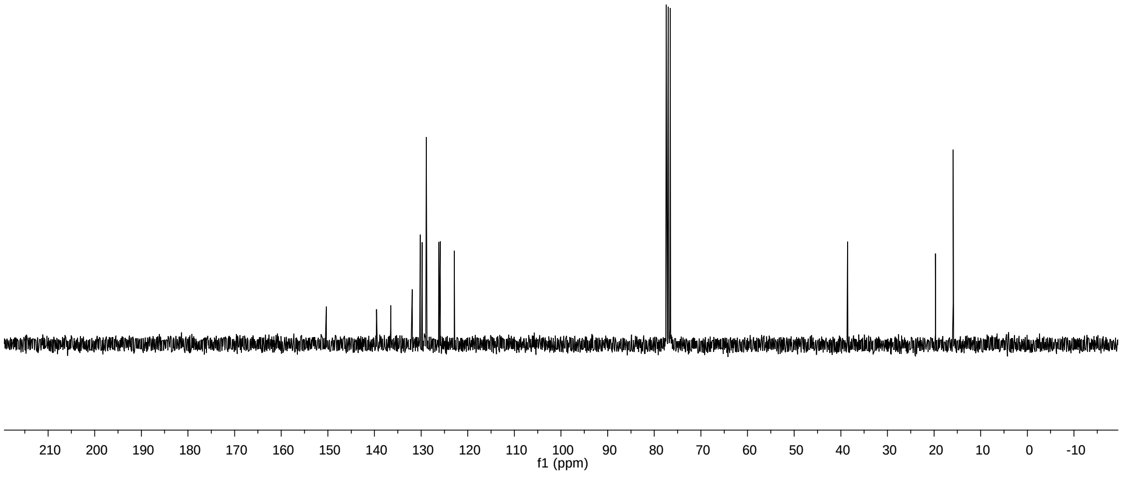


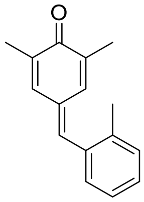
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OH

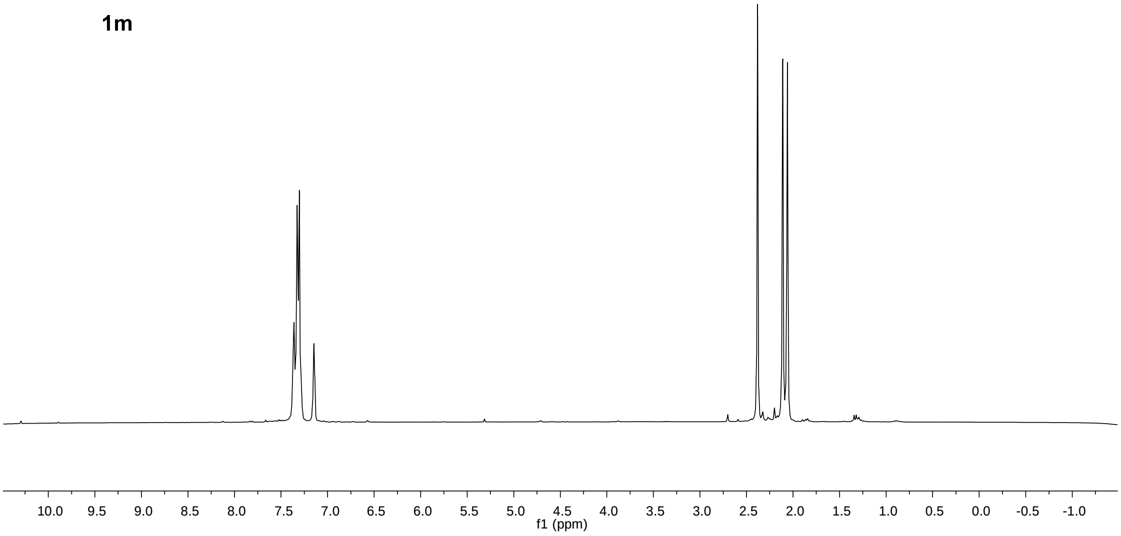
SI-19

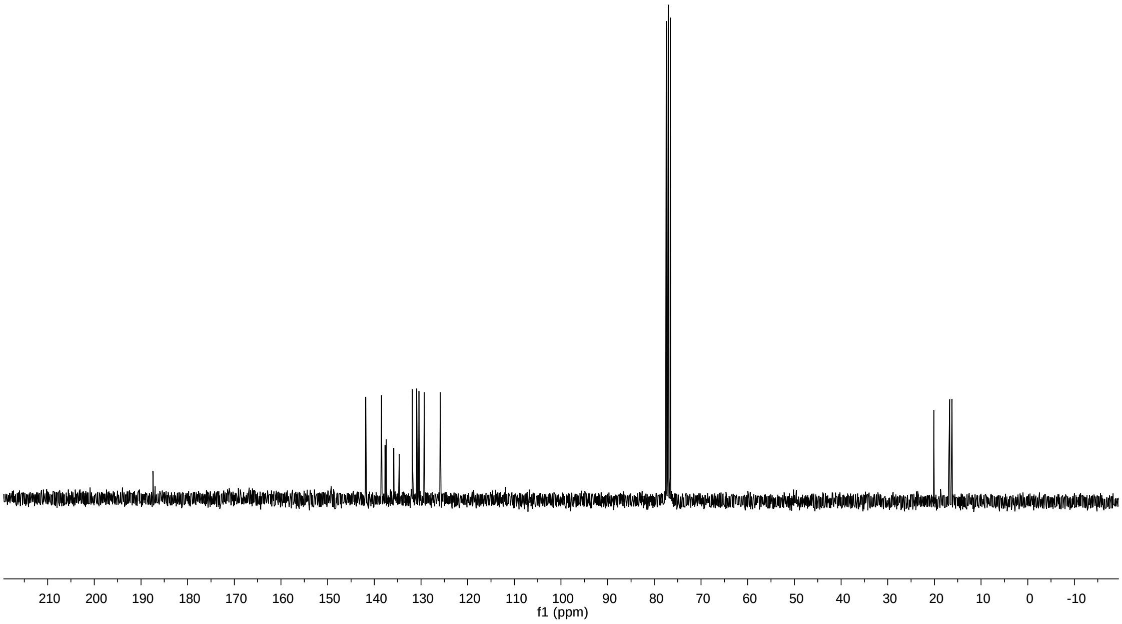
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

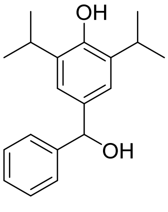

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



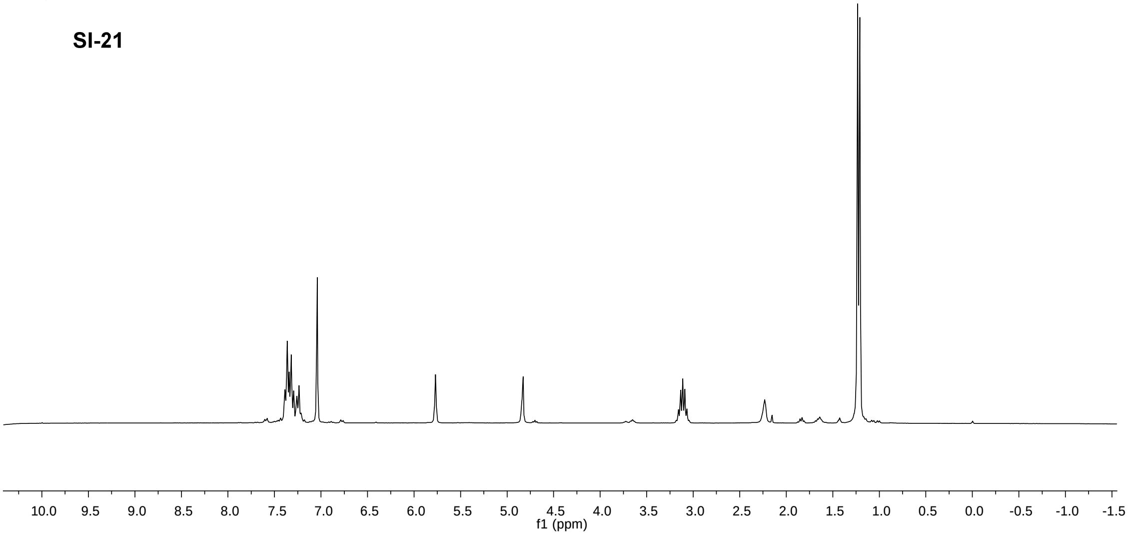
1m

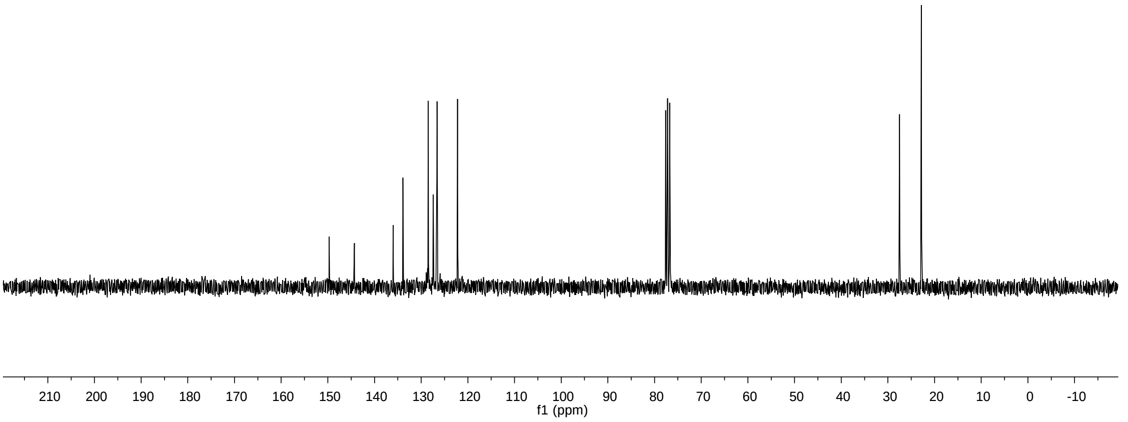

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

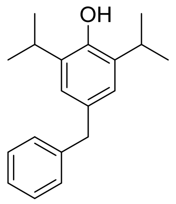

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OH
OH

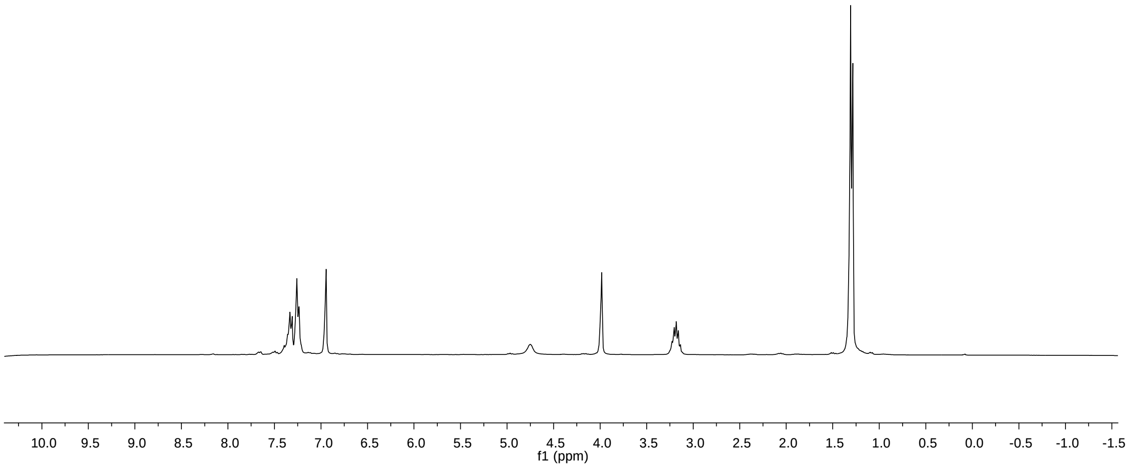
SI-21

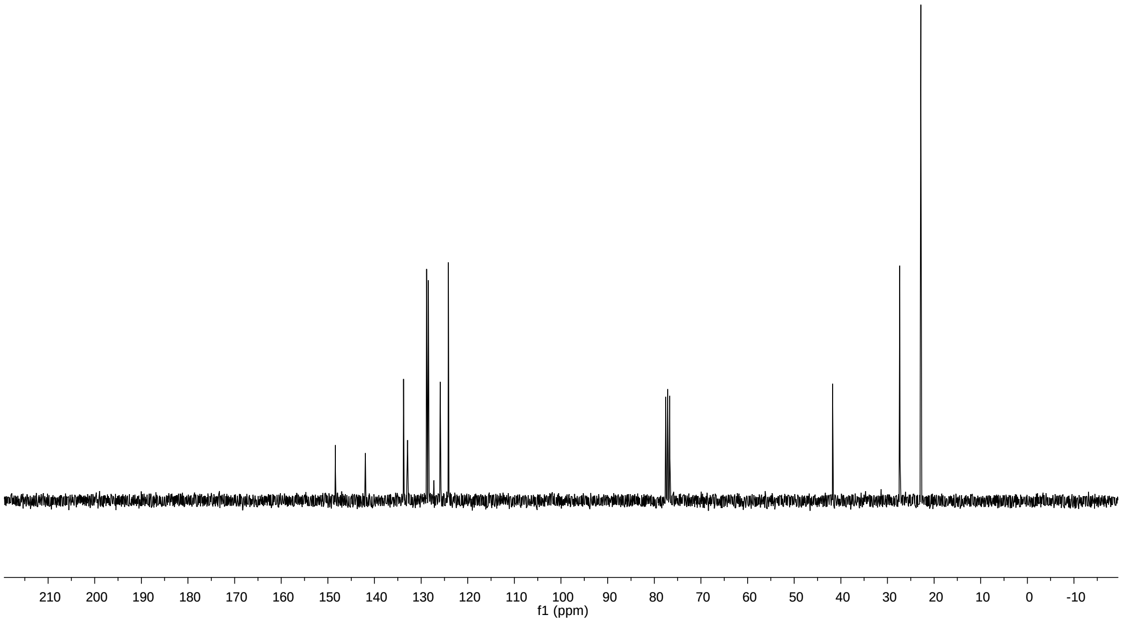

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

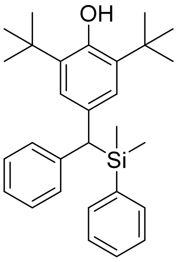

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OH

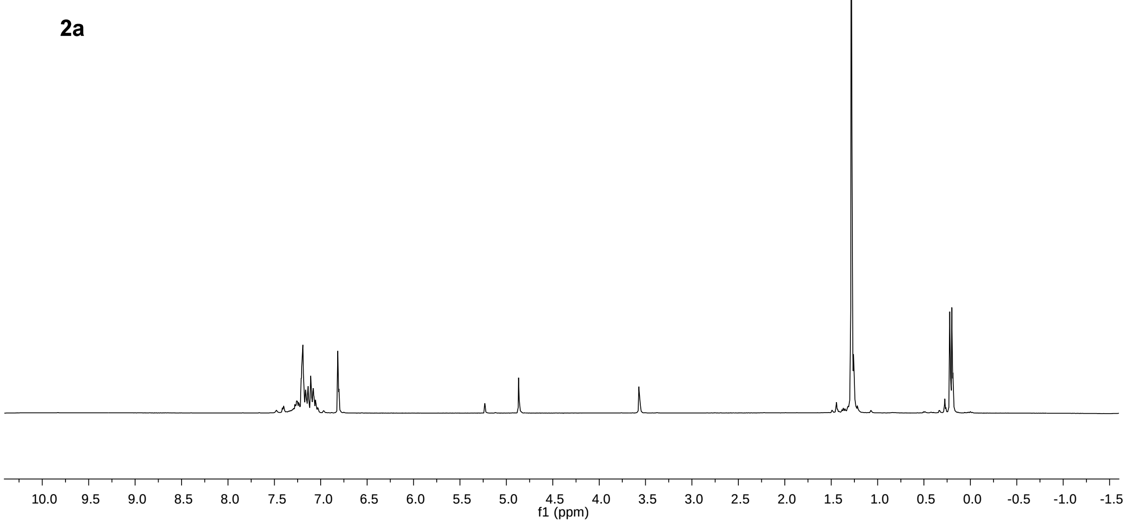
SI-22

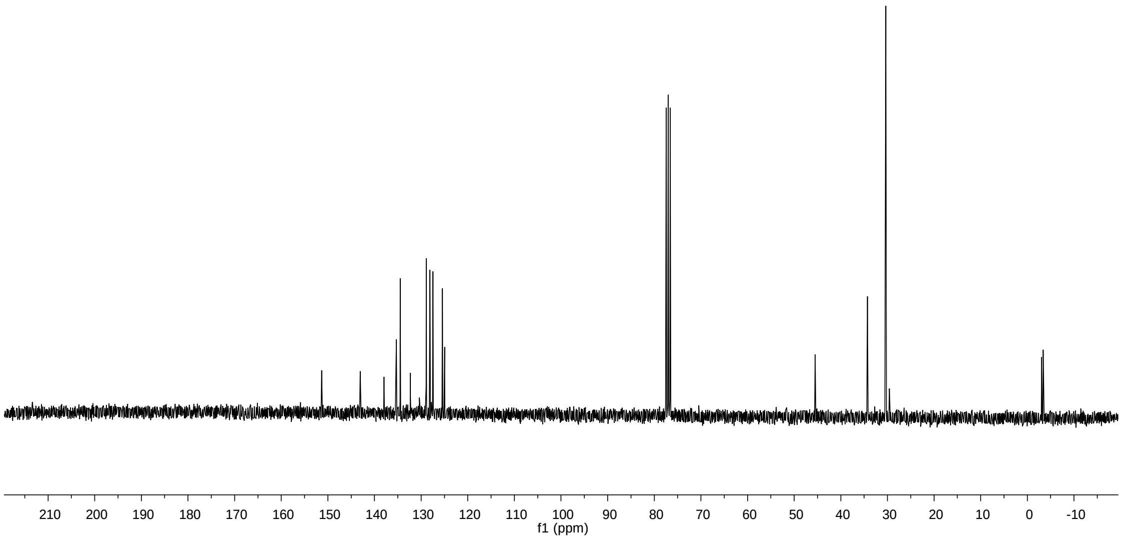

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

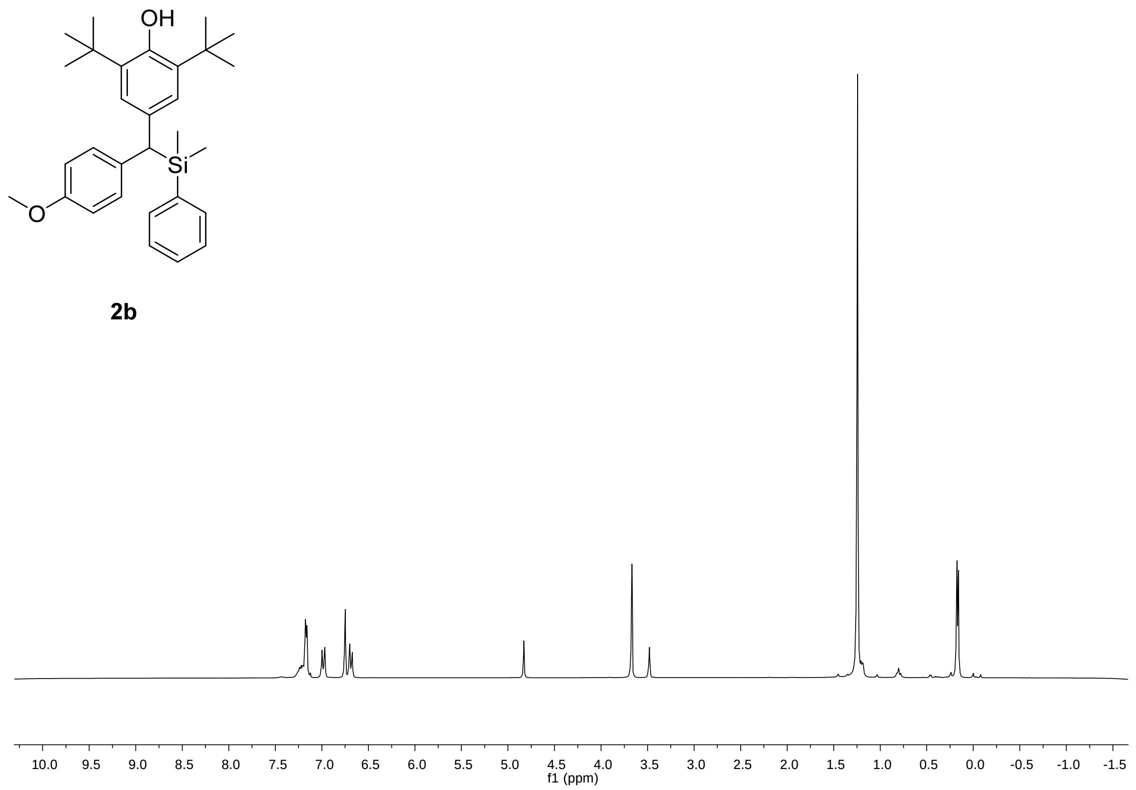

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OH
Si

2a

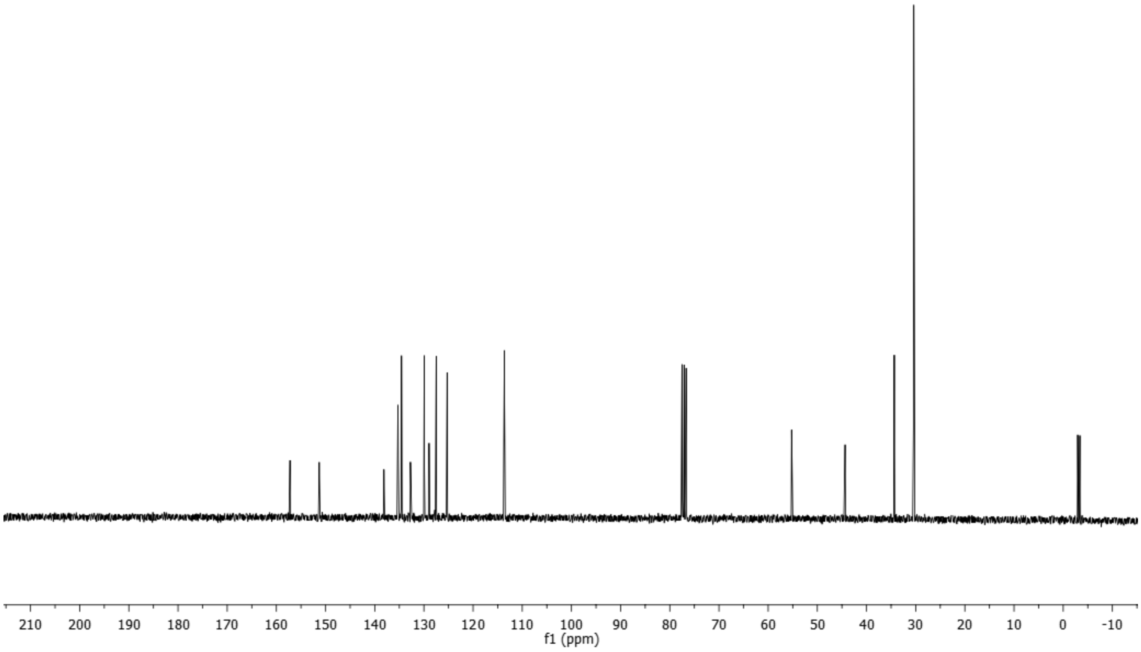

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


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

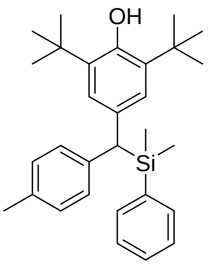


2b

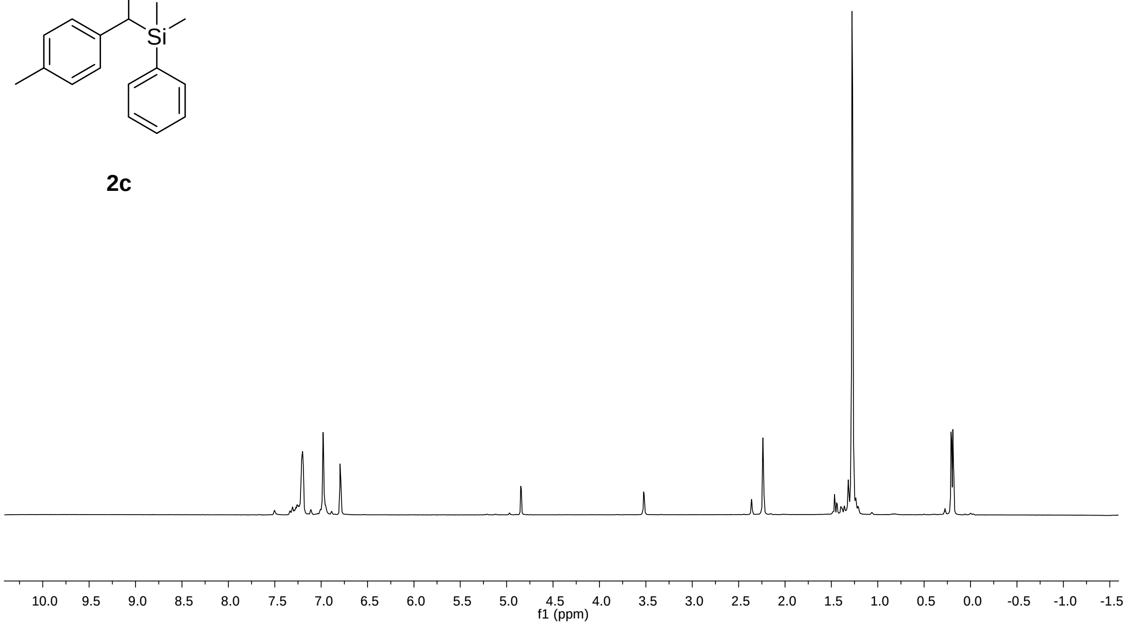
OH
Si
O
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

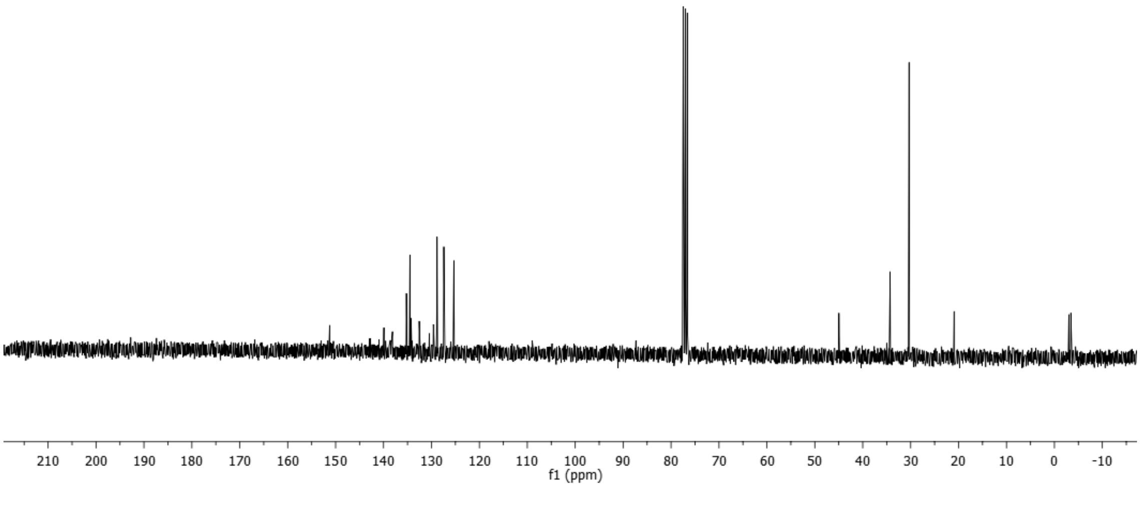


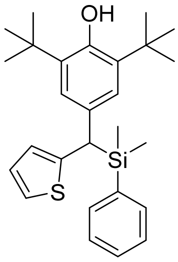
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OH
Si

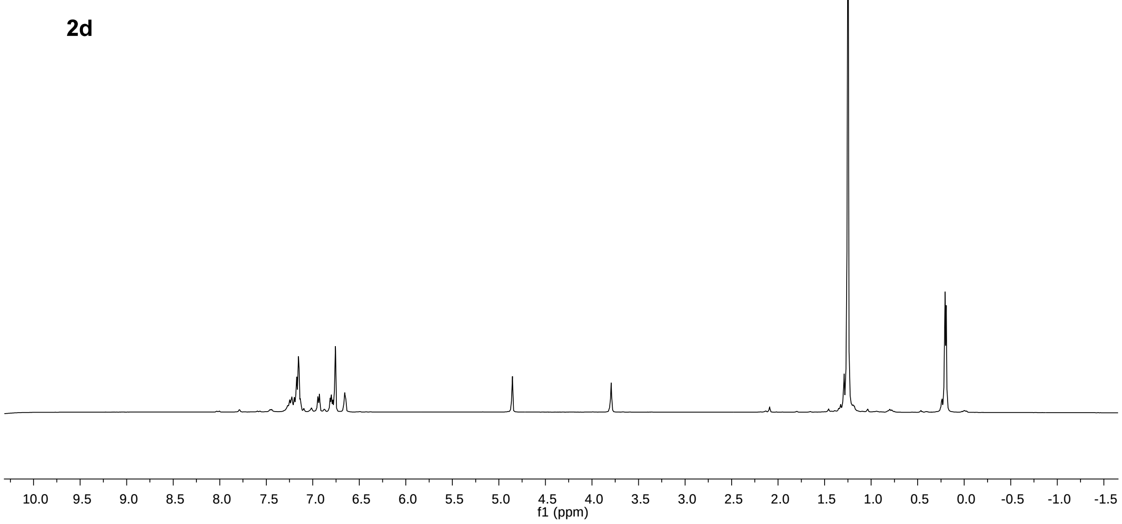
2c

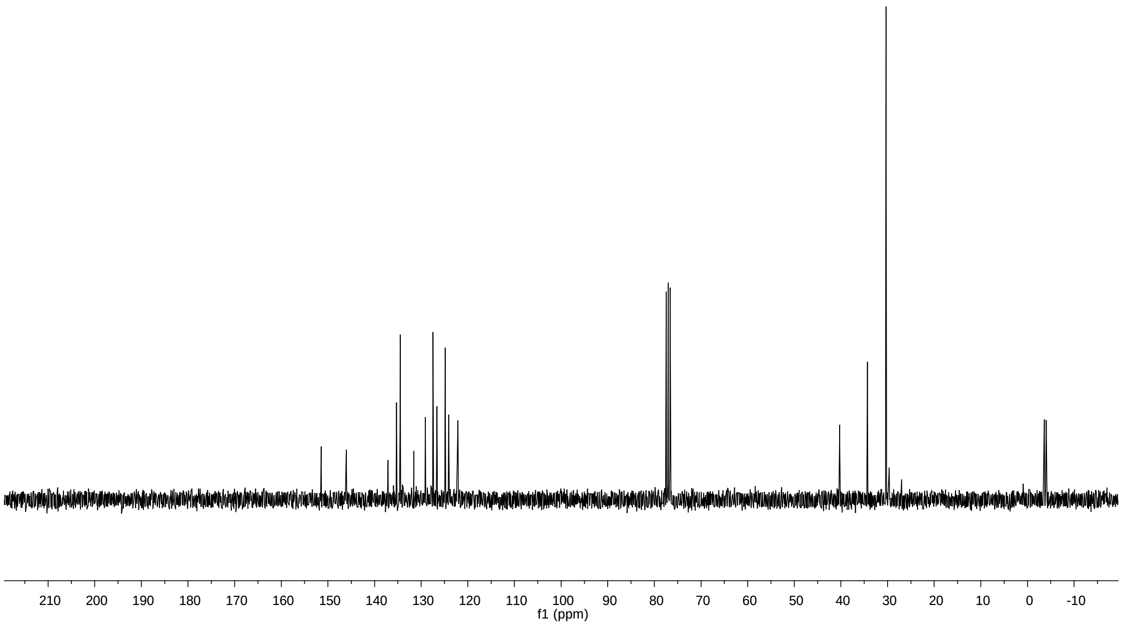

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

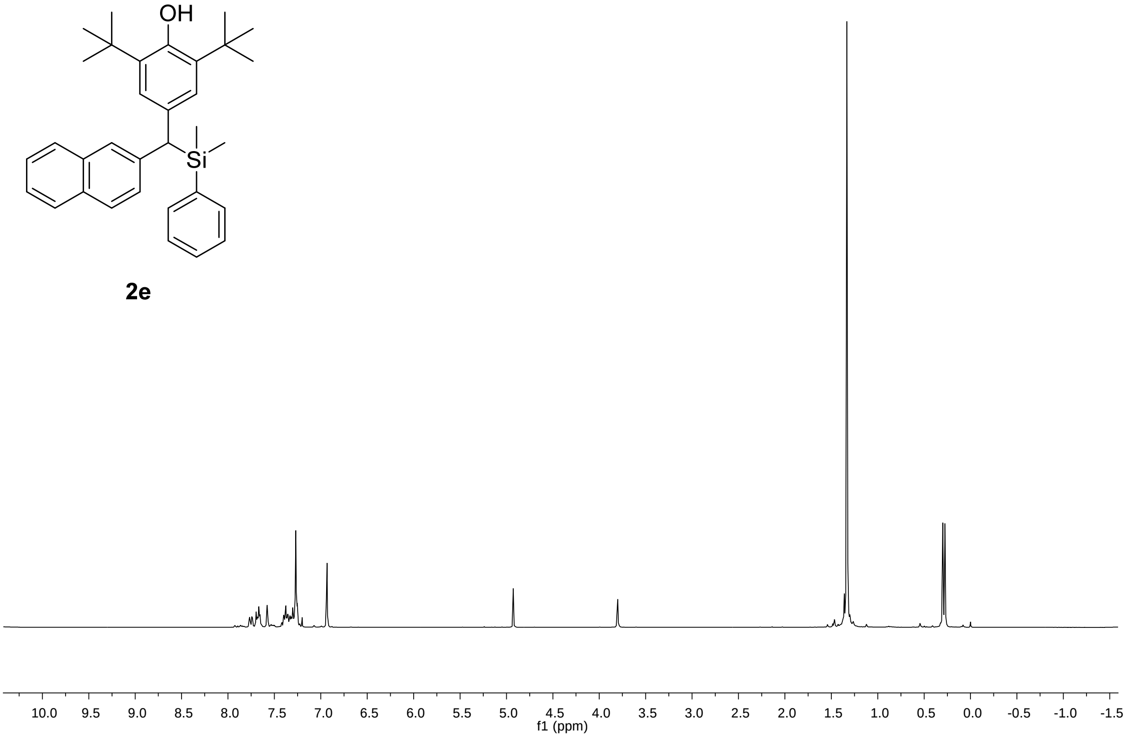

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OH
Si
S

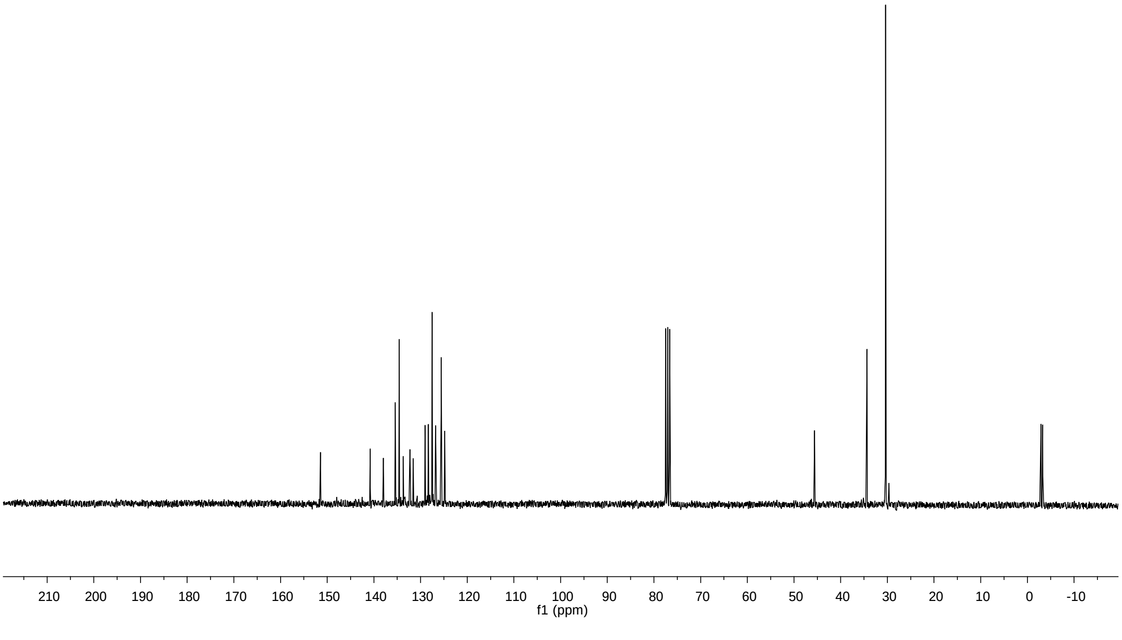
2d

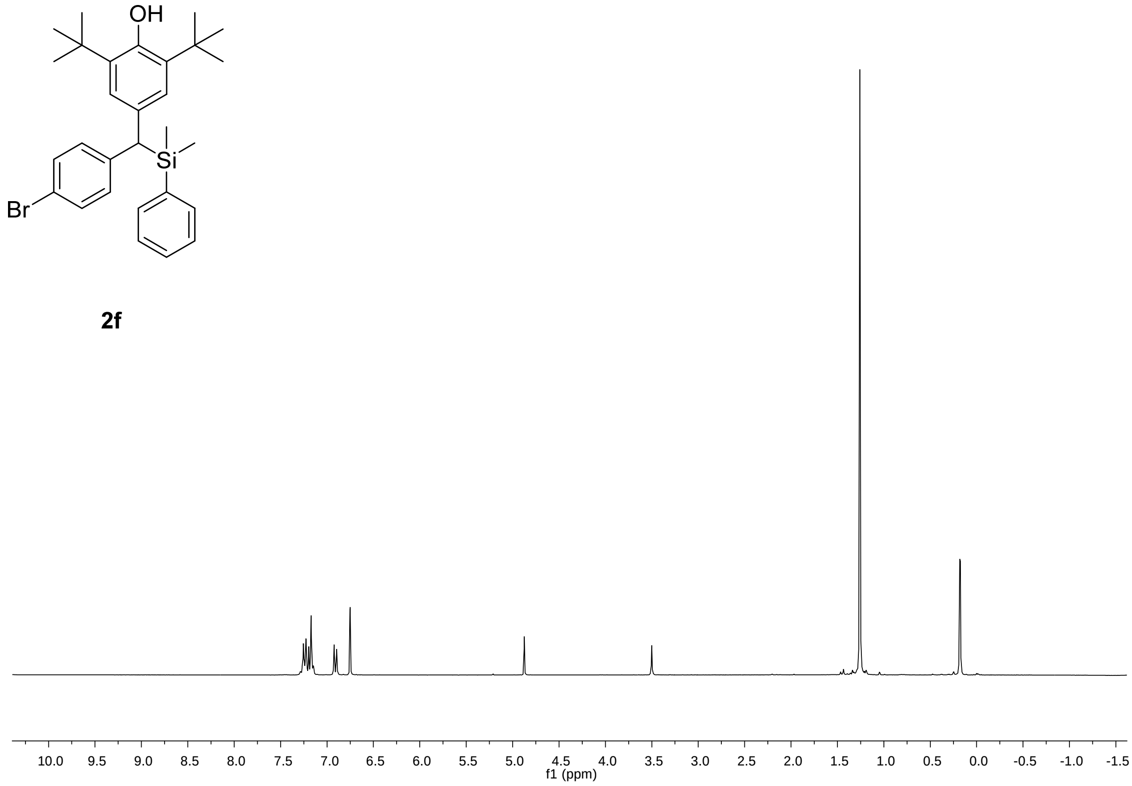

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)


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

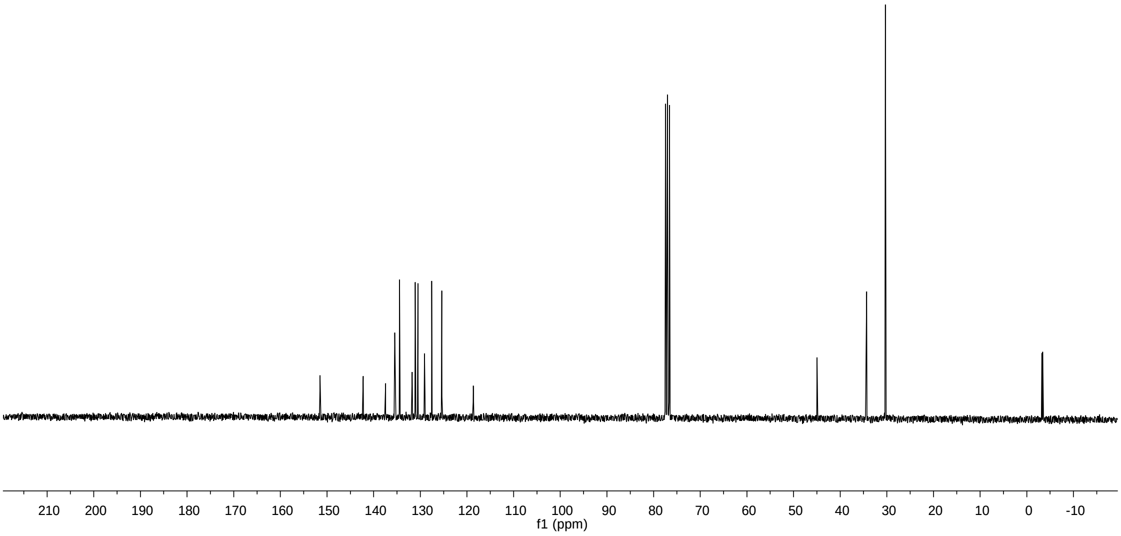

OH
Si
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

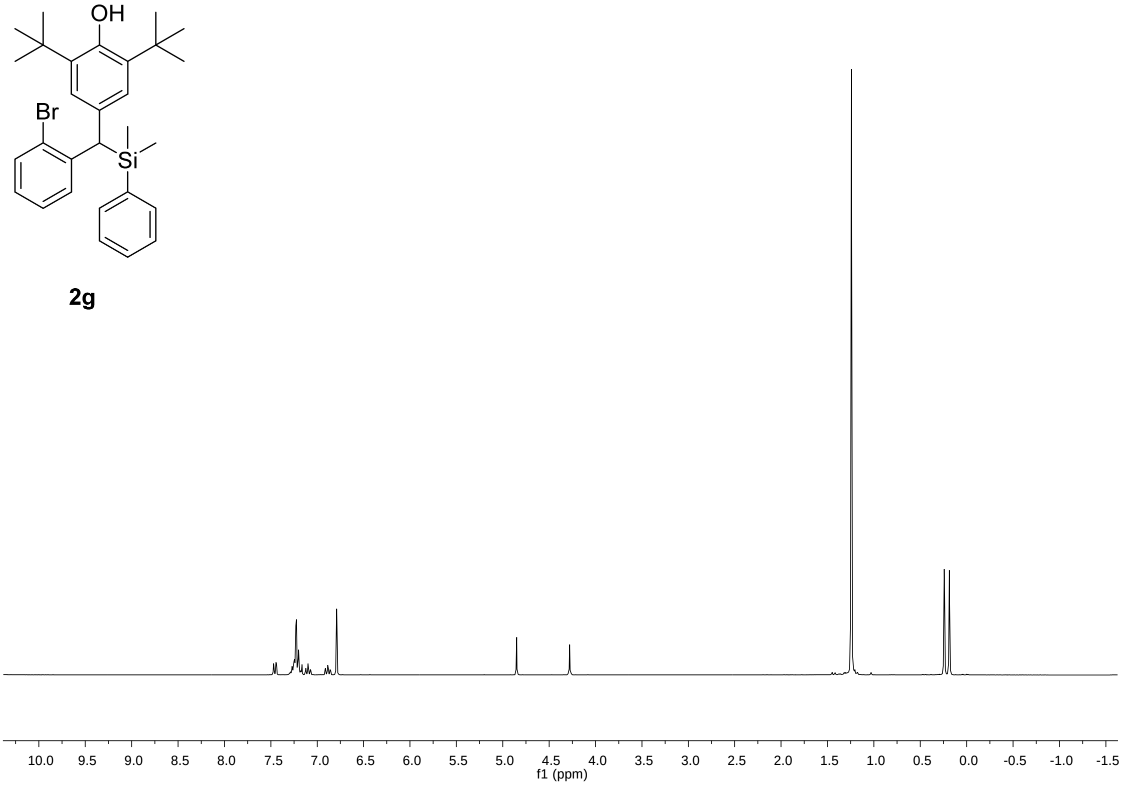
2e


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


OH
Si
Br
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

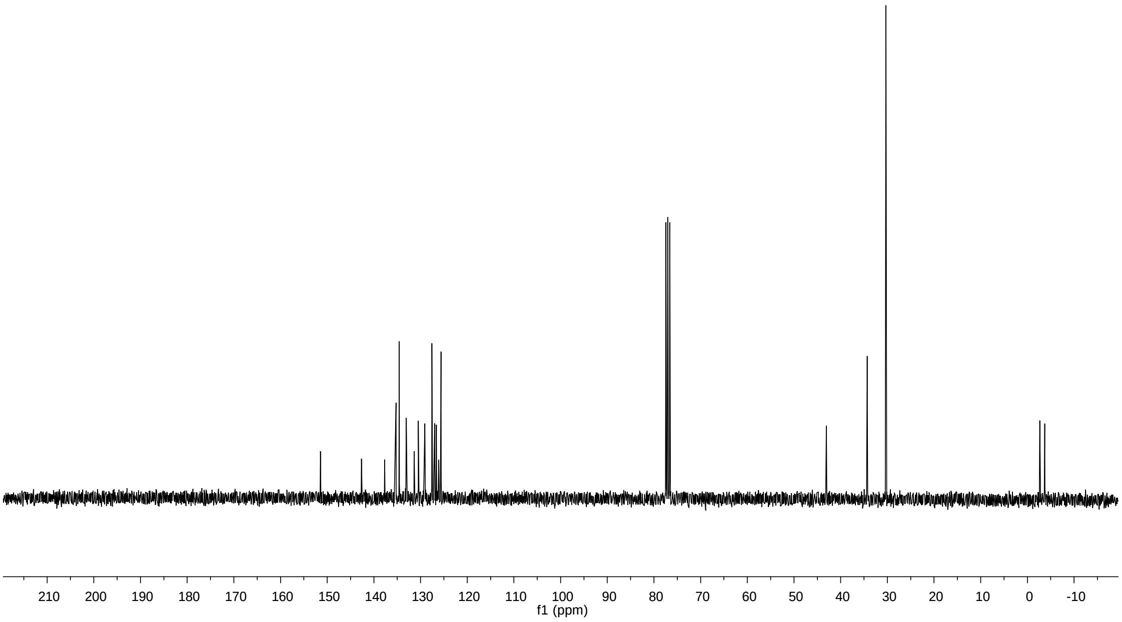
2f

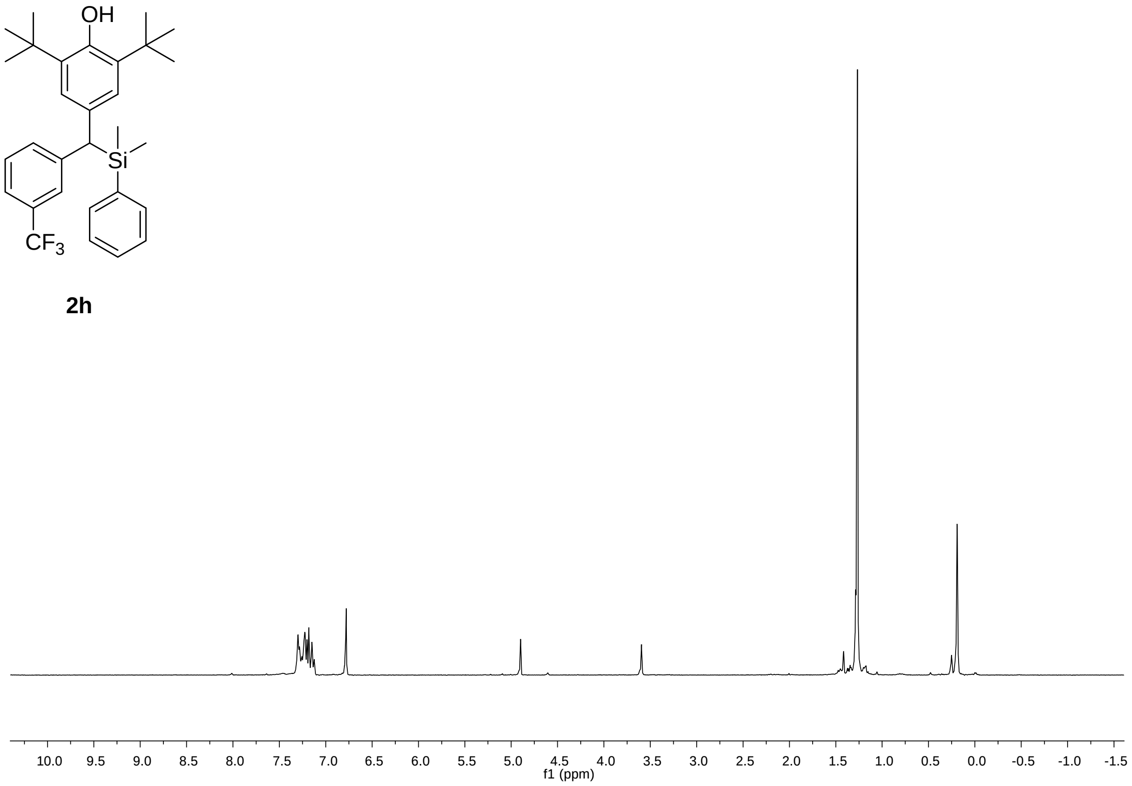

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OH
Br
Si

2g

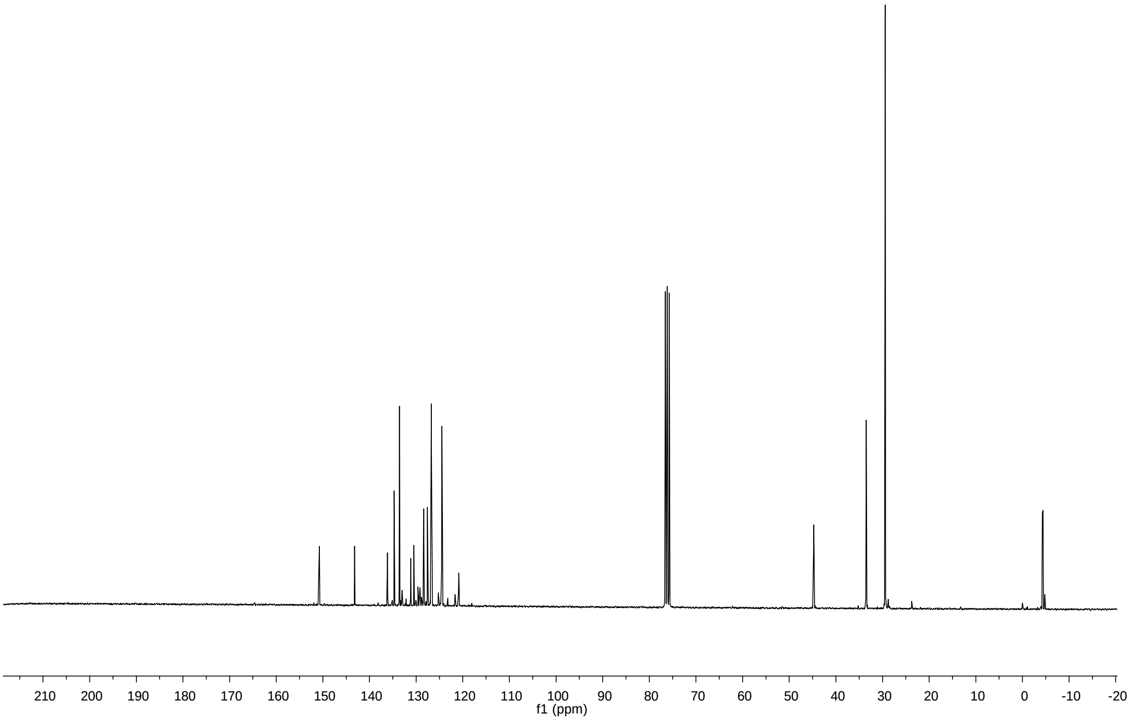
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)


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

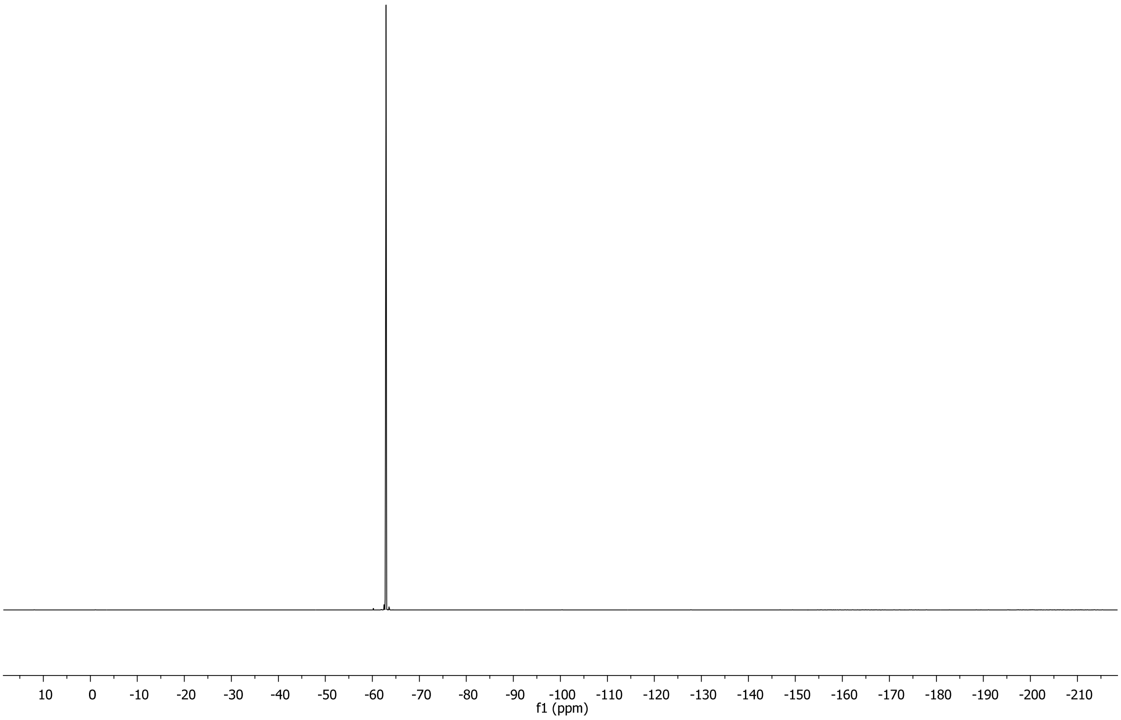


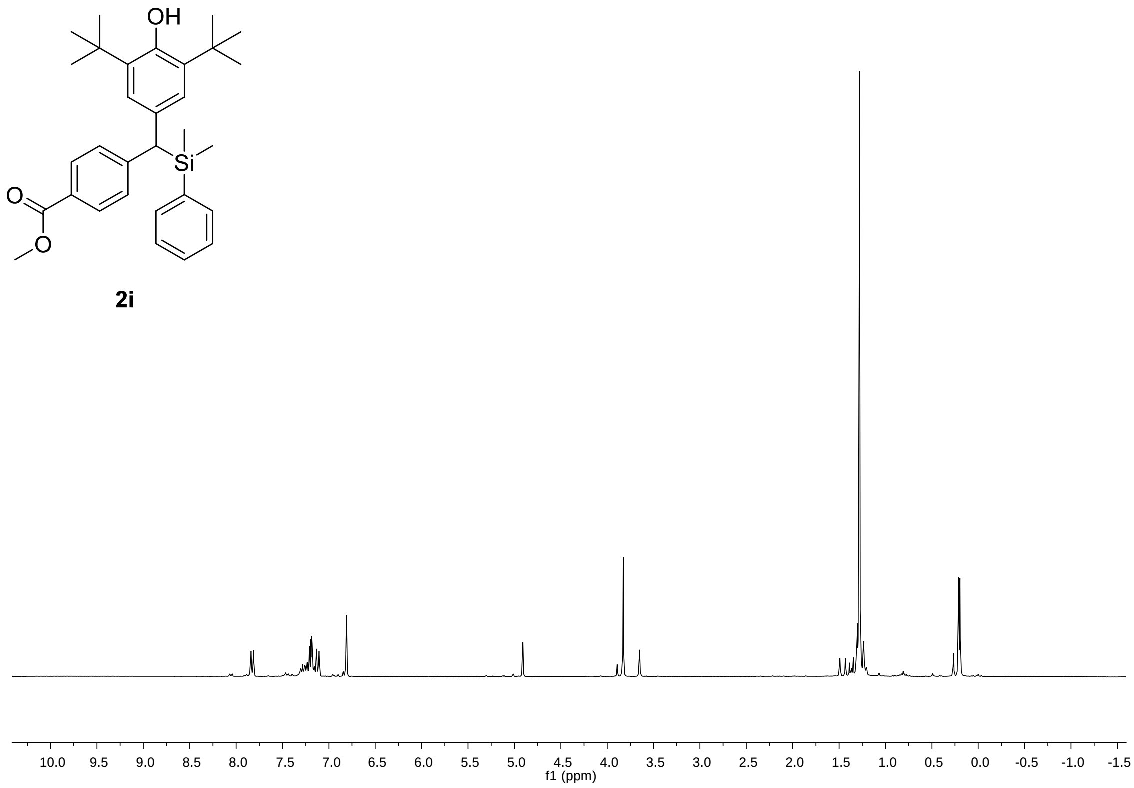
2h

OH
Si
CF3
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)



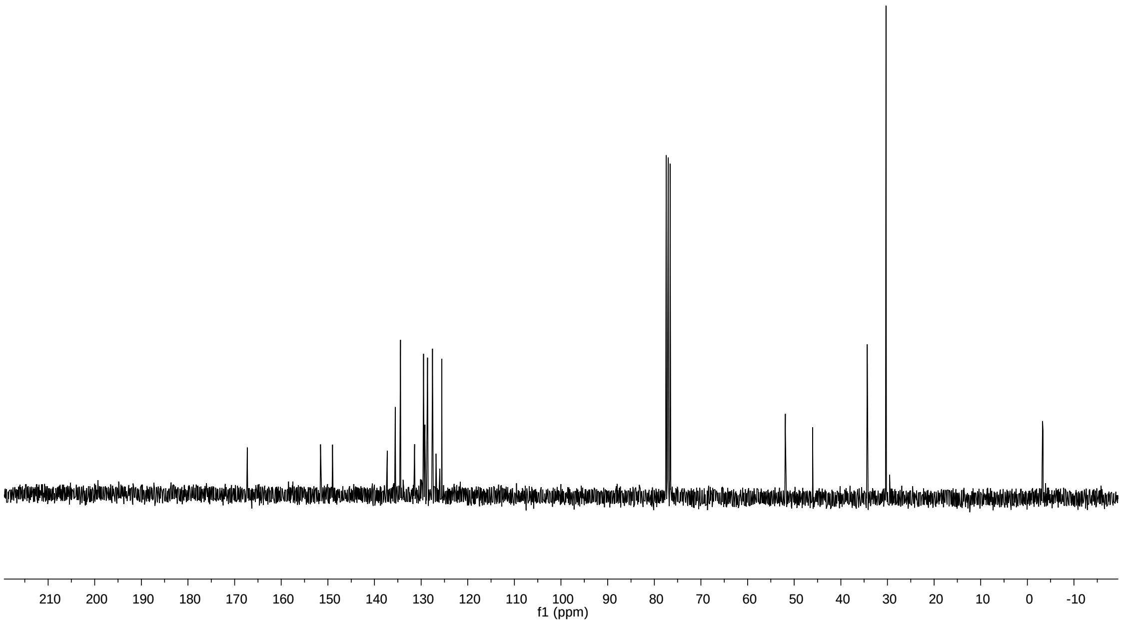
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

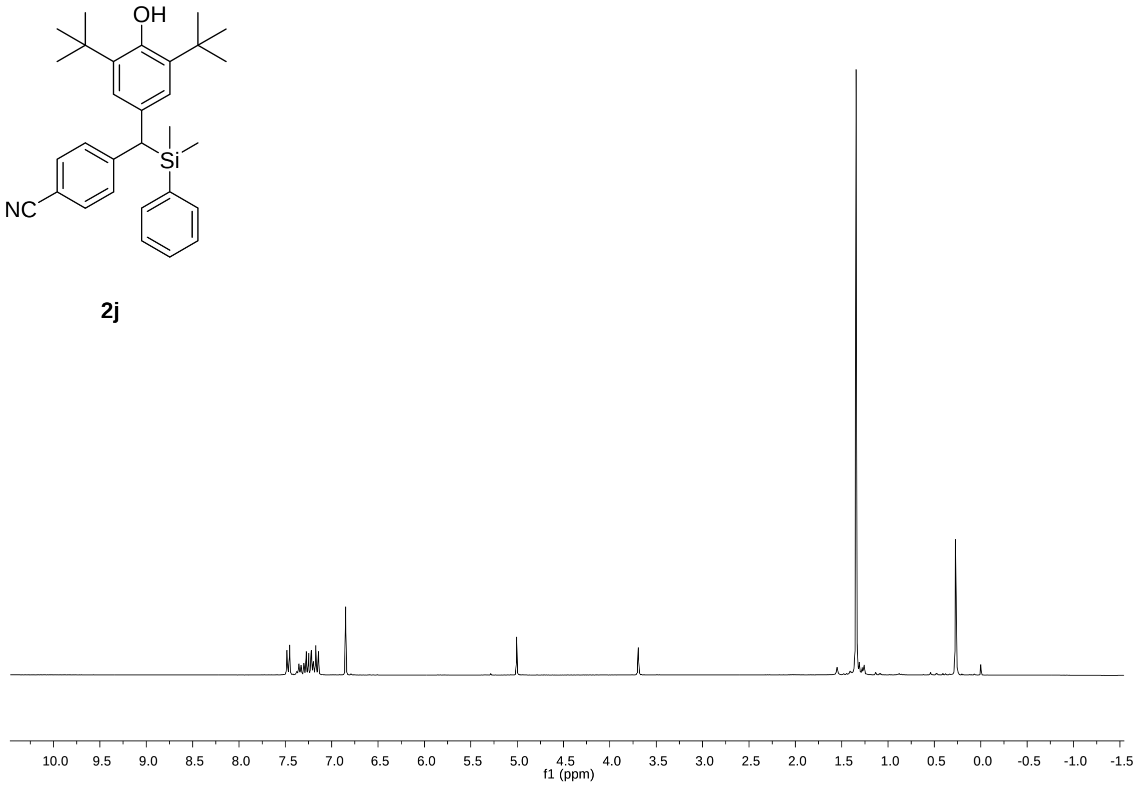

10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
f1 (ppm)


OH
Si
O
O

2i

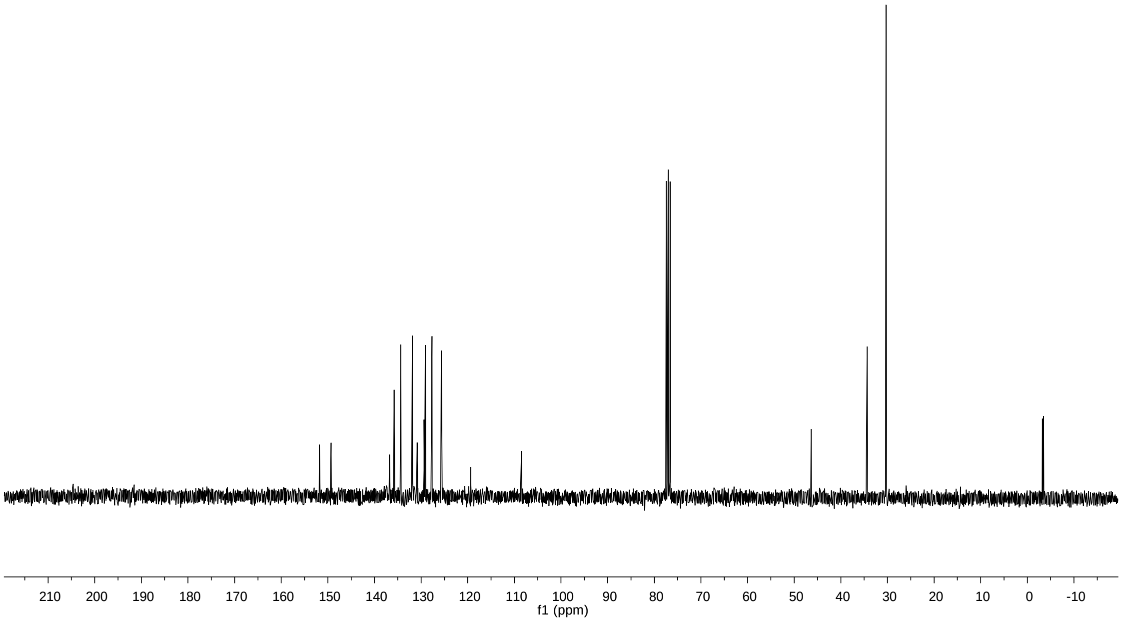
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

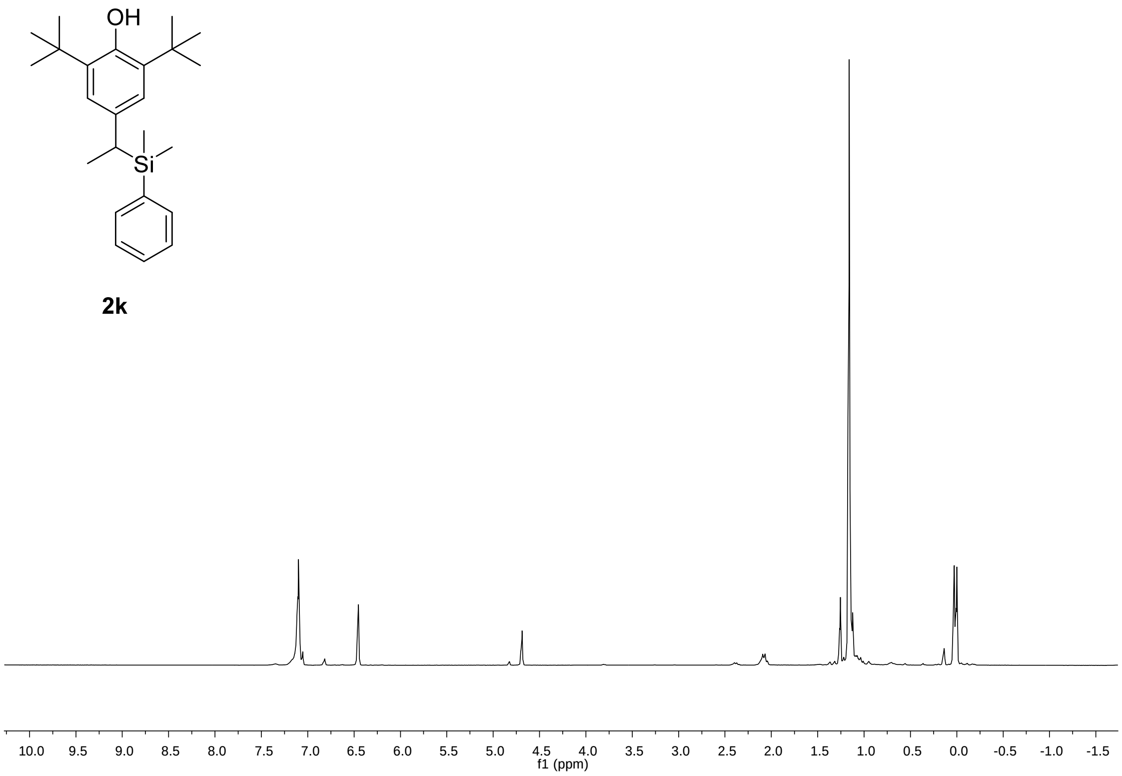

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OH
Si
NC

2j

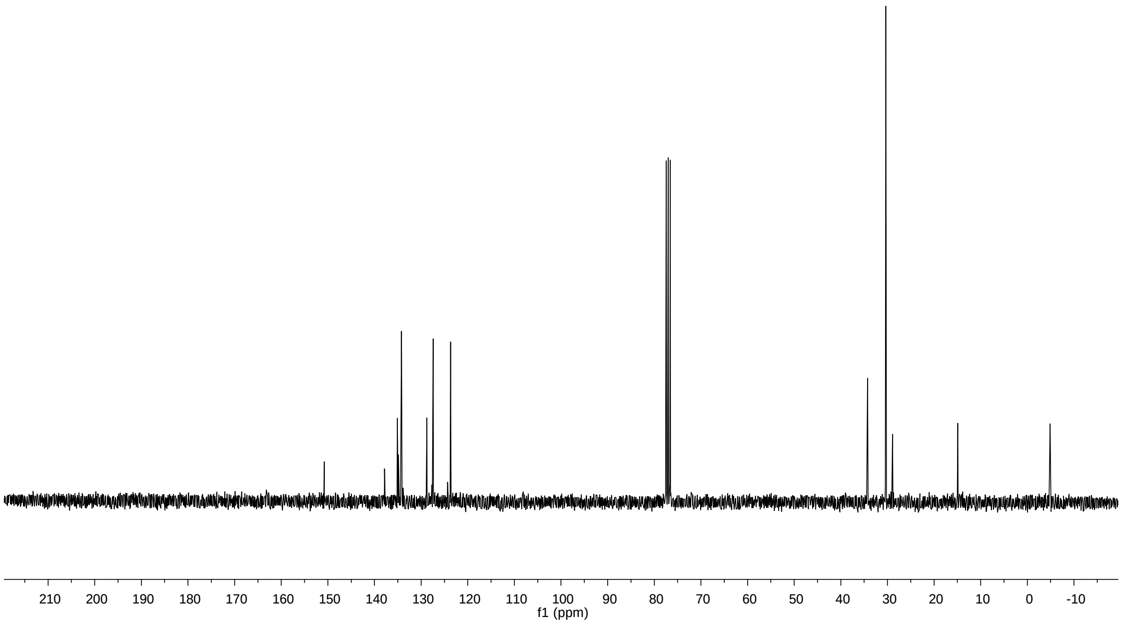
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

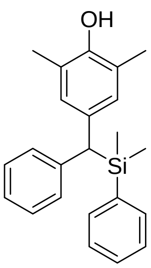

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OH
Si

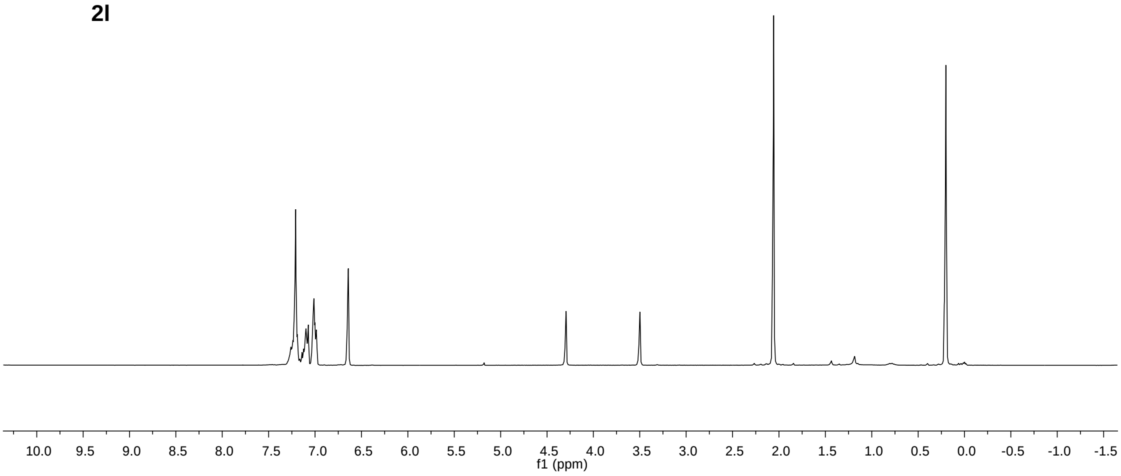
2k

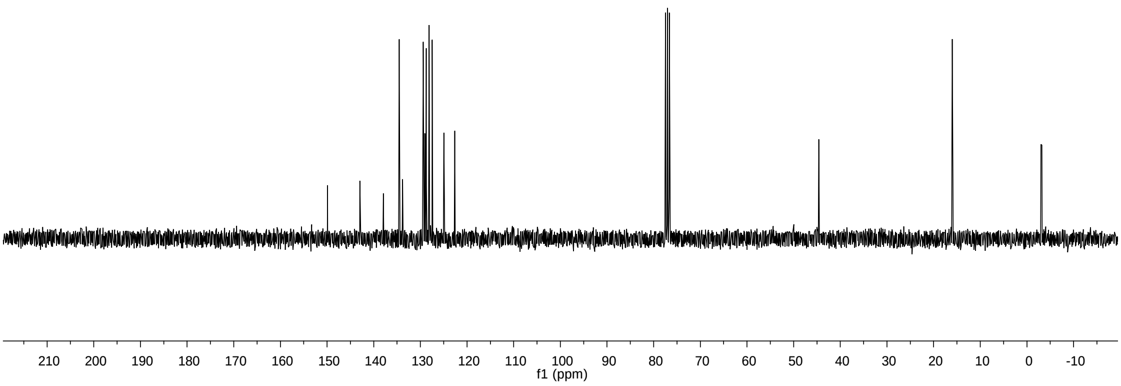
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

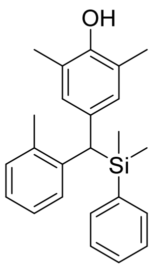

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


OH
Si

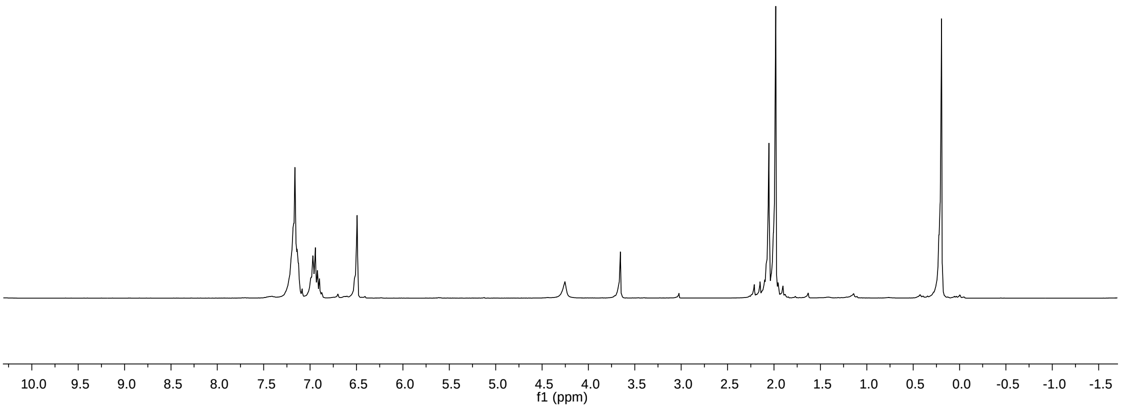
2l

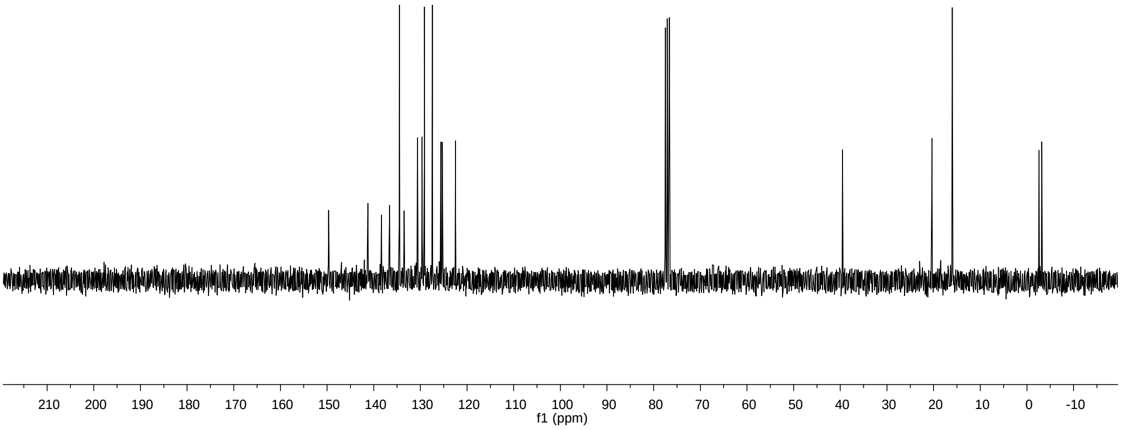

10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

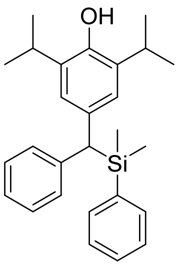

210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



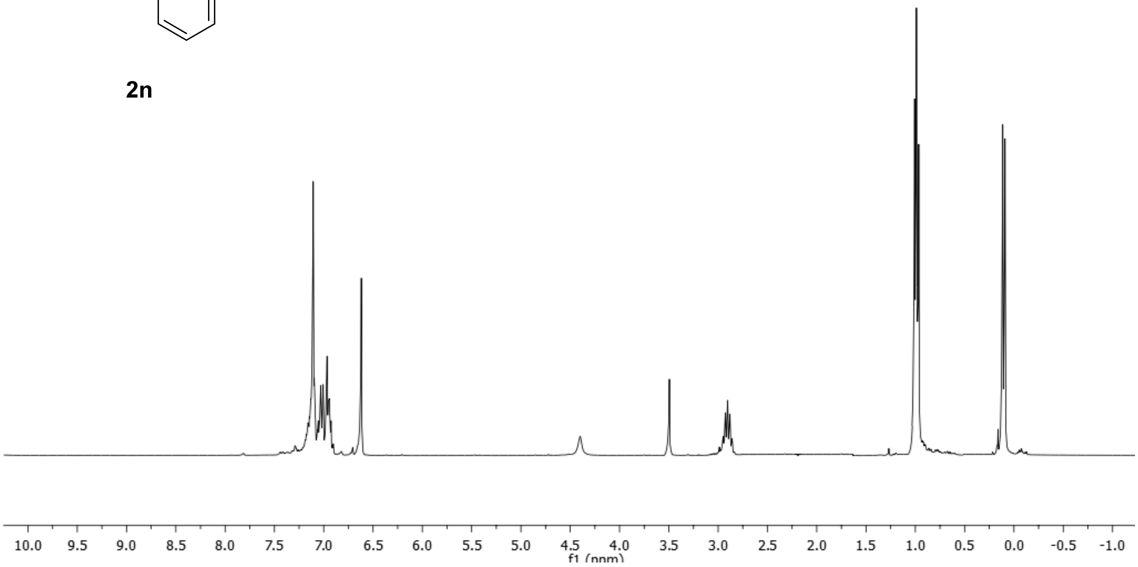
2m

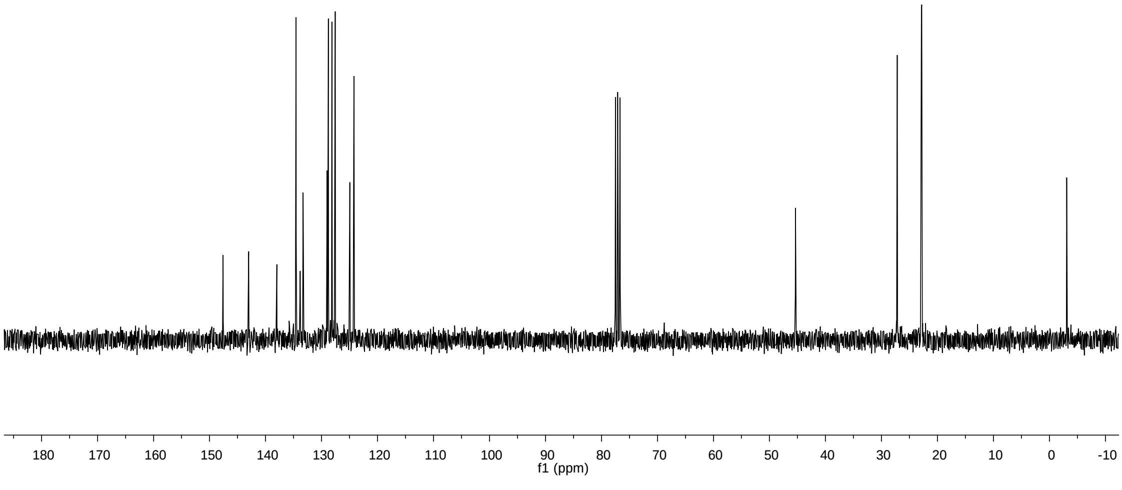

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)

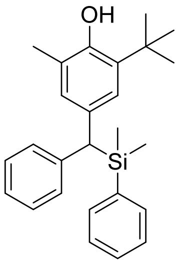

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OH
Si

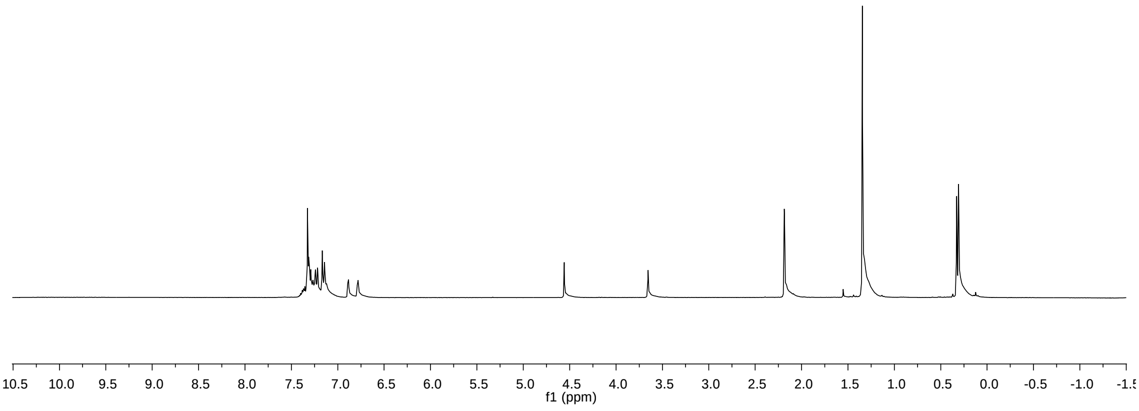
2n

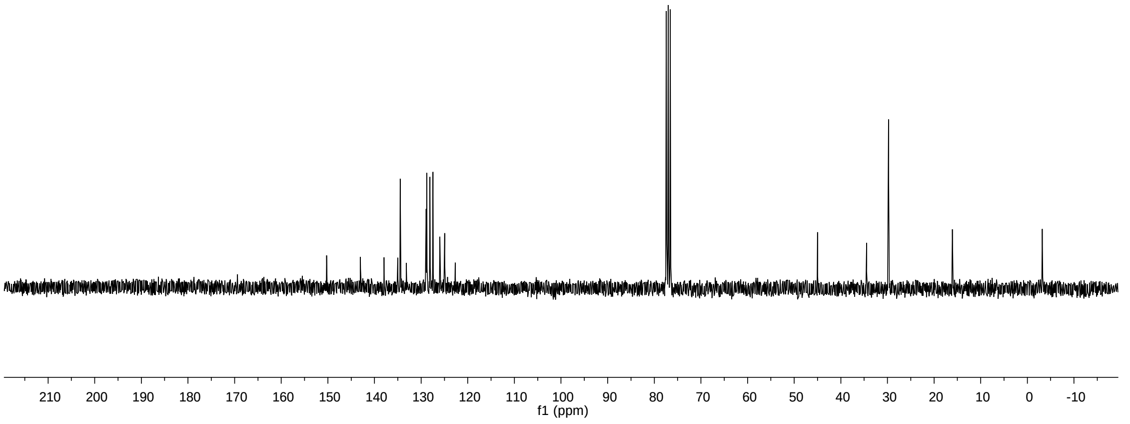

10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

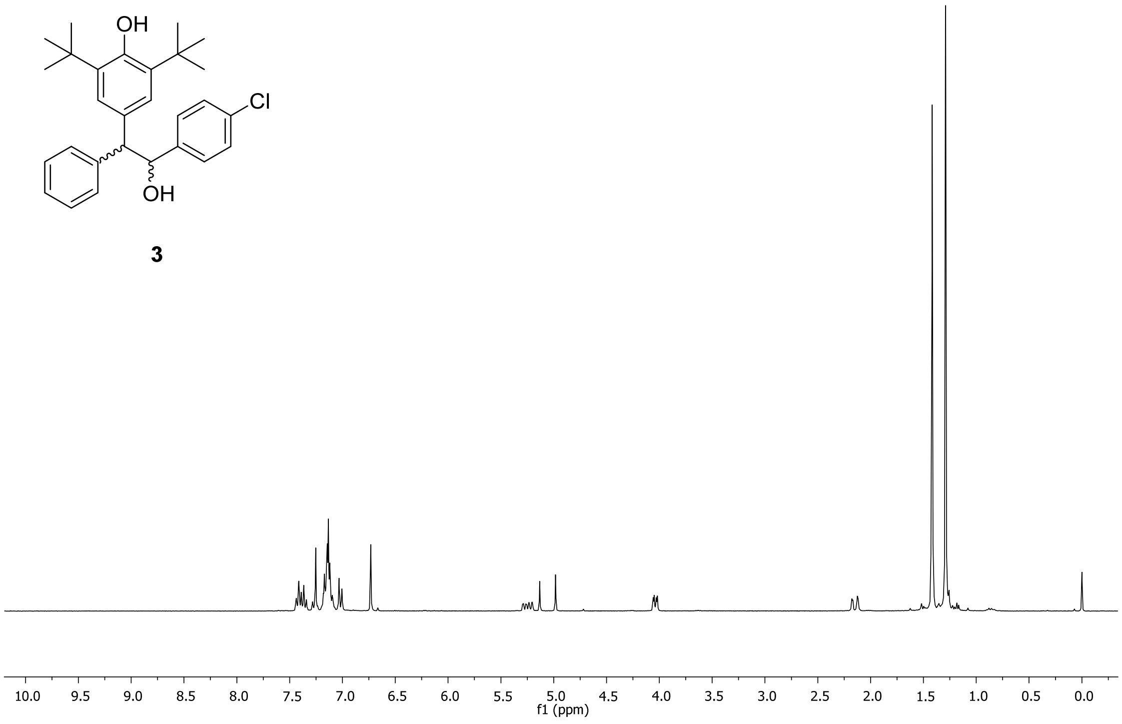

180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


OH
Si

2o

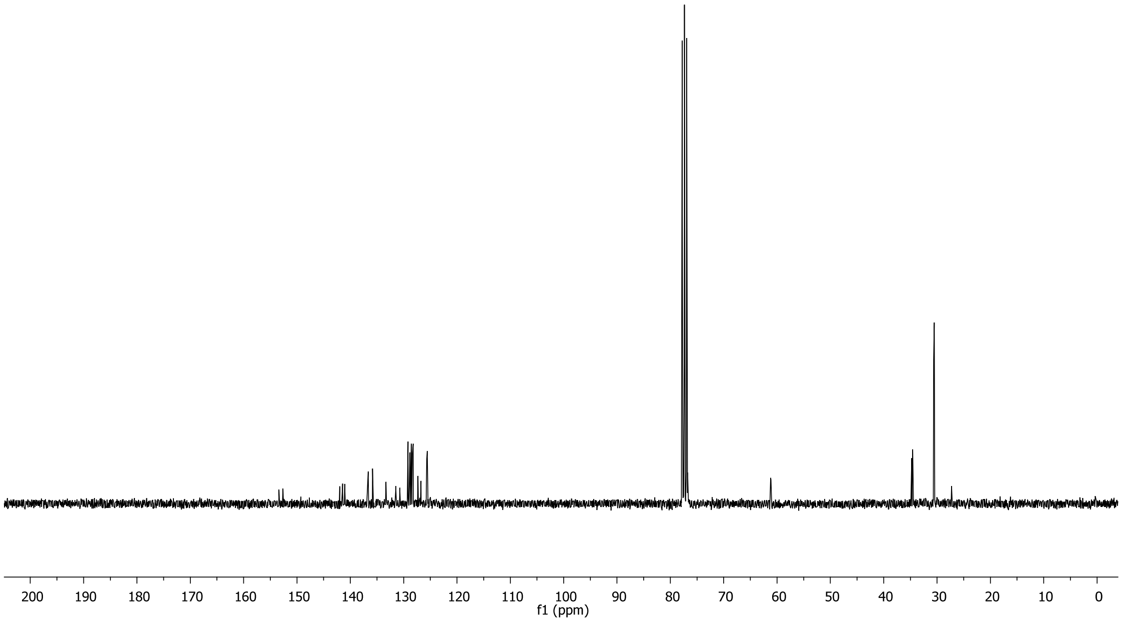

10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
f1 (ppm)


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

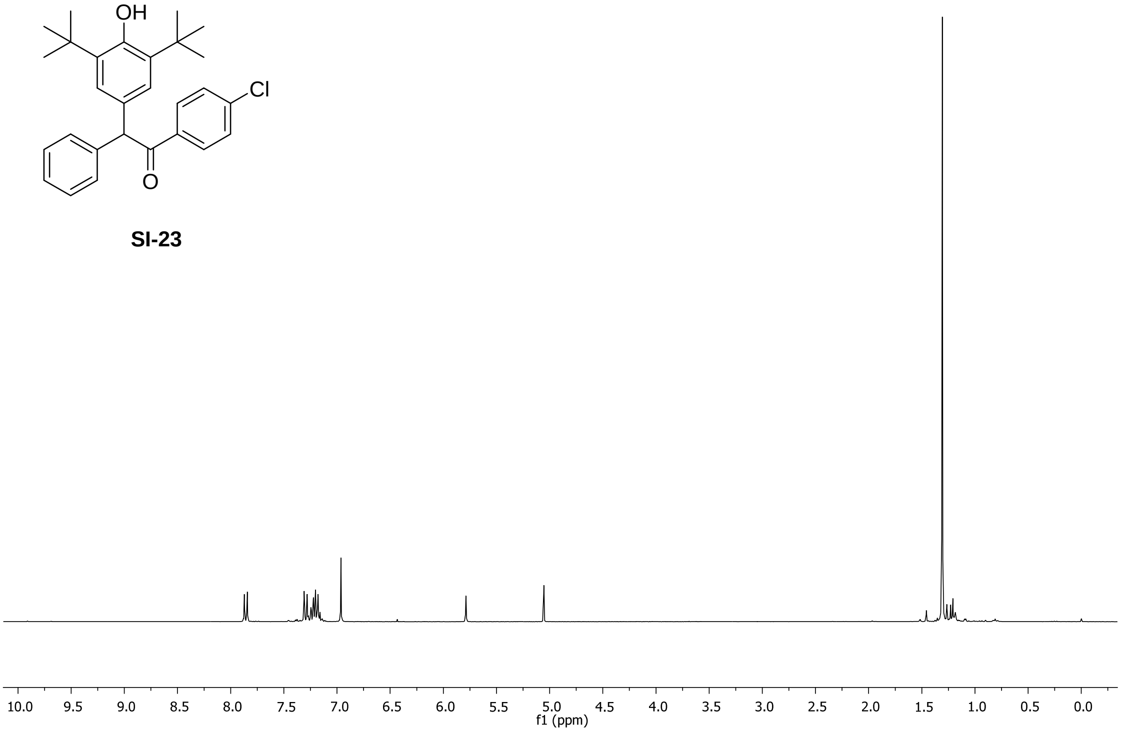


3

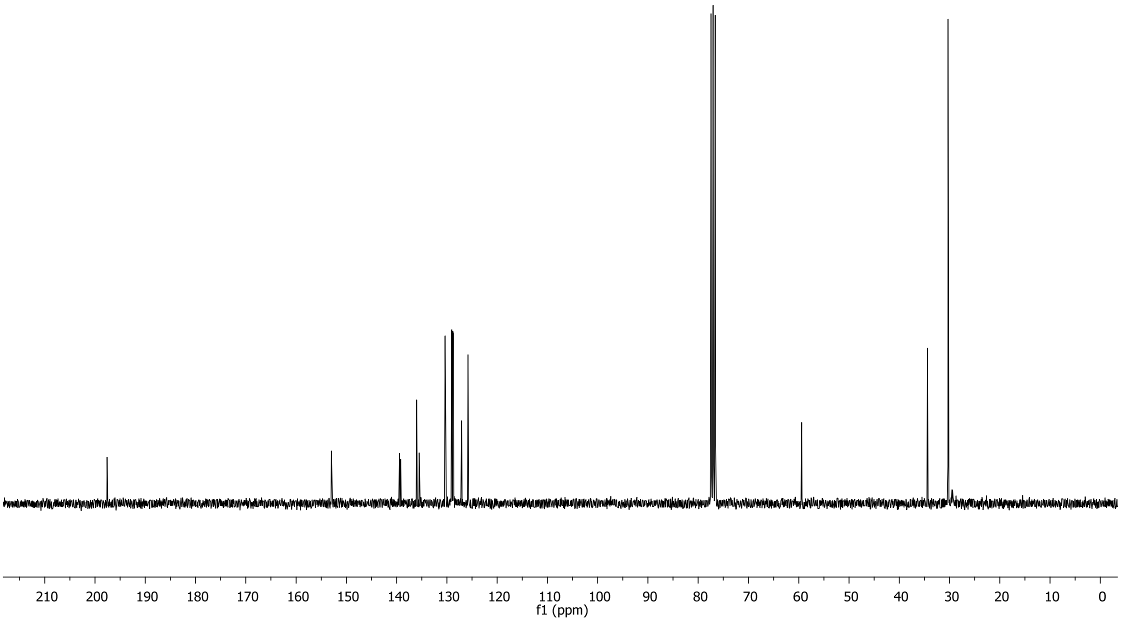
OH
Cl
OH
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

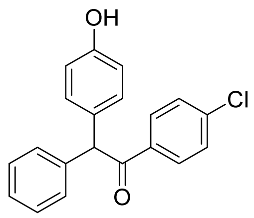


200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

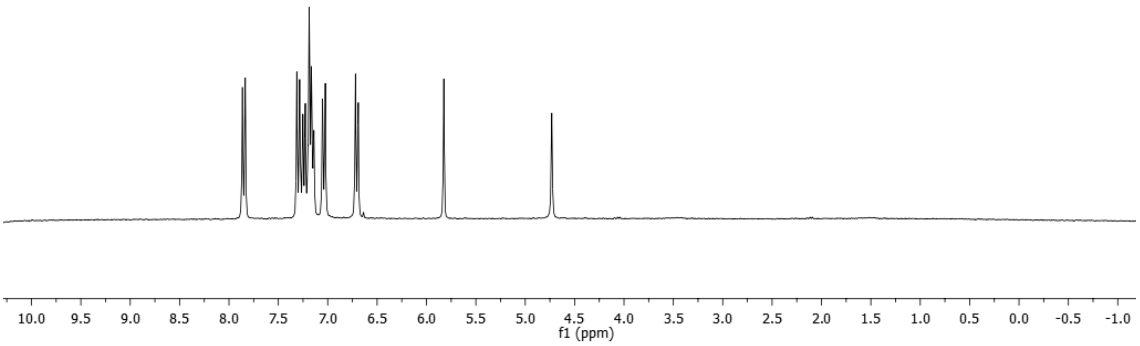

OH
Cl
O
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

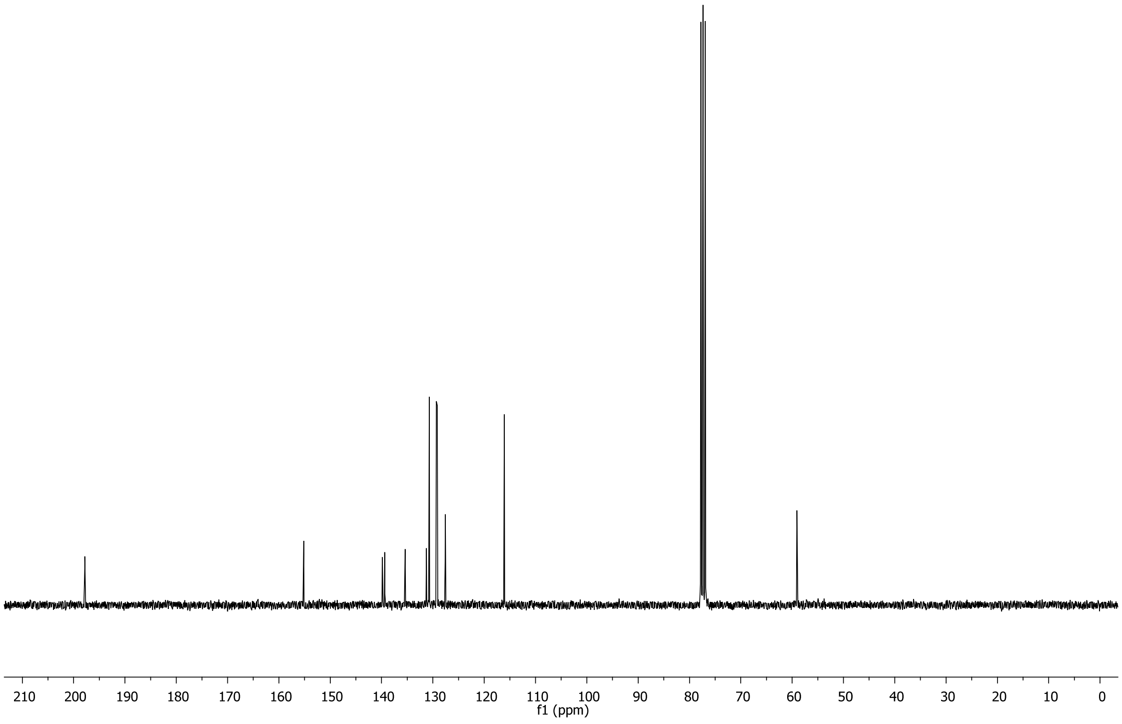
SI-23


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



4


10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)


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

8. X-Ray Data

4-[(2-Bromophenyl)(dimethyl(phenyl)silyl)methyl]-2,6-di-*tert*-butylphenol, 2g[15]

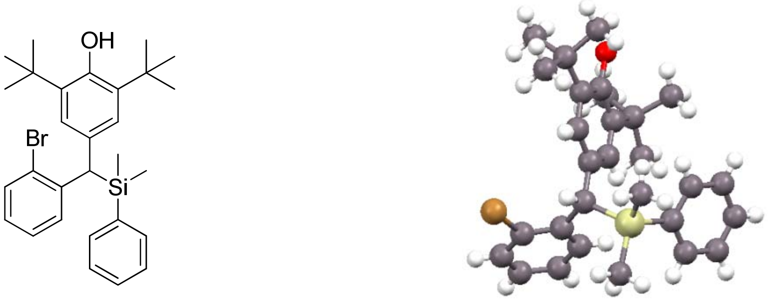


Figure S1. X-ray crystallography of compound **2g**

A clear colourless prismatic-like specimen of $C_{29}H_{36}BrOSi$, approximate dimensions 0.10 mm x 0.21 mm x 0.24 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured.

Table 1: Data collection details for 2g.

Axis	dx/mm	2θ/°	ω/°	ϕ/°	χ/°	Width/°	Frames	Time/s	Wavelength/Å	Voltage/kV	Current/mA	Temperature/K
Phi	35.091	20.50	12.48	-347.51	28.87	0.50	739	10.00	0.71073	50	30.0	n/a
Phi	35.091	13.00	13.95	-39.72	-74.52	0.50	739	10.00	0.71073	50	30.0	n/a
Omega	35.091	23.00	-42.83	-203.37	67.48	0.50	133	10.00	0.71073	50	30.0	n/a
Omega	35.091	15.50	13.78	-105.30	-61.97	0.50	69	10.00	0.71073	50	30.0	n/a
Omega	35.091	5.50	-70.22	-63.39	21.35	0.50	151	10.00	0.71073	50	30.0	n/a
Omega	35.091	-9.50	16.08	-265.18	-44.66	0.50	80	10.00	0.71073	50	30.0	n/a
Omega	35.091	-9.50	-11.00	-36.14	-78.81	0.50	96	10.00	0.71073	50	30.0	n/a
Omega	35.091	8.00	-83.99	-88.37	27.00	0.50	190	10.00	0.71073	50	30.0	n/a
Phi	35.091	8.00	-11.84	40.23	75.11	0.50	427	10.00	0.71073	50	30.0	n/a
Phi	35.091	-4.50	71.78	1.80	-31.85	0.50	658	10.00	0.71073	50	30.0	n/a

A total of 3282 frames were collected. The total exposure time was 9.12 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 87080 reflections to a maximum θ angle of 25.35° (0.83 Å resolution), of which 10052 were independent (average redundancy 8.663, completeness = 99.9%, R_{int} = 7.25%, R_{sig} = 5.44%) and 6124 (60.92%) were greater than $2\sigma(F^2)$. The final cell constants of $\underline{a}$ = 9.5769(3) Å, $\underline{b}$ = 15.5585(5) Å, $\underline{c}$ = 18.7701(6) Å, α = 98.4470(10)°, β = 95.2440(10)°, γ = 94.6910(10)°, volume = 2741.97(15) $Å^3$, are based upon the refinement of the XYZ-centroids of 9838 reflections above 20 σ(I) with 4.614° < 2θ < 42.05°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.895. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7058 and 0.8596.

---

[15] **CCDC 1414585** contains the supplementary crystallographic data. These data can be obtained free of charge at www.ccdc.cam.ac.uk/conts/retrieving.html

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 4 for the formula unit, $C_{29}H_{36}BrOSi$. The final anisotropic full-matrix least-squares refinement on F^2 with 593 variables converged at R1 = 4.90%, for the observed data and wR2 = 15.32% for all data. The goodness-of-fit was 1.052. The largest peak in the final difference electron density synthesis was 0.543 $e^-/Å^3$ and the largest hole was -0.839 $e^-/Å^3$ with an RMS deviation of 0.098 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.232 $g/cm^3$and F(000), 1068 e^-.

Table 2. Sample and crystal data for 2g.

Chemical formula	$C_{29}H_{36}BrOSi$	
Formula weight	508.58	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal size	0.10 x 0.21 x 0.24 mm	
Crystal habit	clear colourless prismatic	
Crystal system	triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.5769(3) Å	α = 98.4470(10)°
	b = 15.5585(5) Å	β = 95.2440(10)°
	c = 18.7701(6) Å	γ = 94.6910(10)°
Volume	2741.97(15) $Å^3$	
Z	4	
Density (calculated)	1.232 Mg/cm^3	
Absorption coefficient	1.561 mm^{-1}	
F(000)	1068	

Table 3. Data collection and structure refinement for 2g

Theta range for data collection	1.33 to 25.35°
Index ranges	-11<=h<=11, -18<=k<=18, -22<=l<=22
Reflections collected	87080
Independent reflections	10052 [R(int) = 0.0725]
Coverage of independent reflections	99.9%
Absorption correction	multi-scan
Max. and min. transmission	0.8596 and 0.7058
Structure solution technique	direct methods
Structure solution program	SHELXS-97 (Sheldrick, 2008)
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-97 (Sheldrick, 2008)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints /	10052 / 0 / 593

parameters		
Goodness-of-fit on F^2	1.052	
Final R indices	6124 data; I>2σ(I)	R1 = 0.0490, wR2 = 0.1227
	all data	R1 = 0.1032, wR2 = 0.1532
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0757P)^2+0.8520P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.543 and -0.839 eÅ^{-3}	
R.M.S. deviation from mean	0.098 eÅ^{-3}	

Table 4. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for 2g

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	**y/b**	**z/c**	**U(eq)**
Br1	0.32464(5)	0.55173(4)	0.48423(3)	0.0881(2)
Br2	0.29069(7)	0.05140(4)	0.01605(3)	0.0982(2)
C1	0.1881(4)	0.5558(2)	0.5513(2)	0.0514(10)
C2	0.0862(5)	0.6111(3)	0.5422(3)	0.0735(13)
C3	0.9822(5)	0.6174(3)	0.5875(3)	0.0760(14)
C4	0.9818(5)	0.5687(3)	0.6426(2)	0.0667(12)
C5	0.0850(4)	0.5133(2)	0.6514(2)	0.0526(10)
C6	0.1917(3)	0.5041(2)	0.60580(17)	0.0378(8)
C7	0.2985(3)	0.4387(2)	0.61290(17)	0.0353(8)
C8	0.2403(3)	0.3461(2)	0.57912(16)	0.0327(7)
C9	0.3050(3)	0.2992(2)	0.52504(17)	0.0361(8)
C10	0.2534(3)	0.2152(2)	0.49170(18)	0.0395(8)
C11	0.1322(4)	0.1781(2)	0.51654(18)	0.0412(8)
C12	0.0609(3)	0.2232(2)	0.57027(18)	0.0376(8)
C13	0.1191(3)	0.3064(2)	0.60003(17)	0.0358(8)
C14	0.3266(4)	0.1673(2)	0.4296(2)	0.0545(10)
C15	0.2234(5)	0.1463(3)	0.3600(2)	0.0784(14)
C16	0.3817(5)	0.0836(3)	0.4508(3)	0.0783(14)
C17	0.4545(5)	0.2236(3)	0.4125(2)	0.0775(14)
C18	0.9257(4)	0.1833(2)	0.5958(2)	0.0494(9)
C19	0.8669(4)	0.2490(3)	0.6523(3)	0.0742(13)
C20	0.9562(4)	0.1044(3)	0.6331(2)	0.0627(11)
C21	0.8094(4)	0.1574(3)	0.5326(3)	0.0799(14)
C22	0.2901(3)	0.3875(2)	0.76899(18)	0.0407(8)
C23	0.2751(4)	0.2975(2)	0.76197(19)	0.0511(9)
C24	0.1980(4)	0.2537(3)	0.8074(2)	0.0640(12)

	x/a	**y/b**	**z/c**	**U(eq)**
C25	0.1345(5)	0.3014(4)	0.8608(2)	0.0723(13)
C26	0.1492(5)	0.3894(3)	0.8696(2)	0.0785(14)
C27	0.2242(4)	0.4324(3)	0.8238(2)	0.0601(11)
C28	0.4360(5)	0.5617(3)	0.7460(2)	0.0768(14)
C29	0.5578(4)	0.3904(3)	0.6945(2)	0.0703(13)
C30	0.1479(5)	0.0380(2)	0.9368(2)	0.0599(11)
C31	0.0401(7)	0.0942(3)	0.9417(3)	0.0837(16)
C32	0.9359(6)	0.0866(3)	0.8852(4)	0.0912(17)
C33	0.9382(5)	0.0274(3)	0.8259(3)	0.0756(13)
C34	0.0433(4)	0.9721(3)	0.8212(2)	0.0583(10)
C35	0.1512(4)	0.9743(2)	0.87738(19)	0.0438(9)
C36	0.2570(3)	0.9068(2)	0.87401(18)	0.0404(8)
C37	0.2054(3)	0.8270(2)	0.90647(17)	0.0369(8)
C38	0.0746(3)	0.7819(2)	0.88170(18)	0.0392(8)
C39	0.0256(3)	0.7063(2)	0.90660(17)	0.0370(8)
C40	0.1144(4)	0.6768(2)	0.95918(18)	0.0417(8)
C41	0.2473(3)	0.7195(2)	0.98657(18)	0.0421(8)
C42	0.2891(3)	0.7948(2)	0.95848(18)	0.0419(8)
C43	0.3453(4)	0.6857(3)	0.0433(2)	0.0577(10)
C44	0.2750(5)	0.6826(3)	0.1139(2)	0.0835(14)
C45	0.3881(6)	0.5961(3)	0.0132(3)	0.0954(17)
C46	0.4825(5)	0.7465(4)	0.0643(3)	0.0908(16)
C47	0.8813(3)	0.6585(2)	0.87537(19)	0.0451(9)
C48	0.7811(4)	0.6591(3)	0.9345(3)	0.0813(14)
C49	0.8966(5)	0.5642(3)	0.8422(2)	0.0698(12)
C50	0.8136(4)	0.7025(3)	0.8146(2)	0.0674(12)
C51	0.2034(5)	0.7924(3)	0.7187(2)	0.0680(12)
C52	0.4858(4)	0.8146(3)	0.8066(2)	0.0631(11)
C53	0.3817(4)	0.9691(2)	0.74200(19)	0.0449(9)
C54	0.3058(5)	0.9921(3)	0.6836(3)	0.0731(13)
C55	0.3485(6)	0.0632(4)	0.6517(3)	0.0925(17)
C56	0.4706(7)	0.1129(3)	0.6792(3)	0.0901(18)
C57	0.5487(6)	0.0922(3)	0.7363(3)	0.0936(17)
C58	0.5049(5)	0.0215(3)	0.7682(2)	0.0745(13)
O1	0.0802(3)	0.09344(16)	0.48600(15)	0.0623(7)
O2	0.0674(3)	0.60149(17)	0.98510(15)	0.0609(7)
Si1	0.39399(10)	0.44474(6)	0.70715(5)	0.0418(3)
Si2	0.32750(10)	0.87071(6)	0.78406(5)	0.0412(2)

Table 5. Bond lengths (Å) for 2g.

Br1-C1	1.895(4)	Br2-C30	1.901(5)
C1-C2	1.368(6)	C1-C6	1.391(5)
C2-C3	1.367(7)	C2-H2	0.93
C3-C4	1.367(7)	C3-H3	0.93
C4-C5	1.378(5)	C4-H4	0.93
C5-C6	1.395(5)	C5-H5	0.93
C6-C7	1.512(5)	C7-C8	1.524(4)
C7-Si1	1.902(3)	C7-H7	0.98
C8-C9	1.385(4)	C8-C13	1.386(4)
C9-C10	1.394(4)	C9-H9	0.93
C10-C11	1.402(5)	C10-C14	1.544(5)
C11-O1	1.390(4)	C11-C12	1.404(5)
C12-C13	1.382(4)	C12-C18	1.537(5)
C13-H13	0.93	C14-C17	1.533(6)
C14-C16	1.535(6)	C14-C15	1.542(6)
C15-H15A	0.96	C15-H15B	0.96
C15-H15C	0.96	C16-H16A	0.96
C16-H16B	0.96	C16-H16C	0.96
C17-H17A	0.96	C17-H17B	0.96
C17-H17C	0.96	C18-C21	1.535(6)
C18-C20	1.535(5)	C18-C19	1.540(5)
C19-H19A	0.96	C19-H19B	0.96
C19-H19C	0.96	C20-H20A	0.96
C20-H20B	0.96	C20-H20C	0.96
C21-H21A	0.96	C21-H21B	0.96
C21-H21C	0.96	C22-C23	1.382(5)
C22-C27	1.387(5)	C22-Si1	1.871(3)
C23-C24	1.392(5)	C23-H23	0.93
C24-C25	1.375(6)	C24-H24	0.93
C25-C26	1.350(6)	C25-H25	0.93
C26-C27	1.382(6)	C26-H26	0.93
C27-H27	0.93	C28-Si1	1.855(4)
C28-H28A	0.96	C28-H28B	0.96
C28-H28C	0.96	C29-Si1	1.859(4)
C29-H29A	0.96	C29-H29B	0.96
C29-H29C	0.96	C30-C35	1.384(5)
C30-C31	1.408(7)	C31-C32	1.373(7)
C31-H31	0.93	C32-C33	1.339(7)
C32-H32	0.93	C33-C34	1.378(6)
C33-H33	0.93	C34-C35	1.402(5)
C34-H34	0.93	C35-C36	1.516(5)

C36-C37	1.527(4)	C36-Si2	1.901(3)
C36-H36	0.98	C37-C42	1.383(5)
C37-C38	1.390(4)	C38-C39	1.391(4)
C38-H38	0.93	C39-C40	1.397(5)
C39-C47	1.537(5)	C40-O2	1.391(4)
C40-C41	1.402(5)	C41-C42	1.398(5)
C41-C43	1.534(5)	C42-H42	0.93
C43-C45	1.530(6)	C43-C46	1.539(6)
C43-C44	1.544(6)	C44-H44A	0.96
C44-H44B	0.96	C44-H44C	0.96
C45-H45A	0.96	C45-H45B	0.96
C45-H45C	0.96	C46-H46A	0.96
C46-H46B	0.96	C46-H46C	0.96
C47-C48	1.531(5)	C47-C49	1.532(5)
C47-C50	1.535(5)	C48-H48A	0.96
C48-H48B	0.96	C48-H48C	0.96
C49-H49A	0.96	C49-H49B	0.96
C49-H49C	0.96	C50-H50A	0.96
C50-H50B	0.96	C50-H50C	0.96
C51-Si2	1.860(4)	C51-H51A	0.96
C51-H51B	0.96	C51-H51C	0.96
C52-Si2	1.857(4)	C52-H52A	0.96
C52-H52B	0.96	C52-H52C	0.96
C53-C54	1.368(5)	C53-C58	1.384(5)
C53-Si2	1.880(4)	C54-C55	1.384(6)
C54-H54	0.93	C55-C56	1.363(8)
C55-H55	0.93	C56-C57	1.344(8)
C56-H56	0.93	C57-C58	1.382(6)
C57-H57	0.93	C58-H58	0.93

Table 6. Bond angles (°) for 2g.

C2-C1-C6	122.6(4)	C2-C1-Br1	116.3(3)
C6-C1-Br1	121.1(3)	C3-C2-C1	120.3(4)
C3-C2-H2	119.9	C1-C2-H2	119.9
C2-C3-C4	119.5(4)	C2-C3-H3	120.2
C4-C3-H3	120.2	C3-C4-C5	119.8(4)
C3-C4-H4	120.1	C5-C4-H4	120.1
C4-C5-C6	122.5(4)	C4-C5-H5	118.8
C6-C5-H5	118.8	C1-C6-C5	115.3(3)
C1-C6-C7	122.6(3)	C5-C6-C7	121.9(3)
C6-C7-C8	112.6(3)	C6-C7-Si1	115.3(2)
C8-C7-Si1	112.9(2)	C6-C7-H7	104.9
C8-C7-H7	104.9	Si1-C7-H7	104.9
C9-C8-C13	117.4(3)	C9-C8-C7	121.1(3)
C13-C8-C7	121.4(3)	C8-C9-C10	122.9(3)
C8-C9-H9	118.6	C10-C9-H9	118.6
C9-C10-C11	116.7(3)	C9-C10-C14	120.7(3)
C11-C10-C14	122.6(3)	O1-C11-C10	118.3(3)
O1-C11-C12	118.9(3)	C10-C11-C12	122.8(3)
C13-C12-C11	116.5(3)	C13-C12-C18	120.9(3)
C11-C12-C18	122.7(3)	C12-C13-C8	123.7(3)
C12-C13-H13	118.2	C8-C13-H13	118.2
C17-C14-C16	106.6(4)	C17-C14-C15	107.3(3)
C16-C14-C15	110.8(3)	C17-C14-C10	111.6(3)
C16-C14-C10	110.7(3)	C15-C14-C10	109.9(3)
C14-C15-H15A	109.5	C14-C15-H15B	109.5
H15A-C15-H15B	109.5	C14-C15-H15C	109.5
H15A-C15-H15C	109.5	H15B-C15-H15C	109.5
C14-C16-H16A	109.5	C14-C16-H16B	109.5
H16A-C16-H16B	109.5	C14-C16-H16C	109.5
H16A-C16-H16C	109.5	H16B-C16-H16C	109.5
C14-C17-H17A	109.5	C14-C17-H17B	109.5
H17A-C17-H17B	109.5	C14-C17-H17C	109.5
H17A-C17-H17C	109.5	H17B-C17-H17C	109.5
C21-C18-C20	110.7(3)	C21-C18-C12	111.2(3)
C20-C18-C12	110.4(3)	C21-C18-C19	106.7(3)
C20-C18-C19	106.3(3)	C12-C18-C19	111.3(3)
C18-C19-H19A	109.5	C18-C19-H19B	109.5
H19A-C19-H19B	109.5	C18-C19-H19C	109.5
H19A-C19-H19C	109.5	H19B-C19-H19C	109.5
C18-C20-H20A	109.5	C18-C20-H20B	109.5
H20A-C20-H20B	109.5	C18-C20-H20C	109.5

H20A-C20-H20C	109.5	H20B-C20-H20C	109.5
C18-C21-H21A	109.5	C18-C21-H21B	109.5
H21A-C21-H21B	109.5	C18-C21-H21C	109.5
H21A-C21-H21C	109.5	H21B-C21-H21C	109.5
C23-C22-C27	116.6(3)	C23-C22-Si1	121.2(3)
C27-C22-Si1	122.3(3)	C22-C23-C24	122.0(4)
C22-C23-H23	119.0	C24-C23-H23	119.0
C25-C24-C23	119.1(4)	C25-C24-H24	120.4
C23-C24-H24	120.4	C26-C25-C24	120.2(4)
C26-C25-H25	119.9	C24-C25-H25	119.9
C25-C26-C27	120.4(4)	C25-C26-H26	119.8
C27-C26-H26	119.8	C26-C27-C22	121.7(4)
C26-C27-H27	119.2	C22-C27-H27	119.2
Si1-C28-H28A	109.5	Si1-C28-H28B	109.5
H28A-C28-H28B	109.5	Si1-C28-H28C	109.5
H28A-C28-H28C	109.5	H28B-C28-H28C	109.5
Si1-C29-H29A	109.5	Si1-C29-H29B	109.5
H29A-C29-H29B	109.5	Si1-C29-H29C	109.5
H29A-C29-H29C	109.5	H29B-C29-H29C	109.5
C35-C30-C31	122.1(4)	C35-C30-Br2	120.3(3)
C31-C30-Br2	117.6(4)	C32-C31-C30	119.0(4)
C32-C31-H31	120.5	C30-C31-H31	120.5
C33-C32-C31	120.4(5)	C33-C32-H32	119.8
C31-C32-H32	119.8	C32-C33-C34	120.6(5)
C32-C33-H33	119.7	C34-C33-H33	119.7
C33-C34-C35	122.3(4)	C33-C34-H34	118.8
C35-C34-H34	118.8	C30-C35-C34	115.4(4)
C30-C35-C36	123.2(4)	C34-C35-C36	121.2(3)
C35-C36-C37	111.5(3)	C35-C36-Si2	118.6(2)
C37-C36-Si2	109.9(2)	C35-C36-H36	105.2
C37-C36-H36	105.2	Si2-C36-H36	105.2
C42-C37-C38	117.9(3)	C42-C37-C36	121.6(3)
C38-C37-C36	120.5(3)	C37-C38-C39	122.9(3)
C37-C38-H38	118.6	C39-C38-H38	118.6
C38-C39-C40	116.8(3)	C38-C39-C47	120.1(3)
C40-C39-C47	123.2(3)	O2-C40-C39	117.8(3)
O2-C40-C41	119.1(3)	C39-C40-C41	123.1(3)
C42-C41-C40	116.6(3)	C42-C41-C43	120.6(3)
C40-C41-C43	122.8(3)	C37-C42-C41	122.8(3)
C37-C42-H42	118.6	C41-C42-H42	118.6
C45-C43-C41	110.5(4)	C45-C43-C46	106.6(4)
C41-C43-C46	111.4(3)	C45-C43-C44	111.0(4)

C41-C43-C44	110.8(3)	C46-C43-C44	106.4(4)
C43-C44-H44A	109.5	C43-C44-H44B	109.5
H44A-C44-H44B	109.5	C43-C44-H44C	109.5
H44A-C44-H44C	109.5	H44B-C44-H44C	109.5
C43-C45-H45A	109.5	C43-C45-H45B	109.5
H45A-C45-H45B	109.5	C43-C45-H45C	109.5
H45A-C45-H45C	109.5	H45B-C45-H45C	109.5
C43-C46-H46A	109.5	C43-C46-H46B	109.5
H46A-C46-H46B	109.5	C43-C46-H46C	109.5
H46A-C46-H46C	109.5	H46B-C46-H46C	109.5
C48-C47-C49	109.7(3)	C48-C47-C50	108.1(3)
C49-C47-C50	106.8(3)	C48-C47-C39	110.4(3)
C49-C47-C39	110.6(3)	C50-C47-C39	111.1(3)
C47-C48-H48A	109.5	C47-C48-H48B	109.5
H48A-C48-H48B	109.5	C47-C48-H48C	109.5
H48A-C48-H48C	109.5	H48B-C48-H48C	109.5
C47-C49-H49A	109.5	C47-C49-H49B	109.5
H49A-C49-H49B	109.5	C47-C49-H49C	109.5
H49A-C49-H49C	109.5	H49B-C49-H49C	109.5
C47-C50-H50A	109.5	C47-C50-H50B	109.5
H50A-C50-H50B	109.5	C47-C50-H50C	109.5
H50A-C50-H50C	109.5	H50B-C50-H50C	109.5
Si2-C51-H51A	109.5	Si2-C51-H51B	109.5
H51A-C51-H51B	109.5	Si2-C51-H51C	109.5
H51A-C51-H51C	109.5	H51B-C51-H51C	109.5
Si2-C52-H52A	109.5	Si2-C52-H52B	109.5
H52A-C52-H52B	109.5	Si2-C52-H52C	109.5
H52A-C52-H52C	109.5	H52B-C52-H52C	109.5
C54-C53-C58	116.2(4)	C54-C53-Si2	122.9(3)
C58-C53-Si2	120.9(3)	C53-C54-C55	122.6(5)
C53-C54-H54	118.7	C55-C54-H54	118.7
C56-C55-C54	119.3(5)	C56-C55-H55	120.4
C54-C55-H55	120.4	C57-C56-C55	120.0(5)
C57-C56-H56	120.0	C55-C56-H56	120.0
C56-C57-C58	120.4(5)	C56-C57-H57	119.8
C58-C57-H57	119.8	C57-C58-C53	121.6(5)
C57-C58-H58	119.2	C53-C58-H58	119.2
C28-Si1-C29	110.9(2)	C28-Si1-C22	110.00(19)
C29-Si1-C22	108.67(18)	C28-Si1-C7	107.88(17)
C29-Si1-C7	106.00(17)	C22-Si1-C7	113.39(14)
C52-Si2-C51	107.8(2)	C52-Si2-C53	109.11(17)
C51-Si2-C53	110.14(19)	C52-Si2-C36	105.54(17)

C51-Si2-C36	114.31(17)	C53-Si2-C36	109.73(15)

Table 7. Anisotropic atomic displacement parameters (Å^2) for 2g

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
Br1	0.0779(3)	0.1145(4)	0.0807(4)	0.0607(3)	0.0072(3)	-0.0190(3)
Br2	0.1267(5)	0.0886(4)	0.0623(3)	-0.0198(3)	0.0048(3)	-0.0282(3)
C1	0.056(2)	0.038(2)	0.056(2)	0.0137(18)	-0.0159(19)	-0.0090(18)
C2	0.087(3)	0.052(3)	0.078(3)	0.026(2)	-0.029(3)	-0.004(3)
C3	0.083(3)	0.048(3)	0.087(4)	-0.005(3)	-0.036(3)	0.025(2)
C4	0.069(3)	0.068(3)	0.058(3)	-0.012(2)	-0.008(2)	0.031(2)
C5	0.060(2)	0.055(2)	0.042(2)	0.0023(18)	-0.0002(19)	0.019(2)
C6	0.045(2)	0.0284(17)	0.0365(19)	0.0007(15)	-0.0056(16)	-0.0009(15)
C7	0.0376(18)	0.0318(18)	0.0365(19)	0.0074(14)	0.0038(15)	-0.0004(14)
C8	0.0330(17)	0.0344(18)	0.0312(18)	0.0087(14)	0.0009(14)	0.0016(14)
C9	0.0356(17)	0.0381(19)	0.0346(18)	0.0075(15)	0.0021(15)	0.0021(15)
C10	0.0421(19)	0.041(2)	0.0362(19)	0.0057(16)	0.0010(15)	0.0111(16)
C11	0.047(2)	0.0306(19)	0.043(2)	0.0012(16)	-0.0013(17)	-0.0002(16)
C12	0.0360(18)	0.0324(18)	0.044(2)	0.0104(16)	-0.0025(15)	0.0020(15)
C13	0.0364(18)	0.0348(19)	0.0372(19)	0.0061(15)	0.0054(15)	0.0063(15)
C14	0.061(2)	0.054(2)	0.047(2)	-0.0057(18)	0.0137(19)	0.0100(19)
C15	0.099(4)	0.083(3)	0.047(3)	-0.008(2)	0.004(2)	0.008(3)
C16	0.088(3)	0.067(3)	0.083(3)	0.001(3)	0.018(3)	0.033(3)
C17	0.079(3)	0.081(3)	0.072(3)	-0.007(2)	0.037(3)	0.006(3)
C18	0.0379(19)	0.044(2)	0.066(3)	0.0126(19)	0.0076(18)	-0.0055(16)
C19	0.053(2)	0.064(3)	0.112(4)	0.018(3)	0.042(3)	-0.001(2)
C20	0.061(3)	0.060(3)	0.068(3)	0.020(2)	0.009(2)	-0.007(2)
C21	0.050(2)	0.085(3)	0.102(4)	0.031(3)	-0.014(2)	-0.016(2)
C22	0.0429(19)	0.043(2)	0.0350(19)	0.0053(16)	0.0010(16)	0.0054(16)
C23	0.059(2)	0.051(2)	0.042(2)	0.0063(18)	0.0016(18)	0.0044(19)
C24	0.070(3)	0.056(3)	0.066(3)	0.026(2)	-0.009(2)	-0.009(2)
C25	0.063(3)	0.101(4)	0.060(3)	0.035(3)	0.015(2)	-0.001(3)

	U_{11}	**U_{22}**	**U_{33}**	**U_{23}**	**U_{13}**	**U_{12}**
C26	0.098(4)	0.088(4)	0.063(3)	0.027(3)	0.038(3)	0.029(3)
C27	0.080(3)	0.057(3)	0.049(2)	0.014(2)	0.015(2)	0.015(2)
C28	0.087(3)	0.067(3)	0.063(3)	0.002(2)	-0.017(2)	-0.025(2)
C29	0.048(2)	0.110(4)	0.062(3)	0.037(3)	0.007(2)	0.021(2)
C30	0.080(3)	0.040(2)	0.058(3)	0.0046(19)	0.023(2)	-0.009(2)
C31	0.121(4)	0.039(3)	0.097(4)	-0.002(3)	0.061(4)	0.006(3)
C32	0.091(4)	0.063(3)	0.135(5)	0.032(4)	0.052(4)	0.028(3)
C33	0.069(3)	0.077(3)	0.095(4)	0.039(3)	0.021(3)	0.030(3)
C34	0.061(3)	0.060(3)	0.061(3)	0.019(2)	0.015(2)	0.021(2)
C35	0.056(2)	0.0322(19)	0.046(2)	0.0099(16)	0.0173(18)	0.0001(16)
C36	0.0392(19)	0.041(2)	0.0382(19)	0.0061(15)	-0.0005(15)	-0.0052(16)
C37	0.0389(19)	0.0380(19)	0.0349(19)	0.0065(15)	0.0070(15)	0.0041(15)
C38	0.0359(18)	0.043(2)	0.040(2)	0.0105(16)	0.0009(15)	0.0079(16)
C39	0.0319(17)	0.043(2)	0.0364(19)	0.0049(16)	0.0075(15)	0.0048(15)
C40	0.045(2)	0.041(2)	0.043(2)	0.0116(16)	0.0145(17)	0.0045(16)
C41	0.040(2)	0.049(2)	0.041(2)	0.0136(17)	0.0063(16)	0.0109(17)
C42	0.0363(18)	0.050(2)	0.038(2)	0.0069(17)	0.0007(16)	0.0037(16)
C43	0.050(2)	0.070(3)	0.058(3)	0.026(2)	-0.0029(19)	0.014(2)
C44	0.093(3)	0.108(4)	0.055(3)	0.038(3)	-0.004(2)	0.008(3)
C45	0.087(4)	0.094(4)	0.114(4)	0.031(3)	0.002(3)	0.047(3)
C46	0.063(3)	0.116(4)	0.095(4)	0.049(3)	-0.026(3)	-0.004(3)
C47	0.0364(19)	0.047(2)	0.050(2)	0.0061(18)	0.0040(17)	-0.0021(16)
C48	0.049(2)	0.107(4)	0.082(3)	0.000(3)	0.020(2)	-0.015(2)
C49	0.074(3)	0.058(3)	0.071(3)	0.003(2)	-0.006(2)	-0.004(2)
C50	0.042(2)	0.067(3)	0.088(3)	0.016(2)	-0.018(2)	-0.004(2)
C51	0.071(3)	0.062(3)	0.064(3)	-0.008(2)	0.012(2)	-0.011(2)
C52	0.066(3)	0.061(3)	0.068(3)	0.017(2)	0.015(2)	0.020(2)
C53	0.049(2)	0.048(2)	0.041(2)	0.0070(17)	0.0153(17)	0.0118(18)
C54	0.055(3)	0.096(4)	0.082(3)	0.048(3)	0.014(2)	0.016(2)
C55	0.085(4)	0.116(4)	0.104(4)	0.071(4)	0.037(3)	0.046(4)
C56	0.117(5)	0.057(3)	0.117(5)	0.038(3)	0.069(4)	0.029(3)
C57	0.112(4)	0.064(3)	0.100(4)	0.010(3)	0.027(4)	-0.029(3)
C58	0.085(3)	0.068(3)	0.066(3)	0.014(2)	0.007(2)	-0.021(3)
O1	0.0720(18)	0.0378(15)	0.0693(18)	-0.0091(13)	0.0071(14)	-0.0085(13)
O2	0.0651(17)	0.0560(16)	0.0669(18)	0.0297(14)	0.0098(14)	-0.0021(13)
Si1	0.0402(5)	0.0450(6)	0.0390(6)	0.0096(4)	-0.0016(4)	-0.0024(4)
Si2	0.0420(5)	0.0397(5)	0.0422(6)	0.0077(4)	0.0056(4)	0.0022(4)

Table 8. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for 2g.

	x/a	y/b	z/c	U(eq)
H2	0.0876	0.6446	0.5051	0.088
H3	-0.0876	0.6544	0.5810	0.091
H4	-0.0880	0.5730	0.6739	0.08
H5	0.0835	0.4809	0.6893	0.063
H7	0.3719	0.4548	0.5828	0.042
H9	0.3864	0.3249	0.5103	0.043
H13	0.0745	0.3374	0.6361	0.043
H15A	0.1416	0.1111	0.3689	0.118
H15B	0.2686	0.1151	0.3220	0.118
H15C	0.1956	0.1997	0.3458	0.118
H16A	0.4490	0.0982	0.4928	0.117
H16B	0.4260	0.0544	0.4114	0.117
H16C	0.3045	0.0457	0.4612	0.117
H17A	0.4241	0.2753	0.3962	0.116
H17B	0.4999	0.1911	0.3752	0.116
H17C	0.5196	0.2396	0.4553	0.116
H19A	-0.0650	0.2648	0.6940	0.111
H19B	-0.2185	0.2229	0.6664	0.111
H19C	-0.1523	0.3003	0.6317	0.111
H20A	-0.0063	0.0614	0.5999	0.094
H20B	-0.1295	0.0796	0.6480	0.094
H20C	0.0235	0.1228	0.6748	0.094
H21A	-0.2031	0.2063	0.5077	0.12
H21B	-0.2772	0.1400	0.5509	0.12
H21C	-0.1643	0.1097	0.4997	0.12
H23	0.3177	0.2651	0.7258	0.061
H24	0.1895	0.1930	0.8017	0.077
H25	0.0812	0.2728	0.8909	0.087
H26	0.1086	0.4213	0.9068	0.094
H27	0.2308	0.4931	0.8298	0.072
H28A	0.3501	0.5888	0.7509	0.115
H28B	0.4912	0.5902	0.7146	0.115
H28C	0.4884	0.5665	0.7928	0.115
H29A	0.6062	0.3870	0.7409	0.105
H29B	0.6176	0.4235	0.6679	0.105
H29C	0.5341	0.3326	0.6681	0.105
H31	0.0393	1.1358	0.9826	0.1

	x/a	**y/b**	**z/c**	**U(eq)**
H32	-0.1366	1.1228	0.8881	0.109
H33	-0.1318	1.0237	0.7875	0.091
H34	0.0427	0.9318	0.7792	0.07
H36	0.3393	0.9343	0.9067	0.048
H38	0.0173	0.8033	0.8469	0.047
H42	0.3768	0.8244	0.9755	0.05
H44A	0.2497	0.7396	1.1318	0.125
H44B	0.3398	0.6642	1.1494	0.125
H44C	0.1920	0.6420	1.1042	0.125
H45A	0.3073	0.5538	1.0064	0.143
H45B	0.4590	0.5794	1.0467	0.143
H45C	0.4249	0.5986	0.9676	0.143
H46A	0.5307	0.7502	1.0220	0.136
H46B	0.5418	0.7237	1.0996	0.136
H46C	0.4606	0.8037	1.0843	0.136
H48A	-0.1825	0.6273	0.9711	0.122
H48B	-0.3100	0.6321	0.9137	0.122
H48C	-0.2268	0.7182	0.9559	0.122
H49A	-0.0328	0.5638	0.8090	0.105
H49B	-0.1917	0.5381	0.8168	0.105
H49C	-0.0759	0.5316	0.8799	0.105
H50A	-0.2017	0.7613	0.8338	0.101
H50B	-0.2750	0.6705	0.7951	0.101
H50C	-0.1250	0.7033	0.7770	0.101
H51A	0.2502	0.7718	0.6773	0.102
H51B	0.1234	0.8212	0.7035	0.102
H51C	0.1726	0.7439	0.7415	0.102
H52A	0.4595	0.7660	0.8303	0.095
H52B	0.5540	0.8547	0.8381	0.095
H52C	0.5258	0.7940	0.7629	0.095
H54	0.2221	0.9586	0.6646	0.088
H55	0.2944	1.0769	0.6119	0.111
H56	0.5000	1.1611	0.6584	0.108
H57	0.6328	1.1257	0.7545	0.112
H58	0.5594	1.0087	0.8082	0.089