Enantioselective Hydroxylation of Dihydrosilanes to Si-Chiral Silanols Catalyzed by In Situ Generated Copper(II) Species

W. Yang+, L. Liu+, J. Guo+, S.-G. Wang, J.-Y. Zhang, L.-W. Fan, Y. Tian, L.-L. Wang, C. Luan, Z.-L. Li, C. He, X. Wang,* Q.-S. Gu,* and X.-Y. Liu*

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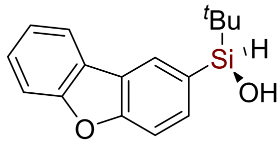


36

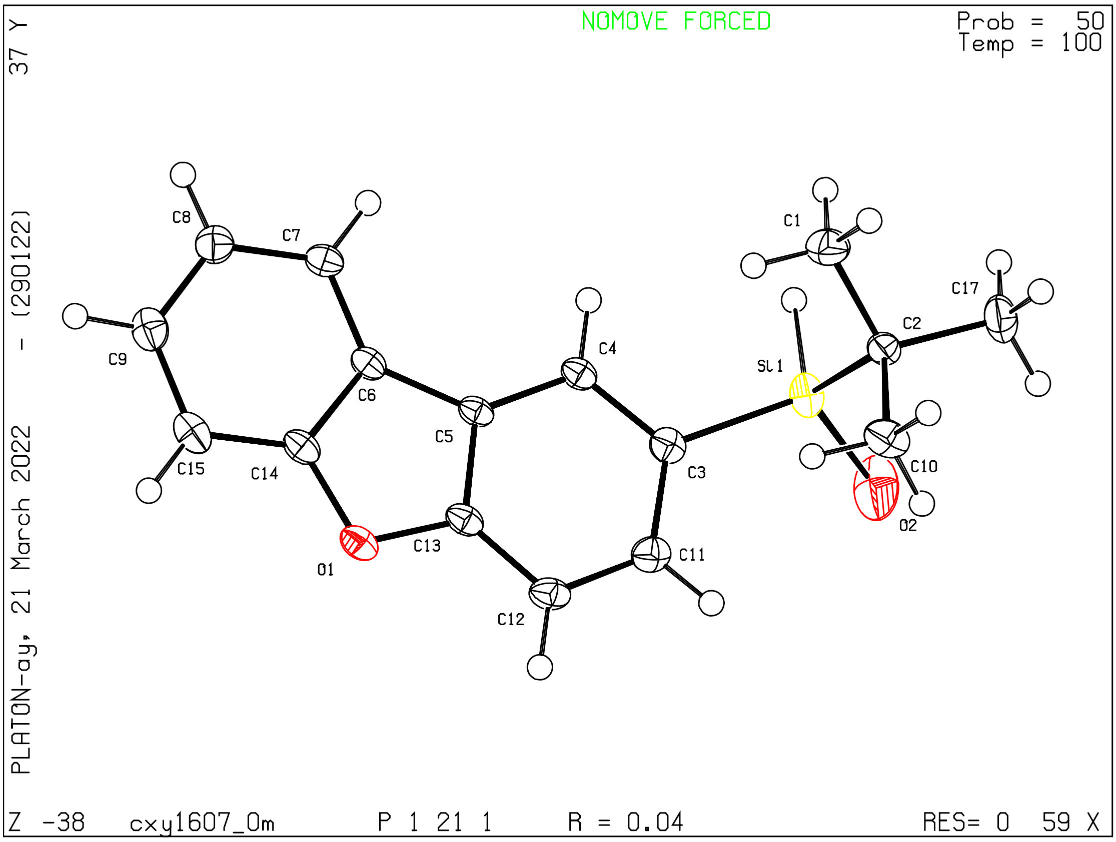
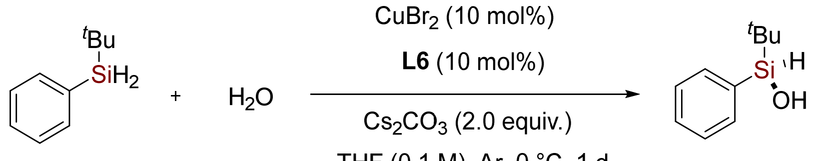


Figure S1. The X-ray structure of (*R*)-*tert*-butyl(dibenzo[*b*,*d*]furan-2-yl)silanol **36** (CCDC 2143892).

Investigation of nonlinear effect:



S1 1

entry	1	2	3	4	5	6	7	8	9	10	11
ee of **L6** (%)	−100	−80	−60	−40	−20	0	+20	+40	+60	+80	+100
ee of **1** (%)	−92	−72	−55	−35	−17	0	+17	+35	+53	+74	+95

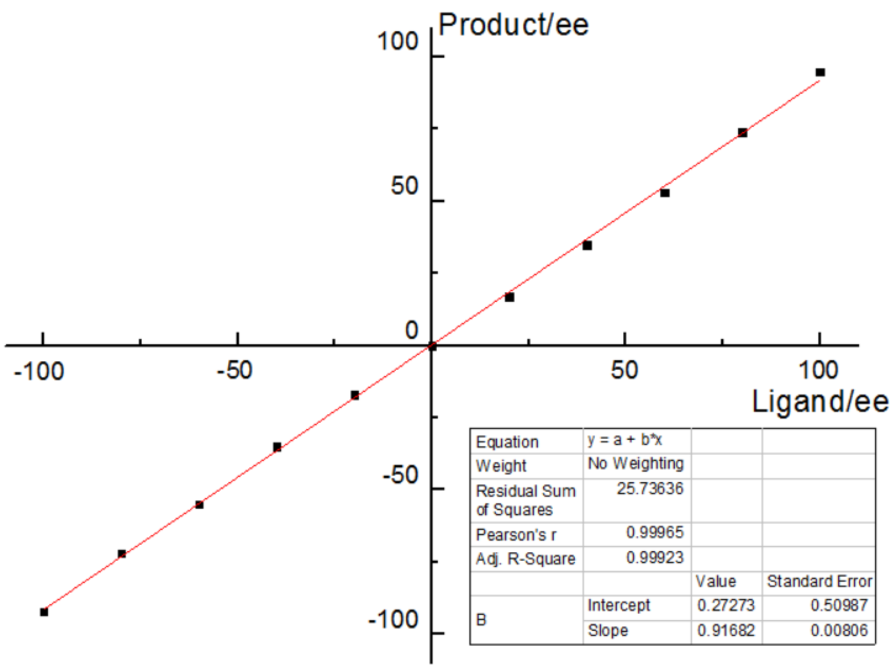


Figure S2. The linear relationship between the ligand ee values and the product ee values.

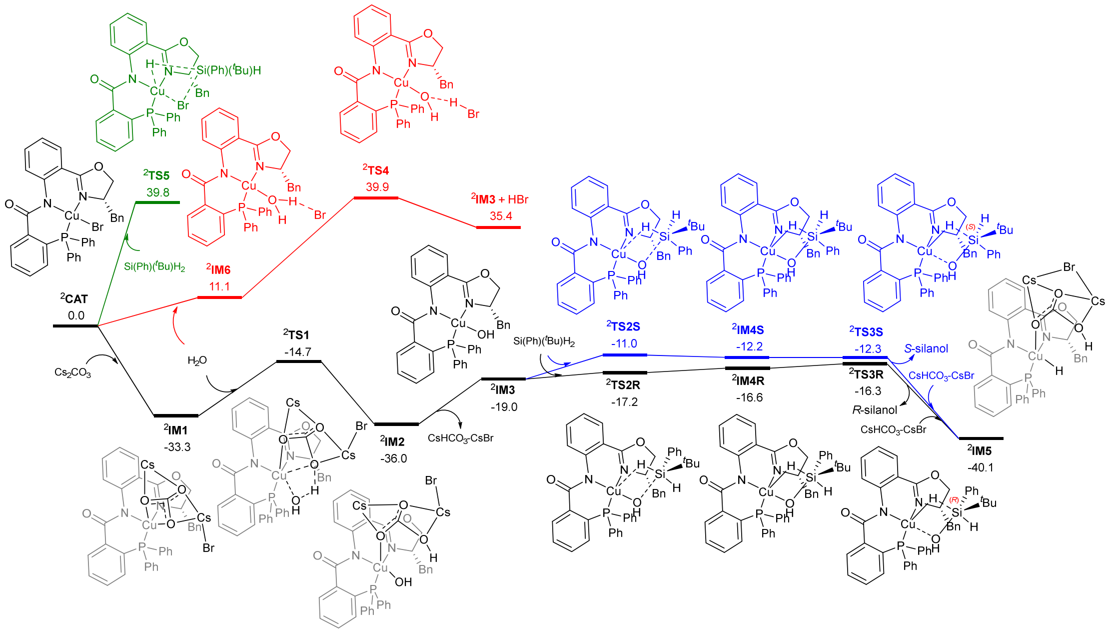
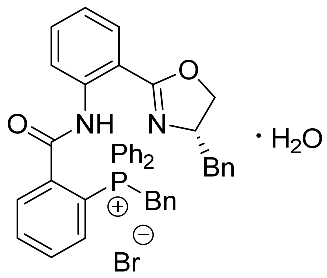


Figure S3. Free energy profile for the complete pathway of ²**CAT**-mediated asymmetric formation of the silanol **1**.



L7·H_2O

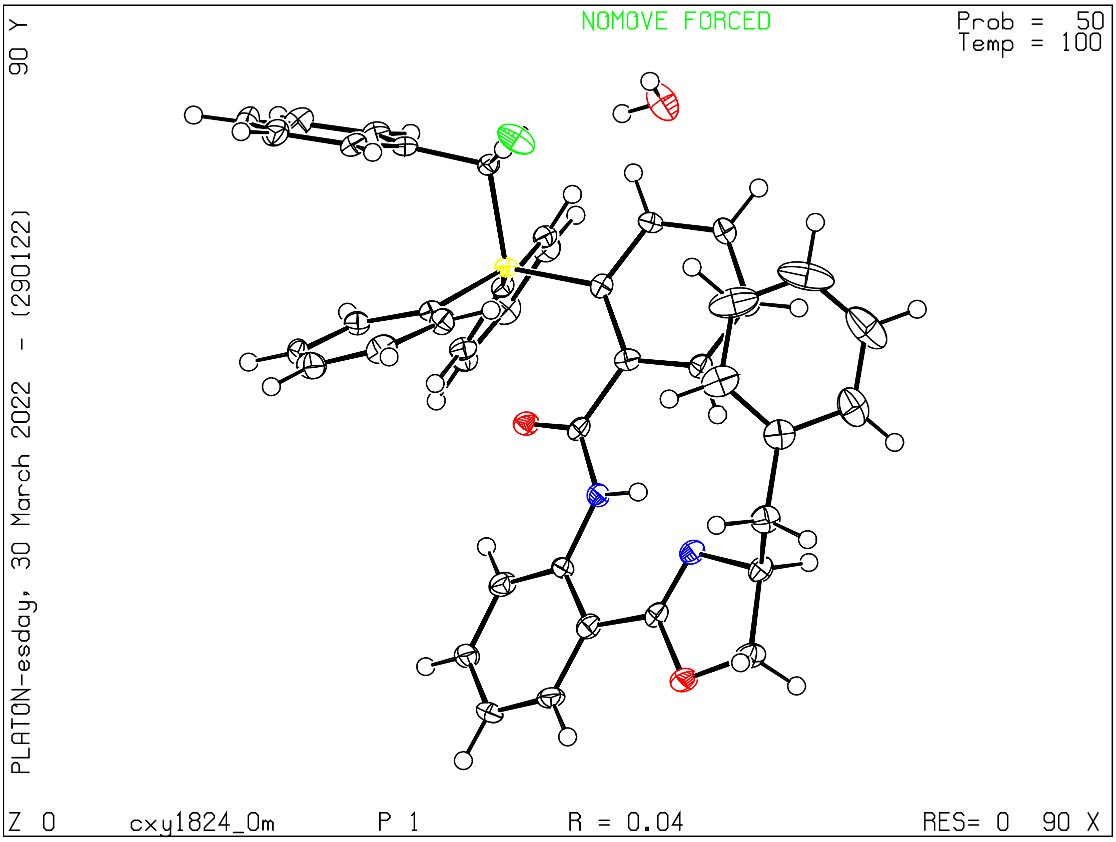
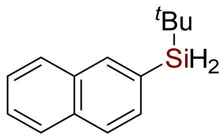


Figure S2. The X-ray structure of **L7**·H_2O (CCDC 2143891).



S32

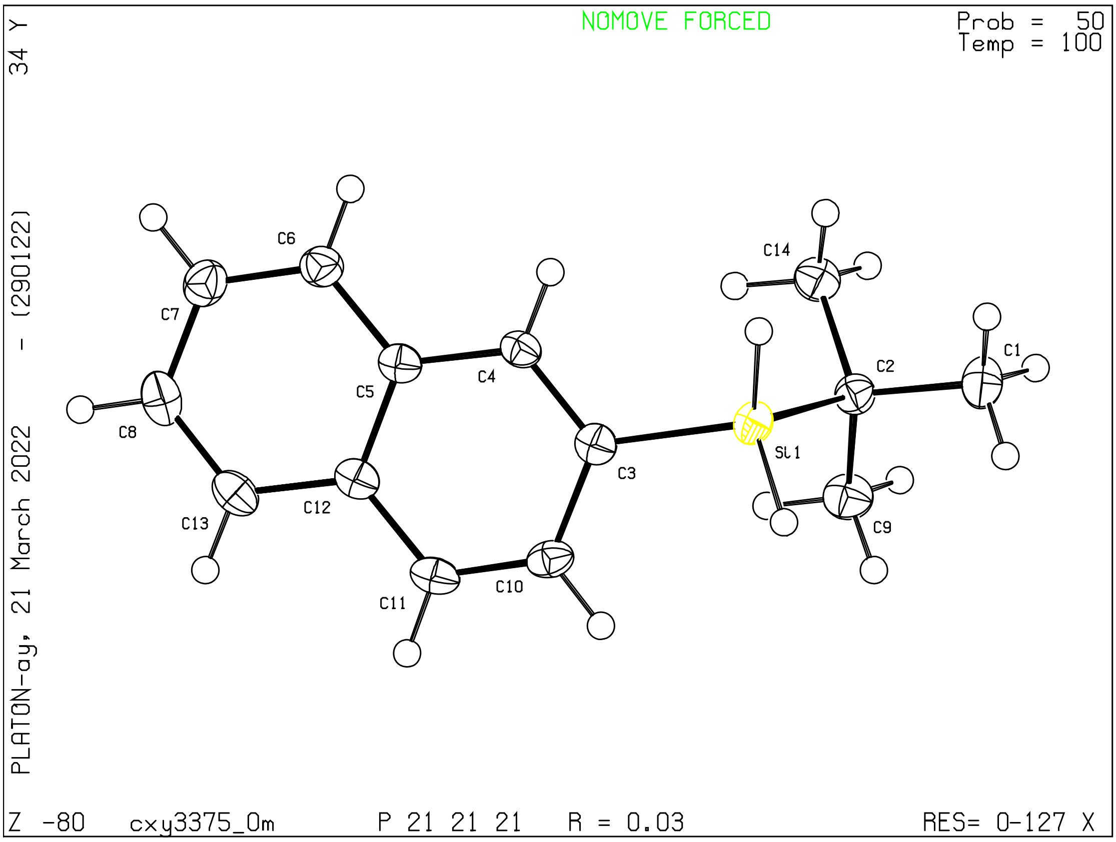
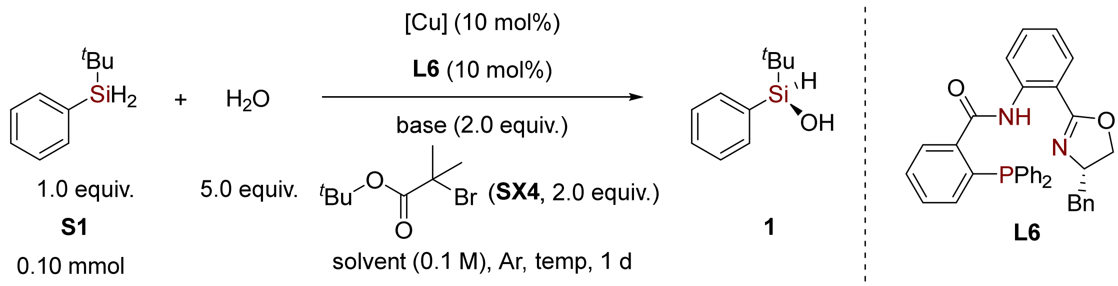


Figure S3. The X-ray structure of *tert*-butyl(naphthalen-2-yl)silane **S32** (CCDC 2143890).

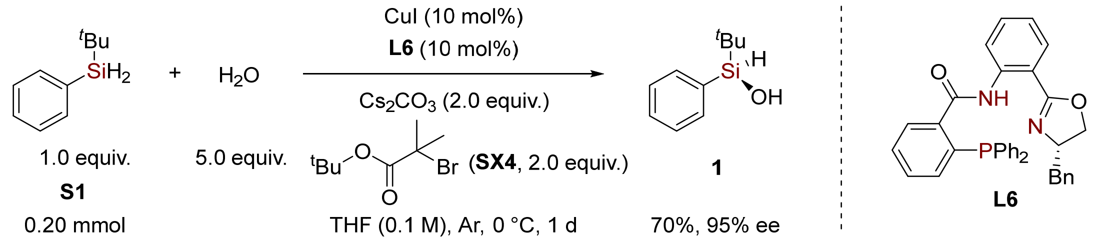
Table S1: Reaction conditions optimization.[a]



entry	[Cu]	base	solvent	temp/°C	**1** NMR yield/%	**1** *ee*/%
1	CuI	Cs_2CO_3	THF	0	68	95
2	$CuBr_2$	Cs_2CO_3	THF	0	70	95
3	$Cu(OTf)_2$	Cs_2CO_3	THF	0	72	95
4	$Cu(hfa)_2$	Cs_2CO_3	THF	0	71	95
5	CuTc	Cs_2CO_3	THF	0	67	95
6	$Cu(PPh_3)_2BH_4$	Cs_2CO_3	THF	0	11	86
7	CuI	K_2CO_3	THF	0	47	91
8	CuI	Na_2CO_3	THF	0	<5	---
9	CuI	Cs_2CO_3	CH_3CN	0	26	89
10	CuI	Cs_2CO_3	DCE	0	13	90
11	CuI	Cs_2CO_3	THF	RT	63	91
12	CuI	Cs_2CO_3	THF (in air)	0	31	59

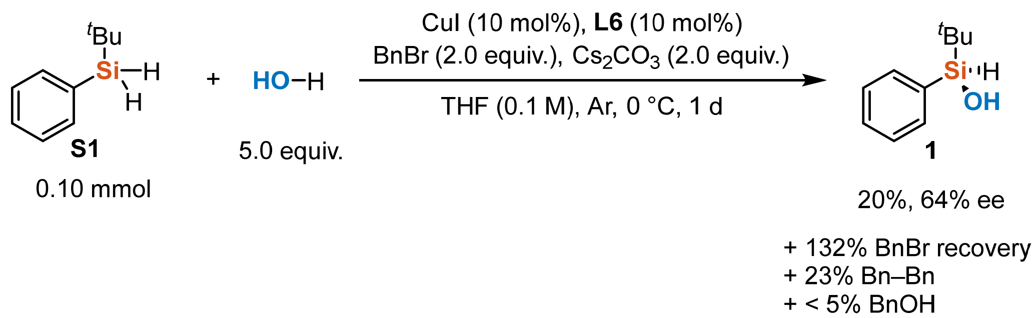
[a] Reaction conditions: **S1** (0.10 mmol), H_2O (0.50 mmol), [Cu] (0.01 mmol), **L6** (0.01 mmol), base (0.20 mmol), **SX4** (0.20 mmol), and solvent (1.0 mL) under Ar for 1 d. Yields were based on ^1H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard. The ee values were based on chiral HPLC analysis. OTf, trifluoromethanesulfonate; Hfa, hexafluoroacetylacetonate; Tc, thiophene-2-carboxylate.

Table S2: Control experiments.[a]

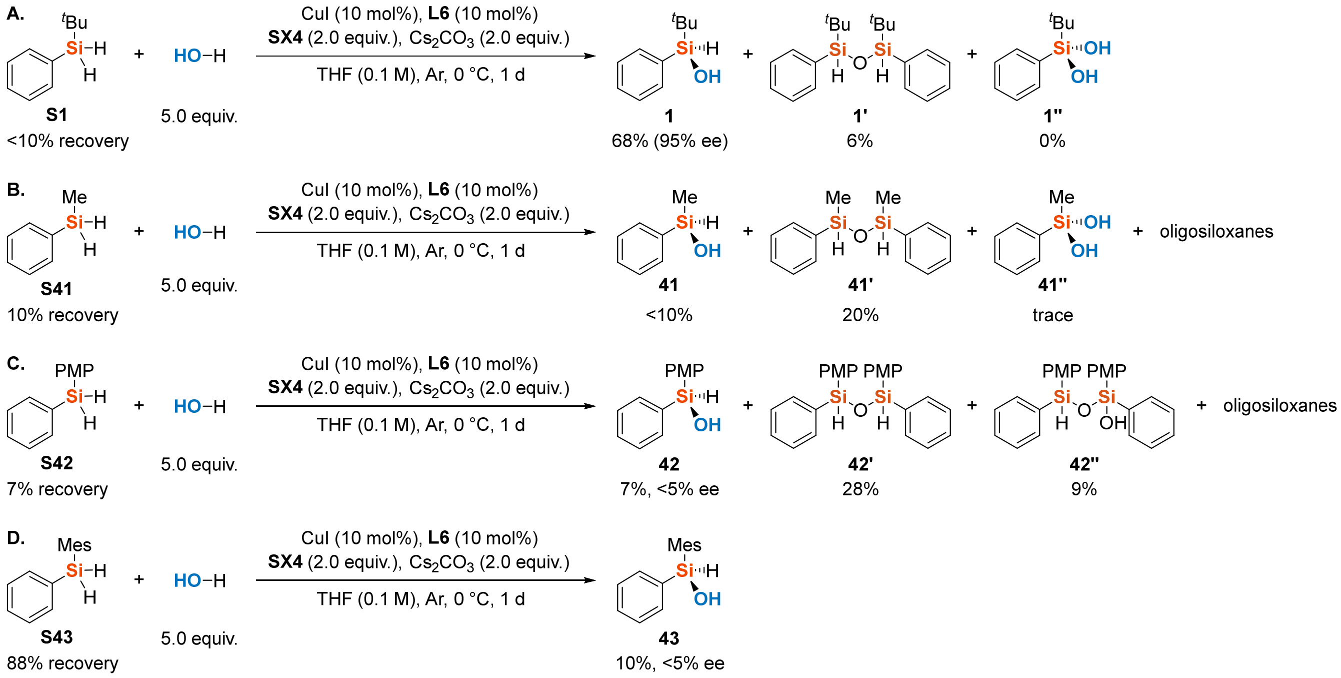


entry	variations	**1** NMR yield/%	**1** *ee*/%
1[a]	none	70	95
2	without CuI	<5	---
3	without **L6**	<5	---
4	without **SX4**	<5	---
5	without H_2O	<5	---
6	without Cs_2CO_3	<5	---

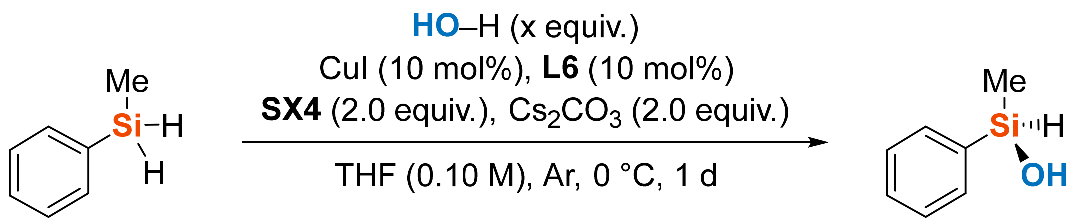
[a] Standard reaction conditions: **S1** (0.20 mmol), H_2O (1.0 mmol), CuI (0.02 mmol), **L6** (0.02 mmol), Cs_2CO_3 (0.40 mmol), **SX4** (0.40 mmol), and THF (2.0 mL) under Ar at 0 °C for 1 d. Yields were isolated yields. The ee values were based on chiral HPLC analysis.



Scheme S1. Results of the enantioselective hydroxylation reaction with BnBr.



Scheme S2. Results of the enantioselective hydroxylation reaction with **S1**, **S41**, **S42**, and **S43**.



S1

1

With 1.0 equiv. H_2O: 52%, 93% ee

With 2.5 equiv. H_2O: 57%, 94% ee

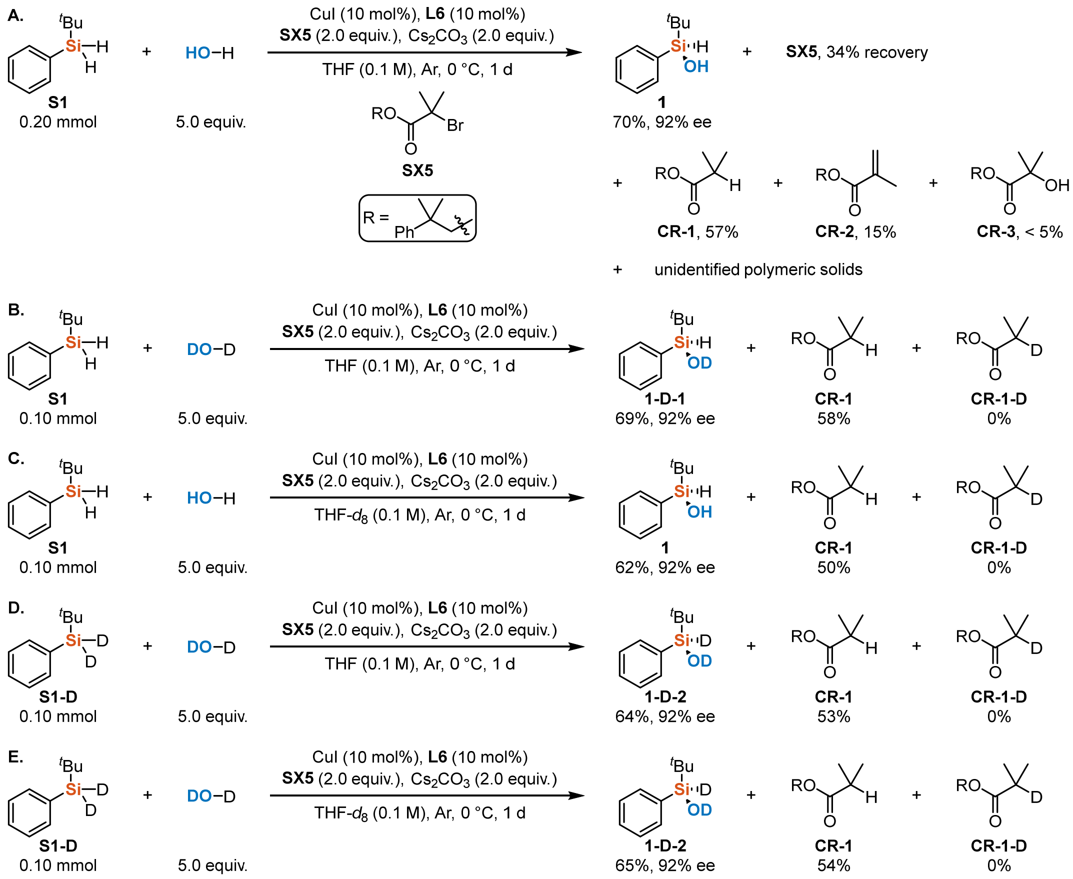
With 5.0 equiv. H_2O: 68%, 95% ee

With 10 equiv. H_2O: 50%, 91% ee

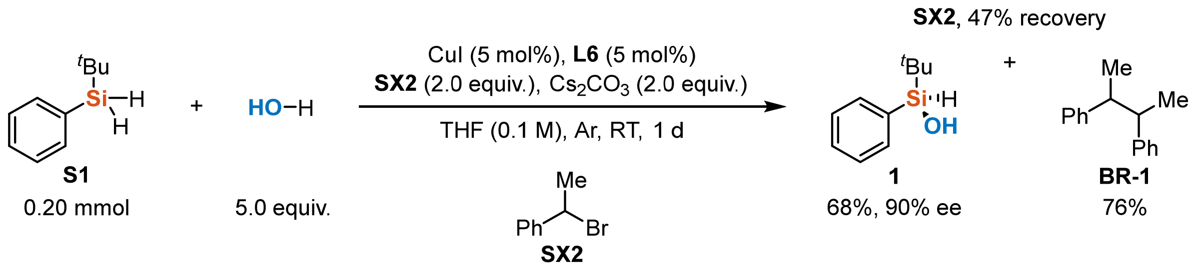
With 20 equiv. H_2O: 35%, 88% ee

With 50 equiv. H_2O: 27%, 81% ee

Scheme S3. Water loading effects on the enantioselective hydroxylation reaction.



Scheme S4. Products of the enantioselective hydroxylation reaction with **SX5** and deuterium-labeling experiments.



Scheme S5. Products of the enantioselective hydroxylation reaction with **SX2**.

1. General Information

Reactions were carried out under an atmosphere of Ar using Schlenk techniques unless otherwise stated. Reactions were monitored by analytical thin-layer chromatography (TLC) on pre-coated silica gel 60 F254 plates. Visualization on TLC was achieved by use of UV light (254 nm), iodine or a basic $KMnO_4$ indicator. Column chromatography was performed using GENERAL-REAGENT silica gel (200-300 mesh) or Tsingdao silica gel (200–300 mesh). As the eluent, petroleum ether (PE), hexane, ethyl acetate (EtOAc), dichloromethane (CH_2Cl_2), and methanol were purchased from Shanghai Titan Scientific Co. Ltd without further purification. Unless otherwise specified, all reagents were purchased from commercial suppliers and directly used without further purification. $PhSiCl_3$ was purchased from Meryer Co. Ltd. Cs_2CO_3 was purchased from Bide Pharmatech Ltd. CH_2Cl_2 and THF were purified and dried using a solvent-purification system that contained activated alumina under argon. Anhydrous diethyl ether (Et_2O) was purchased from Shanghai Lingfeng Chemical Reagent Co. Ltd, which was treated by 4 Å Molecular sieve and distilled after refluxing with sodium and benzophenone.

NMR spectra were recorded on Bruker DRX-400 at 400 MHz for ^1H NMR, 101 MHz for ^{13}C NMR, 376 MHz for ^{19}F NMR, and 162 MHz for ^{31}P NMR respectively, in $CDCl_3$ with tetramethylsilane (TMS) as an internal standard. The chemical shifts are expressed in ppm and coupling constants are given in Hz.

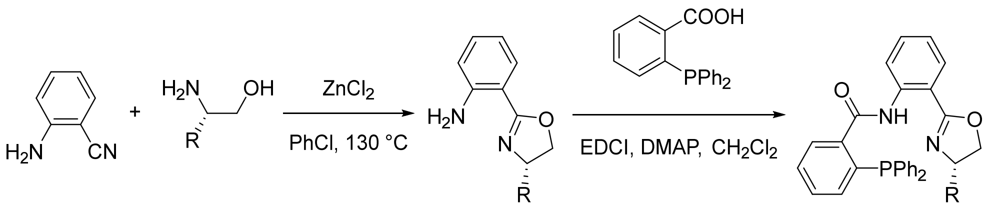
High-resolution mass spectrometry (HRMS) was performed on an Agilent Technologies 6230 TOF LC/MS under the conditions of electrospray ionization (ESI)/ atmospheric pressure chemical ionization (APCI) in a positive/negative mode using CH_2Cl_2 as the solvent.

Enantiomeric excess (ee) was determined using Agilent high-performance liquid chromatography (HPLC) with a Hatachi detector (at appropriate wavelength) or SHIMADZU LC-20AD with SPD-20AV detector.

2. Synthesis of Ligands

The ligands **L1** and **L2** were synthesized according to the literature reports.[1]

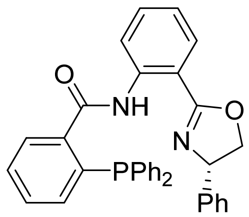
General Procedures for the Synthesis of Chiral Ligand (L3-L6)[1a]



Step A: Under argon atmosphere, a dry 100mL Schlenk flask equipped with a magnetic stir bar was charged with 2-aminobenzonitrile, *L*-amino alcohols (**SSL**), dry $ZnCl_2$ (1.0 equiv.), and 30 mL of chlorobenzene. The reaction mixture was refluxed (ca. 130 °C) for 1–3 d. Upon completion of the reaction monitored by TLC, water and 2 mL ethylenediamine were added. The mixture was extracted with EtOAc three times. The combined organic layer was evaporated under vacuum. The residue was purified by flash chromatography on silica gel to give 2-substituted aniline (**SL**) as a white solid.

Step B: Under argon atmosphere, to a solution of 2-substituted aniline (**SL**, 1 equiv.) in anhydrous CH_2Cl_2 (30 mL) was added 2-(diphenylphosphino)benzoic acid (2 equiv.), 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide hydrochloride (EDCI, 2 equiv.), and 4-dimethylaminopyridine (DMAP, 2 equiv.). The reaction mixture was stirred at ambient temperature for 24 h, concentrated, and purified by flash chromatography (PE/EtOAc = 5/1) to provide the chiral ligand as a white solid.

(S)-2-(diphenylphosphaneyl)-*N*-(2-(4-phenyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (L3)



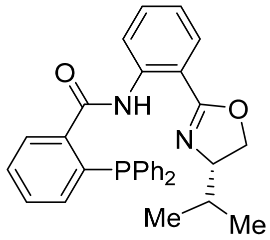
L3

According to the **General Procedures** starting from 2-aminobenzonitrile (2363 mg, 20 mmol) and (*S*)-2-amino-2-phenylethan-1-ol (**SLL3**, 4115 mg, 30 mmol) via **Step A**, 2-substituted aniline was obtained as a white solid (**SL3**, 3372 mg, 14.1 mmol, 71% yield). Through **Step B** with **SL3** (2383 mg, 10 mmol), 2-(diphenylphosphino)benzoic acid (6120 mg, 20 mmol), EDCI (3840 mg, 20 mmol), and DMAP (2440 mg, 20 mmol), the product **L3** was obtained as a white solid (4897 mg, 9.3 mmol, 93% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 12.82 (s, 1H), 8.78 (dd, *J* = 8.4, 1.1 Hz, 1H), 7.90 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.65 (ddd, *J* = 7.9, 3.8, 1.2 Hz, 1H), 7.51 – 7.40 (m, 1H), 7.39 – 7.17 (m, 16H), 7.09 (td, *J* = 7.7, 1.2 Hz, 1H), 7.02 – 6.88 (m,

2H), 5.43 (dd, J = 10.1, 8.6 Hz, 1H), 4.77 (dd, J = 10.1, 8.5 Hz, 1H), 4.26 (t, J = 8.5 Hz, 1H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 167.22, 164.74, 141.68, 141.02, 140.21, 138.91, 138.67, 138.58, 138.26, 134.78, 134.12, 133.91, 133.86, 133.66, 132.88, 130.32, 129.17, 128.87, 128.39, 128.32, 128.27, 127.85, 127.59, 127.55, 126.63, 122.47, 120.26, 113.19, 73.21, 69.91.
^{31}P NMR (162 MHz, $CDCl_3$) δ −7.85.
HRMS (ESI) *m/z* calcd. for $C_{34}H_{28}N_2O_2P$ $[M+H]^+$ 527.1883, found 527.1881.

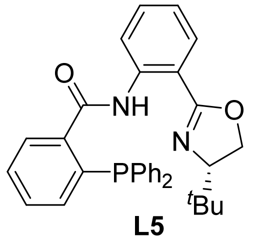
***(S)*-2-(diphenylphosphaneyl)-*N*-(2-(4-isopropyl-4,5-dihydrooxazol-2-yl)phenyl)benzamide (L4)**



L4

According to the **General Procedures** starting from 2-aminobenzonitrile (2363 mg, 20 mmol) and (*S*)-2-amino-3-methylbutan-1-ol (**SLL4**, 3095 mg, 30 mmol) via **Step A**, 2-substituted aniline was obtained as a white solid (**SL4**, 3983 mg, 19.5 mmol, 65% yield). Through **Step B** with **SL4** (2043 mg, 10 mmol), 2-(diphenylphosphino)benzoic acid (6120 mg, 20 mmol), EDCI (3840 mg, 20 mmol), and DMAP (2440 mg, 20 mmol), the product **L4** was obtained as a white solid (4433 mg, 9.0 mmol, 90% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 12.86 (s, 1H), 8.76 (d, J = 7.9 Hz, 1H), 7.88 (ddd, J = 7.5, 3.8, 1.4 Hz, 1H), 7.83 (dd, J = 7.9, 1.6 Hz, 1H), 7.46 – 7.25 (m, 13H), 7.11 – 6.97 (m, 2H), 4.38 (dd, J = 8.8, 7.4 Hz, 1H), 4.17 – 3.91 (m, 2H), 1.71 (dq, J = 13.3, 6.7 Hz, 1H), 0.88 (dd, J = 6.7, 4.0 Hz, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 167.30, 163.51, 141.50, 141.27, 140.01, 138.54, 138.36, 138.31, 138.29, 138.24, 138.18, 134.68, 133.96, 133.88, 133.76, 133.68, 132.42, 130.23, 128.89, 128.38, 128.32, 128.30, 128.26, 128.19, 127.41, 127.37, 122.27, 119.95, 113.28, 72.74, 69.41, 33.12, 18.93, 18.65.
^{31}P NMR (162 MHz, $CDCl_3$) δ −8.26.
HRMS (ESI) *m/z* calcd. for $C_{31}H_{30}N_2O_2P$ $[M+H]^+$ 493.2039, found 493.2038.

(S)-N-(2-(4-(tert-butyl)-4,5-dihydrooxazol-2-yl)phenyl)-2-(diphenylphosphaneyl)benzamide (L5)



L5

According to the **General Procedures** starting from 2-aminobenzonitrile (3544 mg, 30 mmol) and (*S*)-2-amino-3,3-dimethylbutan-1-ol (**SLL5**, 5273 mg, 45 mmol) via **Step A**, 2-substituted aniline was obtained as a white solid (**SL5**, 4960 mg, 22.7 mmol, 76% yield). Through **Step B** with **SL5** (1091 mg, 5 mmol), 2-(diphenylphosphino)benzoic acid (3060 mg, 10 mmol), EDCI (1917 mg, 10 mmol), and DMAP (1222 mg, 10 mmol), the product **L5** was obtained as a white solid (2388 mg, 4.7 mmol, 94% yield).

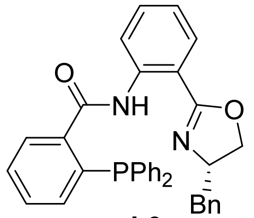
^{1}H NMR (400 MHz, CDCl$_3$) δ 12.83 (s, 1H), 8.82 – 8.62 (m, 1H), 7.96 – 7.67 (m, 2H), 7.50 – 7.26 (m, 13H), 7.14 – 7.01 (m, 2H), 4.30 (dd, *J* = 9.6, 8.1 Hz, 1H), 4.21 – 3.97 (m, 2H), 0.83 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 167.44, 163.52, 141.70, 141.47, 140.09, 138.37, 138.24, 138.20, 138.14, 138.09, 134.63, 134.02, 133.93, 133.82, 133.73, 132.45, 130.21, 128.92, 128.45, 128.36, 128.30, 128.23, 127.49, 127.45, 122.30, 120.02, 113.31, 76.18, 67.36, 33.71, 25.85.

^{31}P NMR (162 MHz, CDCl$_3$) δ −8.42.

HRMS (ESI) *m/z* calcd. for $C_{32}H_{32}N_2O_2P$ $[M+H]^+$ 507.2196, found 507.2194.

(S)-N-(2-(4-benzyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(diphenylphosphanyl)benzamide (L6)

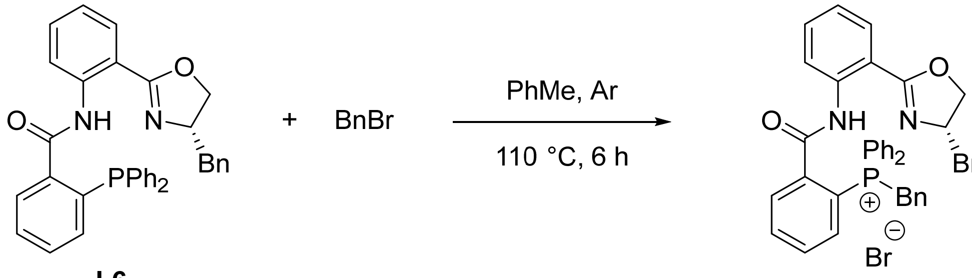


L6

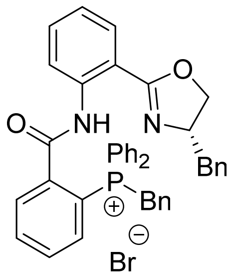
According to the **General Procedures** starting from 2-aminobenzonitrile (3544 mg, 30 mmol) and (*S*)-2-amino-3-phenylpropan-1-ol (**SSL6**, 6804 mg, 45 mmol) via **Step A**, 2-substituted aniline was obtained as a white solid (**SL6**, 5797 mg, 23.0 mmol, 77% yield). Through **Step B** with **SL6** (2523 mg, 10 mmol), 2-(diphenylphosphino)benzoic acid (6120 mg, 20 mmol), EDCI (3840 mg, 20 mmol), and DMAP (2440 mg, 20 mmol), the product **L6** was obtained as a white solid (5260 mg, 9.7 mmol, 97% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 12.70 (s, 1H), 8.77 (d, *J* = 8.4 Hz, 1H), 7.83 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.80 – 7.73 (m, 1H), 7.38 – 7.45 (m, 1H), 7.37 – 7.26 (m, 12H), 7.24 – 7.12 (m, 5H), 7.10 – 7.02 (m, 2H), 4.63 (dq, *J* = 9.4, 7.3 Hz, 1H),

4.36 (dd, J = 9.3, 8.5 Hz, 1H), 4.09 (dd, J = 8.5, 7.5 Hz, 1H), 3.07 (dd, J = 13.9, 6.6 Hz, 1H), 2.80 (dd, J = 13.9, 7.4 Hz, 1H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 167.22, 163.97, 141.23, 141.01, 140.00, 138.76, 138.53, 138.44, 138.32, 137.49, 134.81, 133.93, 133.83, 133.72, 133.63, 132.56, 130.31, 128.94, 128.49, 128.28, 128.25, 128.21, 128.19, 127.31, 127.27, 126.53, 122.30, 120.02, 113.18, 70.67, 67.60, 42.01.
^{31}P NMR (162 MHz, CDCl$_3$) δ −8.09.
HRMS (ESI) *m/z* calcd. for $C_{35}H_{30}N_2O_2P$ $[M+H]^+$ 541.2039, found 541.2038.



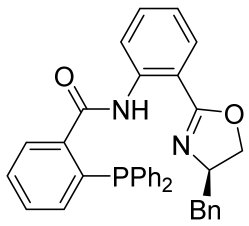
***(S)*-benzyl(2-((2-(4-benzyl-4,5-dihydrooxazol-2-yl)phenyl)carbamoyl)phenyl)diphenylphosphonium bromide (L7)**



L7

The reaction of **L6** (108.1 mg, 0.2 mmol) with BnBr (41.0 mg, 0.24 mmol, 1.2 eq) in PhMe (1 mL) at 110 °C for 6 h gave **L7** as a white solid (65.0 mg, 0.09 mmol, 46% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 13.24 (s, 1H), 8.13 (d, J = 8.4 Hz, 1H), 8.08 (dd, J = 14.4, 7.6 Hz, 1H), 7.93 – 7.74 (m, 3H), 7.67 – 7.55 (m, 7H), 7.55 – 7.44 (m, 4H), 7.35 (ddd, J = 8.7, 7.4, 1.6 Hz, 1H), 7.26 – 7.06 (m, 9H), 7.06 – 6.99 (m, 2H), 5.37 – 5.09 (m, 2H), 4.82 (p, J = 7.4 Hz, 1H), 4.49 (t, J = 8.9 Hz, 1H), 4.20 (dd, J = 8.5, 6.9 Hz, 1H), 3.12 – 2.83 (m, 2H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 164.64, 164.62, 164.10, 139.81, 139.75, 138.36, 138.31, 138.20, 137.45, 135.37, 135.34, 133.68, 133.65, 133.03, 132.93, 132.83, 132.49, 132.35, 131.12, 131.06, 129.53, 129.50, 129.40, 129.38, 129.23, 128.92, 128.72, 128.62, 128.59, 128.49, 128.15, 128.11, 128.05, 127.97, 126.62, 123.65, 121.27, 121.18, 120.38, 120.30, 119.38, 118.80, 117.94, 113.73, 71.34, 67.31, 42.30, 33.34, 32.84.
^{31}P NMR (162 MHz, CDCl$_3$) δ 26.41.
HRMS (ESI) *m/z* calcd. for $C_{42}H_{36}N_2O_2P$ $[M-Br]^+$ 631.2509, found 631.2504.

(*R*)-*N*-(2-(4-benzyl-4,5-dihydrooxazol-2-yl)phenyl)-2-(diphenylphosphanyl)benzamide (*ent*-L6)



***ent*-L6**

According to the **General Procedures** starting from 2-aminobenzonitrile (3544 mg, 30 mmol) and (*R*)-2-amino-3-phenylpropan-1-ol (*ent*-**SSL6**, 6804 mg, 45 mmol) via **Step A**, 2-substituted aniline was obtained as a white solid (*ent*-**SL6**, 6037 mg, 23.9 mmol, 80% yield). Through **Step B** with *ent*-**SL6** (1262 mg, 5 mmol), 2-(diphenylphosphino)benzoic acid (3063 mg, 10 mmol), EDCI (1917 mg, 10 mmol), and DMAP (1222 mg, 10 mmol), the product *ent*-**L6** was obtained as a white solid (2226 mg, 4.12 mmol, 82% yield).

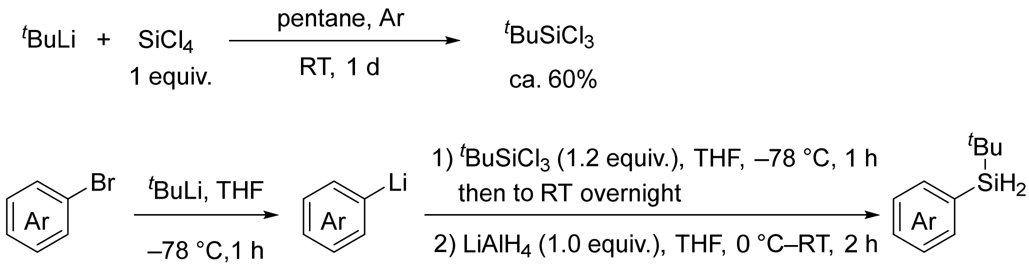
^{1}H NMR (400 MHz, CDCl$_3$) 12.72 (s, 1H), 8.77 (d, *J* = 8.2 Hz, 1H), 7.82 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.80 – 7.73 (m, 1H), 7.45 – 7.38 (m, 1H), 7.36 – 7.23 (m, 12H), 7.23 – 7.12 (m, 5H), 7.10 – 7.01 (m, 2H), 4.61 (dq, *J* = 9.5, 7.2 Hz, 1H), 4.34 (t, *J* = 8.9 Hz, 1H), 4.07 (t, *J* = 8.0 Hz, 1H), 3.05 (dd, *J* = 13.8, 6.6 Hz, 1H), 2.78 (dd, *J* = 13.8, 7.4 Hz, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 167.25, 163.99, 141.26, 141.03, 140.01, 138.78, 138.55, 138.45, 138.33, 137.51, 134.83, 133.95, 133.85, 133.75, 133.65, 132.58, 130.32, 128.96, 128.51, 128.30, 128.27, 128.23, 128.20, 127.33, 127.29, 126.55, 122.32, 120.05, 113.20, 70.68, 67.63, 42.04.

^{31}P NMR (162 MHz, CDCl$_3$) δ −8.12.

3. Synthesis of Substrate and Characterization

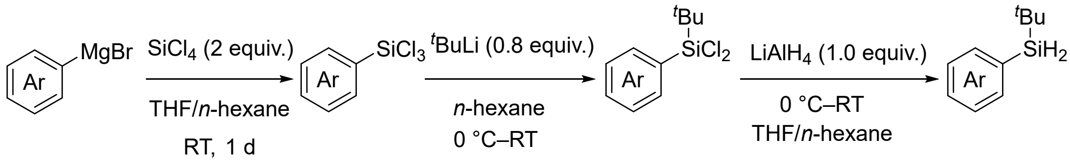
General Procedures A:



The synthesis was adapted from the reported literature.[2] To a stirred solution of $SiCl_4$ (100 mmol) in pentane (30 mL) at RT was added ^tBuLi (77 mL, 1.3 M in pentane) dropwise. The mixture was stirred at RT for 24 h. After the reaction, the mixture was filtered through a pad of Celite eluting with hexane. The filtrate was concentrated under vacuum to give a light yellow oil. It was purified by distillation to give $^tBuSiCl_3$ as a waxy solid in ca. 60% yield.

To a stirred solution of ArBr (2.5 mmol) in THF (10 mL) was added a solution of ^tBuLi in pentane (1.3 M, 2.5–5.0 mmol) dropwise at −78 °C. After the addition, the mixture was stirred at –78 °C for 1 h to give ArLi. A solution of $^tBuSiCl_3$ (575 mg, 3 mmol, 1.2 eq) in THF was added dropwise into the solution of ArLi at −78 °C. The mixture was stirred at −78 °C for 1 h, then warmed to RT overnight to give $Ar(^tBu)SiCl_2$. A solution of $LiAlH_4$ in THF (2.5 M, 1 mL, 2.5 mmol, 1 eq) was directly added dropwise into the solution of $Ar(^tBu)SiCl_2$ at 0 °C. The mixture was stirred at 0 °C for about 1 h, then warmed to RT for 3 h. The reaction was quenched with the careful addition of $Na_2SO_4\cdot 10H_2O$ at 0 °C. The mixture was filtered through a pad of silica eluting with EtOAc/hexane. The filtrate was concentrated under vacuum and further purified by column chromatography on silica gel eluting with PE to afford the desired product of $Ar(^tBu)SiH_2$.[3]

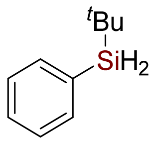
General Procedures B:



To a stirred solution of $SiCl_4$ (3.44 mL, 5.09 g, 30 mmol) in hexane (30 mL) under Ar at RT was added a solution of ArMgBr in THF (prepared by the reaction of 15 mmol ArBr with Mg), and the mixture was stirred at RT for 1 d. After the reaction, the mixture was quickly filtered through a pad of Celite eluting with hexane/CH_2Cl_2. The filtrate was concentrated under vacuum to give $ArSiCl_3$ and used in the next step without further purification.[4]

To the above-prepared $ArSiCl_3$ in hexane (20 mL) under Ar at 0 °C was added a solution of ^{t}BuLi in pentane (1.3 M, 9.23 mL, 12 mmol) dropwise, and the mixture was stirred at 0 °C for about 1 h, then warmed to RT overnight to give Ar(^{t}Bu)$SiCl_2$. A solution of $LiAlH_4$ in THF (2.5 M, 6 mL, 15 mmol, 1 eq) was directly added dropwise into the solution of Ar(^{t}Bu)$SiCl_2$ at 0 °C. The mixture was stirred at 0 °C for about 1 h, then warmed to RT for 3 h. The reaction was quenched with the careful addition of $Na_2SO_4{\cdot}10H_2O$ at 0 °C. The mixture was filtered through a pad of silica eluting with EtOAc/hexane. The filtrate was concentrated under vacuum and further purified by column chromatography on silica gel eluting with PE to afford the desired product of Ar(^{t}Bu)SiH_2.[5]

***tert*-butyl(phenyl)silane (S1)**[3]



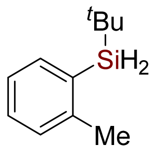
S1

According to the **General Procedures B** starting from $PhSiCl_3$ (10 mmol) with ^{t}BuLi in pentane (1.3 M, 7.69 mL, 10 mmol), the product **S1** was obtained as a colorless oil[3] (1154 mg, 7.0 mmol, 70% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.55 (m, 2H), 7.42-7.33 (m, 3H), 4.15 (s, 2H), 1.02 (s, 9H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.88, 132.21, 129.52, 127.81, 27.42, 16.41.

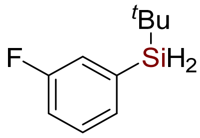
***tert*-butyl(*o*-tolyl)silane (S2)**



S2

According to the **General Procedures B** with 2-bromotoluene (2565 mg, 15 mmol), the product **S2** was obtained as a colorless oil (1357 mg, 7.6 mmol, 51% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.51 (dd, *J* = 7.2, 1.5 Hz, 1H), 7.30 (td, *J* = 7.5, 7.5, 1.6 Hz, 1H), 7.22 – 7.11 (m, 2H), 4.22 (s, 2H), 2.47 (s, 3H), 1.03 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ. 144.14, 137.51, 131.50, 129.93, 129.60, 124.80, 27.89, 23.37, 17.17.
HRMS (APCI) *m/z* calcd. for $C_{11}H_{19}Si$ $[M+H]^+$ 179.1251, found 179.1251.

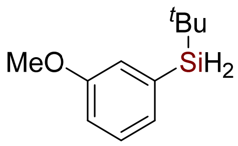
***tert*-butyl(3-fluorophenyl)silane (S3)**



S3

According to the **General Procedures B** using 1-bromo-3-fluorobenzene (2625 mg, 15 mmol), the product **S3** was obtained as a colorless oil (633 mg, 3.5 mmol, 23% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.40 – 7.30 (m, 2H), 7.30 – 7.22 (m, 1H), 7.15 – 7.04 (m, 1H), 4.15 (s, 2H), 1.02 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 162.35 (d, *J* = 248.5 Hz), 135.03 (d, *J* = 4.6 Hz), 131.46 (d, *J* = 3.2 Hz), 129.62 (d, *J* = 6.7 Hz), 122.08 (d, *J* = 18.9 Hz), 116.56 (d, *J* = 21.1 Hz), 27.35, 16.40.
^{19}F NMR (376 MHz, CDCl$_3$) δ −113.49.
HRMS (APCI) *m/z* calcd. for $C_{10}H_{16}FSi$ $[M+H]^+$ 183.1000, found 183.0999.

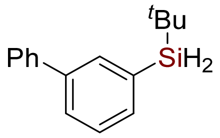
***tert*-butyl(3-methoxyphenyl)silane (S4)**



S4

According to the **General Procedures B** using 1-bromo-3-methoxybenzene (2805 mg, 15 mmol), the product **S4** was obtained as a colorless oil (484 mg, 2.5 mmol, 17% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.30 (t, *J* = 7.7 Hz, 1H), 7.14 (d, *J* = 7.1 Hz, 1H), 7.10 (d, *J* = 2.5 Hz, 1H), 6.94 (dd, *J* = 8.2, 2.2 Hz, 1H), 4.14 (s, 2H), 3.81 (s, 3H), 1.02 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 158.86, 133.64, 129.02, 128.18, 121.08, 115.04, 55.10, 27.45, 16.42.
HRMS (ESI) *m/z* calcd. for $C_{11}H_{19}OSi$ $[M+H]^+$ 195.1200, found 195.1199.

[1,1'-biphenyl]-3-yl(*tert*-butyl)silane (S5)



S5

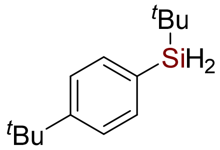
According to the **General Procedures B** using 3-bromo-1,1'-biphenyl (3496 mg, 15 mmol), the product **S5** was obtained as a colorless oil (1230 mg, 5.1 mmol, 34% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.79 (s, 1H), 7.66 – 7.53 (m, 4H), 7.49 – 7.41 (m, 3H), 7.39 – 7.31 (m, 1H), 4.21 (s, 2H), 1.05 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 141.22, 140.62, 134.75, 134.63, 132.76, 128.77, 128.45, 128.21, 127.30, 127.24, 27.47, 16.46.

HRMS (APCI) *m/z* calcd. for $C_{16}H_{21}Si$ $[M+H]^+$ 241.1407, found 241.1407.

***tert*-butyl(4-(*tert*-butyl)phenyl)silane (S6)**



S6

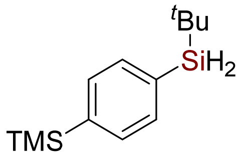
According to the **General Procedures B** using 1-bromo-4-(*tert*-butyl)benzene (3196 mg, 15 mmol), the product **S6** was obtained as a colorless oil (1900 mg, 8.6 mmol, 57% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.56 – 7.47 (m, 2H), 7.42 – 7.34 (m, 2H), 4.14 (s, 2H), 1.32 (s, 9H), 1.02 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 152.53, 135.84, 128.59, 124.82, 34.70, 31.24, 27.51, 16.49.

HRMS (APCI) *m/z* calcd. for $C_{14}H_{25}Si$ $[M+H]^+$ 221.1720, found 221.1720.

(4-(*tert*-butylsilyl)phenyl)trimethylsilane (S7)



S7

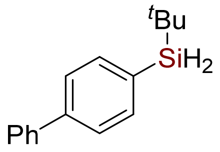
According to the **General Procedures B** using (4-bromophenyl)trimethylsilane (3438 mg, 15 mmol), the product **S7** was obtained as a colorless oil (2103 mg, 8.9 mmol, 59% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.63 – 7.56 (m, 2H), 7.54 (d, J = 7.9 Hz, 2H), 4.17 (s, 2H), 1.05 (s, 9H), 0.30 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 141.92, 135.10, 132.62, 27.47, 16.48, −1.23.

HRMS (APCI) *m/z* calcd. for $C_{13}H_{25}Si_2$ $[M+H]^+$ 237.1489, found 237.1489.

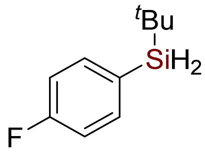
[1,1'-biphenyl]-4-yl(*tert*-butyl)silane (S8)



S8

According to the **General Procedures B** using 4-bromo-1,1'-biphenyl (3496 mg, 15 mmol), the product **S8** was obtained as a colorless oil (1281 mg, 5.3 mmol, 35% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.77 – 7.50 (m, 6H), 7.42 (t, *J* = 7.6, 7.6 Hz, 2H), 7.37 – 7.29 (m, 1H), 4.20 (s, 2H), 1.05 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 142.26, 140.87, 136.39, 130.90, 128.79, 127.50, 127.13, 126.52, 27.48, 16.49.
HRMS (APCI) *m/z* calcd. for $C_{16}H_{21}Si$ [M+H]$^+$ 241.1407, found 241.1407.

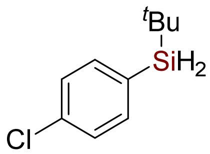
***tert*-butyl(4-fluorophenyl)silane (S9)**



S9

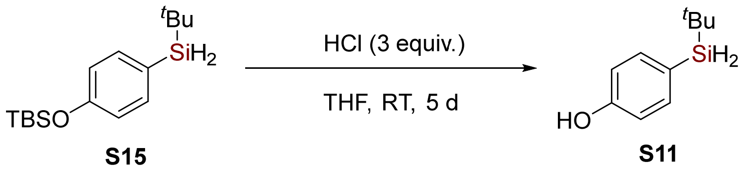
According to the **General Procedures B** using 1-bromo-4-fluorobenzene (2625 mg, 15 mmol), the product **S9** was obtained as a colorless oil (603 mg, 3.3 mmol, 22% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.63 – 7.45 (m, 2H), 7.18 – 6.94 (m, 2H), 4.15 (s, 2H), 1.00 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 164.13 (d, *J* = 249.0 Hz), 137.81 (d, *J* = 7.8 Hz), 127.64 (d, *J* = 4.3 Hz), 115.11 (d, *J* = 19.8 Hz), 27.31, 16.35.
^{19}F NMR (376 MHz, CDCl$_3$) δ −110.97.
HRMS (ESI) *m/z* calcd. for $C_{10}H_{16}FSi$ [M+H]$^+$ 183.1000, found 183.0999.

***tert*-butyl(4-chlorophenyl)silane (S10)**

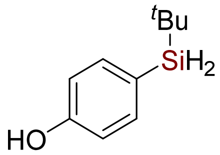


S10

According to the **General Procedures B** using 1-bromo-4-chlorobenzene (2870 mg, 15 mmol), the product **S10** was obtained as a colorless oil (964 mg, 4.85 mmol, 32% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.49 (d, *J* = 8.2 Hz, 2H), 7.34 (d, *J* = 8.2 Hz, 2H), 4.13 (s, 2H), 1.00 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 137.15, 136.07, 130.47, 128.12, 27.31, 16.35.
HRMS (APCI) *m/z* calcd. for $C_{10}H_{16}ClSi$ [M+H]$^+$ 199.0704, found 199.0704.



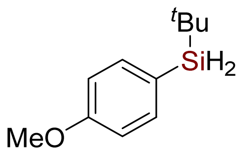
4-(*tert*-butylsilyl)phenol (S11)



S11

The reaction of *tert*-butyl(4-(*tert*-butylsilyl)phenoxy)dimethylsilane (**S15**, 2946 mg, 10 mmol) with aq. HCl (1 M, 30 mmol) in THF (50 mL) at RT for 5 d gave the product **S11** as a white solid (1620 mg, 9.0 mmol, 90% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.52 – 7.42 (m, 2H), 6.92 – 6.73 (m, 2H), 4.91 (s, 1H), 4.11 (s, 2H), 1.00 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 156.87, 137.58, 123.21, 115.05, 27.34, 16.42.
HRMS (APCI) *m/z* calcd. for $C_{10}H_{17}OSi$ $[M+H]^+$ 181.1043, found 181.1043.

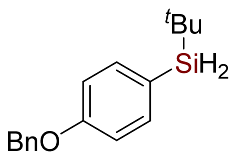
tert-butyl(4-methoxyphenyl)silane (S12)



S12

According to the **General Procedures B** using 1-bromo-4-methoxybenzene (2805 mg, 15 mmol), the product **S12** was obtained as a colorless oil (466 mg, 2.4 mmol, 16% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.49 (d, *J* = 8.0 Hz, 2H), 6.91 (d, *J* = 8.2 Hz, 2H), 4.12 (s, 2H), 3.82 (s, 3H), 1.00 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 160.85, 137.35, 122.91, 113.63, 54.99, 27.36, 16.44.
The obtained NMR spectral data are in good agreement with those reported in literature.[3]

(4-(benzyloxy)phenyl)(*tert*-butyl)silane (S13)



S13

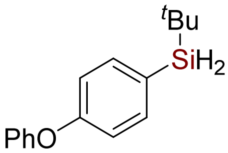
According to the **General Procedures B** using 1-(benzyloxy)-4-bromobenzene (3946 mg, 15 mmol), the product **S13** was obtained as a colorless oil (436 mg, 1.6 mmol, 11% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.65 – 7.25 (m, 7H), 6.98 (d, *J* = 7.9 Hz, 2H), 5.07 (s, 2H), 4.12 (s, 2H), 1.00 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 160.10, 137.38, 136.85, 128.59, 128.00, 127.49, 123.29, 114.50, 69.73, 27.37, 16.44.

HRMS (ESI) *m/z* calcd. for $C_{17}H_{22}NaOSi$ $[M+Na]^+$ 293.1332, found 293.1333.

***tert*-butyl(4-phenoxyphenyl)silane (S14)**



S14

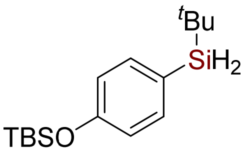
According to the **General Procedures B** using 1-bromo-4-phenoxybenzene (3438 mg, 15 mmol), the product **S14** was obtained as a colorless oil (511 mg, 2.0 mmol, 13% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.52 (d, *J* = 8.5 Hz, 2H), 7.35 (t, *J* = 7.9 Hz, 2H), 7.13 (t, *J* = 7.4 Hz, 1H), 7.04 (d, *J* = 7.8 Hz, 2H), 6.99 (d, *J* = 8.4 Hz, 2H), 4.14 (s, 2H), 1.02 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 158.95, 156.51, 137.52, 129.80, 125.94, 123.66, 119.46, 117.88, 27.37, 16.43.

HRMS (ESI) *m/z* calcd. for $C_{16}H_{21}OSi$ $[M+H]^+$ 257.1356, found 257.1354.

***tert*-butyl(4-(*tert*-butylsilyl)phenoxy)dimethylsilane (S15)**



S15

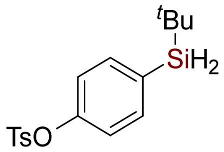
According to the **General Procedures B** using (4-bromophenoxy)(*tert*-butyl)dimethylsilane (4309 mg, 15 mmol), the product **S15** was obtained as a colorless oil in 38% yield (1665 mg, 5.65 mmol).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.48 (d, *J* = 8.0 Hz, 2H), 6.89 (d, *J* = 7.9 Hz, 2H), 4.17 (s, 2H), 1.04 (s, 9H), 1.03 (s, 9H), 0.25 (s, 6H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 157.15, 137.35, 123.71, 119.80, 27.41, 25.68, 18.21, 16.44, −4.36.

HRMS (ESI) *m/z* calcd. for $C_{16}H_{31}OSi_2$ $[M+H]^+$ 295.1908, found 295.1908.

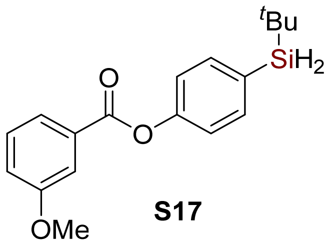
4-(*tert*-butylsilyl)phenyl 4-methylbenzenesulfonate (S16)



S16

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and TsCl (190.6 mg, 1.0 mmol) in the presence of Cs_2CO_3 (325.8 mg, 1.0 mmol) in CH_3CN (5 mL) at RT for 1 d gave the product **S16** as a colorless oil (284.9 mg, 0.85 mmol, 85% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.75 – 7.64 (m, 2H), 7.53 – 7.43 (m, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.03 – 6.94 (m, 2H), 4.11 (s, 2H), 2.45 (s, 3H), 0.98 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 150.90, 145.37, 137.21, 132.40, 131.41, 129.72, 128.47, 121.77, 27.28, 21.69, 16.32.
HRMS (ESI) *m/z* calcd. for $C_{17}H_{23}O_3SSi$ $[M+H]^+$ 335.1132, found 335.1130.

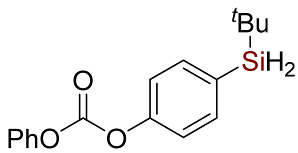
4-(*tert*-butylsilyl)phenyl 3-methoxybenzoate (S17)



S17

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and 3-methoxybenzoic acid (180.2 mg, 1.2 mmol) in the presence of EDCI (249.2 mg, 1.3 mmol) and DMAP (24.4 mg, 0.2 mmol) in DCM (5 mL) at RT for 1 d gave the product **S17** as a white solid (261.0 mg, 0.83 mmol, 83% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (dt, *J* = 7.7, 1.3 Hz, 1H), 7.70 (dd, *J* = 2.7, 1.5 Hz, 1H), 7.67 – 7.58 (m, 2H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.31 – 7.21 (m, 2H), 7.18 (ddd, *J* = 8.3, 2.7, 1.0 Hz, 1H), 4.18 (s, 2H), 3.88 (s, 3H), 1.04 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 164.85, 159.67, 152.29, 137.18, 130.73, 129.60, 122.58, 121.21, 120.20, 114.49, 55.49, 27.36, 16.42.
HRMS (ESI) *m/z* calcd. for $C_{18}H_{23}O_3Si$ $[M+H]^+$ 315.1411, found 315.1407.

4-(*tert*-butylsilyl)phenyl phenyl carbonate (S18)

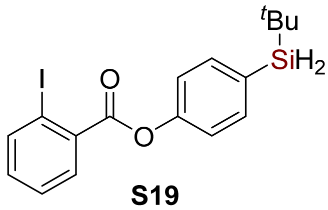


S18

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and phenyl carbonochloridate (0.15 mL, 1.2 mmol) in the presence of NEt_3 (0.28 mL, 2 mmol) in DCM (5 mL) at RT for 4 h gave the product **S18** as a white solid (266.3 mg, 0.89 mmol, 89% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.70 – 7.43 (m, 2H), 7.34 (dd, *J* = 8.7, 7.2 Hz, 2H), 7.25 – 7.16 (m, 5H), 4.09 (s, 2H), 0.94 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 152.24, 151.85, 150.93, 137.24, 130.37, 129.56, 126.32, 120.87, 120.36, 27.32, 16.39.
HRMS (ESI) *m/z* calcd. for $C_{17}H_{20}NaO_3Si$ $[M+Na]^+$ 323.1074, found 323.1072.

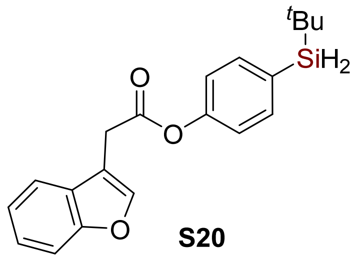
4-(*tert*-butylsilyl)phenyl 2-iodobenzoate (S19)



S19

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and 2-iodobenzoic acid (297.8 mg, 1.2 mmol) in the presence of EDCI (249.2 mg, 1.3 mmol) and DMAP (24.4 mg, 0.2 mmol) in DCM (5 mL) at RT for 1 d gave the product **S19** as a colorless oil (348.1 mg, 0.85 mmol, 85% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.97 (ddd, *J* = 11.7, 7.9, 1.4 Hz, 2H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.39 (td, *J* = 7.6, 1.2 Hz, 1H), 7.29 – 6.76 (m, 3H), 4.09 (s, 2H), 0.94 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 164.66, 152.00, 141.69, 137.19, 133.98, 133.27, 131.55, 130.08, 128.07, 121.09, 94.68, 27.34, 16.42.
HRMS (ESI) *m/z* calcd. for $C_{17}H_{20}IO_2Si$ $[M+H]^+$ 411.0272, found 411.0269.

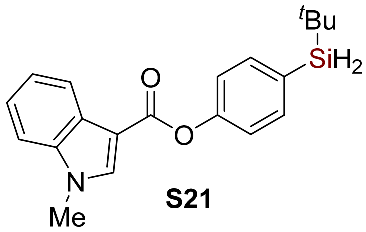
4-(*tert*-butylsilyl)phenyl 2-(benzofuran-3-yl)acetate (S20)



S20

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and 2-(benzofuran-3-yl)acetic acid (211.4 mg, 1.2 mmol) in the presence of EDCI (249.2 mg, 1.3 mmol) and DMAP (24.4 mg, 0.2 mmol) in DCM (5 mL) at RT for 1 d gave the product **S20** as a white solid (273.8 mg, 0.81 mmol, 81% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.72 (d, *J* = 1.2 Hz, 1H), 7.65 (dd, *J* = 7.4, 1.6 Hz, 1H), 7.61 – 7.55 (m, 2H), 7.54 – 7.48 (m, 1H), 7.31 (ddd, *J* = 12.5, 7.7, 1.4 Hz, 2H), 7.14 – 7.04 (m, 2H), 4.14 (s, 2H), 3.97 (d, *J* = 1.1 Hz, 2H), 1.00 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 168.97, 155.24, 151.91, 143.06, 137.14, 129.98, 127.42, 124.62, 122.78, 120.91, 119.61, 112.52, 111.62, 30.01, 27.32, 16.39.
HRMS (ESI) *m/z* calcd. for $C_{20}H_{22}NaO_3Si$ $[M+H]^+$ 361.1230, found 361.1226.

4-(*tert*-butylsilyl)phenyl 1-methyl-1*H*-indole-3-carboxylate (S21)



S21

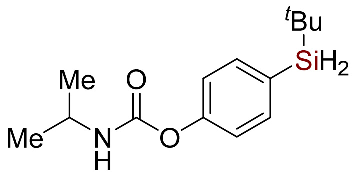
The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and 1-methyl-1*H*-indole-3-carboxylic acid (210.2 mg, 1.2 mmol) in the presence of EDCI (249.2 mg, 1.3 mmol) and DMAP (24.4 mg, 0.2 mmol) in DCM (5 mL) at RT for 1 d gave the product **S21** as a colorless oil (278.5 mg, 0.83 mmol, 83% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.27 – 8.20 (m, 1H), 7.96 (s, 1H), 7.69 – 7.58 (m, 2H), 7.46 – 7.38 (m, 1H), 7.37 – 7.29 (m, 2H), 7.29 – 7.19 (m, 2H), 4.18 (s, 2H), 3.89 (s, 3H), 1.04 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 162.88, 152.34, 137.32, 137.09, 136.15, 129.05, 126.77, 123.11, 122.30, 121.70, 121.58, 109.93, 106.04, 33.59, 27.37, 16.44.

HRMS (ESI) *m/z* calcd. for $C_{20}H_{24}NO_2Si$ [M+H]$^+$ 338.1571, found 338.1566.

4-(*tert*-butylsilyl)phenyl isopropylcarbamate (S22)



S22

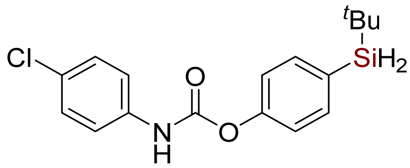
The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and 2-isocyanatopropane (0.12 mL, 1.2 mmol) in the presence of NEt_3 (0.028 mL, 0.2 mmol) in DCM (5 mL) at RT for 4 h gave the product **S22** as a colorless oil (197.8 mg, 0.75 mmol, 75% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.79 – 7.44 (m, 2H), 7.17 – 6.89 (m, 2H), 5.03 – 4.72 (m, 1H), 4.14 (s, 2H), 3.98 – 3.68 (m, 1H), 1.23 (d, *J* = 6.6 Hz, 6H), 1.01 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 153.41, 152.38, 136.98, 128.67, 121.06, 43.43, 27.32, 22.86, 16.40.

HRMS (ESI) *m/z* calcd. for $C_{14}H_{24}NO_2Si$ [M+H]$^+$ 266.1571, found 266.1568.

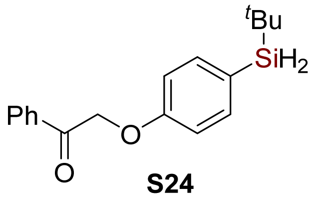
4-(*tert*-butylsilyl)phenyl (4-chlorophenyl)carbamate (S23)



S23

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and 1-chloro-4-isocyanatobenzene (184.3 mg, 1.2 mmol) in the presence of NEt_3 (0.028 mL, 0.2 mmol) in DCM (5 mL) at RT for 4 h gave the product **S23** as a white solid (210.2 mg, 0.63 mmol, 63% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 – 7.57 (m, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.33 – 7.27 (m, 2H), 7.22 – 7.16 (m, 2H), 6.94 (br, 1H), 4.16 (s, 2H), 1.02 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 151.72, 151.29, 137.16, 135.87, 129.73, 129.18, 129.02, 121.03, 119.96, 27.33, 16.40.
HRMS (ESI) *m/z* calcd. for $C_{17}H_{21}ClNO_2Si$ $[M+H]^+$ 334.1025, found 334.1020.

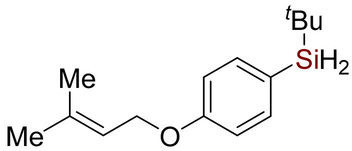
2-(4-(*tert*-butylsilyl)phenoxy)-1-phenylethan-1-one (S24)



S24

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and 2-bromo-1-phenylethan-1-one (239.0 mg, 1.2 mmol) in the presence of K_2CO_3 (193.2 mg, 1.4 mmol) in acetone (5 mL) at RT for 4 h gave the product **S24** as a white solid (194.7 mg, 0.65 mmol, 65% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 – 7.98 (m, 2H), 7.67 – 7.55 (m, 1H), 7.55 – 7.33 (m, 4H), 6.95 (d, *J* = 8.6 Hz, 2H), 5.30 (s, 2H), 4.11 (s, 2H), 1.00 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 194.28, 159.28, 137.43, 134.51, 133.92, 128.85, 128.13, 124.22, 114.40, 70.46, 27.34, 16.43.
HRMS (ESI) *m/z* calcd. for $C_{18}H_{23}O_2Si$ $[M+H]^+$ 299.1462, found 299.1459.

***tert*-butyl(4-((3-methylbut-2-en-1-yl)oxy)phenyl)silane (S25)**

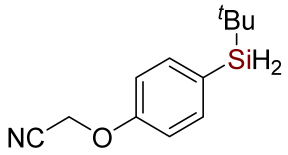


S25

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and 1-bromo-3-methylbut-2-ene (0.14 mL, 1.2 mmol) in the presence of K_2CO_3

(193.2 mg, 1.4 mmol) in acetone (5 mL) at RT for 4 h gave the product **S25** as a colorless oil (153.3 mg, 0.62 mmol, 62% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.49 (d, *J* = 8.6 Hz, 2H), 6.93 (d, *J* = 8.6 Hz, 2H), 5.51 (dddd, *J* = 8.2, 5.4, 2.9, 1.4 Hz, 1H), 4.65 – 4.43 (m, 2H), 4.12 (s, 2H), 1.80 (d, *J* = 1.3 Hz, 3H), 1.75 (s, 3H), 1.00 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 160.16, 138.35, 137.32, 122.77, 119.50, 114.29, 64.45, 27.36, 25.84, 18.18, 16.45.
HRMS (ESI) *m/z* calcd. for $C_{15}H_{25}OSi$ $[M+H]^+$ 249.1669, found 249.1669.

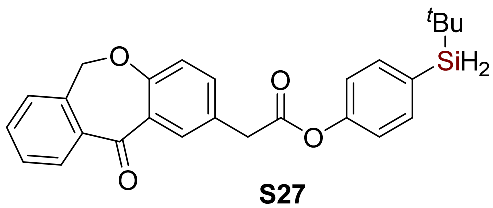
2-(4-(*tert*-butylsilyl)phenoxy)acetonitrile (S26)



S26

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and 2-bromoacetonitrile (0.07 mL, 1.2 mmol) in the presence of K_2CO_3 (193.2 mg, 1.4 mmol) in acetone (5 mL) at RT for 1 d gave the product **S26** as a colorless oil (111.6 mg, 0.51 mmol, 51% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.57 (d, *J* = 8.6 Hz, 2H), 7.00 (d, *J* = 8.6 Hz, 2H), 4.78 (s, 2H), 4.16 (s, 2H), 1.02 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 157.71, 137.61, 126.10, 114.99, 114.33, 53.13, 27.28, 16.36.
HRMS (ESI) *m/z* calcd. for $C_{12}H_{18}NOSi$ $[M+H]^+$ 220.1152, found 220.1155.

4-(*tert*-butylsilyl)phenyl-2-(11-oxo-6,11-dihydrodibenzo[*b,e*]oxepin-2-yl)acetate (S27)

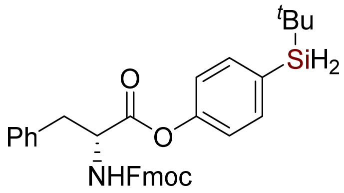


S27

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and Isoxepac (322.0 mg, 1.2 mmol) in the presence of EDCI (249.2 mg, 1.3 mmol) and DMAP (24.4 mg, 0.2 mmol) in DCM (5 mL) at RT for 1 d gave the product **S27** as a white solid (266.6 mg, 0.62 mmol, 62% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.23 (d, *J* = 2.4 Hz, 1H), 7.90 (dd, *J* = 7.7, 1.4 Hz, 1H), 7.62 – 7.55 (m, 3H), 7.53 (dd, *J* = 8.5, 2.4 Hz, 1H), 7.48 (td, *J* = 7.6, 1.3 Hz, 1H), 7.38 (dd, *J* = 7.4, 1.3 Hz, 1H), 7.17 – 7.03 (m, 3H), 5.21 (s, 2H), 4.14 (s, 2H), 3.89 (s, 2H), 1.00 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 190.81, 169.67, 160.63, 151.97, 140.41, 137.09, 136.27, 135.47, 132.82, 132.60, 129.80, 129.49, 129.29, 127.83, 127.12, 125.21, 121.25, 120.94, 73.63, 40.30, 27.32, 16.38.

HRMS (ESI) *m/z* calcd. for $C_{26}H_{27}O_4Si$ $[M+H]^+$ 431.1673, found 431.1670.

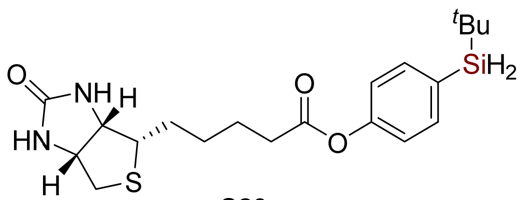
4-(*tert*-butylsilyl)phenyl(((9*H*-fluoren-9-yl)methoxy)carbonyl)-*D*-phenylalaninate (S28)



S28

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 100 mg, 0.55 mmol) and Fmoc-*D*-phenylalanine (236.3 mg, 0.61 mmol) in the presence of EDCI (160.0 mg, 0.83 mmol) and DMAP (13.6 mg, 0.11 mmol) in DCM (3 mL) at RT for 1 d gave the product **S28** as a white solid (216.9 mg, 0.39 mmol, 71% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.67 (d, *J* = 7.6 Hz, 2H), 7.48 (dt, *J* = 8.3, 1.7 Hz, 4H), 7.29 (q, *J* = 8.7 Hz, 2H), 7.28 – 7.16 (m, 5H), 7.15 – 7.09 (m, 2H), 6.91 (d, *J* = 8.0 Hz, 2H), 5.29 (d, *J* = 8.3 Hz, 1H), 4.82 (dt, *J* = 8.2, 6.0 Hz, 1H), 4.38 (dd, *J* = 10.7, 7.2 Hz, 1H), 4.30 (dd, *J* = 10.8, 6.7 Hz, 1H), 4.13 (t, *J* = 6.9 Hz, 1H), 4.05 (s, 2H), 3.17 (d, *J* = 6.1 Hz, 2H), 0.92 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 170.01, 155.58, 151.52, 143.73, 143.63, 141.28, 137.15, 135.37, 130.23, 129.46, 128.74, 127.71, 127.37, 127.04, 125.05, 125.00, 120.73, 119.97, 67.03, 54.92, 47.11, 38.24, 27.31, 25.62, 25.59, 16.37.
HRMS (ESI) *m/z* calcd. for $C_{34}H_{36}NO_4Si$ $[M+H]^+$ 550.2408, found 550.2406.

4-(*tert*-butylsilyl)phenyl-5-((3*aS*,4*S*,6*aR*)-2-oxohexahydro-1*H*-thieno[3,4-*d*]imidazol-4-yl)pentanoate (S29)



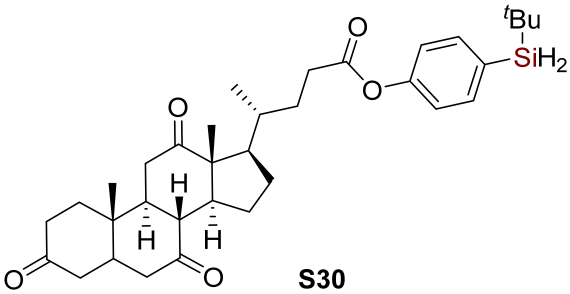
S29

The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and biotin (294.0 mg, 1.2 mmol) in the presence of EDCI (249.2 mg, 1.3 mmol) and DMAP (24.4 mg, 0.2 mmol) in DCM (5 mL) at RT for 1 d gave the product **S29** as a white solid (315.5 mg, 0.78 mmol, 78% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.4 Hz, 2H), 7.09 (d, *J* = 8.4 Hz, 2H), 6.05 (s, 1H), 5.43 (s, 1H), 4.49 (dd, *J* = 7.8, 4.9 Hz, 1H), 4.31 (ddd, *J* = 7.9, 4.6, 1.5 Hz, 1H), 4.14 (s, 2H), 3.17 (ddd, *J* = 8.4, 6.4, 4.5 Hz, 1H), 2.90 (dd, *J* = 12.8, 4.9 Hz, 1H), 2.73 (d, *J* = 12.8 Hz, 1H), 2.59 (t, *J* = 7.5 Hz, 2H), 1.88 – 1.62 (m, 4H), 1.61 – 1.46 (m, 2H), 1.01 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 171.99, 163.70, 151.98, 137.10, 134.40, 129.61, 121.08, 61.96, 60.09, 55.45, 40.53, 34.00, 28.34, 28.27, 27.33, 25.60, 24.72, 16.38.

HRMS (ESI) *m/z* calcd. for $C_{20}H_{31}N_2O_3SSi$ $[M+H]^+$ 407.1819, found 407.1815.

4-(*tert*-butylsilyl)phenyl-(4*R*)-4-((8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-3,7,12-trioxohexadecahydro-1*H*-cyclopenta[a]phenanthren-17-yl)pentanoate (S30)



S30

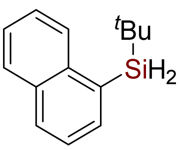
The reaction of 4-(*tert*-butylsilyl)phenol (**S11**, 180.3 mg, 1.0 mmol) and dehydrocholic acid (483.0 mg, 1.2 mmol) in the presence of EDCI (249.2 mg, 1.3 mmol) and DMAP (24.4 mg, 0.2 mmol) in DCM (5 mL) at RT for 1 d gave the product **S30** as a white solid (412.0 mg, 0.73 mmol, 73% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.57 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 8.3 Hz, 2H), 4.14 (s, 2H), 2.96 – 2.80 (m, 3H), 2.65 (ddd, *J* = 15.9, 9.1, 5.3 Hz, 1H), 2.52 (ddd, *J* = 16.0, 8.7, 7.3 Hz, 1H), 2.43 – 2.28 (m, 3H), 2.25 (q, *J* = 4.8 Hz, 1H), 2.20 (dd, *J* = 5.1, 1.7 Hz, 1H), 2.19 – 2.14 (m, 1H), 2.12 (d, *J* = 2.1 Hz, 1H), 2.06 (ddt, *J* = 12.5, 6.3, 3.4 Hz, 2H), 2.02 – 1.92 (m, 2H), 1.86 (td, *J* = 11.5, 7.1 Hz, 1H), 1.73 – 1.59 (m, 2H), 1.68 – 1.42 (m, 1H), 1.40 (s, 3H), 1.41 – 1.19 (m, 3H), 1.09 (s, 3H), 1.01 (s, 9H), 0.91 (d, *J* = 6.6 Hz, 3H), 0.87 (d, *J* = 3.3 Hz, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 211.92, 209.03, 208.66, 172.33, 152.03, 137.08, 129.52, 121.05, 56.88, 51.73, 48.95, 46.81, 45.63, 45.51, 44.94, 42.76, 38.61, 36.46, 35.98, 35.44, 35.24, 31.57, 30.33, 27.62, 27.32, 25.59, 25.10, 21.87, 18.64, 16.38, 11.84.

HRMS (ESI) *m/z* calcd. for $C_{34}H_{49}O_5Si$ $[M+H]^+$ 565.3344, found 565.3340.

***tert*-butyl(naphthalen-1-yl)silane (S31)**

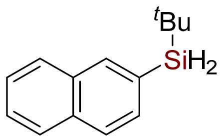


S31

According to the **General Procedures A** using 1-bromonaphthalene (518 mg, 2.5 mmol), the product **S31** was obtained as a colorless oil (109.6 mg, 0.51 mmol, 20% yield).

^{1}H NMR (400 MHz, CDCl$_3$) δ 8.14 (d, *J* = 7.0 Hz, 1H), 7.94 – 7.88 (m, 1H), 7.87 – 7.82 (m, 1H), 7.79 (dd, *J* = 6.7, 1.3 Hz, 1H), 7.57 – 7.40 (m, 3H), 4.52 (s, 2H), 1.05 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 137.45, 137.01, 133.18, 131.13, 130.45, 128.74, 128.70, 125.97, 125.64, 125.00, 28.11, 17.34.
The obtained NMR spectral data are in good agreement with those reported in literature.[3]

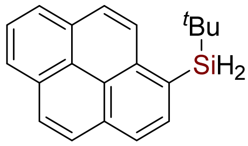
***tert*-butyl(naphthalen-2-yl)silane (S32)**



S32

According to the **General Procedures B** using 2-bromonaphthalene (3106 mg, 15 mmol), the product **S32** was obtained as a semi-solid (712 mg, 3.3 mmol, 22% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.10 (s, 1H), 7.87 – 7.78 (m, 3H), 7.62 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.54 – 7.43 (m, 2H), 4.28 (s, 2H), 1.05 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 136.99, 133.83, 132.86, 131.66, 129.74, 128.05, 127.73, 126.97, 126.60, 126.01, 27.50, 16.65.
HRMS (APCI) *m/z* calcd. for $C_{14}H_{19}Si$ $[M+H]^+$ 215.1251, found 215.1251.

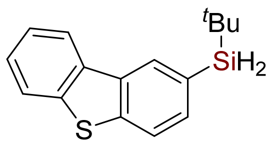
***tert*-butyl(pyren-1-yl)silane (S33)**[3]



S33

According to the **General Procedures A** using 1-bromopyrene (596.0 mg, 2.1 mmol), the product **S33** was prepared as a pale yellow solid (105.9 mg, 0.37 mmol, 18% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.41 (d, *J* = 9.2 Hz, 1H), 8.24 (d, *J* = 7.5 Hz, 1H), 8.22 – 7.98 (m, 7H), 4.73 (s, 2H), 1.09 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 136.45, 135.32, 132.65, 131.23, 130.75, 128.34, 128.23, 128.15, 127.46, 125.90, 125.29, 125.26, 124.63, 124.48, 123.97, 28.06, 17.70.

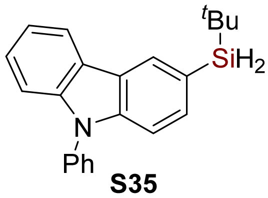
***tert*-butyl(dibenzo[*b,d*]thiophen-2-yl)silane (S34)**



S34

According to the **General Procedures A** using 2-bromodibenzo[*b*,*d*]thiophene (657.9 mg, 2.5 mmol), the product **S34** was obtained as a white solid (202.8 mg, 0.75 mmol, 30% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.46 – 8.39 (m, 1H), 8.24 (dtd, *J* = 7.5, 3.6, 2.4 Hz, 1H), 7.93 – 7.84 (m, 2H), 7.67 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.54 – 7.44 (m, 2H), 4.36 (s, 2H), 1.12 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 141.11, 139.13, 135.24, 135.11, 133.47, 129.13, 127.44, 126.80, 124.44, 122.78, 122.30, 121.56, 27.45, 16.54.
HRMS (APCI) *m/z* calcd. for $C_{16}H_{19}SSi$ [M+H]$^+$ 271.0971, found 271.0971.

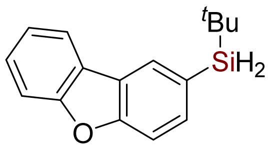
3-(*tert*-butylsilyl)-9-phenyl-9*H*-carbazole (S35)



S35

According to the **General Procedures A** using 3-bromo-9-phenyl-9*H*-carbazole (805.5 mg, 2.5 mmol), the product **S35** was obtained as a white solid (230.6 mg, 0.7 mmol, 28% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.41 (t, *J* = 1.0 Hz, 1H), 8.21 (dt, *J* = 7.8, 1.1 Hz, 1H), 7.67 – 7.55 (m, 5H), 7.53 – 7.46 (m, 1H), 7.48 – 7.38 (m, 3H), 7.33 (ddd, *J* = 8.0, 4.6, 3.5 Hz, 1H), 4.36 (s, 2H), 1.10 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 141.83, 140.83, 137.46, 133.14, 129.88, 128.33, 127.56, 127.09, 126.07, 123.25, 123.09, 121.84, 120.30, 120.18, 109.81, 109.48, 27.49, 16.65.
HRMS (ESI) *m/z* calcd. for $C_{22}H_{24}NSi$ [M+H]$^+$ 330.1673, found 330.1669.

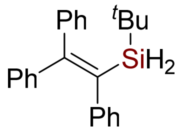
***tert*-butyl(dibenzo[*b,d*]furan-2-yl)silane (S36)**



S36

According to the **General Procedures B** using 2-bromodibenzo[*b*,*d*]furan (3706 mg, 15 mmol), the product **S36** was obtained as a white solid (1020 mg, 4.0 mmol, 27% yield).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.16 (s, 1H), 7.95 (d, *J* = 7.6 Hz, 1H), 7.63 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.58 – 7.50 (m, 2H), 7.48 – 7.39 (m, 1H), 7.38 – 7.27 (m, 1H), 4.29 (s, 2H), 1.05 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 157.33, 156.05, 134.52, 128.42, 127.25, 125.66, 124.18, 123.79, 122.83, 120.65, 111.66, 111.40, 27.43, 16.52.
HRMS (ESI) *m/z* calcd. for $C_{16}H_{19}OS$ [M+H]$^+$ 255.1200, found 255.1193.

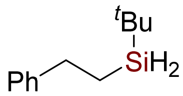
***tert*-butyl(1,2,2-triphenylvinyl)silane (S37)**



S37

According to the **General Procedures A** using (2-bromoethene-1,1,2-triyl)tribenzene (838 mg, 2.5 mmol), the product **S37** was obtained as a colorless oil (343 mg, 0.45 mmol, 18% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.38 – 7.26 (m, 5H), 7.18 – 7.08 (m, 4H), 7.07 – 6.97 (m, 4H), 6.95 – 6.87 (m, 2H), 3.84 (s, 2H), 0.80 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 156.29, 144.47, 143.90, 142.50, 137.52, 130.28, 129.67, 129.63, 127.97, 127.79, 127.36, 127.32, 126.44, 125.59, 28.58, 17.15.
HRMS (ESI) *m/z* calcd. for $C_{24}H_{27}Si$ $[M+H]^+$ 343.1877, found 343.1879.

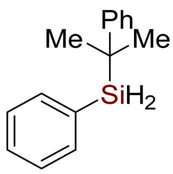
***tert*-butyl(phenethyl)silane (S38)**



S38

According to the **General Procedures B** starting from trichloro(phenethyl)silane (360 mg, 1.5 mmol) with 1 equiv. ^{t}BuLi, the product **S38** was obtained as a colorless oil in 60% yield (174 mg, 0.90 mmol).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32 – 7.25 (m, 2H), 7.23 – 7.13 (m, 3H), 3.57 (t, J = 4.0 Hz, 2H), 2.78 – 2.69 (m, 2H), 1.11 – 1.02 (m, 2H), 1.01 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 144.45, 128.34, 127.81, 125.72, 31.68, 27.89, 15.72, 9.86.
HRMS (APCI) *m/z* calcd. for $C_{12}H_{21}Si$ $[M+H]^+$ 193.1407, found 193.1407.

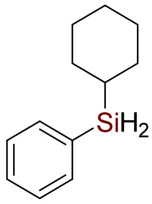
phenyl(2-phenylpropan-2-yl)silane (S39)



S39

According to the literature report[6] using prop-1-en-2-ylbenzene (591 mg, 5 mmol) and $PhSiH_3$ (263 mg, 2.5 mmol), the product **S39** was obtained as a colorless oil in 12% yield (65.3 mg, 0.29 mmol).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 – 7.32 (m, 1H), 7.32 – 7.24 (m, 6H), 7.24 – 7.19 (m, 2H), 7.17 – 7.10 (m, 1H), 4.28 (s, 2H), 1.46 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 147.57, 135.97, 131.39, 129.73, 128.12, 127.66, 126.07, 124.84, 26.04, 25.19.
HRMS (APCI) *m/z* calcd. for $C_{15}H_{19}Si$ $[M+H]^+$ 227.1251, found 227.1251.

cyclohexyl(phenyl)silane (S40)



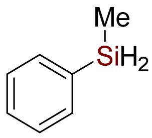
S40

According to the **General Procedures B** starting from trichloro(phenyl)silane (2115 mg, 10 mmol) with cyclohexylmagnesium bromide (2 M in THF, 10 mmol, 1 equiv.), the product **S40** was obtained as a colorless oil[3] in 27% yield (517 mg, 2.7 mmol).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.48 (m, 2H), 7.44 – 7.27 (m, 3H), 4.16 (d, J = 2.9 Hz, 2H), 1.87 – 1.58 (m, 6H), 1.38 – 1.16 (m, 5H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.60, 132.10, 129.43, 127.86, 30.17, 28.82, 27.63, 26.89, 26.59, 22.12.

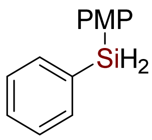
methyl(phenyl)silane (S41)



S41

According to the **General Procedures B** starting from dichloro(methyl)(phenyl)silane (1911 mg, 10 mmol) by the reduction with $LiAlH_4$, the product **S41** was obtained as a colorless oil[7] in 30% yield (364 mg, 3.0 mmol).

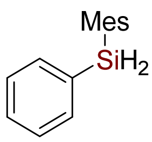
(4-methoxyphenyl)(phenyl)silane (S42)



S42

S42 was prepared according to the literature report.[8]

mesityl(phenyl)silane (S43)

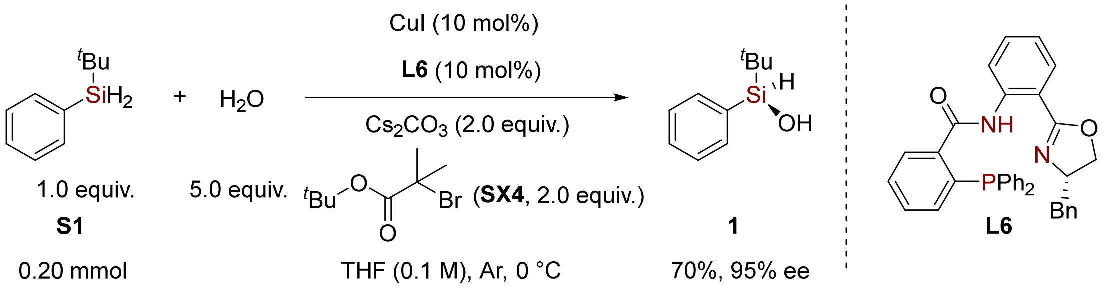


S43

S43 was prepared according to the literature report.[9]

4. Construction of Silicon-Stereogenic Silanols

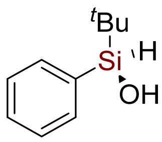
General Procedures:



A 10 mL Schlenk tube equipped with a magnetic stir bar was charged with CuI (3.8 mg, 0.020 mmol, 10 mol%), **L6** (10.8 mg, 0.010 mmol, 10 mol%), silane substrate (0.20 mmol, 1.0 equiv., if solid), and Cs_2CO_3 (130.3 mg, 0.40 mmol, 2 equiv.). The tube was evacuated and backfilled with argon three times. Under the flow of Ar, silane substrate (0.20 mmol, 1.0 equiv., if liquid), anhydrous THF (2.0 mL), H_2O (18.0 mg, 1.0 mmol, 5.0 equiv.), and *tert*-butyl 2-bromo-2-methylpropanoate (**SX4**, 89.2 mg, 0.40 mmol, 2.0 equiv.) were added into the mixture. The reaction mixture was stirred at 0 °C for 10–72 h and monitored by TLC. After the reaction, the mixture was then filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated and the residue was purified by column chromatography on silica gel to afford the desired product.

The racemic samples were synthesized by using the racemic ligand of **L6** or with the following procedures:
A vial equipped with a stirrer was charged with CuI (1.9 mg, 0.010 mmol, 10 mol%), silane substrate (0.10 mmol, 1.0 equiv.), CH_3CN (0.50 mL), and TBHP (*tert*-butyl hydroperoxide, 70% in H_2O, 0.10 mmol, 1.0 equiv.). The mixture was stirred at RT under air for 0.5–12 h. Upon completion, the mixture was then filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated and the residue was purified by preparative TLC or column chromatography on silica gel to afford the desired racemic product.

(*R*)-*tert*-butyl(phenyl)silanol (1)

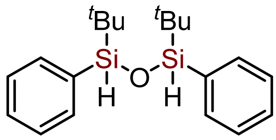


1

According to the general procedures with *tert*-butyl(phenyl)silane (**S1**, 32.9 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **1** as a colorless oil (25.2 mg, 0.14 mmol, 70% yield, 95% ee) and the byproduct **1'** in 6% yield.

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.62–7.59 (m, 2H), 7.45–7.36 (m, 3H), 4.80 (s, 1H), 1.93 (s, 1H), 0.98 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 134.66, 134.12, 130.11, 127.83, 25.39, 17.98.
HRMS (APCI) *m/z* calcd. for $C_{10}H_{17}OSi$ [M+H]$^+$ 181.1043, found 181.1043.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 230 nm, t(major) = 12.1 min, t(minor) = 13.7 min, 95% ee.

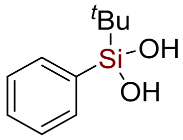
1,3-di-*tert*-butyl-1,3-diphenyldisiloxane (1')



1'

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.61 – 7.50 (m, 4H), 7.43 – 7.30 (m, 6H), 4.86 (s, 1H), 4.86 (s, 1H), 0.94 (s, 9H), 0.93 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 134.71, 134.64, 134.15, 134.13, 129.79, 127.60, 127.57, 25.41, 25.38, 18.61, 18.56.
HRMS (APCI) *m/z* calcd. for $C_{20}H_{31}OSi_2$ [M+H]$^+$ 343.1908, found 343.1901.

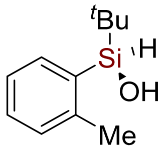
***tert*-butyl(phenyl)silanediol (1'')**



1''

The authentic sample of **1''** was prepared as a white solid according to the procedures for synthesizing the racemic samples with 2.0 equiv. TBHP (*tert*-butyl hydroperoxide).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.70 – 7.59 (m, 2H), 7.47 – 7.39 (m, 1H), 7.39 – 7.30 (m, 2H), 2.88 (br, 2H), 0.97 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 134.62, 133.62, 130.16, 127.74, 25.69, 18.12.
HRMS (ESI) *m/z* calcd. for $C_{10}H_{16}O_2SiNa$ [M+Na]$^+$ 219.0812, found 219.0812.

(*R*)-*tert*-butyl(*o*-tolyl)silanol (2)

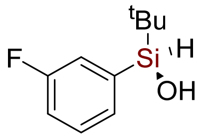


2

According to the general procedures with *tert*-butyl(*o*-tolyl)silane (**S2**, 35.7 mg, 0.20 mmol), CuI (7.6 mg, 0.04 mmol) and **L6** (21.6 mg, 0.04 mmol) at 0 °C for 48 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **2** as a colorless oil (22.2 mg, 0.114 mmol, 57% yield, 94% ee).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.55 (dd, *J* = 7.3, 1.5 Hz, 1H), 7.32 (td, *J* = 7.5, 1.6 Hz, 1H), 7.24 – 7.13 (m, 2H), 4.98 (s, 1H), 2.49 (s, 3H), 1.91 (s, 1H), 0.99 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 143.91, 134.93, 133.39, 129.96, 129.86, 124.71, 25.81, 22.71, 18.71.
HRMS (APCI) *m/z* calcd. for $C_{11}H_{19}OSi$ [M+H]$^+$ 195.1200, found 195.1199.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 220 nm, t_R (major) = 11.0 min, t_R (minor) = 12.3 min, 94% ee.

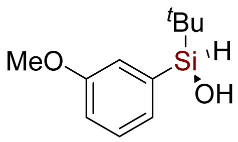
(*R*)-*tert*-butyl(3-fluorophenyl)silanol (3)



3

According to the general procedures with *tert*-butyl(3-fluorophenyl)silane (**S3**, 36.4 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **3** as a colorless oil (21.2 mg, 0.108 mmol, 54% yield, 87% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.42 – 7.32 (m, 2H), 7.29 (ddt, *J* = 8.7, 2.7, 0.7 Hz, 1H), 7.10 (ddt, *J* = 9.2, 4.3, 2.7 Hz, 1H), 4.79 (s, 1H), 0.97 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 162.50 (d, *J* = 248.6 Hz), 137.60 (d, *J* = 4.1 Hz), 129.66 (d, *J* = 4.8 Hz), 129.61, 120.39 (d, *J* = 19.0 Hz), 117.05 (d, *J* = 21.0 Hz), 25.28, 17.93.
^{19}F NMR (376 MHz, CDCl$_3$) δ −113.39.
HRMS (ESI) *m/z* calcd. for $C_{10}H_{16}FOSi$ [M+H]$^+$ 199.0949, found 199.0945.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 220 nm, t_R (major) = 18.4 min, t_R (minor) = 19.8 min, 87% ee.

***(R)-tert*-butyl(3-methoxyphenyl)silanol (4)**

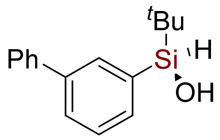


4

According to the general procedures with *tert*-butyl(3-methoxyphenyl)silane (**S4**, 38.9 mg, 0.20 mmol) at 0 °C for 48 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **4** as a colorless oil (26.5 mg, 0.126 mmol, 63% yield, 93% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.33 (t, *J* = 7.9 Hz, 1H), 7.18 (d, *J* = 7.2 Hz, 1H), 7.14 (d, *J* = 2.7 Hz, 1H), 6.97 (ddd, *J* = 8.2, 2.8, 1.0 Hz, 1H), 4.78 (s, 1H), 3.82 (s, 3H), 2.02 (s, 1H), 0.98 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 158.94, 136.19, 129.05, 126.35, 119.20, 115.64, 55.14, 25.39, 17.96.

HRMS (ESI) *m/z* calcd. for $C_{11}H_{19}O_2Si$ $[M+H]^+$ 211.1149, found 211.1149.
HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.8 mL/min. λ = 220 nm, t_R (major) = 8.8 min, t_R (minor) = 9.8 min, 93% ee.

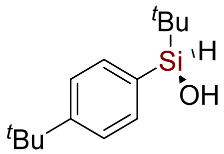
***(R)*-[1,1'-biphenyl]-3-yl(*tert*-butyl)silanol (5)**



5

According to the general procedures with [1,1'-biphenyl]-3-yl(*tert*-butyl)silane (**S5**, 48.0 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **5** as a colorless oil (33.2 mg, 0.13 mmol, 65% yield, 89% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.82 (dd, *J* = 2.0, 1.0 Hz, 1H), 7.65 (ddd, *J* = 7.7, 2.1, 1.3 Hz, 1H), 7.62 – 7.55 (m, 3H), 7.46 (q, *J* = 7.7 Hz, 3H), 7.39 – 7.30 (m, 1H), 4.85 (s, 1H), 1.01 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 141.20, 140.58, 135.22, 133.01, 132.83, 128.96, 128.77, 128.20, 127.31, 127.23, 25.41, 18.00.
HRMS (ESI) *m/z* calcd. for $C_{16}H_{20}NaOSi$ $[M+Na]^+$ 279.1176, found 279.1184.
HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 220 nm, t_R (major) = 14.5 min, t_R (minor) = 16.3 min, 89% ee.

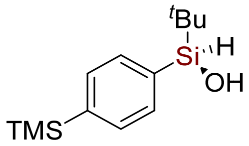
***(R)-tert*-butyl(4-(*tert*-butyl)phenyl)silanol (6)**



6

According to the general procedures with *tert*-butyl(4-(*tert*-butyl)phenyl)silane (**S6**, 44.1 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **6** as a colorless oil (34.1 mg, 0.144 mmol, 72% yield, 94% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.63 – 7.50 (m, 2H), 7.48 – 7.33 (m, 2H), 4.78 (s, 1H), 1.93 (s, 1H), 1.33 (s, 9H), 0.99 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 153.14, 134.05, 131.16, 124.79, 34.75, 31.19, 25.41, 18.01.
HRMS (ESI) *m/z* calcd. for $C_{14}H_{24}NaOSi$ $[M+Na]^+$ 259.1489, found 259.1486.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 220 nm, t_R (major) = 10.5 min, t_R (minor) = 12.7 min, 94% ee.

(*R*)-*tert*-butyl(4-(trimethylsilyl)phenyl)silanol (7)



7

According to the general procedures with *tert*-butyl(4-(trimethylsilyl)phenyl)silane (**S7**, 47.3 mg, 0.20 mmol) at 0 °C for 48 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **7** as a colorless oil (30.4 mg, 0.12 mmol, 60% yield, 93% ee).

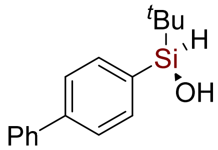
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.59 (d, *J* = 7.9 Hz, 2H), 7.56 – 7.48 (m, 2H), 4.79 (s, 1H), 0.99 (s, 9H), 0.28 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 142.68, 135.04, 133.32, 132.60, 25.39, 18.01, −1.25.

HRMS (APCI) *m/z* calcd. for $C_{13}H_{25}OSi_2$ [M+H]$^+$ 253.1438, found 253.1438.

HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 270 nm, t(major) = 8.3 min, t(minor) = 9.0 min, 93% ee.

(*R*)-[1,1'-biphenyl]-4-yl(*tert*-butyl)silanol (8)



8

According to the general procedures with [1,1'-biphenyl]-4-yl(*tert*-butyl)silane (**S8**, 48.1 mg, 0.20 mmol) at 0 °C for 48 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **8** as a colorless oil (35.0 mg, 0.136 mmol, 68% yield, 92% ee).

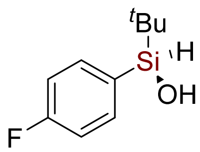
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.72 – 7.65 (m, 2H), 7.65 – 7.56 (m, 4H), 7.45 (dd, *J* = 8.4, 6.8 Hz, 2H), 7.41 – 7.32 (m, 1H), 4.84 (s, 1H), 2.01 (br, 1H), 1.01 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 142.76, 140.86, 134.61, 133.33, 128.79, 127.54, 127.15, 126.51, 25.40, 18.04.

HRMS (ESI) *m/z* calcd. for $C_{16}H_{19}OSi$ [M−H]$^-$ 255.1211, found 255.1205.

HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.8 mL/min. λ = 270 nm, t_R (major) = 14.7 min, t_R (minor) = 16.7 min, 92% ee.

(*R*)-*tert*-butyl(4-fluorophenyl)silanol (9)



9

According to the general procedures with *tert*-butyl(4-fluorophenyl)silane (**S9**, 36.5 mg, 0.20 mmol) at 0 °C for 48 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **9** as a colorless oil (23.8 mg, 0.120 mmol, 60% yield, 90% ee).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.69 – 7.47 (m, 2H), 7.21 – 6.92 (m, 2H), 4.79 (s, 1H), 2.04 (s, 1H), 0.96 (s, 9H).

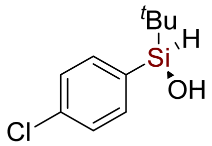
^{13}C NMR (101 MHz, CDCl$_3$) δ 164.34 (d, J = 249.2 Hz), 136.11 (d, J = 7.4 Hz), 130.15 (d, J = 3.8 Hz), 115.07 (d, J = 19.7 Hz), 25.28, 17.92.

^{19}F NMR (376 MHz, CDCl$_3$) δ −110.14.

HRMS (ESI) *m/z* calcd. for $C_{10}H_{16}FOSi$ [M+H]$^+$ 199.0949, found 199.0949.

HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 254 nm, t_R (major) = 10.1 min, t_R (minor) = 11.3 min, 90% ee.

(R)-tert-butyl(4-chlorophenyl)silanol (10)



10

According to the general procedures with *tert*-butyl(4-chlorophenyl)silane (**S10**, 39.8 mg, 0.20 mmol) at 0 °C for 10 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **10** as a colorless oil (17.3 mg, 0.080 mmol, 40% yield, 85% ee).

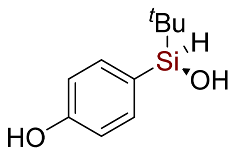
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.57 – 7.49 (m, 2H), 7.40 – 7.34 (m, 2H), 4.78 (s, 1H), 2.05 (s, 1H), 0.96 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 136.46, 135.43, 132.89, 128.10, 25.26, 17.91.

HRMS (ESI) *m/z* calcd. for $C_{10}H_{14}ClOSi$ [M−H]$^-$ 213.0508, found 213.0500.

HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 220 nm, t_R (major) = 12.5 min, t_R (minor) = 14.0 min, 85% ee.

(R)-tert-butyl(4-hydroxyphenyl)silanol (11)



11

According to the general procedures with *tert*-butyl(4-hydroxyphenyl)silane (**S11**, 36.1 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 2/1) to yield the product **11** as a white solid (23.6 mg, 0.12 mmol, 60% yield, 86% ee).

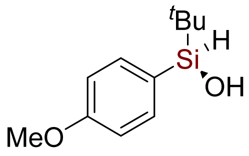
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.57 – 7.43 (m, 2H), 6.95 – 6.75 (m, 2H), 4.91 (s, 1H), 4.76 (s, 1H), 1.87 (s, 1H), 0.96 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 157.31, 135.90, 125.80, 115.03, 25.36, 17.98.

HRMS (ESI) *m/z* calcd. for $C_{10}H_{15}O_2Si$ [M−H]$^-$ 195.0847, found 195.0838

HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 1.0 mL/min. λ = 230 nm, t_R (major) = 27.2 min, t_R (minor) = 34.2 min, 86% ee.

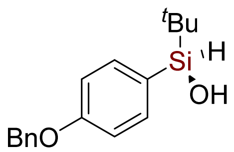
***(R)-tert*-butyl(4-methoxyphenyl)silanol (12)**



12

According to the general procedures with *tert*-butyl(4-methoxyphenyl)silane (**S12**, 38.9 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **12** as a colorless oil (25.7 mg, 0.122 mmol, 61% yield, 91% ee).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 – 7.39 (m, 2H), 7.05 – 6.77 (m, 2H), 4.77 (s, 1H), 3.82 (s, 3H), 2.01 (s, 1H), 0.96 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 161.17, 135.65, 125.60, 113.57, 55.01, 25.36, 17.99.
HRMS (ESI) *m/z* calcd. for $C_{11}H_{18}NaO_2Si$ $[M+Na]^+$ 233.0968, found 233.0967.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 240 nm, t_R (major) = 17.8 min, t_R (minor) = 22.2 min, 91% ee.

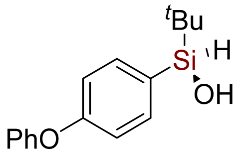
***(R)*-(4-(benzyloxy)phenyl)(*tert*-butyl)silanol (13)**



13

According to the general procedures using (4-(benzyloxy)phenyl)(*tert*-butyl)silane (**S13**, 54.1 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **13** as a colorless oil (40.1 mg, 0.14 mmol, 70% yield, 91% ee).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 – 7.51 (m, 2H), 7.47 – 7.30 (m, 5H), 7.01 (d, *J* = 8.5 Hz, 2H), 5.08 (s, 2H), 4.77 (s, 1H), 1.85 (s, 1H), 0.97 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 160.45, 136.80, 135.69, 128.60, 128.01, 127.50, 125.94, 114.44, 69.74, 25.38, 18.01.
HRMS (ESI) *m/z* calcd. for $C_{17}H_{22}NaO_2Si$ $[M+Na]^+$ 309.1281, found 309.1280.
HPLC conditions:: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min, λ = 220 nm, t_R (major) = 37.0 min, t_R (minor) = 44.6 min, 91% ee.

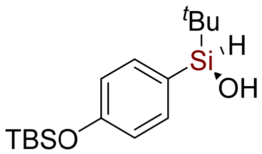
***(R)*-*tert*-butyl(4-phenoxyphenyl)silanol (14)**



14

According to the general procedures with *tert*-butyl(4-phenoxyphenyl)silane (**S14**, 51.3 mg, 0.20 mmol) at 0 °C for 48 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **14** as a colorless oil (34.7 mg, 0.127 mmol, 64% yield, 90% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.61 – 7.53 (m, 2H), 7.41 – 7.31 (m, 2H), 7.18 – 7.10 (m, 1H), 7.07 – 6.93 (m, 4H), 4.79 (s, 1H), 1.97 (s, 1H), 0.98 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 159.31, 156.44, 135.81, 129.81, 128.47, 123.71, 119.50, 117.80, 25.36, 18.00.
HRMS (ESI) *m/z* calcd. for $C_{16}H_{21}O_2Si$ [M+H]$^+$ 273.1305, found 273.1303.
HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.8 mL/min. λ = 254 nm, t_R (major) = 10.3 min, t_R (minor) = 11.1 min, 90% ee.

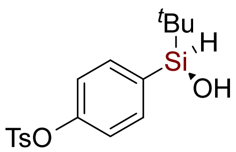
***(R)*-*tert*-butyl(4-((*tert*-butyldimethylsilyl)oxy)phenyl)silanol (15)**



15

According to the general procedures with *tert*-butyl(4-(*tert*-butylsilyl)phenoxy)dimethylsilane (**S15**, 58.8 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 10/1) to yield the product **15** as a colorless oil (31.4 mg, 0.102 mmol, 51% yield, 90% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.55 – 7.42 (m, 2H), 6.94 – 6.78 (m, 2H), 4.76 (s, 1H), 1.91 (s, 1H), 0.98 (s, 9H), 0.96 (s, 9H), 0.21 (s, 6H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 157.46, 135.60, 126.36, 119.72, 25.63, 25.37, 18.18, 17.97, -4.40.
HRMS (ESI) *m/z* calcd. for $C_{16}H_{30}NaO_2Si_2$ [M+Na]$^+$ 333.1677, found 333.1674.
HPLC conditions: Chiralcel AS-3, *n*-hexane/*i*-PrOH = 99.8/0.2, flow rate 0.45 mL/min. λ = 254 nm, t(major) = 77.6 min, t(minor) = 89.1 min, 90% ee.

***(R)*-4-(*tert*-butyl(hydroxy)silyl)phenyl 4-methylbenzenesulfonate (16)**



16

According to the general procedures with the 4-(*tert*-butylsilyl)phenyl 4-methylbenzenesulfonate (**S16**, 66.8 mg, 0.20 mmol) at 0 °C for 16 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 4/1) to yield the product **16** as a white solid (37.8 mg, 0.108 mmol, 54% yield, 91% ee).

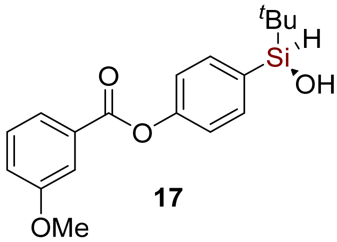
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.71 (d, *J* = 8.3 Hz, 2H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 2H), 7.02 (d, *J* = 8.4 Hz, 2H), 4.77 (s, 1H), 2.45 (s, 3H), 2.02 (s, 1H), 0.94 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 151.19, 145.38, 135.51, 133.78, 132.44, 129.74, 128.48, 121.76, 25.25, 21.70, 17.89.

HRMS (ESI) *m/z* calcd. for $C_{17}H_{23}O_4SSi$ $[M+H]^+$ 351.1081, found 351.1078.

HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min. λ = 254 nm, t(minor) = 7.8 min, t(major) = 9.5 min, 91% ee.

(R)-4-(*tert*-butyl(hydroxy)silyl)phenyl 3-methoxybenzoate (17)



17

According to the general procedures with 4-(*tert*-butylsilyl)phenyl 3-methoxybenzoate (**S17**, 62.8 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 10/1) to yield the product **17** as a colorless oil (39.6 mg, 0.12 mmol, 60% yield, 94% ee).

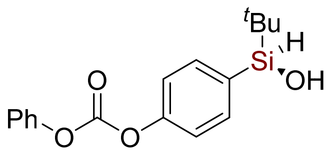
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.81 (d, *J* = 7.7 Hz, 1H), 7.73 – 7.62 (m, 3H), 7.42 (t, *J* = 8.0 Hz, 1H), 7.29 – 7.23 (m, 2H), 7.19 (dd, *J* = 8.3, 2.7 Hz, 1H), 4.83 (s, 1H), 3.89 (s, 3H), 2.11 (s, 1H), 1.00 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 164.89, 159.68, 152.59, 135.48, 132.29, 130.71, 129.62, 122.61, 121.21, 120.24, 114.50, 55.51, 25.32, 17.97.

HRMS (ESI) *m/z* calcd. for $C_{18}H_{23}O_4Si$ $[M+H]^+$ 331.1360, found 331.1357.

HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min. λ = 230 nm, t(major) = 16.4 min, t(minor) = 26.9 min, 94% ee.

(R)-4-(*tert*-butyl(hydroxy)silyl)phenyl phenyl carbonate (18)

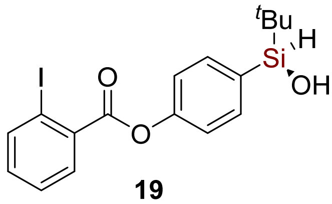


18

According to the general procedures with 4-(*tert*-butylsilyl)phenyl phenyl carbonate (60.0 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 10/1) to yield the product **18** as a colorless oil (26.7 mg, 0.084 mmol, 42% yield, 85% ee).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.70 – 7.63 (m, 2H), 7.47 – 7.39 (m, 2H), 7.35 – 7.22 (m, 5H), 4.81 (s, 1H), 2.07 (s, 1H), 0.98 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 152.52, 151.88, 150.92, 135.55, 132.86, 129.58, 126.35, 120.88, 120.35, 25.28, 17.94.
HRMS (ESI) *m/z* calcd. for $C_{17}H_{21}O_4Si$ [M+H]$^+$ 317.1204, found 317.1203.
HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min. λ = 210 nm, t(major) = 7.7 min, t(minor) = 8.4 min, 85% ee.

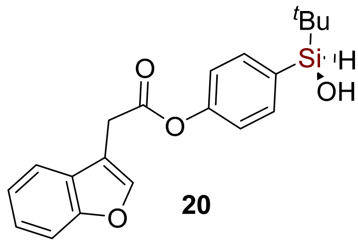
***(R)*-4-(*tert*-butyl(hydroxy)silyl)phenyl 2-iodobenzoate (19)**



19

According to the general procedures with 4-(*tert*-butylsilyl)phenyl 2-iodobenzoate (**S19**, 82.0 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 10/1) to yield the product **19** as a colorless oil (52.2 mg, 0.122 mmol, 61% yield, 94% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.08 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.05 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.73 – 7.63 (m, 2H), 7.49 (td, *J* = 7.6, 1.2 Hz, 1H), 7.35 – 7.26 (m, 2H), 7.23 (td, *J* = 7.7, 1.7 Hz, 1H), 4.83 (s, 1H), 2.09 (br, 1H), 0.99 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 164.70, 152.32, 141.70, 135.50, 134.00, 133.29, 132.60, 131.56, 128.08, 121.09, 94.67, 25.31, 17.96.
HRMS (ESI) *m/z* calcd. for $C_{17}H_{20}IO_3Si$ [M+H]$^+$ 427.0221, found 427.0217.
HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min. λ = 254 nm, t(major) = 21.8 min, t(minor) = 31.9 min, 94% ee.

***(R)*-4-(*tert*-butyl(hydroxy)silyl)phenyl 2-(benzofuran-3-yl)acetate (20)**

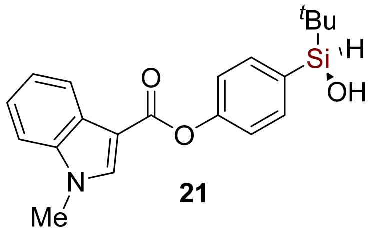


20

According to the general procedures with 4-(*tert*-butylsilyl)phenyl 2-(benzofuran-3-yl)acetate (**S20**, 82.0 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 10/1) to yield the product **20** as a colorless oil (38.2 mg, 0.108 mmol, 54% yield, 93% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.73 (s, 1H), 7.65 (d, *J* = 7.3 Hz, 1H), 7.61 (d, *J* = 8.3 Hz, 2H), 7.51 (d, *J* = 8.1 Hz, 1H), 7.37 – 7.26 (m, 2H), 7.12 (d, *J* = 8.3 Hz, 2H), 4.78 (s, 1H), 3.97 (s, 2H), 2.05 (s, 1H), 0.96 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 168.99, 155.23, 152.21, 143.07, 135.43, 132.47, 127.41, 124.63, 122.78, 120.90, 119.60, 112.50, 111.63, 30.00, 25.28, 17.93.
HRMS (ESI) *m/z* calcd. for $C_{20}H_{23}O_4Si$ [M+H]$^+$ 355.1360, found 355.1357.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min. λ = 254 nm, t(major) = 13.6 min, t(minor) = 16.9 min, 93% ee.

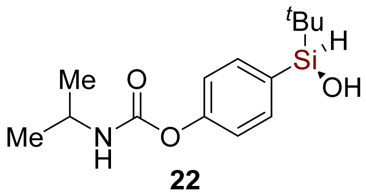
(*R*)-4-(*tert*-butyl(hydroxy)silyl)phenyl 1-methyl-1*H*-indole-3-carboxylate (21)



21

According to the general procedures with 4-(*tert*-butylsilyl)phenyl 1-methyl-1*H*-indole-3-carboxylate (**S21**, 67.5 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 10/1) to yield the product **21** as a white solid (51.6 mg, 0.146 mmol, 73% yield, 93% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.28 – 8.17 (m, 1H), 7.96 (s, 1H), 7.75 – 7.59 (m, 2H), 7.43 – 7.27 (m, 5H), 4.82 (s, 1H), 3.89 (s, 3H), 2.17 (s, 1H), 1.00 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 162.92, 152.64, 137.32, 136.21, 135.37, 131.62, 126.75, 123.12, 122.31, 121.70, 121.57, 109.94, 106.00, 33.60, 25.34, 17.98.
HRMS (ESI) *m/z* calcd. for $C_{20}H_{24}NO_3Si$ [M+H]$^+$ 354.1520, found 354.1515.
HPLC conditions:: Chiralcel OJ-H, n-hexane/*i*-PrOH = 75/25, flow rate 1.0 mL/min, λ = 220 nm, t_R (major) = 24.0 min, t_R (minor) = 32.5 min, 93% ee.

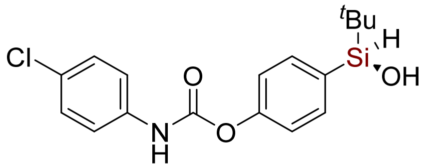
(*R*)-4-(*tert*-butyl(hydroxy)silyl)phenyl isopropylcarbamate (22)



22

According to the general procedures with 4-(*tert*-butylsilyl)phenyl isopropylcarbamate (**S22**, 53.0 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 4/1) to yield the product **22** as a colorless oil (40.2 mg, 0.142 mmol, 71% yield, 92% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.59 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 4.88 (d, *J* = 7.7 Hz, 1H), 4.78 (s, 1H), 4.03 – 3.81 (m, 1H), 2.11 (s, 1H), 1.24 (d, *J* = 6.6 Hz, 6H), 0.97 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 153.43, 152.68, 135.28, 131.29, 121.05, 43.47, 25.31, 22.88, 17.95.
HRMS (ESI) *m/z* calcd. for $C_{14}H_{24}NO_3Si$ [M+H]$^+$ 282.1520, found 282.1517.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min. λ = 230 nm, t(major) = 5.5 min, t(minor) = 6.3 min, 92% ee.

***(R)*-4-(*tert*-butyl(hydroxy)silyl)phenyl (4-chlorophenyl)carbamate (23)**



23

According to the general procedures with 4-(*tert*-butylsilyl)phenyl (4-chlorophenyl)carbamate (**S23**, 66.6 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 4/1) to yield the product **23** as a colorless oil (43.3 mg, 0.124 mmol, 62% yield, 80% ee).

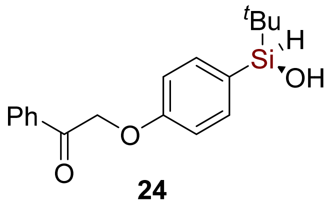
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.64 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 8.5 Hz, 2H), 7.36 – 7.28 (m, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 6.98 (s, 1H), 4.81 (s, 1H), 2.05 (s, 1H), 0.98 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 171.24, 152.03, 151.24, 135.85, 135.46, 132.21, 129.20, 121.02, 119.95, 25.30, 17.96.

HRMS (ESI) *m/z* calcd. for $C_{17}H_{21}ClNO_3Si$ [M+H]$^+$ 350.0974, found 350.0971.

HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 75/25, flow rate 1.0 mL/min. λ = 260 nm, t(minor) = 8.0 min, t(major) = 9.5 min, 80% ee.

***(R)*-2-(4-(*tert*-butyl(hydroxy)silyl)phenoxy)-1-phenylethan-1-one (24)**



24

According to the general procedures with 2-(4-(*tert*-butylsilyl)phenoxy)-1-phenylethan-1-one (**S24**, 59.8 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 10/1) to yield the product **24** as a colorless oil (36.7 mg, 0.116 mmol, 58% yield, 95% ee).

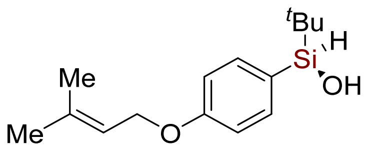
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.06 – 7.95 (m, 2H), 7.69 – 7.59 (m, 1H), 7.57 – 7.44 (m, 4H), 7.02 – 6.90 (m, 2H), 5.30 (s, 2H), 4.76 (s, 1H), 1.95 (s, 1H), 0.96 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 194.28, 159.63, 135.76, 134.51, 133.94, 128.86, 128.13, 126.88, 114.37, 70.46, 25.35, 17.99.

HRMS (ESI) *m/z* calcd. for $C_{18}H_{23}O_3Si$ [M+H]$^+$ 315.1411, found 315.1407.

HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 75/25, flow rate 1.0 mL/min. λ = 254 nm, t(major) = 7.7 min, t(minor) = 8.8 min, 95% ee.

***(R)*-*tert*-butyl(4-((3-methylbut-2-en-1-yl)oxy)phenyl)silanol (25)**



25

According to the general procedures with *tert*-butyl(4-((3-methylbut-2-en-1-yl)oxy)phenyl)silane (**S25**, 49.8 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **25** as a colorless oil (46.2 mg, 0.172 mmol, 86% yield, 91% ee).

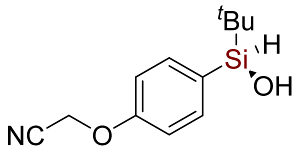
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.58 – 7.46 (m, 2H), 7.01 – 6.89 (m, 2H), 5.64 – 5.38 (m, 1H), 4.76 (s, 1H), 4.53 (d, *J* = 6.8 Hz, 2H), 1.92 (s, 1H), 1.80 (s, 3H), 1.75 (s, 3H), 0.97 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 160.53, 138.38, 135.63, 125.45, 119.47, 114.26, 64.49, 25.83, 25.38, 18.19, 18.01.

HRMS (ESI) *m/z* calcd. for $C_{15}H_{24}NaO_2Si$ [M+Na]$^+$ 287.1438, found 287.1436.

HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 90/10, flow rate 1.0 mL/min. λ = 240 nm, t(major) = 5.4 min, t(minor) = 6.4 min, 91% ee.

(*R*)-2-(4-(*tert*-butyl(hydroxy)silyl)phenoxy)acetonitrile (26)



26

According to the general procedures with 2-(4-(*tert*-butylsilyl)phenoxy)acetonitrile (**S26**, 43.8 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 10/1) to yield the product **26** as a colorless oil (29.9 mg, 0.128 mmol, 64% yield, 92% ee).

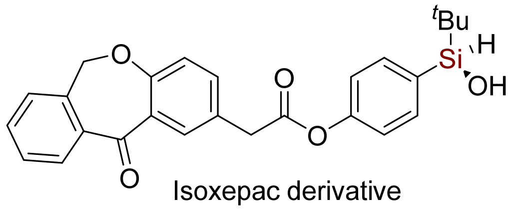
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.60 (d, *J* = 8.7 Hz, 2H), 7.01 (d, *J* = 8.6 Hz, 2H), 4.79 (s, 2H), 4.79 (s, 1H), 0.97 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 158.05, 135.98, 128.76, 114.95, 114.33, 53.18, 25.31, 17.97.

HRMS (ESI) *m/z* calcd. for $C_{12}H_{18}NO_2Si$ [M+H]$^+$ 236.1101, found 236.1106.

HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 80/20, flow rate 0.7 mL/min. λ = 214 nm, t(major) = 8.8 min, t(minor) = 10.1 min, 92% ee.

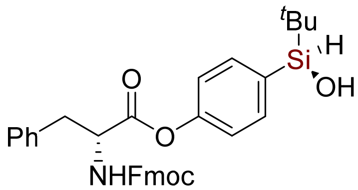
(R)-4-(tert-butyl(hydroxy)silyl)phenyl-2-(11-oxo-6,11-dihydrodibenzo[b,e]oxepin-2-yl)acetate (27)



Isoxepac derivative
27

According to the general procedures with 4-(*tert*-butylsilyl)phenyl-2-(11-oxo-6,11-dihydrodibenzo[*b,e*]oxepin-2-yl)acetate (**S27**, 86.0 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 4/1) to yield the product **27** as a colorless oil (78.4 mg, 0.176 mmol, 88% yield, 92% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.22 (d, *J* = 2.3 Hz, 1H), 7.90 (dd, *J* = 7.7, 1.3 Hz, 1H), 7.63 – 7.42 (m, 5H), 7.37 (d, *J* = 7.4 Hz, 1H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.07 (d, *J* = 8.4 Hz, 1H), 5.20 (s, 2H), 4.78 (s, 1H), 3.89 (s, 2H), 2.20 (s, 1H), 0.96 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 190.87, 169.69, 160.64, 152.26, 140.38, 136.29, 135.47, 135.37, 132.83, 132.60, 132.35, 129.49, 129.29, 127.83, 127.10, 125.20, 121.25, 120.92, 73.62, 40.29, 25.28, 17.92.
HRMS (ESI) *m/z* calcd. for $C_{26}H_{27}O_5Si$ $[M+H]^+$ 447.1622, found 447.1620.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 80/20, flow rate 1.0 mL/min. λ = 254 nm, t_R (major) = 19.2 min, t_R (minor) = 25.1 min, 92% ee.

4-((R)-tert-butyl(hydroxy)silyl)phenyl-(((9H-fluoren-9-yl)methoxy)carbonyl)-D-phenylalaninate (28)

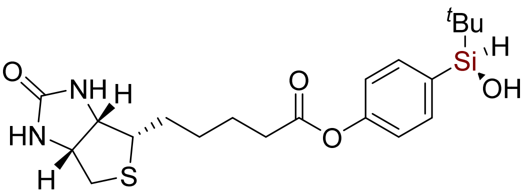


D-phenylalanine derivative
28

According to the general procedures with 4-(*tert*-butylsilyl)phenyl-(((9*H*-fluoren-9-yl)methoxy)carbonyl)-*D*-phenylalaninate (**S28**, 81.2 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 1/1) to yield the product **28** as a colorless oil (53.0 mg, 0.092 mmol, 47% yield, >20:1 dr).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.76 (d, *J* = 7.5 Hz, 2H), 7.66 – 7.52 (m, 4H), 7.39 (td, *J* = 7.5, 1.0 Hz, 2H), 7.36 – 7.25 (m, 5H), 7.23 – 7.17 (m, 2H), 7.01 (d, *J* = 7.9 Hz, 2H), 5.38 (d, *J* = 8.3 Hz, 1H), 4.97 – 4.86 (m, 1H), 4.79 (s, 1H), 4.46 (dd, *J* = 10.7, 7.1 Hz, 1H), 4.38 (dd, *J* = 10.7, 6.8 Hz, 1H), 4.21 (t, *J* = 6.8 Hz, 1H), 3.26 (d, *J* = 6.1 Hz, 2H), 0.96 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 170.02, 155.63, 151.78, 143.73, 143.63, 141.29, 135.45, 135.36, 132.84, 129.45, 128.74, 127.72, 127.38, 127.05, 125.05, 125.00, 120.68, 119.98, 67.06, 54.92, 47.11, 38.23, 25.28, 17.92.
HRMS (ESI) *m/z* calcd. for $C_{34}H_{36}NO_5Si$ [M+H]$^+$ 566.2357, found 566.2355.

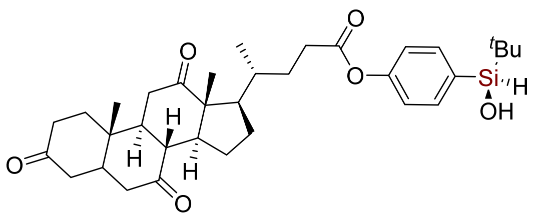
4-(*(R)-tert*-butyl(hydroxy)silyl)phenyl-5-((3*aS*,4*S*,6*aR*)-2-oxohexahydro-1*H*-thieno[3,4-*d*]imidazol-4-yl)pentanoate (29)



biotin derivative
29

According to the general procedures with 4-(*tert*-butylsilyl)phenyl 5-((3*aS*,4*S*,6*aR*)-2-oxohexahydro-1*H*-thieno[3,4-*d*]imidazol-4-yl)pentanoate (**S29**, 81.2 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 1/4) to yield the product **29** as a colorless oil (42.3 mg, 0.1 mmol, 50% yield, >20:1 dr).
^{1}H NMR (400 MHz, DMSO-*d*$_6$) δ 7.58 (d, *J* = 8.4 Hz, 2H), 7.15 (d, *J* = 8.3 Hz, 2H), 6.53 – 6.40 (m, 2H), 6.38 (s, 1H), 4.67 (d, *J* = 1.7 Hz, 1H), 4.32 (dd, *J* = 7.7, 5.0 Hz, 1H), 4.16 (ddd, *J* = 7.8, 4.4, 1.8 Hz, 1H), 3.14 (ddd, *J* = 8.5, 6.2, 4.3 Hz, 1H), 2.83 (dd, *J* = 12.4, 5.1 Hz, 1H), 2.63 – 2.55 (m, 3H), 1.78 – 1.59 (m, 3H), 1.58 – 1.34 (m, 3H), 0.89 (s, 9H).
^{13}C NMR (101 MHz, DMSO-*d*$_6$) δ 172.11, 163.24, 152.28, 135.63, 133.43, 121.66, 61.51, 59.68, 55.80, 33.80, 28.46, 28.40, 25.90, 24.85, 18.22.
HRMS (ESI) *m/z* calcd. for $C_{20}H_{31}N_2O_4SSi$ [M+H]$^+$ 423.1768, found 423.1766.

4-(*(R)-tert*-butyl(hydroxy)silyl)phenyl-(4*R*)-4-((8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-3,7,12-trioxohexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentanoate (30)

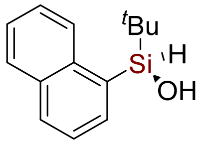


dehydrocholic acid derivative
30

According to the general procedures with 4-(*tert*-butylsilyl)phenyl (4*R*)-4-((8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-3,7,12-trioxohexadecahydro-1*H*-cyclopenta[*a*]phenanthren-17-yl)pentanoate (**S30**, 112.8 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 2/1) to yield the product **30** as a white solid (70.2 mg, 0.122 mmol, 61% yield, >20:1 dr).

¹H NMR (400 MHz, $CDCl_3$) δ 7.77 – 7.42 (m, 2H), 7.24 – 6.89 (m, 2H), 4.77 (s, 1H), 3.15-2.95 (m, 1H), 2.95 – 2.78 (m, 3H), 2.72 – 2.59 (m, 1H), 2.53 (ddd, *J* = 15.9, 8.7, 7.2 Hz, 1H), 2.41 – 1.73 (m, 14H), 1.67 – 1.46 (m, 2H), 1.46-1.32 (m, 1H), 1.39 (s, 3H), 1.34 – 1.17 (m, 2H), 1.08 (s, 3H), 0.96 (s, 9H), 0.91 (d, *J* = 6.6 Hz, 3H).
¹³C NMR (101 MHz, $CDCl_3$) δ 212.20, 209.37, 208.84, 172.34, 152.19, 135.32, 132.29, 120.92, 56.82, 51.67, 48.86, 46.71, 45.54, 45.44, 44.85, 42.65, 38.50, 36.35, 35.90, 35.38, 35.12, 31.50, 30.25, 27.56, 25.26, 25.03, 21.76, 18.58, 17.87, 11.76.
HRMS (ESI) *m/z* calcd. for $C_{34}H_{48}NaO_6Si$ $[M+Na]^+$ 603.3112, found 603.3107.

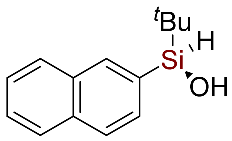
***(R)-tert*-butyl(naphthalen-1-yl)silanol (31)**



31

According to the general procedures with *tert*-butyl(naphthalen-1-yl)silane (**S31**, 42.8 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **31** as a colorless oil (24.2 mg, 0.106 mmol, 53% yield, 93% ee).
¹H NMR (400 MHz, $CDCl_3$) δ 8.32 – 8.21 (m, 1H), 7.91 (d, *J* = 8.2 Hz, 1H), 7.88 – 7.83 (m, 1H), 7.81 (dd, *J* = 6.8, 1.3 Hz, 1H), 7.55 – 7.39 (m, 3H), 5.23 (s, 1H), 1.01 (s, 9H).
¹³C NMR (101 MHz, $CDCl_3$) δ 137.23, 134.63, 133.26, 132.90, 130.60, 128.74, 128.40, 125.96, 125.63, 124.87, 26.07, 18.84.
HRMS (ESI) *m/z* calcd. for $C_{14}H_{19}OSi$ $[M+H]^+$ 231.1200, found 231.1198.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 254 nm, t_R (major) = 13.5 min, t_R (minor) = 15.1 min, 93% ee.

***(R)-tert*-butyl(naphthalen-2-yl)silanol (32)**

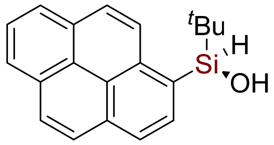


32

According to the general procedures with *tert*-butyl(naphthalen-2-yl)silane (**S32**, 42.9 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **32** as a colorless oil (28.9 mg, 0.126 mmol, 63% yield, 87% ee).
¹H NMR (400 MHz, $CDCl_3$) δ 8.13 (s, 1H), 7.90 – 7.80 (m, 3H), 7.65 (dd, *J* = 8.1, 1.2 Hz, 1H), 7.55 – 7.45 (m, 2H), 4.93 (s, 1H), 2.09 (s, 1H), 1.01 (s, 9H).
¹³C NMR (101 MHz, $CDCl_3$) δ 135.33, 134.23, 132.73, 132.18, 129.81, 128.23, 127.75, 127.00, 126.70, 126.01, 25.45, 18.15.

HRMS (APCI) *m/z* calcd. for $C_{14}H_{19}OSi$ [M+H]$^+$ 231.1200, found 231.1199.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 254 nm, t_R (major) = 18.5 min, t_R (minor) = 22.6 min, 87% ee.

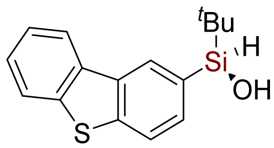
***(R)-tert*-butyl(pyren-1-yl)silanol (33)**



33

According to the general procedures with *tert*-butyl(pyren-1-yl)silane (**S33**, 28.8 mg, 0.10 mmol) at 0 °C for 72 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **33** as a light yellow solid (22.4 mg, 0.074 mmol, 74% yield, 84% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.55 (d, *J* = 9.2 Hz, 1H), 8.27 (d, *J* = 7.6 Hz, 1H), 8.24 – 8.14 (m, 3H), 8.15 – 7.95 (m, 4H), 5.46 (s, 1H), 2.32 (s, 1H), 1.05 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 136.37, 132.75, 132.62, 131.23, 130.69, 129.98, 128.34, 127.75, 127.45, 127.44, 125.90, 125.31, 125.27, 124.65, 124.49, 123.96, 26.04, 19.15.
HRMS (ESI) *m/z* calcd. for $C_{20}H_{19}OSi$ [M−H]$^-$ 303.1211, found 303.1207.
HPLC conditions: Chiralcel OD-H, *n*-hexane/*i*-PrOH = 98/2, flow rate 1.0 mL/min. λ = 270 nm, t_R (major) = 25.2 min, t_R (minor) = 29.2 min, 84% ee.

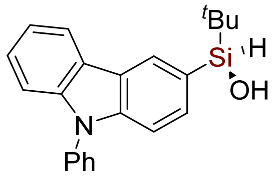
***(R)-tert*-butyl(dibenzo[*b,d*]thiophen-2-yl)silanol (34)**



34

According to the general procedures with *tert*-butyl(dibenzo[*b,d*]thiophen-2-yl)silane (**S34**, 27.0 mg, 0.10 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **34** as a white solid (14.3 mg, 0.05 mmol, 50% yield, 89% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.41 (t, *J* = 0.9 Hz, 1H), 8.27 – 8.18 (m, 1H), 7.92 – 7.82 (m, 2H), 7.67 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.52 – 7.43 (m, 2H), 4.95 (s, 1H), 1.03 (s, 9H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 139.14, 135.29, 135.03, 131.74, 129.99, 127.42, 126.85, 124.49, 122.81, 122.33, 121.63, 25.43, 18.09.
HRMS (APCI) *m/z* calcd. for $C_{16}H_{19}OSSi$ [M+H]$^+$ 287.0920, found 287.0920.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 254 nm, t(major) = 17.0 min, t(minor) = 19.4 min, 89% ee.

***(R)-tert*-butyl(9-phenyl-9*H*-carbazol-3-yl)silanol (35)**



35

According to the general procedures with 3-(*tert*-butylsilyl)-9-phenyl-9*H*-carbazole (**S35**, 32.9 mg, 0.10 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **35** as a colorless oil (20.1 mg, 0.058 mmol, 58% yield, 94% ee).

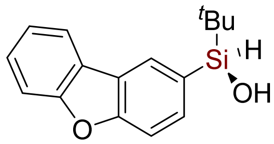
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.41 (d, *J* = 1.0 Hz, 1H), 8.18 (dd, *J* = 7.7, 1.0 Hz, 1H), 7.68 – 7.52 (m, 5H), 7.48 (ddt, *J* = 8.7, 6.6, 1.5 Hz, 1H), 7.45 – 7.35 (m, 3H), 7.31 (ddd, *J* = 8.0, 5.1, 2.9 Hz, 1H), 4.96 (s, 1H), 1.03 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 142.19, 140.88, 137.43, 131.38, 129.89, 127.60, 127.10, 126.66, 126.09, 124.51, 123.13, 120.33, 120.21, 109.82, 109.46, 25.52, 18.18.

HRMS (ESI) *m/z* calcd. for $C_{22}H_{23}NNaOSi$ [M+Na]$^+$ 368.1441, found 368.1439.

HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.8 mL/min. λ = 254 nm, t(major) = 15.3 min, t(minor) = 29.8 min, 94% ee.

***(R)-tert*-butyl(dibenzo[*b,d*]furan-2-yl)silanol (36)**



36

According to the general procedures with *tert*-butyl(dibenzo[*b,d*]furan-2-yl)silane (**S36**, 50.9 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **36** as a white solid (31.2 mg, 0.115 mmol, 58% yield, 84% ee).

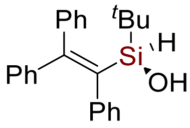
^{1}H NMR (400 MHz, CDCl$_3$) δ 8.21 (s, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.68 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.62 – 7.53 (m, 2H), 7.46 (td, *J* = 7.8, 1.4 Hz, 1H), 7.35 (td, *J* = 7.5, 1.0 Hz, 1H), 4.93 (s, 1H), 2.28 (br, 1H), 1.01 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 157.59, 156.05, 132.79, 128.26, 127.28, 126.76, 124.07, 123.82, 122.87, 120.70, 111.67, 111.37, 25.42, 18.07.

HRMS (ESI) *m/z* calcd. for $C_{16}H_{17}O_2Si$ [M−H]$^-$ 269.1003, found 269.0998.

HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 220 nm, t_R (major) = 15.3 min, t_R (minor) = 16.8 min, 84% ee.

***(R)-tert*-butyl(1,2,2-triphenylvinyl)silanol (37)**



37

According to the general procedures with *tert*- butyl(1,2,2-triphenylvinyl)silane (**S37**, 34.2 mg, 0.10 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **37** as a colorless oil (7.2 mg, 0.02 mmol, 20% yield, 59% ee).

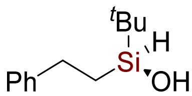
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.43 – 7.30 (m, 5H), 7.18 – 7.11 (m, 4H), 7.09 – 6.98 (m, 4H), 6.91 (dd, *J* = 7.5, 2.1 Hz, 2H), 4.50 (s, 1H), 2.01 (br, 1H), 0.74 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 155.86, 143.35, 142.68, 142.50, 139.47, 130.60, 130.08, 129.98, 129.56, 129.47, 128.76, 128.07, 127.97, 127.79, 127.74, 127.39, 127.19, 126.53, 125.84, 125.77, 26.55, 19.05.

HRMS (ESI) *m/z* calcd. for $C_{24}H_{26}NaOSi$ [M+Na]$^+$ 381.1645, found 381.1645.

HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 97/3, flow rate 0.5 mL/min. λ = 230 nm, t(minor) = 13.3 min, t(major) = 17.0 min, 59% ee.

***(S)-tert*-butyl(phenethyl)silanol (38)**



38

According to the general procedures with *tert*-butyl(phenethyl)silane (**S38**, 38.4 mg, 0.20 mmol) at 0 °C for 36 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **38** as a colorless oil (12.5 mg, 0.06 mmol, 30% yield, 53% ee).

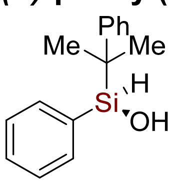
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.65 – 6.67 (m, 5H), 4.36 (dd, *J* = 3.6, 1.8 Hz, 1H), 3.28 – 2.54 (m, 2H), 1.11 – 1.00 (m, 2H), 0.96 (s, 9H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 144.45, 128.44, 127.83, 125.77, 29.67, 25.61, 17.75, 14.46.

HRMS (ESI) *m/z* calcd. for $C_{12}H_{20}NaOSi$ [M+Na]$^+$ 231.1176, found 231.1174.

HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 98/2, flow rate 0.35 mL/min. λ = 230 nm, t(minor) = 25.3 min, t(major) = 26.9 min, 53% ee.

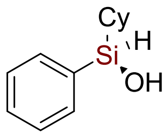
***(S)*-phenyl(2-phenylpropan-2-yl)silanol (39)**



39

According to the general procedures with phenyl(2-phenylpropan-2-yl)silane (**S39**, 22.6 mg, 0.10 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 20/1) to yield the product **39** as a colorless oil (8.5 mg, 0.035 mmol, 35% yield, 81% ee).
H NMR (400 MHz, $CDCl_3$) δ 7.43 – 7.28 (m, 7H), 7.26 – 7.22 (m, 2H), 7.19 – 7.12 (m, 1H), 4.86 (s, 1H), 1.96 (s, 1H), 1.42 (s, 3H), 1.41 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 146.55, 134.26, 133.47, 130.20, 128.20, 127.64, 126.40, 124.95, 28.16, 23.26, 22.88.
HRMS (APCI) *m/z* calcd. for $C_{15}H_{19}OSi$ [M+H]$^+$ 243.1200, found 243.1200.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 220 nm, t(major) = 12.9 min, t(minor) = 14.7 min, 81% ee.

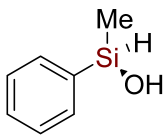
(R)-cyclohexyl(phenyl)silanol (40)



40

According to the general procedures with cyclohexyl(phenyl)silane (**S40**, 38.0 mg, 0.20 mmol) at 0 °C for 24 h, the reaction mixture was purified by column chromatography (PE/EtOAc = 30/1) to yield the product **40** as a colorless oil (10.2 mg, 0.05 mmol, 25% yield, 67% ee).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.53 (m, 2H), 7.47 – 7.33 (m, 3H), 4.87 (d, *J* = 2.0 Hz, 1H), 1.83 – 1.79 (m, 1H), 1.75 – 1.67 (m, 3H), 1.31 – 1.16 (m, 8H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 135.28, 133.90, 130.06, 127.91, 27.48, 26.70, 26.46, 26.40, 25.56.
HRMS (APCI) *m/z* calcd. for $C_{12}H_{19}OSi$ [M+H]$^+$ 207.1200, found 207.1199.
HPLC conditions: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 214 nm, t(major) = 12.0 min, t(minor) = 13.4 min, 67% ee.

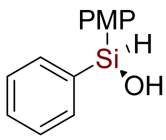
(*R*)-methyl(phenyl)silanol (41)[10]



41

According to the general procedures with methyl(phenyl)silane (**S41**, 27.5 mg, 0.20 mmol) at 0 °C for 24 h, the reaction gave **41** in <10% yield.

(*S*)-(4-methoxyphenyl)(phenyl)silanol (42)



42

According to the general procedures with (4-methoxyphenyl)(phenyl)silane (**S42**, 21.4 mg, 0.10 mmol) at 0 °C for 24 h, the reaction gave **42** in <10% yield.

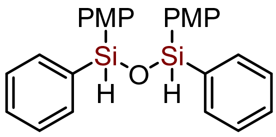
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.69 – 7.61 (m, 2H), 7.57 (d, *J* = 8.1 Hz, 2H), 7.47 – 7.34 (m, 3H), 6.95 (d, *J* = 8.2 Hz, 2H), 5.50 (s, 1H), 3.82 (s, 3H), 2.36 (s, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 161.45, 135.98, 135.25, 134.25, 130.31, 128.02, 125.87, 113.83, 55.07.

HRMS (APCI) *m/z* calcd. for $C_{13}H_{15}O_2Si$ [M+H]$^+$ 231.0836, found 231.0830.

HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 1.0 mL/min. λ = 240 nm, t(major) = 17.8 min, t(minor) = 21.3 min, 2% ee.

1,3-bis(4-methoxyphenyl)-1,3-diphenyldisiloxane (42')



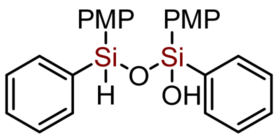
42'

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.54 (d, *J* = 6.9 Hz, 4H), 7.47 (d, *J* = 8.3 Hz, 4H), 7.44 – 7.37 (m, 2H), 7.37 – 7.29 (m, 4H), 6.88 (d, *J* = 8.4 Hz, 4H), 5.55 (s, 2H), 3.81 (s, 6H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 161.24, 135.98, 135.40, 134.27, 130.05, 127.87, 126.08, 113.66, 55.04.

HRMS (APCI) *m/z* calcd. for $C_{26}H_{27}O_3Si_2$ [M+H]$^+$ 443.1493, found 443.1481.

1,3-bis(4-methoxyphenyl)-1,3-diphenyldisiloxan-1-ol (42'')



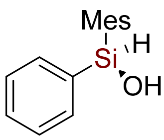
42''

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.65 – 7.46 (m, 8H), 7.44 – 7.29 (m, 6H), 6.88 (t, *J* = 8.1 Hz, 4H), 5.61 (s, 1H), 3.81 (s, 3H), 3.81 (s, 3H), 2.70 (s, 1H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 161.28, 135.99, 135.98, 135.42, 134.93, 134.27, 130.16, 130.11, 127.93, 127.79, 126.10, 125.61, 113.72, 113.55, 55.04, 55.03.

HRMS (ESI) *m/z* calcd. for $C_{26}H_{26}O_4Si_2Na$ [M+Na]$^+$ 481.1262, found 481.1255.

(*S*)-mesityl(phenyl)silanol (43)



43

According to the general procedures with mesityl(phenyl)silane (**S43**, 22.6 mg, 0.10 mmol) at 0 °C for 24 h, the reaction gave **43** in 10% yield with <5% ee. 88% **S43** was recovered.

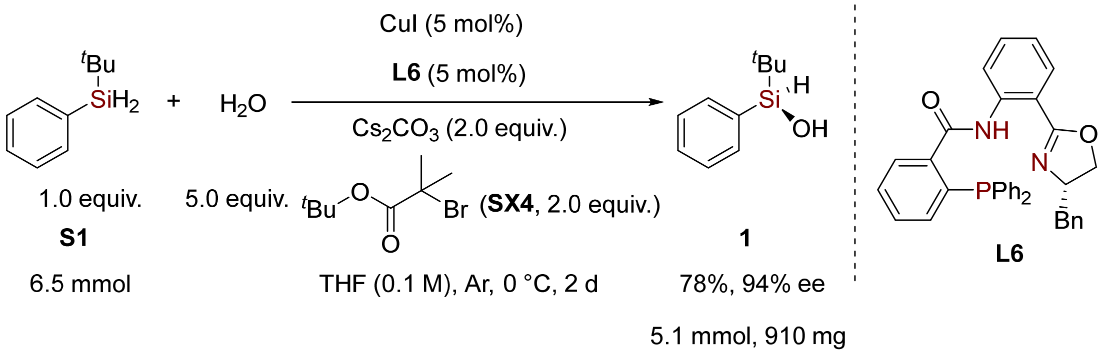
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 – 7.53 (m, 2H), 7.44 – 7.29 (m, 3H), 6.85 (s, 2H), 5.85 (s, 1H), 2.42 (s, 6H), 2.29 (s, 3H), 2.24 (br, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 144.96, 140.42, 136.03, 133.94, 129.97, 128.75, 128.12, 128.03, 23.27, 21.20.

HRMS (APCI) *m/z* calcd. for $C_{15}H_{18}OSiNa$ $[M+Na]^+$ 265.1019, found 265.1013.

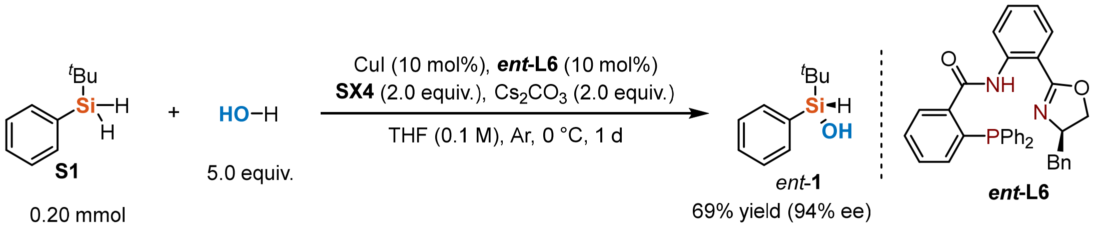
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 98/2, flow rate 0.6 mL/min. λ = 220 nm, t(major) = 23.5 min, t(minor) = 25.3 min, 3% ee.

Procedures for large-scale synthesis:



A 250 mL Schlenk flask equipped with a magnetic stir bar was charged with CuI (61.9 mg, 0.325 mmol, 5 mol%), **L6** (175.7 mg, 0.325 mmol, 5 mol%), Cs_2CO_3 (4235 mg, 13 mmol, 2 equiv.), The flask was evacuated and backfilled with argon three times. Under the flow of Ar, *tert*-butyl(phenyl)silane (**S1**, 1068 mg, .6.5 mmol, 1.0 equiv.), anhydrous THF (65 mL), H_2O (586 mg, 32.5 mmol, 5.0 equiv.), and *tert*-butyl 2-bromo-2-methylpropanoate (**SX4**, 2900 mg, 13 mmol, 2.0 equiv.) were added into the mixture. The reaction mixture was stirred at 0 °C for 2 d. After the reaction, the mixture was filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated and the residue was purified by column chromatography on silica gel eluting with 30/1 PE/EtOAc to afford the desired product of *tert*-butyl(phenyl)silanol (**1**, 910 mg, 5.1 mmol) in 78% isolated yield with 94% ee.

Procedures for the enantiomer of 1 (*ent*-1) synthesis:

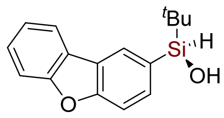


A 10 mL Schlenk tube equipped with a magnetic stir bar was charged with CuI (3.8 mg, 0.020 mmol, 10 mol%), *ent*-**L6** (10.8 mg, 0.010 mmol, 10 mol%), and Cs_2CO_3 (130.3 mg, 0.40 mmol, 2.0 equiv.). The tube was evacuated and backfilled with argon three times. Under the flow of Ar, **S1** (32.9 mg, 0.20 mmol, 1.0 equiv.), anhydrous THF (2.0 mL), H_2O (18.0 mg, 1.0 mmol, 5.0 equiv.), and *tert*-butyl 2-bromo-2-methylpropanoate (**SX4**, 89.2 mg, 0.40 mmol, 2.0 equiv.) were added into the mixture. The reaction mixture was stirred at 0 °C for 1 d and then was filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated and the residue was purified by column chromatography on silica gel to afford *ent*-**1** (24.9 mg, 0.138 mmol) in 69% yield with 94% ee.

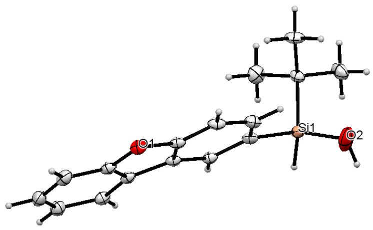
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 95/5, flow rate 0.5 mL/min. λ = 220 nm, t(minor) = 10.6 min, t(major) = 11.8 min, 94% ee.

5. Assignment of Absolute Stereochemistry

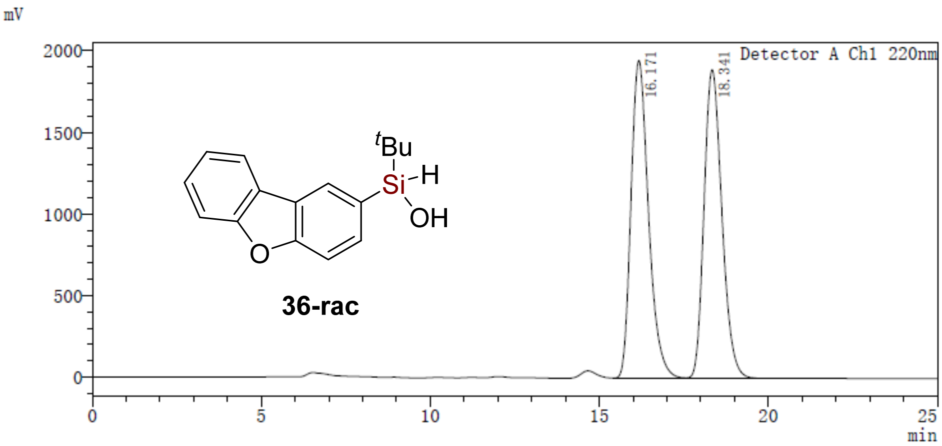
1) The absolute configuration of Si-chiral silanols was determined to be *R* through the X-ray structure of **36**.



36



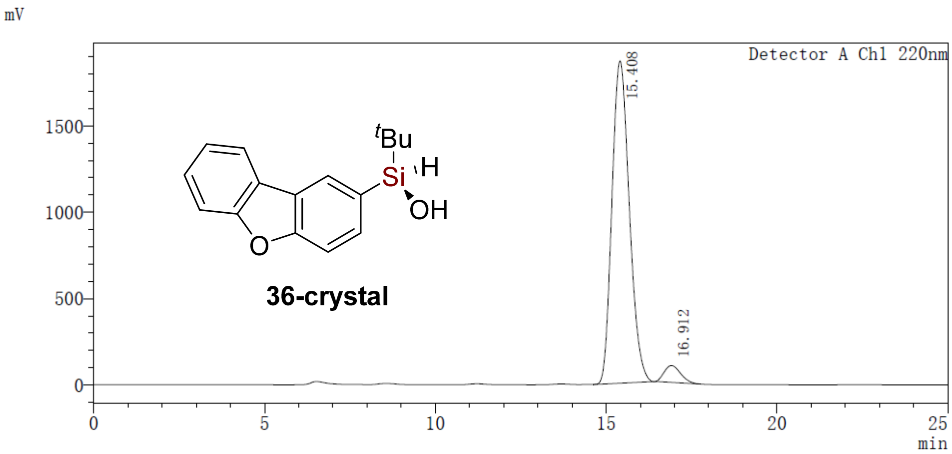
90% ee for crystal (R)



Peak Table

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Area%
1	16.171	70331878	50.284
2	18.341	69536846	49.716

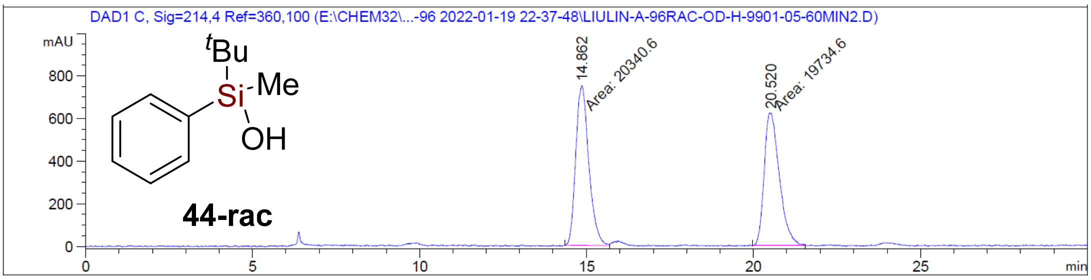


Peak Table

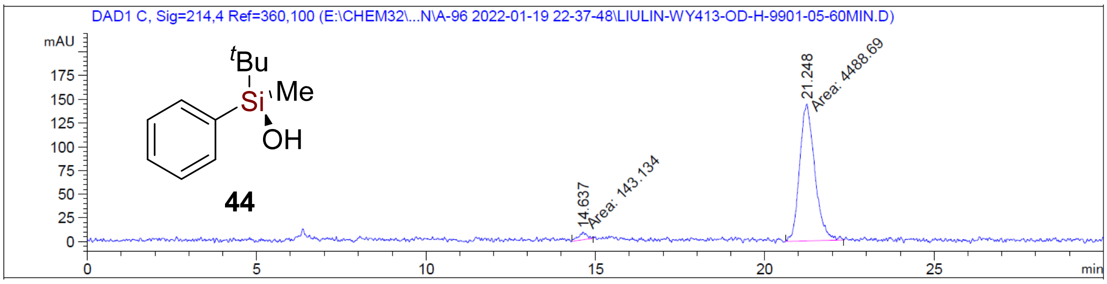
Detector A Ch1 220nm

Peak#	Ret. Time	Area	Area%
1	15.408	66055399	95.258
2	16.912	3288420	4.742

2) The absolute configuration of the tertiary Si-chiral silanol **44** was assigned to be *R* by comparing its chiral HPLC spectrum with that of the reported highly enantiopure silanol (>98% ee)[11] under the same HPLC conditions: Chiralcel OD-H, *n*-hexane/*i*-PrOH = 99/1, flow rate 0.5 mL/min. λ = 214 nm, t(minor) = 14.6 min, t(major) = 21.2 min, 94% ee.



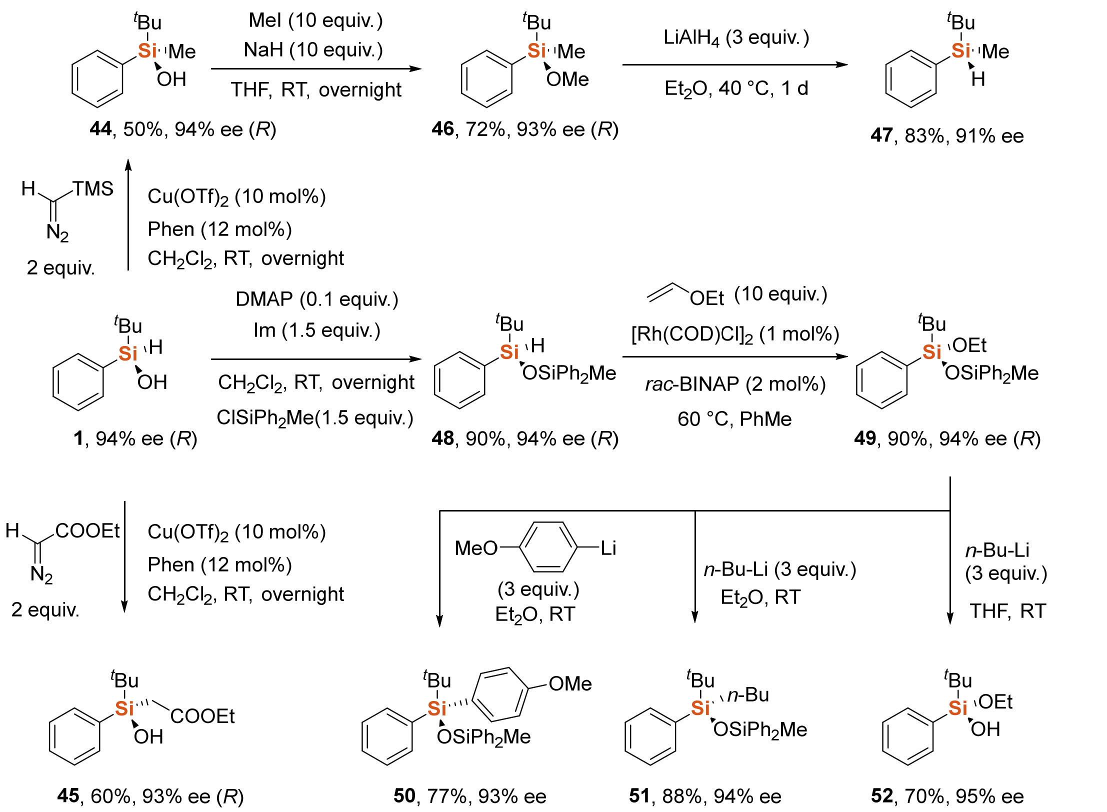
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.862	MM	0.4523	2.03406e4	749.55762	50.7562
2	20.520	MM	0.5283	1.97346e4	622.59058	49.2438
Totals :				4.00752e4	1372.14819	



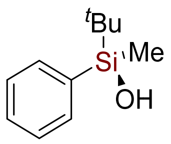
Signal 3: DAD1 C, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.637	MM	0.2879	143.13380	8.28679	3.0902
2	21.248	MM	0.5173	4488.68994	144.60741	96.9098
Totals :				4631.82375	152.89420	

6. Derivatizations of Silicon-Stereogenic Silanols



(*R*)-*tert*-butyl(methyl)(phenyl)silanol (44)



44

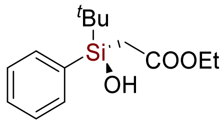
To a 10 mL Schlenk tube was added $Cu(OTf)_2$ (3.6 mg, 0.01 mmol) and 1,10-phenanthroline (Phen, 2.2 mg, 0.012 mmol). The tube was evaculated and refilled with Ar three times. Under Ar, CH_2Cl_2 (1 mL) was added to the tube. The mixture was stirred at RT for 15 min. To the resulting mixture was further added the silanol **1** (18.0 mg, 0.10 mmol) and 1 equiv. (diazomethyl)trimethylsilane (2 M in hexane, 0.05 mL, 0.10 mmol). After stirring at RT for 0.5 h, another 1 equiv. (diazomethyl)trimethylsilane (0.05 mL, 0.10 mmol) was added. The resulting mixture was reacted overnight and filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated and the residue was purified by column chromatography (PE/EtOAc = 10/1) on silica gel to yield **44** as a colorless oil[11] (9.7 mg, 0.050 mmol, 50% yield, 94% ee).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.62 – 7.56 (m, 2H), 7.44 – 7.33 (m, 3H), 1.79 (s, 1H), 0.94 (s, 9H), 0.39 (s, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 136.77, 133.98, 129.42, 127.59, 25.80, 18.28, −4.71.

HPLC conditions: Chiralcel OD-H, *n*-hexane/*i*-PrOH = 99/1, flow rate 0.5 mL/min, λ = 214 nm, t_R (minor) = 14.6 min, t_R (major) = 21.2 min, 94% ee.

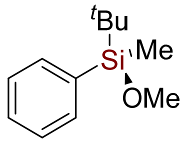
ethyl (*R*)-2-(*tert*-butyl(hydroxy)(phenyl)silyl)acetate (45)



45

To a 10 mL Schlenk tube was added $Cu(OTf)_2$ (3.6 mg, 0.01 mmol) and Phen (2.2 mg, 0.012 mmol). The tube was evacuated and refilled with Ar three times. Under Ar, CH_2Cl_2 (1 mL) was added to the tube. The mixture was stirred at RT for 15 min. To the resulting mixture was further added the silanol **1** (18.0 mg, 0.10 mmol) and 1 equiv. ethyl 2-diazoacetate (11.4 mg, 0.10 mmol). After stirring at RT for 0.5 h, another 1 equiv. ethyl 2-diazoacetate (11.4 mg, 0.10 mmol) was added. The resulting mixture was reacted overnight and filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated and the residue was purified by column chromatography (PE/EtOAc = 5/1) on silica gel to yield **45** as a colorless oil (16.0 mg, 0.060 mmol, 60% yield, 93% ee).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 – 7.55 (m, 2H), 7.47 – 7.29 (m, 3H), 3.98 (q, *J* = 7.1 Hz, 2H), 3.07 (br, 1H), 2.29 (s, 2H), 1.06 (t, *J* = 7.1 Hz, 3H), 0.97 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 172.86, 134.18, 133.74, 129.87, 127.59, 60.45, 25.61, 22.75, 18.67, 14.04.
HRMS (ESI) *m/z* calcd. for $C_{14}H_{22}NaO_3Si$ $[M+Na]^+$ 289.1230, found 289.1227.
HPLC conditions: Chiralcel AS-3, *n*-hexane/*i*-PrOH = 98/2, flow rate 0.5 mL/min, λ = 220 nm, t_R (minor) = 35.0 min, t_R (major) = 37.5 min, 93% ee.

(*R*)-*tert*-butyl(methoxy)(methyl)(phenyl)silane (46)



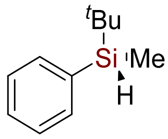
46

To a 10 mL Schlenk tube was added NaH (60 wt% dispersion, 68.8 mg, 1.72 mmol). The tube was evacuated and refilled with Ar three times. The THF (2.0 mL) was added to the tube, followed by the silanol **44** (33.5 mg, 0.17 mmol). At last, MeI (244.1 mg, 1.72 mmol) was added. The resulting mixture was stirred at RT overnight and filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated and the residue was purified by column chromatography (PE) on silica gel to yield **46** as a colorless oil[11] (25.7 mg, 0.123 mmol, 72% yield, 93% ee).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.48 (m, 2H), 7.43 – 7.29 (m, 3H), 3.49 (s, 3H), 0.91 (s, 9H), 0.37 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 135.52, 134.45, 129.34, 127.57, 51.30, 25.88, 18.24, −7.88.

HPLC conditions:: Chiralcel OJ-H, *n*-hexane/*i*-PrOH = 100/0, flow rate 0.5 mL/min, λ = 220 nm, t_R (major) = 8.1 min, t_R (minor) = 9.3 min, 93% ee.

***(S)-tert*-butyl(methyl)(phenyl)silane (47)**



47

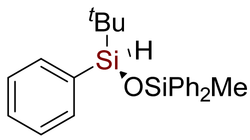
To a 10 mL Schlenk tube was added $LiAlH_4$ (11.4 mg, 0.30 mmol). The tube was evaculated and refilled with Ar three times. Then Et_2O (1.0 mL) was added to the tube, followed by silyl ether **46** (20.8 mg, 0.10 mmol). The resulting mixture was reacted at 40 °C for 24 h and filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated to dryness to yield **47** as a colorless oil[11] (14.8 mg, 0.083 mmol, 83% yield, 91% ee). Enantiomeric excess was established as 91% ee by chiral HPLC analysis of the oxidation product of *tert*-butyl(methyl)(phenyl)silanol through methyltrioxorhenium catalyzed oxidation of **47** with H_2O_2.[3]

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (dt, *J* = 7.6, 1.7 Hz, 2H), 7.42 – 7.32 (m, 3H), 4.16 (dd, *J* = 3.9, 1.7 Hz, 1H), 0.96 (s, 9H), 0.35 (d, *J* = 3.8 Hz, 3H).

^{1}H NMR (400 MHz, $CDCl_3$) δ 135.49, 135.05, 129.19, 127.61, 26.82, 16.60, −8.47.

HPLC conditions: Chiralcel OD-H, *n*-hexane/*i*-PrOH = 99/1, flow rate 0.5 mL/min, λ = 214 nm, t_R (minor) = 14.7 min, t_R (major) = 21.2 min, 91% ee.

***(R)*-3-(*tert*-butyl)-1-methyl-1,1,3-triphenyldisiloxane (48)**



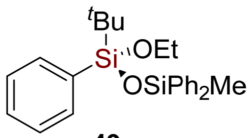
48

To the CH_2Cl_2 (10 mL) solution of **1** (180 mg, 1.0 mmol) was added imidazole (102.1 mg, 1.5 mmol), DMAP (12.2 mg, 0.1 mmol), and $Ph_2MeSiCl$ (315 μL, 1.5 mmol). The mixture was reacted at room temperature overnight. The mixture was poured into H_2O and extracted with CH_2Cl_2. The combined organic layer was washed with brine, dried over Na_2SO_4, and evaporated to dryness in vacuo. The residue was purified by column chromatography on silica gel (PE) to give **48** as a colorless oil (340.1 mg, 0.9 mmol, 90% yield, 94% ee).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.47 (m, 6H), 7.42 – 7.26 (m, 9H), 4.86 (s, 1H), 0.91 (s, 9H), 0.62 (s, 3H).

^{13}C NMR (101 MHz, CDCl$_3$) δ 137.42, 137.37, 134.94, 134.16, 133.97, 129.73, 129.60, 127.72, 127.56, 25.41, 18.30, −0.89.
HRMS (ESI) *m/z* calcd. for $C_{23}H_{28}NaOSi_2$ [M+Na]$^+$ 399.1571, found 399.1570.
HPLC conditions: Chiralcel OD-3, *n*-hexane/*i*-PrOH = 100/0, flow rate 0.3 mL/min, λ = 220 nm, t_R (minor) = 50.2 min, t_R (major) = 52.1 min, 94% ee.

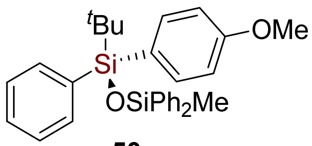
***(R)*-1-(*tert*-butyl)-1-ethoxy-3-methyl-1,3,3-triphenyldisiloxane (49)**



49

Inside an argon-filled glovebox, an oven-dried 10 mL tube was charged with $[Rh(cod)Cl]_2$ (1.3 mg, 0.0027 mmol), *rac*-BINAP (3.4 mg, 0.0054 mmol), and anhydrous toluene (2 mL). The mixture was stirred at room temperature for 5 min, followed by the addition of **48** (102.2 mg, 0.27 mmol) and ethyl vinyl ether (260 μL, 2.7 mmol). The tube was capped and taken outside of the glovebox. The resulting mixture was heated to 60 °C and stirred for 12 h. Then the reaction mixture was concentrated and purified by preparative TLC (PE) to afford **49** as a colorless oil (103 mg, 0.243 mmol, 90% yield, 94% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.83 – 7.47 (m, 6H), 7.40-7.29 (m, 9H), 3.65 – 3.61 (m, 2H), 1.09 (t, J = 6.9 Hz, 3H), 0.89 (s, 9H), 0.70 (s, 3H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 137.59, 137.52, 135.06, 134.05, 134.03, 133.54, 129.63, 129.60, 127.75, 127.74, 127.47, 58.73, 25.93, 18.43, 18.22, −0.48.
HRMS (ESI) *m/z* calcd. for $C_{25}H_{32}NaO_2Si_2$ [M+Na]$^+$ 443.1833, found 443.1845.
HPLC conditions: Chiralcel OD-3, *n*-hexane/*i*-PrOH = 100/0, flow rate 0.25 mL/min. λ = 214 nm, t(minor) = 18.2 min, t(major) = 19.6 min, 94% ee.

***(R)*-1-(*tert*-butyl)-1-(4-methoxyphenyl)-3-methyl-1,3,3-triphenyldisiloxane (50)**

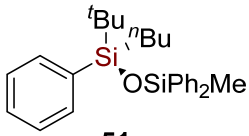


50

4-Bromoanisole (41.3 μL, 0.33 mmol) was dissolved in anhydrous Et_2O (1 mL) and cooled to 0 °C under Ar. *n*-Butyllithium (125 μL, 2.4 M in hexanes, 0.3 mmol) was added dropwise and the reaction was stirred for 30 min. **49** (42.0 mg, 0.1 mmol) was dissolved in anhydrous Et_2O (0.5 mL) and added dropwise to the reaction. The reaction mixture was then warmed to room temperature and stirred overnight. The reaction was quenched with H_2O and extracted with EtOAc. The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by preparative TLC (PE) to afford **50** as a colorless oil (37.1 mg, 0.077 mmol, 77% yield, 93% ee).

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.63 – 7.55 (m, 2H), 7.51 (dt, *J* = 6.7, 1.6 Hz, 6H), 7.41 – 7.32 (m, 3H), 7.32 – 7.21 (m, 6H), 6.87 – 6.78 (m, 2H), 3.80 (s, 3H), 1.00 (s, 9H), 0.56 (s, 3H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 160.59, 137.69, 136.77, 135.70, 135.19, 134.15, 129.47, 129.27, 127.64, 127.40, 126.28, 113.20, 54.93, 26.85, 19.37, −0.57.
HRMS (ESI) *m/z* calcd. for $C_{30}H_{34}NaO_2Si_2$ [M+Na]$^+$ 505.1990, found 505.1988.
HPLC conditions: Chiralcel OD-H, *n*-hexane/*i*-PrOH = 100/0, flow rate 0.3 mL/min. λ = 230 nm, t(major) = 82.4 min, t(minor) = 91.3 min, 93% ee.

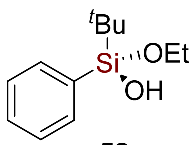
(R)-1-(*tert*-butyl)-1-butyl-3-methyl-1,3,3-triphenyldisiloxane (51)



51

49 (42.0 mg, 0.1 mmol) was dissolved in anhydrous Et_2O (1 mL) under Ar. *n*-Butyllithium (125 μL, 2.4 M in hexanes, 0.3 mmol) was added dropwise and the reaction was stirred at room temperature overnight. The reaction was quenched with H_2O and extracted with EtOAc. The combined organic layer was washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by preparative TLC (PE) to afford **51** as a colorless oil (38.0 mg, 0.088 mmol, 88% yield, 94% ee).
^{1}H NMR (400 MHz, CDCl$_3$) δ 7.59 (dd, *J* = 7.9, 1.6 Hz, 4H), 7.55 – 7.43 (m, 2H), 7.41 – 7.27 (m, 9H), 1.23 – 1.07 (m, 4H), 0.85 (s, 9H), 0.92 – 0.78 (m, 2H), 0.75 – 0.69 (m, 3H), 0.69 (s, 3H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 137.95, 137.92, 136.13, 134.41, 134.09, 129.52, 128.99, 127.69, 127.35, 26.63, 26.28, 25.43, 18.88, 13.51, 11.83, −0.39.
HRMS (ESI) *m/z* calcd. for $C_{27}H_{36}NaOSi_2$ [M+Na]$^+$ 455.2197, found 455.2196.
HPLC conditions: Chiralcel OD-3, *n*-hexane/*i*-PrOH = 100/0, flow rate 0.25 mL/min. λ = 254 nm, t(minor) = 16.6 min, t(major) = 17.4 min, 94% ee.

(S)-*tert*-butyl(ethoxy)(phenyl)silanol (52)



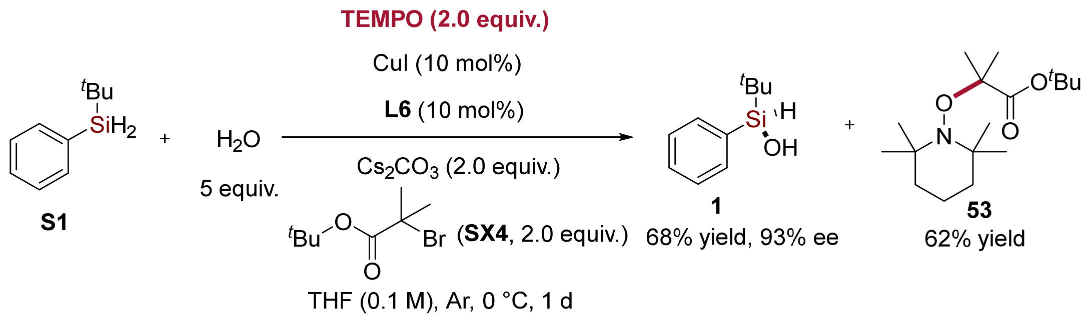
52

49 (42.0 mg, 0.1 mmol) was dissolved in anhydrous THF (1 mL) under Ar. *n*-Butyllithium (125 μL, 2.4 M in hexanes, 0.3 mmol) was added dropwise and the reaction was stirred at room temperature overnight. The reaction was quenched with H_2O and extracted with EtOAc. The organic layer was washed with brine, dried over Na_2SO_4, and concentrated. The residue was purified by preparative TLC (PE/EtOAc = 10/1) to afford **52** as a colorless oil (15.6 mg, 0.07 mmol, 70% yield, 95% ee).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.94 – 7.56 (m, 2H), 7.55 – 7.31 (m, 3H), 3.82 (qd, *J* = 7.0, 1.2 Hz, 2H), 1.23 (t, *J* = 7.0 Hz, 3H), 0.96 (s, 9H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 134.91, 133.06, 129.93, 127.68, 58.72, 25.82, 18.48, 18.20.
HRMS (ESI) *m/z* calcd. for $C_{12}H_{21}O_2Si$ $[M+H]^+$ 225.1305, found 225.1304.
HPLC conditions: Chiralcel AD, *n*-hexane/*i*-PrOH = 98/2, flow rate 0.7 mL/min. λ = 214 nm, t(major) = 13.1 min, t(minor) = 15.7 min, 95% ee.

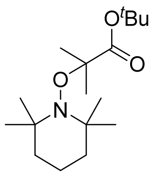
7. Mechanistic Studies

Radical-trapping experiment:



A 10 mL Schlenk tube equipped with a magnetic stir bar was charged with CuI (3.8 mg, 0.020 mmol, 10 mol%), **L6** (10.8 mg, 0.010 mmol, 10 mol%), TEMPO (62.5 mg, 0.20 mmol, 2.0 equiv.), and Cs_2CO_3 (130.3 mg, 0.40 mmol, 2 equiv.). The tube was evacuated and backfilled with argon three times. Under the flow of Ar, **S1** (32 mg, 0.20 mmol, 1.0 equiv.), anhydrous THF (2.0 mL), H_2O (18.0 mg, 1.0 mmol, 5.0 equiv.), and *tert*-butyl 2-bromo-2-methylpropanoate (**SX4**, 89.2 mg, 0.40 mmol, 2 equiv.) were added into the mixture. The reaction mixture was stirred at 0 °C for 1 d and then was filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated and the residue was purified by column chromatography on silica gel to afford the desired product **1** (24.4 mg, 0.136 mmol, 68% yield, 93% ee) and **53** (37.0 mg, 0.124 mmol, 62% yield).

***tert*-butyl 2-methyl-2-((2,2,6,6-tetramethylpiperidin-1-yl)oxy)propanoate (53)**



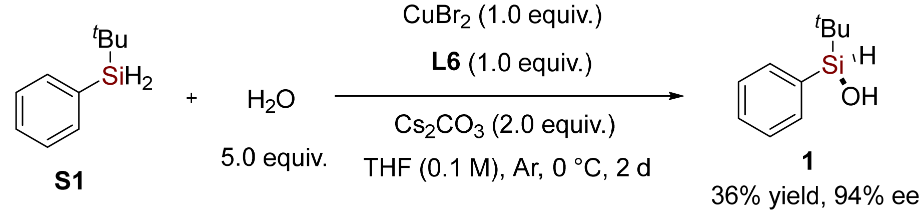
53

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.54 (d, *J* = 13.0 Hz, 1H), 1.45 (s, 9H), 1.50 – 1.42 (m, 3H), 1.40 (s, 6H), 1.43 – 1.35 (m, 1H), 1.30 – 1.23 (m, 1H), 1.13 (s, 6H), 1.02 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 175.27, 81.28, 80.25, 59.44, 40.56, 33.45, 27.88, 24.45, 20.35, 17.01.

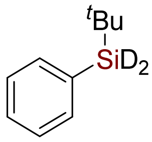
HRMS (ESI) *m/z* calcd. for $C_{17}H_{34}NO_3$ $[M+H]^+$ 300.2533, found 300.2530.

A stoichiometric catalyst reaction:



A 10 mL Schlenk tube equipped with a magnetic stir bar was charged with $CuBr_2$ (44.7 mg, 0.20 mmol, 1.0 equiv.), **L6** (108 mg, 0.20 mmol, 1.0 equiv.), and Cs_2CO_3 (130.3 mg, 0.40 mmol, 2.0 equiv.). The tube was evacuated and backfilled with argon three times. Under the flow of Ar, **S1** (32 mg, 0.20 mmol, 1.0 equiv.), anhydrous THF (2.0 mL), and H_2O (18.0 mg, 1.0 mmol, 5.0 equiv.) were added to the mixture. The reaction mixture was stirred at 0 °C for 2 d. The mixture was then filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated and the residue was purified by column chromatography on silica gel to afford the desired product **1** (13.0 mg, 0.072 mmol, 36% yield, 94% ee).

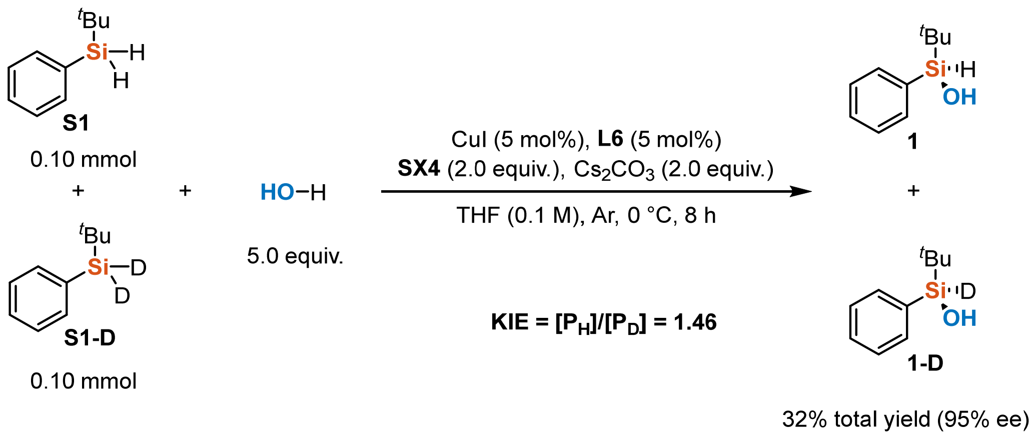
KIE experiments:
Synthesis of S1-D
***tert*-butyl(phenyl)silane (S1-D)**



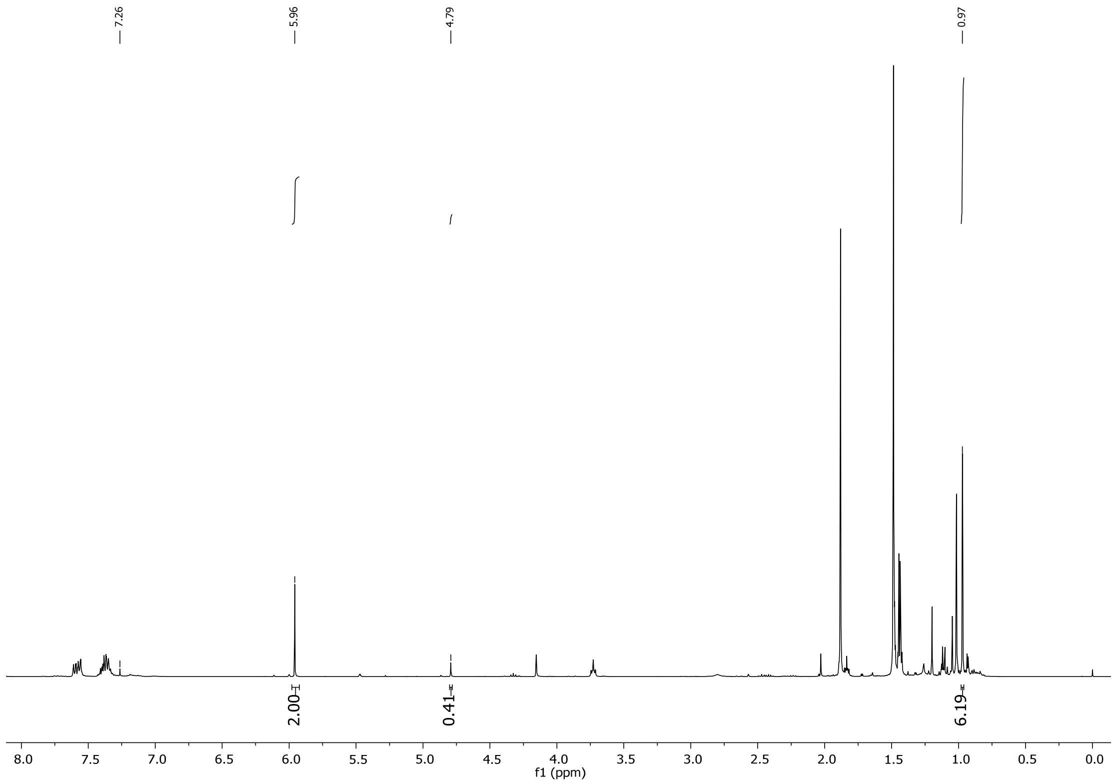
S1-D

According to the **General Procedures B** for the synthesis of substrates using $PhSiCl_3$ (5.0 mmol), ^{t}BuLi in pentane (1.3 M, 3.27 mL, 4.25 mmol), and $LiAlD_4$ (209.9 mg, 5.0 mmol), the product **S1-D** was obtained as a colorless oil[3] (218.3 mg, 1.3 mmol, 26% yield).
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59-7.55 (m, 2H), 7.42-7.33 (m, 3H), 1.02 (s, 9H).
^{2}H NMR (61 MHz, $CHCl_3$) δ 4.20 (s, 2D).
^{13}C NMR (101 MHz, $CDCl_3$) δ 135.87, 132.16, 129.52, 127.80, 27.39, 16.25.

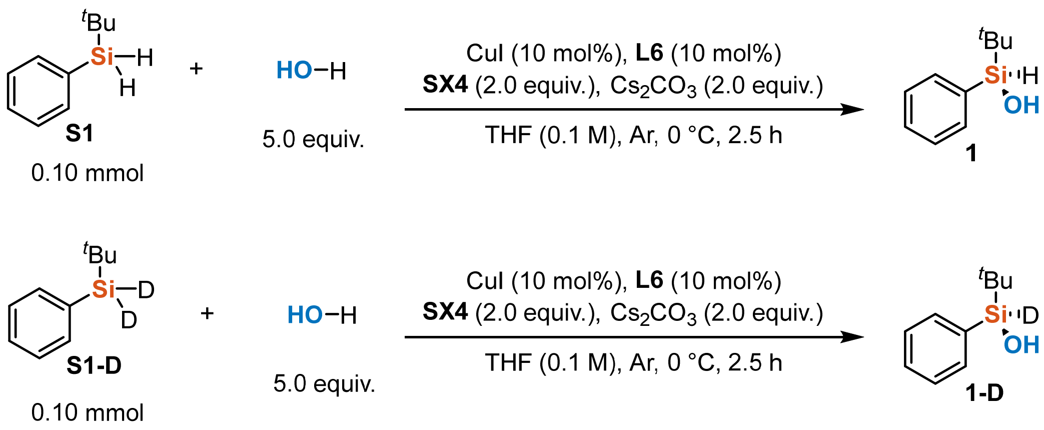
KIE determined from an intermolecular competition



A 10 mL Schlenk tube equipped with a magnetic stir bar was charged with CuI (1.9 mg, 0.010 mmol, 5 mol%), **L6** (5.4 mg, 0.010 mmol, 5 mol%), and Cs_2CO_3 (130.3 mg, 0.40 mmol, 2.0 equiv.). The tube was evacuated and backfilled with argon three times. Under the flow of Ar, **S1** (16.4 mg, 0.10 mmol), **S1-D** (16.6 mg, 0.10 mmol), anhydrous THF (2.0 mL), H_2O (18.0 mg, 1.0 mmol, 5.0 equiv.), and *tert*-butyl 2-bromo-2-methylpropanoate (**SX4**, 89.2 mg, 0.40 mmol, 2.0 equiv.) were added into the mixture. The reaction mixture was stirred at 0 °C for 8 h and then was filtered through a pad of celite eluting with CH_2Cl_2. The filtrate was evaporated and taken for ^{1}H NMR analysis with 1,1,2,2-tetrachloroethane as the internal standard. **1** and **1-D** were obtained in 32% total NMR yield with 95% ee.
The molar ratio of **1**/**1-D** = 0.41/(6.19/9 – 0.41) =0.41/0.28 = 1.46.


7.26
5.96
4.79
0.97
2.00
0.41
6.19
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)

KIE determined from two parallel reactions



KIE = k_H/k_D = 1.84

A 10 mL Schlenk tube equipped with a magnetic stir bar was charged with CuI (1.9 mg, 0.010 mmol, 10 mol%), **L6** (5.4 mg, 0.010 mmol, 10 mol%), and Cs_2CO_3 (65.2 mg, 0.20 mmol, 2.0 equiv.). The tube was evacuated and backfilled with argon three times. Under the flow of Ar, **S1** (16.4 mg, 0.10 mmol) or **S1-D** (16.6 mg, 0.10 mmol), anhydrous THF (1.0 mL), H_2O (9.0 mg, 0.50 mmol, 5.0 equiv.), and *tert*-butyl 2-bromo-2-methylpropanoate (**SX4**, 44.6 mg, 0.20 mmol, 2.0 equiv.) were added into the mixture. The reaction mixture was stirred at 0 °C. The yield of **1** or **1-D** was determined by ^1H NMR analysis of the crude reaction mixture with 1,1,2,2-tetrachloroethane as the internal standard at the indicated time intervals to obtain the individual reaction rate and the KIE value.

	0.5 h	1 h	1.5 h	2.0 h	2.5 h
1 yield/%	1.58	5.25	9.87	13.86	18.80
1-D yield/%	0.94	2.62	5.04	7.56	10.18

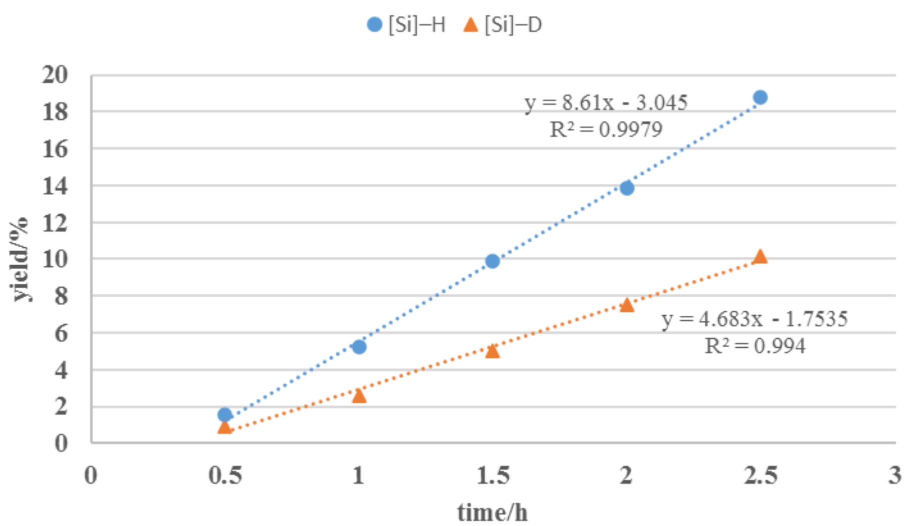
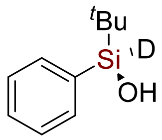


Figure S6. The linear model fitted plot of the yield of product vs time

Both the intermolecular competition and two parallel reactions revealed small but significant isotope effects, which indicates Si–H bond cleavage might not be the only rate-determining step.

***(R)-tert*-butyl(phenyl)silan-*d*-ol (1-D)**

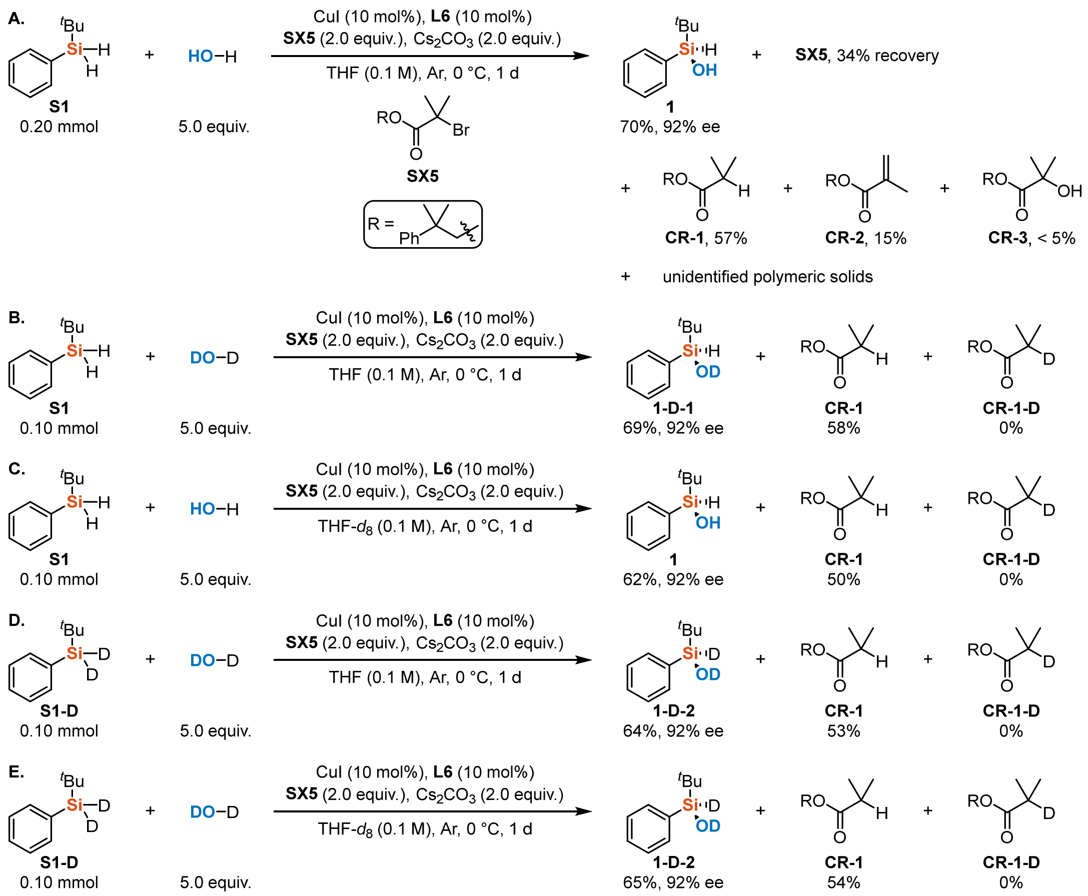


1-D

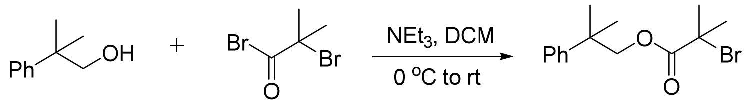
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.56 (m, 2H), 7.47 – 7.34 (m, 3H), 1.97 (br, 1H), 0.98 (s, 9H).

^{2}H NMR (61 MHz, $CHCl_3$) δ 4.86 (s, 1D).
^{13}C NMR (101 MHz, $CDCl_3$) δ 134.58, 134.10, 130.08, 127.79, 25.35, 17.87.

Deuterium-Labeling studies



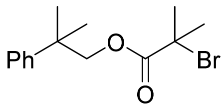
Scheme S4. Products of the enantioselective hydroxylation reaction with **SX5** and deuterium-labeling experiments.



SX5

A mixture of 2-methyl-2-phenylpropan-1-ol (0.75 g, 5 mmol) and trimethylamine (1.4 mL, 10 mmol) in DCM (20 mL) was treated slowly with 2-bromo-2-methylpropanoyl bromide (0.60 mL, 5 mmol) at 0 °C. After completion of the addition, the reaction mixture was stirred for another 2 h at rt. After completion of the reaction, the reaction mixture was poured into water and extracted with DCM. The extract was washed with water and brine solution, dried over $MgSO_4$, and concentrated. The crude compound was subjected to column chromatography on silica gel to obtain **SX5** (1.36 g, 4.55 mmol, 91% yield).

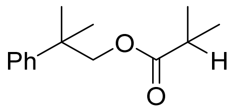
2-methyl-2-phenylpropyl 2-bromo-2-methylpropanoate (SX5)



SX5

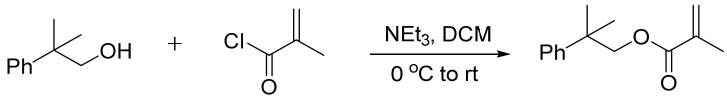
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 2H), 7.34 – 7.26 (m, 2H), 7.24 – 7.13 (m, 1H), 4.19 (s, 2H), 1.82 (s, 6H), 1.40 (s, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 171.25, 145.60, 128.11, 126.20, 125.82, 74.12, 55.71, 38.42, 30.59, 25.56.
HRMS (ESI) *m/z* calcd. for $C_{14}H_{19}BrNaO_2$ $[M+Na]^+$ 321.0461, found 321.0459.

2-methyl-2-phenylpropyl isobutyrate (CR-1)



CR-1

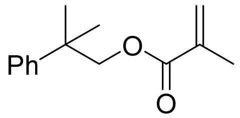
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.41 – 7.34 (m, 2H), 7.34 – 7.26 (m, 2H), 7.22 – 7.16 (m, 1H), 4.12 (s, 2H), 2.48 (m, 1H), 1.36 (s, 6H), 1.08 (d, J = 7.0 Hz, 6H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 176.87, 146.13, 128.09, 126.09, 125.86, 72.59, 38.27, 34.00, 25.75, 18.83.
HRMS (ESI) *m/z* calcd. for $C_{14}H_{20}NaO_2$ $[M+Na]^+$ 243.1356, found 243.1354.



CR-2

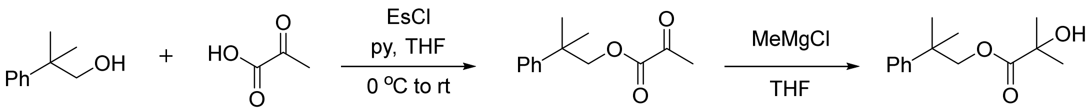
A mixture of 2-methyl-2-phenylpropan-1-ol (30.1 mg, 0.2 mmol) and trimethylamine (40.5 mg, 0.4 mmol) in DCM (1.0 mL) was treated slowly with methacryloyl chloride (41.8 mg, 0.4 mmol) at 0 °C. After completion of the addition, the reaction mixture was stirred for another 1 h at rt. After completion of the reaction, the reaction mixture was passed through a pad of silica eluting with EtOAc. The eluent was concentrated and purified by preparative TLC to obtain **CR-2** (27.1 mg, 0.124 mmol, 62% yield).

2-methyl-2-phenylpropyl methacrylate (CR-2)



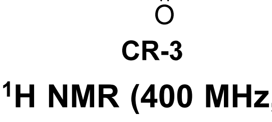
CR-2

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.39 (dd, *J* = 8.3, 1.4 Hz, 2H), 7.33 (t, *J* = 7.6 Hz, 2H), 7.25 – 7.17 (m, 1H), 6.02 (s, 1H), 5.51 (q, *J* = 1.7 Hz, 1H), 4.18 (s, 2H), 1.89 (s, 3H), 1.40 (s, 6H).
^{13}C NMR (101 MHz, CDCl$_3$) δ 167.33, 146.20, 136.29, 128.20, 126.20, 125.91, 125.41, 73.24, 38.33, 25.82, 18.25.
HRMS (ESI) *m/z* calcd. for $C_{14}H_{18}O_2Na$ $[M+Na]^+$ 241.1199, found 241.1194.



A mixture of 2-methyl-2-phenylpropan-1-ol (75.0 mg, 0.5 mmol), 2-oxopropanoic acid (52.8 mg, 0.6 mmol, 1.2 equiv.), and pyridine (py, 98.9 mg, 1.25 mmol, 2.5 equiv.) in THF (1.0 mL) was treated with ethanesulfonyl chloride (EsCl, 77.1 mg, 0.6 mmol, 1.2 equiv.) at 0 °C. The reaction mixture was stirred at rt overnight and passed through a pad of silica eluting with EtOAc. The eluent was concentrated and purified by preparative TLC to obtain **MCO** (21.6 mg, 0.1 mmol, 20% yield).
To a solution of **MCO** (0.1 mmol) in THF (2 mL) at 0 °C was added MeMgCl solution (3 M in THF, 35 μL, 1 equiv). The mixture was stirred at 0 °C for 1 h and quenched with drops of NH_4Cl (sat. aq). The mixture was passed through a pad of silica eluting with EtOAc. The eluent was concentrated and purified by preparative TLC to obtain **CR-3** (8.1 mg, 0.034 mmol, 34% yield) mixed with the impurity of 2-methyl-2-phenylpropan-1-ol (**SMOH**) with the same R_f value.

2-methyl-2-phenylpropyl 2-hydroxy-2-methylpropanoate (CR-3)



CR-3

^{1}H NMR (400 MHz, CDCl$_3$) δ 7.40 – 7.29 (m, 4H), 7.25 – 7.19 (m, 1H), 4.22 (s, 2H), 3.03 (s, 1H), 1.39 (s, 6H), 1.30 (s, 6H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 177.37, 145.59, 128.30, 126.41, 125.88, 74.13, 71.99, 38.43, 27.08, 25.72.
HRMS (ESI) *m/z* calcd. for $C_{14}H_{20}O_3Na$ $[M+Na]^+$ 259.1305, found 259.1300.

8. DFT Calculations

Computational methods

All calculations were performed with Gaussian 09[12] with the ultrafine integration grid and the keywords acc2e=11 and 5D 7F. The hybrid functional B3LYP[13] was combined with the dispersion correction D3[14] to improve computational accuracy. Structures were optimized and characterized by frequency calculations to be energy minima (zero imaginary frequencies) or transition states (only one imaginary frequency) at the B3LYP-D3/BS1 level in the gas phase, BS1 designating a mixed basis set of SDD[15] for copper, bromine, cesium and 6-31G(d,p) for other atoms. The energies were then refined by B3LYP-D3/BS2// B3LYP-D3/BS1 single-point energy calculations with the solvent (tetrahydrofuran) effects included using the SMD solvation model,[16] BS2 denoting a mixed basis set of SDD for copper, bromine, cesium and 6-311++G(d,p) for other atoms. The refined energies were converted to zero-point energy-corrected Gibbs free energies at 298.15 K and 1 atm, using the B3LYP-D3/BS1 harmonic frequencies.

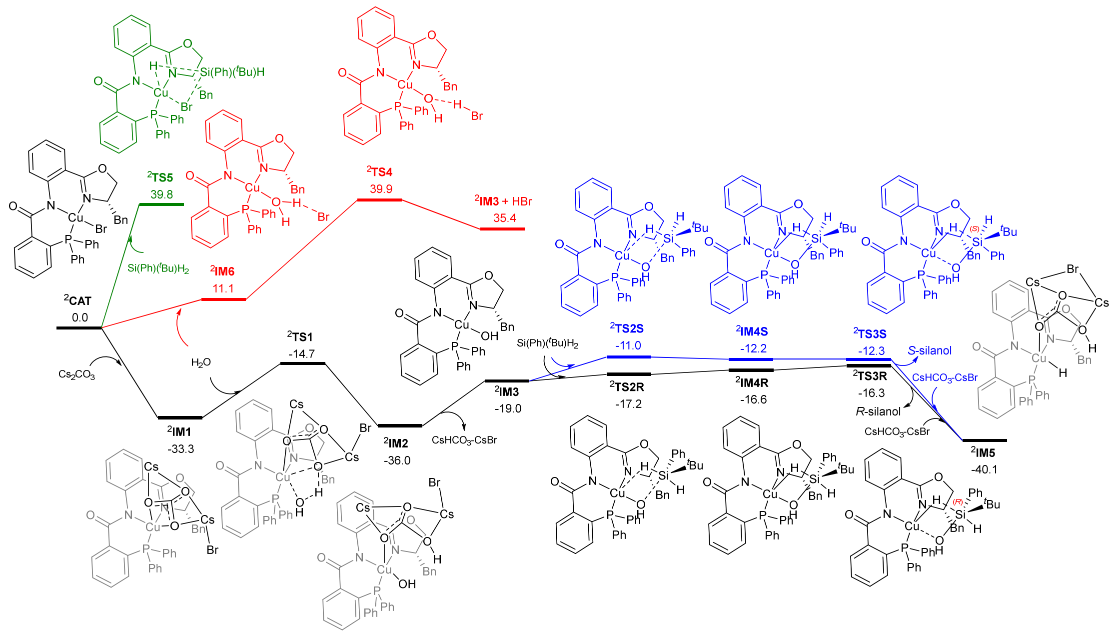
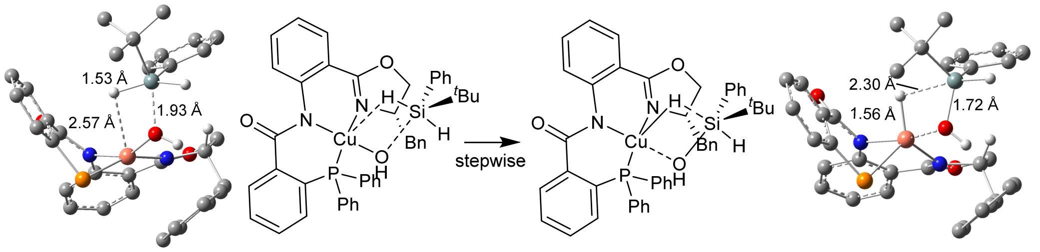
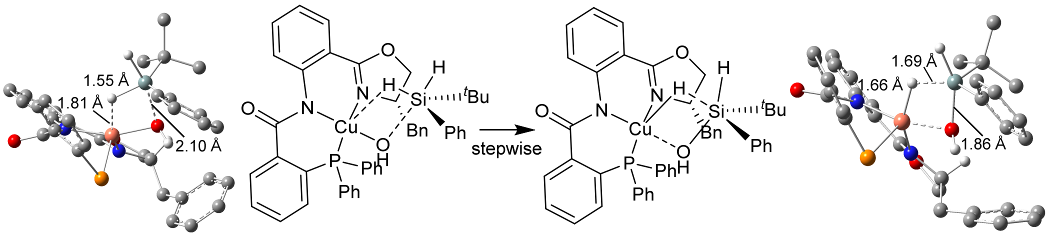


Figure S3. Free energy profile for the complete pathway of ^{2}**CAT**-catalyzed asymmetric chiral silanol formation.



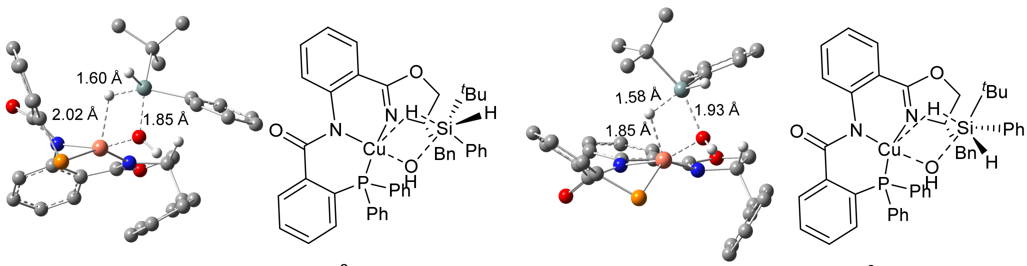
^{2}**TS2R**
-17.2

^{2}**TS3R**
-16.3



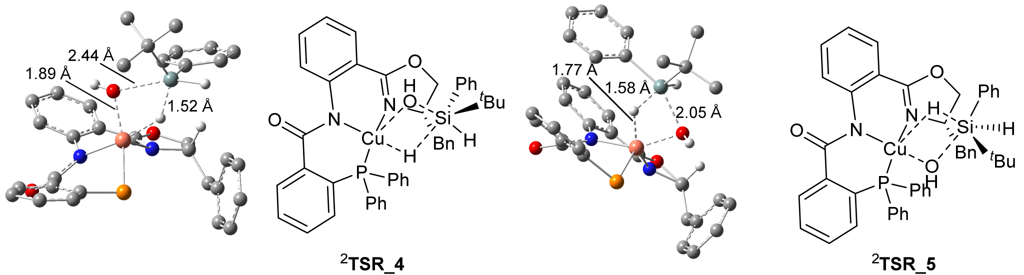
^{2}**TSR_3/1**
-5.0

^{2}**TSR_3/2**
-5.4



^{2}**TSR_1**
-8.9
concerted

^{2}**TSR_2**
-6.7
concerted



^{2}**TSR_4**
0.7
concerted

^{2}**TSR_5**
1.1
concerted

Figure S7. Located conformers of *σ*-metathesis transition state leading to major product *R*-silanol. Free energies are compared to ^{2}**CAT**. Trivial hydrogen atoms in the 3D diagram are omitted for clarity.

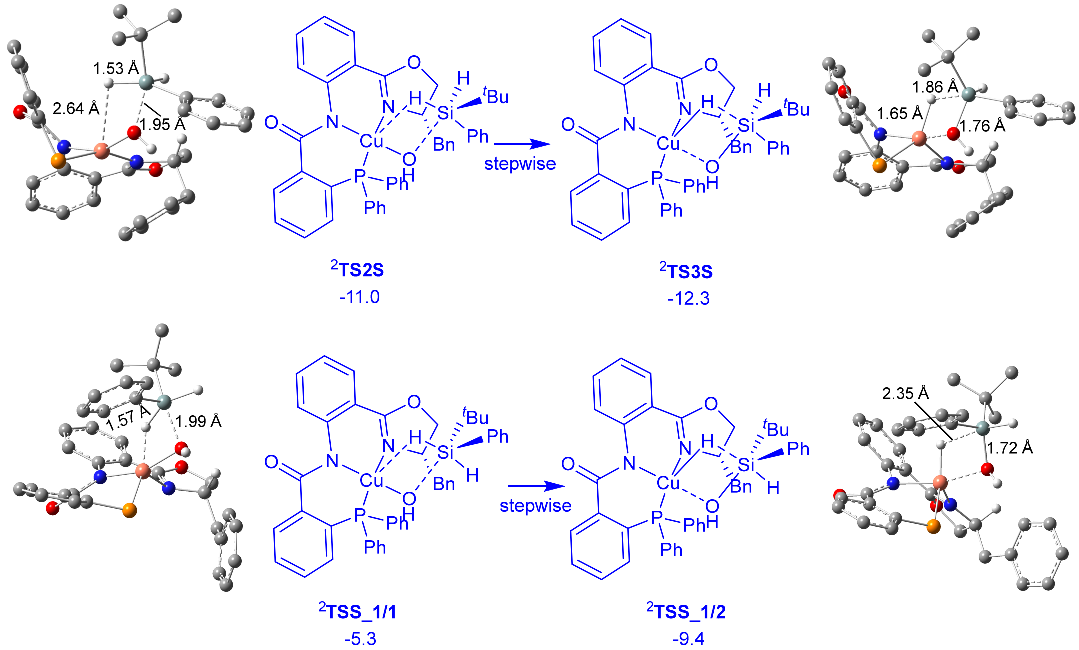


Figure S8. Located conformers of σ-metathesis transition state leading to major product *S*-silanol. Free energies are compared to ^{2}**CAT**. Trivial hydrogen atoms in the 3D diagram are omitted for clarity.

Cartesian Coordinates (Å), SCF Energies, and Free Energies at 298.15 K and 1 atm for the Optimized Structures

^{2}CAT

E_{gas} optimization: -2162.84246415a.u.

E_{sol} single-point: -2163.30475325a.u.

G_{sol} thermo-corrected: -2162.83395025a.u.

C	2.732684	0.713531	1.917004
C	2.738057	-0.591021	1.375415
C	3.639423	-1.554522	1.862458
C	4.537613	-1.252002	2.879165
H	5.229745	-2.008346	3.237312
C	4.529637	0.029272	3.432755
H	5.219397	0.285435	4.231798
C	3.637991	0.985853	2.961079
C	1.897374	1.934163	1.517499
O	1.822097	2.843826	2.350189
N	1.368613	2.042711	0.250433
C	1.048373	3.381204	-0.102910
C	2.096330	4.319379	-0.167210
H	3.097067	3.980132	0.076587
C	1.872095	5.642538	-0.518548
H	2.710489	6.332072	-0.562254
C	0.578851	6.090922	-0.818501
H	0.402223	7.125065	-1.096015
C	-0.473004	5.191723	-0.764018
H	-1.483705	5.508077	-0.997517
C	-0.254441	3.843611	-0.417029
C	-1.392501	2.938295	-0.413568
O	-2.634241	3.456232	-0.323207
C	-3.570393	2.347107	-0.462986
H	-4.134172	2.501750	-1.386299
H	-4.253825	2.372146	0.389197
C	-2.676212	1.083747	-0.495178
H	-2.823265	0.505700	-1.410351
N	-1.325461	1.656106	-0.533002
H	3.635249	-2.551811	1.434891
H	3.616317	1.980465	3.389165
P	1.526788	-1.115619	0.119851
C	2.397883	-2.245072	-1.012868
C	2.504100	-3.622485	-0.771709
C	2.994760	-1.689740	-2.154047
C	3.215434	-4.432298	-1.657888
H	2.021197	-4.062364	0.095586
C	3.710635	-2.502057	-3.031787
H	2.873702	-0.631739	-2.364696
C	3.821752	-3.872678	-2.784545
H	3.292420	-5.499136	-1.469486
H	4.166275	-2.067852	-3.916424
H	4.371732	-4.505571	-3.474938
C	0.279014	-2.109010	1.016394
C	0.103776	-1.978165	2.401819
C	-0.634170	-2.876047	0.269456
C	-0.973746	-2.604995	3.031212
H	0.798703	-1.382614	2.985199
C	-1.699801	-3.506540	0.908532
H	-0.523591	-2.947929	-0.808016
C	-1.876973	-3.366081	2.288007
H	-1.106850	-2.493145	4.103238
H	-2.408580	-4.086413	0.325974
H	-2.722248	-3.840417	2.777212
Cu	0.367100	0.636712	-0.742625
Br	-0.421193	-0.580693	-2.728664
C	-2.826980	0.150605	0.720391
H	-1.989405	-0.553663	0.696607
H	-2.723707	0.741927	1.637642
C	-4.132908	-0.606790	0.706134
C	-4.350603	-1.601077	-0.260797
C	-5.151698	-0.328412	1.624032
C	-5.556089	-2.299602	-0.304175
H	-3.562926	-1.827605	-0.975163
C	-6.361078	-1.027928	1.584081
H	-4.993124	0.434726	2.382490
C	-6.566271	-2.015145	0.619924
H	-5.708303	-3.067253	-1.057888
H	-7.139908	-0.801401	2.306921
H	-7.505260	-2.560222	0.587377

^{2}IM1

E_{gas} optimization: -2467.14610069a.u.

E_{sol} single-point: -2467.74527644a.u.

G_{sol} thermo-corrected: -2467.27140244a.u.

C	-1.916824	3.514244	1.488483
C	-0.667373	3.618640	0.830959
C	-0.100993	4.884411	0.592996
C	-0.747015	6.053954	0.974161
H	-0.292146	7.019633	0.773562
C	-1.980181	5.963188	1.620781
H	-2.504986	6.862388	1.931026

C	-2.540558	4.717372	1.876855
C	-2.743557	2.275978	1.876937
O	-3.604795	2.450666	2.750318
N	-2.569339	1.076152	1.243282
C	-3.597824	0.136393	1.415967
C	-4.944274	0.516484	1.191392
H	-5.142252	1.554568	0.954804
C	-5.993761	-0.385631	1.279336
H	-7.009205	-0.040820	1.100312
C	-5.756692	-1.729511	1.616349
H	-6.579371	-2.431064	1.720017
C	-4.449887	-2.136596	1.848275
H	-4.233860	-3.163628	2.123970
C	-3.368455	-1.234954	1.739875
C	-2.018657	-1.773615	1.916061
O	-1.889820	-2.999270	2.489429
C	-0.487483	-3.375736	2.339554
H	-0.438846	-4.208310	1.630740
H	-0.115723	-3.706745	3.311194
C	0.201728	-2.087653	1.824081
H	0.762097	-2.261984	0.901718
N	-0.936887	-1.221316	1.502328
H	0.862904	4.945687	0.096796
H	-3.485182	4.636899	2.400090
P	0.307883	2.164631	0.301608
C	0.956129	2.602977	-1.361685
C	2.255476	3.071110	-1.604665
C	0.083396	2.396851	-2.446929
C	2.678670	3.325920	-2.912955
H	2.947387	3.214884	-0.781719
C	0.502935	2.672663	-3.748758
H	-0.909719	1.989790	-2.269948
C	1.804327	3.132525	-3.985324
H	3.691976	3.674777	-3.088496
H	-0.181830	2.517503	-4.578265
H	2.133717	3.340280	-4.999917
C	1.737417	2.082526	1.433422
C	1.680126	2.664594	2.709981
C	2.847402	1.293238	1.084257
C	2.721897	2.458498	3.615941
H	0.826398	3.270487	2.996951
C	3.893760	1.107497	1.986461
H	2.926069	0.809110	0.115687
C	3.828087	1.684546	3.256864
H	2.667114	2.907668	4.603692
H	4.735663	0.496583	1.676185
H	4.635001	1.526805	3.966485
Cu	-1.070998	0.357000	0.139658
Br	5.058720	-0.869113	-1.015953
C	1.128180	-1.420252	2.857986
H	1.370908	-0.419030	2.492361
H	0.574880	-1.296866	3.796936
C	2.392476	-2.220483	3.069286
C	3.373152	-2.242361	2.066686
C	2.600797	-2.972974	4.231600
C	4.539416	-2.989510	2.222296
H	3.253779	-1.656625	1.159921
C	3.766283	-3.728589	4.390446
H	1.854289	-2.955535	5.023334
C	4.737118	-3.737958	3.386887
H	5.283161	-2.959622	1.431027
H	3.916558	-4.303035	5.300897
H	5.646283	-4.319279	3.514592
O	-0.018559	-0.672167	-1.204016
O	-2.129293	-0.173413	-1.568196
C	-1.070936	-0.830053	-1.987446
O	-1.059386	-1.556969	-3.008440
Cs	-4.137745	-2.125959	-1.997268
Cs	2.215618	-0.904388	-3.118919

Cs_2CO_3

E_{gas} optimization: -304.167543546a.u.

E_{sol} single-point: -304.362312853a.u.

G_{sol} thermo-corrected: -304.384349853a.u.

O	1.126125	1.829459	0.001993
O	-1.125775	1.829448	-0.001547
C	0.000159	1.201660	-0.000507
O	0.000176	-0.136441	-0.002050
Cs	-2.828217	-0.321699	0.000247
Cs	2.828123	-0.321750	0.000042

^{2}TS1

E_{gas} optimization: -2543.57044219a.u.

E_{sol} single-point: -2544.19944859a.u.

G_{sol} thermo-corrected: -2543.70357859a.u.

C	0.315789	-2.031968	3.648750
C	-0.621394	-0.982541	3.512926
C	-1.218806	-0.435466	4.658805
C	-0.880423	-0.899316	5.928990
H	-1.349687	-0.460560	6.804732

C	0.052522	-1.927719	6.066733
H	0.321378	-2.295132	7.052768
C	0.627866	-2.496716	4.933465
C	0.926494	-2.814794	2.502509
O	1.237029	-3.989806	2.719373
N	1.101227	-2.189784	1.288580
C	1.377019	-3.014075	0.194360
C	0.621167	-4.192311	-0.021230
H	-0.160037	-4.434213	0.686827
C	0.863255	-5.028447	-1.099701
H	0.260993	-5.924691	-1.222576
C	1.882888	-4.733659	-2.020660
H	2.097008	-5.405304	-2.846656
C	2.618854	-3.569938	-1.853062
H	3.401896	-3.308680	-2.556015
C	2.369128	-2.693208	-0.772967
C	3.119731	-1.441692	-0.727471
O	4.092468	-1.286443	-1.645375
C	4.476542	0.118330	-1.618687
H	4.053072	0.589960	-2.505836
H	5.566991	0.170084	-1.622504
C	3.825788	0.653206	-0.329650
H	3.223597	1.529984	-0.570990
N	2.906552	-0.431066	0.049349
H	-1.948406	0.360066	4.556488
H	1.319948	-3.327334	5.014223
P	-0.953145	-0.269608	1.861435
C	-1.988962	-1.446516	0.929842
C	-2.416600	-2.665867	1.475083
C	-2.380297	-1.085577	-0.368546
C	-3.231609	-3.514539	0.725268
H	-2.119115	-2.950414	2.479289
C	-3.239671	-1.915883	-1.091930
H	-2.031282	-0.157184	-0.812030
C	-3.654527	-3.135466	-0.552089
H	-3.560798	-4.457489	1.152327
H	-3.635080	-1.568431	-2.041379
H	-4.334933	-3.772010	-1.110359
C	-1.999373	1.199999	2.148949
C	-1.382449	2.385484	2.594276
C	-3.386006	1.175930	1.928539
C	-2.155986	3.520834	2.835112
H	-0.305062	2.416947	2.720151
C	-4.152208	2.322875	2.160948
H	-3.879452	0.295765	1.532533
C	-3.541223	3.490652	2.622153
H	-1.677771	4.431513	3.186144
H	-5.214454	2.292565	1.941559
H	-4.138793	4.379340	2.807902
Cu	1.149232	-0.191065	0.962039
Br	-5.382393	0.985771	-1.225694
C	4.818363	0.947400	0.813102
H	4.244564	1.136817	1.729074
H	5.408868	0.044744	1.005971
C	5.719674	2.117840	0.492992
C	5.209096	3.424222	0.477293
C	7.065389	1.924425	0.156993
C	6.019303	4.506496	0.136831
H	4.166422	3.599224	0.735419
C	7.881577	3.005256	-0.184858
H	7.478798	0.918815	0.171197
C	7.360433	4.299417	-0.196706
H	5.605912	5.511017	0.133964
H	8.923942	2.834860	-0.438747
H	7.993412	5.141495	-0.460628
O	0.181987	1.431065	-0.531830
O	-0.659906	1.079605	-2.568137
C	0.379855	1.070231	-1.822075
O	1.524763	0.676722	-2.202994
Cs	-0.129744	-1.664502	-3.395650
Cs	-2.464158	3.058307	-1.308735
H	2.433172	2.139998	1.337107
H	1.044324	1.896250	0.432214
O	1.509503	1.878897	1.411010

^{2}IM2

E_{gas} optimization: -2543.61995869a.u.

E_{sol} single-point: -2544.23673456a.u.

G_{sol} thermo-corrected: -2543.73761756a.u.

C	0.839085	-3.330169	2.431918
C	0.139361	-2.227126	2.975265
C	0.104447	-2.043236	4.364358
C	0.767369	-2.927699	5.214576
H	0.738560	-2.766578	6.288422
C	1.453474	-4.020563	4.682663
H	1.965636	-4.717407	5.339779
C	1.468534	-4.226104	3.304858
C	0.861931	-3.707861	0.957811
O	0.855023	-4.911275	0.677237
N	0.897216	-2.686633	0.048590
C	0.730245	-2.988365	-1.304153

C	-0.304401	-3.852769	-1.730321
H	-0.925064	-4.316829	-0.975672
C	-0.533157	-4.103114	-3.076181
H	-1.340725	-4.771830	-3.363049
C	0.270685	-3.508709	-4.062254
H	0.106447	-3.721718	-5.114355
C	1.296102	-2.657959	-3.671498
H	1.930903	-2.189565	-4.415036
C	1.536669	-2.380154	-2.308995
C	2.591608	-1.422058	-1.978881
O	3.267855	-0.887108	-3.024232
C	4.225890	0.055697	-2.475379
H	4.130964	0.993669	-3.023900
H	5.230654	-0.355566	-2.624392
C	3.836229	0.153742	-0.985637
H	3.258345	1.063241	-0.791695
N	2.907259	-0.969753	-0.809831
H	-0.438945	-1.202451	4.782581
H	1.957548	-5.092209	2.872430
P	-0.620462	-1.012516	1.830725
C	-2.099801	-1.837711	1.125449
C	-2.340957	-3.212749	1.273884
C	-2.999097	-1.071814	0.365085
C	-3.447124	-3.803866	0.660260
H	-1.671472	-3.832108	1.859025
C	-4.117213	-1.659445	-0.229350
H	-2.869040	0.000051	0.243452
C	-4.336723	-3.032394	-0.090529
H	-3.615075	-4.870186	0.782254
H	-4.801516	-1.021160	-0.781737
H	-5.204900	-3.494906	-0.551896
C	-1.272404	0.356535	2.870849
C	-0.354981	1.336780	3.298434
C	-2.628526	0.483335	3.217582
C	-0.796937	2.418202	4.064983
H	0.687608	1.246906	2.996260
C	-3.064267	1.578375	3.968515
H	-3.347990	-0.261713	2.896434
C	-2.150574	2.546026	4.397380
H	-0.080252	3.163356	4.400900
H	-4.115886	1.666231	4.226185
H	-2.490343	3.387923	4.995145
Cu	1.339351	-0.786245	0.509518
Br	-4.473475	1.828949	-1.403601
C	5.022821	0.095064	-0.014620
H	4.630123	-0.141397	0.980664
H	5.677543	-0.739677	-0.289466
C	5.786247	1.400564	0.014569
C	5.168674	2.555999	0.519438
C	7.088916	1.497869	-0.486398
C	5.841887	3.776412	0.523405
H	4.151888	2.495163	0.901244
C	7.766079	2.720204	-0.482479
H	7.578982	0.609452	-0.877773
C	7.144119	3.862453	0.022275
H	5.350303	4.661446	0.917527
H	8.778281	2.777780	-0.872940
H	7.668832	4.813500	0.026112
O	0.990888	2.498187	0.039271
O	-0.249730	2.527058	-1.814301
C	0.417880	1.838579	-1.014378
O	0.562751	0.566995	-1.072721
Cs	-1.659726	-0.077870	-3.015473
Cs	-1.979157	3.673830	0.470824
H	2.971386	0.608641	1.754317
H	1.477544	1.835615	0.632717
O	2.033437	0.705270	1.557868

[2]**IM3**

E_{gas} optimization: -2225.23095005a.u.

E_{sol} single-point: -2225.72352678a.u.

G_{sol} thermo-corrected: -2225.23824878a.u.

C	3.022955	-0.321528	1.338004
C	2.502982	-1.517740	0.797609
C	3.169052	-2.737850	1.009998
C	4.343221	-2.797006	1.752565
H	4.848005	-3.747284	1.900098
C	4.855223	-1.622779	2.307426
H	5.767982	-1.647709	2.895918
C	4.198491	-0.413331	2.108290
C	2.514930	1.117924	1.196807
O	2.831582	1.894415	2.102997
N	1.860901	1.532585	0.051334
C	2.021973	2.916531	-0.195954
C	3.333711	3.433283	-0.287347
H	4.160289	2.747749	-0.137644
C	3.583570	4.769388	-0.552141
H	4.611270	5.115369	-0.620948
C	2.525561	5.672289	-0.735013
H	2.719568	6.719523	-0.943181
C	1.227613	5.202407	-0.653068

H	0.387914	5.873850	-0.795669
C	0.960929	3.840303	-0.395588
C	-0.425681	3.414852	-0.359537
O	-1.387412	4.344210	-0.162646
C	-2.669549	3.662384	-0.257208
H	-3.214880	4.090554	-1.102230
H	-3.222237	3.856954	0.665625
C	-2.305691	2.167600	-0.451409
H	-2.696490	1.791846	-1.400241
N	-0.842284	2.207987	-0.543385
H	2.759414	-3.647813	0.582981
H	4.580541	0.499833	2.548135
P	0.926487	-1.512921	-0.108991
C	1.085638	-2.757903	-1.433678
C	0.780119	-4.111803	-1.234578
C	1.541812	-2.326616	-2.687362
C	0.951343	-5.027087	-2.274113
H	0.398264	-4.446394	-0.274510
C	1.716973	-3.245144	-3.721116
H	1.731338	-1.270789	-2.852740
C	1.424026	-4.595721	-3.515339
H	0.712213	-6.074687	-2.115059
H	2.067975	-2.905069	-4.690996
H	1.553926	-5.308979	-4.324313
C	-0.335675	-2.179555	1.036382
C	-0.061780	-2.564791	2.355393
C	-1.656801	-2.223541	0.555163
C	-1.102696	-2.994536	3.182779
H	0.953529	-2.526978	2.736733
C	-2.688737	-2.653733	1.386412
H	-1.857190	-1.889947	-0.459131
C	-2.412515	-3.039530	2.701914
H	-0.887003	-3.290549	4.205482
H	-3.707628	-2.662681	1.011427
H	-3.218532	-3.366822	3.352509
Cu	0.310631	0.588432	-0.805728
C	-2.761709	1.212953	0.672177
H	-2.029715	0.400775	0.718432
H	-2.720485	1.732074	1.636567
C	-4.125717	0.612229	0.426053
C	-4.302069	-0.246492	-0.672286
C	-5.213640	0.866372	1.266225
C	-5.540221	-0.838513	-0.916229
H	-3.451003	-0.452476	-1.319085
C	-6.455957	0.273290	1.022842
H	-5.086388	1.523990	2.122978
C	-6.622096	-0.581090	-0.067530
H	-5.661052	-1.505492	-1.765469
H	-7.291208	0.477999	1.686865
H	-7.586369	-1.044336	-0.256151
O	-0.915663	-0.264733	-1.978482
H	-1.363584	0.418551	-2.495259

$CsHCO_3$-CsBr

E_{gas} optimization: -318.300889598a.u.

E_{sol} single-point: -318.457171575a.u.

G_{sol} thermo-corrected: -318.472234575a.u.

Br	0.031219	2.465218	0.352253
O	1.068412	-2.864026	0.787070
O	-1.186670	-2.671092	0.809830
C	-0.131337	-2.384793	0.206672
O	0.051053	-1.684279	-0.819478
Cs	-2.518688	-0.090589	-0.193189
Cs	2.508892	-0.106589	-0.194859
H	0.771797	-3.373933	1.554348

^{2}TS2R

E_{gas} optimization: -2905.51158980a.u.

E_{sol} single-point: -2906.11820430a.u.

G_{sol} thermo-corrected: -2905.4107983a.u.

C	0.789044	-0.346180	-2.807091
C	1.557956	-1.171309	-1.955219
C	1.921699	-2.458720	-2.371788
C	1.509827	-2.948403	-3.610971
H	1.785741	-3.954693	-3.911732
C	0.741016	-2.143552	-4.450470
H	0.405450	-2.518899	-5.412466
C	0.404067	-0.851034	-4.055101
C	0.407338	1.102524	-2.548560
O	0.203584	1.816006	-3.533425
N	0.293035	1.552148	-1.247504
C	0.280684	2.939735	-1.056633
C	1.195072	3.762271	-1.752440
H	1.893533	3.291342	-2.431670
C	1.203879	5.138640	-1.595404
H	1.928861	5.730946	-2.146784
C	0.289514	5.768191	-0.738906
H	0.289491	6.847327	-0.623877
C	-0.608788	4.989310	-0.029773
H	-1.315411	5.448355	0.652660

C	-0.612285	3.584047	-0.156223
C	-1.509355	2.840467	0.717037
O	-2.582651	3.484650	1.216417
C	-3.346772	2.490307	1.963891
H	-4.183262	2.171978	1.338576
H	-3.707194	2.967579	2.877451
C	-2.327756	1.364574	2.200941
H	-2.764756	0.378035	2.046285
N	-1.333522	1.630061	1.145729
H	2.510426	-3.091965	-1.717275
H	-0.166771	-0.199717	-4.706620
P	1.934106	-0.591695	-0.265083
C	2.615845	-2.014942	0.651645
C	3.927428	-2.031359	1.146788
C	1.753064	-3.087997	0.937174
C	4.371967	-3.109954	1.915014
H	4.600588	-1.206569	0.936822
C	2.207666	-4.166344	1.692588
H	0.728058	-3.059477	0.587982
C	3.515773	-4.179163	2.186370
H	5.389321	-3.115016	2.295589
H	1.534980	-4.992576	1.902973
H	3.865397	-5.018335	2.780895
C	3.275581	0.637369	-0.420594
C	4.329803	0.470043	-1.330343
C	3.221638	1.792551	0.371882
C	5.323628	1.443924	-1.433350
H	4.362299	-0.411328	-1.964363
C	4.216166	2.764407	0.266872
H	2.382715	1.939021	1.044933
C	5.268727	2.589076	-0.634091
H	6.135931	1.312674	-2.142176
H	4.159050	3.663176	0.873402
H	6.039705	3.348950	-0.722479
Cu	-0.092825	0.329629	0.276824
C	-1.665702	1.460443	3.599524
H	-1.343618	2.498759	3.747350
H	-2.439253	1.251613	4.348089
C	-0.494930	0.525473	3.774178
C	0.792694	0.918964	3.382348
C	-0.678576	-0.780505	4.249314
C	1.862131	0.024089	3.434866
H	0.945973	1.930353	3.015948
C	0.391748	-1.678367	4.304240
H	-1.668542	-1.099711	4.567245
C	1.663247	-1.281472	3.888021
H	2.847454	0.339701	3.104689
H	0.227922	-2.691117	4.660460
H	2.488392	-1.985663	3.897769
Si	-2.232217	-2.035130	-0.117263
H	-1.208915	-1.511707	-1.128609
C	-2.662888	-3.578125	-1.249252
C	-3.954674	-4.265716	-0.785713
C	-2.800580	-3.140896	-2.715870
C	-1.478811	-4.556967	-1.121141
H	-3.892471	-4.575878	0.264309
H	-4.818866	-3.596785	-0.881874
H	-4.167250	-5.164969	-1.383921
H	-1.898059	-2.629079	-3.068850
H	-2.969535	-4.006008	-3.375444
H	-3.644856	-2.454193	-2.851069
H	-1.636960	-5.459992	-1.730907
H	-0.541359	-4.096915	-1.461046
H	-1.337926	-4.890443	-0.083323
O	-0.886695	-1.288367	1.043435
H	-1.021154	-1.380051	1.998443
C	-3.583177	-0.707704	-0.317188
C	-3.395327	0.377401	-1.194732
C	-4.806668	-0.771639	0.373849
C	-4.383030	1.347077	-1.386212
H	-2.455799	0.465318	-1.734770
C	-5.805320	0.189323	0.186994
H	-4.981742	-1.592507	1.066408
C	-5.596272	1.251832	-0.698165
H	-4.206660	2.173001	-2.070612
H	-6.746488	0.108673	0.725836
H	-6.370533	1.999935	-0.847620
H	-2.650782	-2.739066	1.184553

^{2}IM4R

E_{gas} optimization: -2905.51464627a.u.

E_{sol} single-point: -2906.11601861a.u.

G_{sol} thermo-corrected: -2905.40987461a.u.

C	-1.267713	0.336620	2.822203
C	-2.185964	-0.286838	1.940999
C	-3.122619	-1.192324	2.462488
C	-3.137497	-1.512807	3.819897
H	-3.867182	-2.223891	4.196548
C	-2.212212	-0.924808	4.680842
H	-2.205051	-1.178458	5.736737
C	-1.301999	0.003277	4.182094

C	-0.313424	1.456613	2.446395
O	0.124421	2.174626	3.345596
N	-0.033343	1.635519	1.107083
C	0.238631	2.922536	0.652626
C	-0.448189	4.025254	1.221453
H	-1.140416	3.836904	2.031336
C	-0.263421	5.319099	0.771439
H	-0.826103	6.125181	1.234440
C	0.630145	5.594849	-0.274086
H	0.780360	6.610203	-0.626425
C	1.316583	4.542925	-0.851695
H	2.011007	4.725783	-1.663864
C	1.125968	3.209981	-0.422223
C	1.858643	2.183003	-1.154774
O	2.999668	2.583873	-1.762696
C	3.612006	1.397228	-2.327933
H	4.465273	1.126670	-1.701656
H	3.946278	1.640479	-3.339534
C	2.487845	0.344454	-2.276964
H	2.855470	-0.596886	-1.865344
N	1.517828	0.947661	-1.342490
H	-3.834683	-1.670549	1.799374
H	-0.598678	0.505349	4.836690
P	-2.025973	-0.065347	0.116671
C	-3.084954	-1.383734	-0.584062
C	-4.299073	-1.141098	-1.240901
C	-2.592058	-2.698330	-0.505458
C	-5.012611	-2.199830	-1.809120
H	-4.685891	-0.129370	-1.311346
C	-3.320074	-3.752726	-1.051683
H	-1.631434	-2.882949	-0.033930
C	-4.528715	-3.506021	-1.710430
H	-5.950652	-2.003384	-2.320644
H	-2.935102	-4.765922	-0.979395
H	-5.089136	-4.327979	-2.146638
C	-2.822536	1.523935	-0.301758
C	-3.949102	2.008842	0.377340
C	-2.242017	2.296554	-1.318257
C	-4.492770	3.247425	0.033222
H	-4.387476	1.425342	1.182102
C	-2.785704	3.534548	-1.658302
H	-1.338393	1.942499	-1.806142
C	-3.912753	4.009353	-0.984437
H	-5.362798	3.621471	0.565283
H	-2.314601	4.137557	-2.428568
H	-4.330889	4.978292	-1.241506

Cu	0.324113	-0.033565	0.060436
C	1.843509	0.089057	-3.656210
H	1.394634	1.025314	-4.007764
H	2.651930	-0.162950	-4.354184
C	0.825046	-1.023729	-3.650106
C	-0.549188	-0.763079	-3.586577
C	1.254438	-2.360195	-3.673467
C	-1.473709	-1.808573	-3.561830
H	-0.895506	0.266036	-3.554299
C	0.332017	-3.409926	-3.643323
H	2.318757	-2.578646	-3.721258
C	-1.035692	-3.133732	-3.591271
H	-2.535169	-1.593125	-3.497912
H	0.683426	-4.437445	-3.663018
H	-1.758612	-3.941779	-3.559367
Si	2.067083	-2.140119	0.711927
H	1.216567	-0.749287	1.307429
C	1.631340	-2.974074	2.402830
C	2.478098	-4.249408	2.574027
C	1.909686	-2.017528	3.577539
C	0.134772	-3.339959	2.390831
H	2.289884	-4.973642	1.774444
H	3.551648	-4.025549	2.570528
H	2.246993	-4.737922	3.531358
H	1.319376	-1.099955	3.499330
H	1.650056	-2.498758	4.530969
H	2.966624	-1.732445	3.626242
H	-0.153167	-3.812582	3.340491
H	-0.491997	-2.452326	2.265000
H	-0.107754	-4.045689	1.586557
O	0.748430	-1.940203	-0.464322
H	0.871615	-2.296086	-1.358178
C	3.629421	-1.040198	0.647167
C	3.664211	0.264873	1.176068
C	4.805455	-1.526882	0.048380
C	4.820379	1.045067	1.119741
H	2.765597	0.677599	1.627045
C	5.967298	-0.751538	-0.018579
H	4.809057	-2.529237	-0.374513
C	5.977419	0.537610	0.520558
H	4.815608	2.049347	1.534734
H	6.863015	-1.152528	-0.486565
H	6.878101	1.143885	0.470764
H	2.635508	-3.326566	-0.063996

^{2}**TS3R**

E_{gas} optimization: -2905.51260965a.u.
E_{sol} single-point: -2906.11404722a.u.
G_{sol} thermo-corrected: -2905.40935322a.u.

C	-1.463523	0.070207	2.799701
C	-2.175649	-0.703321	1.846009
C	-2.939341	-1.791185	2.299116
C	-2.971122	-2.147844	3.647197
H	-3.566289	-2.999953	3.963638
C	-2.237592	-1.411755	4.575791
H	-2.243232	-1.687220	5.626424
C	-1.510333	-0.304170	4.149111
C	-0.734653	1.372672	2.514415
O	-0.483583	2.122196	3.458412
N	-0.436696	1.649717	1.194418
C	-0.423819	2.969623	0.776413
C	-1.319693	3.905492	1.361219
H	-1.952034	3.571716	2.172651
C	-1.418006	5.209432	0.917859
H	-2.136910	5.874161	1.389537
C	-0.611289	5.676890	-0.131621
H	-0.683964	6.702748	-0.478031
C	0.280512	4.799584	-0.716731
H	0.915450	5.133261	-1.529478
C	0.381121	3.450996	-0.299218
C	1.324613	2.620997	-1.036654
O	2.334078	3.284329	-1.658208
C	3.219377	2.282995	-2.209884
H	4.111119	2.230981	-1.579403
H	3.493165	2.592240	-3.221771
C	2.387616	0.987036	-2.154134
H	2.973537	0.164243	-1.740503
N	1.301466	1.336372	-1.218376
H	-3.504702	-2.382743	1.588444
H	-0.968339	0.314889	4.855224
P	-1.945454	-0.425431	0.028709
C	-2.796214	-1.866033	-0.736184
C	-3.977215	-1.771981	-1.485651
C	-2.140471	-3.107826	-0.651740
C	-4.491784	-2.896715	-2.137496
H	-4.493902	-0.820816	-1.564786
C	-2.669849	-4.232644	-1.279638
H	-1.205426	-3.181161	-0.104083
C	-3.843988	-4.129031	-2.032559
H	-5.404619	-2.809527	-2.720309
H	-2.157232	-5.187109	-1.197193
H	-4.249331	-5.002799	-2.534774
C	-2.987102	1.020946	-0.394686
C	-4.190930	1.315095	0.260606
C	-2.520746	1.886078	-1.395504
C	-4.919211	2.453966	-0.087682
H	-4.547251	0.661331	1.051762
C	-3.247999	3.024550	-1.740697
H	-1.561121	1.687690	-1.864147
C	-4.449331	3.308342	-1.088318
H	-5.848393	2.678993	0.428374
H	-2.862878	3.702908	-2.496092
H	-5.011085	4.201059	-1.347917
Cu	0.446675	0.102766	0.217155
C	1.830236	0.582165	-3.536336
H	1.155775	1.373739	-3.882336
H	2.676466	0.552003	-4.234645
C	1.133561	-0.755895	-3.546801
C	-0.262416	-0.861097	-3.537932
C	1.895393	-1.936354	-3.535903
C	-0.884888	-2.110738	-3.532197
H	-0.865731	0.041967	-3.529784
C	1.275745	-3.189928	-3.521888
H	2.981128	-1.871299	-3.543787
C	-0.118243	-3.277096	-3.522408
H	-1.967396	-2.176474	-3.511155
H	1.881874	-4.091124	-3.511476
H	-0.608442	-4.244729	-3.501565
Si	2.571219	-2.003843	0.667635
H	1.117011	-0.436444	1.524216
C	2.073932	-2.811221	2.335107
C	3.014957	-4.020260	2.546738
C	2.221966	-1.855793	3.536554
C	0.615451	-3.303148	2.252748
H	2.922004	-4.759860	1.744214
H	4.067699	-3.716642	2.599683
H	2.772303	-4.521983	3.492947
H	1.529971	-1.012736	3.464631
H	2.000539	-2.394640	4.467639
H	3.238582	-1.455289	3.617701
H	0.332911	-3.801834	3.189502
H	-0.074546	-2.470340	2.098696
H	0.471214	-4.025469	1.440000
O	1.254085	-1.733372	-0.407066
H	1.390748	-1.970071	-1.338938
C	3.838178	-0.598633	0.682272
C	3.654602	0.648552	1.312969

C	5.042013	-0.799703	-0.021107
C	4.626009	1.647403	1.240202
H	2.728982	0.841967	1.845104
C	6.016624	0.199201	-0.102983
H	5.220733	-1.750529	-0.517954
C	5.809872	1.426637	0.529628
H	4.454519	2.600352	1.732984
H	6.935045	0.017544	-0.655003
H	6.564908	2.206016	0.470402
H	3.300032	-3.070759	-0.097264

[2]TSR_1

E_{gas} optimization: -2905.49841688a.u.

E_{sol} single-point: -2906.10421680a.u.

G_{sol} thermo-corrected: -2905.3975878a.u.

C	1.885120	0.443094	2.678311
C	1.478341	1.616481	2.000604
C	1.125841	2.757230	2.734171
C	1.144176	2.740500	4.128627
H	0.856645	3.629672	4.682109
C	1.529375	1.581477	4.801295
H	1.539315	1.555970	5.886925
C	1.913980	0.454799	4.077844
C	2.424000	-0.820086	2.025385
O	3.238950	-1.484368	2.668865
N	1.982341	-1.158795	0.762993
C	2.733107	-2.093246	0.042619
C	4.145807	-2.037285	0.055196
H	4.622788	-1.258212	0.634775
C	4.919051	-2.952521	-0.639619
H	6.001515	-2.865223	-0.605586
C	4.321441	-3.982631	-1.379950
H	4.928166	-4.705568	-1.915638
C	2.940167	-4.056460	-1.427246
H	2.451229	-4.832077	-2.006235
C	2.136251	-3.115542	-0.748961
C	0.698046	-3.203168	-0.953007
O	0.183286	-4.392925	-1.344209
C	-1.263179	-4.223462	-1.340375
H	-1.647685	-4.639245	-0.403508
H	-1.668293	-4.772997	-2.192037
C	-1.438458	-2.699950	-1.424054
H	-2.254576	-2.329723	-0.804111
N	-0.150774	-2.227187	-0.883953
H	0.817954	3.658157	2.214613
H	2.254274	-0.442714	4.581578
P	1.280942	1.561392	0.183483
C	0.431455	3.097161	-0.320182
C	1.020358	4.025405	-1.190922
C	-0.900210	3.284518	0.091924
C	0.288938	5.127064	-1.640644
H	2.045751	3.889373	-1.519450
C	-1.620472	4.390484	-0.353248
H	-1.369687	2.559523	0.745930
C	-1.030453	5.312785	-1.222705
H	0.753727	5.841361	-2.314206
H	-2.648815	4.523498	-0.029939
H	-1.596810	6.170658	-1.573688
C	2.959371	1.621579	-0.531193
C	3.990910	2.371636	0.051681
C	3.218954	0.863032	-1.681465
C	5.264281	2.367560	-0.518830
H	3.799962	2.942036	0.956068
C	4.491809	0.862842	-2.250905
H	2.428294	0.252842	-2.107268
C	5.514473	1.616217	-1.670380
H	6.062146	2.945090	-0.061182
H	4.688701	0.261652	-3.133389
H	6.508694	1.609557	-2.107611
Cu	0.241841	-0.497422	0.075222
C	-1.631895	-2.225879	-2.888234
H	-0.855530	-2.704793	-3.497973
H	-2.598516	-2.613267	-3.231470
C	-1.576243	-0.728165	-3.060853
C	-0.347671	-0.082610	-3.255696
C	-2.735153	0.053387	-2.947118
C	-0.271028	1.309911	-3.303881
H	0.554918	-0.681145	-3.345861
C	-2.660758	1.449102	-2.996317
H	-3.696082	-0.423460	-2.776273
C	-1.426735	2.081346	-3.165527
H	0.692599	1.794806	-3.429125
H	-3.566945	2.033124	-2.870221
H	-1.359910	3.164061	-3.168134
Si	-2.341321	-0.184049	1.613000
H	-0.803672	-0.564861	1.806768
C	-2.748733	-1.664928	2.844089
C	-4.214091	-1.699211	3.313139
C	-2.376689	-3.006526	2.177718
C	-1.842968	-1.477559	4.078332
H	-4.506569	-0.750618	3.779140

H	-4.912639	-1.885196	2.493138
H	-4.363582	-2.491260	4.062228
H	-1.346737	-2.988898	1.798190
H	-2.448397	-3.837601	2.894991
H	-3.043400	-3.253062	1.341258
H	-1.963356	-2.317779	4.777855
H	-0.783907	-1.425111	3.802791
H	-2.089739	-0.558150	4.622194
O	-1.584653	0.208618	-0.032552
H	-2.104561	0.442126	-0.814847
C	-4.031179	0.003020	0.626518
C	-4.697994	-1.045554	-0.035426
C	-4.523060	1.300466	0.389835
C	-5.781244	-0.819266	-0.889791
H	-4.373439	-2.072527	0.117607
C	-5.602252	1.545595	-0.464081
H	-4.044396	2.146008	0.882518
C	-6.234133	0.483195	-1.114842
H	-6.273353	-1.657477	-1.378183
H	-5.952621	2.563506	-0.620516
H	-7.073741	0.666134	-1.779994
H	-2.354296	1.099135	2.388952

^{2}**TSR_2**

E_{gas} optimization: -2905.49371656a.u.

E_{sol} single-point: -2906.09831946a.u.

G_{sol} thermo-corrected: -2905.39417046a.u.

C	-1.030691	2.180947	2.025382
C	-1.980560	1.159976	1.845634
C	-2.773951	0.741503	2.922164
C	-2.609020	1.313668	4.182941
H	-3.216707	0.971089	5.015121
C	-1.664325	2.324264	4.367300
H	-1.529108	2.774088	5.346424
C	-0.900678	2.769096	3.289727
C	-0.188207	2.809059	0.925796
O	-0.345492	4.017310	0.754929
N	0.750054	2.022194	0.276781
C	1.921607	2.654357	-0.159826
C	2.395190	3.817667	0.509273
H	1.801927	4.237560	1.307273
C	3.582911	4.440080	0.176844
H	3.887088	5.321635	0.734815
C	4.393785	3.942959	-0.852679
H	5.323486	4.433197	-1.122167
C	3.988313	2.796866	-1.503578
H	4.609186	2.369481	-2.280475
C	2.777186	2.135418	-1.179215
C	2.532992	0.886642	-1.882053
O	3.514263	0.479525	-2.719701
C	3.207113	-0.870363	-3.130741
H	3.957829	-1.531161	-2.690121
H	3.266199	-0.909549	-4.222181
C	1.787035	-1.127212	-2.579601
H	1.772075	-1.981430	-1.901032
N	1.524702	0.079658	-1.768517
H	-3.510744	-0.041606	2.779600
H	-0.194358	3.582977	3.416518
P	-2.030939	0.400018	0.185006
C	-3.231828	-0.970565	0.353384
C	-4.522826	-0.938562	-0.190423
C	-2.821704	-2.106214	1.073544
C	-5.387424	-2.020564	-0.015840
H	-4.852989	-0.075185	-0.757132
C	-3.686192	-3.186690	1.242026
H	-1.833463	-2.142615	1.519722
C	-4.971783	-3.147055	0.696414
H	-6.386385	-1.982325	-0.440872
H	-3.354026	-4.056036	1.801620
H	-5.646052	-3.988167	0.828560
C	-2.767366	1.685759	-0.884408
C	-3.940537	2.376224	-0.541889
C	-2.071608	2.038490	-2.049592
C	-4.430741	3.377907	-1.378088
H	-4.456384	2.141268	0.384818
C	-2.561956	3.045925	-2.881189
H	-1.135055	1.540770	-2.282092
C	-3.744382	3.709482	-2.550023
H	-5.338612	3.909948	-1.109425
H	-2.013334	3.321711	-3.776883
H	-4.123253	4.497487	-3.194367
Cu	0.321625	0.097721	-0.134915
C	0.750974	-1.332734	-3.701747
H	0.618814	-0.383685	-4.234425
H	1.193921	-2.036401	-4.419806
C	-0.583657	-1.885800	-3.259588
C	-1.767232	-1.162118	-3.434115
C	-0.662154	-3.170508	-2.700063
C	-2.999433	-1.702053	-3.057248
H	-1.728223	-0.169740	-3.872969
C	-1.889255	-3.710647	-2.316706

H	0.247507	-3.748267	-2.559336
C	-3.064706	-2.977095	-2.497654
H	-3.905234	-1.118631	-3.191459
H	-1.930048	-4.704714	-1.880356
H	-4.018195	-3.387839	-2.184176
Si	1.243826	-1.966185	1.622084
H	0.652092	-3.360657	1.714141
H	0.838800	-0.437845	1.560621
C	1.441412	-1.744747	3.561443
C	2.186401	-2.961027	4.134044
C	2.194024	-0.452379	3.911883
C	0.019939	-1.678277	4.150191
H	1.679633	-3.901140	3.882878
H	3.211173	-3.022134	3.748382
H	2.249150	-2.907696	5.231352
H	1.693318	0.429463	3.493024
H	2.250204	-0.310379	5.001325
H	3.221052	-0.467123	3.529340
H	0.046654	-1.582929	5.246059
H	-0.536584	-0.814427	3.766239
H	-0.557991	-2.584116	3.920592
C	2.971215	-1.990453	0.853419
C	3.565624	-3.173510	0.382398
C	3.682649	-0.789368	0.672726
C	4.816877	-3.160557	-0.241156
H	3.041928	-4.119817	0.498556
C	4.929750	-0.764435	0.045228
H	3.243651	0.147380	1.005655
C	5.502013	-1.954213	-0.413048
H	5.257404	-4.090162	-0.593201
H	5.442097	0.182999	-0.097222
H	6.472921	-1.941687	-0.901358
O	0.351534	-1.878984	-0.087666
H	-0.442470	-2.401809	-0.259405

[2]**TSR_3/1**

E_{gas} optimization: -2905.49398290a.u.

E_{sol} single-point: -2906.09851890a.u.

G_{sol} thermo-corrected: -2905.3913679a.u.

C	0.737918	1.741433	2.447748
C	-0.518192	1.876038	1.825252
C	-1.660979	2.075717	2.612369
C	-1.567774	2.119625	4.003052
H	-2.465301	2.263733	4.597664
C	-0.324161	1.988263	4.621239
H	-0.242066	2.025328	5.703502
C	0.820120	1.825934	3.843176
C	2.074436	1.635870	1.732373
O	2.882564	2.533479	1.971597
N	2.318758	0.523975	0.946239
C	3.653026	0.147895	0.749722
C	4.633333	0.437656	1.737491
H	4.337938	0.993644	2.613967
C	5.952053	0.043089	1.615336
H	6.649996	0.291367	2.410447
C	6.389637	-0.673830	0.492968
H	7.426877	-0.974944	0.389049
C	5.461911	-1.007220	-0.471047
H	5.766167	-1.586558	-1.333330
C	4.100300	-0.625929	-0.365493
C	3.221476	-1.115872	-1.413029
O	3.802348	-1.912728	-2.345682
C	2.790611	-2.264003	-3.306578
H	2.833523	-3.342459	-3.473549
H	3.017282	-1.743197	-4.244829
C	1.469441	-1.780348	-2.672893
H	0.901689	-2.605236	-2.231333
N	1.941924	-0.939653	-1.553191
H	-2.630560	2.189365	2.142150
H	1.797846	1.766524	4.310023
P	-0.573278	1.622753	0.007555
C	-2.288318	2.076449	-0.469831
C	-2.581666	3.228225	-1.215512
C	-3.337489	1.220218	-0.096721
C	-3.900876	3.523364	-1.566401
H	-1.785179	3.897444	-1.521658
C	-4.654778	1.528980	-0.432643
H	-3.132833	0.311963	0.457170
C	-4.941187	2.679607	-1.170412
H	-4.113884	4.418379	-2.144137
H	-5.447348	0.855530	-0.123927
H	-5.966905	2.915489	-1.439167
C	0.485580	2.954297	-0.672174
C	0.512990	4.250175	-0.135833
C	1.324077	2.634803	-1.749915
C	1.353220	5.216935	-0.686014
H	-0.110073	4.493072	0.719796
C	2.161947	3.604972	-2.300275
H	1.345213	1.615622	-2.123612
C	2.174955	4.896403	-1.769989
H	1.376813	6.216263	-0.261571

H	2.815251	3.348810	-3.129431
H	2.835473	5.649336	-2.190237
Cu	0.817852	-0.467214	0.079560
C	0.590776	-1.045939	-3.701946
H	1.000768	-0.041774	-3.856273
H	0.711798	-1.574527	-4.658262
C	-0.889422	-0.979870	-3.403466
C	-1.566516	0.242711	-3.370961
C	-1.628428	-2.160369	-3.225683
C	-2.948478	0.290271	-3.172497
H	-1.009445	1.167653	-3.497287
C	-3.005042	-2.116075	-3.011424
H	-1.121952	-3.121528	-3.248711
C	-3.670233	-0.886966	-2.985557
H	-3.452820	1.249179	-3.135945
H	-3.557822	-3.040061	-2.866593
H	-4.740312	-0.846136	-2.807745
Si	-0.621858	-2.271599	1.756051
H	-0.533989	-2.266427	3.280284
H	0.348214	-1.064655	1.722697
C	0.159834	-3.995284	1.363894
C	-0.622293	-4.761219	0.278528
C	1.613819	-3.786781	0.885249
C	0.175864	-4.841407	2.653260
H	-1.653262	-4.965217	0.590488
H	-0.654887	-4.196137	-0.656365
H	-0.144282	-5.731330	0.079843
H	2.214249	-3.234187	1.617811
H	2.106702	-4.755804	0.720600
H	1.645317	-3.231888	-0.056720
H	0.614321	-5.829706	2.454525
H	0.763551	-4.366806	3.445340
H	-0.834759	-5.001542	3.046663
C	-2.493081	-1.956303	1.655166
C	-3.107622	-1.238139	2.697624
C	-3.312471	-2.391662	0.596224
C	-4.472877	-0.943331	2.673694
H	-2.503762	-0.893121	3.532653
C	-4.682748	-2.124875	0.577909
H	-2.875260	-2.942415	-0.230399
C	-5.266477	-1.393903	1.615960
H	-4.918255	-0.368741	3.481577
H	-5.292352	-2.479112	-0.249331
H	-6.331823	-1.178786	1.601685
O	-0.491050	-1.843297	-0.293194
H	-1.275347	-1.483678	-0.727523

[2]**TSR_3/2**

E_{gas} optimization: -2905.49236215a.u.

E_{sol} single-point: -2906.09793804a.u.

G_{sol} thermo-corrected: -2905.39208304a.u.

C	2.083703	1.799542	2.119614
C	0.966124	2.412287	1.512544
C	0.221371	3.364963	2.222917
C	0.551960	3.693376	3.536438
H	-0.042758	4.424021	4.077135
C	1.652651	3.087680	4.143144
H	1.922614	3.338583	5.164793
C	2.421185	2.171905	3.428533
C	3.087096	0.857653	1.459269
O	4.270487	1.193314	1.559148
N	2.642377	-0.299555	0.859409
C	3.578558	-1.311472	0.601654
C	4.660630	-1.530309	1.490932
H	4.758033	-0.885343	2.351804
C	5.599203	-2.526200	1.284130
H	6.404087	-2.648797	2.003819
C	5.518452	-3.373233	0.170323
H	6.259319	-4.148220	0.002951
C	4.459746	-3.214634	-0.702077
H	4.353690	-3.875929	-1.553629
C	3.479149	-2.214309	-0.503781
C	2.358035	-2.217222	-1.427386
O	2.395231	-3.100353	-2.459787
C	1.202752	-2.872784	-3.248432
H	0.783425	-3.843732	-3.519270
H	1.495345	-2.334847	-4.158700
C	0.301061	-2.024069	-2.331909
H	-0.397913	-2.654994	-1.773151
N	1.270577	-1.520731	-1.344285
H	-0.627955	3.846096	1.749475
H	3.309015	1.735333	3.873018
P	0.510671	1.852449	-0.171443
C	-1.095461	2.639134	-0.559335
C	-1.303451	3.444754	-1.689461
C	-2.203798	2.270164	0.225174
C	-2.593308	3.866576	-2.023721
H	-0.463438	3.737158	-2.311010
C	-3.488067	2.695598	-0.106906
H	-2.070466	1.648721	1.103475
C	-3.685964	3.493314	-1.237885

H	-2.741907	4.488188	-2.902156
H	-4.324733	2.382985	0.509857
H	-4.686183	3.821688	-1.505632
C	1.755549	2.626979	-1.264989
C	2.059585	3.996522	-1.209195
C	2.453390	1.798522	-2.155360
C	3.034005	4.531164	-2.049751
H	1.540107	4.636191	-0.501161
C	3.432594	2.336990	-2.992497
H	2.243885	0.733391	-2.166817
C	3.719704	3.701552	-2.942913
H	3.267071	5.590986	-2.002690
H	3.977814	1.689257	-3.672883
H	4.485198	4.119362	-3.590491
Cu	0.730168	-0.546863	0.337410
C	-0.494995	-0.895199	-3.028395
H	-0.181669	0.056119	-2.590057
H	-0.209925	-0.846194	-4.088169
C	-2.002305	-1.020893	-2.923591
C	-2.787253	0.105271	-2.643169
C	-2.646976	-2.251943	-3.113912
C	-4.177248	0.004762	-2.549729
H	-2.312842	1.069289	-2.492345
C	-4.034808	-2.356570	-3.017489
H	-2.062396	-3.141076	-3.337795
C	-4.806223	-1.225882	-2.736448
H	-4.756989	0.890435	-2.311422
H	-4.513503	-3.320898	-3.161818
H	-5.886476	-1.307656	-2.658715
Si	-1.399159	-1.322871	1.981118
H	-1.188408	-0.880863	3.424032
H	0.165435	-0.685829	1.888026
C	-1.204122	-3.236014	2.029470
C	-2.182131	-3.902533	1.040754
C	0.236977	-3.635389	1.645277
C	-1.507082	-3.733229	3.456608
H	-3.225968	-3.697824	1.301668
H	-2.019250	-3.548543	0.017749
H	-2.046788	-4.993370	1.049643
H	0.983716	-3.169098	2.297069
H	0.364487	-4.725075	1.715337
H	0.471810	-3.341933	0.615957
H	-1.433186	-4.828830	3.505516
H	-0.805553	-3.318131	4.187847
H	-2.519197	-3.456991	3.775083
C	-3.209029	-0.685672	1.901787
C	-3.709318	0.106319	2.950368
C	-4.082167	-0.958068	0.828139
C	-5.011878	0.614009	2.931607
H	-3.062175	0.333438	3.794612
C	-5.388890	-0.469910	0.807747
H	-3.743309	-1.560362	-0.009524
C	-5.857834	0.322553	1.859224
H	-5.366724	1.231216	3.753005
H	-6.035698	-0.701861	-0.033750
H	-6.873842	0.708385	1.843092
O	-1.190130	-1.144655	0.145218
H	-1.794934	-0.532744	-0.299106

^{2}TSR_4

E_{gas} optimization: -2905.47849928a.u.

E_{sol} single-point: -2906.08643990a.u.

G_{sol} thermo-corrected: -2905.3823199a.u.

C	1.015087	0.024546	2.591385
C	-0.208835	-0.652258	2.424346
C	-0.442709	-1.834522	3.142907
C	0.526181	-2.354258	4.001177
H	0.327688	-3.275573	4.541160
C	1.733941	-1.678571	4.174732
H	2.492234	-2.069728	4.846494
C	1.961437	-0.489039	3.488495
C	1.395674	1.360889	1.979092
O	1.729481	2.240774	2.773646
N	1.438411	1.479775	0.602617
C	2.284460	2.475312	0.092412
C	3.512694	2.759058	0.744127
H	3.757361	2.216270	1.645660
C	4.403478	3.702045	0.268100
H	5.332661	3.868414	0.806240
C	4.125377	4.429727	-0.898431
H	4.818738	5.177501	-1.269273
C	2.958493	4.156499	-1.580813
H	2.735698	4.680247	-2.501821
C	2.036132	3.183508	-1.119661
C	0.896968	2.917408	-1.978918
O	0.824826	3.657662	-3.114036
C	-0.377040	3.265992	-3.802401
H	-0.145207	3.146911	-4.862608
H	-1.117893	4.066472	-3.679777
C	-0.809343	1.964456	-3.102808
H	-0.462162	1.077068	-3.641116

N	-0.029941	2.015444	-1.845366
H	-1.389457	-2.351983	3.043379
H	2.882626	0.062948	3.638224
P	-1.398831	0.046977	1.204349
C	-2.923583	-0.951471	1.457095
C	-4.102161	-0.418693	1.998590
C	-2.912663	-2.297234	1.054444
C	-5.237456	-1.219928	2.144967
H	-4.137745	0.619438	2.309864
C	-4.040686	-3.099292	1.215825
H	-2.016278	-2.721355	0.618098
C	-5.209651	-2.562026	1.760825
H	-6.142918	-0.792798	2.566624
H	-4.008198	-4.139582	0.905400
H	-6.092309	-3.183215	1.881498
C	-1.797774	1.692437	1.911279
C	-1.965111	1.899274	3.289322
C	-1.901964	2.780530	1.033933
C	-2.253652	3.172957	3.776201
H	-1.854683	1.066202	3.977207
C	-2.191923	4.054641	1.523747
H	-1.711108	2.630382	-0.023223
C	-2.370528	4.250799	2.893943
H	-2.374863	3.327848	4.844264
H	-2.261456	4.894604	0.838446
H	-2.585717	5.244010	3.277367
Cu	0.311577	0.408410	-0.654084
C	-2.336338	1.905453	-2.936600
H	-2.631541	2.601486	-2.143800
H	-2.767837	2.305863	-3.865691
C	-2.947599	0.542145	-2.700720
C	-3.835457	0.328832	-1.642180
C	-2.694697	-0.518021	-3.585591
C	-4.459168	-0.908741	-1.468012
H	-4.038228	1.135250	-0.941854
C	-3.295844	-1.762721	-3.401310
H	-2.010334	-0.375635	-4.416589
C	-4.184554	-1.960514	-2.340109
H	-5.135867	-1.055507	-0.633997
H	-3.071762	-2.575097	-4.086626
H	-4.654167	-2.928169	-2.191309
Si	1.706414	-1.848194	-1.389996
H	2.349136	-1.024785	-2.447998
H	1.096657	-1.161320	-0.139779
C	0.936888	-3.541021	-1.956049
C	1.950392	-4.687191	-1.751987
C	-0.326985	-3.863238	-1.133914
C	0.566811	-3.479212	-3.453697
H	2.886910	-4.507417	-2.290204
H	2.207913	-4.826679	-0.698313
H	1.526331	-5.629820	-2.125783
H	-1.127456	-3.136901	-1.308350
H	-0.725797	-4.848553	-1.413929
H	-0.115334	-3.889807	-0.057829
H	0.122370	-4.433165	-3.772139
H	-0.147940	-2.680979	-3.667101
H	1.451245	-3.305763	-4.077000
C	3.262397	-2.305871	-0.354823
C	4.551033	-2.308429	-0.914759
C	3.146809	-2.650782	1.003759
C	5.675261	-2.653834	-0.159742
H	4.682495	-2.028571	-1.959054
C	4.262010	-2.998274	1.767743
H	2.170255	-2.633657	1.483588
C	5.531954	-3.002766	1.185118
H	6.661950	-2.645449	-0.616649
H	4.140656	-3.253733	2.817608
H	6.404571	-3.267305	1.776711
O	-0.015669	-0.810574	-2.128088
H	-0.879224	-1.233235	-2.022054

^{2}TSR_5

E_{gas} optimization: -2905.48154549a.u.

E_{sol} single-point: -2906.08781460a.u.

G_{sol} thermo-corrected: -2905.3816086a.u.

C	0.568670	-0.467429	2.809489
C	-0.630537	-1.040973	2.341336
C	-1.078999	-2.255822	2.883280
C	-0.344163	-2.916202	3.865846
H	-0.699920	-3.862779	4.262352
C	0.838046	-2.347465	4.340528
H	1.417259	-2.847496	5.111354
C	1.272184	-1.127317	3.830216
C	1.225471	0.831656	2.362620
O	1.685733	1.550099	3.252006
N	1.391136	1.071323	1.015492
C	2.527025	1.799173	0.642522
C	3.747870	1.601704	1.333030
H	3.766937	0.905263	2.158877
C	4.914759	2.239091	0.958745
H	5.829099	2.027103	1.505594

C	4.932419	3.129467	-0.125991
H	5.847585	3.635021	-0.416696
C	3.766247	3.330722	-0.835999
H	3.759973	3.988906	-1.696192
C	2.564089	2.669812	-0.483605
C	1.426033	2.860331	-1.362908
O	1.578397	3.770773	-2.356603
C	0.340466	3.805592	-3.093576
H	0.573577	3.811895	-4.160022
H	-0.188736	4.730443	-2.830356
C	-0.415831	2.550090	-2.620760
H	-0.255651	1.709683	-3.303627
N	0.300216	2.209158	-1.374215
H	-2.006979	-2.692082	2.530302
H	2.172856	-0.659485	4.210876
P	-1.563024	-0.166082	1.023548
C	-2.864212	-1.371690	0.572479
C	-4.185976	-1.343101	1.032863
C	-2.459915	-2.414727	-0.276033
C	-5.082216	-2.345536	0.655385
H	-4.521100	-0.536900	1.675985
C	-3.353688	-3.414870	-0.652144
H	-1.433143	-2.450664	-0.624239
C	-4.670323	-3.381663	-0.185030
H	-6.105751	-2.314047	1.018109
H	-3.020706	-4.214984	-1.306794
H	-5.371149	-4.159255	-0.474673
C	-2.341898	1.226562	1.917356
C	-3.030605	1.065612	3.129967
C	-2.167326	2.513464	1.388964
C	-3.578108	2.173022	3.776421
H	-3.119106	0.078867	3.575545
C	-2.709387	3.621277	2.042603
H	-1.582081	2.638825	0.483816
C	-3.423368	3.450448	3.229913
H	-4.112053	2.042638	4.713205
H	-2.562817	4.616200	1.632175
H	-3.842987	4.312394	3.740535
Cu	0.233508	0.398363	-0.469332
C	-1.916003	2.824168	-2.464873
H	-2.060801	3.495647	-1.610946
H	-2.223030	3.399173	-3.351508
C	-2.842566	1.629996	-2.356283
C	-3.925684	1.665305	-1.469315
C	-2.719070	0.526523	-3.213712
C	-4.865910	0.633834	-1.444391
H	-4.035196	2.507914	-0.792518
C	-3.648005	-0.513797	-3.176958
H	-1.886372	0.468497	-3.906067
C	-4.731273	-0.459840	-2.298211
H	-5.694951	0.679099	-0.744859
H	-3.527395	-1.365201	-3.841098
H	-5.447275	-1.273851	-2.260849
Si	1.696443	-1.466807	-1.634462
H	2.275407	-0.547997	-2.658678
H	0.920152	-1.223557	-0.282470
C	1.308451	-3.246953	-2.279129
C	2.548076	-3.708570	-3.080090
C	1.106780	-4.201741	-1.083440
C	0.079063	-3.320655	-3.204172
H	2.712061	-3.084674	-3.966215
H	3.458203	-3.676429	-2.473261
H	2.412479	-4.743391	-3.424672
H	0.238806	-3.925368	-0.473271
H	0.944709	-5.229236	-1.438666
H	1.980578	-4.212045	-0.424956
H	-0.013807	-4.330794	-3.627090
H	-0.857442	-3.115866	-2.672833
H	0.148457	-2.612071	-4.035422
C	3.294881	-1.634300	-0.556727
C	4.560398	-1.306600	-1.070722
C	3.226555	-1.991396	0.802245
C	5.708450	-1.345714	-0.274407
H	4.650051	-0.994229	-2.109990
C	4.364687	-2.036310	1.608676
H	2.260321	-2.211319	1.251307
C	5.612864	-1.712043	1.069586
H	6.673851	-1.079226	-0.697691
H	4.275293	-2.309082	2.657621
H	6.501620	-1.733942	1.694991
O	-0.015916	-0.517291	-2.231159
H	-0.843080	-1.018422	-2.193564

Si(Ph)(^{t}Bu)H$_2$

E_{gas} optimization: -680.240330010a.u.

E_{sol} single-point: -680.366384861a.u.

G_{sol} thermo-corrected: -680.175490861a.u.

Si	-0.868982	-0.000003	-1.180380
H	-1.097790	-1.216144	-2.010969
C	0.906186	-0.000102	-0.564080
C	1.580322	1.204992	-0.292708

C	1.580403	-1.205075	-0.292490
C	2.873101	1.208209	0.233914
H	1.091901	2.155130	-0.497389
C	2.873211	-1.208100	0.234136
H	1.092064	-2.155316	-0.496879
C	3.521479	0.000096	0.499064
H	3.375184	2.150812	0.434240
H	3.375338	-2.150649	0.434601
H	4.528360	0.000204	0.907285
C	-2.103219	0.000099	0.281855
C	-1.875587	-1.258413	1.143987
C	-1.876589	1.258915	1.143714
C	-3.544300	-0.000563	-0.265938
H	-2.047402	-2.179048	0.573836
H	-0.856770	-1.296002	1.545334
H	-2.568438	-1.266532	1.996606
H	-2.049056	2.179256	0.573313
H	-2.569390	1.266671	1.996376
H	-0.857809	1.297391	1.545165
H	-4.266620	-0.000421	0.562194
H	-3.748744	0.885420	-0.878229
H	-3.748157	-0.887139	-0.877536
H	-1.096962	1.216054	-2.011344

[2]TS2S

E_{gas} optimization: -2905.49994023a.u.

E_{sol} single-point: -2906.10739396a.u.

G_{sol} thermo-corrected: -2905.40095196a.u.

C	-1.603501	-1.586029	2.322386
C	-1.033619	-2.308973	1.249606
C	-0.357486	-3.510987	1.497730
C	-0.212886	-3.988130	2.800055
H	0.329779	-4.911609	2.978561
C	-0.762431	-3.272750	3.863664
H	-0.647547	-3.631949	4.881885
C	-1.468635	-2.097188	3.618780
C	-2.459397	-0.334209	2.201342
O	-3.348391	-0.178896	3.040679
N	-2.184034	0.565485	1.191514
C	-3.124112	1.573131	0.945131
C	-4.507107	1.284165	0.942453
H	-4.818988	0.267010	1.137010
C	-5.456136	2.267379	0.711267
H	-6.508731	1.998014	0.711804
C	-5.073091	3.596152	0.481402
H	-5.817949	4.366933	0.311715
C	-3.724791	3.910247	0.462009
H	-3.400161	4.926737	0.269156
C	-2.743658	2.917389	0.665925
C	-1.351881	3.315724	0.512201
O	-1.044711	4.626073	0.645798
C	0.408907	4.707132	0.568569
H	0.795658	4.762862	1.591236
H	0.665200	5.614628	0.018964
C	0.798574	3.401424	-0.139824
H	1.701407	2.948171	0.270326
N	-0.365752	2.549717	0.166359
H	0.076473	-4.066786	0.673795
H	-1.935184	-1.548044	4.428585
P	-1.061450	-1.562174	-0.416515
C	-0.009690	-2.581772	-1.503125
C	-0.517844	-3.230475	-2.637594
C	1.371383	-2.622793	-1.242075
C	0.344787	-3.912726	-3.498478
H	-1.581217	-3.201542	-2.851946
C	2.224090	-3.313630	-2.099369
H	1.767386	-2.090802	-0.386165
C	1.714676	-3.957005	-3.231316
H	-0.056473	-4.412396	-4.375475
H	3.289163	-3.340153	-1.888186
H	2.382737	-4.489275	-3.902238
C	-2.772067	-1.702099	-1.036150
C	-3.562805	-2.831969	-0.781780
C	-3.310436	-0.626635	-1.757119
C	-4.874211	-2.885866	-1.255079
H	-3.157614	-3.656671	-0.202585
C	-4.620981	-0.684082	-2.230039
H	-2.709195	0.262958	-1.918405
C	-5.402432	-1.814449	-1.980500
H	-5.485548	-3.760076	-1.051494
H	-5.035717	0.158375	-2.775144
H	-6.426143	-1.856642	-2.340859
Cu	-0.457584	0.557310	0.213658
C	0.940741	3.601281	-1.672023
H	0.076231	4.184482	-2.013581
H	1.833603	4.214416	-1.840622
C	1.031774	2.313314	-2.453737
C	-0.135334	1.654895	-2.869787
C	2.270921	1.708541	-2.708543
C	-0.069373	0.411867	-3.501273
H	-1.100653	2.115521	-2.676150

C	2.337064	0.465796	-3.346474
H	3.188732	2.187720	-2.377599
C	1.168708	-0.190032	-3.736195
H	-0.984023	-0.094489	-3.796091
H	3.305912	0.004545	-3.504976
H	1.218438	-1.170591	-4.197989
Si	2.489030	0.326989	1.675105
H	1.160833	-0.291859	2.124151
C	3.481301	-0.767299	2.975450
C	2.724745	-0.719424	4.315248
C	3.479353	-2.224231	2.465317
C	4.931834	-0.306651	3.197238
H	2.718677	0.292163	4.739431
H	1.682916	-1.040906	4.203980
H	3.198014	-1.382416	5.055562
H	4.049819	-2.332633	1.534196
H	3.939726	-2.901566	3.201150
H	2.458609	-2.586547	2.286434
H	5.431489	-0.934928	3.950506
H	5.523945	-0.359668	2.278441
H	4.974758	0.729289	3.555438
O	1.455412	0.267283	0.020994
H	1.883149	0.573190	-0.792961
C	3.944362	0.672281	0.399646
C	4.510315	1.958206	0.338538
C	4.426182	-0.268947	-0.530629
C	5.489387	2.297197	-0.601438
H	4.177731	2.717082	1.045232
C	5.410599	0.050695	-1.468732
H	4.015739	-1.276069	-0.539878
C	5.942376	1.342388	-1.514563
H	5.900969	3.303945	-0.619665
H	5.760151	-0.705280	-2.168750
H	6.703200	1.598201	-2.247025
H	2.360915	1.722184	2.226842

[2]IM4S

E_{gas} optimization: -2905.50454704a.u.

E_{sol} single-point: -2906.10780969a.u.

G_{sol} thermo-corrected: -2905.40286769a.u.

C	-1.864930	-1.599488	2.248761
C	-1.535537	-2.282566	1.052000
C	-1.273198	-3.660133	1.100219
C	-1.288327	-4.351895	2.311299
H	-1.069790	-5.415781	2.325704
C	-1.577870	-3.672829	3.494180
H	-1.579137	-4.199988	4.443618
C	-1.884614	-2.314919	3.452125
C	-2.358324	-0.163233	2.326743
O	-3.117426	0.129666	3.251595
N	-1.959231	0.702971	1.334514
C	-2.768273	1.800988	1.037099
C	-4.177756	1.678629	1.110853
H	-4.595370	0.731527	1.424358
C	-5.024872	2.725543	0.794281
H	-6.098921	2.573232	0.856634
C	-4.512714	3.966789	0.391581
H	-5.175059	4.792100	0.150884
C	-3.140691	4.118805	0.300039
H	-2.716320	5.064827	-0.017395
C	-2.259605	3.054821	0.592887
C	-0.839618	3.312321	0.373949
O	-0.429502	4.603858	0.479329
C	1.017333	4.575327	0.382938
H	1.425569	4.654567	1.396126
H	1.336193	5.431865	-0.214995
C	1.306442	3.210017	-0.263341
H	2.159664	2.713301	0.201132
N	0.066960	2.460218	0.023953
H	-1.032851	-4.194717	0.188119
H	-2.163544	-1.775943	4.350656
P	-1.283423	-1.328962	-0.504597
C	-0.508497	-2.516656	-1.663548
C	-1.143993	-2.975326	-2.825485
C	0.815174	-2.912762	-1.400013
C	-0.468921	-3.823802	-3.706836
H	-2.163406	-2.672074	-3.042526
C	1.475507	-3.776157	-2.270909
H	1.322998	-2.530322	-0.521848
C	0.837149	-4.231781	-3.428759
H	-0.969232	-4.172935	-4.605667
H	2.494737	-4.082684	-2.053172
H	1.356178	-4.898590	-4.111344
C	-2.941408	-0.957416	-1.171156
C	-4.041117	-1.804033	-0.971823
C	-3.110723	0.242746	-1.876235
C	-5.292517	-1.454037	-1.480883
H	-3.919623	-2.724114	-0.407489
C	-4.361456	0.588296	-2.386193
H	-2.266820	0.915745	-1.990964
C	-5.452694	-0.260382	-2.189598

H	-6.143237	-2.109603	-1.318659
H	-4.488118	1.528395	-2.914495
H	-6.429958	0.013203	-2.576713
Cu	-0.149673	0.433825	0.547437
C	1.544146	3.323928	-1.786461
H	0.732603	3.926599	-2.212361
H	2.476078	3.883039	-1.933695
C	1.618095	1.989467	-2.485027
C	0.470119	1.426089	-3.056950
C	2.817229	1.262552	-2.526211
C	0.511198	0.166967	-3.654888
H	-0.461928	1.983294	-3.026263
C	2.860415	-0.000300	-3.127195
H	3.717779	1.672224	-2.075263
C	1.708115	-0.551523	-3.691509
H	-0.391586	-0.262775	-4.077688
H	3.795523	-0.551389	-3.133480
H	1.732865	-1.539628	-4.137672
Si	2.452545	0.275871	1.658621
H	0.757439	0.337364	2.015989
C	2.654075	-1.179426	2.913959
C	1.782708	-0.920872	4.160207
C	2.186716	-2.488788	2.248682
C	4.125231	-1.321732	3.356430
H	2.057772	0.014295	4.661368
H	0.720352	-0.867134	3.906159
H	1.912358	-1.735557	4.886390
H	2.800321	-2.750224	1.377996
H	2.257211	-3.324599	2.958848
H	1.144182	-2.423425	1.924590
H	4.218714	-2.125399	4.100324
H	4.787130	-1.561895	2.519576
H	4.501935	-0.401537	3.818110
O	1.699343	-0.184520	0.103313
H	2.156692	0.054006	-0.719947
C	4.160128	0.488895	0.742583
C	4.841323	1.715548	0.793141
C	4.705365	-0.504273	-0.096773
C	5.992816	1.957118	0.035406
H	4.456730	2.507329	1.435021
C	5.859752	-0.283907	-0.849392
H	4.207405	-1.468936	-0.177476
C	6.503848	0.956397	-0.792602
H	6.490217	2.922501	0.091168
H	6.256403	-1.072709	-1.484493
H	7.397013	1.137062	-1.384548
H	2.484292	1.644408	2.289341

^{2}TS3S

E_{gas} optimization: -2905.50435220a.u.

E_{sol} single-point: -2906.10763945a.u.

G_{sol} thermo-corrected: -2905.40310645a.u.

C	1.816371	-1.723633	-2.208188
C	1.492052	-2.338523	-0.972551
C	1.207635	-3.712839	-0.951537
C	1.194933	-4.464594	-2.126402
H	0.961760	-5.524706	-2.083573
C	1.475902	-3.850519	-3.346184
H	1.454849	-4.424170	-4.268117
C	1.803646	-2.497473	-3.375041
C	2.331303	-0.301844	-2.365002
O	3.030927	-0.047326	-3.346006
N	2.019936	0.589621	-1.363888
C	2.901232	1.633073	-1.091232
C	4.296966	1.434468	-1.250311
H	4.640258	0.482476	-1.631416
C	5.222826	2.408614	-0.926463
H	6.280529	2.194045	-1.053308
C	4.812193	3.655180	-0.432878
H	5.536523	4.424047	-0.184043
C	3.458763	3.885433	-0.268324
H	3.111398	4.839383	0.112629
C	2.496361	2.895139	-0.567879
C	1.106996	3.246897	-0.287812
O	0.798772	4.570582	-0.356878
C	-0.636784	4.664854	-0.203708
H	-1.072092	4.847226	-1.191921
H	-0.856164	5.507485	0.456421
C	-1.033641	3.292655	0.375402
H	-1.913559	2.883574	-0.126663
N	0.145535	2.460675	0.069615
H	0.972014	-4.199350	-0.011883
H	2.075656	-2.006210	-4.302604
P	1.251918	-1.310476	0.543893
C	0.462511	-2.457414	1.736548
C	1.099128	-2.927931	2.893105
C	-0.876630	-2.813063	1.494990
C	0.408780	-3.744975	3.792402
H	2.131215	-2.657013	3.092270
C	-1.552353	-3.647707	2.381843
H	-1.383999	-2.422564	0.618739

C	-0.913763	-4.111858	3.536199
H	0.909601	-4.102397	4.687757
H	-2.583924	-3.923307	2.181189
H	-1.445123	-4.754477	4.232403
C	2.910898	-0.939057	1.209117
C	3.997003	-1.814238	1.069078
C	3.095624	0.296093	1.847252
C	5.249649	-1.458578	1.571509
H	3.864379	-2.761863	0.554779
C	4.347942	0.648738	2.348089
H	2.264910	0.992552	1.908874
C	5.425095	-0.229266	2.212154
H	6.089921	-2.137115	1.455388
H	4.487847	1.617294	2.818313
H	6.403907	0.049359	2.591737
Cu	0.166326	0.444299	-0.597959
C	-1.292438	3.352836	1.896177
H	-0.405170	3.784785	2.374496
H	-2.121166	4.052631	2.061527
C	-1.622388	2.017071	2.515059
C	-0.635539	1.255169	3.154071
C	-2.923846	1.498464	2.432927
C	-0.939801	0.013383	3.712413
H	0.377380	1.642512	3.215189
C	-3.231930	0.253889	2.992263
H	-3.701961	2.061835	1.923930
C	-2.240808	-0.488629	3.636867
H	-0.162117	-0.572330	4.191549
H	-4.243132	-0.129540	2.906030
H	-2.470322	-1.459248	4.062415
Si	-2.495216	0.409319	-1.652124
H	-0.669132	0.496212	-2.015942
C	-2.572979	-1.009350	-2.959399
C	-1.660206	-0.700786	-4.164070
C	-2.096565	-2.317864	-2.297269
C	-4.019438	-1.186831	-3.470515
H	-1.936360	0.240279	-4.653530
H	-0.610110	-0.630973	-3.869272
H	-1.747126	-1.500466	-4.912421
H	-2.741045	-2.616153	-1.461570
H	-2.107606	-3.138516	-3.027352
H	-1.073892	-2.226863	-1.922637
H	-4.050075	-1.974305	-4.235987
H	-4.710167	-1.470079	-2.671603
H	-4.406448	-0.269081	-3.928685
O	-1.741198	-0.061287	-0.134333
H	-2.187465	0.197472	0.689390
C	-4.240384	0.563949	-0.838353
C	-4.957048	1.768963	-0.919335
C	-4.810575	-0.467576	-0.065948
C	-6.176825	1.948733	-0.258308
H	-4.549783	2.590305	-1.507146
C	-6.032181	-0.306799	0.589331
H	-4.284005	-1.414688	0.035935
C	-6.717340	0.909034	0.499972
H	-6.704498	2.896173	-0.335543
H	-6.449733	-1.123727	1.173197
H	-7.664889	1.041802	1.014987
H	-2.428683	1.804156	-2.194496

^{2}TSS_1/1

E_{gas} optimization: -2905.49530326a.u.

E_{sol} single-point: -2906.09775732a.u.

G_{sol} thermo-corrected: -2905.39189632a.u.

C	0.110627	1.223247	2.895092
C	1.116755	1.624386	1.995285
C	1.772365	2.851594	2.170537
C	1.423677	3.699436	3.218773
H	1.929234	4.653636	3.334642
C	0.428872	3.309644	4.117240
H	0.151280	3.958783	4.942642
C	-0.202037	2.077332	3.964956
C	-0.692689	-0.072307	2.880272
O	-0.912206	-0.594584	3.975327
N	-1.238195	-0.508382	1.691006
C	-2.439543	-1.235535	1.787421
C	-3.423976	-0.803574	2.708944
H	-3.187166	0.025463	3.362495
C	-4.671432	-1.394821	2.793156
H	-5.393139	-1.011009	3.508849
C	-5.010564	-2.463505	1.953022
H	-5.989040	-2.928990	2.009814
C	-4.077663	-2.906743	1.036137
H	-4.324519	-3.720634	0.366432
C	-2.795193	-2.315811	0.930727
C	-1.920321	-2.842239	-0.112180
O	-2.441996	-3.851278	-0.860455
C	-1.427896	-4.249565	-1.802602
H	-1.886406	-4.322625	-2.790848
H	-1.051546	-5.235499	-1.502772
C	-0.349802	-3.148800	-1.687575

H	-0.434186	-2.434791	-2.513405
N	-0.743389	-2.429713	-0.460887
H	2.549082	3.150741	1.475141
H	-0.948167	1.747070	4.678743
P	1.557083	0.481552	0.641645
C	2.559575	1.481626	-0.511108
C	3.910073	1.242491	-0.789591
C	1.893211	2.530253	-1.173450
C	4.586773	2.046499	-1.709970
H	4.428591	0.417942	-0.316117
C	2.572250	3.324092	-2.094989
H	0.852189	2.739468	-0.955820
C	3.922969	3.084079	-2.365251
H	5.634379	1.850917	-1.920132
H	2.039144	4.128449	-2.592352
H	4.453866	3.702792	-3.082994
C	2.616393	-0.764558	1.455717
C	3.812692	-0.418911	2.105016
C	2.157396	-2.087634	1.502822
C	4.560066	-1.397325	2.757311
H	4.151789	0.612887	2.109791
C	2.900893	-3.059643	2.174752
H	1.217806	-2.346543	1.025531
C	4.105013	-2.719411	2.790999
H	5.488251	-1.127382	3.252483
H	2.535283	-4.081560	2.216981
H	4.683980	-3.477818	3.310149
Cu	-0.475811	-0.321747	-0.133713
C	1.059458	-3.750546	-1.642298
H	1.179846	-4.260828	-0.678748
H	1.089918	-4.544209	-2.404247
C	2.247977	-2.844709	-1.900359
C	3.492199	-3.194701	-1.357501
C	2.183284	-1.738800	-2.759152
C	4.647272	-2.484742	-1.683676
H	3.556428	-4.035060	-0.671734
C	3.337770	-1.025709	-3.086401
H	1.230317	-1.414460	-3.160562
C	4.574940	-1.403266	-2.562788
H	5.599772	-2.776889	-1.250547
H	3.267760	-0.162075	-3.741326
H	5.469804	-0.844780	-2.821248
Si	-2.196441	0.886621	-2.047160
H	-2.052020	0.854217	-3.546089
H	-2.170776	-0.060200	-0.797942
C	-4.153087	0.770576	-2.006742
C	-4.697168	1.015713	-0.590802
C	-4.735334	1.806080	-2.982156
C	-4.538352	-0.649796	-2.461215
H	-4.288056	0.300960	0.132108
H	-4.457336	2.024772	-0.235729
H	-5.791686	0.909405	-0.566483
H	-4.355249	1.662815	-4.001152
H	-5.832029	1.731306	-3.029351
H	-4.489396	2.829859	-2.675020
H	-5.631139	-0.773638	-2.488255
H	-4.162145	-0.870966	-3.468848
H	-4.145864	-1.413093	-1.776751
C	-1.722898	2.593695	-1.381490
C	-1.633530	2.822201	0.006052
C	-1.373058	3.652989	-2.237667
C	-1.189053	4.042800	0.518650
H	-1.885254	2.022805	0.698174
C	-0.934973	4.881244	-1.732832
H	-1.429850	3.513178	-3.314932
C	-0.832812	5.075115	-0.352547
H	-1.100267	4.175556	1.592982
H	-0.667991	5.684316	-2.415492
H	-0.476432	6.023346	0.040625
O	-0.354469	0.139049	-2.038153
H	0.347122	0.743594	-2.321278

^{2}TSS_1/2

E_{gas} optimization: -2905.50177680a.u.

E_{sol} single-point: -2906.10427372a.u.

G_{sol} thermo-corrected: -2905.39837772a.u.

C	-0.892029	0.958407	3.033744
C	0.309336	1.428839	2.461041
C	0.927831	2.576741	2.986184
C	0.340985	3.310033	4.011739
H	0.828247	4.205783	4.385941
C	-0.868620	2.875355	4.554921
H	-1.344155	3.434256	5.355902
C	-1.453716	1.704000	4.087002
C	-1.676869	-0.317866	2.719948
O	-2.316296	-0.802751	3.664472
N	-1.685009	-0.830588	1.457098
C	-2.738777	-1.708467	1.143934
C	-4.064016	-1.395417	1.516212
H	-4.233147	-0.497829	2.097518
C	-5.132437	-2.207340	1.170565

H	-6.137618	-1.921396	1.468205
C	-4.923552	-3.386814	0.443716
H	-5.756841	-4.028179	0.174664
C	-3.633932	-3.721790	0.067085
H	-3.449874	-4.626447	-0.501052
C	-2.538597	-2.891763	0.389506
C	-1.230688	-3.303760	-0.123507
O	-1.083206	-4.649514	-0.305619
C	0.290511	-4.852175	-0.685001
H	0.332464	-5.615850	-1.463910
H	0.845291	-5.198815	0.197687
C	0.750883	-3.458227	-1.142799
H	0.606384	-3.368030	-2.227703
N	-0.237203	-2.563075	-0.492906
H	1.873405	2.911370	2.573233
H	-2.360442	1.320379	4.539246
P	1.115199	0.521699	1.081123
C	2.077981	1.778893	0.158485
C	3.271445	1.441986	-0.500723
C	1.501479	3.041008	-0.084947
C	3.900993	2.367330	-1.336391
H	3.705951	0.455695	-0.383634
C	2.129493	3.953491	-0.930238
H	0.557368	3.310528	0.374173
C	3.337759	3.625378	-1.550445
H	4.824686	2.086890	-1.831388
H	1.659781	4.915888	-1.107258
H	3.827706	4.339370	-2.206066
C	2.276581	-0.585348	1.967651
C	3.597697	-0.258777	2.301982
C	1.737777	-1.811542	2.394328
C	4.378974	-1.160485	3.026539
H	4.018467	0.694385	1.998884
C	2.517102	-2.699623	3.136182
H	0.712825	-2.062099	2.134821
C	3.841759	-2.380411	3.444146
H	5.405403	-0.904450	3.273633
H	2.090271	-3.642048	3.467011
H	4.451295	-3.076219	4.013473
Cu	-0.622811	-0.365335	-0.207781
C	2.216563	-3.189655	-0.798037
H	2.280848	-2.932941	0.263573
H	2.759341	-4.139411	-0.907419
C	2.954058	-2.157086	-1.628130
C	4.335632	-2.003057	-1.429383
C	2.336383	-1.387715	-2.620054
C	5.084272	-1.133490	-2.221850
H	4.827263	-2.583094	-0.651591
C	3.082675	-0.508856	-3.410906
H	1.266113	-1.446284	-2.772078
C	4.459510	-0.389509	-3.227313
H	6.154630	-1.041211	-2.059404
H	2.579550	0.079446	-4.173550
H	5.039832	0.283040	-3.852220
Si	-1.248524	1.485423	-2.585262
H	-0.588278	2.290109	-3.665310
H	-1.942294	-0.069440	-0.966129
C	-2.606265	0.455076	-3.467935
C	-2.839631	1.103032	-4.852853
C	-2.115398	-0.995333	-3.661809
C	-3.941012	0.450251	-2.694837
H	-3.179904	2.142214	-4.767530
H	-1.932273	1.100590	-5.466488
H	-3.614400	0.549648	-5.400049
H	-1.934838	-1.481686	-2.698489
H	-2.873761	-1.575333	-4.205350
H	-1.186302	-1.038553	-4.242989
H	-4.701758	-0.096020	-3.268692
H	-3.837968	-0.036700	-1.721041
H	-4.317634	1.465970	-2.527997
C	-1.692057	2.820960	-1.324638
C	-1.367861	4.149021	-1.665764
C	-2.186559	2.587258	-0.025935
C	-1.501518	5.192966	-0.747425
H	-0.978297	4.368762	-2.656623
C	-2.303030	3.622837	0.902722
H	-2.444347	1.577459	0.274063
C	-1.954496	4.927913	0.546765
H	-1.238054	6.207131	-1.036580
H	-2.641455	3.402782	1.910798
H	-2.034431	5.731649	1.273653
O	0.078176	0.512924	-2.070063
H	0.940226	0.954766	-2.074029

***S*-silanol**

E_{gas} optimization: -755.514560454a.u.

E_{sol} single-point: -755.672266995a.u.

G_{sol} thermo-corrected: -755.476586995a.u.

Si	-0.810480	0.445621	0.844482
H	-0.984832	-0.058238	2.240087
C	-1.997749	-0.473666	-0.313601

C	-3.449847	-0.209290	0.134564
C	-1.800908	0.027504	-1.758808
C	-1.696079	-1.984609	-0.242464
H	-3.628084	-0.558544	1.158576
H	-3.694484	0.857116	0.094840
H	-4.153141	-0.740739	-0.521393
H	-0.777375	-0.145392	-2.110100
H	-2.479533	-0.502668	-2.440877
H	-2.011531	1.098819	-1.842798
H	-2.374764	-2.538582	-0.904901
H	-0.670507	-2.209655	-0.556544
H	-1.833078	-2.381534	0.770736
C	0.986677	0.184022	0.374290
C	1.766183	-0.800438	1.007273
C	1.581557	0.934733	-0.657294
C	3.086354	-1.036917	0.619196
H	1.338548	-1.388483	1.816809
C	2.902146	0.706113	-1.046586
H	1.004391	1.708640	-1.158119
C	3.655528	-0.283113	-0.409557
H	3.671760	-1.803006	1.120348
H	3.344026	1.296774	-1.844531
H	4.683537	-0.463364	-0.711694
O	-1.208981	2.065098	0.708871
H	-0.619531	2.683344	1.153771

***R*-silanol**

E_{gas} optimization: -755.514560454a.u.

E_{sol} single-point: -755.672266995a.u.

G_{sol} thermo-corrected: -755.476586995a.u.

Si	-0.810480	0.445621	-0.844482
H	-0.984832	-0.058238	-2.240087
C	-1.997749	-0.473666	0.313601
C	-3.449847	-0.209290	-0.134564
C	-1.800908	0.027504	1.758808
C	-1.696079	-1.984609	0.242464
H	-3.628084	-0.558544	-1.158576
H	-3.694484	0.857116	-0.094840
H	-4.153141	-0.740739	0.521393
H	-0.777375	-0.145392	2.110100
H	-2.479533	-0.502668	2.440877
H	-2.011531	1.098819	1.842798
H	-2.374764	-2.538582	0.904901
H	-0.670507	-2.209655	0.556544
H	-1.833078	-2.381534	-0.770736
C	0.986677	0.184022	-0.374290
C	1.766183	-0.800438	-1.007273
C	1.581557	0.934733	0.657294
C	3.086354	-1.036917	-0.619196
H	1.338548	-1.388483	-1.816809
C	2.902146	0.706113	1.046586
H	1.004391	1.708640	1.158119
C	3.655528	-0.283113	0.409557
H	3.671760	-1.803006	-1.120348
H	3.344026	1.296774	1.844531
H	4.683537	-0.463364	0.711694
O	-1.208981	2.065098	-0.708871
H	-0.619531	2.683344	-1.153771

^{2}IM5

E_{gas} optimization: -2468.34478811a.u.

E_{sol} single-point: -2468.93559919a.u.

G_{sol} thermo-corrected: -2468.44299119a.u.

C	-0.686808	3.518672	2.340757
C	-0.022841	2.409960	2.915702
C	0.064963	2.297174	4.310323
C	-0.513684	3.258661	5.137847
H	-0.445313	3.153263	6.216807
C	-1.165845	4.356846	4.574901
H	-1.612720	5.113492	5.213295
C	-1.230200	4.490747	3.189835
C	-0.753334	3.821807	0.849269
O	-0.705236	5.010841	0.512202
N	-0.874793	2.759047	0.000319
C	-0.757184	2.986561	-1.369938
C	0.289530	3.786895	-1.886393
H	0.961586	4.261408	-1.183711
C	0.463628	3.965767	-3.251544
H	1.281348	4.587832	-3.607079
C	-0.410902	3.362047	-4.170089
H	-0.290846	3.521305	-5.237644
C	-1.450080	2.575139	-3.691625
H	-2.139359	2.102367	-4.382025
C	-1.634431	2.366311	-2.307860
C	-2.700391	1.455726	-1.891238
O	-3.489387	0.953818	-2.878228
C	-4.474473	0.108106	-2.225478
H	-4.604120	-0.792667	-2.825437
H	-5.421455	0.660104	-2.176100
C	-3.865370	-0.130955	-0.836748

H	-3.244558	-1.035542	-0.846204
N	-2.929806	0.995219	-0.705294
H	0.584659	1.453074	4.751659
H	-1.691949	5.358136	2.730972
P	0.630702	1.105560	1.807230
C	2.138498	1.811216	1.034610
C	2.442548	3.180800	1.101299
C	2.981753	0.967653	0.291827
C	3.557321	3.688485	0.431768
H	1.814968	3.860056	1.665847
C	4.110558	1.472462	-0.356545
H	2.795257	-0.100335	0.221039
C	4.394393	2.839257	-0.295169
H	3.773599	4.751381	0.491497
H	4.750779	0.777002	-0.892405
H	5.270524	3.237074	-0.799787
C	1.218831	-0.258849	2.891399
C	0.249281	-1.141797	3.404390
C	2.573134	-0.487800	3.189852
C	0.628069	-2.225911	4.198291
H	-0.796650	-0.973619	3.165558
C	2.949617	-1.583516	3.972029
H	3.336136	0.181587	2.808404
C	1.980127	-2.454126	4.479846
H	-0.133294	-2.890626	4.597516
H	4.000679	-1.746155	4.193561
H	2.274671	-3.295370	5.101747
Cu	-1.353141	0.862788	0.586559
Br	4.285342	-2.046351	-1.441275
C	-4.859349	-0.231371	0.320441
H	-4.271897	-0.181927	1.243911
H	-5.524508	0.639676	0.308209
C	-5.650039	-1.520206	0.260867
C	-4.993803	-2.752260	0.416917
C	-7.028573	-1.521246	0.019044
C	-5.702482	-3.950107	0.334127
H	-3.920384	-2.770512	0.593388
C	-7.741208	-2.720432	-0.061463
H	-7.549294	-0.574264	-0.102384
C	-7.079772	-3.938749	0.095467
H	-5.179422	-4.894733	0.456090
H	-8.811622	-2.700828	-0.246920
H	-7.631343	-4.872457	0.032373
O	-1.058991	-2.350720	0.269338
O	0.077090	-2.628138	-1.636150
C	-0.497359	-1.818471	-0.887119
O	-0.583475	-0.557918	-1.035092
Cs	1.545517	-0.024555	-3.060820
Cs	1.861083	-3.731073	0.632629
H	-1.434778	-1.589302	0.776347
H	-1.942688	-0.271801	1.508635

^{2}IM6

E_{gas} optimization: -2239.27698542a.u.

E_{sol} single-point: -2239.77317231a.u.

G_{sol} thermo-corrected: -2239.27814931a.u.

C	3.297794	0.466450	1.489492
C	3.012038	-0.858154	1.096228
C	3.904100	-1.899448	1.406849
C	5.084213	-1.646120	2.098038
H	5.767708	-2.458805	2.324493
C	5.368314	-0.341301	2.506127
H	6.280611	-0.126708	3.054881
C	4.482078	0.690948	2.215416
C	2.500900	1.743621	1.226470
O	2.603580	2.642007	2.060874
N	1.835063	1.903633	0.019563
C	1.678745	3.251093	-0.394658
C	2.822242	4.078486	-0.415094
H	3.761221	3.666351	-0.065088
C	2.772183	5.388472	-0.863607
H	3.681614	5.982650	-0.867583
C	1.567444	5.944974	-1.314245
H	1.527372	6.970160	-1.667206
C	0.428044	5.161066	-1.306289
H	-0.519476	5.560872	-1.649562
C	0.464845	3.822761	-0.860345
C	-0.780299	3.072259	-0.878774
O	-1.939196	3.758275	-0.889385
C	-2.999841	2.769185	-1.075265
H	-3.309759	2.805903	-2.124177
H	-3.833653	3.040534	-0.426664
C	-2.324275	1.442628	-0.696883
H	-2.601964	0.621108	-1.360925
N	-0.896238	1.783872	-0.884859
H	3.663955	-2.913541	1.102578
H	4.686759	1.701955	2.546831
P	1.435031	-1.266429	0.298143
C	1.777050	-2.643020	-0.853096
C	0.987325	-3.796824	-0.914570
C	2.792162	-2.442338	-1.809120

C	1.216985	-4.744209	-1.914712
H	0.185649	-3.953566	-0.203252
C	3.015621	-3.393188	-2.803082
H	3.411003	-1.549131	-1.765378
C	2.224663	-4.545784	-2.857818
H	0.591033	-5.629427	-1.961926
H	3.802445	-3.233706	-3.534293
H	2.390949	-5.281168	-3.639037
C	0.307857	-1.839928	1.614979
C	0.712882	-1.891937	2.957952
C	-1.022184	-2.143076	1.271755
C	-0.206285	-2.251869	3.944278
H	1.732697	-1.647946	3.235288
C	-1.930339	-2.505957	2.265862
H	-1.356936	-2.094057	0.236525
C	-1.525524	-2.557148	3.601736
H	0.110355	-2.288059	4.982458
H	-2.957966	-2.720416	1.990163
H	-2.238374	-2.826747	4.375472
Cu	0.660824	0.575434	-0.813048
Br	-2.249857	-2.061568	-2.231406
C	-2.544565	1.035850	0.775066
H	-1.863979	0.207275	0.992285
H	-2.236435	1.872739	1.413722
C	-3.968644	0.633848	1.079651
C	-4.513126	-0.529945	0.513201
C	-4.771474	1.416421	1.918966
C	-5.829333	-0.899505	0.790340
H	-3.910635	-1.136911	-0.158191
C	-6.089662	1.045568	2.197094
H	-4.358125	2.317573	2.366657
C	-6.621425	-0.115056	1.633909
H	-6.236455	-1.801368	0.341711
H	-6.697276	1.662522	2.853437
H	-7.646071	-0.405743	1.848127
O	0.289556	-0.321587	-2.604877
H	-0.612959	-0.778820	-2.590636
H	0.895996	-1.054817	-2.796177

^{2}**TS4**

E_{gas} optimization: -2239.22439729a.u.

E_{sol} single-point: -2239.72111519a.u.

G_{sol} thermo-corrected: -2239.23223919a.u.

C	2.838217	-2.082936	1.155275
C	1.595085	-2.671020	0.835944
C	1.383543	-4.045253	1.046854
C	2.381656	-4.850605	1.584667
H	2.204578	-5.911312	1.736350
C	3.605459	-4.274207	1.929924
H	4.396040	-4.884197	2.357554
C	3.821046	-2.915694	1.723844
C	3.324883	-0.644005	0.940302
O	4.228522	-0.261693	1.689072
N	2.863814	0.103682	-0.126495
C	3.800431	1.066497	-0.573686
C	5.095379	0.622703	-0.923038
H	5.323108	-0.429563	-0.795133
C	6.063380	1.482788	-1.413731
H	7.041774	1.089578	-1.675973
C	5.786859	2.847504	-1.580029
H	6.542242	3.523768	-1.967051
C	4.529379	3.317719	-1.248337
H	4.285054	4.366812	-1.371425
C	3.531720	2.450648	-0.751967
C	2.229229	3.018486	-0.449213
O	2.100434	4.365972	-0.429969
C	0.716087	4.655803	-0.089231
H	0.330801	5.364857	-0.824423
H	0.707227	5.119744	0.902933
C	0.012558	3.277174	-0.114231
H	-0.588143	3.152642	-1.017759
N	1.145724	2.352668	-0.240753
H	0.425529	-4.482485	0.782168
H	4.764313	-2.459183	1.998178
P	0.229971	-1.647778	0.215820
C	-0.675258	-2.671474	-0.998442
C	-1.756435	-3.488114	-0.639481
C	-0.267492	-2.611381	-2.340603
C	-2.412644	-4.244817	-1.610491
H	-2.095429	-3.517057	0.391503
C	-0.928406	-3.366775	-3.308329
H	0.558656	-1.963867	-2.623708
C	-2.001178	-4.184580	-2.943605
H	-3.252079	-4.872784	-1.326885
H	-0.612262	-3.310725	-4.345631
H	-2.519456	-4.768445	-3.698628
C	-0.942139	-1.401500	1.601234
C	-0.890431	-2.110836	2.808636
C	-1.929105	-0.418199	1.413555
C	-1.826192	-1.841226	3.810710
H	-0.124331	-2.862297	2.970436

C	-2.859334	-0.153304	2.416107
H	-1.928697	0.146813	0.486061
C	-2.809040	-0.867982	3.616638
H	-1.782336	-2.391051	4.746475
H	-3.604268	0.622142	2.262827
H	-3.528595	-0.660366	4.403441
Cu	0.926013	0.387504	-0.562684
Br	-4.050384	-0.757231	-1.827983
C	-0.843885	2.931578	1.119640
H	-0.690495	1.865162	1.313643
H	-0.459109	3.456642	2.001703
C	-2.330990	3.170267	0.969388
C	-3.019771	2.695592	-0.161527
C	-3.062630	3.803355	1.980080
C	-4.402611	2.856305	-0.269521
H	-2.454995	2.187831	-0.941564
C	-4.448515	3.954823	1.877467
H	-2.544673	4.175188	2.860953
C	-5.123865	3.481534	0.752181
H	-4.919981	2.493809	-1.154047
H	-4.997337	4.446746	2.675769
H	-6.199844	3.602473	0.667303
O	-0.739692	0.728414	-1.421233
H	-3.611352	0.353330	-1.040506
H	-1.097273	-0.061295	-1.848736
H	-2.723897	-3.044271	5.204660
C	-1.137121	-3.970360	4.066642
H	-1.318365	-4.968561	4.452659
C	-0.123373	-3.750671	3.148649
H	0.494159	-4.573443	2.807569
C	0.119789	-2.463956	2.623382
C	1.176265	-2.334581	1.620595
O	2.091501	-3.339411	1.573389
C	2.869982	-3.136613	0.366718
H	2.573164	-3.899819	-0.359575
H	3.926476	-3.259368	0.613641
C	2.497539	-1.704052	-0.076602
H	2.223008	-1.672371	-1.134765
N	1.301247	-1.410499	0.725649
H	-0.251847	4.877811	0.627729
H	-0.859111	2.780207	5.045814
P	0.103346	2.088907	0.186436
C	-0.959013	2.864400	-1.094561
C	-0.563537	3.937138	-1.906587
C	-2.247105	2.329843	-1.242563
C	-1.448022	4.463459	-2.849974
H	0.434523	4.353864	-1.813098
C	-3.132754	2.862636	-2.177825
H	-2.551261	1.483839	-0.635207
C	-2.731659	3.929345	-2.985788
H	-1.132800	5.291553	-3.478593
H	-4.122297	2.429278	-2.280619
H	-3.414945	4.340530	-3.723527

^{2}TS5

E_{gas} optimization: -2843.05246685a.u.

E_{sol} single-point: -2843.63204615a.u.

G_{sol} thermo-corrected: -2842.94608215a.u.

C	-0.457048	2.407360	2.985517
C	-0.282841	3.019116	1.721159
C	-0.393193	4.417654	1.600356
C	-0.692452	5.222949	2.691951
H	-0.779405	6.298586	2.568621
C	-0.878580	4.627216	3.940167
H	-1.116909	5.234349	4.808972
C	-0.750443	3.250579	4.076280
C	-0.339586	0.934278	3.403951
O	-0.097596	0.727395	4.602869
N	-0.527803	-0.070751	2.507287
C	-0.677999	-1.364482	3.040727
C	-1.692655	-1.616642	3.985258
H	-2.290883	-0.777318	4.319939
C	-1.924358	-2.888990	4.485338
C	1.816083	2.559997	-0.254018
C	2.719997	3.028062	0.709702
C	2.278221	2.290745	-1.555806
C	4.064096	3.216751	0.378935
H	2.377027	3.235579	1.718385
C	3.616627	2.497872	-1.883596
H	1.588455	1.916381	-2.307299
C	4.515440	2.952489	-0.914417
H	4.757589	3.570004	1.136499
H	3.964463	2.285589	-2.889821
H	5.562131	3.091074	-1.167114
Cu	-0.414832	-0.131687	0.509547
Br	-0.405563	-0.741514	-2.422057
C	3.604768	-0.666647	0.195681
H	3.189159	0.325473	0.009451
H	3.866698	-0.710214	1.258989
C	4.825987	-0.894635	-0.664074
C	4.753872	-0.719267	-2.054976

C	6.041435	-1.311192	-0.108136
C	5.865319	-0.949042	-2.864301
H	3.819665	-0.388412	-2.500371
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H	6.114734	-1.448710	0.968065
C	7.074350	-1.360854	-2.295858
H	5.790091	-0.805563	-3.938796
H	8.094290	-1.859923	-0.463235
H	7.941526	-1.539034	-2.925229
Si	-2.338132	-2.033578	-2.139289
H	-2.527527	-2.414650	-3.563662
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C	-2.053822	-3.656669	-1.150166
C	-0.553582	-3.990792	-1.061553
C	-2.662542	-3.628283	0.266589
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H	-0.090573	-4.077091	-2.051338
H	-0.019040	-3.220831	-0.504453
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H	-2.166481	-2.895124	0.905798
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C	-3.831093	-0.979132	-1.724600
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H	-4.415853	-0.922022	-3.808226
C	-5.347344	0.194529	-0.218725
H	-3.554335	-0.808784	0.410779
C	-6.163767	0.549650	-1.296615
H	-6.453552	0.413028	-3.430363
H	-5.605600	0.511435	0.787693
H	-7.059952	1.140760	-1.129568

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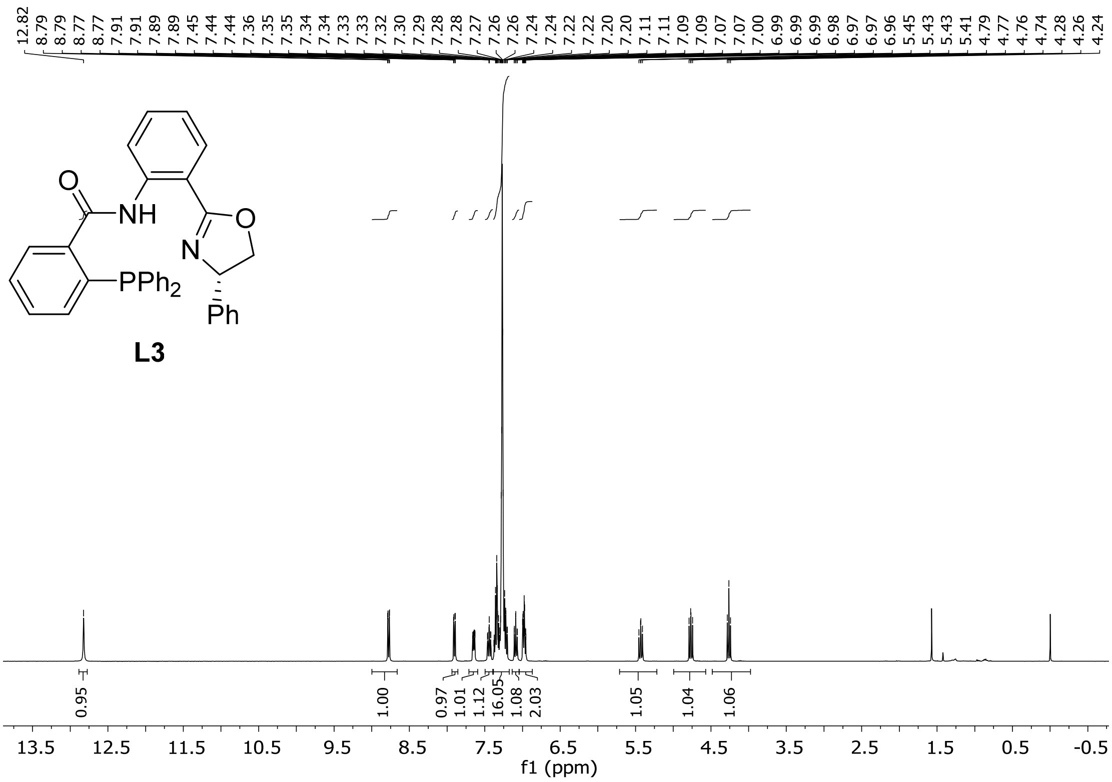
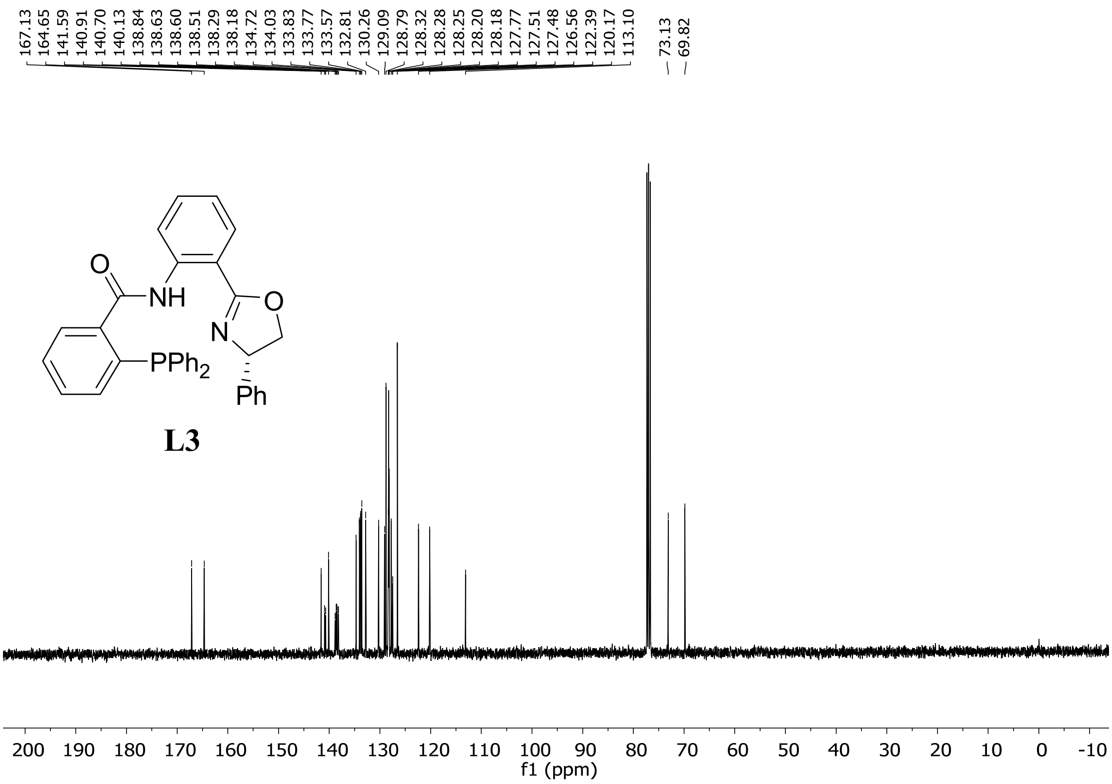
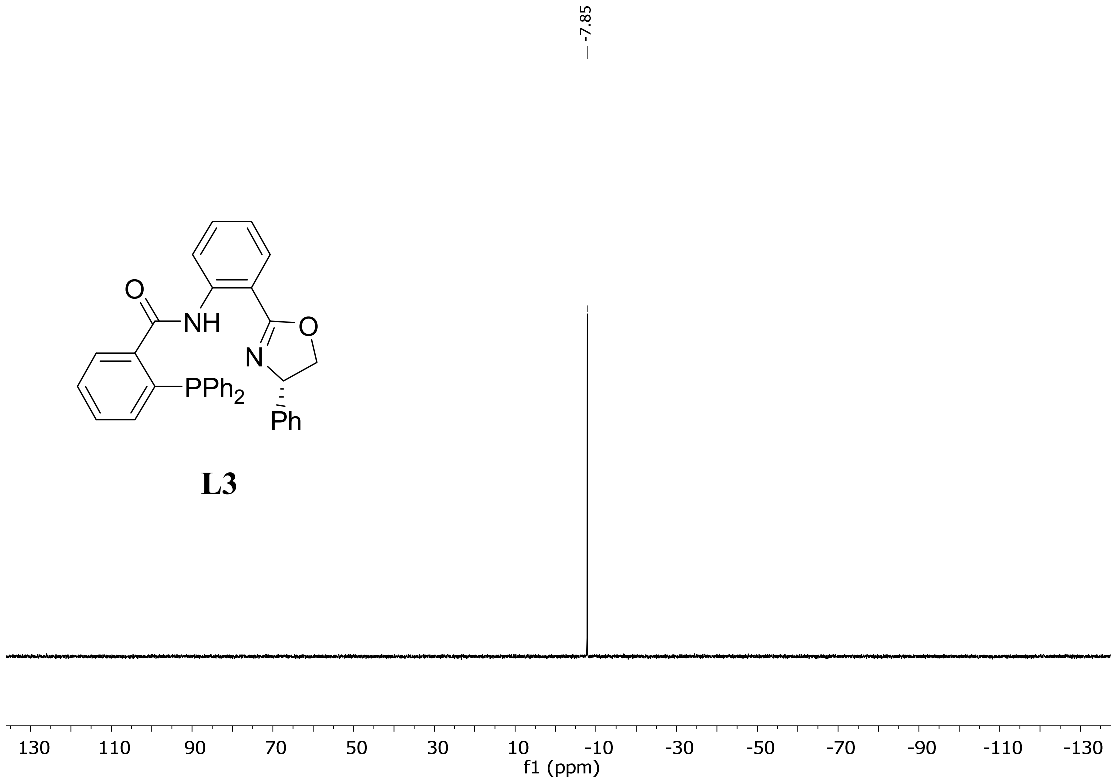
10. NMR Spectra



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Ph
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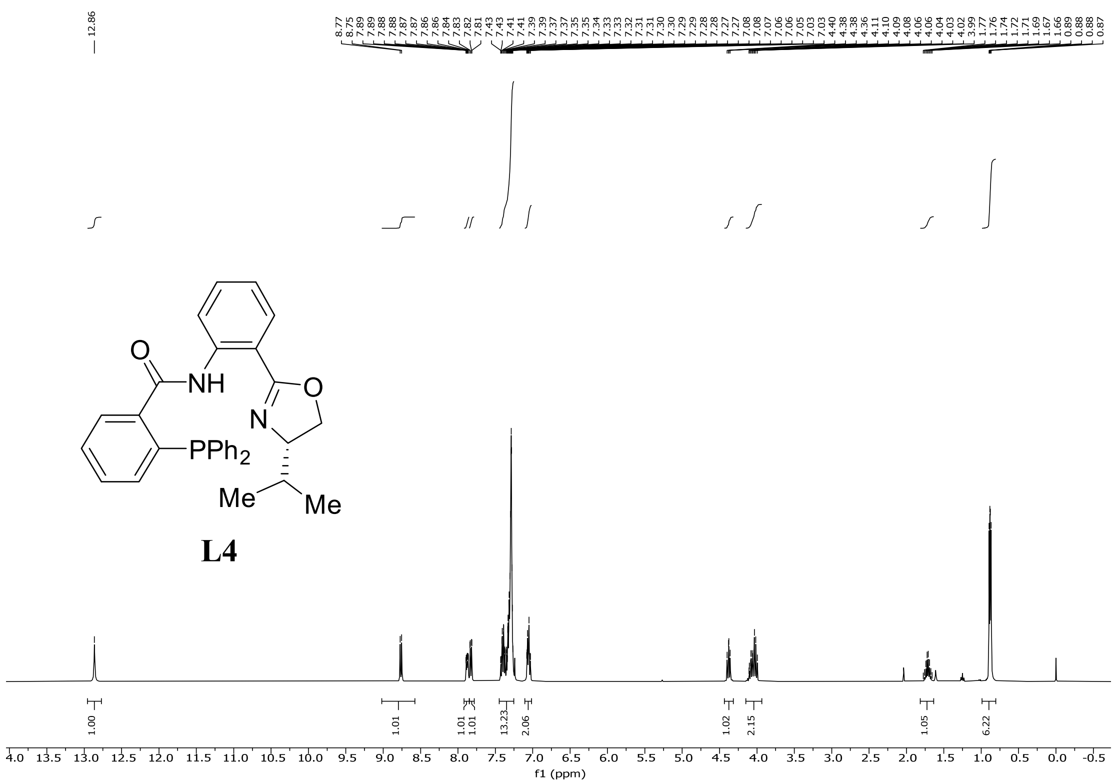
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Me
Me
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14.0 13.5 13.0 12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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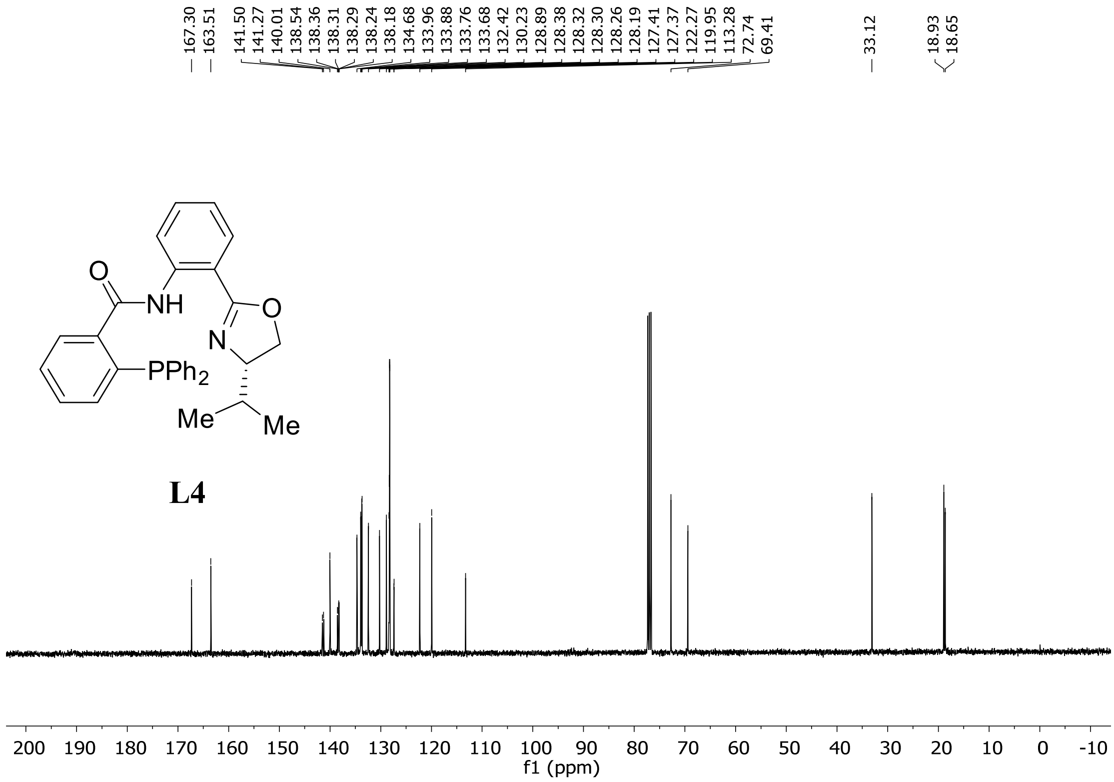
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138.24
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133.96
133.88
133.76
133.68
132.42
130.23
128.89
128.38
128.32
128.30
128.26
128.19
127.41
127.37
122.27
119.95
113.28
72.74
69.41
33.12
18.93
18.65
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O
N
PPh2
Me
Me
L4
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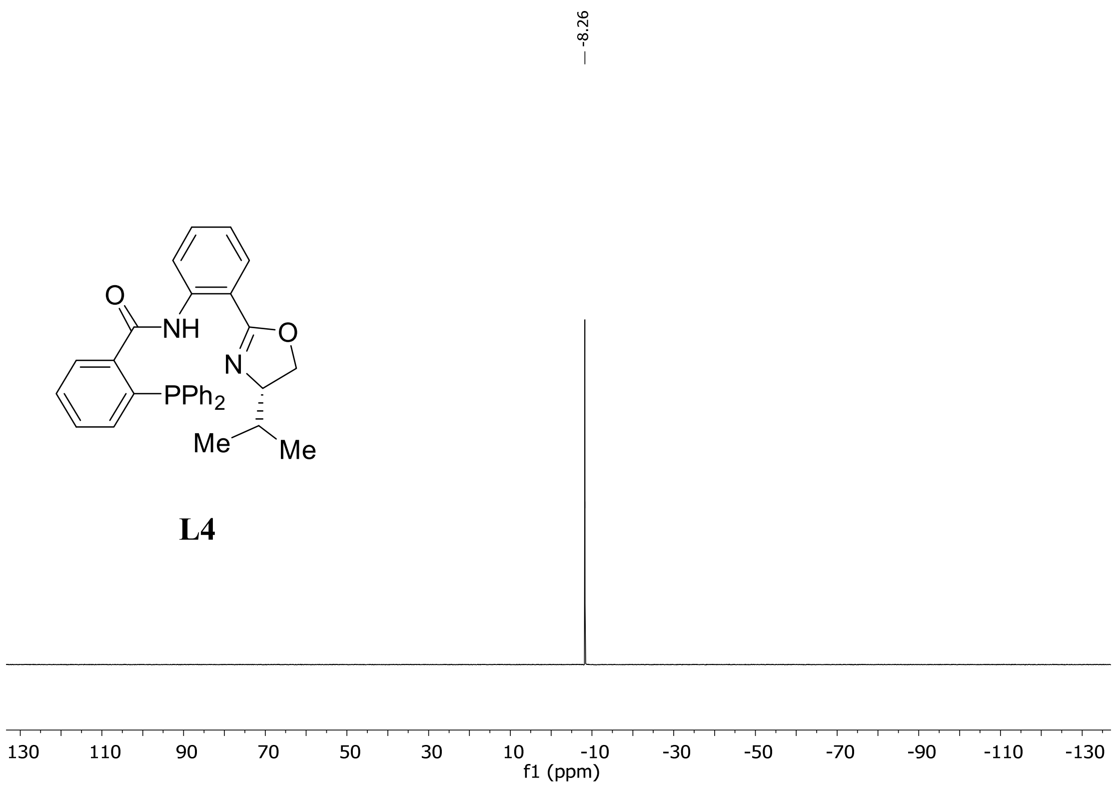
f1 (ppm)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Me
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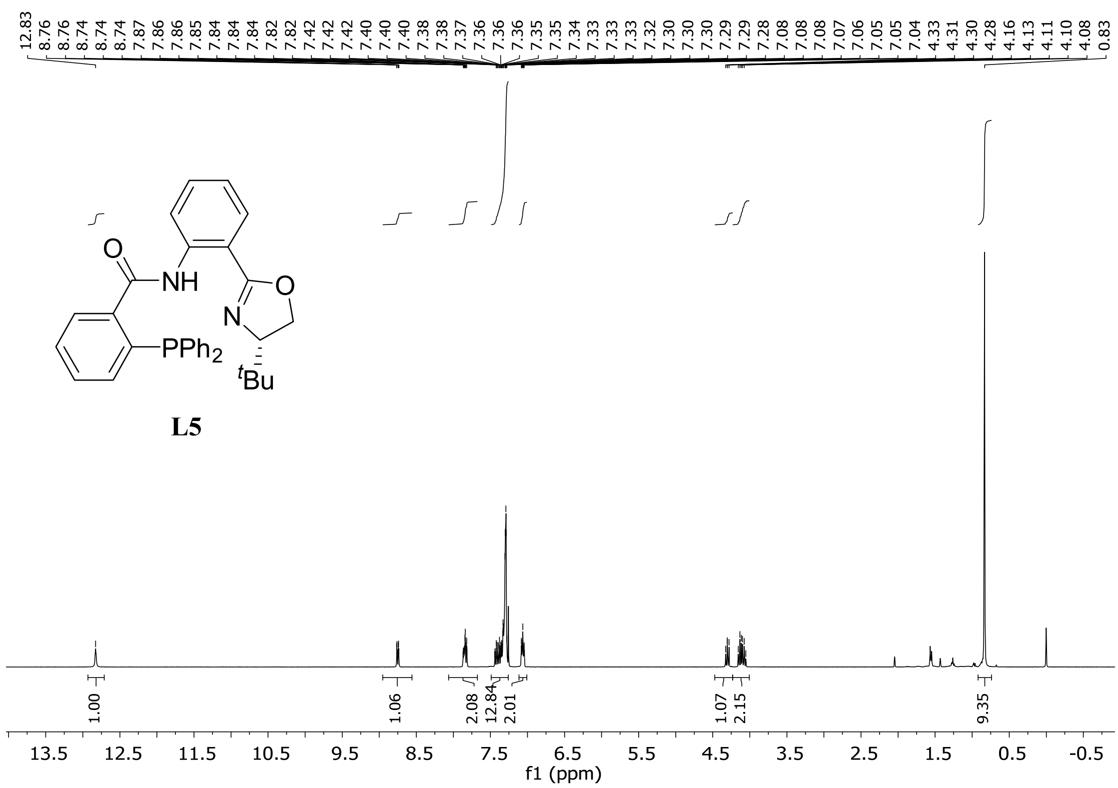
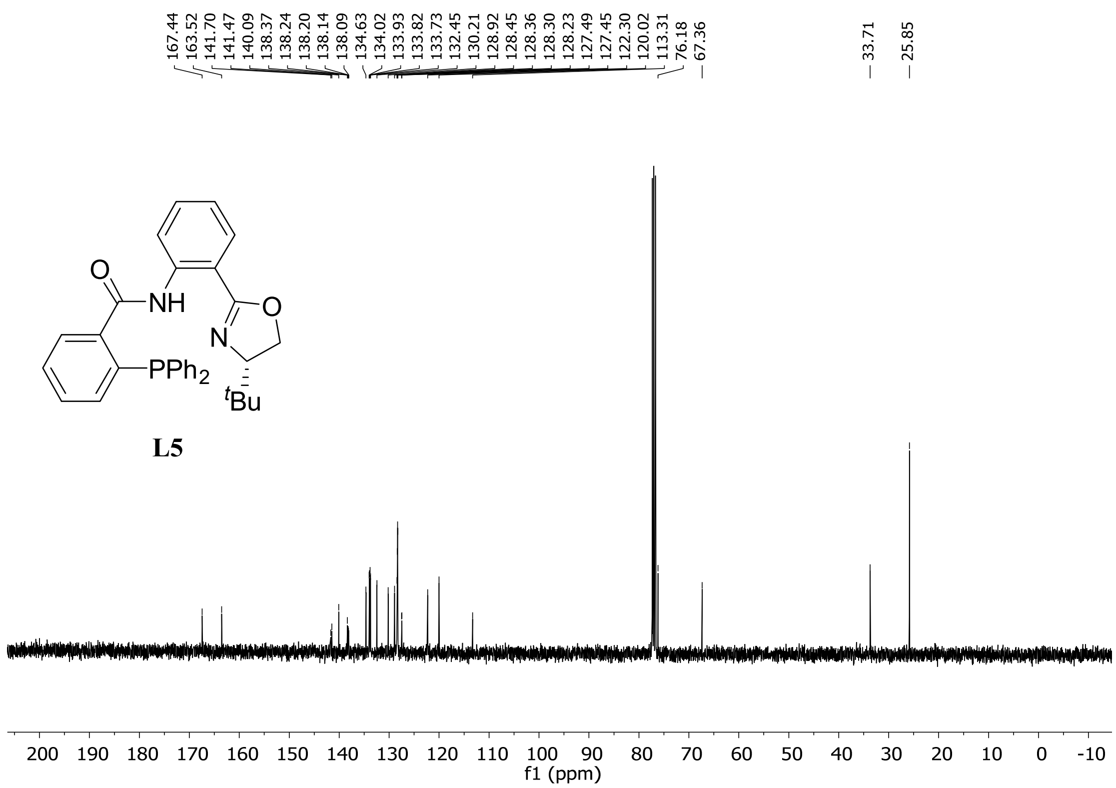


L5



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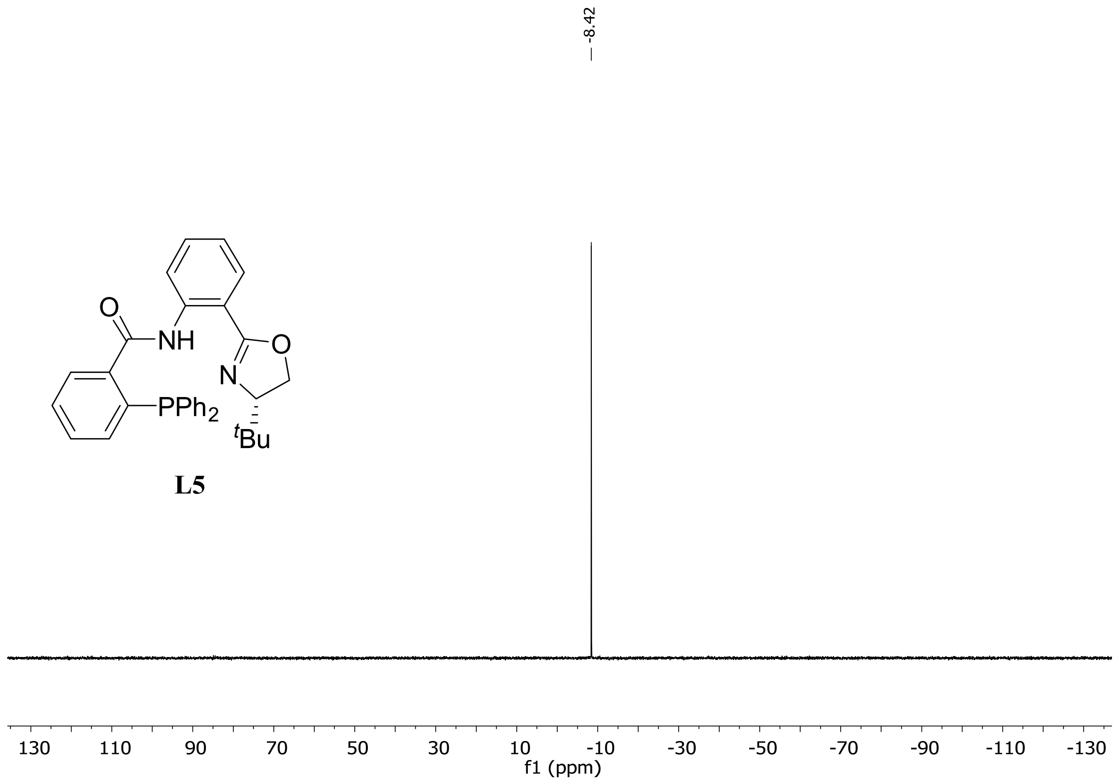

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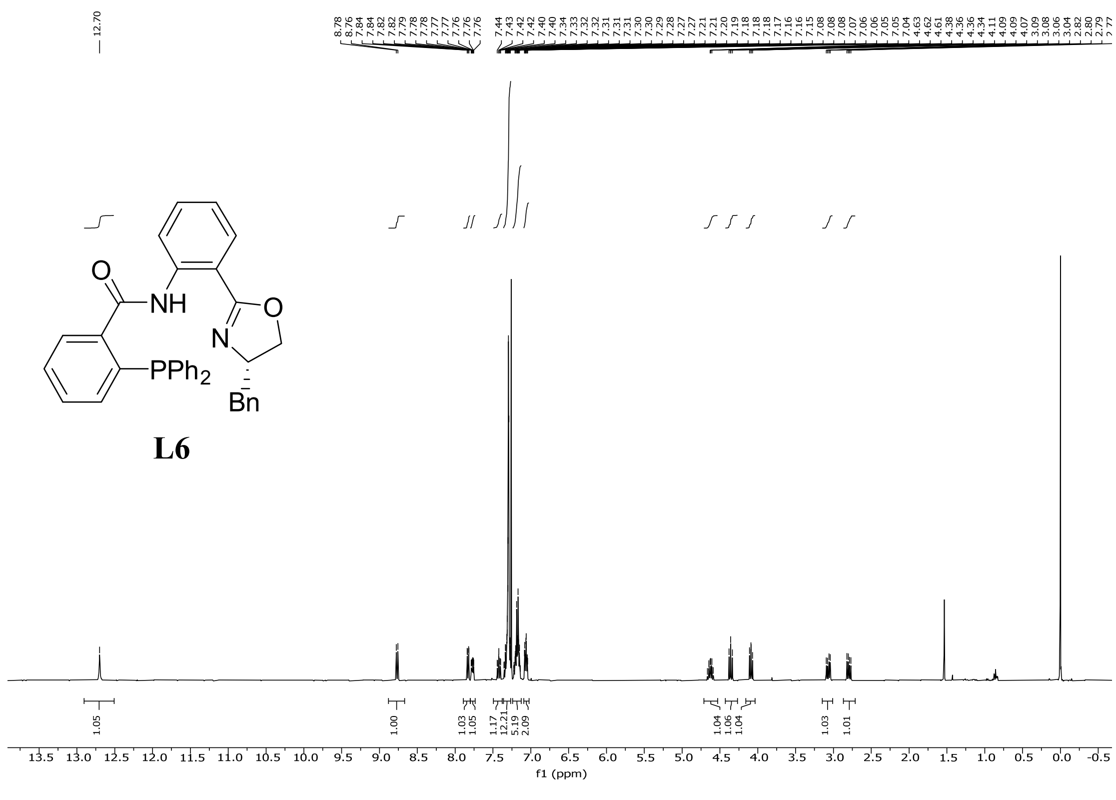

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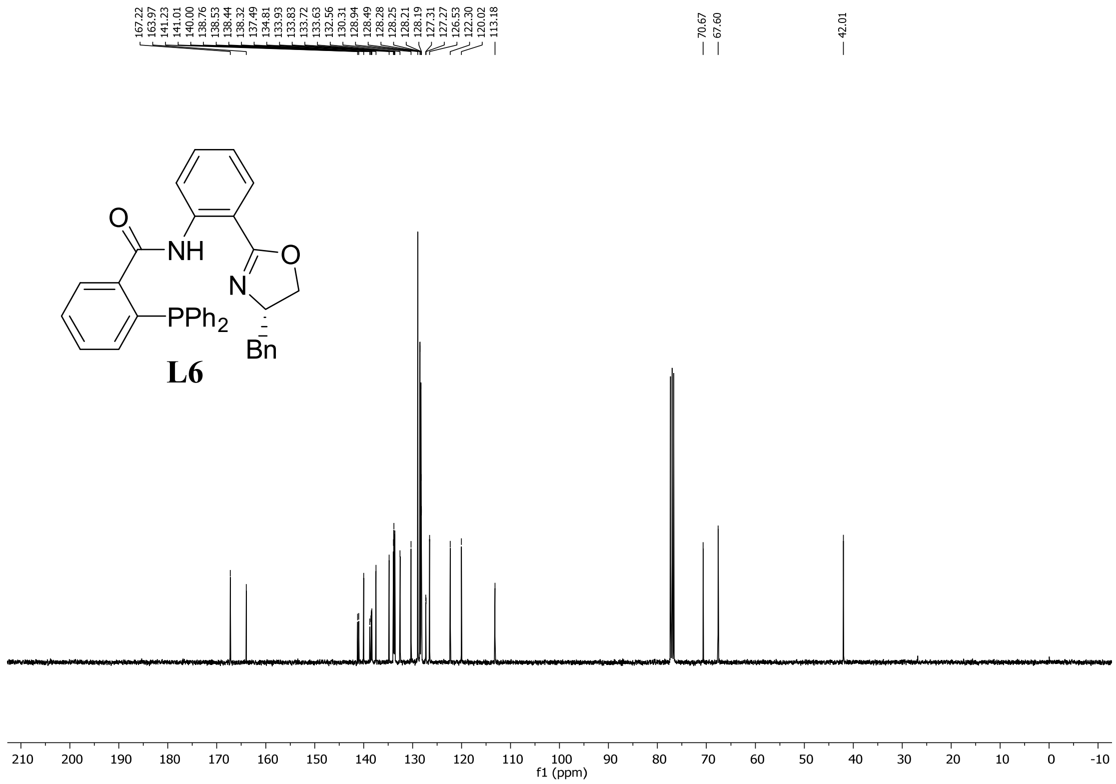
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133.63
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128.49
128.28
128.25
128.21
128.19
127.31
127.27
126.53
122.30
120.02
113.18
70.67
67.60
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O
N
PPh2
Bn
L6
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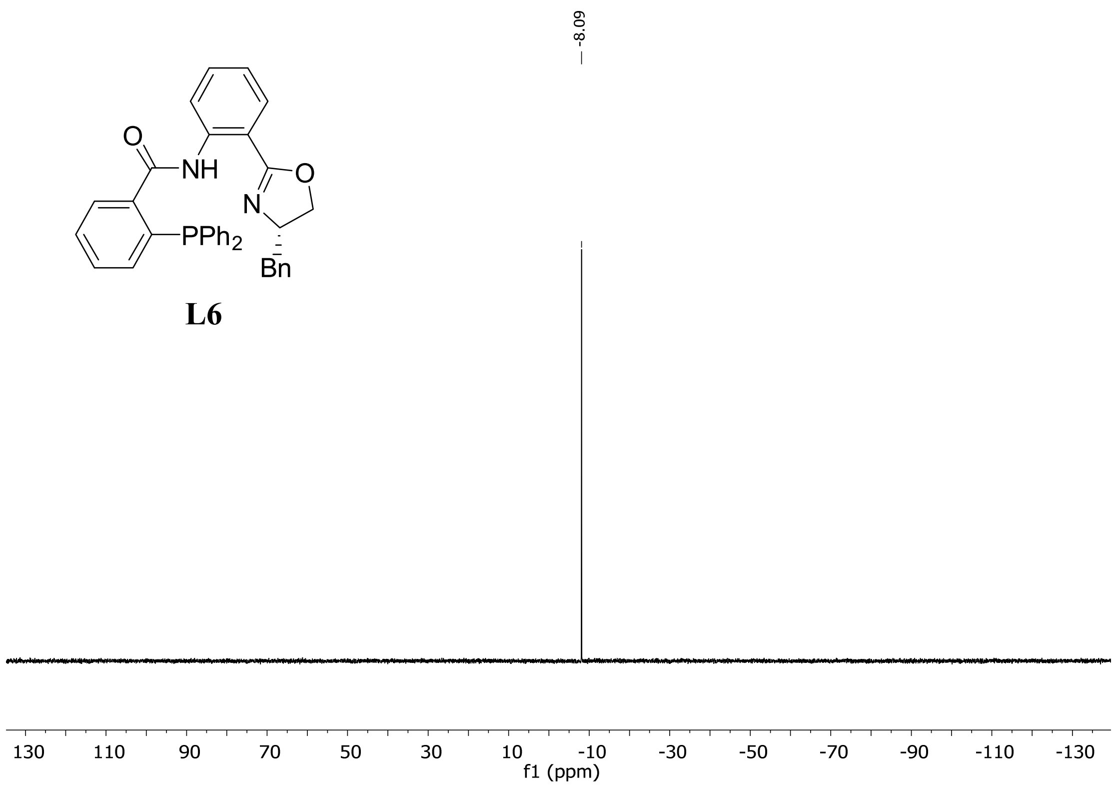
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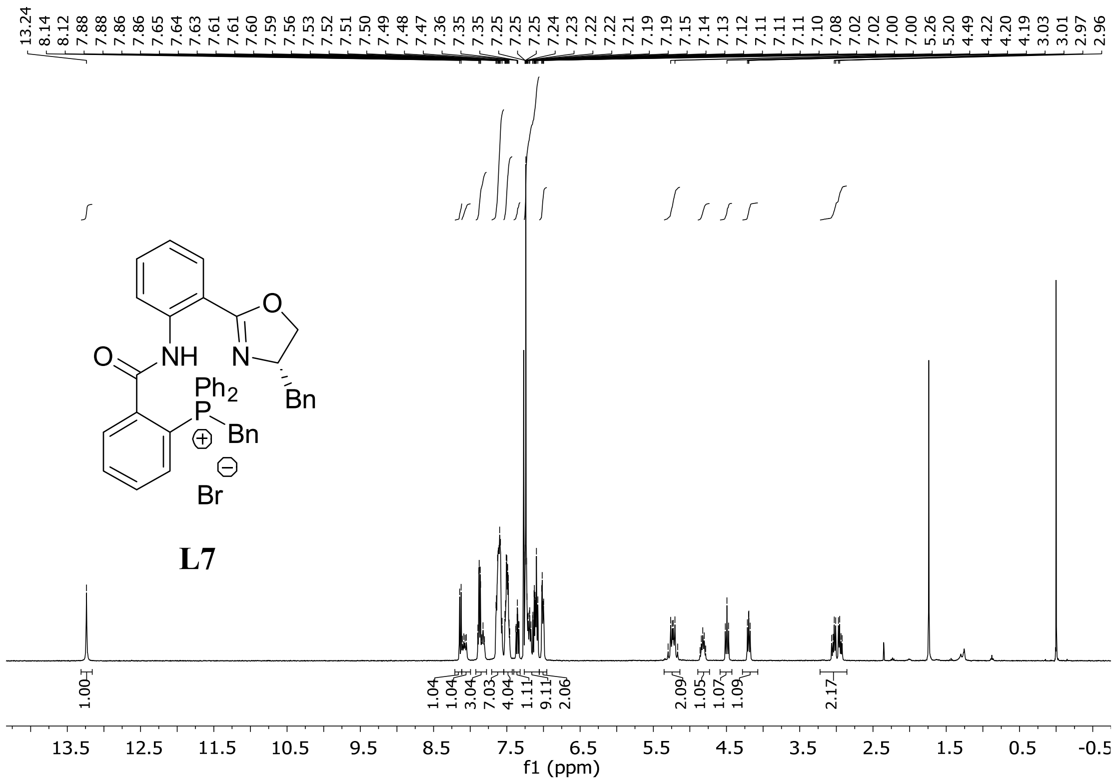

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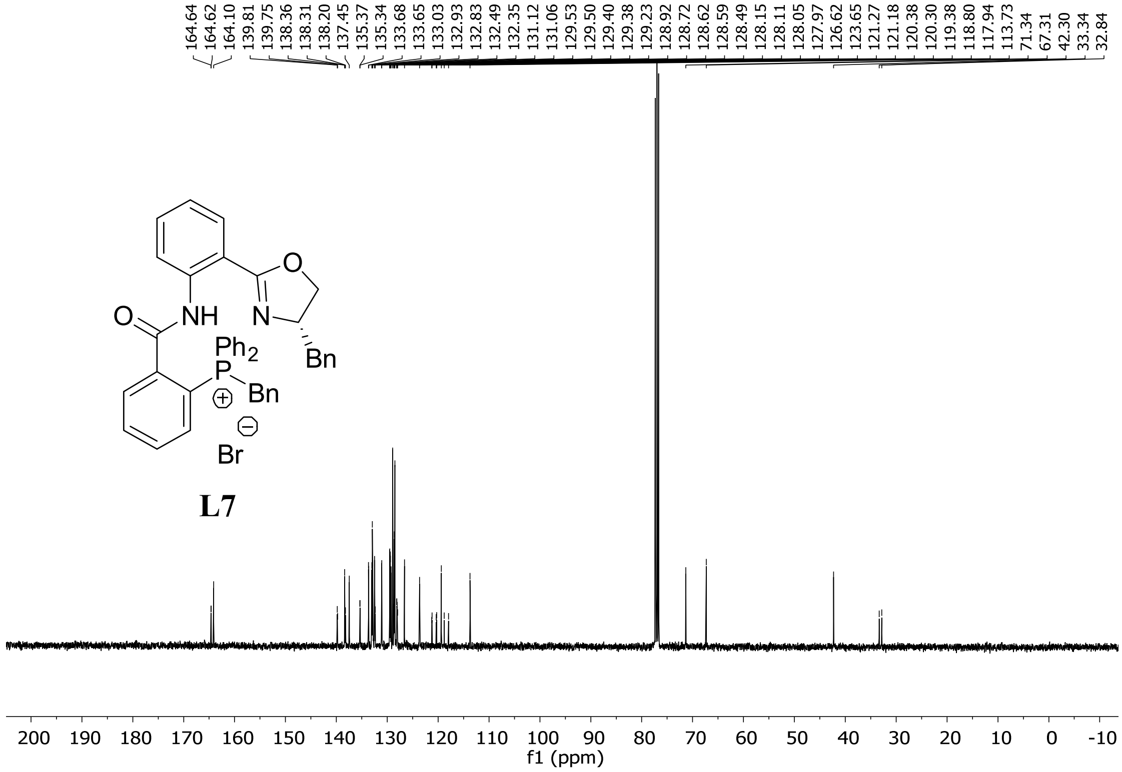

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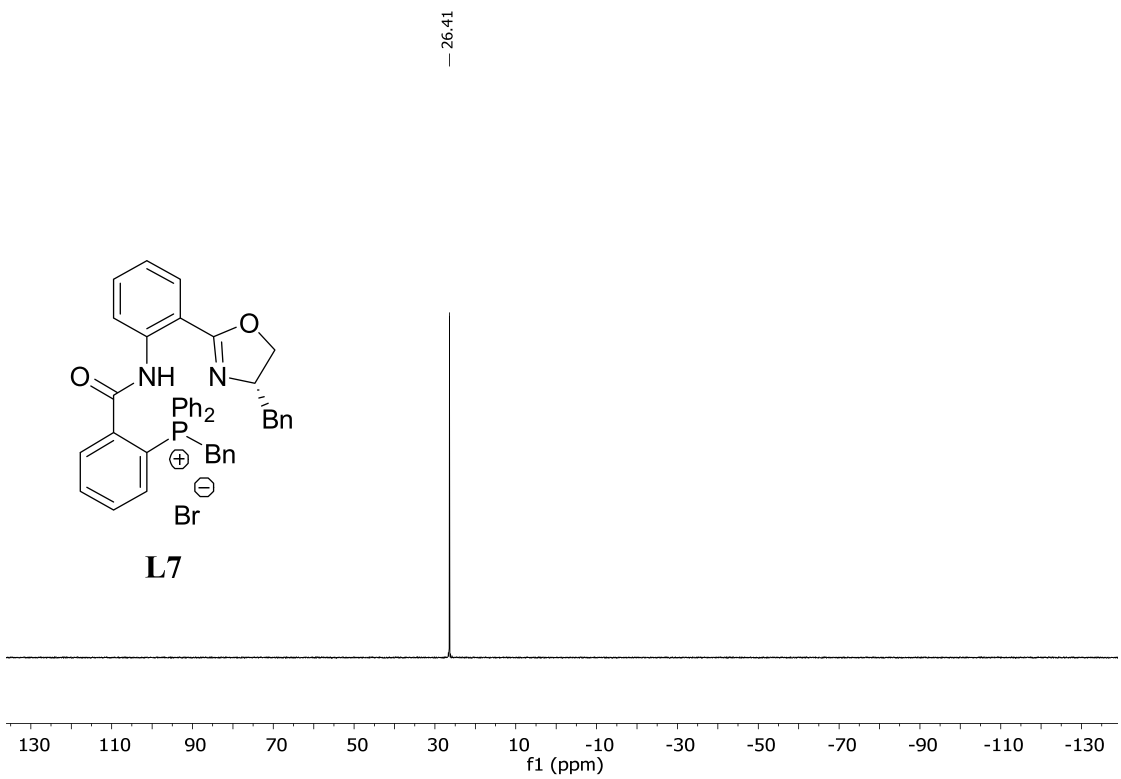
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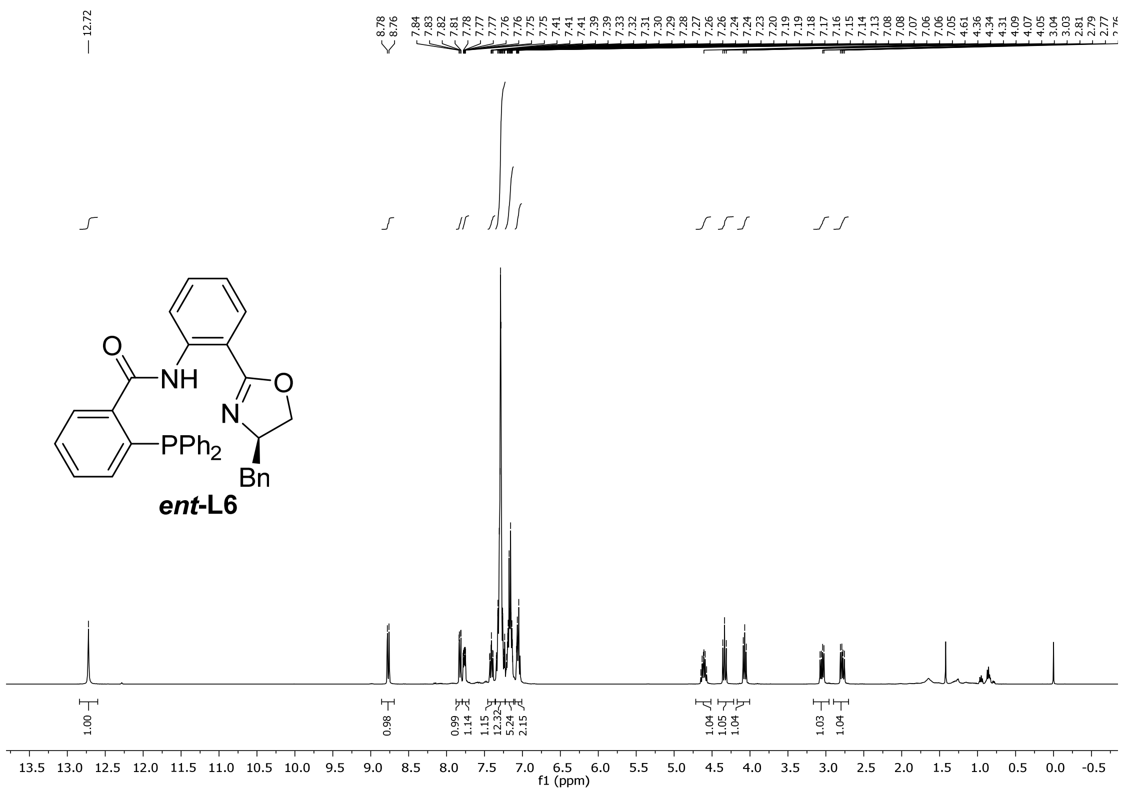
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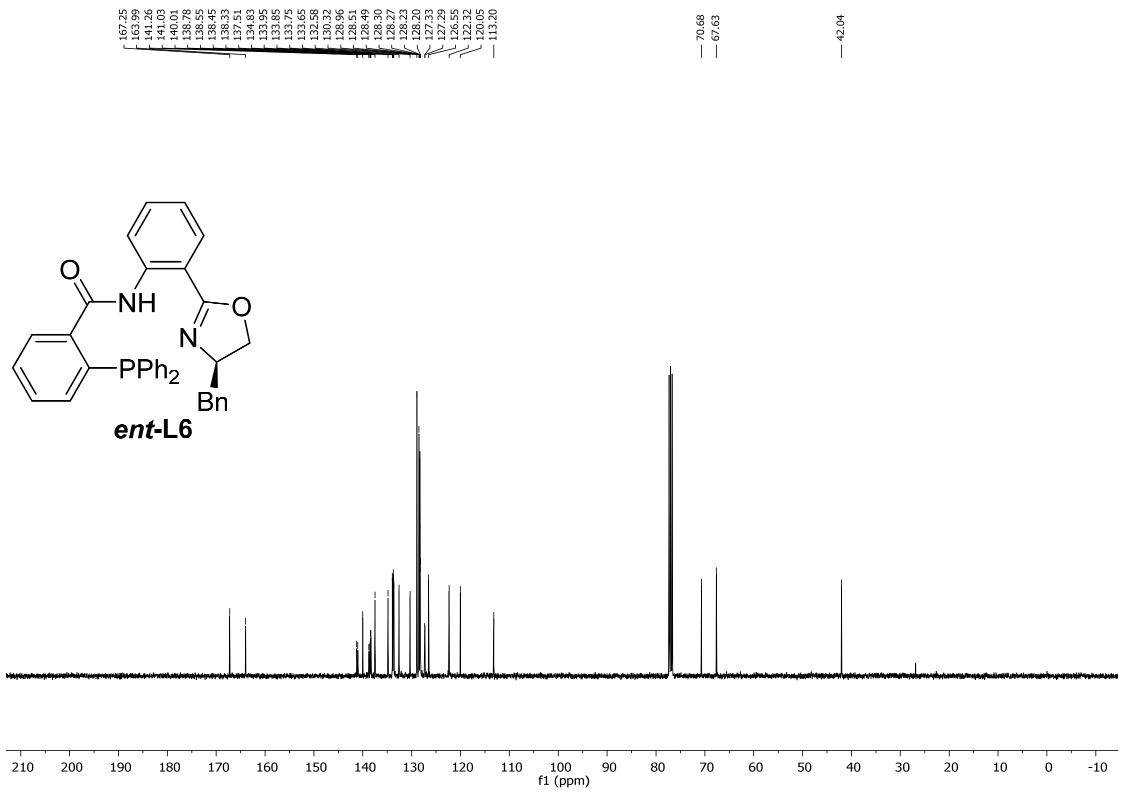
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127.33
127.29
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122.32
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O
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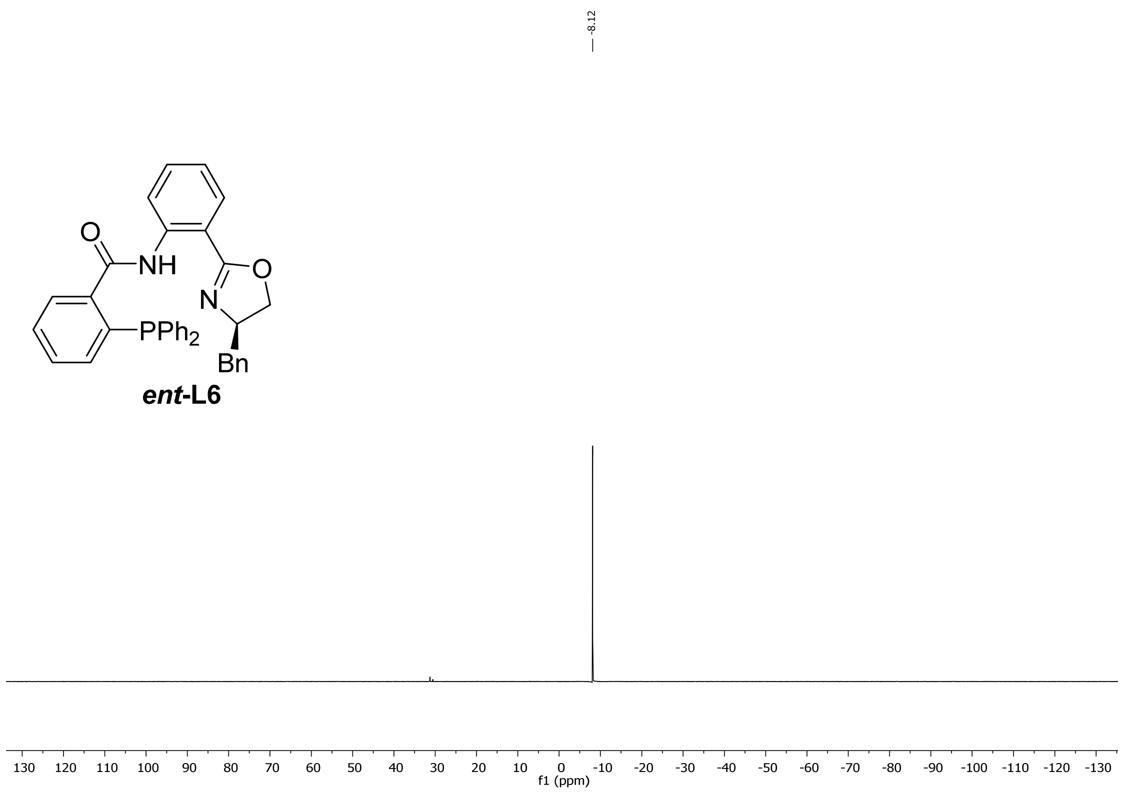
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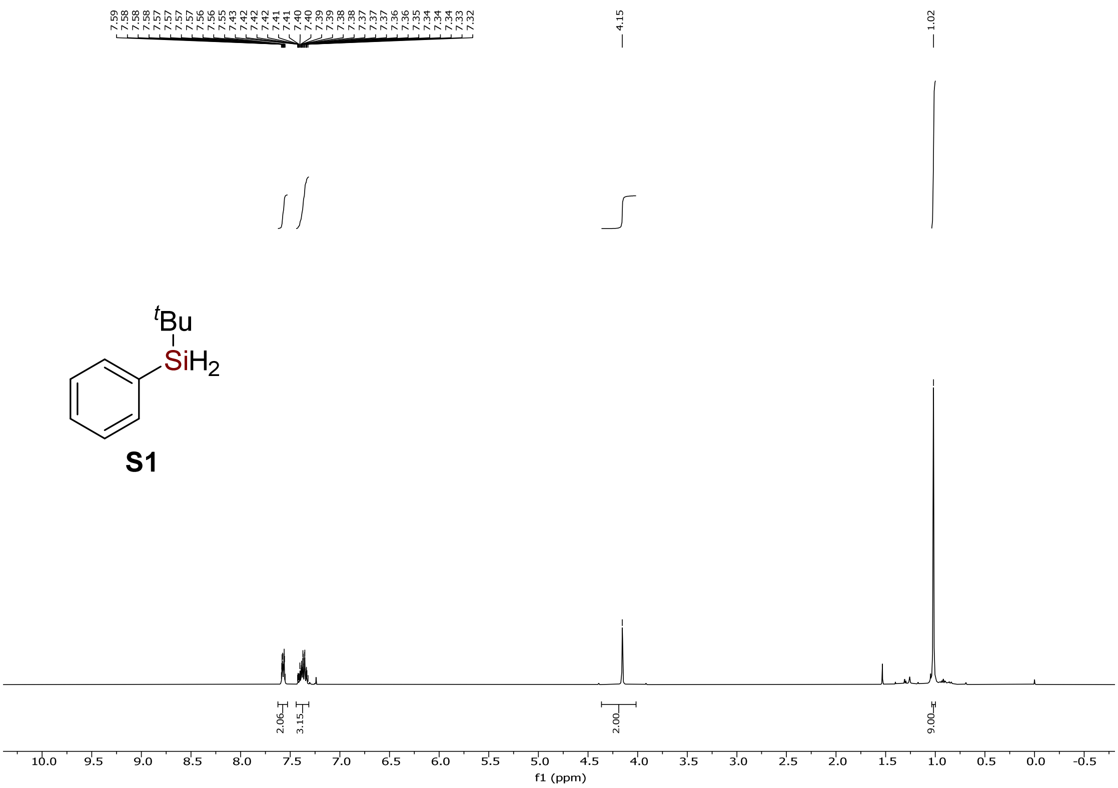
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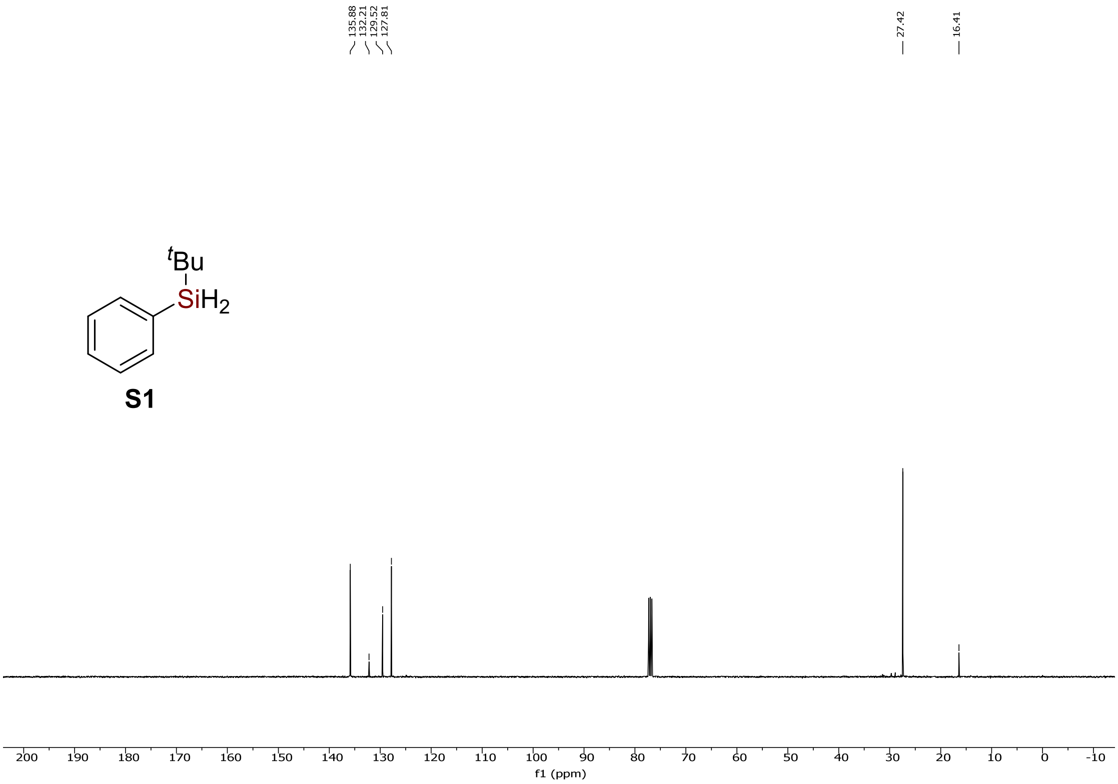
4.15
1.02
tBu
SiH2
S1
2.06
3.15
2.00
9.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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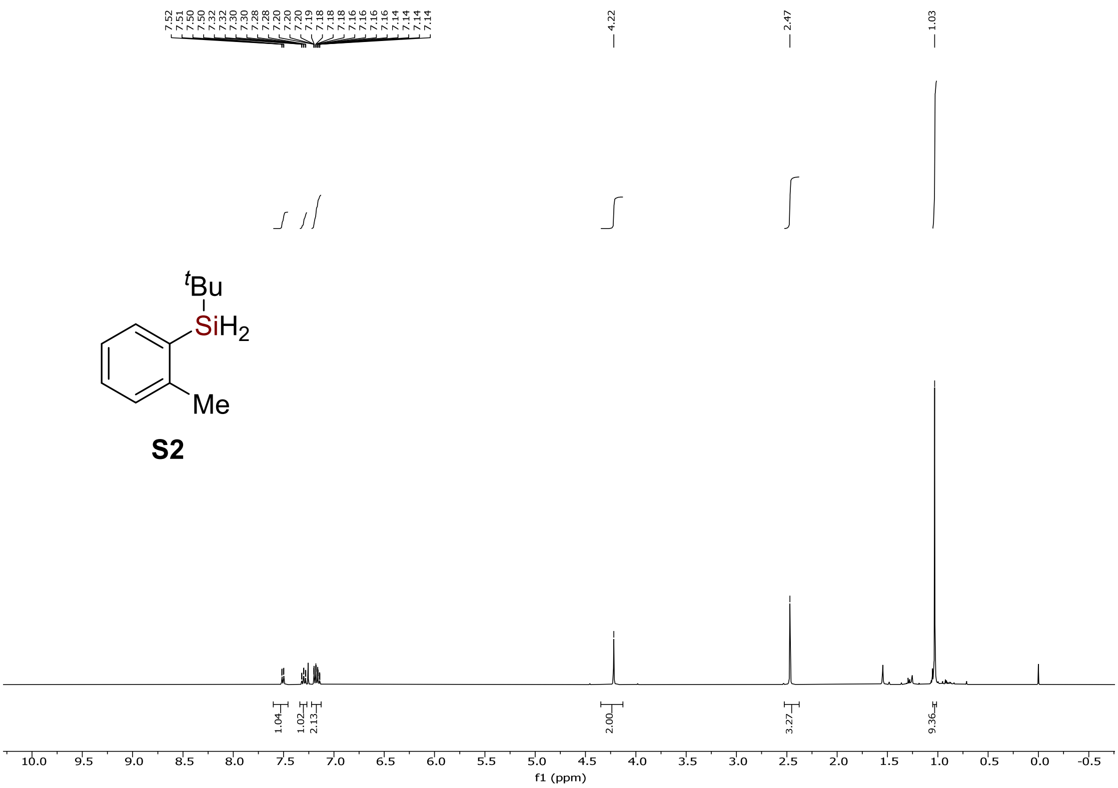
f1 (ppm)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7.18
7.18
7.16
7.16
7.16
7.14
7.14
7.14
7.14
4.22
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Me
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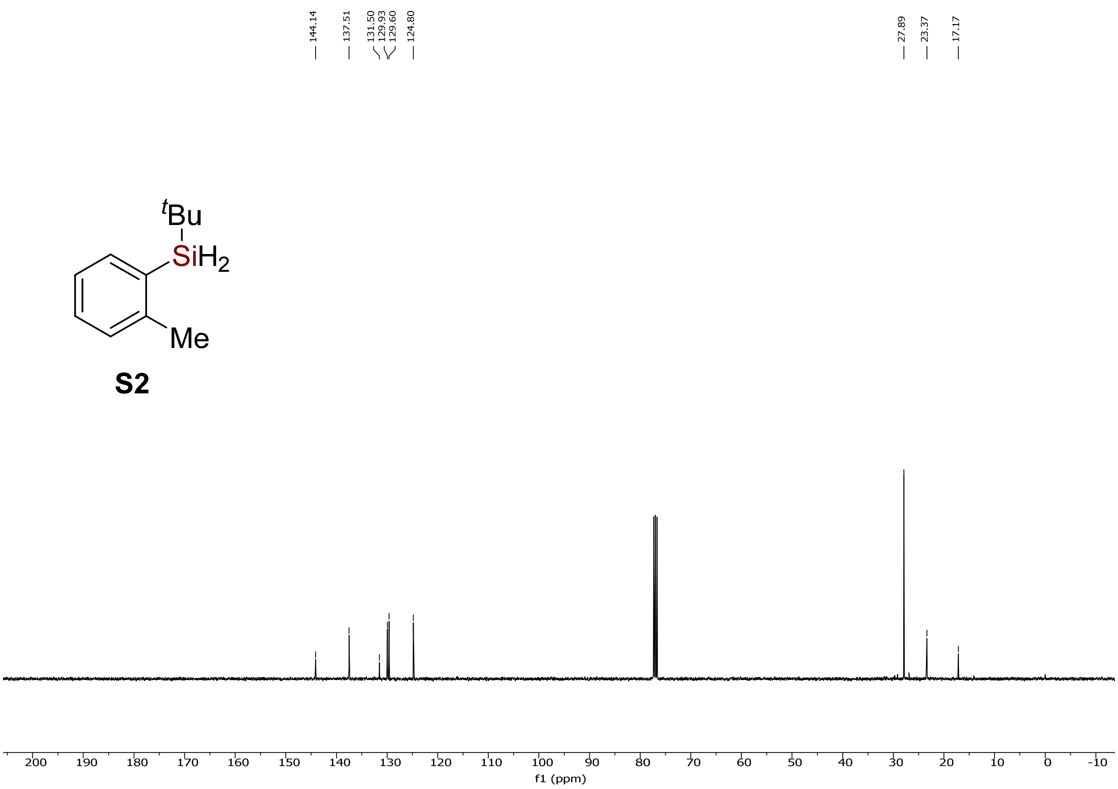
f1 (ppm)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S2
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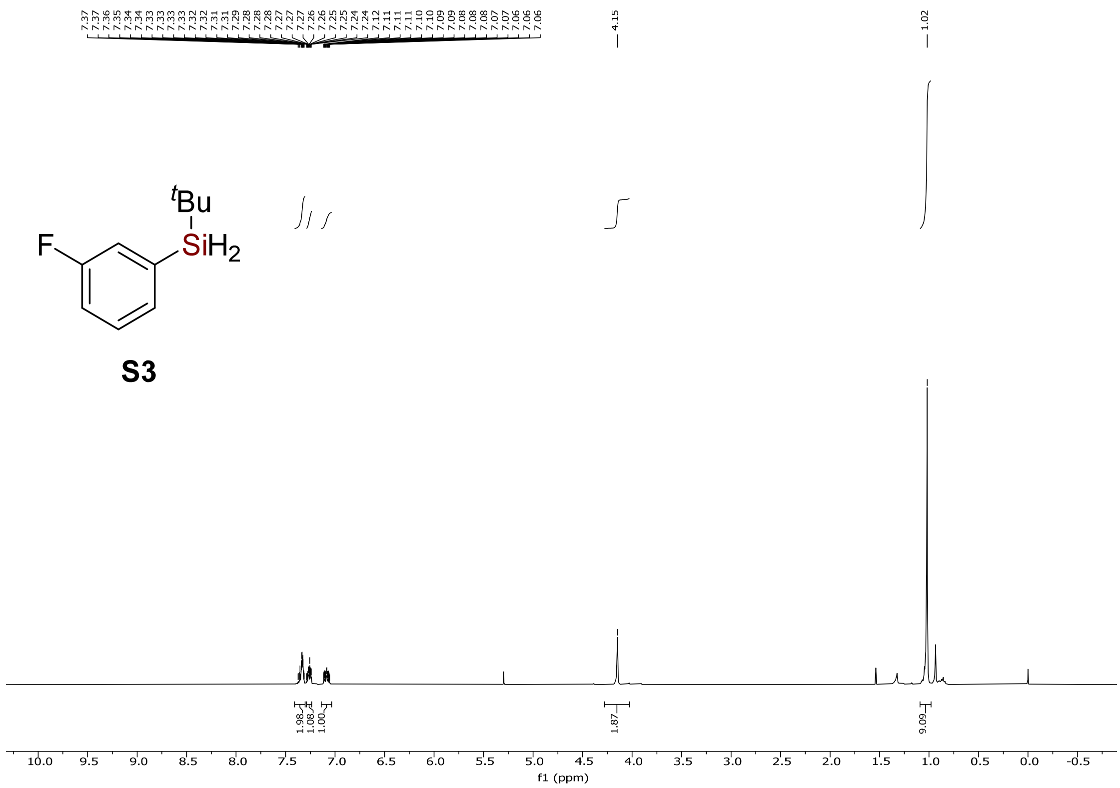

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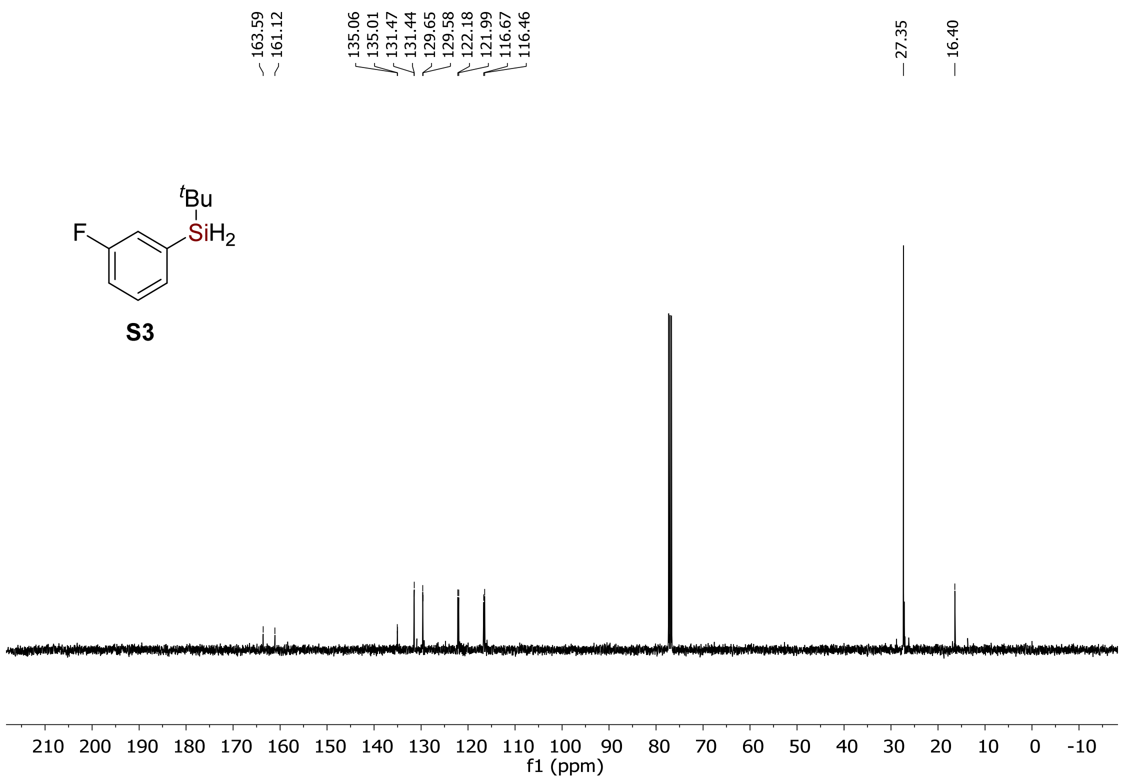

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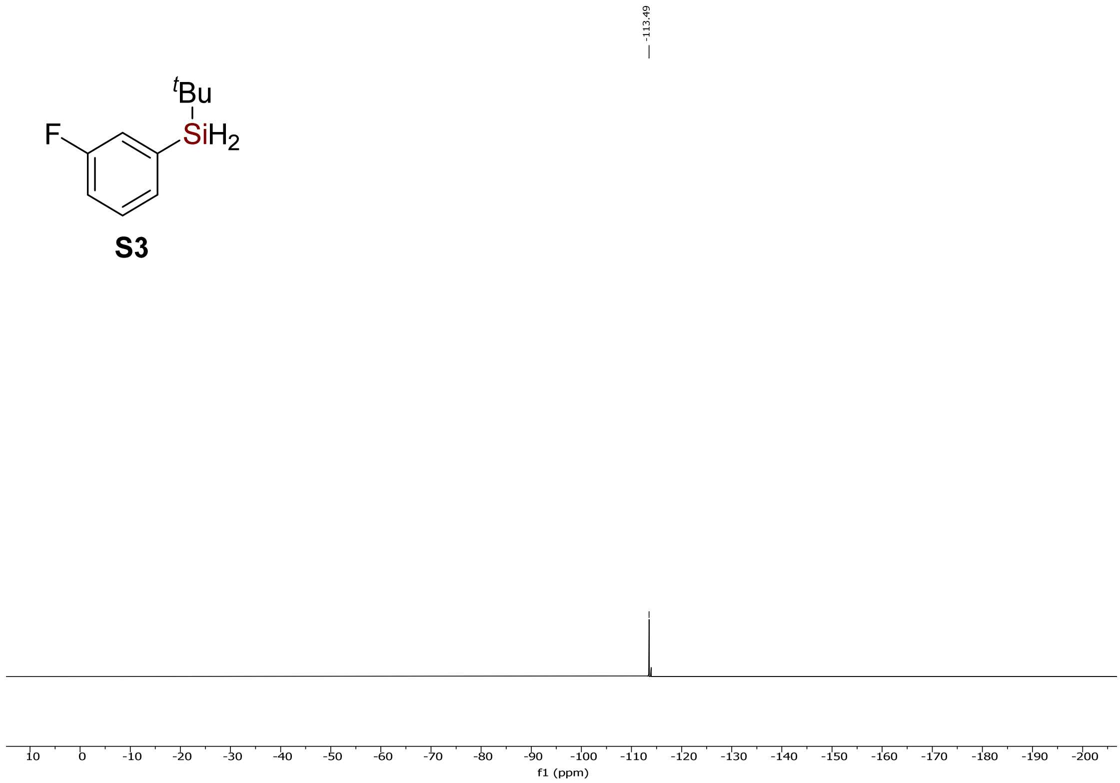
F
S3
f1 (ppm)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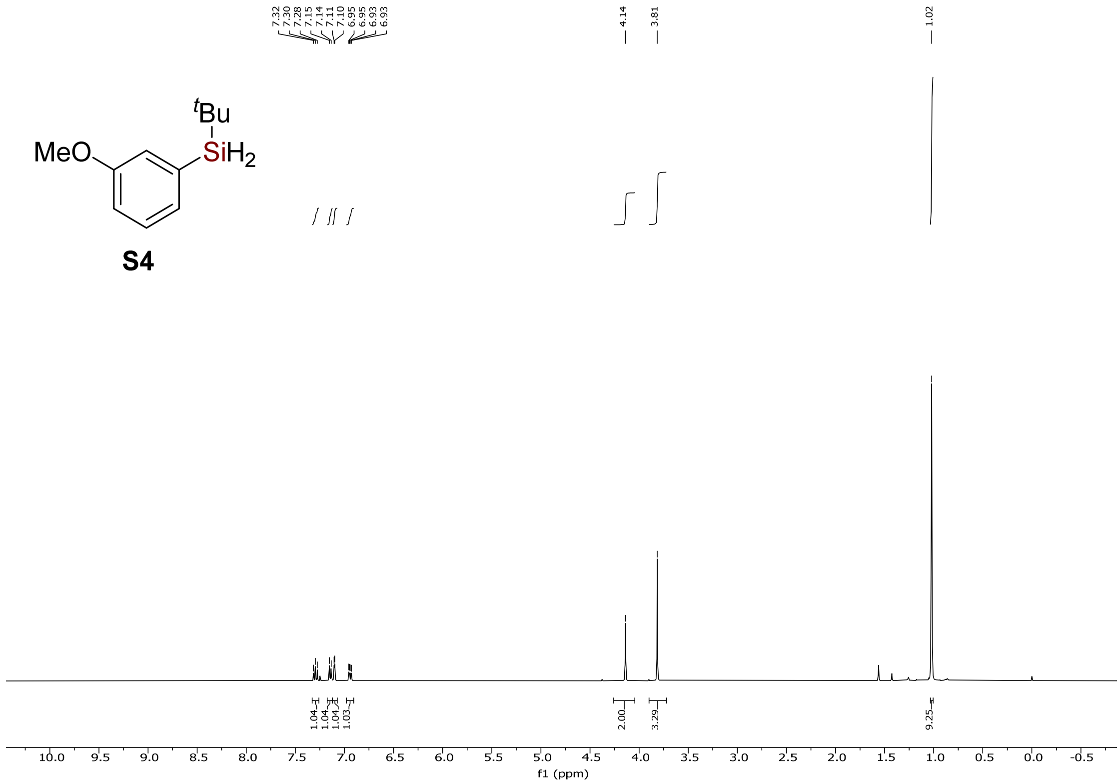
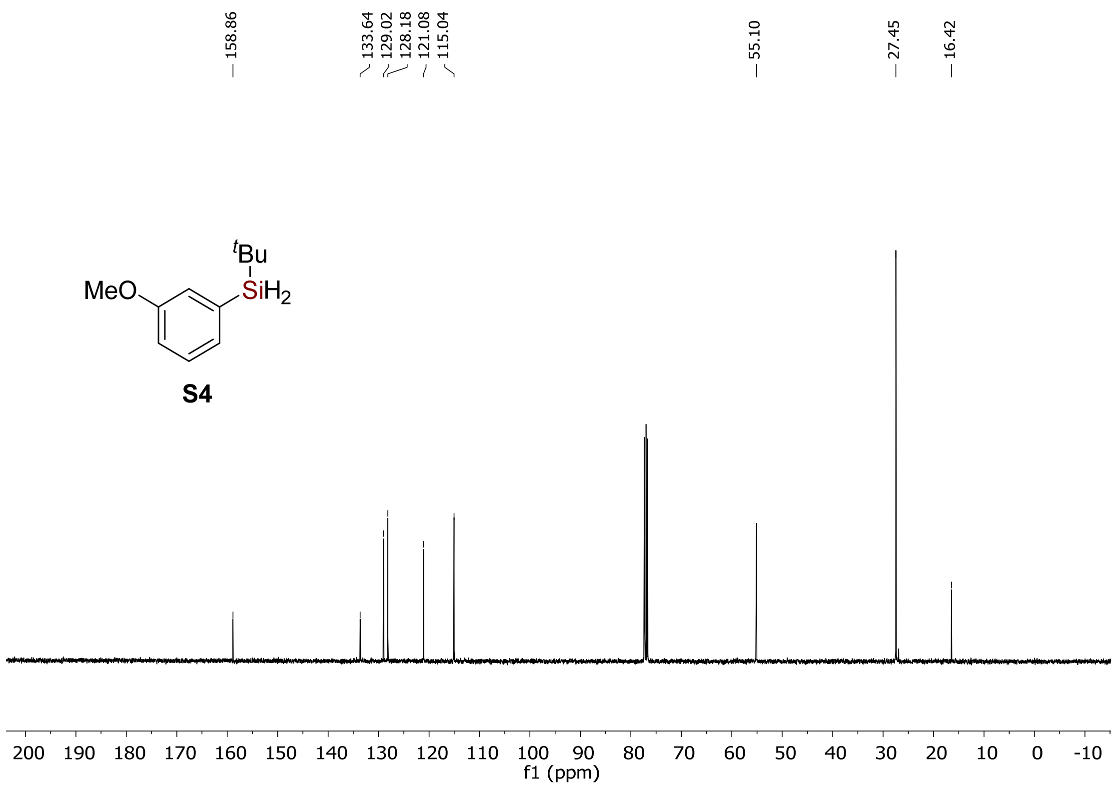
f1 (ppm)

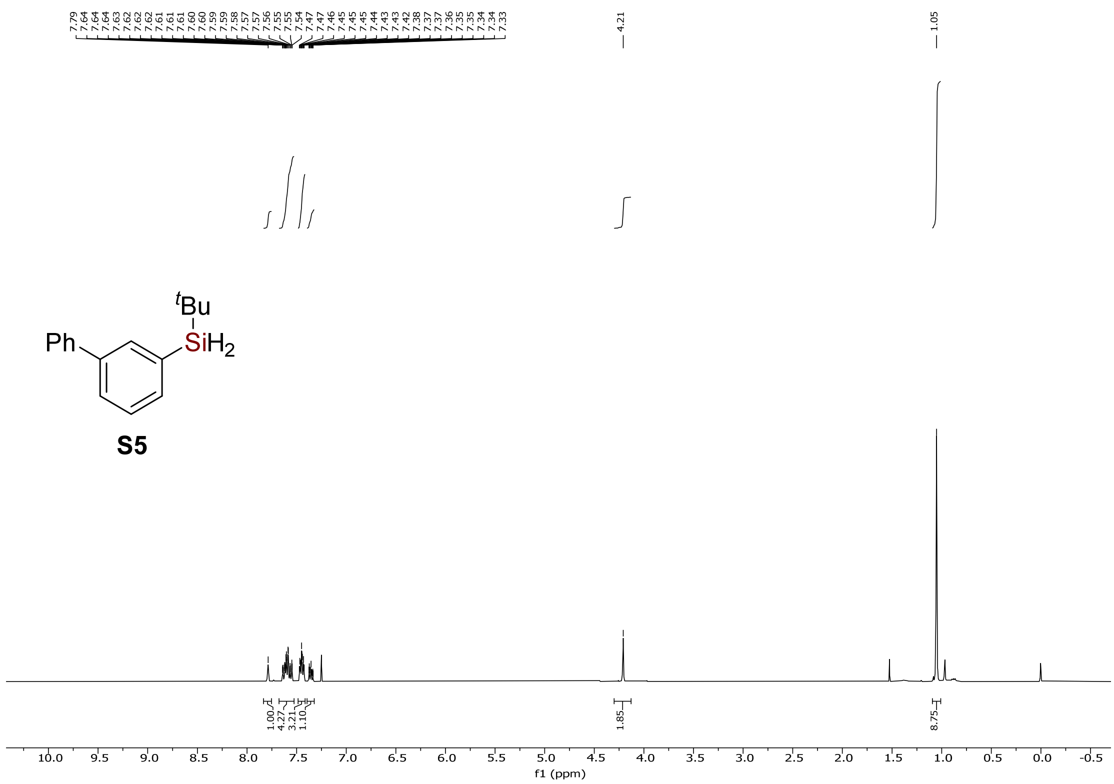
S3


7.32
7.30
7.28
7.15
7.14
7.11
7.10
6.95
6.95
6.93
6.93
4.14
3.81
1.02
MeO
tBu
SiH2
1.04
1.04
1.04
1.03
2.00
3.29
9.25
f1 (ppm)

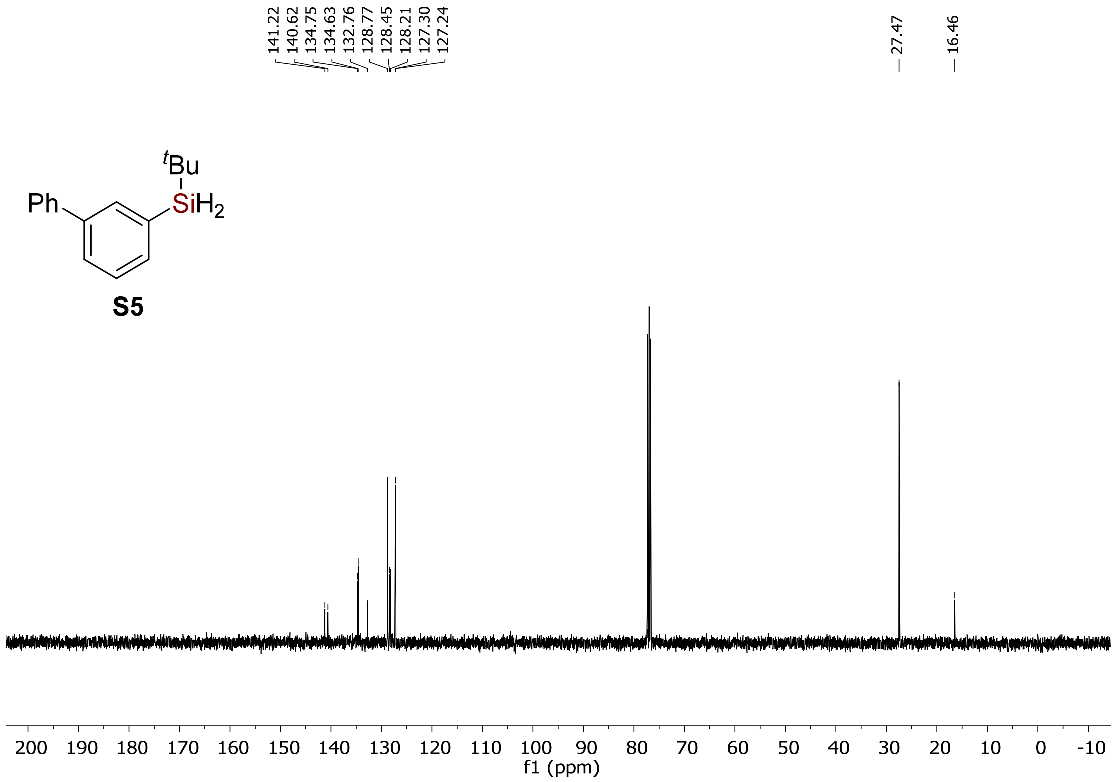
S4

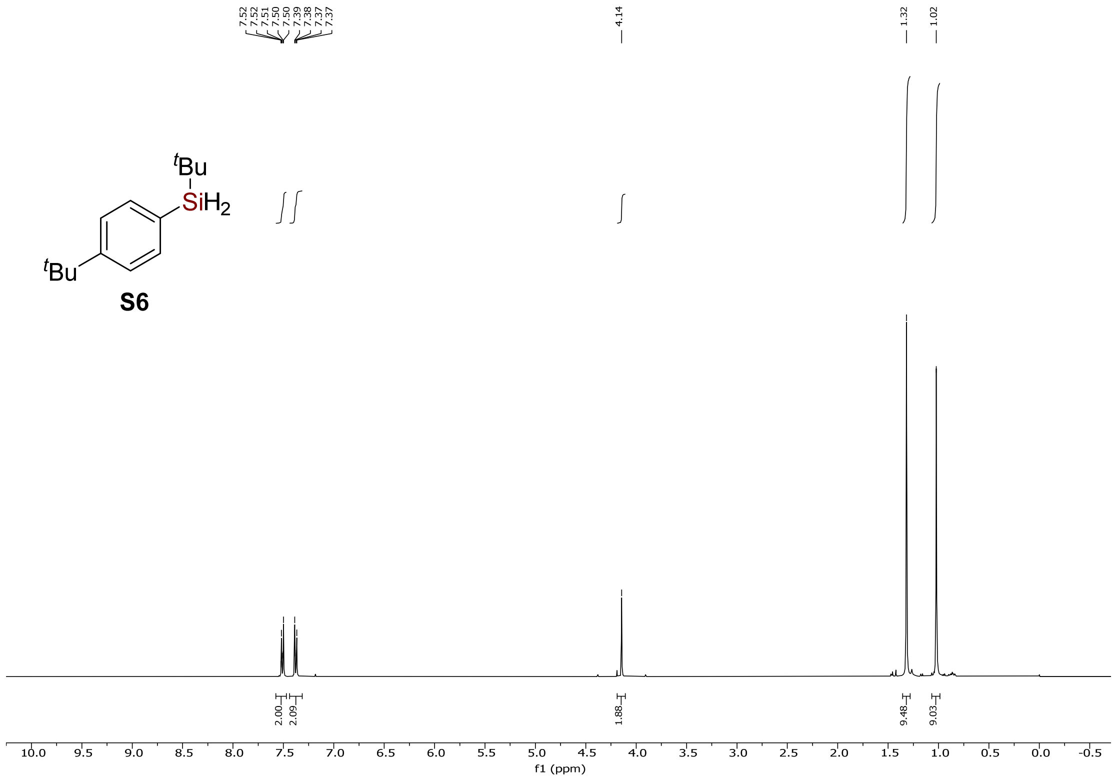


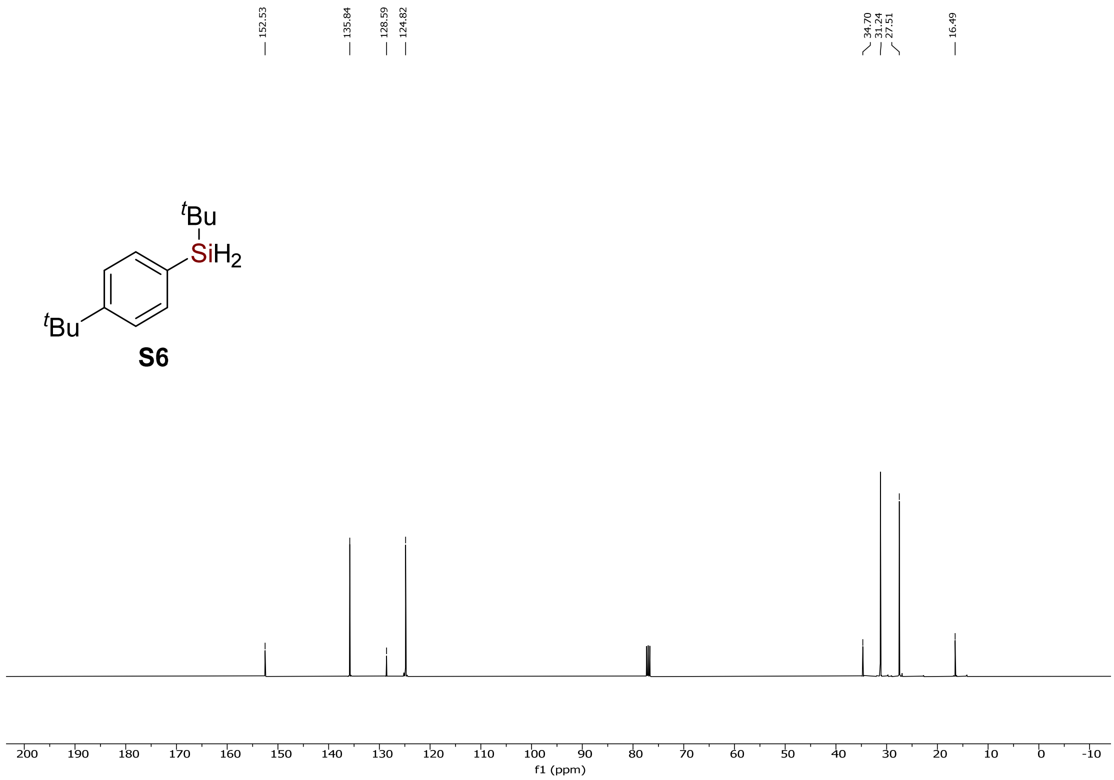
S4

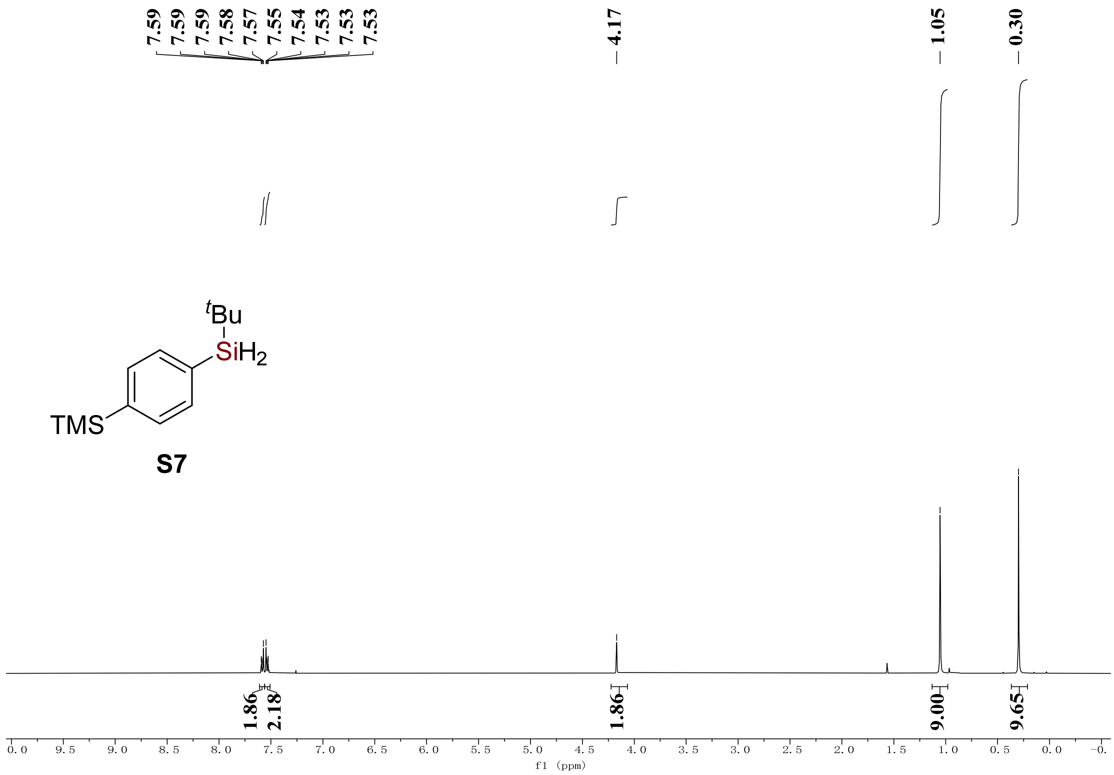


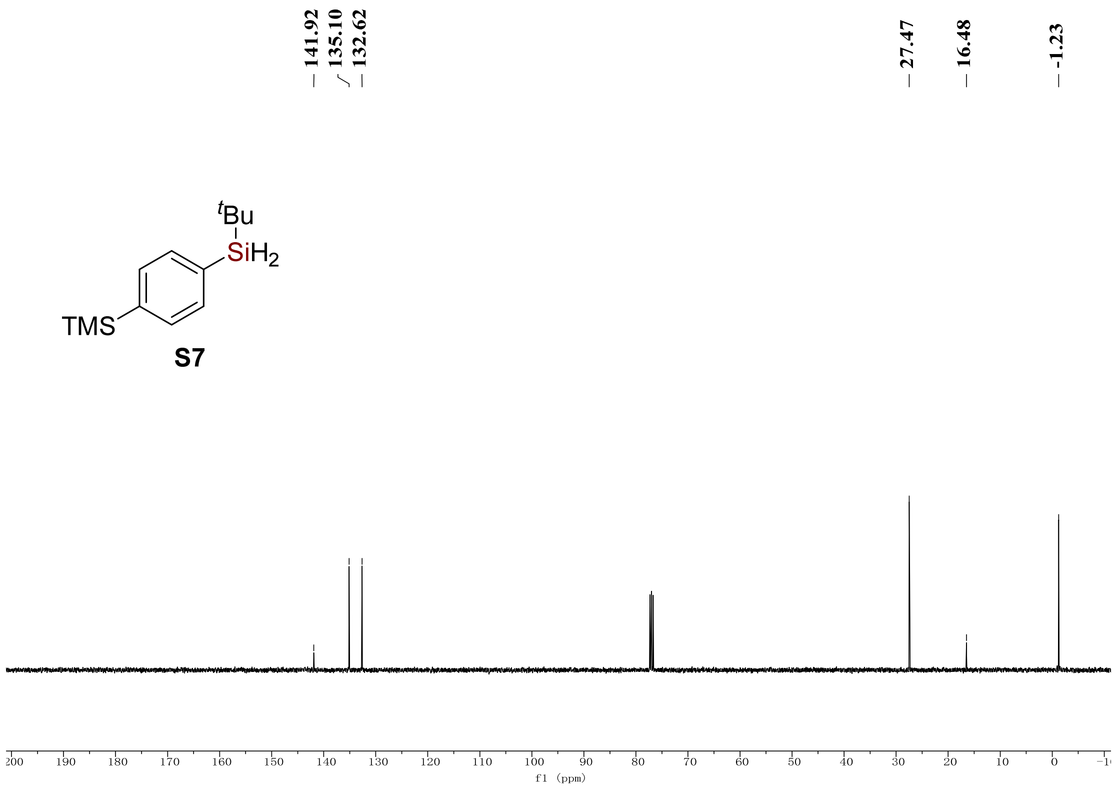
S5


141.22
140.62
134.75
134.63
132.76
128.77
128.45
128.21
127.30
127.24
27.47
16.46
tBu
Ph
SiH2
S5
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

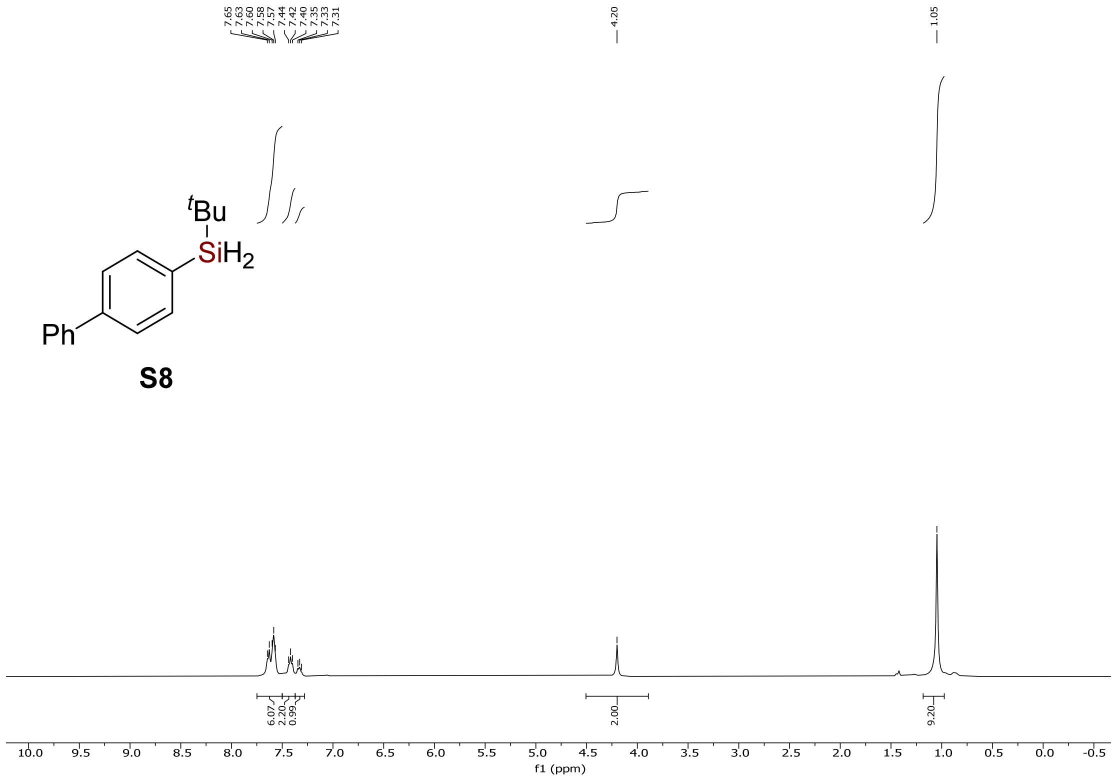

7.52
7.52
7.51
7.50
7.39
7.38
7.37
7.37
4.14
1.32
1.02
tBu
SiH2
tBu
S6
2.00
2.09
1.88
9.48
9.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


152.53
135.84
128.59
124.82
34.70
31.24
27.51
16.49
tBu
SiH2
tBu
S6
f1 (ppm)

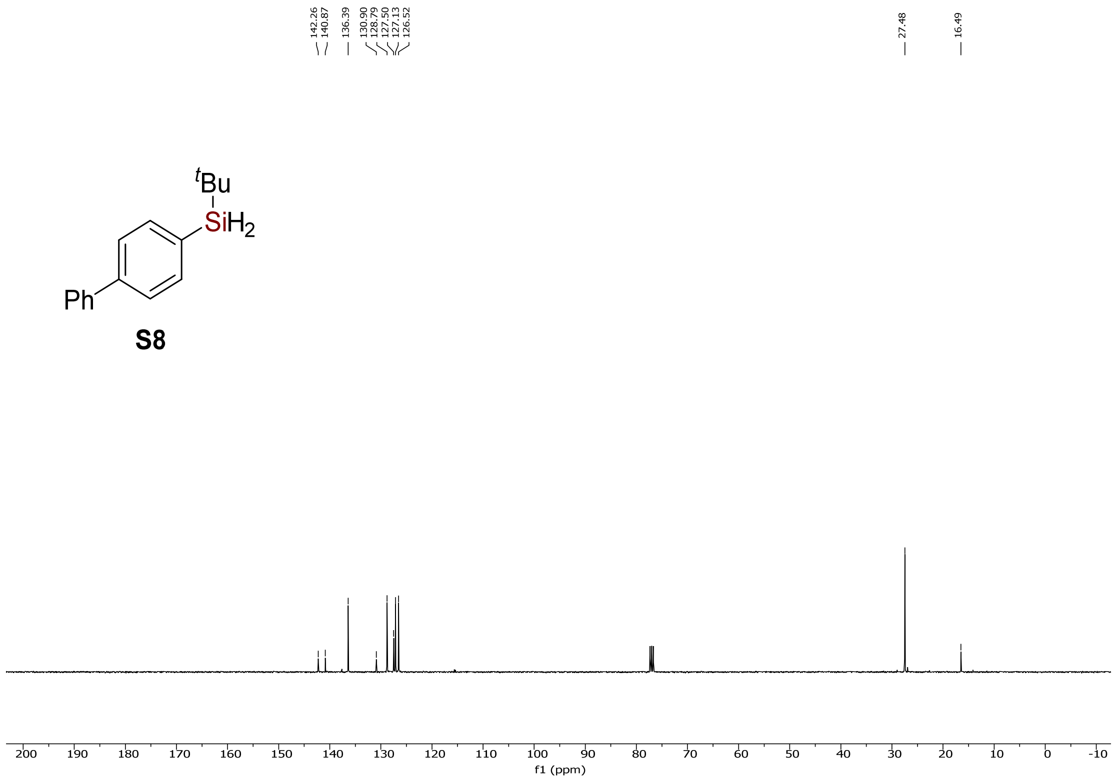

7.59
7.59
7.59
7.58
7.57
7.55
7.54
7.53
7.53
7.53
4.17
1.05
0.30
tBu
SiH2
TMS
S7
1.86
2.18
1.86
9.00
9.65
f1 (ppm)


141.92
135.10
132.62
27.47
16.48
-1.23
^{t}Bu
SiH$_2$
TMS
f1 (ppm)

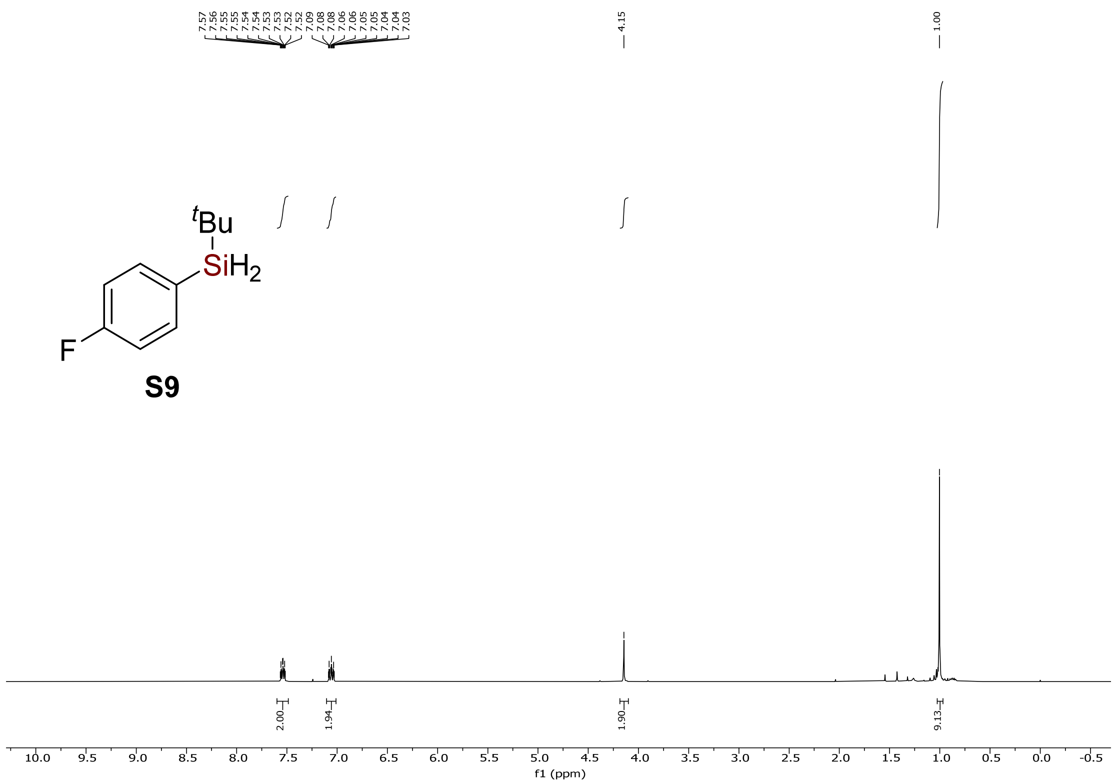
S7


7.65
7.63
7.60
7.58
7.57
7.44
7.42
7.40
7.35
7.33
7.31
4.20
1.05
^{t}Bu
SiH$_2$
Ph
6.07
2.20
0.99
2.00
9.20
f1 (ppm)

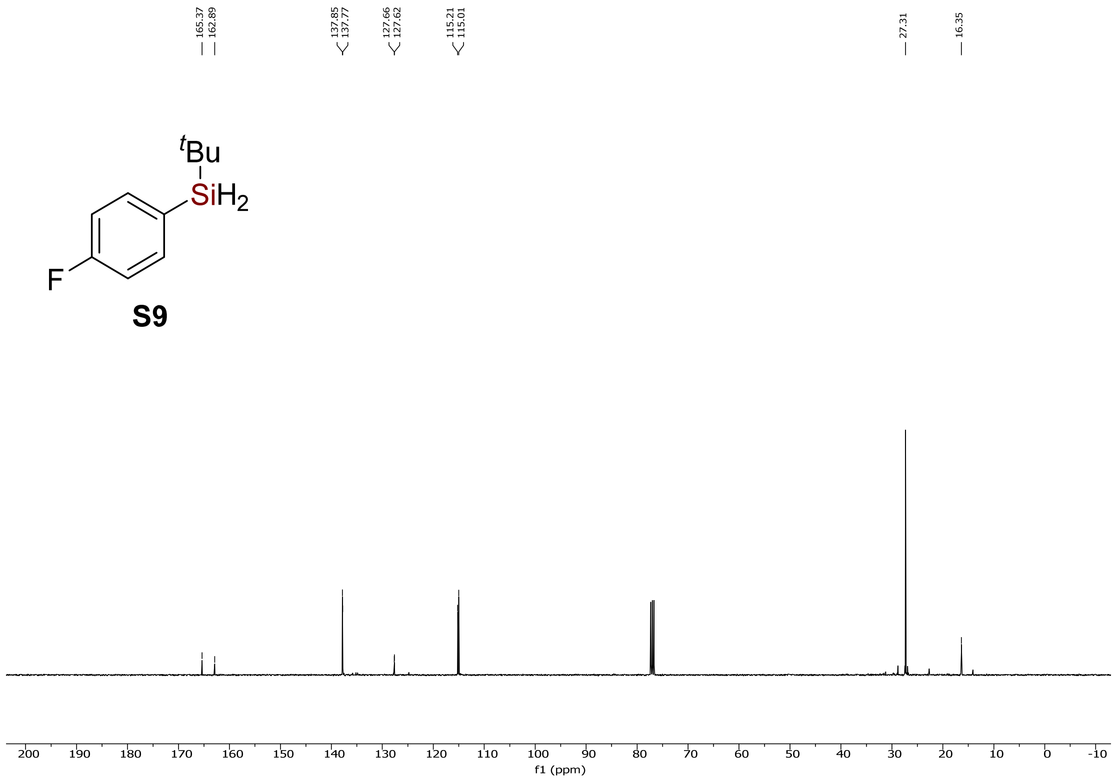
S8

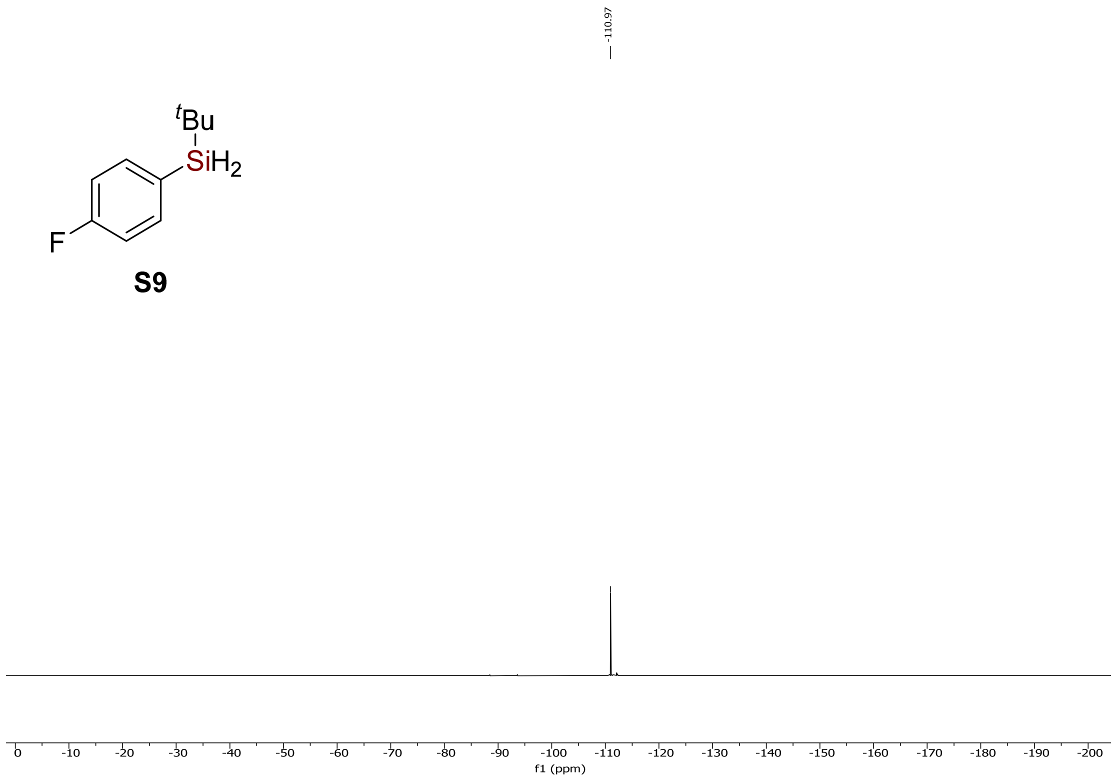

142.26
140.87
136.39
130.90
128.79
127.50
127.13
126.52
27.48
16.49
tBu
SiH2
Ph
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

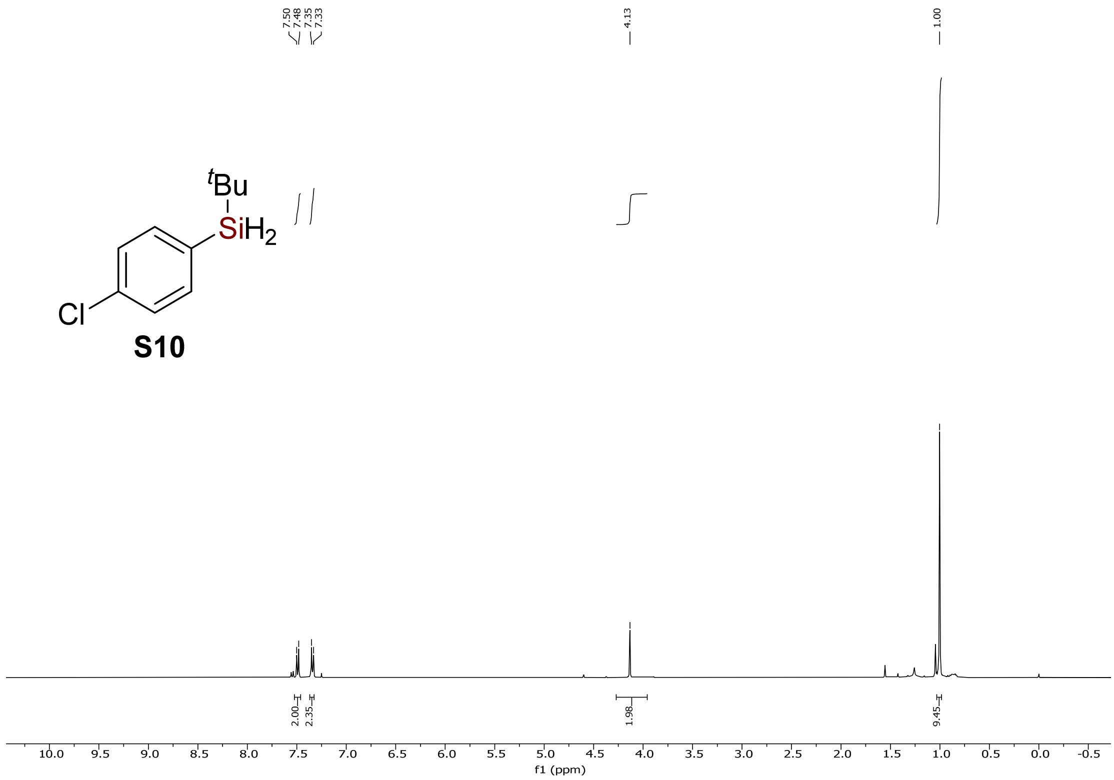
S8


7.57
7.56
7.55
7.55
7.54
7.53
7.53
7.52
7.52
7.09
7.08
7.08
7.06
7.06
7.05
7.05
7.04
7.04
7.03
4.15
1.00
tBu
SiH2
F
2.00
1.94
1.90
9.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

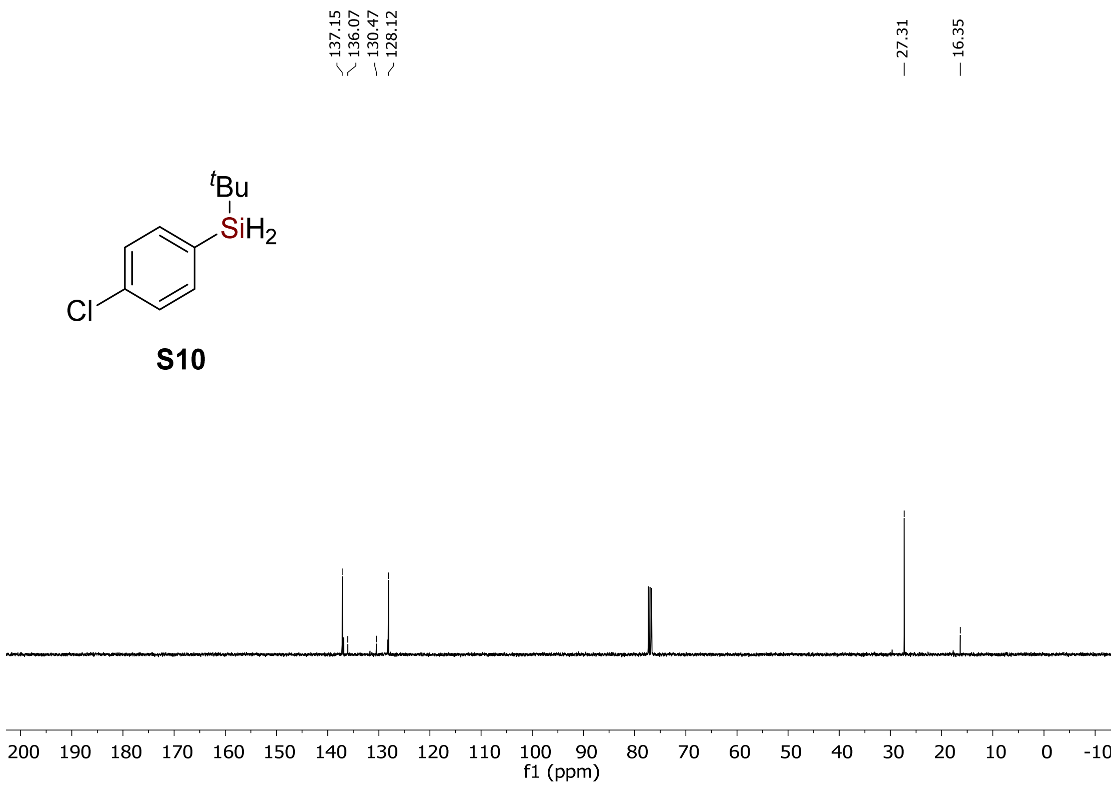
S9


165.37
162.89
137.85
137.77
127.66
127.62
115.21
115.01
27.31
16.35
tBu
SiH2
F
S9
f1 (ppm)

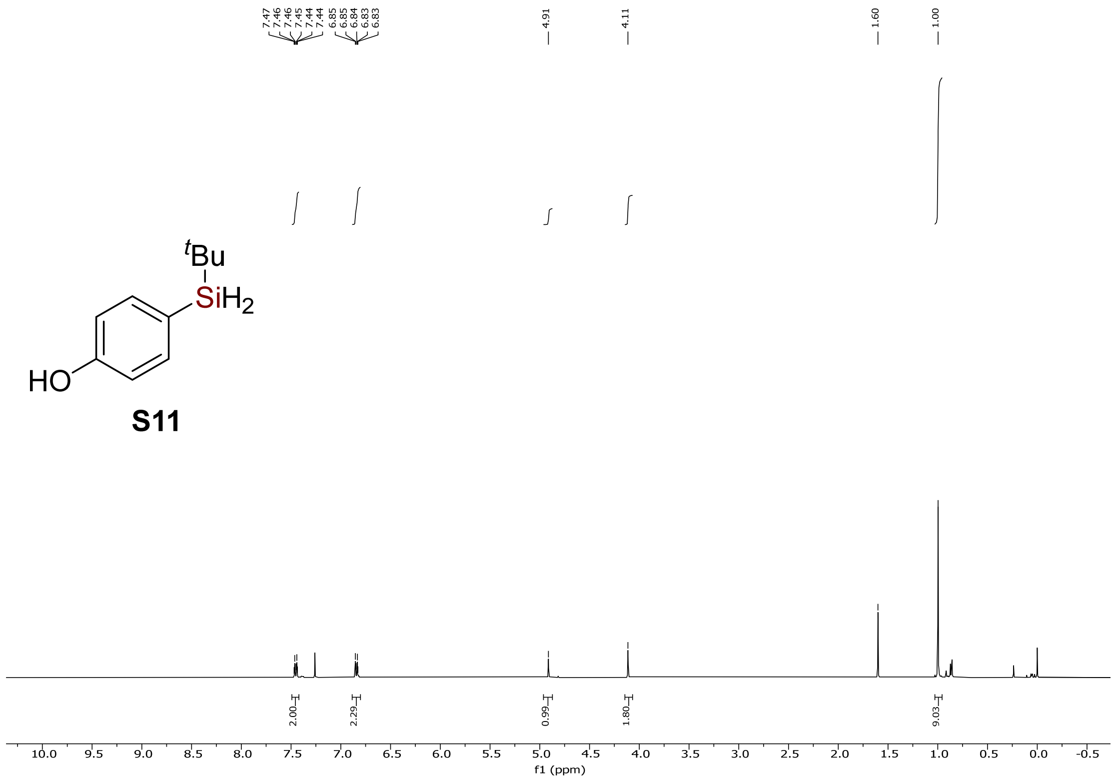

-110.97
tBu
SiH2
F
S9
f1 (ppm)

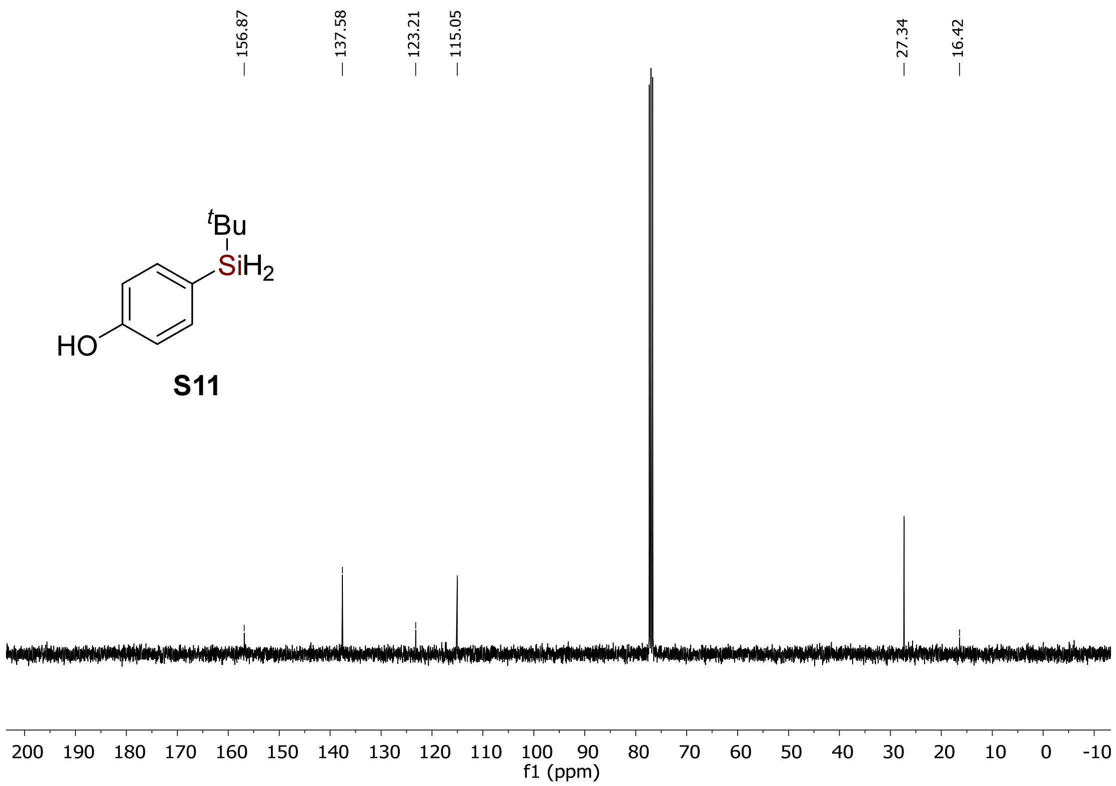


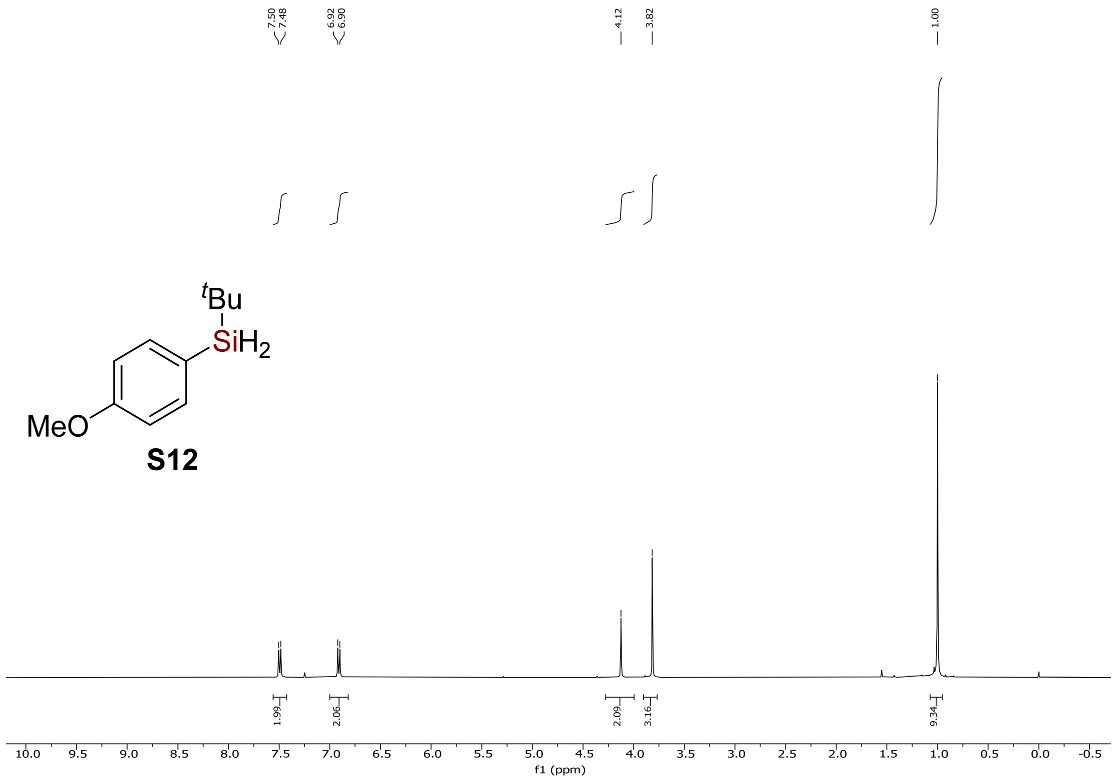
7.50
7.48
7.35
7.33
4.13
1.00
tBu
SiH2
Cl
S10
2.00
2.35
1.98
9.45
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



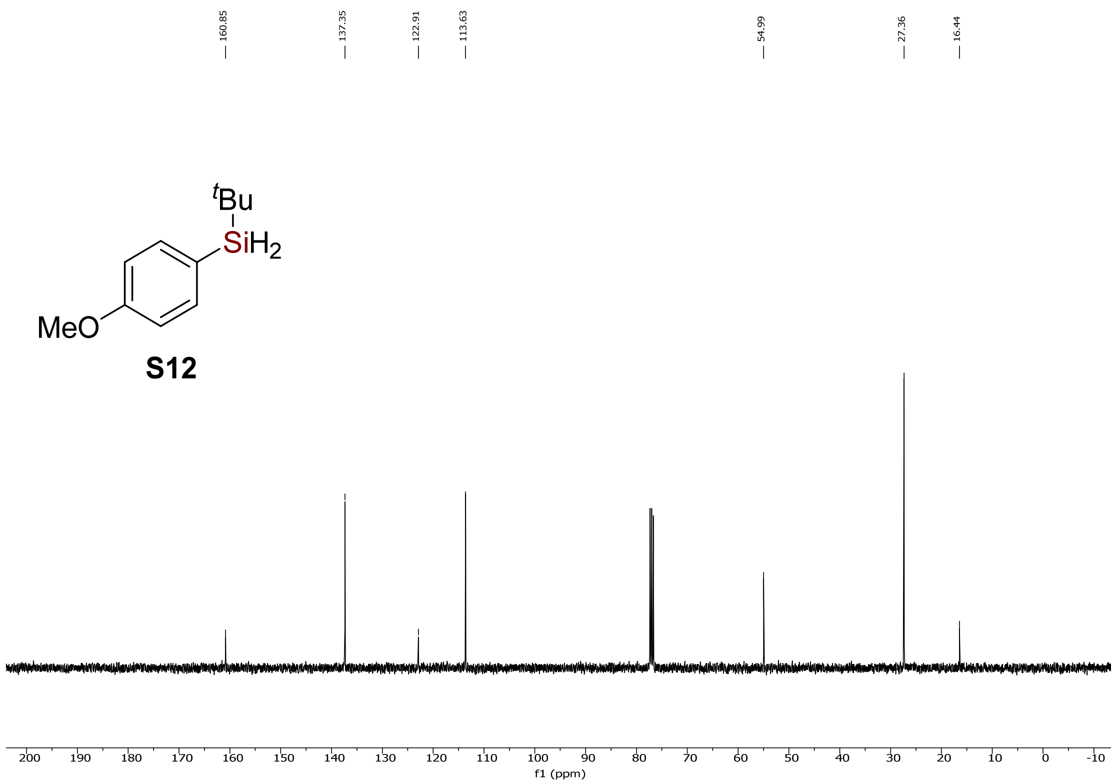
137.15
136.07
130.47
128.12
27.31
16.35
tBu
SiH2
Cl
S10
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.47
7.46
7.46
7.45
7.44
7.44
6.85
6.85
6.84
6.83
6.83
4.91
4.11
1.60
1.00
tBu
SiH2
HO
S11
2.00
2.29
0.99
1.80
9.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

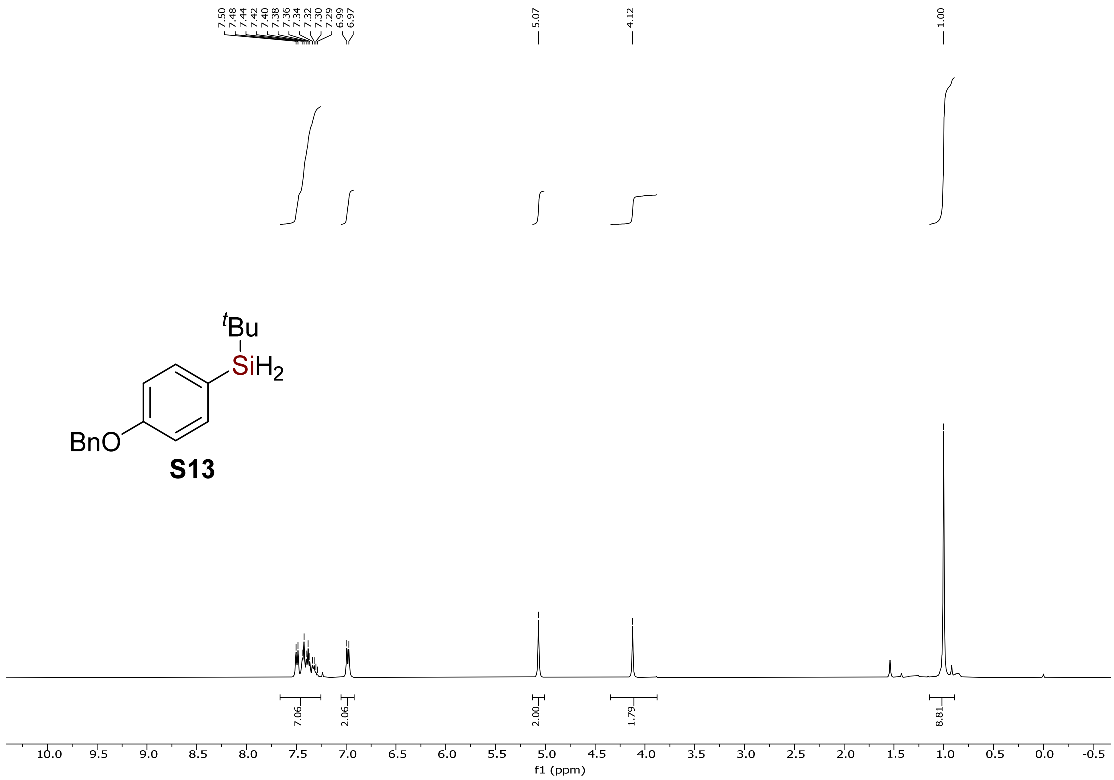

156.87
137.58
123.21
115.05
27.34
16.42
tBu
SiH2
HO
S11
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



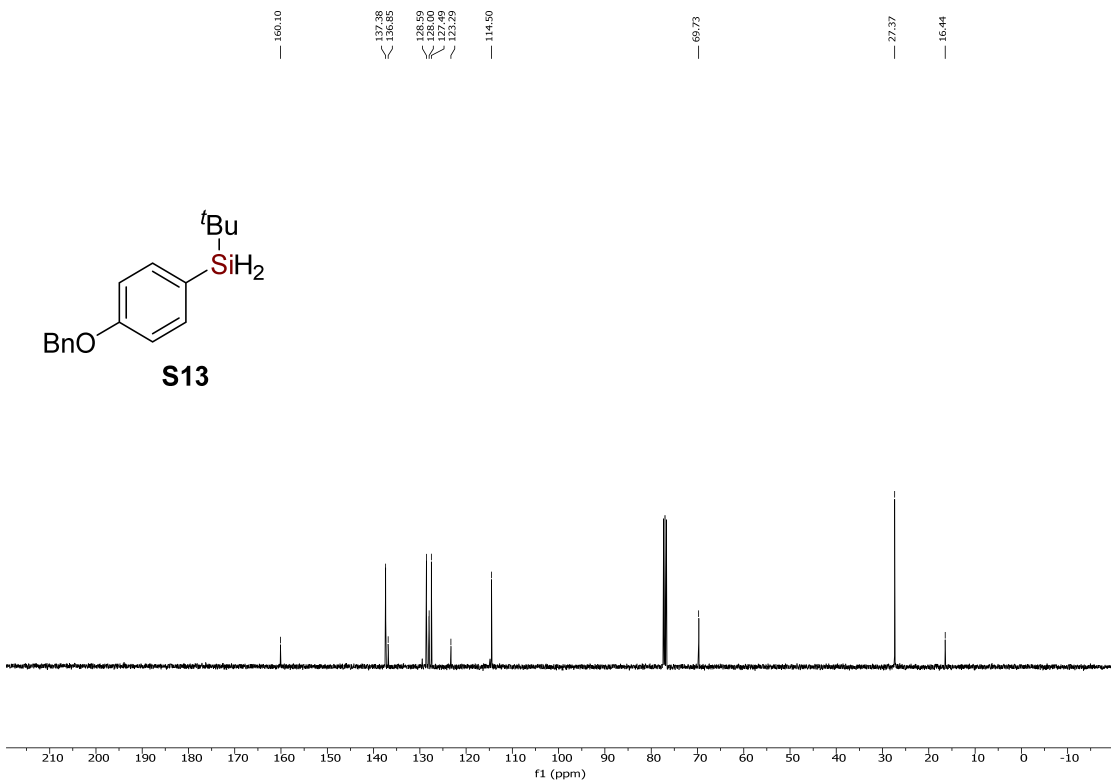
S12



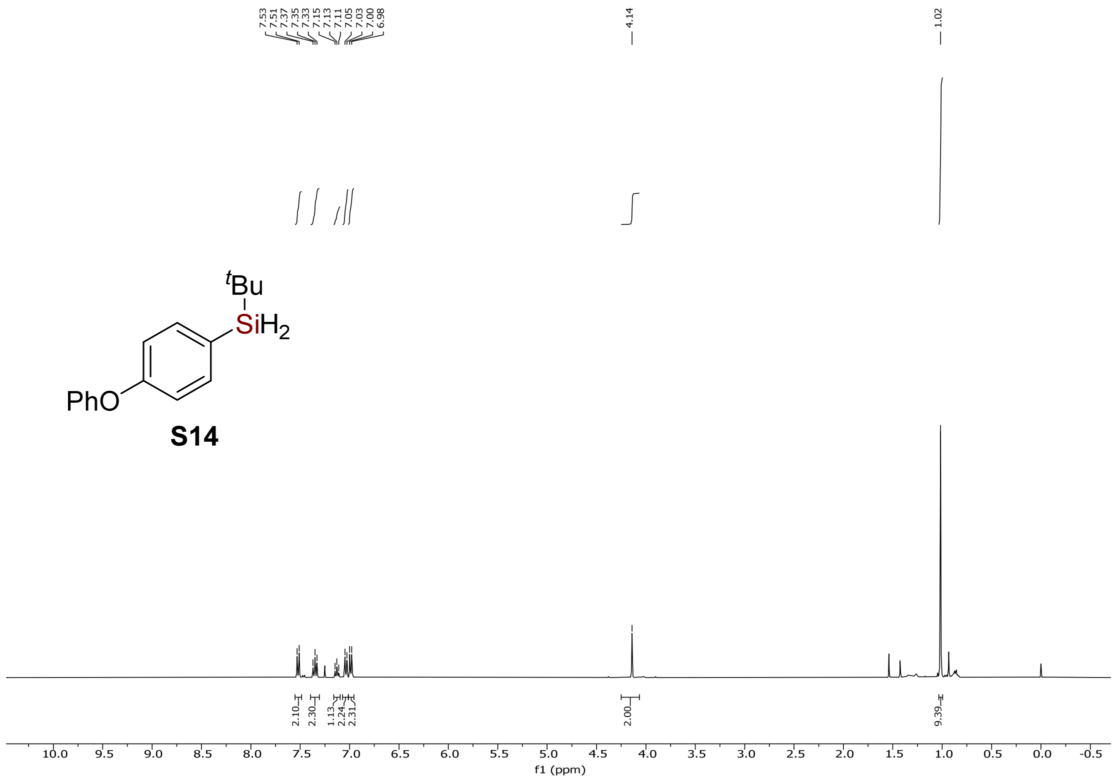
S12


7.50
7.48
7.44
7.42
7.40
7.38
7.36
7.34
7.32
7.30
7.29
6.99
6.97
5.07
4.12
1.00
tBu
SiH2
BnO
7.06
2.06
2.00
1.79
8.81
f1 (ppm)

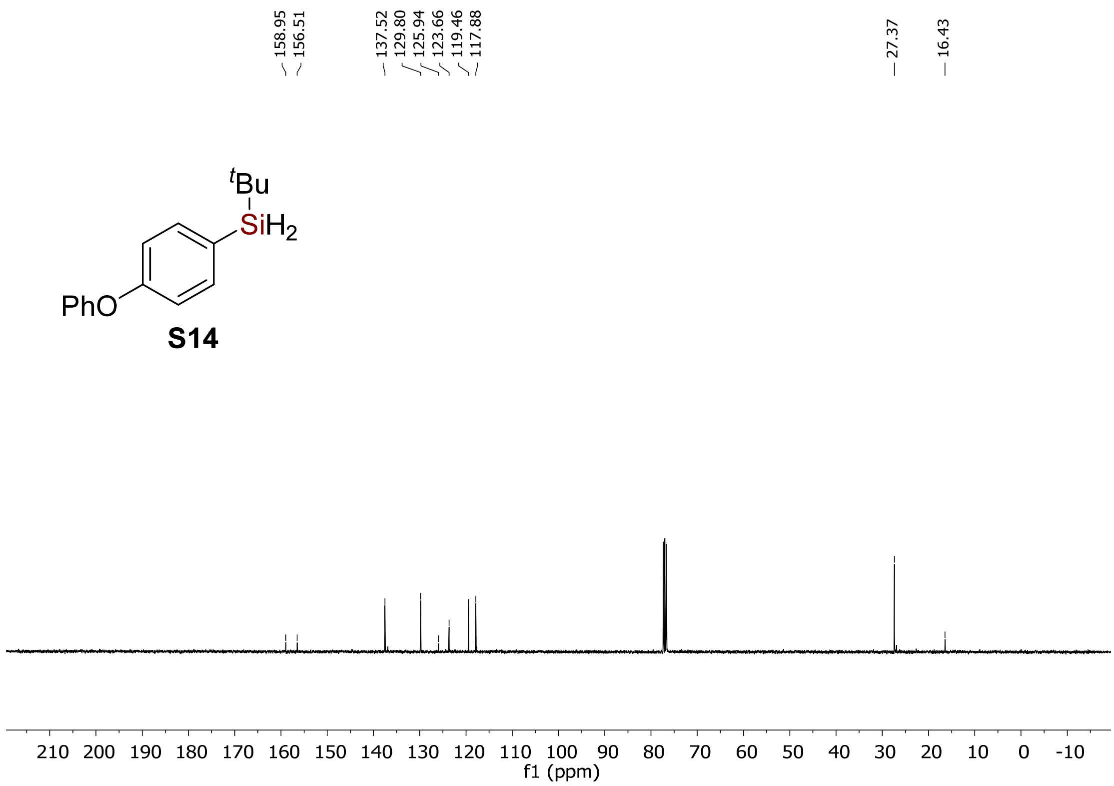
S13


160.10
137.38
136.85
128.59
128.00
127.49
123.29
114.50
69.73
27.37
16.44
tBu
SiH2
BnO
f1 (ppm)

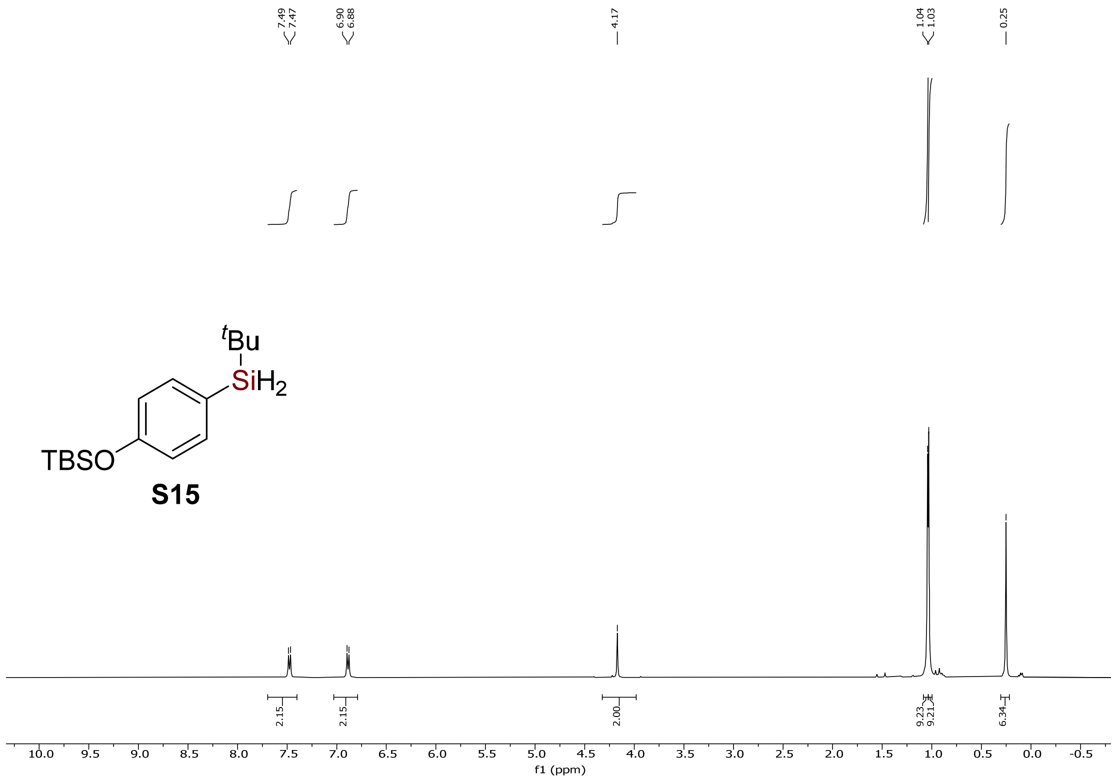
S13

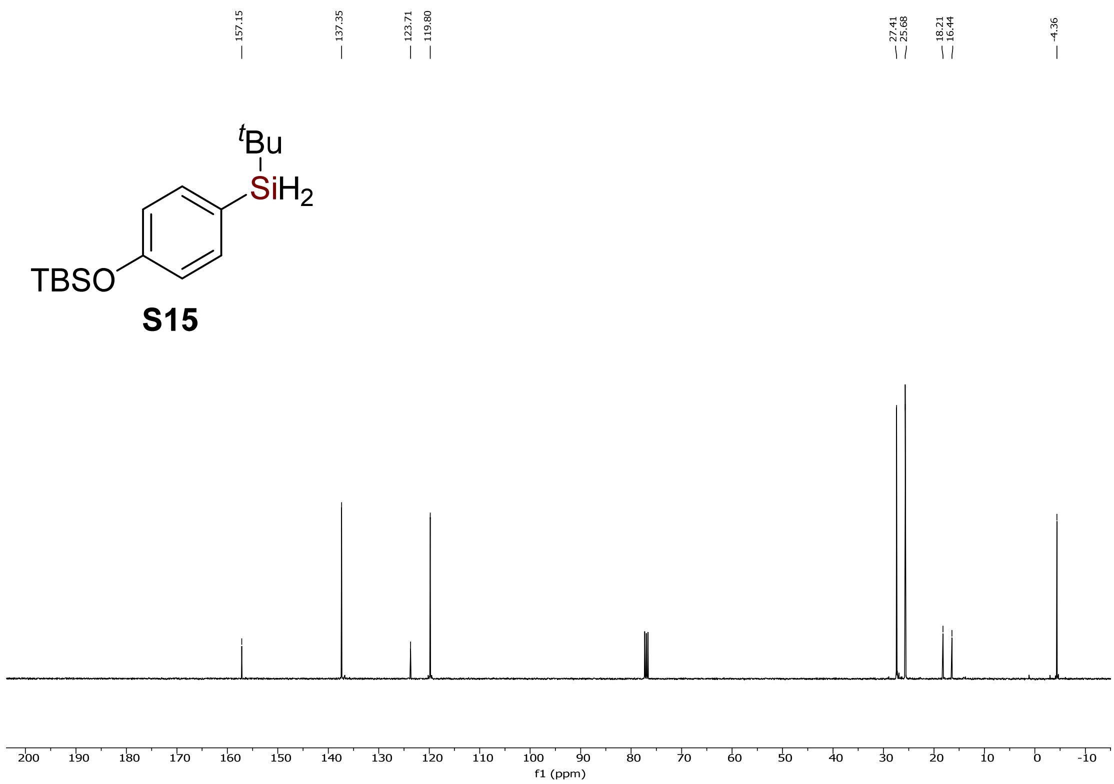


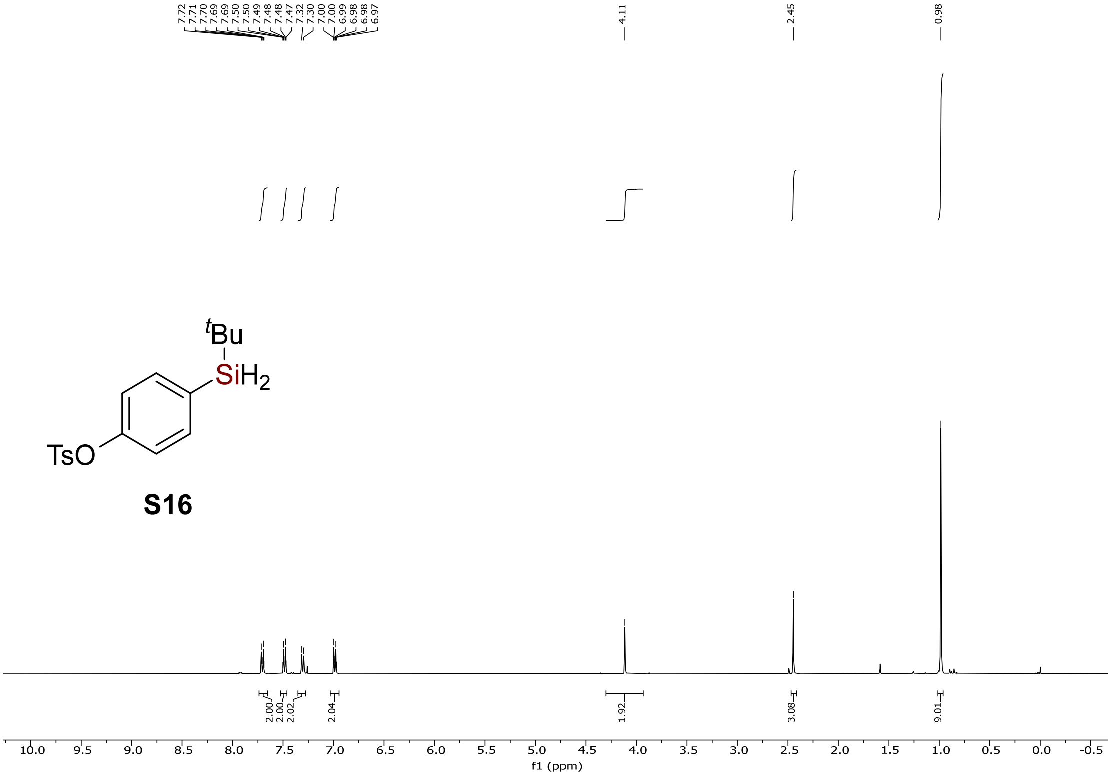
S14



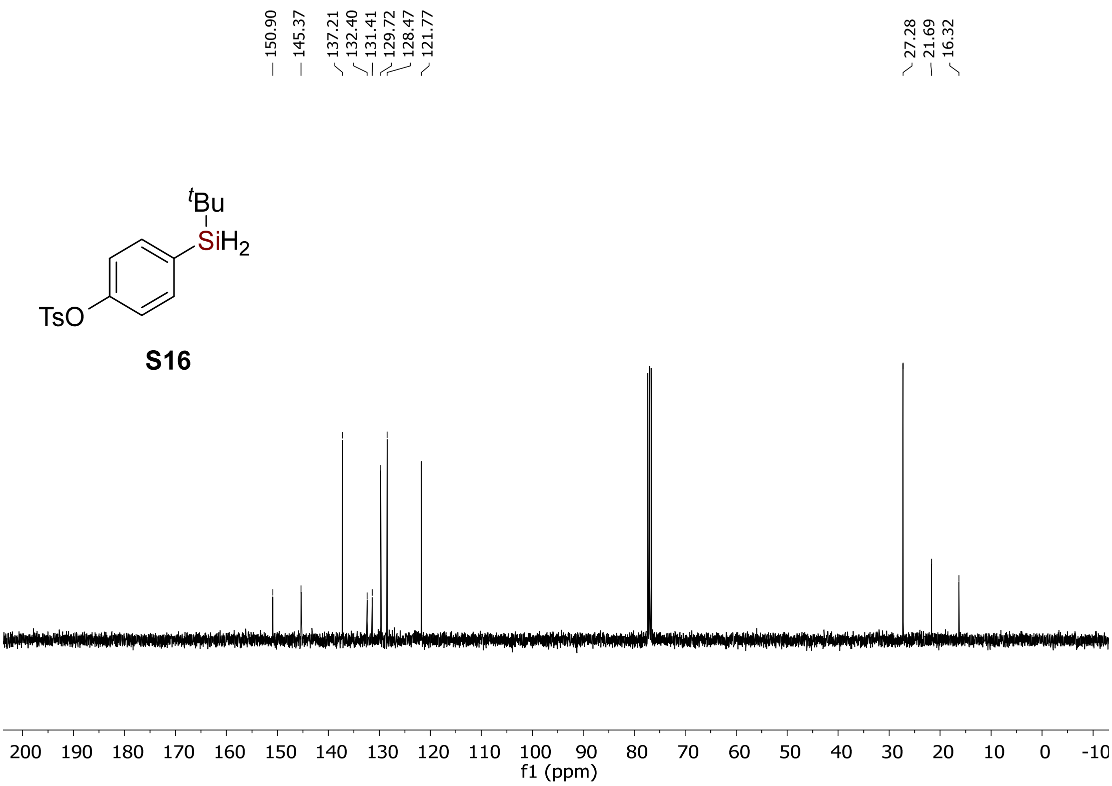
S14


7.49
7.47
6.90
6.88
4.17
1.04
1.03
0.25
tBu
SiH2
TBSO
S15
2.15
2.15
2.00
9.23
9.21
6.34
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

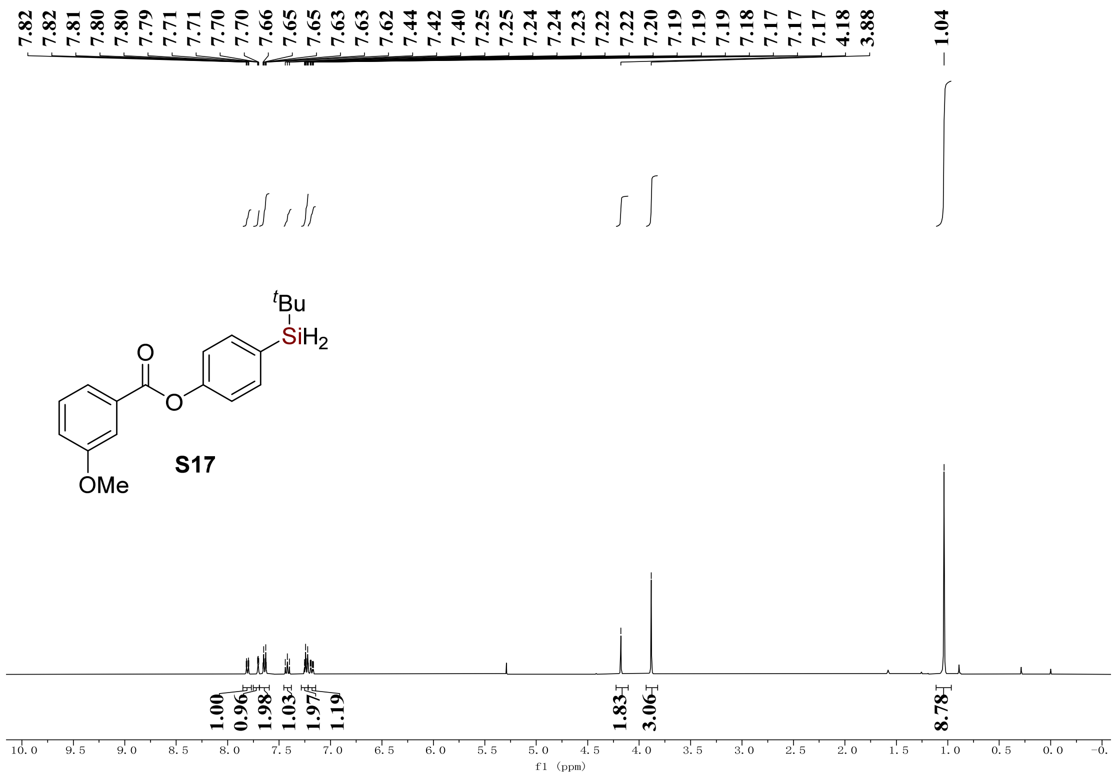

157.15
137.35
123.71
119.80
27.41
25.68
18.21
16.44
-4.36
tBu
SiH2
TBSO
S15
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

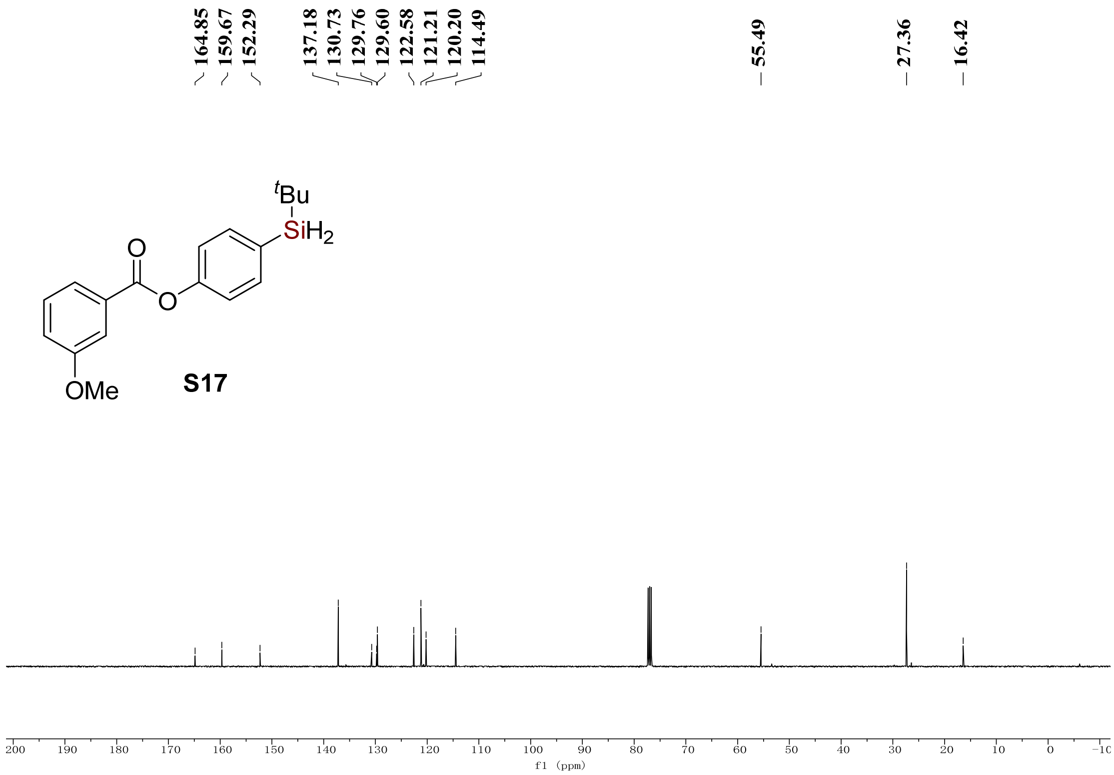


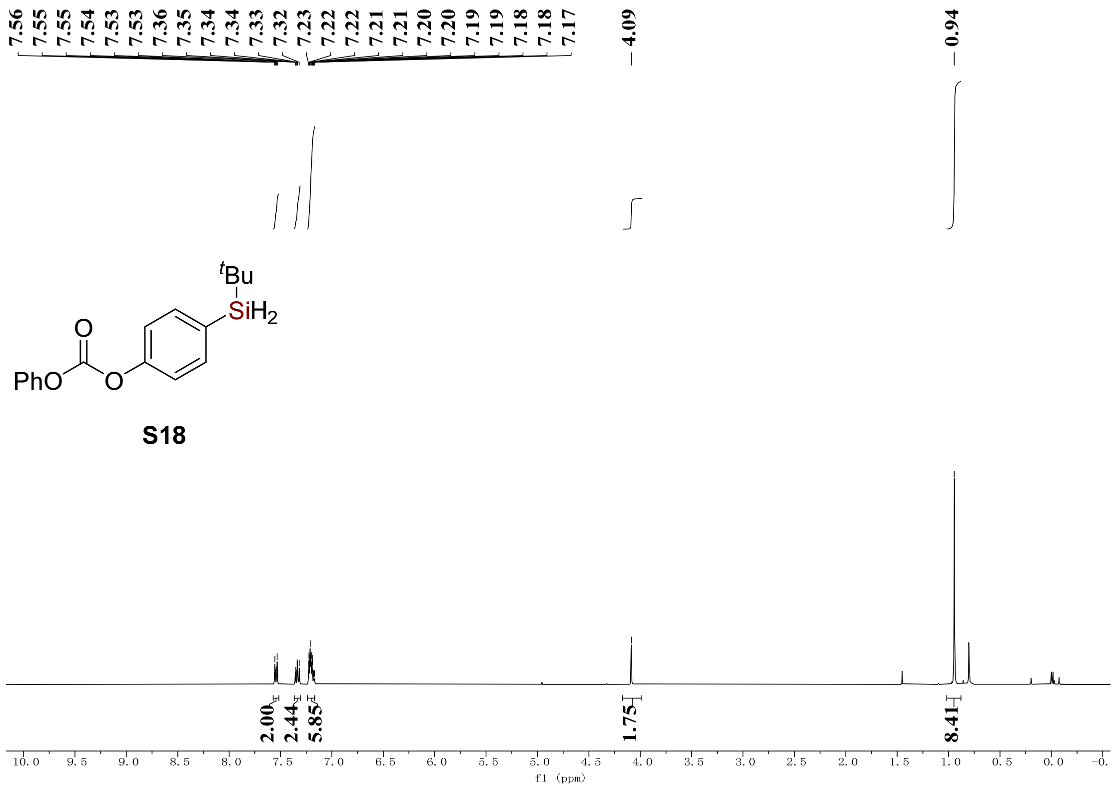
7.72 7.71 7.70 7.69 7.50 7.50 7.49 7.48 7.48 7.47 7.32 7.30 7.00 7.00 6.99 6.98 6.98 6.97
4.11
2.45
0.98
tBu
SiH2
TsO
S16
2.00 2.00 2.02 2.04
1.92
3.08
9.01
f1 (ppm)



150.90
145.37
137.21 132.40 131.41 129.72 128.47 121.77
27.28 21.69 16.32
tBu
SiH2
TsO
S16
f1 (ppm)






7.56
7.55
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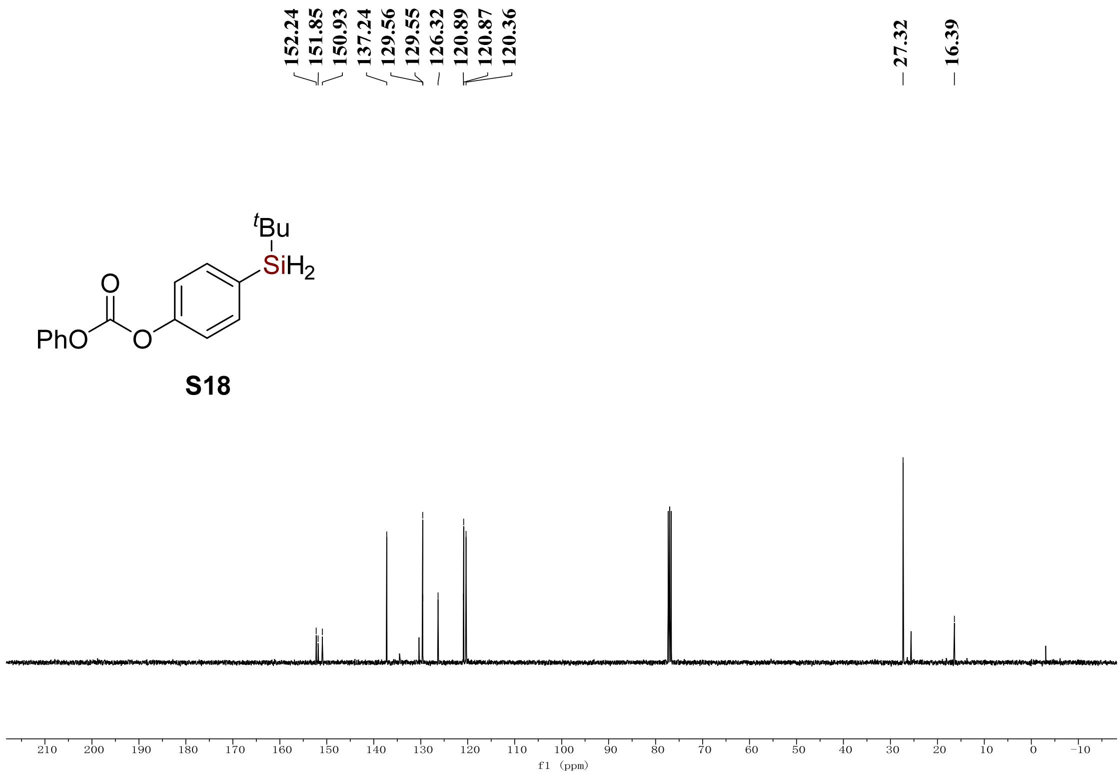
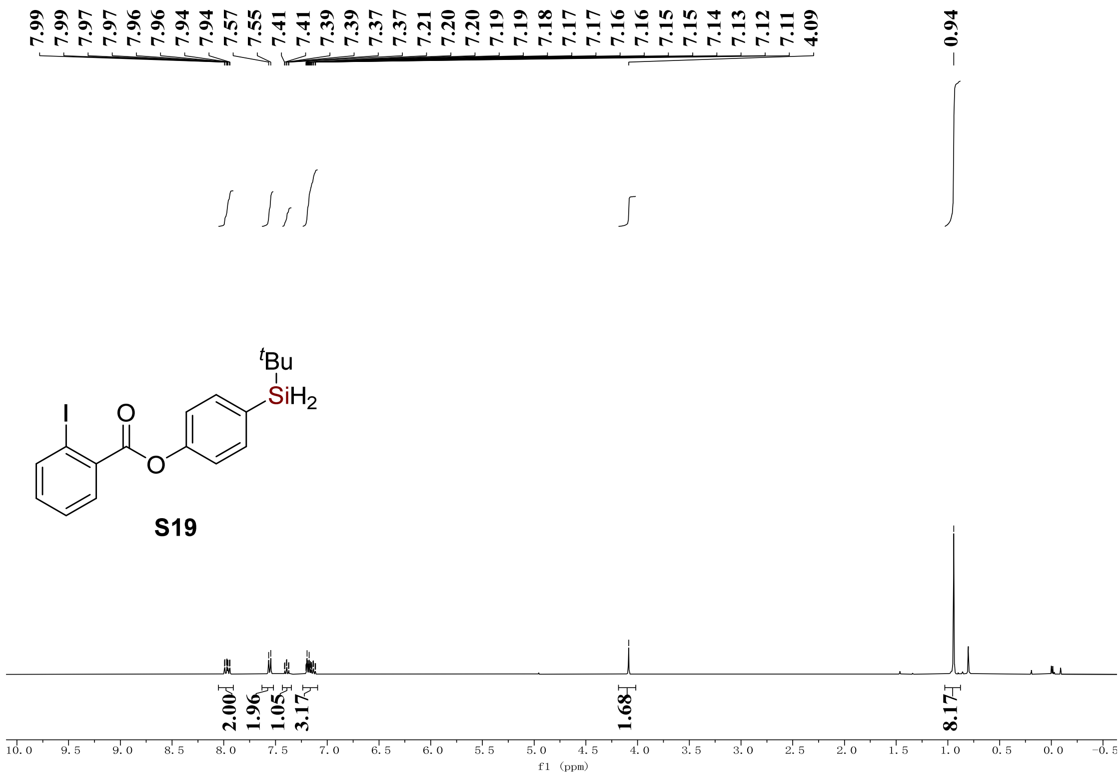
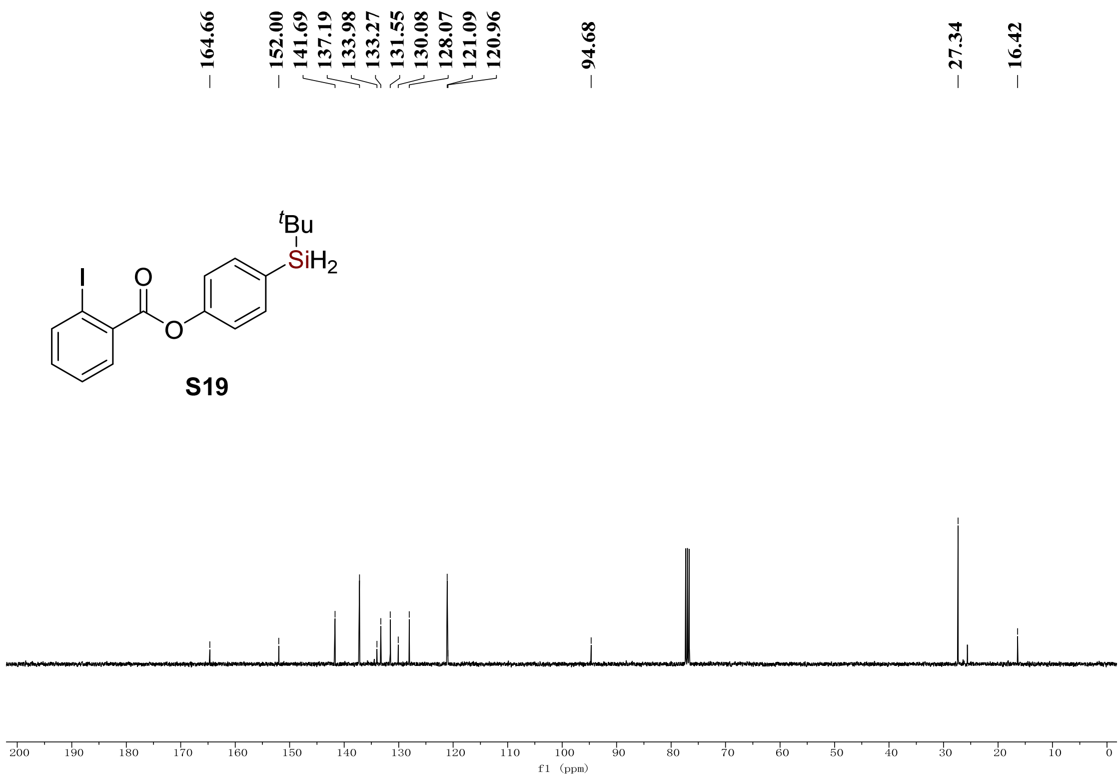
7.54
7.53
7.53
7.36
7.35
7.34
7.34
7.33
7.32
7.23
7.22
7.22
7.21
7.21
7.20
7.20
7.19
7.19
7.18
7.18
7.17
4.09
0.94
tBu
SiH2
O
PhO
O
2.00
2.44
5.85
1.75
8.41
f1 (ppm)

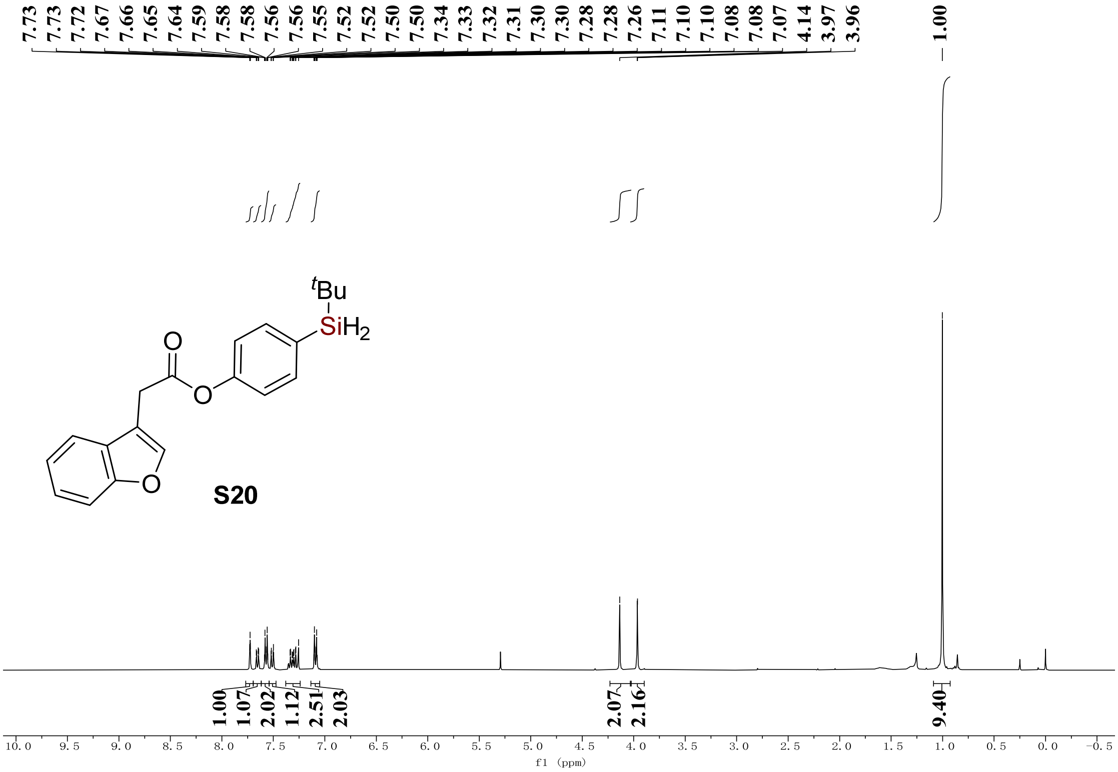
S18

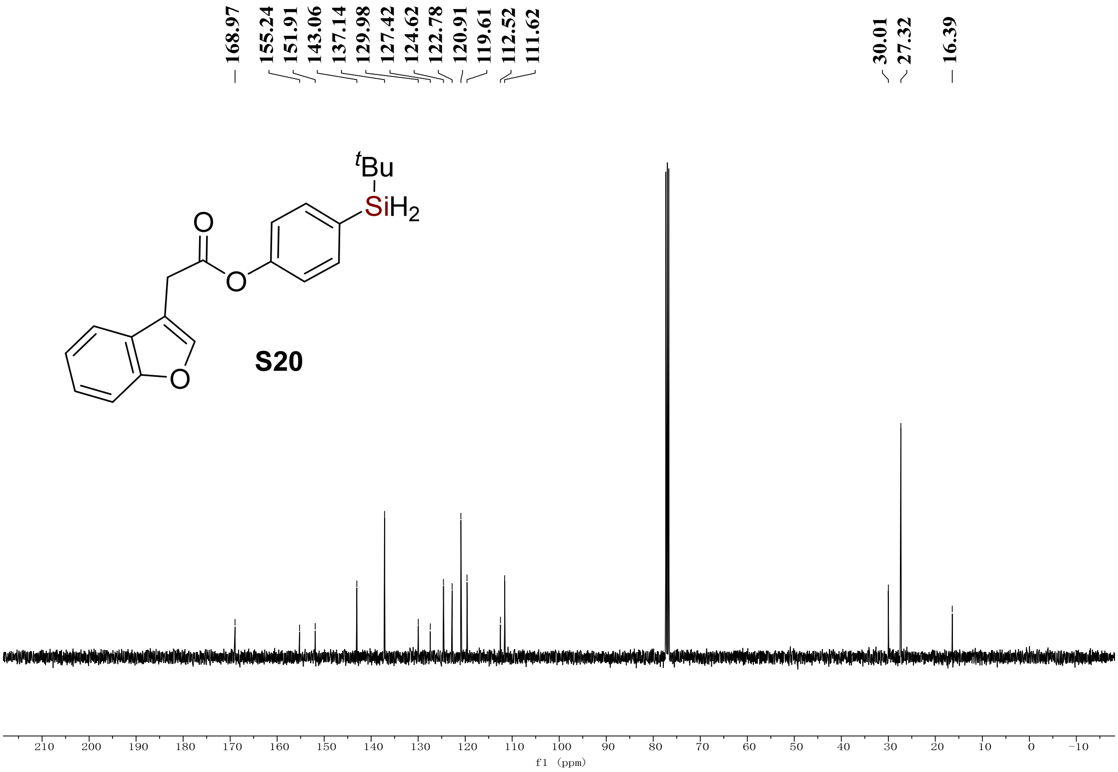

152.24
151.85
150.93
137.24
129.56
129.55
126.32
120.89
120.87
120.36
27.32
16.39
tBu
SiH2
O
PhO
O
f1 (ppm)

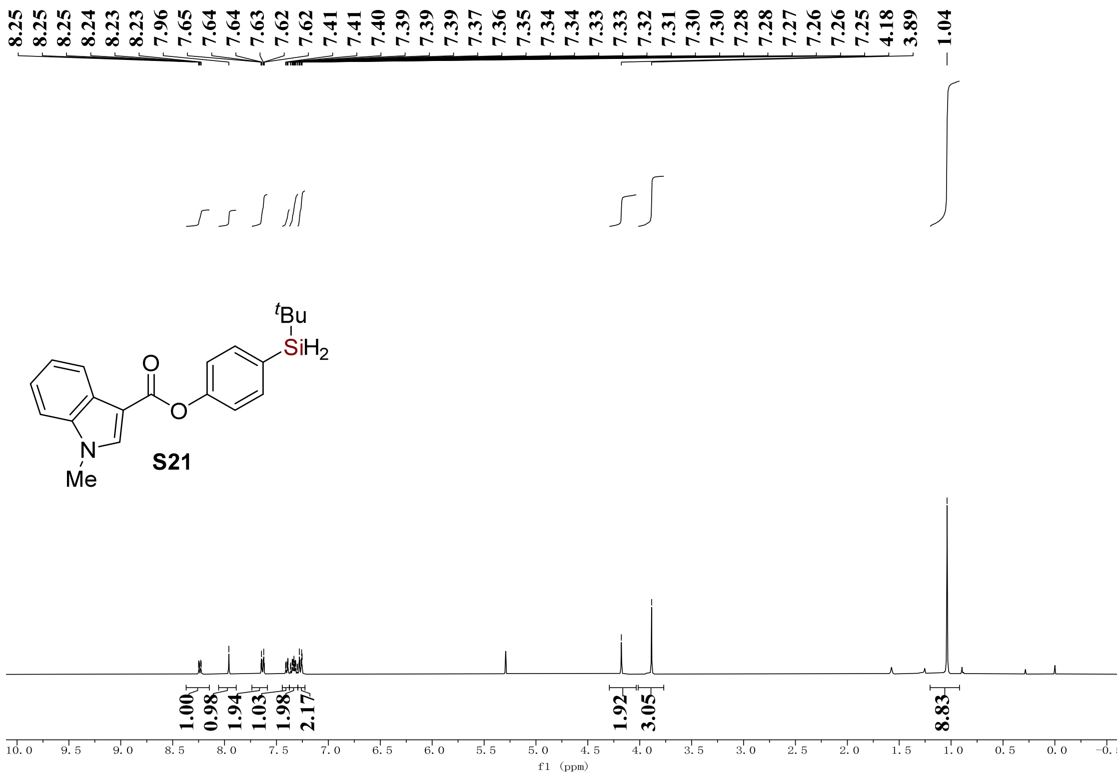
S18

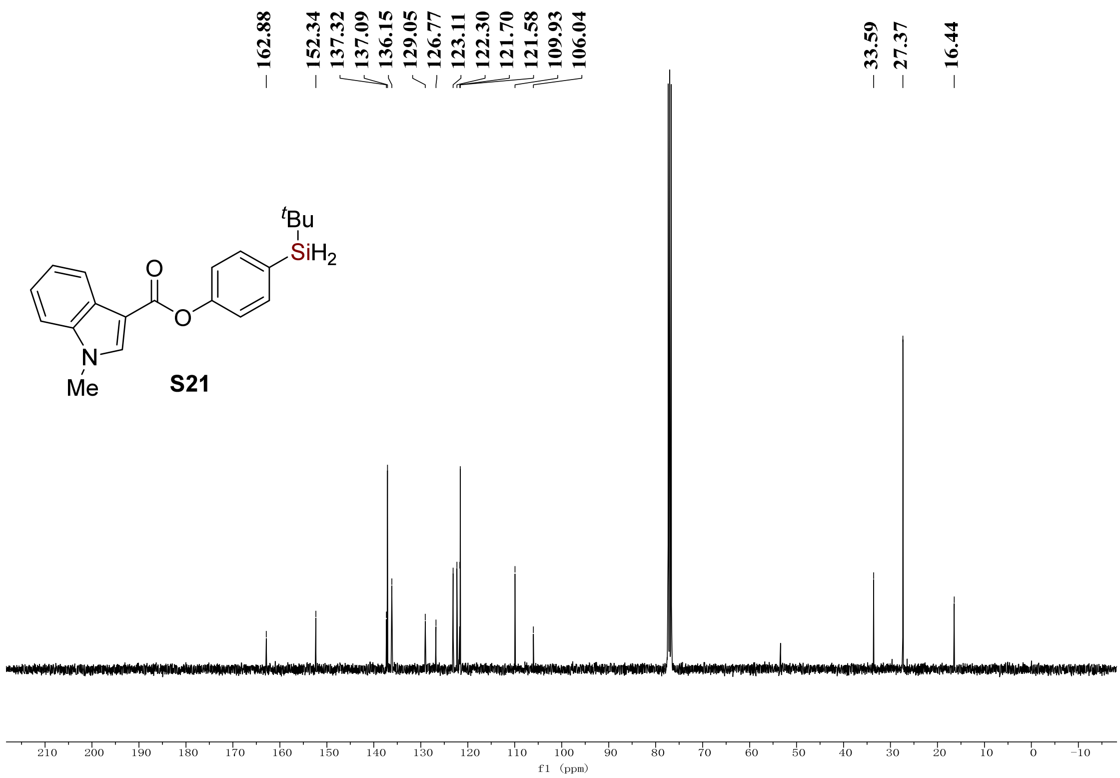

7.99
7.99
7.97
7.97
7.96
7.96
7.94
7.94
7.57
7.55
7.41
7.41
7.39
7.39
7.37
7.37
7.21
7.20
7.20
7.19
7.19
7.18
7.17
7.17
7.16
7.16
7.15
7.15
7.14
7.13
7.12
7.11
4.09
0.94
tBu
SiH2
I
O
O
S19
2.00
1.96
1.05
3.17
1.68
8.17
f1 (ppm)

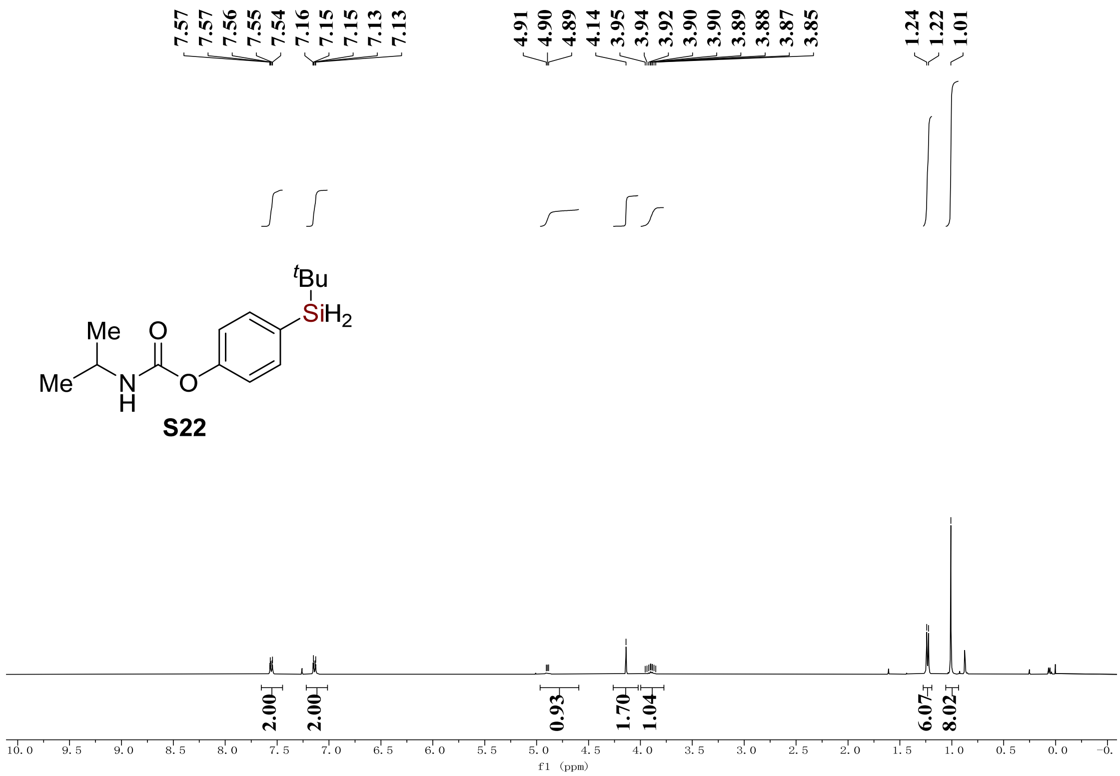

164.66
152.00
141.69
137.19
133.98
133.27
131.55
130.08
128.07
121.09
120.96
94.68
27.34
16.42
tBu
SiH2
I
O
O
S19
f1 (ppm)

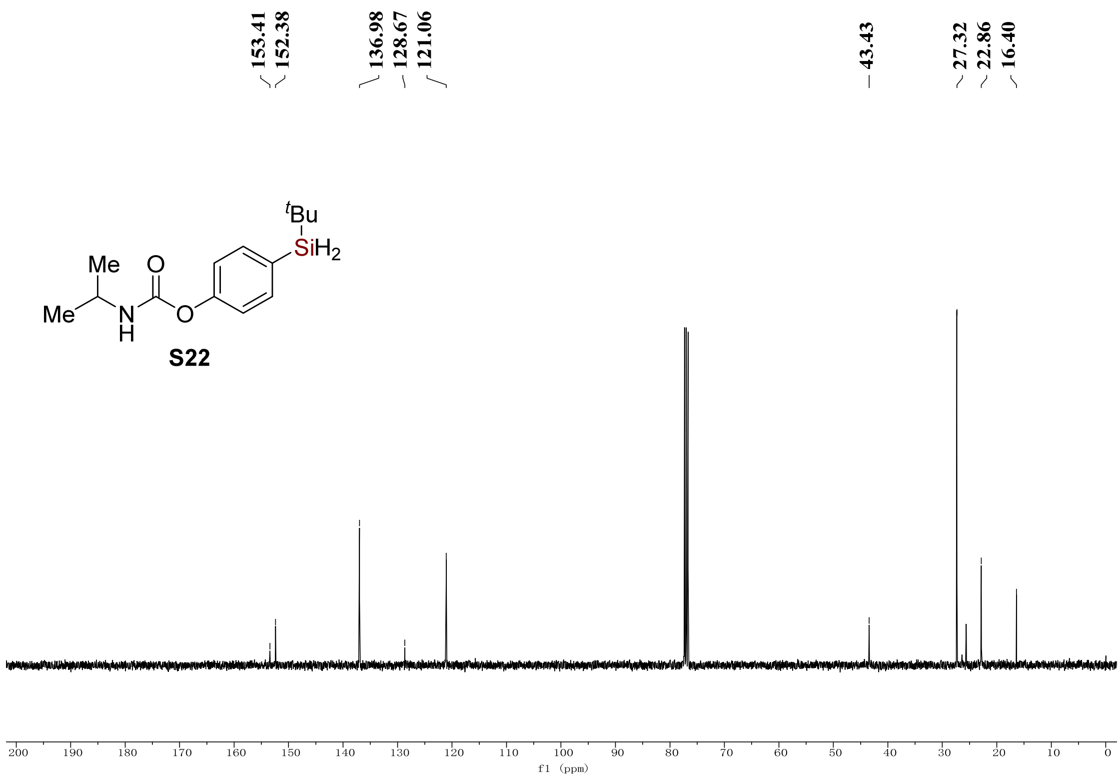

7.73
7.73
7.72
7.67
7.66
7.65
7.64
7.59
7.58
7.56
7.56
7.55
7.52
7.52
7.50
7.50
7.34
7.33
7.32
7.31
7.30
7.30
7.28
7.28
7.26
7.11
7.10
7.10
7.08
7.08
7.07
4.14
3.97
3.96
1.00
tBu
SiH2
O
O
O
S20
1.00
1.07
2.02
1.12
2.51
2.03
2.07
2.16
9.40
f1 (ppm)

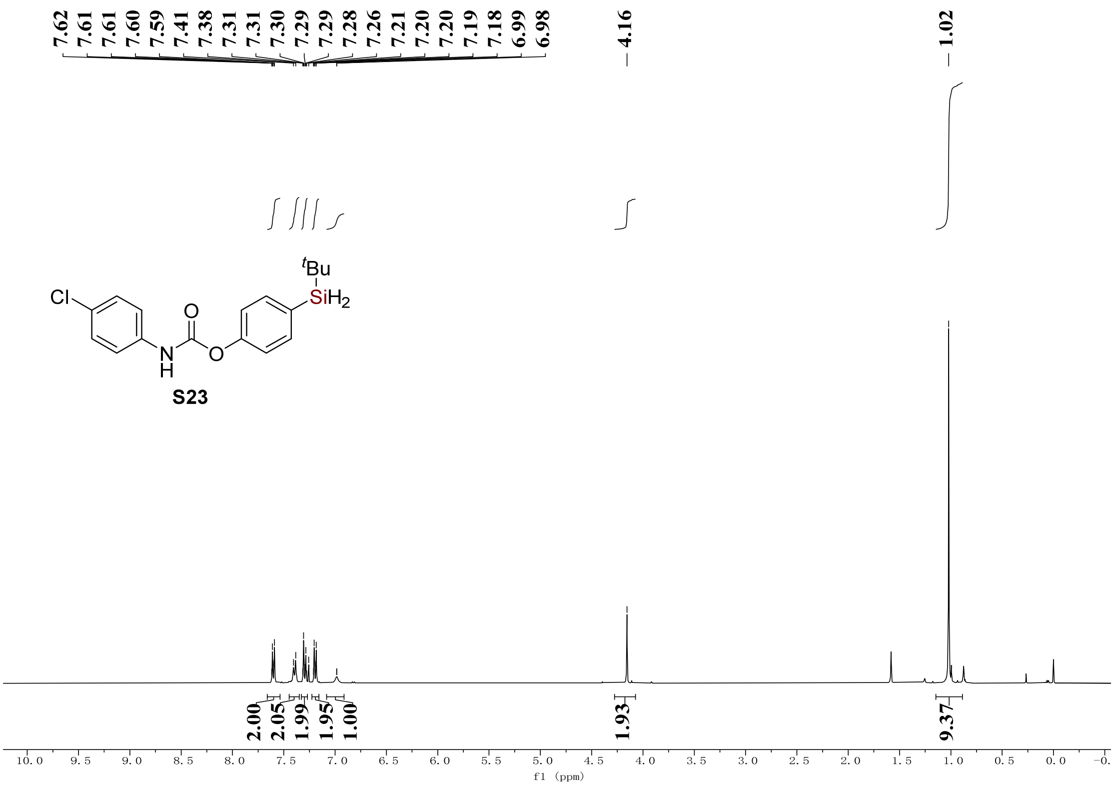

168.97
155.24
151.91
143.06
137.14
129.98
127.42
124.62
122.78
120.91
119.61
112.52
111.62
30.01
27.32
16.39
tBu
SiH2
O
O
O
S20
f1 (ppm)


8.25 8.25 8.25 8.24 8.23 8.23 7.96 7.65 7.64 7.64 7.63 7.62 7.62 7.41 7.41 7.40 7.39 7.39 7.39 7.37 7.36 7.35 7.34 7.34 7.33 7.33 7.32 7.31 7.30 7.30 7.28 7.28 7.27 7.26 7.26 7.25 4.18 3.89
1.04
tBu
SiH2
O
O
N
Me
S21
1.00 0.98 1.94 1.03 1.98 2.17
1.92 3.05
8.83
f1 (ppm)

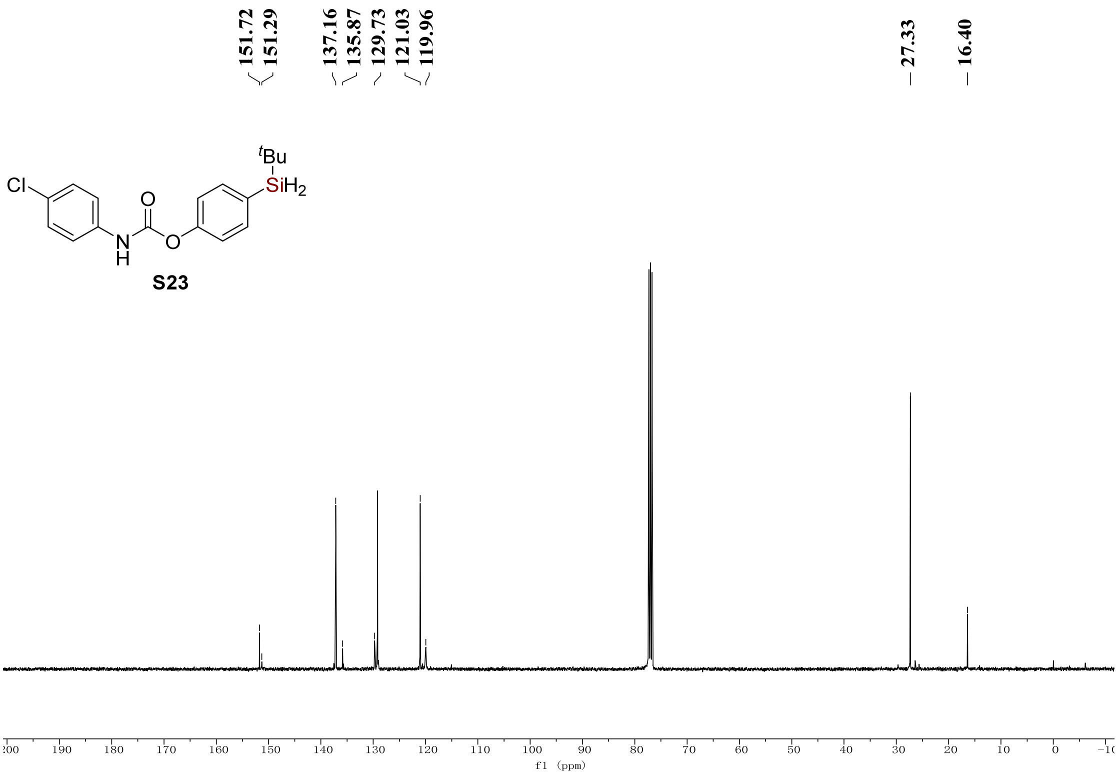

162.88
152.34 137.32 137.09 136.15 129.05 126.77 123.11 122.30 121.70 121.58 109.93 106.04
33.59 27.37 16.44
tBu
SiH2
O
O
N
Me
S21
f1 (ppm)



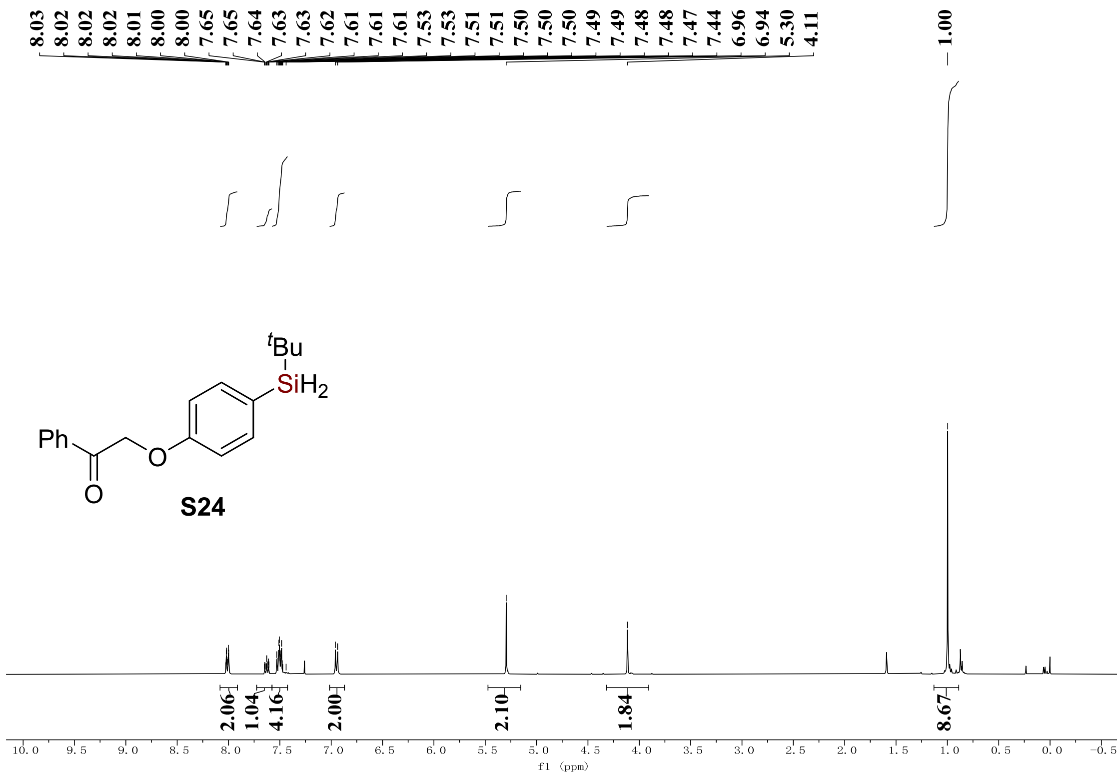




7.62 7.61 7.61 7.60 7.59 7.41 7.38 7.31 7.31 7.30 7.29 7.29 7.28 7.26 7.21 7.20 7.20 7.19 7.18 6.99 6.98
4.16
1.02
Cl
O
N
H
O
^{t}Bu
SiH$_2$
S23
2.00 2.05 1.99 1.95 1.00
1.93
9.37
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)



151.72 151.29
137.16 135.87 129.73 121.03 119.96
27.33
16.40
Cl
O
N
H
O
^{t}Bu
SiH$_2$
S23
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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8.02
8.02
8.01
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8.00
7.65
7.65
7.64
7.63
7.63
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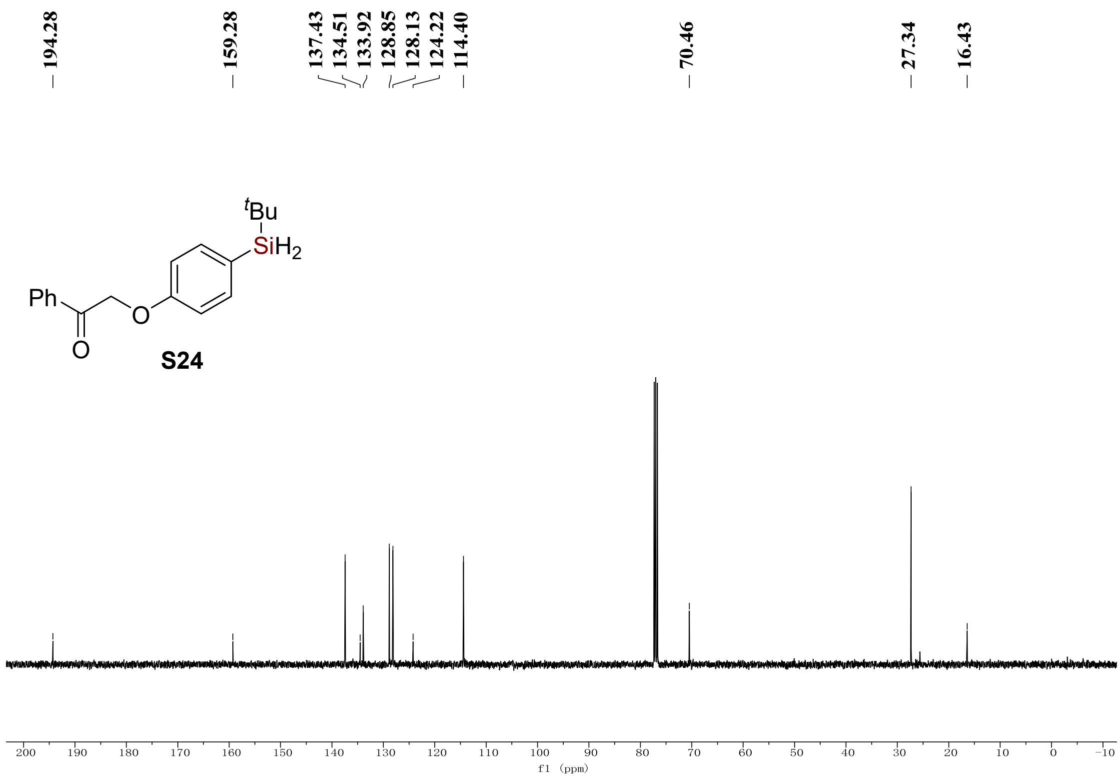
7.61
7.61
7.61
7.53
7.53
7.51
7.51
7.50
7.50
7.50
7.49
7.49
7.48
7.48
7.47
7.44
6.96
6.94
5.30
4.11
1.00
^{t}Bu
SiH_2
Ph
O
O
S24
2.06
1.04
4.16
2.00
2.10
1.84
8.67
f1 (ppm)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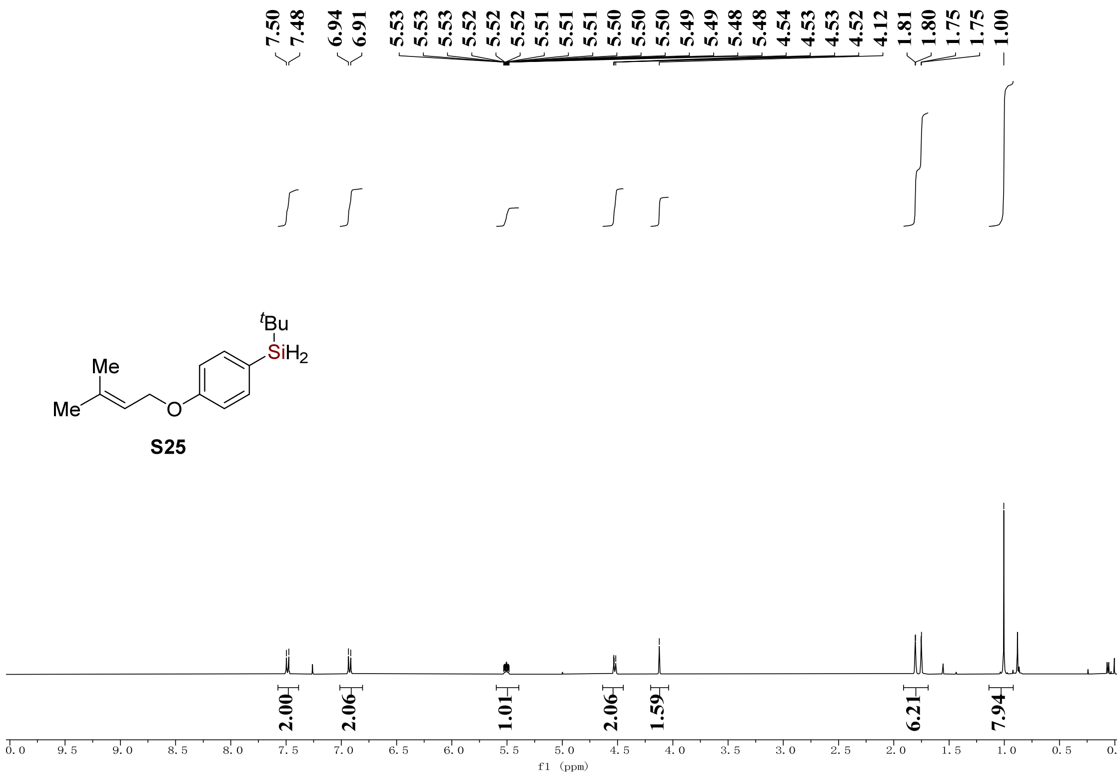
133.92
128.85
128.13
124.22
114.40
70.46
27.34
16.43
^{t}Bu
SiH_2
Ph
O
O
S24
f1 (ppm)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6.94
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5.53
5.53
5.53
5.52
5.52
5.52
5.51
5.51
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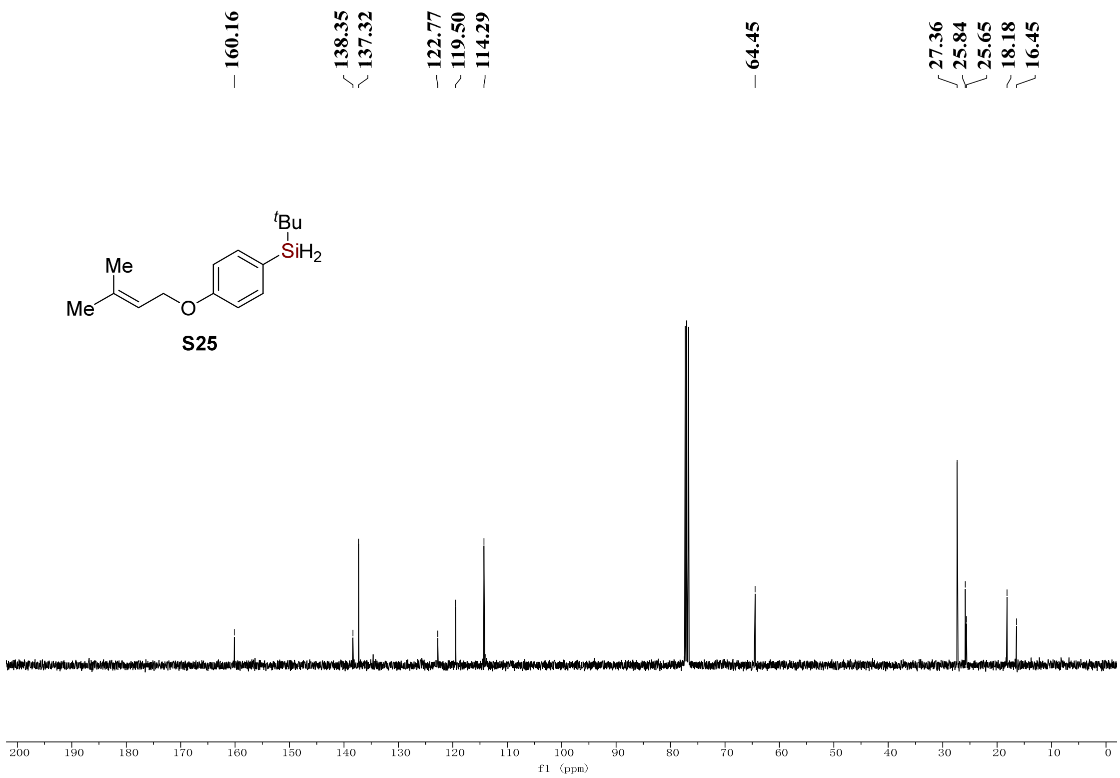
5.50
5.50
5.50
5.49
5.49
5.48
5.48
4.54
4.53
4.53
4.52
4.12
1.81
1.80
1.75
1.75
1.00
tBu
SiH2
Me
Me
O
S25
2.00
2.06
1.01
2.06
1.59
6.21
7.94
f1 (ppm)


160.16
138.35
137.32
122.77
119.50
114.29
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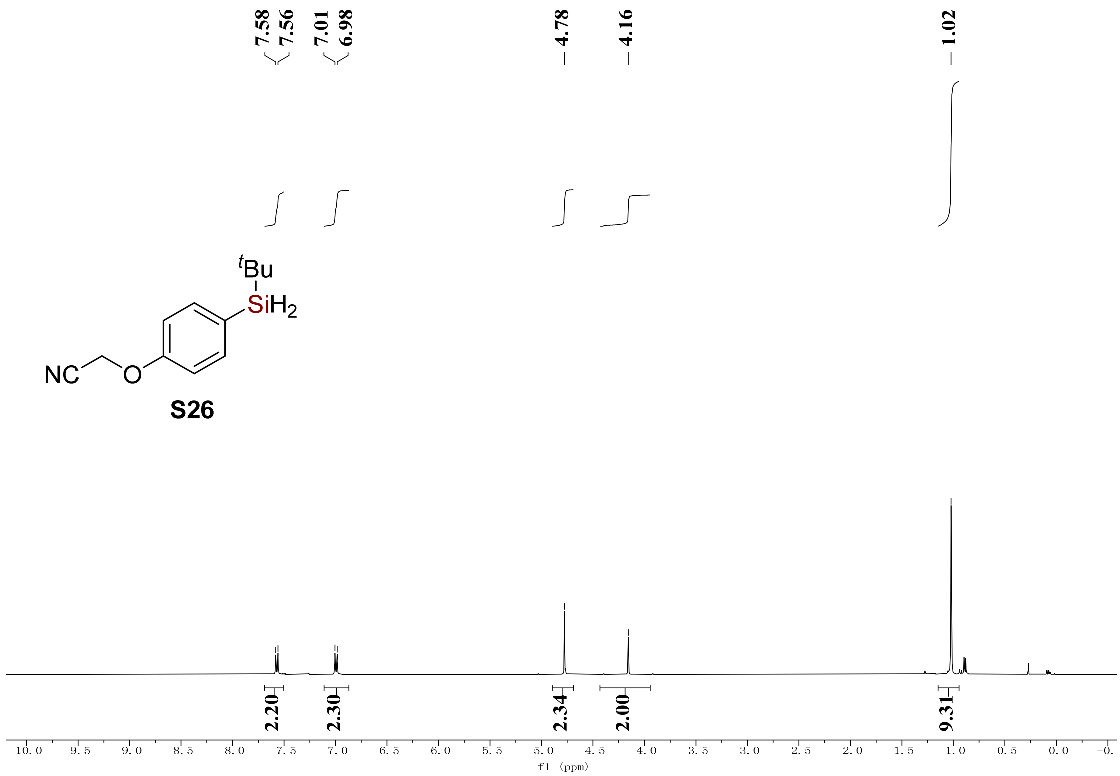
27.36
25.84
25.65
18.18
16.45
tBu
SiH2
Me
Me
O
S25
f1 (ppm)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7.56
7.01
6.98
4.78
4.16
1.02
tBu
SiH2
NC
O
S26
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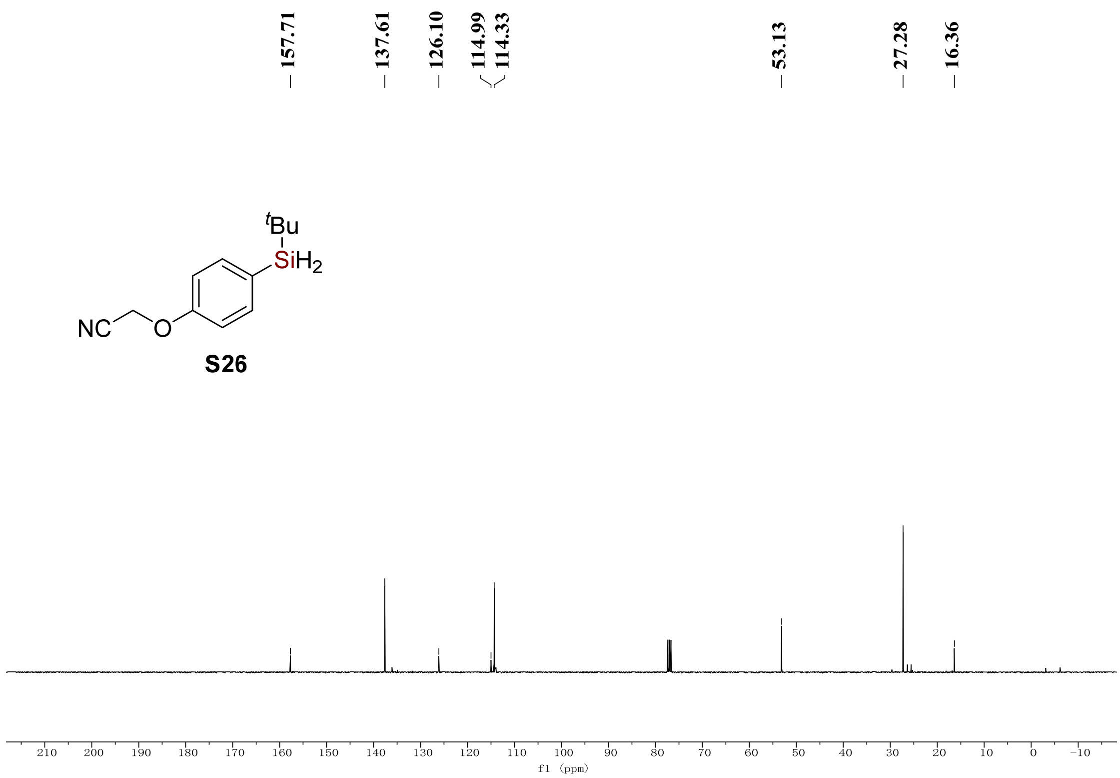
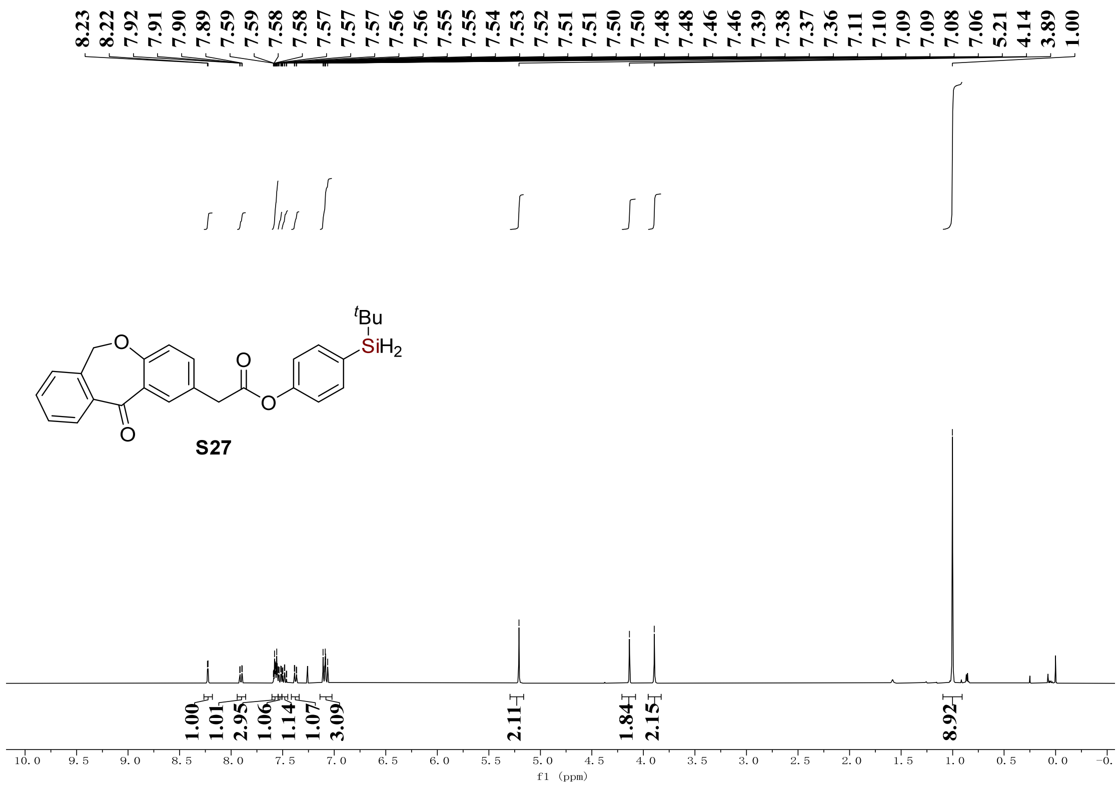
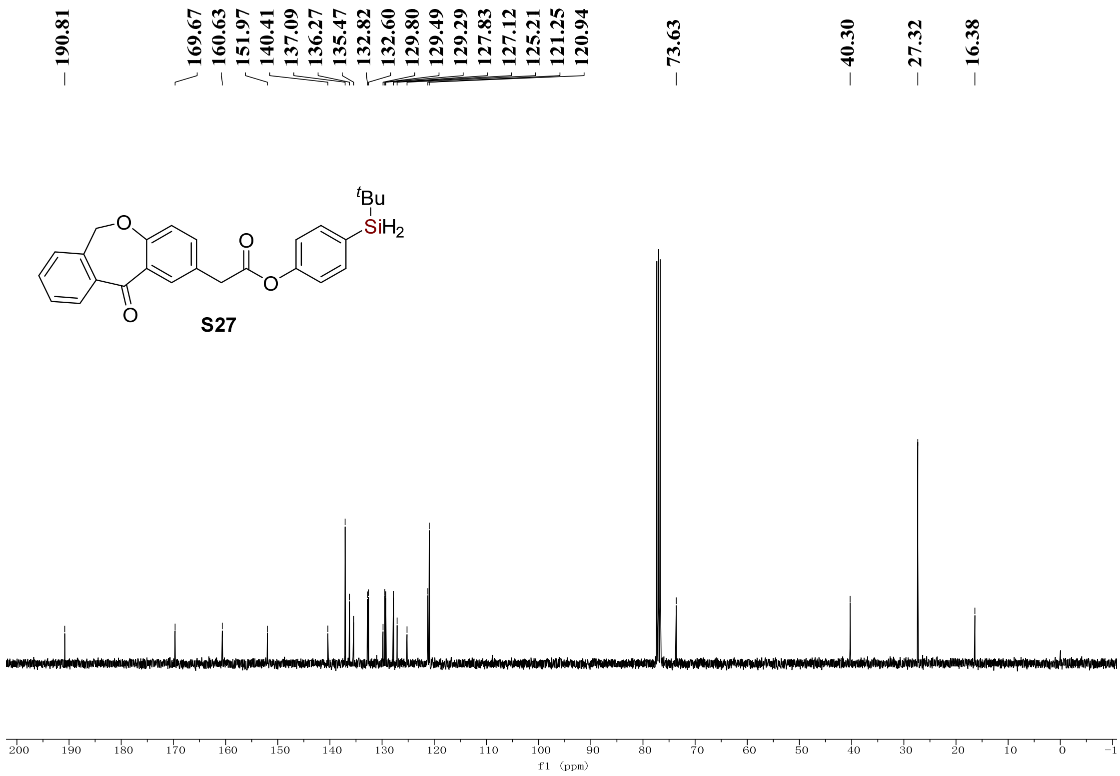
2.30
2.34
2.00
9.31
f1 (ppm)


157.71
137.61
126.10
114.99
114.33
53.13
27.28
16.36
tBu
SiH2
NC
O
S26
f1 (ppm)


8.23 8.22 7.92 7.91 7.90 7.89 7.59 7.59 7.58 7.58 7.57 7.57 7.57 7.56 7.56 7.55 7.55 7.54 7.53 7.52 7.51 7.51 7.50 7.50 7.48 7.48 7.46 7.46 7.39 7.38 7.37 7.36 7.11 7.10 7.09 7.09 7.08 7.06 5.21 4.14 3.89 1.00
tBu
SiH2
O
O
O
O
S27
1.00 1.01 2.95 1.06 1.14 1.07 3.09 2.11 1.84 2.15 8.92
f1 (ppm)


190.81 169.67 160.63 151.97 140.41 137.09 136.27 135.47 132.82 132.60 129.80 129.49 129.29 127.83 127.12 125.21 121.25 120.94 73.63 40.30 27.32 16.38
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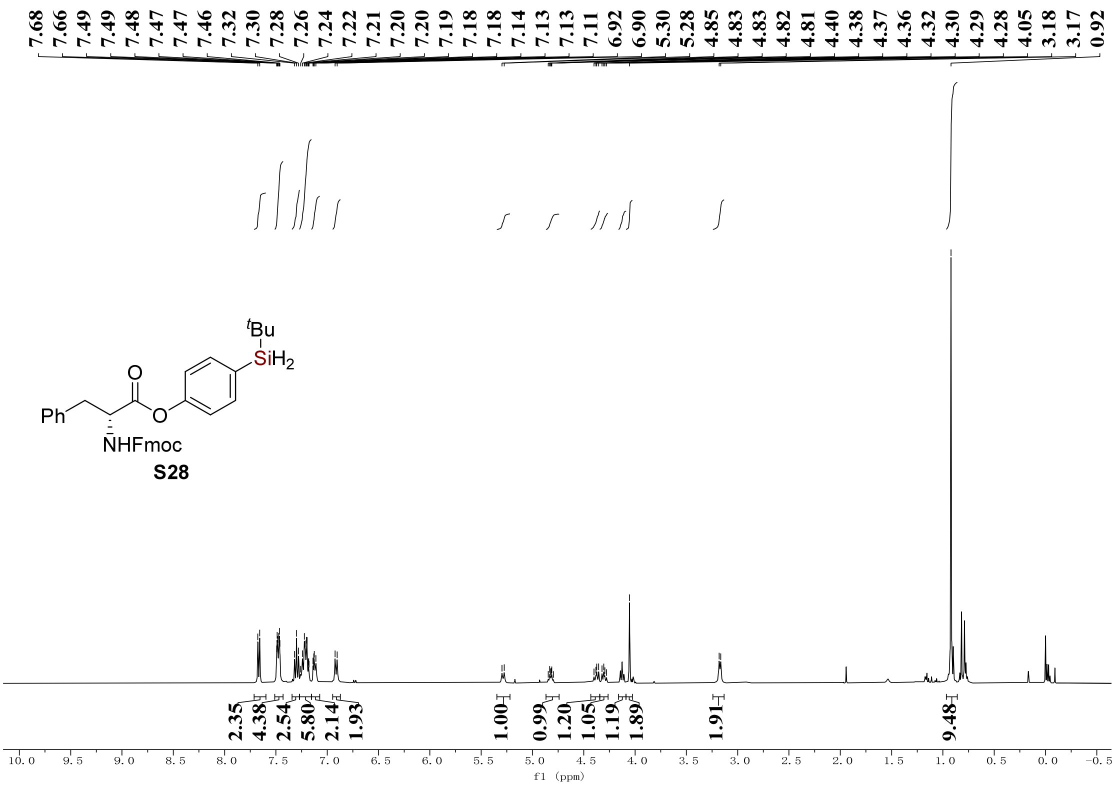
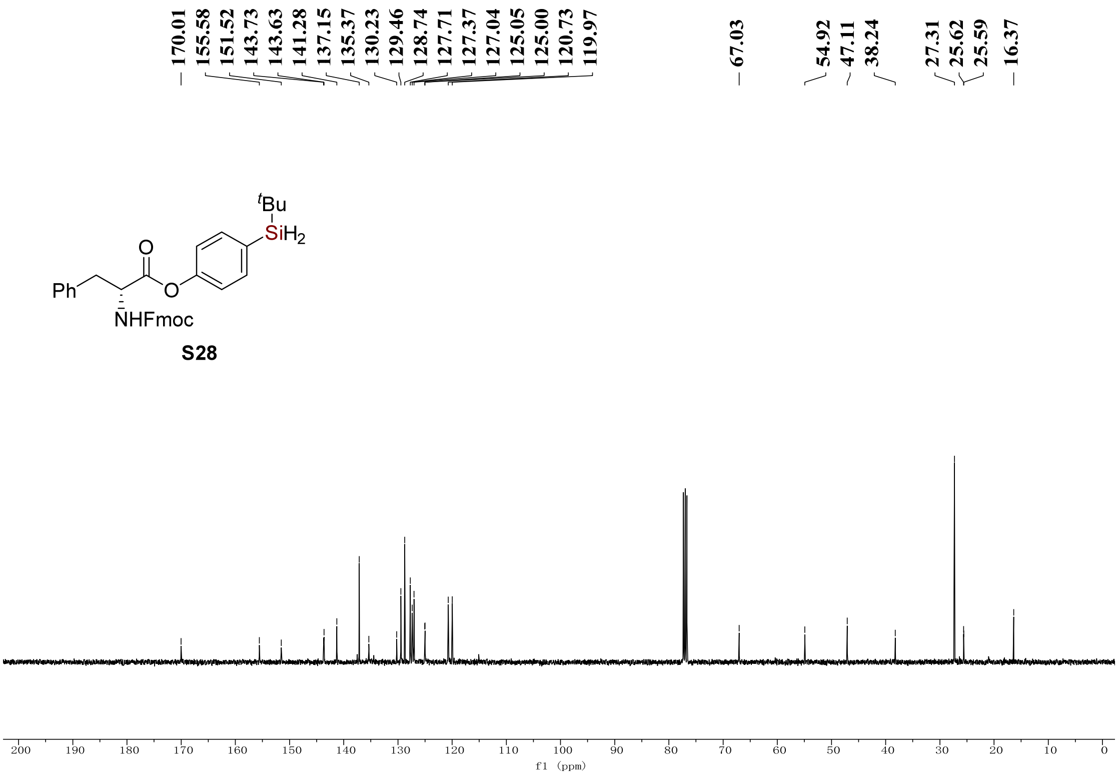
O
O
O
O
S27
f1 (ppm)


7.68 7.66 7.49 7.49 7.48 7.47 7.47 7.46 7.32 7.30 7.28 7.26 7.24 7.22 7.21 7.20 7.20 7.19 7.18 7.18 7.14 7.13 7.13 7.11 6.92 6.90 5.30 5.28 4.85 4.83 4.83 4.82 4.81 4.40 4.38 4.37 4.36 4.32 4.30 4.29 4.28 4.05 3.18 3.17 0.92
tBu
SiH2
O
Ph
O
NHFmoc
S28
2.35 4.38 2.54 5.80 2.14 1.93 1.00 0.99 1.20 1.05 1.19 1.89 1.91 9.48
f1 (ppm)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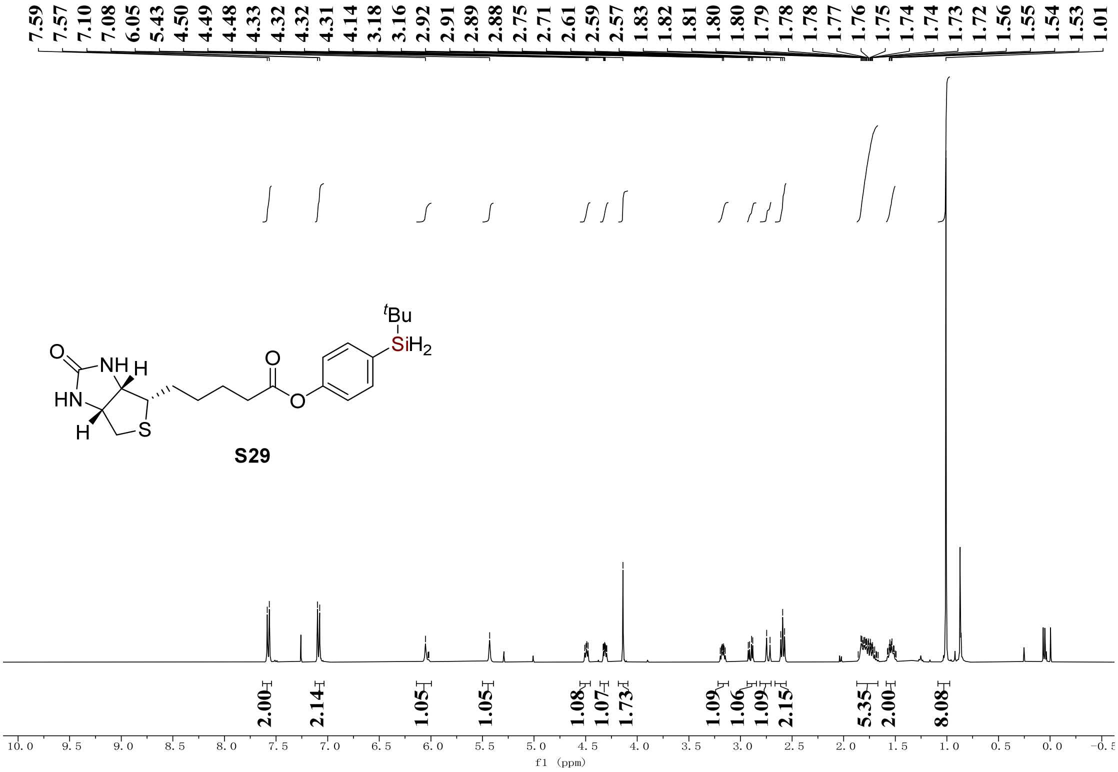
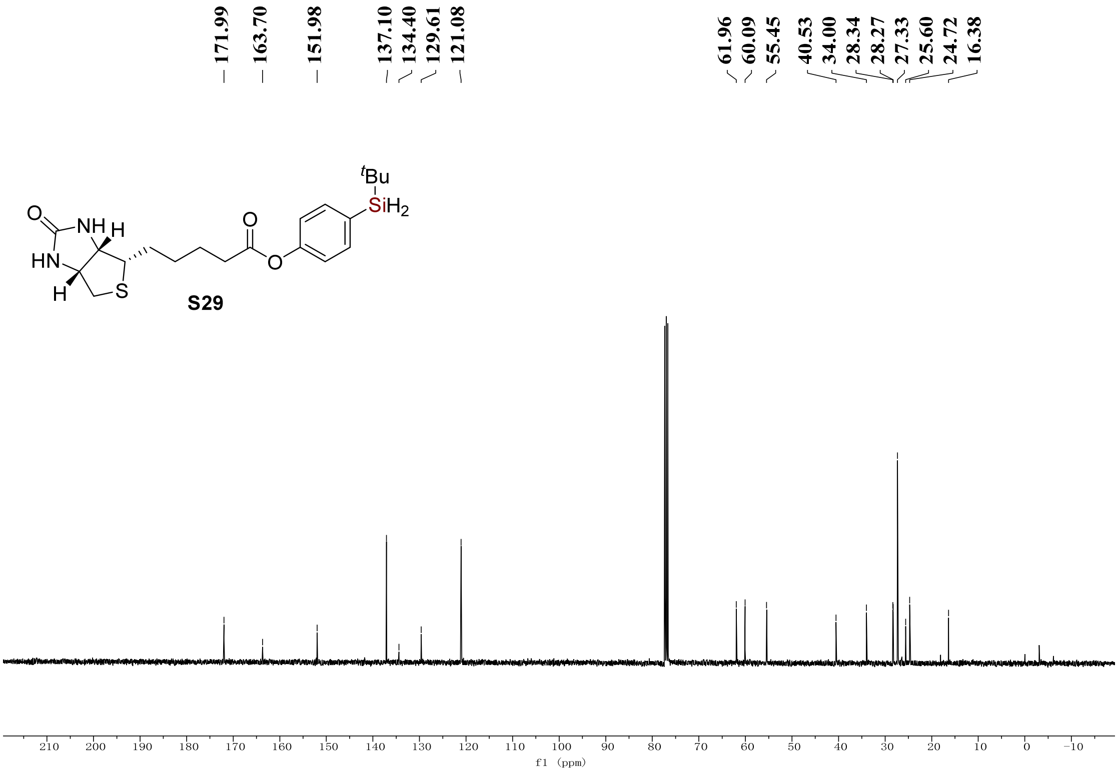
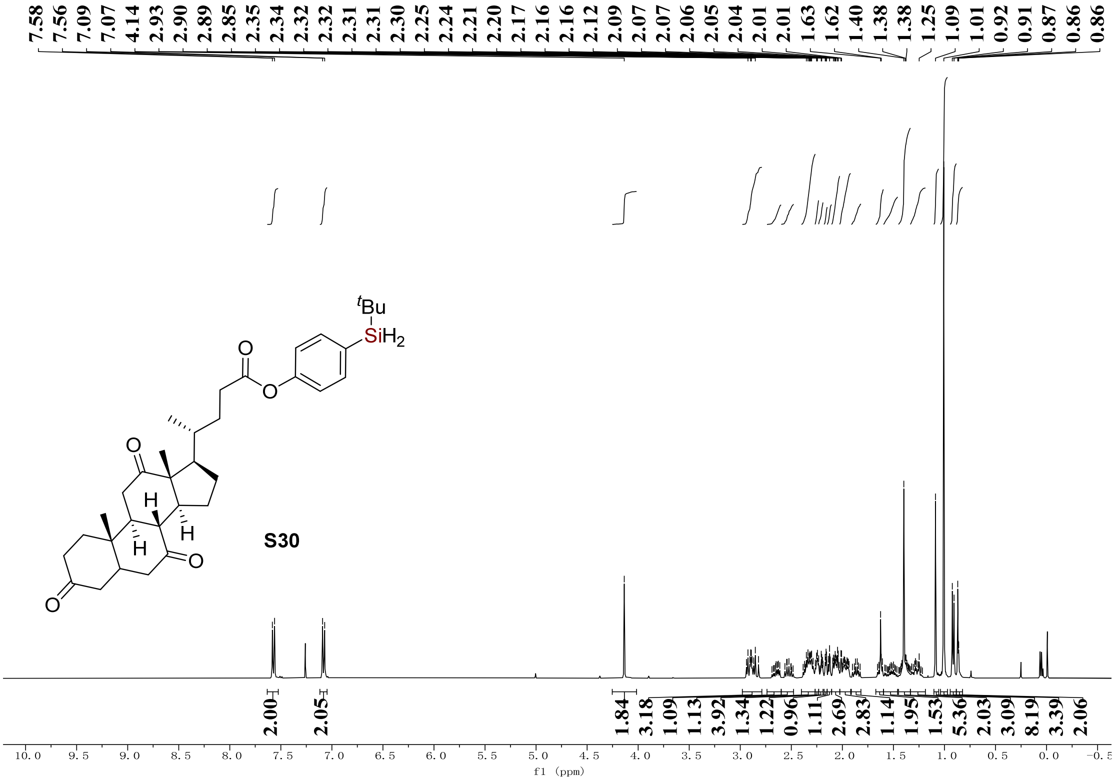
tBu
SiH2
O
Ph
O
NHFmoc
S28
f1 (ppm)



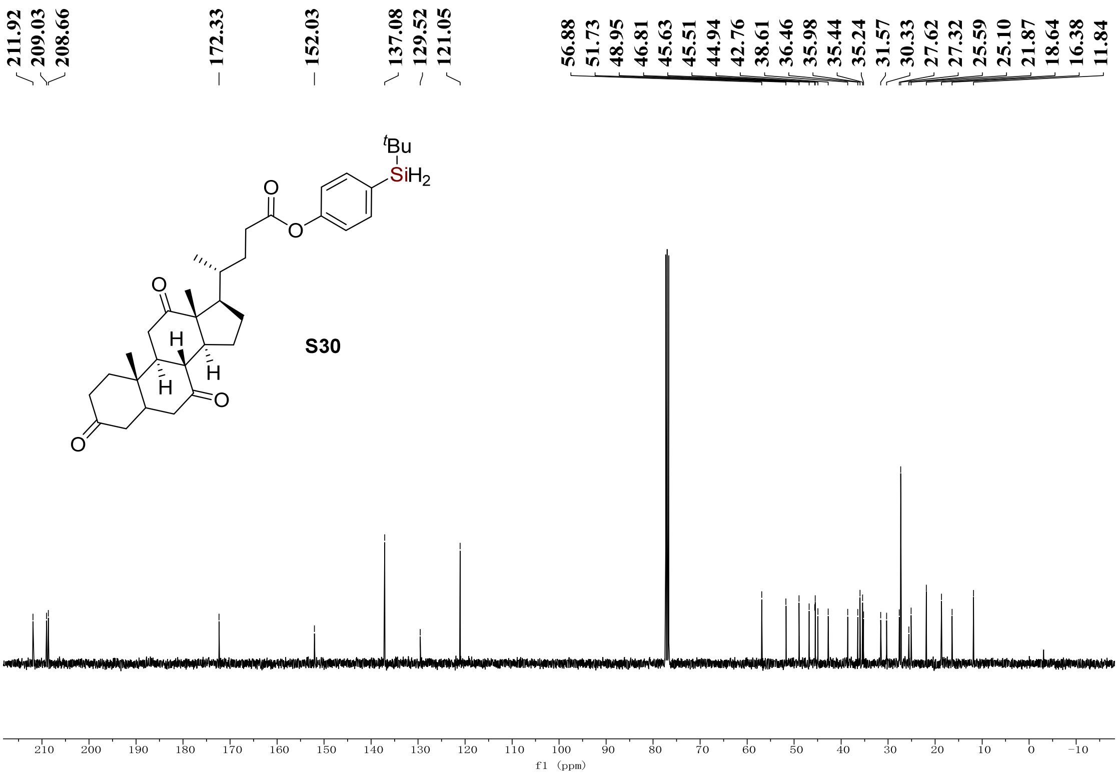
S29



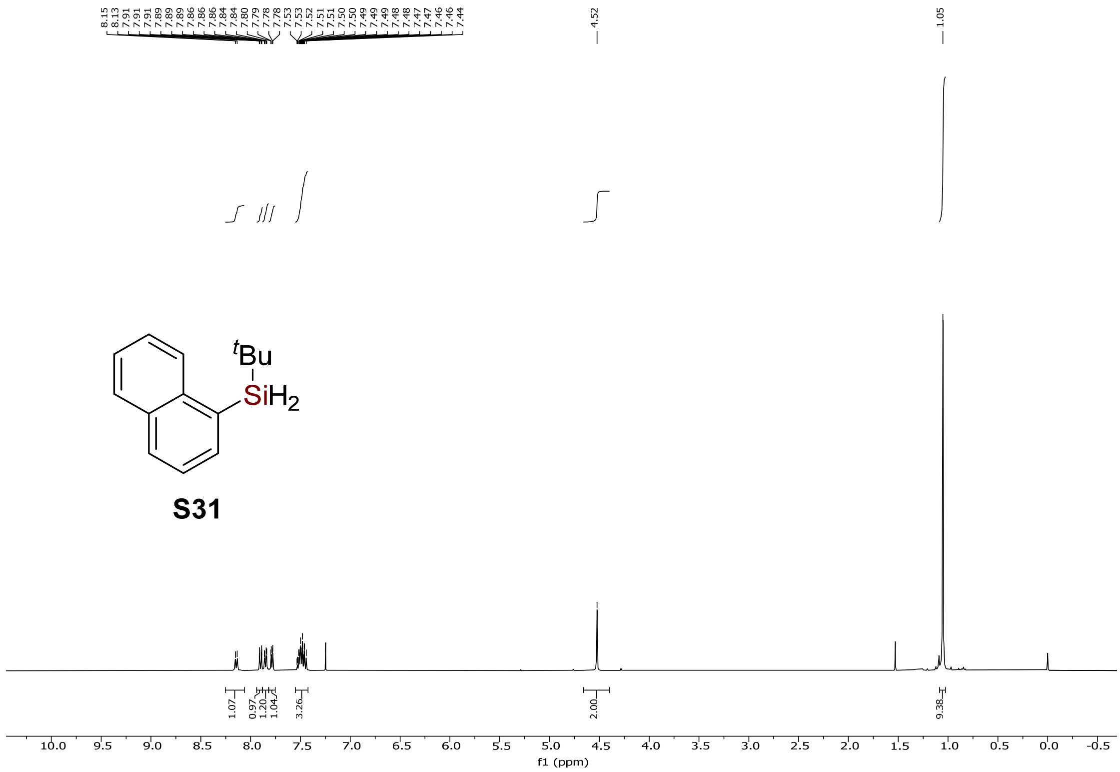
S29



S30



S30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7.79
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7.78
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7.50
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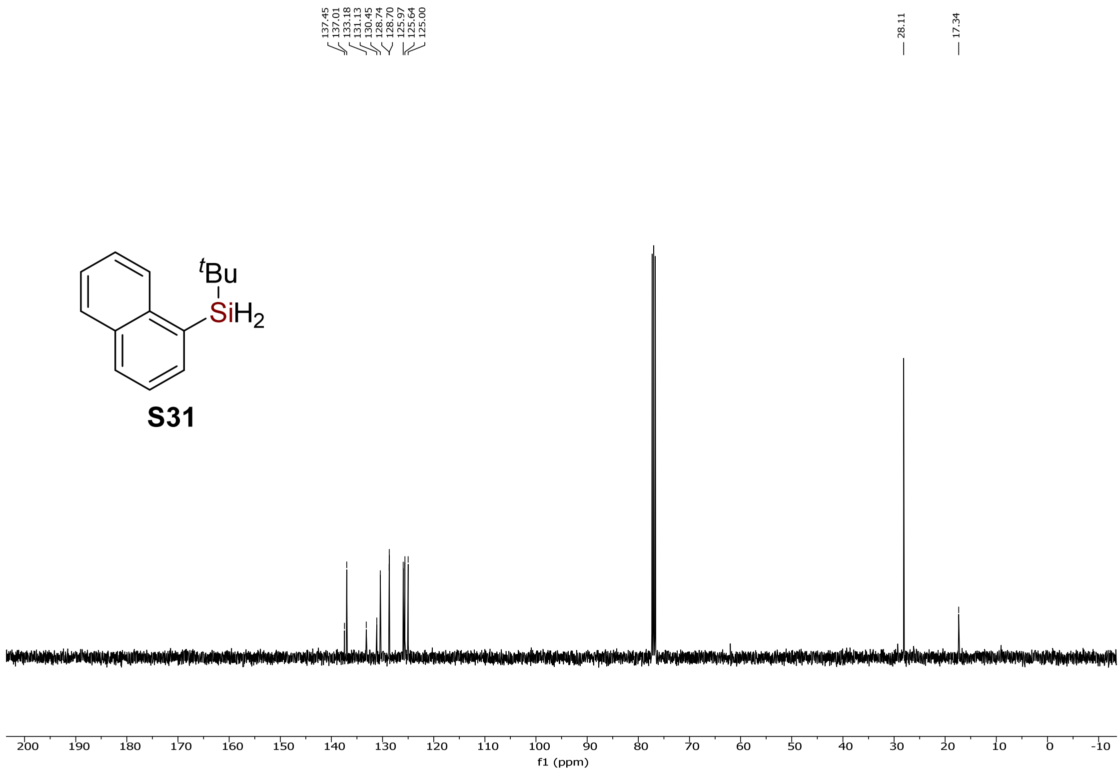
7.49
7.49
7.48
7.48
7.47
7.47
7.46
7.46
7.44
4.52
1.05
tBu
SiH2
S31
1.07
0.97
1.20
1.04
3.26
2.00
9.38
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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133.18
131.13
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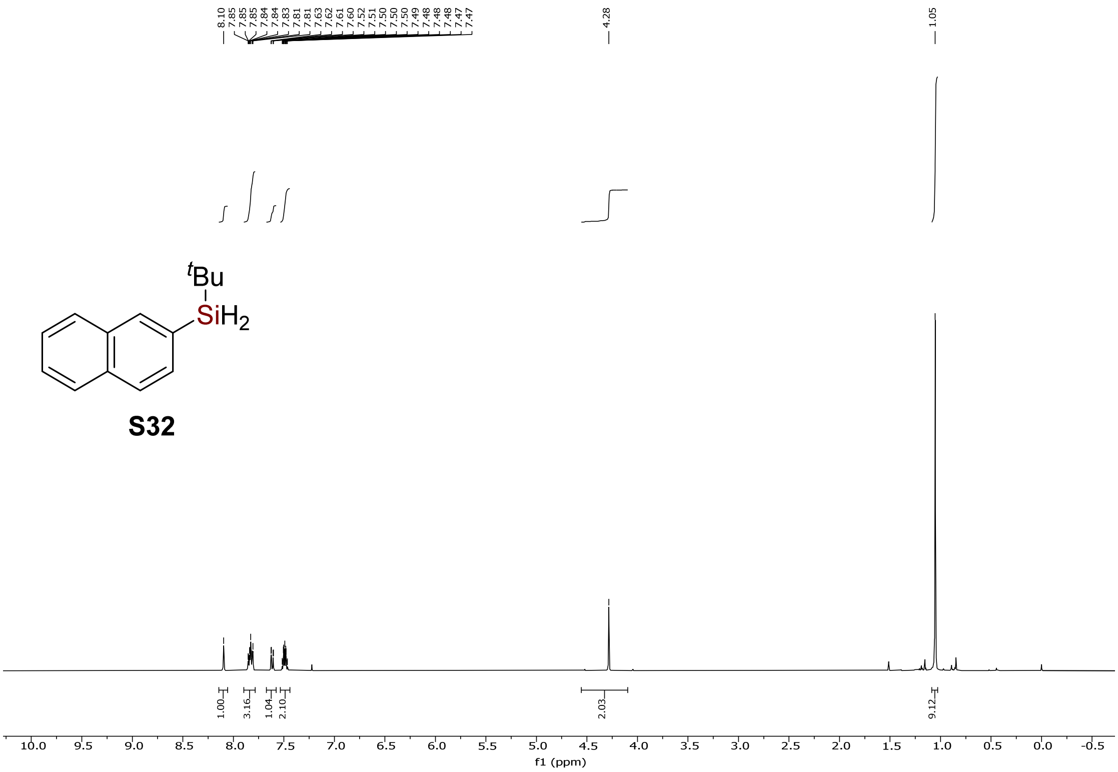
128.74
128.70
125.97
125.64
125.00
28.11
17.34
tBu
SiH2
S31
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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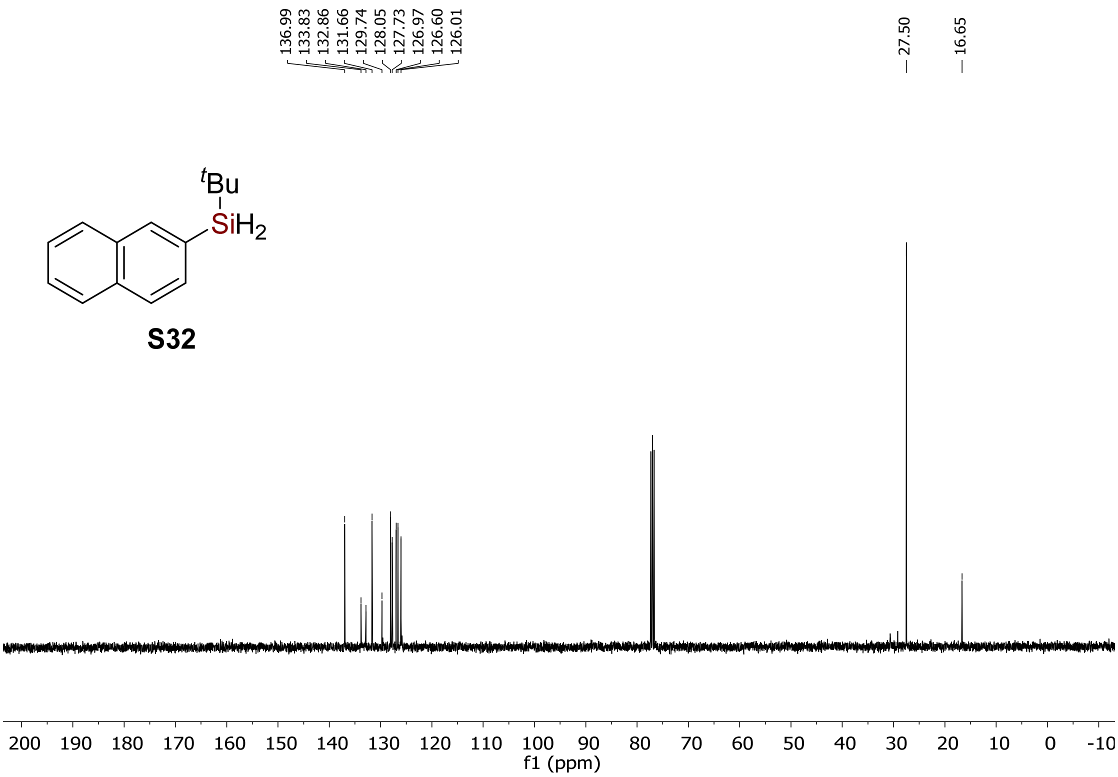
7.85
7.85
7.84
7.84
7.83
7.81
7.81
7.63
7.62
7.61
7.60
7.52
7.51
7.50
7.50
7.50
7.49
7.48
7.48
7.48
7.47
7.47
4.28
1.05
^{t}Bu
SiH$_2$
S32
1.00
3.16
1.04
2.10
2.03
9.12
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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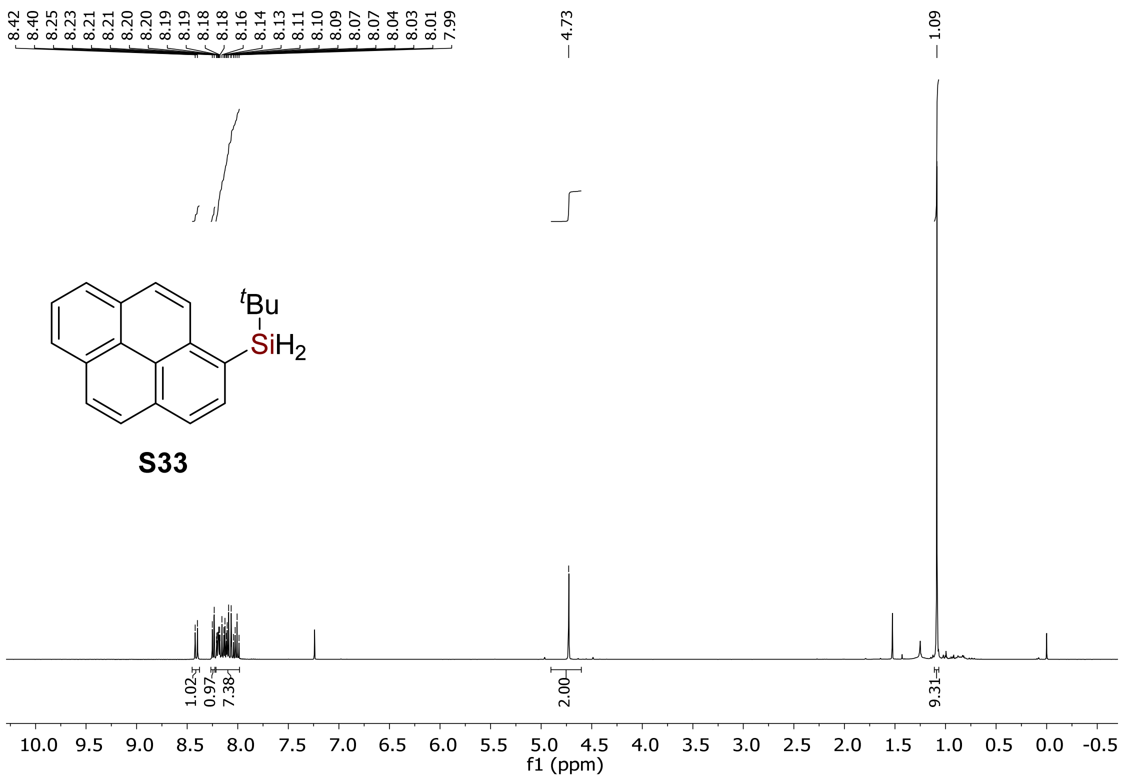
127.73
126.97
126.60
126.01
27.50
16.65
^{t}Bu
SiH$_2$
S32
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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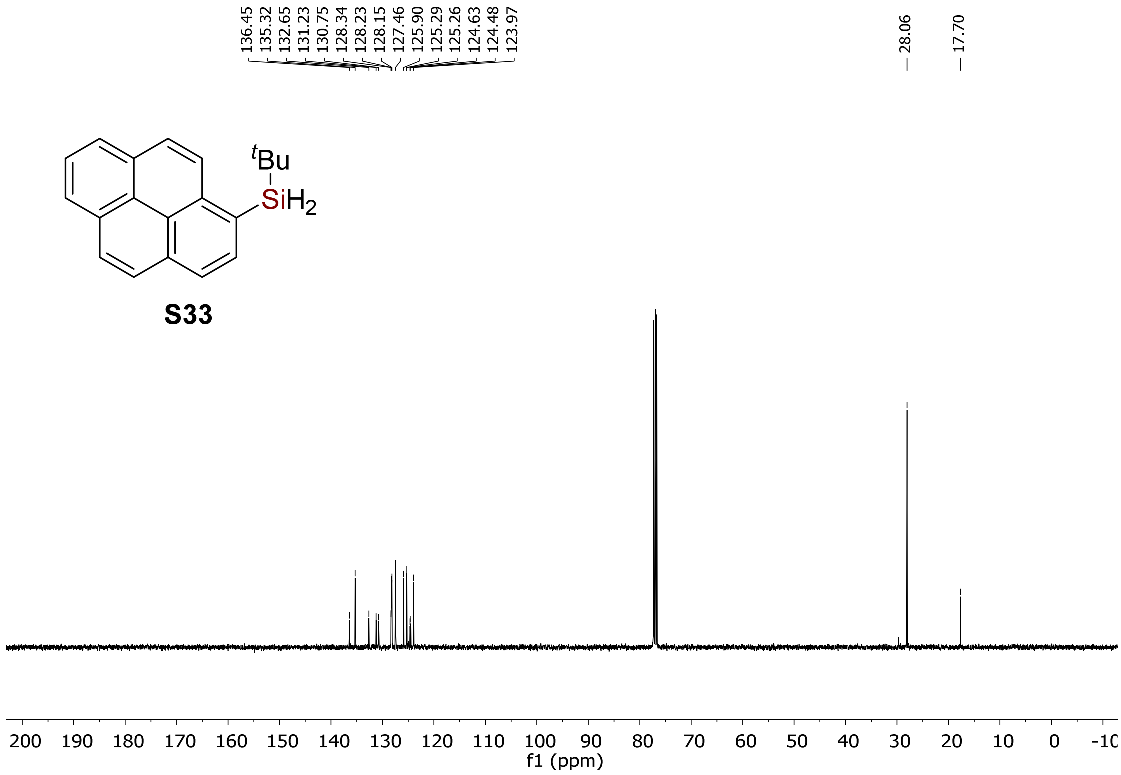
8.16
8.14
8.13
8.11
8.10
8.09
8.07
8.07
8.04
8.03
8.01
7.99
4.73
1.09
tBu
SiH2
S33
1.02
0.97
7.38
2.00
9.31
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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128.15
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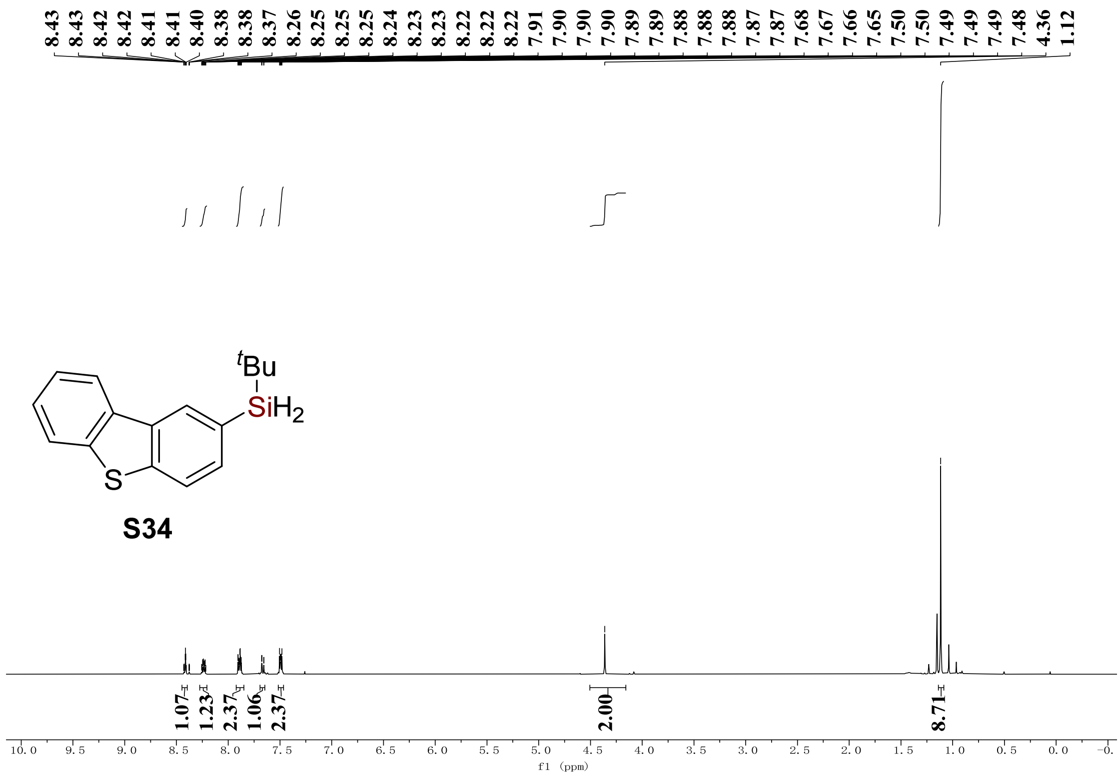
125.90
125.29
125.26
124.63
124.48
123.97
28.06
17.70
tBu
SiH2
S33
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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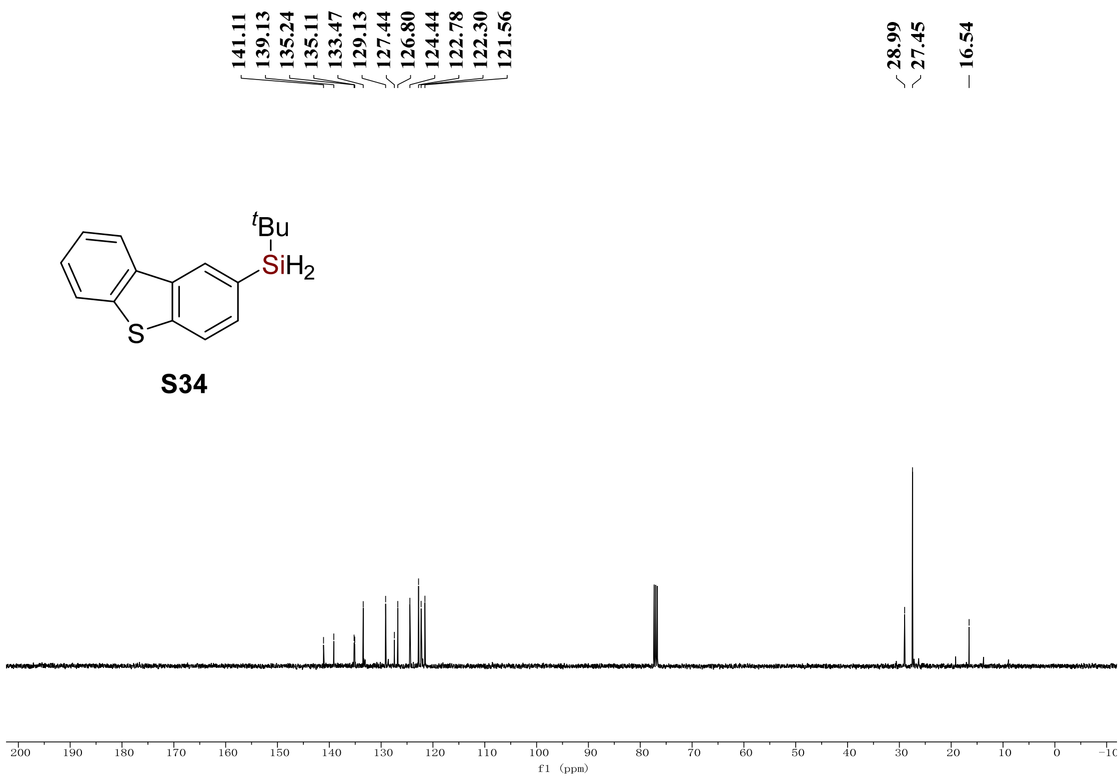
^{t}Bu
SiH$_2$
S
S34
1.07
1.23
2.37
1.06
2.37
2.00
8.71
f1 (ppm)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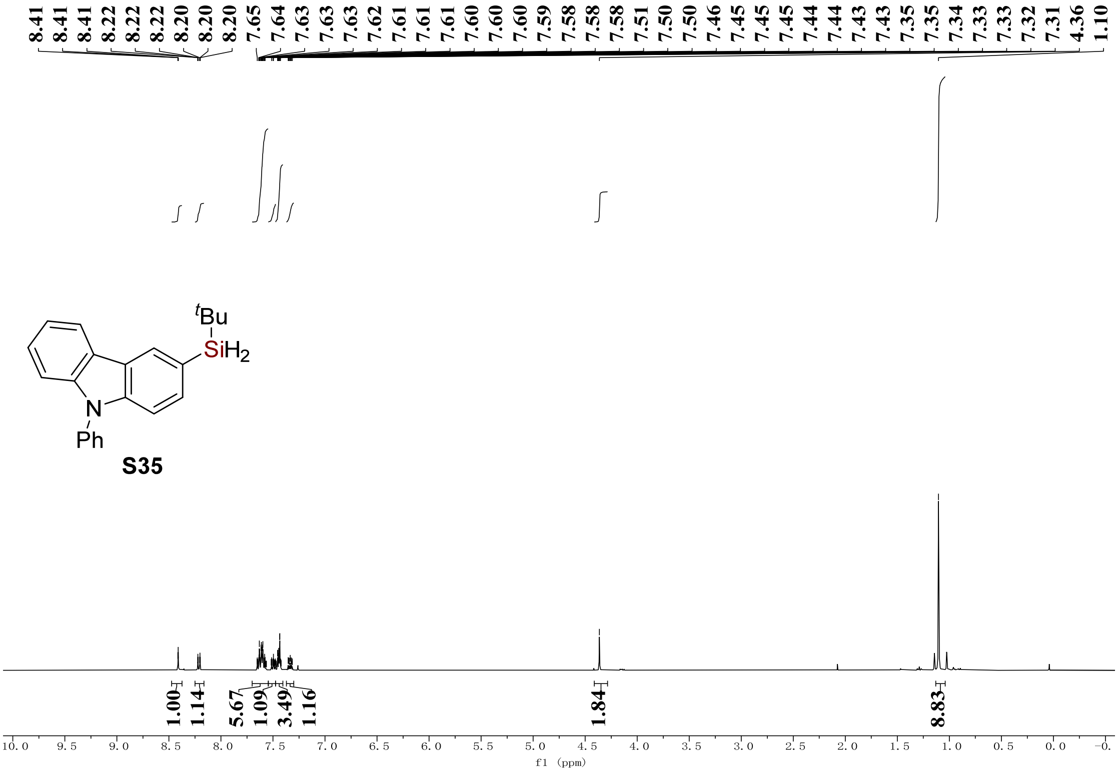
28.99 27.45
16.54
^{t}Bu
SiH$_2$
S
S34
f1 (ppm)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7.43
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7.33
7.33
7.32
7.31
4.36
1.10
tBu
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Ph
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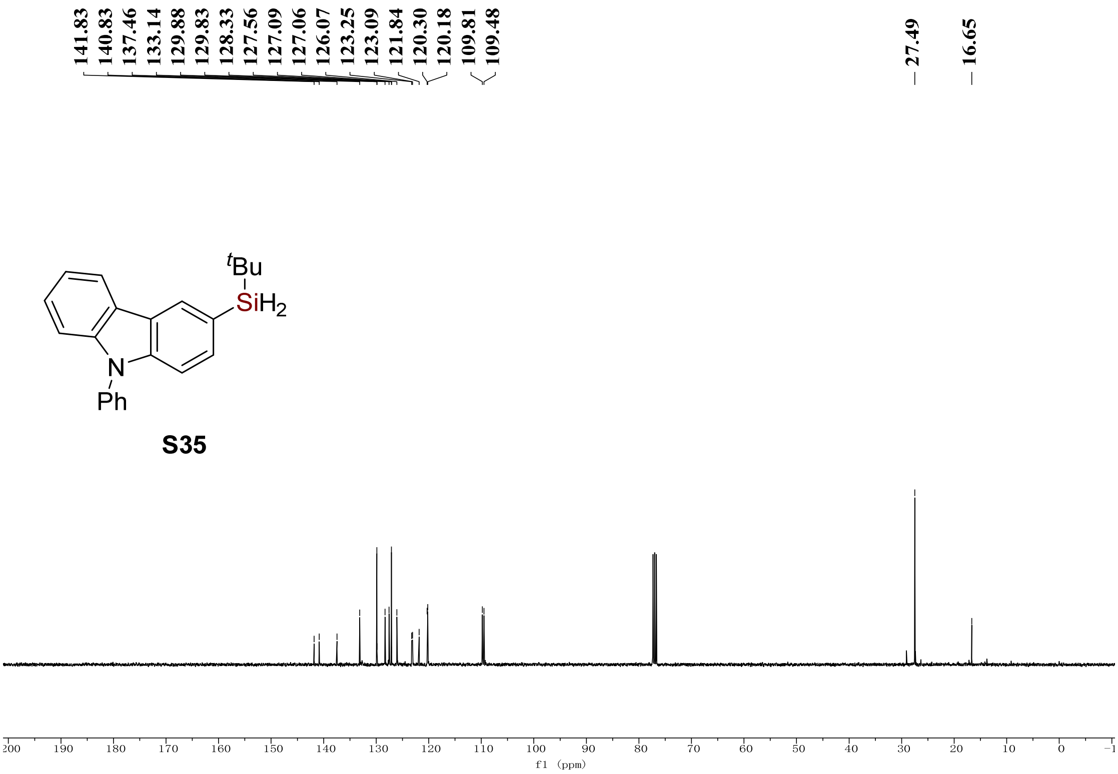
1.84
8.83
f1 (ppm)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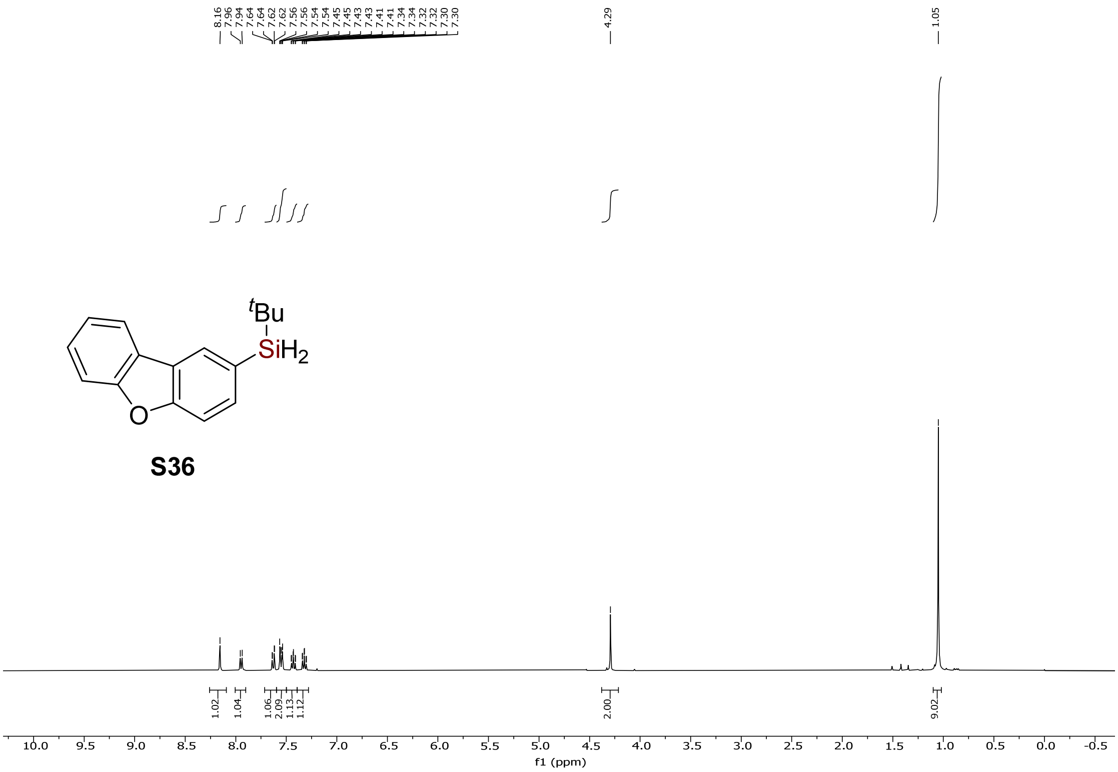
tBu
SiH2
N
Ph
S35
f1 (ppm)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7.45
7.43
7.43
7.41
7.34
7.34
7.32
7.32
7.30
7.30
4.29
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1.06
2.09
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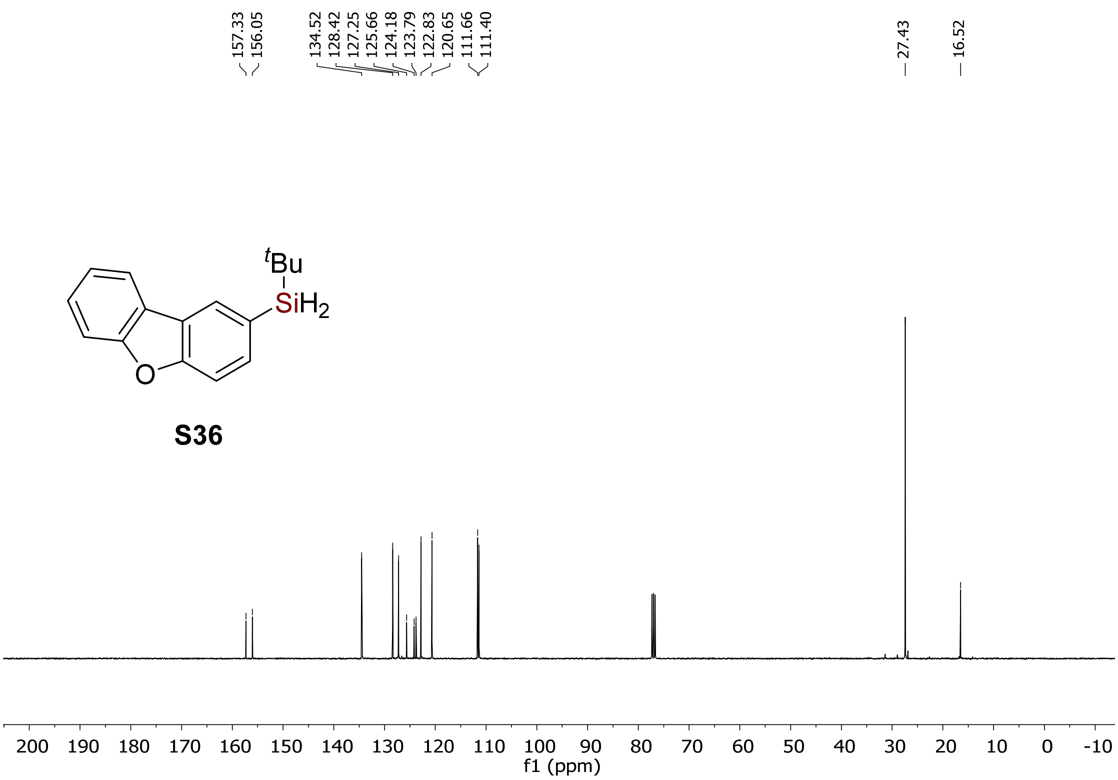
1.12
2.00
9.02
f1 (ppm)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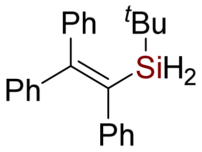
tBu
SiH2
O
S36
f1 (ppm)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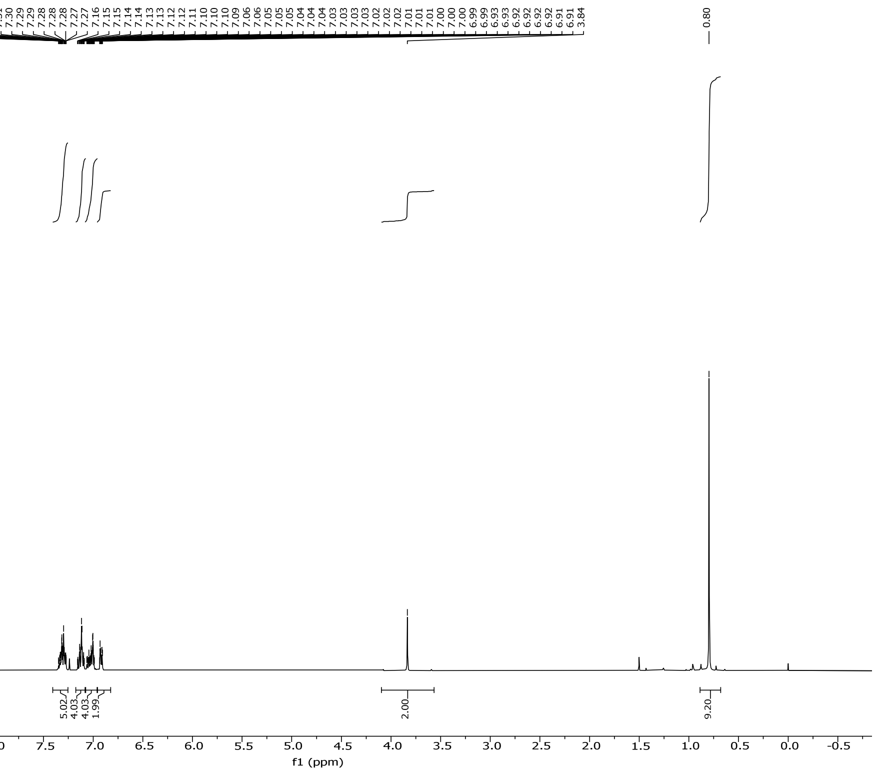
tBu
Ph
SiH2
Ph

S37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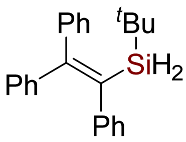
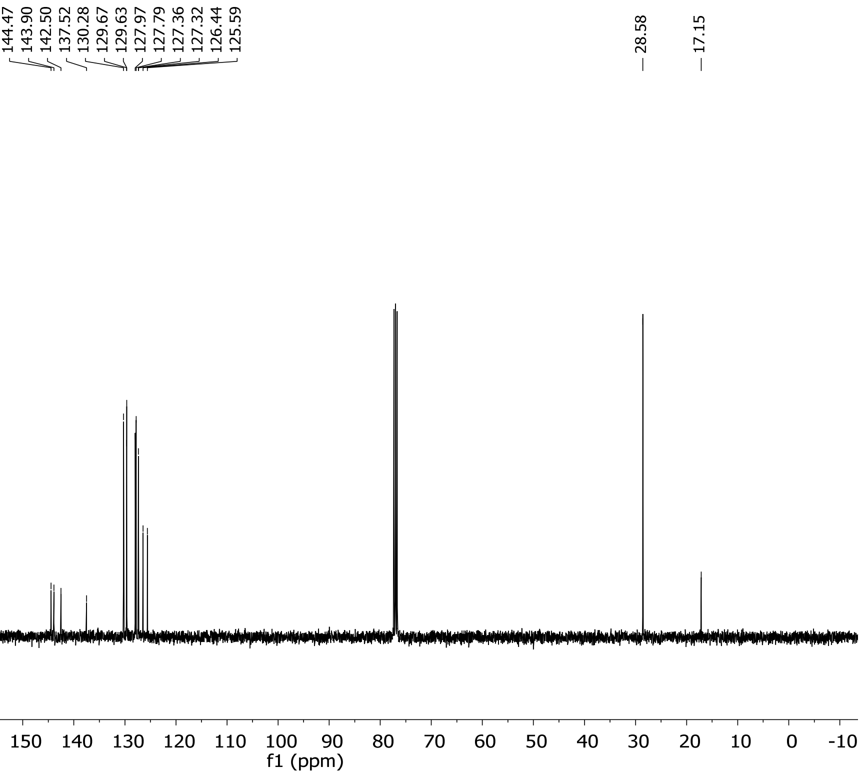
6.91
6.91
3.84
0.80
5.02
4.03
4.03
1.99
2.00
9.20
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


Ph
tBu
Ph
SiH2
Ph

S37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137.52
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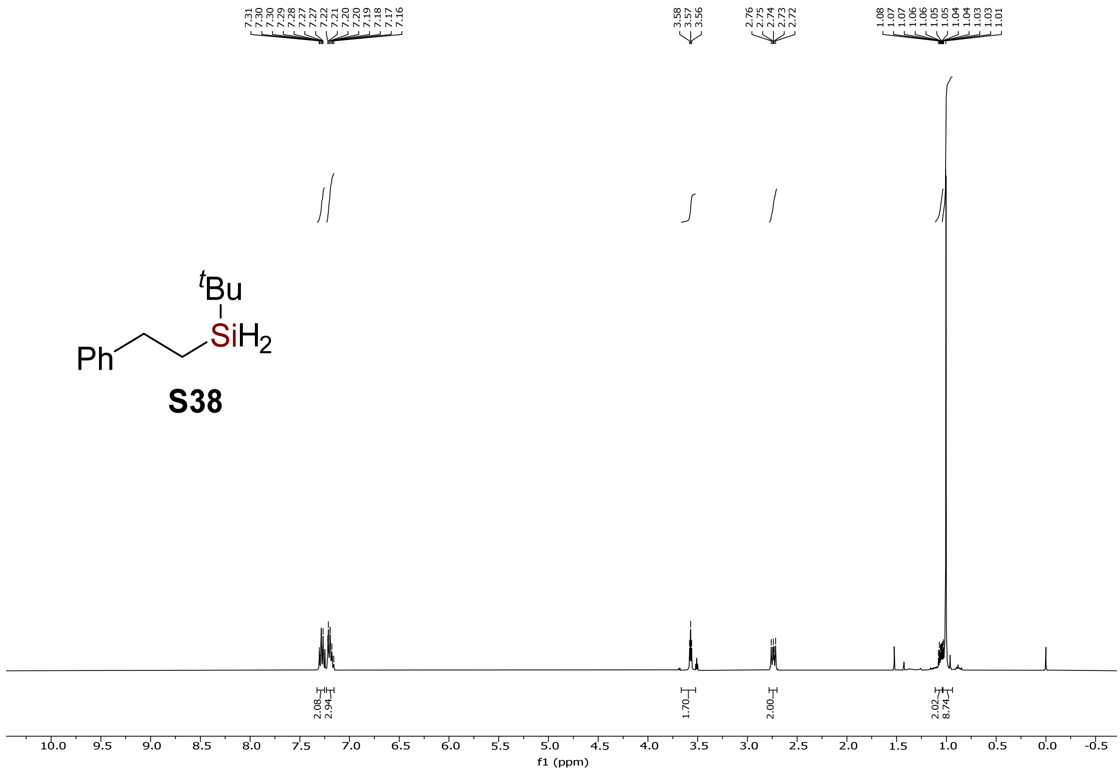
129.63
127.97
127.79
127.36
127.32
126.44
125.59
28.58
17.15
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



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7.30
7.30
7.29
7.28
7.27
7.27
7.22
7.21
7.20
7.20
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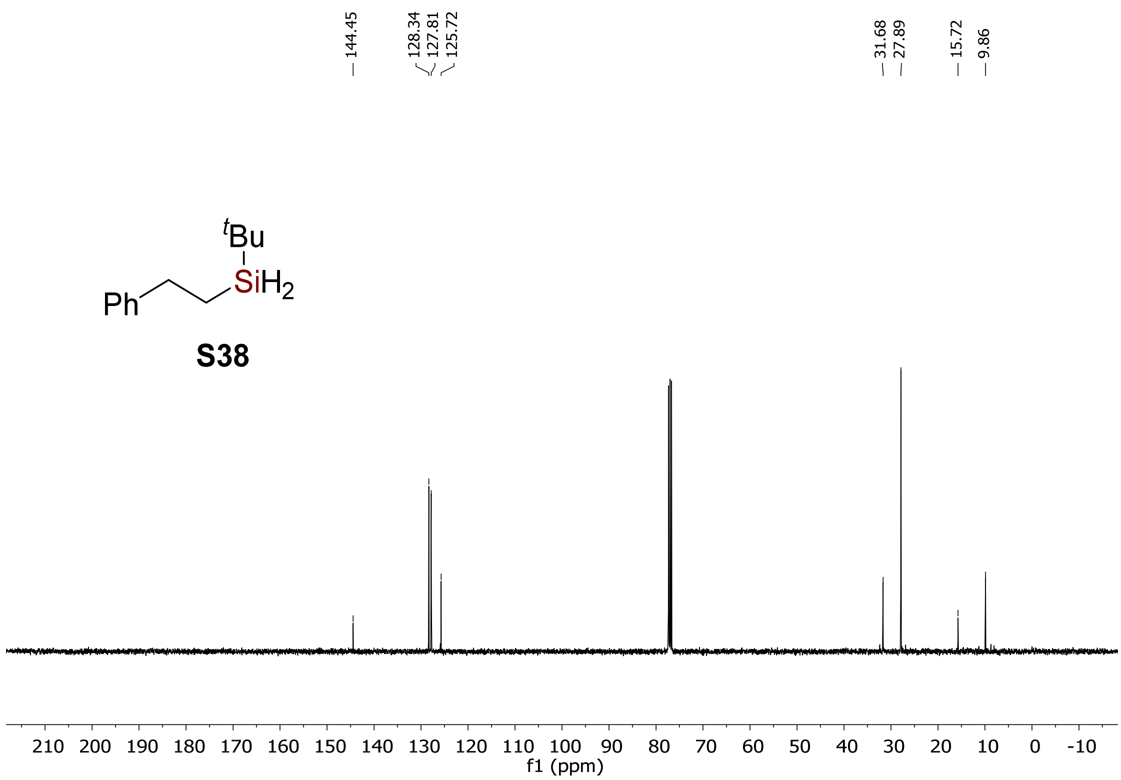
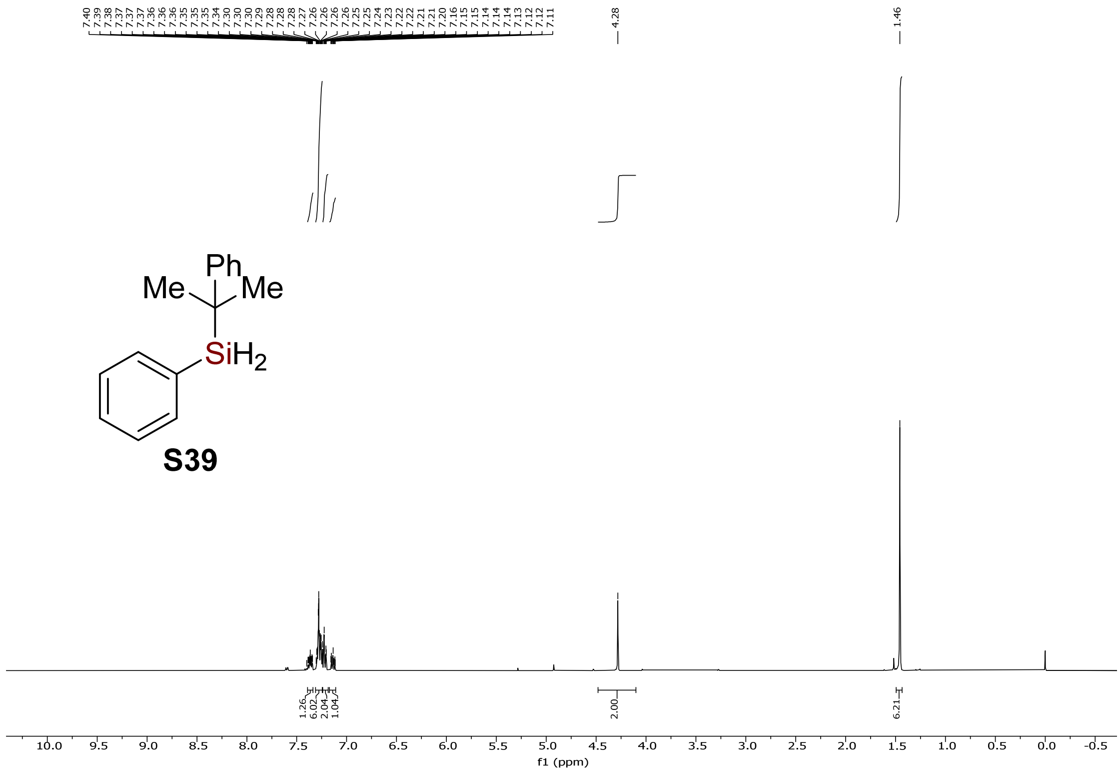
7.18
7.17
7.16
3.58
3.57
3.56
2.76
2.75
2.74
2.73
2.72
1.08
1.07
1.07
1.06
1.06
1.05
1.05
1.04
1.04
1.03
1.03
1.01
tBu
SiH2
Ph
S38
2.08
2.94
1.70
2.00
2.02
8.74
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)



144.45
128.34
127.81
125.72
31.68
27.89
15.72
9.86
tBu
SiH2
Ph
S38
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)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1.46
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Me
Me
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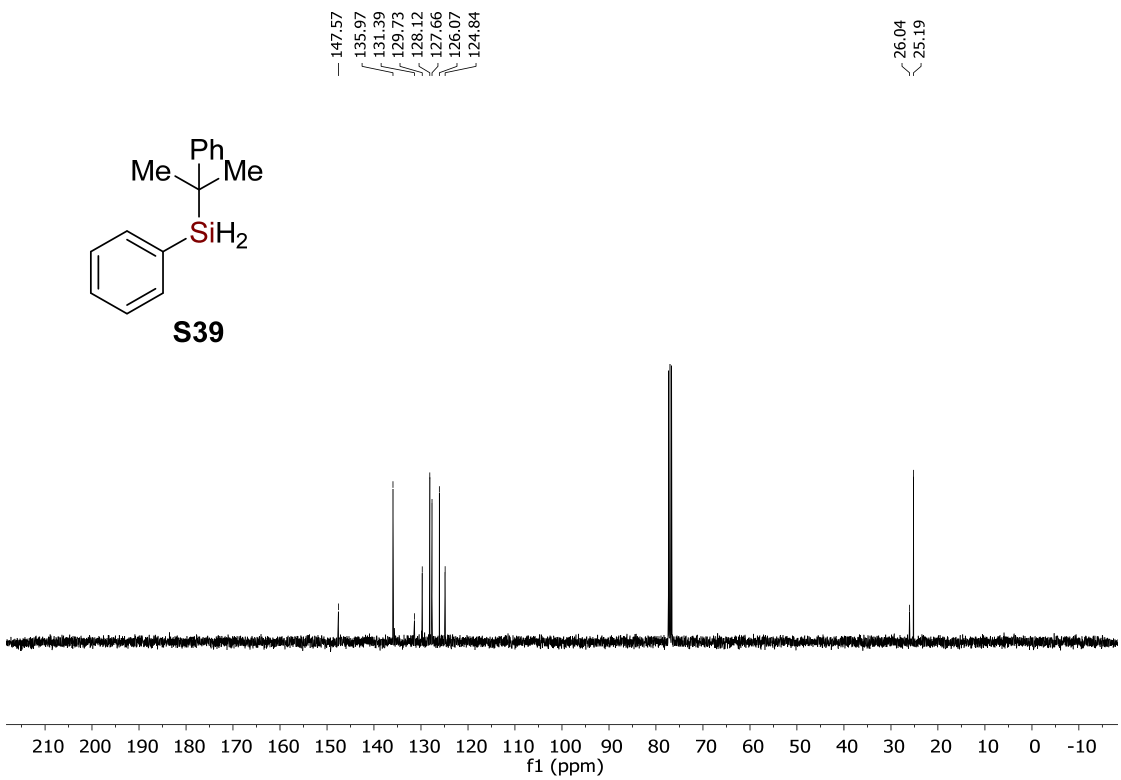
S39
2.00
6.21
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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135.97
131.39
129.73
128.12
127.66
126.07
124.84
26.04
25.19
Ph
Me
Me
SiH2
S39
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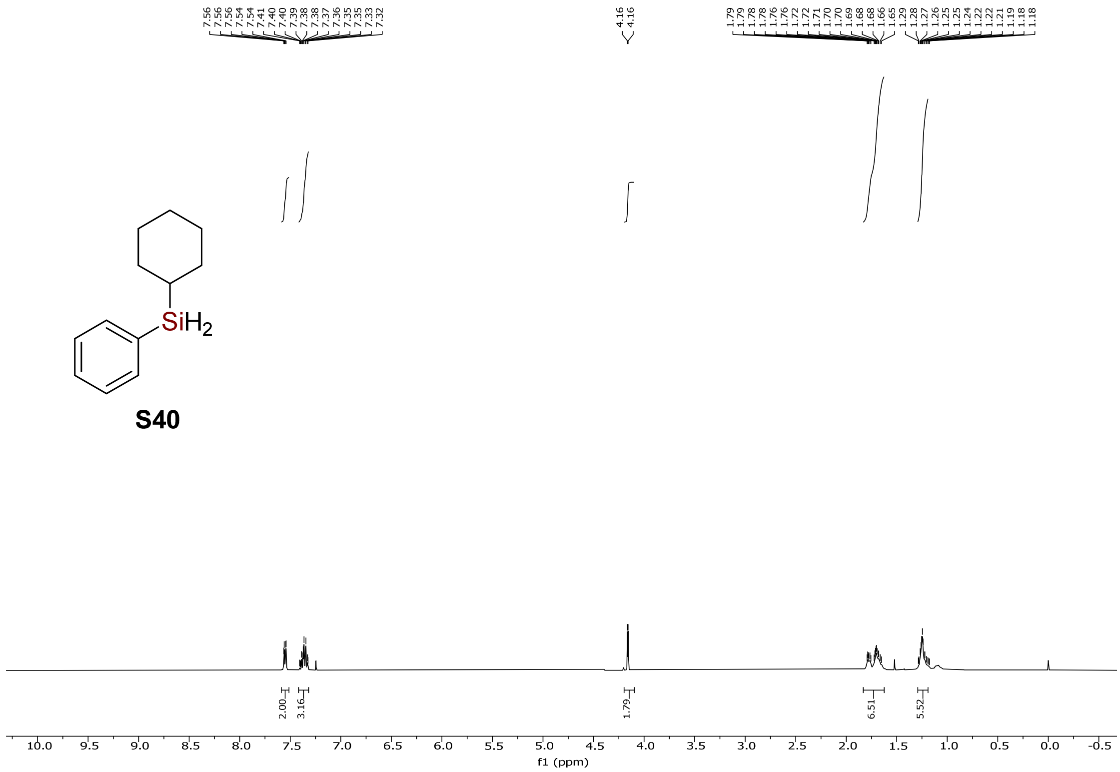
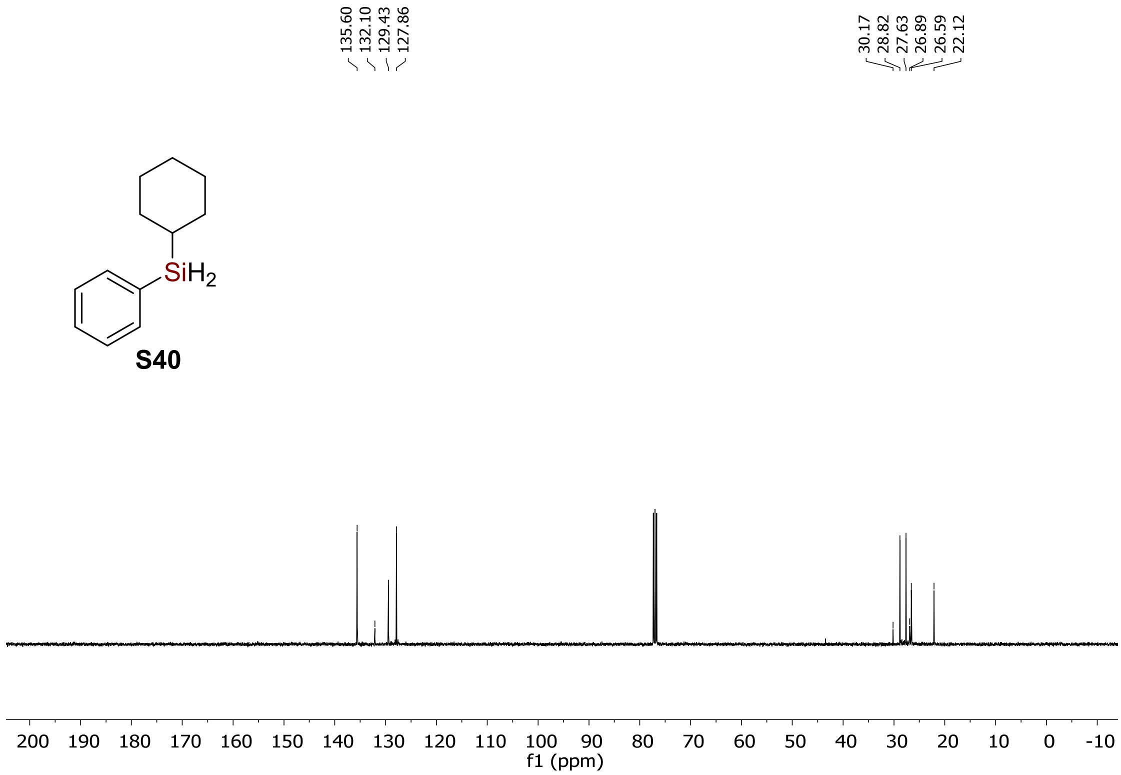
f1 (ppm)



S40



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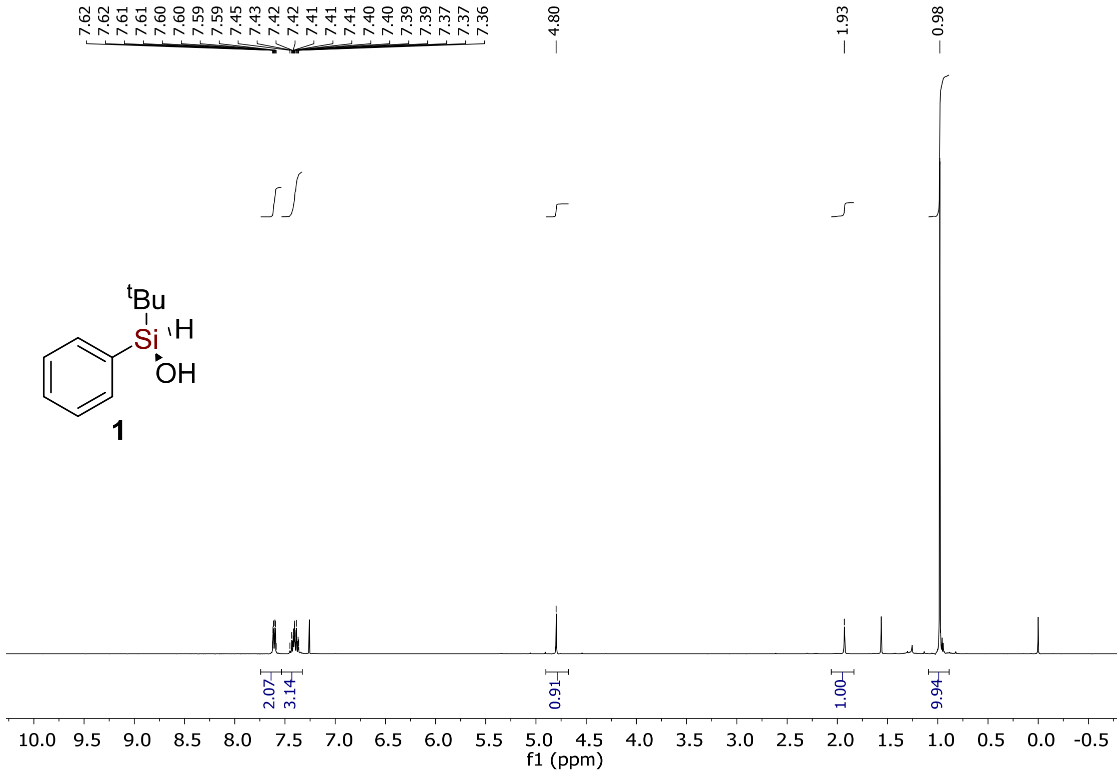
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4.80
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tBu
Si
H
OH
1
2.07
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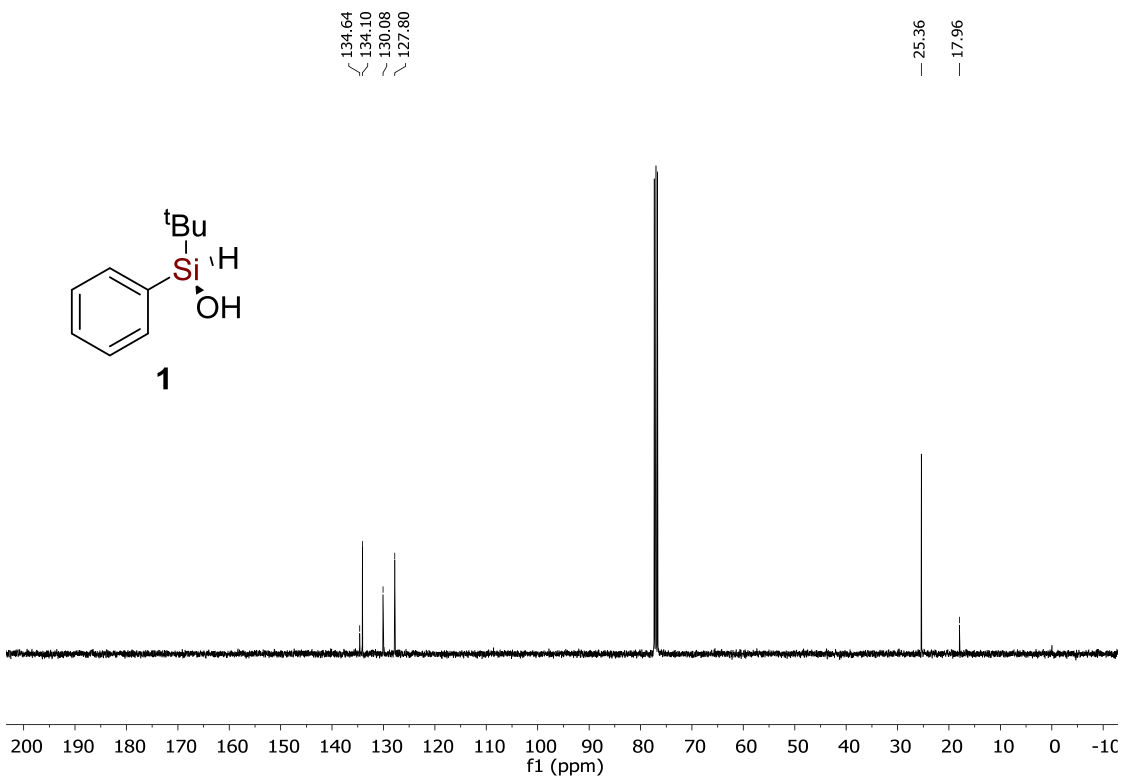
0.91
1.00
9.94
f1 (ppm)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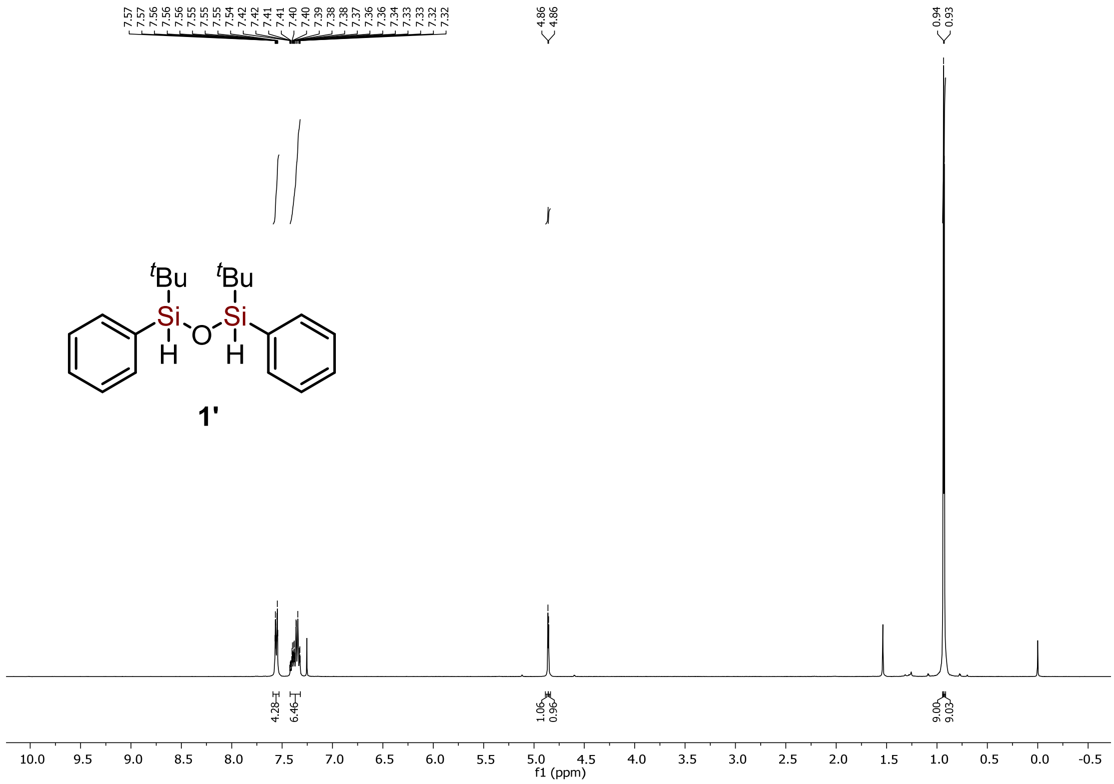
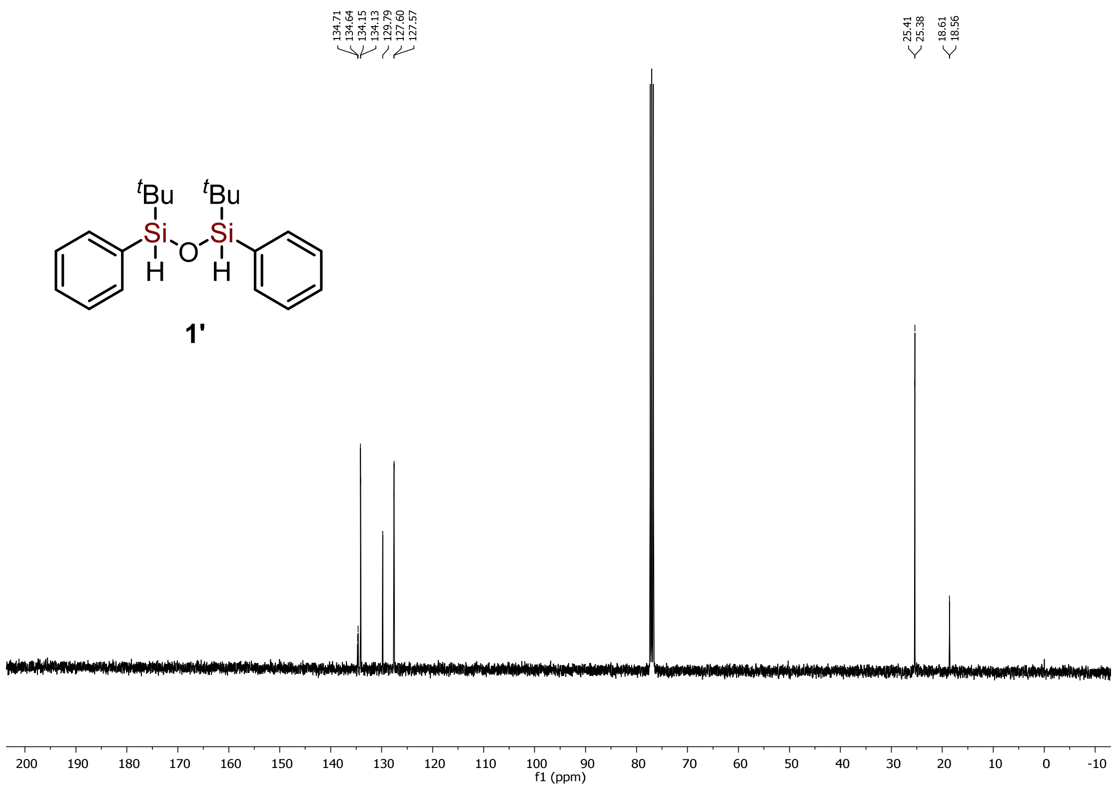
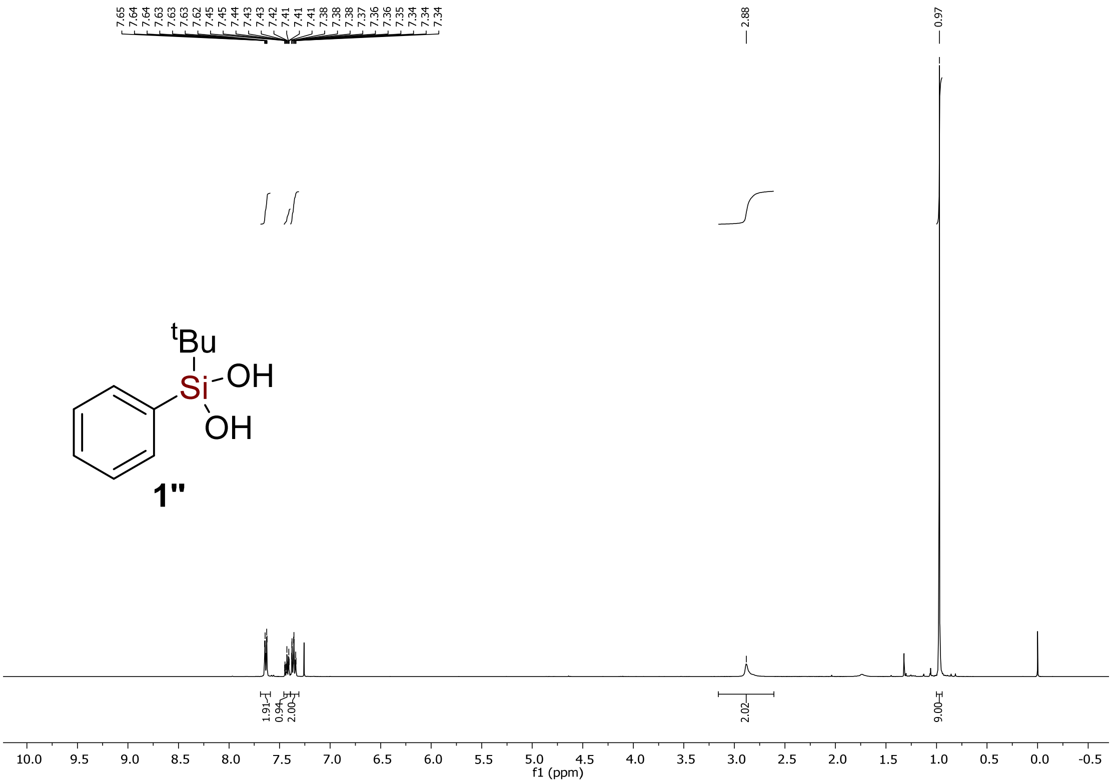
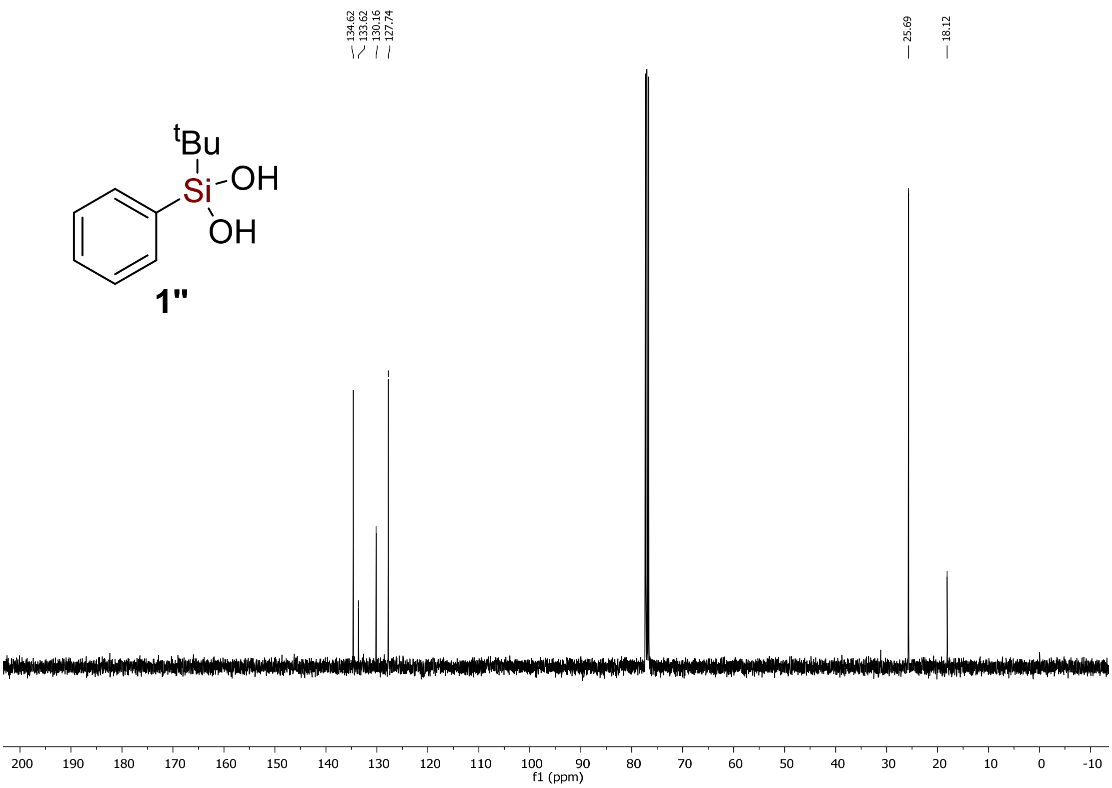
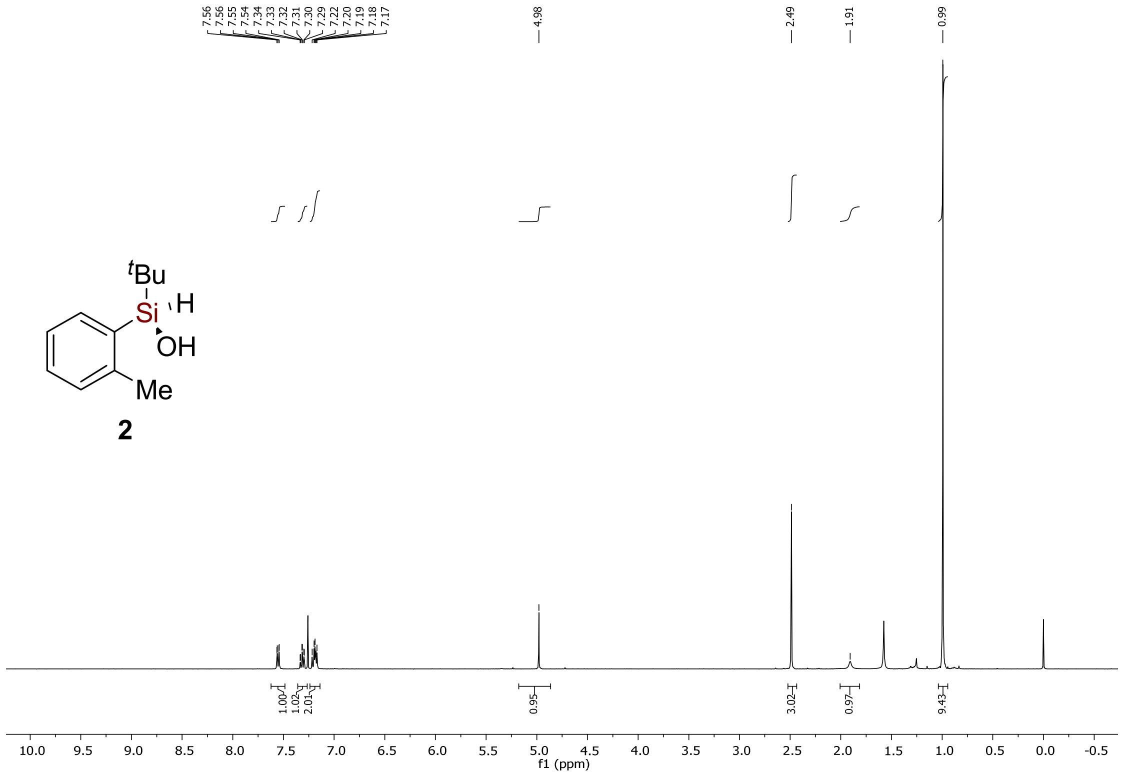
Si
H
OH
1
f1 (ppm)







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7.22
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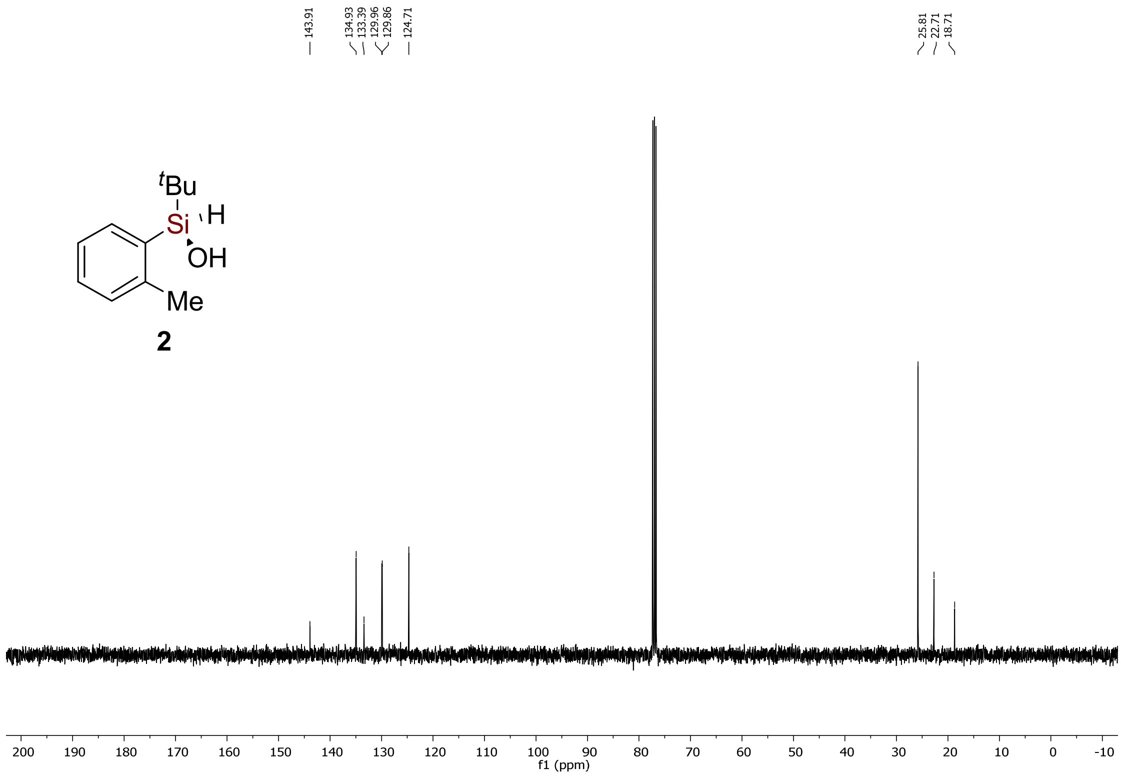
7.19
7.18
7.17
4.98
2.49
1.91
0.99
tBu
Si
H
OH
Me
2
1.00
1.02
2.01
0.95
3.02
0.97
9.43
f1 (ppm)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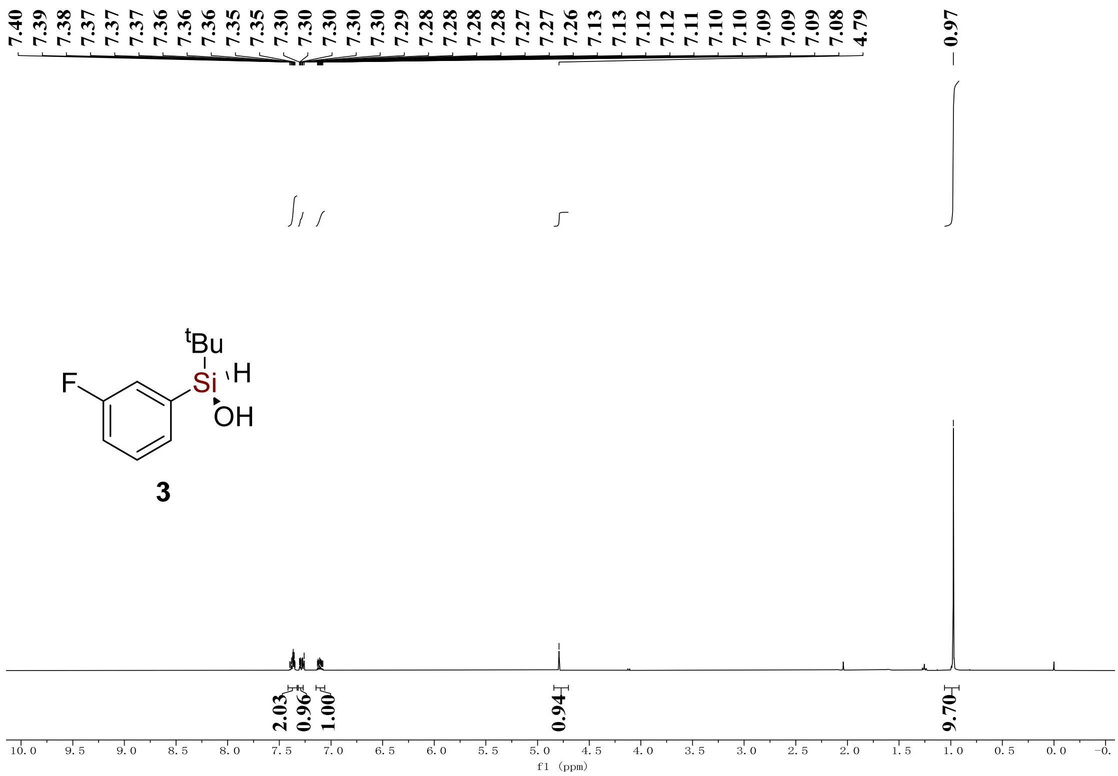
22.71
18.71
tBu
Si
H
OH
Me
2
f1 (ppm)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7.30
7.30
7.29
7.28
7.28
7.28
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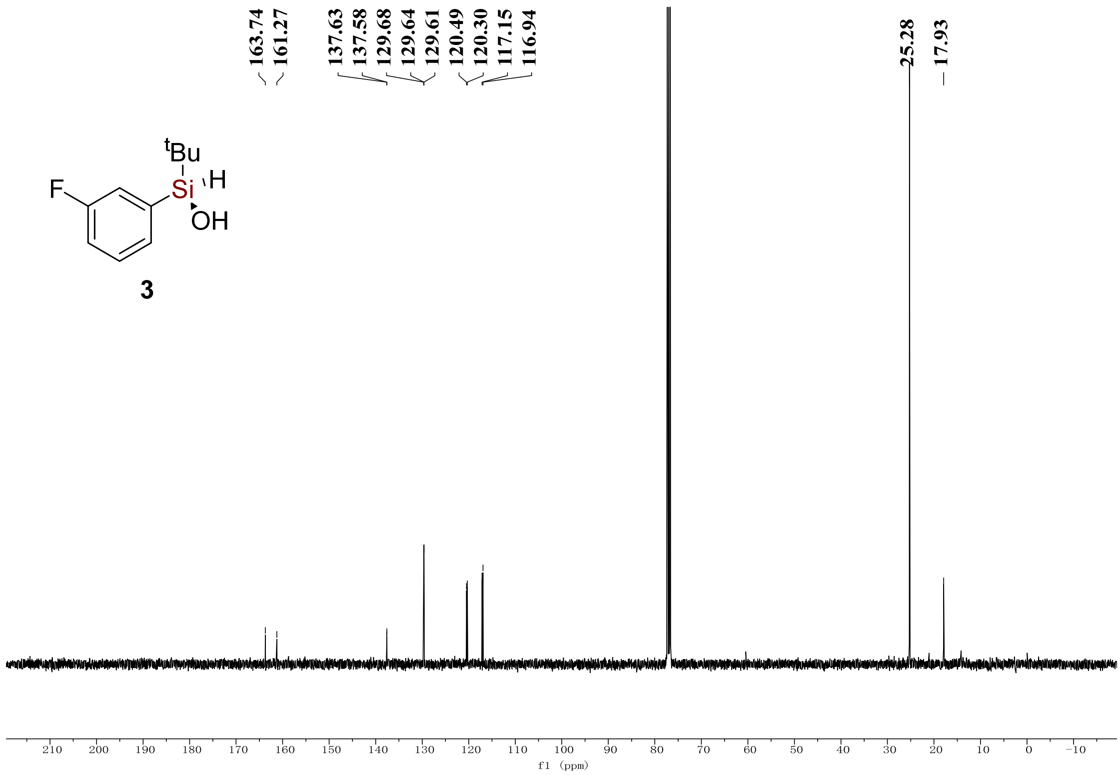
7.27
7.27
7.26
7.13
7.13
7.12
7.12
7.11
7.10
7.10
7.09
7.09
7.09
7.08
4.79
0.97
tBu
Si
H
F
OH
3
2.03
0.96
1.00
0.94
9.70
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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116.94
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17.93
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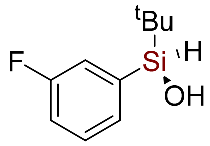
Si
H
F
OH
3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



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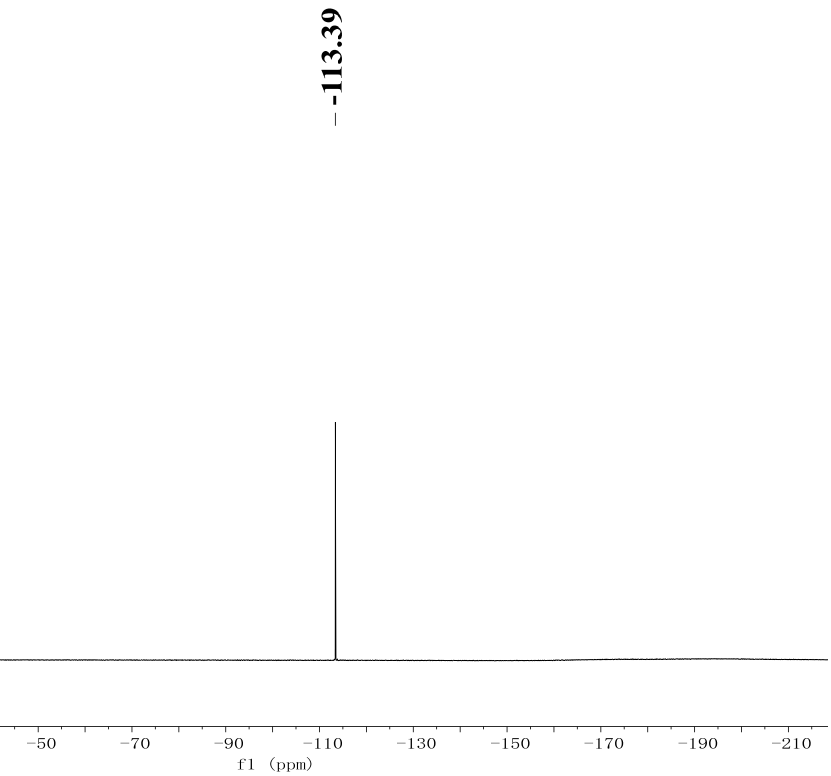

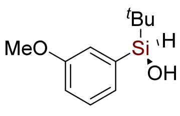

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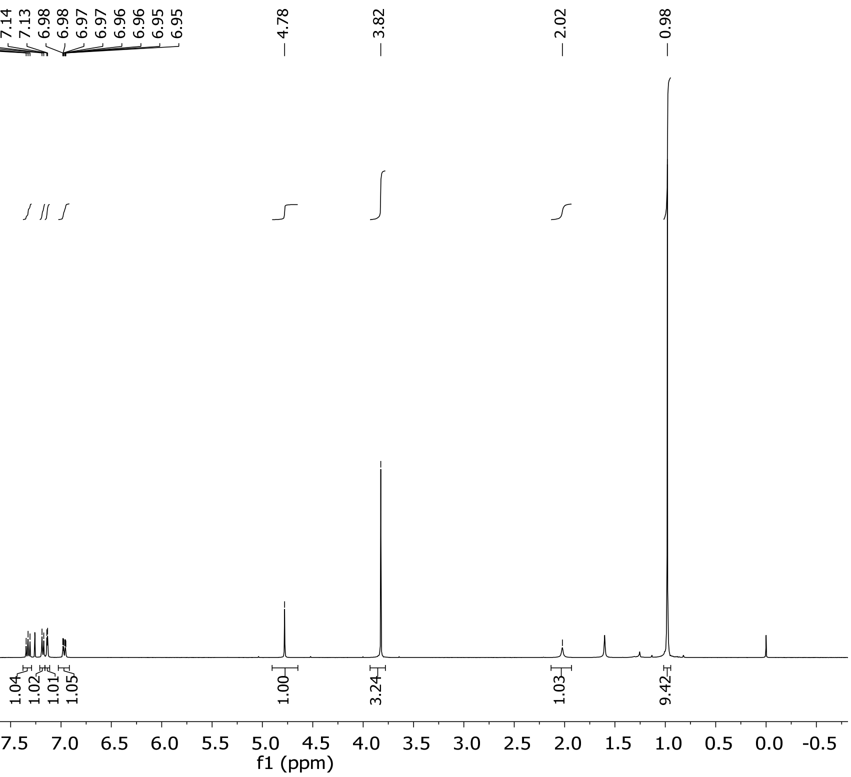

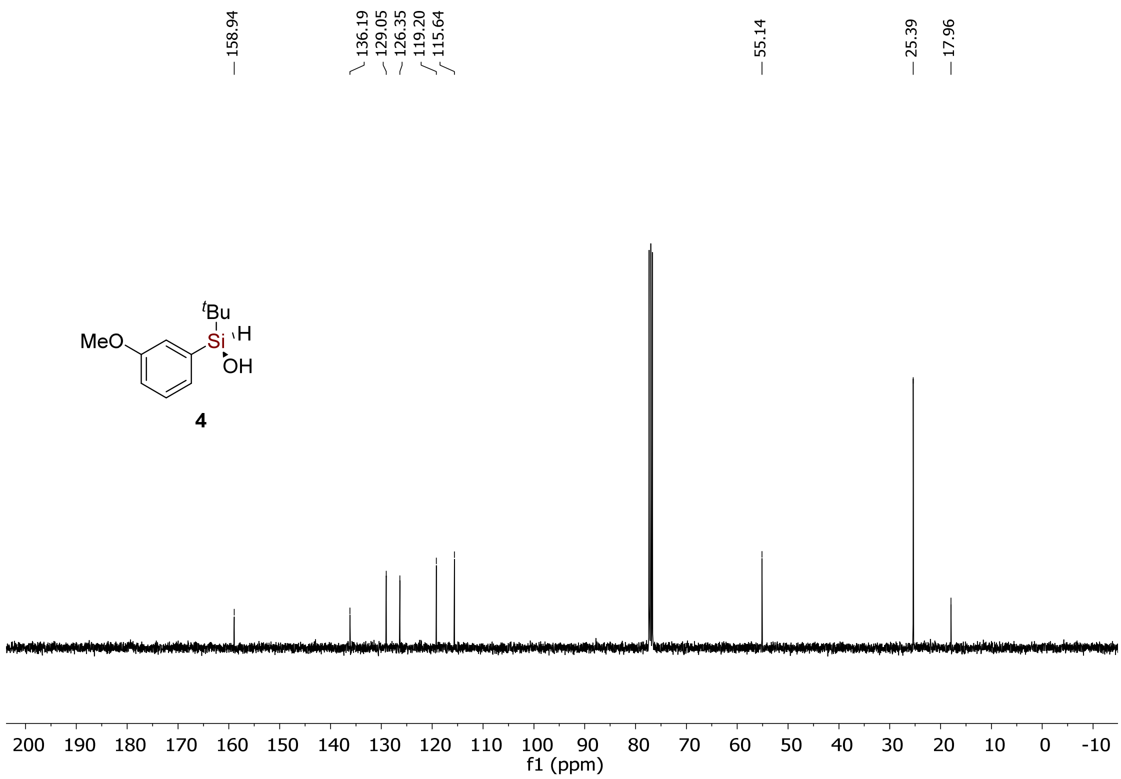
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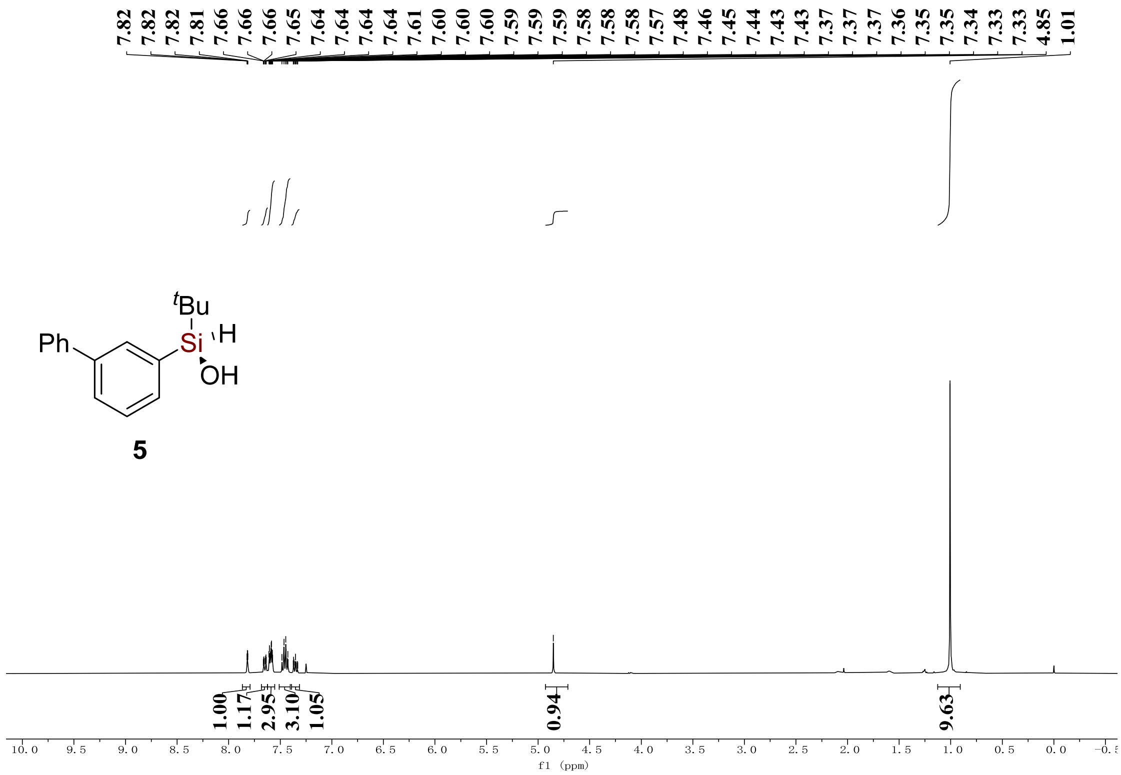
115.64
55.14
25.39
17.96
MeO
tBu
Si
H
OH
4
f1 (ppm)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7.45
7.44
7.43
7.43
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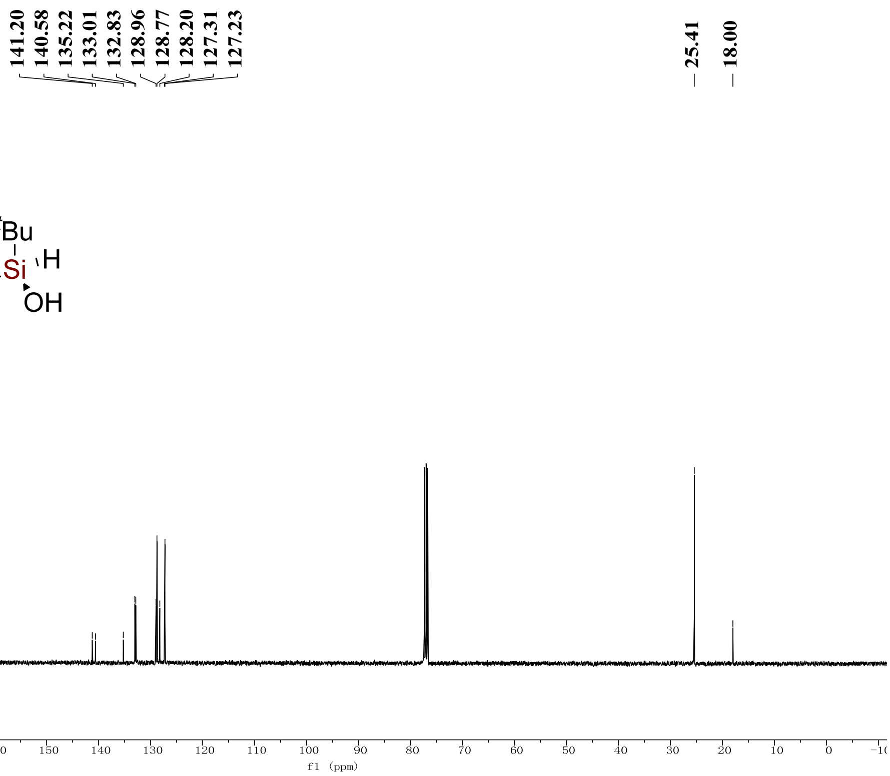
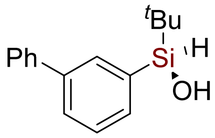
7.37
7.37
7.36
7.35
7.35
7.34
7.33
7.33
4.85
1.01
Ph
tBu
Si
H
OH
5
1.00
1.17
2.95
3.10
1.05
0.94
9.63
f1 (ppm)


141.20
140.58
135.22
133.01
132.83
128.96
128.77
128.20
127.31
127.23
25.41
18.00
f1 (ppm)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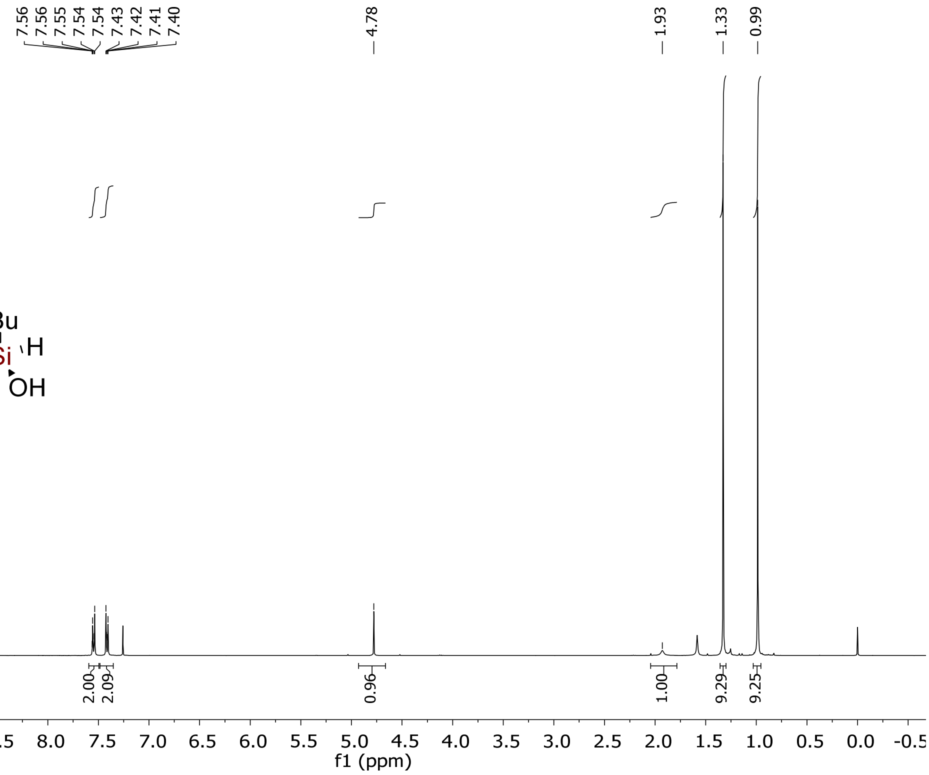
Ph
Si
H
OH

5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7.41
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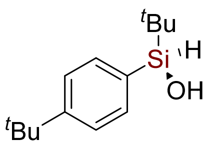
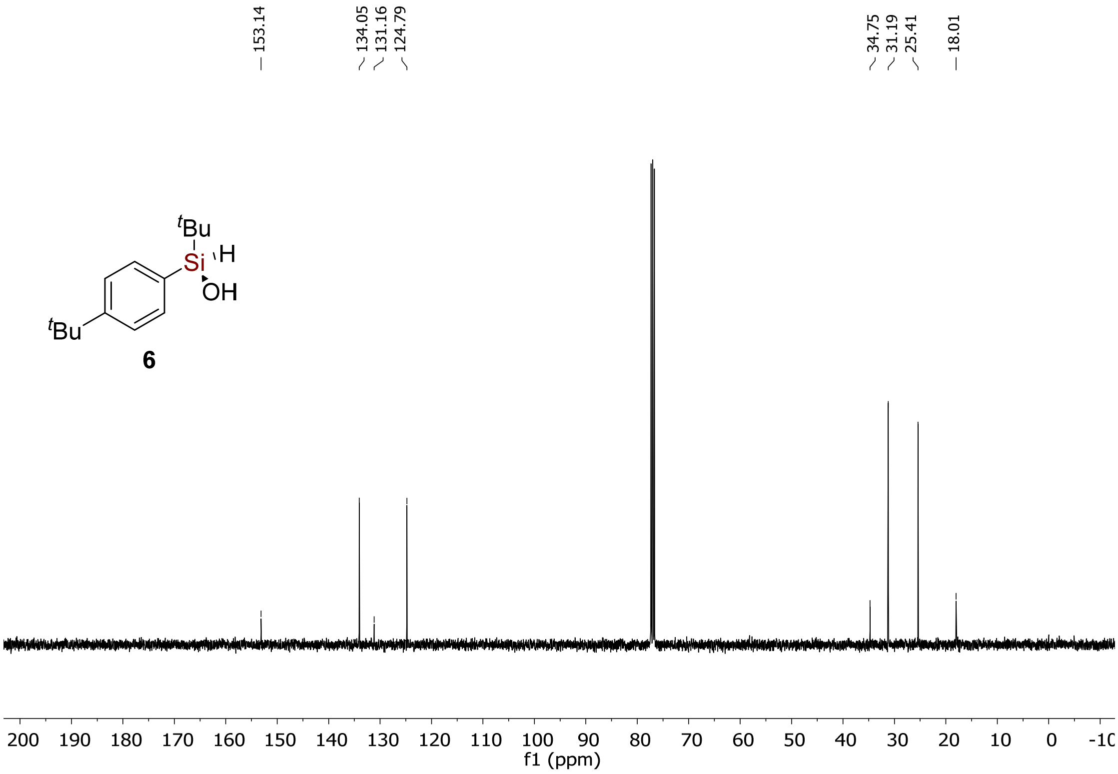
1.33
0.99
2.00
2.09
0.96
1.00
9.29
9.25
f1 (ppm)


tBu
Si
H
OH
tBu

6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31.19
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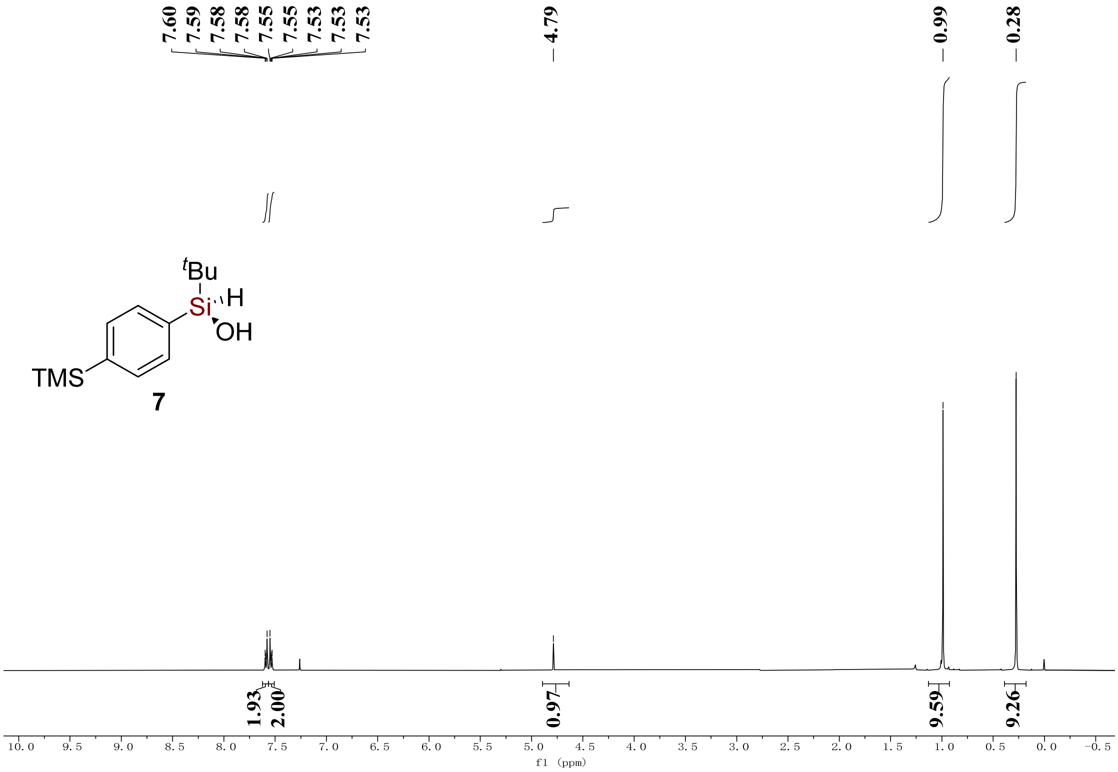
6
f1 (ppm)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7.55
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7.53
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0.28
TMS
7
1.93
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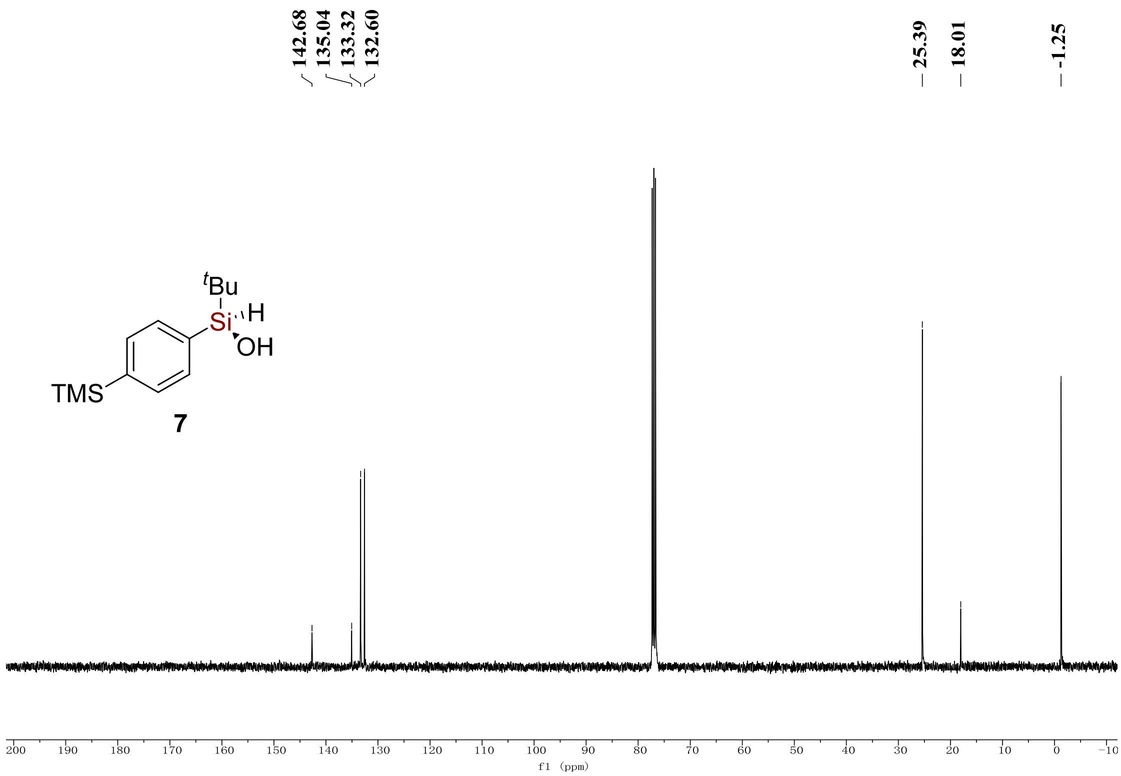
0.97
9.59
9.26
f1 (ppm)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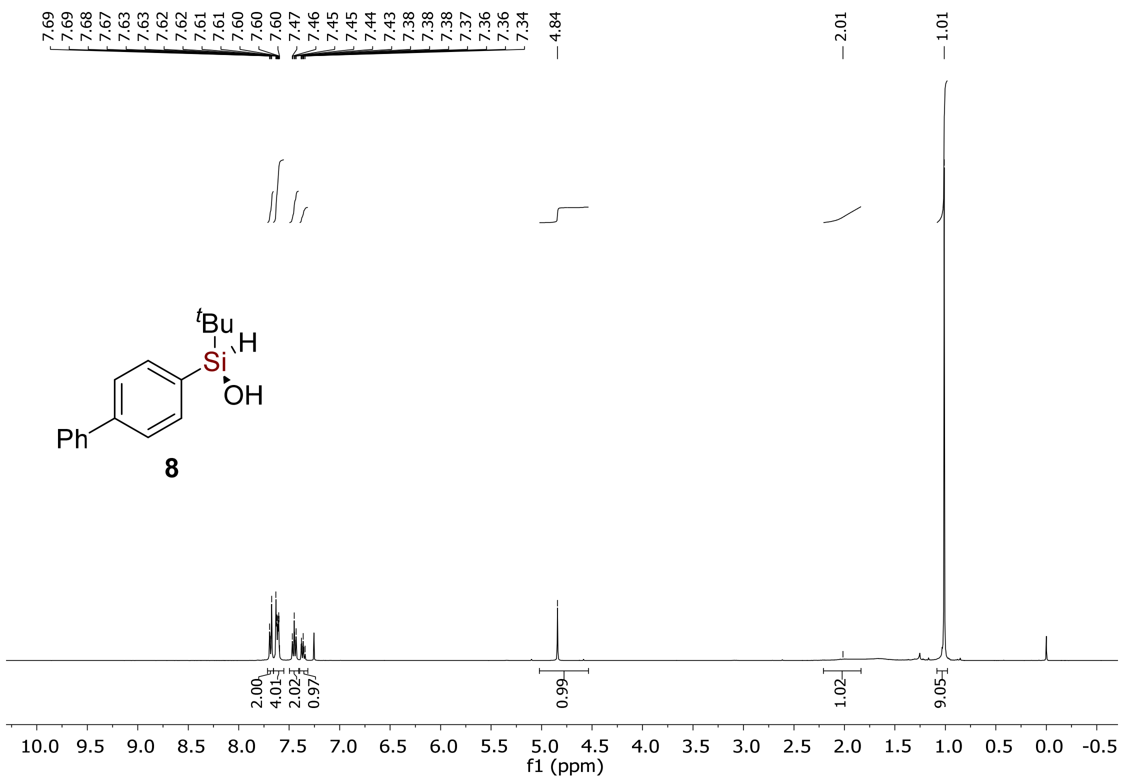
tBu
Si
H
OH
TMS
7
f1 (ppm)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7.60
7.47
7.46
7.45
7.45
7.44
7.43
7.38
7.38
7.38
7.37
7.36
7.36
7.34
4.84
2.01
1.01
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Si
H
OH
Ph
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4.01
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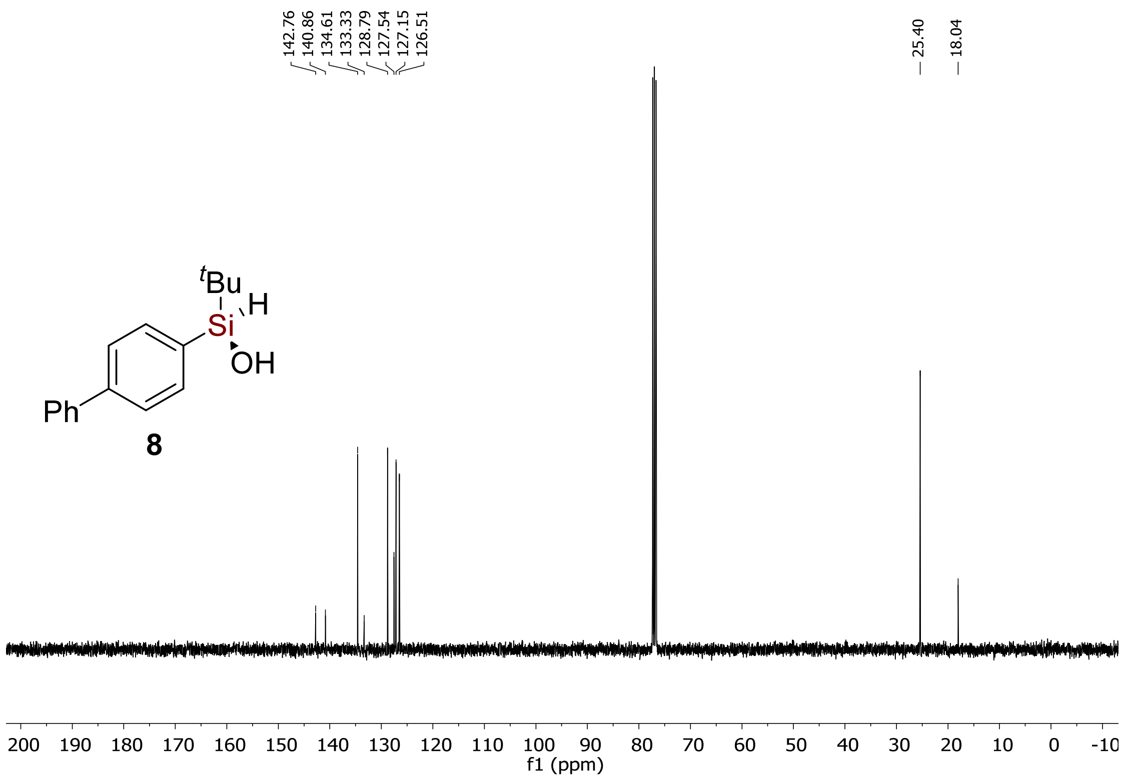
0.99
1.02
9.05
f1 (ppm)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H
Si
OH
Ph
8
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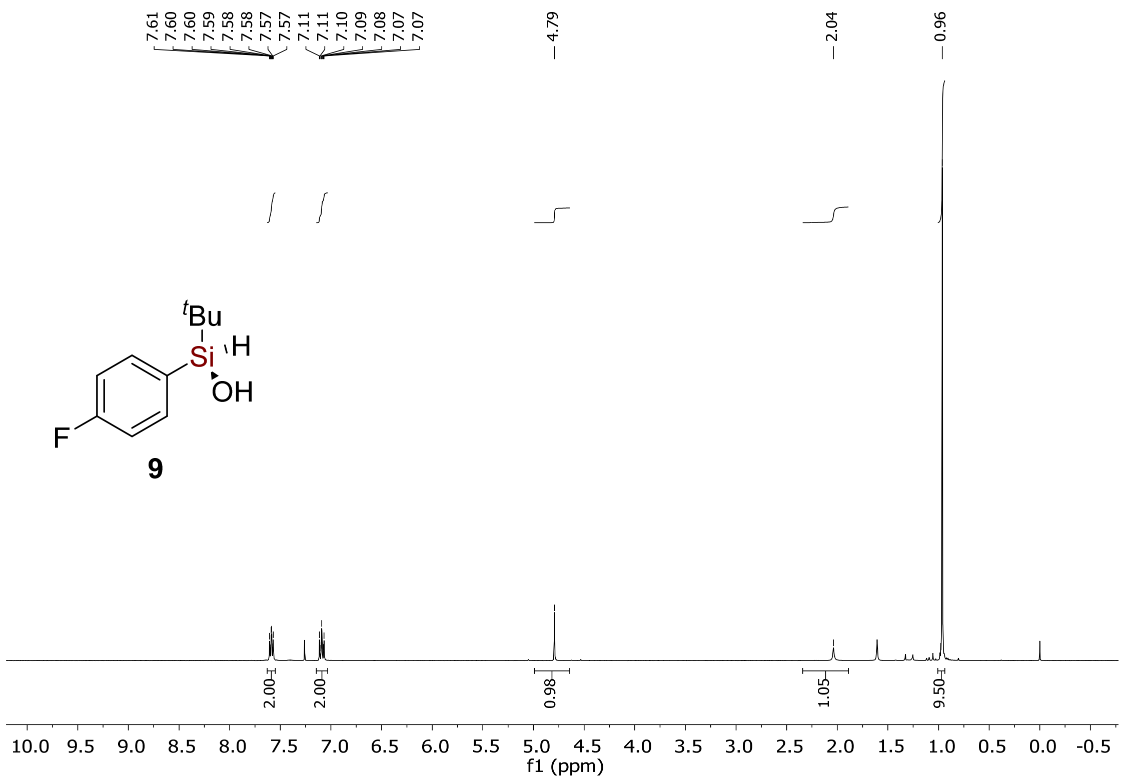
f1 (ppm)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7.10
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7.08
7.07
7.07
4.79
2.04
0.96
tBu
H
Si
OH
F
9
2.00
2.00
0.98
1.05
9.50
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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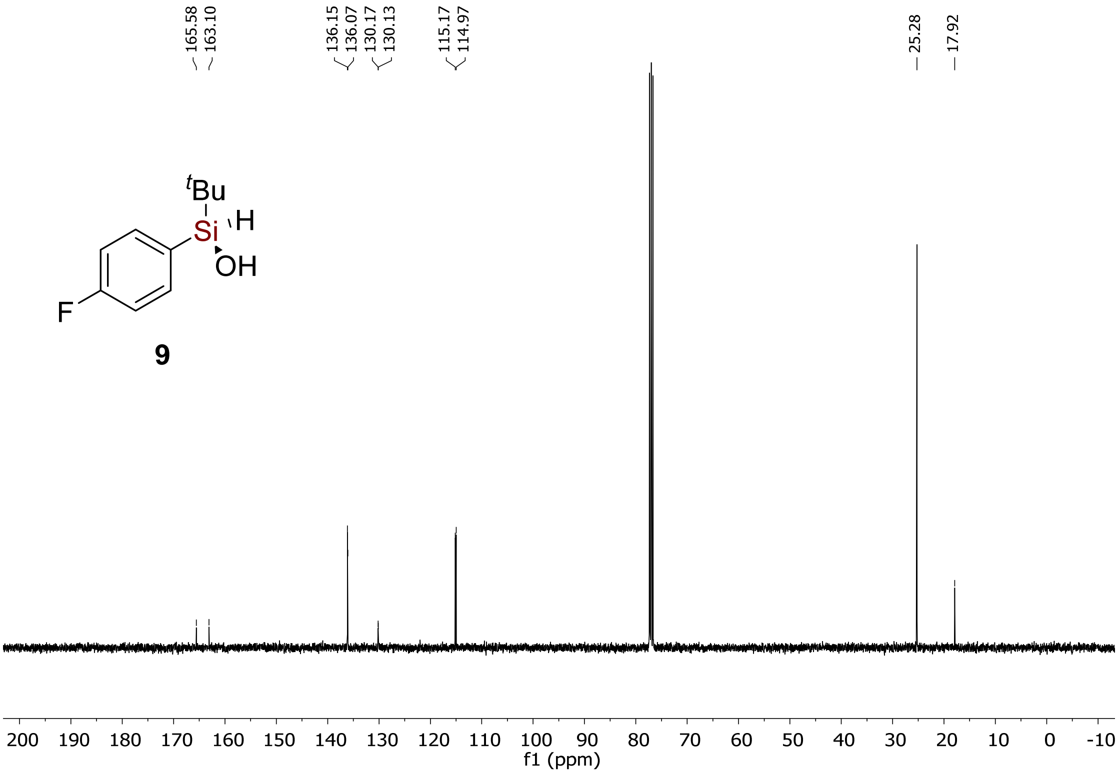
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F
9
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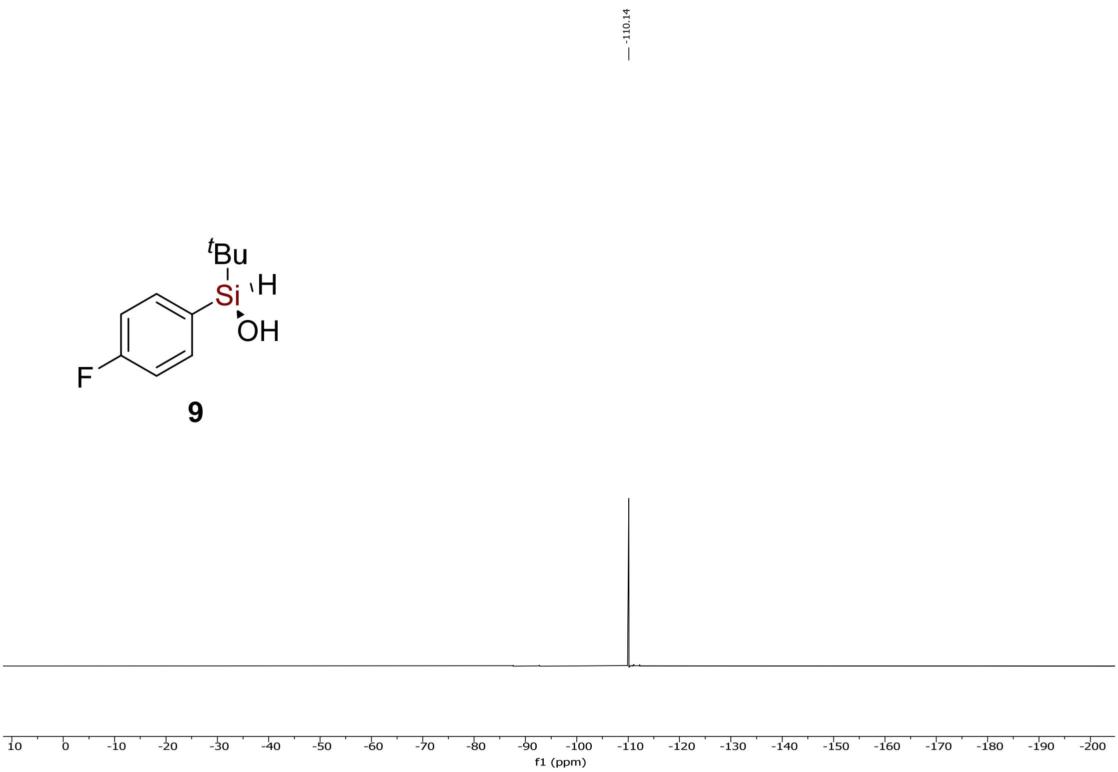
f1 (ppm)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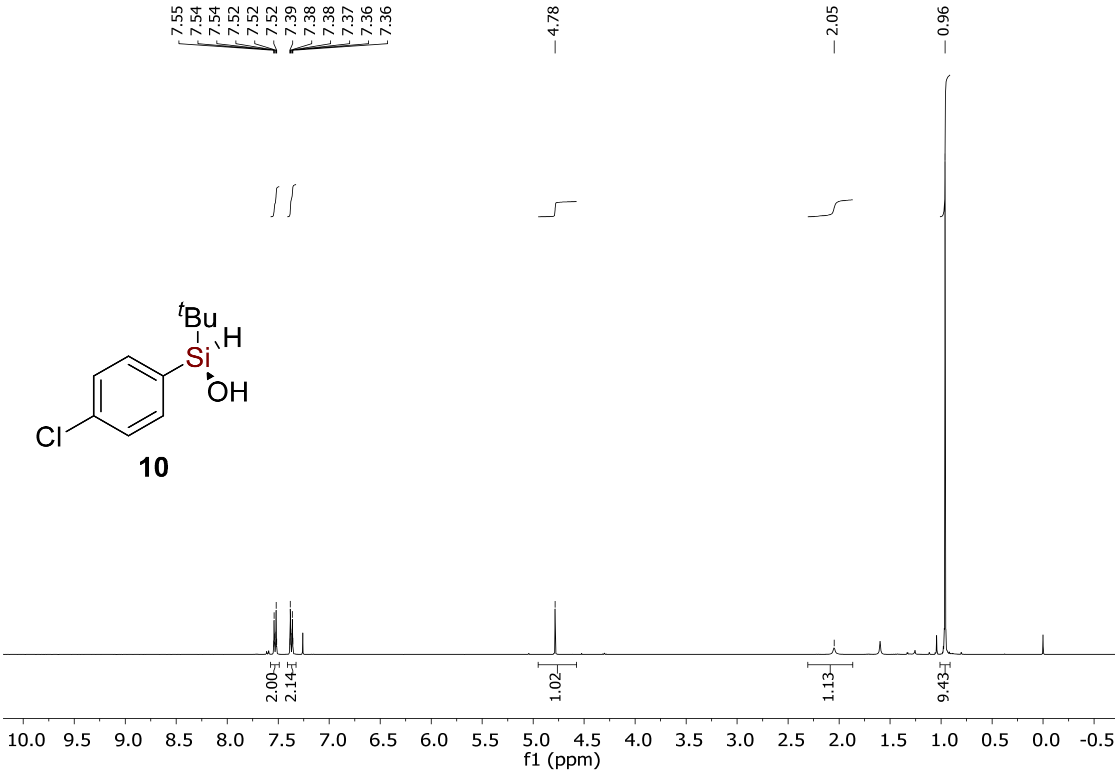
f1 (ppm)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7.36
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4.78
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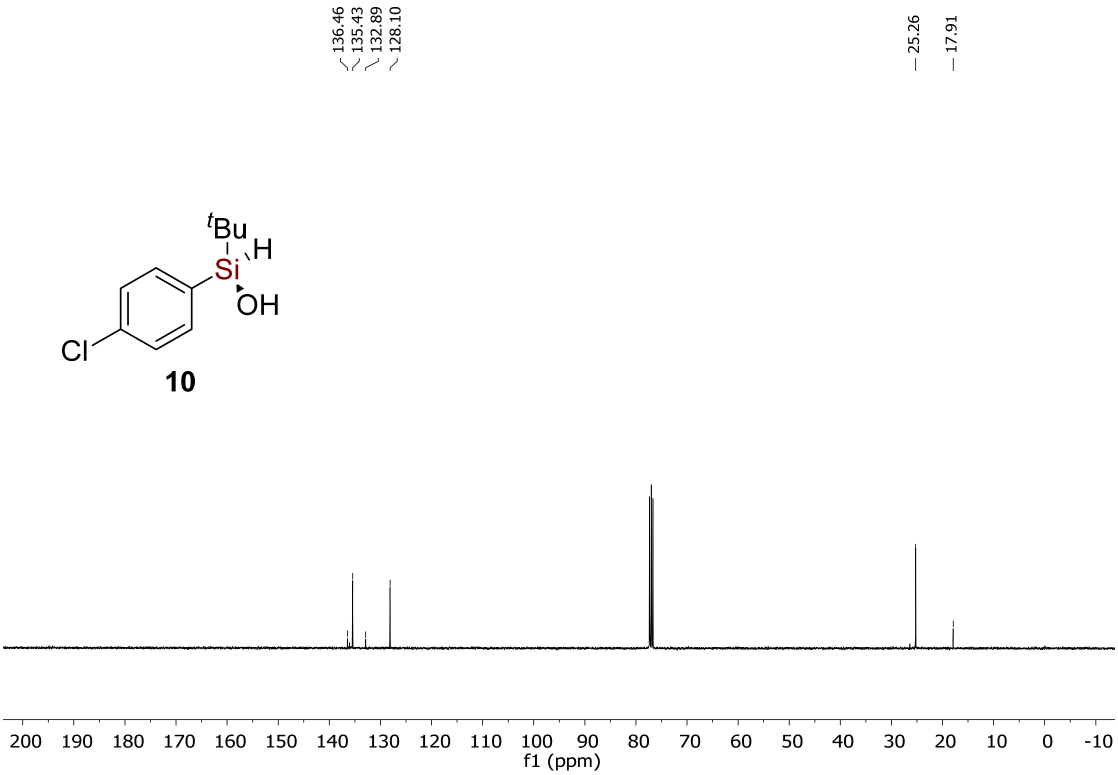
H
Si
OH
Cl
10
2.00
2.14
1.02
1.13
9.43
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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Si
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Cl
10
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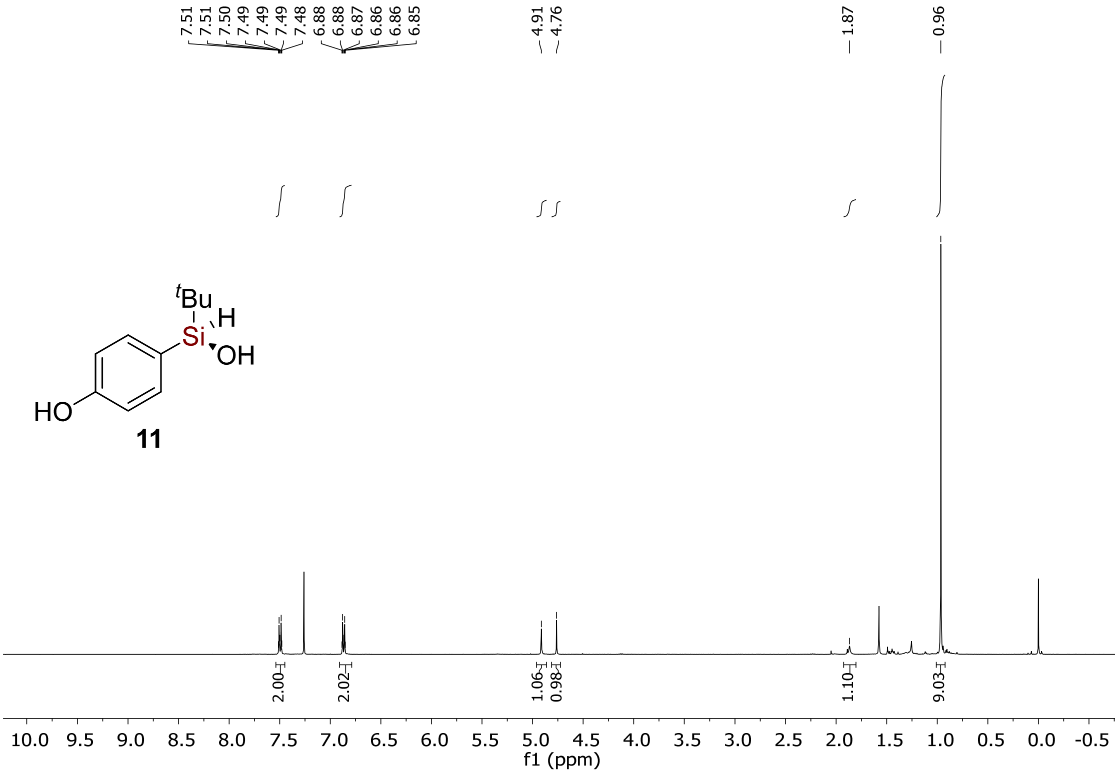
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OH
HO
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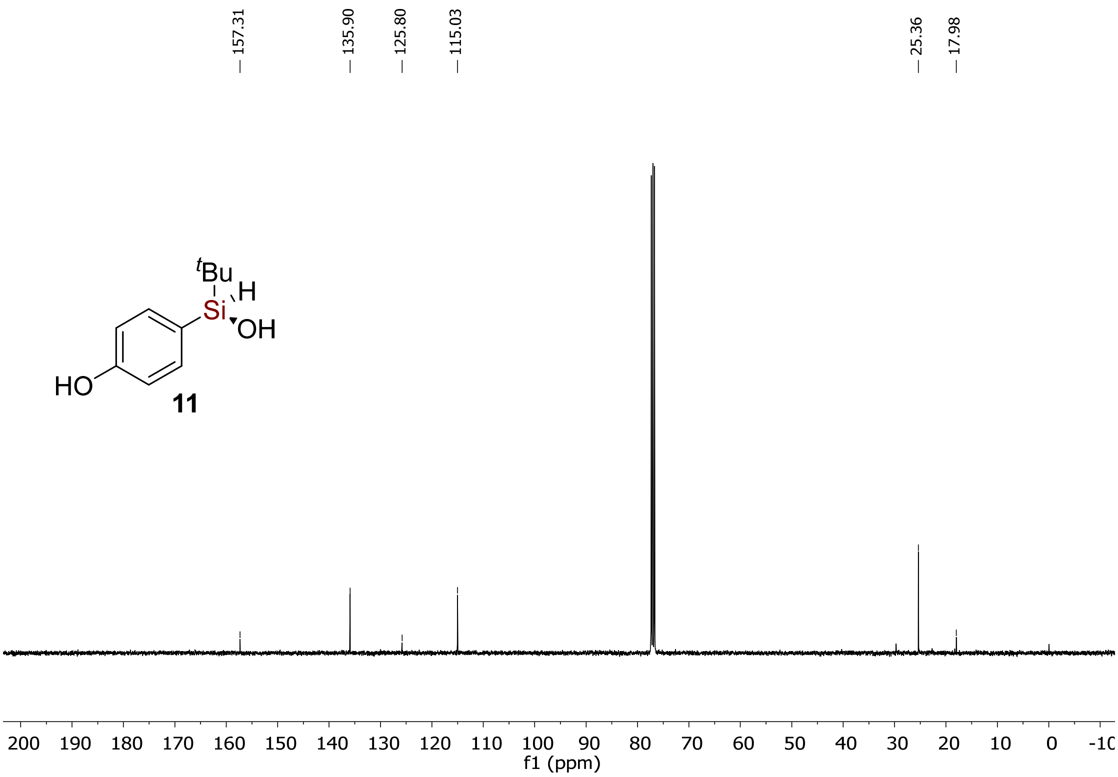
2.00
2.02
1.06
0.98
1.10
9.03
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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Si
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HO
11
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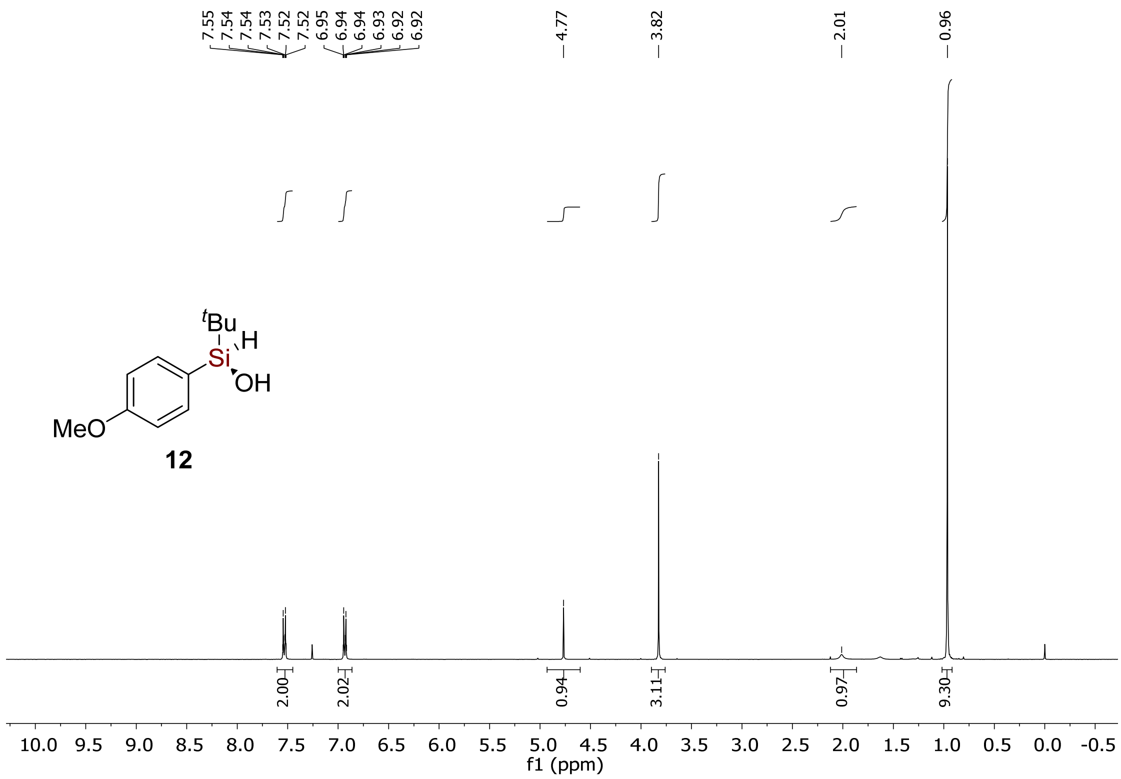
f1 (ppm)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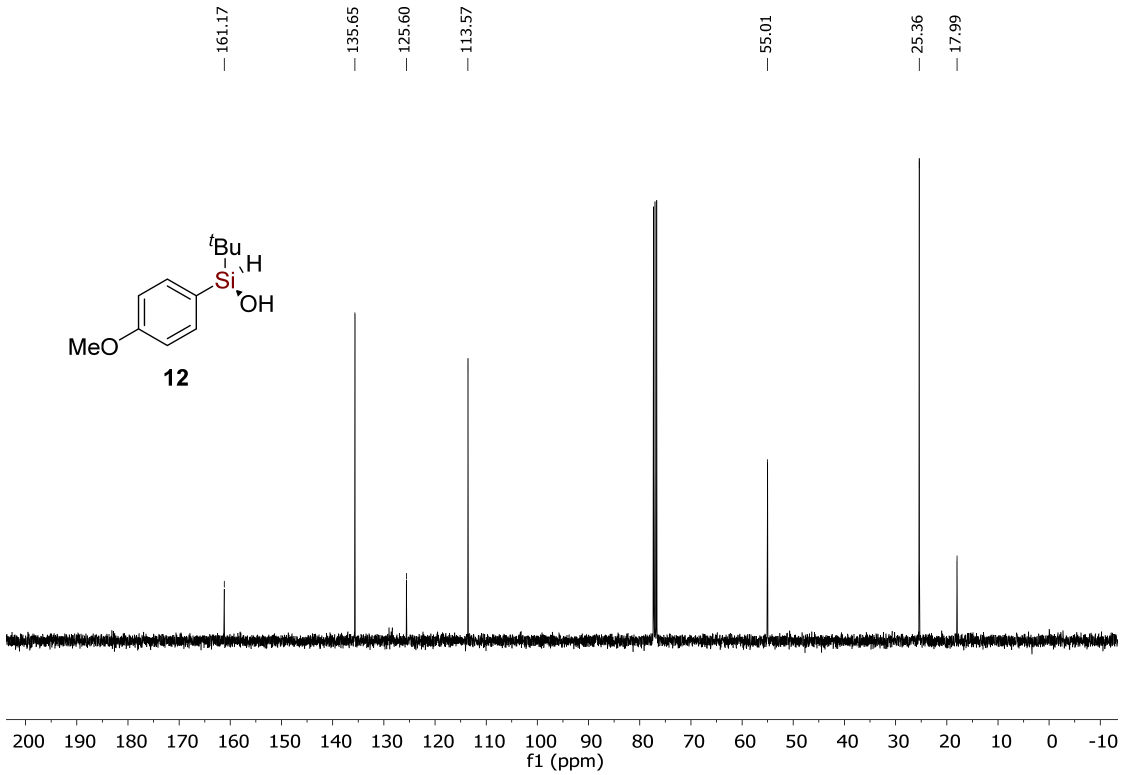
6.94
6.94
6.93
6.92
6.92
4.77
3.82
2.01
0.96
tBu
H
Si
OH
MeO
12
2.00
2.02
0.94
3.11
0.97
9.30
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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OH
MeO
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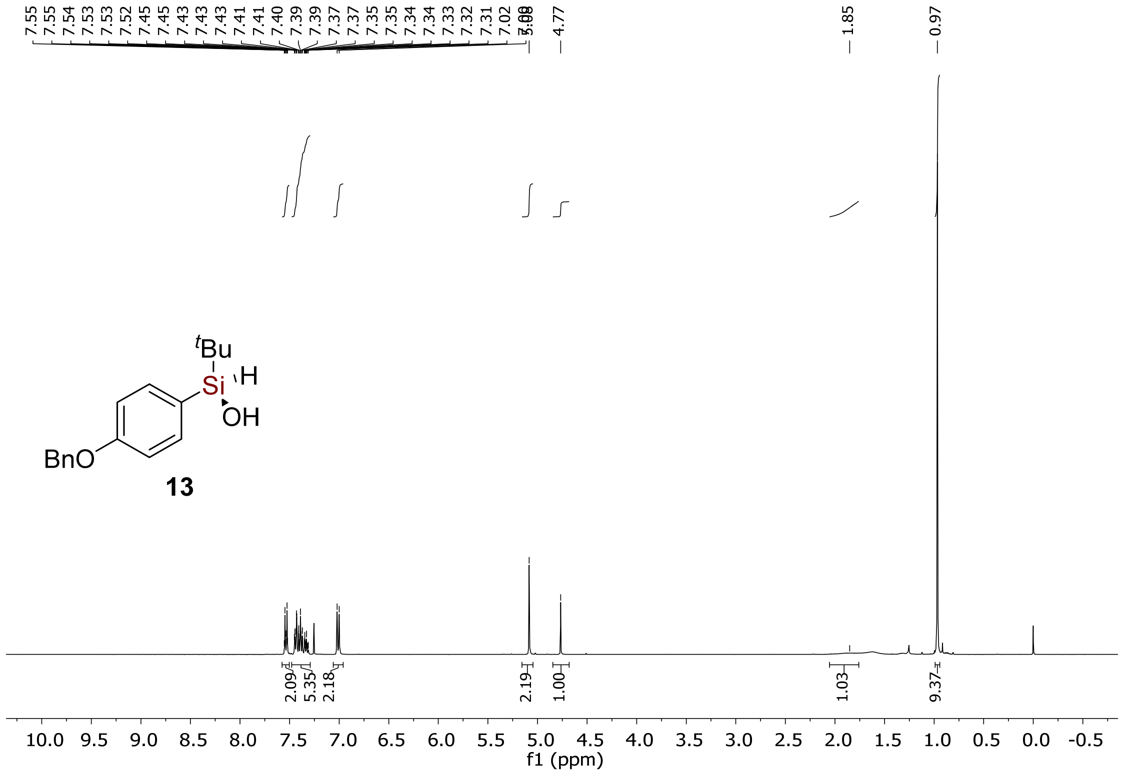
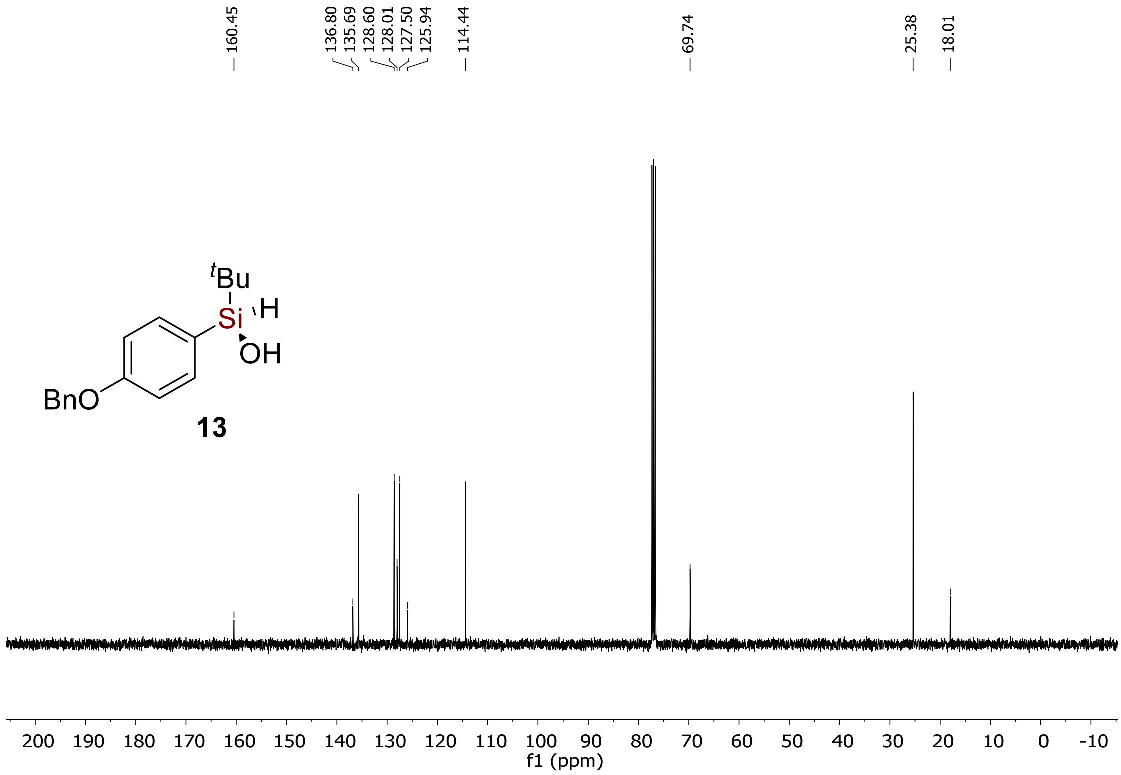
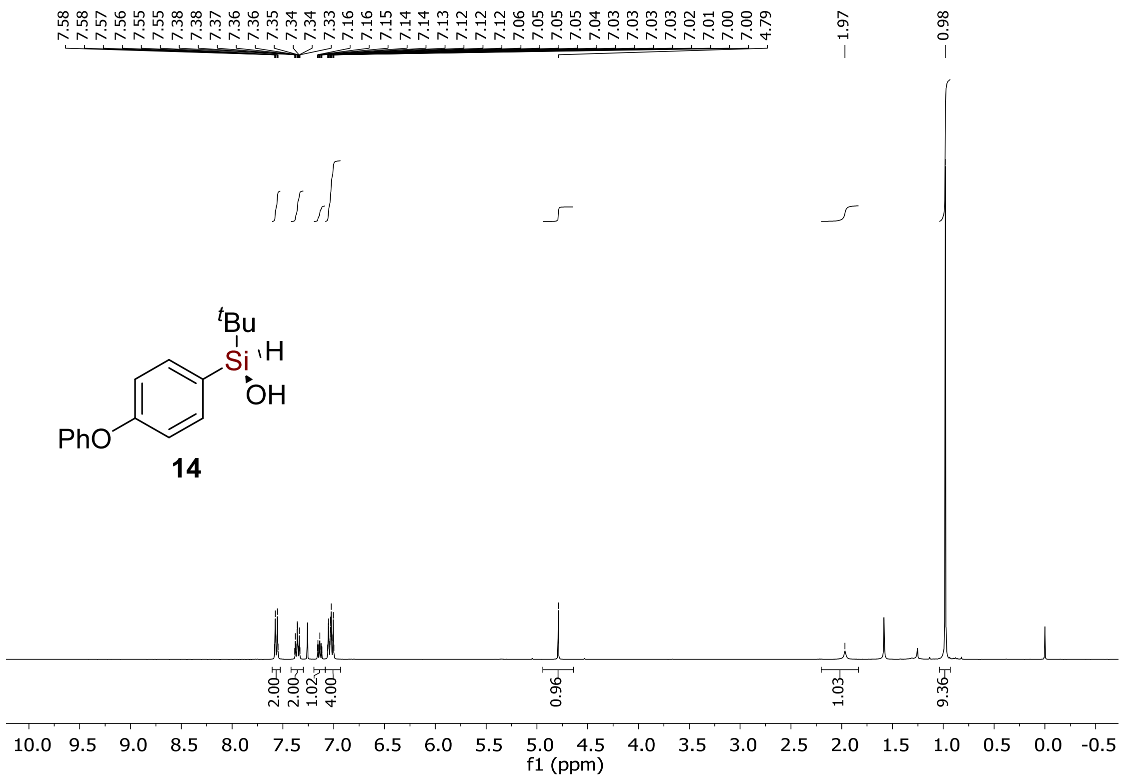
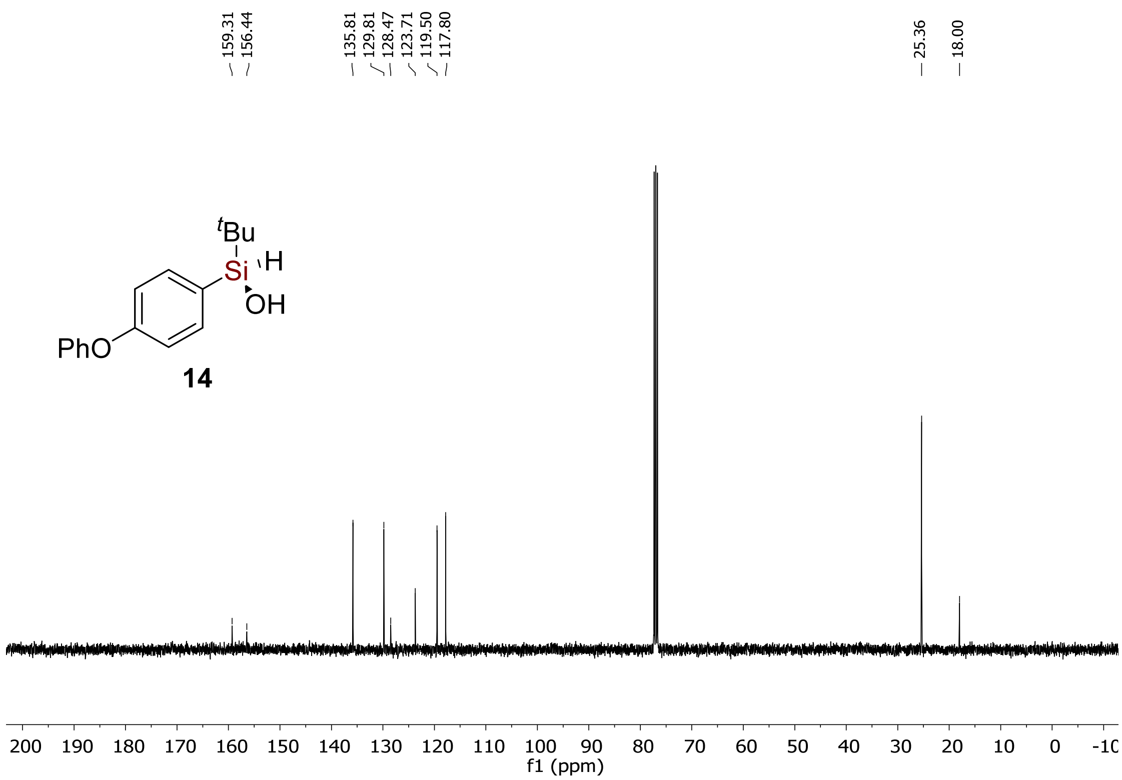
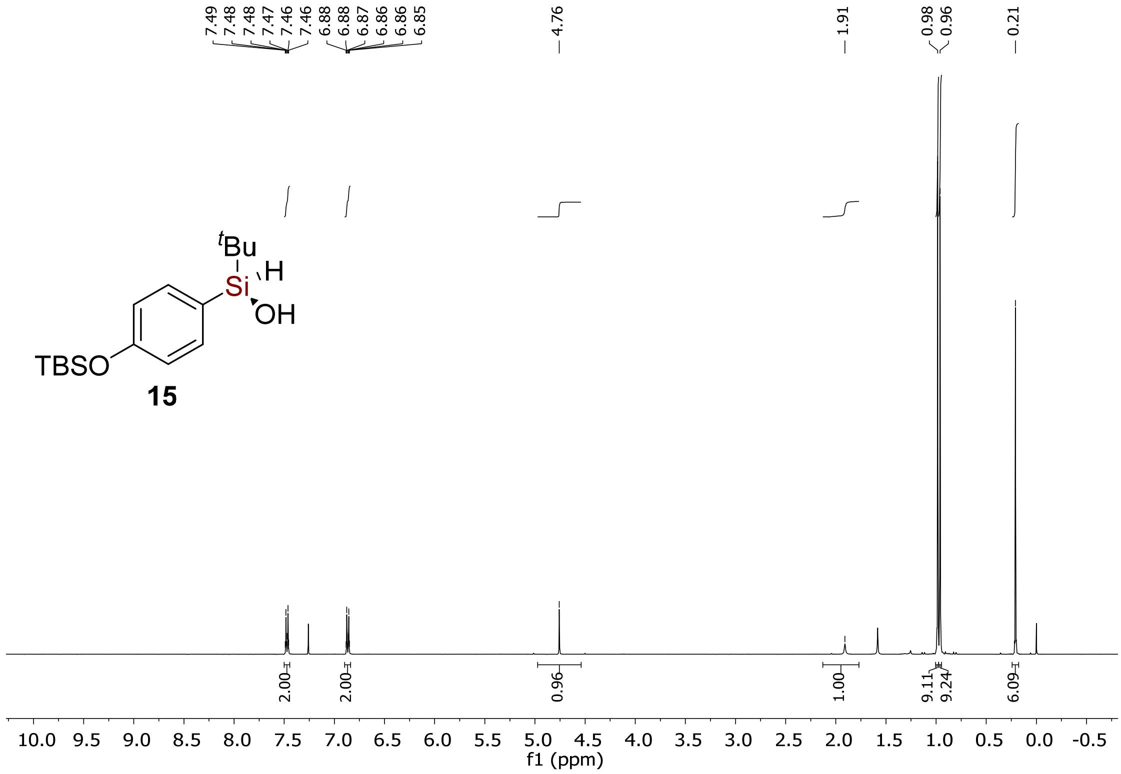
f1 (ppm)







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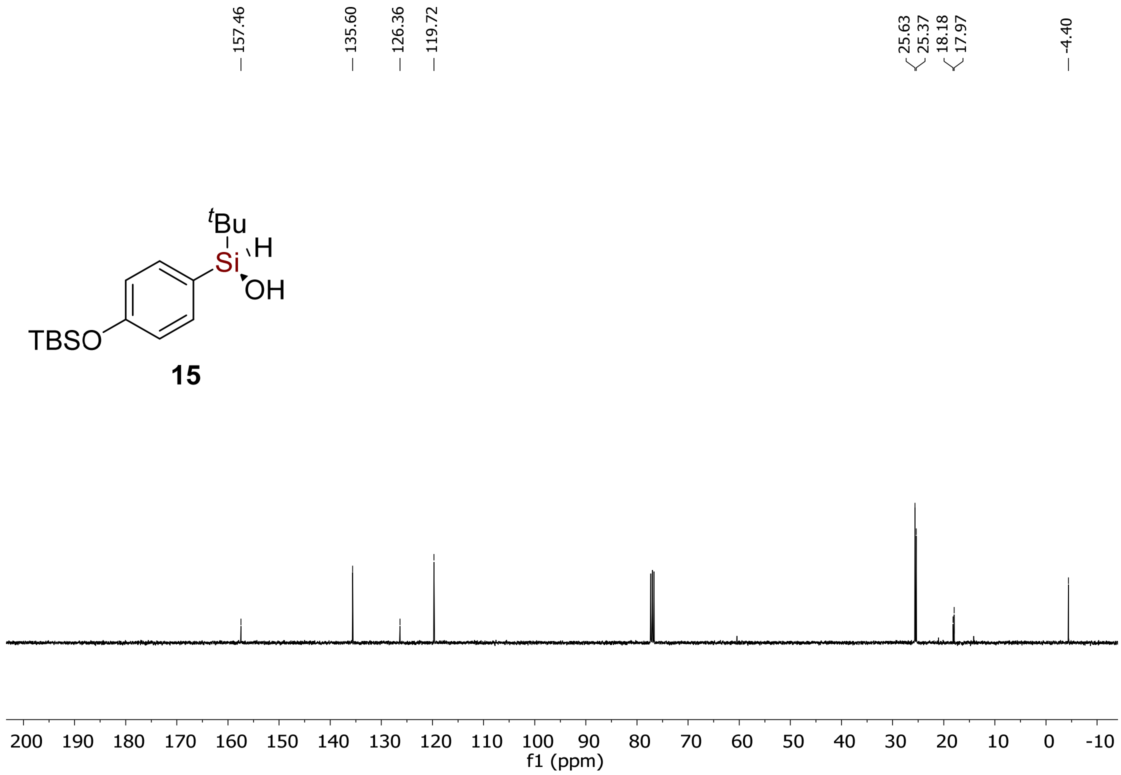
4.76
1.91
0.98
0.96
0.21
tBu
Si
H
OH
TBSO
15
2.00
2.00
0.96
1.00
9.11
9.24
6.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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Si
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OH
TBSO
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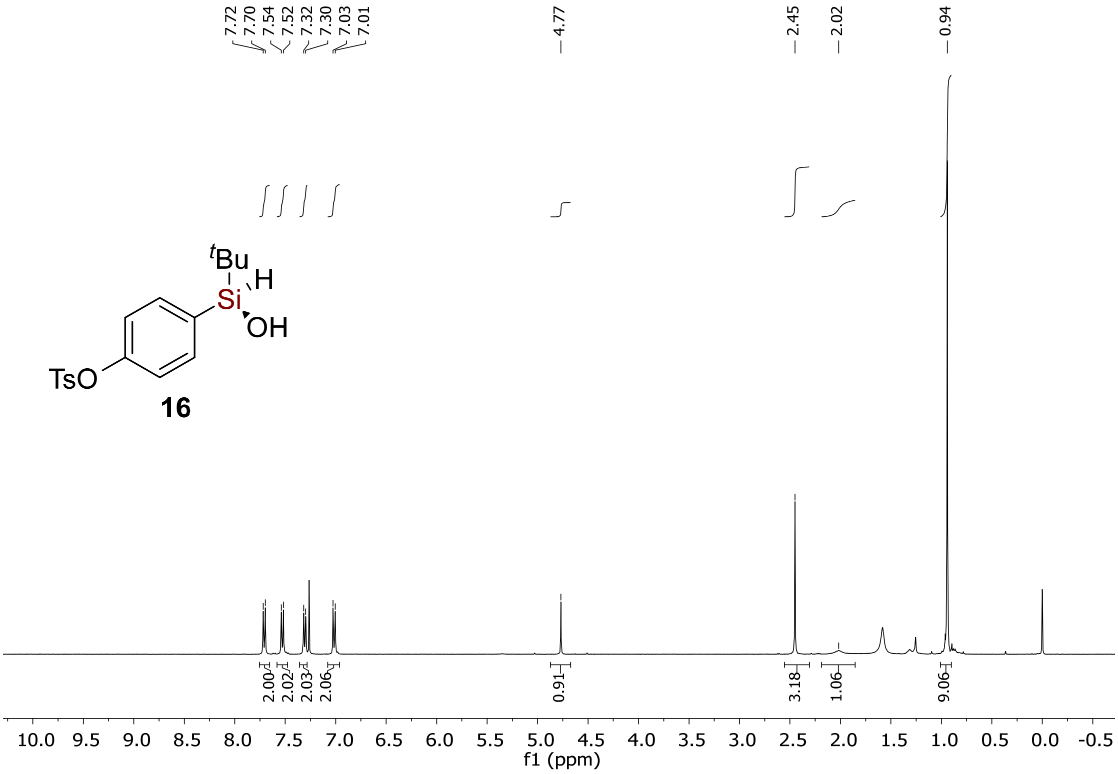
f1 (ppm)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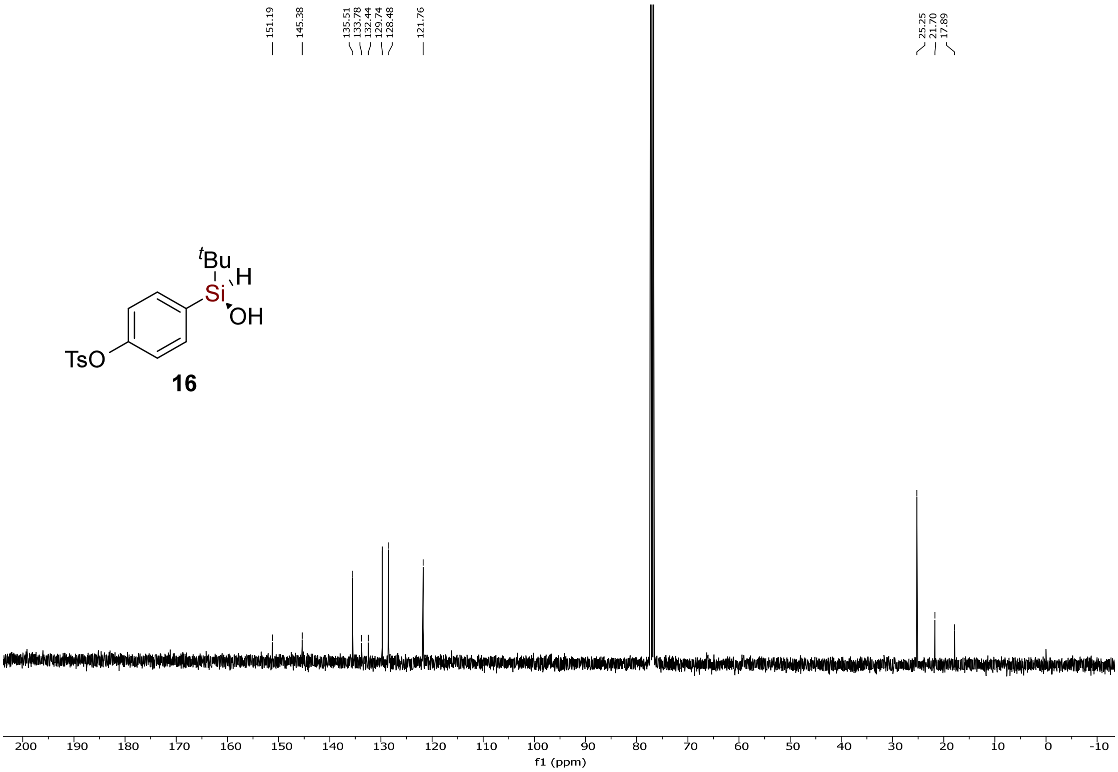
0.94
tBu
H
Si
OH
TsO
16
2.00
2.02
2.03
2.06
0.91
3.18
1.06
9.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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H
Si
OH
TsO
16
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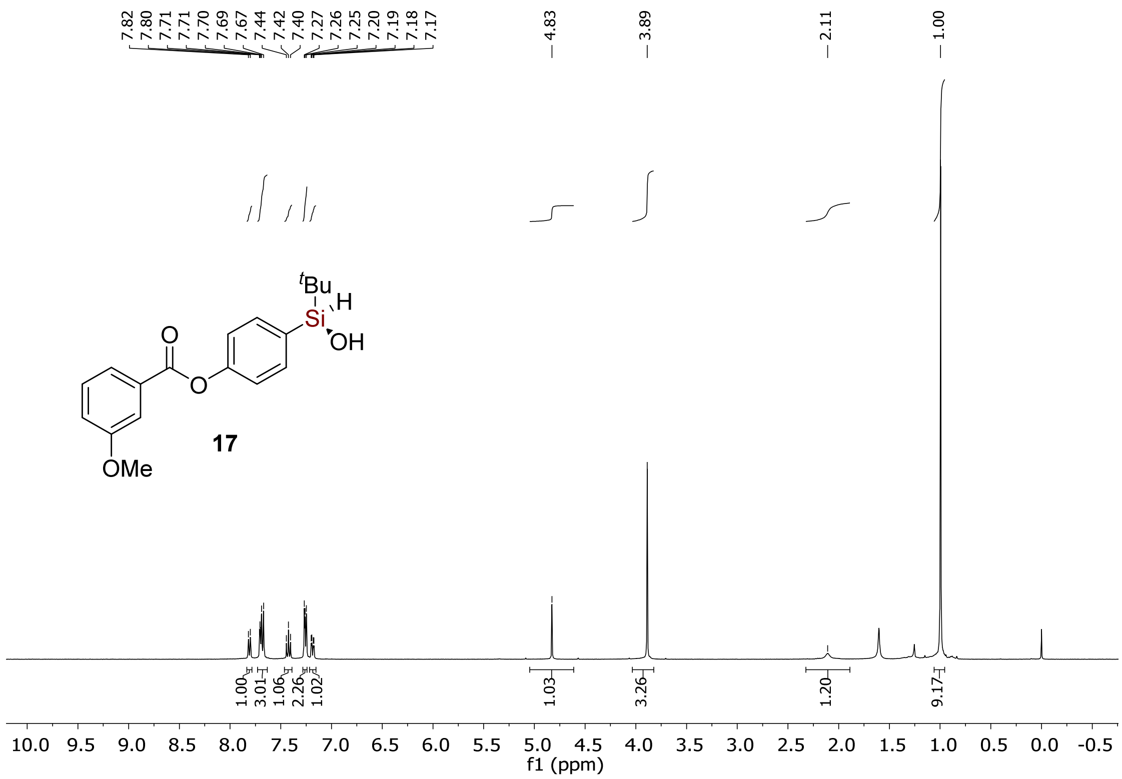
f1 (ppm)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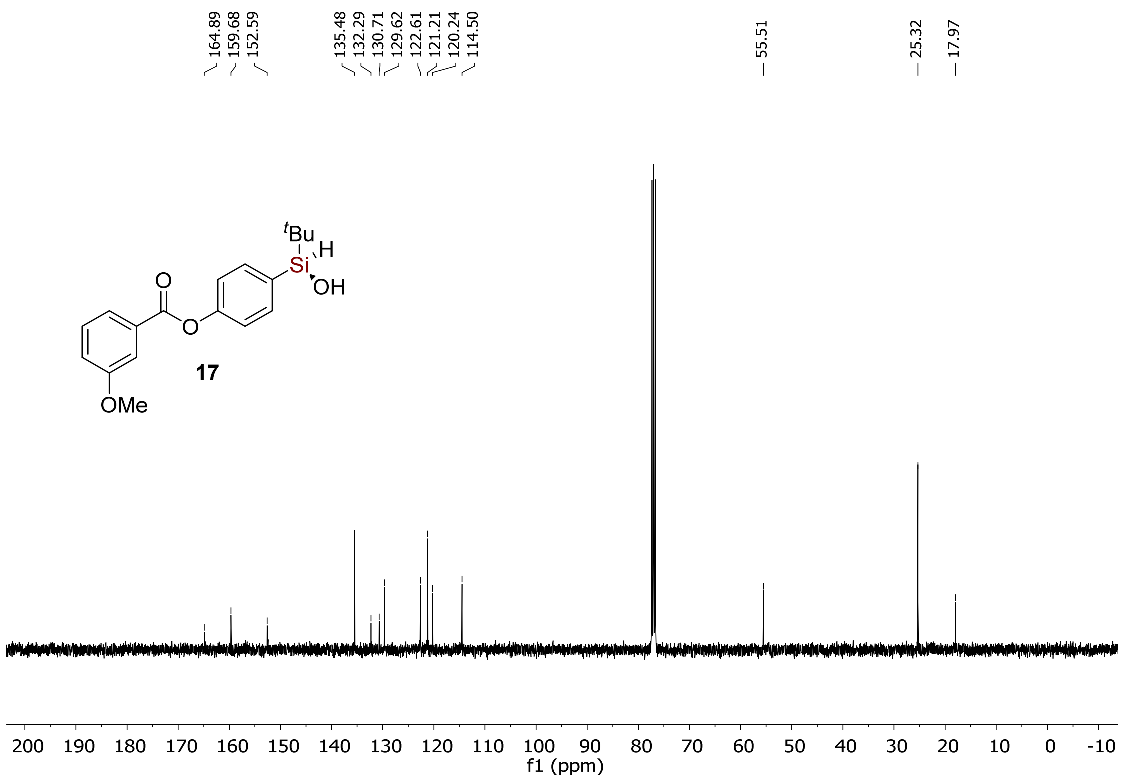
7.20
7.19
7.18
7.17
4.83
3.89
2.11
1.00
tBu
H
Si
OH
O
O
OMe
17
1.00
3.01
1.06
2.26
1.02
1.03
3.26
1.20
9.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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55.51
25.32
17.97
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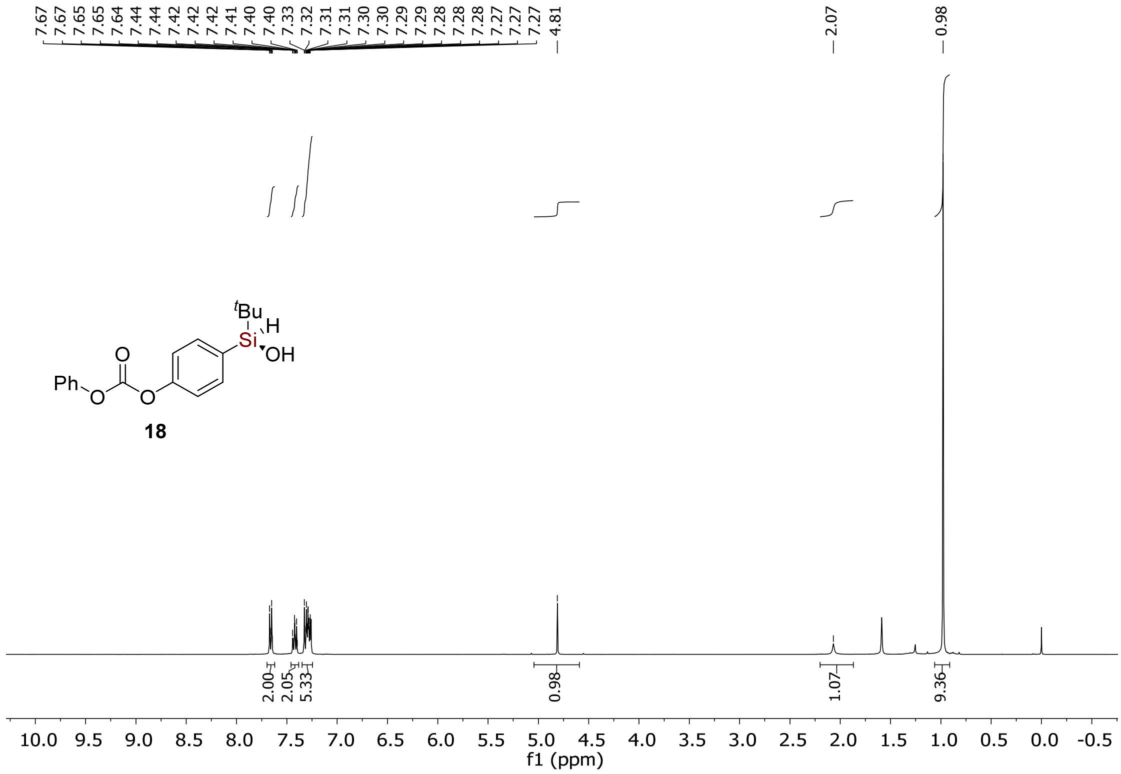
OH
O
O
OMe
17
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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7.32
7.31
7.31
7.30
7.30
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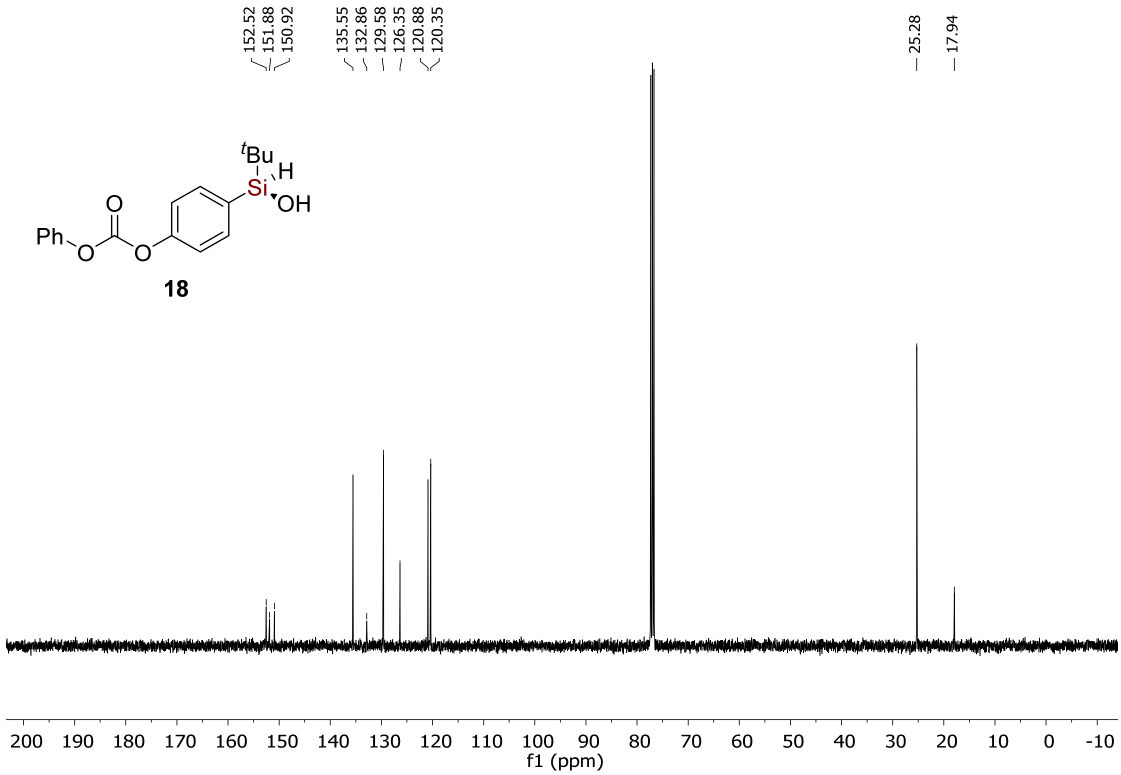
7.29
7.28
7.28
7.28
7.27
7.27
7.27
4.81
2.07
0.98
tBu
H
Si
OH
O
Ph
O
O
18
2.00
2.05
5.33
0.98
1.07
9.36
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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O
Ph
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O
18
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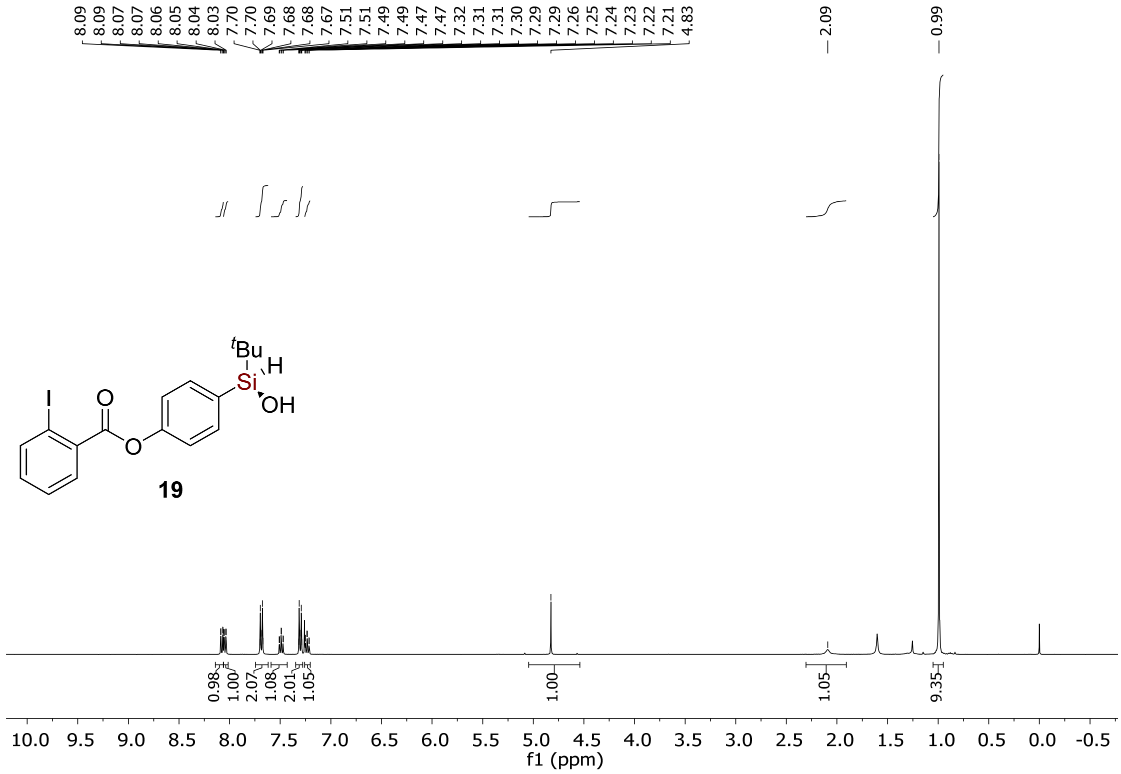
f1 (ppm)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7.31
7.30
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7.29
7.26
7.25
7.24
7.23
7.22
7.21
4.83
2.09
0.99
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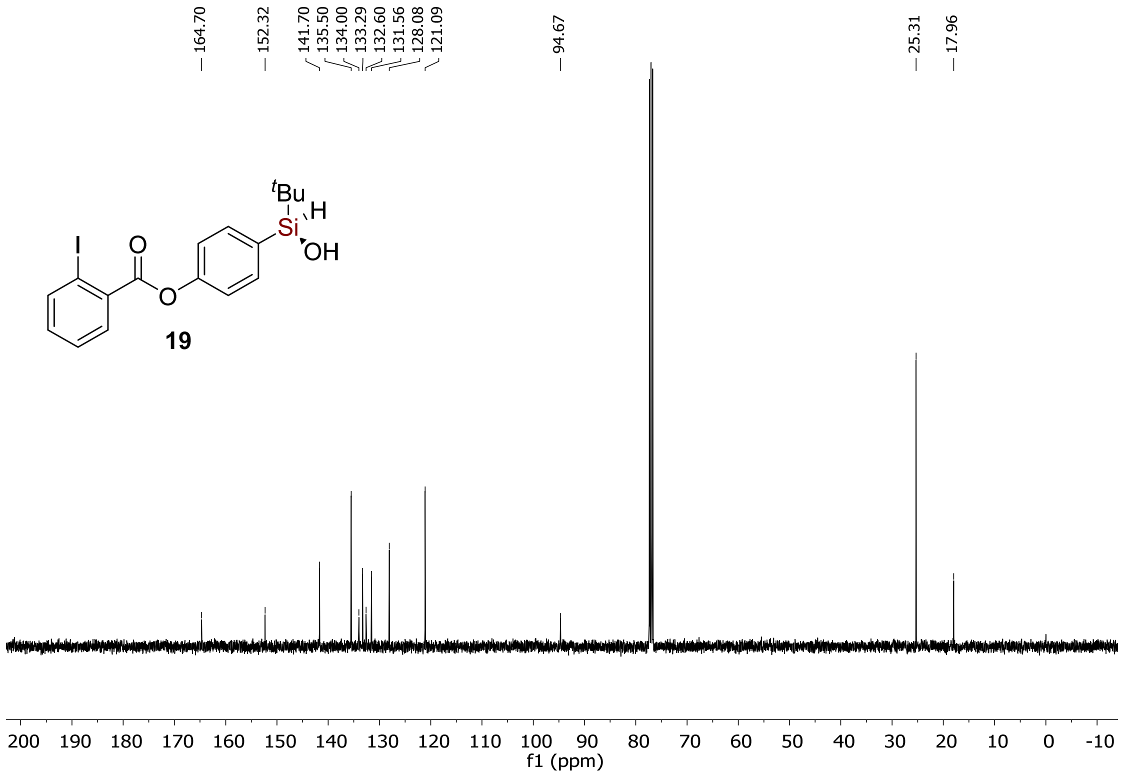
H
Si
OH
I
O
O
19
0.98
1.00
2.07
1.08
2.01
1.05
1.00
1.05
9.35
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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OH
I
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O
19
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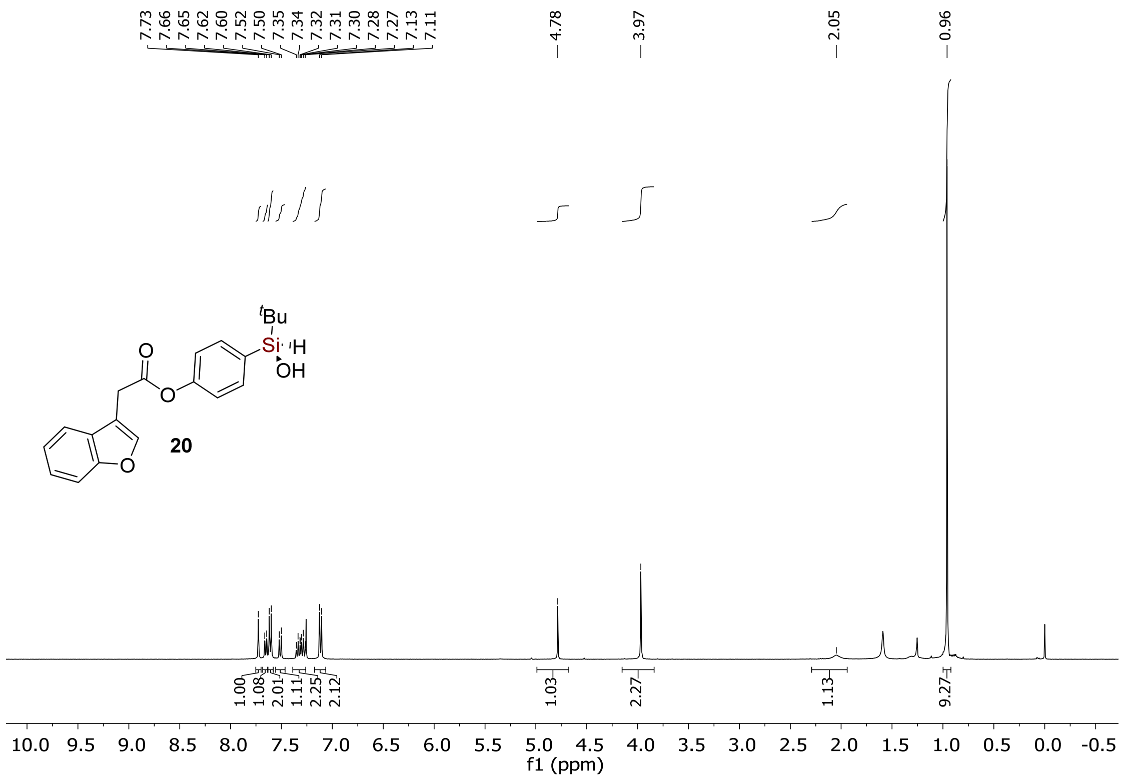
f1 (ppm)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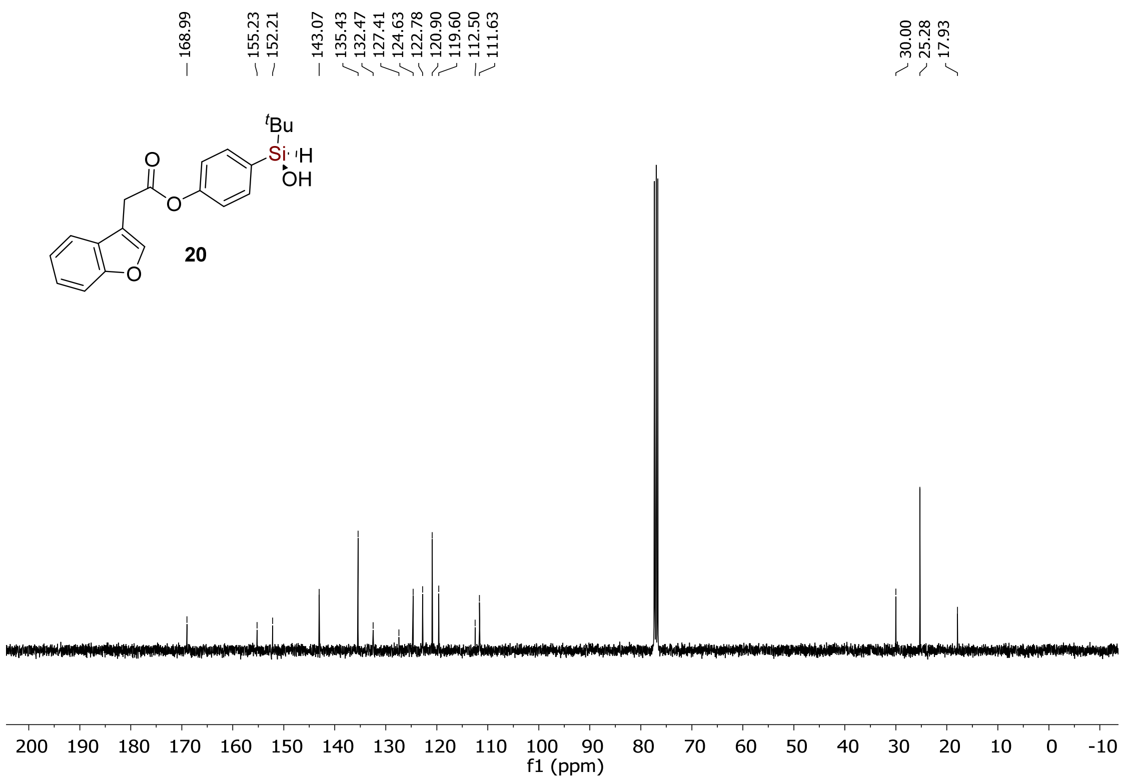
7.31
7.30
7.28
7.27
7.13
7.11
4.78
3.97
2.05
0.96
tBu
Si
H
O
OH
O
O
20
1.00
1.08
2.01
1.11
2.25
2.12
1.03
2.27
1.13
9.27
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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124.63
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120.90
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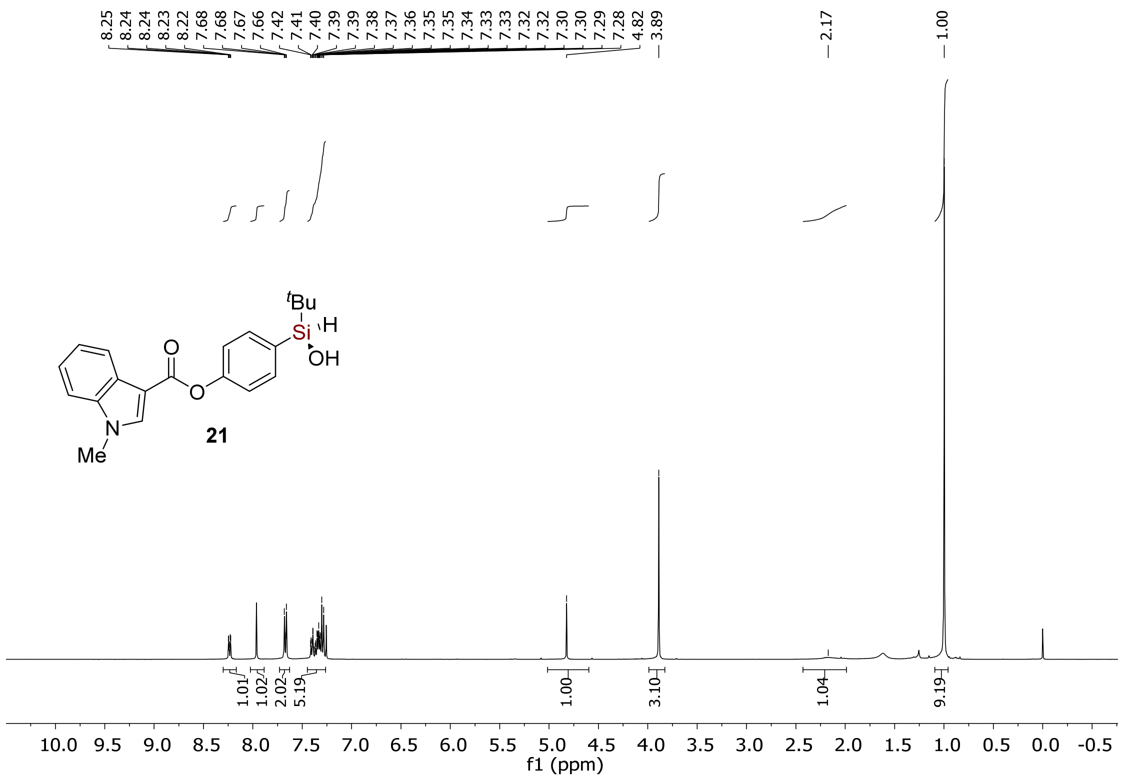
112.50
111.63
30.00
25.28
17.93
tBu
Si
H
O
OH
O
O
20
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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8.24
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7.66
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7.41
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7.37
7.36
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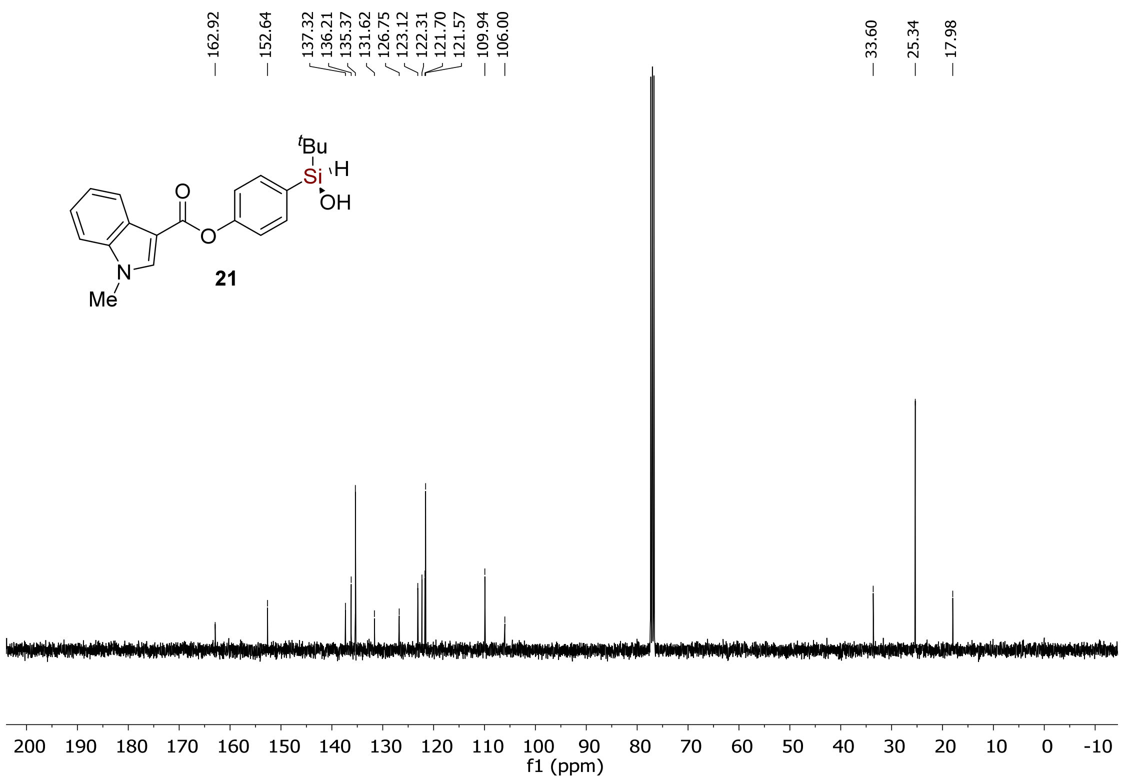
7.35
7.34
7.33
7.33
7.32
7.32
7.30
7.30
7.29
7.28
4.82
3.89
2.17
1.00
tBu
Si
H
OH
O
O
N
Me
21
1.01
1.02
2.02
5.19
1.00
3.10
1.04
9.19
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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121.70
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109.94
106.00
33.60
25.34
17.98
tBu
Si
H
OH
O
O
N
Me
21
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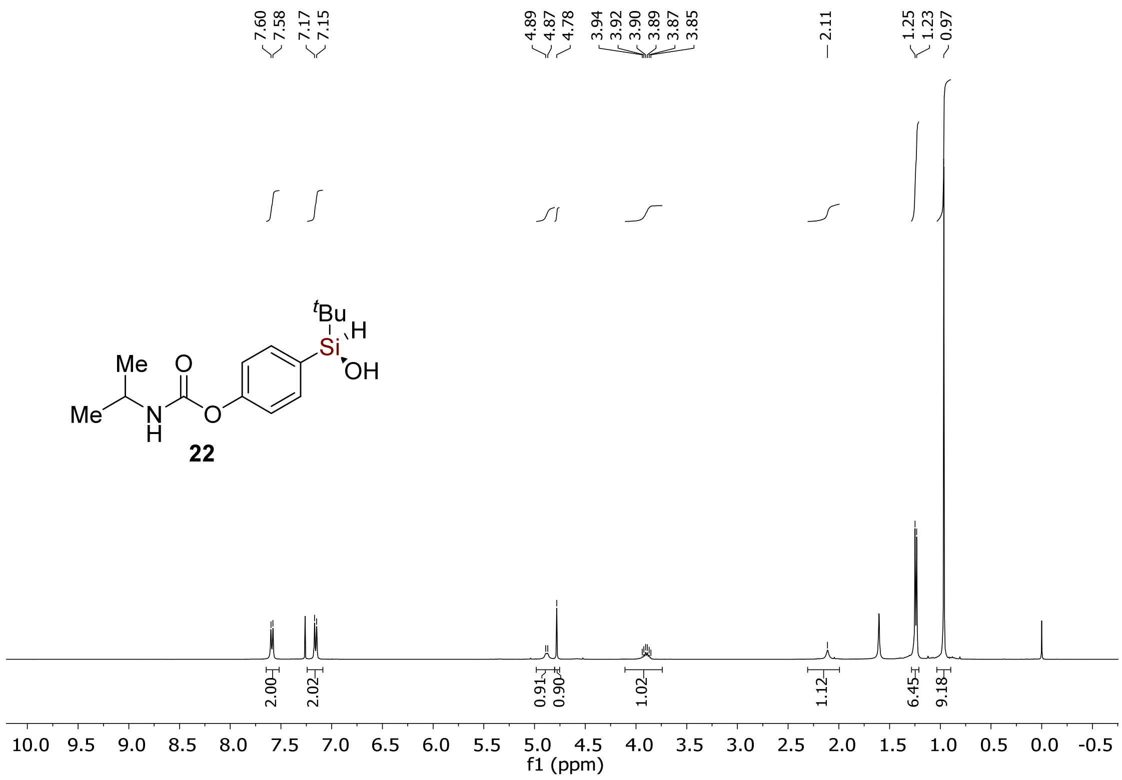
f1 (ppm)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4.87
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3.94
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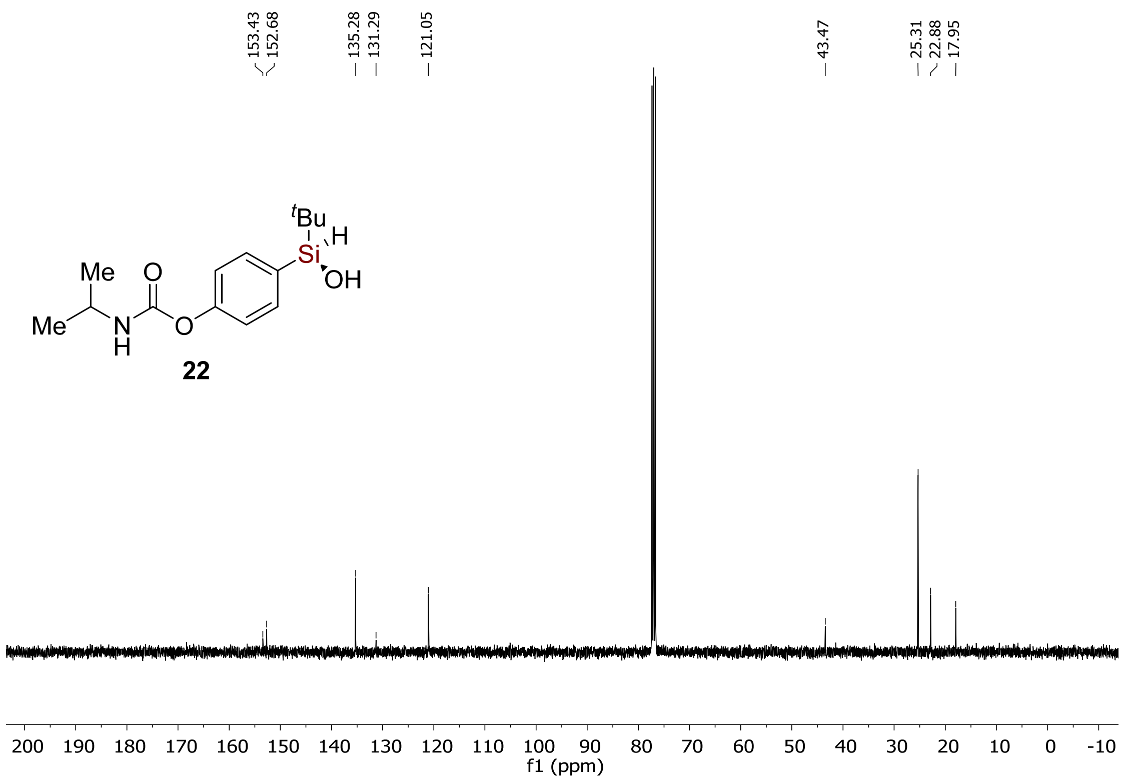
3.90
3.89
3.87
3.85
2.11
1.25
1.23
0.97
^tBu
H
Si
OH
Me
O
Me
N
H
O
22
2.00
2.02
0.91
0.90
1.02
1.12
6.45
9.18
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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22.88
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Si
OH
Me
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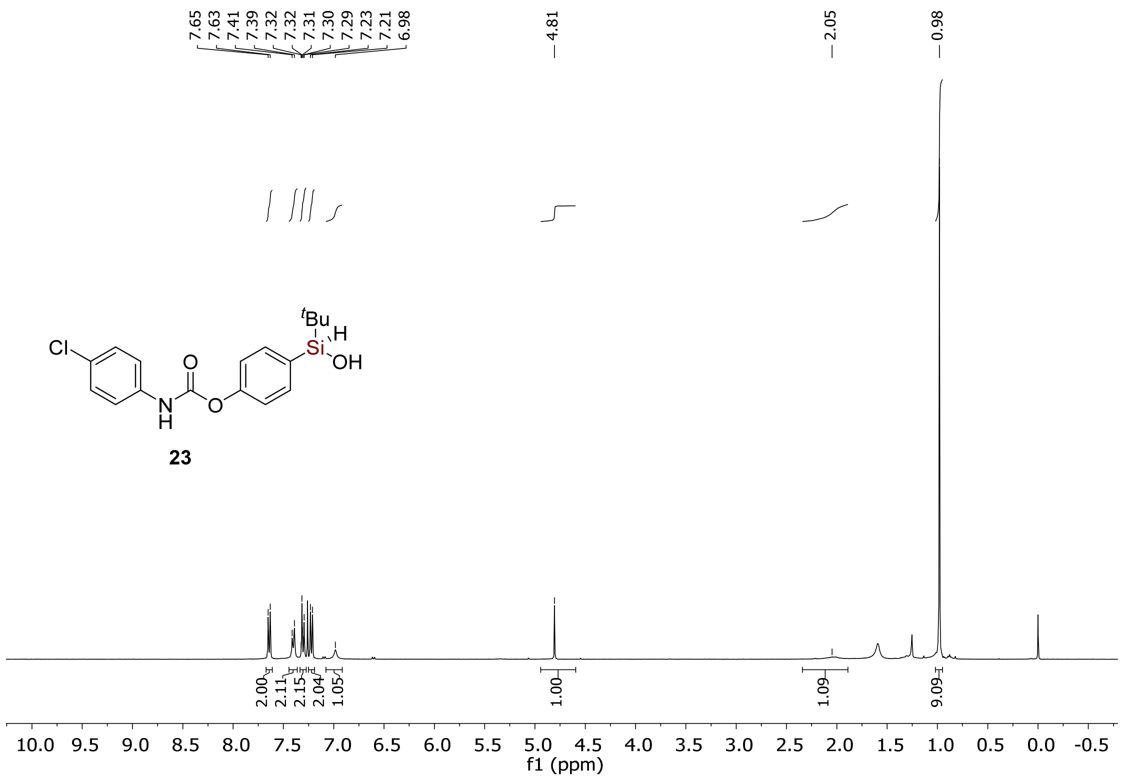
Me
N
H
O
22
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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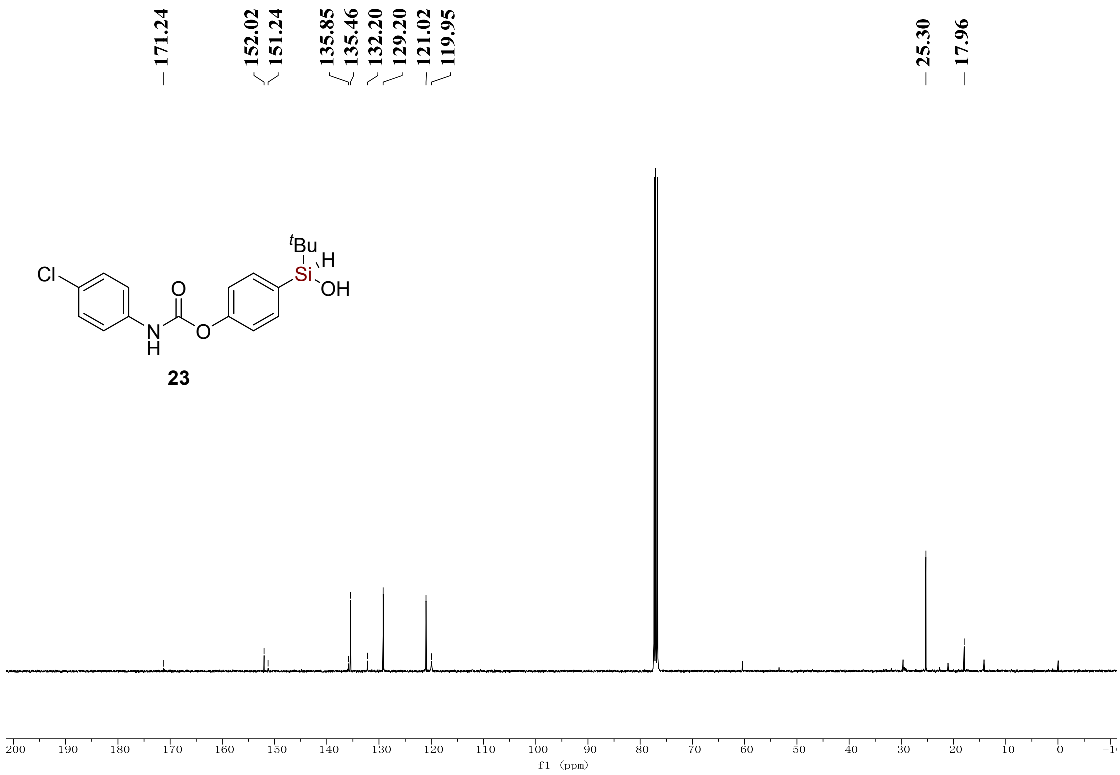
7.31
7.30
7.29
7.23
7.21
6.98
4.81
2.05
0.98
tBu
H
Si
OH
Cl
O
N
H
O
23
2.00
2.11
2.15
2.04
1.05
1.00
1.09
9.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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17.96
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OH
Cl
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N
H
O
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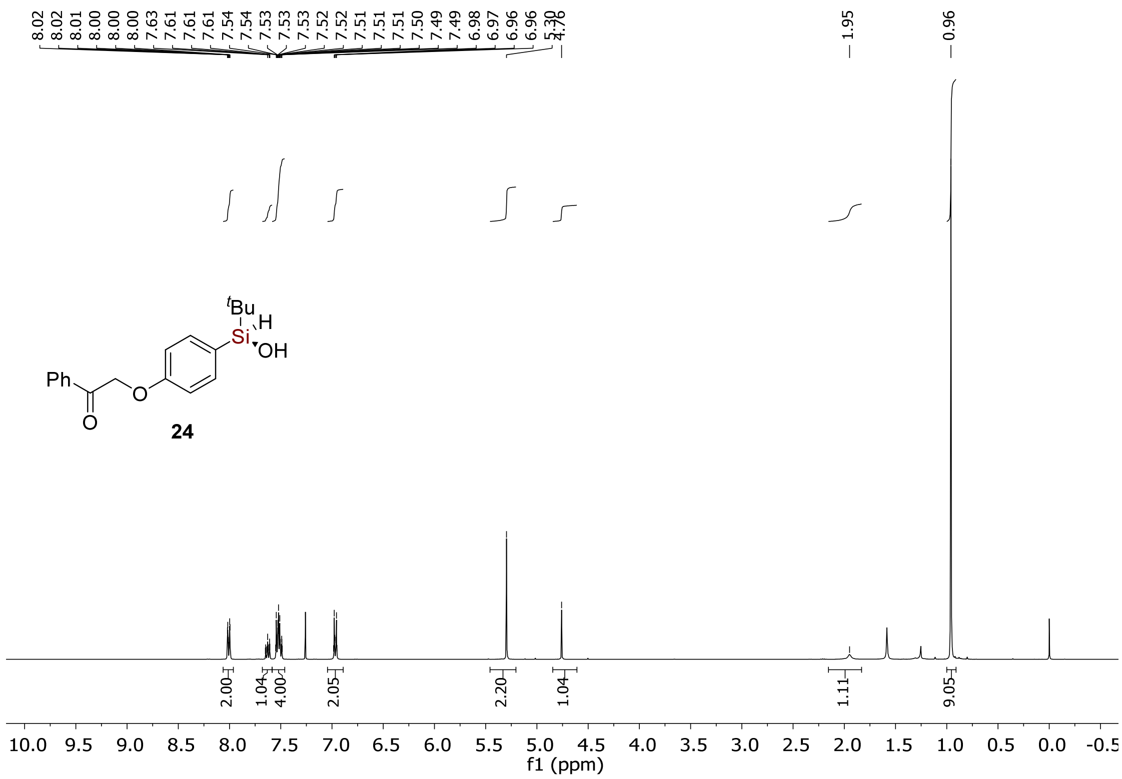
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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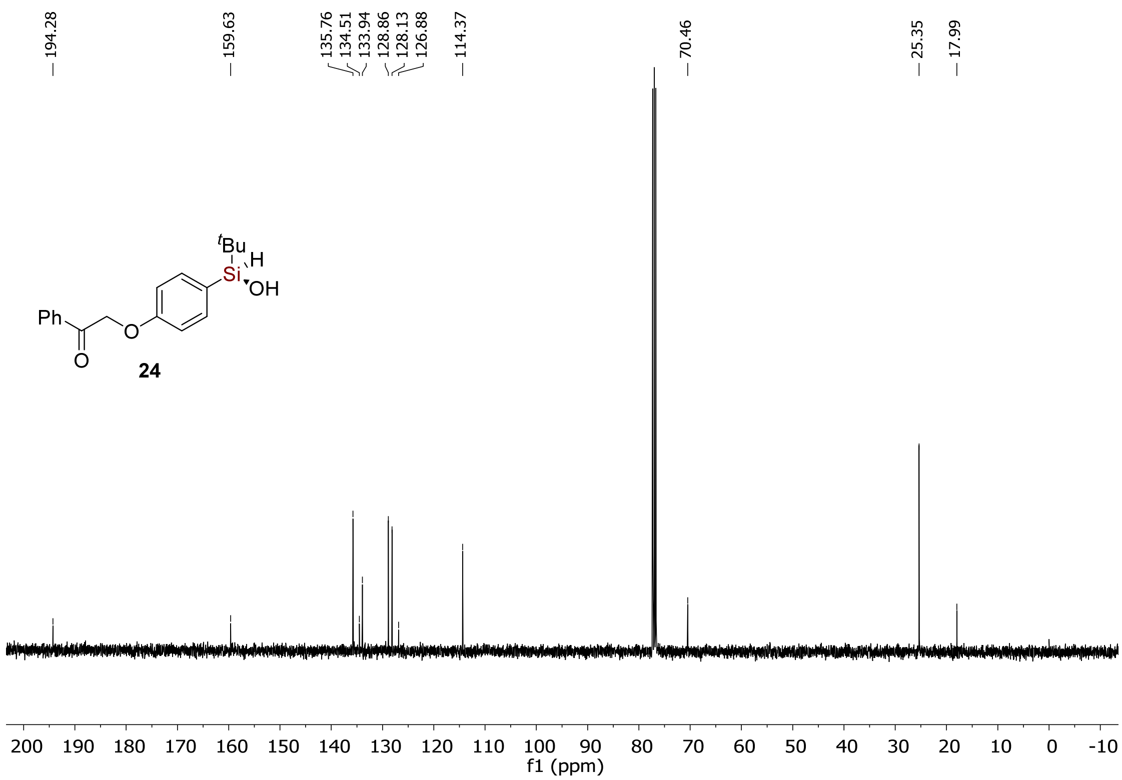
1.95
0.96
tBu
H
Si
OH
Ph
O
O
24
2.00
1.04
4.00
2.05
2.20
1.04
1.11
9.05
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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135.76 134.51 133.94 128.86 128.13 126.88
114.37
70.46
25.35
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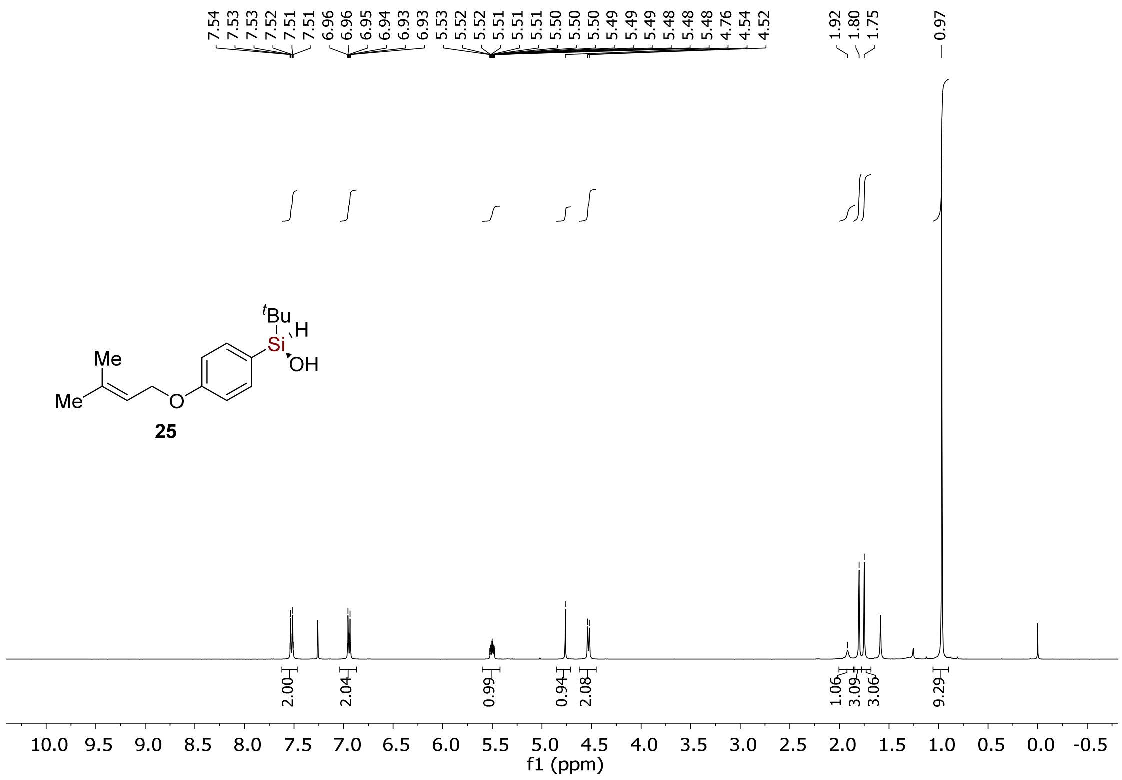
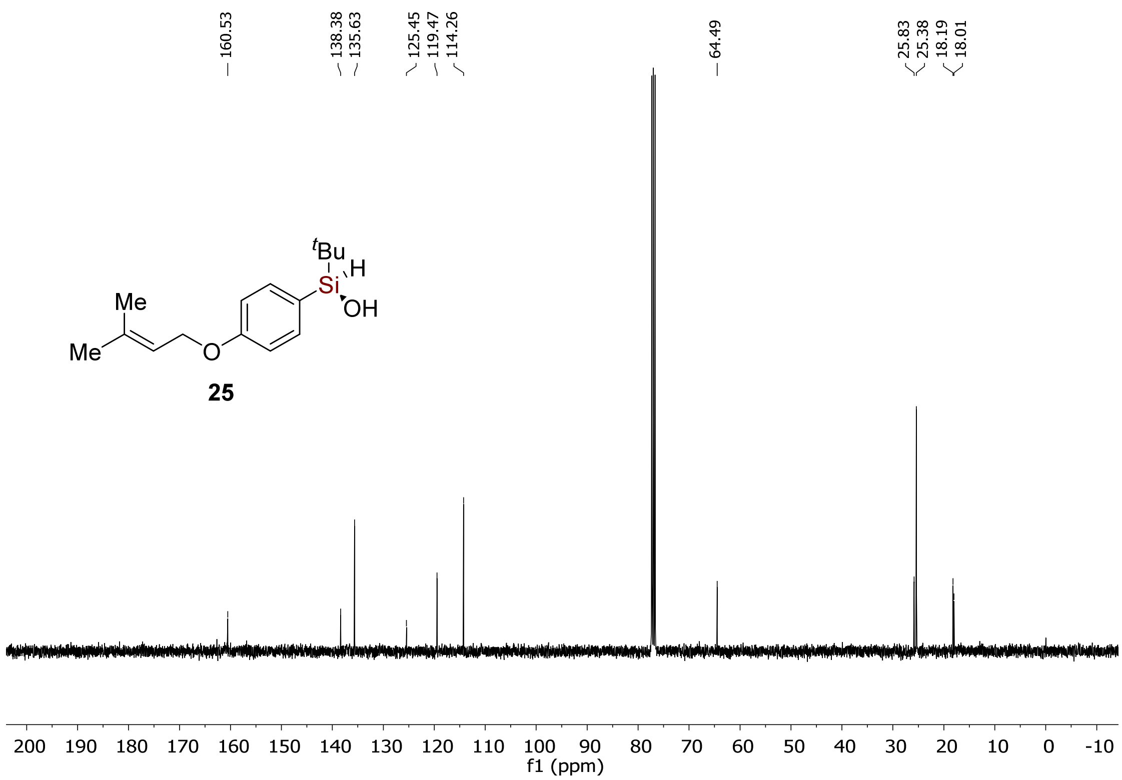
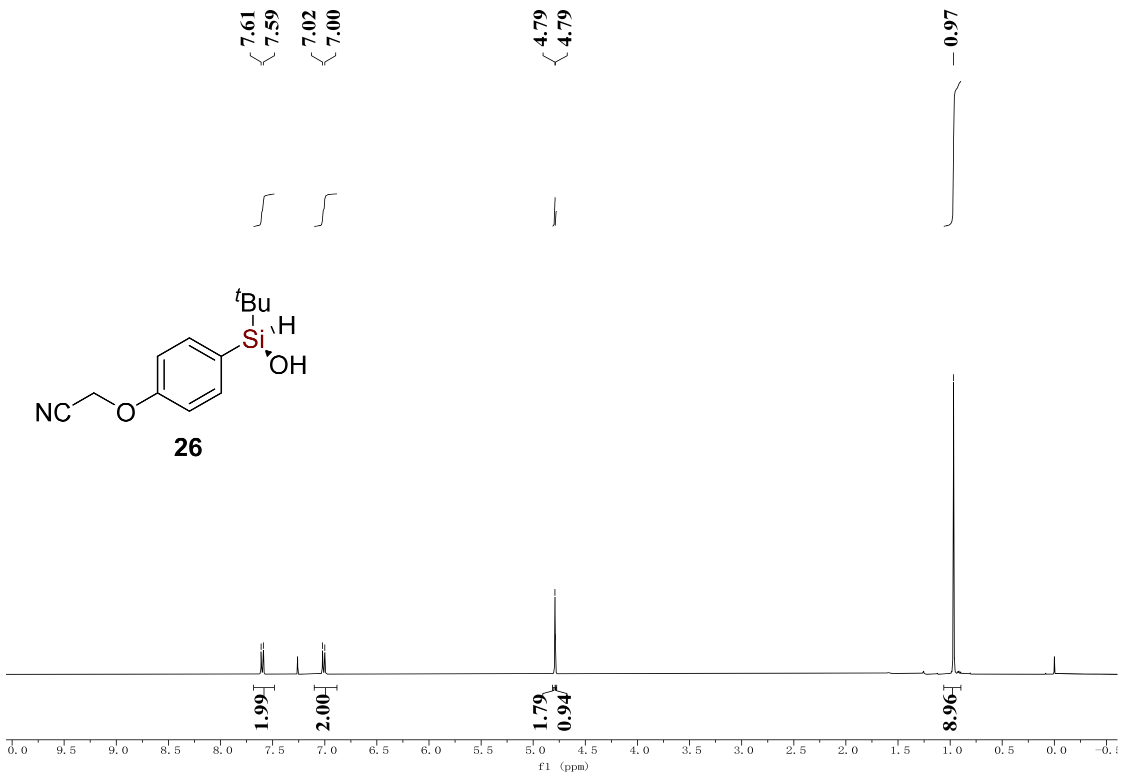
Si
OH
Ph
O
O
24
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



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OH
NC
O
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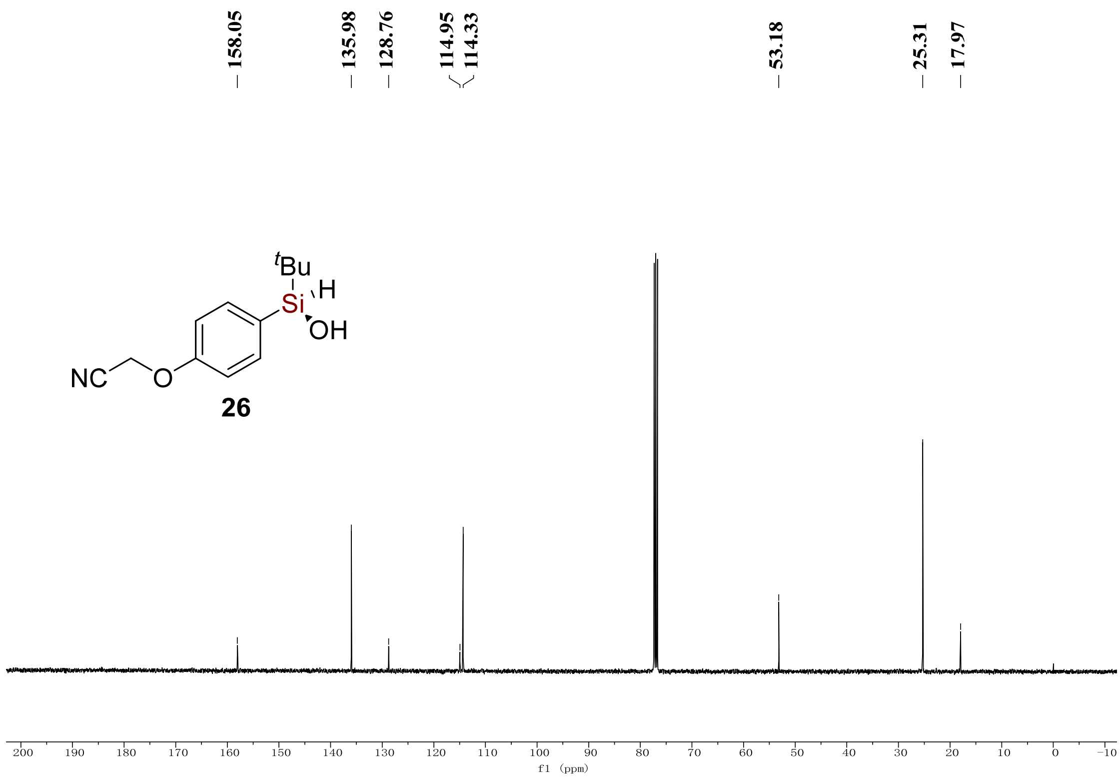
8.96
f1 (ppm)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OH
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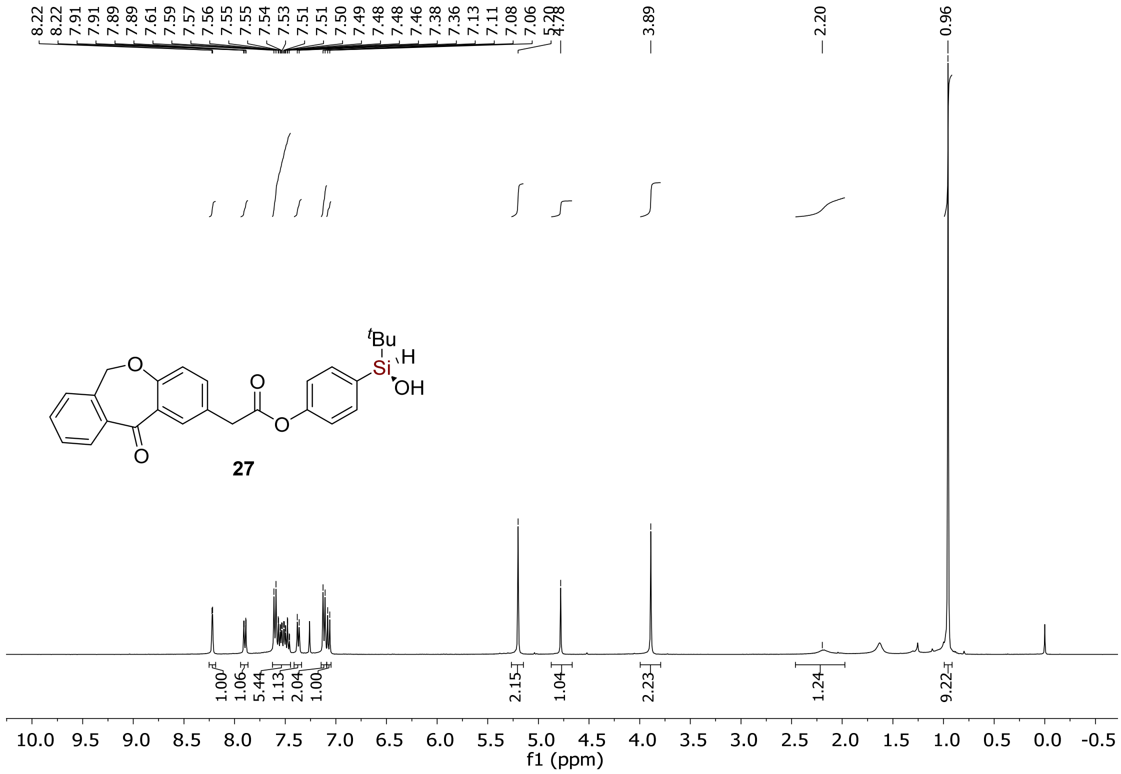
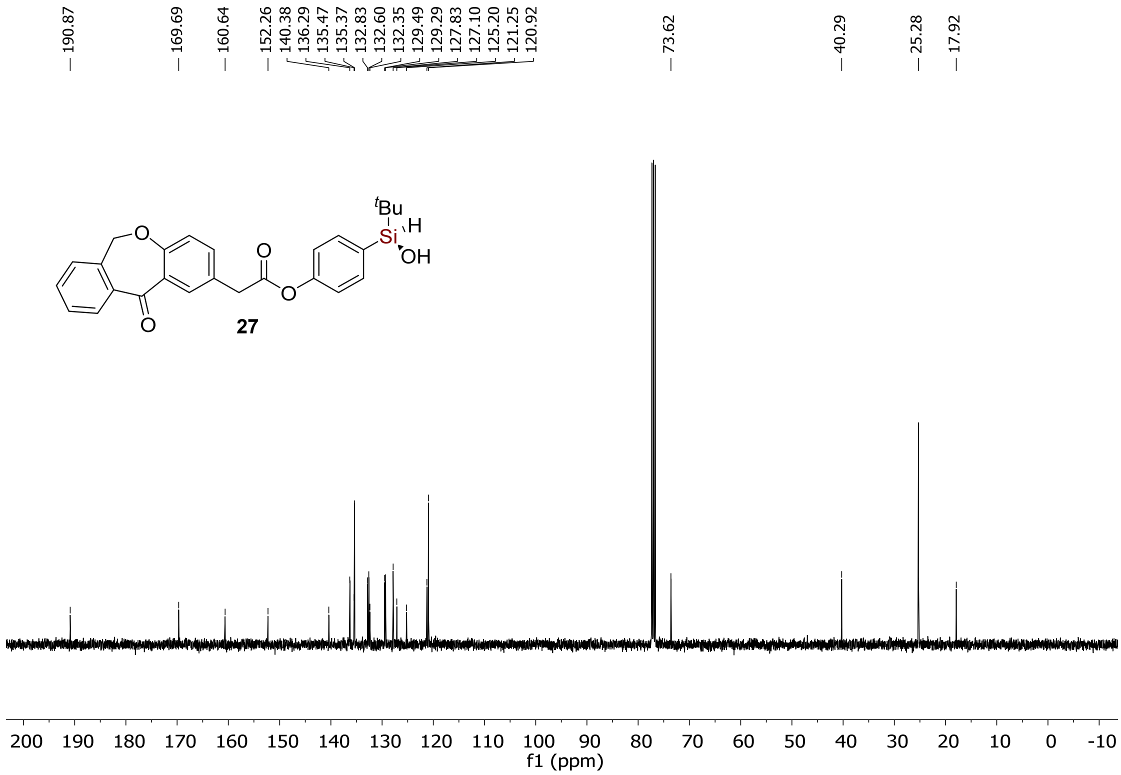
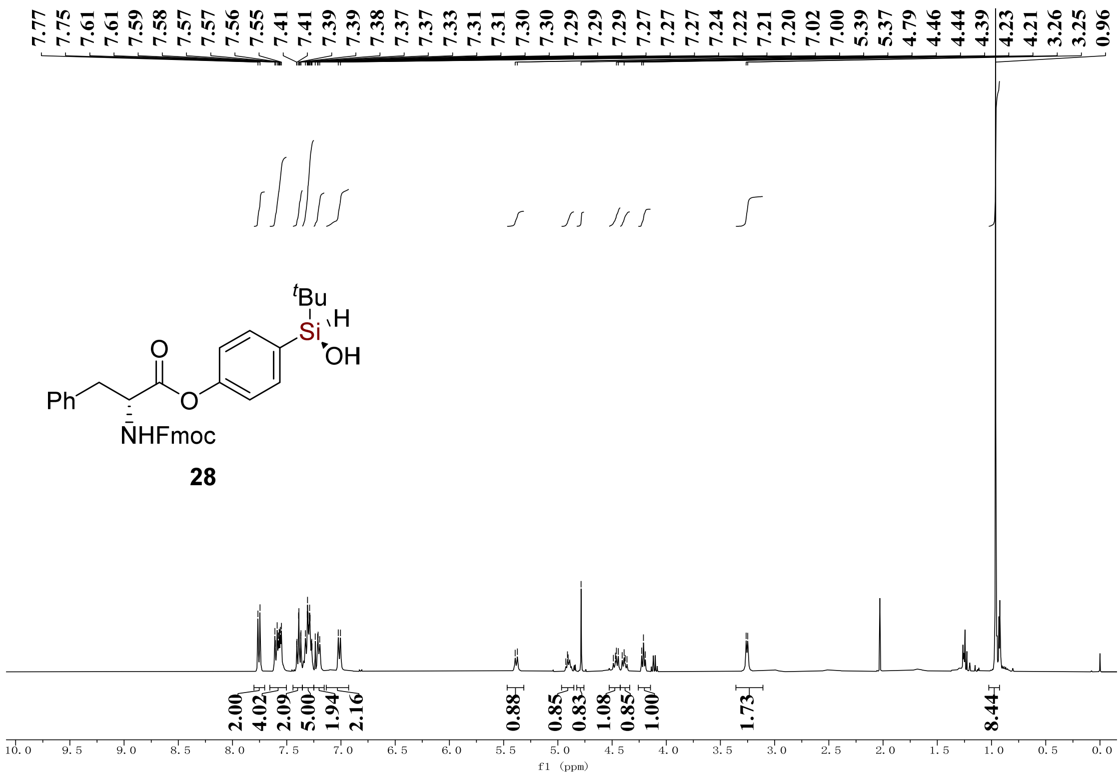
f1 (ppm)



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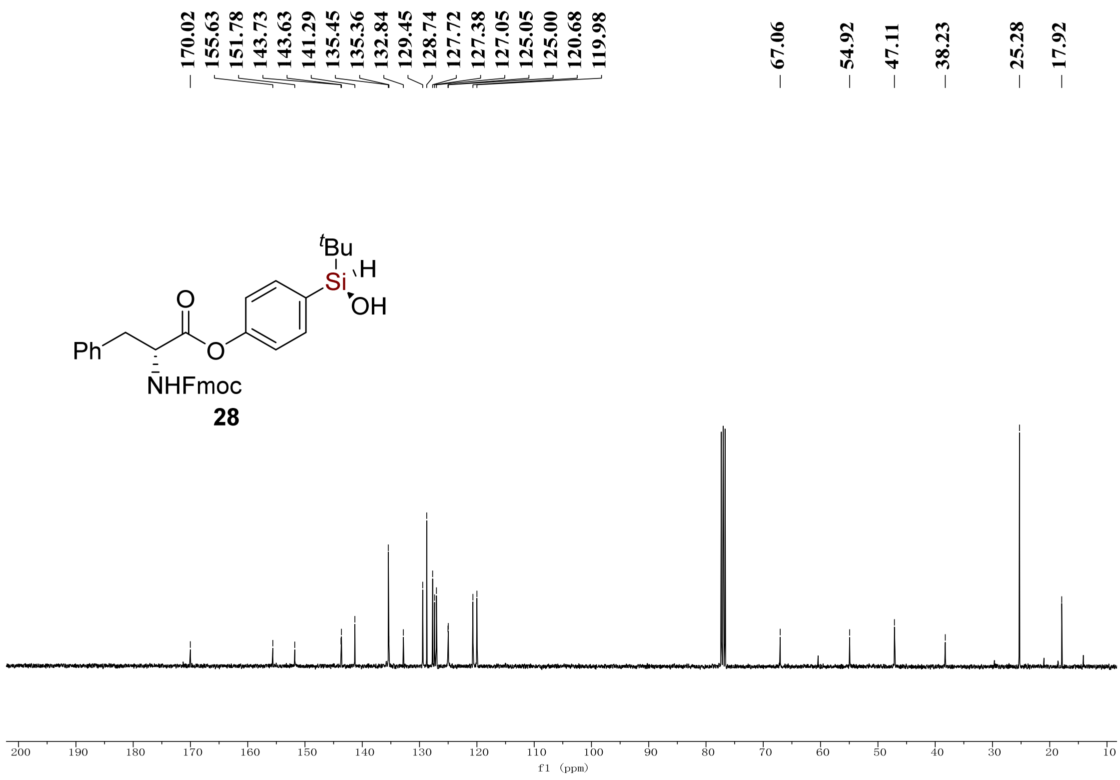
7.31
7.30
7.30
7.29
7.29
7.29
7.27
7.27
7.27
7.24
7.22
7.21
7.20
7.02
7.00
5.39
5.37
4.79
4.46
4.44
4.39
4.23
4.21
3.26
3.25
0.96
tBu
Si
H
OH
O
Ph
O
NHFmoc
28
2.00
4.02
2.09
5.00
1.94
2.16
0.88
0.85
0.83
1.08
0.85
1.00
1.73
8.44
f1 (ppm)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127.38
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125.05
125.00
120.68
119.98
67.06
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25.28
17.92
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Si
H
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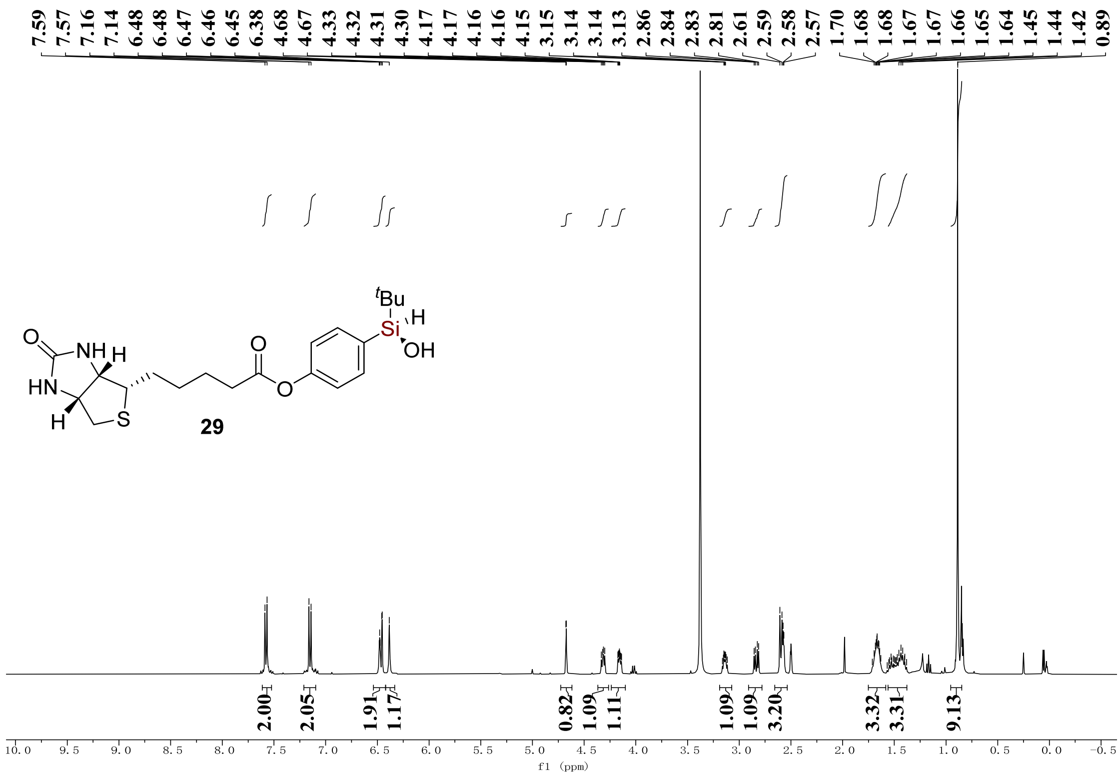
O
Ph
O
NHFmoc
28
f1 (ppm)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tBu
H
Si
OH
O
NH
H
HN
H
S
O
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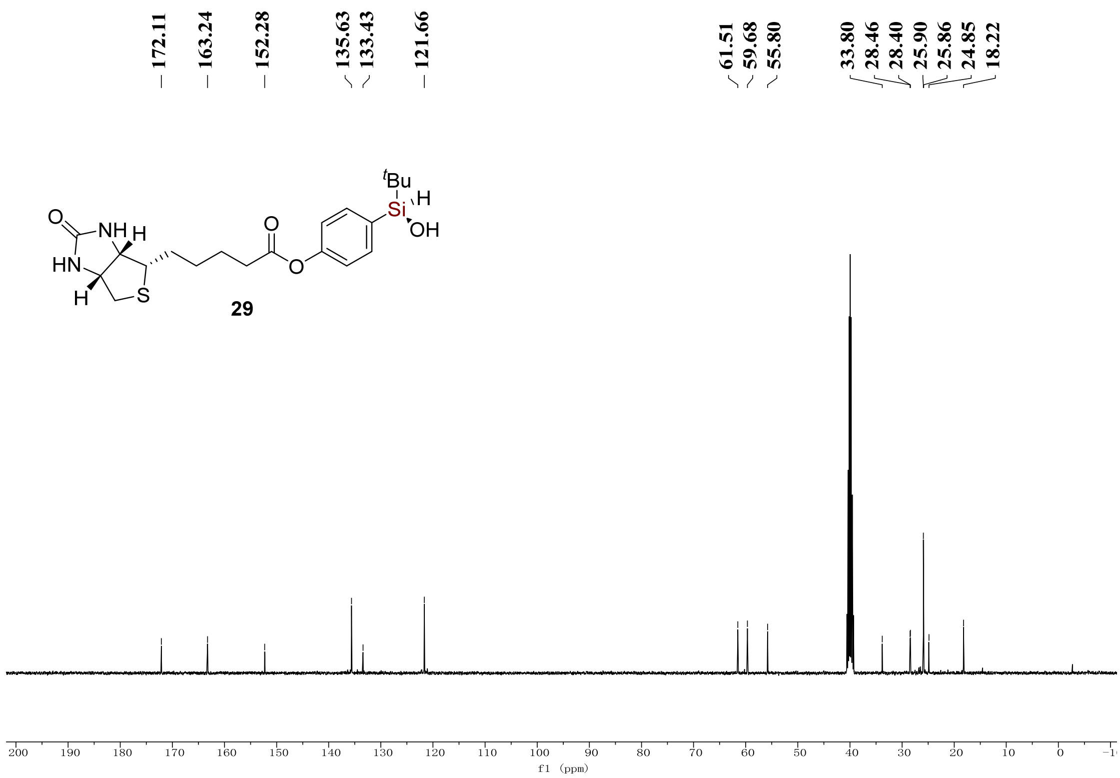
2.00 2.05 1.91 1.17 0.82 1.09 1.11 1.09 1.09 3.20 3.32 3.31 9.13
f1 (ppm)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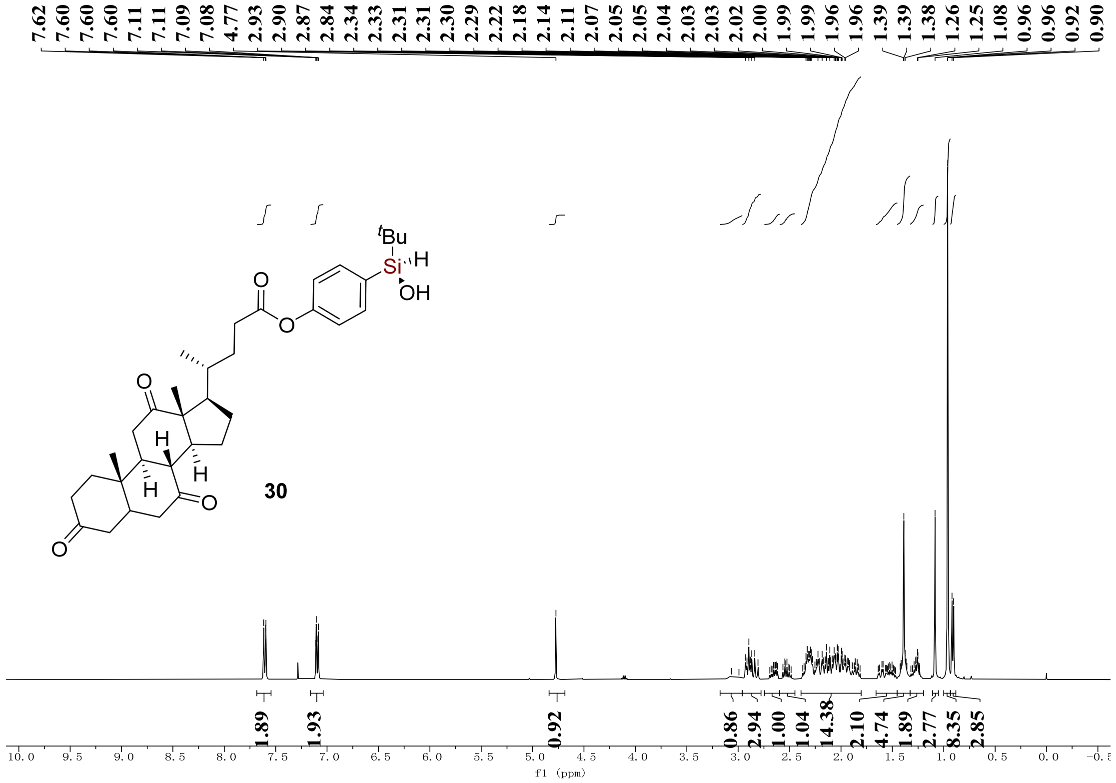
tBu
H
Si
OH
O
NH
H
HN
H
S
O
O
29
f1 (ppm)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2.84
2.34
2.33
2.31
2.31
2.30
2.29
2.22
2.18
2.14
2.11
2.07
2.05
2.05
2.04
2.03
2.03
2.02
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1.99
1.99
1.96
1.96
1.39
1.39
1.38
1.26
1.25
1.08
0.96
0.96
0.92
0.90
tBu
Si
H
OH
O
O
O
O
H
H
H
O
30
1.89
1.93
0.92
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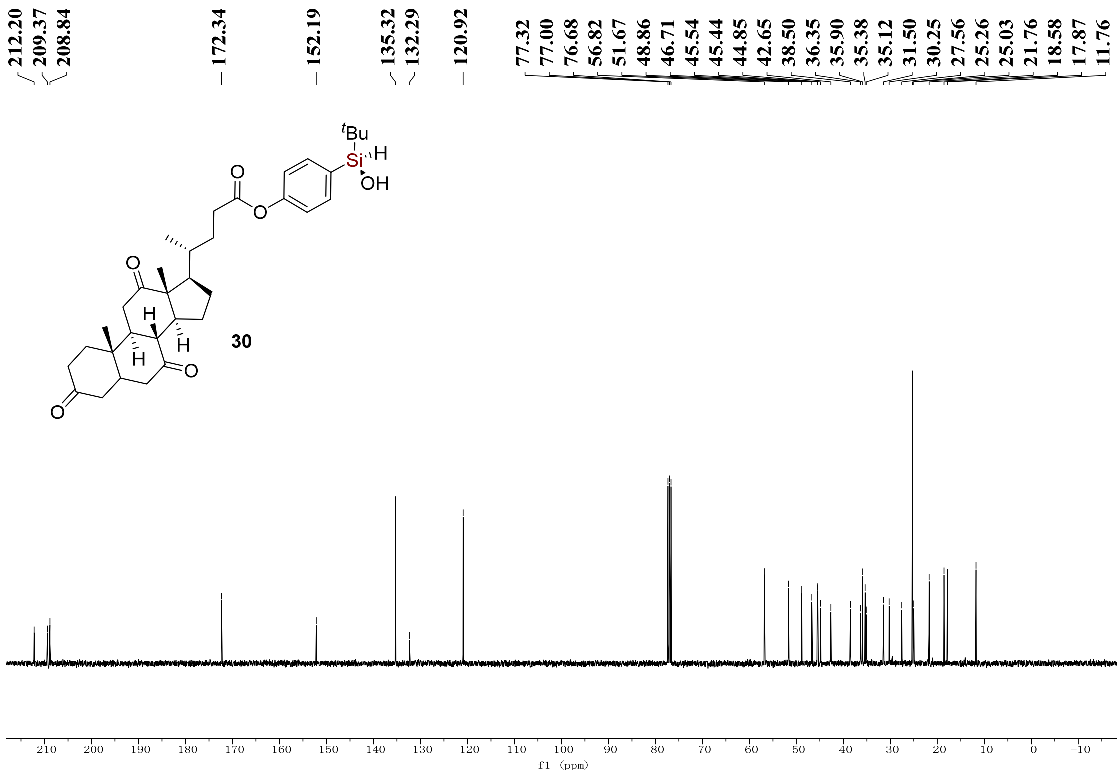
2.77
8.35
2.85
f1 (ppm)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120.92
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77.00
76.68
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48.86
46.71
45.54
45.44
44.85
42.65
38.50
36.35
35.90
35.38
35.12
31.50
30.25
27.56
25.26
25.03
21.76
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17.87
11.76
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Si
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O
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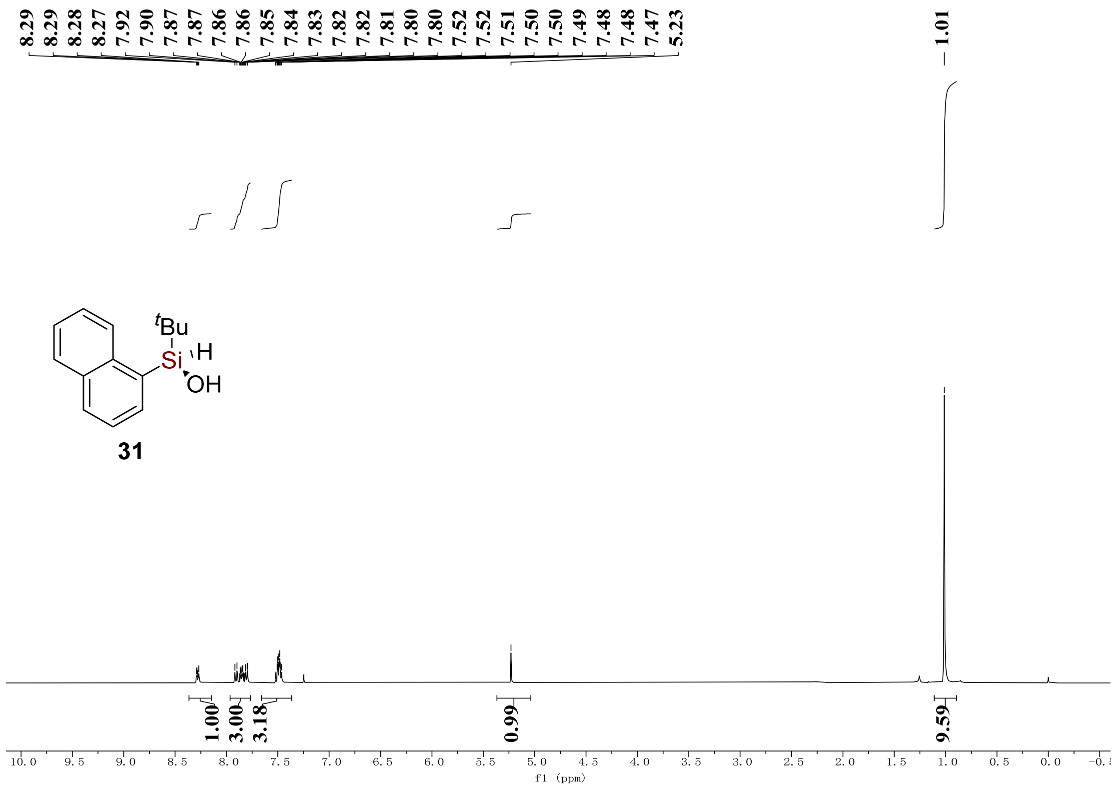
H
H
H
O
O
30
f1 (ppm)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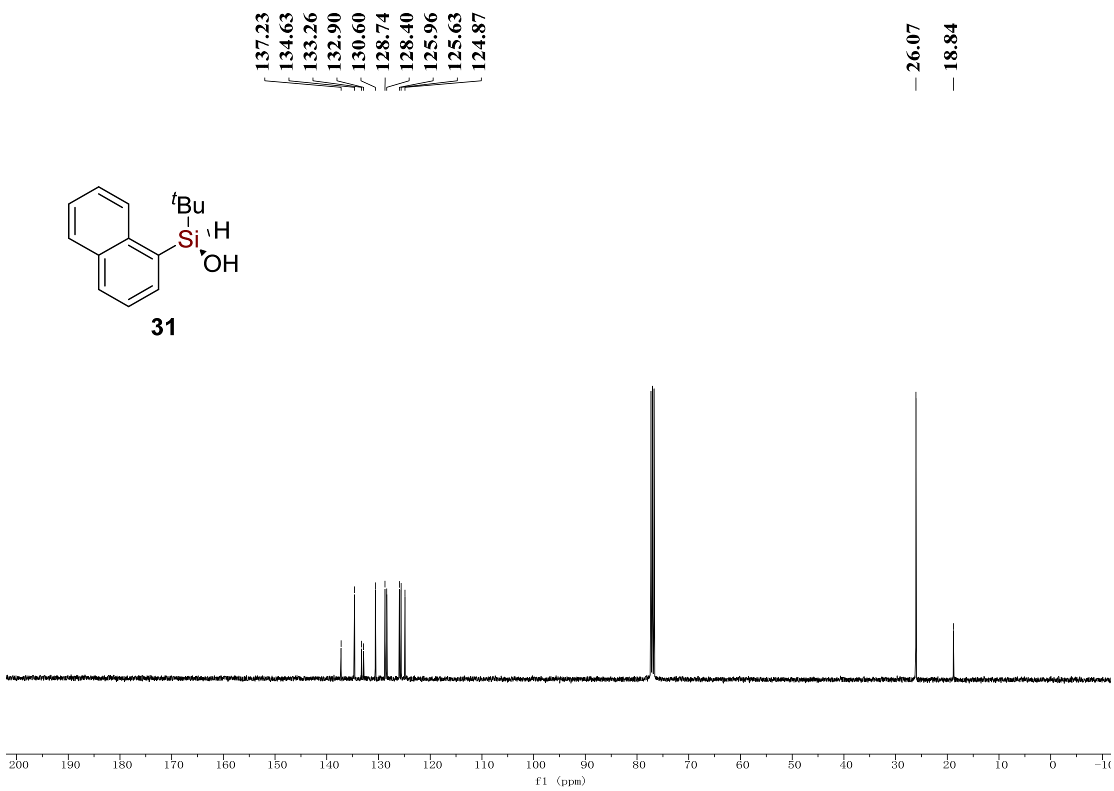
7.49
7.48
7.48
7.47
5.23
1.01
tBu
Si
H
OH
31
1.00
3.00
3.18
0.99
9.59
f1 (ppm)


137.23
134.63
133.26
132.90
130.60
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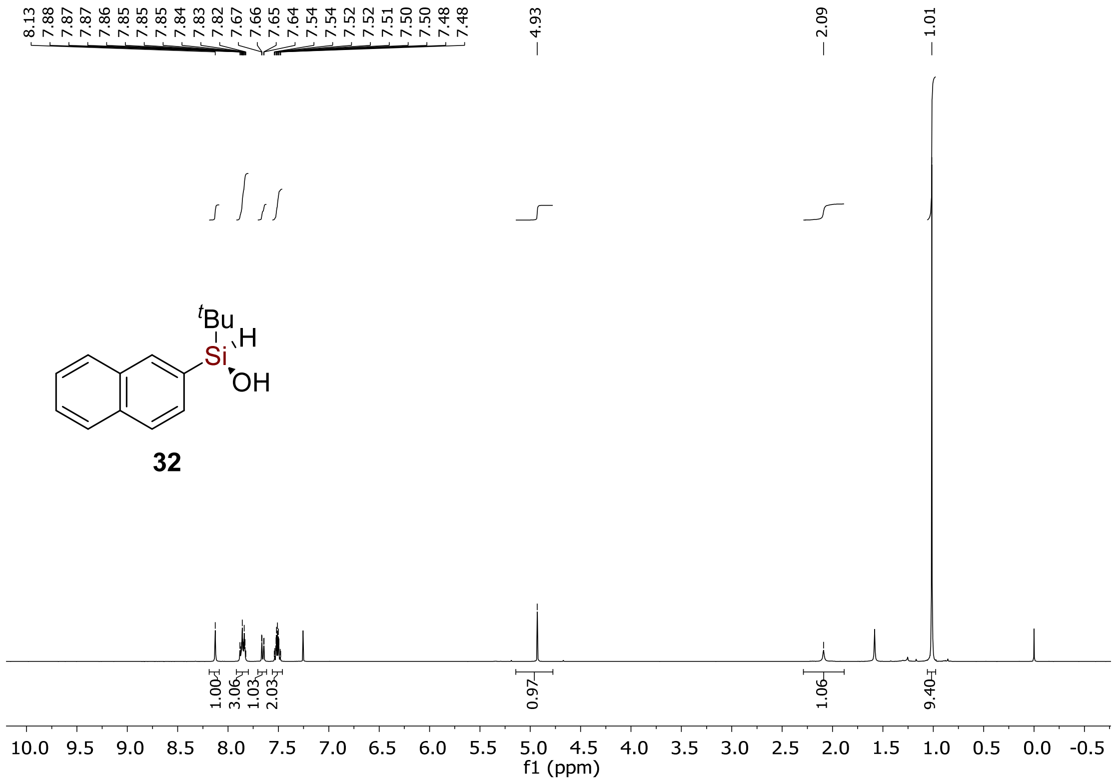
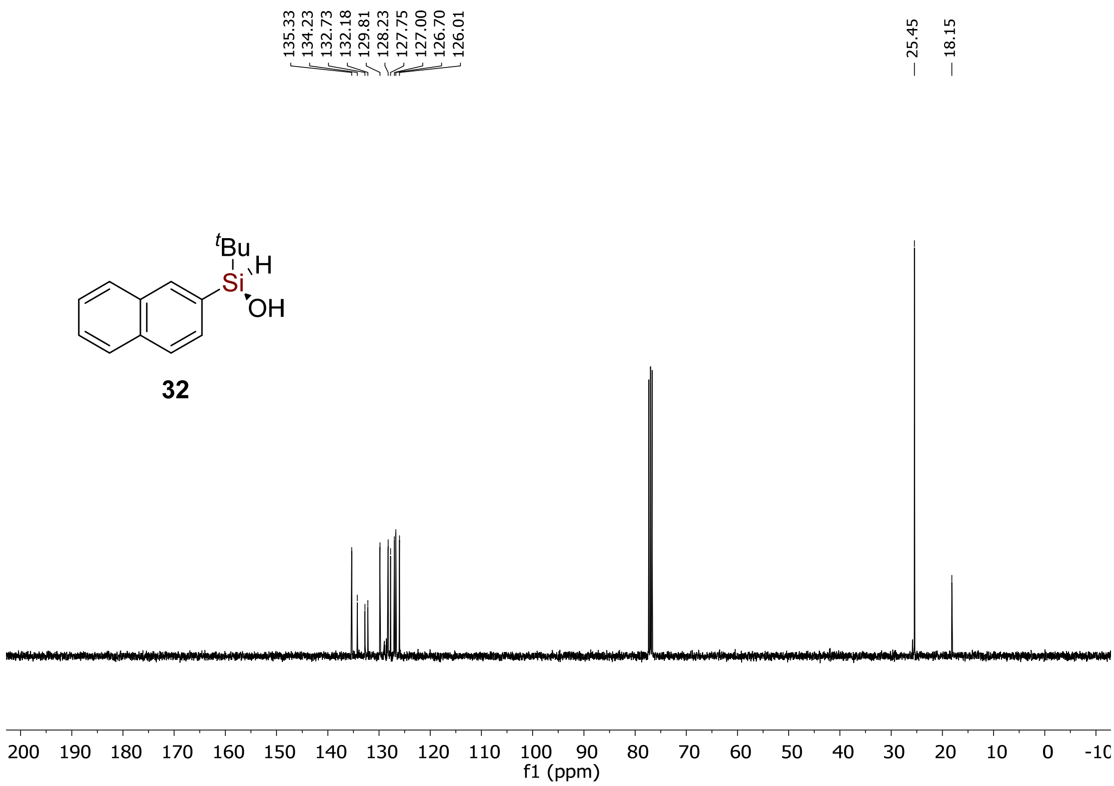
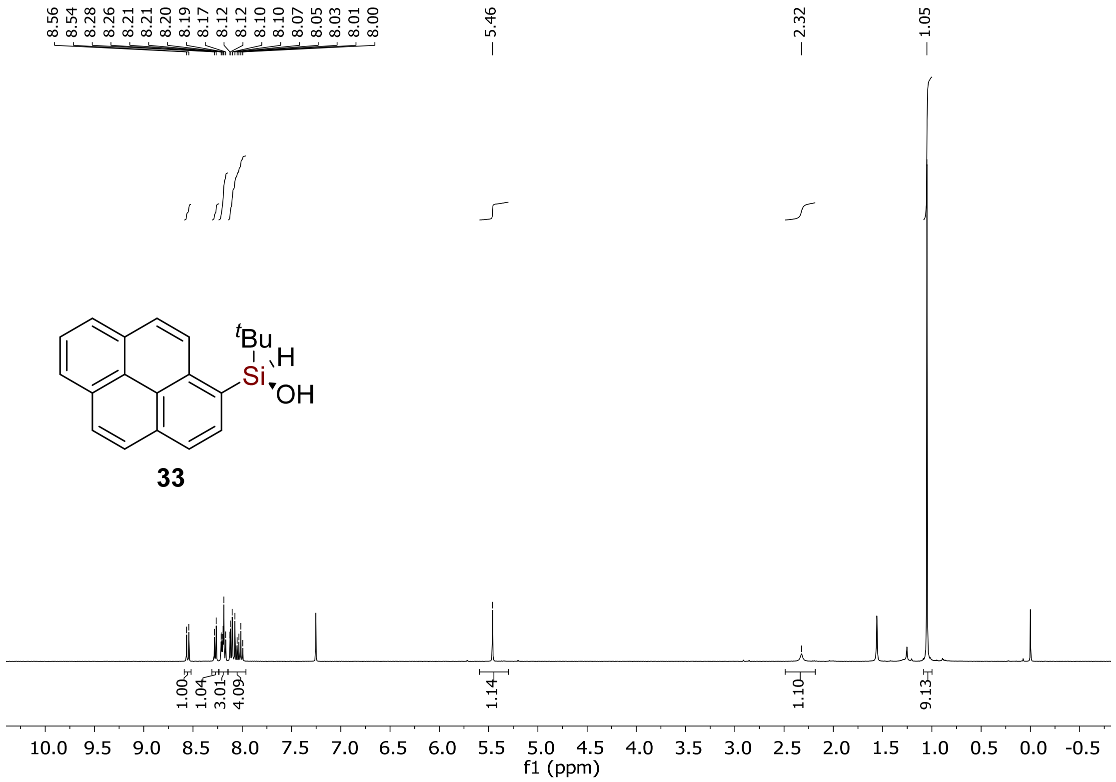
128.40
125.96
125.63
124.87
26.07
18.84
tBu
Si
H
OH
31
f1 (ppm)



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8.28
8.26
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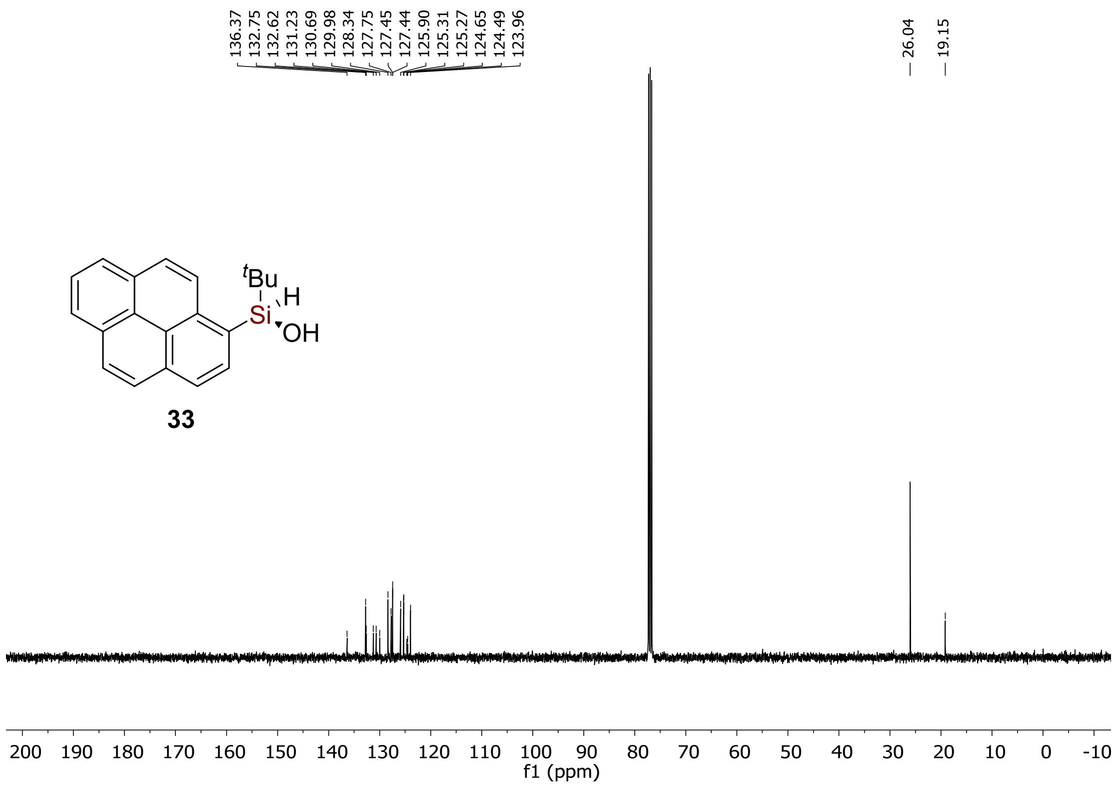
8.21
8.20
8.19
8.17
8.12
8.12
8.10
8.10
8.07
8.05
8.03
8.01
8.00
5.46
2.32
1.05
tBu
H
Si
OH
33
1.00
1.04
3.01
4.09
1.14
1.10
9.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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132.75
132.62
131.23
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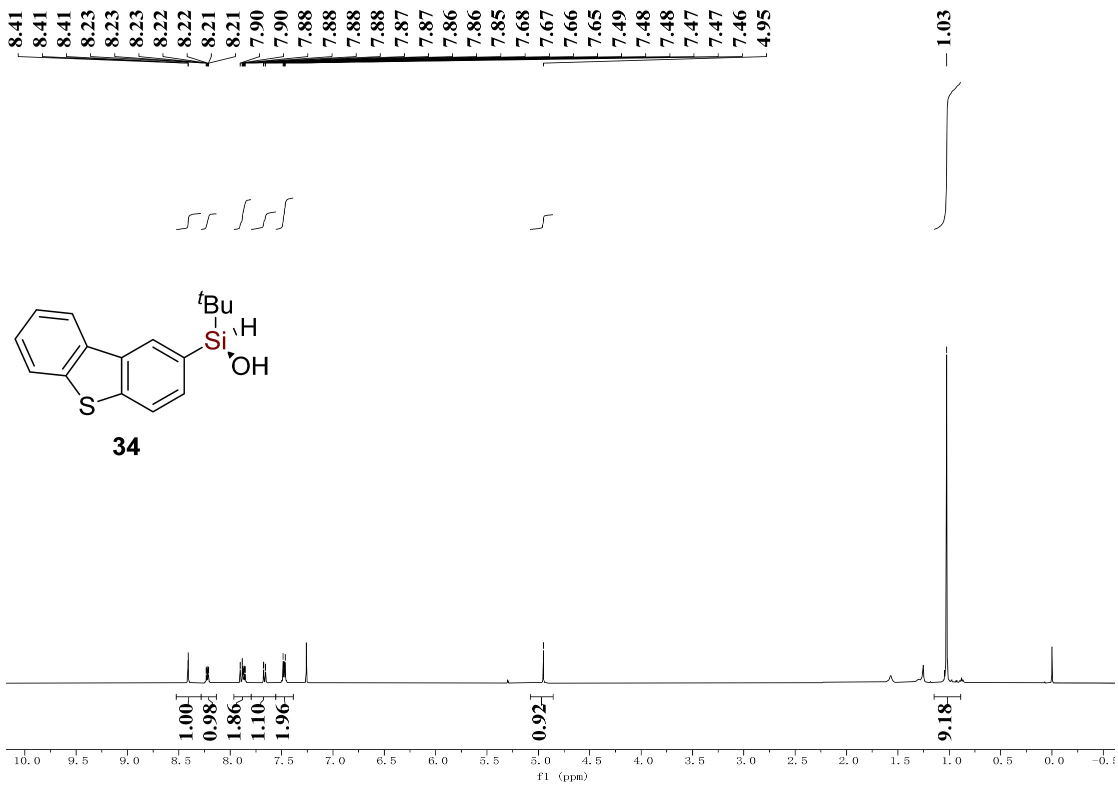
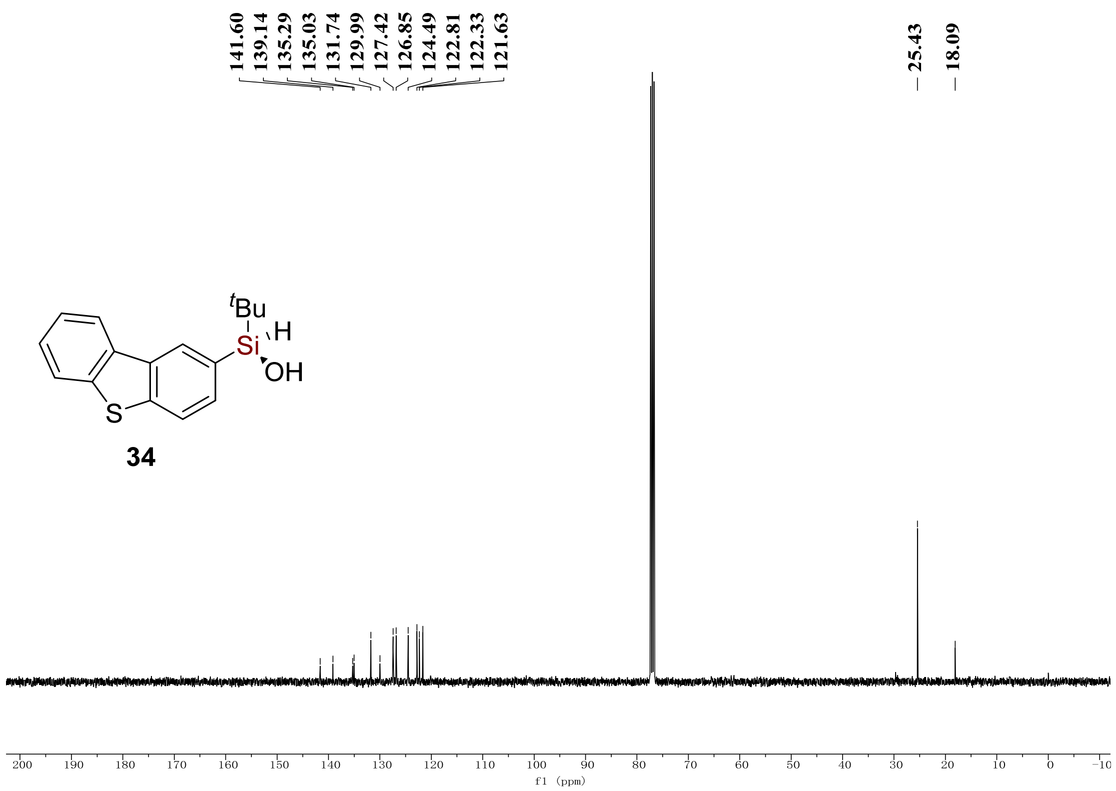
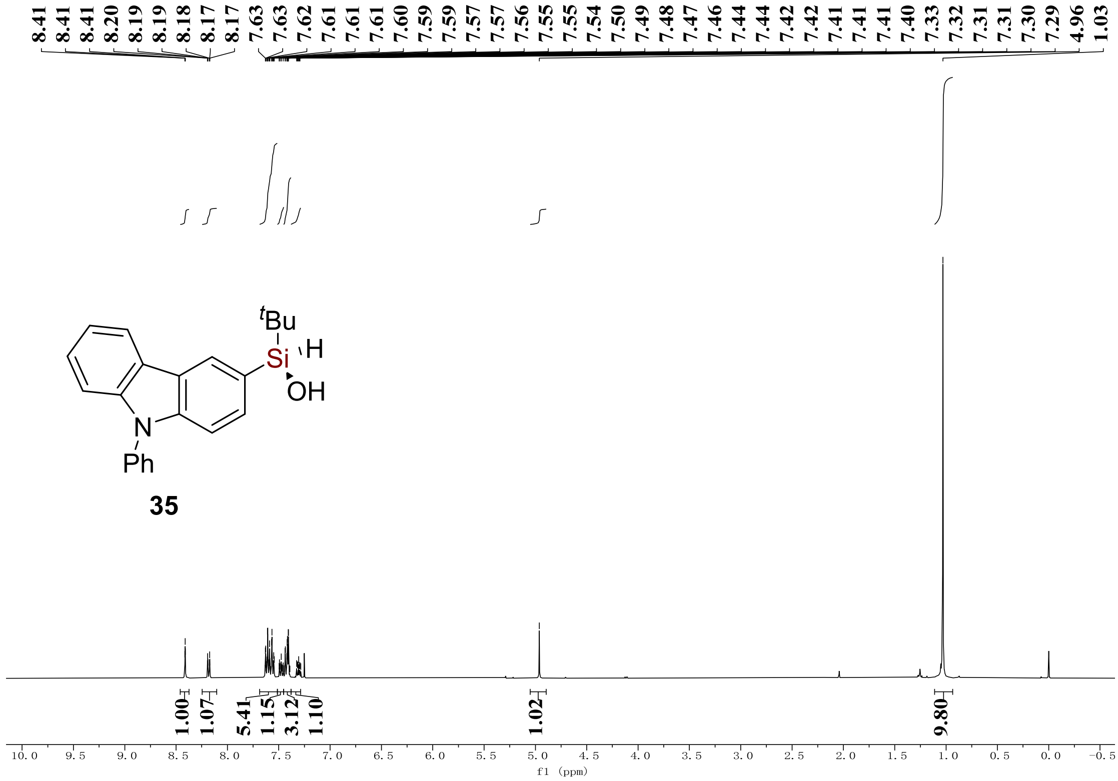
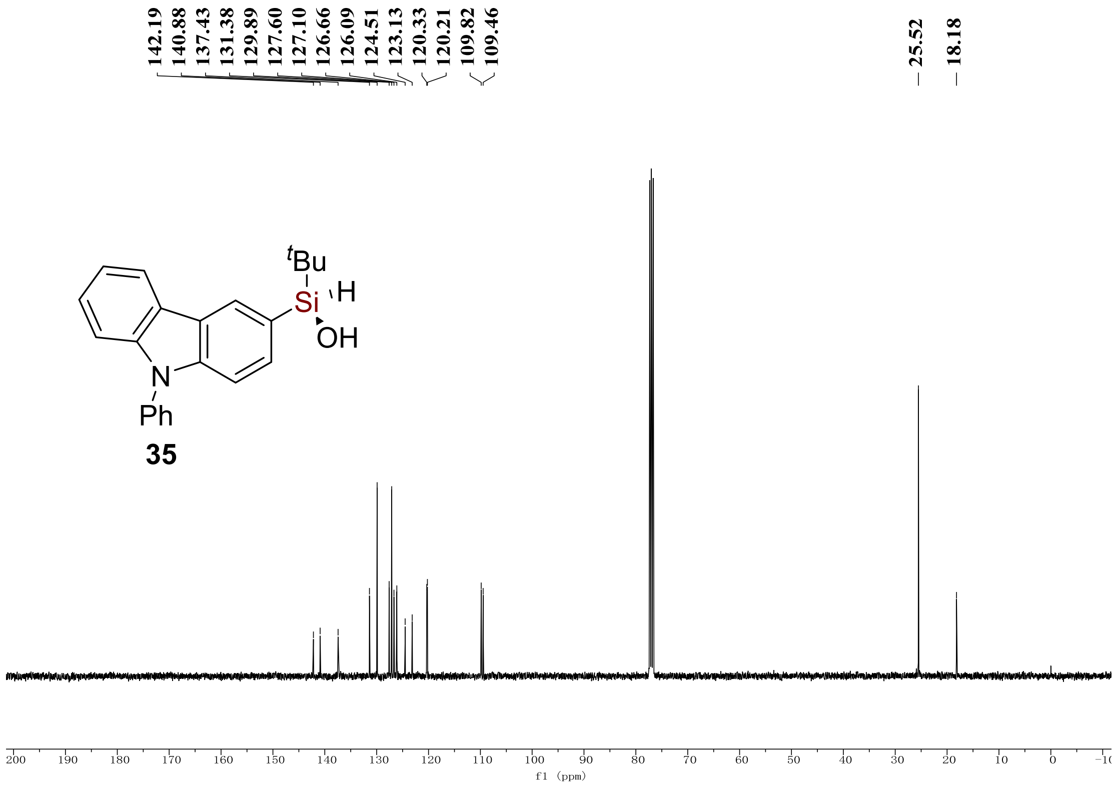
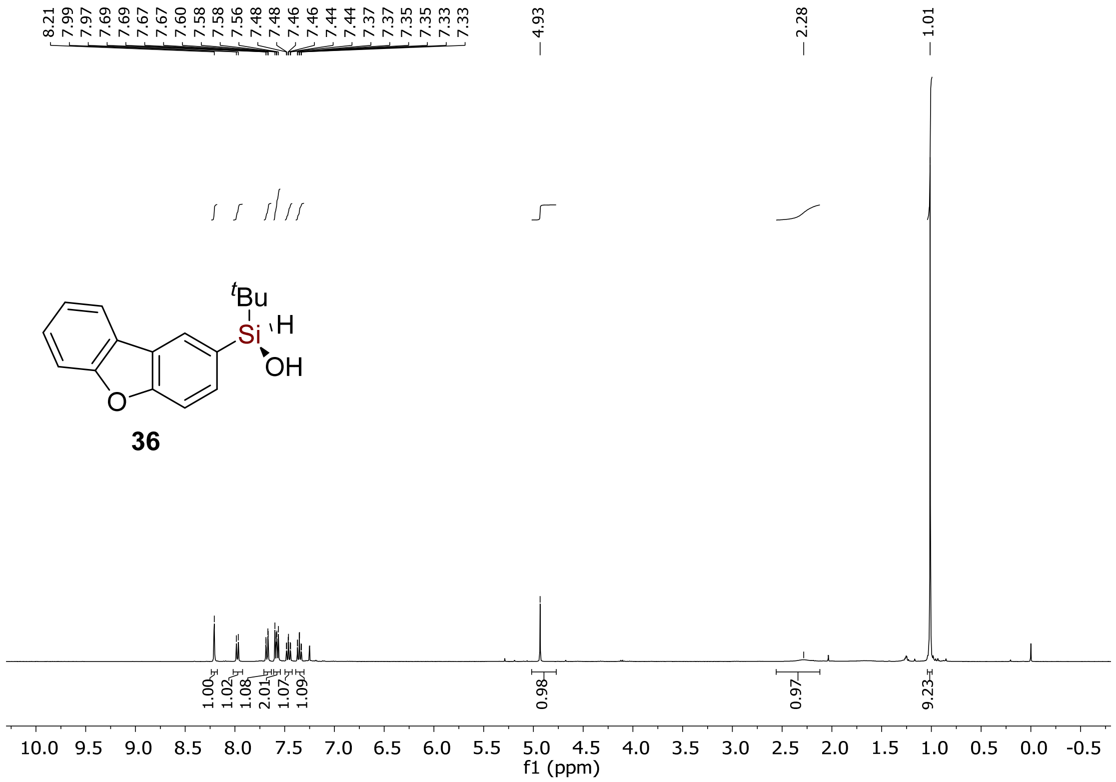
129.98
128.34
127.75
127.45
127.44
125.90
125.31
125.27
124.65
124.49
123.96
26.04
19.15
tBu
H
Si
OH
33
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

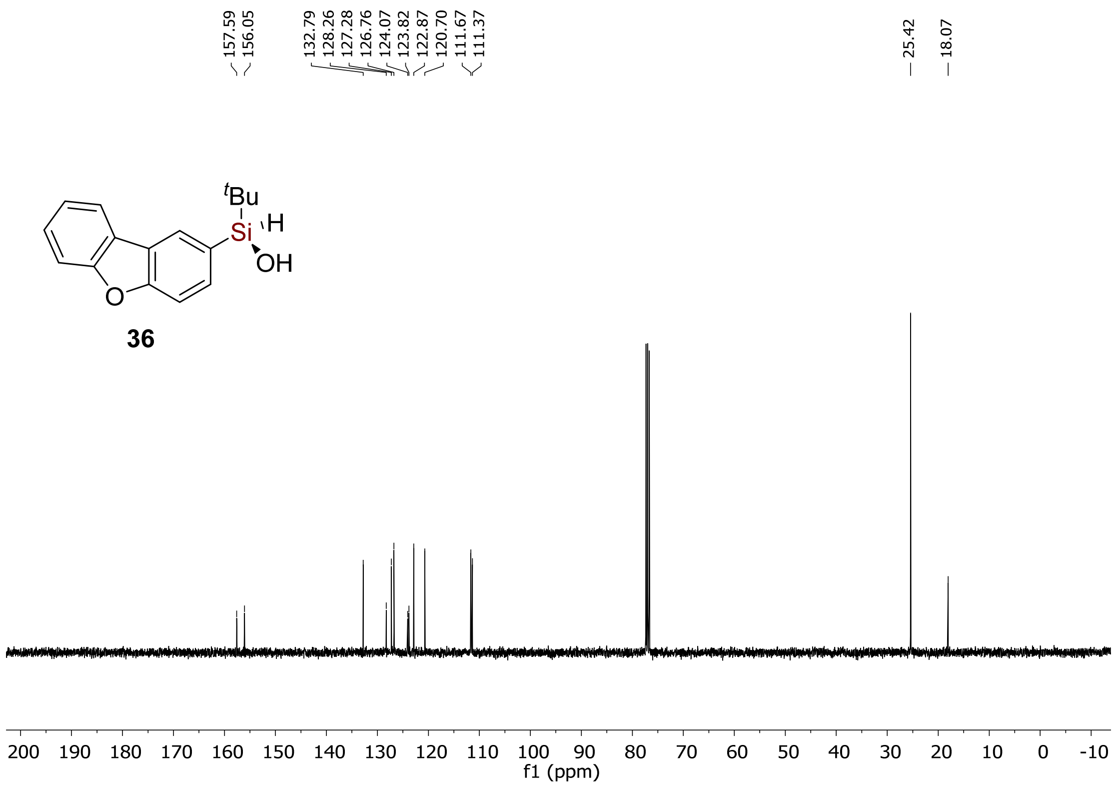


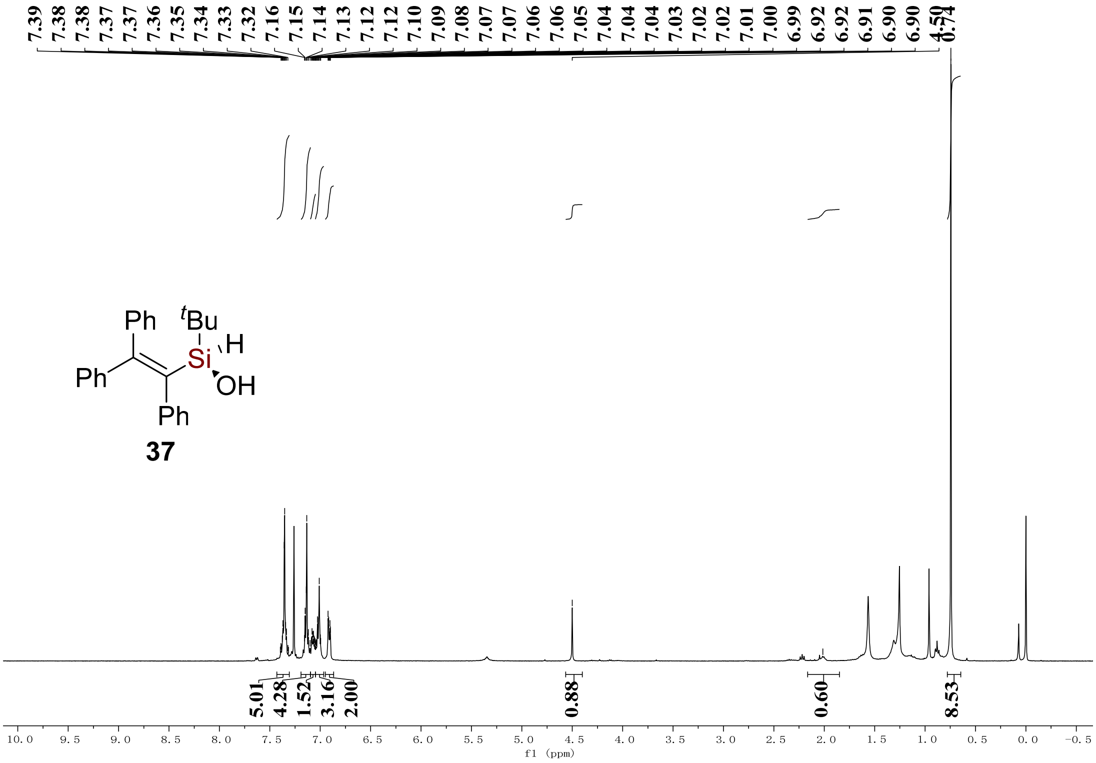


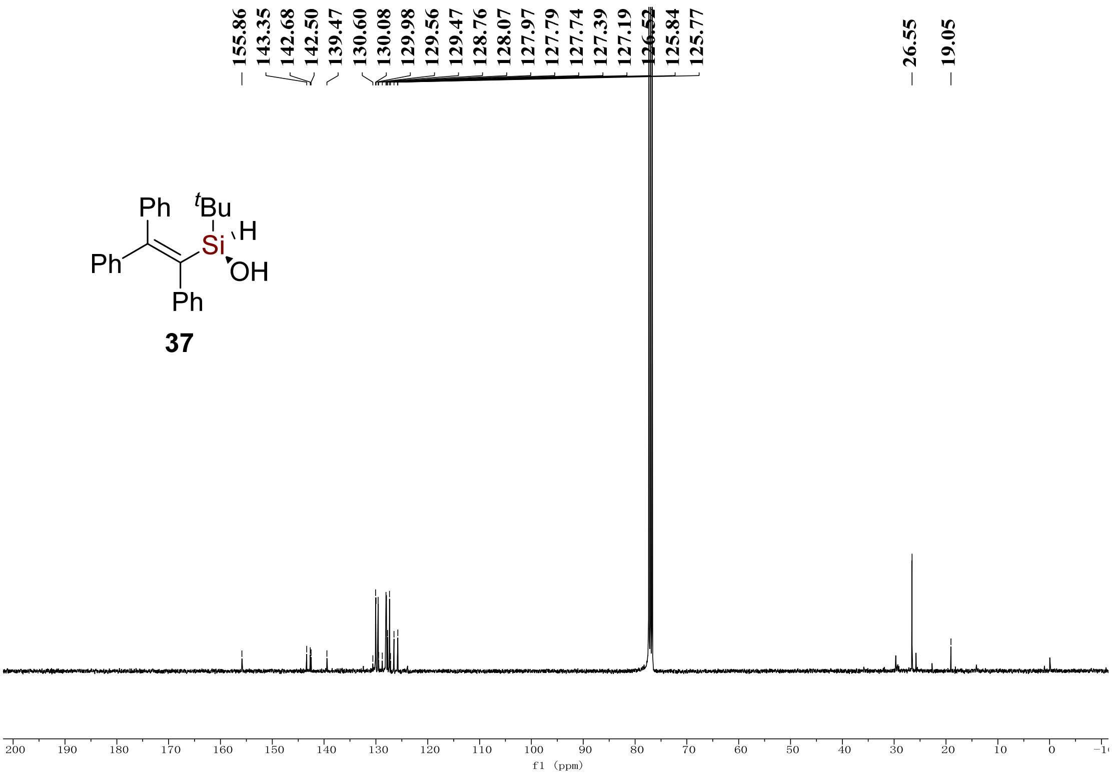

8.41
8.41
8.41
8.20
8.19
8.19
8.18
8.17
8.17
7.63
7.63
7.62
7.61
7.61
7.61
7.60
7.59
7.59
7.57
7.57
7.56
7.55
7.55
7.54
7.50
7.49
7.48
7.47
7.46
7.44
7.44
7.42
7.42
7.41
7.41
7.41
7.40
7.33
7.32
7.31
7.31
7.30
7.29
4.96
1.03
tBu
Si
H
OH
N
Ph
35
1.00
1.07
5.41
1.15
3.12
1.10
1.02
9.80
f1 (ppm)


142.19
140.88
137.43
131.38
129.89
127.60
127.10
126.66
126.09
124.51
123.13
120.33
120.21
109.82
109.46
25.52
18.18
tBu
Si
H
OH
N
Ph
35
f1 (ppm)


8.21
7.99
7.97
7.69
7.69
7.67
7.67
7.60
7.58
7.58
7.56
7.48
7.48
7.46
7.46
7.44
7.44
7.37
7.37
7.35
7.35
7.33
7.33
4.93
2.28
1.01
tBu
Si
H
OH
O
36
1.00
1.02
1.08
2.01
1.07
1.09
0.98
0.97
9.23
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


157.59
156.05
132.79
128.26
127.28
126.76
124.07
123.82
122.87
120.70
111.67
111.37
25.42
18.07
tBu
Si
H
OH
O
36
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.39
7.38
7.38
7.37
7.37
7.36
7.35
7.34
7.33
7.32
7.16
7.15
7.14
7.13
7.12
7.12
7.10
7.09
7.08
7.07
7.07
7.06
7.06
7.05
7.04
7.04
7.04
7.03
7.02
7.02
7.01
7.00
6.99
6.92
6.92
6.91
6.90
6.90
4.50
0.74
Ph
tBu
H
Si
Ph
OH
Ph
37
5.01
4.28
1.52
3.16
2.00
0.88
0.60
8.53
f1 (ppm)


155.86
143.35
142.68
142.50
139.47
130.60
130.08
129.98
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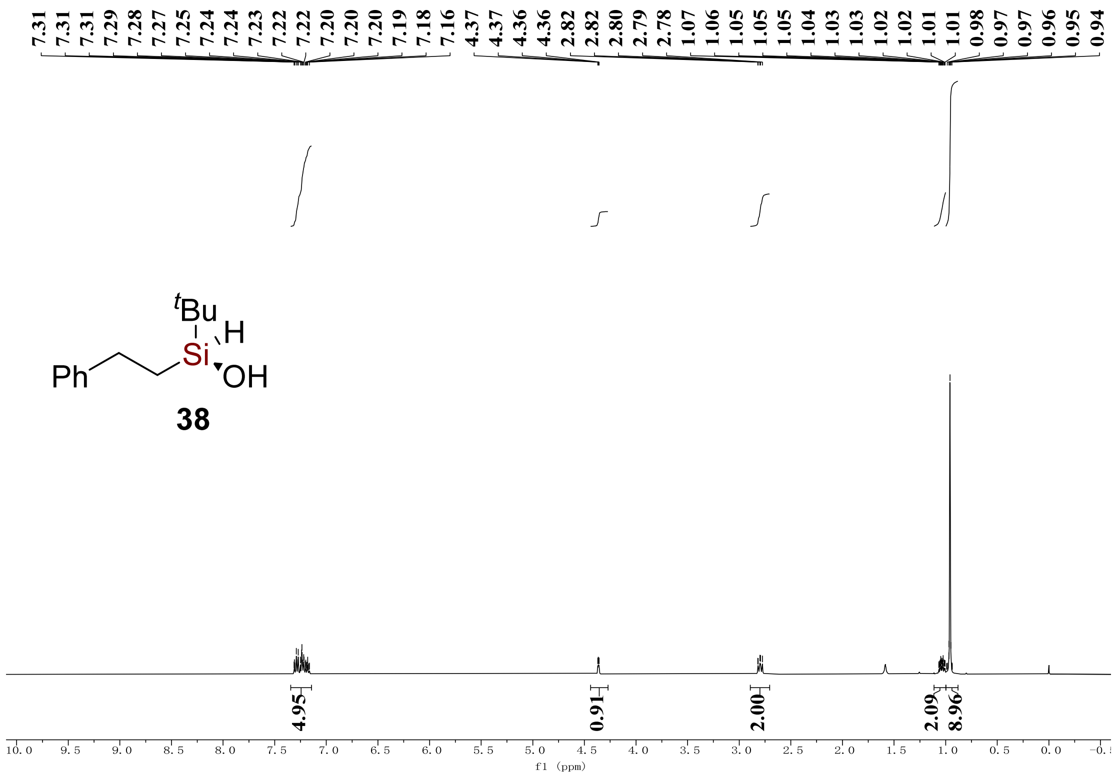
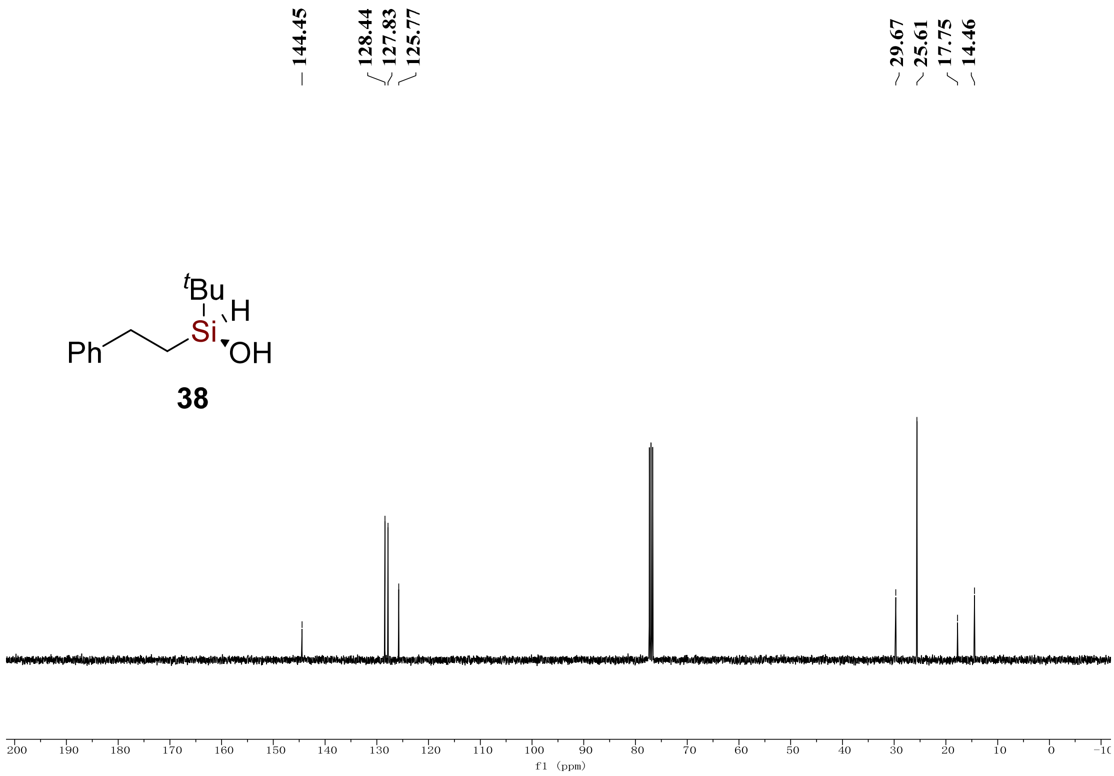
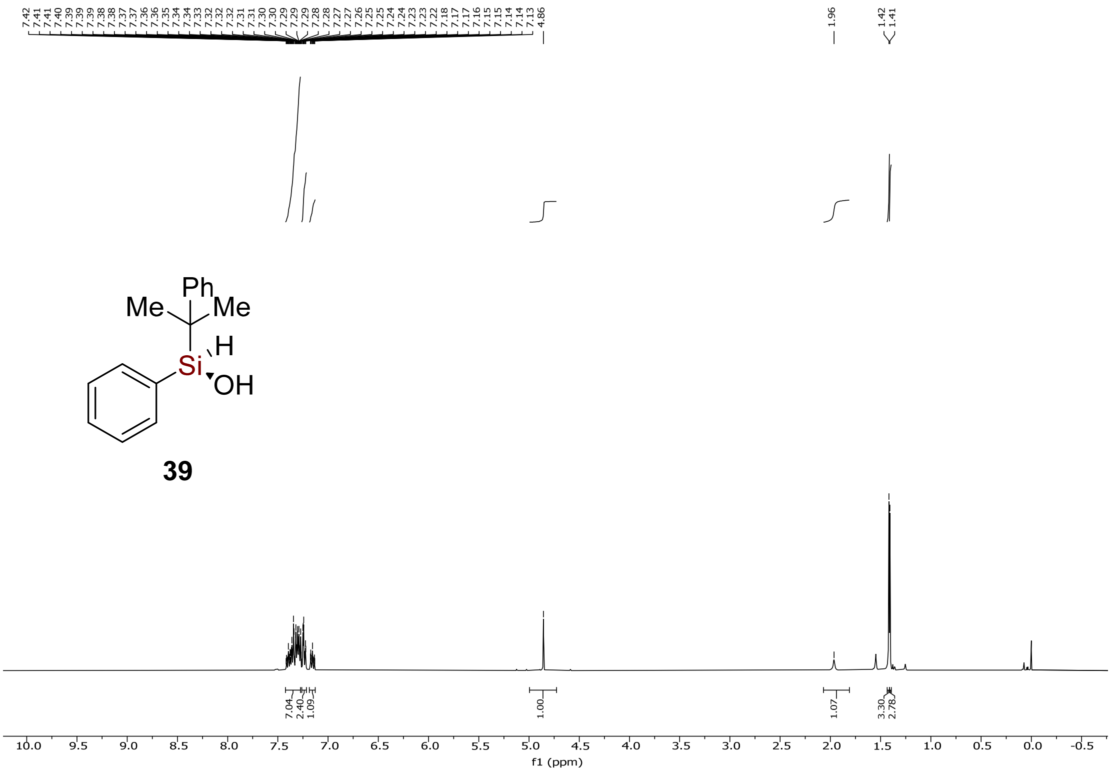
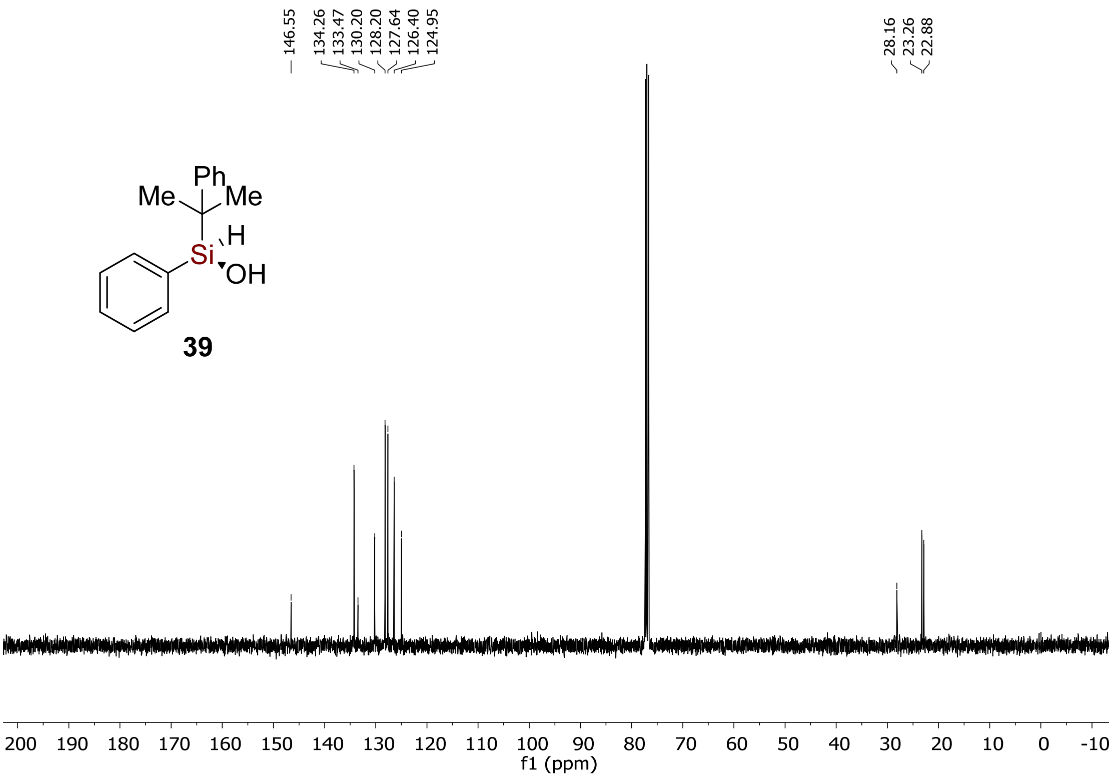
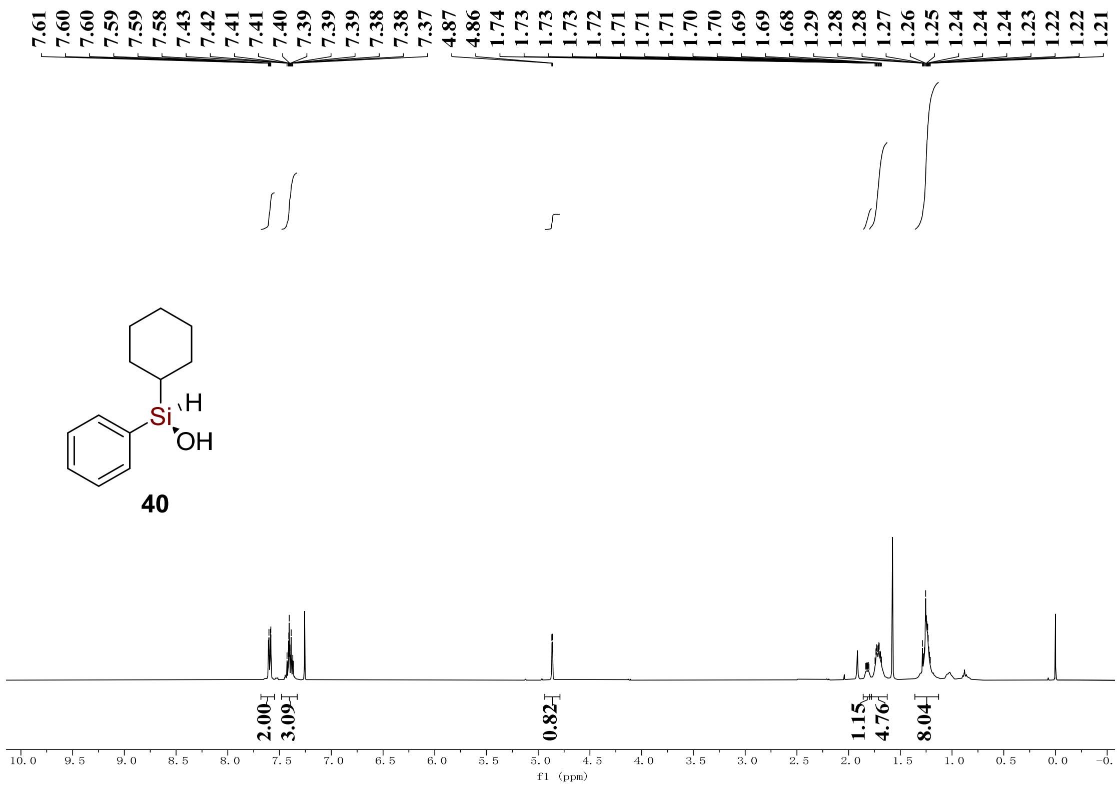
129.47
128.76
128.07
127.97
127.79
127.74
127.39
127.19
126.52
125.84
125.77
26.55
19.05
Ph
tBu
H
Si
Ph
OH
Ph
37
f1 (ppm)


7.31 7.31 7.31 7.29 7.28 7.27 7.25 7.24 7.24 7.23 7.22 7.22 7.20 7.20 7.20 7.19 7.18 7.16 4.37 4.37 4.36 4.36 2.82 2.82 2.80 2.79 2.78 1.07 1.06 1.05 1.05 1.05 1.04 1.03 1.03 1.02 1.02 1.01 1.01 0.98 0.97 0.97 0.96 0.95 0.94
tBu
H
Ph
Si
OH
38
4.95
0.91
2.00
2.09
8.96
f1 (ppm)


144.45
128.44
127.83
125.77
29.67
25.61
17.75
14.46
tBu
H
Ph
Si
OH
38
f1 (ppm)



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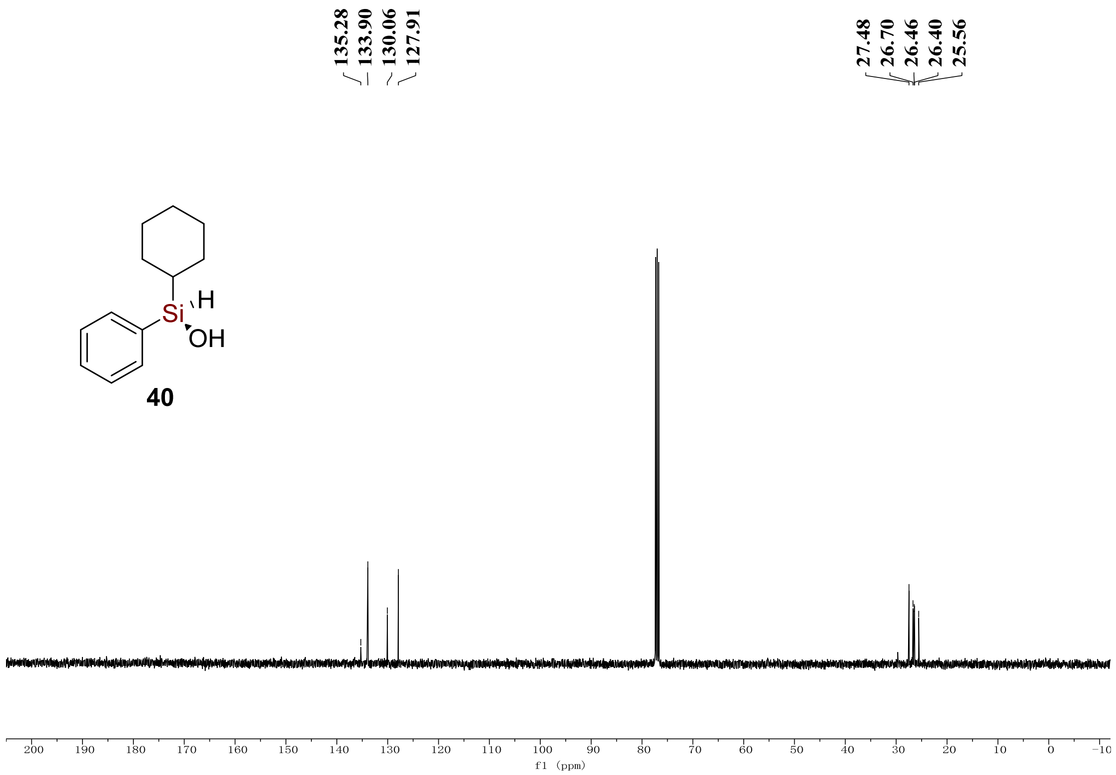
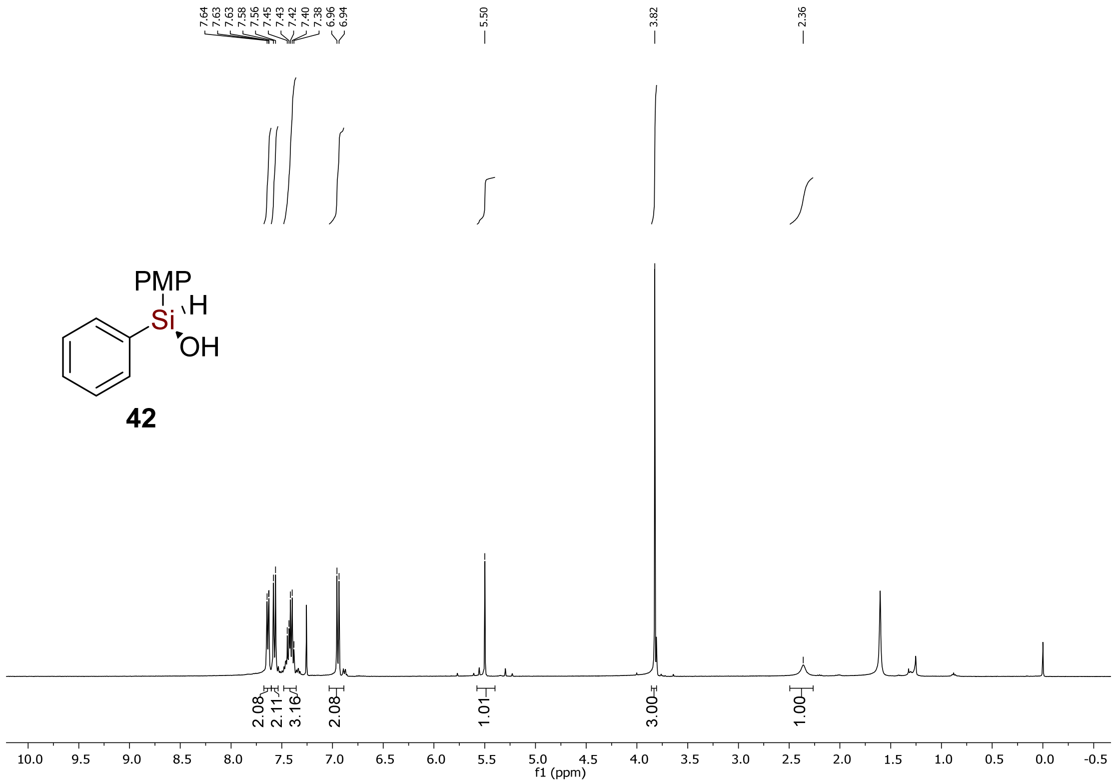
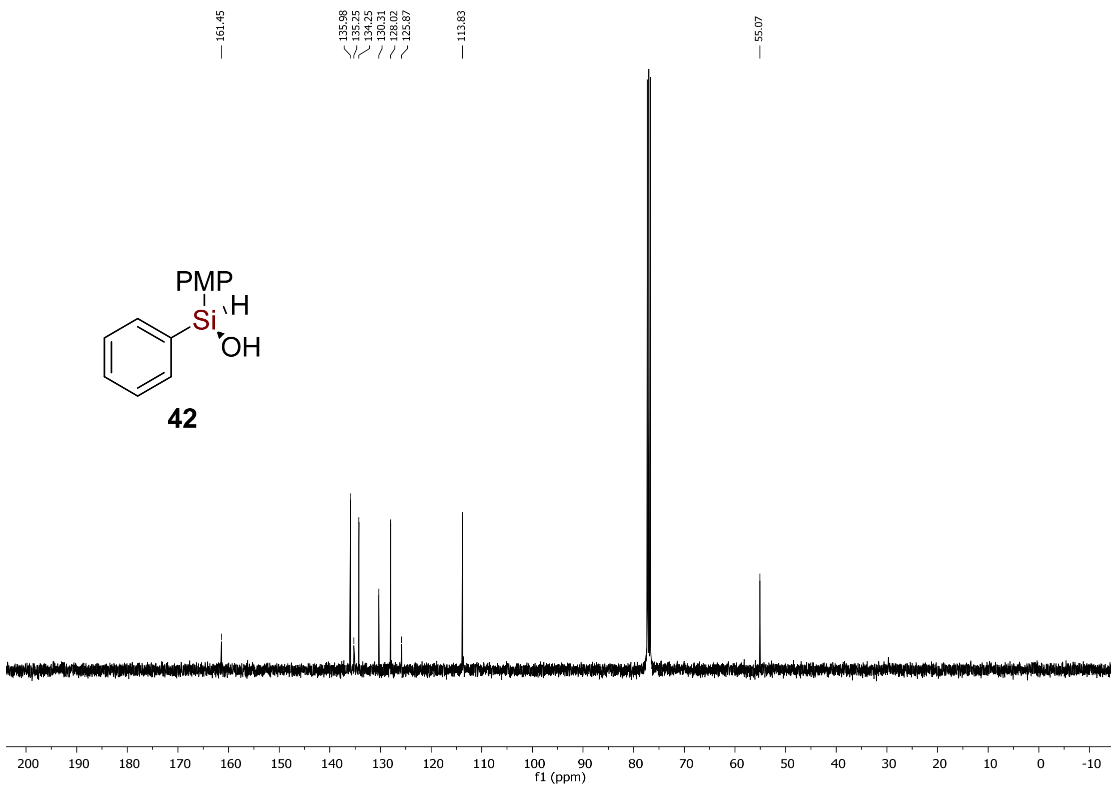
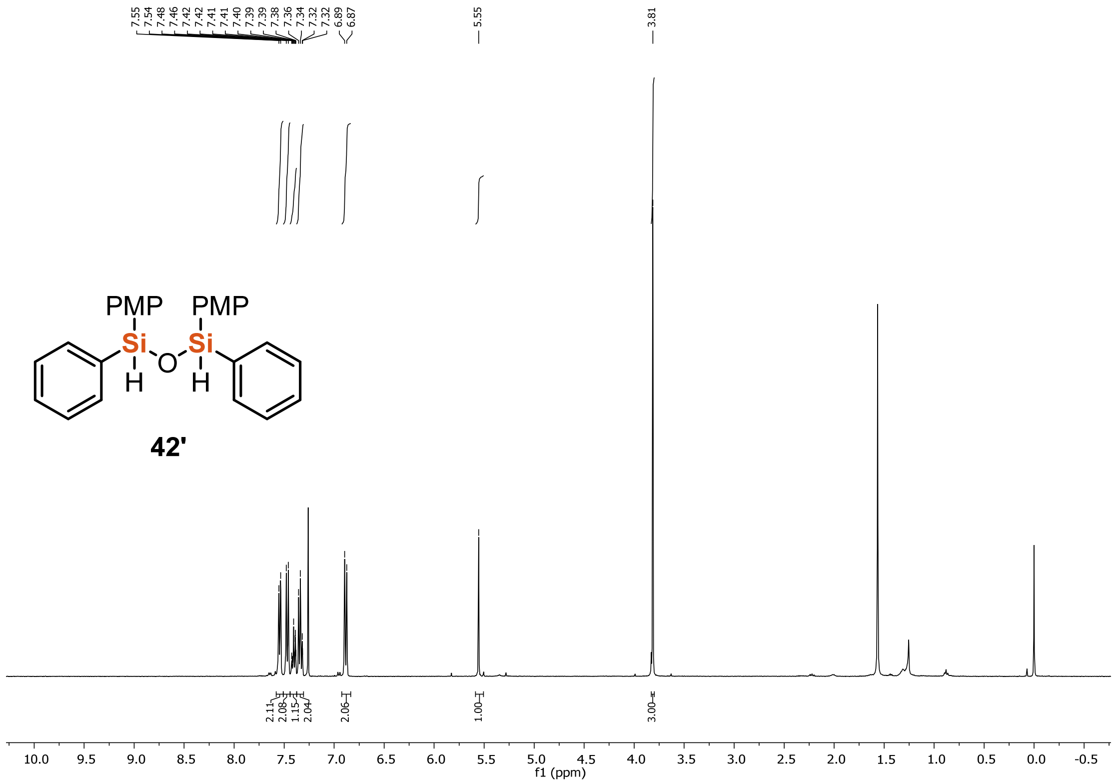
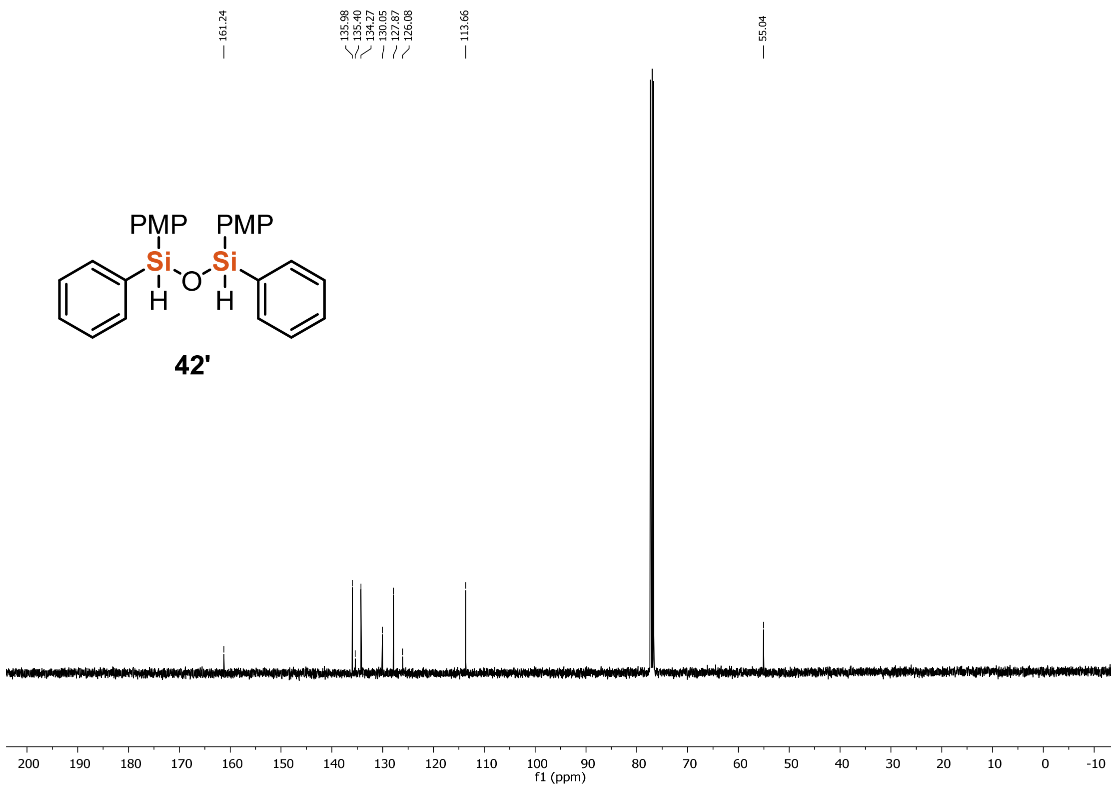
7.60
7.60
7.59
7.59
7.58
7.43
7.42
7.41
7.41
7.40
7.39
7.39
7.39
7.38
7.38
7.37
4.87
4.86
1.74
1.73
1.73
1.73
1.72
1.71
1.71
1.71
1.70
1.70
1.69
1.69
1.68
1.29
1.28
1.28
1.27
1.26
1.25
1.24
1.24
1.24
1.23
1.22
1.22
1.21
Si
H
OH
40
2.00
3.09
0.82
1.15
4.76
8.04
f1 (ppm)

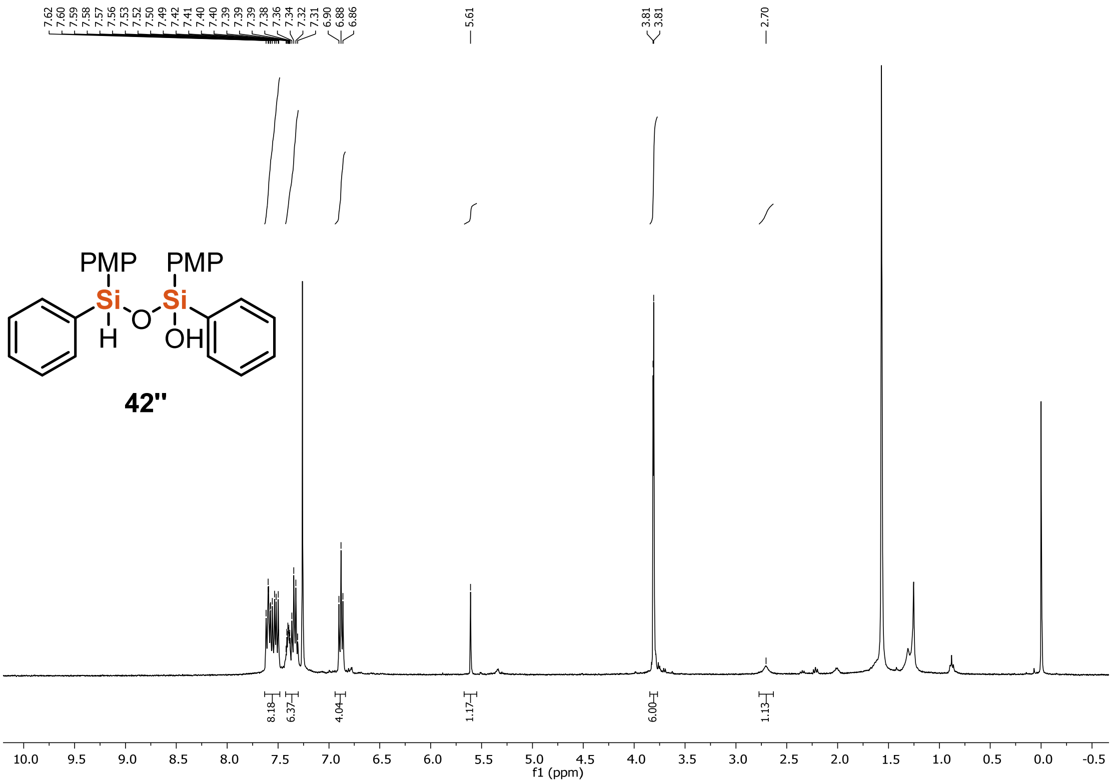

135.28
133.90
130.06
127.91
27.48
26.70
26.46
26.40
25.56
Si
H
OH
40
f1 (ppm)

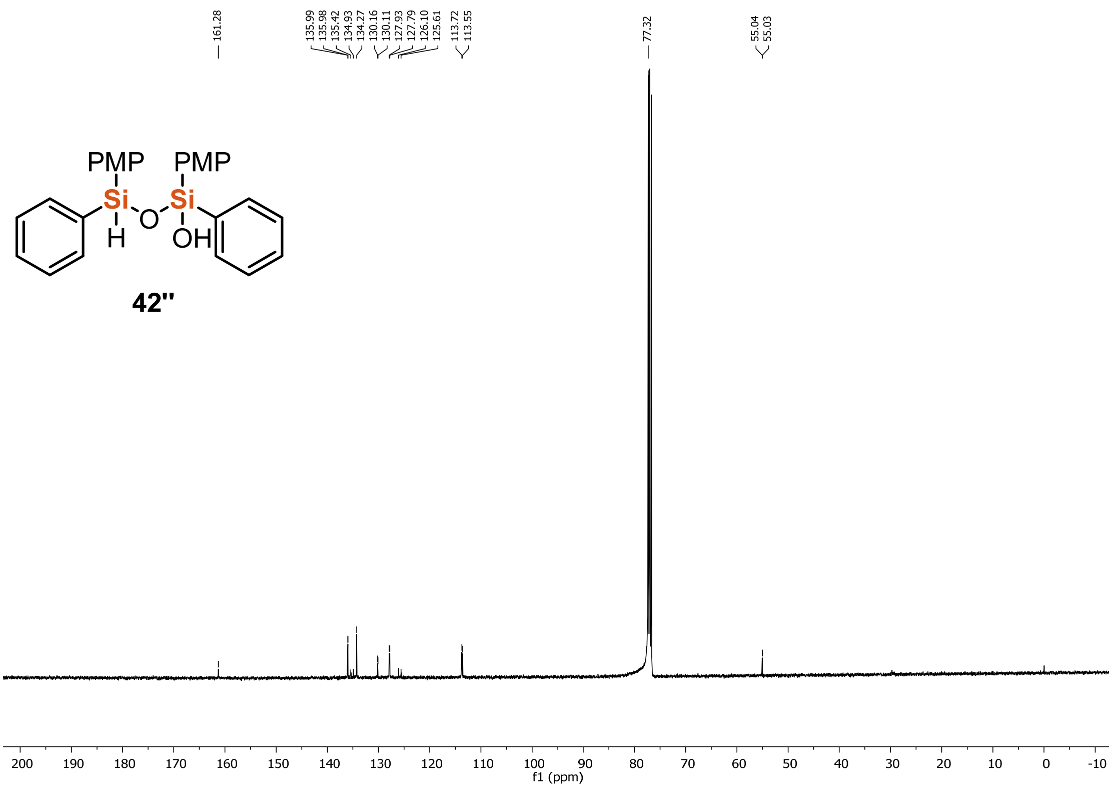


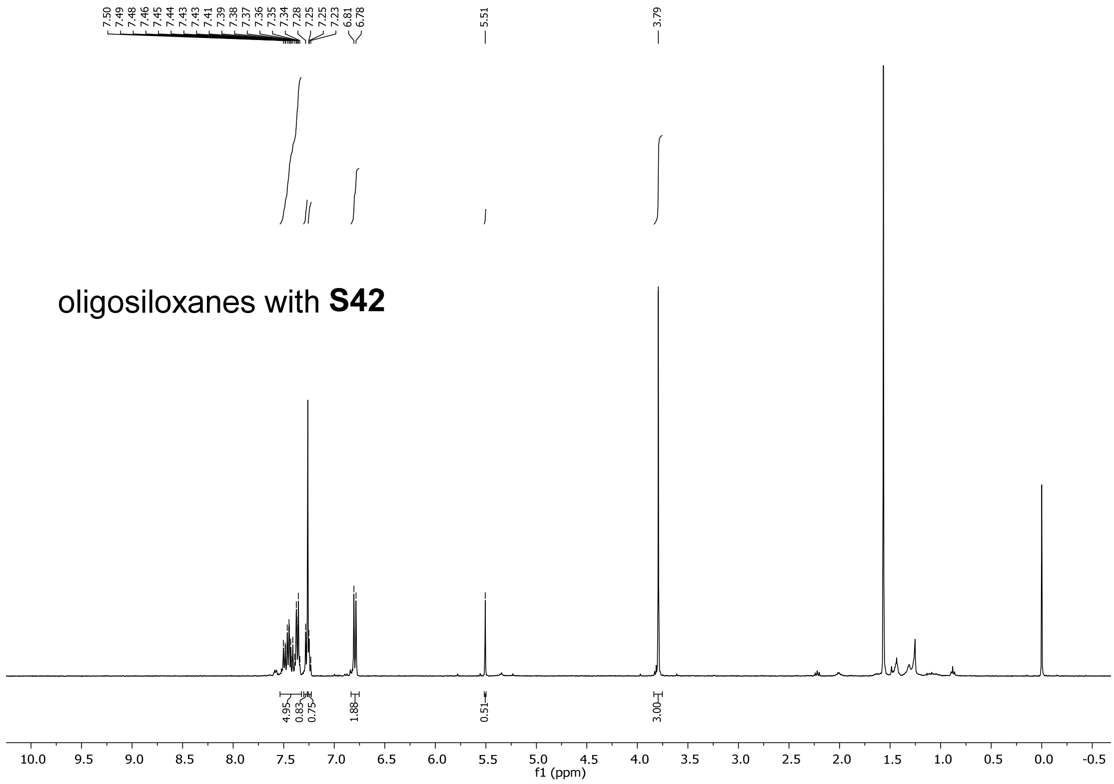


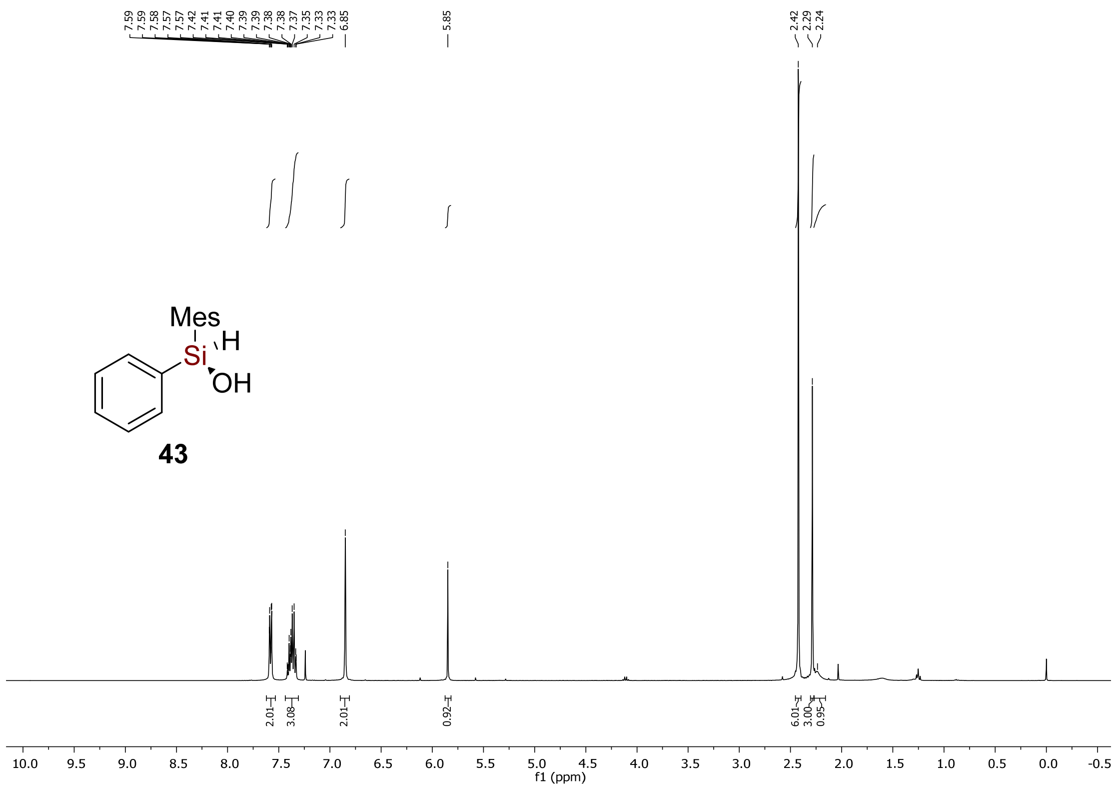

PMP PMP
Si O Si
H H
42'
f1 (ppm)

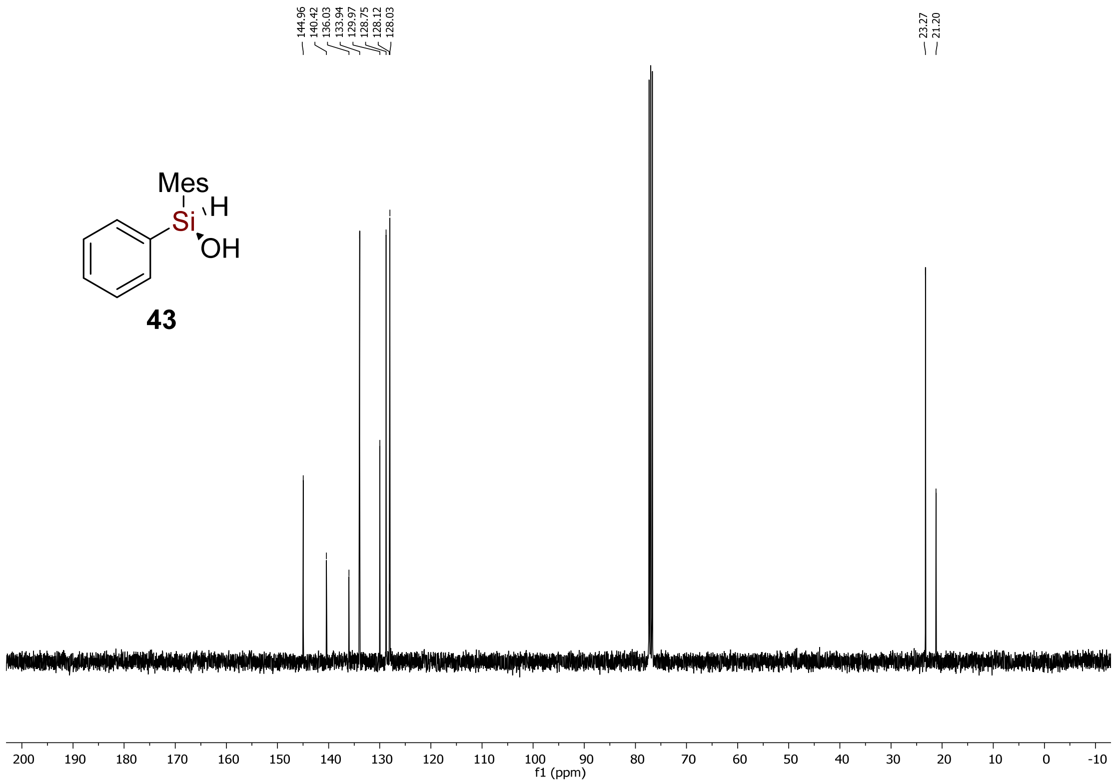

PMP PMP
Si O Si
H H
42'
f1 (ppm)

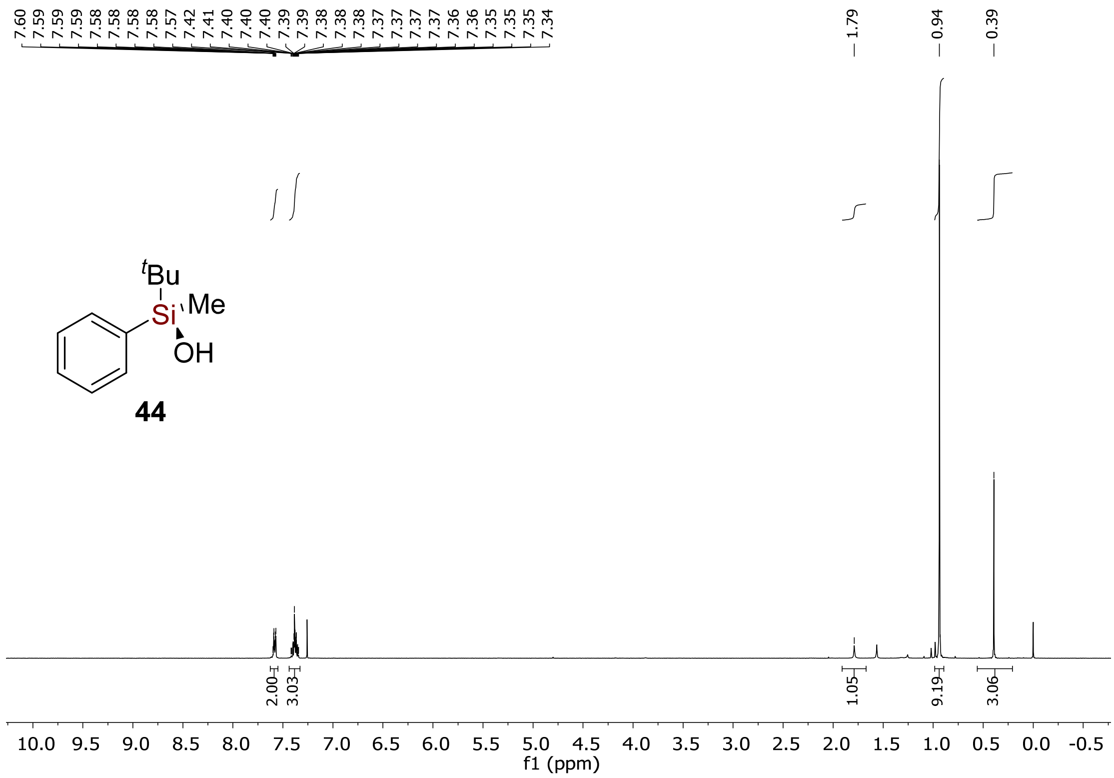

PMP
PMP
Si
O
Si
H
OH
42''
7.62 7.60 7.59 7.58 7.57 7.56 7.53 7.52 7.50 7.49 7.42 7.41 7.40 7.40 7.39 7.39 7.39 7.39 7.38 7.36 7.34 7.32 7.31 6.90 6.88 6.86
5.61
3.81 3.81
2.70
8.18 6.37 4.04 1.17 6.00 1.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

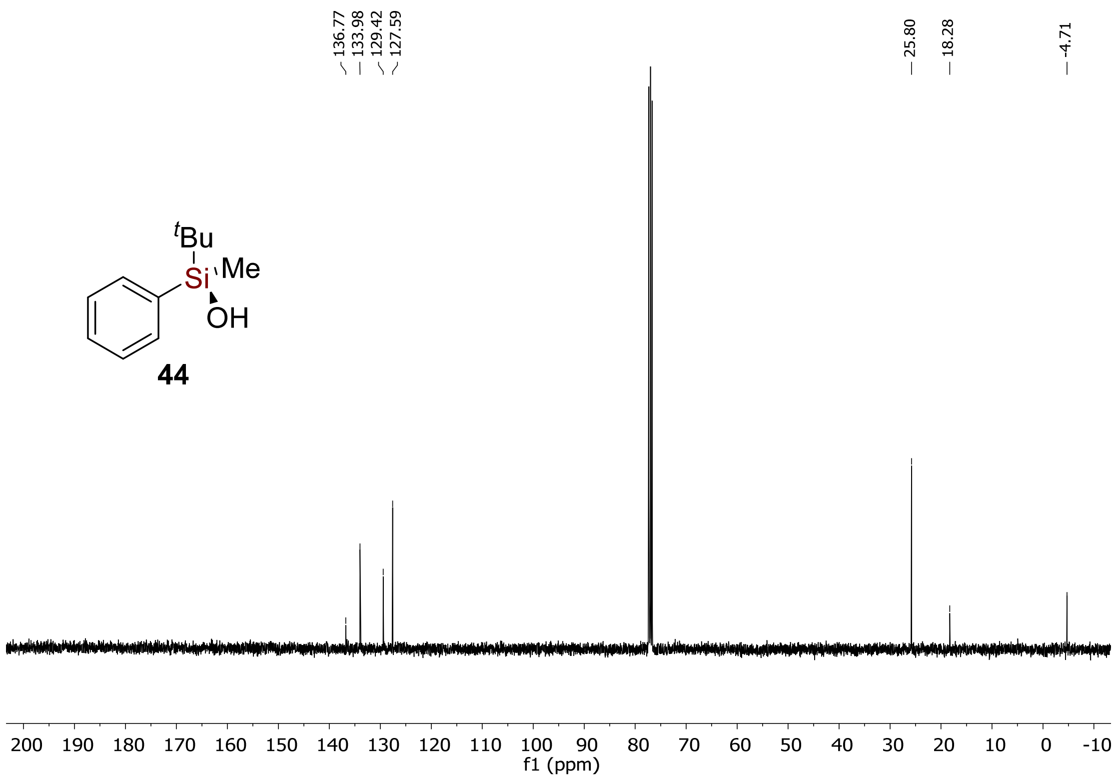

161.28
135.99 135.98 135.42 134.93 134.27 130.16 130.11 127.93 127.79 126.10 125.61 113.72 113.55
77.32
55.04 55.03
PMP
PMP
Si
O
Si
H
OH
42''
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

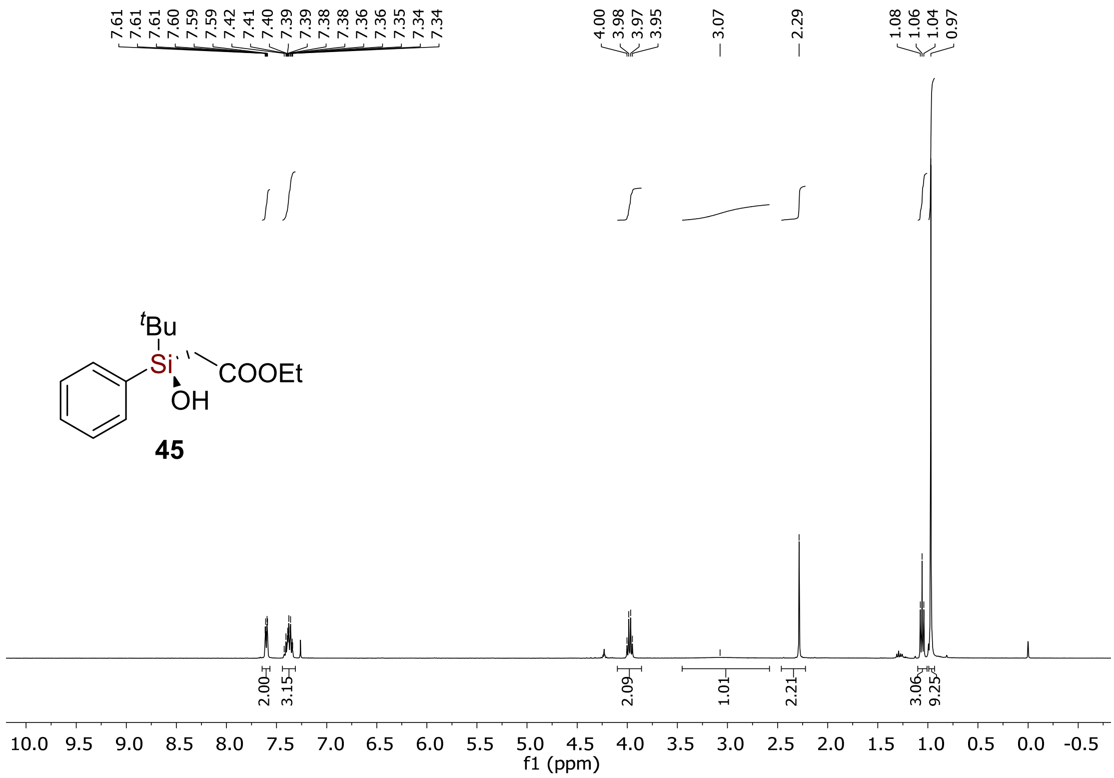

oligosiloxanes with **S42**
f1 (ppm)

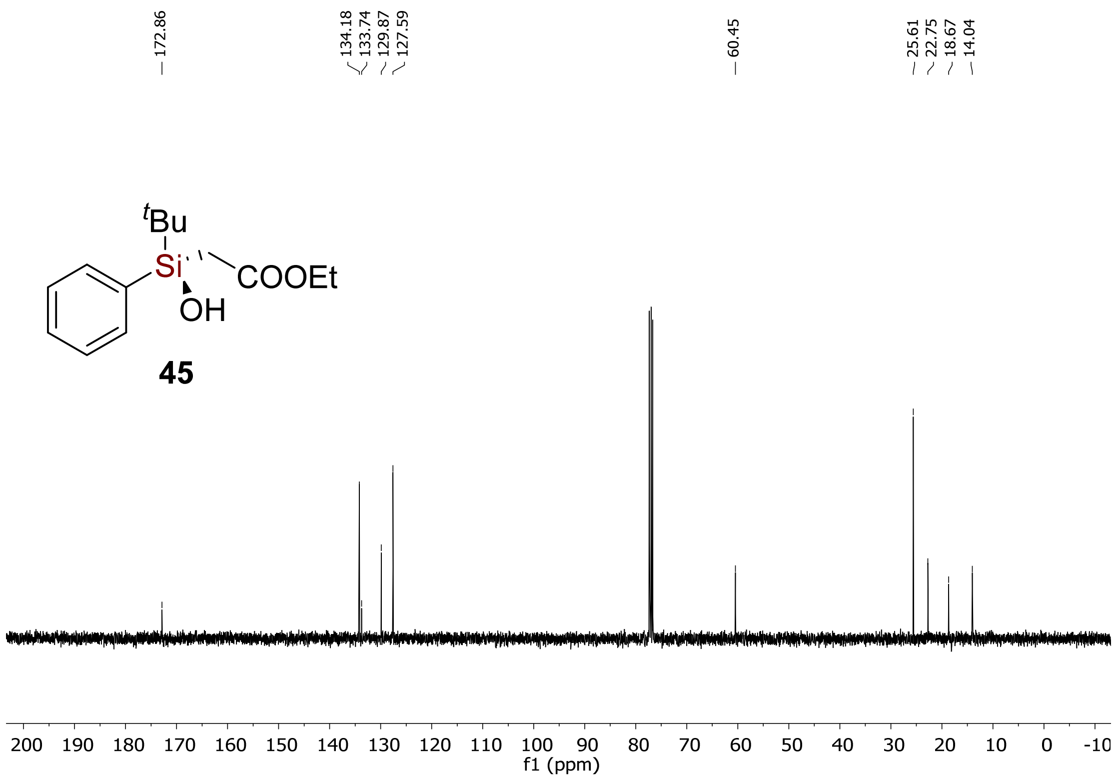

Mes
Si
H
OH
43
f1 (ppm)

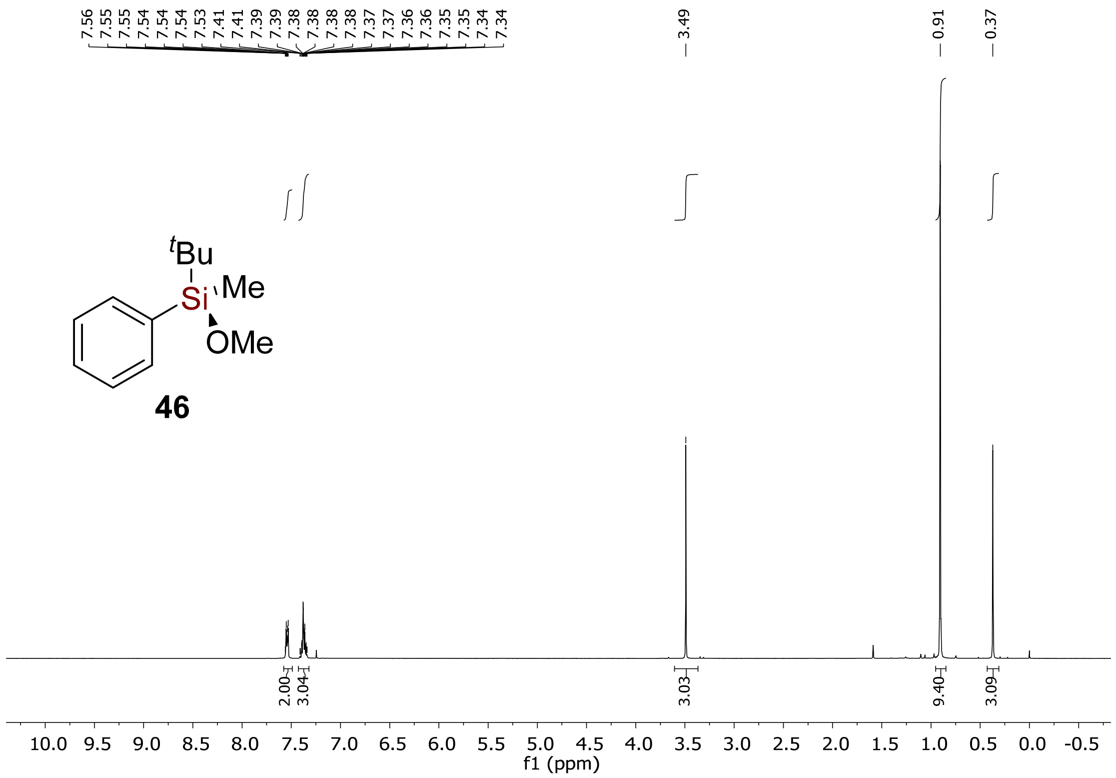

144.96
140.42
136.03
133.94
129.97
128.75
128.12
128.03
23.27
21.20
Mes
Si
H
OH
43
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

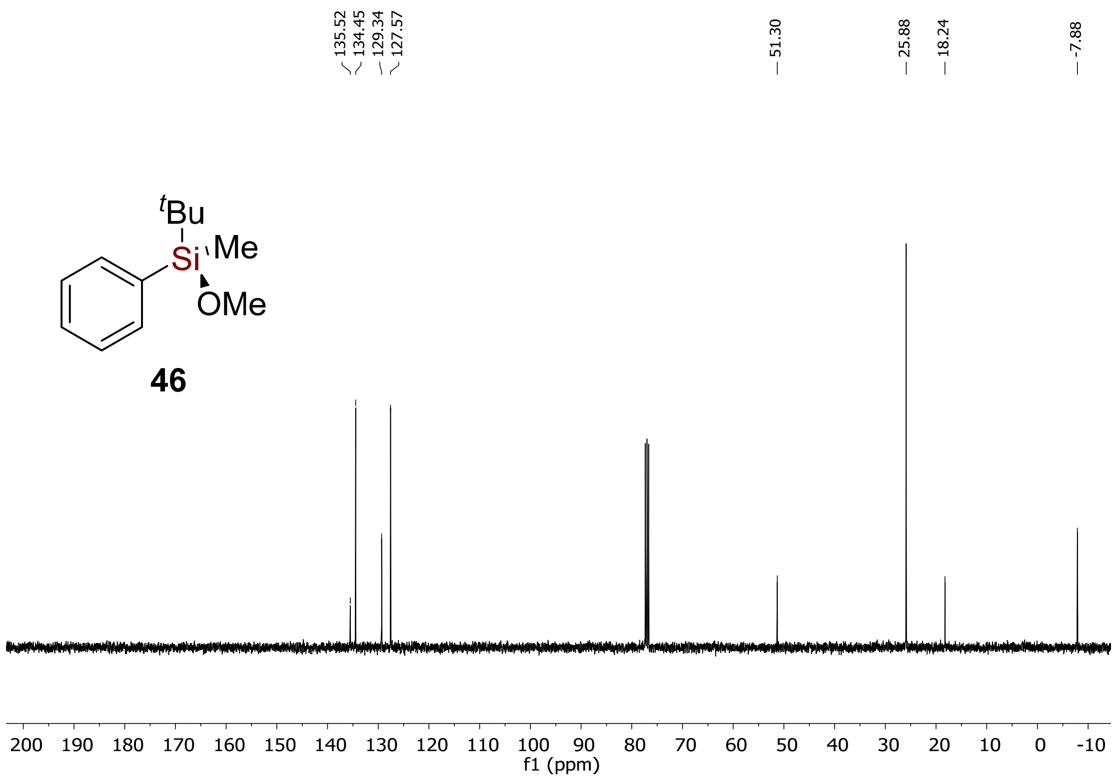

7.60 7.59 7.59 7.59 7.58 7.58 7.58 7.58 7.57 7.42 7.41 7.40 7.40 7.40 7.39 7.39 7.38 7.38 7.38 7.37 7.37 7.37 7.37 7.36 7.36 7.35 7.35 7.35 7.35 7.34
1.79
0.94
0.39
tBu
Si
Me
OH
44
2.00
3.03
1.05
9.19
3.06
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


136.77
133.98
129.42
127.59
25.80
18.28
-4.71
tBu
Si
Me
OH
44
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.61 7.61 7.61 7.60 7.59 7.59 7.42 7.41 7.40 7.39 7.39 7.38 7.38 7.36 7.35 7.34 7.34
4.00 3.98 3.97 3.95
3.07
2.29
1.08 1.06 1.04 0.97
tBu
Si
COOEt
OH
45
2.00
3.15
2.09
1.01
2.21
3.06
9.25
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


172.86
134.18
133.74
129.87
127.59
60.45
25.61
22.75
18.67
14.04
tBu
Si
COOEt
OH
45
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


7.56 7.55 7.55 7.54 7.54 7.54 7.53 7.41 7.41 7.39 7.39 7.38 7.38 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.35 7.34 7.34
3.49
0.91
0.37
tBu
Si
Me
OMe
46
2.00
3.04
3.03
9.40
3.09
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


135.52
134.45
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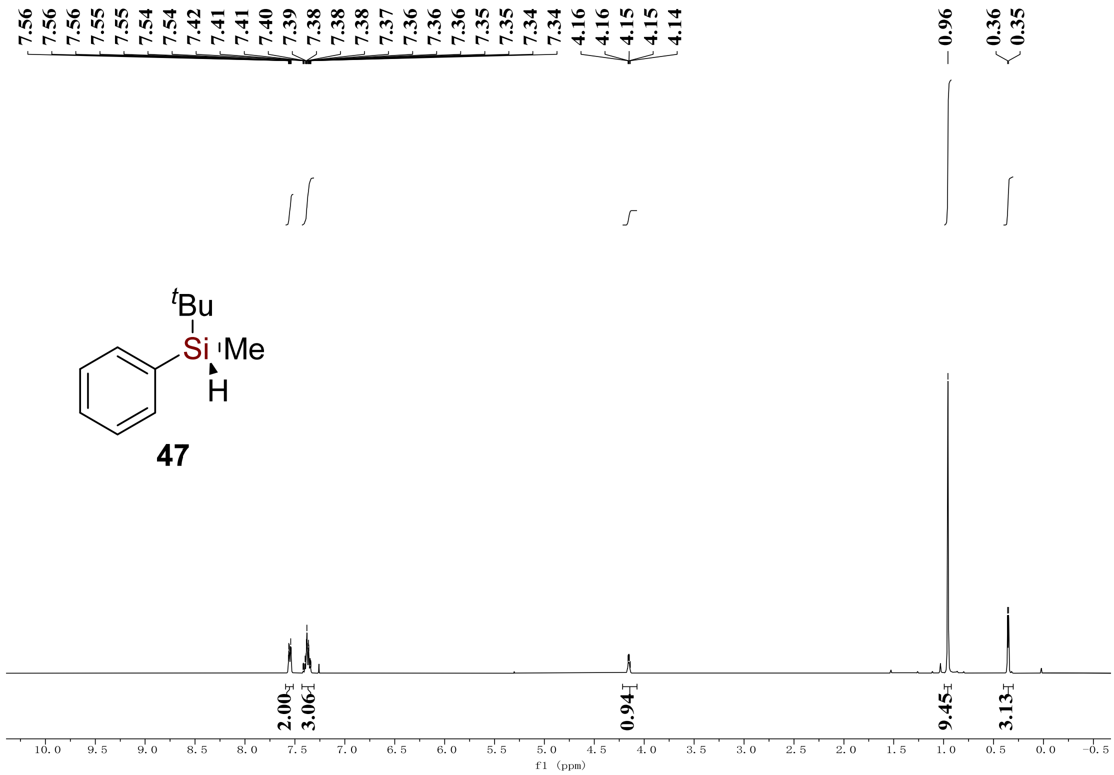
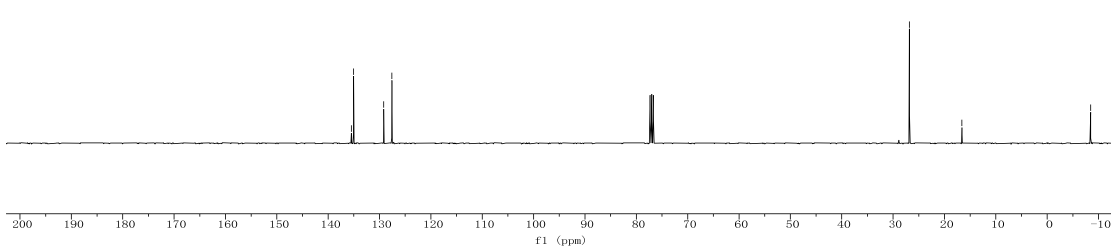
127.57
51.30
25.88
18.24
-7.88
tBu
Si
Me
OMe
f1 (ppm)

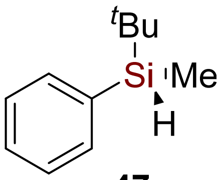
46


7.56
7.56
7.56
7.55
7.55
7.54
7.54
7.42
7.41
7.41
7.40
7.39
7.38
7.38
7.38
7.37
7.36
7.36
7.36
7.35
7.35
7.34
7.34
4.16
4.16
4.15
4.15
4.14
0.96
0.36
0.35
tBu
Si
Me
H
2.00
3.06
0.94
9.45
3.13
f1 (ppm)

47

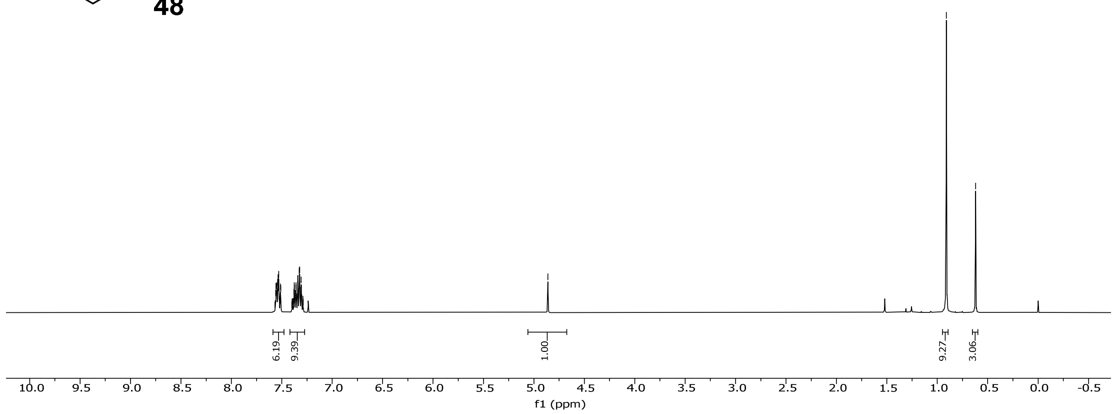


135.49
135.05
129.19
127.61
26.82
16.60
-8.47
f1 (ppm)

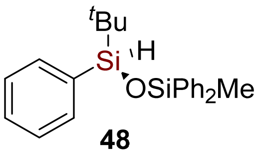


tBu
Si
Me
H

47

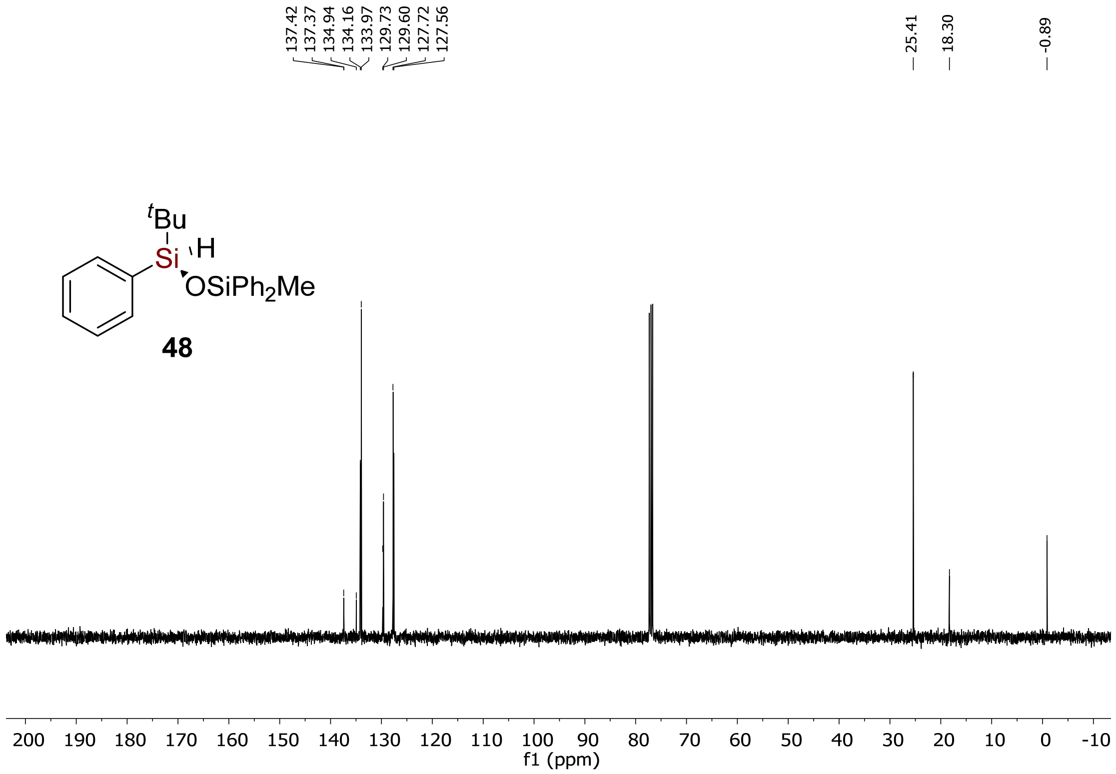


7.57 7.56 7.56 7.55 7.55 7.54 7.54 7.53 7.53 7.53 7.52 7.51 7.51 7.40 7.40 7.40 7.39 7.39 7.39 7.38 7.38 7.37 7.37 7.36 7.36 7.35 7.34 7.34 7.33 7.32 7.31 7.30 7.29 7.29 7.29
4.86
0.91
0.62
6.19
9.39
1.00
9.27
3.06
f1 (ppm)



tBu
Si
H
OSiPh2Me

48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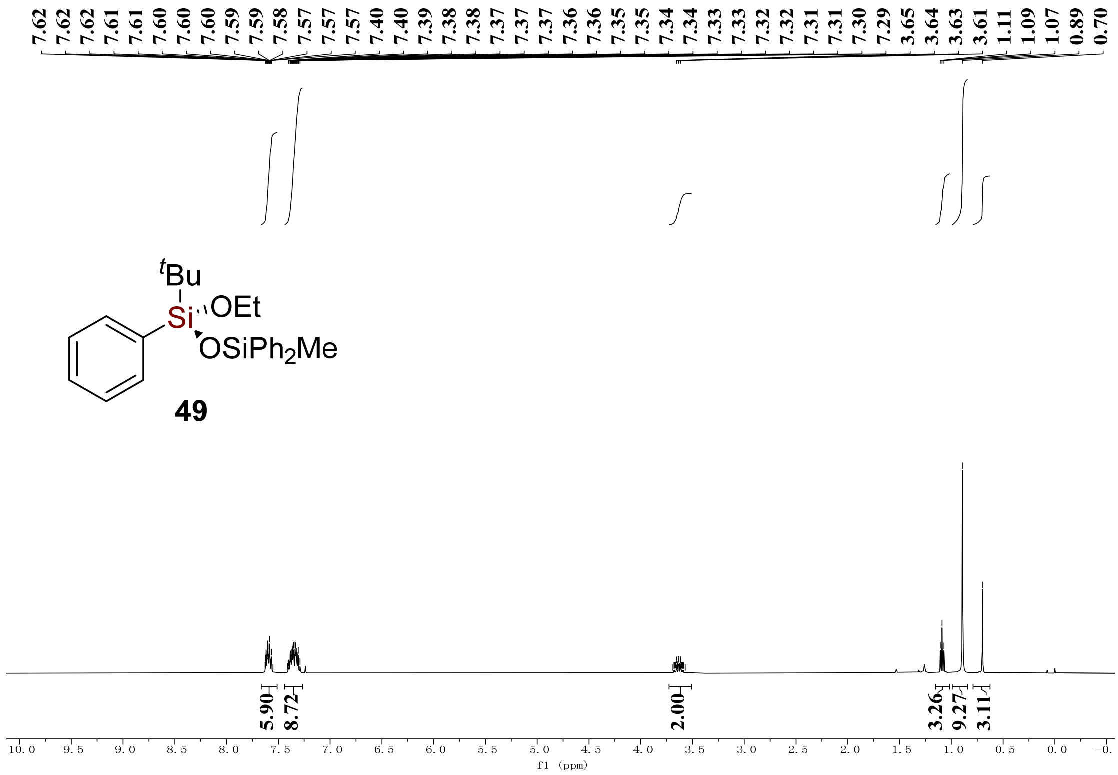
134.16
133.97
129.73
129.60
127.72
127.56
25.41
18.30
-0.89
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)
^{t}Bu
Si
H
OSiPh$_2$Me

48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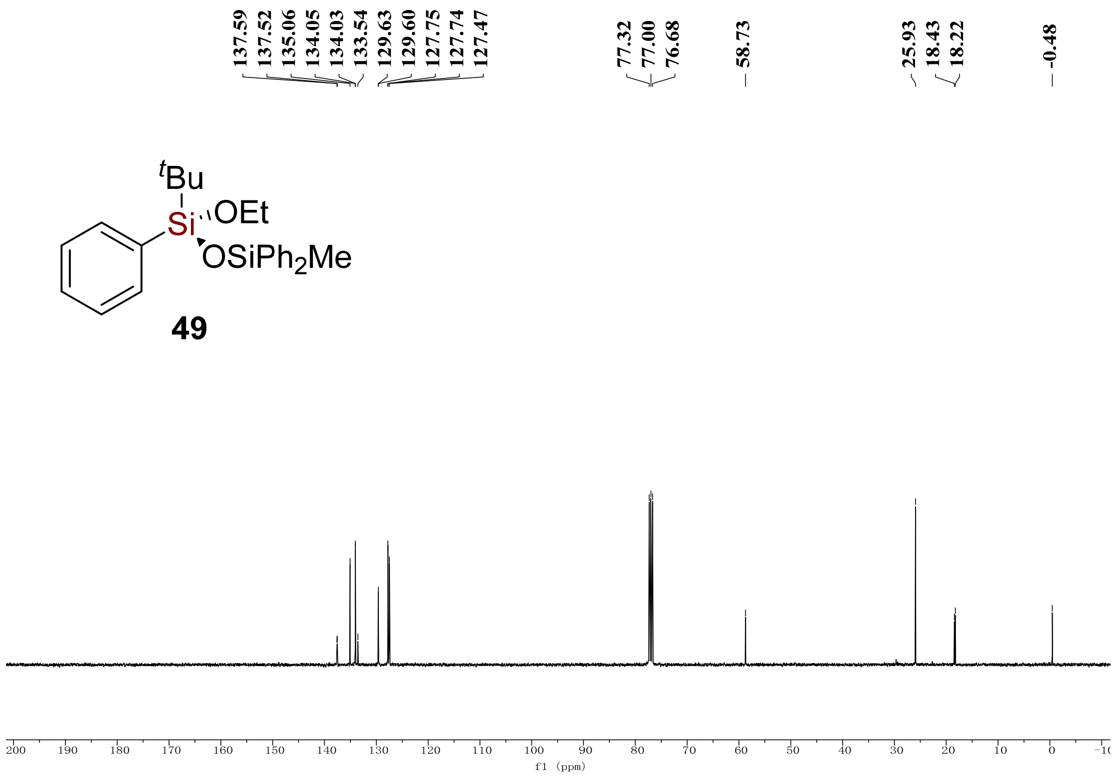
5.90
8.72
2.00
3.26
9.27
3.11
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)
^{t}Bu
Si
OEt
OSiPh$_2$Me

49



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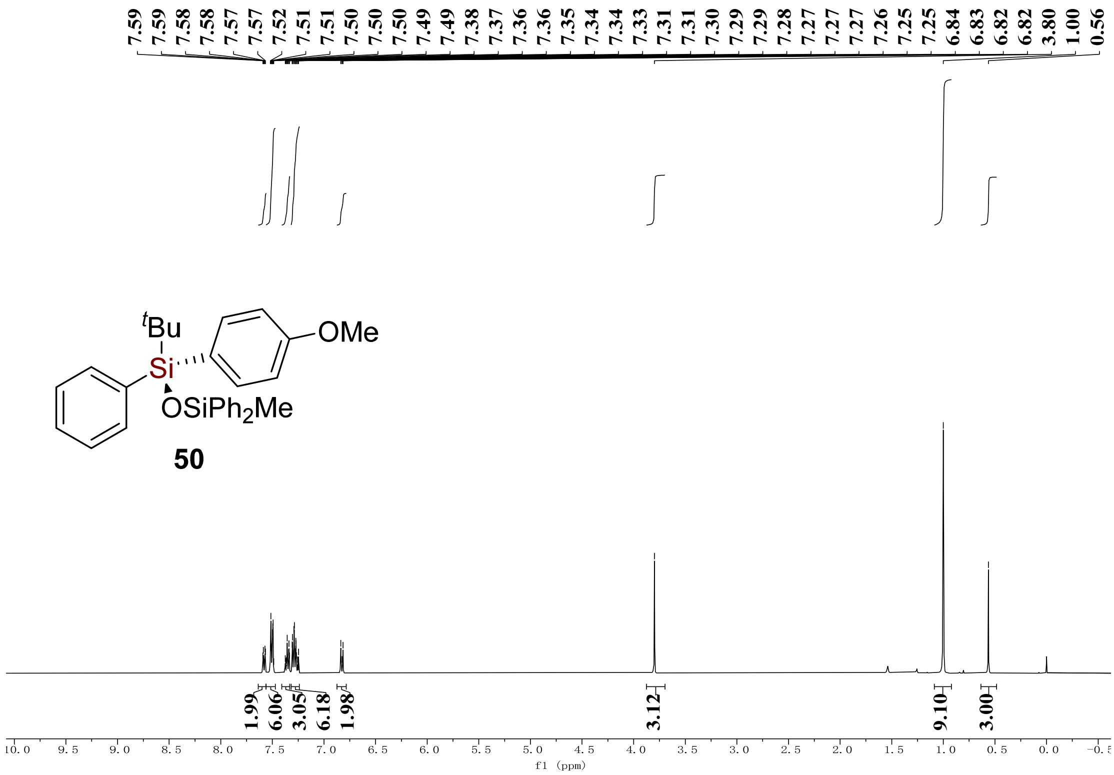
135.06
134.05
134.03
133.54
129.63
129.60
127.75
127.74
127.47
77.32
77.00
76.68
58.73
25.93
18.43
18.22
-0.48
tBu
Si
OEt
OSiPh2Me
f1 (ppm)

49



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7.58
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7.57
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7.51
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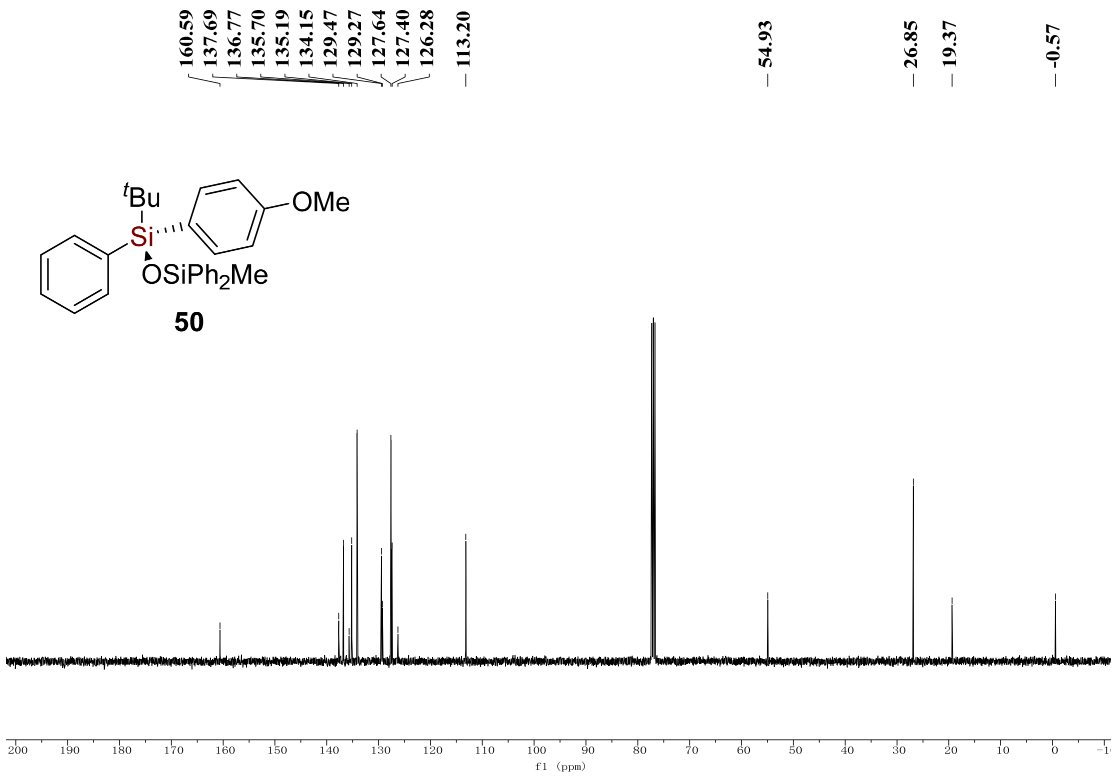
7.50
7.50
7.49
7.49
7.38
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.31
7.31
7.30
7.29
7.29
7.28
7.27
7.27
7.27
7.26
7.25
7.25
6.84
6.83
6.82
6.82
3.80
1.00
0.56
tBu
Si
OMe
OSiPh2Me
1.99
6.06
3.05
6.18
1.98
3.12
9.10
3.00
f1 (ppm)

50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135.70
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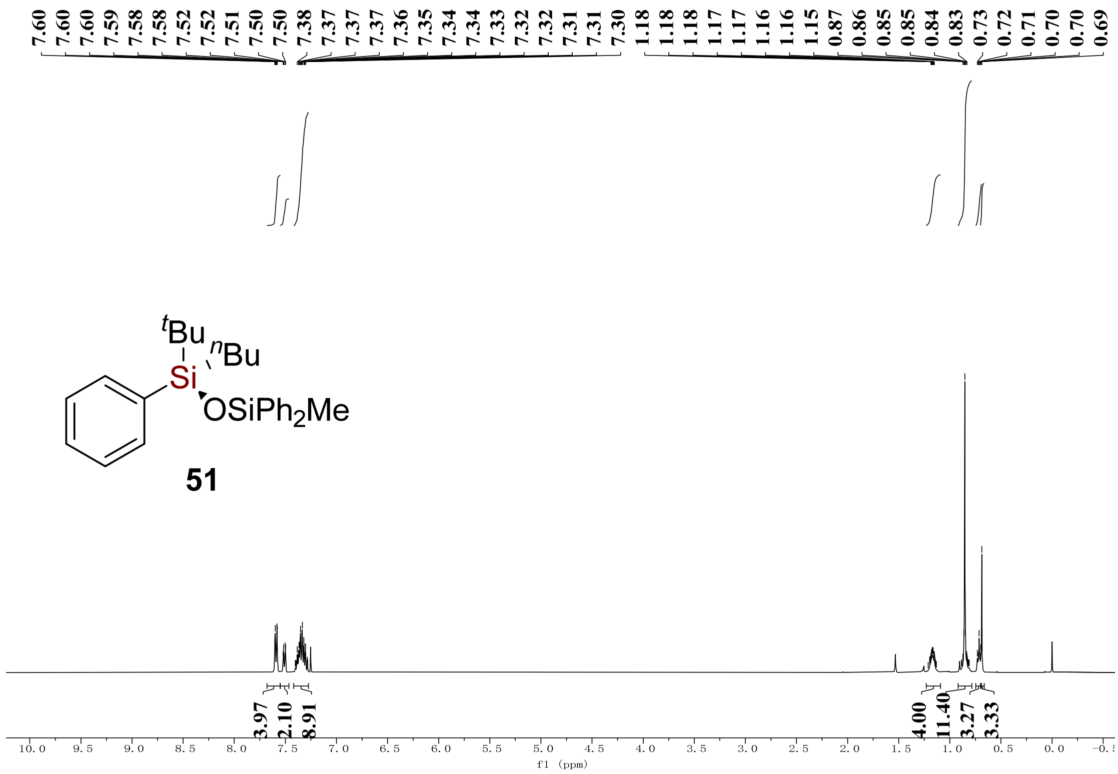
129.47
129.27
127.64
127.40
126.28
113.20
54.93
26.85
19.37
-0.57
tBu
Si
OMe
OSiPh2Me
50
f1 (ppm)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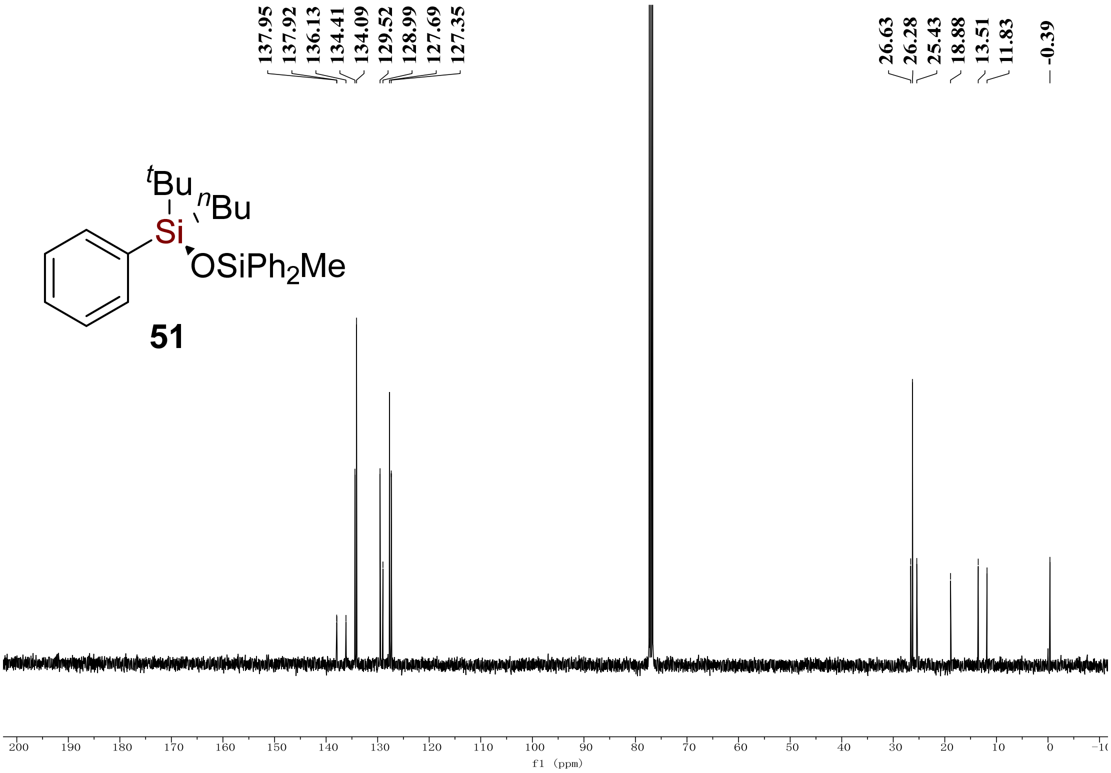
7.37
7.37
7.36
7.35
7.34
7.33
7.32
7.32
7.31
7.31
7.30
1.18
1.18
1.18
1.17
1.17
1.16
1.16
1.15
0.87
0.86
0.85
0.85
0.84
0.83
0.73
0.72
0.71
0.70
0.70
0.69
tBu
nBu
Si
OSiPh2Me
51
3.97
2.10
8.91
4.00
11.40
3.27
3.33
f1 (ppm)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134.41
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129.52
128.99
127.69
127.35
26.63
26.28
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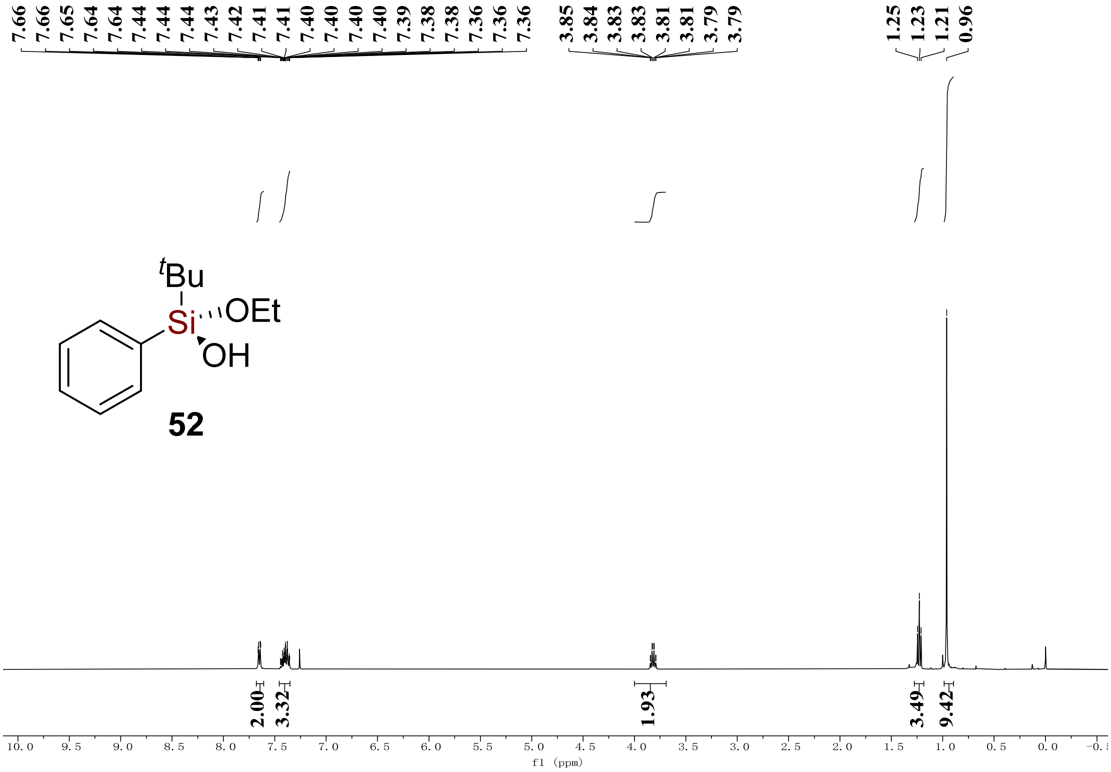
18.88
13.51
11.83
-0.39
tBu
nBu
Si
OSiPh2Me
51
f1 (ppm)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7.44
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7.42
7.41
7.41
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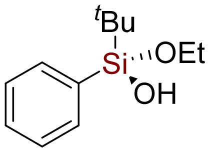
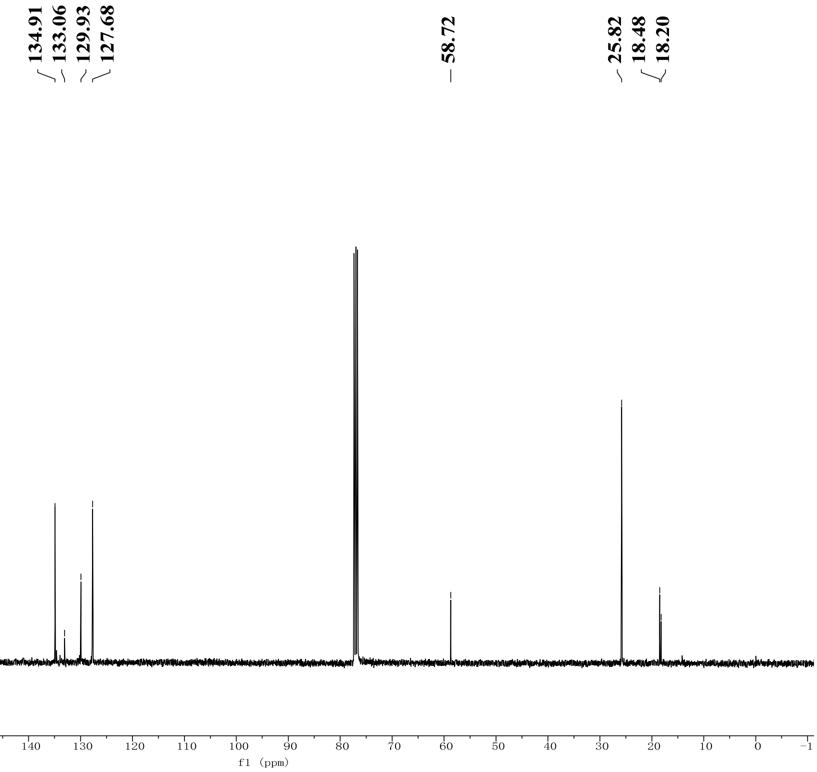
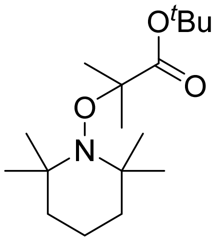
7.40
7.40
7.40
7.39
7.38
7.38
7.36
7.36
7.36
3.85
3.84
3.83
3.83
3.81
3.81
3.79
3.79
1.25
1.23
1.21
0.96
tBu
Si
OEt
OH
52
2.00
3.32
1.93
3.49
9.42
f1 (ppm)

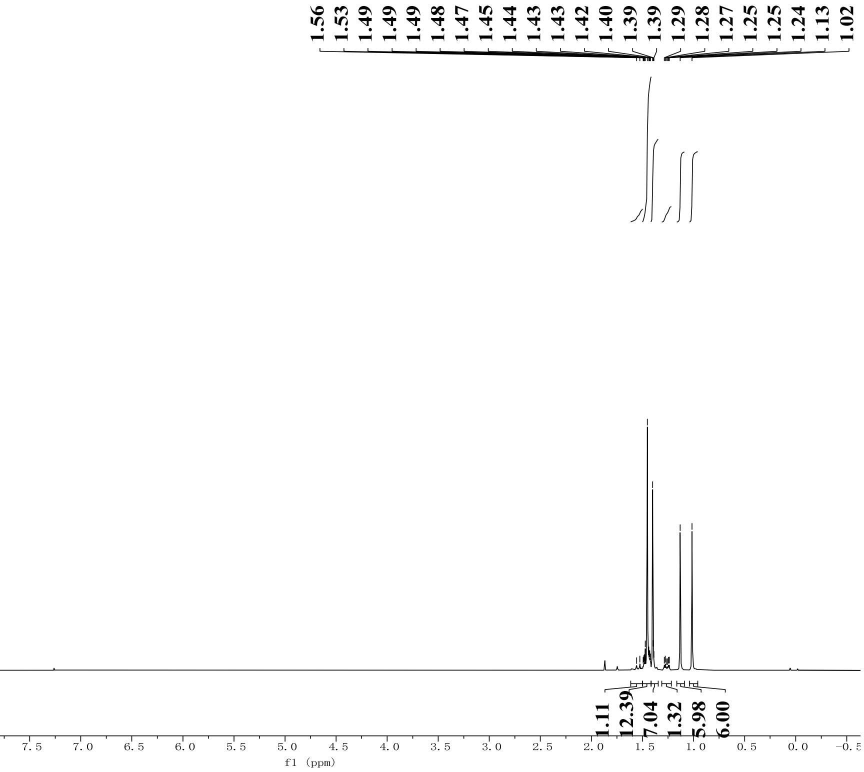

tBu
Si
OEt
OH

52


134.91
133.06
129.93
127.68
58.72
25.82
18.48
18.20
f1 (ppm)


OtBu
O
O
N

53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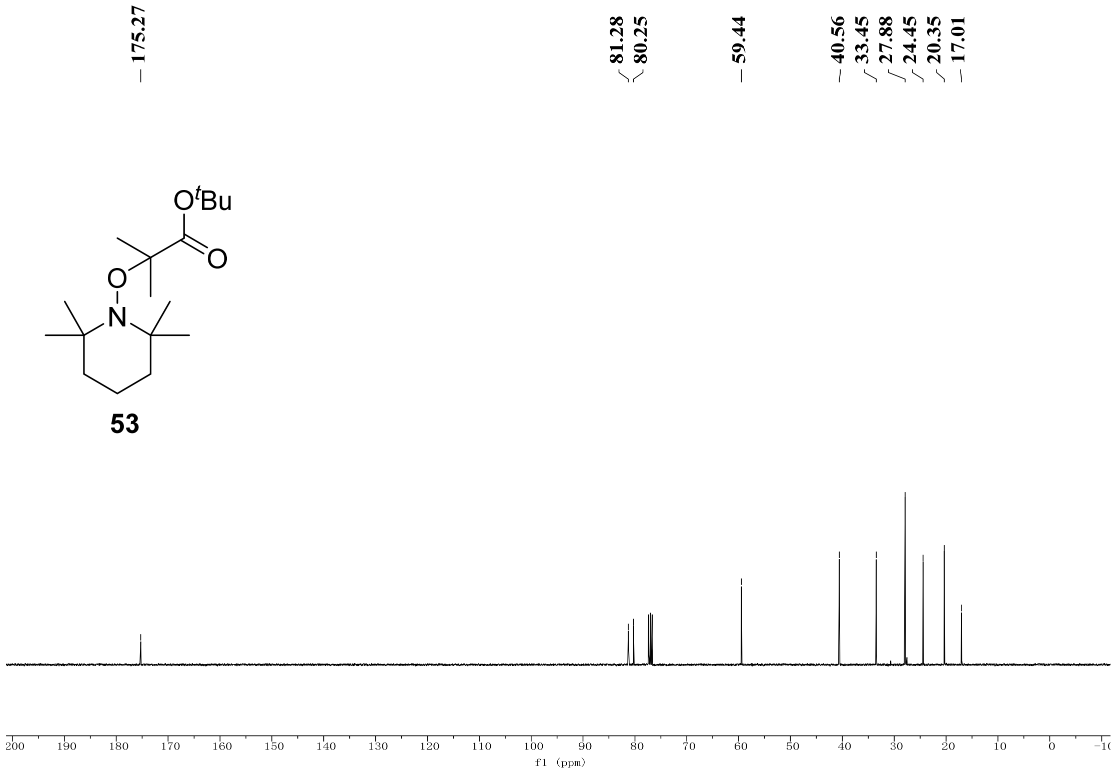
1.47
1.45
1.44
1.43
1.43
1.42
1.40
1.39
1.39
1.29
1.28
1.27
1.25
1.25
1.24
1.13
1.02
1.11
12.39
7.04
1.32
5.98
6.00
f1 (ppm)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81.28
80.25
59.44
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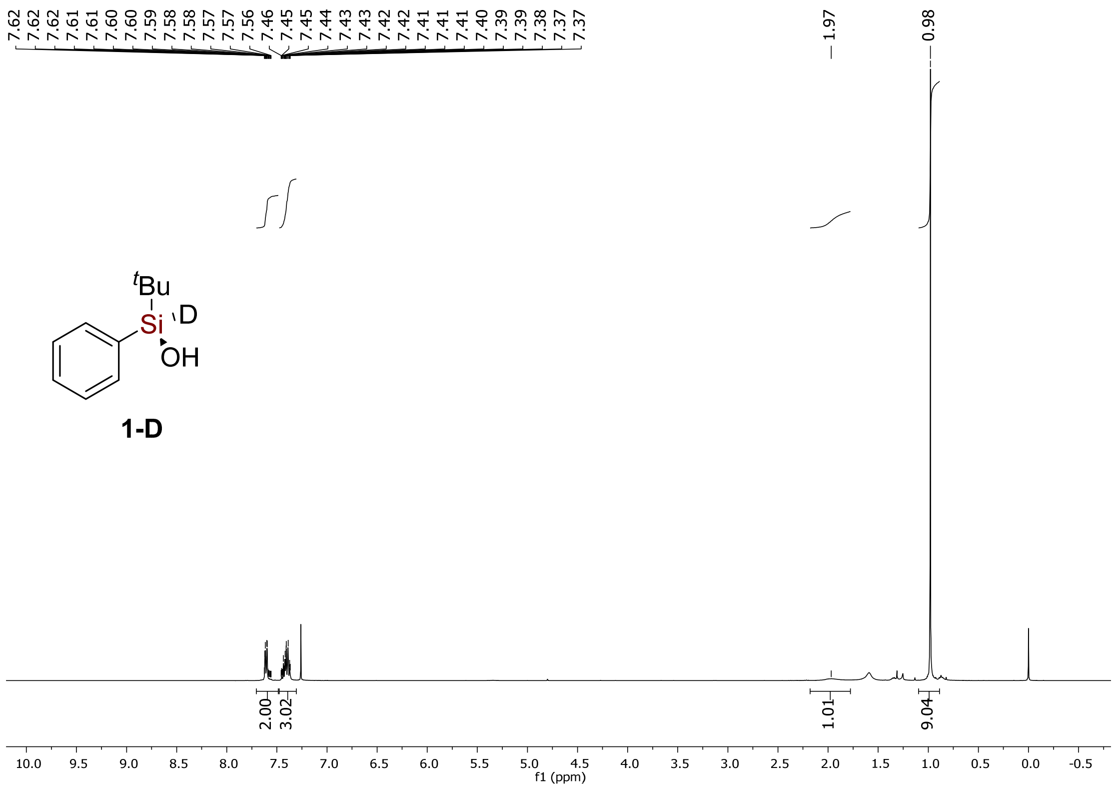
33.45
27.88
24.45
20.35
17.01
f1 (ppm)

53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7.62
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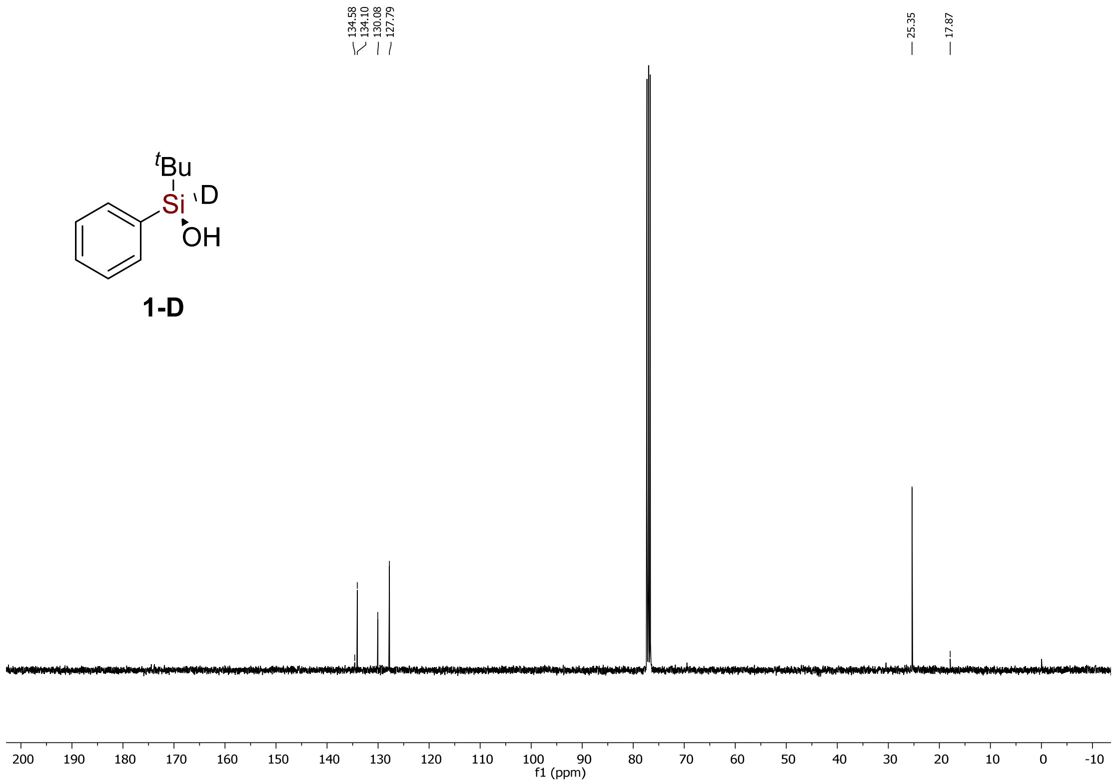
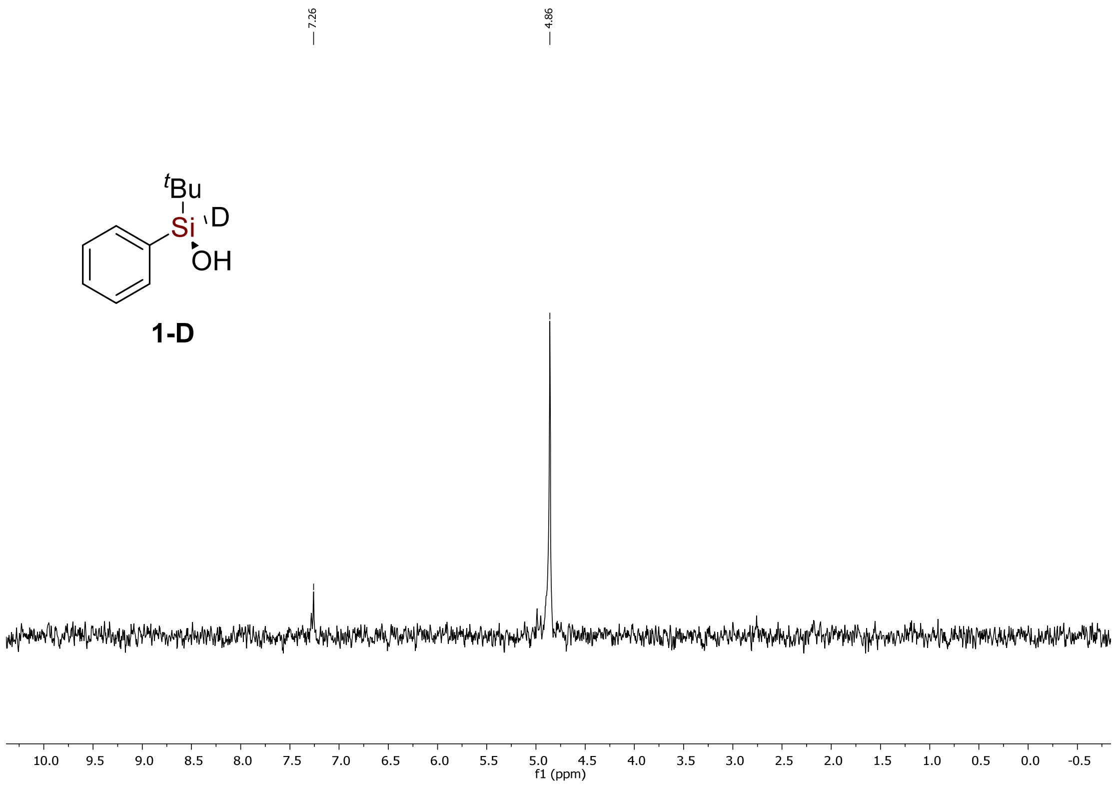
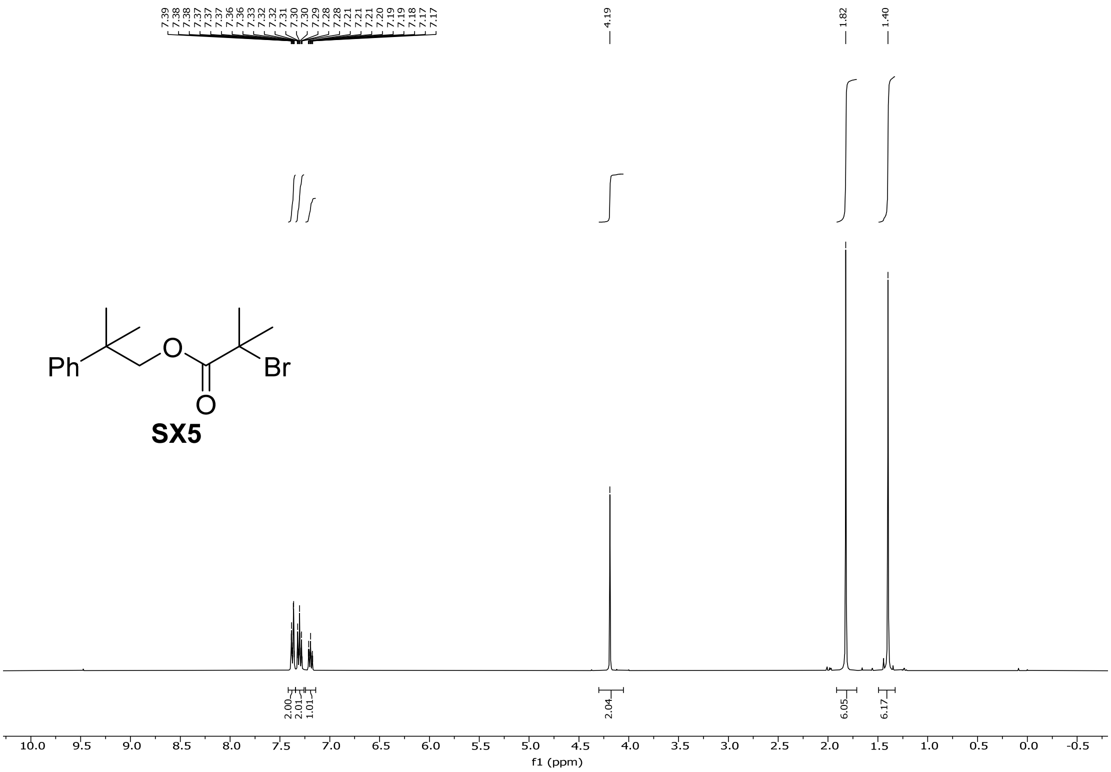
7.60
7.59
7.58
7.58
7.57
7.56
7.46
7.45
7.45
7.44
7.43
7.43
7.42
7.42
7.41
7.41
7.41
7.40
7.39
7.39
7.38
7.37
7.37
1.97
0.98
2.00
3.02
1.01
9.04
f1 (ppm)

1-D

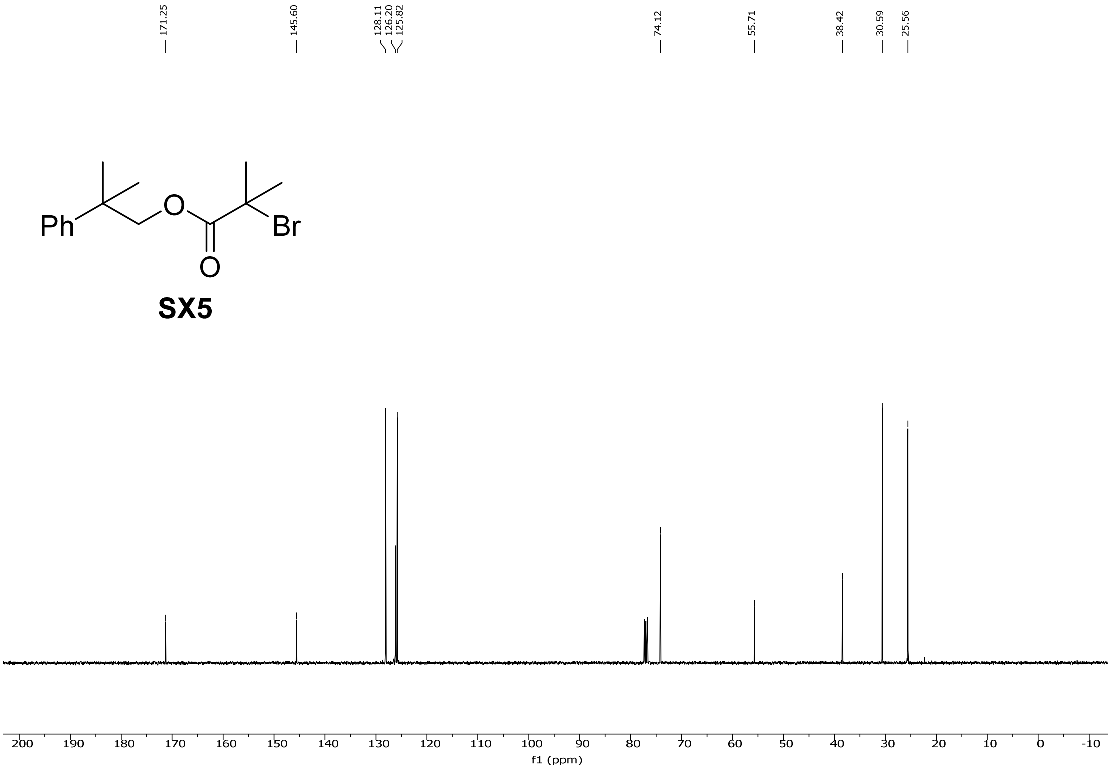


^{2}H NMR (61 MHz, $CHCl_3$) spectrum of 1-D

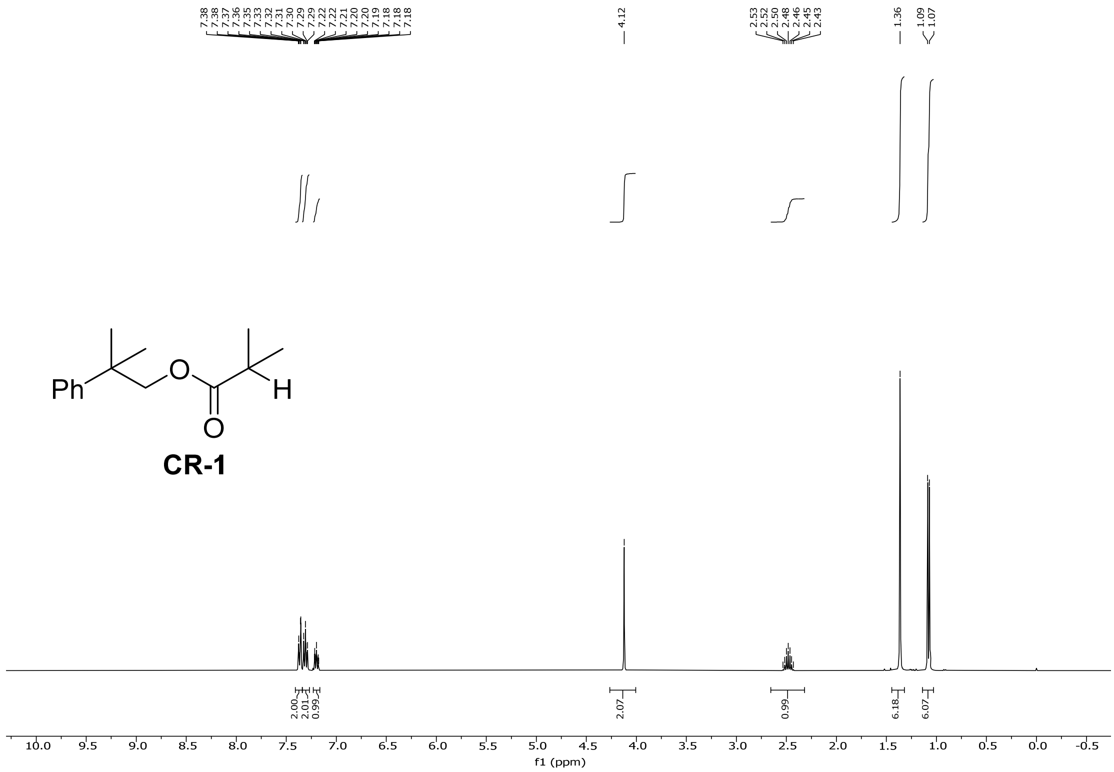




SX5



SX5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7.38
7.37
7.36
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7.33
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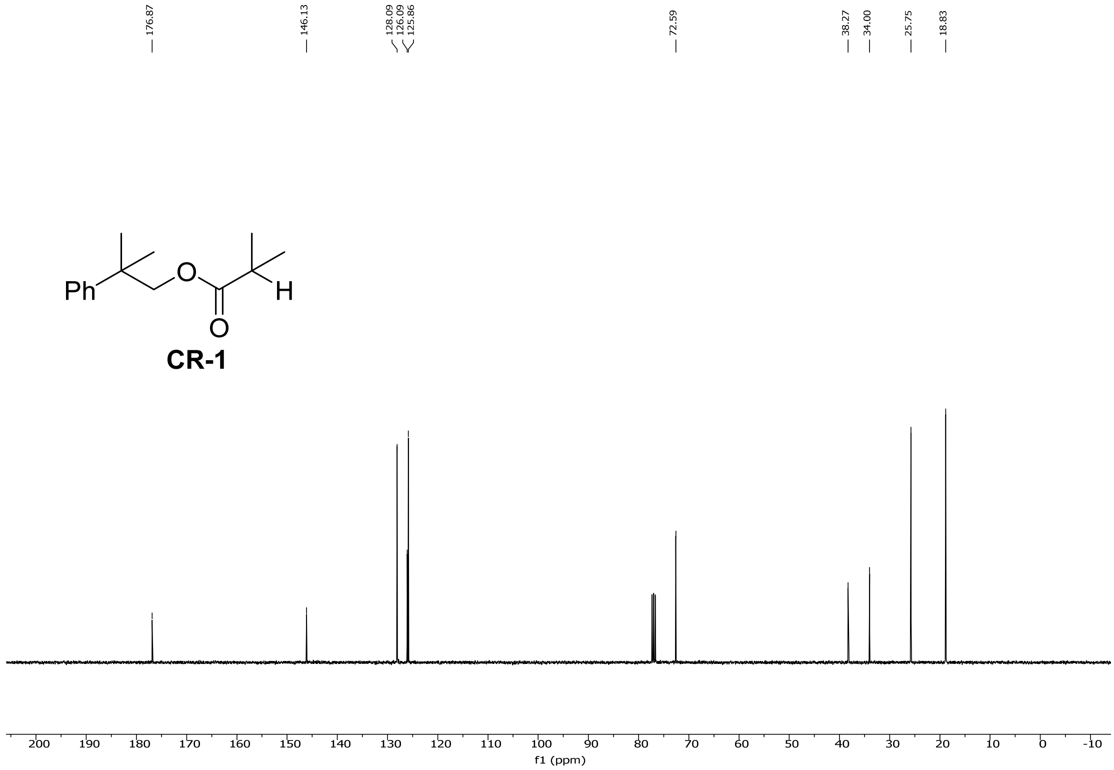
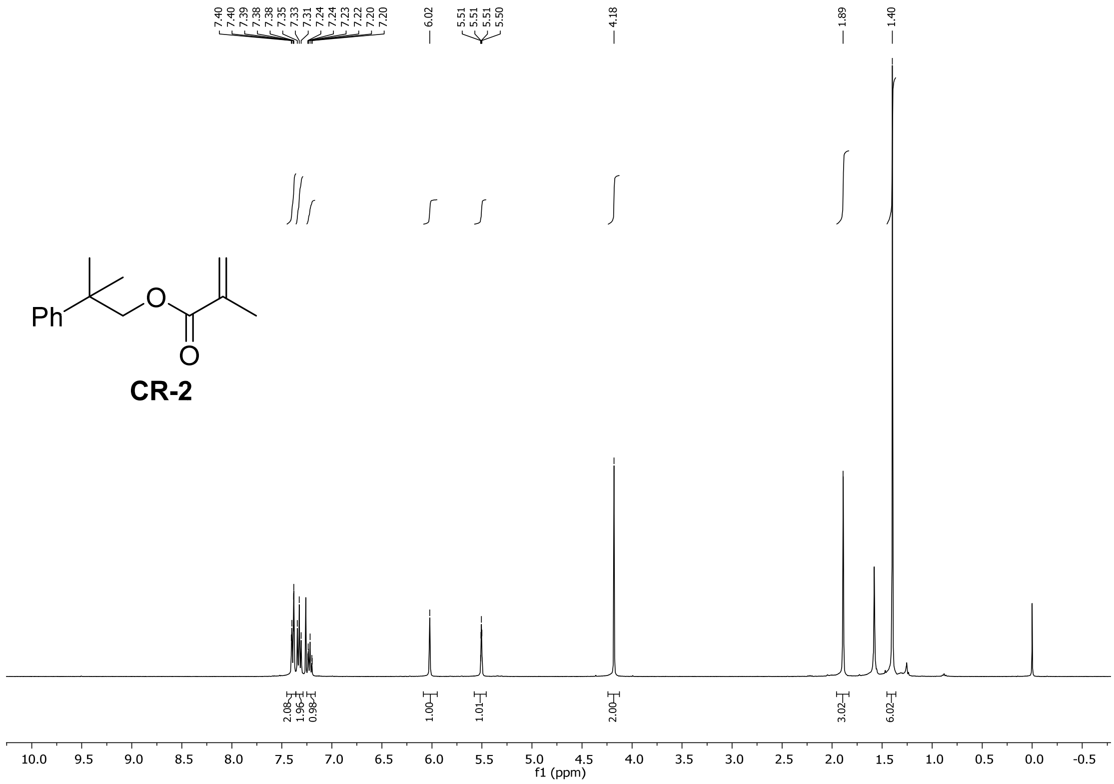
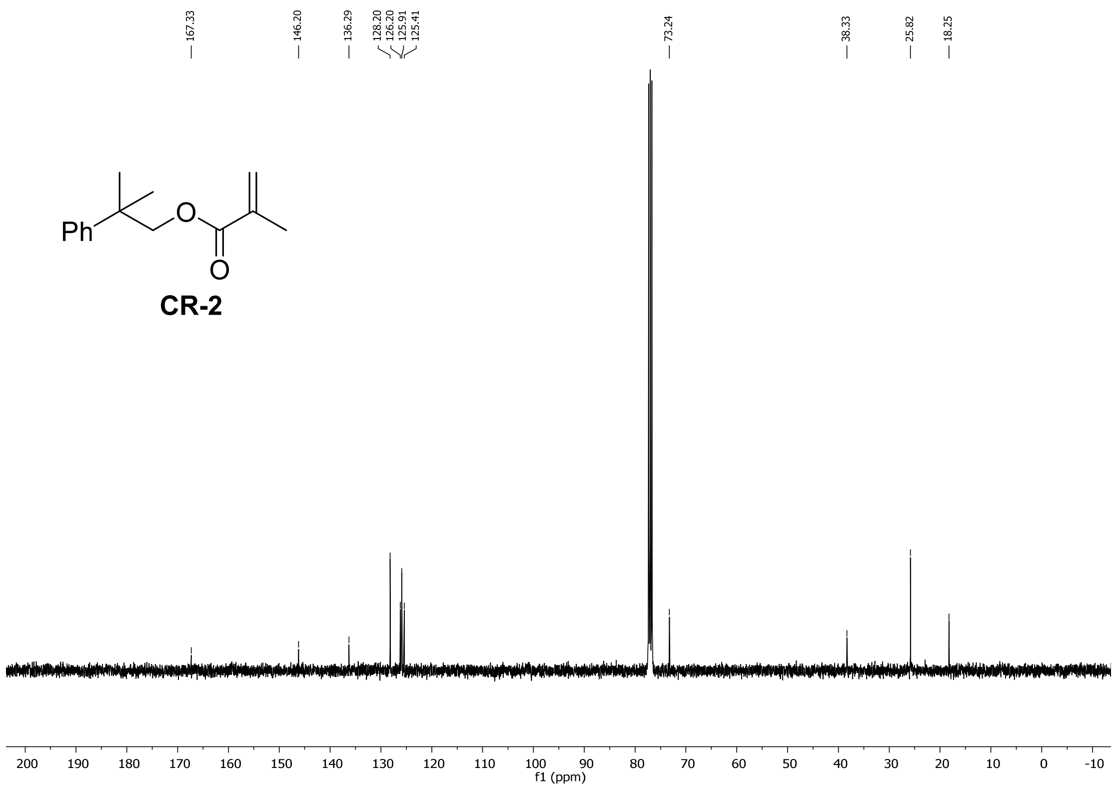
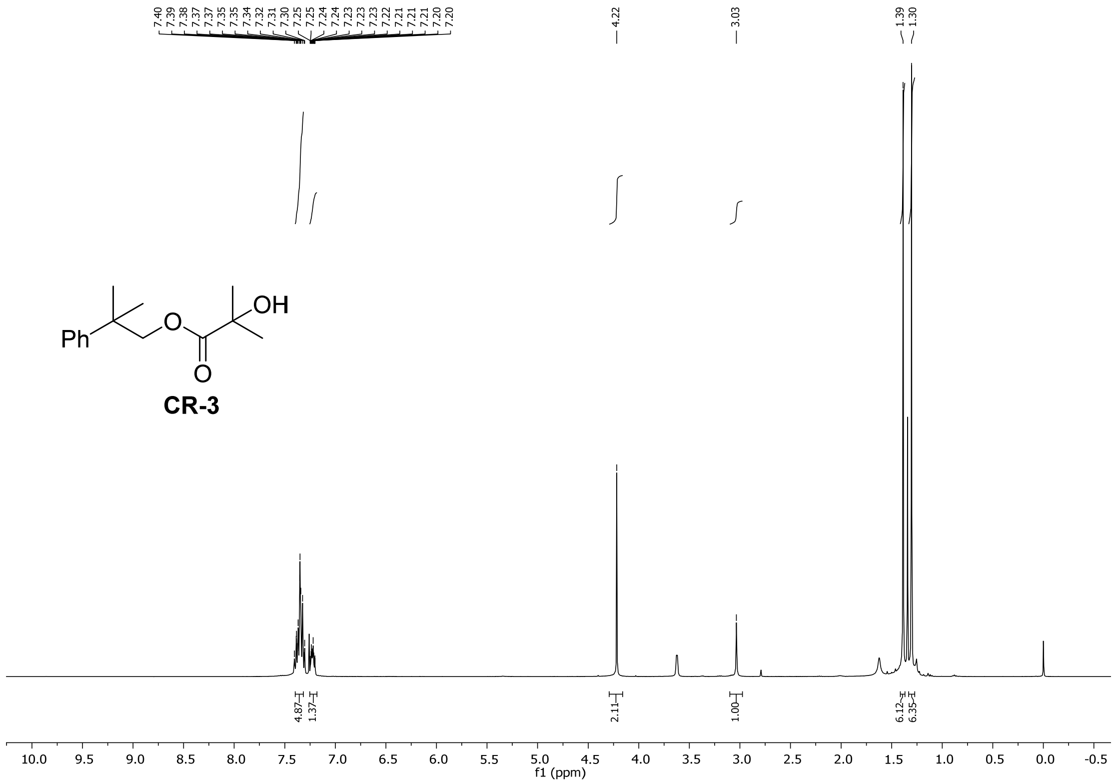
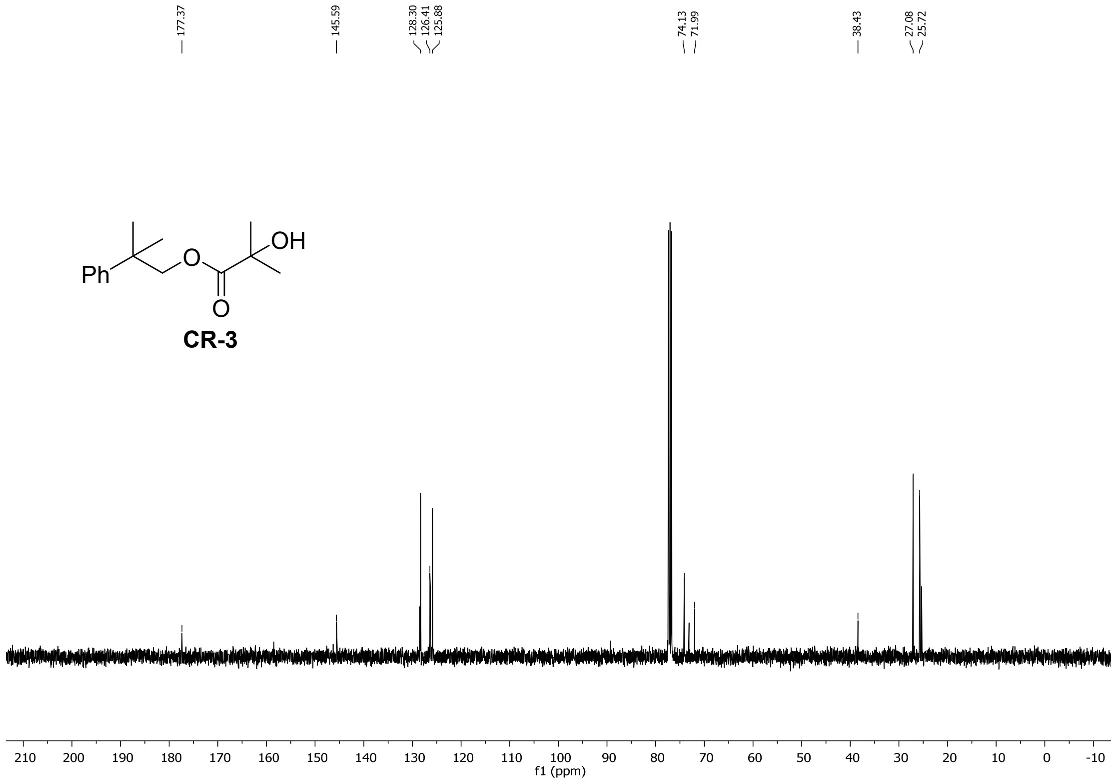
7.31
7.30
7.29
7.29
7.22
7.22
7.21
7.20
7.19
7.18
7.18
7.18
4.12
2.53
2.52
2.50
2.48
2.46
2.45
2.43
1.36
1.09
1.07
Ph
O
H
O
CR-1
2.00
2.01
0.99
2.07
0.99
6.18
6.07
f1 (ppm)


176.87
146.13
128.09
126.09
125.86
72.59
38.27
34.00
25.75
18.83
Ph
O
H
O
CR-1
f1 (ppm)

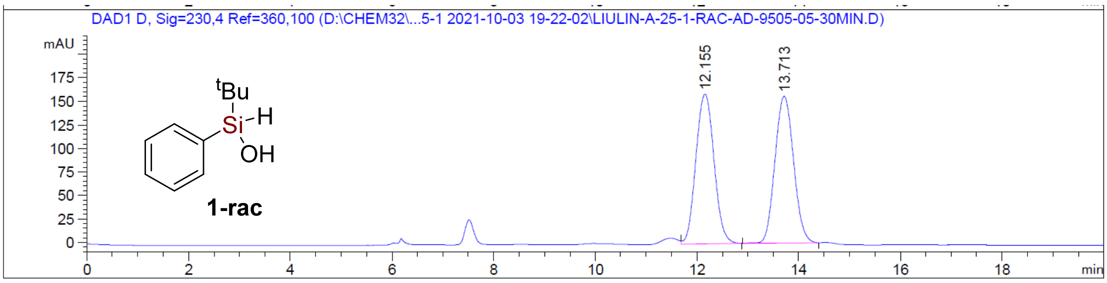

7.40
7.40
7.39
7.38
7.38
7.35
7.33
7.31
7.24
7.24
7.23
7.22
7.20
7.20
6.02
5.51
5.51
5.51
5.50
4.18
1.89
1.40
Ph
O
O
CR-2
2.08
1.96
0.98
1.00
1.01
2.00
3.02
6.02
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


167.33
146.20
136.29
128.20
126.20
125.91
125.41
73.24
38.33
25.82
18.25
Ph
O
O
CR-2
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


CR-3
f1 (ppm)


CR-3
f1 (ppm)

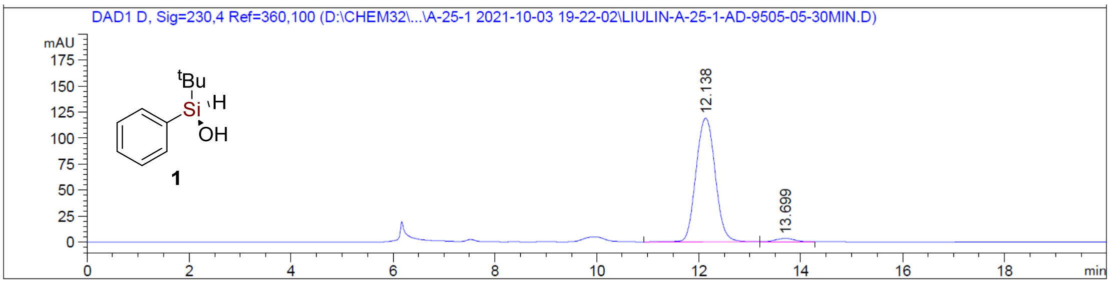
11. HPLC Spectra



Signal 4: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.155	VB	0.3958	3957.72656	159.30977	49.9158
2	13.713	BB	0.4028	3971.07813	156.08057	50.0842

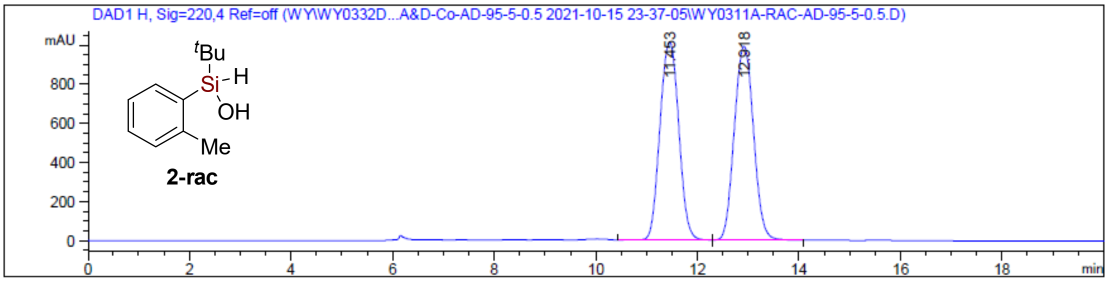
Totals : 7928.80469 315.39034



Signal 4: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.138	BB	0.4191	3111.39331	118.98605	97.3946
2	13.699	BB	0.3970	83.23408	3.26942	2.6054

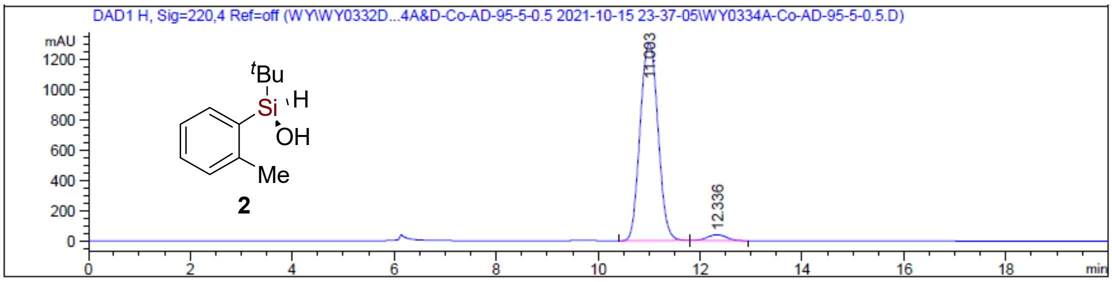
Totals : 3194.62739 122.25546



Signal 8: DAD1 H, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.453	BB	0.4164	2.61426e4	1015.13513	49.9548
2	12.918	BB	0.4237	2.61899e4	993.09174	50.0452

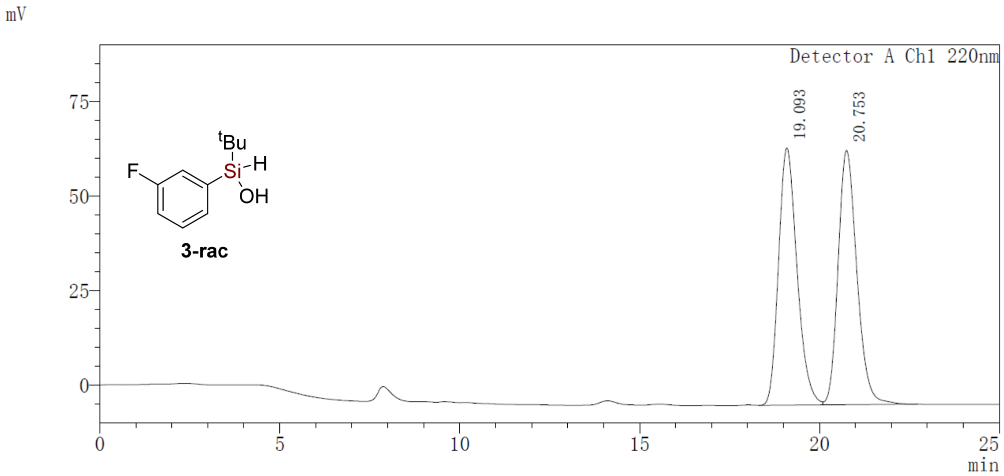
Totals : 5.23325e4 2008.22687



Signal 8: DAD1 H, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.003	BB	0.3898	3.18133e4	1308.03271	97.0551
2	12.336	BB	0.4022	965.29504	38.54086	2.9449

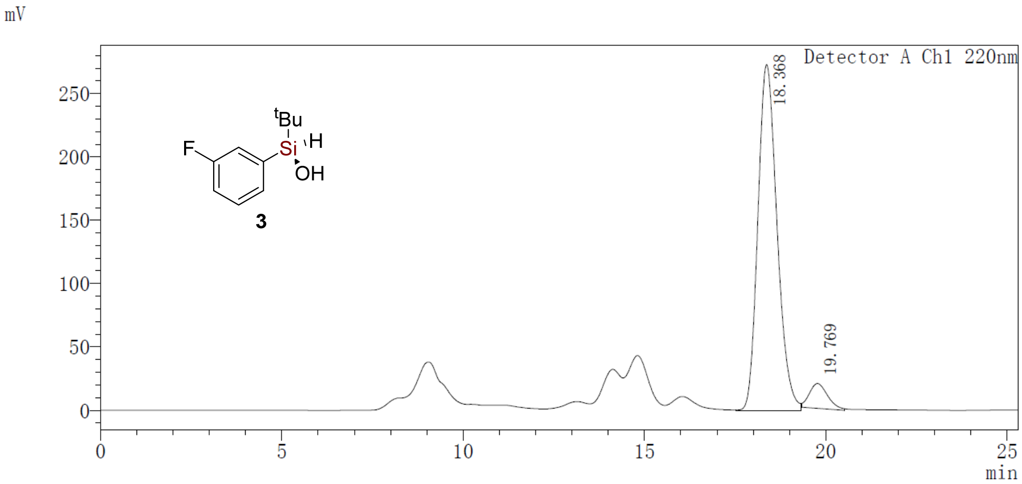
Totals : 3.27786e4 1346.57358



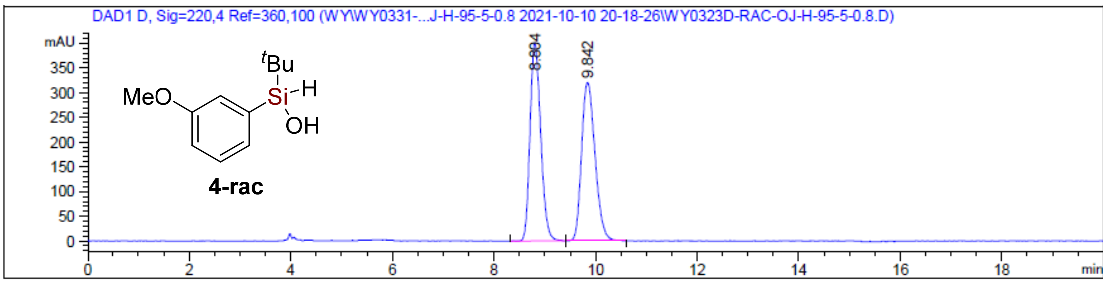
Peak Table

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Area%
1	19.093	2438942	49.966
2	20.753	2442291	50.034



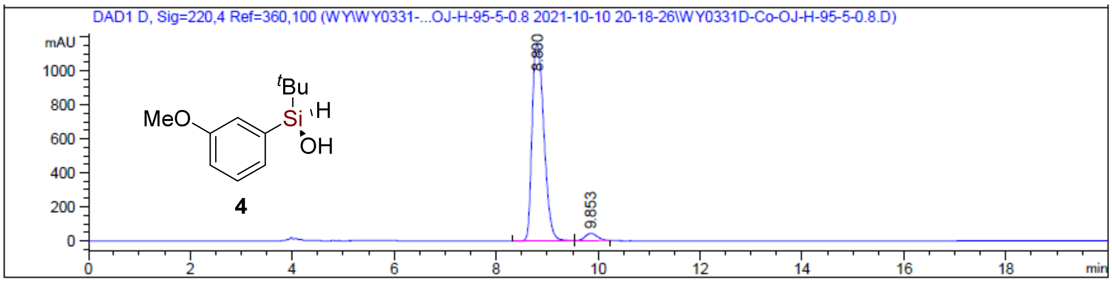
Peak#	Ret. Time	Area	Area%
1	18.368	10042059	93.579
2	19.769	689076	6.421



Signal 4: DAD1 D, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.804	VB R	0.2306	5867.77637	401.17209	49.8672
2	9.842	BB	0.2903	5890.37012	320.63400	50.0593
3	29.936	VV	0.1027	8.64928	1.11281	0.0735

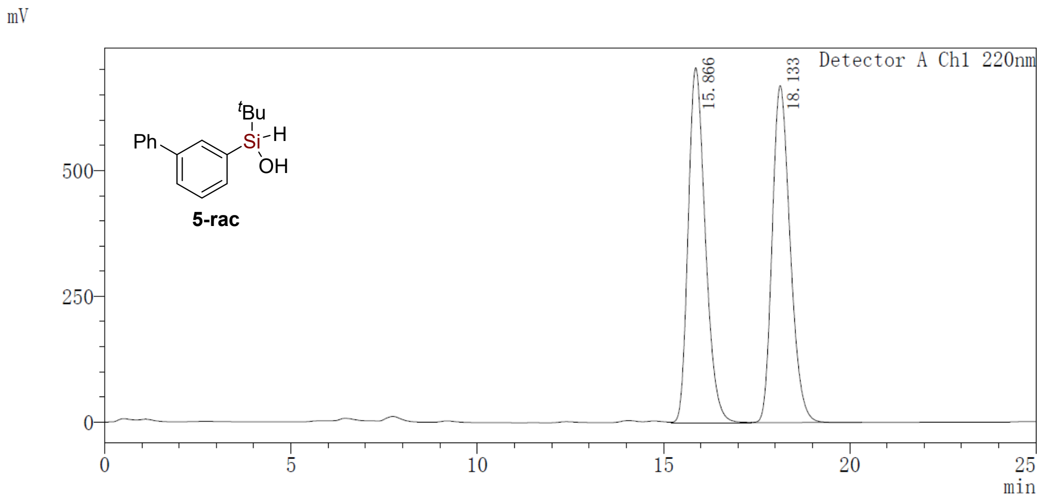
Totals : 1.17668e4 722.91890



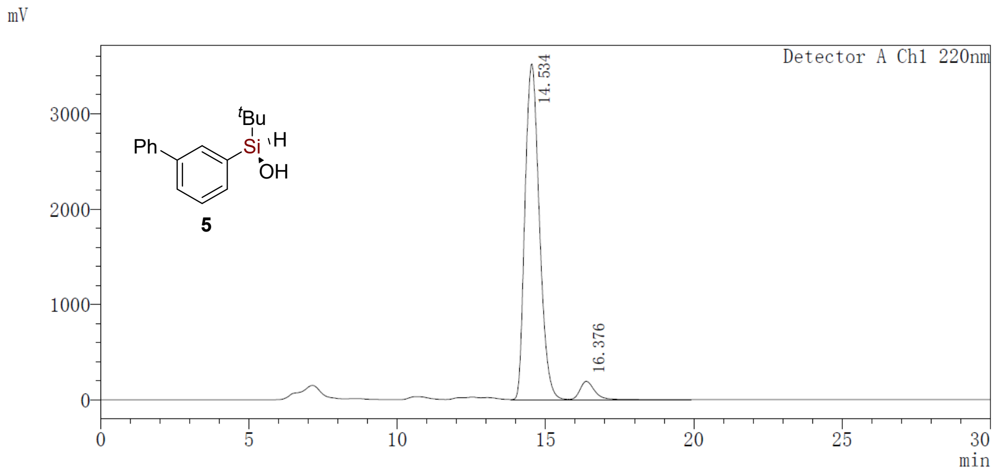
Signal 4: DAD1 D, Sig=220,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.800	VV R	0.2575	1.86447e4	1159.91406	96.2724
2	9.853	VB	0.2496	721.90790	42.61866	3.7276

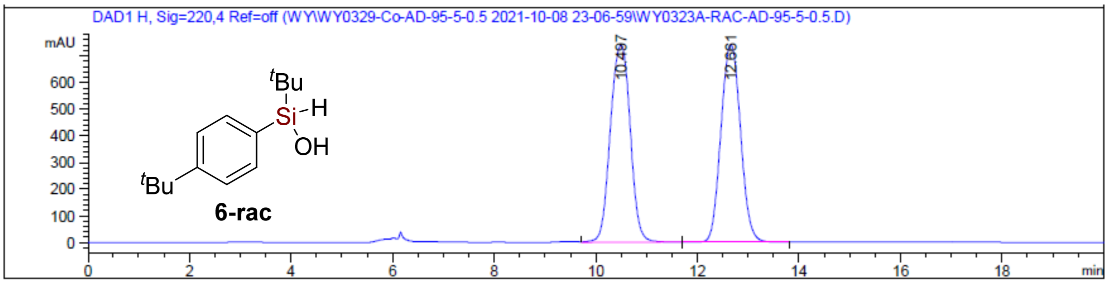
Totals : 1.93666e4 1202.53273



Peak#	Ret. Time	Area	Area%
1	15.866	22554847	50.128
2	18.133	22439887	49.872



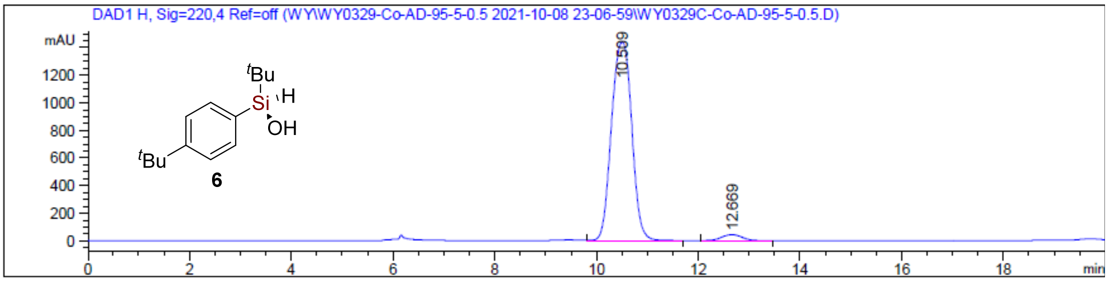
Peak#	Ret. Time	Area	Area%
1	14.534	118510343	94.660
2	16.376	6684872	5.340



Signal 8: DAD1 H, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.497	VB	0.4382	2.01522e4	738.83752	50.3487
2	12.661	BB	0.4283	1.98730e4	742.39508	49.6513

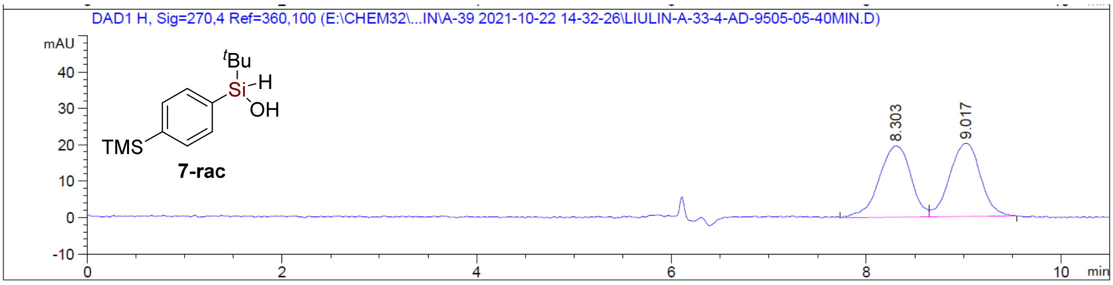
Totals : 4.00253e4 1481.23260



Signal 8: DAD1 H, Sig=220,4 Ref=off

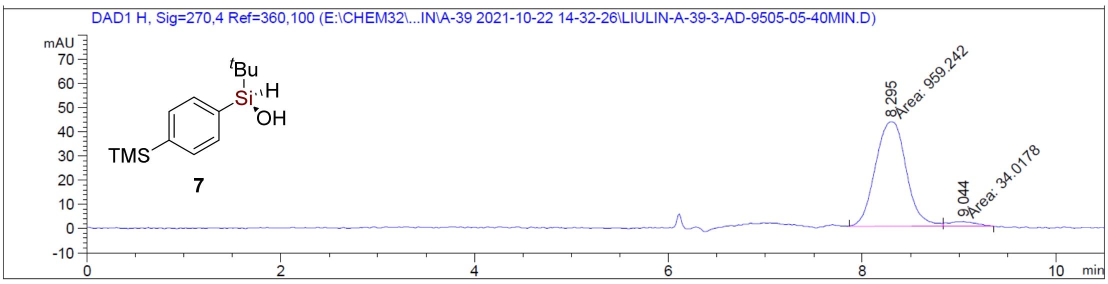
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.509	VB	0.4493	3.96788e4	1440.58594	97.1406
2	12.669	BB	0.4355	1167.98865	42.91240	2.8594

Totals : 4.08467e4 1483.49834



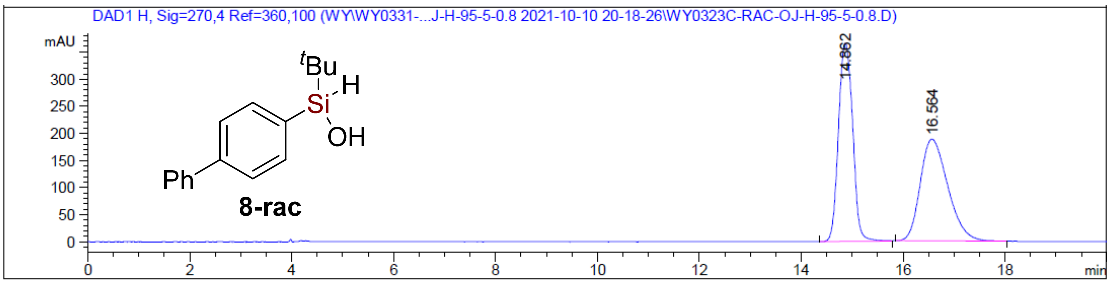
Signal 8: DAD1 H, Sig=270,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.303	BV	0.3153	442.85382	19.62187	50.0853
2	9.017	VV R	0.2721	441.34464	20.10712	49.9147
Totals :				884.19846	39.72899	



Signal 8: DAD1 H, Sig=270,4 Ref=360,100

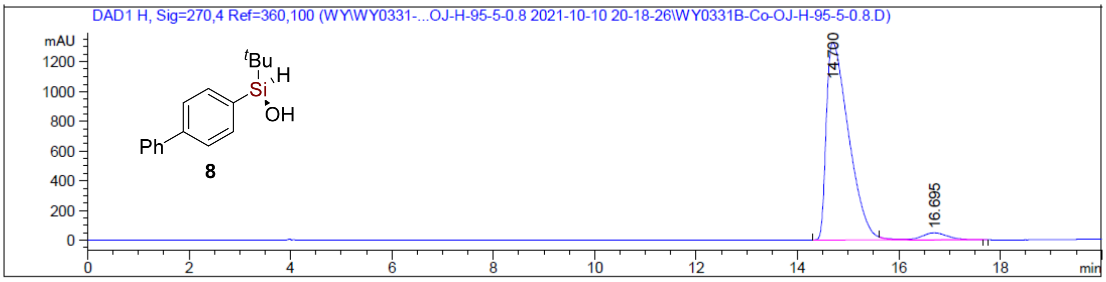
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.295	MF	0.3693	959.24170	43.28731	96.5751
2	9.044	FM	0.3135	34.01783	1.80852	3.4249
Totals :				993.25953	45.09583	



Signal 8: DAD1 H, Sig=270,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.862	BB	0.3175	7068.21143	365.69183	49.9818
2	16.564	BV R	0.5613	7073.35791	187.86169	50.0182

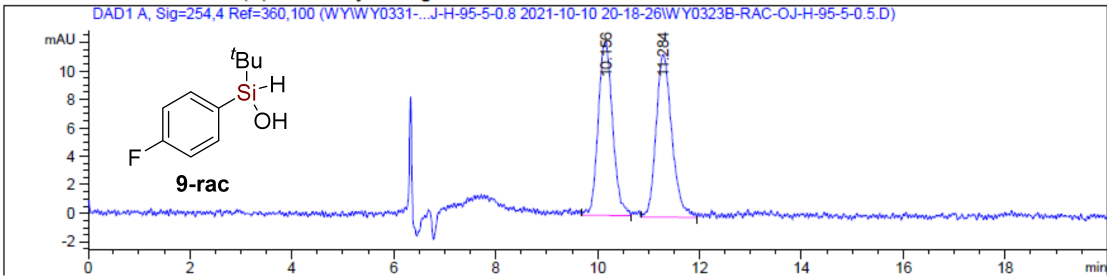
Totals : 1.41416e4 553.55353



Signal 8: DAD1 H, Sig=270,4 Ref=360,100

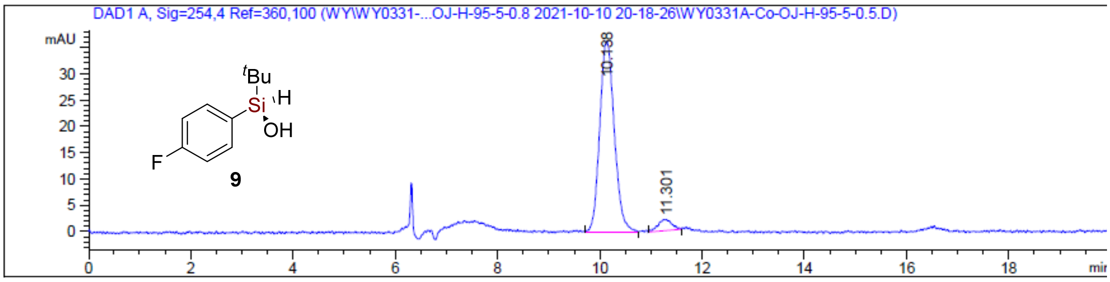
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.700	BV R	0.4261	4.05529e4	1328.55151	95.8807
2	16.695	VV E	0.4990	1742.25439	47.15537	4.1193

Totals : 4.22951e4 1375.70688



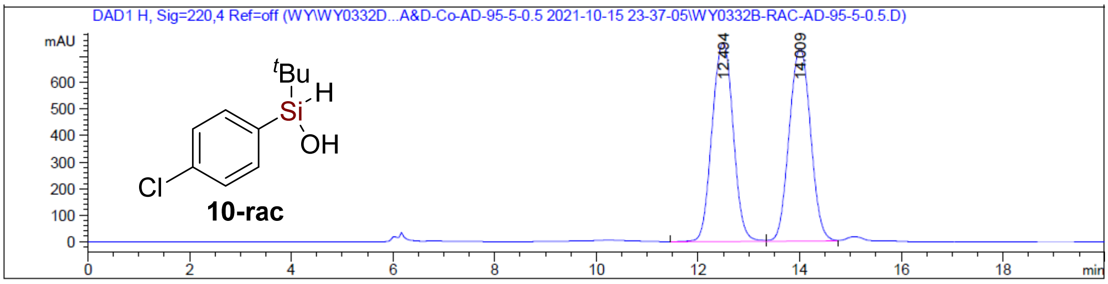
Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.156	VB R	0.2422	239.22018	12.22811	49.3798
2	11.284	BV R	0.2849	245.22902	11.40441	50.6202
Totals :				484.44920	23.63252	



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

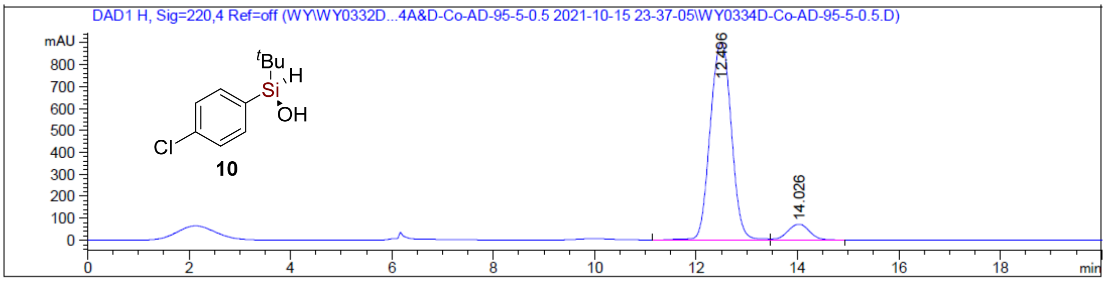
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.138	BB	0.2852	720.23761	36.35097	94.8063
2	11.301	VV R	0.2329	39.45634	2.08400	5.1937
Totals :				759.69395	38.43497	



Signal 8: DAD1 H, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.494	BV	0.4645	2.16267e4	749.78351	50.3527
2	14.009	VV	0.4716	2.13237e4	728.25806	49.6473

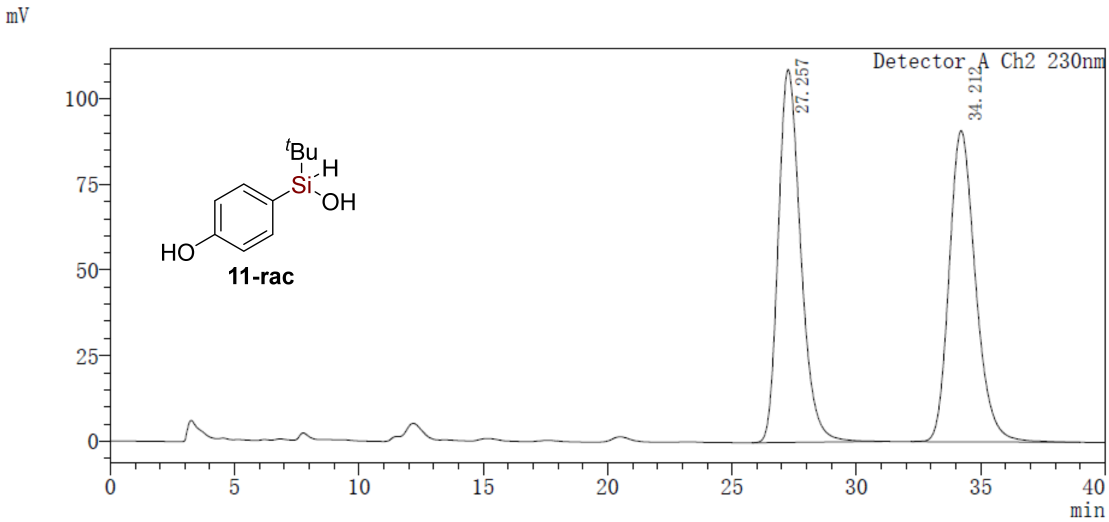
Totals : 4.29505e4 1478.04156



Signal 8: DAD1 H, Sig=220,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.496	BV	0.4696	2.60590e4	900.47961	92.4360
2	14.026	VB	0.4700	2132.41357	71.90397	7.5640

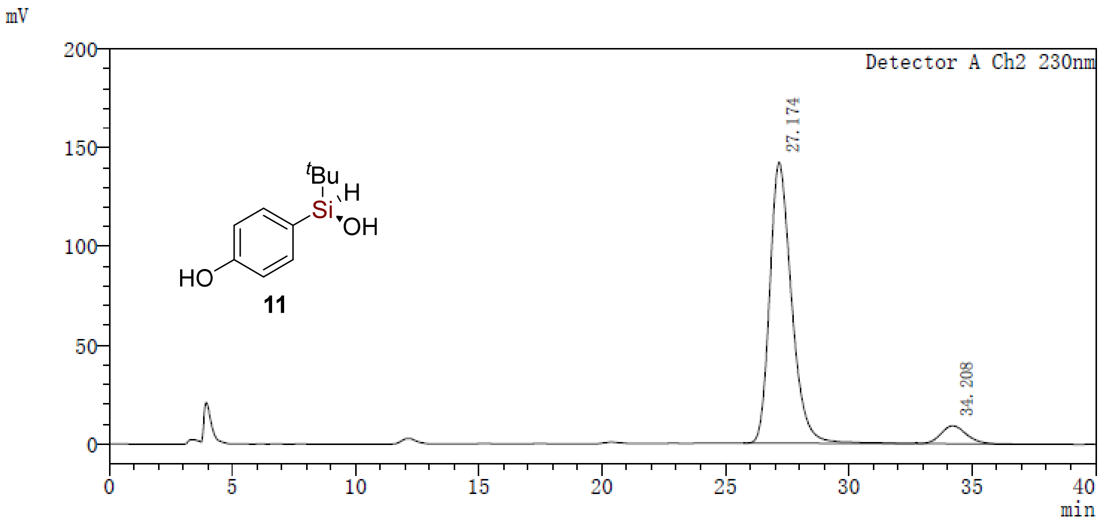
Totals : 2.81915e4 972.38358



Peak Table

Detector A Ch2 230nm

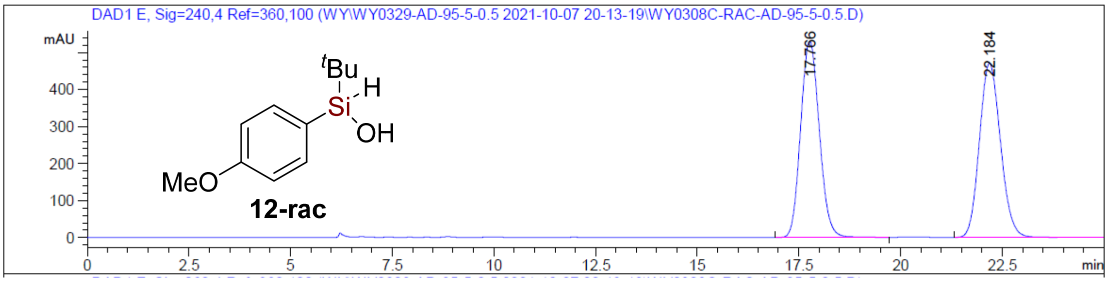
Peak#	Ret. Time	Area	Area%
1	27.257	6837842	50.480
2	34.212	6707707	49.520



Peak Table

Detector A Ch2 230nm

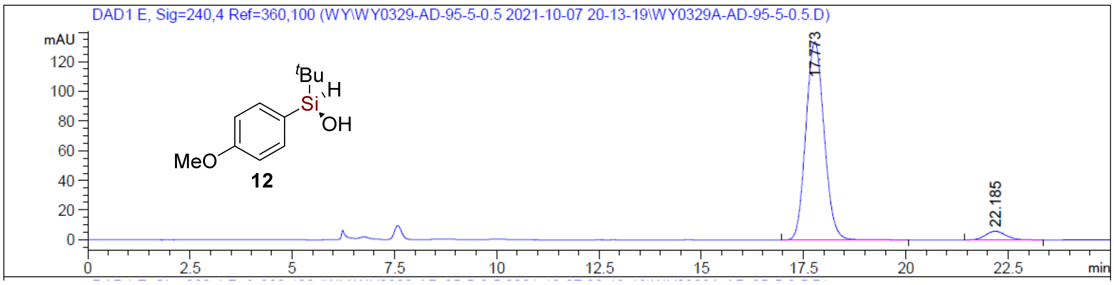
Peak#	Ret. Time	Area	Area%
1	27.174	8868619	93.043
2	34.208	663173	6.957



Signal 5: DAD1 E, Sig=240,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.766	BB	0.5035	1.68970e4	530.60211	49.9195
2	22.184	BBA	0.5602	1.69515e4	470.65051	50.0805

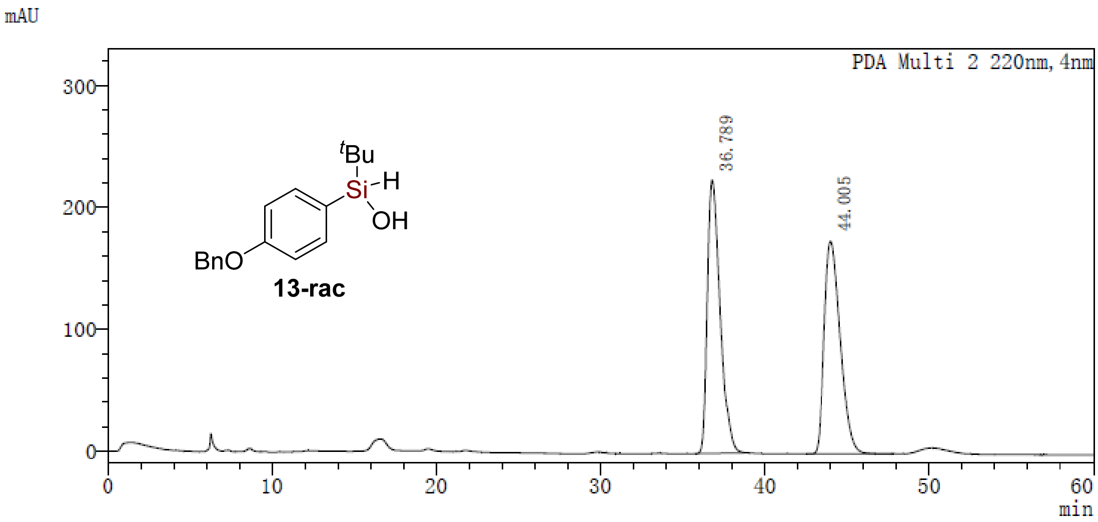
Totals : 3.38485e4 1001.25262



Signal 5: DAD1 E, Sig=240,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.773	BB	0.4843	4156.77100	133.85883	95.3223
2	22.185	BB	0.5222	203.98459	5.88711	4.6777

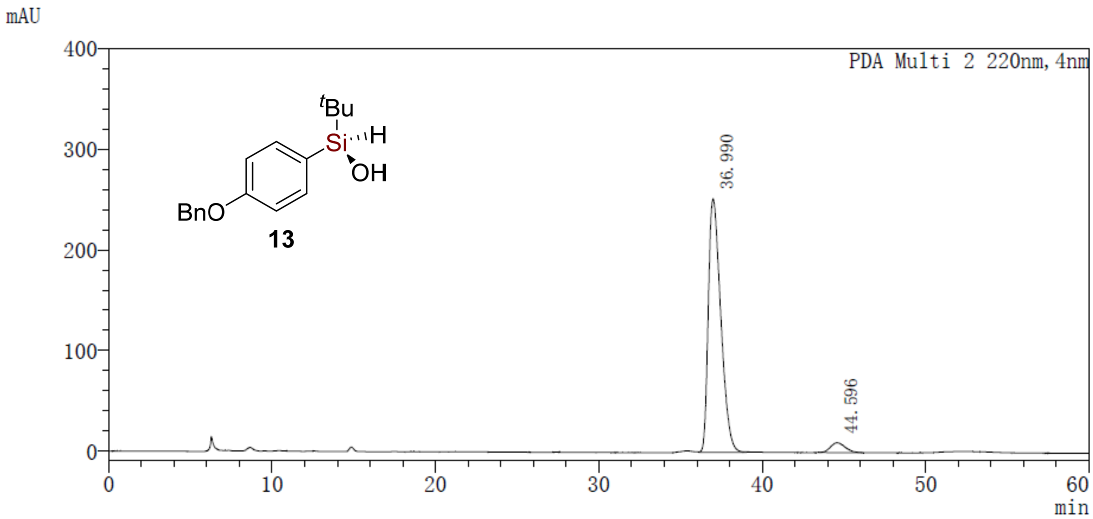
Totals : 4360.75558 139.74593



Peak Table

PDA Ch2 220nm

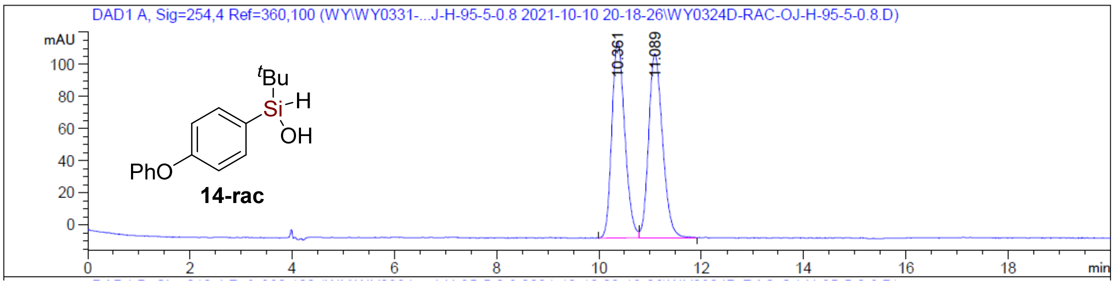
Peak#	Ret. Time	Area	Area%
1	36.789	12031288	50.406
2	44.005	11837508	49.594



Peak Table

PDA Ch2 220nm

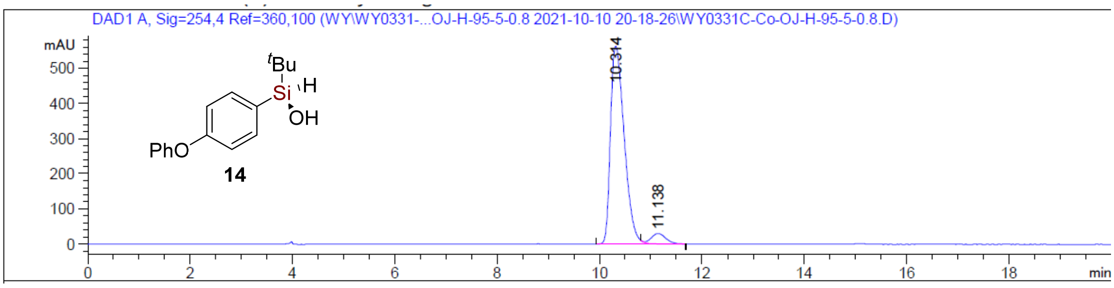
Peak#	Ret. Time	Area	Area%
1	36.990	13361514	95.591
2	44.596	616220	4.409



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.361	BV	0.2753	2156.39453	122.55605	49.6630
2	11.089	VB	0.2979	2185.65942	114.91826	50.3370

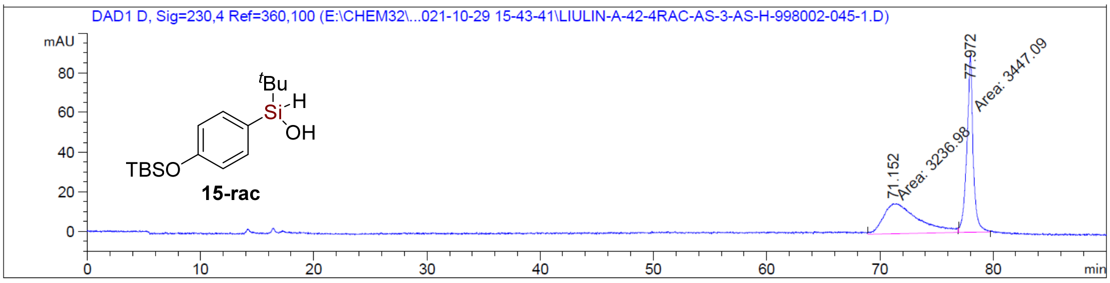
Totals : 4342.05396 237.47430



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.314	BV R	0.2913	1.04854e4	562.94366	94.8183
2	11.138	VB E	0.3098	573.00952	29.09576	5.1817

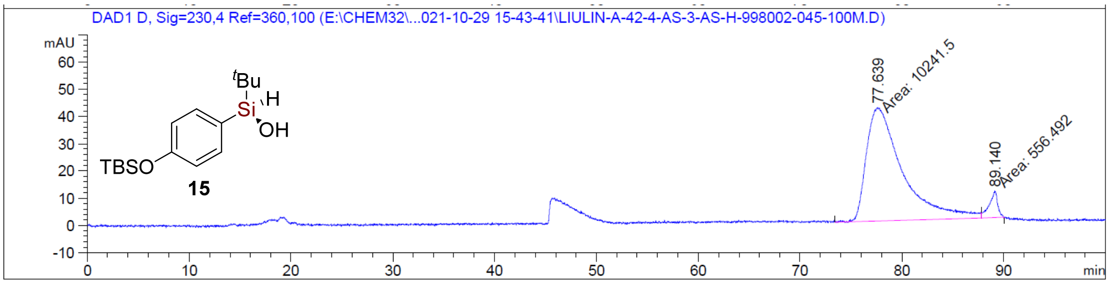
Totals : 1.10584e4 592.03942



Signal 4: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	71.152	MF	3.5356	3236.98169	15.25890	48.4283
2	77.972	FM	0.6446	3447.09033	89.12873	51.5717

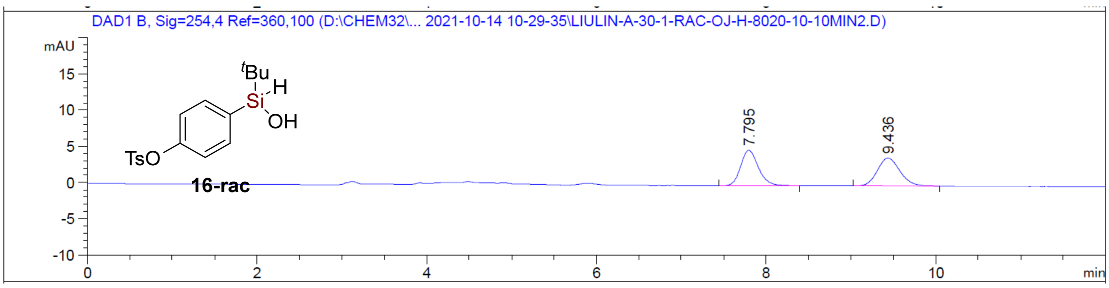
Totals : 6684.07202 104.38763



Signal 4: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	77.639	MF	4.0916	1.02415e4	41.71748	94.8463
2	89.140	FM	0.9525	556.49188	9.73747	5.1537

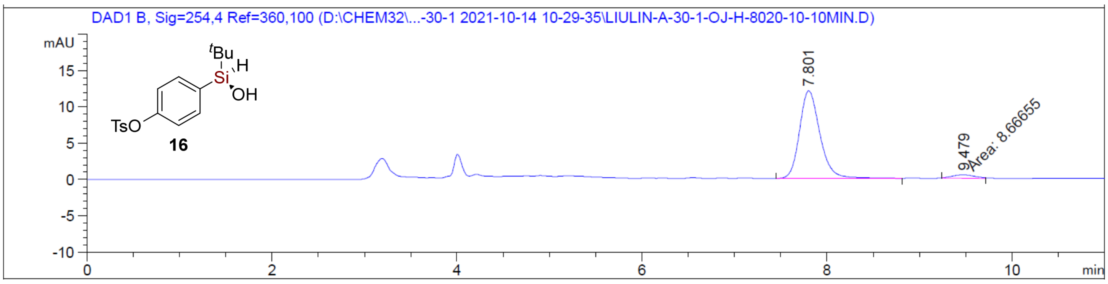
Totals : 1.07980e4 51.45495



Signal 2: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.795	BB	0.2263	71.61598	4.90689	50.2924
2	9.436	BB	0.2796	70.78314	3.83089	49.7076

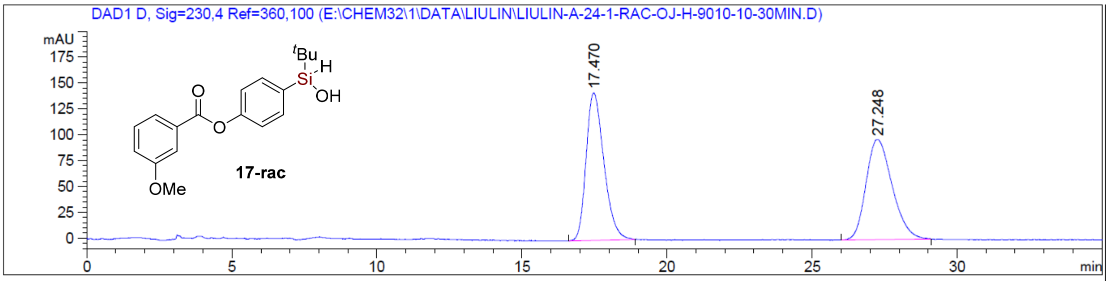
Totals : 142.39912 8.73778



Signal 2: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.801	BB	0.2343	184.72519	12.08609	95.5187
2	9.479	MM	0.2939	8.66655	4.91515e-1	4.4813

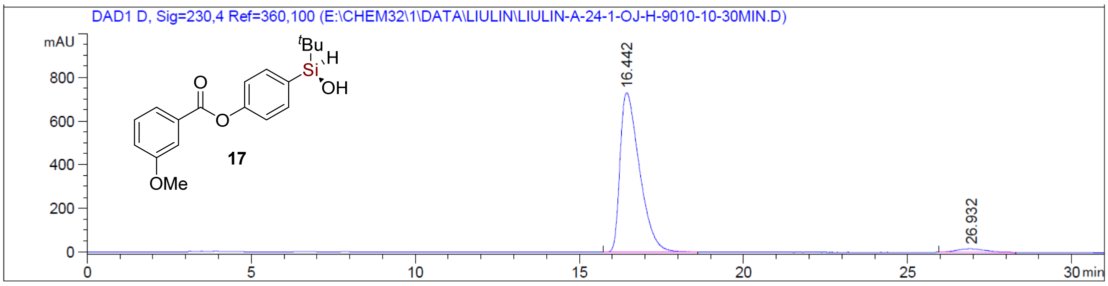
Totals : 193.39174 12.57761



Signal 4: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.470	BB	0.5836	6079.16943	142.52798	50.1065
2	27.248	VV R	0.7377	6053.31543	96.77784	49.8935

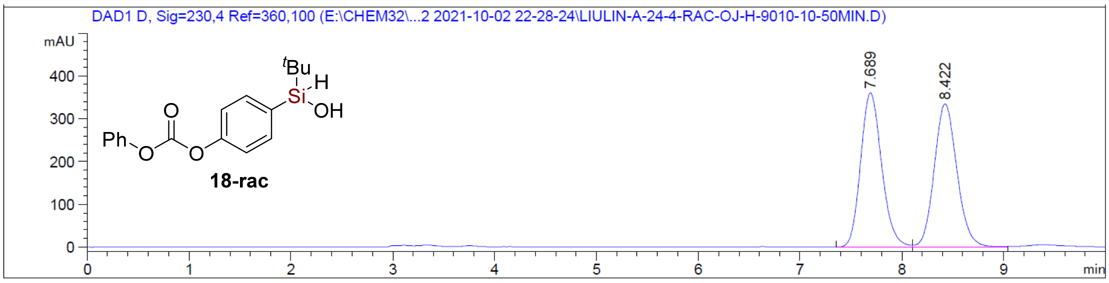
Totals : 1.21325e4 239.30582



Signal 4: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.442	VV R	0.5798	2.99935e4	729.31799	96.9656
2	26.932	VV R	0.7188	938.59338	15.44885	3.0344

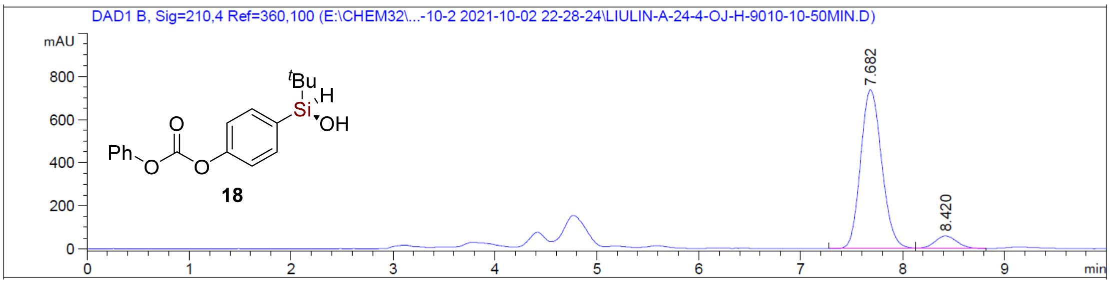
Totals : 3.09321e4 744.76684



Signal 4: DAD1 D, Sig=230,4 Ref=360,100

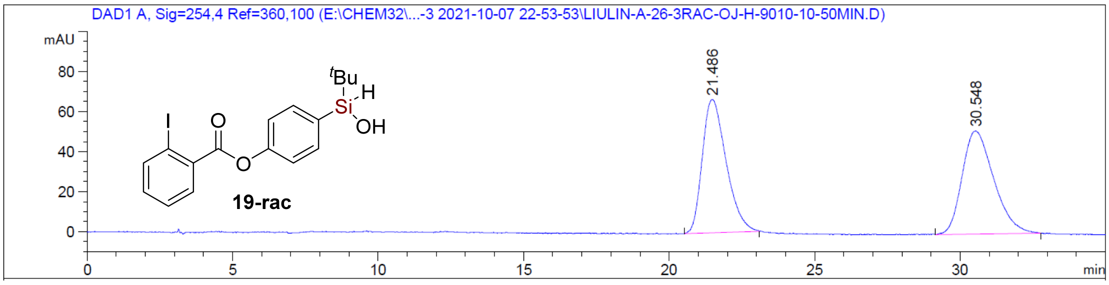
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.689	BV	0.2219	5185.41504	360.40762	49.9942
2	8.422	VV	0.2389	5186.62256	334.48621	50.0058

Totals : 1.03720e4 694.89383



Signal 2: DAD1 B, Sig=210,4 Ref=360,100

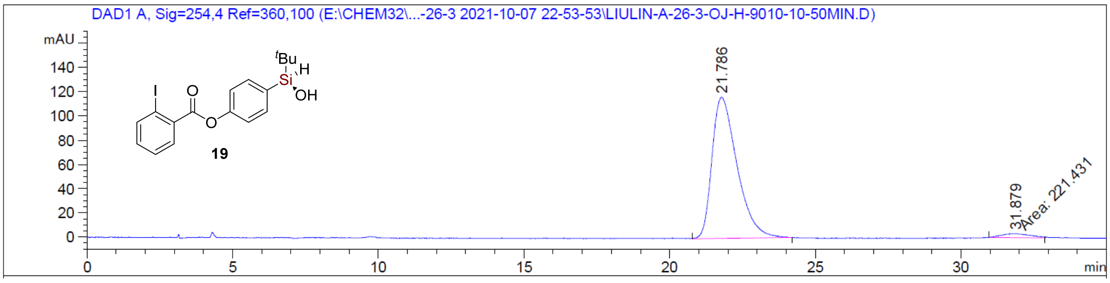
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.682	VV R	0.2283	1.06188e4	736.14056	92.2630
2	8.420	VB	0.2341	890.46210	58.34136	7.7370



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.486	BB	0.7044	3792.69727	66.59971	49.2784
2	30.548	BV R	0.8999	3903.78027	51.41168	50.7216

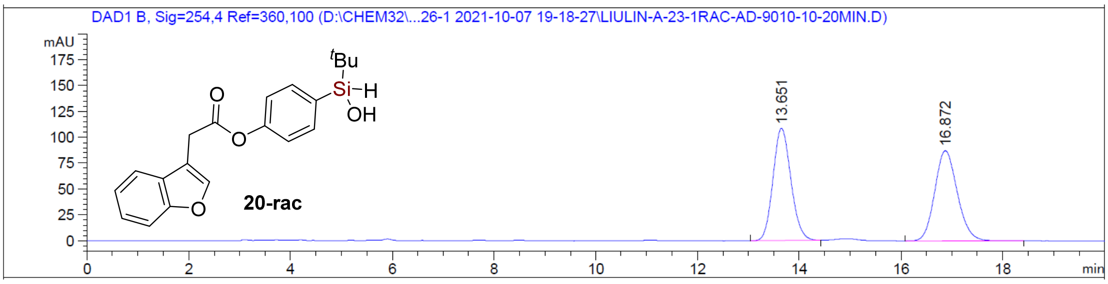
Totals : 7696.47754 118.01139



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	21.786	VB R	0.7980	6961.46777	116.36109	96.9172
2	31.879	MM	1.1036	221.43103	3.34411	3.0828

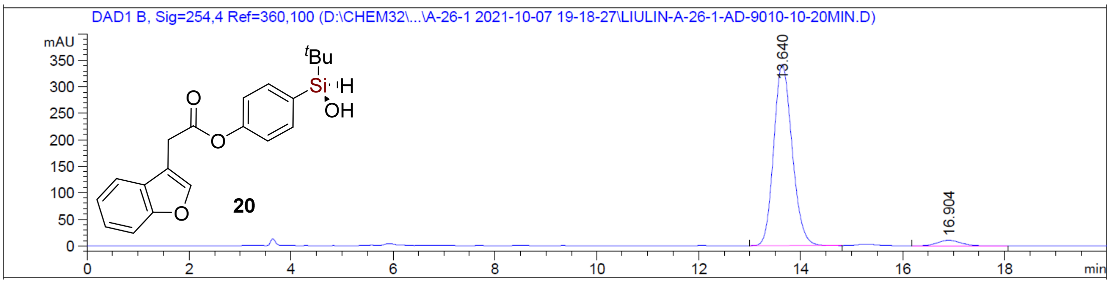
Totals : 7182.89880 119.70520



Signal 2: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.651	BB	0.3800	2663.31616	108.63986	49.7850
2	16.872	BB	0.4775	2686.32349	87.17942	50.2150

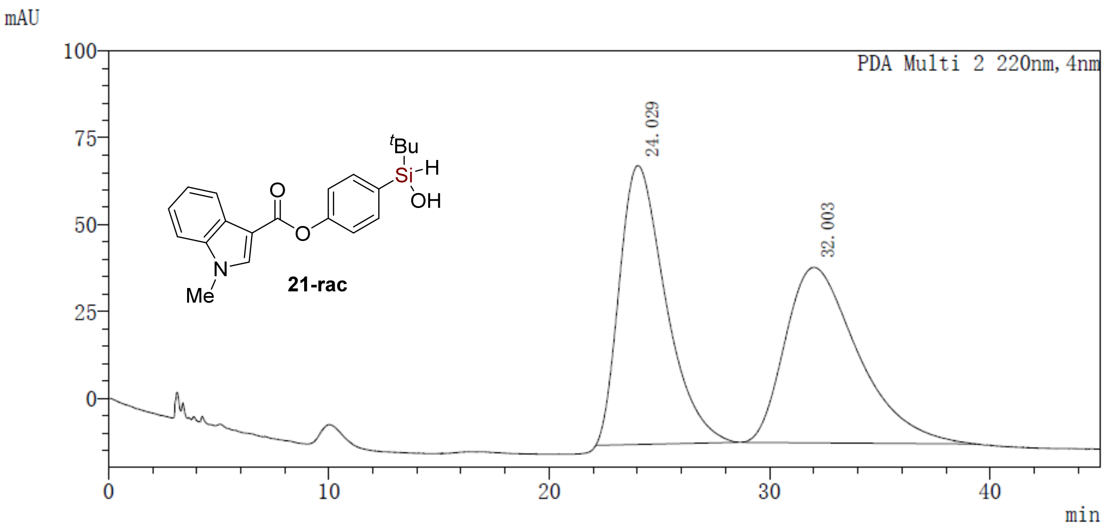
Totals : 5349.63965 195.81928



Signal 2: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.640	BB	0.3863	8558.94629	341.62067	96.3982
2	16.904	BB	0.4802	319.79294	10.30107	3.6018

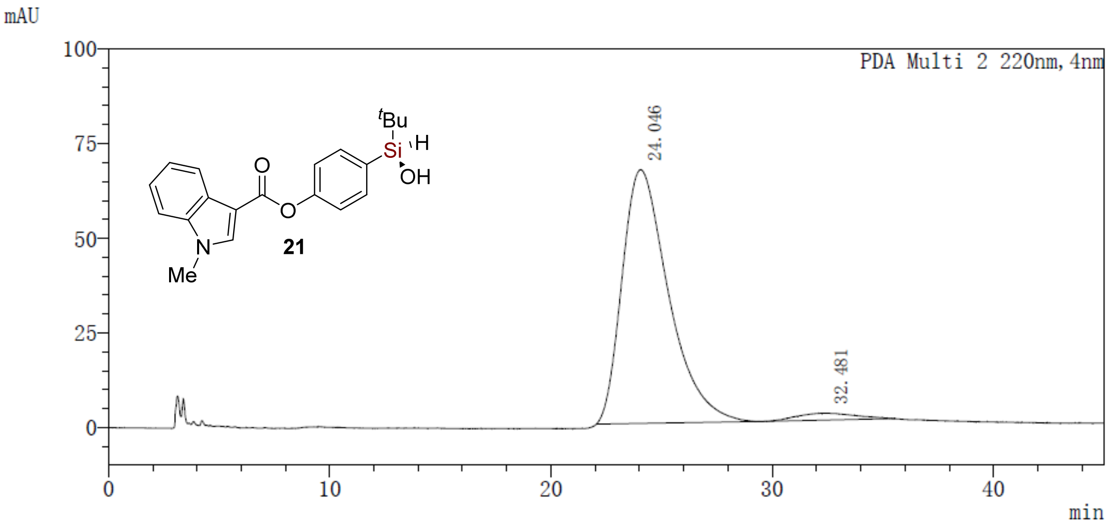
Totals : 8878.73923 351.92174



Peak Table

PDA Ch2 220nm

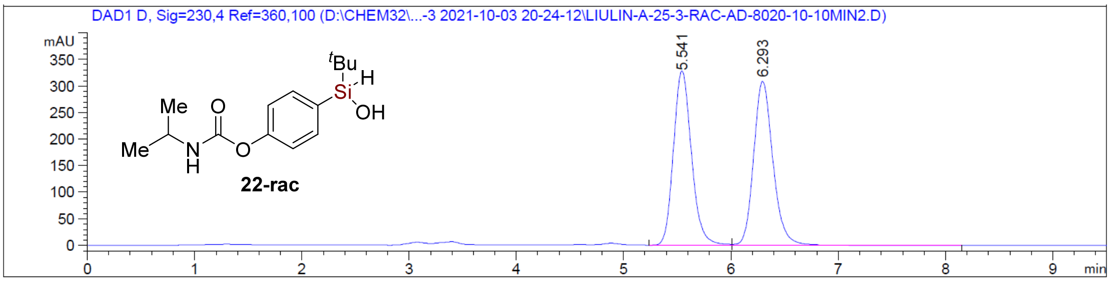
Peak#	Ret. Time	Area	Area%
1	24.029	11691945	50.074
2	32.003	11657381	49.926



Peak Table

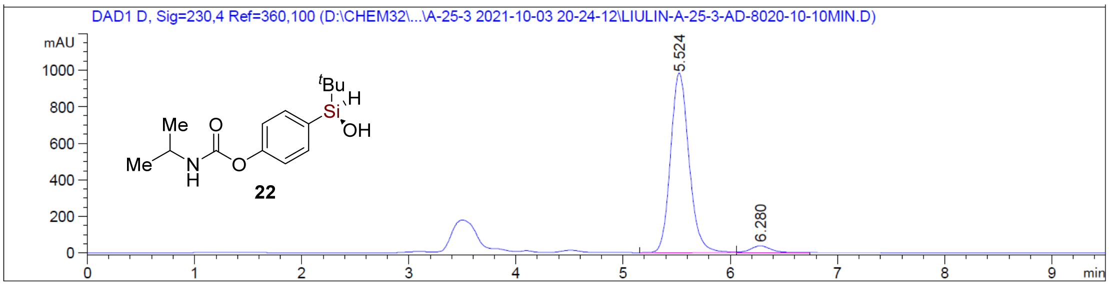
PDA Ch2 220nm

Peak#	Ret. Time	Area	Area%
1	24.046	9787199	96.631
2	32.481	341247	3.369



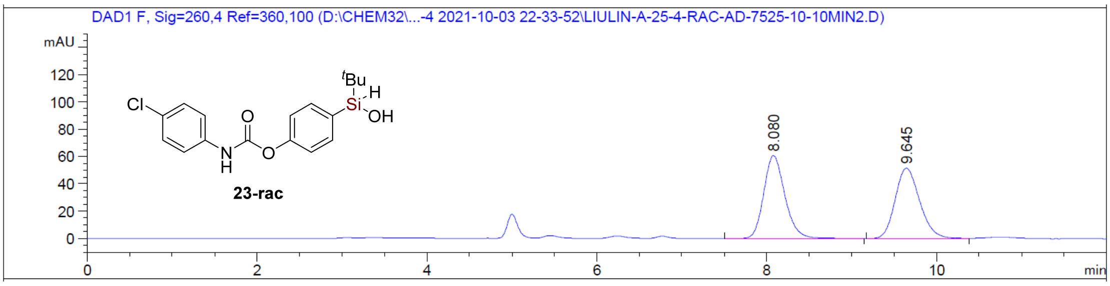
Signal 4: DAD1 D, Sig=230,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.541	BV	0.1803	3826.93384	327.57690	49.7789
2	6.293	VB	0.1921	3860.92798	308.34769	50.2211
Totals :				7687.86182	635.92459	



Signal 4: DAD1 D, Sig=230,4 Ref=360,100

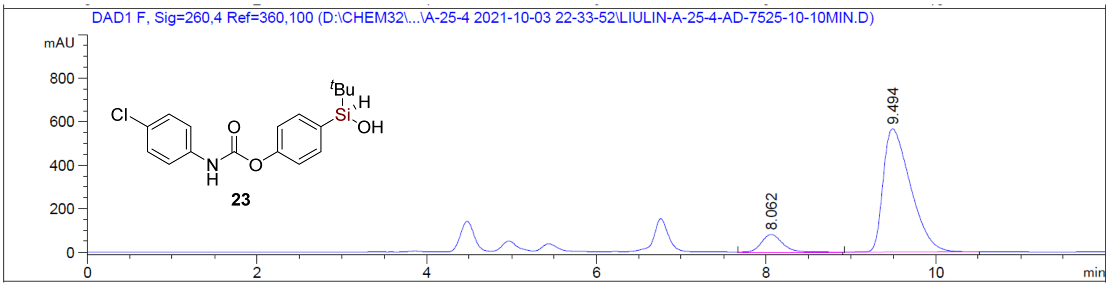
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.524	BV	0.1836	1.17916e4	985.54431	96.0385
2	6.280	VB	0.1984	486.38962	37.23679	3.9615
Totals :				1.22780e4	1022.78111	



Signal 6: DAD1 F, Sig=260,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.080	BB	0.2669	1056.84619	60.76555	50.6322
2	9.645	BB	0.3095	1030.45483	51.49400	49.3678

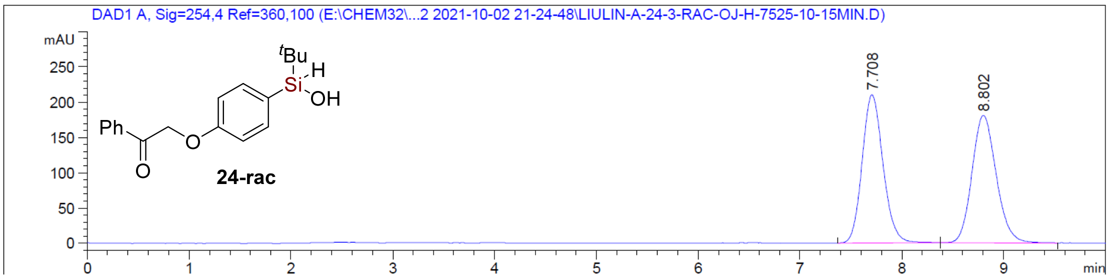
Totals : 2087.30103 112.25955



Signal 6: DAD1 F, Sig=260,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.062	BB	0.2620	1374.94080	81.01470	9.7781
2	9.494	BB	0.3455	1.26864e4	565.99469	90.2219

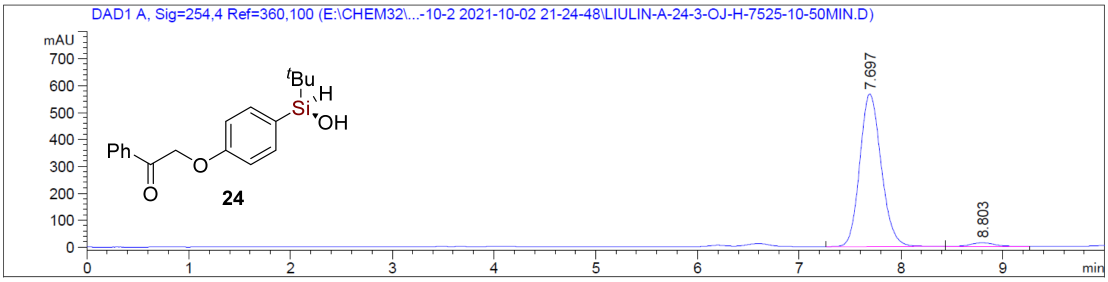
Totals : 1.40614e4 647.00939



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.708	BB	0.2205	2997.83057	210.11287	50.0290
2	8.802	BB	0.2575	2994.35571	180.56339	49.9710

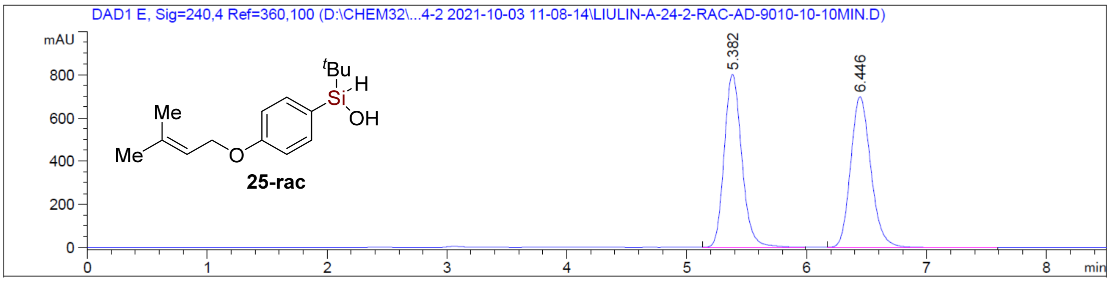
Totals : 5992.18628 390.67625



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.697	BV	0.2248	8299.66699	566.87201	97.2618
2	8.803	VB	0.2572	233.66165	13.96835	2.7382

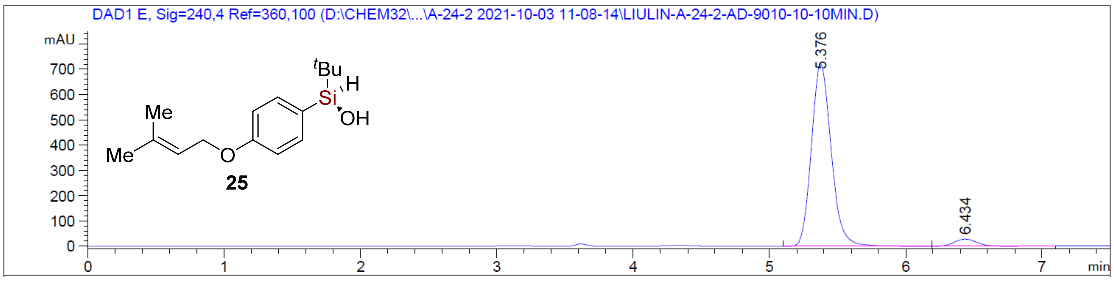
Totals : 8533.32864 580.84036



Signal 5: DAD1 E, Sig=240,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.382	VV	0.1573	8187.52979	800.97247	50.0288
2	6.446	VB	0.1808	8178.10547	697.49506	49.9712

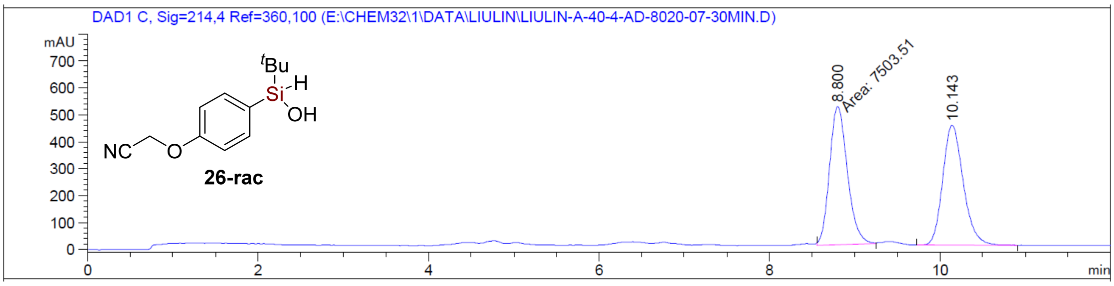
Totals : 1.63656e4 1498.46753



Signal 5: DAD1 E, Sig=240,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	5.376	BV	0.1558	7280.82617	721.01025	95.6639
2	6.434	VB	0.1767	330.01443	28.57535	4.3361

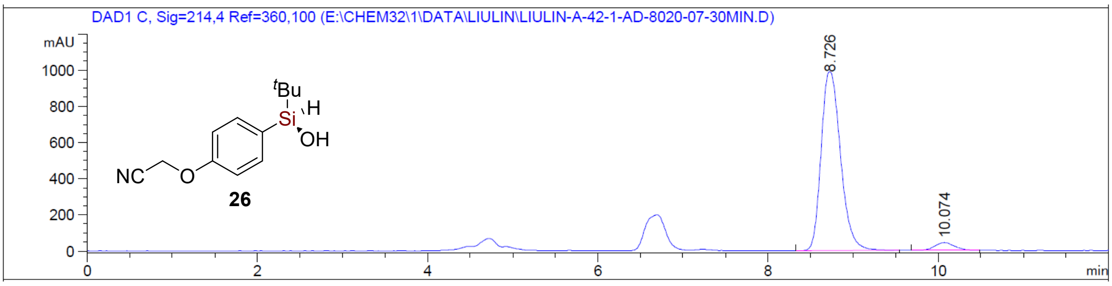
Totals : 7610.84061 749.58560



Signal 3: DAD1 C, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.800	MM	0.2438	7503.50977	512.90289	50.0742
2	10.143	BV R	0.2601	7481.27832	444.80173	49.9258

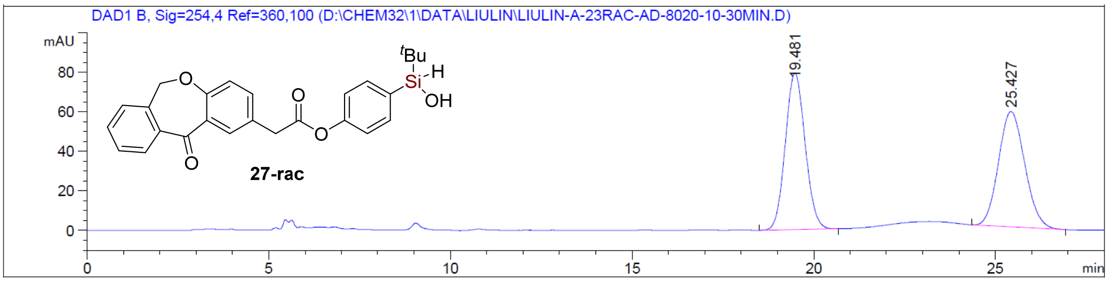
Totals : 1.49848e4 957.70462



Signal 3: DAD1 C, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.726	VV R	0.2485	1.56579e4	990.07709	95.7652
2	10.074	VV R	0.2310	692.40930	43.18921	4.2348

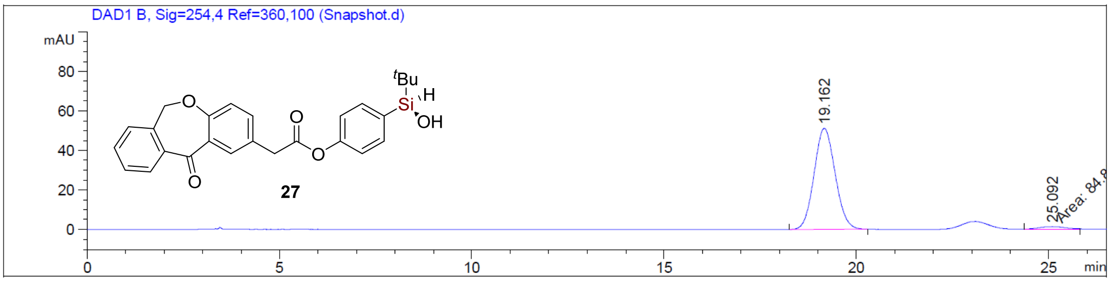
Totals : 1.63503e4 1033.26630



Signal 2: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.481	BB	0.5923	3002.62256	79.19407	50.5418
2	25.427	BB	0.7673	2938.25122	58.36754	49.4582

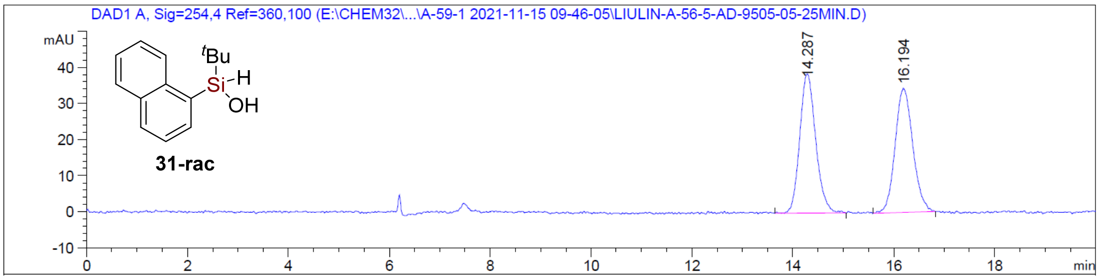
Totals : 5940.87378 137.56161



Signal 2: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.162	BB	0.5981	1945.62134	51.11383	95.8188
2	25.092	MM	0.8939	84.89960	1.58303	4.1812

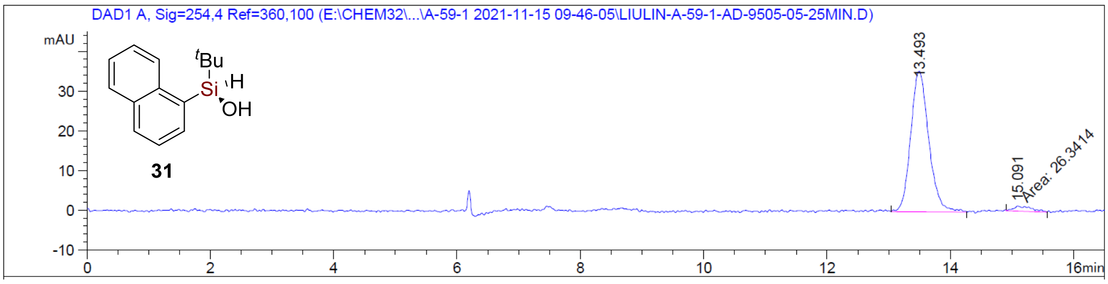
Totals : 2030.52094 52.69686



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.287	VV R	0.3197	853.03021	38.62123	50.2855
2	16.194	VB R	0.3014	843.34314	34.47982	49.7145

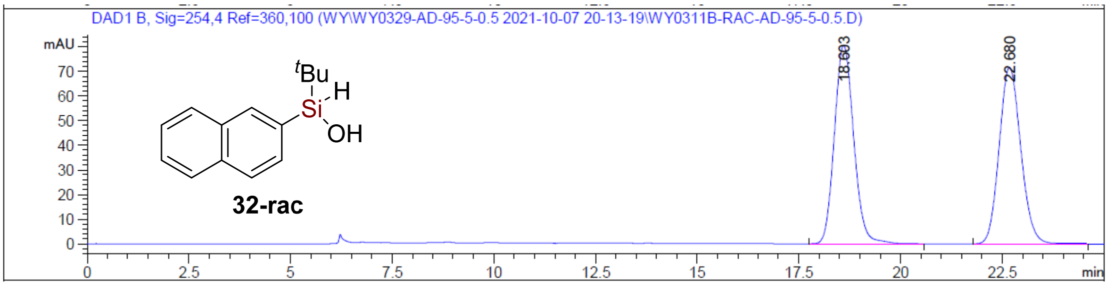
Totals : 1696.37335 73.10105



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.493	VV R	0.3052	719.55383	35.38477	96.4685
2	15.091	MM	0.3337	26.34145	1.31556	3.5315

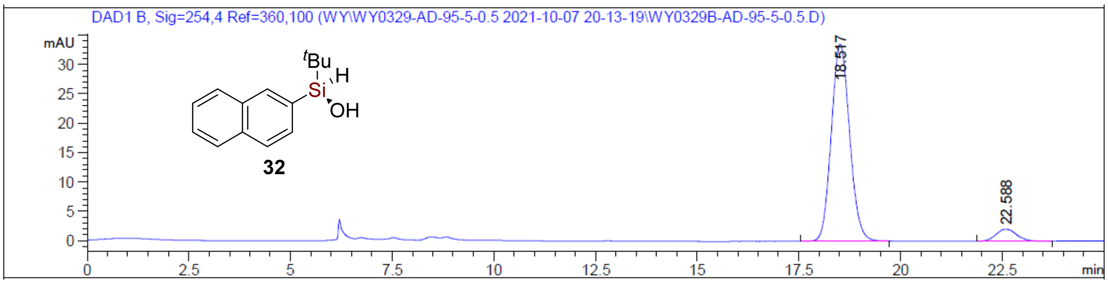
Totals : 745.89528 36.70032



Signal 2: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.603	BB	0.5179	2664.50879	80.56169	50.1919
2	22.680	BB	0.5703	2644.13232	71.69299	49.8081

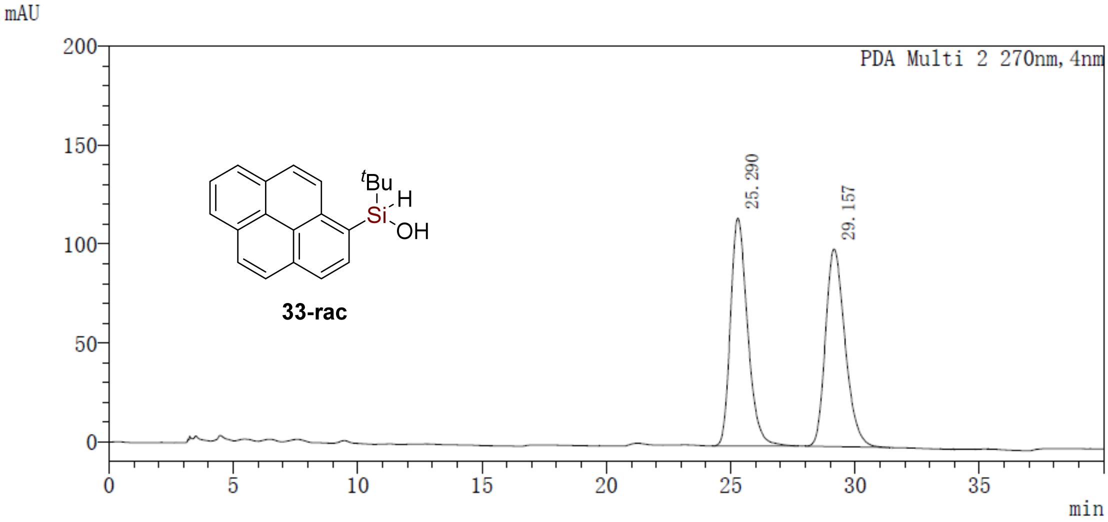
Totals : 5308.64111 152.25468



Signal 2: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	18.517	BB	0.4866	1048.37610	33.54225	93.4389
2	22.588	BB	0.4578	73.61546	2.08580	6.5611

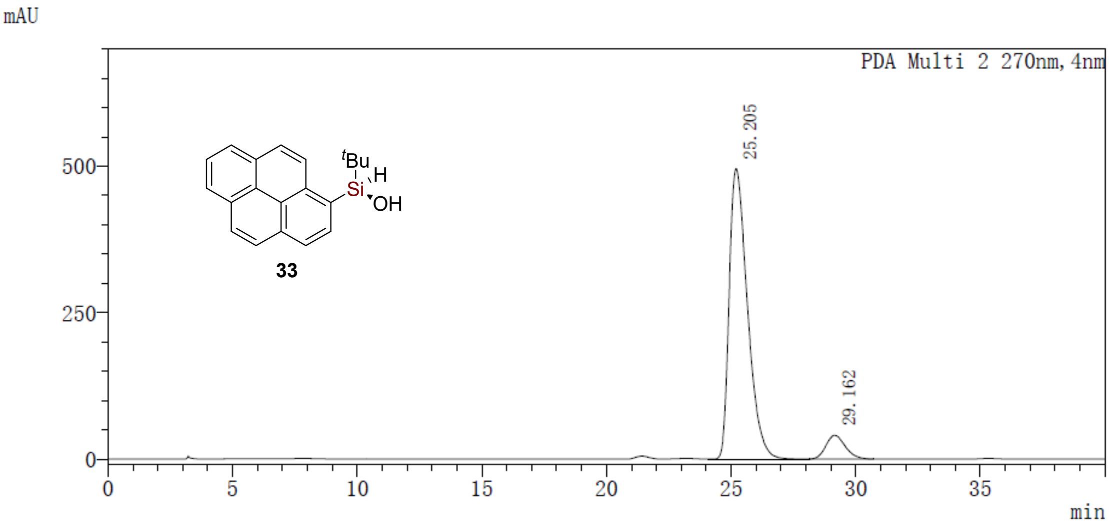
Totals : 1121.99155 35.62805



Peak Table

PDA Ch2 270nm

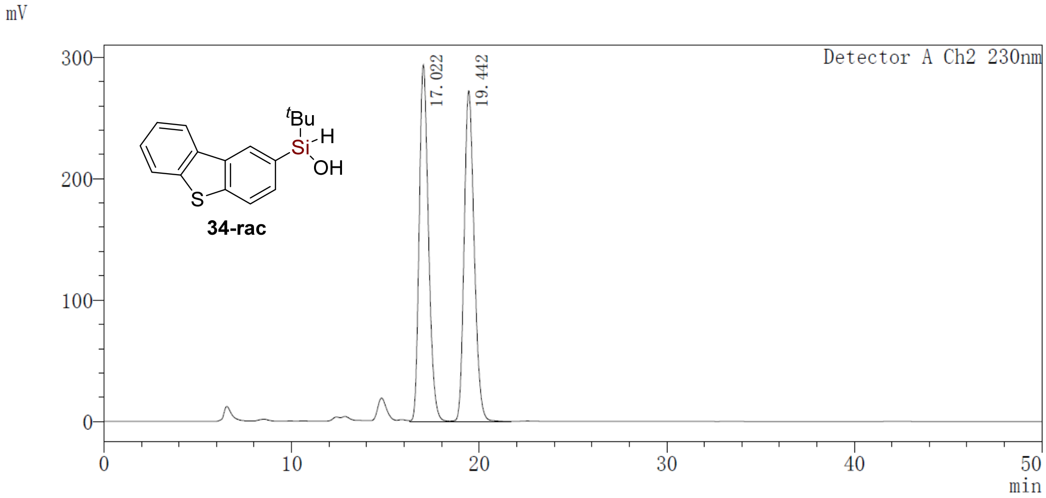
Peak#	Ret. Time	Area	Area%
1	25.290	5499466	50.107
2	29.157	5476040	49.893



Peak Table

PDA Ch2 270nm

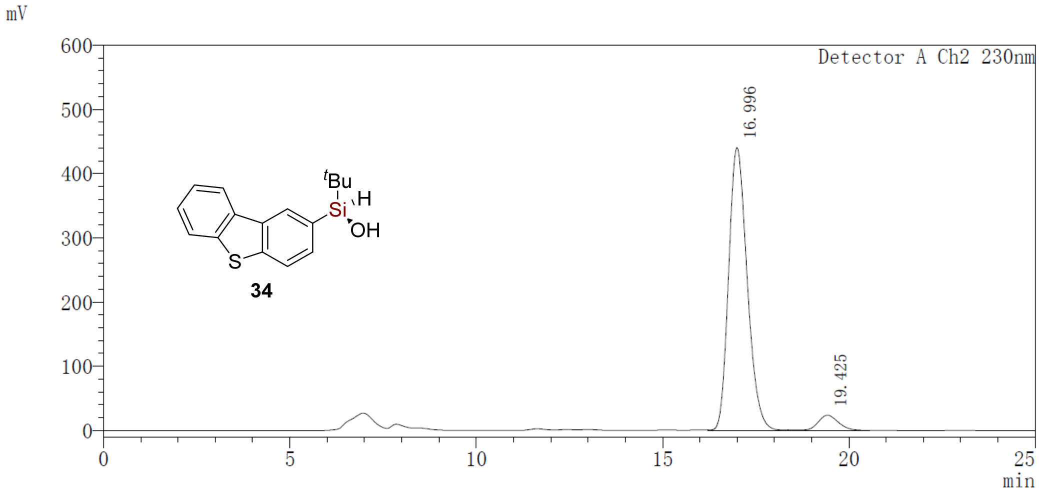
Peak#	Ret. Time	Area	Area%
1	25.205	25249043	91.983
2	29.162	2200538	8.017



Peak Table

Detector A Ch2 230nm

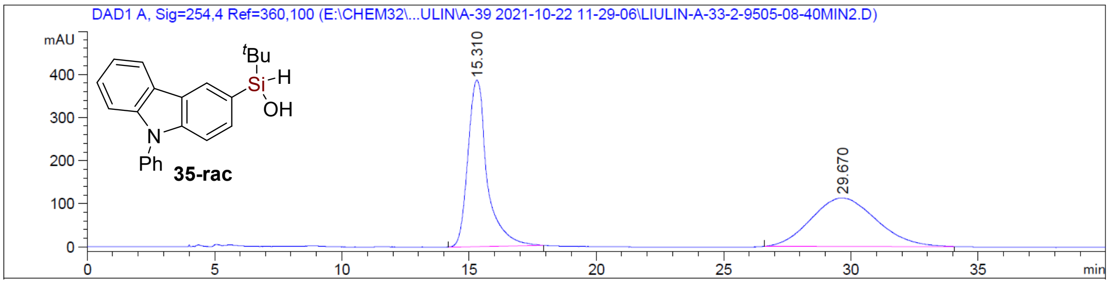
Peak#	Ret. Time	Area	Area%
1	17.022	10089100	49.927
2	19.442	10118423	50.073



Peak Table

Detector A Ch2 230nm

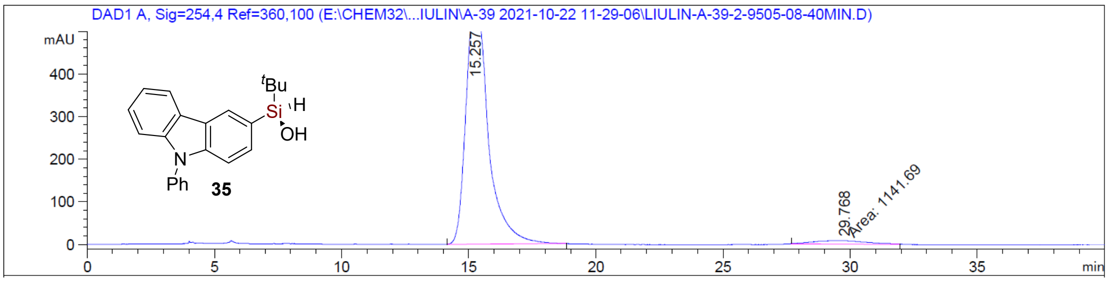
Peak#	Ret. Time	Area	Area%
1	16.996	15259452	94.551
2	19.425	879457	5.449



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.310	BV R	0.7695	2.02188e4	385.74930	50.2725
2	29.670	BV R	2.0905	1.99996e4	112.39199	49.7275

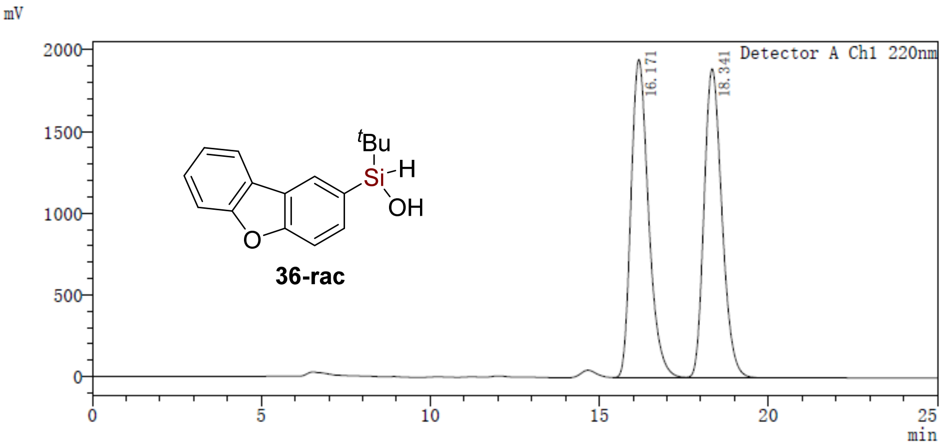
Totals : 4.02184e4 498.14129



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.257	BB	0.8350	3.46937e4	577.44342	96.8141
2	29.768	MM	2.4289	1141.68665	7.83421	3.1859

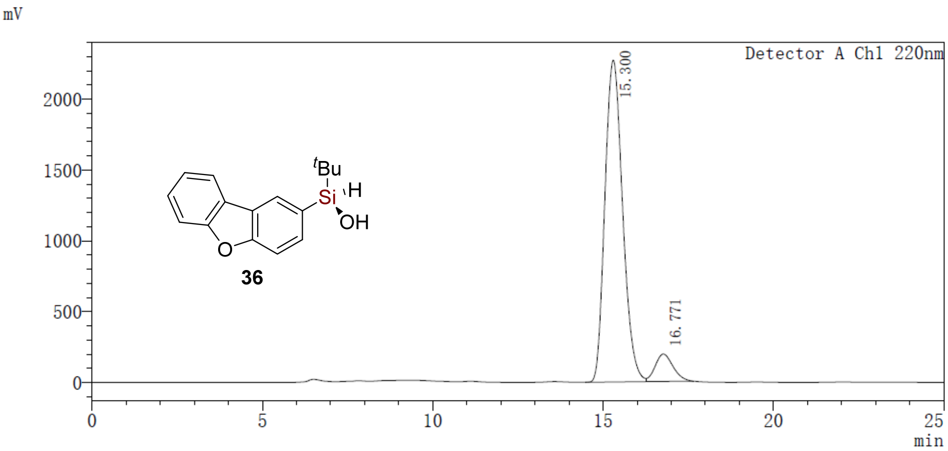
Totals : 3.58354e4 585.27763



Peak Table

Detector A Ch1 220nm

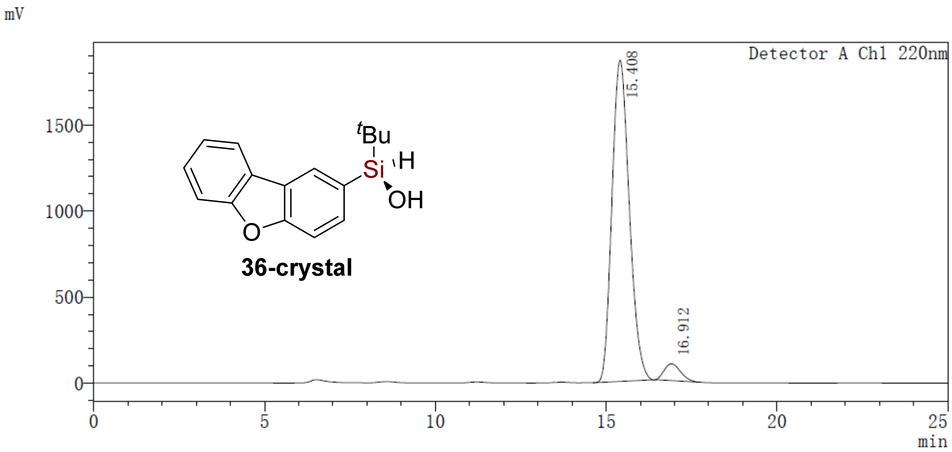
Peak#	Ret. Time	Area	Area%
1	16.171	70331878	50.284
2	18.341	69536846	49.716



Peak Table

Detector A Ch1 220nm

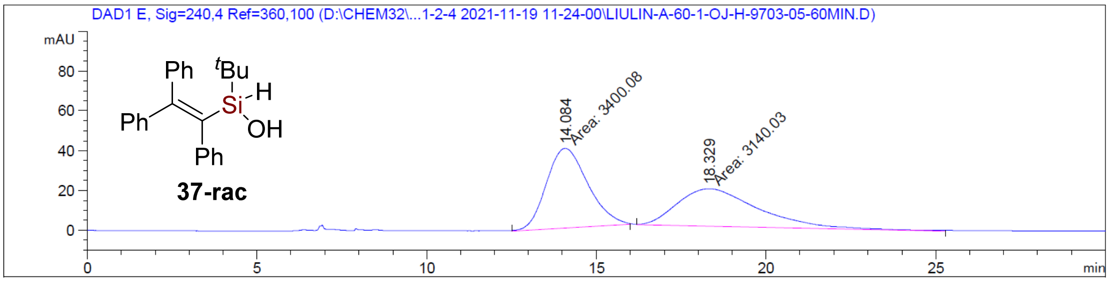
Peak#	Ret. Time	Area	Area%
1	15.300	82250171	92.040
2	16.771	7112884	7.960



Peak Table

Detector A Ch1 220nm

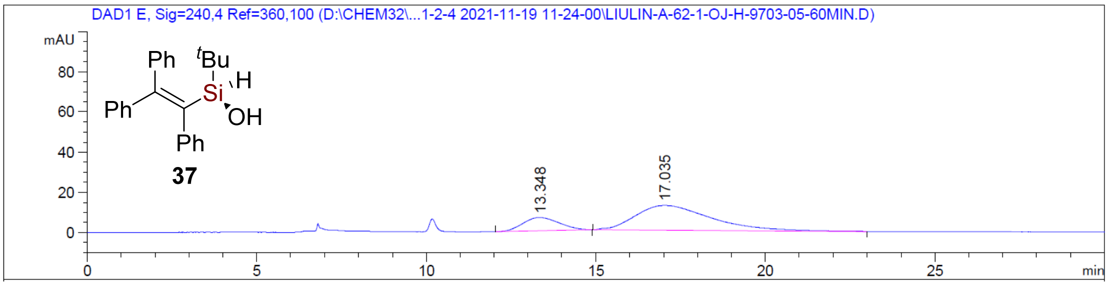
Peak#	Ret. Time	Area	Area%
1	15.408	66055399	95.258
2	16.912	3288420	4.742



Signal 5: DAD1 E, Sig=240,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.084	MM	1.4169	3400.07983	39.99426	51.9881
2	18.329	MM	2.7775	3140.03149	18.84240	48.0119

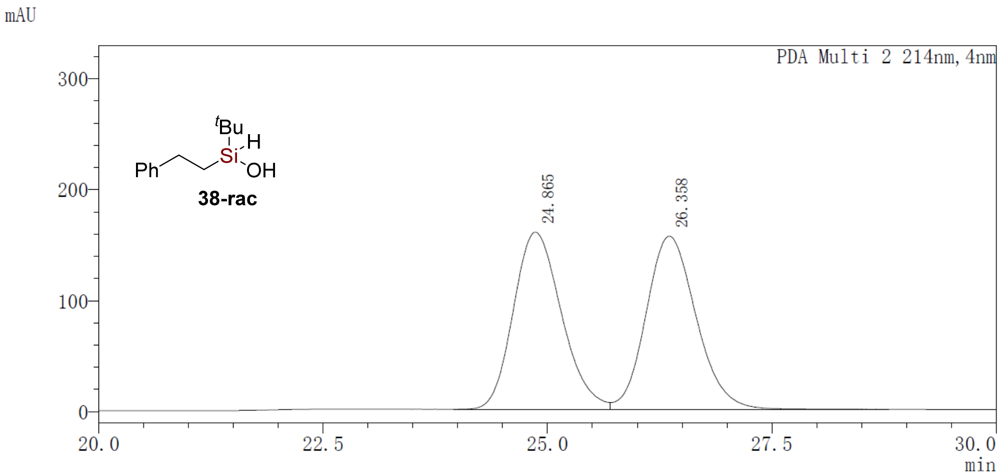
Totals : 6540.11133 58.83666



Signal 5: DAD1 E, Sig=240,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.348	BB	0.8918	497.86670	6.67780	20.4821
2	17.035	BB	1.8271	1932.86829	12.39635	79.5179

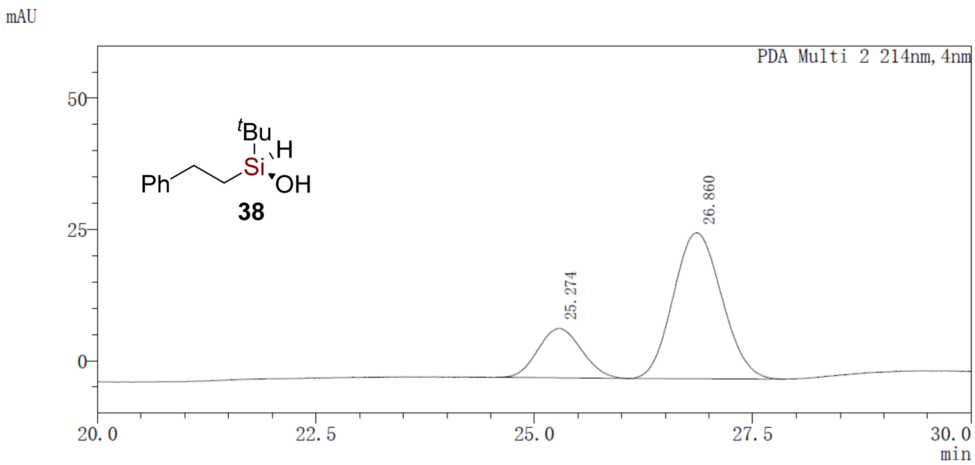
Totals : 2430.73499 19.07416



Peak Table

PDA Ch2 214nm

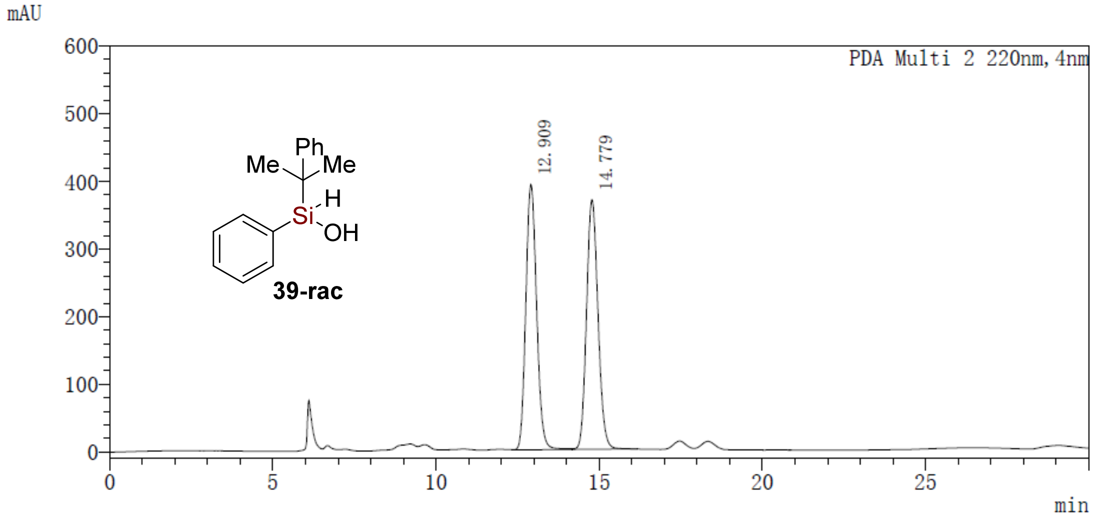
Peak#	Ret. Time	Area	Area%
1	24.865	5963418	49.615
2	26.358	6055992	50.385



Peak Table

PDA Ch2 214nm

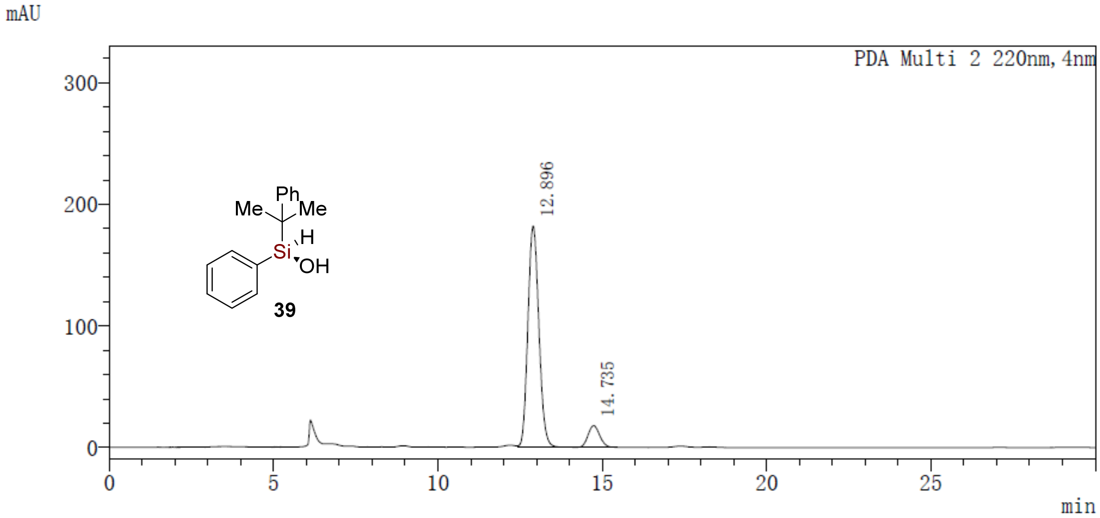
Peak#	Ret. Time	Area	Area%
1	25.274	327503	23.358
2	26.860	1074593	76.642



Peak Table

PDA Ch2 220nm

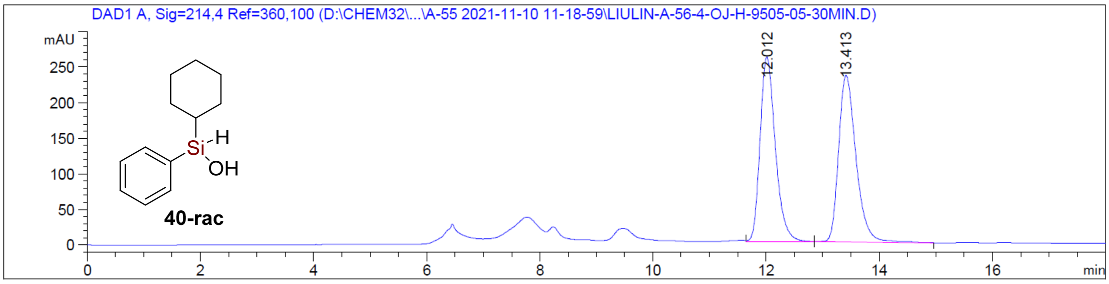
Peak#	Ret. Time	Area	Area%
1	12.909	9040376	49.995
2	14.779	9042323	50.005



Peak Table

PDA Ch2 220nm

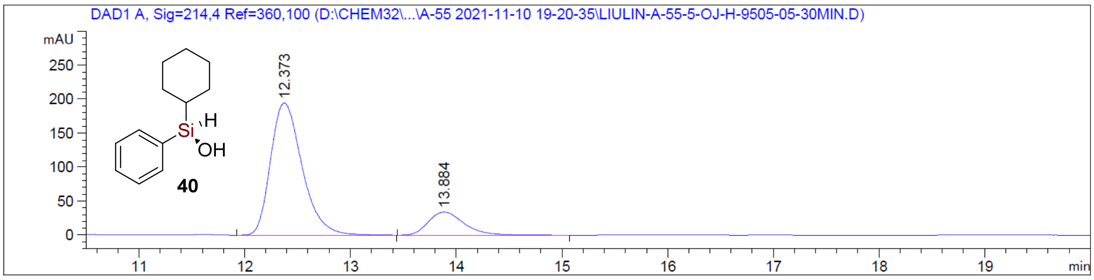
Peak#	Ret. Time	Area	Area%
1	12.896	4242208	90.549
2	14.735	442779	9.451



Signal 1: DAD1 A, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.012	VB	0.2869	4855.69336	258.76569	49.3849
2	13.413	BB	0.3264	4976.64307	233.70210	50.6151

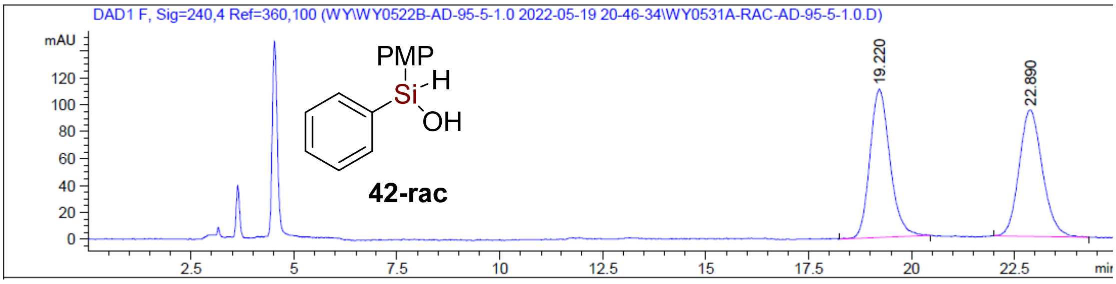
Totals : 9832.33643 492.46779



Signal 1: DAD1 A, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	11.970	BB	0.3138	4005.60498	198.17380	83.4967
2	13.394	BB	0.3676	791.71826	33.50994	16.5033

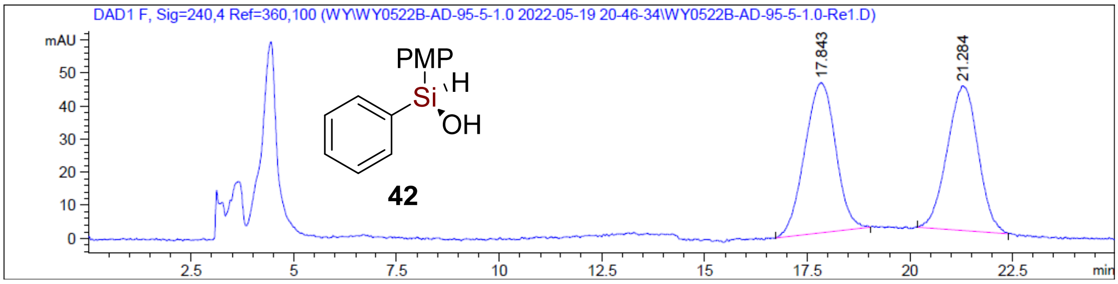
Totals : 4797.32324 231.68373



Signal 6: DAD1 F, Sig=240,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	19.220	VV R	0.4928	3727.48242	110.15948	50.0627
2	22.890	BV R	0.5372	3718.14185	94.06375	49.9373

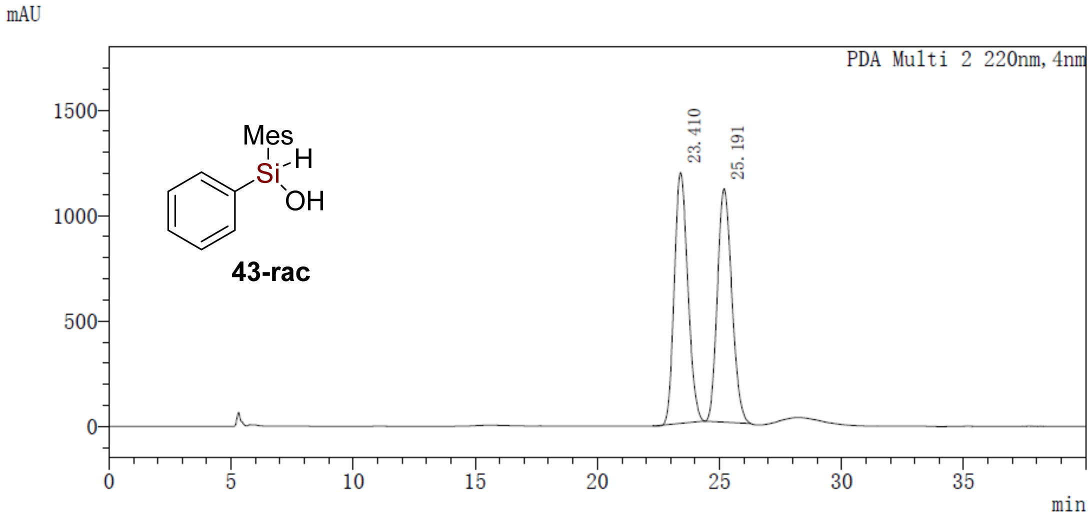
Totals : 7445.62427 204.22323



Signal 6: DAD1 F, Sig=240,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	17.843	BV R	0.6299	2383.03320	45.43306	51.0503
2	21.284	VV R	0.6238	2284.97241	43.71924	48.9497

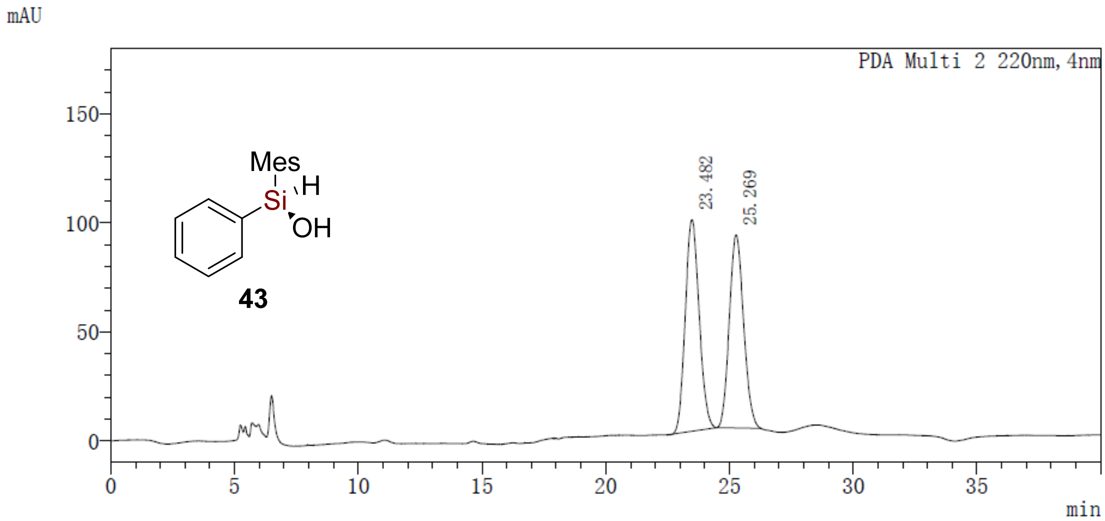
Totals : 4668.00562 89.15230



Peak Table

PDA Ch2 220nm

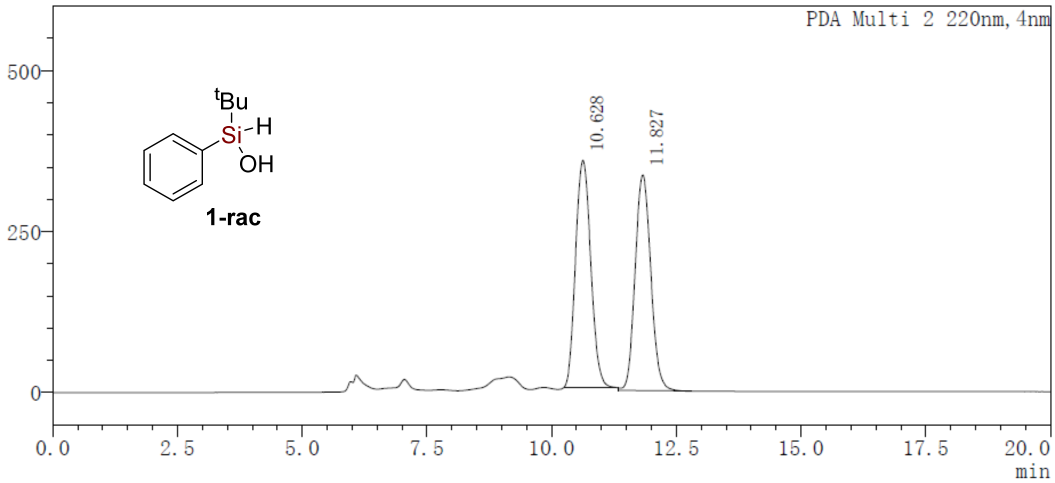
Peak#	Ret. Time	Area	Area%
1	23.410	45749429	50.096
2	25.191	45574871	49.904



Peak Table

PDA Ch2 220nm

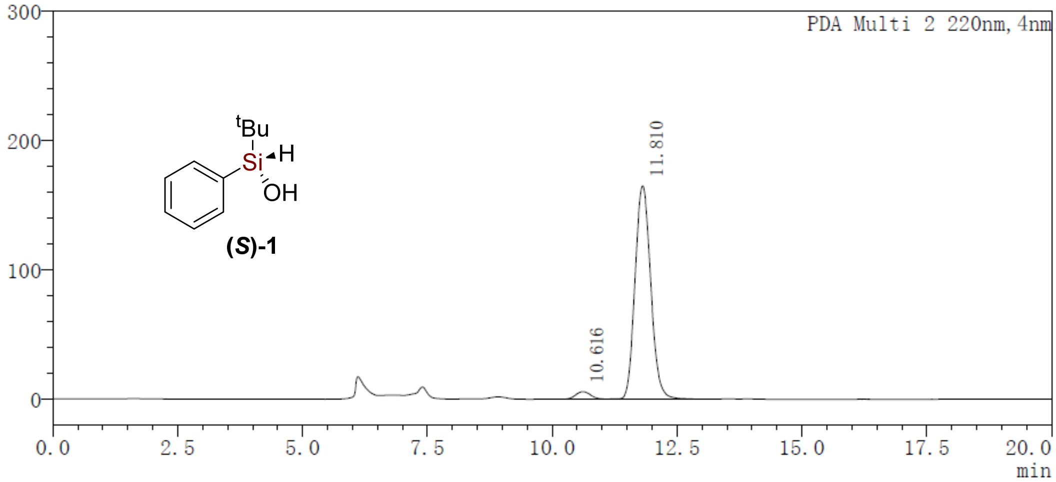
Peak#	Ret. Time	Area	Area%
1	23.482	3789588	51.587
2	25.269	3556393	48.413



Peak Table

PDA Ch2 220nm

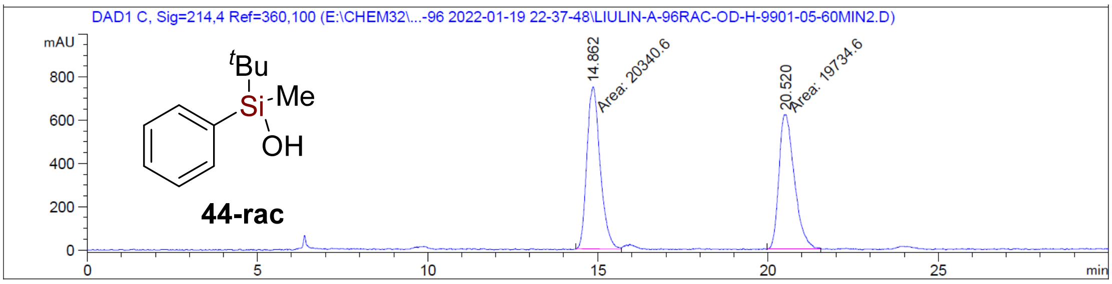
Peak#	Ret. Time	Area	Area%
1	10.628	7462966	50.408
2	11.827	7342025	49.592



Peak Table

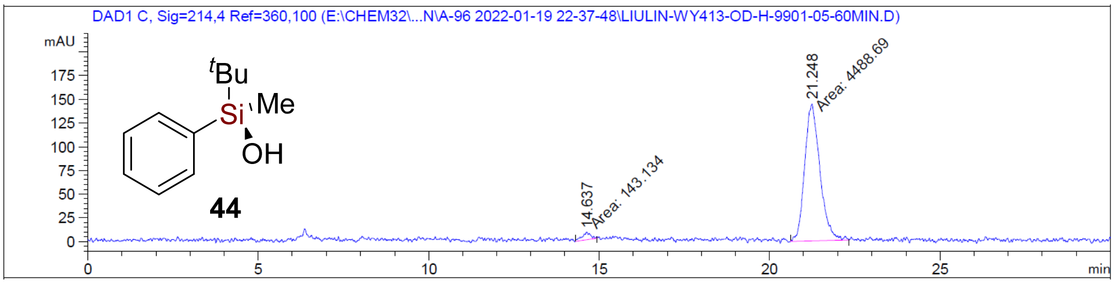
PDA Ch2 220nm

Peak#	Ret. Time	Area	Area%
1	10.616	118657	3.176
2	11.810	3617174	96.824



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.862	MM	0.4523	2.03406e4	749.55762	50.7562
2	20.520	MM	0.5283	1.97346e4	622.59058	49.2438

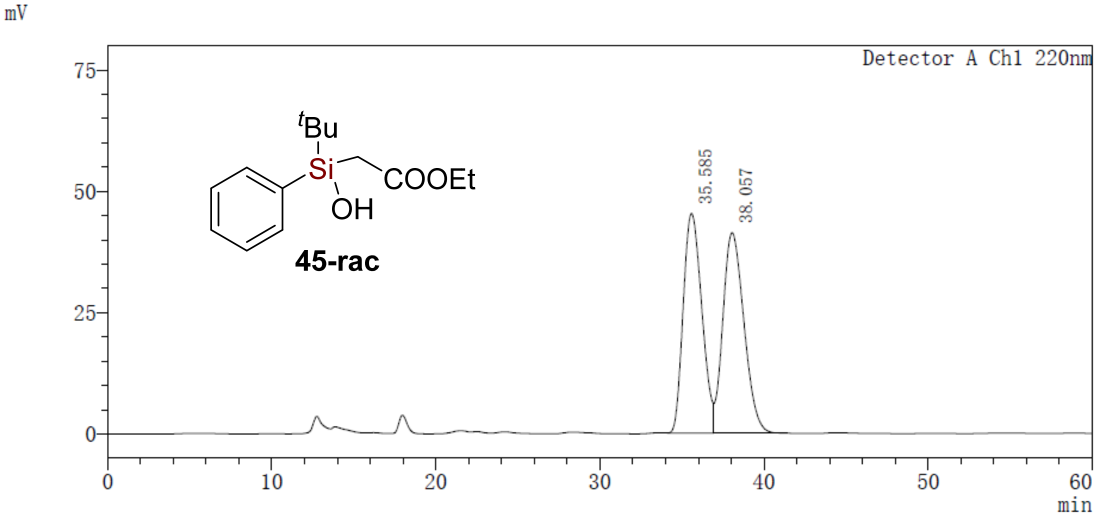
Totals : 4.00752e4 1372.14819



Signal 3: DAD1 C, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.637	MM	0.2879	143.13380	8.28679	3.0902
2	21.248	MM	0.5173	4488.68994	144.60741	96.9098

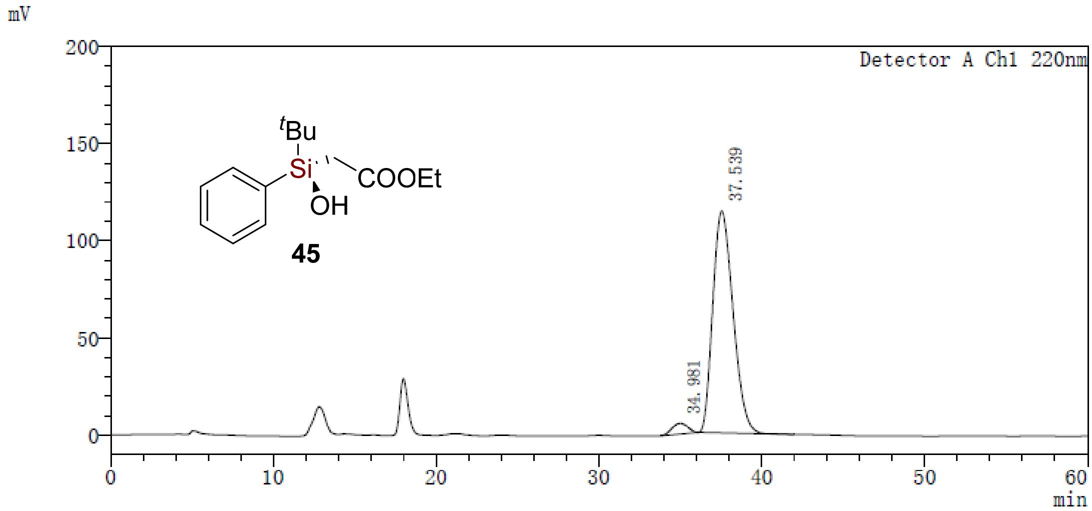
Totals : 4631.82375 152.89420



Peak Table

Detector A Ch1 220nm

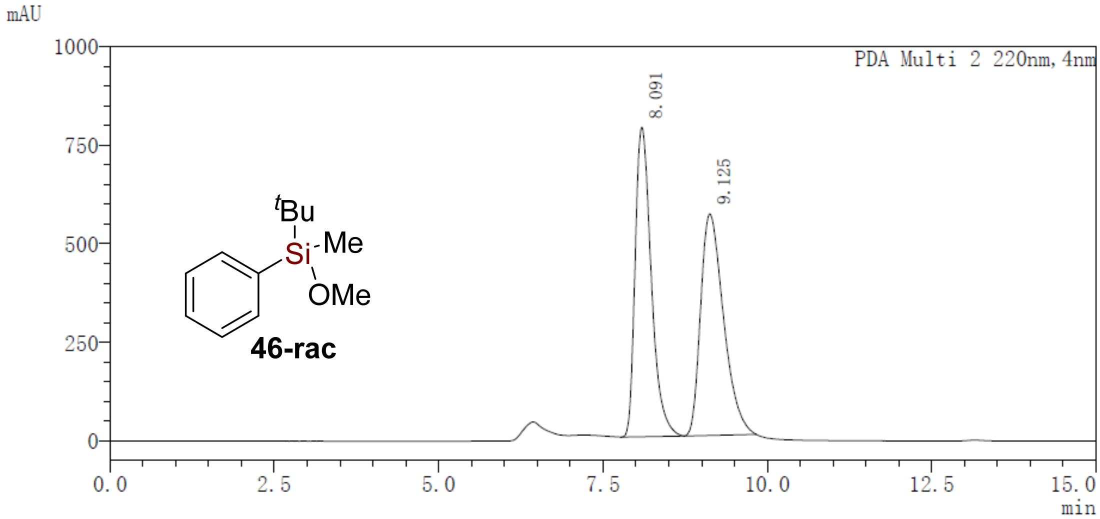
Peak#	Ret. Time	Area	Area%
1	35.585	3565850	49.074
2	38.057	3700396	50.926



Peak Table

Detector A Ch1 220nm

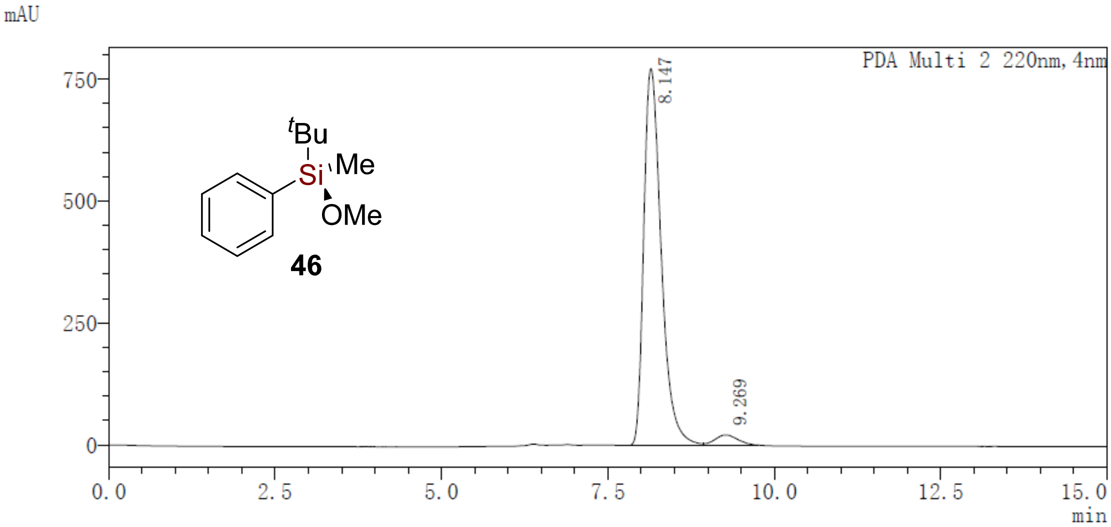
Peak#	Ret. Time	Area	Area%
1	34.981	373886	3.614
2	37.539	9971935	96.386



Peak Table

PDA Ch2 220nm

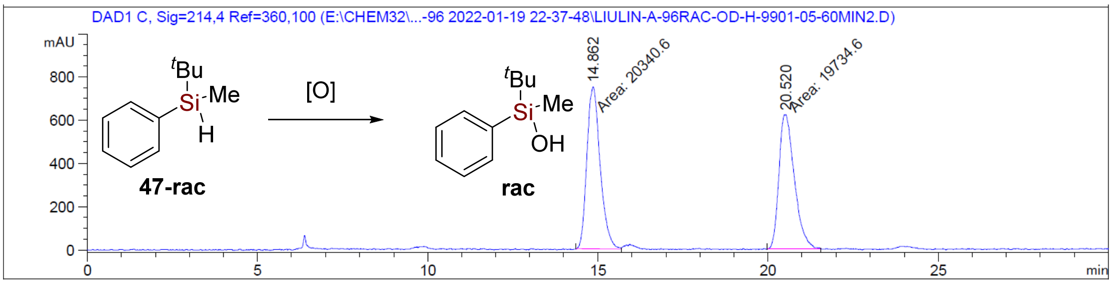
Peak#	Ret. Time	Area	Area%
1	8.091	13369164	49.445
2	9.125	13669432	50.555



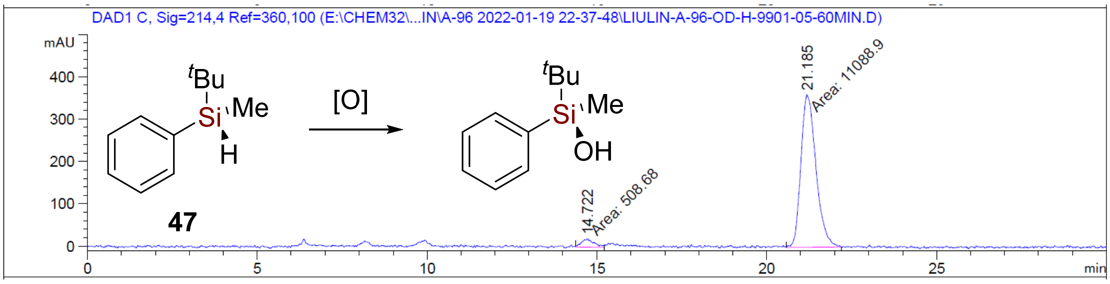
Peak Table

PDA Ch2 220nm

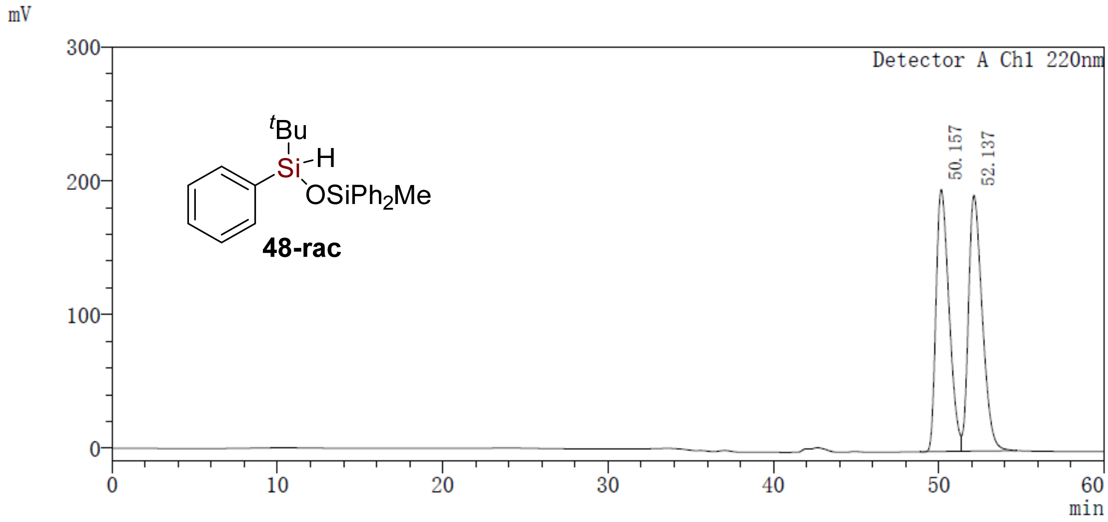
Peak#	Ret. Time	Area	Area%
1	8.147	14095749	96.490
2	9.269	512721	3.510



Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.862	MM	0.4523	2.03406e4	749.55762	50.7562
2	20.520	MM	0.5283	1.97346e4	622.59058	49.2438
Totals :				4.00752e4	1372.14819	



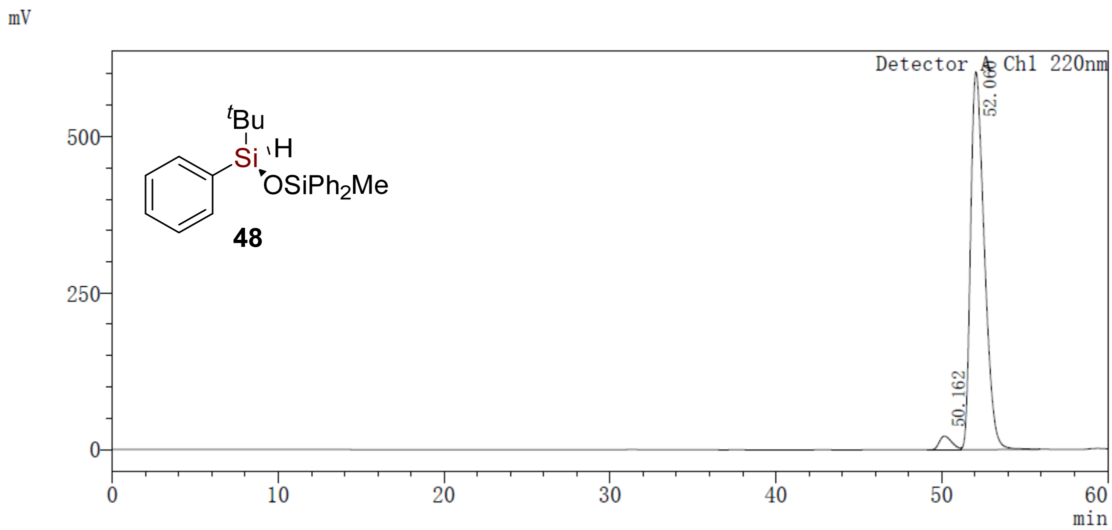
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.722	MM	0.4231	508.68011	20.03715	4.3861
2	21.185	MM	0.5135	1.10889e4	359.93124	95.6139
Totals :				1.15976e4	379.96839	



Peak Table

Detector A Ch1 220nm

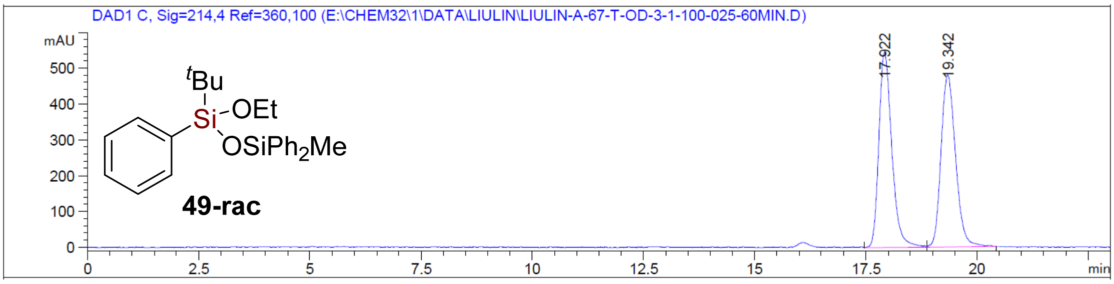
Peak#	Ret. Time	Area	Area%
1	50.157	10709897	49.034
2	52.137	11131772	50.966



Peak Table

Detector A Ch1 220nm

Peak#	Ret. Time	Area	Area%
1	50.162	1143117	3.181
2	52.060	34794685	96.819

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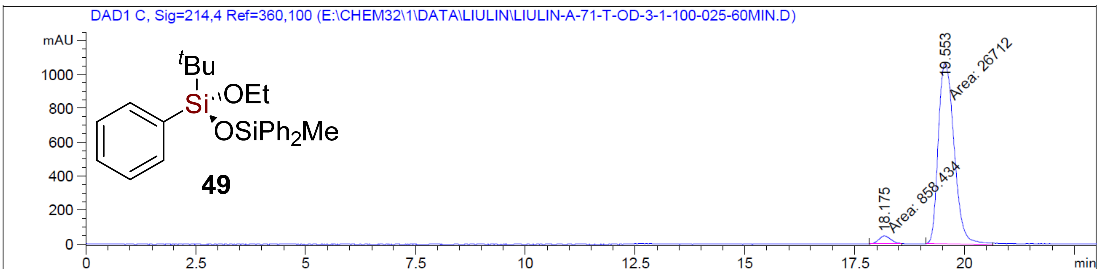
Signal 3: DAD1 C, Sig=214,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1  17.922 BV R  0.3041 1.10293e4  544.53638  50.2963
   2  19.342 VV R  0.3385 1.08993e4  480.14175  49.7037

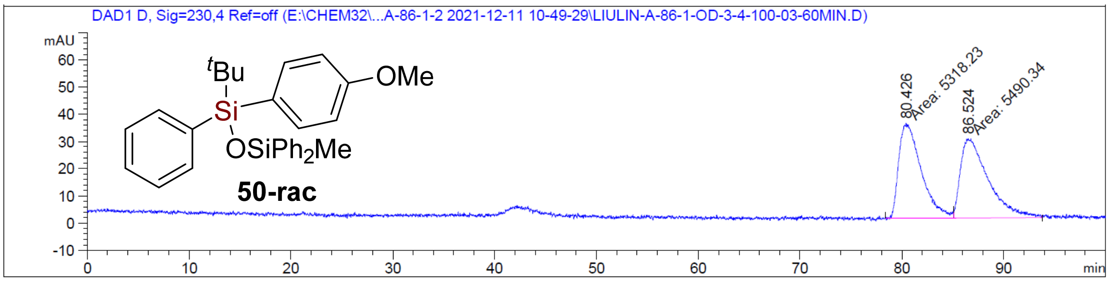
Totals :                  2.19286e4 1024.67813
```




```
Signal 3: DAD1 C, Sig=214,4 Ref=360,100

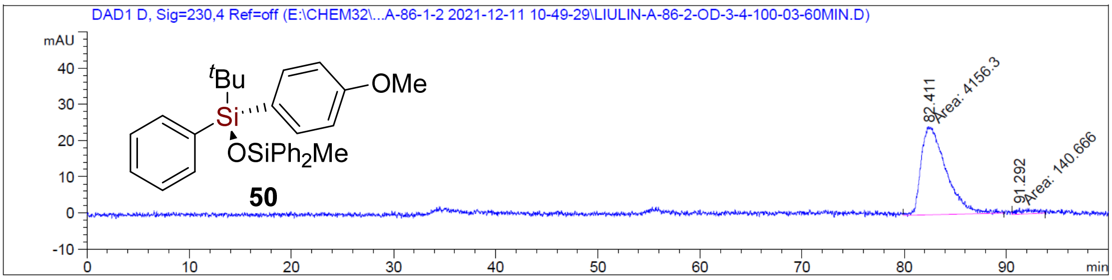
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]        %
----|-------|----|-------|----------|----------|--------|
   1  18.175 MM    0.3125  858.43420   45.78785   3.1136
   2  19.553 MM    0.4182 2.67120e4 1064.52698  96.8864

Totals :                  2.75704e4 1110.31483
```



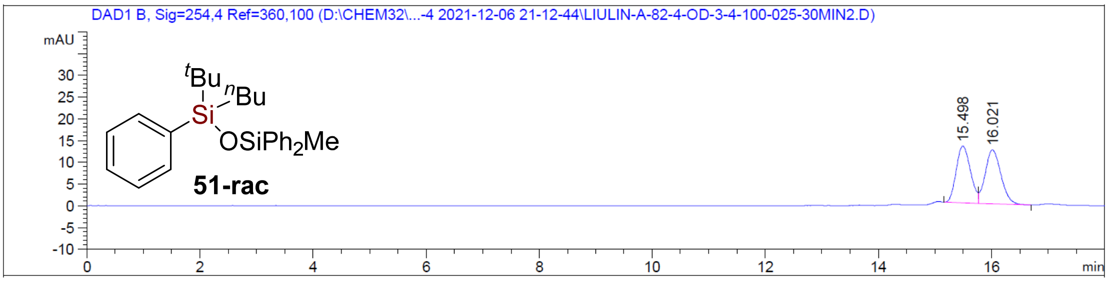
Signal 4: DAD1 D, Sig=230,4 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	80.426	MF	2.5399	5318.22852	34.89820	49.2038
2	86.524	FM	3.1339	5490.34375	29.19869	50.7962



Signal 4: DAD1 D, Sig=230,4 Ref=off

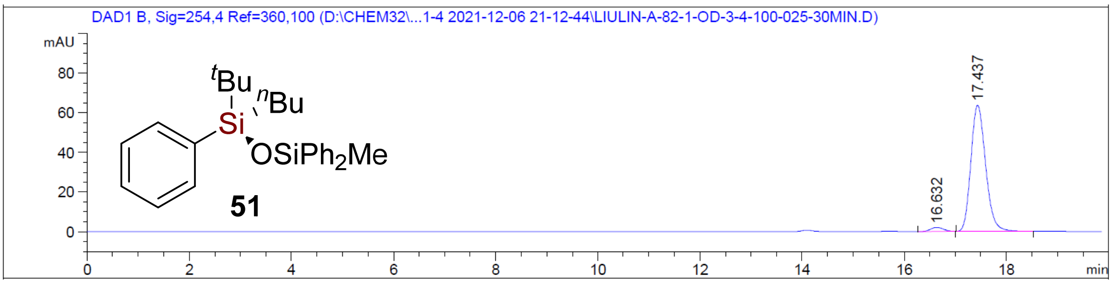
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	82.411	MM	2.8362	4156.30078	24.42392	96.7264
2	91.292	MM	1.3466	140.66612	1.74106	3.2736
Totals :				4296.96690	26.16498	



Signal 2: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	15.498	BV	0.2724	229.23476	13.08289	48.7636
2	16.021	VB	0.3021	240.85896	12.42871	51.2364

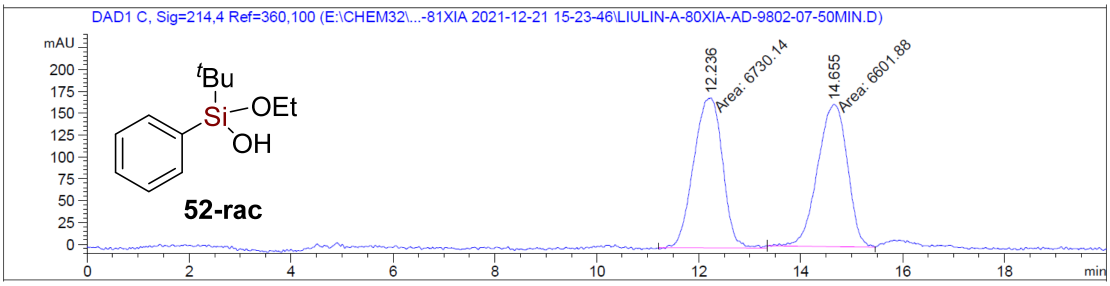
Totals : 470.09372 25.51160



Signal 2: DAD1 B, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	16.632	BB	0.2468	37.59529	2.10066	2.8526
2	17.437	BB	0.3126	1280.32446	63.68105	97.1474

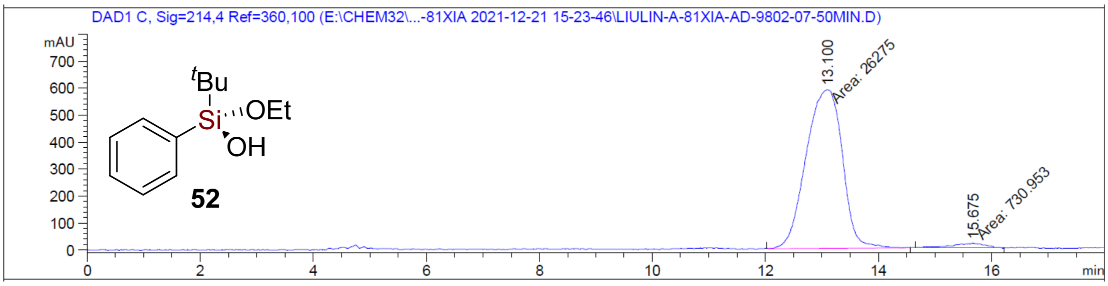
Totals : 1317.91975 65.78171



Signal 3: DAD1 C, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.236	MF	0.6541	6730.13965	171.49753	50.4810
2	14.655	MM	0.6756	6601.87598	162.86983	49.5190

Totals : 1.33320e4 334.36736



Signal 3: DAD1 C, Sig=214,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.100	MM	0.7447	2.62750e4	588.01056	97.2934
2	15.675	MM	0.7118	730.95349	17.11424	2.7066

Totals : 2.70060e4 605.12480