Supporting Information

Radical 1,2-aryl migration in *α*, *α*-diaryl allylic alcohols toward *β*-silyl ketones

*Haibo Peng, Jin-Tao Yu, Yan Jiang and Jiang Cheng**

School of Petrochemical Engineering, Jiangsu Province Key Laboratory of Fine Petrochemical Engineering, Changzhou University, Changzhou 213164, P. R. China

Email: jiangcheng@cczu.edu.cn

Table of Contents

1 General experimental detail

Chemicals were used as received without special purification unless stated otherwise. ^{1}H and ^{13}C NMR spectra were recorded at ambient temperature on a 400 MHz NMR spectrometer (100 MHz for ^{13}C NMR). NMR results were reported in δ units, parts per million (ppm), and were referenced to $CDCl_3$ (δ 7.26 or 77.0 ppm) as the internal standard. The coupling constants J are given in Hz. IR spectra were recorded on a spectrometer using KBr discs.

General Procedure:

A sealed tube was charged with α, α-diaryl allylic alcohol (0.2 mmol), silane (1.4 mmol), DTBP (0.8 mmol), Cu_2O (0.01 mmol), Et_3N (0.25 equiv), benzene (1.5 mL). The mixture was purged with nitrogen and kept stirring under nitrogen at 110 ^{o}C for 15 h. The mixture was concentrated in vacuum and the residue was purified by preparative TLC on GF254 (petroleum/ethyl acetate) to afford the desired product.

2 Screening the Conditions

Table 2. Screening the Optimal Conditions.[a]

1a **2a** **3aa**

Entry	Catalyst (mol%)	Base (equiv)	Peroxide (equiv)	T (^{o}C)	Yield (%)[b]
1	Cu_2O (5.0)	Et_3N (0.25)	DTBP (4.0)	110	67
2	Cu_2O (15)	Et_3N (0.25)	DTBP (4.0)	110	77
3	Cu_2O (10)	Et_3N (0.25)	DTBP (3.0)	110	62
4	Cu_2O (10)	Et_3N (0.25)	DTBP (5.0)	110	76
5	Cu_2O (10)	Et_3N (0.15)	DTBP (4.0)	110	60
6	Cu_2O (10)	Et_3N (0.35)	DTBP (4.0)	110	64
7	Cu_2O (10)	Et_3N (0.25)	DTBP (4.0)	100	68
8	Cu_2O (10)	Et_3N (0.25)	DTBP (4.0)	120	75
9	Cu_2O (10)	Et_3N (0.25)	TBHP (4.0)	110	< 5
10	Cu_2O (10)	Et_3N (0.25)	BPO (4.0)	110	< 5

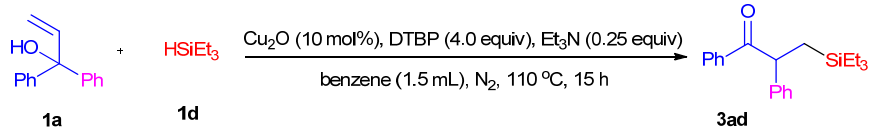
11	Cu_2O (10)	Et_3N (0.25)	$K_2S_2O_8$ (4.0)	110	< 5
12	Cu_2O (10)	Et_3N (0.25)	DDQ (4.0)	110	< 5

[a] Reaction conditions: **1a** (0.2 mmol), **2a** (1.4 mmol), Et_3N, Cu_2O, oxidant in benzene (1.5 mL) at 110 °C under N_2 for 15 h in sealed tube. [b] Isolated yields.

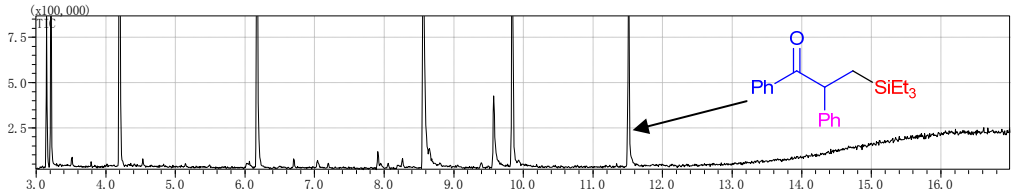
3 Mechanistic Experiments

3.1 Free radical capture experiments

General Procedure:



1a **1d** **3ad**



Residual time of 3ad: 11.511 min.

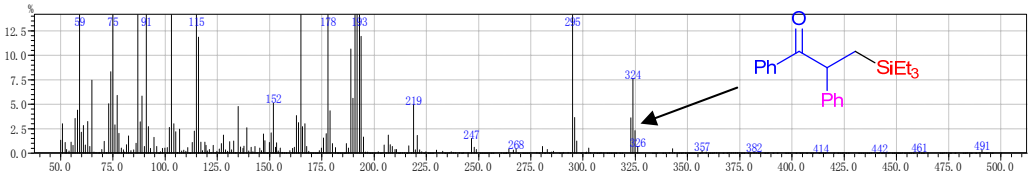


Figure 1

Add 2.0 equiv of TEMPO to the reaction mixture

1a **2** **3ad**, not detect

A sealed reaction tube was charged with **1a** (0.2 mmol), triethylsilane (1.4 mmol), DTBP (0.8 mmol), Cu_2O (0.01 mmol), Et_3N (0.25 equiv), TEMPO (2.0 equiv.), benzene (1.5 mL). The mixture was purged with nitrogen and kept stirring under nitrogen at 110 °C for 15 h. The reaction mixture was analyzed using GC-MS spectrometer, as shown in Figure S2.

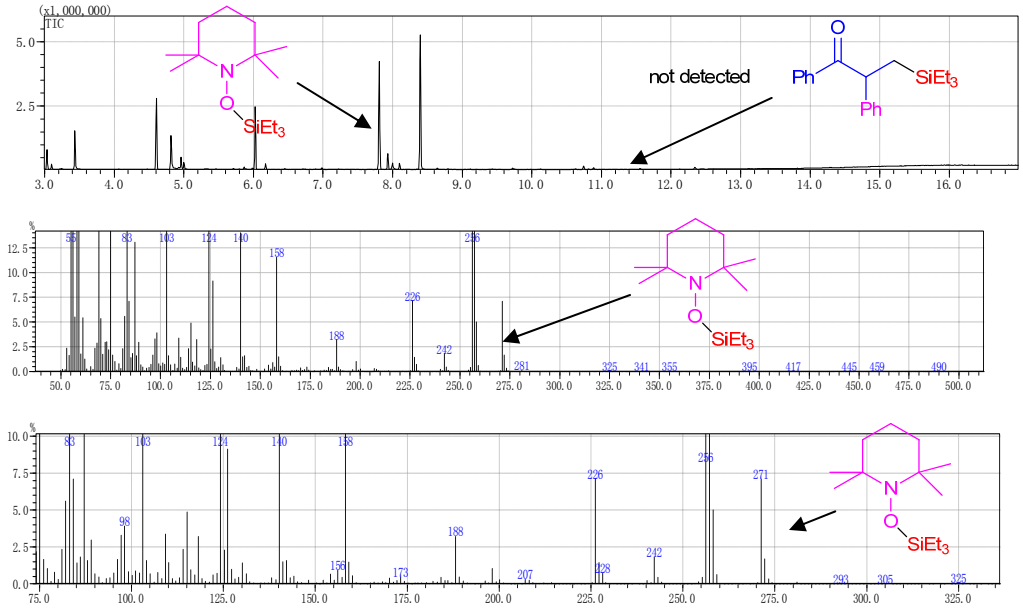
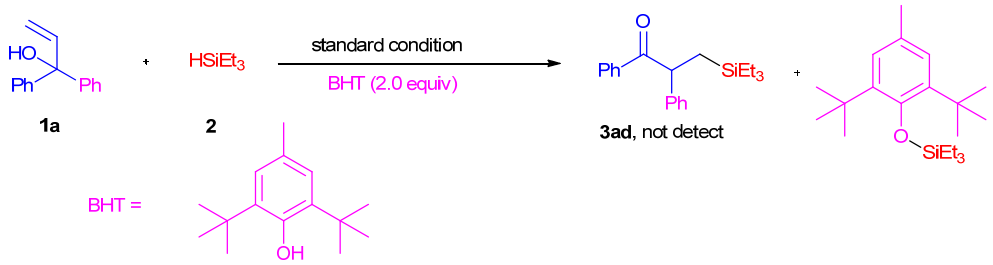


Figure S2

Add 2.0 equiv of BHT to the reaction mixture



A sealed reaction tube was charged with **1a** (0.2 mmol), triethylsilane (1.4 mmol), DTBP (0.8 mmol), Cu_2O (0.01 mmol), Et_3N (0.25 equiv), BHT (2.0 equiv), benzene (1.5 mL). The mixture was purged with nitrogen and kept stirring under nitrogen at 110 °C for 15 h. The reaction mixture was analyzed using GC-MS spectrometer, as shown in Figure S3.

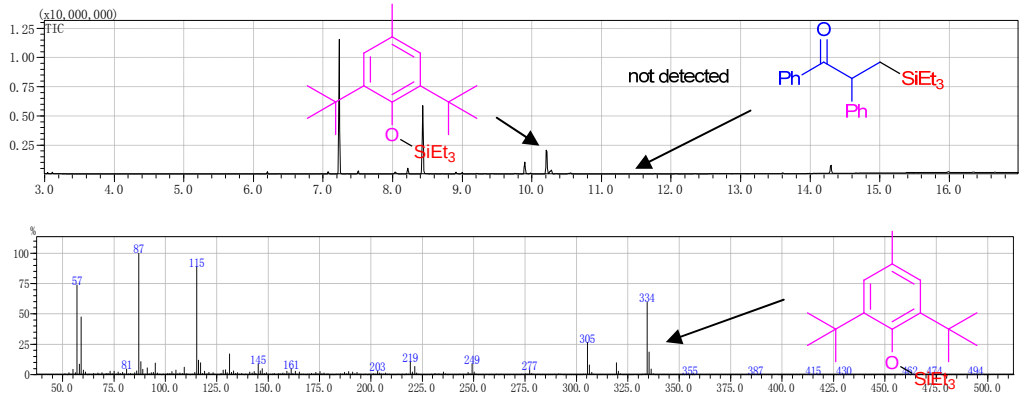


Figure S3

3.2 Competitive experiments

A sealed tube were charged with **1a**/ 1,1-bis(3-(trifluoromethyl)phenyl)prop-2-en-1-ol (1: 1, 0.2 mmol), **2a** (1.4 mmol), DTBP (0.8 mmol), Cu_2O (0.01 mmol), Et_3N (0.25 equiv), benzene (1.5 mL). The mixture was purged with nitrogen and kept stirring under nitrogen at 110 ^oC for 2 h. The mixture was concentrated in vacuum and the residue was purified by preparative TLC on GF254 (petroleum/ethyl acetate) to afford the desired product. The mixture was analyzed using ^1H NMR spectrometer. As shown in Figure S4, the ratio of **3ea** and **3aa** is nearly 1.05.

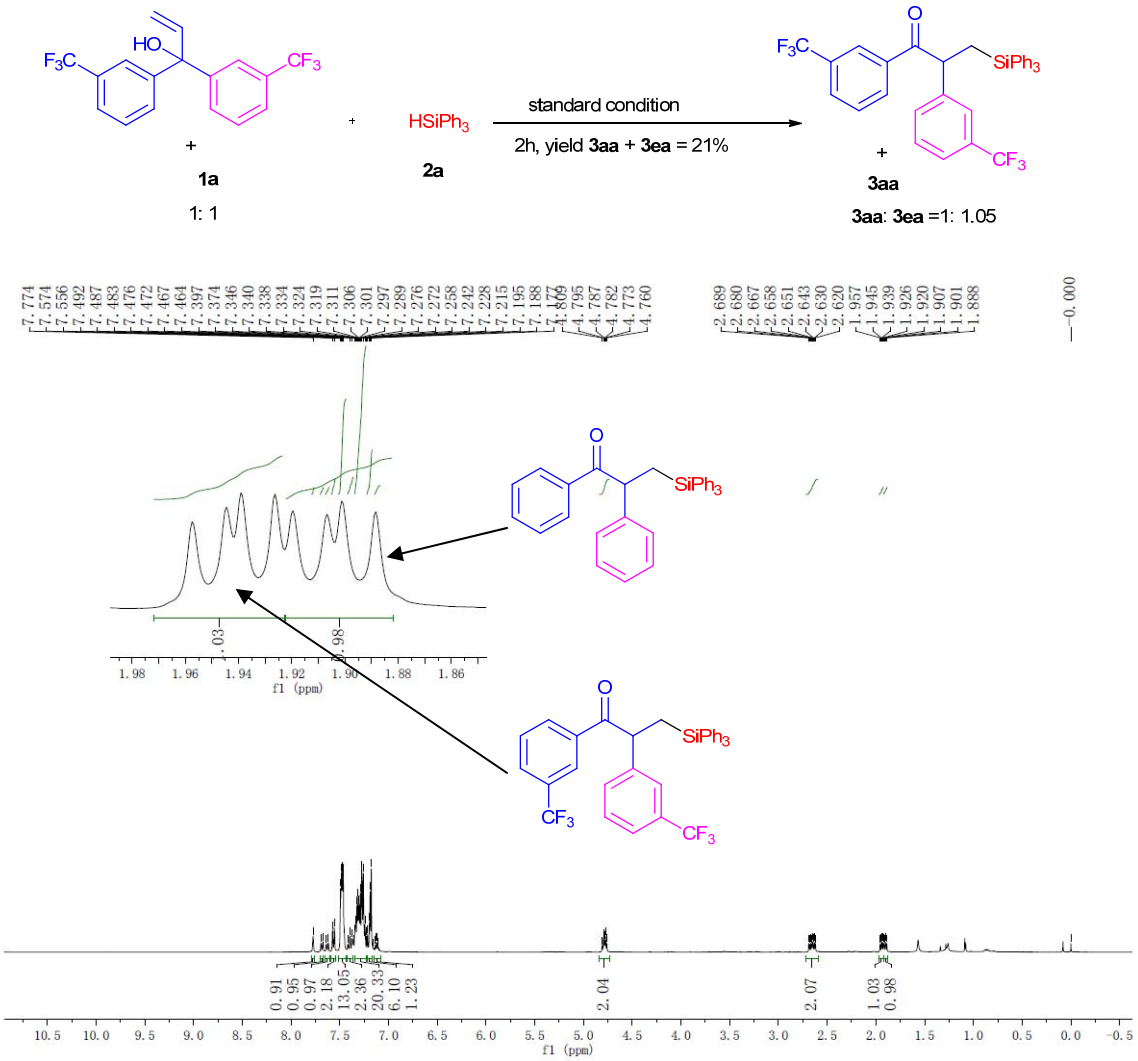


Figure S4

A sealed tube were charged with **1a**/ 1,1-di-*p*-tolylprop-2-en-1-ol (1: 1, 0.2 mmol), **2a** (1.4 mmol), DTBP (0.8 mmol), Cu_2O (0.01 mmol), Et_3N (0.25 equiv), benzene (1.5 mL). The mixture was purged with nitrogen and kept stirring under nitrogen at 110 ^oC for

2 h. The mixture was concentrated in vacuum and the residue was purified by preparative TLC on GF254 (petroleum/ethyl acetate) to afford the desired product. The mixture was analyzed using ^{1}H NMR spectrometer. As shown in Figure S5, the ratio of **3aa** and **3ba** is nearly 1.03.

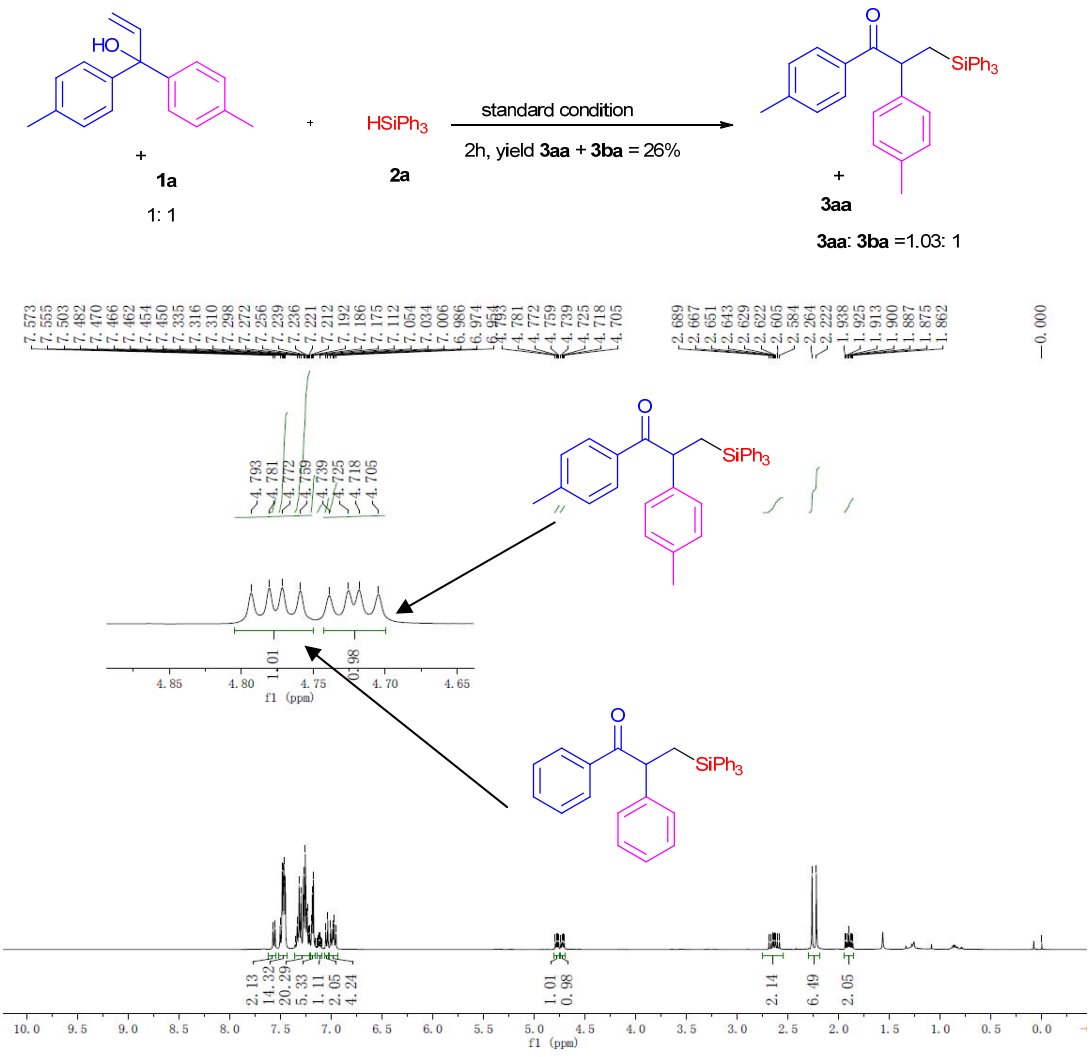
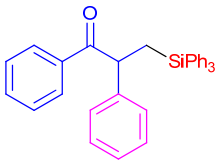


Figure S5

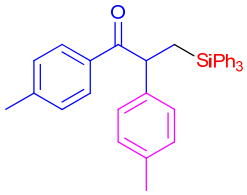
4 Characterization data for the products

1,2-diphenyl-3-(triphenylsilyl)propan-1-one (**3aa**):



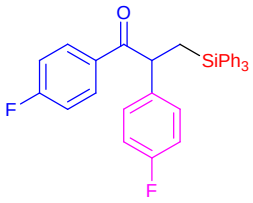
TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (73.0 mg, 78% yield) as a yellowish oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58-7.56 (m, 2H), 7.49-7.46 (m, 6H), 7.34-7.24 (m, 10H), 7.20-7.18 (m, 6H), 7.14-7.10 (m, 1H), 4.80-4.76 (m, 1H), 2.70-2.63 (m, 1H), 1.94-1.89 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 199.4, 141.8, 136.4, 135.7, 134.5, 132.3, 129.4, 128.9, 128.4, 128.0, 128.0, 127.8, 126.8, 49.1, 18.6. MS (EI): 468 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{33}H_{28}NaOSi$ $(M+Na)^+$ 491.1802, found 491.1808. IR (KBr) v 3068, 2926, 1682, 1597, 1492, 1447, 1428, 1332, 1257, 1223, 1176, 1110, 1028 cm^{-1}.

1,2-di-*p*-tolyl-3-(triphenylsilyl)propan-1-one (**3ba**):



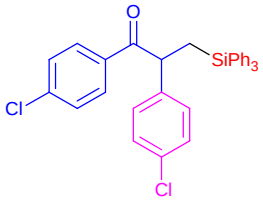
TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (73.4 mg, 74% yield) as a yellowish oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.51-7.45 (m, 8H), 7.32-7.29 (m, 3H), 7.26-7.23 (m, 6H), 7.06-7.04 (m, 2H), 7.00-6.96 (m, 4H), 4.73 (q, J = 5.2 Hz, 1H), 2.62 (dd, J_1 = 8.4 Hz, J_2 = 6.8 Hz, 1H), 2.25 (s, 3H), 2.21 (s, 3H), 1.89 (dd, J_1 = 5.2 Hz, J_2 = 10.0 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 199.1, 142.9, 139.0, 136.3, 135.7, 134.7, 134.0, 129.5, 129.3, 128.7, 128.6, 127.9, 127.7, 48.5, 21.5, 21.0, 18.5. MS (EI): 496 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{35}H_{32}NaOSi$ $(M+Na)^+$ 519.2115, found 519.2123. IR (KBr) v 3068, 2855, 1682, 1607, 1511, 1455, 1428, 1256, 1229, 1175, 1110, 1029 cm^{-1}.

1,2-bis(4-fluorophenyl)-3-(triphenylsilyl)propan-1-one (**3ca**)**:**



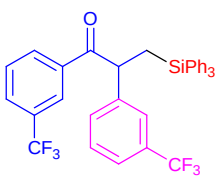
TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (71.6, mg, 71% yield) as a colorless oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.48-7.45 (m, 7H), 7.36-7.25 (m, 8H), 7.19-7.11 (m, 6H), 7.08-7.06 (m, 2H), 4.67 (q, J = 5.2 Hz, 1H), 2.61-2.55 (m, 1H), 1.90-1.85 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 198.0, 139.7, 139.0, 135.7, 135.4 (d, $J_{C\text{-}F}$ = 30.6 Hz), 134.2, 132.9, 132.7 (d, $J_{C\text{-}F}$ = 147.6 Hz), 129.5, 129.2 (d, $J_{C\text{-}F}$ = 23.1 Hz), 129.1 (d, $J_{C\text{-}F}$ = 131.1 Hz), 127.9, 127.5 (d, $J_{C\text{-}F}$ = 13.5 Hz), 48.5, 18.5. MS (EI): 504 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{33}H_{26}F_2NaOSi$ $(M+Na)^+$ 527.1613, found 527.1619. IR (KBr) v 3069, 2925, 1683, 1589, 1489, 1428, 1400, 1253, 1174, 1013 cm^{-1}.

1,2-bis(4-chlorophenyl)-3-(triphenylsilyl)propan-1-one (3da):



TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (60.0 mg, 56% yield) as a colorless oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.59-7.55 (M, 2H), 7.48-7.46 (m, 5H), 7.35-7.24 (m, 10H), 7.13-7.10 (m, 2H), 6.91-6.84 (m, 4H), 4.70 (q, J = 5.6 Hz, 1H), 2.58 (dd, J_1 = 8.4 Hz, J_2 = 6.8 Hz, 1H), 1.89 (dd, J_1 = 5.6 Hz, J_2 = 9.6 Hz, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.9, 135.7, 134.3, 131.0, 130.9, 129.5, 129.5, 129.4, 127.9, 115.9, 115.6, 115.3, 115.1, 48.2, 18.7. MS (EI): 536 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{33}H_{27}Cl_2OSi$ $(M+H)^+$ 537.1203, found 537.1202. IR (KBr) v 3069, 2923, 1683, 1597, 1428, 1229, 1155, 1110, 1014 cm^{-1}.

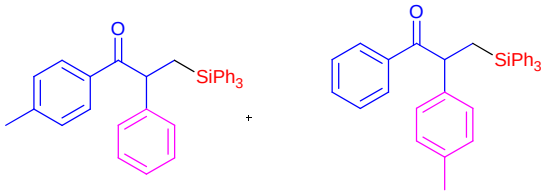
1,2-bis(3-(trifluoromethyl)phenyl)-3-(triphenylsilyl)propan-1-one (3ea):



TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (80.9 mg, 67% yield) as a

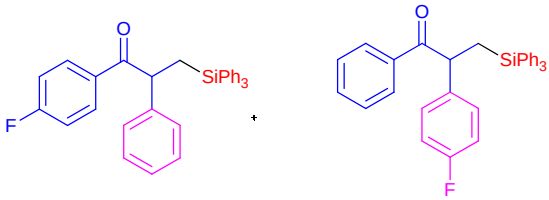
colorless oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.80 (s, 1H), 7.70 (d, J = 7.6 Hz, 1H), 7.62 (d, J = 7.6 Hz, 1H), 7.51-7.49 (m, 6H), 7.41-7.39 (m, 2H), 7.35-7.21 (m, 12H), 4.83-4.80 (m, 1H), 2.71-2.63 (m, 1H), 1.98-1.93 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.8, 141.9, 136.5, 135.7, 135.2, 133.9, 131.4 (d, $J_{C\text{-}F}$ = 32.0 Hz), 131.3, 130.8 (d, $J_{C\text{-}F}$ = 32.8 Hz), 129.7, 129.2 (d, $J_{C\text{-}F}$ = 66.9 Hz), 128.0, 125.2 (m), 124.8 (m), 124.1 (m), 49.2, 18.8. MS (EI): 604 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{35}H_{25}F_6OSi$ $(M\text{-}H)^-$ 603.1584, found 603.1581. IR (KBr) v 3070, 2928, 1691, 1611, 1590, 1487, 1429, 1328, 1167, 1127, 1073 cm^{-1}.

2-phenyl-1-(*p*-tolyl)-3-(triphenylsilyl)propan-1-one (3fa + 3fa'):



TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (**3fa** + **3fa**' = 68.4 mg, 2.3: 1, 71% yield) as a colorless oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58-7.55 (m, 1H), 7.50-7.46 (m, 7H), 7.34-7.23 (m, 10H), 7.21-7.16 (m, 4H), 7.13-7.05 (m, 2H), 7.01-6.97 (m, 2H), 4.77-4.73 (m, 1H), 2.67-2.61 (m, 1H), 2.26 (s, 2.08H), 2.23 (s, 0.92H), 1.93-1.87 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 199.5, 199.1, 143.0, 142.0, 138.8, 136.5, 135.7, 134.6, 133.9, 132.3, 129.6, 129.3, 129.3, 128.8, 128.7, 128.6, 128.4, 128.0, 128.0, 127.9, 127.8, 126.7, 48.9, 48.7, 21.5, 20.9, 18.6, 18.5. MS (EI): 482 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{34}H_{30}NaOSi$ $(M+Na)^+$ 505.1958, found 505.1961. IR (KBr) v 3067, 2922, 1679, 1605, 1428, 1457, 1227, 1175, 1110, 1028 cm^{-1}.

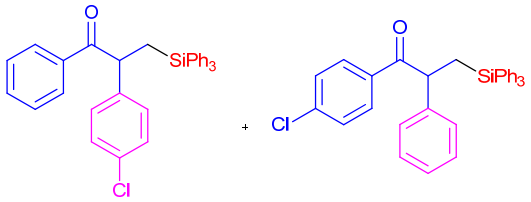
1-(4-fluorophenyl)-2-phenyl-3-(triphenylsilyl)propan-1-one (3ga + 3ga'):



TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (**3ga** + **3ga**' = 70.0 mg, 2.5: 1, 72% yield) as a yellow oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.59-7.55 (m, 2H), 7.50-7.46 (m, 6H), 7.34-7.24 (m, 10H), 7.21-7.17 (m, 3H), 7.15-7.10 (m, 2H), 6.87-6.81 (m, 2H), 4.76 (q, J = 6.0 Hz, 0.27H), 4.72 (q, J = 4.8 Hz, 0.68H), 2.68 (q, J = 9.2 Hz, 0.67H), 2.60 (q, J = 8.0 Hz,

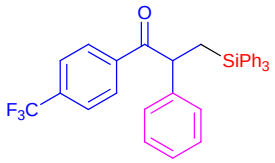
0.3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.8, 166.4, 141.7, 135.7, 135.7, 134.4, 134.4, 132.7 (d, $J_{C\text{-}F}$ = 25.9 Hz), 131.0 (d, $J_{C\text{-}F}$ = 9.1 Hz), 129.7 (d, $J_{C\text{-}F}$ = 8.0 Hz), 129.5, 129.4, 129.0, 128.3 (d, $J_{C\text{-}F}$ = 42.7 Hz), 127.9, 127.8, 127.8, 127.0, 115.6 (d, $J_{C\text{-}F}$ = 21.3 Hz), 115.1 (d, $J_{C\text{-}F}$ = 21.6 Hz), 49.2, 48.2, 18.6, 18.6. MS (EI): 486 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{33}H_{27}FNaOSi$ $(M+Na)^+$ 509.1707, found 509.1714. IR (KBr) ν 3068, 2922, 1683, 1598, 1505, 1428, 1335, 1229, 1156, 1110 cm^{-1}.

2-(4-chlorophenyl)-1-phenyl-3-(triphenylsilyl)propan-1-one (3ha + 3ha'):



TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (**3ha + 3ha'** = 77.3 mg, 3.0: 1, 77% yield) as a yellowish oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58-7.56 (m, 1H), 7.50-7.46 (m, 6H), 7.35-7.14 (m, 13H), 7.13-7.07 (m, 3H), 4.77 (q, J = 5.6 Hz, 0.73H), 4.71 (q, J = 4.8 Hz, 0.24H), 2.71-2.65 (m, 0.23H), 2.63-2.57 (m, 0.74H), 1.94-1.88 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 199.2, 198.1, 141.5, 140.0, 138.6, 136.1, 135.7, 135.6, 134.7, 134.4, 134.2, 132.7, 132.6, 129.8, 129.4, 129.4, 129.0, 128.9, 128.4, 128.3, 128.1, 127.8, 127.8, 127.0, 49.3, 48.3, 18.5. MS (EI): 502 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{33}H_{27}ClNaOSi$ $(M+Na)^+$ 525.1412, found 525.1418. IR (KBr) ν 3068, 1683, 1589, 1489, 1428, 1253, 1222, 1110, 1014 cm^{-1}.

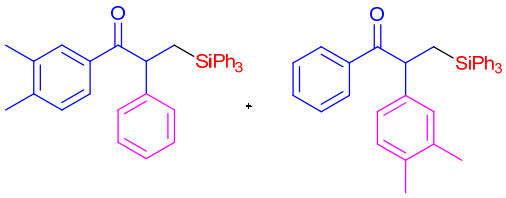
2-phenyl-1-(4-(trifluoromethyl)phenyl)-3-(triphenylsilyl)propan-1-one (3ia + 3ia'):



TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (61.1 mg, 57% yield) as a yellow oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.60-7.58 (m, 2H), 7.47-7.45 (m, 5H), 7.41-7.31 (m, 7H), 7.28-7.23 (m, 9H), 7.21-7.20 (m, 1H), 4.87-4.84 (m, 1H), 2.62-2.57 (m, 1H), 1.97-1.92 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 199.0, 145.3, 136.0, 135.6 134.1, 132.8, 129.6, 129.1 (d, $J_{C\text{-}F}$ = 32.3 Hz), 128.5, 128.4, 128.3, 127.9, 125.7 (m), 124.0 (d, $J_{C\text{-}F}$ = 270.4 Hz), 48.7, 18.6. MS (EI): 536 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{34}H_{27}F_3NaOSi$ $(M+Na)^+$ 559.1675, found 559.1675.

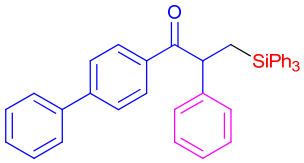
IR (KBr) *v* 3069, 2926, 1683, 1616, 1428, 1325, 1259, 1166, 1109, 1069, 1018 cm^{-1}.

1-(3,4-dimethylphenyl)-2-phenyl-3-(triphenylsilyl)propan-1-one (3ja + 3ja'):



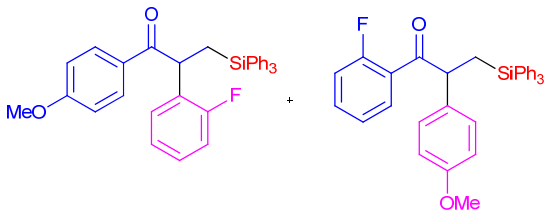
TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (**3ja** + **3ja'** = 67.5 mg, 1.1: 1, 68% yield) as a yellow oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.60-7.58 (m, 1H), 7.47-7.46 (m, 6H), 7.34-7.20 (m, 11H), 7.19-7.07 (m, 5H), 6.95-6.89 (m, 2H), 4.77-4.70 (m, 1H), 2.65-2.59 (d, 1H), 2.17 (s, 2H), 2.14-2.13 (m, 3H), 2.11 (s, 1H), 1.94-1.91 (m, 0.51H), 1.90-1.88 (m, 0.54H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 199.6, 199.5, 142.0, 141.8, 139.1, 137.0, 136.5, 136.3, 135.8, 135.1, 134.7, 134.6, 134.4, 132.2, 130.1, 129.6, 129.3, 129.2, 129.1, 128.8, 128.5, 128.0, 127.9, 127.7, 127.7, 126.7, 126.2, 125.4, 48.9, 48.7, 19.8, 19.7, 19.6, 19.3, 18.6, 18.5. MS (EI): 496 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{35}H_{32}NaOSi$ $(M+Na)^+$ 519.2115, found 519.2124. IR (KBr) *v* 3068, 2920, 1679, 1605, 1491, 1428, 1257, 1110, 1029 cm^{-1}.

1-([1,1'-biphenyl]-4-yl)-2-phenyl-3-(triphenylsilyl)propan-1-one (3ka):



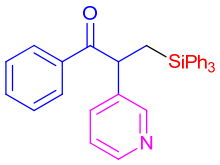
TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (58.8 mg, 54% yield) as a colorless oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.58 (d, J = 7.2 Hz, 2H), 7.49-7.47 (m, 4H), 7.42-7.36 (m, 2H), 7.35-7.24 (m, 12H), 7.22-7.13 (m, 5H), 7.09-7.05 (m, 2H), 6.80-6.73 (m, 2H), 5.08-5.05 (m, 1H), 2.63-2.57 (m, 1H), 2.09-2.04 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 198.3, 144.3, 136.1, 136.0, 135.7, 135.4, 135.2, 132.6, 129.5, 128.5, 128.1, 127.8, 127.6, 127.5, 126.8, 125.3, 124.7, 43.5, 19.5. MS (EI): 544 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{39}H_{33}OSi$ $(M+H)^+$ 545.2295, found 545.2296. IR (KBr) *v* 3068, 2922, 1684, 1596, 1428, 1233, 1110, 1028 cm^{-1}.

2-(2-fluorophenyl)-1-(4-methoxyphenyl)-3-(triphenylsilyl)propan-1-one (3la + 3la'):



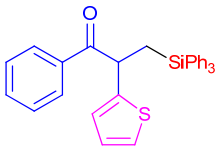
TLC on GF254 (ethyl acetate: petroleum, 1:10) give the product (**3la** + **3la**' = 46.4 mg, 2.1: 1, 45% yield) as a colorless oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.64-7.61 (m, 2H), 7.50-7.46 (m, 4H), 7.41-7.21 (m, 16H), 7.06-6.93 (m, 3H), 6.89-6.83 (m, 1H), 6.71-6.64 (m, 2H), 5.18-5.15 (m, 0.68H), 4.72-4.68 (m, 0.29H), 3.74 (s, 2H), 3.69 (s, 1H), 2.63-2.54 (m, 1H), 1.91-1.86 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 197.5, 197.5, 163.1, 160.5, 158.3 (d, $J_{C\text{-}F}$ = 47.6 Hz), 136.1 (d, $J_{C\text{-}F}$ = 20.8 Hz), 135.7, 135.2, 135.0, 134.7, 134.4, 133.6, 131.0 (dd), 130.6, 130.1, 129.5, 129.3, 129.1, 129.1, 129.0, 128.9, 128.8, 128.4, 128.3, 127.9, 127.7, 127.4, 124.6 (dd), 123.9 (dd), 116.2 (d, $J_{C\text{-}F}$ = 23.7 Hz), 115.4 (d, $J_{C\text{-}F}$ = 22.7 Hz), 114.0, 113.3, 55.3, 55.1, 39.6, 39.5, 18.0, 17.8. MS (EI): 516 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{34}H_{29}FNaO_2Si$ $(M+Na)^+$ 539.1813, found 539.1814. IR (KBr) ν 3068, 2930, 1677, 1600, 1510, 1487, 1428, 1254, 1176, 1110,1030 cm^{-1}.

1-phenyl-2-(pyridin-3-yl)-3-(triphenylsilyl)propan-1-one: (3ma):



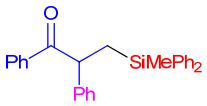
TLC on GF254 (ethyl acetate: petroleum, 1:10) give the product (51.6 mg, 55% yield) as a yellowish oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 8.40-8.35 (m, 2H), 7.58-7.53 (m, 3H), 7.51-7.47 (m, 6H), 7.41-7.32 (m, 4H), 7.30-7.21 (m, 8H), 7.10-7.07 (m, 1H), 4.84-4.80 (m, 1H), 2.61 (dd, J_1 = 8.0 Hz, J_2 = 7.2 Hz ,1H), 1.95-1.90 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 198.9, 149.5, 148.2, 137.1, 135.8, 135.6, 135.3, 134.0, 132.8, 129.6, 128.4, 128.3, 127.9, 123.7, 46.1, 18.5. MS (EI): 469 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{32}H_{28}NOSi$ $(M+H)^+$ 470.1935, found 470.1954. IR (KBr) ν 3068, 2924, 1682, 1596, 1427, 1229, 1110, 1024 cm^{-1}.

1-phenyl-2-(thiophen-2-yl)-3-(triphenylsilyl)propan-1-one (3na):



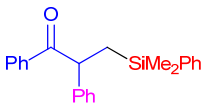
TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (71.1 mg, 75% yield) as a colorless oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.66-7.62 (m, 2H), 7.51-7.47 (m, 6H), 7.39-7.34 (m, 3H), 7.33-7.19 (m, 12H), 4.85-4.82 (m, 1H), 2.67-2.62 (m, 1H), 2.02-1.97 (m, 1H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 199.5, 140.7, 139.8, 135.7, 134.5, 132.4, 129.4, 128.7, 128.5, 128.1, 127.8, 127.6, 126.9, 48.7, 18.6. MS (EI): 474 (M+); HRMS (ESI-TOF) m/z calcd for $C_{31}H_{25}OSSi$ $(M-H)^-$ 473.1401, found 473.1401. IR (KBr) ν 3068, 2924, 1682, 1597, 1485, 1427, 1326, 1252, 1223, 1174, 1109, 1028 cm^{-1}.

3-(methyldiphenylsilyl)-1,2-diphenylpropan-1-one (3ab):



TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (50.3 mg, 62% yield) as a colorless oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.74-7.72 (m, 2H), 7.50-7.44 (m, 4H), 7.42-7.32 (m, 4H), 7.31-7.26 (m, 5H), 7.22-7.11 (m, 5H), 4.64 (t, J = 7.2 Hz, 1H), 2.19-2.13 (m, 1H), 1.74-1.69 (m, 1H), 0.29 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 200.0, 141.2, 136.7, 136.5, 136.5, 134.6, 134.4, 132.6, 129.3, 129.2, 128.8, 128.6, 128.3, 128.2, 127.8, 127.8, 126.9, 49.0, 19.5, -0.40. MS (EI): 406 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{28}H_{26}NaOSi$ $(M+Na)^+$ 429.1645, found 429.1648. IR (KBr) ν 3067, 2955, 1683, 1598, 1447, 1250, 1226, 1112 cm^{-1}.

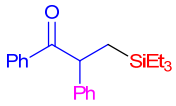
3-(dimethyl(phenyl)silyl)-1,2-diphenylpropan-1-one (3ac):



TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (50.9 mg, 74% yield) as a yellow oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.83-7.79 (m, 2H), 7.46-7.41 (m, 3H), 7.33-7.30 (m, 5H) 7.23-7.21 (m, 4H), 7.17-7.12 (m, 1H), 4.60 (t, J = 7.6 Hz, 1H), 1.79 (dd, J_1 = 7.6 Hz, J_2 = 7.2 Hz ,1H), 1.42 (dd, J_1 = 7.6 Hz, J_2 = 7.2 Hz ,1H), 0.13 (s, 3H), 0.12 (s, 3H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 200.2, 141.3, 138.5, 136.5, 133.6, 132.6, 128.9, 128.8, 128.6, 128.4, 128.2, 127.6, 126.9,

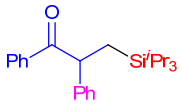
49.2, 21.2, -2.5, -2.7. MS (EI): 344 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{23}H_{23}OSi$ $(M-H)^-$ 343.1524, found 343.1523. IR (KBr) ν 3067, 2956, 1682, 1597, 1491, 1427, 1254, 1176, 1111, 1028 cm^{-1}.

1,2-diphenyl-3-(triethylsilyl)propan-1-one (3ad):



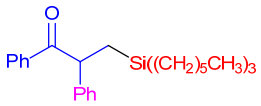
TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (43.4 mg, 67% yield) as a yellow oily liquid. ^1H NMR ($CDCl_3$, 400 MHz): δ 7.97-7.95 (m, 2H), 7.48-7.45 (m, 1H), 7.40-7.36 (m, 2H), 7.34-7.32 (m, 2H), 7.27-7.24 (m, 2H), 7.18-7.14 (m, 1H), 4.69 (t, J = 7.2 Hz, 1H), 1.58 (dd, J_1 = 7.6 Hz, J_2 = 7.2 Hz, 1H), 1.18 (dd, J_1 = 7.2 Hz, J_2 = 8.0 Hz, 1H), 0.88 (t, J = 8.0 Hz, 9H), 0.49-0.33 (m, 6H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 200.3, 141.9, 136.7, 132.7, 128.8, 128.6, 128.5, 128.1, 126.8, 49.0, 17.0, 7.3, 3.5. MS (EI): 324 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{21}H_{29}OSi$ $(M+H)^+$ 325.1982, found 325.1986. IR (KBr) ν 3062, 2952, 1683, 1598, 1447, 1415, 1224, 1175, 1016 cm^{-1}.

1,2-diphenyl-3-(triisopropylsilyl)propan-1-one (3ae):



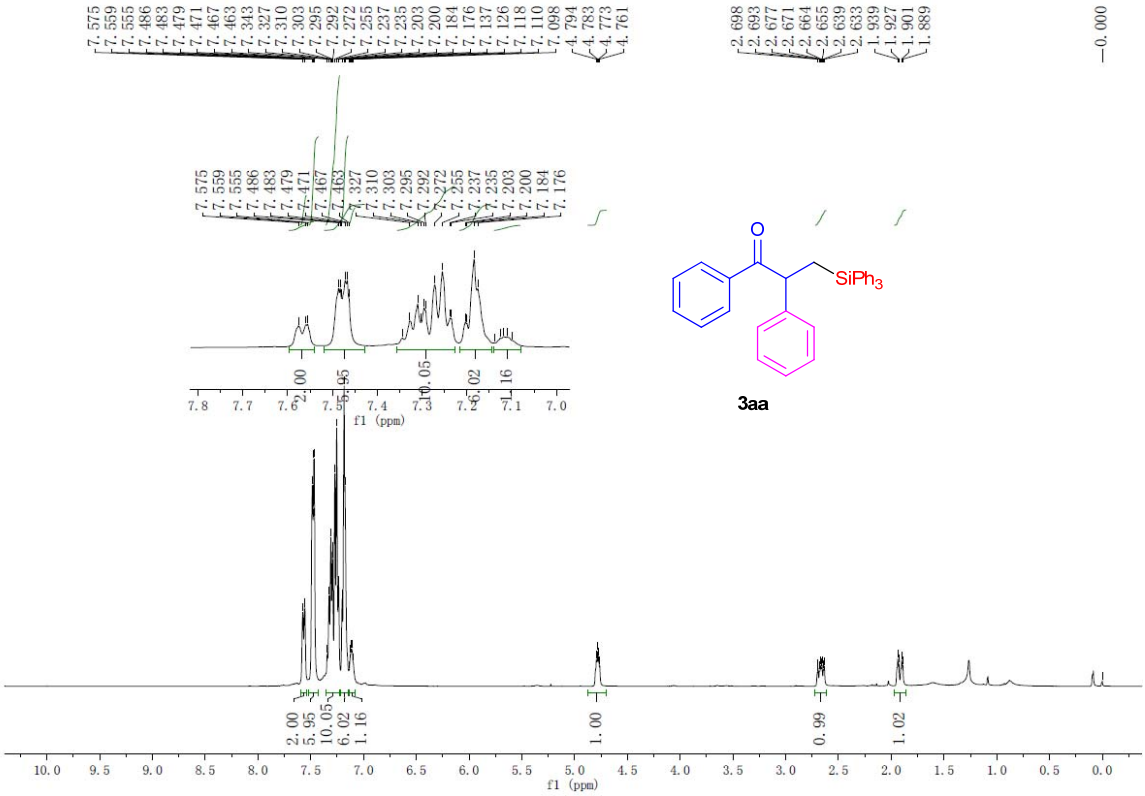
TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (46.8 mg, 64% yield) as a colorless oily liquid. ^1H NMR ($CDCl_3$, 400 MHz): δ 7.96-7.94 (m, 2H), 7.46-7.42 (m, 1H), 7.38-7.33 (m, 4H), 7.27-7.23 (m, 2H), 7.16-7.12 (m, 1H), 4.84-4.81 (m, 1H), 1.90 (dd, J_1 = 8.4 Hz, J_2 = 6.8 Hz, 1H), 1.05-0.97 (m, 22H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 199.9, 142.7, 136.8, 132.6, 128.9, 128.5, 128.5, 127.9, 126.7, 49.0, 18.7, 14.9, 11.2. MS (EI): 366 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{24}H_{35}OSi$ $(M+H)^+$ 367.2452, found 367.2452. IR (KBr) ν 2941, 2865, 1683, 1598, 1463, 1447, 1400, 1366, 1354, 1223, 1176, 1028, 1015 cm^{-1}.

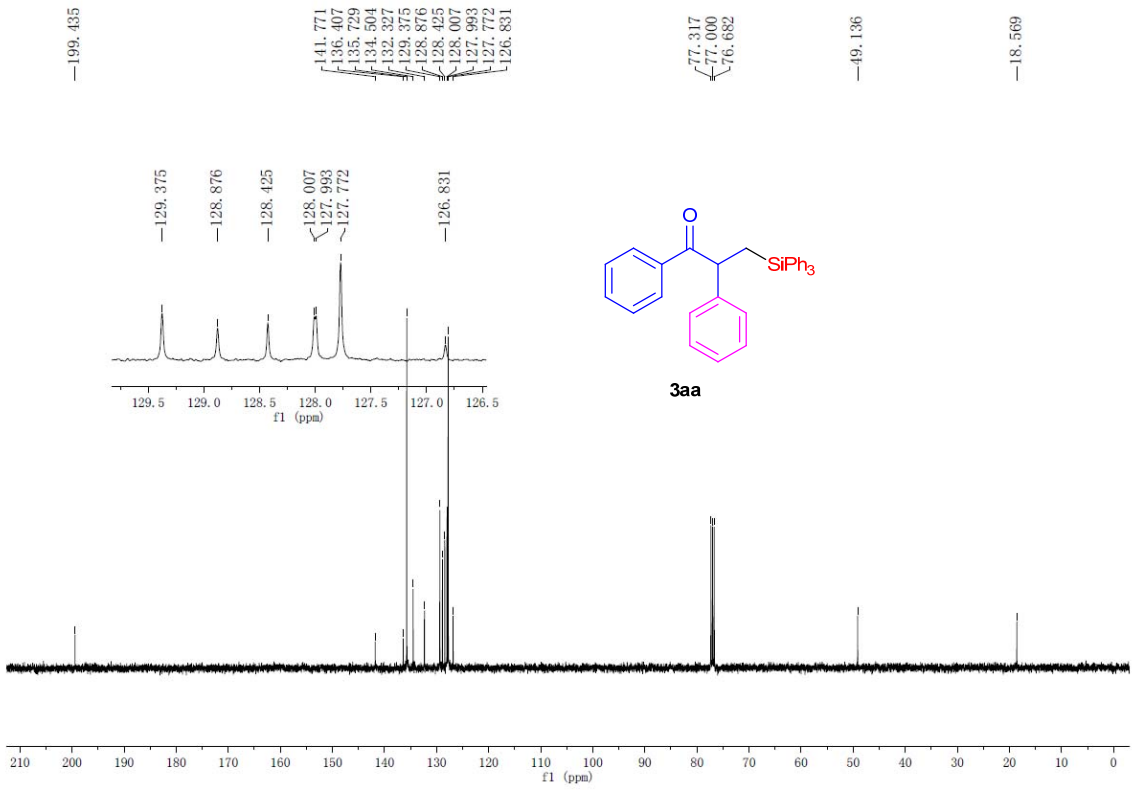
1,2-diphenyl-3-(trihexylsilyl)propan-1-one (3af):

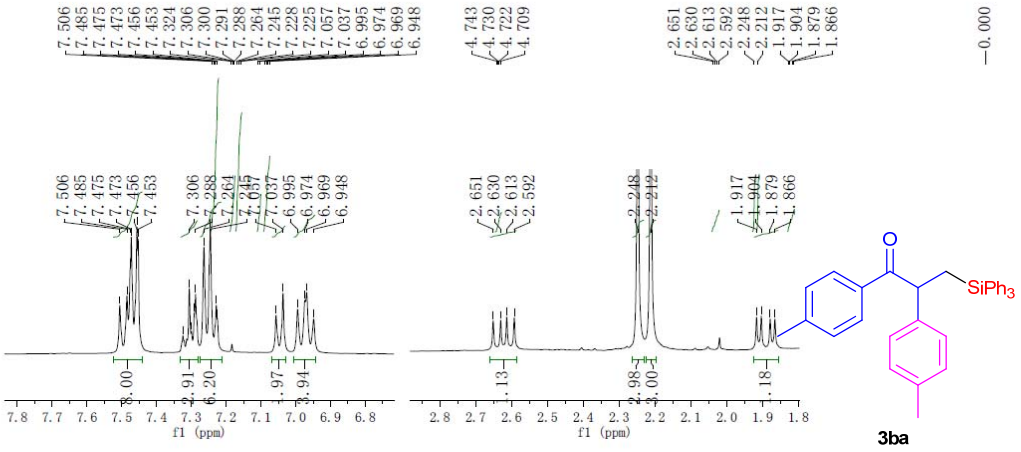


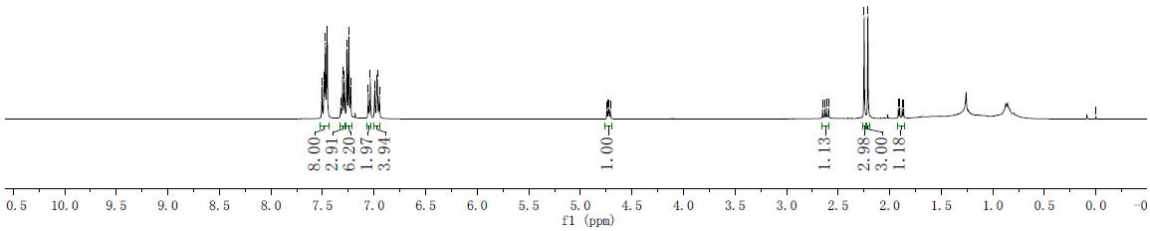
TLC on GF254 (ethyl acetate: petroleum, 1:30) give the product (60.0 mg, 61% yield) as a colorless oily liquid. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 7.97-7.95 (m, 2H), 7.49-7.45 (m, 1H), 7.40-7.36 (m, 2H), 7.34-7.32 (m, 2H), 7.27-7.24 (m, 2H), 7.18-7.14 (m, 1H), 4.68 (t, J = 7.2 Hz, 1H), 1.54 (dd, J_1 = 7.2 Hz, J_2 = 7.6 Hz, 1H), 1.28-1.14 (m, 31H), 0.85 (t, J = 6.8 Hz, 9H); ^{13}C NMR ($CDCl_3$, 100 MHz): δ 200.4, 144.8, 136.7, 132.6, 128.8, 128.6, 128.5, 128.1, 126.8, 49.1, 33.5, 31.5, 23.7, 22.6, 18.0, 14.1, 12.7. MS (EI): 492 (M^+); HRMS (ESI-TOF) m/z calcd for $C_{33}H_{52}NaOSi$ $(M+Na)^+$ 515.3680, found 515.3690. IR (KBr) v 3061, 2922, 1685, 1598, 1454, 1410, 1377, 1224, 1177, 1100 cm^{-1}.

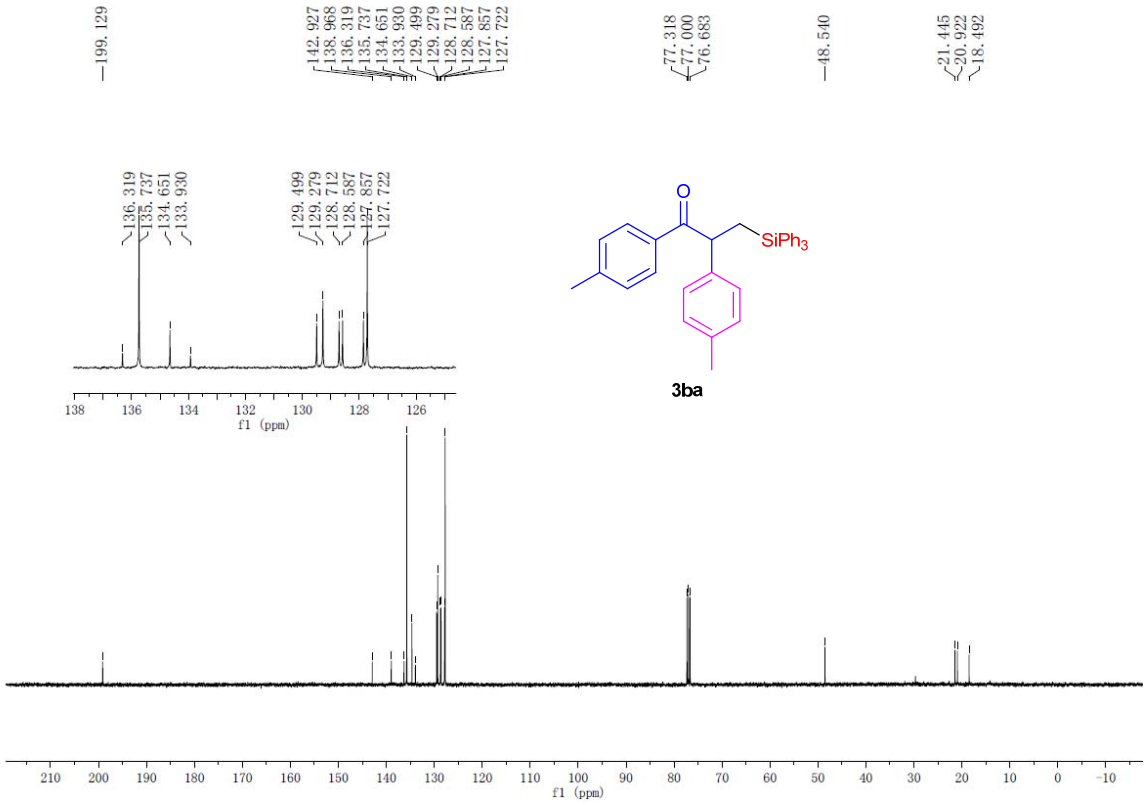
5 Copies of ^{1}H NMR and ^{13}C NMR spectra

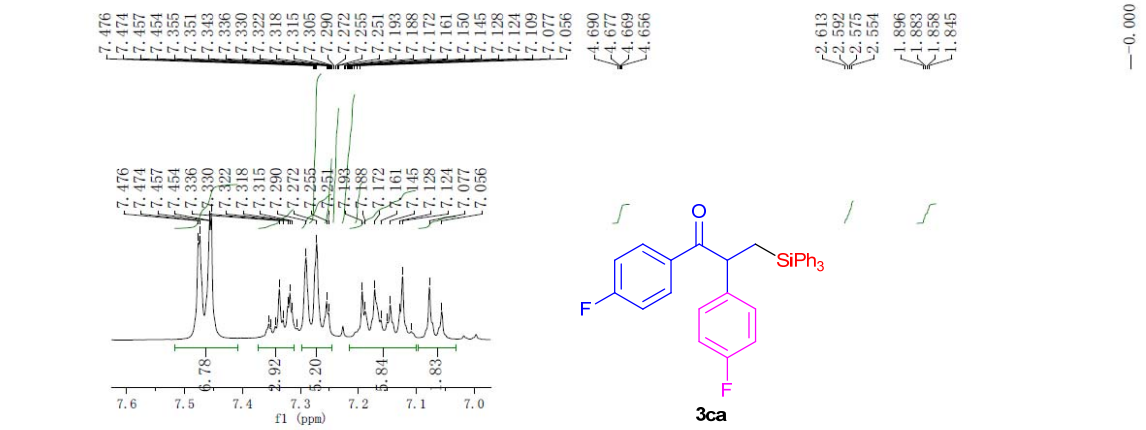


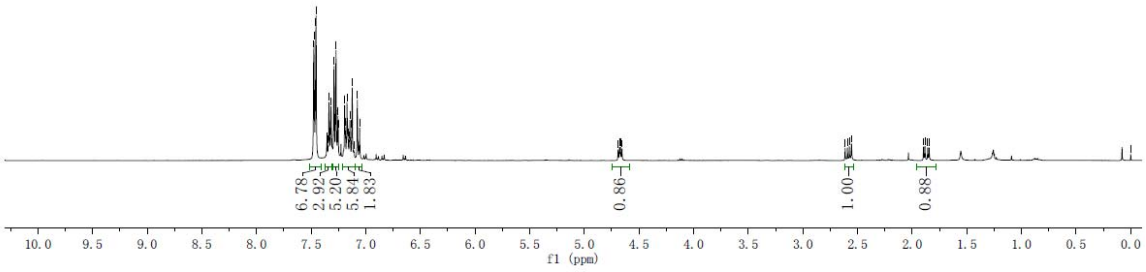


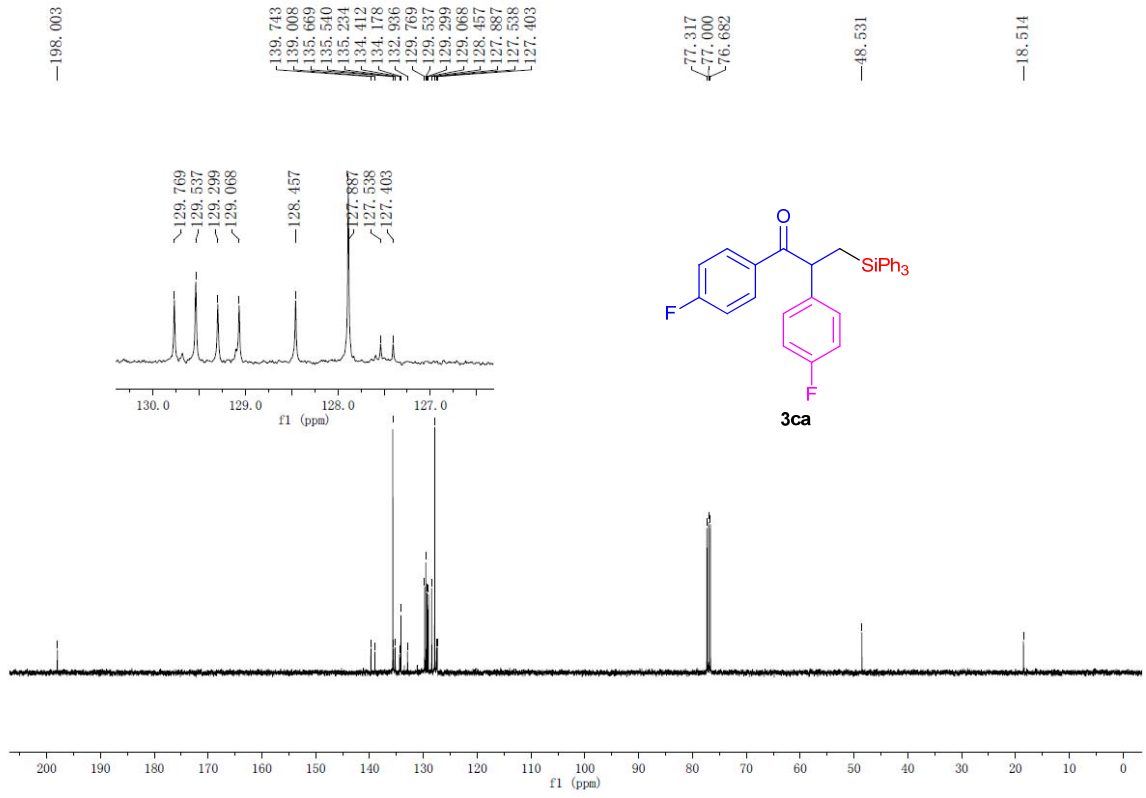

SiPh3
3ba
f1 (ppm)

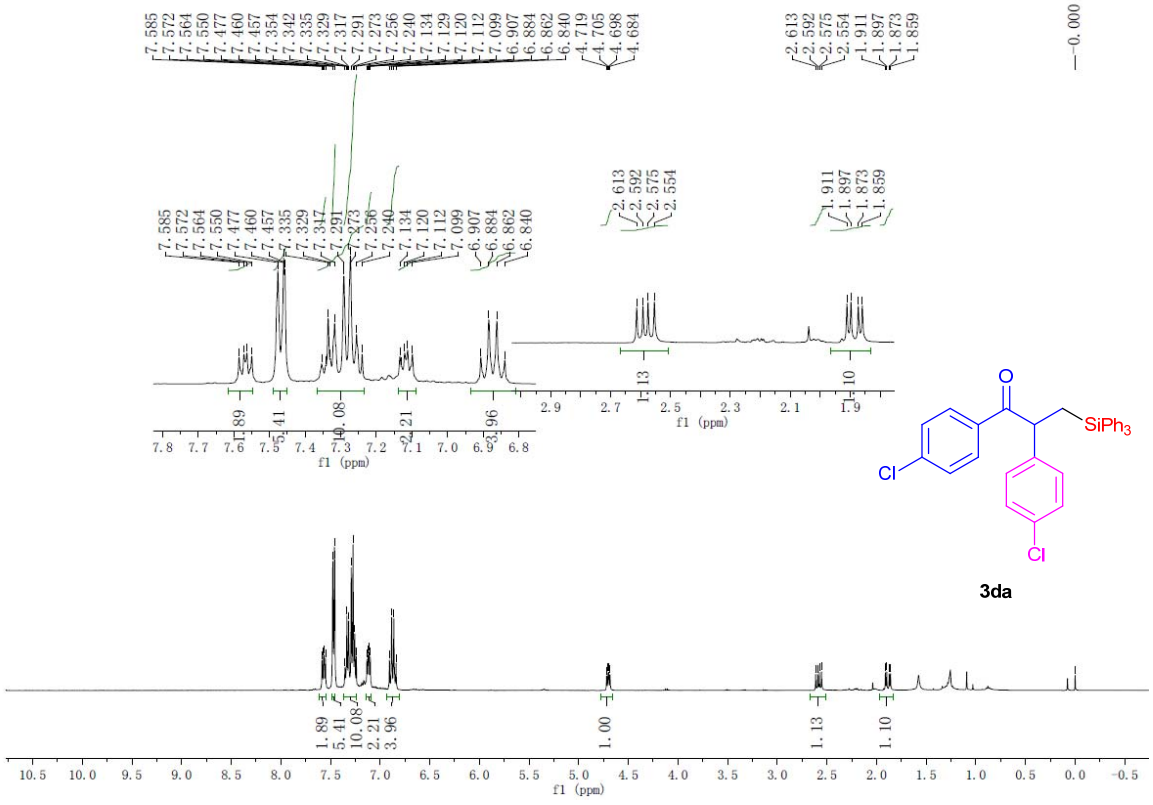

f1 (ppm)


SiPh3
3ba
f1 (ppm)

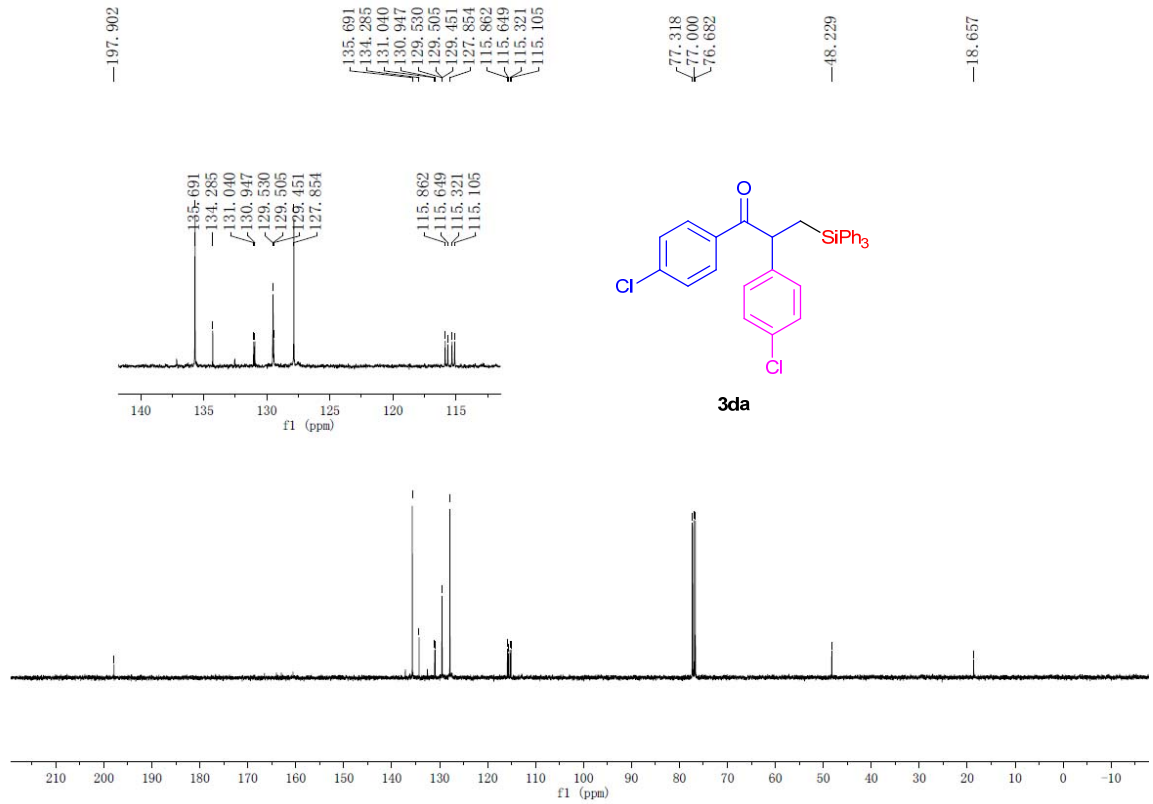

7.476
7.474
7.457
7.454
7.355
7.351
7.343
7.336
7.330
7.322
7.318
7.315
7.305
7.290
7.272
7.255
7.251
7.193
7.188
7.172
7.161
7.150
7.145
7.128
7.124
7.109
7.077
7.056
4.690
4.677
4.669
4.656
2.613
2.592
2.575
2.554
1.896
1.883
1.858
1.845
0.000
6.78
2.92
5.20
5.84
1.83
7.6
7.5
7.4
7.3
7.2
7.1
7.0
f1 (ppm)
SiPh3
F
F
O
3ca


6.78
2.92
5.20
5.84
1.83
0.86
1.00
0.88
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)

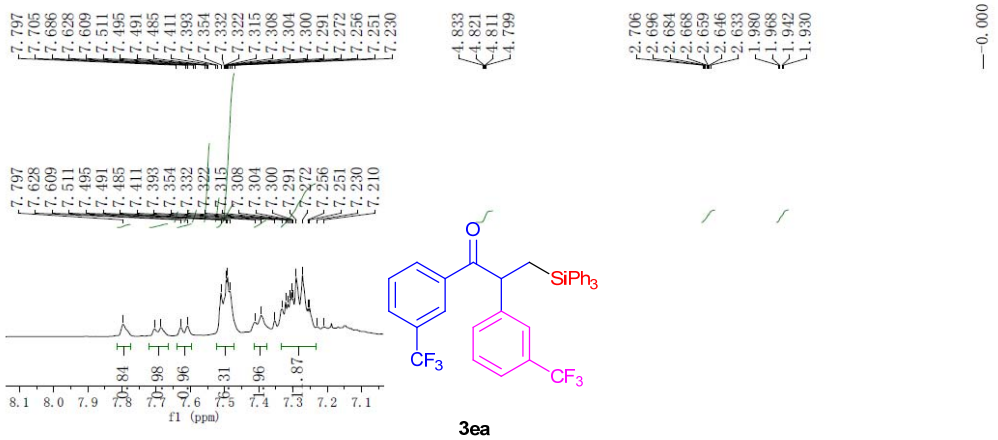

198.003
139.743
139.008
135.669
135.540
135.234
134.412
134.178
132.936
129.769
129.537
129.299
129.068
128.457
127.887
127.538
127.403
77.317
77.000
76.682
48.531
18.514
130.0
129.0
128.0
127.0
f1 (ppm)
SiPh3
F
F
O
3ca
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.585 7.572 7.564 7.550 7.477 7.460 7.457 7.354 7.342 7.335 7.329 7.317 7.291 7.273 7.256 7.240 7.134 7.129 7.120 7.112 7.099 6.907 6.884 6.862 6.840 4.719 4.705 4.698 4.684
2.613 2.592 2.575 2.554 1.911 1.897 1.873 1.859
0.000
1.89 5.41 10.08 2.21 3.96 1.00 1.13 1.10
f1 (ppm)
O
SiPh3
Cl
Cl

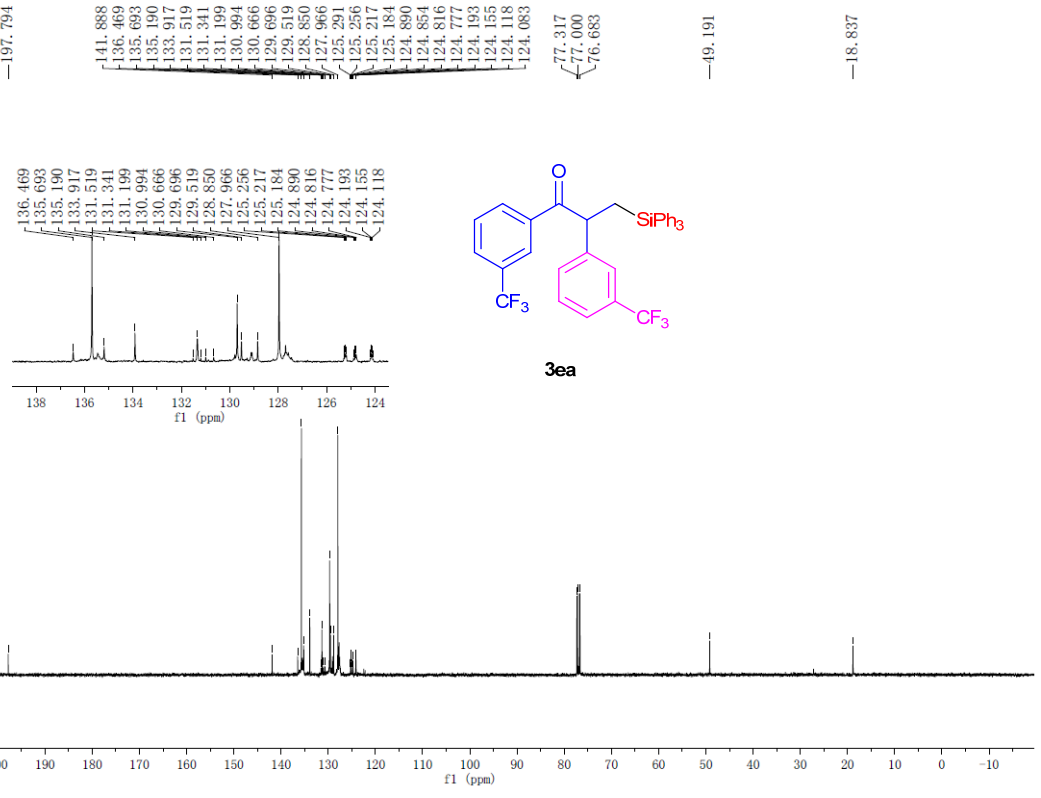
3da


197.902
135.691 134.285 131.040 130.947 129.530 129.505 129.451 127.854 115.862 115.649 115.321 115.105
77.318 77.000 76.682
48.229
18.657
f1 (ppm)
O
SiPh3
Cl
Cl

3da

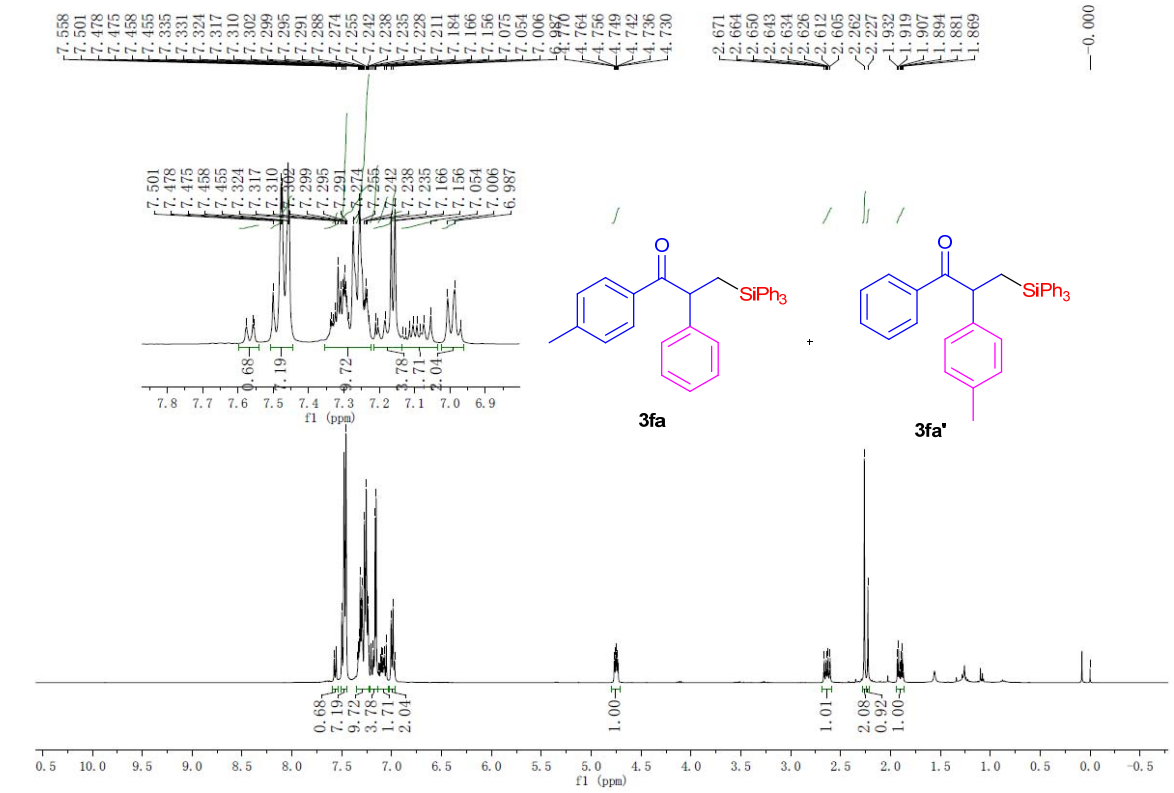

7.797
7.705
7.686
7.628
7.609
7.511
7.495
7.491
7.485
7.411
7.393
7.354
7.332
7.322
7.315
7.308
7.304
7.300
7.291
7.272
7.256
7.251
7.230
4.833
4.821
4.811
4.799
2.706
2.696
2.684
2.668
2.659
2.646
2.633
1.980
1.968
1.942
1.930
0.000
0.84
0.98
0.96
6.31
1.96
11.87
0.91
0.98
0.99
f1 (ppm)
O
SiPh3
CF3
CF3

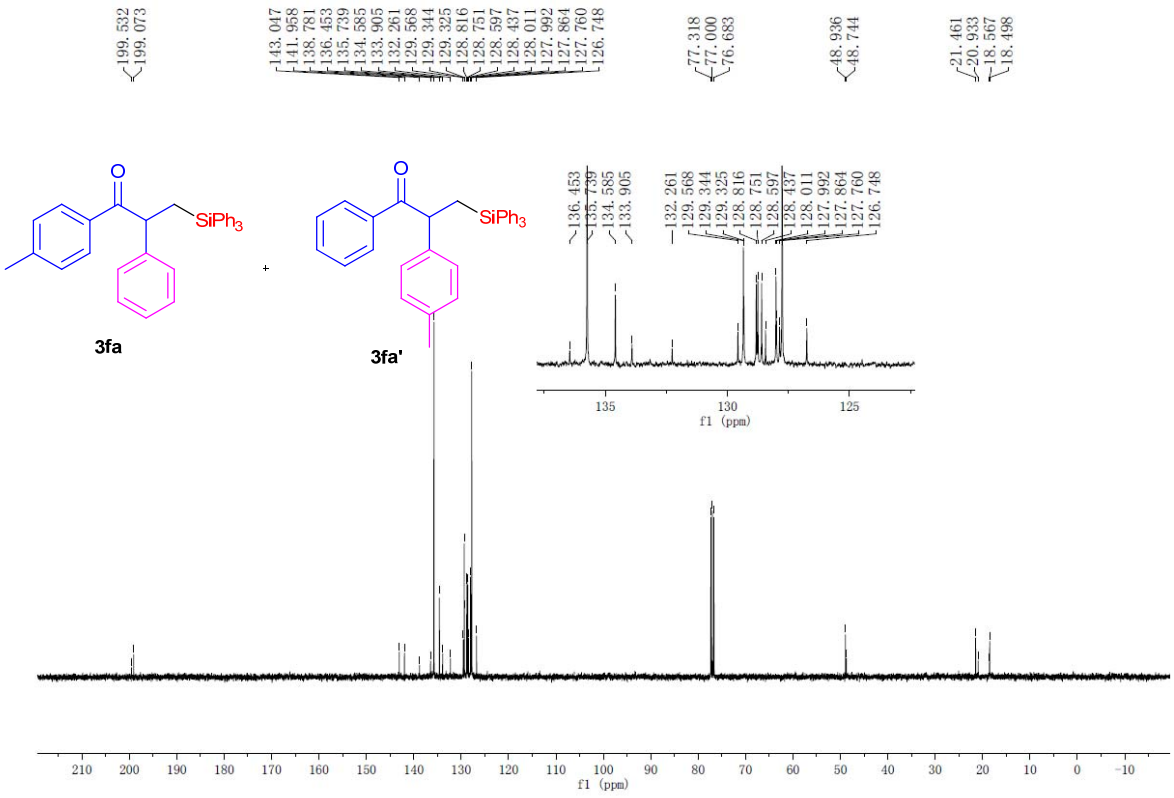
3ea

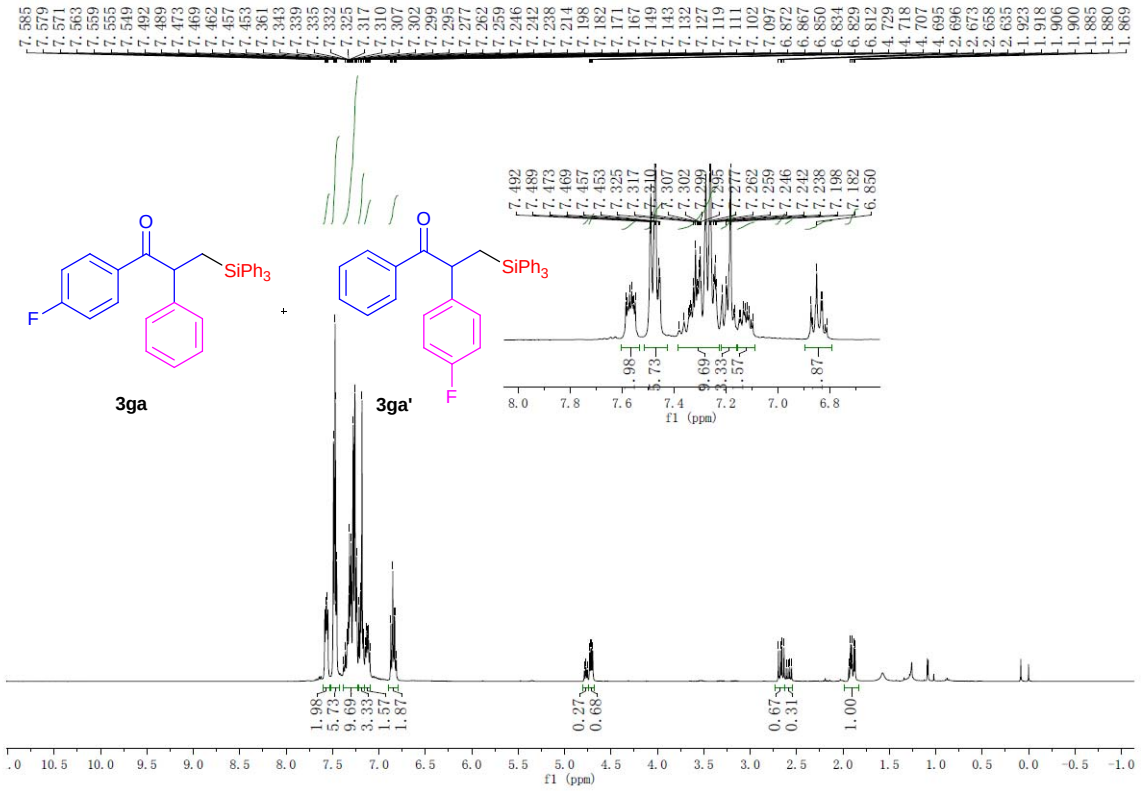

197.794
141.888
136.469
135.693
135.190
133.917
131.519
131.341
131.199
130.994
130.666
129.696
129.519
128.850
127.966
125.291
125.256
125.217
125.184
124.890
124.854
124.816
124.777
124.193
124.155
124.118
124.083
77.317
77.000
76.683
49.191
18.837
f1 (ppm)

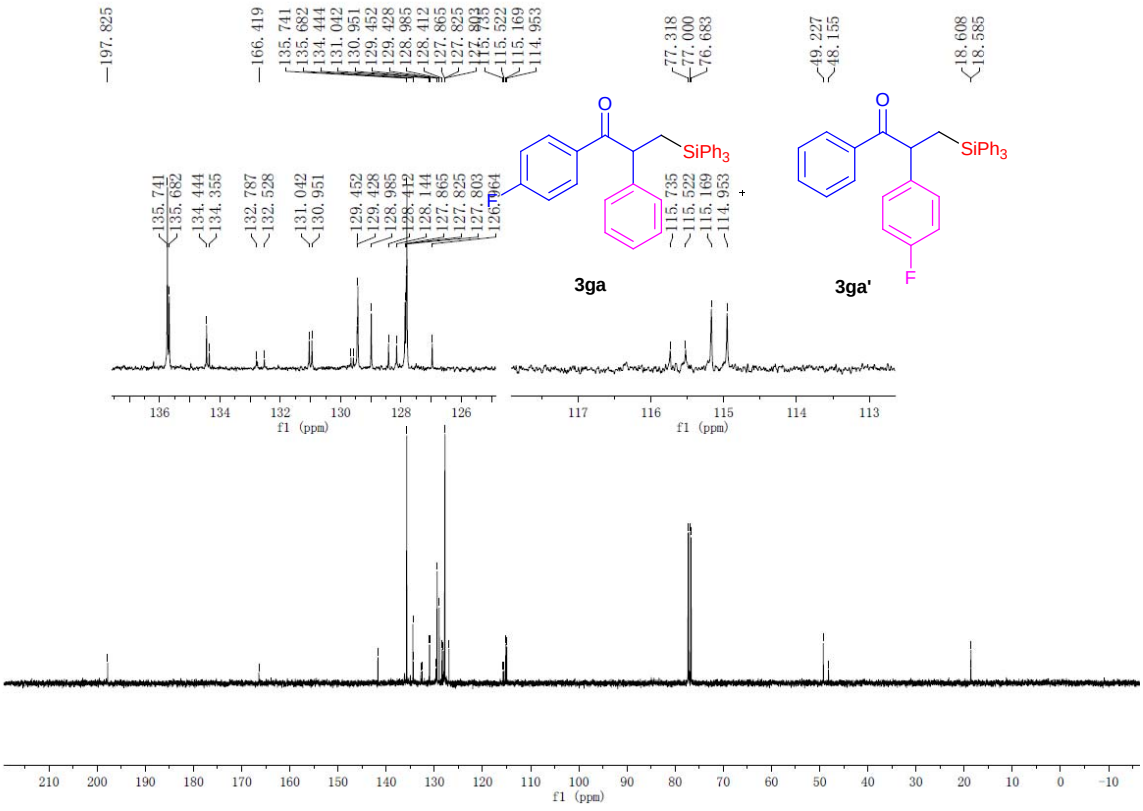
O
SiPh3
CF3
CF3

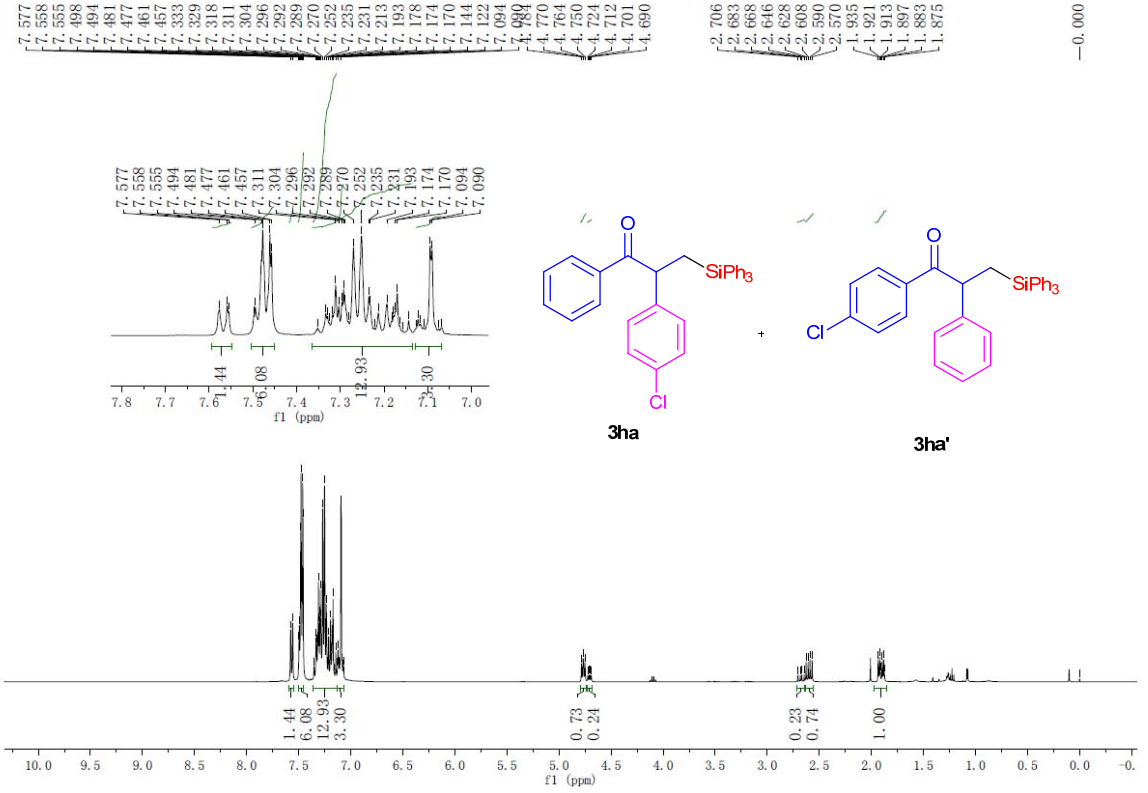
3ea

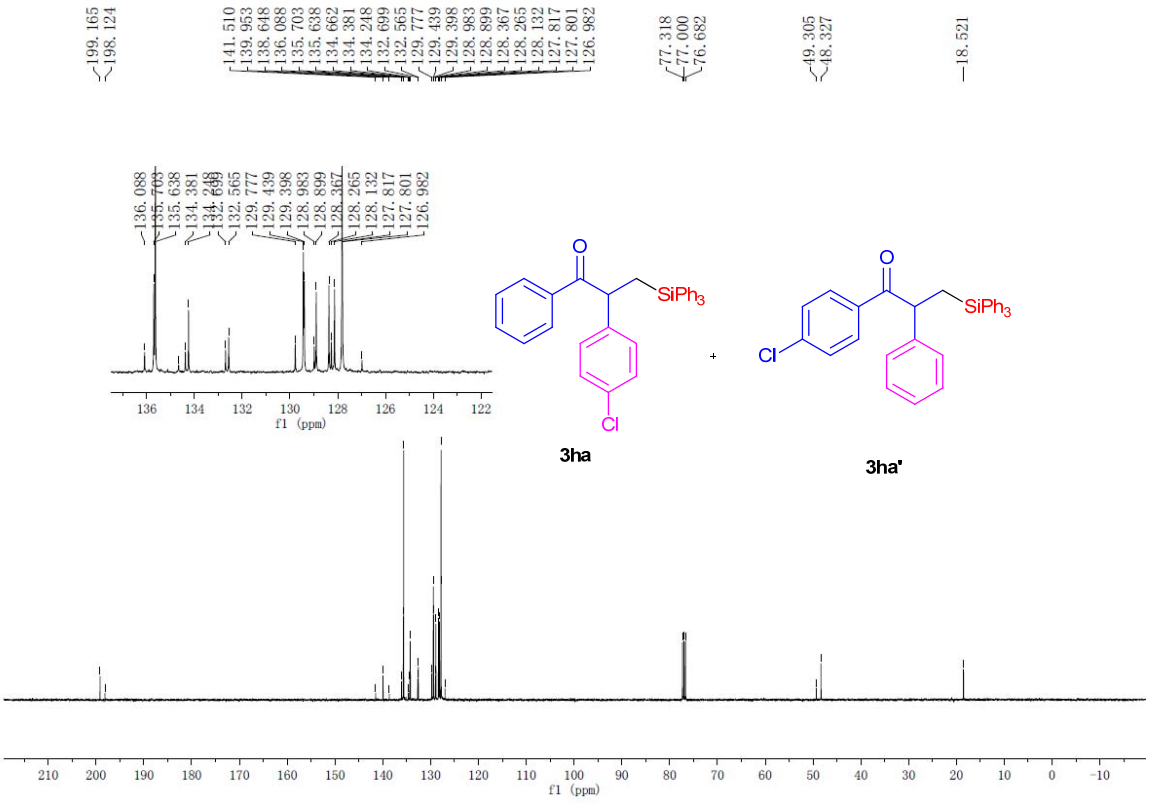

SiPh3
3fa
3fa'
f1 (ppm)

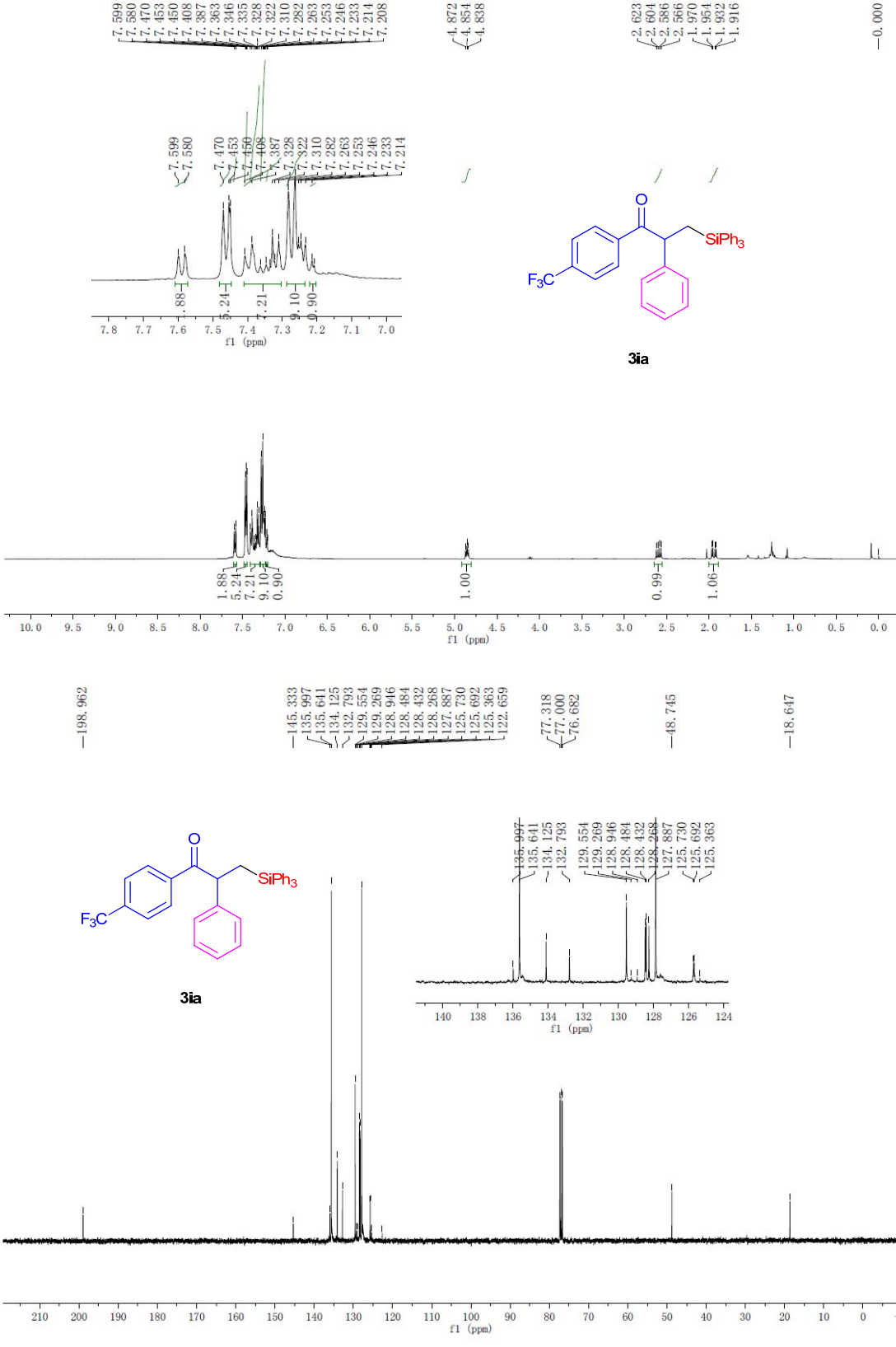

SiPh3
3fa
3fa'
f1 (ppm)

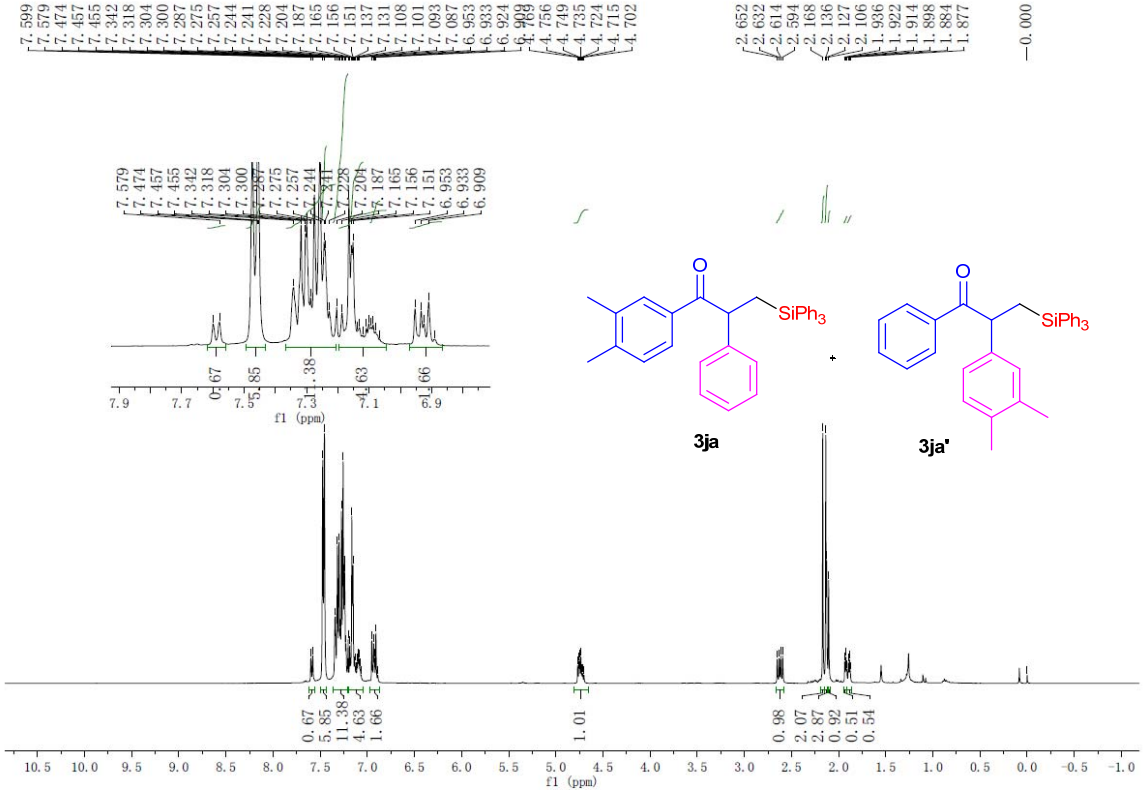

3ga
3ga'
SiPh3
F
f1 (ppm)

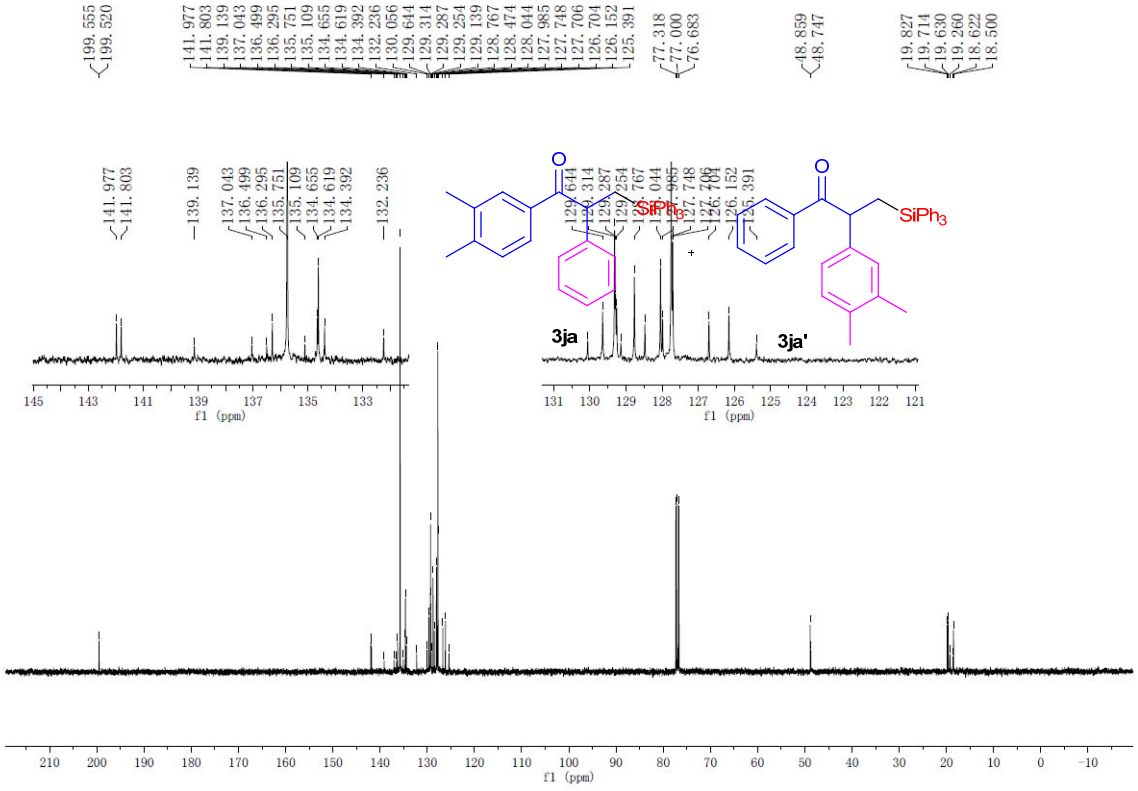

3ga
3ga'
SiPh3
F
f1 (ppm)

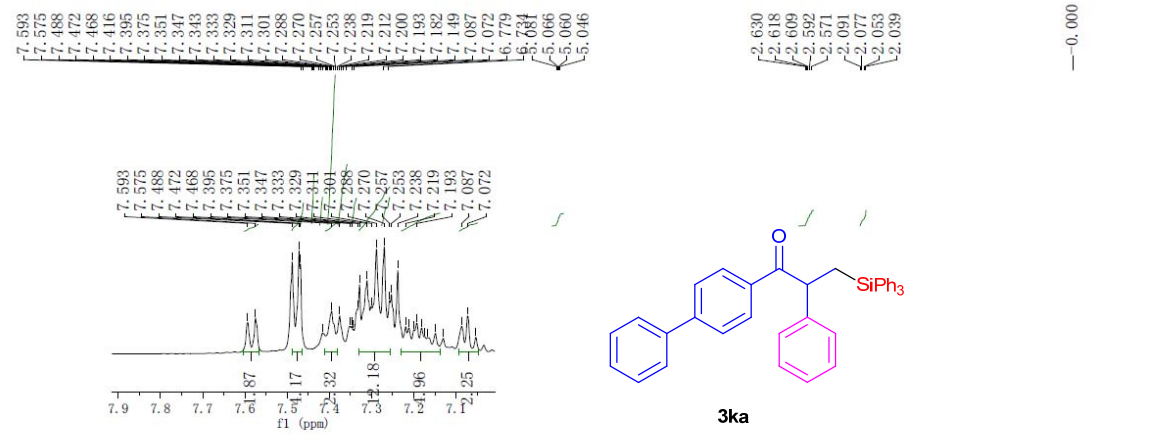

SiPh3
Cl
3ha
3ha'
f1 (ppm)

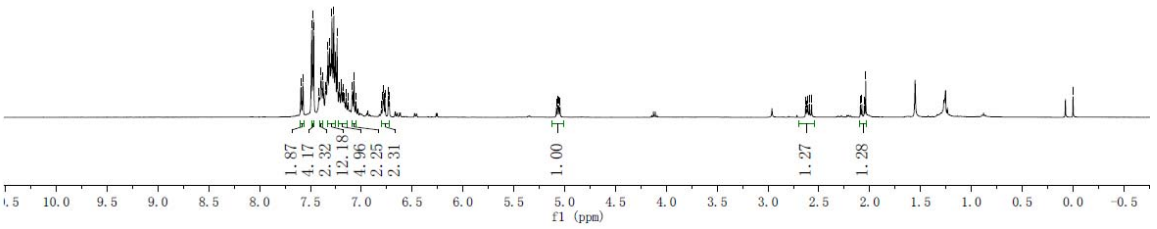

SiPh3
Cl
3ha
3ha'
f1 (ppm)

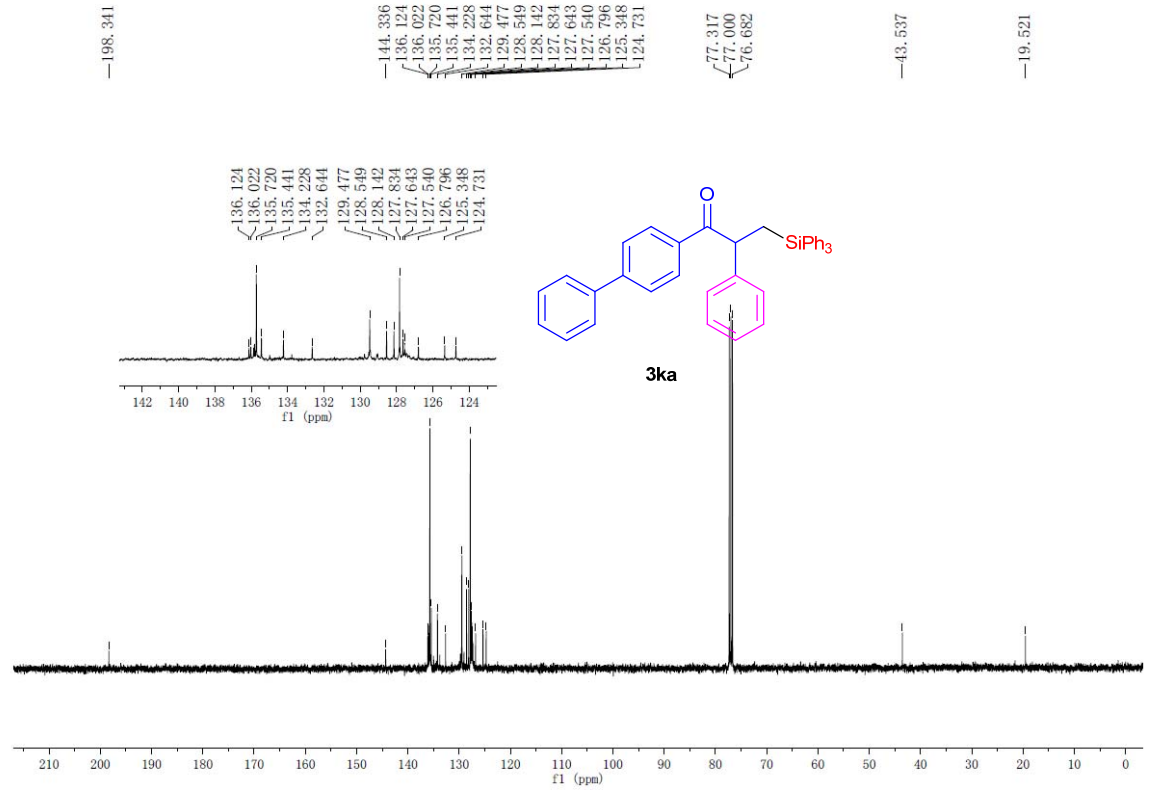

7.599
7.580
7.470
7.453
7.450
7.408
7.387
7.363
7.346
7.335
7.328
7.322
7.310
7.282
7.263
7.253
7.246
7.233
7.214
7.208
4.872
4.854
4.838
2.623
2.604
2.586
2.566
1.970
1.954
1.932
1.916
0.000
SiPh3
F3C
O
3ia
1.88
5.24
7.21
9.10
0.90
1.00
0.99
1.06
f1 (ppm)
198.962
145.333
135.997
135.641
134.125
132.793
129.554
129.269
128.946
128.484
128.432
128.268
127.887
125.730
125.692
125.363
122.659
77.318
77.000
76.682
48.745
18.647

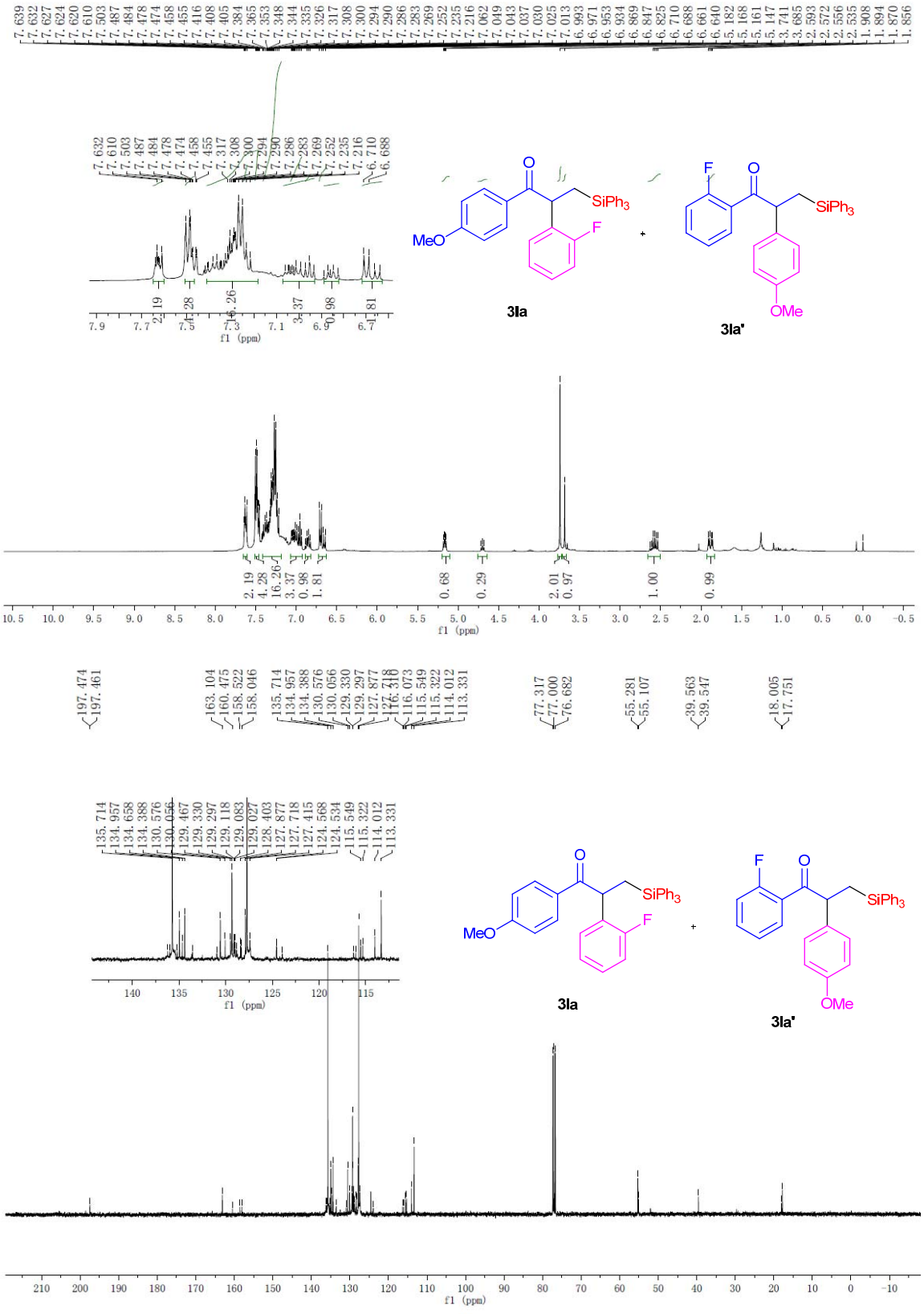

3ja
3ja'
SiPh3
f1 (ppm)

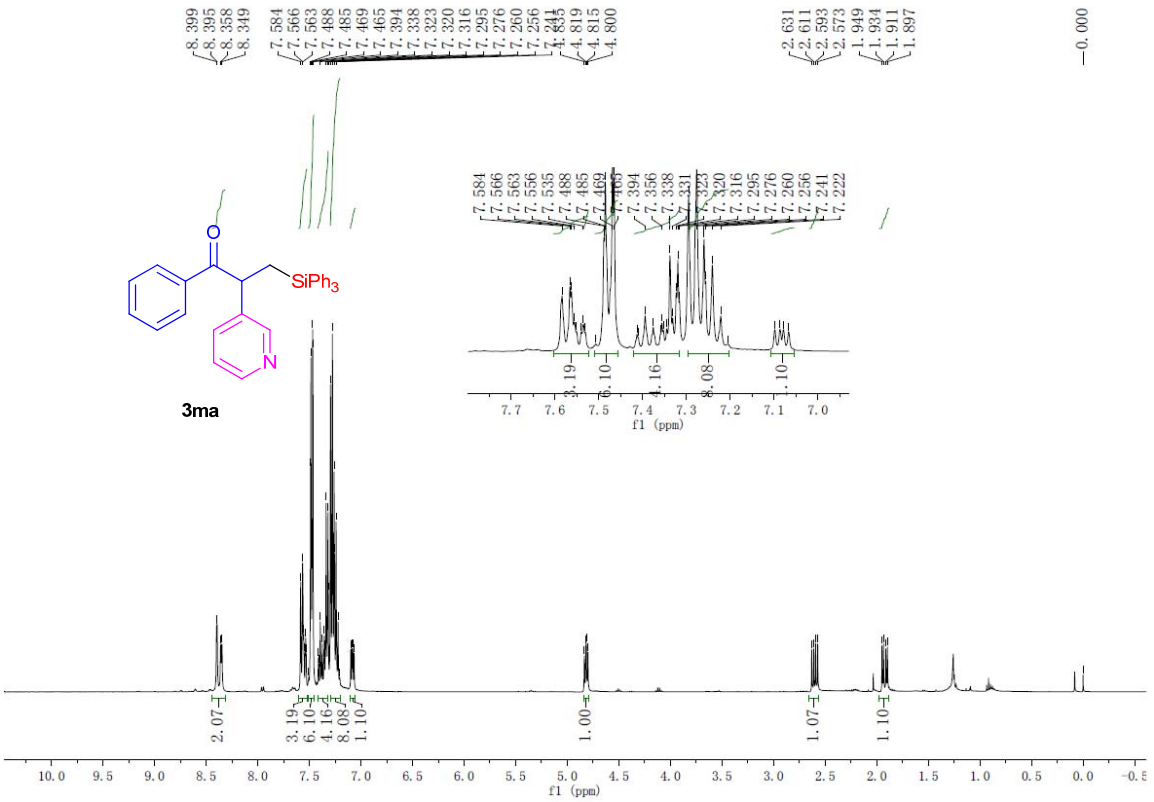

3ja
3ja'
SiPh3
f1 (ppm)

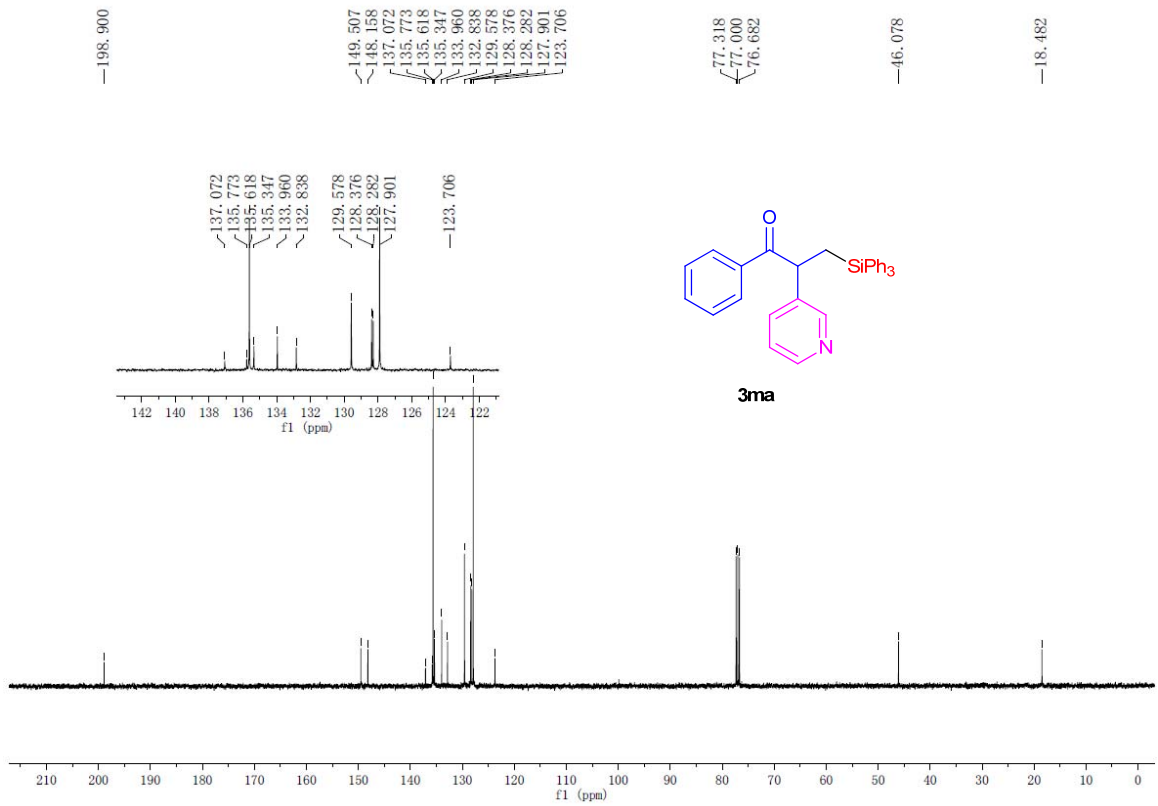

SiPh3
O
3ka
f1 (ppm)

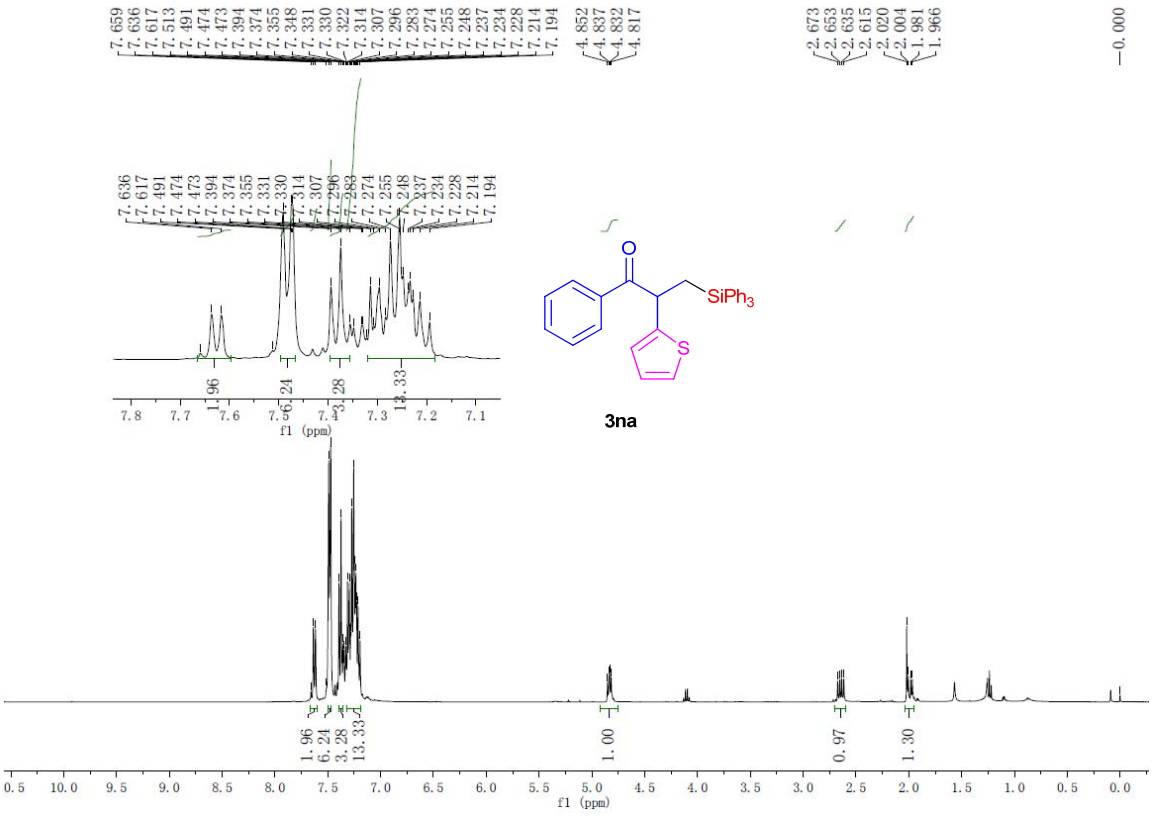

f1 (ppm)

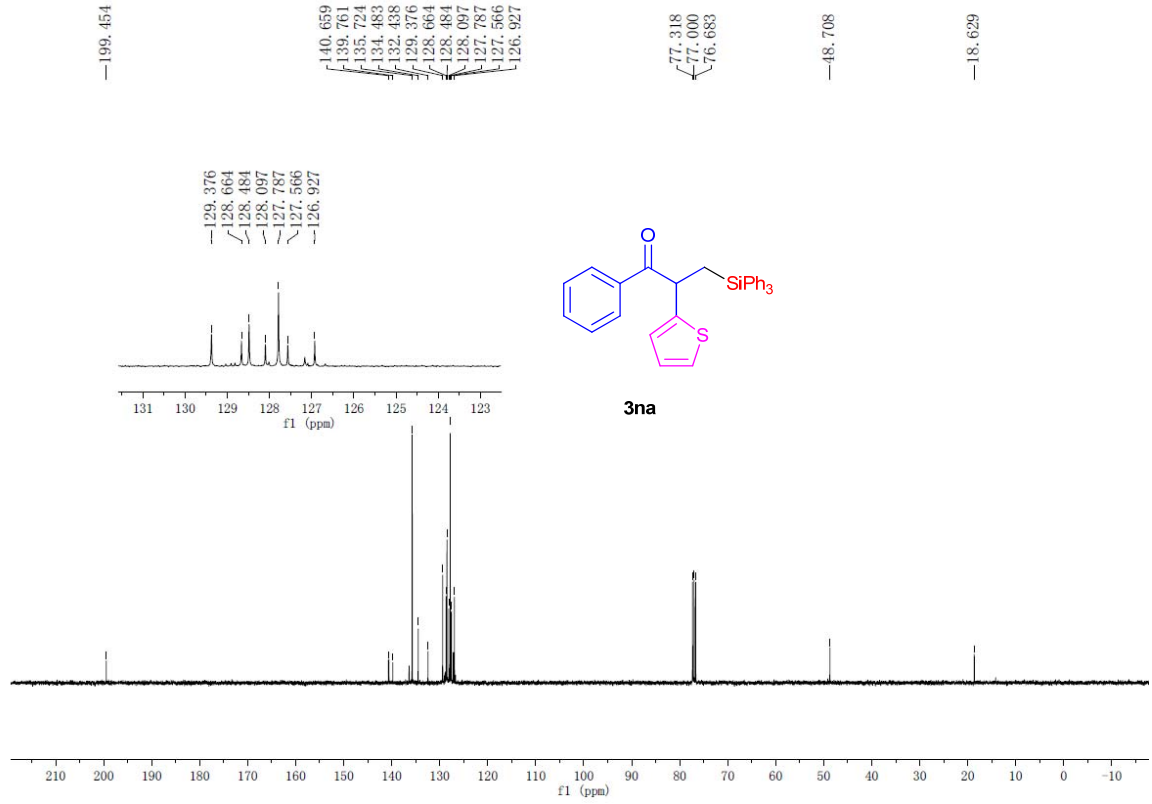

SiPh3
O
3ka
f1 (ppm)

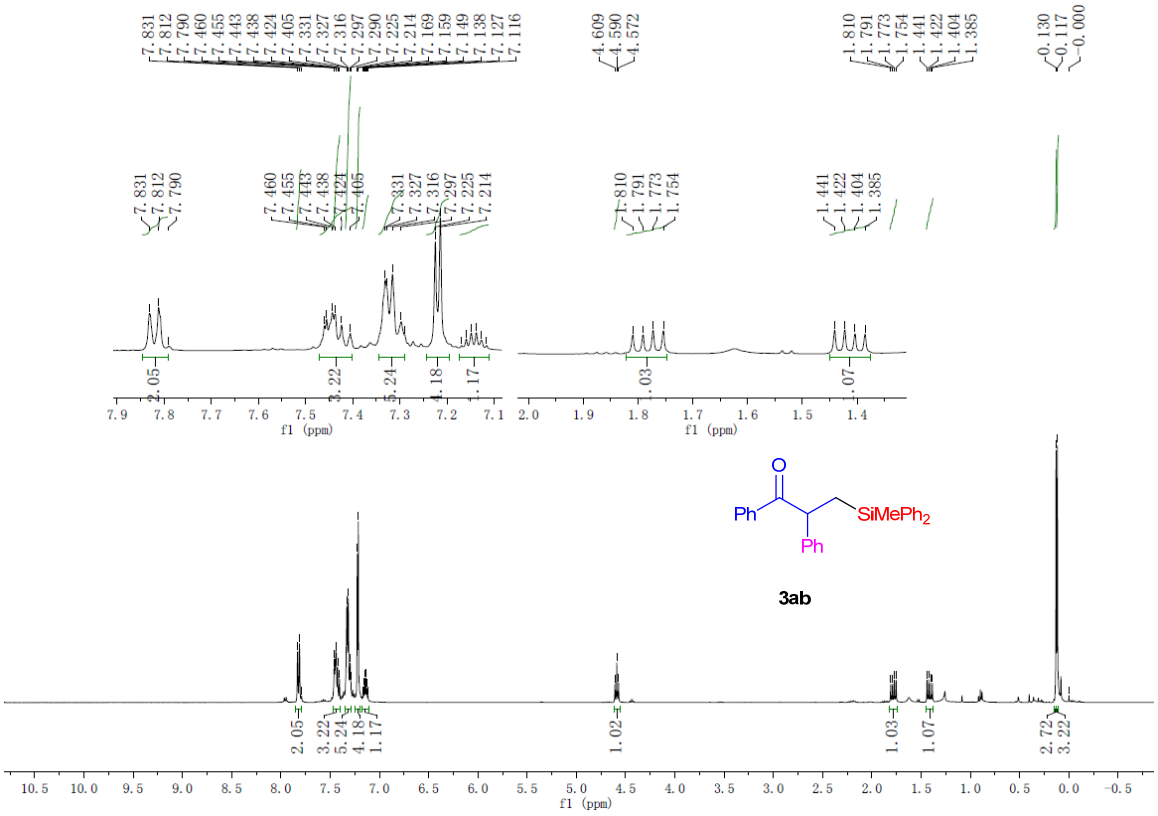

MeO
SiPh3
F
3la
OMe
3la'
f1 (ppm)

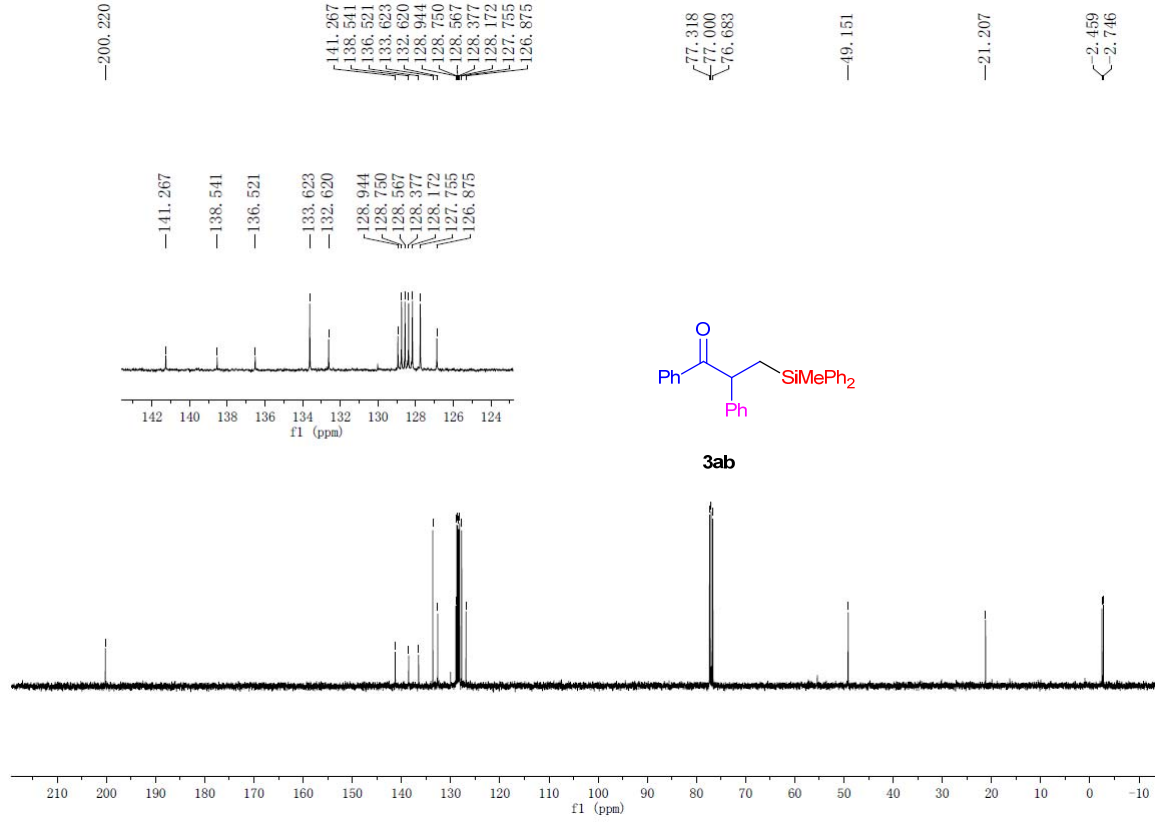

3ma
SiPh3
O
N
f1 (ppm)

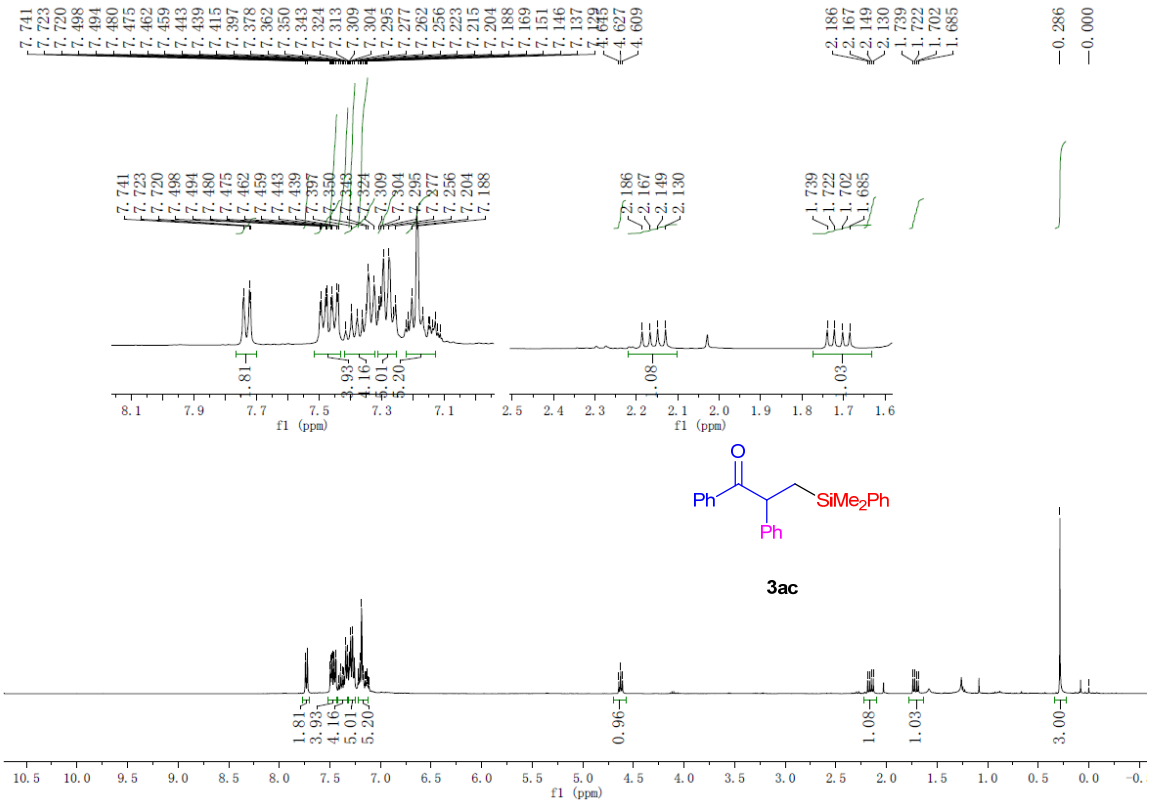

3ma
SiPh3
O
N
f1 (ppm)

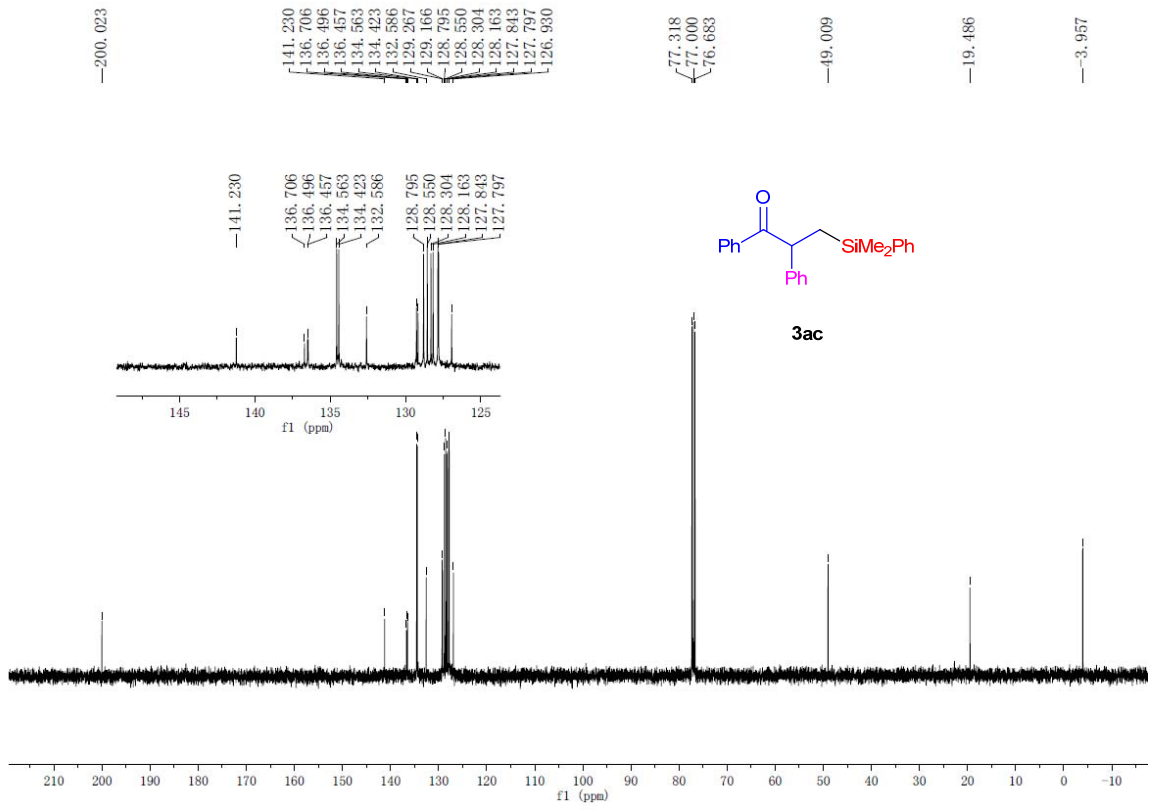

7.659
7.636
7.617
7.513
7.491
7.474
7.473
7.394
7.374
7.355
7.348
7.331
7.330
7.322
7.314
7.307
7.296
7.283
7.274
7.255
7.248
7.237
7.234
7.228
7.214
7.194
4.852
4.837
4.832
4.817
2.673
2.653
2.635
2.615
2.020
2.004
1.981
1.966
0.000
SiPh3
S
3na
1.96
6.24
3.28
13.33
1.00
0.97
1.30
f1 (ppm)

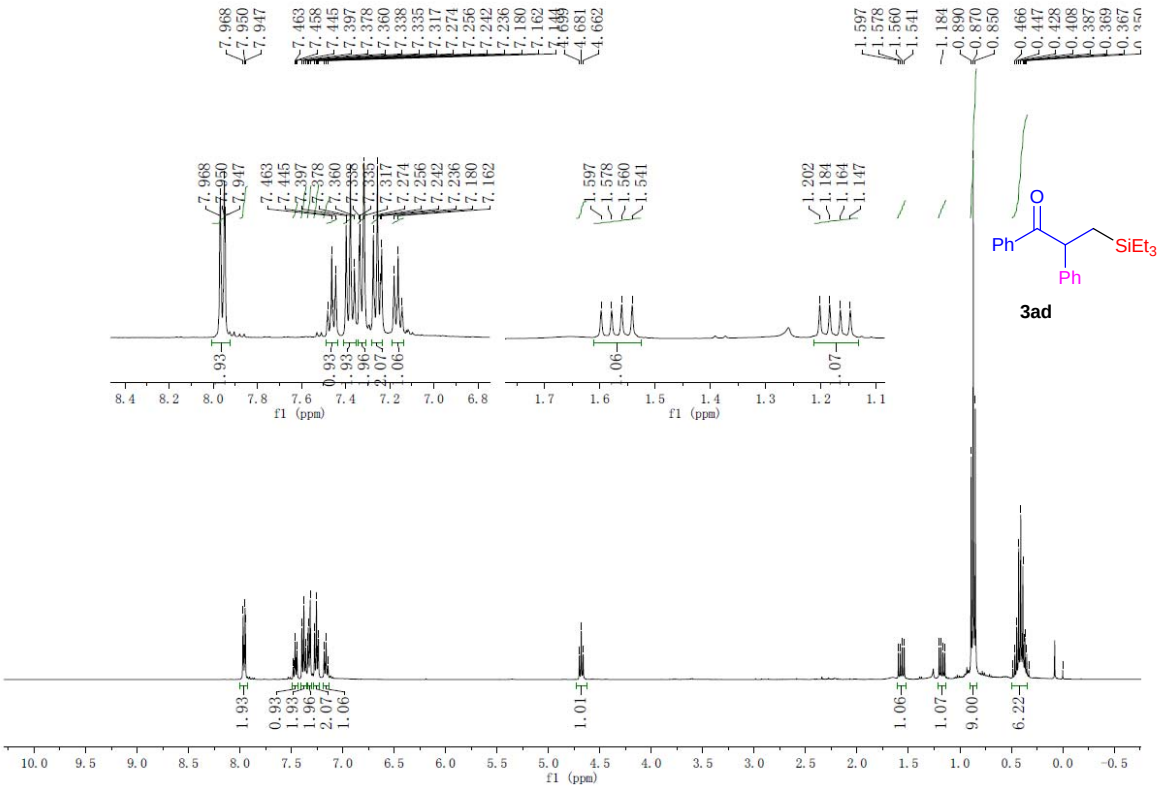

199.454
140.659
139.761
135.724
134.483
132.438
129.376
128.664
128.484
128.097
127.787
127.566
126.927
77.318
77.000
76.683
48.708
18.629
SiPh3
S
3na
f1 (ppm)

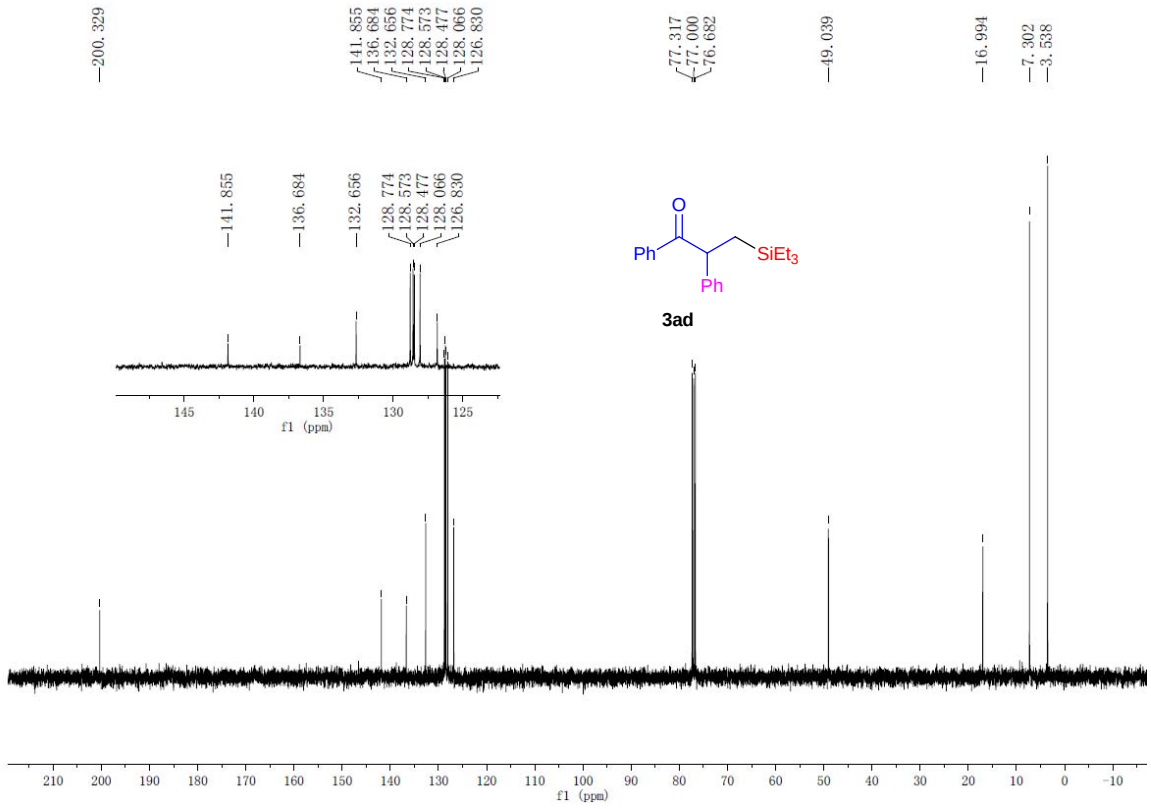

7.831
7.812
7.790
7.460
7.455
7.443
7.438
7.424
7.405
7.331
7.327
7.316
7.297
7.290
7.225
7.214
7.169
7.159
7.149
7.138
7.127
7.116
4.609
4.590
4.572
1.810
1.791
1.773
1.754
1.441
1.422
1.404
1.385
0.130
0.117
-0.000
2.05
3.22
5.24
4.18
1.17
1.03
1.07
f1 (ppm)
Ph
SiMePh2
Ph
3ab
2.05
3.22
5.24
4.18
1.17
1.02
1.03
1.07
2.72
3.22
f1 (ppm)

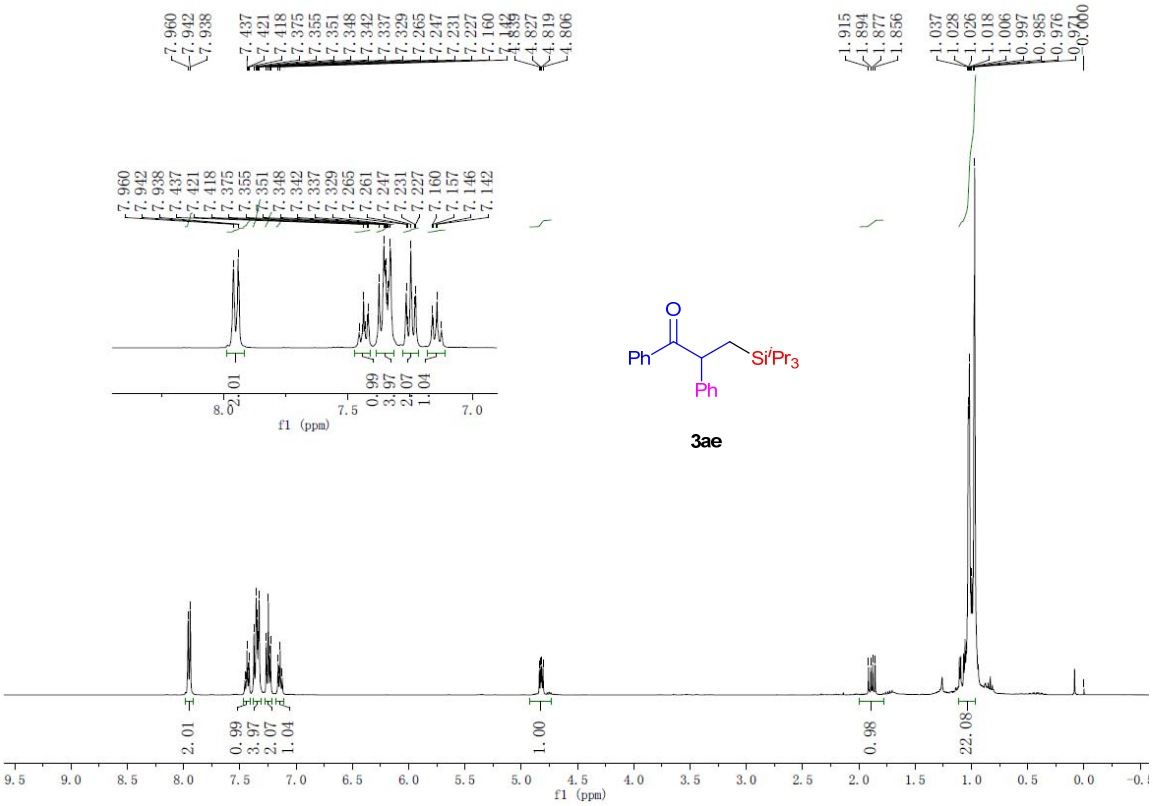

200.220
141.267
138.541
136.521
133.623
132.620
128.944
128.750
128.567
128.377
128.172
127.755
126.875
77.318
77.000
76.683
49.151
21.207
2.459
2.746
f1 (ppm)
Ph
SiMePh2
Ph
3ab
f1 (ppm)

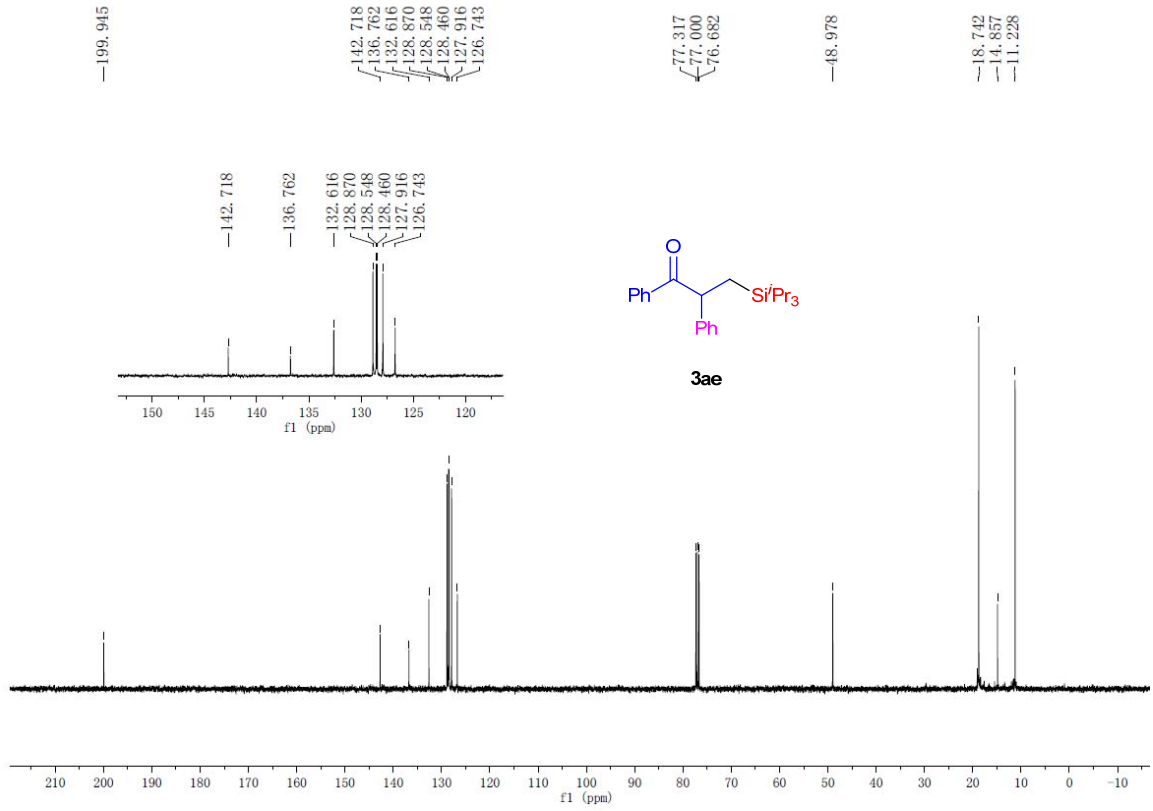

Ph
SiMe2Ph
Ph
3ac

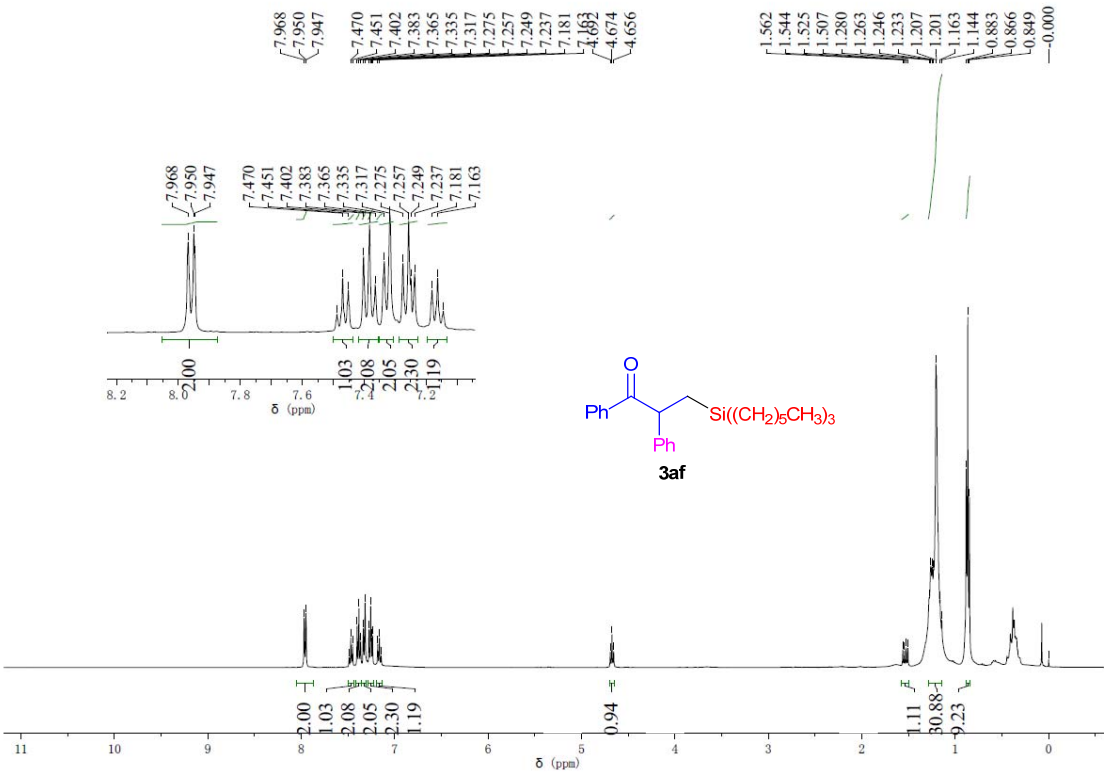

Ph
SiMe2Ph
Ph
3ac

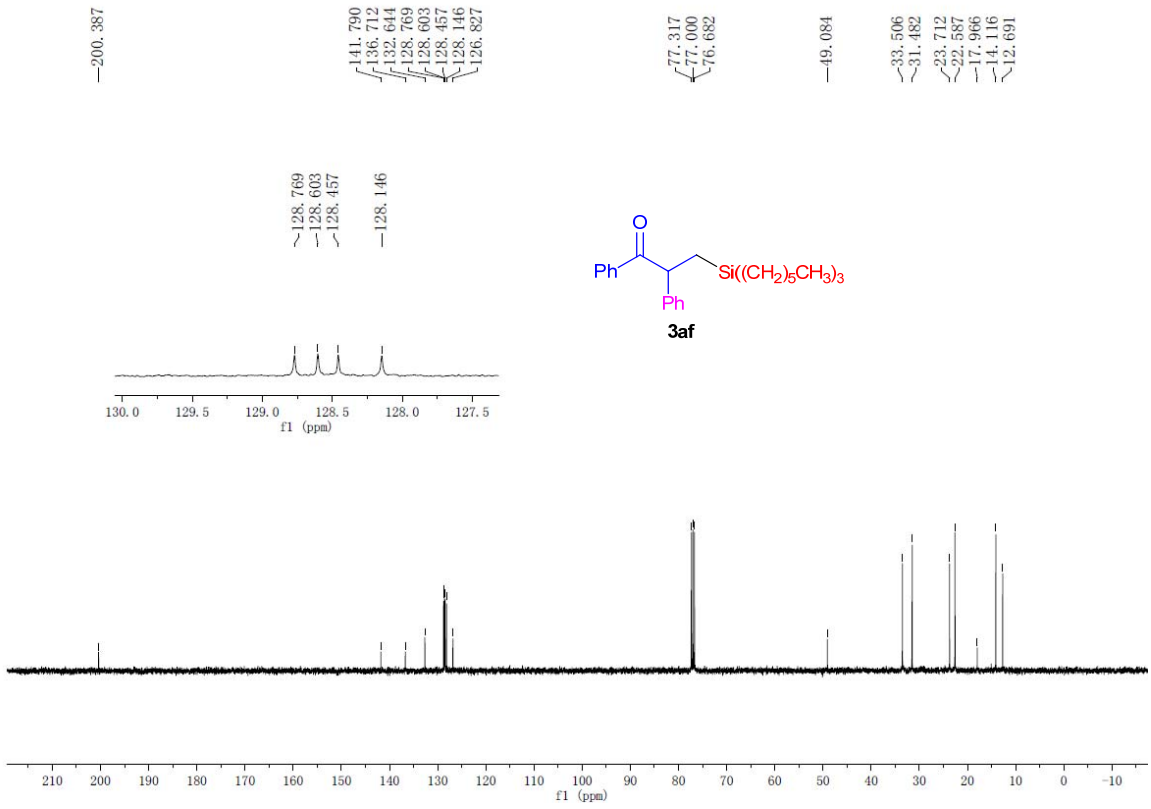

Ph
SiEt3
Ph
3ad
f1 (ppm)


Ph
SiEt3
Ph
3ad
f1 (ppm)


7.960
7.942
7.938
7.437
7.421
7.418
7.375
7.355
7.351
7.348
7.342
7.337
7.329
7.265
7.247
7.231
7.227
7.160
7.157
7.146
7.142
4.827
4.819
4.806
1.915
1.894
1.877
1.856
1.037
1.028
1.026
1.018
1.006
0.997
0.985
0.976
0.000
2.01
0.99
3.97
2.07
1.04
1.00
0.98
22.08
f1 (ppm)
Ph
O
Si^{i}Pr$_3$
Ph
3ae


199.945
142.718
136.762
132.616
128.870
128.548
128.460
127.916
126.743
77.317
77.000
76.682
48.978
18.742
14.857
11.228
f1 (ppm)
Ph
O
Si^{i}Pr$_3$
Ph
3ae


7.968
7.950
7.947
7.470
7.451
7.402
7.383
7.365
7.335
7.317
7.275
7.257
7.249
7.237
7.181
7.163
4.674
4.656
1.562
1.544
1.525
1.507
1.280
1.263
1.246
1.233
1.207
1.201
1.163
1.144
0.883
0.866
0.849
-0.000
2.00
1.03
2.08
2.05
2.30
1.19
0.94
1.11
30.88
9.23
δ (ppm)
Ph
O
Ph
Si((CH2)5CH3)3
3af


200.387
141.790
136.712
132.644
128.769
128.603
128.457
128.146
126.827
77.317
77.000
76.682
49.084
33.506
31.482
23.712
22.587
17.966
14.116
12.691
128.769
128.603
128.457
128.146
f1 (ppm)
Ph
O
Ph
Si((CH2)5CH3)3
3af