Supplementary information

An Entry to 1,3-Azasiline-Fused Quinolinones by Oxidative Heteroannulation Involving Silyl C(sp^3)-H Functionalization

Li-Jun Wu, Yuan Yang, Ren-Jie Song*, Jiang-Xi Yu, Jin-Heng Li,* and De-Liang He*

State Key Laboratory of Chemo/Biosensing and Chemometrics, College of Chemistry and Chemical Engineering, Hunan University, Changsha 410082, China, state Key Laboratory of Jiangxi Province for Persistent Pollutants Control and Resources Recycle, Nanchang Hangkong University, Nanchang 330063, China, and State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000, China

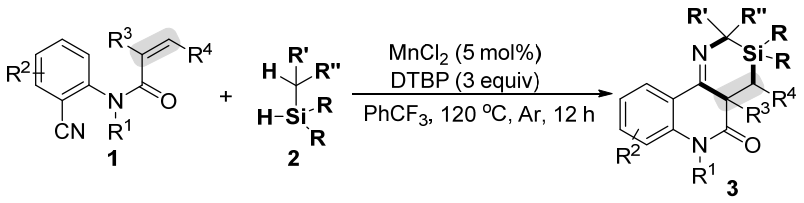
Email: srj0731@hnu@hnu.edu.cn, jhli@hnu.edu.cn and delianghe@hnu.edu.cn

List of Contents

(A) Typical experimental procedure

^{1}H NMR,^{13}C NMR and ^{19}F NMR spectra were recorded on a Bruker 400 MHz advance spectrometer at room temperature in $CDCl_3$ with tetramethylsilane as internal standard. Low-resolution mass spectra (LRMS) data were measured on GCMS-QP2010 Ultra. High-resolution mass spectra (HRMS) was recorded on an electrospray ionization (ESI) apparatus using time-of-flight (TOF) mass spectrometry. Melting Point were recorded on Hanon MP100 Apparatus. All products were identified by ^{1}H and ^{13}C NMR, LRMS, HRMS. Unless otherwise noted, all reactions were carried out using standard Schlenk techniques, and all starting materials and solvents were commercially available and were used without further purification. Column chromatography was performed on silica gel (300-400 mesh) using petroleum ether (PE)/ethyl acetate (EA). Substrates **1a-r** were prepared according to the literatures.[1]

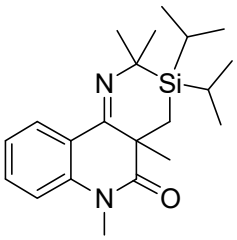
(a) Typical Experimental Procedure for Synthesis of 1,3-Azasiline-Fused Quinolinones 3：



To a Schlenk tube were added alkenes **1** (0.2 mmol), silanes **2** (0.6 mol), $MnCl_2$ (5 mol%; 0.01 mmol), DTBP (3 equiv; 0.6 mmol) and $PhCF_3$ (2 mL). Then the tube was charged with argon, and was stirred at 120 ^{o}C for 12 h until complete consumption of starting material as monitored by TLC and/or GC-MS analysis. After the reaction was finished, the concentrated in vacuum, and the resulting residue was purified by silica gel column chromatography (hexane/ethyl acetate) to afford the desired products **3**.

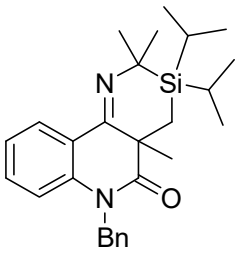
(B) Analytical data

3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3aa):



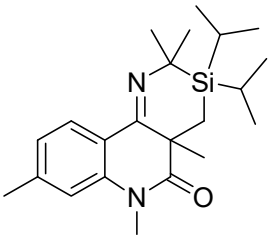
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.84 (d, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.97 (d, *J* = 8.0 Hz, 1H), 3.41 (s, 3H), 2.38 (d, *J* = 15.6 Hz, 1H), 1.44 (s, 3H), 1.33 (s, 3H), 1.21 (s, 3H), 1.18-1.12 (m, 6H), 1.08-1.05 (m, 5H), 0.84 (s, 3H), 0.76 (d, *J* = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.4, 161.2, 139.2, 130.3, 127.1, 126.6, 123.3, 113.5, 48.4, 45.8, 31.1, 30.7, 29.1, 28.4, 19.5, 19.0, 18.9, 18.9, 11.6, 10.7, 10.5; LRMS (EI, 70 eV) *m/z* (%): 356 (M^+, 24), 299 (100), 170 (13); HRMS *m/z* (ESI) calcd for $C_{21}H_{33}N_2OSi$ ($[M+H]^+$) 357.2357, found 357.2371.

6-benzyl-3,3-diisopropyl-2,2,4a-trimethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ba):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.85 (d, *J* = 7.6 Hz, 1H), 7.30-7.18 (m, 6H), 7.05 (t, *J* = 7.2 Hz, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 5.42 (d, *J* = 16.4 Hz, 1H), 4.98 (d, *J* = 16.4 Hz, 1H), 2.47 (d, *J* = 15.6 Hz, 1H), 1.47 (s, 6H), 1.23 (s, 3H), 1.19-1.15 (m, 6H), 1.10-1.05 (m, 5H), 0.89 (s, 3H), 0.79 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.6, 161.1, 138.5, 136.9, 130.3, 128.7, 127.3, 127.1, 126.7, 126.3, 123.4, 114.4, 48.5, 47.2, 46.0, 31.3, 29.1, 28.5, 19.6, 19.0, 18.9, 18.9, 11.7, 10.7, 10.6; LRMS (EI, 70 eV) *m/z* (%): 432 (M^+, 6), 91 (100), 59 (18); HRMS *m/z* (ESI) calcd for $C_{27}H_{37}N_2OSi$ ($[M+H]^+$) 433.2670, found 433.2683.

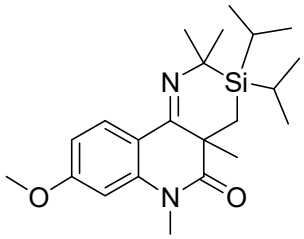
3,3-diisopropyl-2,2,4a,6,8-pentamethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3da):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.73 (d, *J* = 8.0 Hz, 1H), 6.89 (d, *J* = 7.6 Hz, 1H), 6.78 (s, 1H), 3.40 (s, 3H), 2.38 (s, 3H), 2.36 (d, *J* = 15.6 Hz, 1H), 1.43 (s, 3H), 1.33 (s, 3H), 1.20 (s, 3H), 1.17-1.13 (m, 6H), 1.09-1.04 (m, 5H), 0.83 (s,

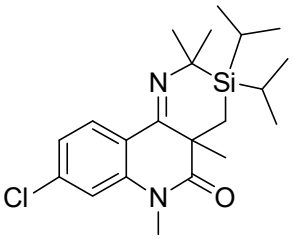
3H), 0.75 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.6, 161.1, 140.6, 139.0, 127.1, 124.0, 124.0, 114.2, 48.3, 45.6, 31.2, 30.7, 29.1, 28.4, 21.7, 19.6, 19.0, 18.9, 11.6, 10.7, 10.5; LRMS (EI, 70 eV) *m/z* (%): 370 (M^+, 29), 313 (100), 170 (10); HRMS *m/z* (ESI) calcd for $C_{22}H_{35}N_2OSi$ ($[M+H]^+$) 371.2513, found 371.2527.

3,3-diisopropyl-8-methoxy-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ea):



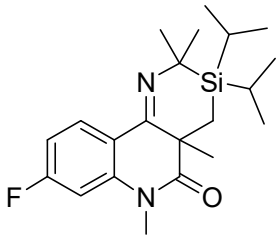
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.80 (d, *J* = 8.4 Hz, 1H), 6.63 (d, *J* = 8.4 Hz, 1H), 6.51 (s, 1H), 3.84 (s, 3H), 2.39 (s, 3H), 2.34 (d, *J* = 15.6 Hz, 1H), 1.43 (s, 3H), 1.34 (s, 3H), 1.19 (s, 3H), 1.17-1.13 (m, 6H), 1.09-1.04 (m, 5H), 0.83 (s, 3H), 0.75 (d, *J* = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.8, 173.2, 161.6, 140.5, 128.6, 119.7, 107.6, 100.5, 55.5, 48.4, 45.5, 31.4, 30.7, 29.2, 28.5, 19.6, 19.0, 18.9, 18.9, 11.7, 10.8, 10.6; LRMS (EI, 70 eV) *m/z* (%): 386 (M^+, 0.4), 213 (100), 155 (1); HRMS *m/z* (ESI) calcd for $C_{22}H_{35}N_2O_2Si$ ($[M+H]^+$) 387.2462, found 387.2473.

8-chloro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3fa):



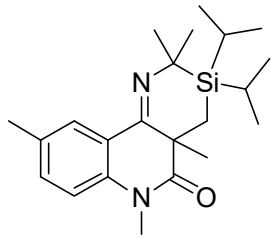
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.80 (d, *J* = 8.4 Hz, 1H), 7.06 (d, *J* = 8.4 Hz, 1H), 6.97 (s, 1H), 3.39 (s, 3H), 2.35 (d, *J* = 16.0 Hz, 1H), 1.43 (s, 3H), 1.33 (s, 3H), 1.20 (s, 3H), 1.17-1.13 (m, 6H), 1.07-1.04 (m, 5H), 0.82 (s, 3H), 0.76 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.4, 160.1, 140.2, 136.2, 128.5, 124.8, 123.2, 113.8, 48.4, 46.0, 31.1, 30.8, 29.0, 28.4, 19.6, 19.0, 18.9, 18.8, 11.6, 10.7, 10.5; LRMS (EI, 70 eV) *m/z* (%): 393 (M^++2, 3), 391 (M^+, 10), 333 (100), 170 (34); HRMS *m/z* (ESI) calcd for $C_{21}H_{32}ClN_2OSi$ ($[M+H]^+$) 391.1967, found 391.1981.

8-fluoro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino-[5,6-c]quinolin-5(3H)-one (3ga):



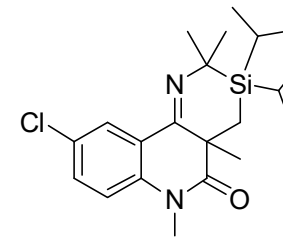
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.84 (t, *J* = 7.6 Hz, 1H), 6.78 (t, *J* = 7.6 Hz, 1H), 6.70 (d, *J* = 10.4 Hz, 1H), 3.38 (s, 3H), 2.35 (d, *J* = 15.6 Hz, 1H), 1.43 (s, 3H), 1.34 (s, 3H), 1.20 (s, 3H), 1.18-1.14 (m, 6H), 1.10-1.04 (m, 5H), 0.83 (s, 3H), 0.77 (d, *J* = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.5, 164.2 (d, *J* = 246.0 Hz), 160.0, 140.7 (d, *J* = 10.5 Hz), 129.1 (d, *J* = 9.7 Hz), 122.5 (d, *J* = 3.0 Hz), 109.7 (d, *J* = 21.2 Hz), 101.2 (d, *J* = 27.0 Hz), 48.4, 45.8, 31.2, 30.8, 29.1, 28.4, 19.6, 19.0, 18.9, 11.6, 10.7, 10.5; LRMS (EI, 70 eV) *m/z* (%): 374 (M^+, 24), 317 (100), 218 (24); HRMS *m/z* (ESI) calcd for $C_{21}H_{32}FN_2OSi$ ($[M+H]^+$) 375.2262, found 375.2273.

3,3-diisopropyl-2,2,4a,6,9-pentamethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ha):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.62 (s, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 6.86 (d, *J* = 8.4 Hz, 1H), 3.38 (s, 3H), 2.38 (d, *J* = 16.4 Hz, 1H), 2.34 (s, 3H), 1.44 (s, 3H), 1.32 (s, 3H), 1.21 (s, 3H), 1.18-1.14 (m, 6H), 1.10-1.05 (m, 5H), 0.84 (s, 3H), 0.75 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.1, 161.6, 136.9, 132.7, 131.0, 127.4, 126.4, 113.5, 48.3, 45.8, 31.0, 30.7, 29.1, 28.5, 20.6, 19.5, 19.0, 18.9, 18.9, 11.6, 10.8, 10.5; LRMS (EI, 70 eV) *m/z* (%): 370 (M^+, 2), 197 (100), 103 (5); HRMS *m/z* (ESI) calcd for $C_{22}H_{35}N_2OSi$ ($[M+H]^+$) 371.2513, found 371.2521.

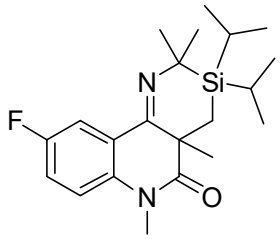
9-chloro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ia):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.82 (s, 1H), 7.32 (d, *J* = 7.6 Hz, 1H), 6.91 (d, *J* = 8.8 Hz, 1H), 3.39 (s, 3H), 2.36 (d, *J* = 15.6 Hz, 1H), 1.44 (s, 3H), 1.33 (s, 3H), 1.21 (s, 3H), 1.17-1.14 (m, 6H), 1.08-1.04 (m, 5H), 0.82 (s, 3H), 0.76 (d, *J* = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.0, 160.0, 137.8, 130.0, 128.6, 127.8, 126.9, 114.9, 48.3, 46.2, 31.0, 30.8, 28.9, 28.3, 19.5, 18.9, 18.8,

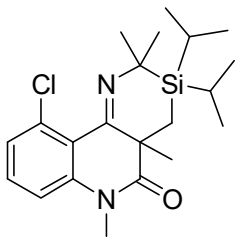
18.8, 11.6, 10.6, 10.5; LRMS (EI, 70 eV) *m/z* (%): 393 (M^++2, 3), 391 (M^+, 8), 333 (100), 170 (36); HRMS *m/z* (ESI) calcd for $C_{21}H_{32}ClN_2OSi$ ($[M+H]^+$) 391.1967, found 391.1983.

9-fluoro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ja):



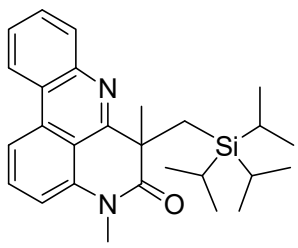
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.57 (d, *J* = 11.6 Hz, 1H), 7.08-7.04 (m, 1H), 6.94-6.91 (m, 1H), 3.40 (s, 3H), 2.37 (d, *J* = 18.0 Hz, 1H), 1.44 (s, 3H), 1.34 (s, 3H), 1.20 (s, 3H), 1.18-1.14 (m, 6H), 1.06-1.04 (m, 5H), 0.82 (s, 3H), 0.76 (d, *J* = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.0, 160.4, 158.9 (d, *J* = 235.4 Hz), 135.4 (d, *J* = 10.5 Hz), 128.2 (d, *J* = 6.9 Hz), 116.8 (d, *J* = 23.1 Hz), 114.9 (d, *J* = 7.4 Hz), 113.7 (d, *J* = 23.8 Hz), 48.2, 46.1, 31.0, 30.9, 29.0, 28.3, 19.5, 19.0, 18.8,18.8, 11.6, 10.7, 10.5; LRMS (EI, 70 eV) *m/z* (%): 374 (M^+, 10), 317 (100), 116 (36); HRMS *m/z* (ESI) calcd for $C_{21}H_{32}FN_2OSi$ ($[M+H]^+$) 375.2262, found 375.2289.

10-chloro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ka):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.22 (d, *J* = 8.0 Hz, 1H), 7.16 (d, *J* = 8.0 Hz, 1H), 6.90 (d, *J* = 8.0 Hz, 1H), 3.35 (s, 3H), 2.21 (d, *J* = 15.6 Hz, 1H), 1.40 (s, 3H), 1.37 (s, 3H), 1.27 (s, 3H), 1.18-1.14 (m, 6H), 1.09-1.05 (m, 5H), 0.91 (s, 3H), 0.84 (d, *J* = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.1, 158.7, 141.0, 132.8, 129.4, 126.2, 125.2, 112.4, 48.7, 47.1, 31.2, 30.9, 29.3, 28.5, 28.5, 19.0, 18.9, 18.6, 11.7, 11.4, 10.5; HRMS *m/z* (ESI) calcd for $C_{21}H_{32}ClN_2OSi$ ($[M+H]^+$) 391.1967, found 391.1974.

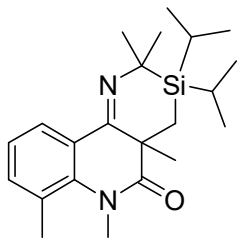
4,6-dimethyl-6-((triisopropylsilyl)methyl)-4H-pyrido[4,3,2-gh]phenanthridin-5(6H)-one (4la):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.51 (d, *J* = 8.4 Hz, 1H), 8.24 (d, *J* = 8.4 Hz, 1H), 8.12 (d, *J* = 8.4 Hz, 1H), 7.80 (t, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 7.6 Hz, 1H), 7.62 (t, *J* =

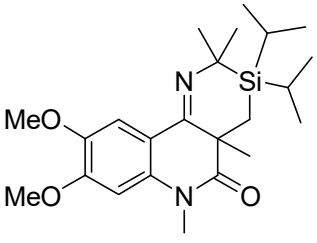
8.0 Hz, 1H), 7.19 (d, *J* = 7.6 Hz, 1H), 3.56 (s, 3H), 2.52 (d, *J* = 14.0 Hz, 1H), 1.78 (d, *J* = 14.0 Hz, 1H), 1.75 (s, 3H), 1.05 (s, 2H), 0.86-0.83 (m, 16H), 0.81-0.74 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.8, 160.7, 144.7, 139.0, 133.3, 131.6, 129.6, 129.0, 126.4, 122.8, 122.5, 115.9, 111.7, 110.6, 49.7, 35.6, 29.7, 21.4, 18.7, 18.6, 11.5; LRMS (EI, 70 eV) *m/z* (%): 432 (M^+, 0.1), 389 (100), 152 (8); HRMS *m/z* (ESI) calcd for $C_{27}H_{37}N_2OSi$ ($[M+H]^+$) 433.2670, found 433.2682.

3,3-diisopropyl-2,2,4a,6,7-pentamethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ma):



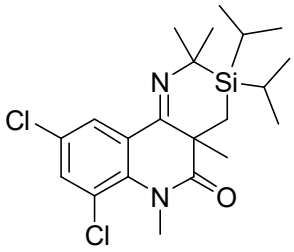
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.54 (d, *J* = 7.6 Hz, 1H), 7.18 (d, *J* = 7.6 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 1H), 3.33 (s, 3H), 2.40 (d, *J* = 15.6 Hz, 1H), 2.40 (s, 3H), 1.43 (s, 3H), 1.26 (s, 3H), 1.18 (s, 3H), 1.16-1.13 (m, 6H), 1.09-1.05 (m, 5H), 0.85 (s, 3H), 0.68 (d, *J* = 15.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.6, 162.4, 139.9, 133.9, 130.2, 126.0, 124.8, 124.5, 48.4, 45.8, 37.5, 30.1, 28.8, 28.6, 21.1, 19.2, 19.0, 18.9, 18.6, 11.6, 11.1, 10.5; LRMS (EI, 70 eV) *m/z* (%): 370 (M^+, 43), 313 (100), 157 (11); HRMS *m/z* (ESI) calcd for $C_{22}H_{35}N_2OSi$ ($[M+H]^+$) 371.2513, found 371.2519.

3,3-diisopropyl-8,9-dimethoxy-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3na):



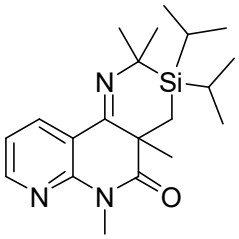
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.42 (s, 1H), 6.52 (s, 1H), 3.95 (s, 3H), 3.93 (s, 3H), 3.41 (s, 3H), 2.36 (d, *J* = 16.0 Hz, 1H), 1.44 (s, 3H), 1.35 (s, 3H), 1.21 (s, 3H), 1.18-1.14 (m, 6H), 1.10-1.04 (m, 5H), 0.84 (s, 3H), 0.76 (d, *J* = 16.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.4, 160.9, 150.8, 145.0, 133.3, 118.7, 109.9, 98.4, 56.1, 56.1, 48.2, 45.5, 31.5, 30.8, 29.2, 28.4, 19.6, 19.0, 18.9, 18.8, 11.7, 10.7, 10.6; LRMS (EI, 70 eV) *m/z* (%): 416 (M^+, 34), 359 (100), 170 (20); HRMS *m/z* (ESI) calcd for $C_{23}H_{37}N_2OSi$ ($[M+H]^+$) 417.2568, found 417.2583.

7,9-dichloro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3oa):



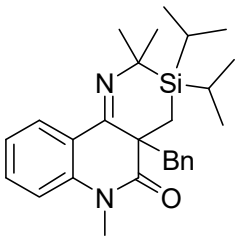
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.61 (s, 1H), 7.39 (s, 1H), 3.44 (s, 3H), 2.39 (d, *J* = 15.6 Hz, 1H), 1.44 (s, 3H), 1.28 (s, 3H), 1.19 (s, 3H), 1.16-1.13 (m, 6H), 1.10-1.06 (m, 5H), 0.83 (s, 3H), 0.69 (d, *J* = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.8, 160.3, 136.8, 132.7, 132.1, 130.0, 125.7, 122.7, 48.4, 46.5, 37.4, 30.0, 28.6, 28.5, 19.1, 18.9, 18.8, 18.5, 11.5, 11.1, 10.4; HRMS *m/z* (ESI) calcd for $C_{21}H_{37}Cl_2N_2OSi$ ($[M+H]^+$) 425.1577, found 425.1584.

3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c][1,8]naphthyridin-5(3H)-one (3pa):



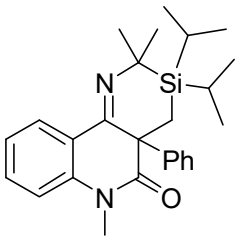
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.37 (d, *J* = 3.6 Hz, 1H), 8.17 (d, *J* = 7.6 Hz, 1H), 7.02 (t, *J* = 6.0 Hz, 1H), 3.54 (s, 3H), 2.39 (d, *J* = 16.0 Hz, 1H), 1.44 (s, 3H), 1.37 (s, 3H), 1.20 (s, 3H), 1.18-1.14 (m, 6H), 1.11-1.04 (m, 5H), 0.80 (s, 3H), 0.78 (d, *J* = 15.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.0, 159.7, 150.9, 148.9, 135.3, 121.3, 118.8, 48.6, 46.4, 31.5, 29.3, 29.1, 28.3, 19.6, 18.9, 18.8, 18.8, 11.6, 10.5, 10.4; LRMS (EI, 70 eV) *m/z* (%): 357 (M^+, 28), 300 (100), 201 (24); HRMS *m/z* (ESI) calcd for $C_{20}H_{32}N_3OSi$ ($[M+H]^+$) 358. 2309, found 358. 2315.

4a-benzyl-3,3-diisopropyl-2,2,6-trimethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3qa):



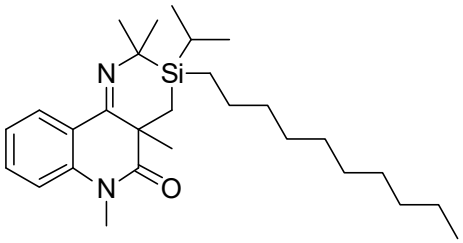
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.91 (d, *J* = 7.2 Hz, 1H), 7.40 (t, *J* = 3.6 Hz, 1H), 7.21-7.16 (m, 4H), 7.00-6.97 (m, 3H), 3.44 (s, 3H), 3.03 (d, *J* = 13.2 Hz, 1H), 2.65 (d, *J* = 13.2 Hz, 1H), 2,20 (d, *J* = 15.2 Hz, 1H), 1.33 (s, 3H), 1.08-1.01 (m, 12H), 0.75-0.74 (m, 3H), 0.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.0, 159.8, 139.2, 136.1, 130.6, 130.3, 127.9, 127.5, 127.4, 127.1, 123.6, 113.6, 54.9, 47.3, 45.6, 30.8, 29.2, 27.2, 19.3, 18.7, 17.7, 12.3, 11.6, 10.1, 5.8; LRMS (EI, 70 eV) *m/z* (%): 432 (M^+, 17), 299 (100), 91 (61); HRMS *m/z* (ESI) calcd for $C_{27}H_{37}N_2OSi$ ($[M+H]^+$) 433.2670, found 433.2685.

3,3-diisopropyl-2,2,6-trimethyl-4a-phenyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ra):



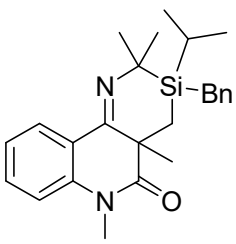
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.90 (d, *J* = 7.6 Hz, 1H), 7.21 (t, *J* = 7.6 Hz, 1H), 7.14-7.01 (m, 6H), 6.75 (d, *J* = 8.4 Hz, 1H), 3.38 (s, 3H), 2.69 (d, *J* = 15.6 Hz, 1H), 1.51 (s, 3H), 1.24 (s, 3H), 1.12-1.05 (m, 8H), 0.98-0.92 (m, 7H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 170.8, 159.1, 144.4, 138.7, 130.2, 128.5, 128.2, 127.0, 126.6, 126.1, 123.3, 113.9, 57.9, 46.1, 31.0, 29.2, 28.1, 19.4, 19.0, 18.8, 18.6, 17.7, 15.1, 11.9, 10.6; LRMS (EI, 70 eV) *m/z* (%): 418 (M^+, 32), 299 (100), 144 (56); HRMS *m/z* (ESI) calcd for $C_{26}H_{35}N_2OSi$ ($[M+H]^+$) 419.2513, found 419.2519.

3-decyl-3-isopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ab):



dr = >20:1; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.81 (d, *J* = 7.6 Hz, 1H), 7.37 (t, *J* = 7.6 Hz, 1H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.96 (d, *J* = 8.0 Hz, 1H), 3.40 (s, 3H), 2.62 (d, *J* = 15.6 Hz, 1H), 1.37 (s, 3H), 1.32 (s, 3H), 1.21-0.99 (m, 25H), 0.88-0.0.80 (m, 5H), 0.65-0.57 (m, 1H), 0.48-0.41(m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.2, 161.4, 139.3, 130.4, 127.0, 126.8, 123.3, 113.5, 48.5, 45.5, 34.1, 31.9, 30.7, 30.7, 29.6, 29.5, 29.3, 29.1, 29.0, 27.8, 24.2, 22.7, 18.7, 18.5, 14.1, 11.9, 11.4, 8.6; LRMS (EI, 70 eV) *m/z* (%): 454 (M^+, 2), 313 (100),218 (10); HRMS *m/z* (ESI) calcd for $C_{28}H_{47}N_2OSi$ ($[M+H]^+$) 455.3452, found 455.3463.

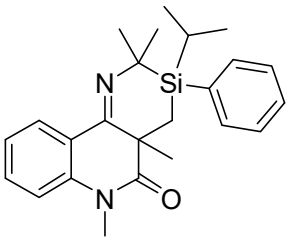
3-benzyl-3-isopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ac):



dr = >20:1; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.86 (d, *J* = 8.0 Hz, 1H), 7.60-7.58 (m, 2H), 7.41-7.58 (m, 4H), 7.12 (t, *J* = 7.6 Hz, 1H), 7.00 (d, *J* = 8.0 Hz, 1H), 3.34 (s, 3H), 2.62 (d, *J* = 15.6 Hz, 1H), 1.53 (s, 3H), 1.35 (s, 3H), 1.30-1.24 (m, 1H), 1.19 (d, *J* = 15.6 Hz, 1H), 1.12 (s, 3H), 1.01-0.96 (m, 5H), 0.88-0.85 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.2, 161.5, 139.2, 134.7, 134.2, 130.5,

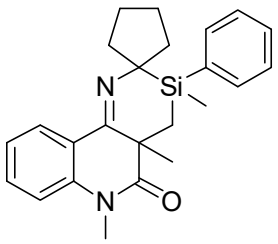
129.2, 127.8, 127.2, 126.6, 123.4, 113.6, 48.7, 45.4, 31.1, 30.8, 28.7, 28.4, 18.5, 18.1, 10.9, 10.3; LRMS (EI, 70 eV) *m/z* (%): 404 (M^+, 42), 313 (100), 91 (64); HRMS *m/z* (ESI) calcd for $C_{25}H_{33}N_2OSi$ ($[M+H]^+$) 405.2357, found 405.2363.

3-isopropyl-2,2,4a,6-tetramethyl-3-phenyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ad)：



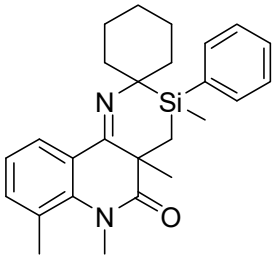
dr = 1.1:1**;** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.88-7.82 (m, 1H), 7.39-7.34 (m, 1H), 7.26-7.21 (m, 1H), 7.12-7.03 (m, 4H), 6.70-6.92 (m, 2H), 3.40 (s, 1.4H), 3.35 (s, 1.6H), 2.35-2.28 (m, 1H), 2.15-2.14 (m, 1H), 1.49 (s, 1H), 1.35-1.19 (m, 7H), 1.11-1.09 (m, 1H), 1.03-0.93 (m, 6H), 0.79-0.77 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.2, 173.1, 161.3, 161.3, 139.3, 139.2, 130.5, 130.2, 128.8, 128.6, 128.5, 128.4, 128.3, 128.1, 128.0, 127.7, 127.2, 127.1, 124.5, 123.9, 123.3, 123.1, 113.6, 113.4, 48.6, 48.1, 45.5, 45.5, 30.9, 30.8, 30.7, 30.6, 30.5, 19.8, 18.6, 18.4, 18.1, 18.0, 17.8, 11.20, 11.7, 11.6, 10.9; LRMS (EI, 70 eV) *m/z* (%): 390 (M^+, 0.1), 183 (100), 218 (10); HRMS *m/z* (ESI) calcd for $C_{24}H_{31}N_2OSi$ ($[M+H]^+$) 391.2200, found 391.2215.

3',4a',6'-trimethyl-3'-phenyl-4',4a'-dihydro-3'H-spiro[cyclopentane-1,2'-[1,3]azasilino[5,6-c]quinolin]-5'(6'H)-one (3ae) :



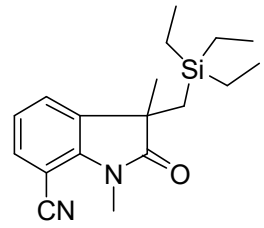
dr = 1.1:1; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.02-7.95 (m, 1H), 7.75-7.68 (m, 2H), 7.54-7.42 (m, 4H), 7.29-7.24 (m, 1H), 7.16-7.14 (m, 1H), 3.57 (s, 1.6H), 3.54 (s, 1.4H), 2.48 (d, *J* = 15.2 Hz, 0.5H), 2.30 (d, *J* = 15.2 Hz, 0.5H), 2.12 - 1.94 (m, 5H), 1.74-1.67 (m, 1H), 1.53-1.39 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.0, 173.2, 160.7, 159.8, 139.5, 139.3, 135.3, 135.0, 134.6, 134.4, 134.2, 133.9, 133.5, 130.4, 129.5, 129.4, 129.4, 127.0, 126.8, 126.3, 123.3, 123.2, 113.7, 113.7, 56.2, 55.6, 48.8, 48.5, 39.7, 38.7, 30.7, 30.5, 30.2, 29.0, 27.5, 27.4, 27.0, 26.1, 25.3, 25.0, 24.8, 15.3, 14.8, -3.1, -5.0, -6.9; LRMS (EI, 70 eV) *m/z* (%): 388 (M^+, 22), 322 (100), 186 (37); HRMS *m/z* (ESI) calcd for $C_{24}H_{29}N_2OSi$ ($[M+H]^+$) 389.2044, found 389.2051.

3',4a',6',7'-tetramethyl-3'-phenyl-4',4a'-dihydro-3'H-spiro[cyclohexane-1,2'-[1,3]azasilino[5,6-c]quinolin]-5'(6'H)-one (3mf):



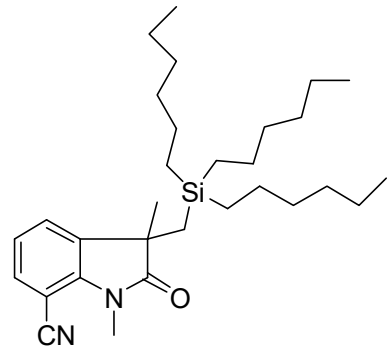
dr = 6:1; Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.62-7.50 (m, 3H), 7.40-7.37 (m, 3H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.11-7.09 (m, 1H), 3.33 (s, 2.6H), 3.54 (s, 0.4H), 2.47-2.37 (m, 4H), 1.76-1.62 (m, 4H), 1.35-1.13 (m, 7H), 0.40-0.36 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.0, 173.7, 162.6, 162.3, 140.4, 137.6, 134.9, 134.6, 134.0, 133.9, 133.5, 130.9, 129.5, 129.4, 129.3, 128.3, 127.8, 127.7, 127.6, 126.2, 124.9, 124.7, 124.7, 124.4, 49.3, 48.9, 48.8, 48.6, 37.5, 37.4, 33.5, 30.0, 27.8, 27.7, 26.8, 26.7, 26.6, 26.6, 26.5, 21.6, 20.9, 20.2, 14.1, 12.7, -3.7, -8.5; LRMS (EI, 70 eV) *m/z* (%): 416 (M^+, 32), 121 (100), 72 (9); HRMS *m/z* (ESI) calcd for $C_{26}H_{33}N_2OSi$ ($[M+H]^+$) 417.2357, found 417.2363.

1,3-dimethyl-2-oxo-3-((triethylsilyl)methyl)indoline-7-carbonitrile (5af):



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.47 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 7.2 Hz, 1H), 7.08 (t, *J* = 7.6 Hz, 1H),3.57 (s, 3H), 1.41 (s, 3H), 1.39 (d, *J* = 15.2 Hz, 1H), 1.17 (d, *J* = 14.8 Hz, 1H), 0.77 (t, *J* = 8.0 Hz, 9H), 0.25-0.04 (m, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 180.9, 144.6, 137.4, 132.2, 126.9, 122.2, 117.2, 92.9, 44.9, 28.5, 27.7, 22.3, 7.1, 3.5; LRMS (EI, 70 eV) *m/z* (%): 314 (M^+, 0.5), 183 (100), 115 (3); HRMS *m/z* (ESI) calcd for $C_{18}H_{27}N_2OSi$ ($[M+H]^+$) 315.1887, found 315.1902.

1,3-dimethyl-2-oxo-3-((trihexylsilyl)methyl)indoline-7-carbonitrile (5ag):



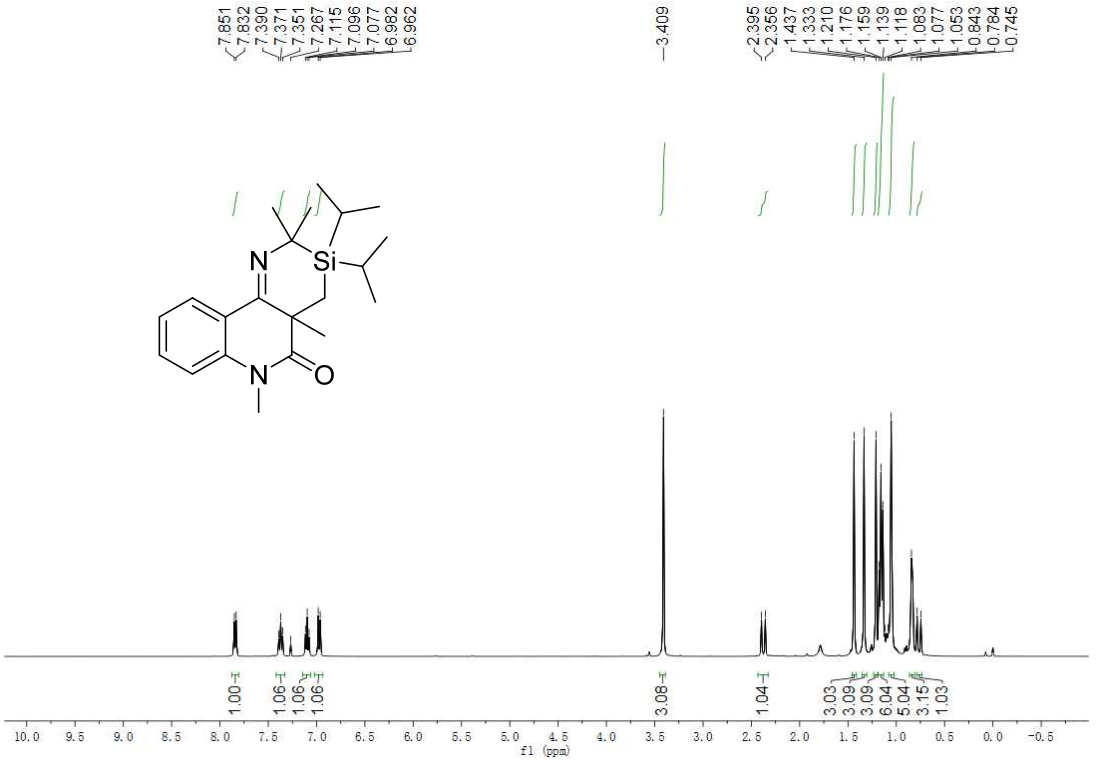
Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46 (d, *J* = 8.0 Hz, 1H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.06 (t, *J* = 7.6 Hz, 1H), 3.56 (s, 3H), 1.39 (s, 3H), 1.35-1.04 (m, 23H), 0.89-0.85 (m, 12H), 0.21-0.13 (m, 3H), 0.07-0.01 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 180.8, 144.7, 137.4, 132.1, 126.9, 122.2, 117.2, 92.9, 45.0, 33.5, 31.4, 28.6, 27.7, 23.4, 22.58, 14.1, 12.7; HRMS *m/z* (ESI) calcd for $C_{30}H_{51}N_2OSi$ ($[M+H]^+$) 483.3765, found 483.3778.

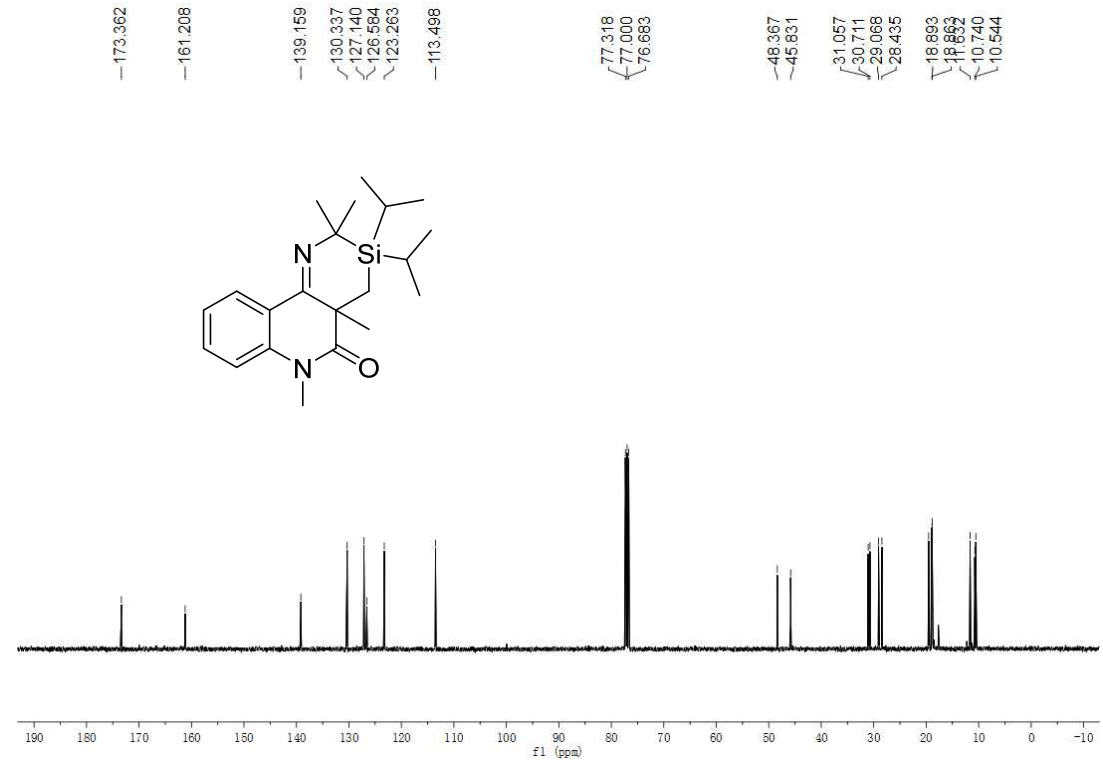
(C) Reference

(1) S. -S. Wang, H. Fu, Y. Shen, M. Sun and Y.-M. Li, *J. Org. Chem.,* 2016, **81**, 2920.

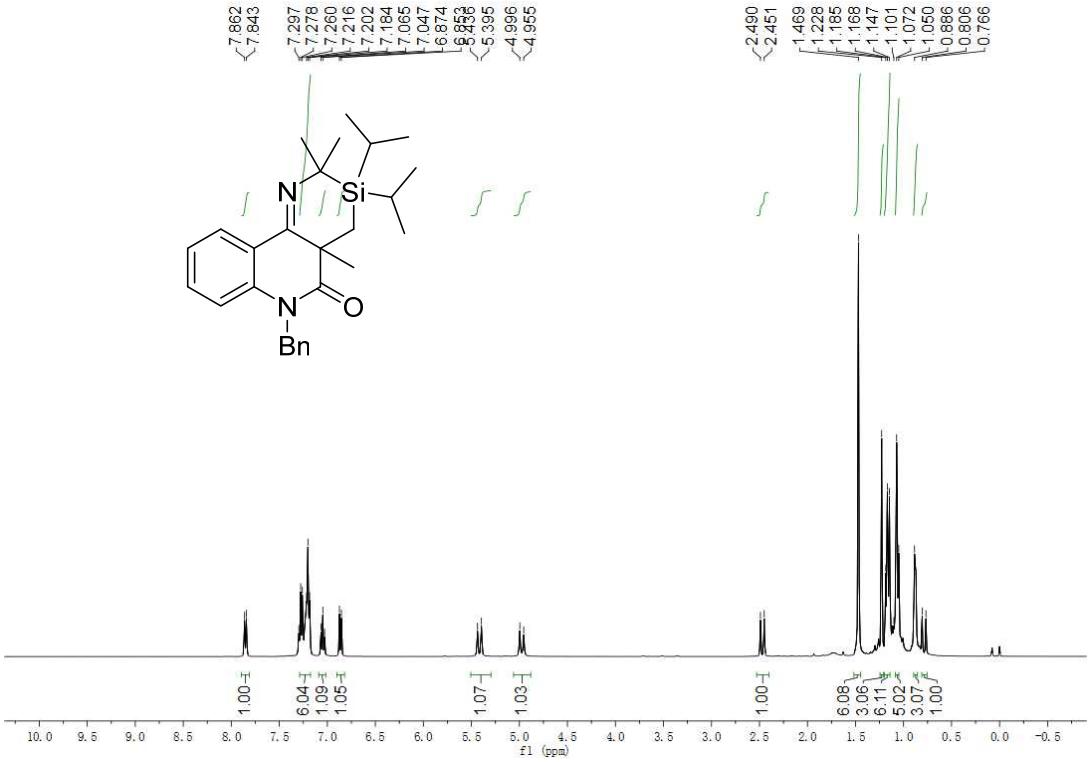
(D) Spectra

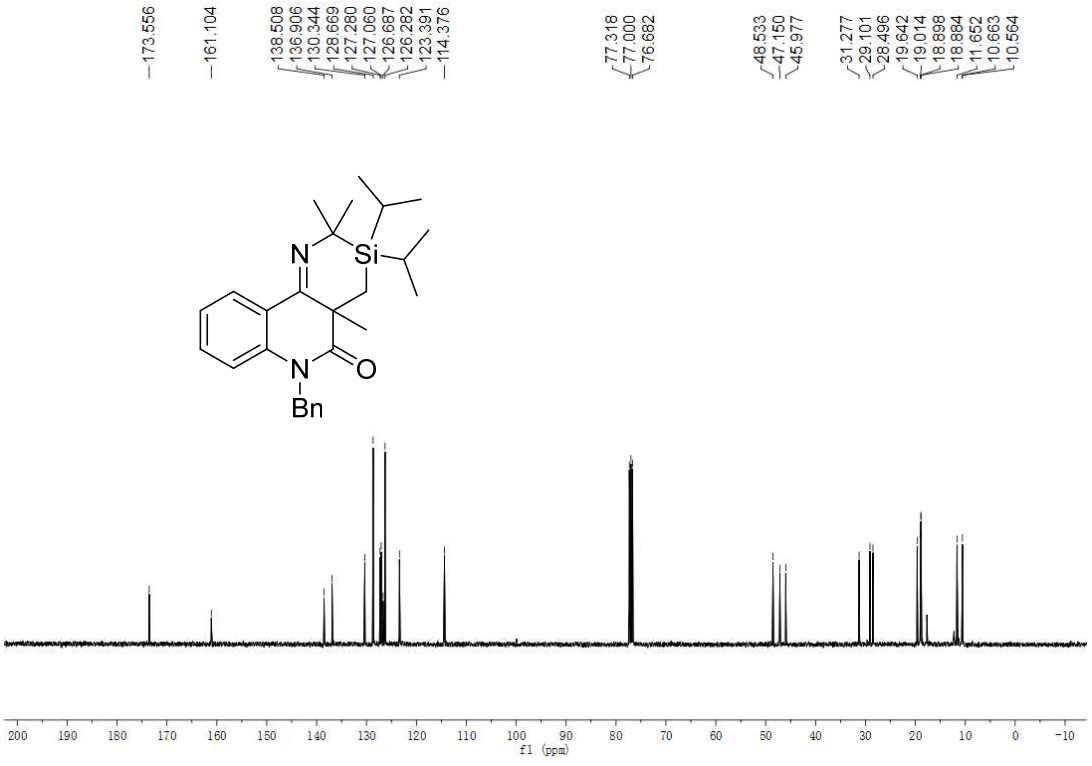
3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3aa)



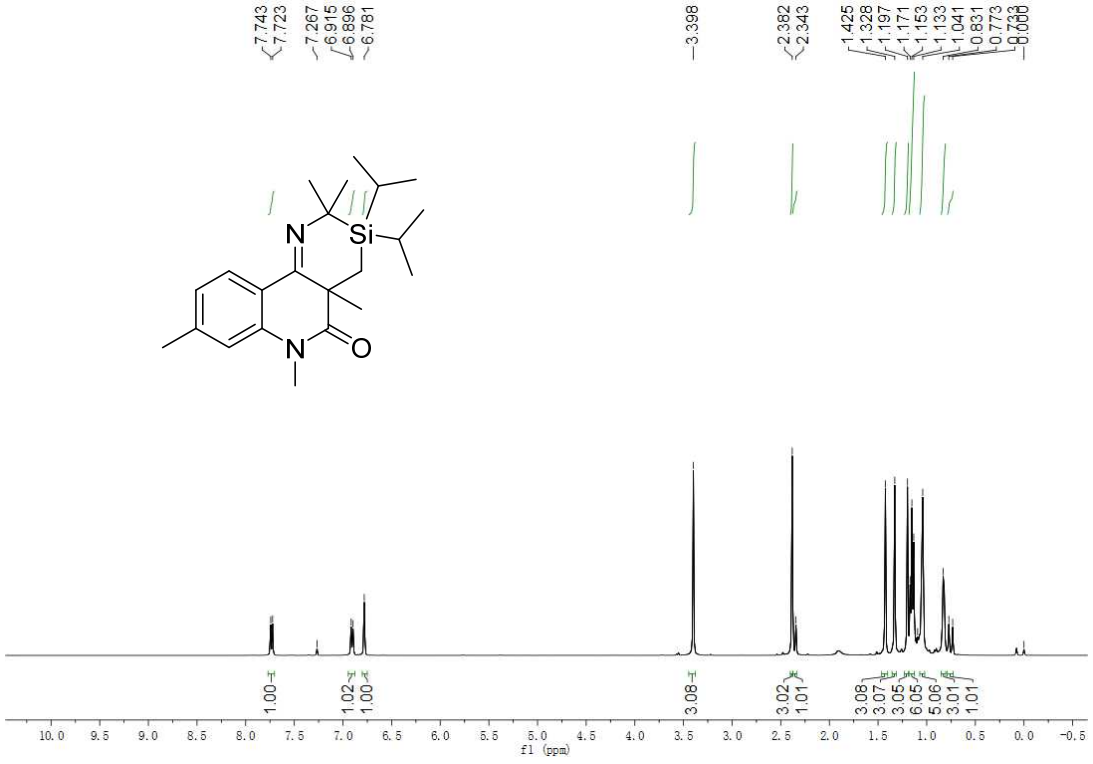


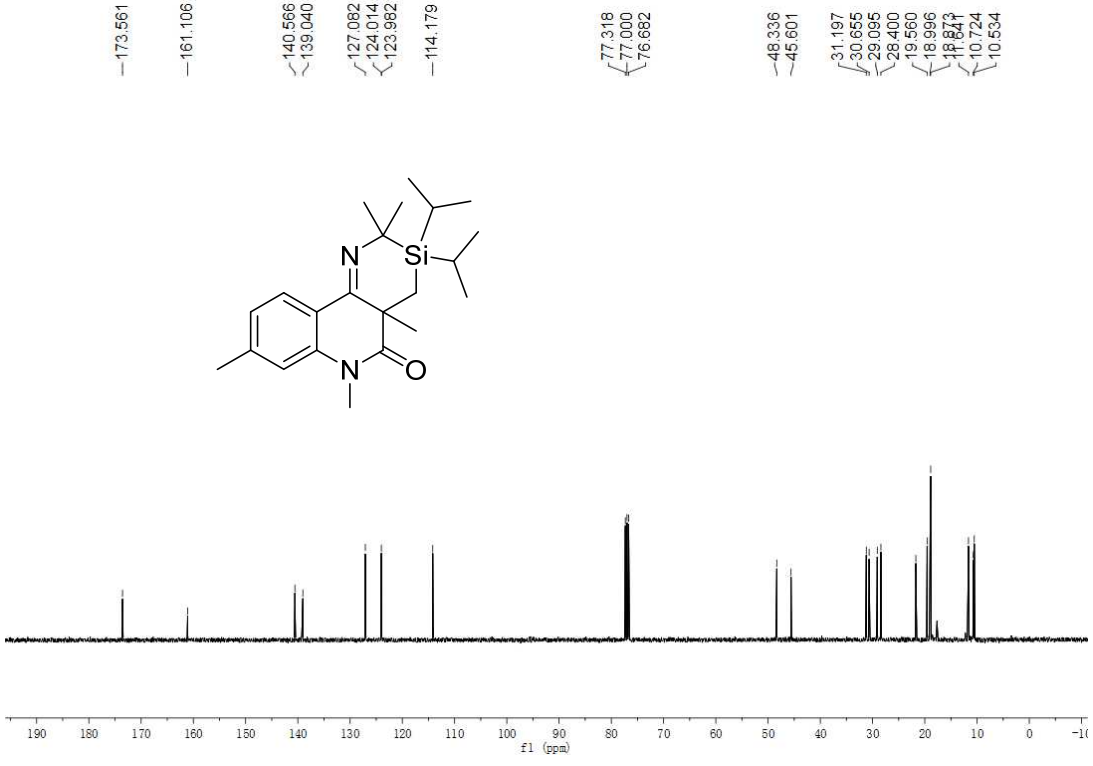
6-benzyl-3,3-diisopropyl-2,2,4a-trimethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ba)



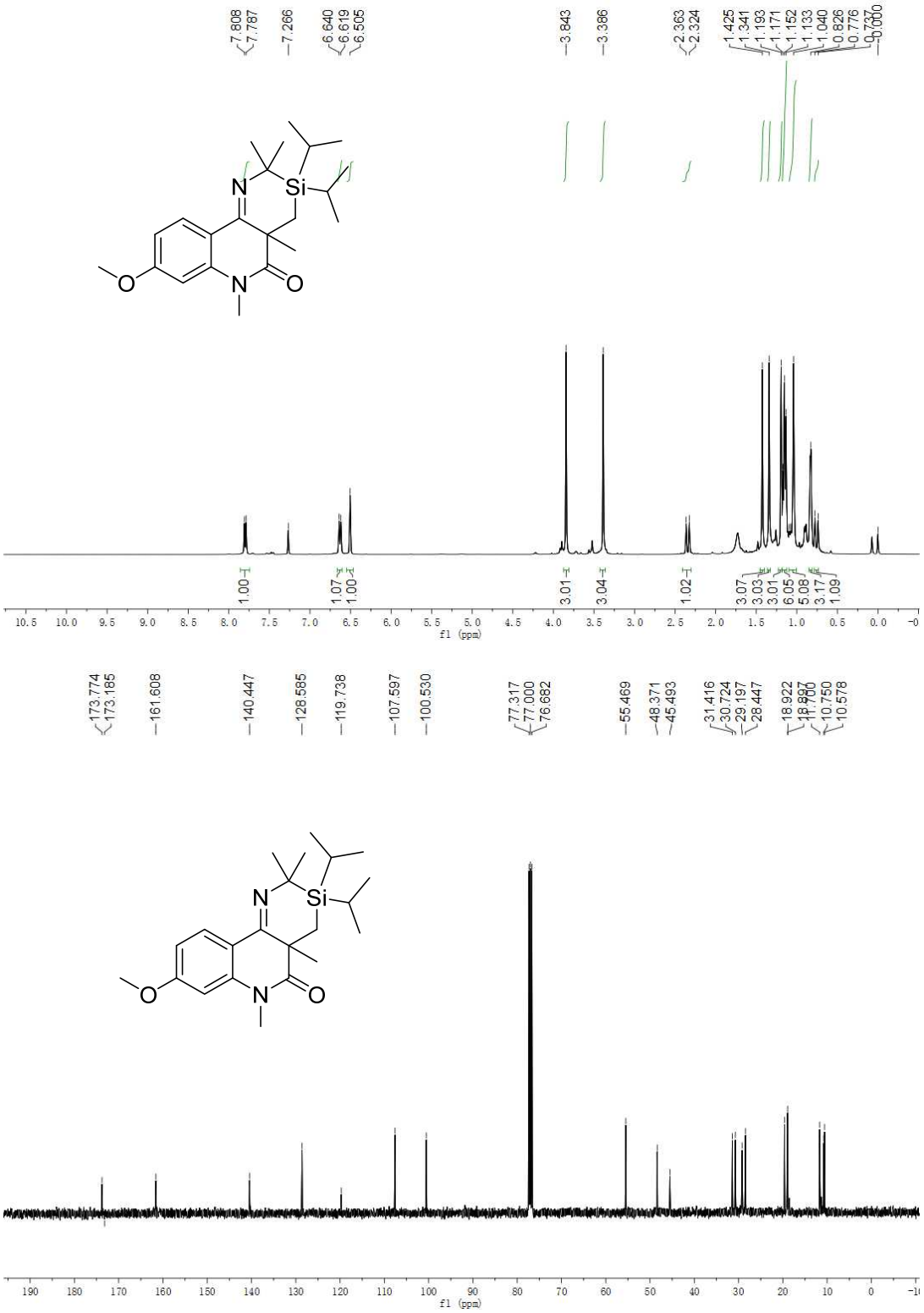


3,3-diisopropyl-2,2,4a,6,8-pentamethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3da)

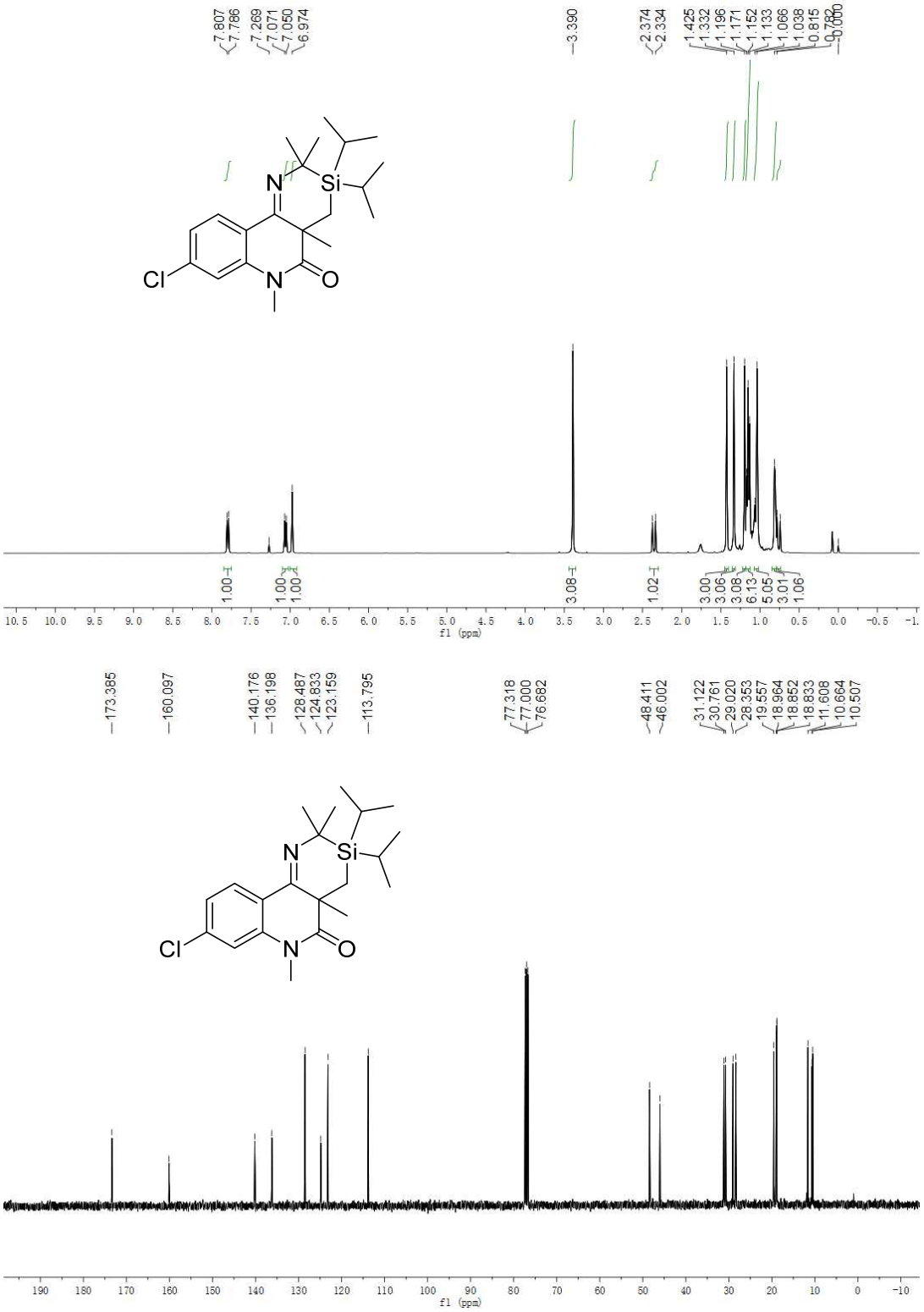




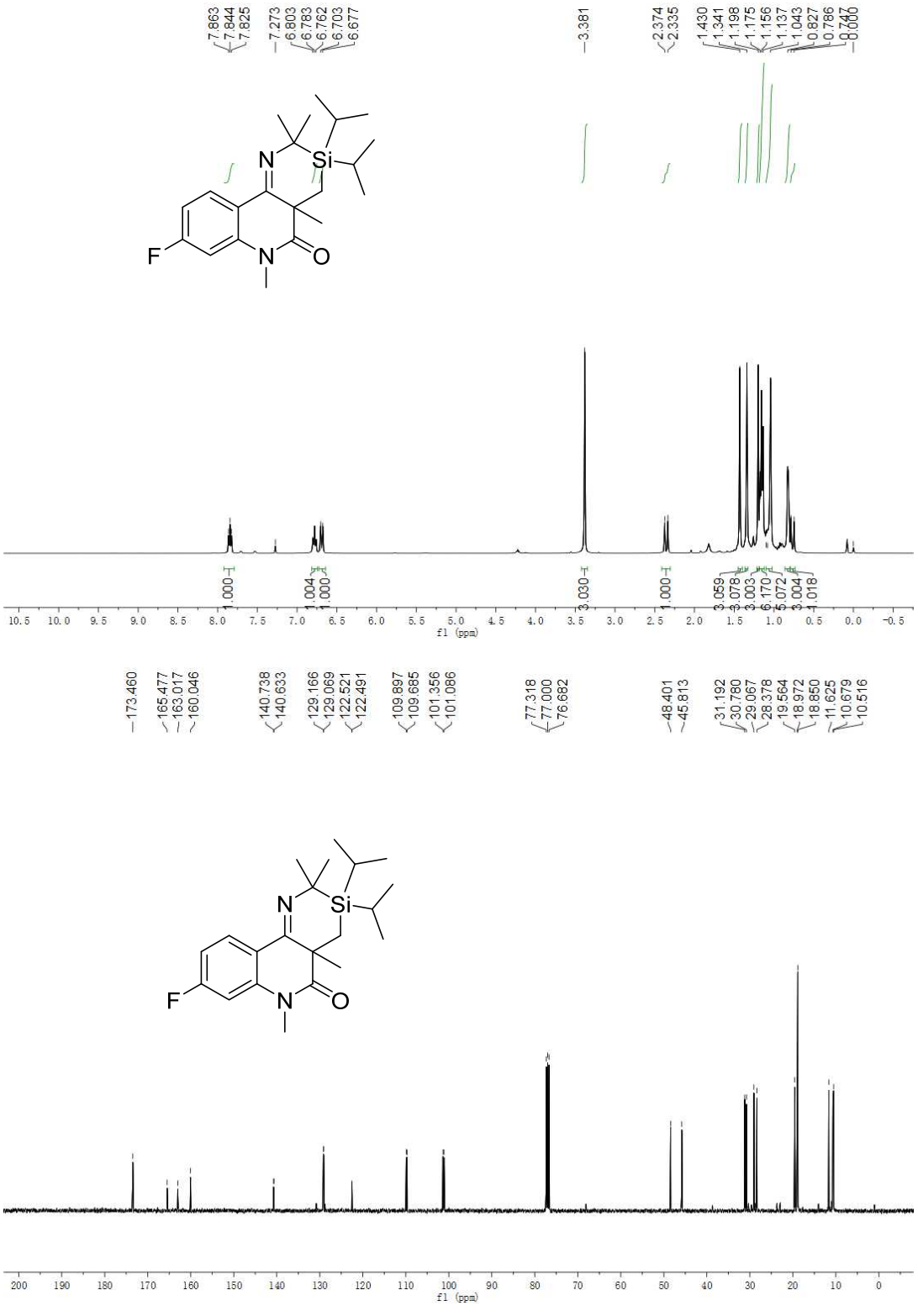
3,3-diisopropyl-8-methoxy-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasili-no[5,6-c]quinolin-5(3H)-one (3ea)



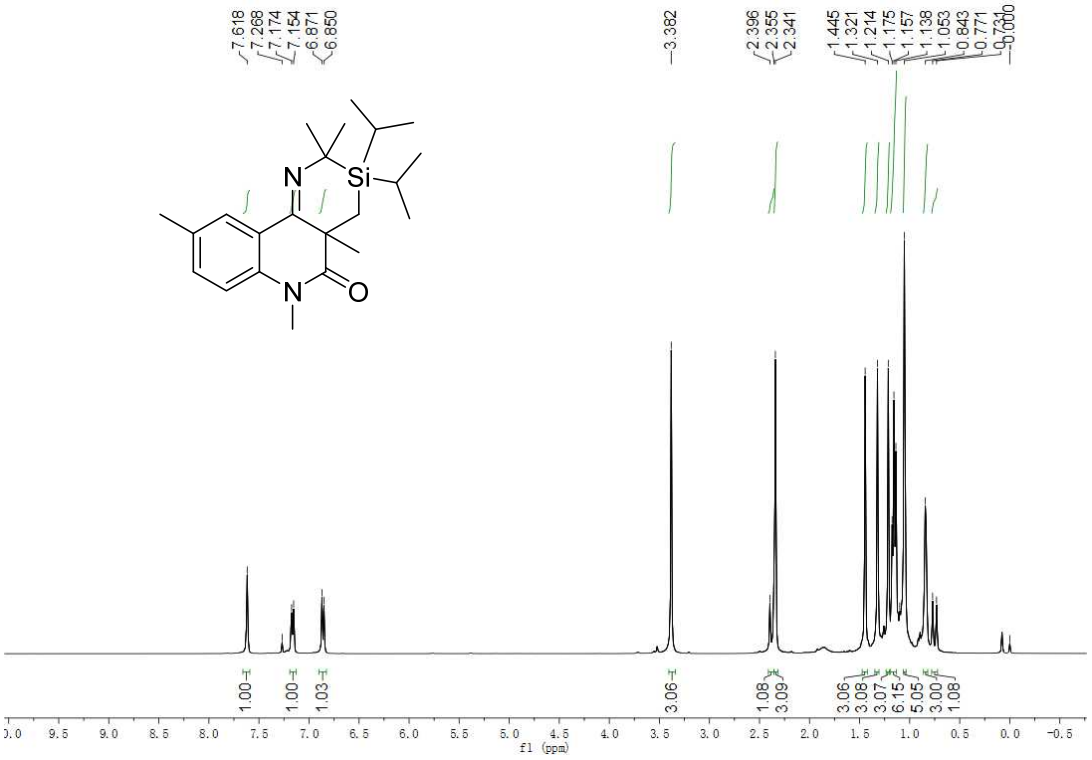
8-chloro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3fa)

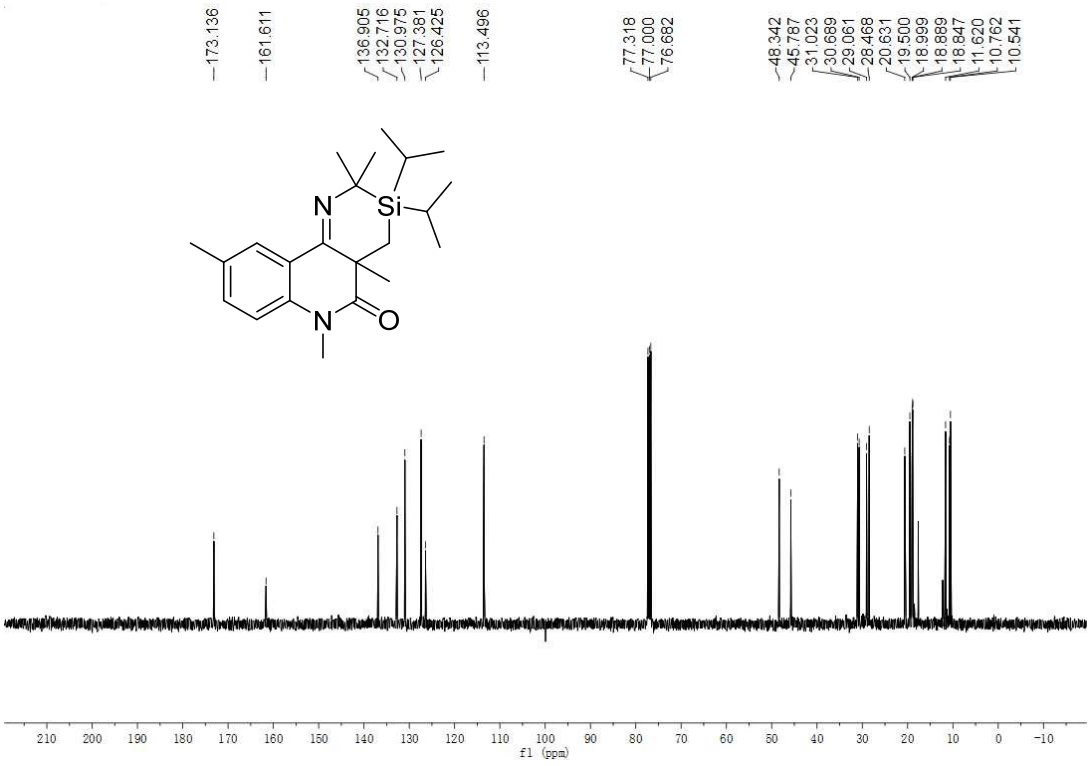


8-fluoro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino-[5,6-c]quinolin-5(3H)-one (3ga)

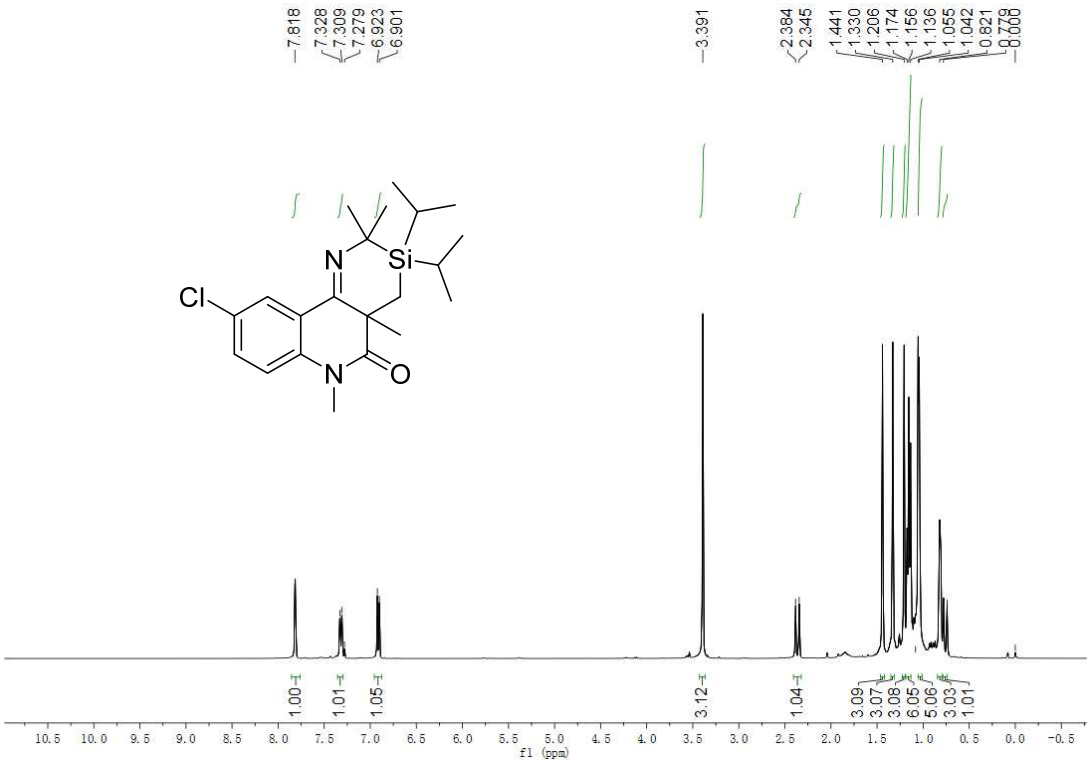


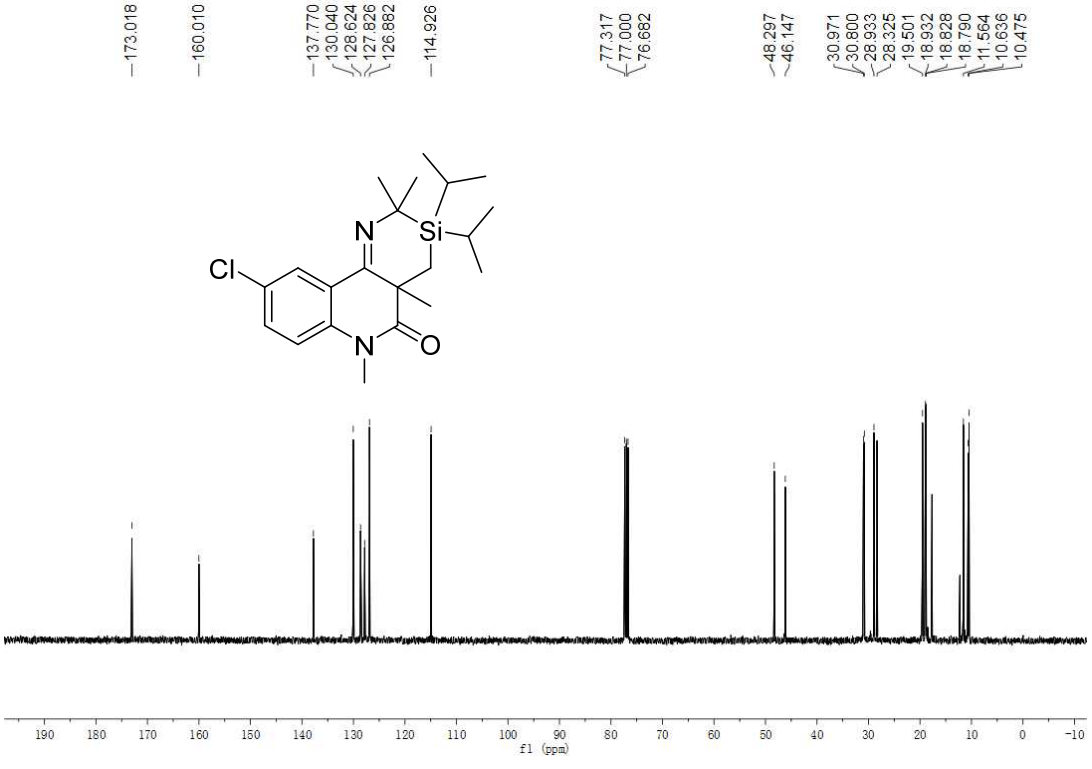
3,3-diisopropyl-2,2,4a,6,9-pentamethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ha)



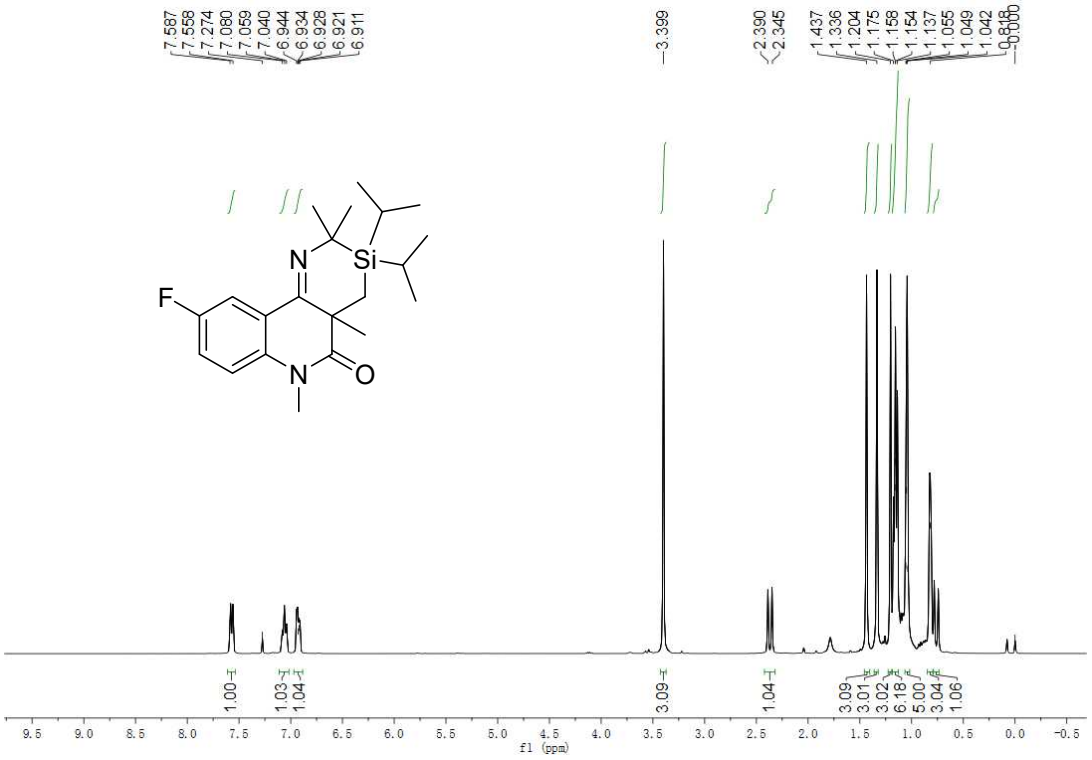


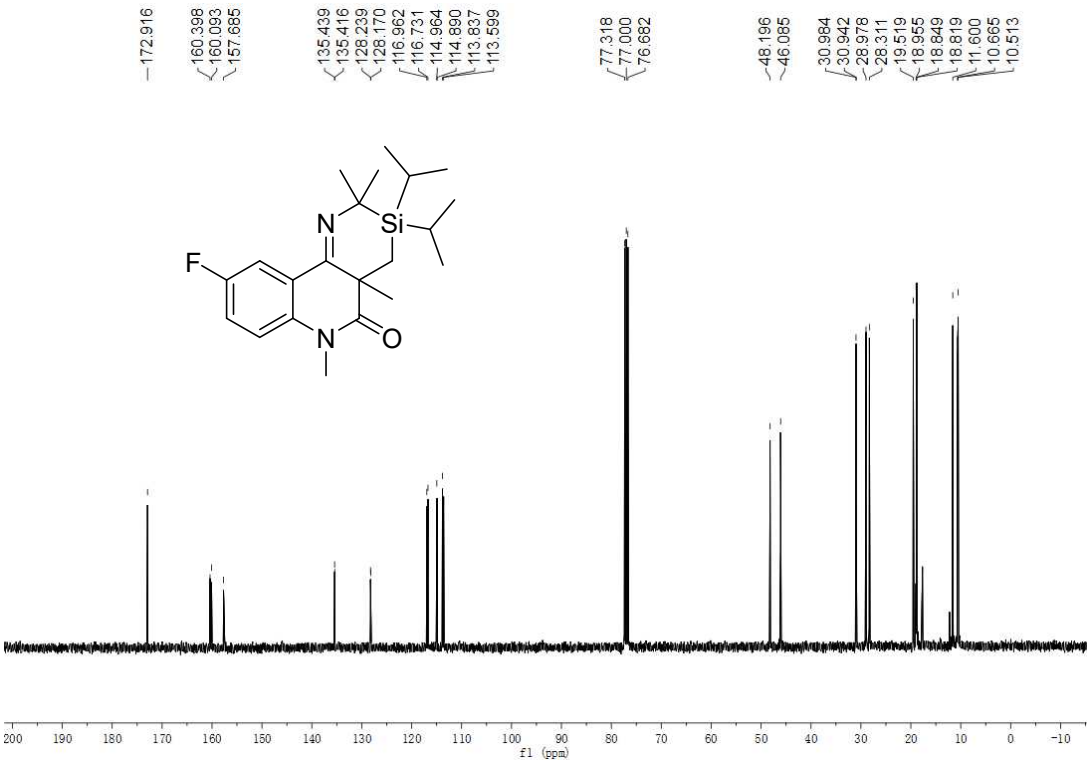
9-chloro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ia)



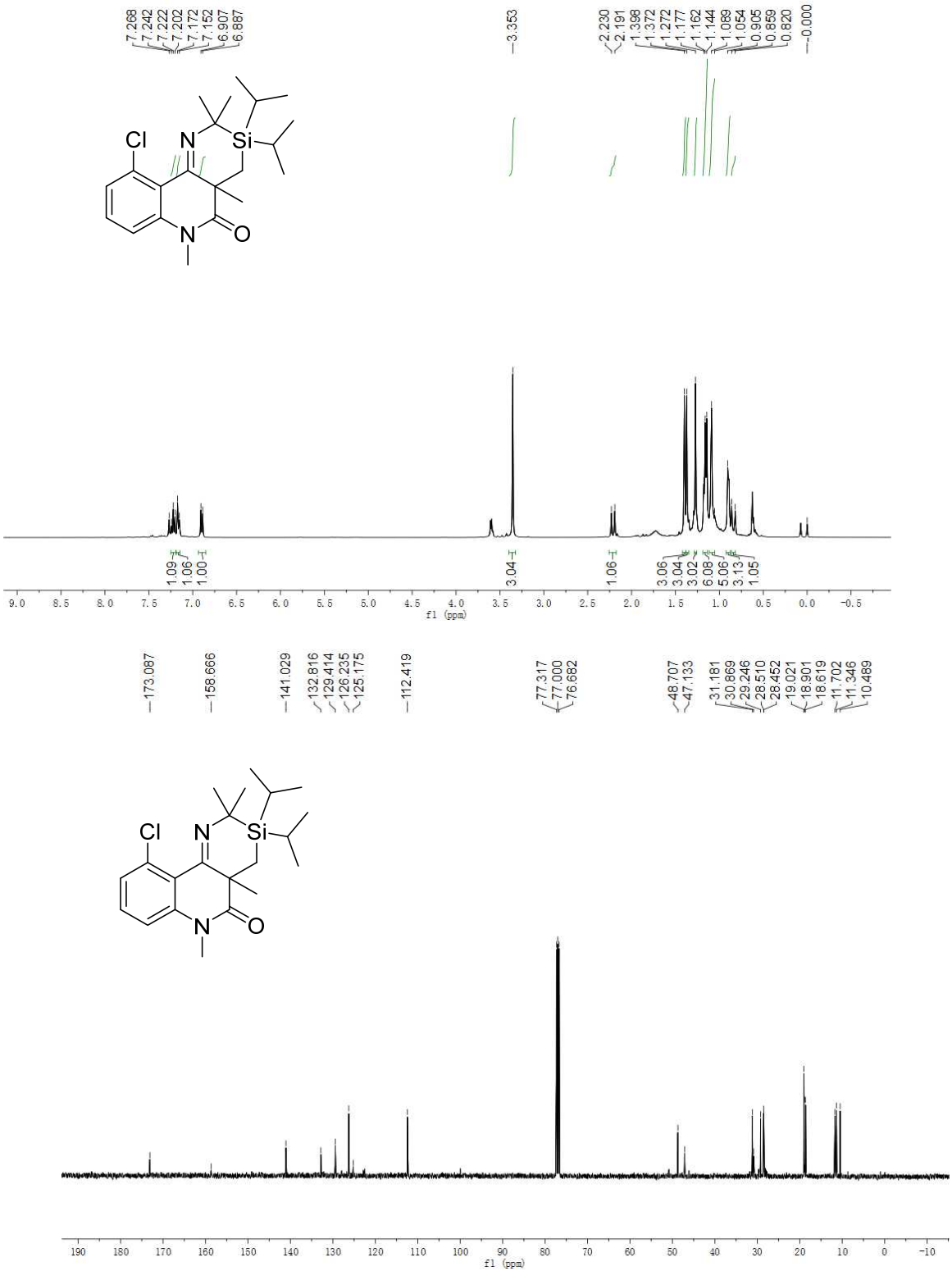


9-fluoro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ja)



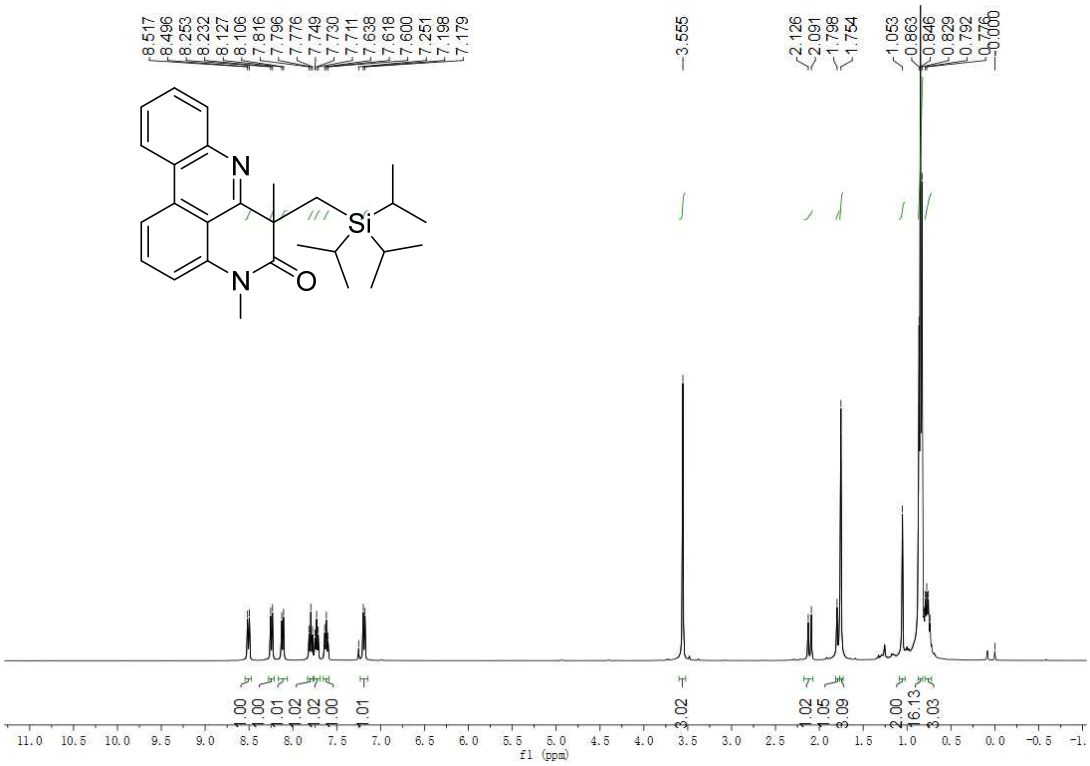


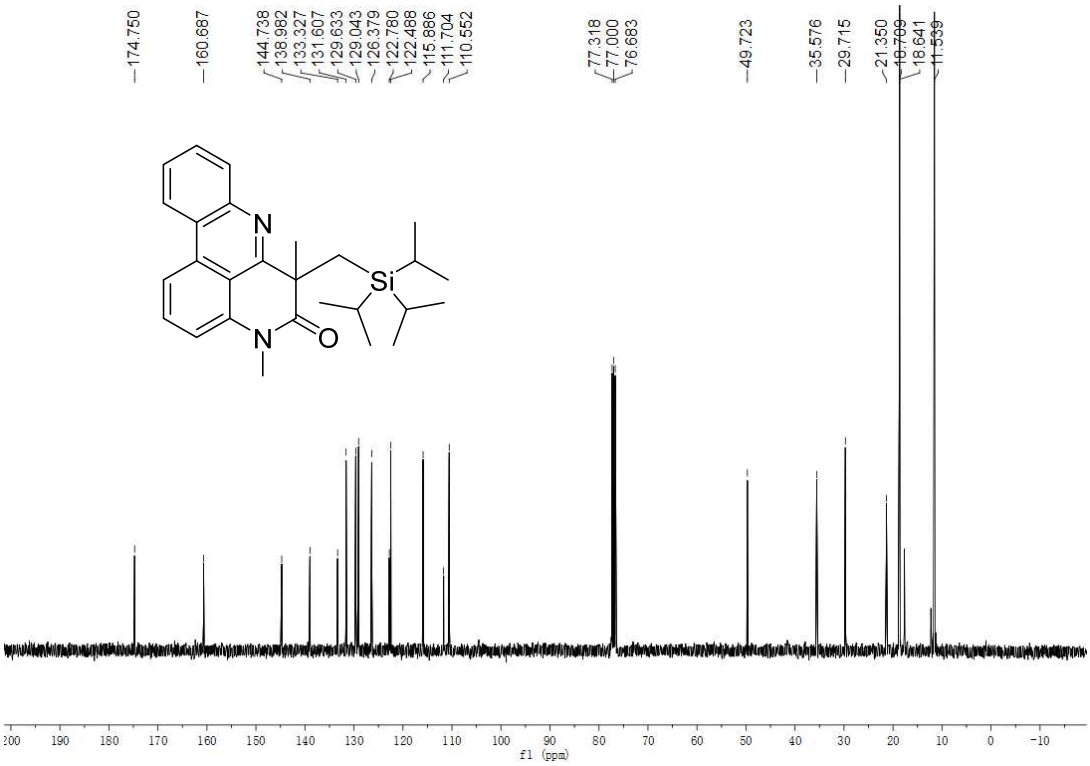
10-chloro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ka)



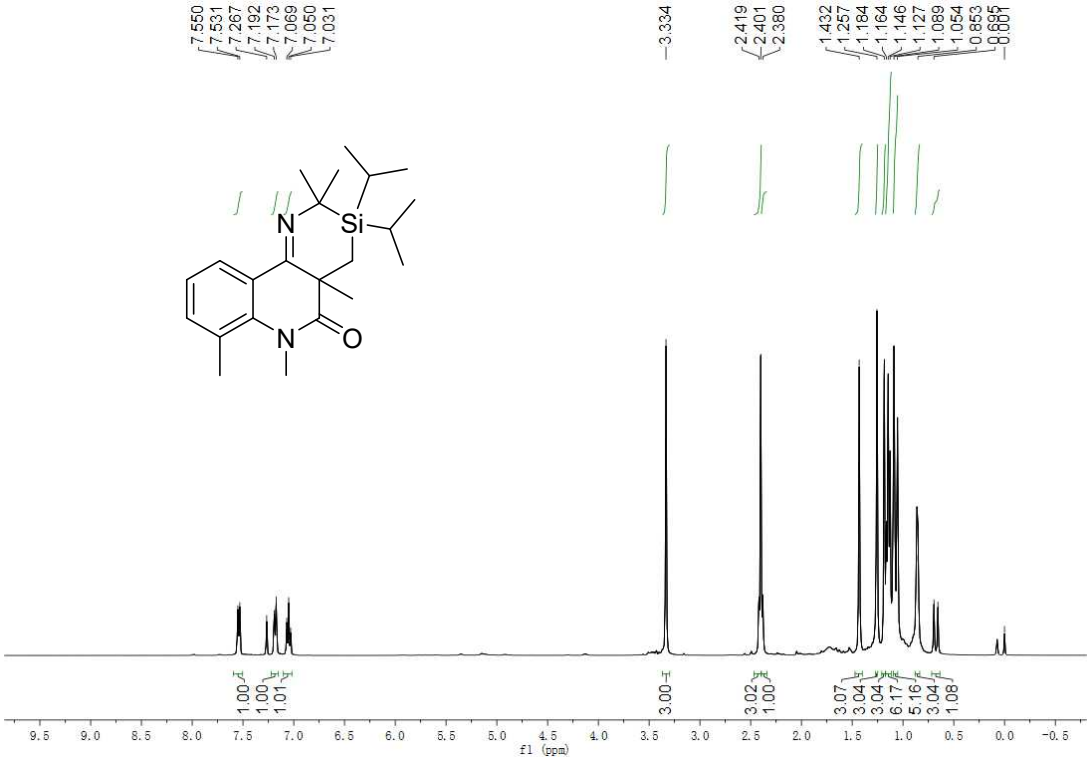
4,6-dimethyl-6-((triisopropylsilyl)methyl)-4H-pyrido[4,3,2-gh]phenanthridin-5(6H)-one

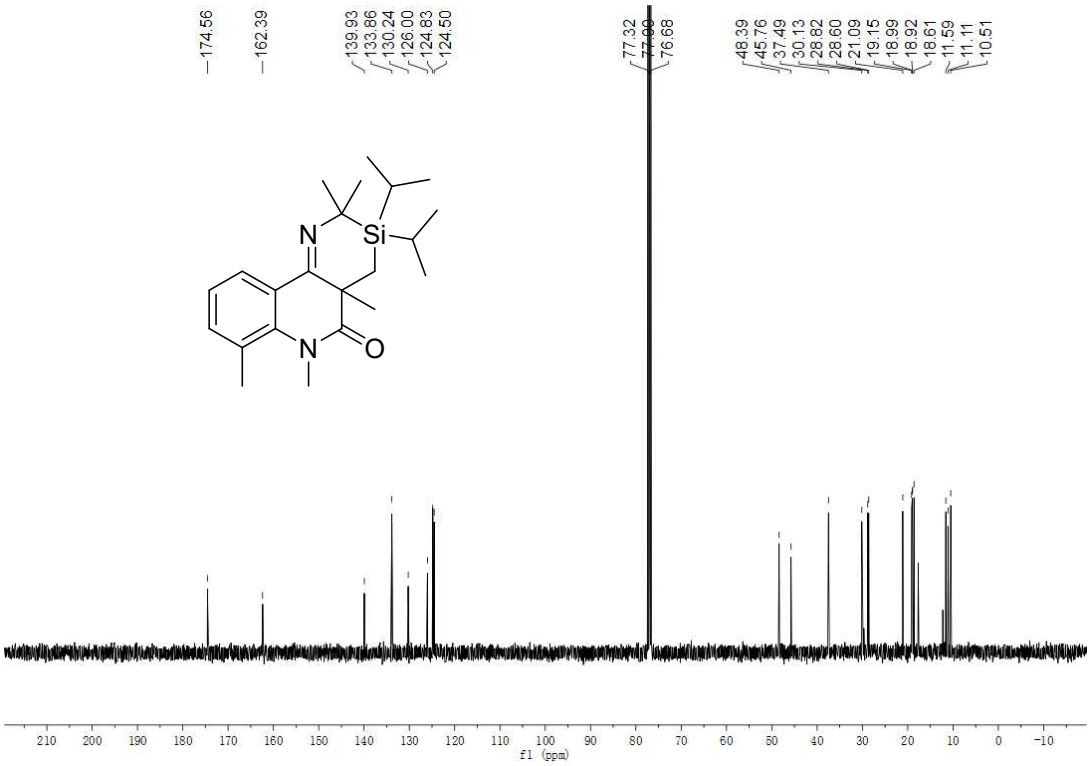
(4la)



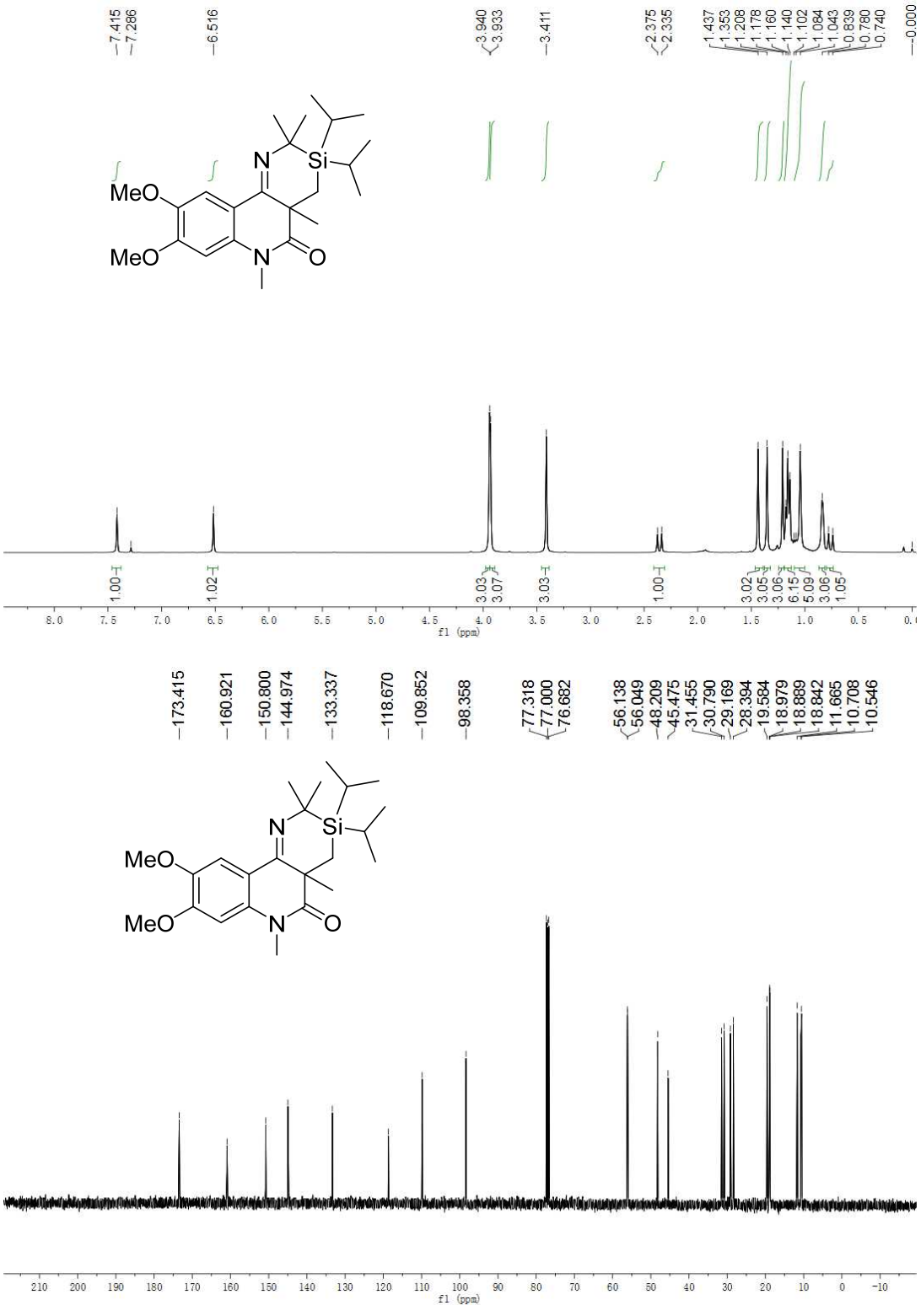


3,3-diisopropyl-2,2,4a,6,7-pentamethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ma)

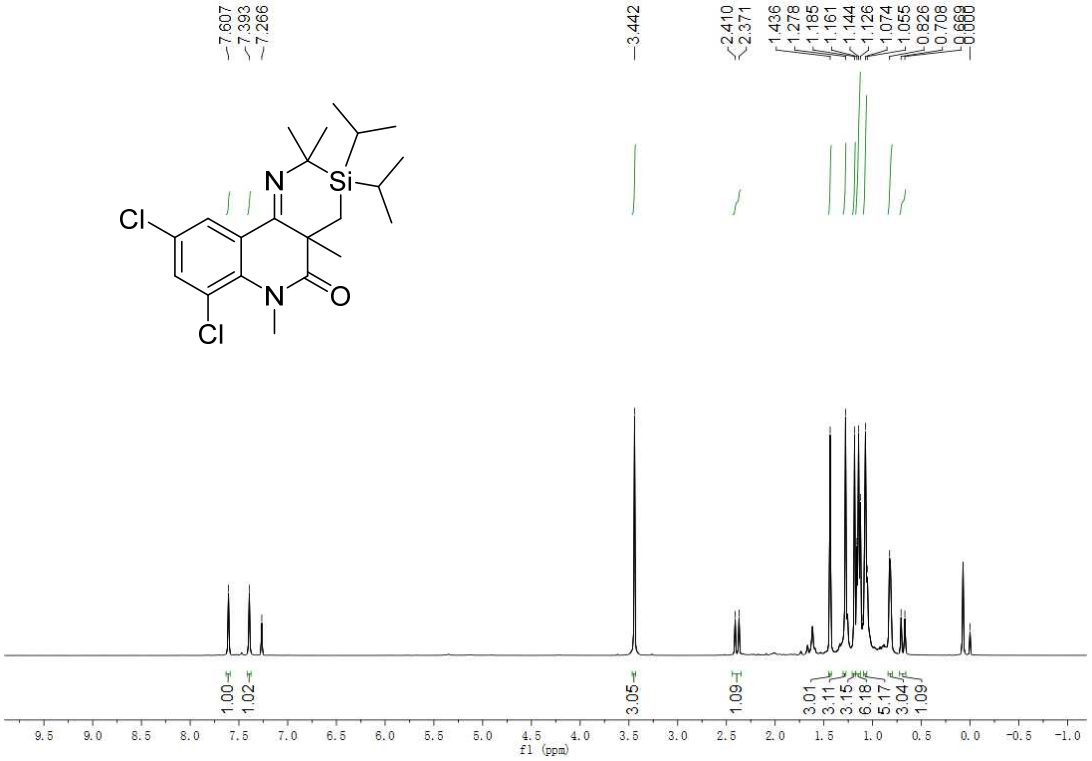


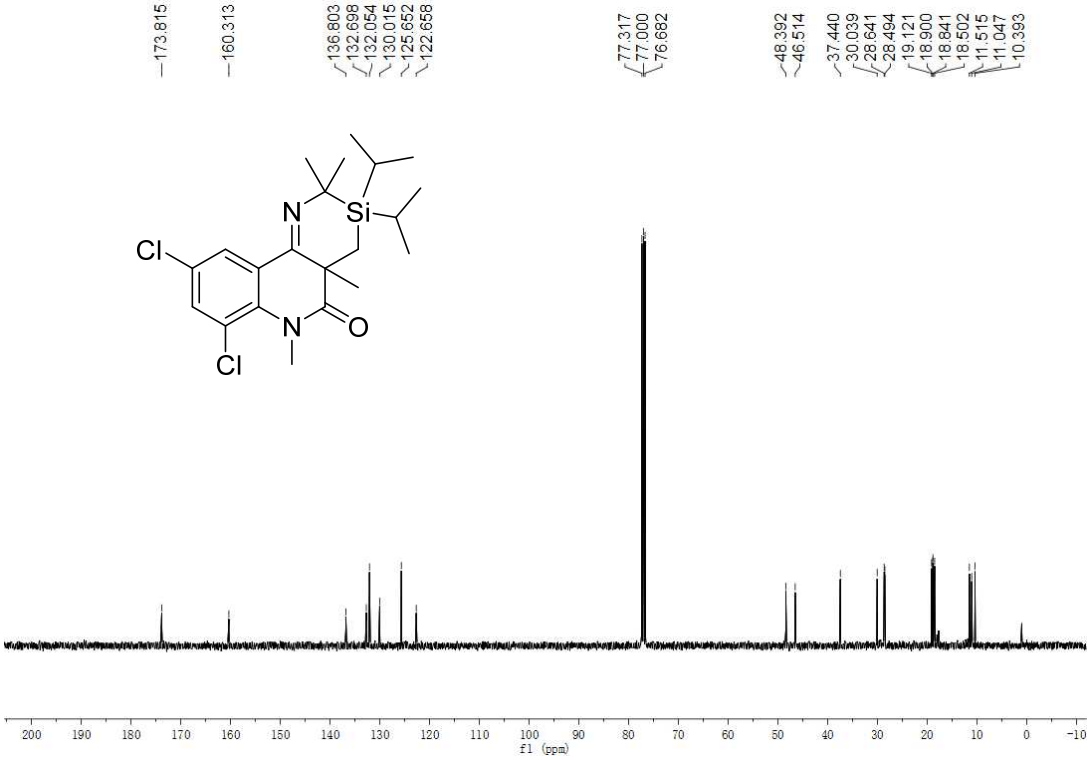


3,3-diisopropyl-8,9-dimethoxy-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3na)

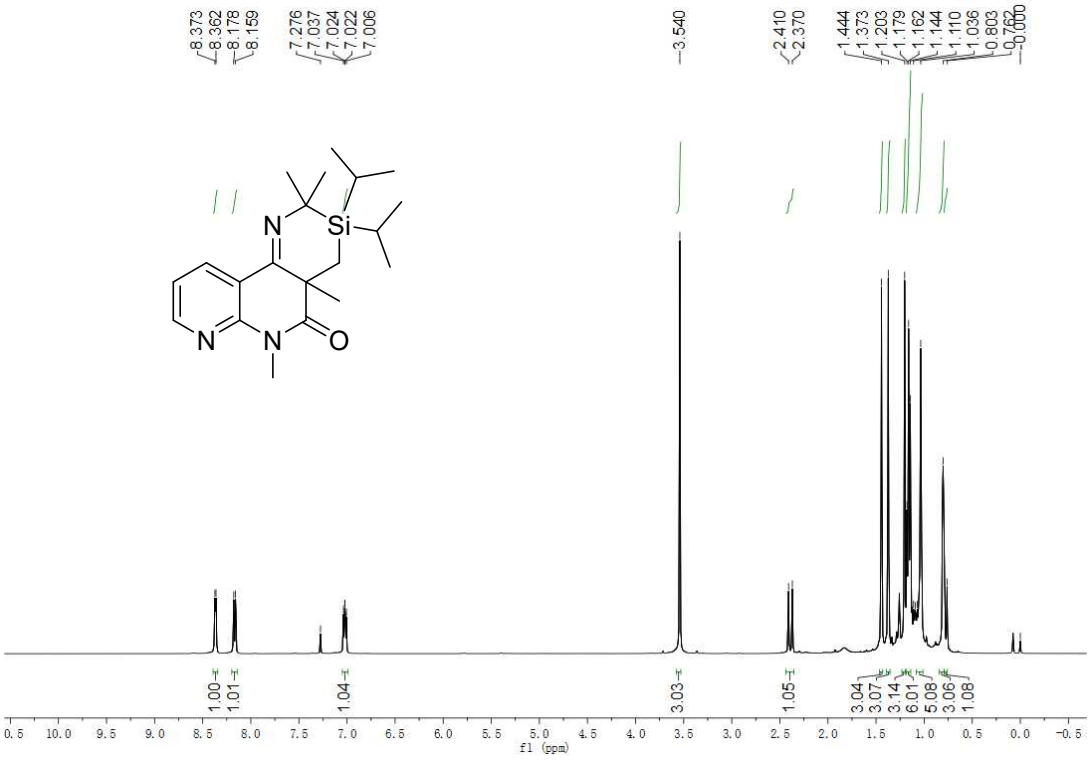


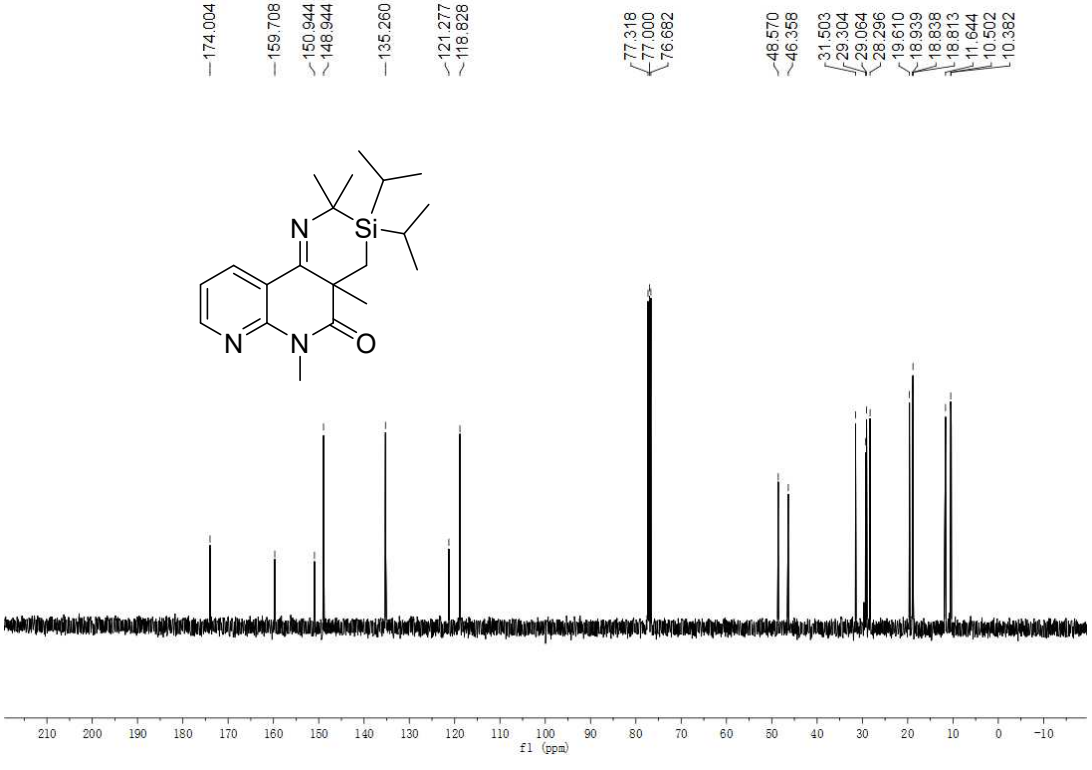
7,9-dichloro-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3oa)



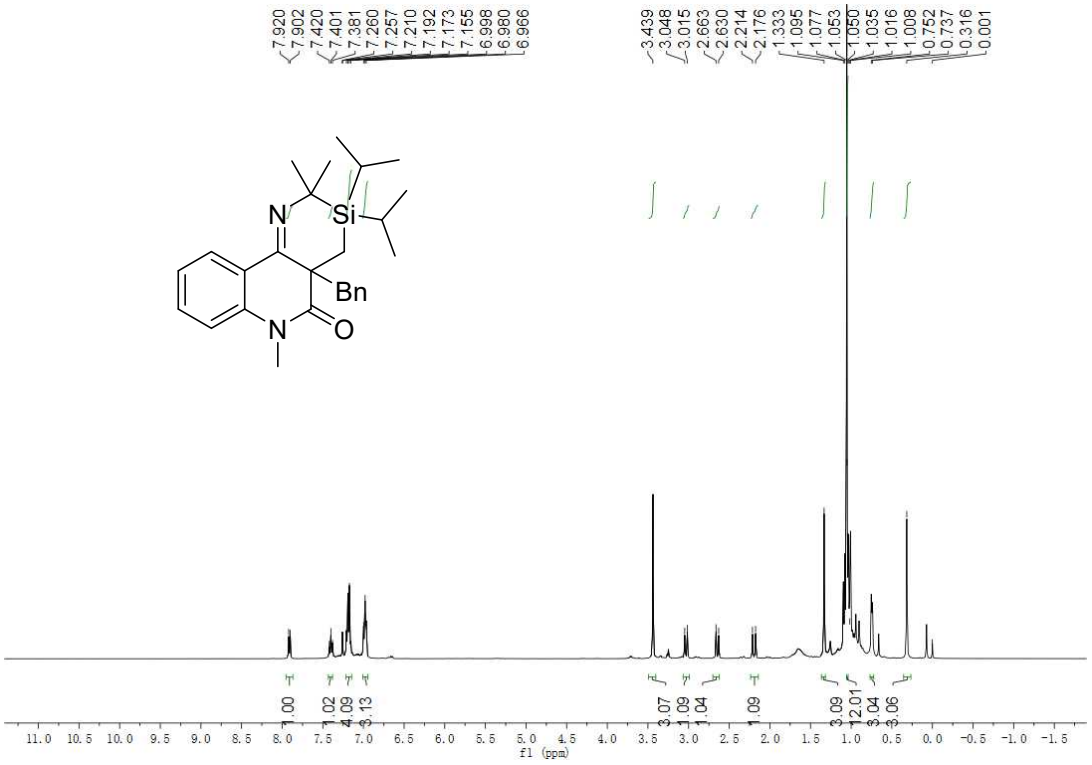


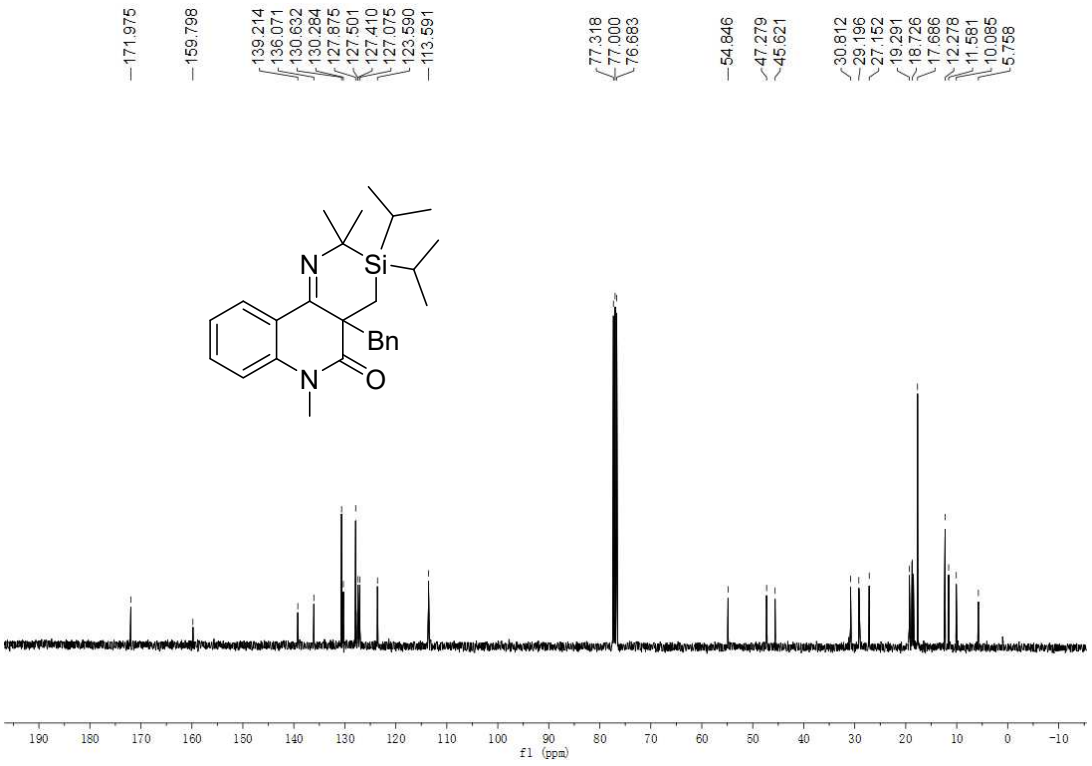
3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c][1,8]naphthyridin-5(3H)-one (3pa)



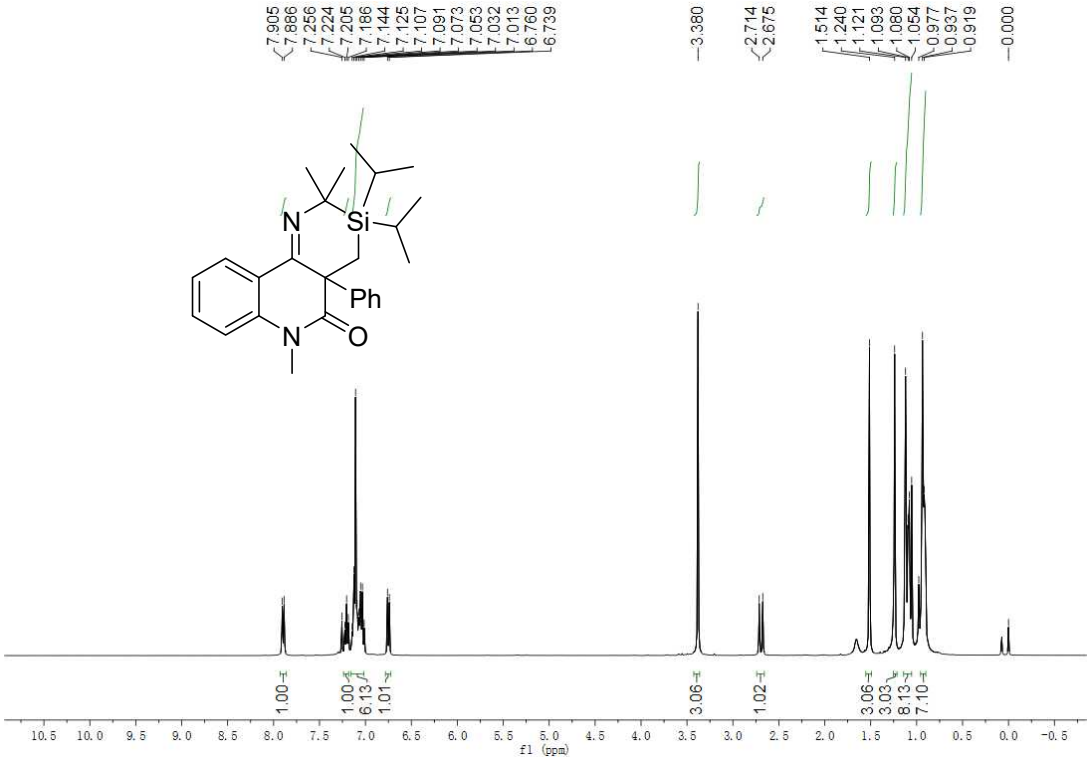


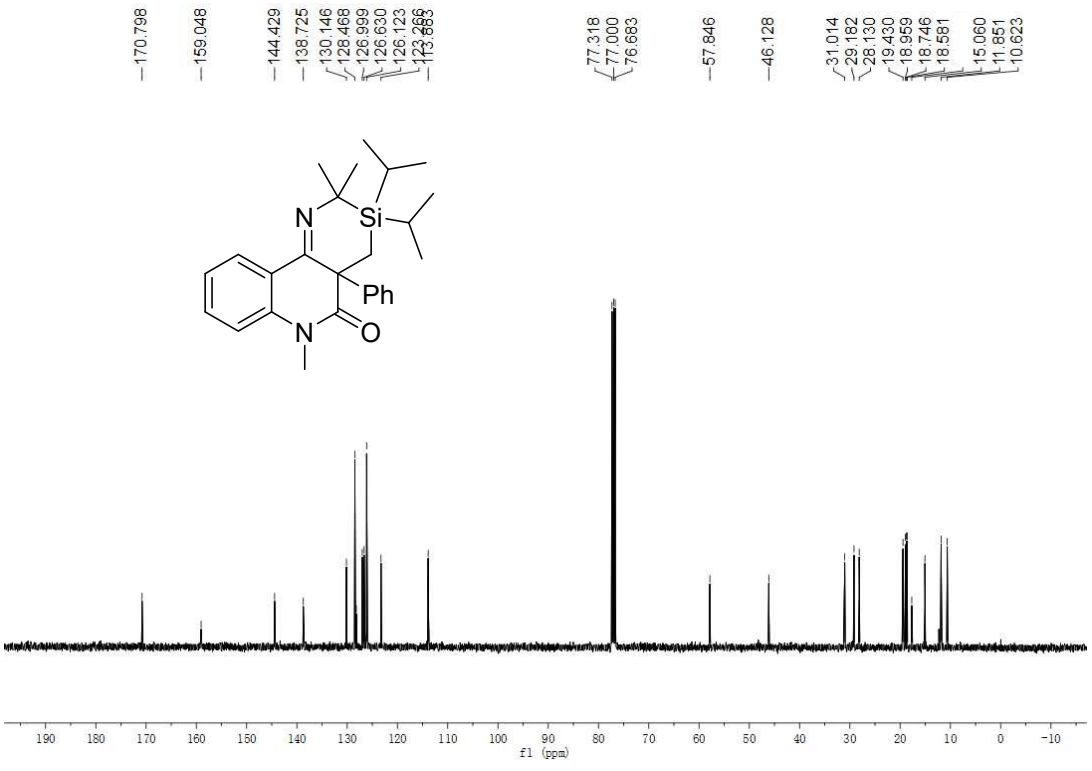
4a-benzyl-3,3-diisopropyl-2,2,6-trimethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3qa)



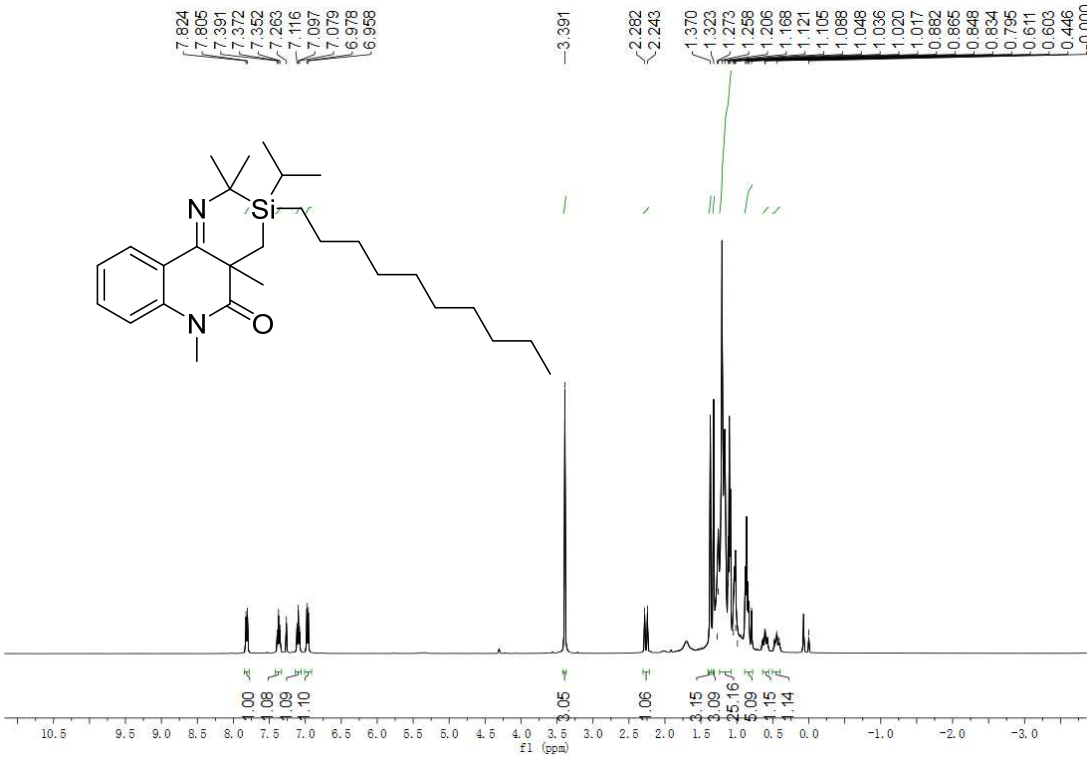


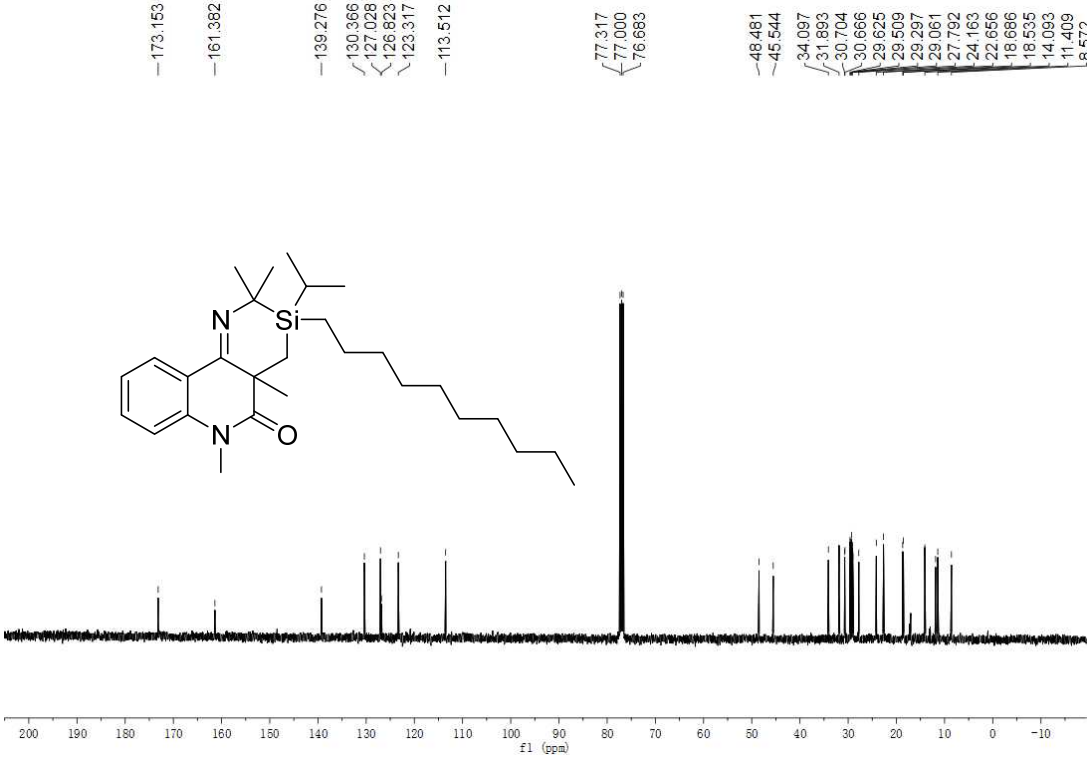
3,3-diisopropyl-2,2,6-trimethyl-4a-phenyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ra)



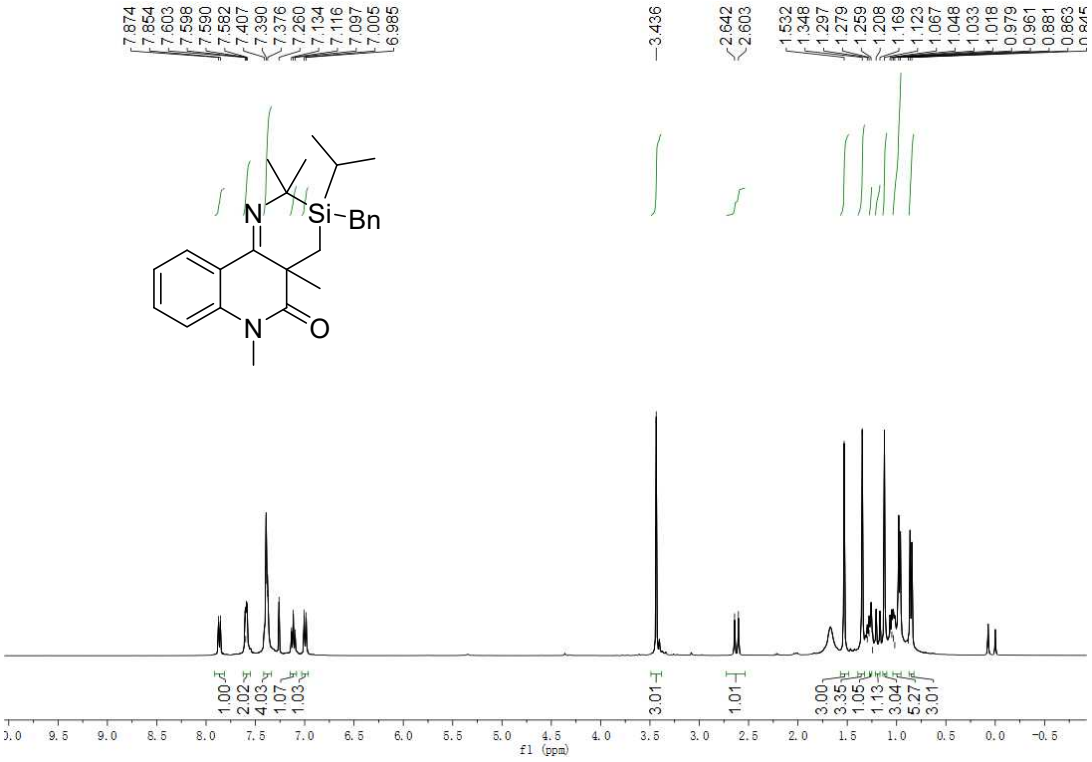


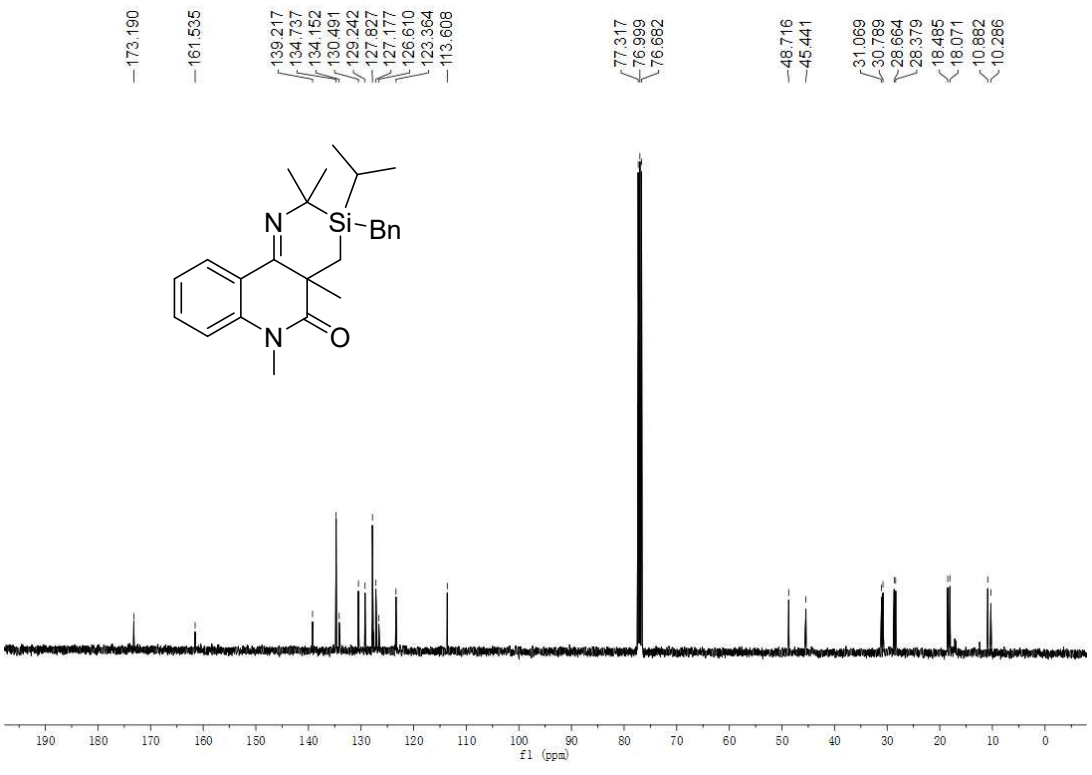
3-decyl-3-isopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ab)



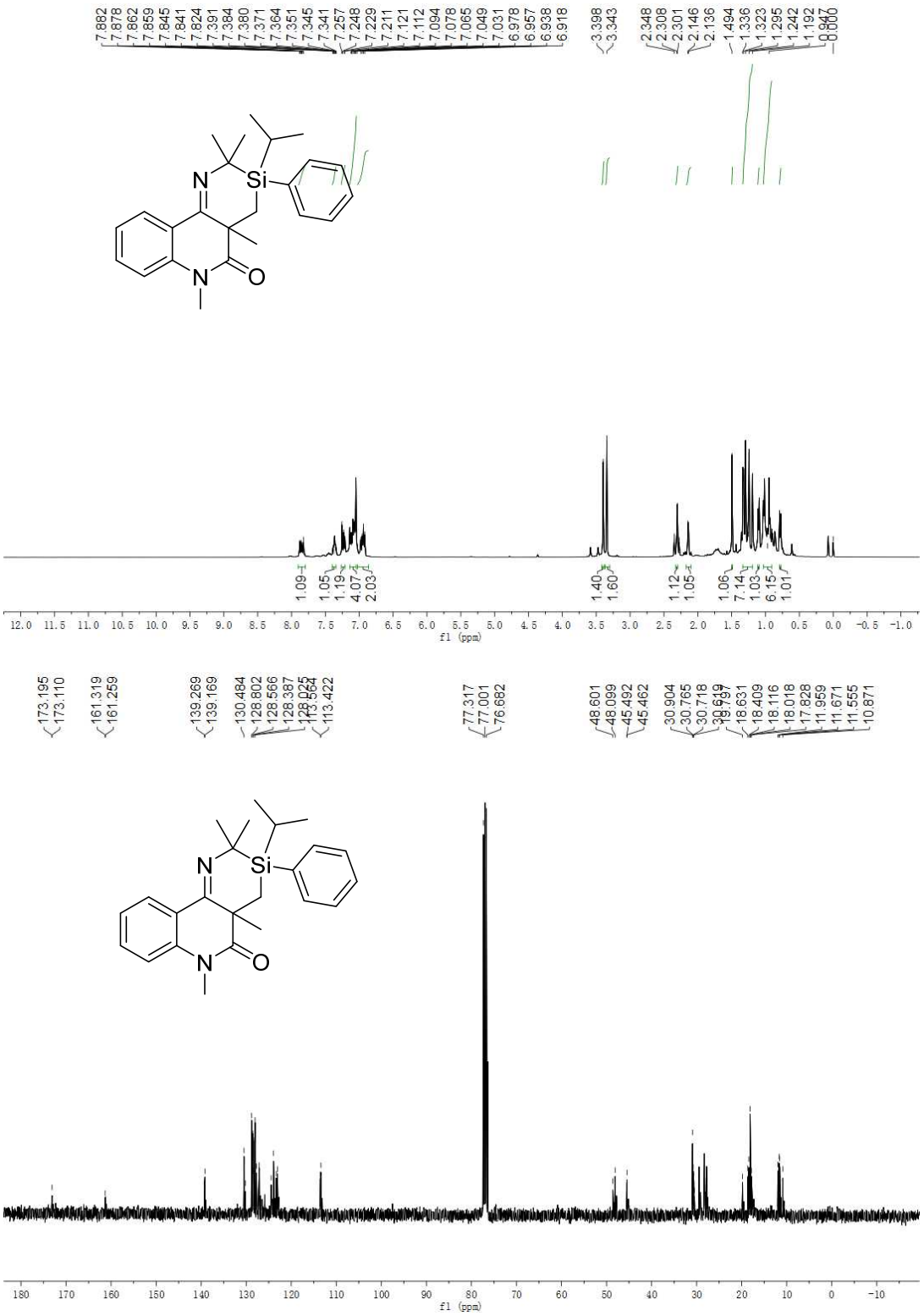


3-benzyl-3-isopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (3ac)

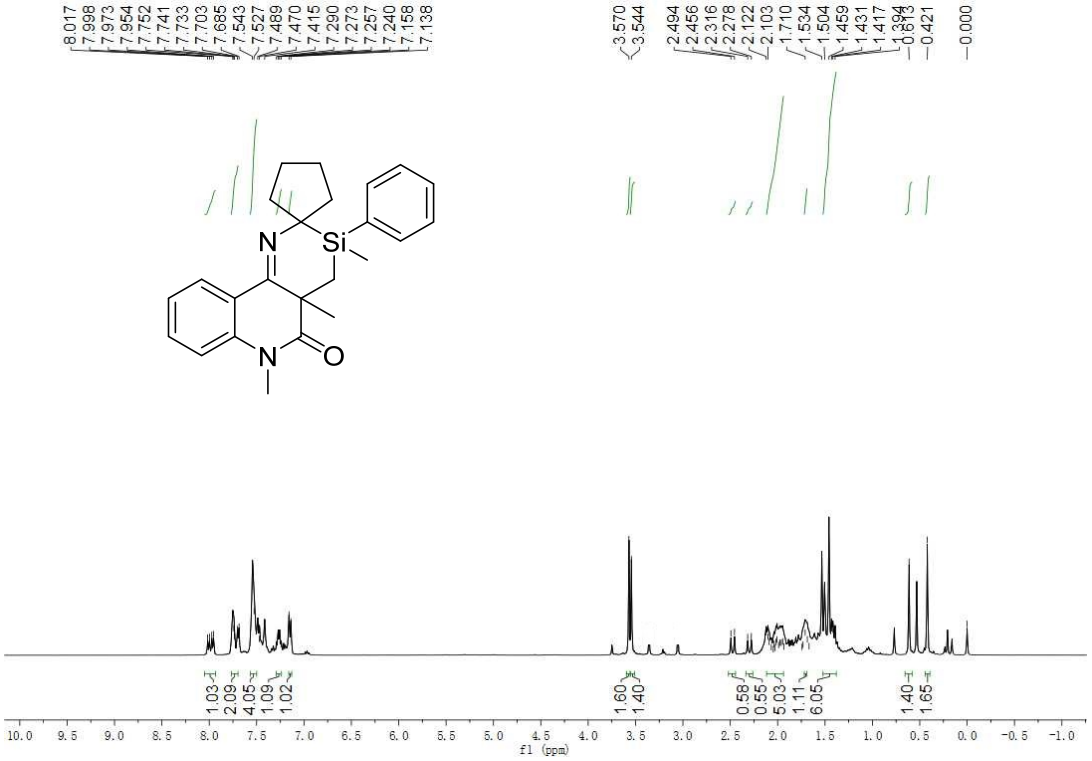


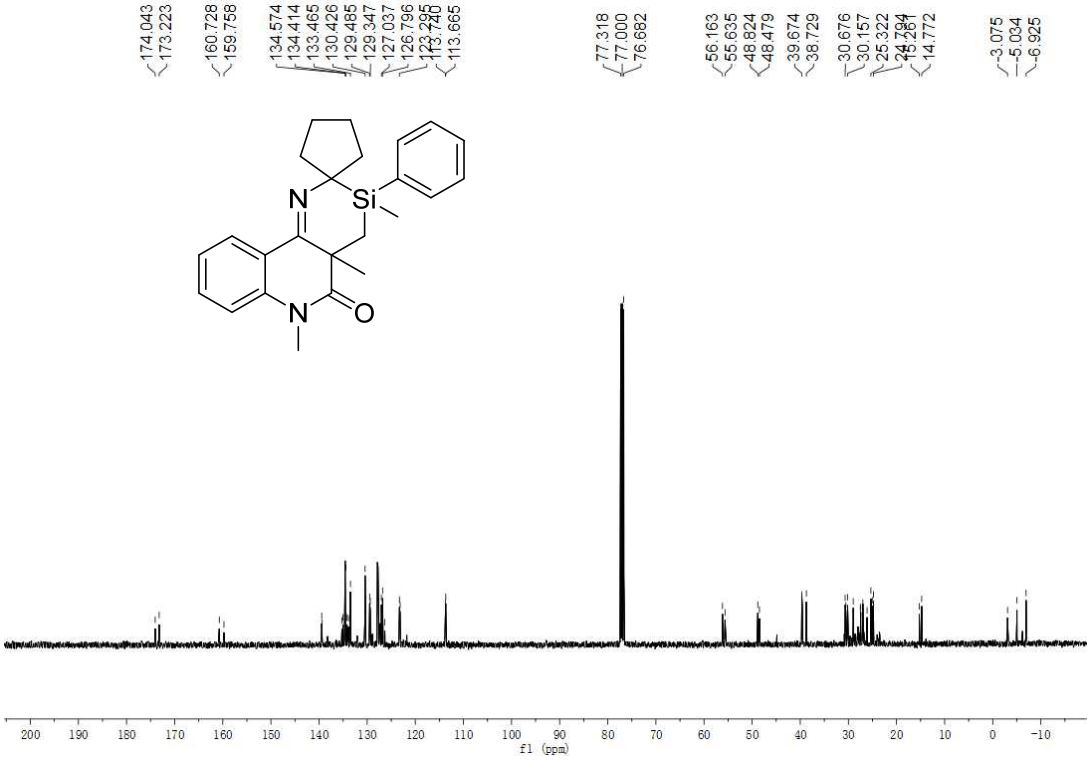


3-isopropyl-2,2,4a,6-tetramethyl-3-phenyl-2,4,4a,6-tetrahydro-[1,3]azasilino[5,6-c]quinolin-5(3H)-one (dr = 1.1 : 1) (3ad)

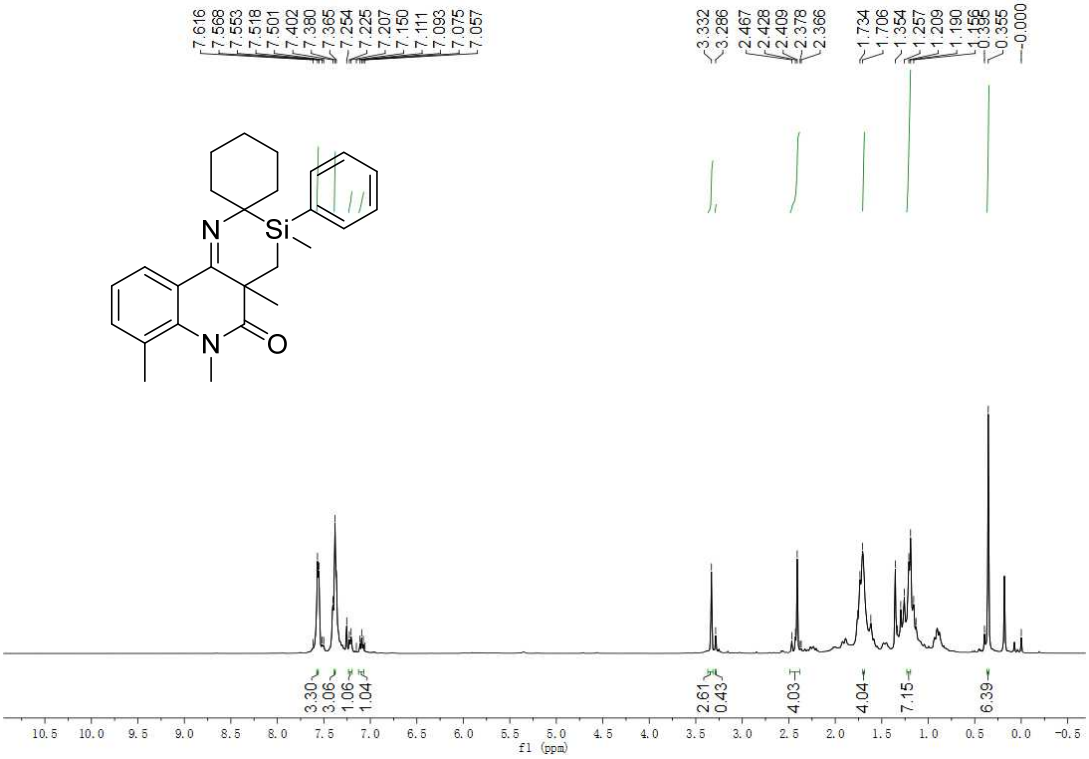


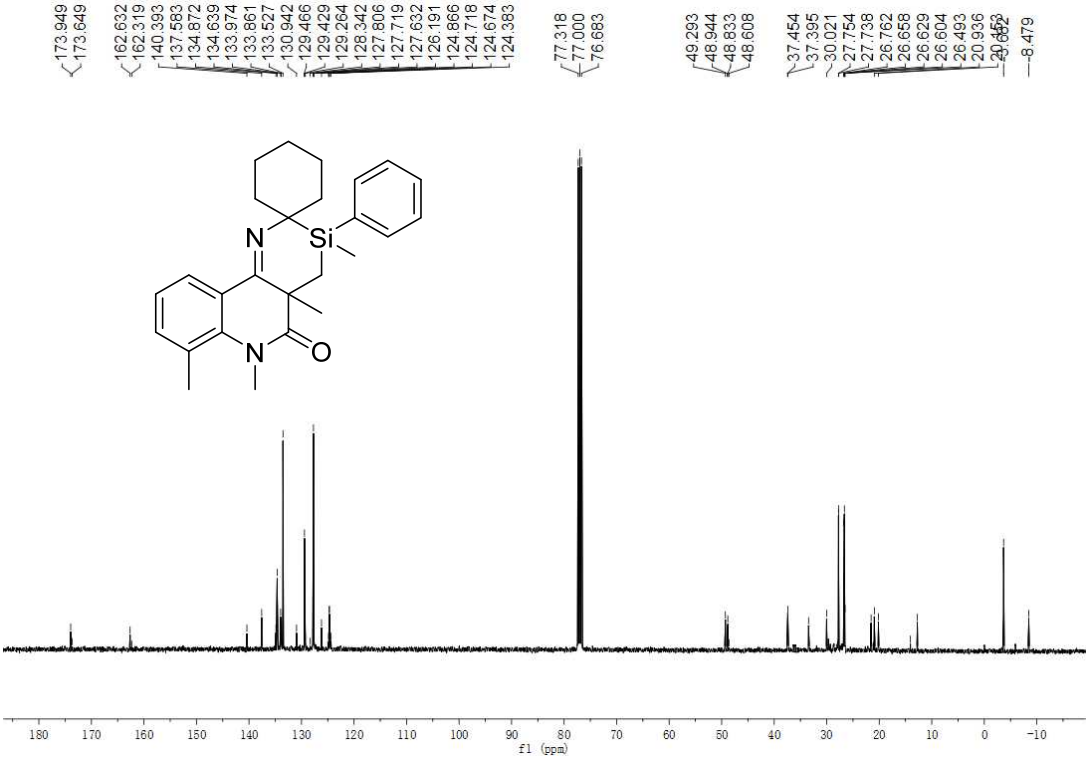
3',4a',6'-trimethyl-3'-phenyl-4',4a'-dihydro-3'H-spiro[cyclopentane-1,2'-[1,3]azasilino[5,6-c]quinolin]-5'(6'H)-one (dr = 1.1 : 1) (3ae)



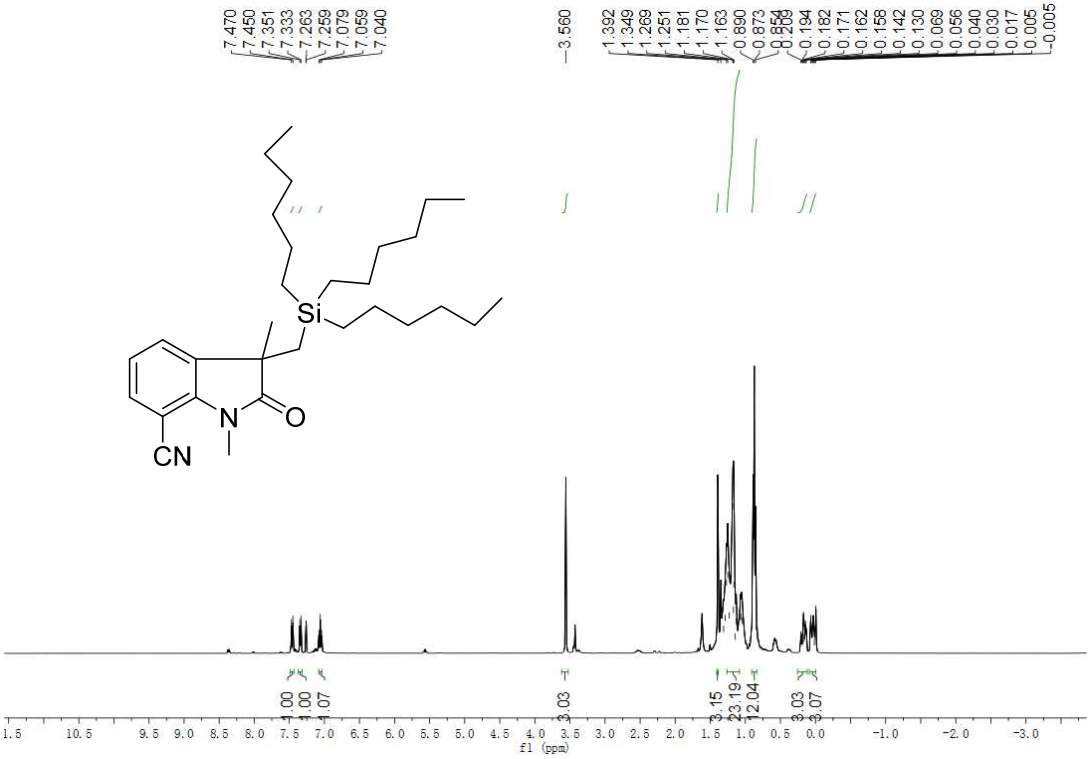


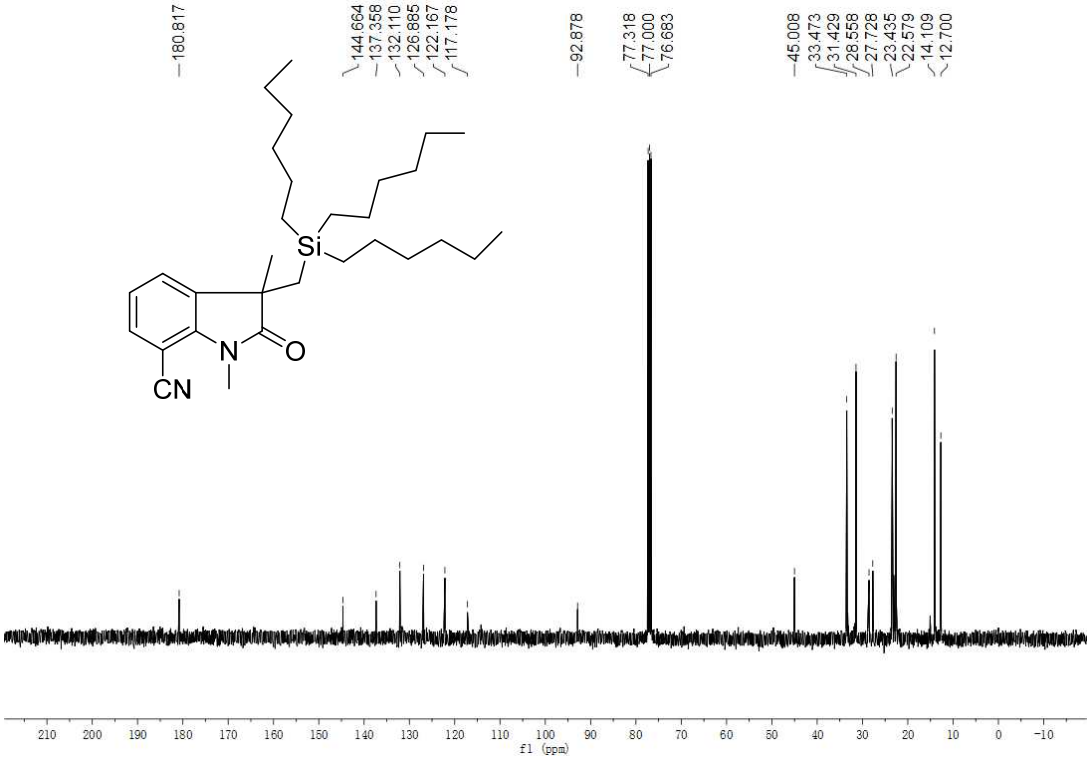
3',4a',6',7'-tetramethyl-3'-phenyl-4',4a'-dihydro-3'H-spiro[cyclohexane-1,2'-[1,3]azasilino[5,6-c]quinolin]-5'(6'H)-one (dr = 6 : 1) (3mf)



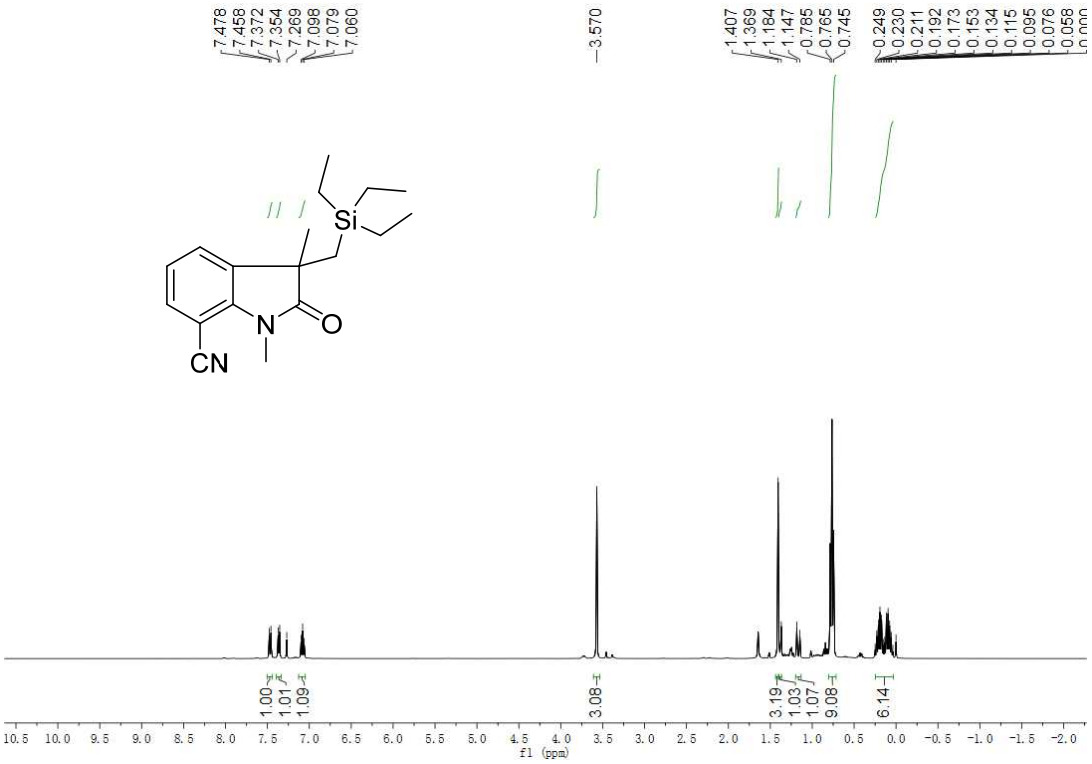


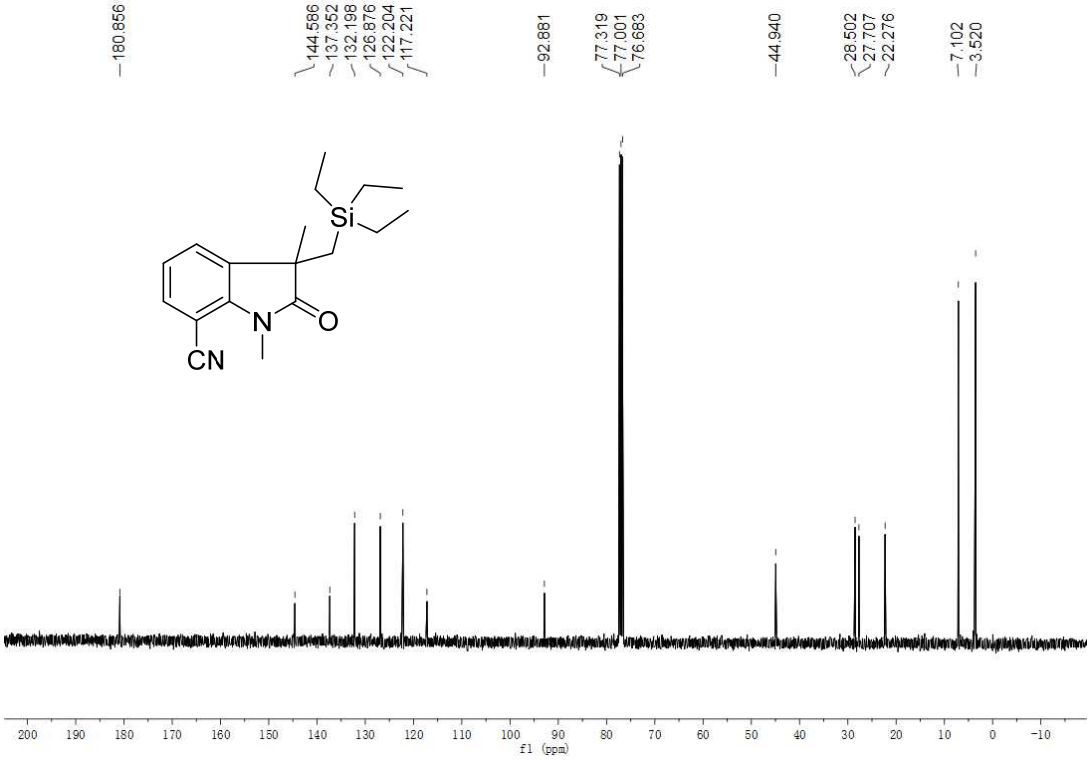
1,3-dimethyl-2-oxo-3-((trihexylsilyl)methyl)indoline-7-carbonitrile (5af)



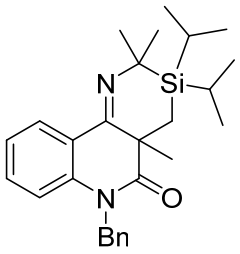


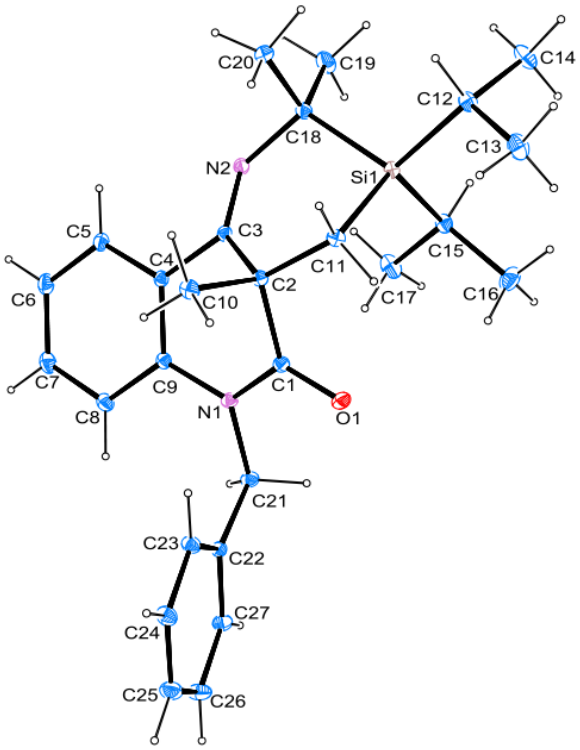
1,3-dimethyl-2-oxo-3-((triethylsilyl)methyl)indoline-7-carbonitrile (5ag)





(E) The X-ray single-crystal diffraction analysis of 3ba





CCDC: 1584738

Table 1. Crystal data and structure refinement for ljh055.

Identification code	ljh055
Empirical formula	C27 H36 N2 O Si
Formula weight	432.67
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 12.787(2) A alpha = 90 deg.

	b = 16.559(3) A beta = 95.643(3) deg.
	c = 11.9492(18) A gamma = 90 deg.
Volume	2517.9(7) A^3
Z, Calculated density	4, 1.141 Mg/m^3
Absorption coefficient	0.114 mm^-1
F(000)	936
Crystal size	0.23 x 0.20 x 0.20 mm
Theta range for data collection	1.60 to 27.49 deg.
Limiting indices	-15<=h<=16, -20<=k<=21, -15<=l<=7
Reflections collected / unique	15140 / 5726 [R(int) = 0.0254]
Completeness to theta = 27.49	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9776 and 0.9744
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5726 / 0 / 288
Goodness-of-fit on F^2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0443, wR2 = 0.1123
R indices (all data)	R1 = 0.0691, wR2 = 0.1267
Extinction coefficient	0.0051(9)
Largest diff. peak and hole	0.219 and -0.203 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ljh055. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Si(1)	3756(1)	1274(1)	7867(1)	47(1)
N(2)	2243(1)	245(1)	6830(1)	54(1)

C(4)	480(1)	296(1)	7231(1)	48(1)
N(1)	233(1)	1130(1)	8850(1)	49(1)
C(1)	1079(1)	1613(1)	8700(1)	49(1)
O(1)	1411(1)	2088(1)	9427(1)	70(1)
C(9)	-159(1)	550(1)	8044(1)	48(1)
C(12)	5002(2)	1821(1)	7590(2)	63(1)
C(21)	-206(2)	1182(1)	9933(2)	57(1)
C(27)	-1634(2)	1763(1)	10923(2)	63(1)
C(5)	121(2)	-316(1)	6495(2)	63(1)
C(7)	-1483(2)	-393(1)	7339(2)	78(1)
C(11)	2618(1)	1977(1)	7662(2)	53(1)
C(10)	756(2)	2044(1)	6738(2)	63(1)
C(3)	1524(1)	681(1)	7180(1)	44(1)
C(13)	5077(2)	2672(1)	8084(2)	90(1)
C(22)	-1048(1)	1805(1)	10018(1)	47(1)
C(18)	3337(1)	520(1)	6720(2)	59(1)
C(6)	-850(2)	-665(1)	6554(2)	79(1)
C(2)	1537(1)	1565(1)	7566(1)	45(1)
C(23)	-1221(1)	2441(1)	9277(2)	61(1)
C(19)	4010(2)	-253(1)	6783(2)	96(1)
C(16)	4156(2)	1377(2)	10248(2)	104(1)
C(26)	-2369(2)	2346(2)	11080(2)	87(1)
C(25)	-2530(2)	2976(2)	10340(2)	83(1)
C(14)	6004(2)	1338(1)	7944(2)	90(1)
C(8)	-1153(1)	218(1)	8082(2)	64(1)
C(24)	-1958(2)	3025(1)	9440(2)	71(1)
C(20)	3336(2)	887(2)	5539(2)	89(1)
C(15)	3933(2)	773(1)	9290(2)	62(1)
C(17)	3050(2)	202(2)	9558(2)	91(1)

Table 3. Selected bond lengths [A] and angles [deg] for ljh055.

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [A] and angles [deg] for ljh055.

Si(1)-C(11)	1.8603(17)
Si(1)-C(15)	1.8859(19)
Si(1)-C(12)	1.8897(19)
Si(1)-C(18)	1.8926(19)
N(2)-C(3)	1.272(2)
N(2)-C(18)	1.489(2)
C(4)-C(5)	1.390(2)
C(4)-C(9)	1.395(2)
C(4)-C(3)	1.486(2)
N(1)-C(1)	1.370(2)
N(1)-C(9)	1.418(2)
N(1)-C(21)	1.462(2)
C(1)-O(1)	1.217(2)
C(1)-C(2)	1.530(2)
C(9)-C(8)	1.390(2)
C(12)-C(13)	1.527(3)
C(12)-C(14)	1.534(3)
C(12)-H(12)	0.9800
C(21)-C(22)	1.502(2)
C(21)-H(21A)	0.9700

C(21)-H(21B)	0.9700
C(27)-C(26)	1.374(3)
C(27)-C(22)	1.377(2)
C(27)-H(27)	0.9300
C(5)-C(6)	1.377(3)
C(5)-H(5)	0.9300
C(7)-C(6)	1.374(3)
C(7)-C(8)	1.384(3)
C(7)-H(7)	0.9300
C(11)-C(2)	1.537(2)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(10)-C(2)	1.554(2)
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(3)-C(2)	1.534(2)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(22)-C(23)	1.379(2)
C(18)-C(20)	1.536(3)
C(18)-C(19)	1.540(3)
C(6)-H(6)	0.9300
C(23)-C(24)	1.379(3)
C(23)-H(23)	0.9300
C(19)-H(19A)	0.9600
C(19)-H(19B)	0.9600
C(19)-H(19C)	0.9600
C(16)-C(15)	1.526(3)

C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(26)-C(25)	1.370(3)
C(26)-H(26)	0.9300
C(25)-C(24)	1.360(3)
C(25)-H(25)	0.9300
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(8)-H(8)	0.9300
C(24)-H(24)	0.9300
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(15)-C(17)	1.529(3)
C(15)-H(15)	0.9800
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(11)-Si(1)-C(15)	114.67(9)
C(11)-Si(1)-C(12)	109.79(8)
C(15)-Si(1)-C(12)	109.88(9)
C(11)-Si(1)-C(18)	98.97(8)
C(15)-Si(1)-C(18)	111.31(9)
C(12)-Si(1)-C(18)	111.88(9)
C(3)-N(2)-C(18)	124.87(14)
C(5)-C(4)-C(9)	118.74(16)
C(5)-C(4)-C(3)	121.96(16)
C(9)-C(4)-C(3)	119.29(14)

C(1)-N(1)-C(9)	122.50(14)
C(1)-N(1)-C(21)	117.32(14)
C(9)-N(1)-C(21)	119.97(14)
O(1)-C(1)-N(1)	120.53(16)
O(1)-C(1)-C(2)	121.86(16)
N(1)-C(1)-C(2)	117.50(14)
C(8)-C(9)-C(4)	120.25(16)
C(8)-C(9)-N(1)	120.68(16)
C(4)-C(9)-N(1)	119.04(15)
C(13)-C(12)-C(14)	110.79(18)
C(13)-C(12)-Si(1)	113.38(15)
C(14)-C(12)-Si(1)	113.46(13)
C(13)-C(12)-H(12)	106.2
C(14)-C(12)-H(12)	106.2
Si(1)-C(12)-H(12)	106.2
N(1)-C(21)-C(22)	116.07(14)
N(1)-C(21)-H(21A)	108.3
C(22)-C(21)-H(21A)	108.3
N(1)-C(21)-H(21B)	108.3
C(22)-C(21)-H(21B)	108.3
H(21A)-C(21)-H(21B)	107.4
C(26)-C(27)-C(22)	120.27(19)
C(26)-C(27)-H(27)	119.9
C(22)-C(27)-H(27)	119.9
C(6)-C(5)-C(4)	121.09(19)
C(6)-C(5)-H(5)	119.5
C(4)-C(5)-H(5)	119.5
C(6)-C(7)-C(8)	120.93(19)
C(6)-C(7)-H(7)	119.5
C(8)-C(7)-H(7)	119.5

C(2)-C(11)-Si(1)	114.67(11)
C(2)-C(11)-H(11A)	108.6
Si(1)-C(11)-H(11A)	108.6
C(2)-C(11)-H(11B)	108.6
Si(1)-C(11)-H(11B)	108.6
H(11A)-C(11)-H(11B)	107.6
C(2)-C(10)-H(10A)	109.5
C(2)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(2)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
N(2)-C(3)-C(4)	116.84(14)
N(2)-C(3)-C(2)	130.80(15)
C(4)-C(3)-C(2)	112.36(13)
C(12)-C(13)-H(13A)	109.5
C(12)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(12)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(27)-C(22)-C(23)	118.54(16)
C(27)-C(22)-C(21)	117.83(15)
C(23)-C(22)-C(21)	123.51(15)
N(2)-C(18)-C(20)	106.64(15)
N(2)-C(18)-C(19)	105.44(16)
C(20)-C(18)-C(19)	108.91(18)
N(2)-C(18)-Si(1)	109.80(11)
C(20)-C(18)-Si(1)	112.30(15)
C(19)-C(18)-Si(1)	113.33(14)

C(7)-C(6)-C(5)	119.5(2)
C(7)-C(6)-H(6)	120.2
C(5)-C(6)-H(6)	120.2
C(1)-C(2)-C(3)	108.79(13)
C(1)-C(2)-C(11)	109.32(14)
C(3)-C(2)-C(11)	115.46(13)
C(1)-C(2)-C(10)	105.03(13)
C(3)-C(2)-C(10)	107.98(14)
C(11)-C(2)-C(10)	109.75(14)
C(24)-C(23)-C(22)	120.92(18)
C(24)-C(23)-H(23)	119.5
C(22)-C(23)-H(23)	119.5
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(25)-C(26)-C(27)	120.6(2)
C(25)-C(26)-H(26)	119.7
C(27)-C(26)-H(26)	119.7
C(24)-C(25)-C(26)	119.8(2)
C(24)-C(25)-H(25)	120.1
C(26)-C(25)-H(25)	120.1

C(12)-C(14)-H(14A)	109.5
C(12)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(12)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(7)-C(8)-C(9)	119.39(19)
C(7)-C(8)-H(8)	120.3
C(9)-C(8)-H(8)	120.3
C(25)-C(24)-C(23)	119.9(2)
C(25)-C(24)-H(24)	120.1
C(23)-C(24)-H(24)	120.1
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(16)-C(15)-C(17)	109.66(19)
C(16)-C(15)-Si(1)	112.60(15)
C(17)-C(15)-Si(1)	115.74(13)
C(16)-C(15)-H(15)	106.0
C(17)-C(15)-H(15)	106.0
Si(1)-C(15)-H(15)	106.0
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5
H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters (A^2 x 10^3) for ljh055.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

	U11	U22	U33	U23	U13	U12
Si(1)	47(1)	41(1)	51(1)	4(1)	2(1)	-1(1)
N(2)	46(1)	55(1)	60(1)	-14(1)	0(1)	5(1)
C(4)	47(1)	48(1)	46(1)	2(1)	-4(1)	5(1)
N(1)	55(1)	51(1)	42(1)	4(1)	9(1)	6(1)
C(1)	52(1)	45(1)	49(1)	0(1)	3(1)	10(1)
O(1)	73(1)	73(1)	66(1)	-25(1)	13(1)	-5(1)
C(9)	48(1)	49(1)	46(1)	9(1)	-1(1)	5(1)
C(12)	58(1)	58(1)	72(1)	14(1)	7(1)	-6(1)
C(21)	65(1)	62(1)	44(1)	8(1)	11(1)	11(1)
C(27)	74(1)	62(1)	56(1)	3(1)	19(1)	1(1)
C(5)	60(1)	68(1)	60(1)	-11(1)	-5(1)	-1(1)
C(7)	58(1)	87(2)	88(2)	8(1)	-3(1)	-19(1)
C(11)	58(1)	40(1)	61(1)	3(1)	10(1)	2(1)
C(10)	65(1)	60(1)	63(1)	20(1)	4(1)	16(1)
C(3)	47(1)	46(1)	39(1)	0(1)	-2(1)	6(1)
C(13)	80(2)	64(1)	126(2)	7(1)	5(1)	-24(1)
C(22)	47(1)	50(1)	44(1)	-2(1)	5(1)	-4(1)
C(18)	47(1)	62(1)	68(1)	-15(1)	5(1)	6(1)
C(6)	70(1)	80(2)	83(2)	-14(1)	-12(1)	-14(1)
C(2)	50(1)	41(1)	45(1)	5(1)	4(1)	8(1)
C(23)	56(1)	70(1)	58(1)	13(1)	14(1)	8(1)

C(19)	60(1)	76(2)	149(2)	-49(2)	1(1)	18(1)
C(16)	129(2)	125(2)	54(1)	2(1)	-6(1)	-16(2)
C(26)	94(2)	98(2)	76(2)	0(1)	40(1)	19(1)
C(25)	79(2)	83(2)	88(2)	-6(1)	18(1)	27(1)
C(14)	54(1)	83(2)	134(2)	30(2)	14(1)	-5(1)
C(8)	54(1)	70(1)	67(1)	10(1)	7(1)	-1(1)
C(24)	66(1)	68(1)	78(1)	11(1)	6(1)	15(1)
C(20)	69(1)	143(2)	57(1)	-22(1)	14(1)	-11(1)
C(15)	58(1)	66(1)	62(1)	16(1)	0(1)	-1(1)
C(17)	73(1)	99(2)	98(2)	56(2)	4(1)	-8(1)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ljh055.

	x	y	z	U(eq)
H(12)	4974	1886	6773	75
H(21A)	364	1294	10510	68
H(21B)	-492	657	10098	68
H(27)	-1531	1338	11430	76
H(5)	543	-493	5953	76
H(7)	-2143	-623	7372	94
H(11A)	2657	2352	8289	63
H(11B)	2678	2290	6985	63
H(10A)	995	2036	6001	94
H(10B)	716	2593	6990	94
H(10C)	72	1800	6710	94
H(13A)	5148	2640	8890	136
H(13B)	4452	2968	7835	136

H(13C)	5678	2942	7837	136
H(6)	-1075	-1081	6067	95
H(23)	-834	2476	8659	73
H(19A)	3958	-516	7492	144
H(19B)	4730	-115	6714	144
H(19C)	3761	-611	6183	144
H(16A)	3570	1738	10263	156
H(16B)	4776	1682	10133	156
H(16C)	4264	1093	10950	156
H(26)	-2761	2313	11694	105
H(25)	-3028	3370	10452	100
H(14A)	6603	1628	7731	135
H(14B)	5964	821	7579	135
H(14C)	6072	1263	8745	135
H(8)	-1593	404	8601	76
H(24)	-2065	3452	8936	85
H(20A)	3013	516	4993	134
H(20B)	4046	990	5383	134
H(20C)	2948	1384	5504	134
H(15)	4565	438	9292	74
H(17A)	3238	-54	10270	136
H(17B)	2947	-202	8981	136
H(17C)	2413	504	9589	136

Table 7. Selected torsion angles [deg] for ljh055.

Symmetry transformations used to generate equivalent atoms:

Table 8. Torsion angles [deg] for ljh055.

C(9)-N(1)-C(1)-O(1)	-177.88(15)
C(21)-N(1)-C(1)-O(1)	-3.2(2)
C(9)-N(1)-C(1)-C(2)	5.7(2)
C(21)-N(1)-C(1)-C(2)	-179.67(13)
C(5)-C(4)-C(9)-C(8)	-2.6(2)
C(3)-C(4)-C(9)-C(8)	177.77(15)
C(5)-C(4)-C(9)-N(1)	175.33(15)
C(3)-C(4)-C(9)-N(1)	-4.3(2)
C(1)-N(1)-C(9)-C(8)	-163.88(15)
C(21)-N(1)-C(9)-C(8)	21.6(2)
C(1)-N(1)-C(9)-C(4)	18.2(2)
C(21)-N(1)-C(9)-C(4)	-156.26(15)
C(11)-Si(1)-C(12)-C(13)	41.94(18)
C(15)-Si(1)-C(12)-C(13)	-85.05(17)
C(18)-Si(1)-C(12)-C(13)	150.79(16)
C(11)-Si(1)-C(12)-C(14)	169.47(16)
C(15)-Si(1)-C(12)-C(14)	42.48(19)

C(18)-Si(1)-C(12)-C(14)	-81.68(18)
C(1)-N(1)-C(21)-C(22)	89.05(19)
C(9)-N(1)-C(21)-C(22)	-96.18(18)
C(9)-C(4)-C(5)-C(6)	0.4(3)
C(3)-C(4)-C(5)-C(6)	-179.93(17)
C(15)-Si(1)-C(11)-C(2)	-70.55(15)
C(12)-Si(1)-C(11)-C(2)	165.19(13)
C(18)-Si(1)-C(11)-C(2)	47.95(14)
C(18)-N(2)-C(3)-C(4)	-179.99(15)
C(18)-N(2)-C(3)-C(2)	0.4(3)
C(5)-C(4)-C(3)-N(2)	-30.0(2)
C(9)-C(4)-C(3)-N(2)	149.69(15)
C(5)-C(4)-C(3)-C(2)	149.69(16)
C(9)-C(4)-C(3)-C(2)	-30.66(19)
C(26)-C(27)-C(22)-C(23)	-0.3(3)
C(26)-C(27)-C(22)-C(21)	176.0(2)
N(1)-C(21)-C(22)-C(27)	166.61(16)
N(1)-C(21)-C(22)-C(23)	-17.4(3)
C(3)-N(2)-C(18)-C(20)	-88.4(2)
C(3)-N(2)-C(18)-C(19)	155.89(18)
C(3)-N(2)-C(18)-Si(1)	33.5(2)
C(11)-Si(1)-C(18)-N(2)	-51.50(14)

C(15)-Si(1)-C(18)-N(2)	69.50(14)
C(12)-Si(1)-C(18)-N(2)	-167.15(12)
C(11)-Si(1)-C(18)-C(20)	66.96(15)
C(15)-Si(1)-C(18)-C(20)	-172.04(14)
C(12)-Si(1)-C(18)-C(20)	-48.68(16)
C(11)-Si(1)-C(18)-C(19)	-169.11(16)
C(15)-Si(1)-C(18)-C(19)	-48.11(18)
C(12)-Si(1)-C(18)-C(19)	75.25(18)
C(8)-C(7)-C(6)-C(5)	-1.0(3)
C(4)-C(5)-C(6)-C(7)	1.4(3)
O(1)-C(1)-C(2)-C(3)	144.41(16)
N(1)-C(1)-C(2)-C(3)	-39.22(18)
O(1)-C(1)-C(2)-C(11)	17.5(2)
N(1)-C(1)-C(2)-C(11)	-166.11(13)
O(1)-C(1)-C(2)-C(10)	-100.19(18)
N(1)-C(1)-C(2)-C(10)	76.18(17)
N(2)-C(3)-C(2)-C(1)	-130.19(18)
C(4)-C(3)-C(2)-C(1)	50.23(17)
N(2)-C(3)-C(2)-C(11)	-6.9(2)
C(4)-C(3)-C(2)-C(11)	173.53(13)
N(2)-C(3)-C(2)-C(10)	116.34(19)
C(4)-C(3)-C(2)-C(10)	-63.24(17)

Si(1)-C(11)-C(2)-C(1)	99.42(14)
Si(1)-C(11)-C(2)-C(3)	-23.59(18)
Si(1)-C(11)-C(2)-C(10)	-145.88(13)
C(27)-C(22)-C(23)-C(24)	0.4(3)
C(21)-C(22)-C(23)-C(24)	-175.59(18)
C(22)-C(27)-C(26)-C(25)	0.0(4)
C(27)-C(26)-C(25)-C(24)	0.1(4)
C(6)-C(7)-C(8)-C(9)	-1.1(3)
C(4)-C(9)-C(8)-C(7)	2.9(3)
N(1)-C(9)-C(8)-C(7)	-174.93(17)
C(26)-C(25)-C(24)-C(23)	0.0(4)
C(22)-C(23)-C(24)-C(25)	-0.3(3)
C(11)-Si(1)-C(15)-C(16)	-62.60(18)
C(12)-Si(1)-C(15)-C(16)	61.62(18)
C(18)-Si(1)-C(15)-C(16)	-173.89(16)
C(11)-Si(1)-C(15)-C(17)	64.65(19)
C(12)-Si(1)-C(15)-C(17)	-171.13(16)
C(18)-Si(1)-C(15)-C(17)	-46.64(19)

Symmetry transformations used to generate equivalent atoms

Table 9. Hydrogen bonds for ljh055 [A and deg.].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)