Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Si-coumarin of hydrogen-bonding inducted bathochromic effect for monitoring adipogenic differentiation

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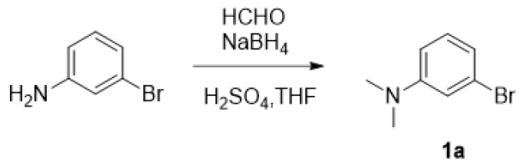
1. Experimental details

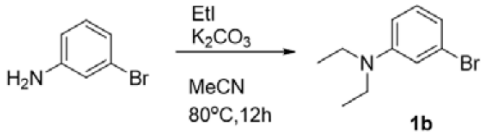
Materials and instruments. Unless otherwise stated, all reagents were purchased from commercial suppliers (including Sigma-Aldrich, Adamas-beta and TCI) and used without further purification. The composition of mixed solvents is given by the volume ratio (*v*/*v*). Thin layer chromatography (TLC) was performed on TLC-aluminum sheets (Silica gel 60 F254). Flash column chromatography was performed with General-Reagent silica gel (200-300 mesh and type H). ^{1}H NMR spectra and ^{13}C NMR were recorded using Bruker Avance spectrometer (500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR) with tetramethylsilane (TMS) as internal standard. The chemical shifts in ^{1}H NMR spectra are reported in δ ppm using the residual proton of the solvents, $CDCl_3$ (7.26ppm) as an internal standard and those in ^{13}C NMR spectra are reported using the solvent signal of $CDCl_3$ (77.16 ppm), as an internal standard. The HRMS were recorded using A Bruker maXis impact. A SHIMADZU UV-2600 UV-vis spectrophotometer was used for absorption measurement and a SHIMADZU RF-6000 spetcrofluorophotometer was used for fluorescent measurement. A Leica SP8 confocal laser scanning microscope was applied for cell imaging.

Scheme S1. Synthesis of Si-Coumarins



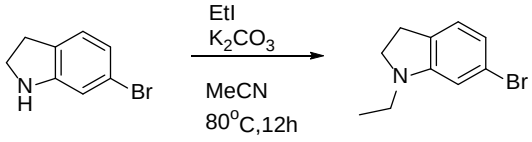
1a

To a dried flask was added M-bromoaniline (4 g, 23.26 mmol), 3M H_2SO_4 (1.8 eq,14 mL), and formaldehyde solution (3 eq), the mixture was stirred in an ice bath for 30 min. $NaBH_4$ (4 eq, 3.4 g) was added in portions under the ice bath. Then stirred at room temperature for 2 hours. After the reaction was completed, saturated $NaHCO_3$ solution was added and extracted with ethyl acetate. The organic phase was combined, washed with saturated brine for 2 times, then dried with anhydrous Na_2SO_4, and the solvent was removed under vacuum. The residue was further purified by column chromatography to afford 1a (3.95 g, 85 %).



1b

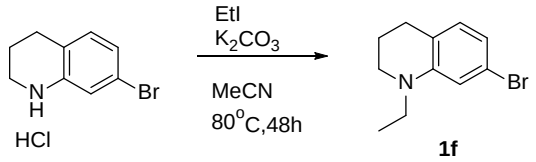
To a dried flask was added m-bromoaniline (4 g, 23.26 mmol), potassium carbonate (3.16 g, 1 eq), iodoethane (8 g, 2.2 eq) and acetonitrile solution (40 mL). The mixture was stirred at 80 ^oC for 12 hours. After the reaction was completed, filtrated and extracted with ethyl acetate. The organic phase was combined, washed with saturated brine, and then dried with anhydrous Na_2SO_4, and the solvent was removed under vacuum. The residue was further purified by column chromatography sto afford 1b (4.2 g, 80 %).



1e

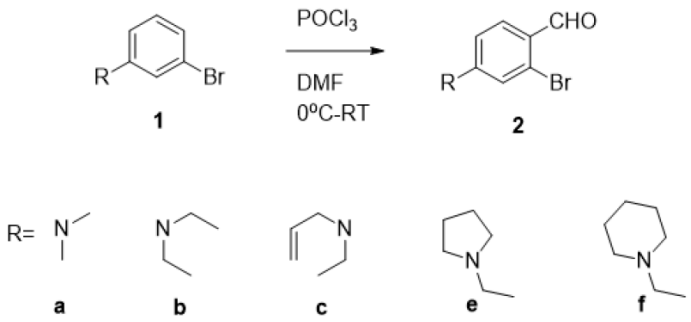
To a dried flask was added 6-bromindoline (2 g, 10 mmol), potassium carbonate (1.36 g, 1 eq), iodoethane (3.43 g, 2.2 eq) and acetonitrile (20 mL). The mixture was stirred at 80 ^oC for

12 hours. After the reaction was completed, filtrated and extracted with ethyl acetate. The organic phase was combined, washed with saturated brine, and then dried with anhydrous Na_2SO_4, the solvent was removed under vacuum. The residue was further purified by column chromatography to afford 1e (1.85 g, 82 %).

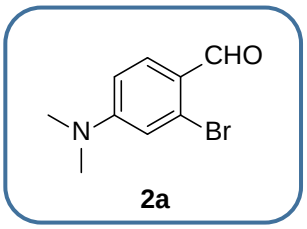


To a dried flask was added 7-bromo-1,2,3,4-tetrahydroquinoline hydrochloride (2 g, 8 mmol), potassium carbonate (6.66 g, 6 eq), iodoethane (5 g, 4 eq) and acetonitrile 40 mL). The mixture was stirred at 80 ^oC for 48 hours. After the reaction was completed, filtrated and extracted with ethyl acetate. The organic phase was combined, washed with saturated brine, and then dried with anhydrous Na_2SO_4, the solvent was removed under vacuum. The residue was further purified by column chromatography to afford 1e (1.34 g, 70 %).

General procedures for synthesizing 2a-2f

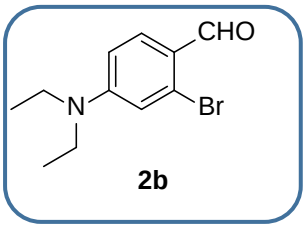


To a dried flask filled with argon was added DMF (10mL) and $POCl_3$ (2.8 ml, 3 eq) in an ice bath, and stirred for 30 min at 0 ^oC. Then the DMF solution of compound **1** (10 mmol) was added to the flask and stirred for 6 h at room temperature. When the reaction was completed, the solution was poured into ice water and the precipitate was filtrated and washed with water for three times, then the solid was dissolved with dichloromethane and dried over Na_2SO_4, and evaporated. The residue was purified by column chromatography to obtain **2a-2f**. Yield is 80 %.



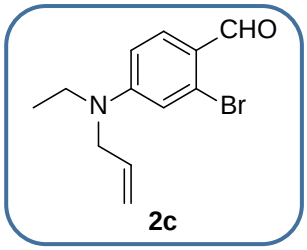
2a

White solid, ^{1}H NMR (500 MHz, Chloroform-*d*) δ 10.09 (s, 1H), 7.79 (d, *J* = 8.9 Hz, 1H), 6.79 (d, *J* = 2.4 Hz, 1H), 6.63 (dd, *J* = 8.9, 2.0 Hz, 1H), 3.08 (s, 6H).^{13}C NMR (126 MHz, Chloroform-*d*) δ 190.22 ,154.49 ,131.04 , 129.71 , 122.01 , 114.83 , 110.58 , 40.09 .



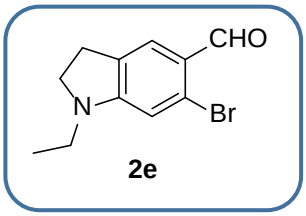
2b

White solid, ^{1}H NMR (500 MHz, Chloroform-*d*) δ 10.00 (s, 1H), 7.72 (d, *J* = 9.0 Hz, 1H), 6.72 (d, *J* = 2.4 Hz, 1H), 6.56 (dd, *J* = 9.0, 2.1 Hz, 1H), 3.36 (q, *J* = 7.1 Hz, 4H), 1.17 (t, *J* = 7.2 Hz, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 189.75 , 152.47 , 130.02 , 121.44 , 114.30 , 110.25 , 44.77 , 12.41 .



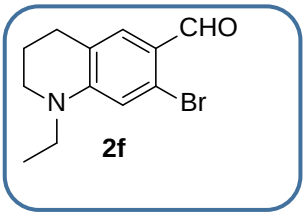
2c

Colorless oil, ^{1}H NMR (500 MHz, Chloroform-*d*) δ 10.06 (s, 1H), 7.77 (d, *J* = 8.9 Hz, 1H), 6.79 (d, *J* = 2.4 Hz, 1H), 6.62 (dd, *J* = 8.9, 2.2 Hz, 1H), 5.82 (ddt, *J* = 16.8, 10.2, 4.6 Hz, 1H), 5.32 – 5.11 (m, 2H), 3.99 – 3.95 (m, 2H), 3.44 (q, *J* = 7.1 Hz, 2H), 1.23 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 190.02 , 153.03 , 131.96 , 131.21 , 129.88 , 122.00 , 116.84 , 114.76 , 110.63 , 52.47 , 45.29 , 12.25 .



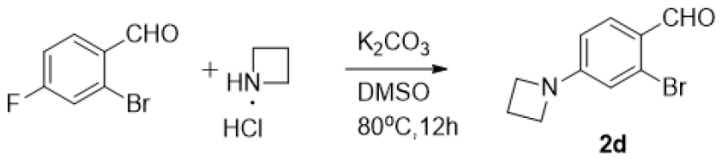
2e

White solid, ^{1}H NMR (500 MHz, Chloroform-*d*) δ 10.04 (s, 1H), 7.57 (s, 1H), 6.47 (s, 1H), 3.62 (t, *J* = 8.6 Hz, 2H), 3.28 (q, *J* = 7.2 Hz, 2H), 2.99 (t, *J* = 8.4 Hz, 2H), 1.21 (t, *J* = 7.2 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 189.97 , 157.08 , 130.37 , 129.86 , 124.78 , 122.63 , 108.44 , 51.41 , 41.06 , 26.70 , 11.65 .

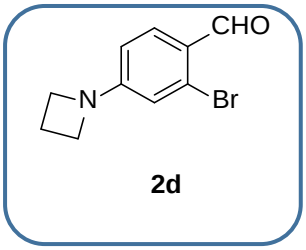


2f

White solid, ^{1}H NMR (500 MHz, Chloroform-*d*) δ 10.02 (s, 1H), 7.52 (s, 1H), 6.68 (s, 1H), 3.44 – 3.33 (m, 4H), 2.71 (t, *J* = 6.3 Hz, 2H), 1.94 (p, *J* = 6.1 Hz, 2H), 1.22 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 190.03 , 150.40 , 129.73 , 128.02 , 121.44 , 121.24 , 112.81 , 48.56 , 45.68 , 27.42 , 21.28 , 11.10 .

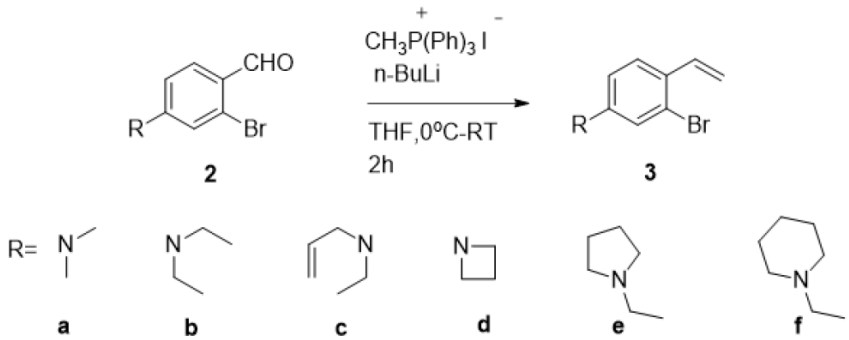


To a dried flask was added 2-bromo-4-fluorobenzaldehyde (2 g, 8 mmol), potassium carbonate (6.66 g, 6 eq), iodoethane (5 g, 4 eq) and acetonitrile 40 mL). The mixture was stirred at 80 °C for 48 hours. After the reaction was completed, filtrated and extracted with ethyl acetate. The organic phase was combined, washed with saturated brine, and then dried with anhydrous Na_2SO_4, the solvent was removed under vacuum. The residue was further purified by column chromatography to afford **2d** (1.34 g, 70 %).



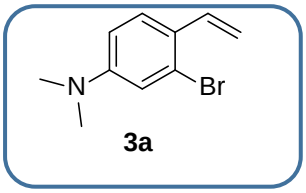
White solid, ^{1}H NMR (500 MHz, Chloroform-*d*) δ 10.07 (s, 1H), 7.76 (d, *J* = 8.6 Hz, 1H), 6.46 (d, *J* = 2.2 Hz, 1H), 6.29 (dd, *J* = 8.6, 1.8 Hz, 1H), 4.03 (t, *J* = 7.4 Hz, 4H), 2.44 (q, *J* = 7.4 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 190.20 , 154.95 , 131.16 , 129.58 , 122.33 , 113.34 , 109.21 , 51.33 , 16.35 .

General procedures for synthesizing 3a-3f



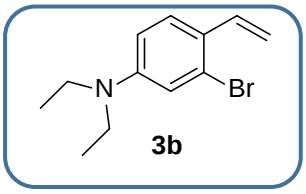
To a dried and argon protected flask was added methyl triphenyl phosphor iodide (4.8 g, 1.2 eq), anhydrous THF (20 mL) and *n*-BuLi (6.8 mL, 1.1eq) then stirred in an ice bath for 30 min. Then the compound **2** (10 mmol) of THF solution was added in drops and stirred at room temperature for 1.5 h. After the reaction was completed, the mixture was filtered by silica gel (200-300 mesh). Then the filtrate was wash with water and dried over Na_2SO_4, the solvent was

removed under vacuum. The residue was directly used in following steps without further purification. Colorless oil, yield 60%.



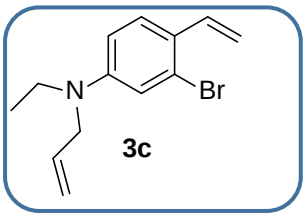
3a

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.47 (d, *J* = 8.8 Hz, 1H), 7.01 (dd, *J* = 17.4, 10.9 Hz, 1H), 6.89 (d, *J* = 2.5 Hz, 1H), 6.67 (dd, *J* = 8.8, 2.5 Hz, 1H), 5.55 (d, *J* = 17.4 Hz, 1H), 5.16 (d, *J* = 10.9 Hz, 1H), 2.98 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 126.77 , 124.85 , 115.53 , 112.17 , 111.78 , 40.31 .



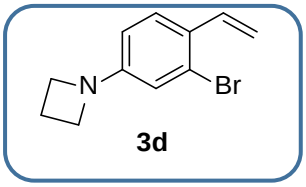
3b

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.41 (d, *J* = 8.8 Hz, 1H), 6.96 (dd, *J* = 17.4, 10.9 Hz, 1H), 6.80 (d, *J* = 2.7 Hz, 1H), 6.59 (dd, *J* = 8.8, 2.6 Hz, 1H), 5.49 (d, *J* = 17.4 Hz, 1H), 5.09 (d, *J* = 10.9 Hz, 1H), 3.33 (q, *J* = 7.1 Hz, 4H), 1.16 (t, *J* = 7.1 Hz, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 135.33 , 126.94 , 114.73 , 111.54 , 111.16 , 77.29 , 44.40 , 12.53 .



3c

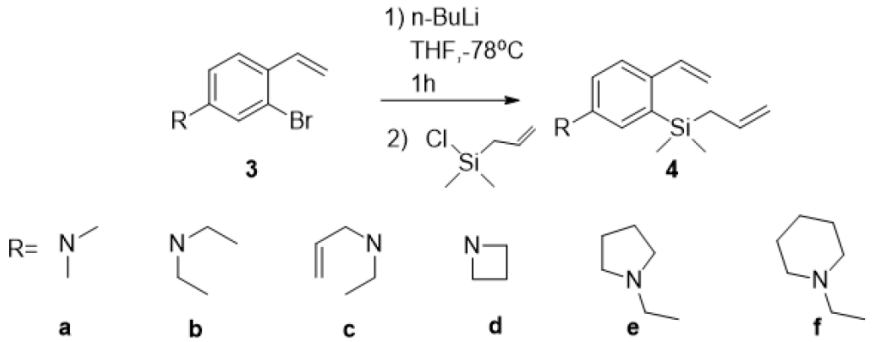
^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.46 (d, *J* = 8.8 Hz, 1H), 7.02 (dd, *J* = 17.4, 10.9 Hz, 1H), 6.88 (d, *J* = 2.4 Hz, 1H), 6.65 (dd, *J* = 8.8, 2.4 Hz, 1H), 5.87 (ddd, *J* = 16.2, 10.3, 4.7 Hz, 1H), 5.55 (d, *J* = 17.4 Hz, 1H), 5.22 (s, 1H), 5.19 (d, *J* = 5.8 Hz, 1H), 5.16 (d, *J* = 11.0 Hz, 1H), 3.95 – 3.90 (m, 2H), 3.41 (q, *J* = 7.1 Hz, 2H), 1.22 (t, *J* = 7.1 Hz, 3H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 148.59, 135.33, 133.52, 126.90 , 125.02 , 124.61 , 116.19 , 115.11 , 111.85 , 111.50 , 52.50 , 44.92 , 12.33 .



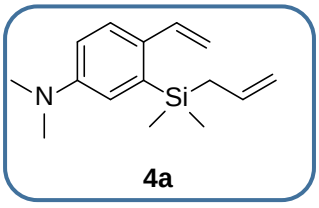
3d

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.40 (d, *J* = 8.5 Hz, 1H), 6.96 (dd, *J* = 17.4, 10.9 Hz, 1H), 6.57 (d, *J* = 2.4 Hz, 1H), 6.34 (dd, *J* = 8.5, 2.3 Hz, 1H), 5.50 (dd, *J* = 17.4, 1.1 Hz, 1H), 5.13 (dd, *J* = 10.9, 1.1 Hz, 1H), 3.89 – 3.85 (m, 4H), 2.37 (q, *J* = 7.3 Hz, 2H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 152.27, 135.42, 126.81, 125.92 , 124.48 , 114.59 , 112.39 , 110.73 , 77.05 , 52.26 , 16.81 .

General procedures for synthesizing 4a-4f:

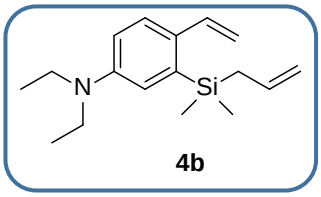


To a dried and argon protected flask was added compound 3 (5 mmol,1.0 eq) and anhydrous THF (10 mL), the mixture stirred at -78 °C for 5 min, then the *n*-BuLi (1.2 eq, 3.75 mL, 1.6 M in hexane solution) was added, and the mixture was stirred for 1h at -78 °C. After 1h, the allyldimethylchlorosilane (0.98 mL,1.3 eq) was added in drops and stirred for overnight from -78 °C to room temperature. After the reaction was completed, quenched reaction with water and extracted with ethyl acetate then washed the organic phase with water and brine, and dried over Na_2SO_4, the solvent was removed under vacuum. The residue was further purified by column chromatography to afford compound **4**, colorless oil, yield 85%.



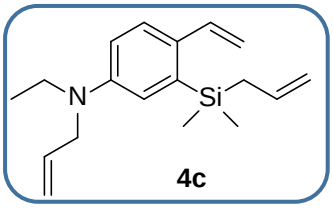
4a

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 8.6 Hz, 1H), 7.01 (dd, *J* = 17.1, 10.9 Hz, 1H), 6.88 (s, 1H), 6.78 (d, *J* = 8.5 Hz, 1H), 5.84 (dq, *J* = 17.3, 8.9 Hz, 1H), 5.56 – 5.49 (m, 1H), 5.12 (d, *J* = 10.8 Hz, 1H), 4.92 (dd, *J* = 26.2, 13.5 Hz, 2H), 2.99 (s, 6H), 1.90 (d, *J* = 8.0 Hz, 2H), 0.38 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 149.18, 137.59 , 135.01 , 126.07 , 118.30 , 113.76 , 113.50 , 111.16 , 40.56 ,



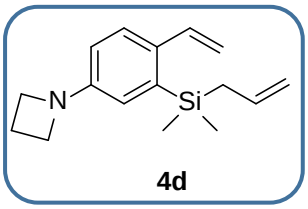
4b

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.54 (d, *J* = 8.7 Hz, 1H), 7.00 (dd, *J* = 17.2, 10.8 Hz, 1H), 6.84 (d, *J* = 2.6 Hz, 1H), 6.74 (dd, *J* = 8.6, 2.4 Hz, 1H), 5.92 – 5.79 (m, 1H), 5.51 (d, *J* = 17.2 Hz, 1H), 5.09 (d, *J* = 11.7 Hz, 1H), 4.93 (dd, *J* = 25.2, 12.7 Hz, 2H), 3.43 – 3.39 (m, 4H), 1.90 (d, *J* = 8.1 Hz, 2H), 1.22 (t, *J* = 7.1 Hz, 6H), 0.38 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 137.53, 135.05, 126.21, 117.41, 113.41, 112.87, 110.42, 44.46 , 24.31 , 12.66 , -1.86 .



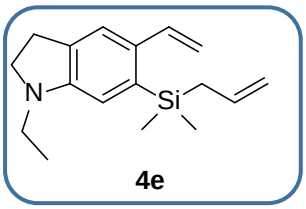
4c

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.55 (d, *J* = 8.7 Hz, 1H), 7.02 (dd, *J* = 17.2, 10.8 Hz, 1H), 6.86 (d, *J* = 2.6 Hz, 1H), 6.76 (dd, *J* = 8.7, 2.6 Hz, 1H), 5.95 – 5.83 (m, 2H), 5.56 – 5.50 (m, 1H), 5.25 (dd, *J* = 17.2, 1.6 Hz, 1H), 5.23 – 5.20 (m, 1H), 5.14 – 5.09 (m, 1H), 5.00 – 4.90 (m, 2H), 3.97 (d, *J* = 4.9 Hz, 2H), 3.48 – 3.44 (m, 2H), 1.91 (d, *J* = 8.1 Hz, 2H), 1.24 (d, *J* = 7.1 Hz, 3H), 0.40 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 146.78, 137.54 , 135.05 , 134.43 , 127.31 , 126.11 , 117.78 , 115.95 , 113.43 , 113.14 , 110.66 , 52.80 , 44.88 , 24.30 , 12.43 , -1.85 .



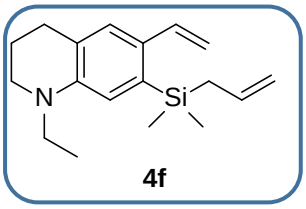
4d

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.53 (d, *J* = 8.4 Hz, 1H), 7.02 (dd, *J* = 17.2, 10.8 Hz, 1H), 6.59 (d, *J* = 2.5 Hz, 1H), 6.51 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.85 (td, *J* = 17.6, 8.1 Hz, 1H), 5.54 (d, *J* = 17.2 Hz, 1H), 5.14 (d, *J* = 10.8 Hz, 1H), 5.00 – 4.88 (m, 2H), 3.94 (t, *J* = 7.2 Hz, 4H), 2.41 (p, *J* = 7.2 Hz, 2H), 1.90 (d, *J* = 8.1 Hz, 2H), 0.39 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.73 , 137.73 , 137.37 , 134.94 , 132.92 , 125.85 , 116.98 , 113.48 , 112.46 , 111.28 , 52.41 , 24.24 , 17.01 , -1.90 .



4e

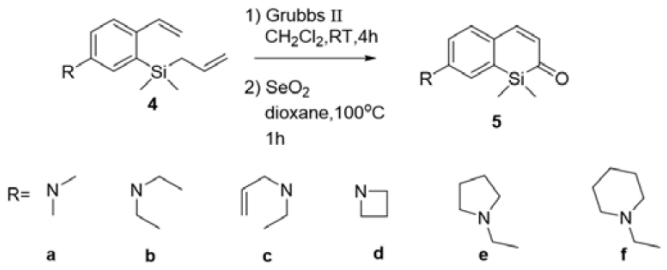
^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.43 (s, 1H), 7.03 (dd, *J* = 17.2, 10.8 Hz, 1H), 6.61 (s, 1H), 5.92 – 5.81 (m, 1H), 5.53 (d, *J* = 17.1 Hz, 1H), 5.11 (d, *J* = 10.9 Hz, 1H), 4.99 – 4.89 (m, 2H), 3.40 (t, *J* = 8.3 Hz, 2H), 3.21 (q, *J* = 7.2 Hz, 2H), 3.01 (t, *J* = 8.2 Hz, 2H), 1.90 (d, *J* = 8.1 Hz, 2H), 1.25 (t, *J* = 7.2 Hz, 3H), 0.39 (s, 6H). ^{13}C NMR (126MHz, Chloroform-*d*) δ 151.25 , 137.89 , 135.82 , 135.09 , 133.57 , 132.24 , 121.41 , 113.37 , 112.05 , 110.49 , 52.10 , 42.92 , 28.34 , 24.43 , 12.06 , -1.72 .



4f

^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.53 (d, *J* = 8.4 Hz, 1H), 7.02 (dd, *J* = 17.2, 10.8 Hz, 1H), 6.59 (d, *J* = 2.5 Hz, 1H), 6.51 (dd, *J* = 8.4, 2.4 Hz, 1H), 5.85 (td, *J* = 17.6, 8.1 Hz, 1H), 5.54 (d, *J* = 17.2 Hz, 1H), 5.14 (d, *J* = 10.8 Hz, 1H), 5.00 – 4.88 (m, 2H), 3.94 (t, *J* = 7.2 Hz, 4H), 2.41 (p, *J* = 7.2 Hz, 2H), 1.90 (d, *J* = 8.1 Hz, 2H), 0.39 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 150.73 , 137.73 , 134.94 , 125.85 , 116.98 , 113.48 , 112.46 , 111.28 , 76.84 , 52.41 , 24.24 , 17.01 , -1.90 .

General procedures for synthesizing 5a-5f:



To a dried and argon protected flask was added compound4 (1 mmol, 1.0 eq) and Grubbs II catalyst (5 %mol) and anhydrous CH_2Cl_2(10 mL) ,the mixture was stirred at room temperature for 4h, After the reaction was completed, the solvent was removed under vacuum and then the crude product was further dried under high vacuum pump. The residue was directly used in next step without further purified. To a dried flask was added the residue and SeO_2(122 mg, 1.1 eq) and dioxane (10 mL), the solution was refluxed at 100°C for 1h. After the reaction was completed, filtered with kieselguhr, the filtrate was removed under vacuum. The residue was further purified by column chromatography to afford compound **5**, orange solid, yield 50% for two steps.

Compound 5a (SiC A): ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.30 (d, *J* = 10.9 Hz, 1H), 7.24 (d, *J* = 8.6 Hz, 1H), 6.83 (d, *J* = 2.8 Hz, 1H), 6.65 (dd, *J* = 8.6, 2.8 Hz, 1H), 5.97 (d, *J* = 10.9 Hz, 1H), 3.05 (s, 6H), 0.35 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 190.24 , 150.55 , 148.72 , 139.68 , 133.98 , 129.18 , 118.52 , 112.33 , 76.83 , 40.10 , -4.01 . HRMS (ESI+) Calcd for $[M+H]^+$:232.1152 ,Found: 232.1152

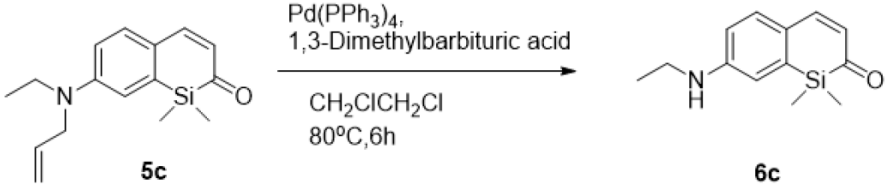
Compound 5b (SiC B): ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.29 (d, *J* = 10.9 Hz, 1H), 7.22 (d, *J* = 8.6 Hz, 1H), 6.80 (s, 1H), 6.62 (d, *J* = 7.3 Hz, 1H), 5.95 (d, *J* = 10.9 Hz, 1H), 3.43 (q, *J* = 7.1 Hz, 4H), 1.21 (t, *J* = 7.1 Hz, 6H), 0.35 (s, 6H). ^{13}C NMR (500MHz, Chloroform-*d*) δ 148.75 , 134.27 , 128.76 , 126.03 , 118.08 , 111.70 , 76.80 , 44.44 , 12.58 , -4.06 . HRMS (ESI+) Calcd for $[M+H]^+$:260.1465 ,Found: 260.1465.

Compound 5c: ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.29 (d, *J* = 10.9 Hz, 1H), 7.22 (d, *J* = 8.6 Hz, 1H), 6.81 (d, *J* = 2.5 Hz, 1H), 6.64 (dd, *J* = 8.6, 2.6 Hz, 1H), 5.95 (d, *J* = 10.9 Hz, 1H), 5.85 (s, 1H), 5.17 (d, *J* = 22.2 Hz, 2H), 3.97 (d, *J* = 4.4 Hz, 2H), 3.45 (q, *J* = 7.1 Hz, 2H), 1.22 (t, *J* = 7.1 Hz, 3H), 0.34 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 148.65 , 134.08 , 133.18 , 129.03 , 126.58 , 118.51 , 116.39 , 112.14 , 76.78 , 52.50 , 44.96 , 12.37 , -4.10 .

Compound 5d (SiC D): ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.29 (d, *J* = 11.0 Hz, 1H), 7.21 (d, *J* = 8.3 Hz, 1H), 6.52 (d, *J* = 2.5 Hz, 1H), 6.37 (dd, *J* = 8.3, 2.5 Hz, 1H), 5.97 (d, *J* = 11.0 Hz, 1H), 3.99 (t, *J* = 7.3 Hz, 4H), 2.43 (p, *J* = 7.3 Hz, 2H), 0.34 (s, 6H). ^{13}C NMR (126MHz, Chloroform-*d*) δ 151.63 , 148.83 , 133.81 , 129.31 , 117.41 , 111.27 , 77.05 , 51.82 , 16.66 , -4.10. HRMS (ESI+) Calcd for $[M+H]^+$:244.1152, Found: 244.1145.

Compound 5e (SiC E): ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.29 – 7.24 (m, 1H), 7.06 (s, 1H), 6.56 (s, 1H), 5.94 (d, *J* = 11.0 Hz, 1H), 3.49 (t, *J* = 8.6 Hz, 2H), 3.26 (q, *J* = 7.2 Hz, 2H), 3.00 (t, *J* = 9.0 Hz, 2H), 1.21 (t, *J* = 7.2 Hz, 3H), 0.33 (s, 6H). ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.29 – 7.24 (m, 1H), 7.06 (s, 1H), 6.56 (s, 1H), 5.94 (d, *J* = 11.0 Hz, 1H), 3.49 (t, *J* = 8.6 Hz, 2H), 3.26 (q, *J* = 7.2 Hz, 2H), 3.00 (t, *J* = 9.0 Hz, 2H), 1.21 (t, *J* = 7.2 Hz, 3H), 0.33 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 153.10 , 149.13 , 139.04 , 129.12 , 128.83 , 128.24 , 112.36 , 77.30 , 51.34 , 41.91 , 27.76 , 11.88 , -4.06. HRMS (ESI+) Calcd for $[M+H]^+$:258.1309, Found: 258.1308.

Compound 5f (SiC F): ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.25 (d, *J* = 10.9 Hz, 1H), 6.97 (s, 1H), 6.73 (s, 1H), 5.95 (d, *J* = 10.9 Hz, 1H), 3.44 (q, *J* = 7.1 Hz, 2H), 3.40 – 3.33 (m, 2H), 2.76 (t, *J* = 6.3 Hz, 2H), 1.98 (dt, *J* = 11.6, 6.1 Hz, 2H), 1.20 (t, *J* = 7.1 Hz, 3H), 0.36 (s, 6H). ^{13}C NMR (126 MHz, Chloroform-*d*) δ 148.87 , 146.05 , 137.55 , 133.70 , 128.75 , 126.17 , 122.98 , 116.92 , 48.77 , 45.33 , 27.96 , 21.72 , 11.16 , -3.98 . HRMS (ESI+) Calcd for $[M+H]^+$:272.1465, Found: 272.1463.



5c **6c**

y.65%

To a dried and argon protected reaction tube was added compound 5c (100 mg, 0.37 mmol), $Pd(PPh_3)_4$ (21 mg, 5 %mol) and 1,3-Dimethylbarbituric acid(68 mg, 1.2 eq). Then the CH_2ClCH_2Cl (2 mL) was added, the mixture was stirred at 80 ℃ for 6h. The reaction was quenched with saturated $NaHCO_3$ aqueous solution, and the aqueous layer was extracted with CH_2Cl_2. The combined organic layer was washed with saturated $NaHCO_3$ aqueous solution and

brine, dried over Na_2SO_4, and concentrated in vacuo. The residue was purified by column chromatography to afford 6c (55 mg, 65 %).

Compound 6c (SiC C): ^{1}H NMR (500 MHz, Chloroform-*d*) δ 7.29 (d, *J* = 11.0 Hz, 1H), 7.21 (d, *J* = 8.4 Hz, 1H), 6.74 (d, *J* = 2.6 Hz, 1H), 6.56 (dd, *J* = 8.4, 2.6 Hz, 1H), 5.96 (d, *J* = 10.9 Hz, 1H), 3.32 (s, 1H), 3.23 (q, *J* = 7.2 Hz, 2H), 1.29 (t, *J* = 7.2 Hz, 3H), 0.33 (s, 6H). ^{13}C NMR (126MHz, Chloroform-*d*) δ 149.19 , 148.87 , 134.41 , 129.39 , 128.04 , 120.16 , 112.44 , 77.16 , 38.14 , 14.75 , -4.04 . HRMS (ESI+) Calcd for $[M+H]^+$: 232.1152, Found:232.1155

2. Photophysical Properties

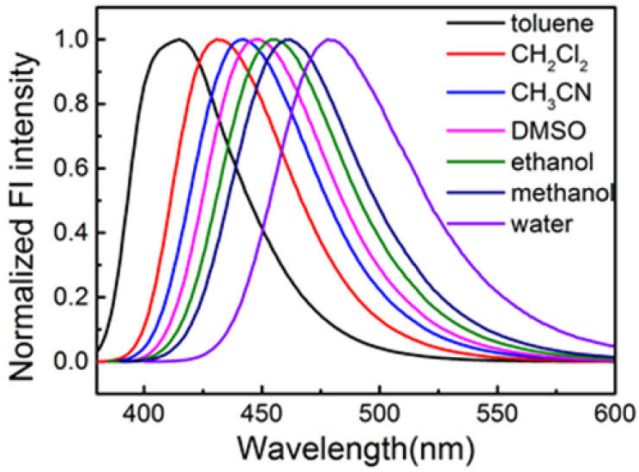


Figure S1. Fluorescence spectra of **Coumarin** in different solvents.

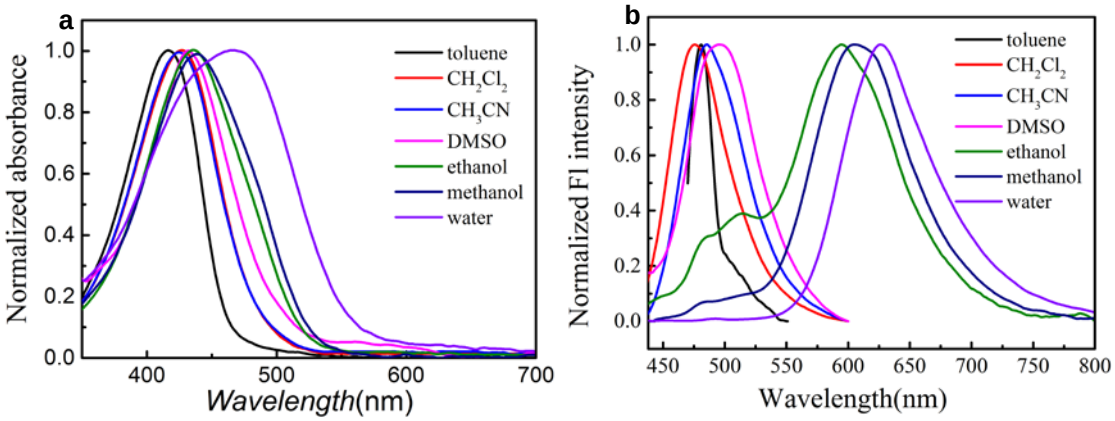


Figure S2. (a) UV–vis absorption spectra and (b) fluorescence spectra of **SiC A** (10 μM) in different solvents.

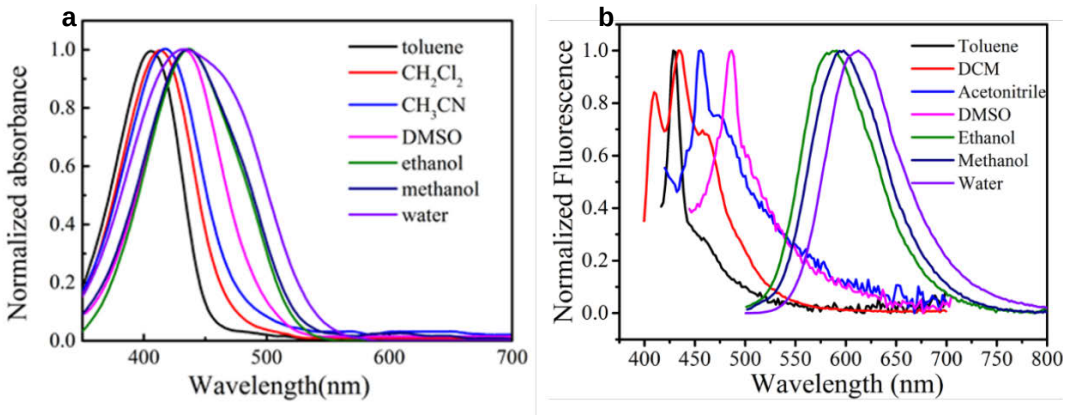


Figure S3. (a) UV–vis absorption spectra and (b) fluorescence spectra of **SiC C** (10 μM) in different solvents.

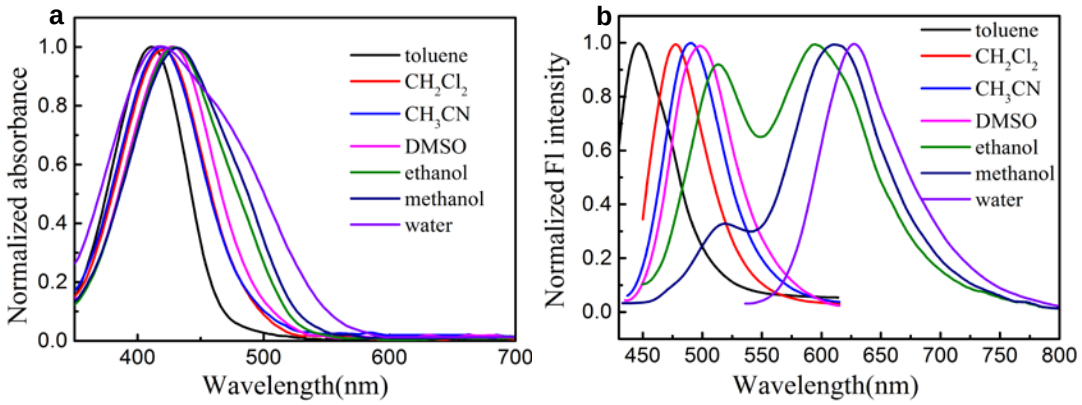


Figure S4. (a) UV–vis absorption spectra and (b) fluorescence spectra of **SiC D** (10 μM) in different solvents.

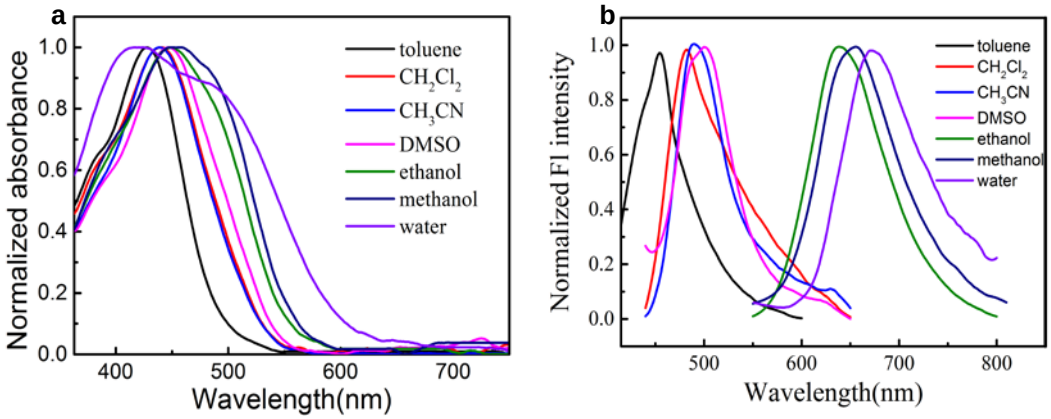


Figure S5. (a) UV–vis absorption spectra and (b) fluorescence spectra of **SiC E** (10 μM) in different solvents.

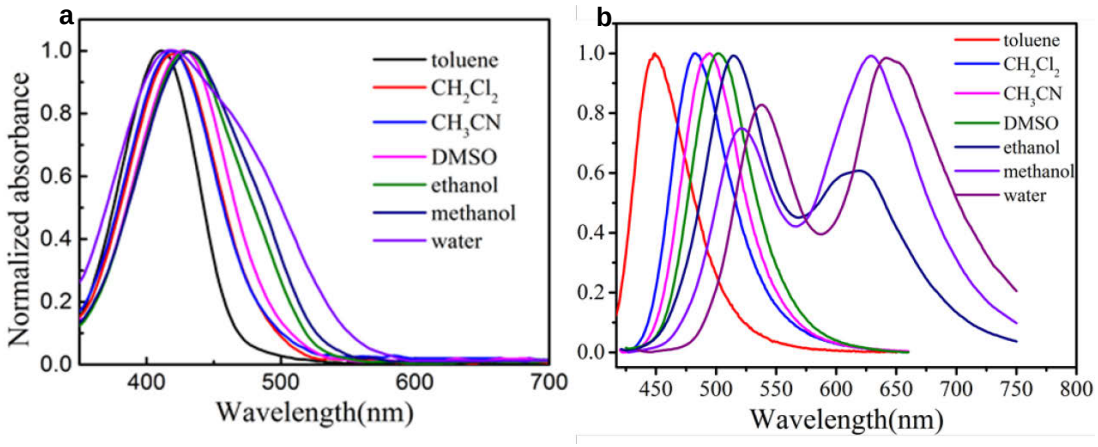


Figure S6. (a) UV–vis absorption spectra and (b) fluorescence spectra of **SiC F** (10 μM) in different solvents.

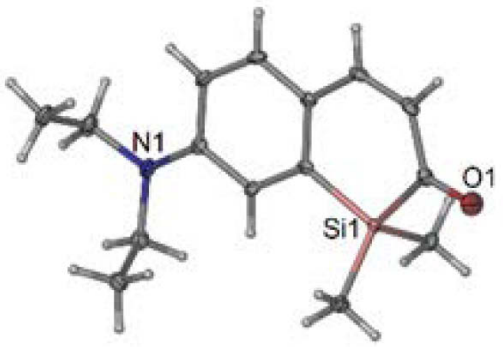


Figure S7. The crystal structure of **SiC B**. The CCDC number is 1939522.

Table S1 Spectroscopic data of Si-coumarins

		Toluene	CH_2Cl_2	MeCN	DMSO	EtOH
SiC A	λ_{max} (nm)	417	427	426	431	434
	ε ($M^{-1}cm^{-1}$)	10300	7200	9300	11100	10000
	λ_{em} (nm)	443	475	484	495	594
	Φ (%)	1.0	6.0	5.6	7.1	1.3
SiC B	λ_{max} (nm)	425	436	436	445	445
	ε ($M^{-1}cm^{-1}$)	15800	16100	19600	19500	18100
	λ_{em} (nm)	445	480	489	497	598
	Φ (%)	0.8	3.2	1.5	4.0	2.3
SiC C	λ_{max} (nm)	406	414	418	434	438
	ε ($M^{-1}cm^{-1}$)	12300	10500	9300	13000	9500
	λ_{em} (nm)	430	434	456	482	590
	Φ (%)	0.3	3.1	1.0	5.0	2.1
SiC D	λ_{max} (nm)	413	420	419	427	428
	ε ($M^{-1}cm^{-1}$)	10900	5700	9500	10500	11000
	λ_{em} (nm)	446	470	491	499	599
	Φ (%)	0.6	3.1	1.0	5.4	2.0
SiC E	λ_{max} (nm)	429	441	440	448	446
	ε ($M^{-1}cm^{-1}$)	7200	4800	6600	6231	3147
	λ_{em} (nm)	454	483	488	501	638
	Φ (%)	2.3	4.5	1.9	12	3.6
SiC F	λ_{max} (nm)	429	441	438	447	449
	ε ($M^{-1}cm^{-1}$)	10400	8900	8600	10800	10200
	λ_{em} (nm)	449	481	494	502	622
	Φ (%)	1.1	4.6	5.5	5.0	5.2

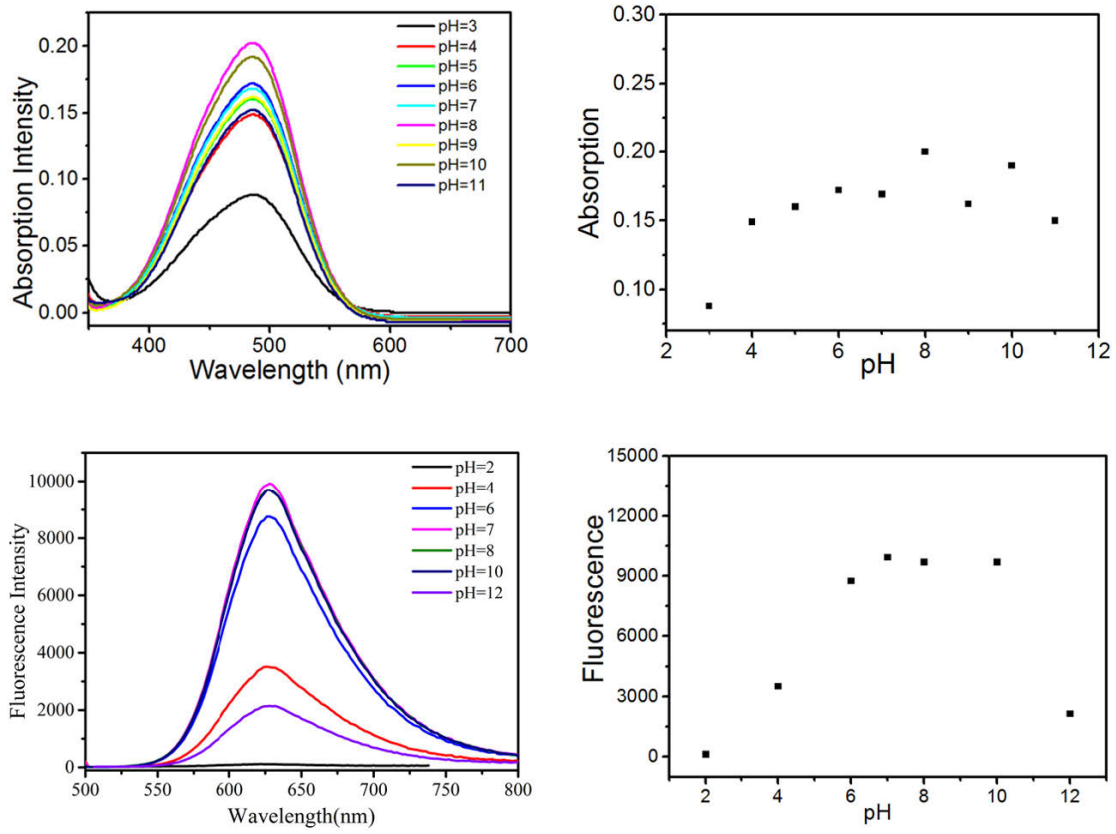


Figure S8. Absorption and fluorescence spectra of **SiC B** in various pH.

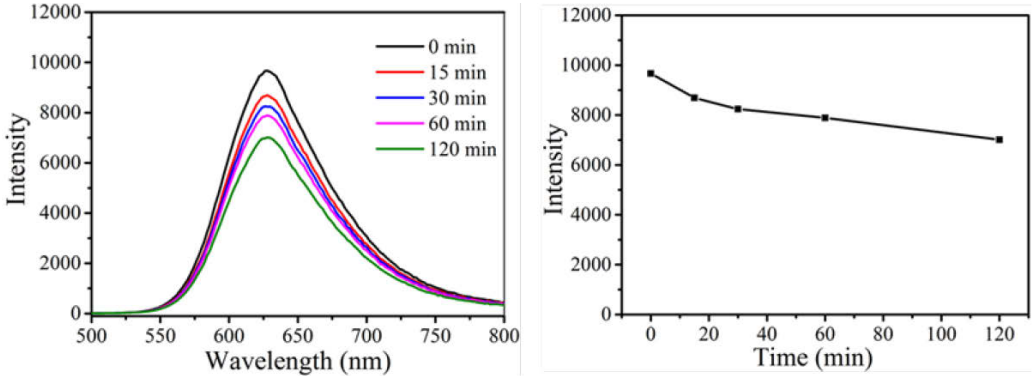


Figure S9. Photostability of **SiC B**. Fluorescence spectra of **SiC B** after continuous irradiation.

3. Biological experiment

MTT assay for the evaluation of cytotoxicity.

MTT assay was performed to evaluate the cytotoxicity of **SiC B**, HeLa cells were seeded into a 96- well plate and incubated in Dulbecco's Modified Eagle's Medium (DMEM) containing various concentration of **SiC B** (0, 0.1, 1, 2, 5, 10 μM) at 37 °C for 24 h. MTT reagent 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide was added to each well, the plates were incubated for another 4 h in a 5% CO_2 / 95% air incubator. DMSO were added to each well to dissolve the formazan, the absorbance of each well was at wavelength of 540 nm.

Culture and white adipogenic differentiation of 3T3-L1 cells.

The mesenchymal stem cell line 3T3-L1 were cultured in DMEM containing 10% fetal bovine serum (FBS) and 1% AA at 37 °C in a 5% CO_2/95% air incubator. After the cells become overgrown, they were cultured for another two days before the addition of differentiation inducers in the DMEM. The cells were cultured with DMEM containing 10% FBS, 50 ng/ml insulin, 0.5 mM IBMX (3-Isobutyl-1-methylxanthine) and 5 μM Dex (dexamethasone) for 2 days. Cells were then changed to the maintenance media of DMEM containing 10% FBS supplemented with 5 ng/ml insulin. The cells were incubated with **SiC B** (5 μM) for 30 mins before washed with PBS for three times for confocal experiments.

Culture and brown adipogenic differentiation of C3H10T1/2 cells.

The mesenchymal stem cell line *C3H10T1/2* were cultured in DMEM (Invitrogen 12430) containing 10% fetal bovine serum (FBS, Gibco) and 1% Antibiotic-Antimycotic (AA, Sigma) at 37 °C in a 5% CO_2 / 95% air incubator. After the cells grew to confluency, brown adipogenic differentiation were induced in the media of DMEM containing 10% FBS, 50 ng/mL insulin, 1 μM Rosi (rosiglitazone), 50 nM T3 (3,3',5-Triiodo-L-Thyronine), 0.5 mM IBMX (3-Isobutyl-1-methylxanthine), 5 μM Dex (dexamethasone) and 125 nM Indo (indomethacin) for 2 days. Cells were then changed to the maintenance media of DMEM containing 10% FBS supplemented with 1 μM rosiglitazone, 5 ng/ml insulin and 50 nM T3. The differentiation process was monitored by confocal microscope on the first, third and eighth days of differentiation. The cells were incubated with **SiC B** (5 μM) for 30 mins before washed with PBS for three times for confocal experiments.

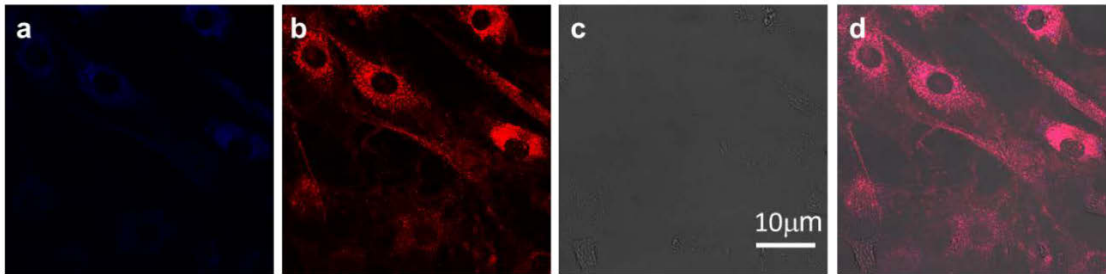


Figure S10. *C3H10T1/2* cells, stained with 5μm **SiC B** before the adipogenic differentiation process.

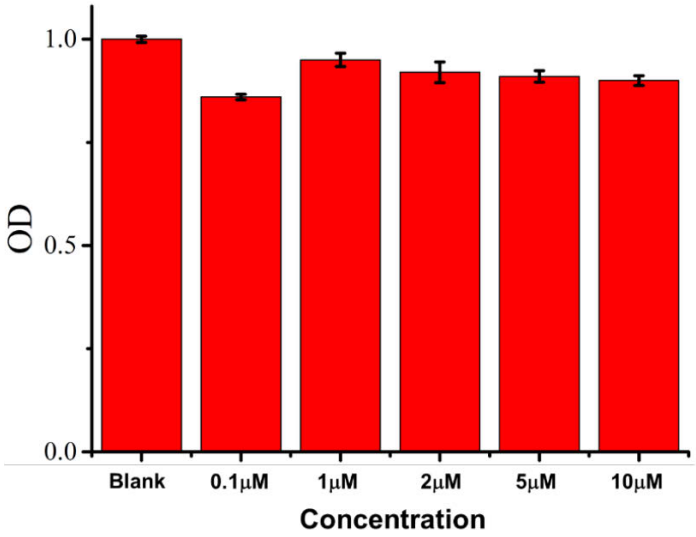


Figure S11. Cell viability results of the HeLa cells with **SiC B** by MTT assay. All data are presented as mean ± standard deviation (n = 3).

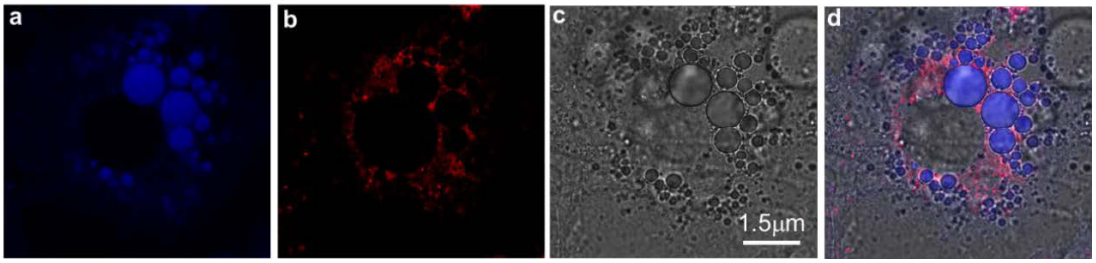


Figure S12. Confocal microphotographs of 3T3-L1 preadipocytes. (a) (b) fluorescence image, λ_{ex} = 405 nm, λ_{em} = 420 – 490 nm for **a**, λ_{em} = 530 - 630 nm for **b**; (c) phase image; (d) merged image of **a**, **b** and **c**.

4. Theoretical calculations

Computational Method. Geometry optimizations and TDDFT were performed at the B3LYP/6-31G(d) level in vacuum by Gaussian 16 program. In the TDDFT calculation, 50 excited states were calculated for each fluorophore.

Table S2. HOMO, LUMO energy level, the energy gap between HOMO and LUMO (ΔE), frontier molecular orbital overlap indexes (Λ), molecular orbitals of HOMO and LUMO for **SiC A-F**, O-coumarin and C-coumarin in Vacuo

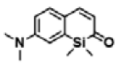
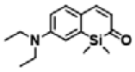
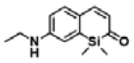
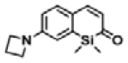
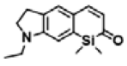
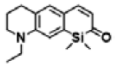
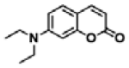
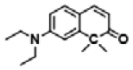
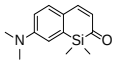
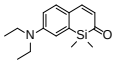
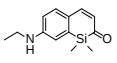
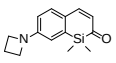
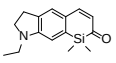
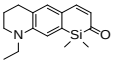
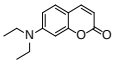
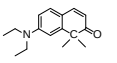
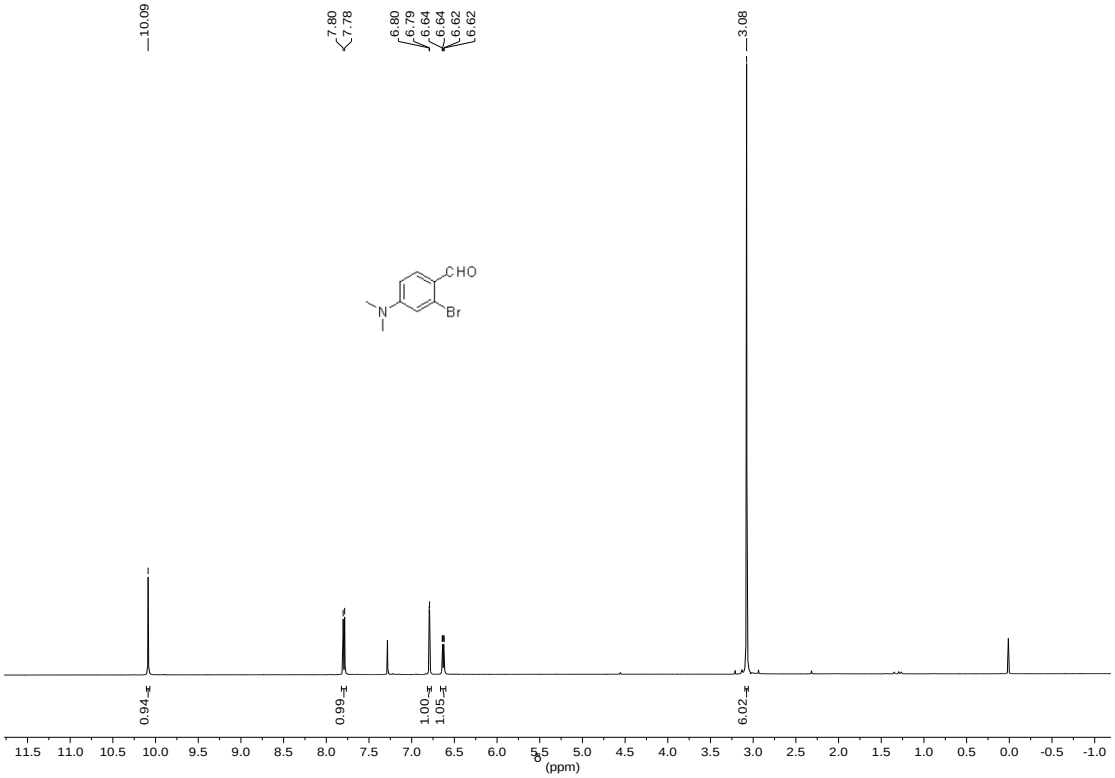
								
LUMO (a.u.)	-0.0620	-0.0627	-0.0625	-0.0627	-0.0633	-0.0614	-0.0505	-0.0530
HOMO (a.u.)	-0.192	-0.192	-0.195	-0.193	-0.190	-0.189	-0.1974	-0.191
ΔE (ev)	3.52	3.52	3.62	3.54	3.46	3.46	4.00	3.73
ΔE (nm)	352	353	344	350	359	359	311	333
Λ	0.646	0.639	0.659	0.652	0.644	0.640	0.671	0.634
LUMO								
HOMO								

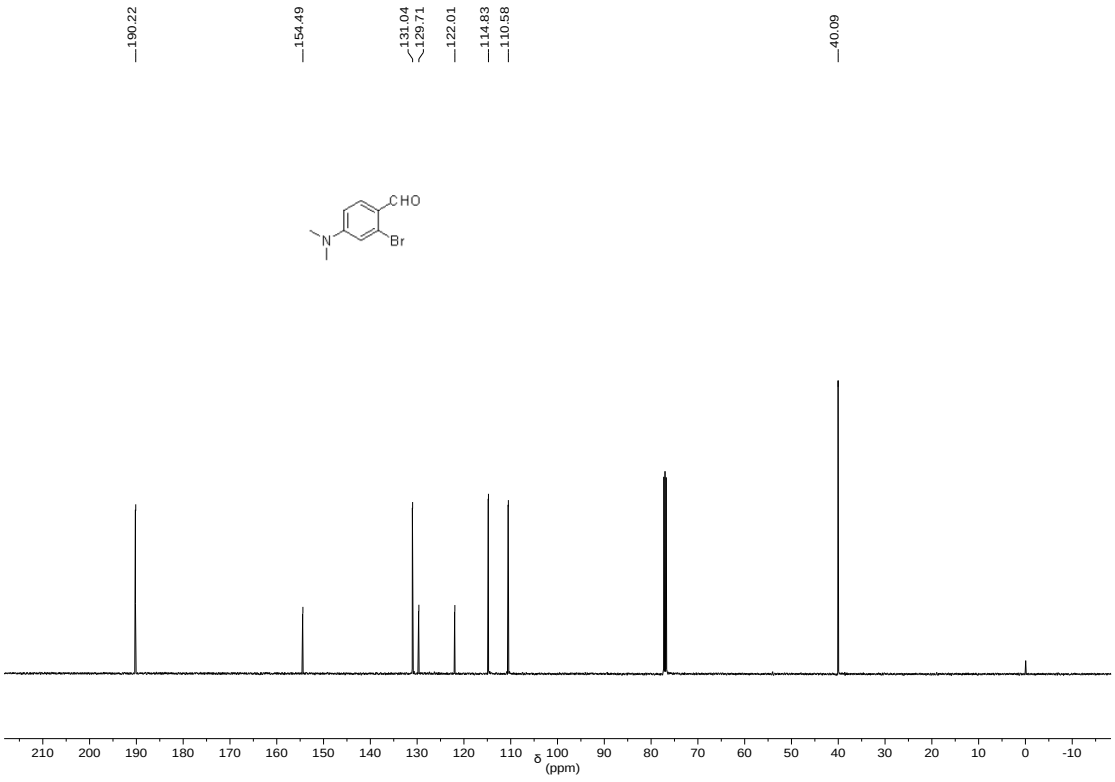
Table S3. TDDFT results for the oscillator strength (*f*) of the major excited state and the contribution of HOMO→LUMO to the excited state.

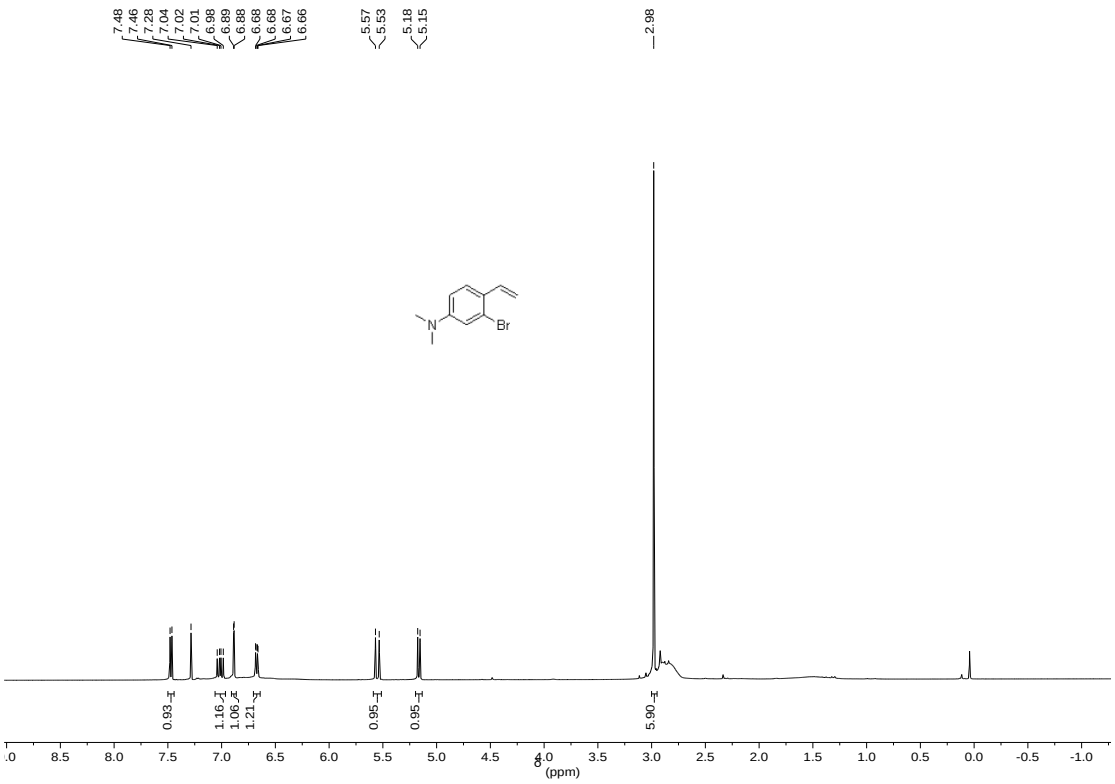
								
f	0.2892	0.3124	0.2969	0.3092	0.2425	0.2605	0.4366	0.3527
Contribution	0.9759	0.9721	0.9706	0.9753	0.9771	0.9764	0.9667	0.9445

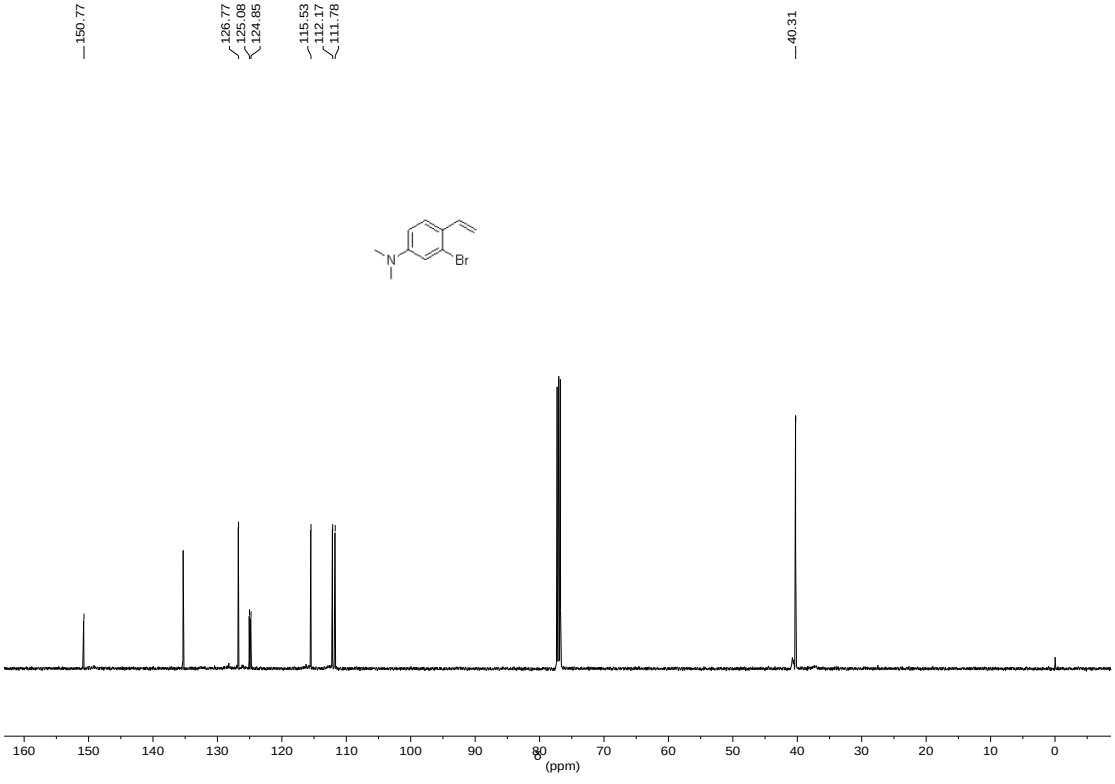
5. NMR and HRMS Spectra

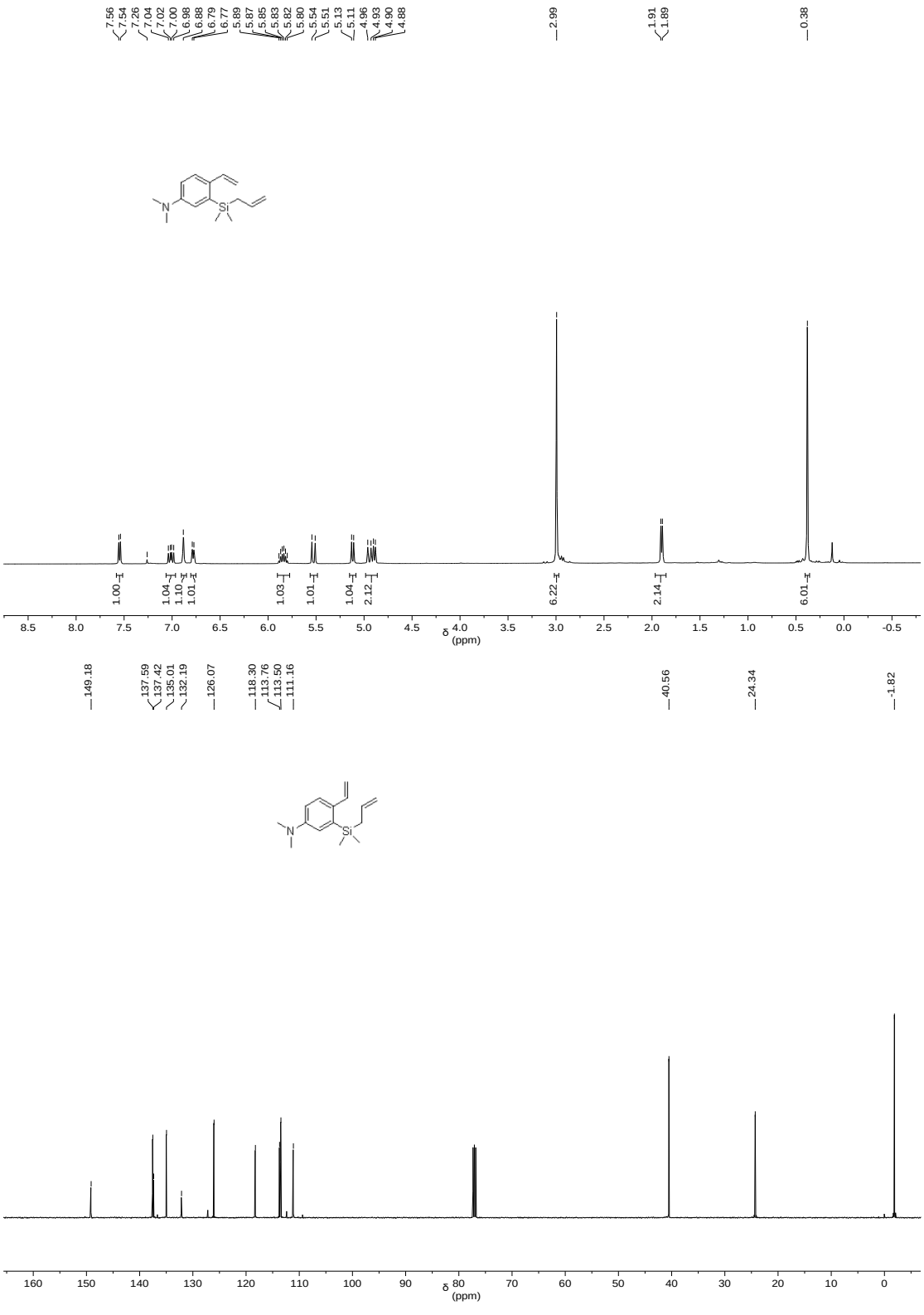
Compound 2a-5a:

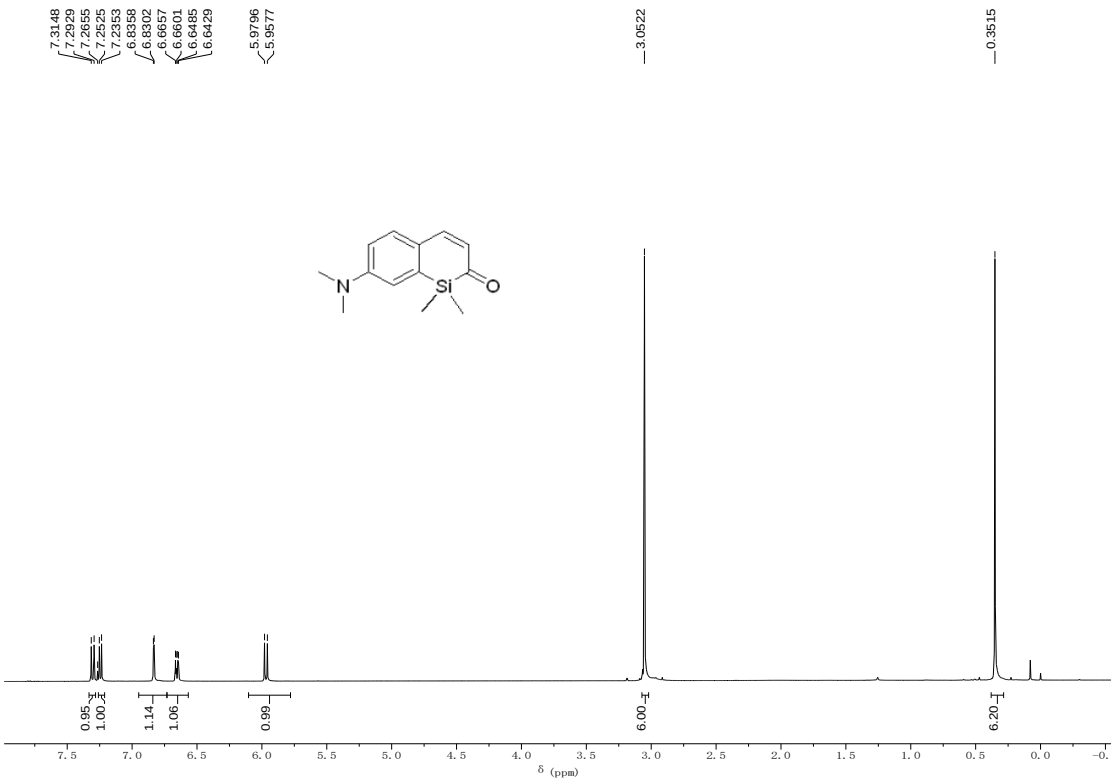


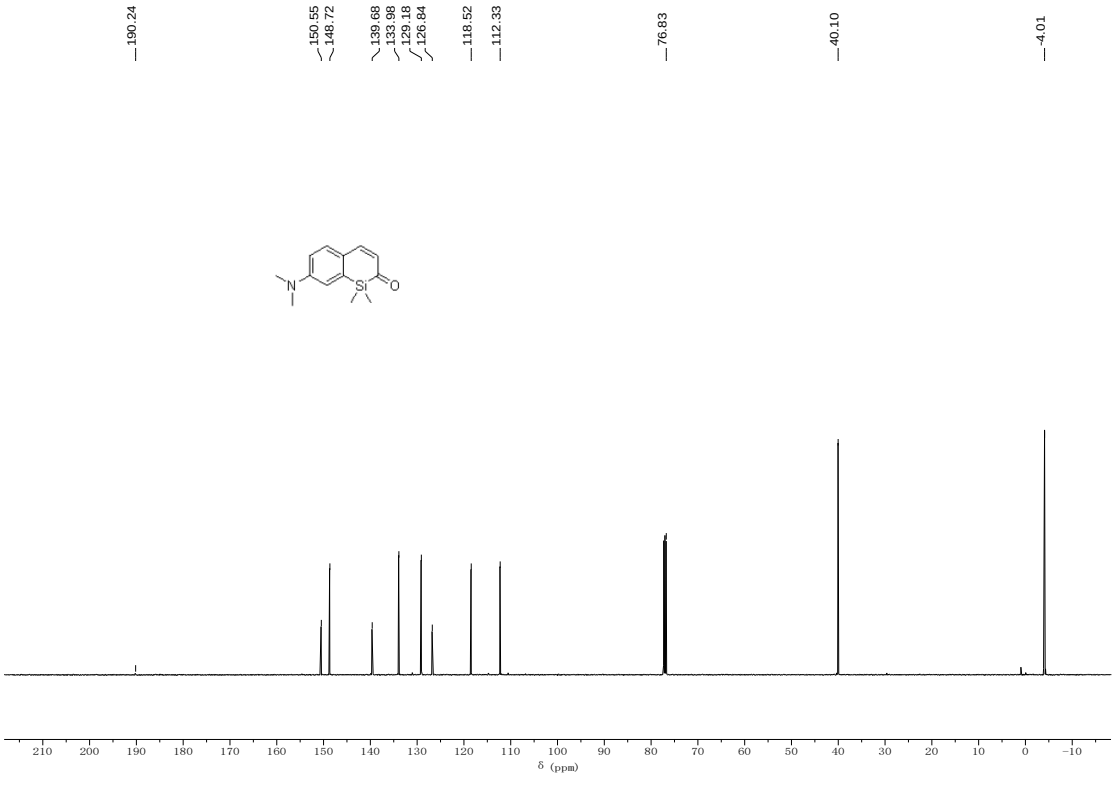



7.48
7.46
7.28
7.04
7.02
7.01
6.98
6.89
6.88
6.68
6.68
6.67
6.66
5.57
5.53
5.18
5.15
2.98
N
Br
0.93
1.16
1.06
1.21
0.95
0.95
5.90
(ppm)

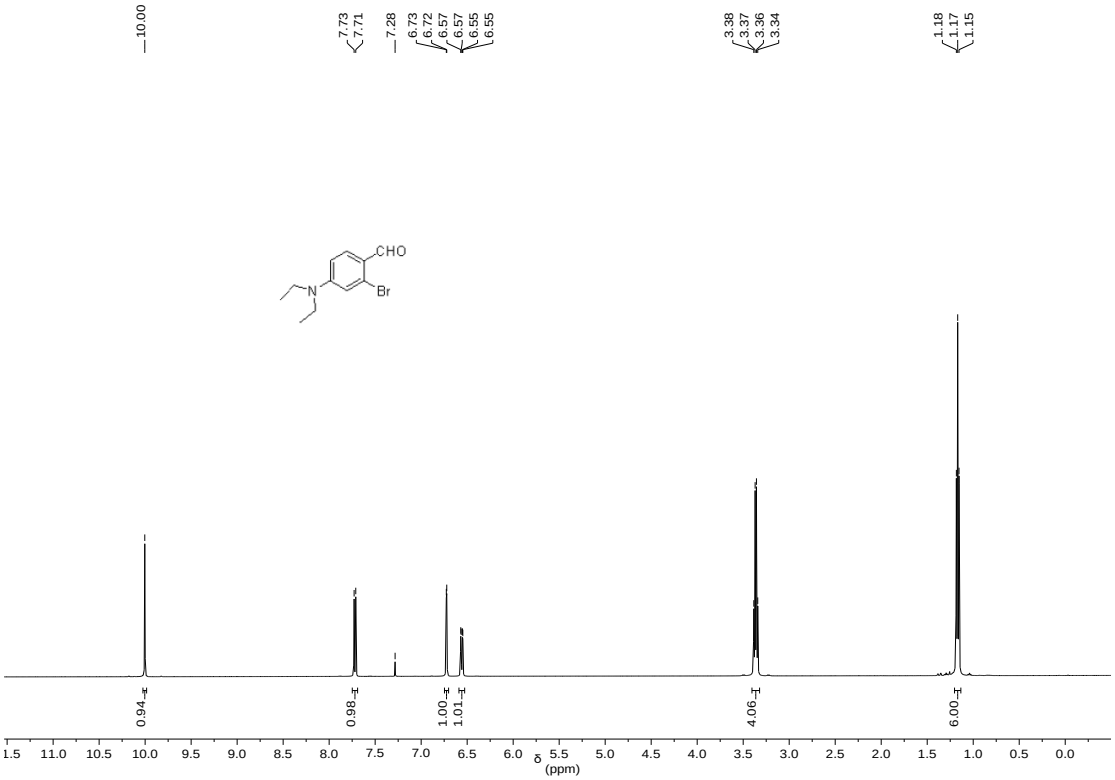

150.77
126.77
125.08
124.85
115.53
112.17
111.78
40.31
N
Br
(ppm)

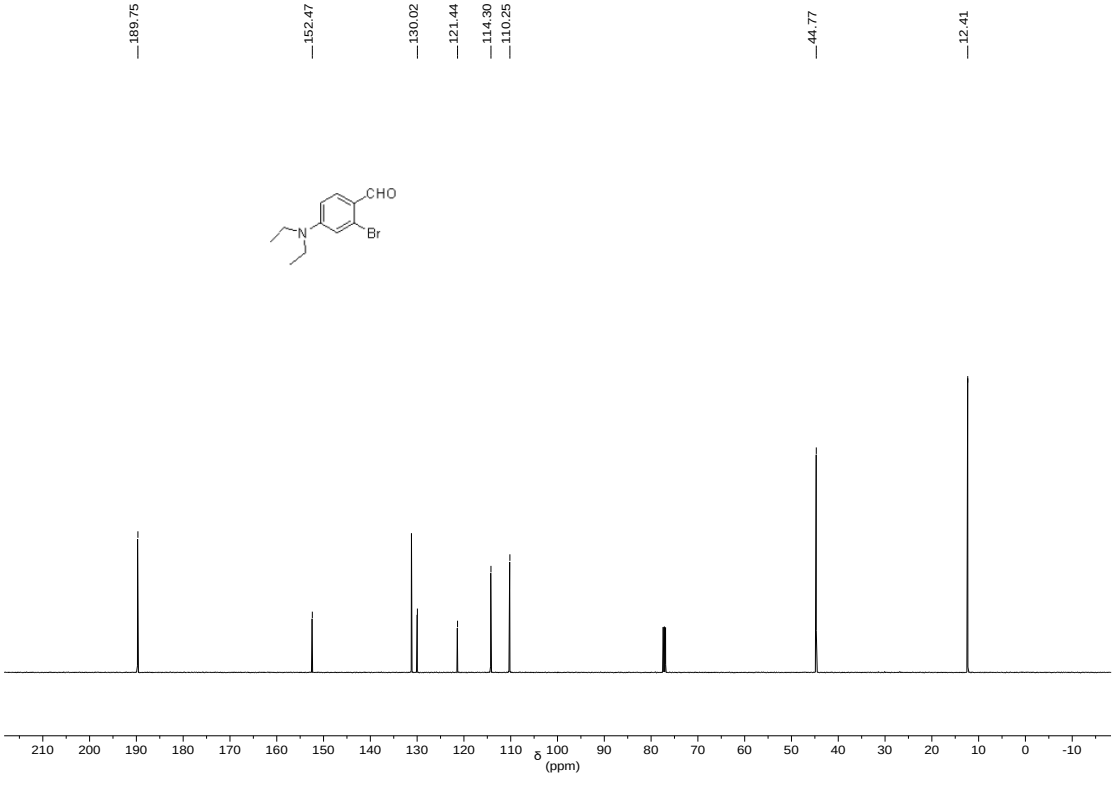

7.56
7.54
7.26
7.04
7.02
7.00
6.98
6.88
6.79
6.77
5.89
5.87
5.85
5.83
5.82
5.80
5.54
5.51
5.13
5.11
4.96
4.93
4.90
4.88
2.99
1.91
1.89
0.38
Si
N
1.00
1.04
1.10
1.01
1.03
1.01
1.04
2.12
6.22
2.14
6.01
δ (ppm)
149.18
137.59
137.42
135.01
132.19
126.07
118.30
113.76
113.50
111.16
40.56
24.34
-1.82
Si
N
δ (ppm)

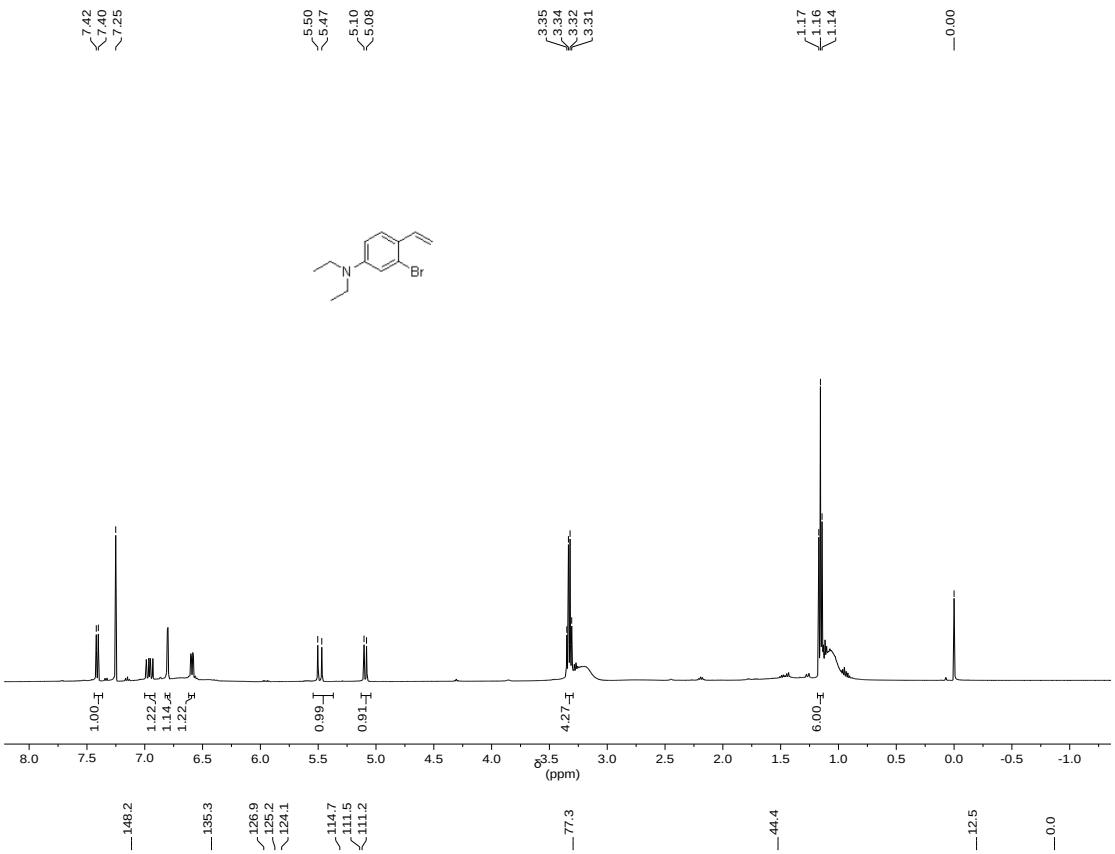

7.3148
7.2929
7.2655
7.2525
7.2353
6.8358
6.8302
6.6657
6.6601
6.6485
6.6429
5.9796
5.9577
3.0522
0.3515
N
Si
O
0.95
1.00
1.14
1.06
0.99
6.00
6.20
δ (ppm)

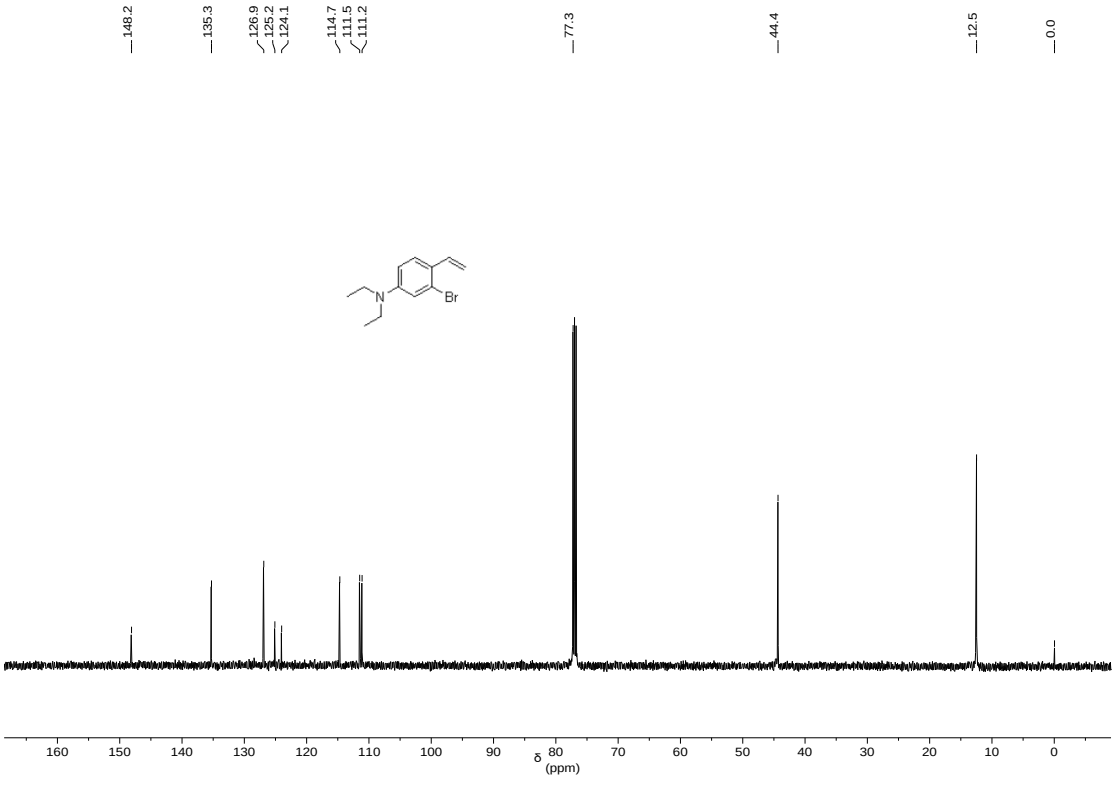

190.24
150.55
148.72
139.68
133.98
129.18
126.84
118.52
112.33
76.83
40.10
-4.01
N
Si
O
δ (ppm)

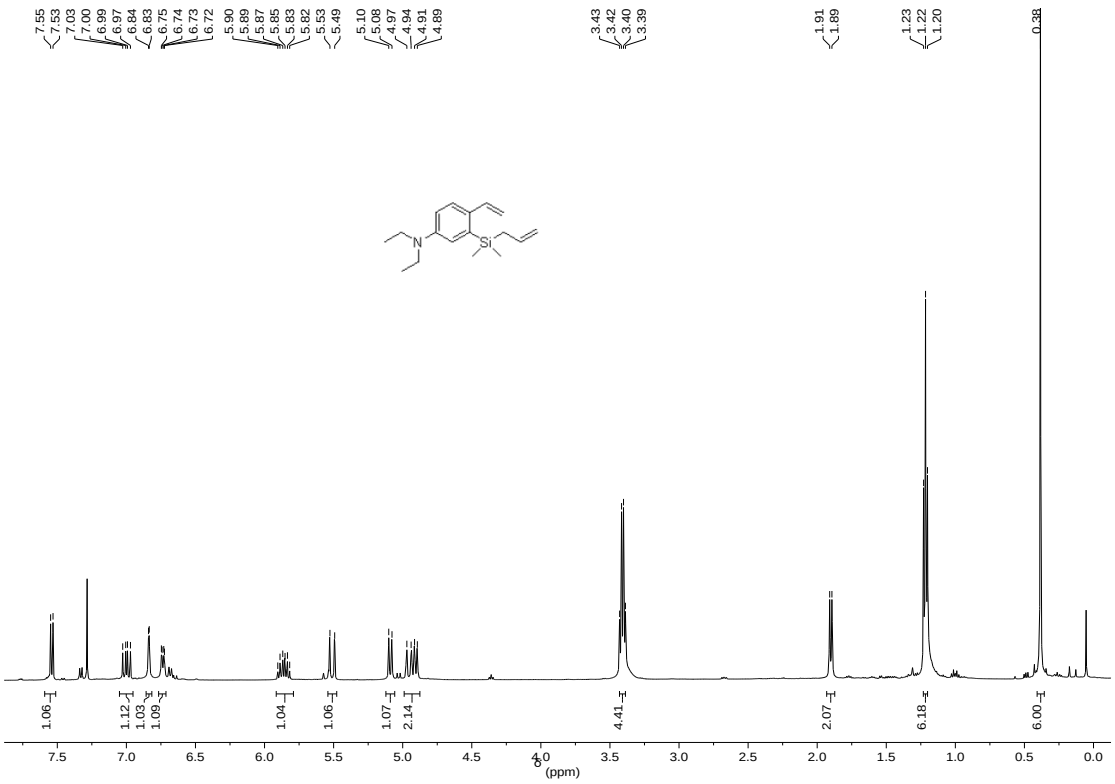
Compound 2b-5b:

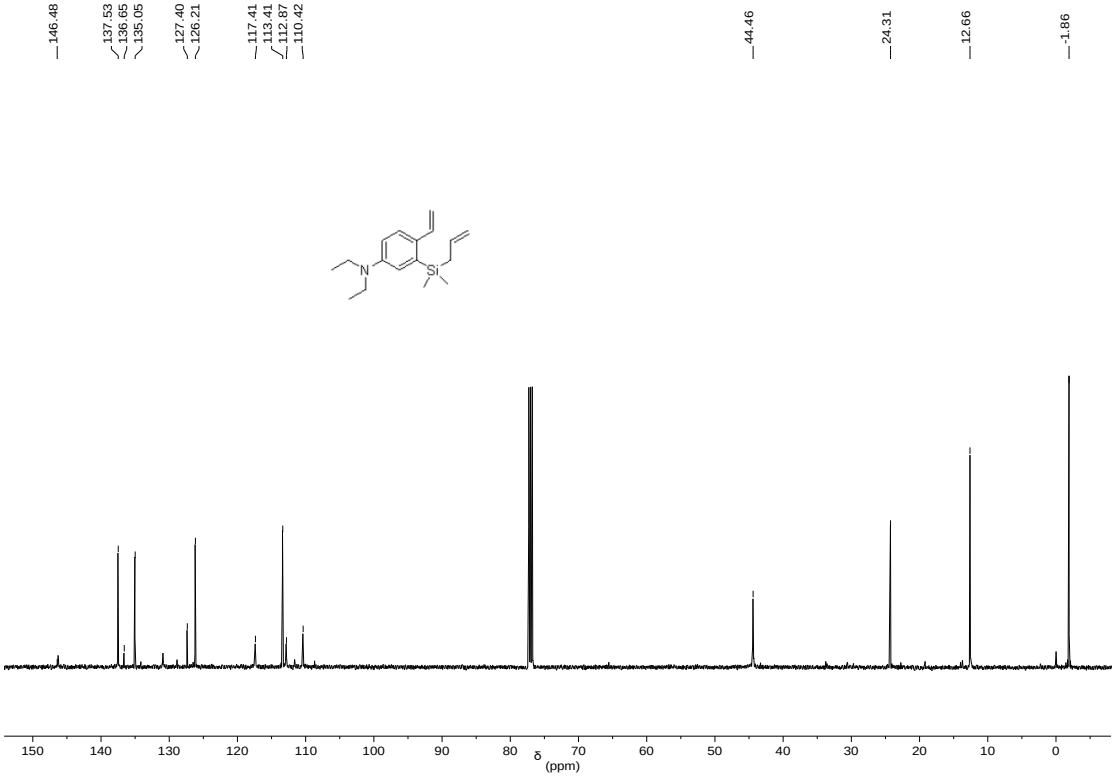


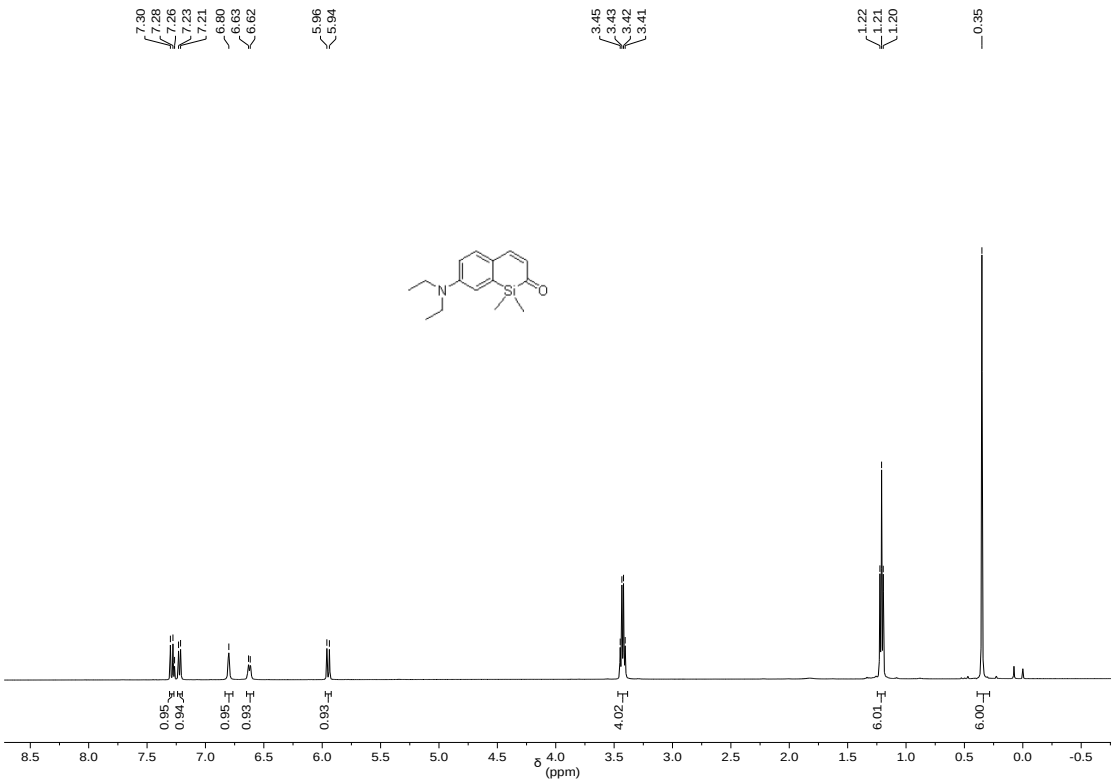


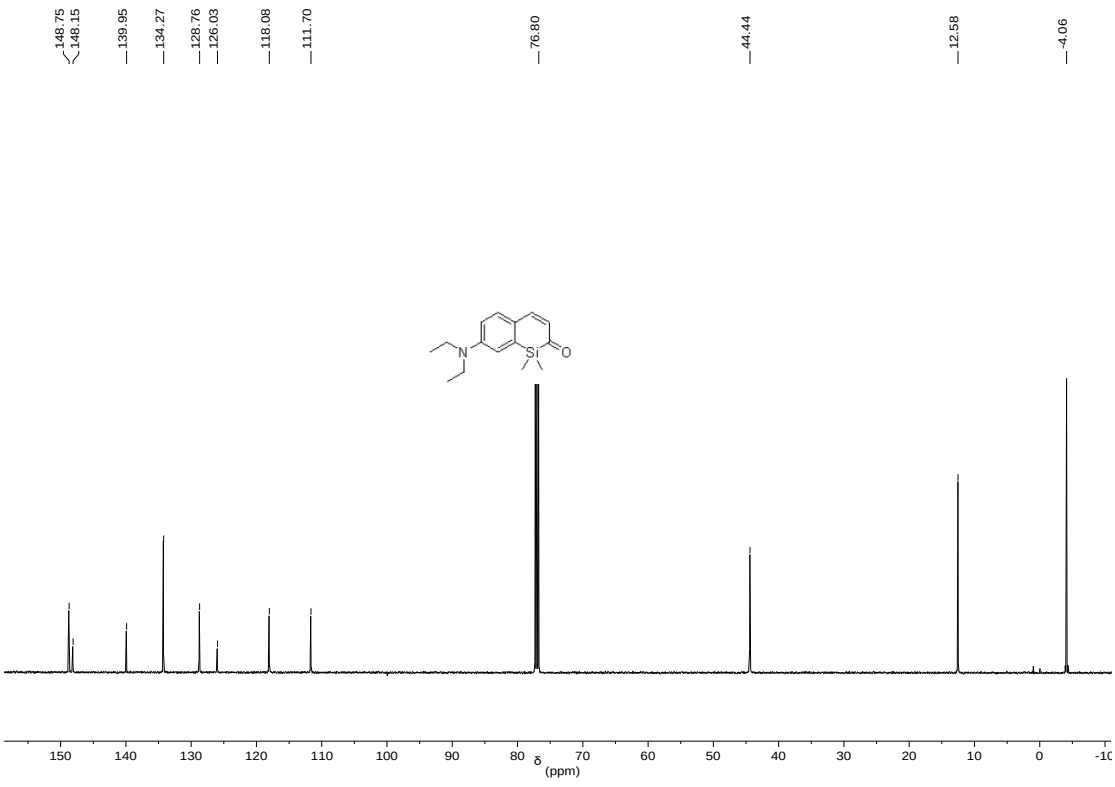

7.42
7.40
7.25
5.50
5.47
5.10
5.08
3.35
3.34
3.32
3.31
1.17
1.16
1.14
0.00
Br
1.00
1.22
1.14
1.22
0.99
0.91
4.27
6.00
δ (ppm)


148.2
135.3
126.9
125.2
124.1
114.7
111.5
111.2
77.3
44.4
12.5
0.0
Br
δ (ppm)

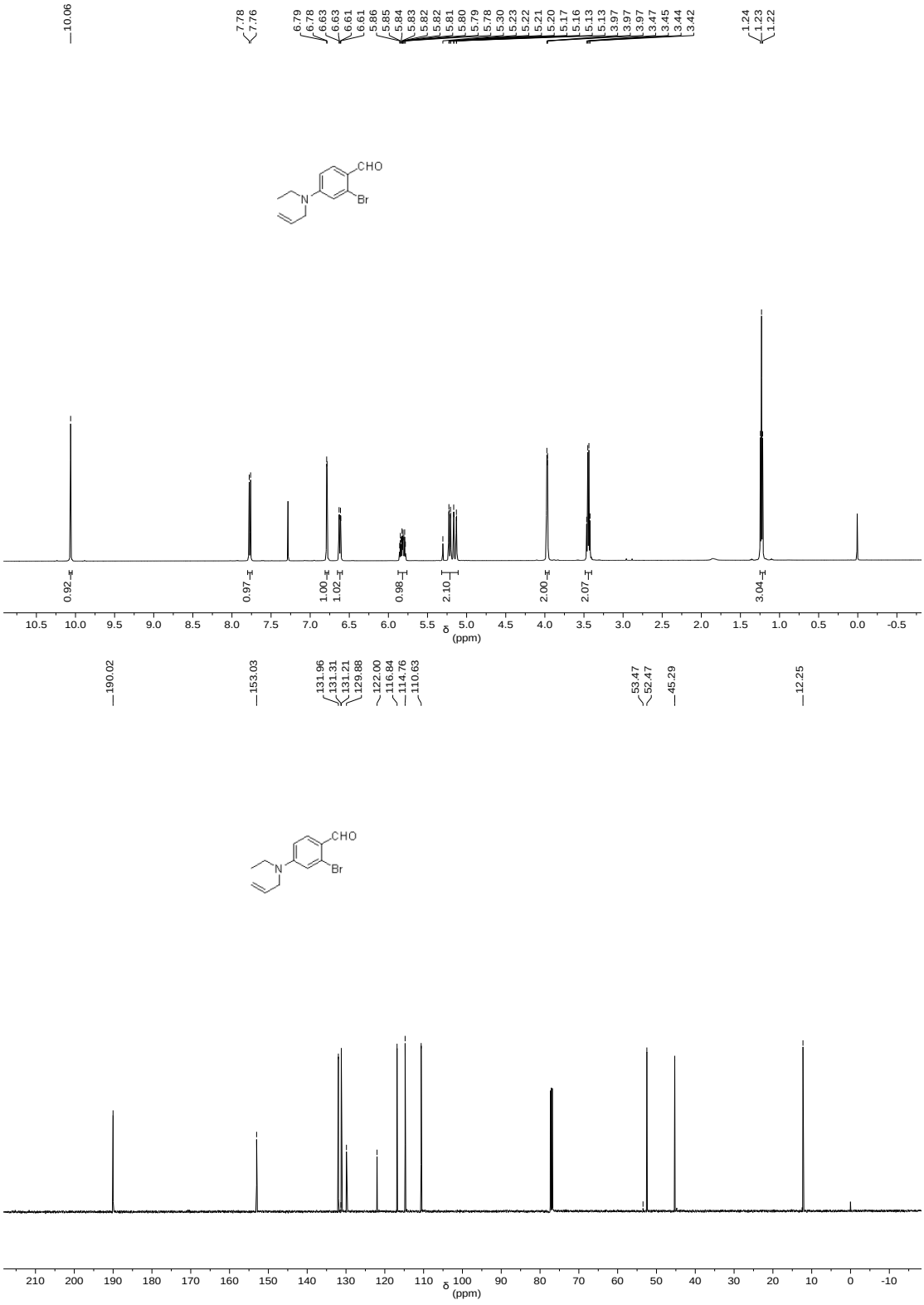

7.55
7.53
7.03
7.00
6.99
6.97
6.84
6.83
6.75
6.74
6.73
6.72
5.90
5.89
5.87
5.85
5.83
5.82
5.53
5.49
5.10
5.08
4.97
4.94
4.91
4.89
3.43
3.42
3.40
3.39
1.91
1.89
1.23
1.22
1.20
0.38
N
Si
1.06
1.12
1.03
1.09
1.04
1.06
1.07
2.14
4.41
2.07
6.18
6.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ
(ppm)

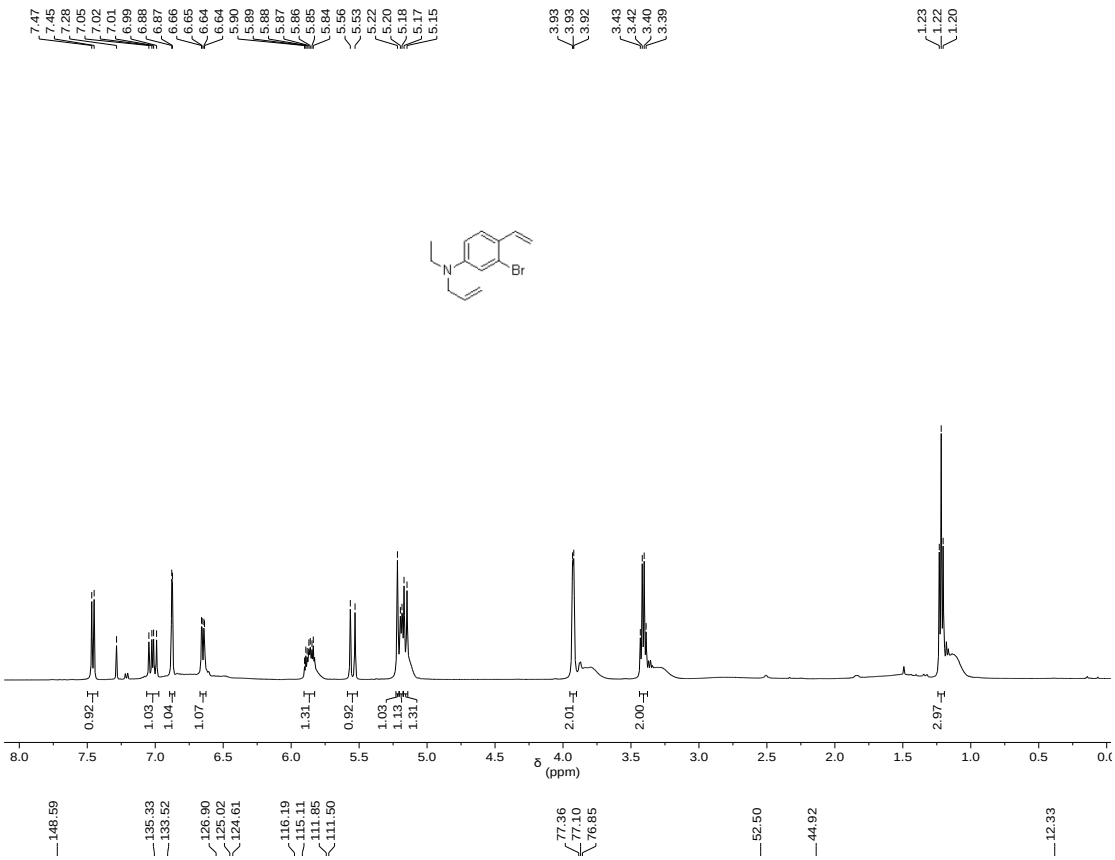

146.48
137.53
136.65
135.05
127.40
126.21
117.41
113.41
112.87
110.42
44.46
24.31
12.66
-1.86
N
Si
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
δ
(ppm)

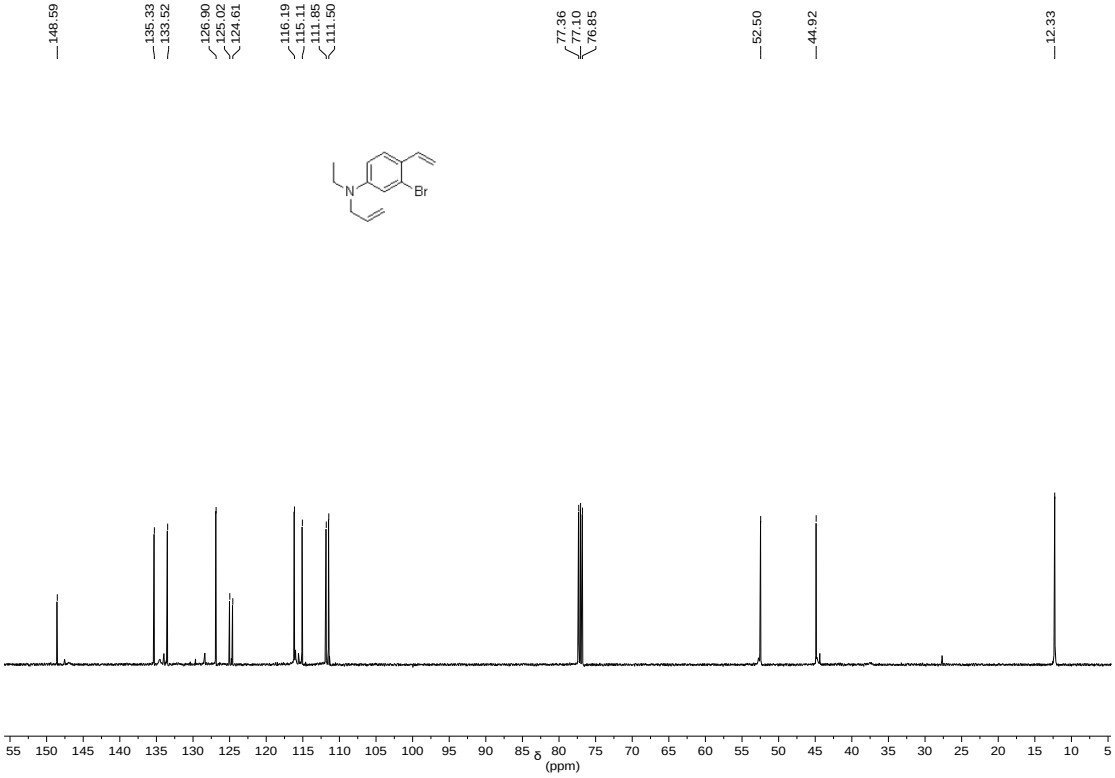

7.30
7.28
7.26
7.23
7.21
6.80
6.63
6.62
5.96
5.94
3.45
3.43
3.42
3.41
1.22
1.21
1.20
0.35
N
Si
O
0.95
0.94
0.95
0.93
0.93
4.02
6.01
6.00
δ (ppm)

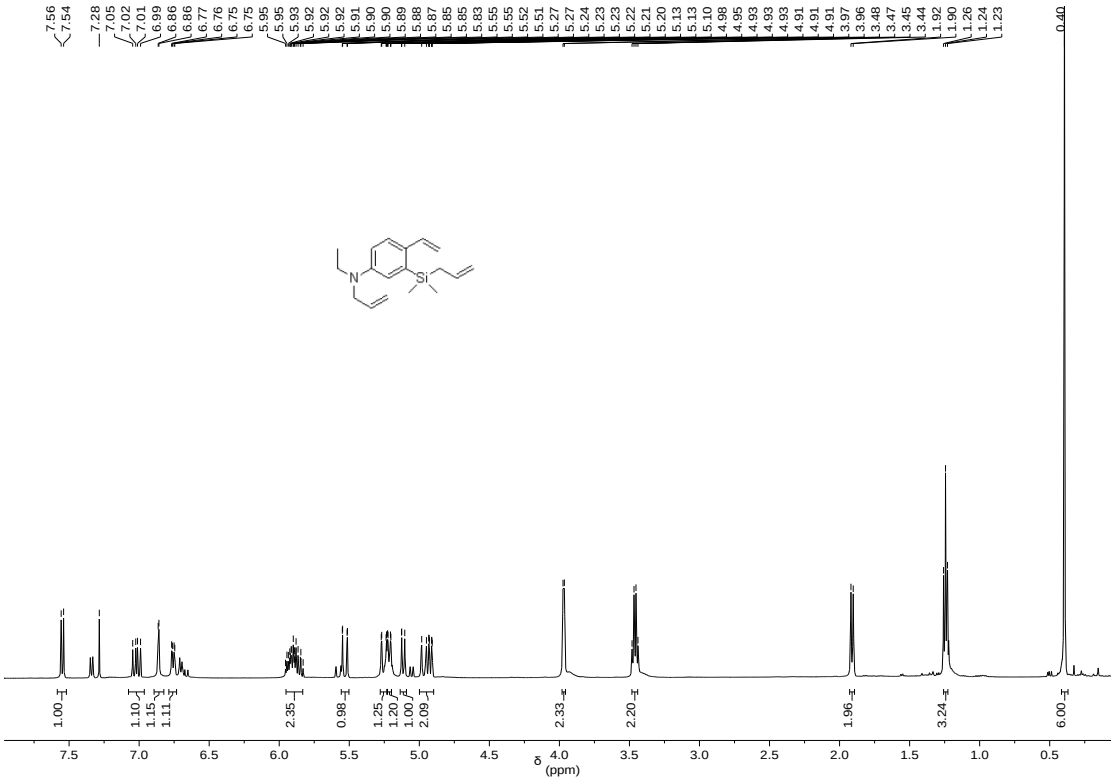

148.75
148.15
139.95
134.27
128.76
126.03
118.08
111.70
76.80
44.44
12.58
-4.06
N
Si
O
δ (ppm)

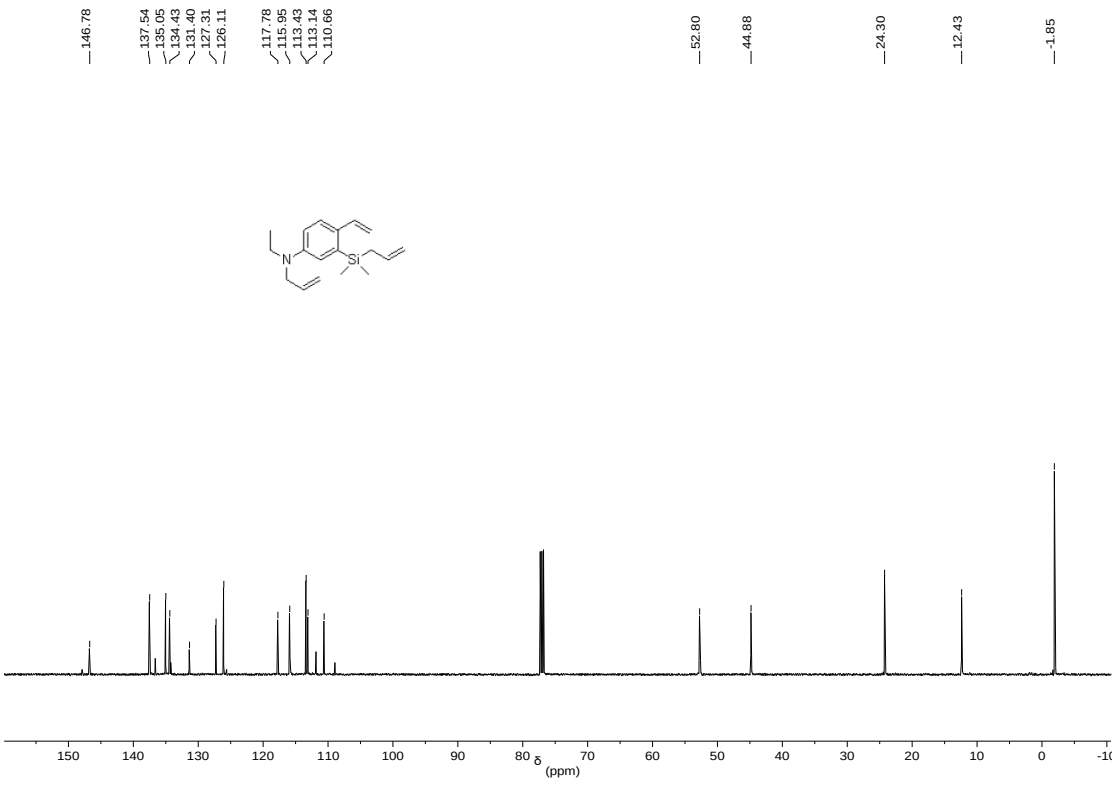
Compound 2c-6c:

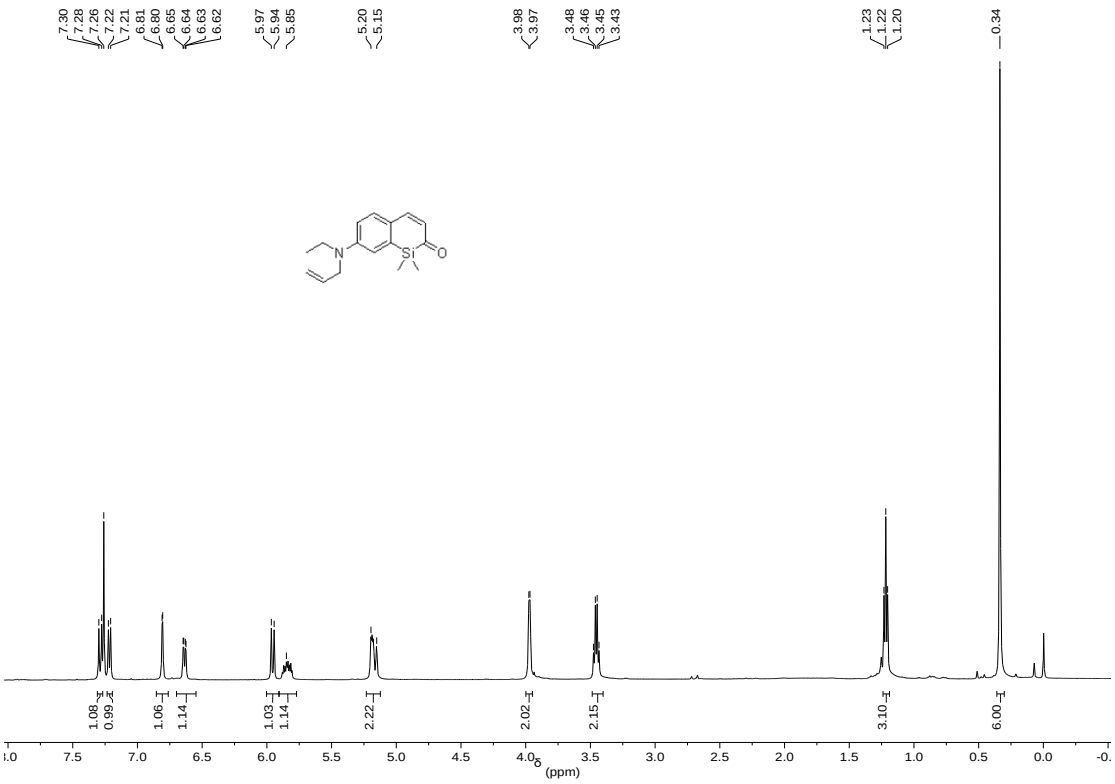


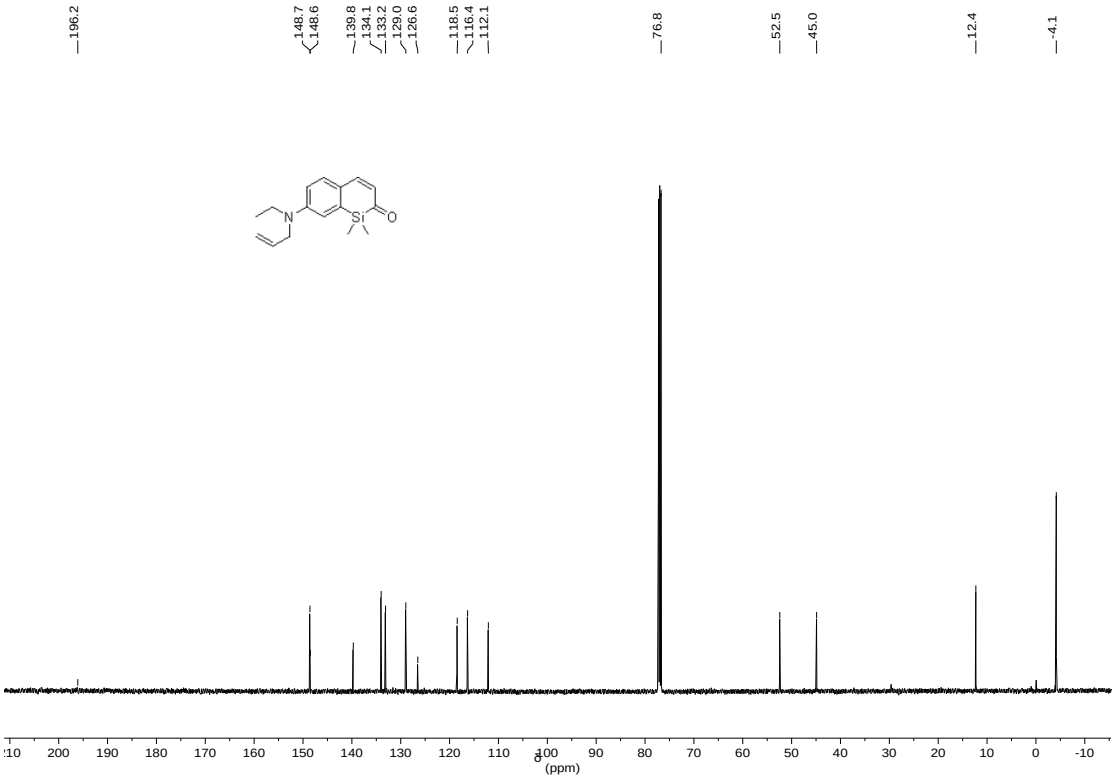

7.47
7.45
7.28
7.05
7.02
7.01
6.99
6.88
6.87
6.66
6.65
6.64
6.64
5.90
5.89
5.88
5.87
5.86
5.85
5.84
5.56
5.53
5.22
5.20
5.18
5.17
5.15
3.93
3.93
3.92
3.43
3.42
3.40
3.39
1.23
1.22
1.20
N
Br
0.92
1.03
1.04
1.07
1.31
0.92
1.03
1.13
1.31
2.01
2.00
2.97
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
δ (ppm)

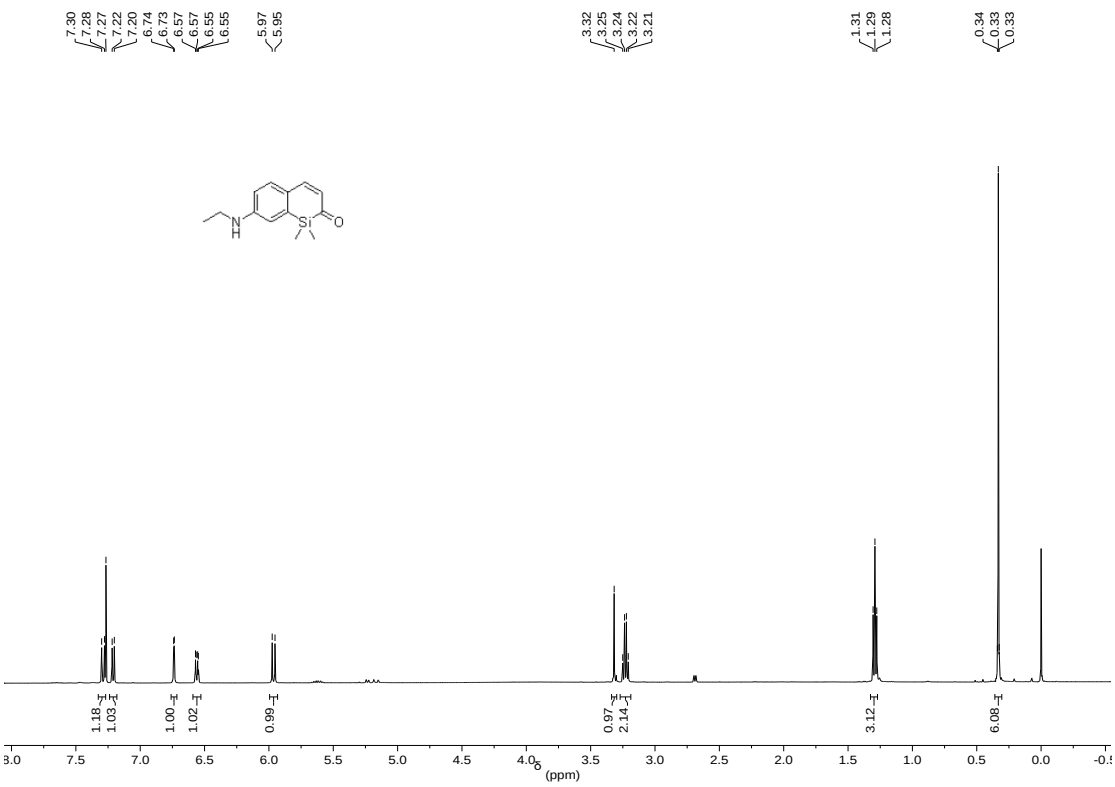

148.59
135.33
133.52
126.90
125.02
124.61
116.19
115.11
111.85
111.50
77.36
77.10
76.85
52.50
44.92
12.33
N
Br
55
150
145
140
135
130
125
120
115
110
105
100
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
15
10
5
δ (ppm)

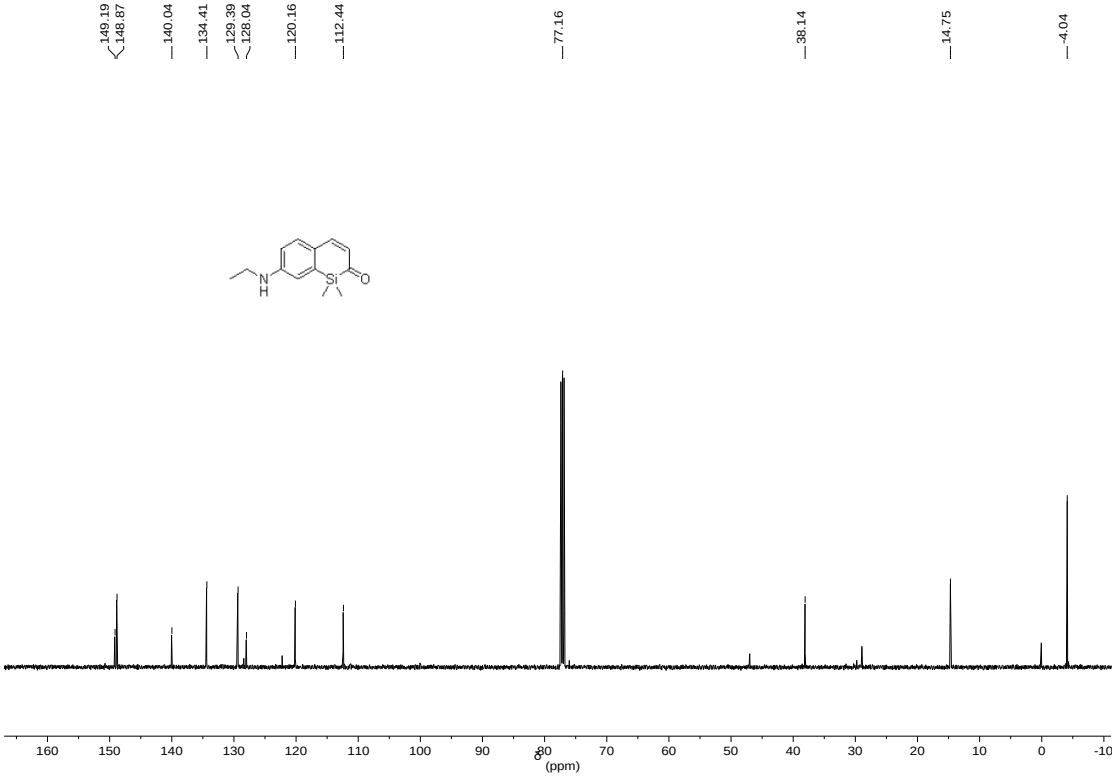

7.56 7.54 7.28 7.05 7.02 7.01 6.99 6.86 6.86 6.77 6.76 6.75 6.75 5.95 5.93 5.92 5.92 5.91 5.90 5.90 5.89 5.88 5.87 5.85 5.85 5.83 5.55 5.55 5.52 5.51 5.27 5.27 5.24 5.23 5.23 5.22 5.21 5.20 5.13 5.10 4.98 4.95 4.93 4.93 4.91 4.91 3.97 3.96 3.48 3.47 3.45 3.44 1.92 1.90 1.26 1.24 1.23 0.40
1.00 1.10 1.15 1.11 2.35 0.98 1.25 1.20 1.00 2.09 2.33 2.20 1.96 3.24 6.00
δ (ppm)


146.78 137.54 135.05 134.43 131.40 127.31 126.11 117.78 115.95 113.43 113.14 110.66 52.80 44.88 24.30 12.43 -1.85
δ (ppm)

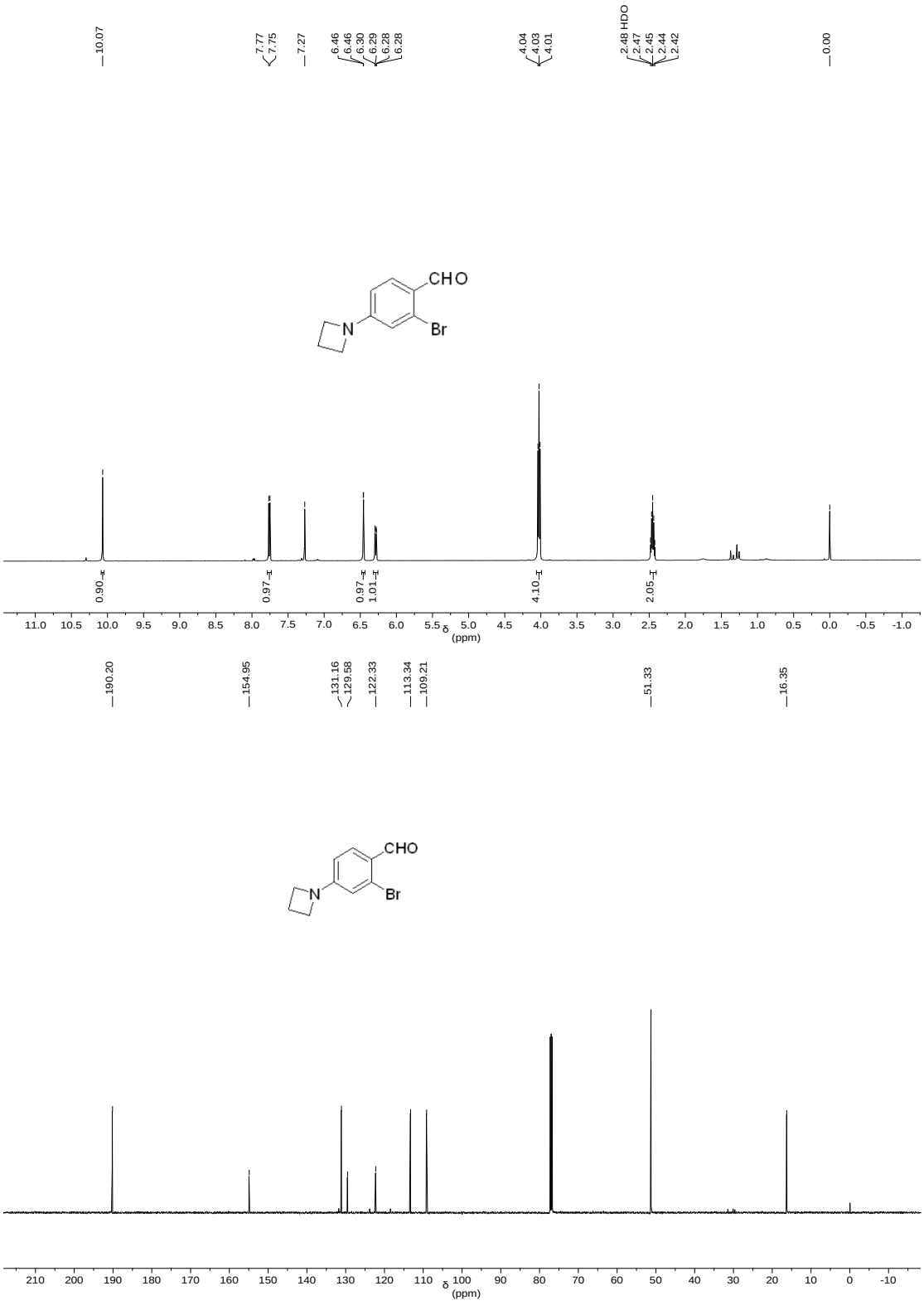

7.30
7.28
7.26
7.22
7.21
6.81
6.80
6.65
6.64
6.63
6.62
5.97
5.94
5.85
5.20
5.15
3.98
3.97
3.48
3.46
3.45
3.43
1.23
1.22
1.20
0.34
1.08
0.99
1.06
1.14
1.03
1.14
2.22
2.02
2.15
3.10
6.00
δ (ppm)

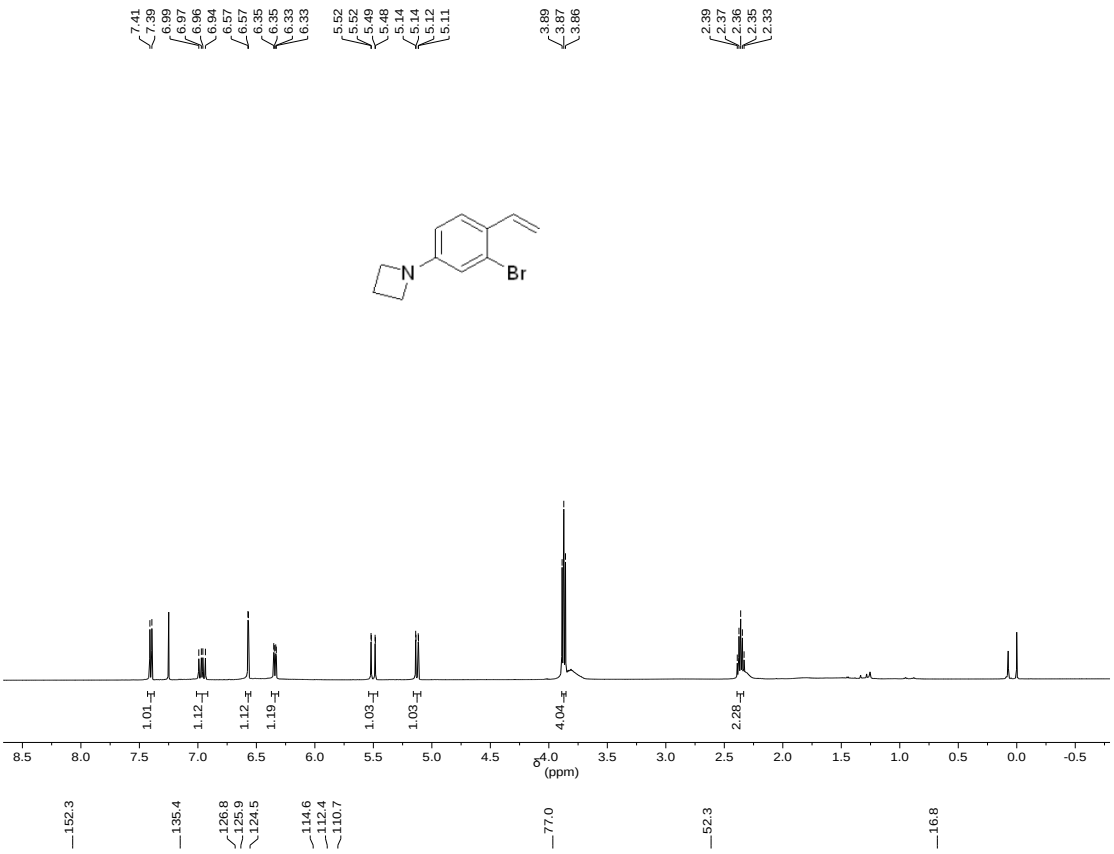

196.2
148.7
148.6
139.8
134.1
133.2
129.0
126.6
118.5
116.4
112.1
76.8
52.5
45.0
12.4
-4.1
δ (ppm)

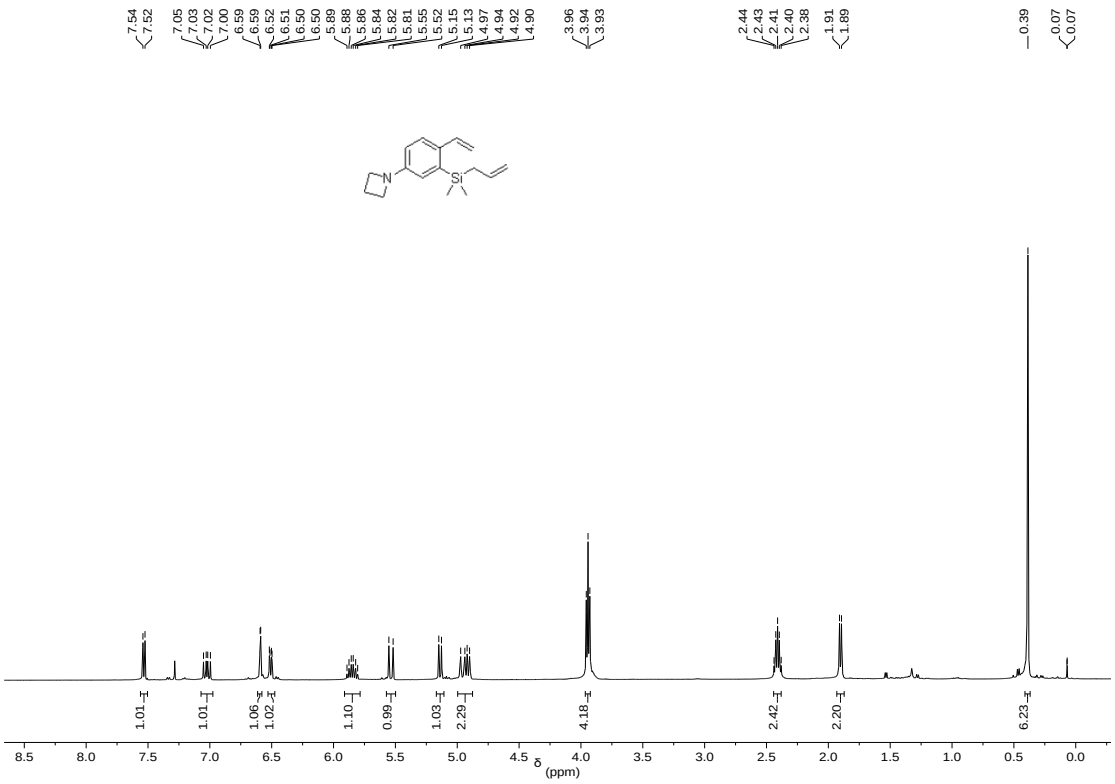

7.30
7.28
7.27
7.22
7.20
6.74
6.73
6.57
6.57
6.55
6.55
6.55
5.97
5.95
3.32
3.25
3.24
3.22
3.21
1.31
1.29
1.28
0.34
0.33
0.33
1.18
1.03
1.00
1.02
0.99
0.97
2.14
3.12
6.08
(ppm)

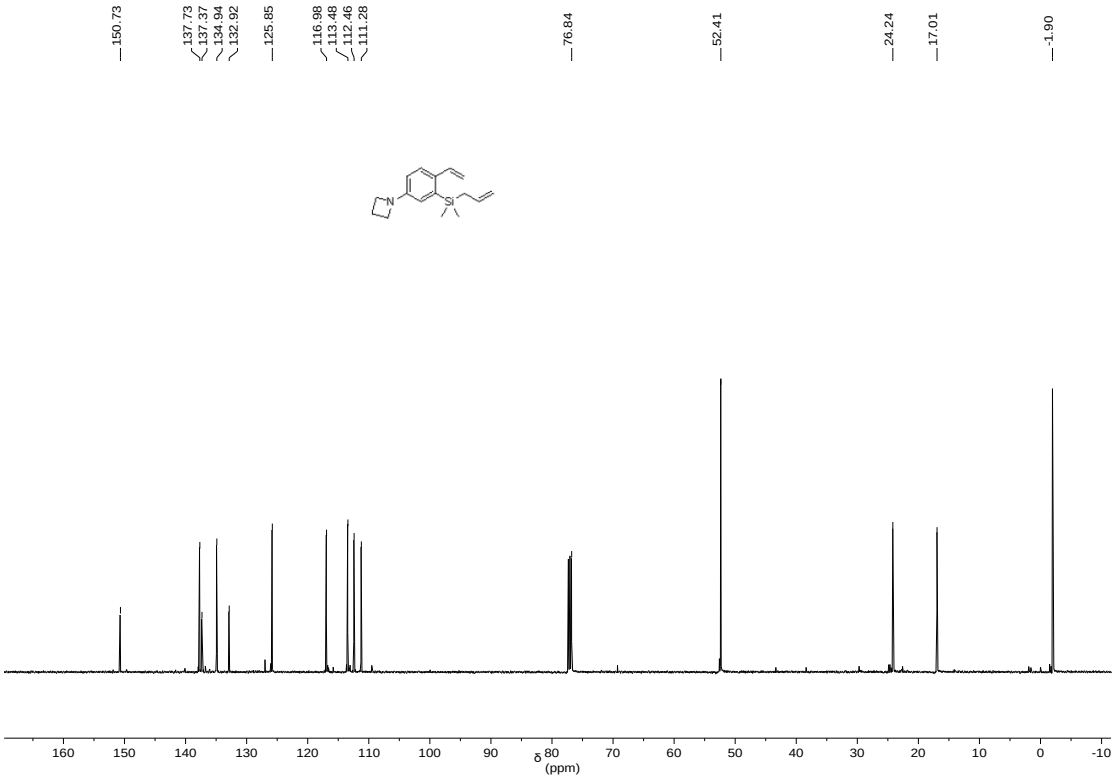

149.19
148.87
140.04
134.41
129.39
128.04
120.16
112.44
77.16
38.14
14.75
-4.04
(ppm)

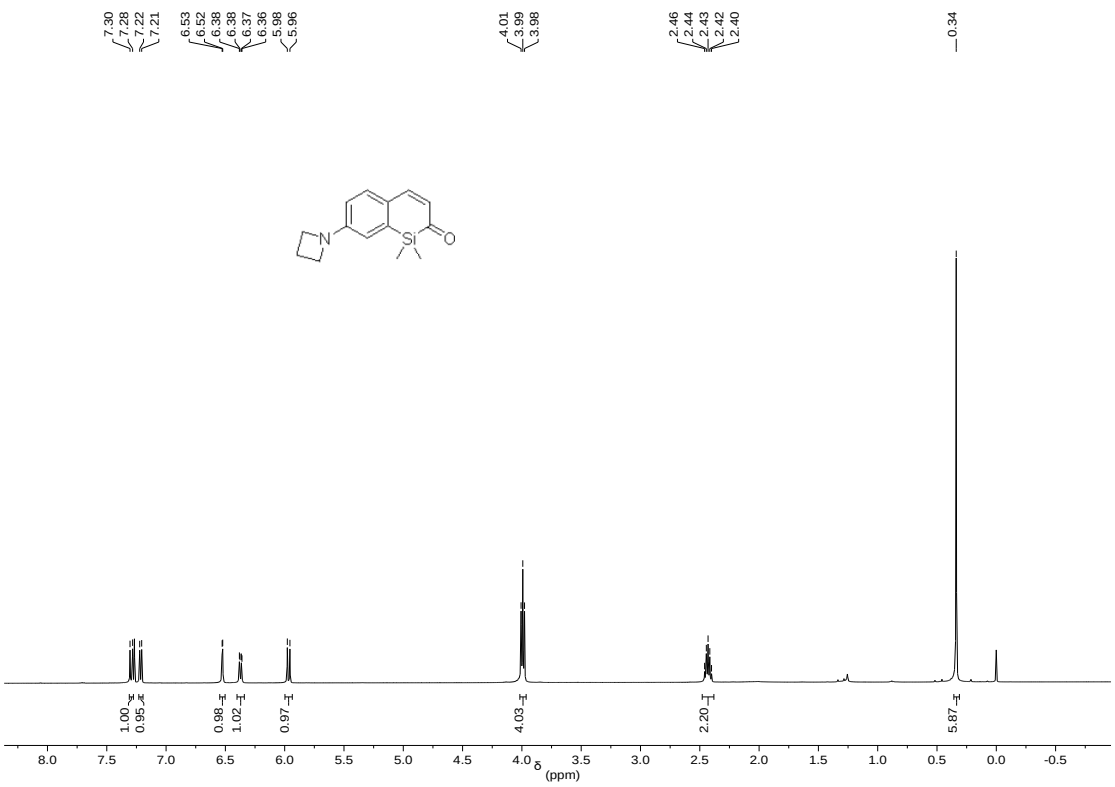
Compound 2d-5d:

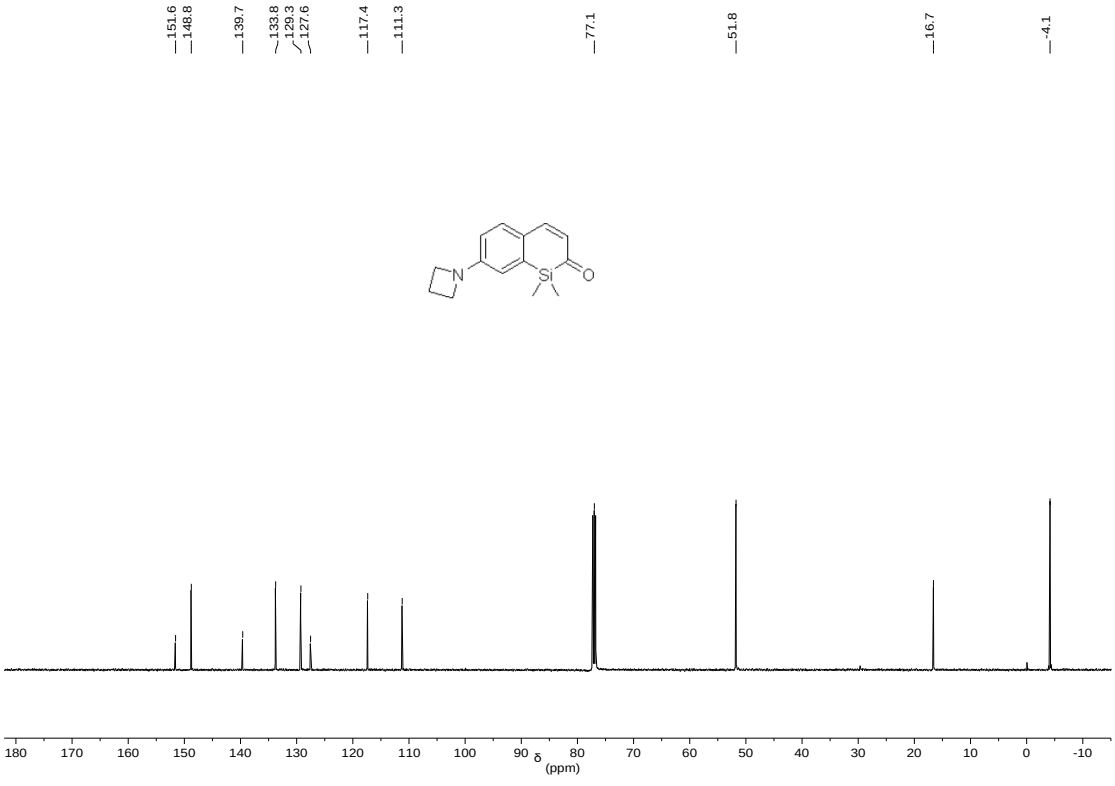



7.41
7.39
6.99
6.97
6.96
6.94
6.57
6.57
6.35
6.35
6.33
6.33
5.52
5.52
5.49
5.48
5.14
5.12
5.11
3.89
3.87
3.86
2.39
2.37
2.36
2.35
2.33
N
Br
1.01
1.12
1.12
1.19
1.03
1.03
4.04
2.28
δ (ppm)
152.3
135.4
126.8
125.9
124.5
114.6
112.4
110.7
77.0
52.3
16.8
N
Br
δ (ppm)

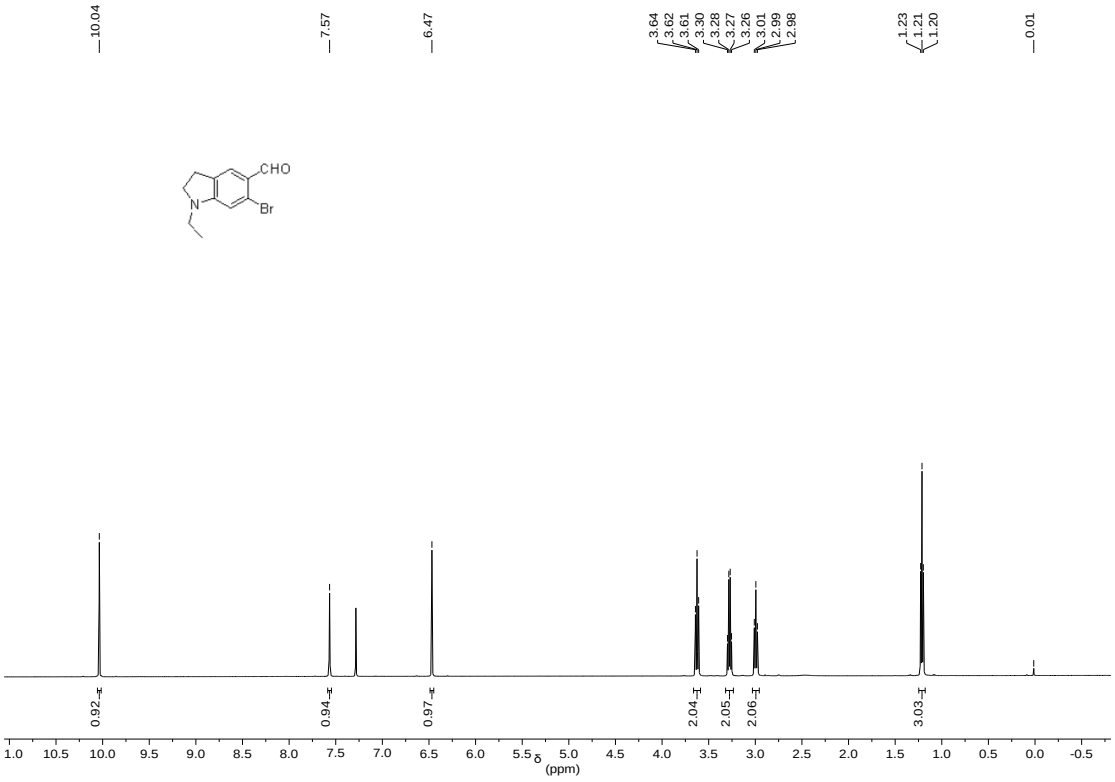

7.54
7.52
7.05
7.03
7.02
7.00
6.59
6.59
6.52
6.51
6.50
6.50
5.89
5.88
5.86
5.84
5.82
5.81
5.55
5.52
5.15
5.13
4.97
4.94
4.92
4.90
3.96
3.94
3.93
2.44
2.43
2.41
2.40
2.38
1.91
1.89
0.39
0.07
0.07
N
Si
1.01
1.01
1.06
1.02
1.10
0.99
1.03
2.29
4.18
2.42
2.20
6.23
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
δ
(ppm)

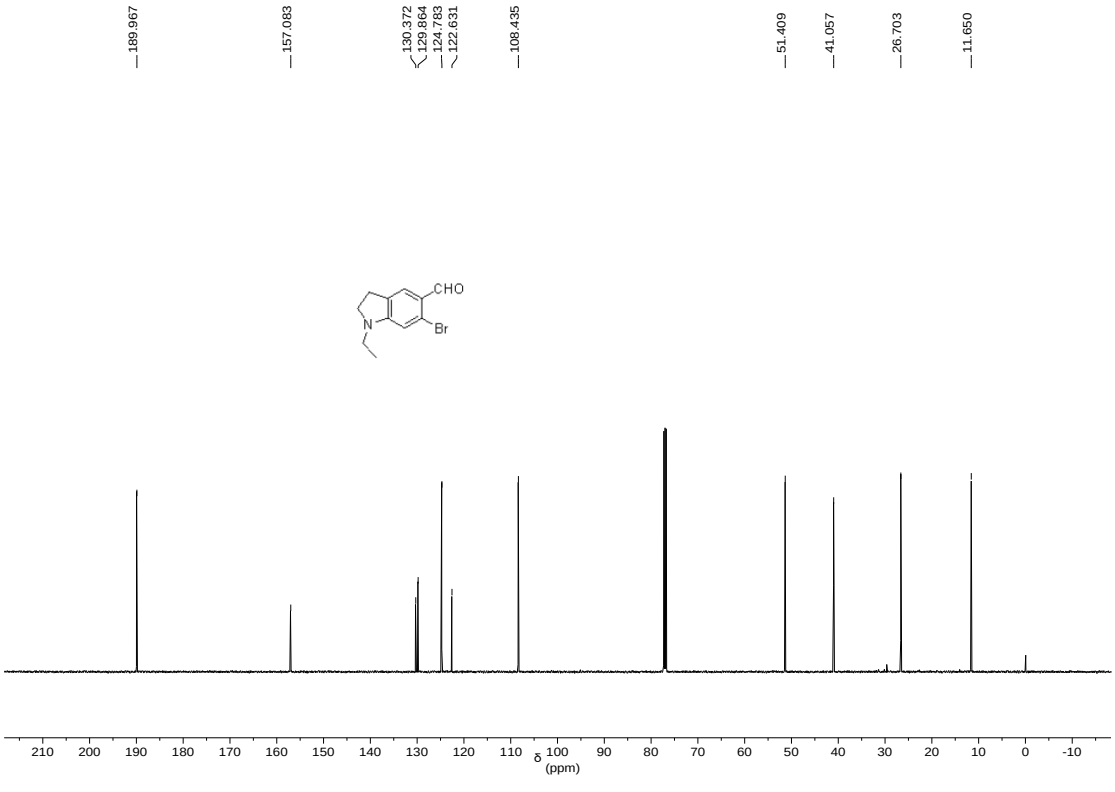

150.73
137.73
137.37
134.94
132.92
125.85
116.98
113.48
112.46
111.28
76.84
52.41
24.24
17.01
-1.90
N
Si
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
δ
(ppm)

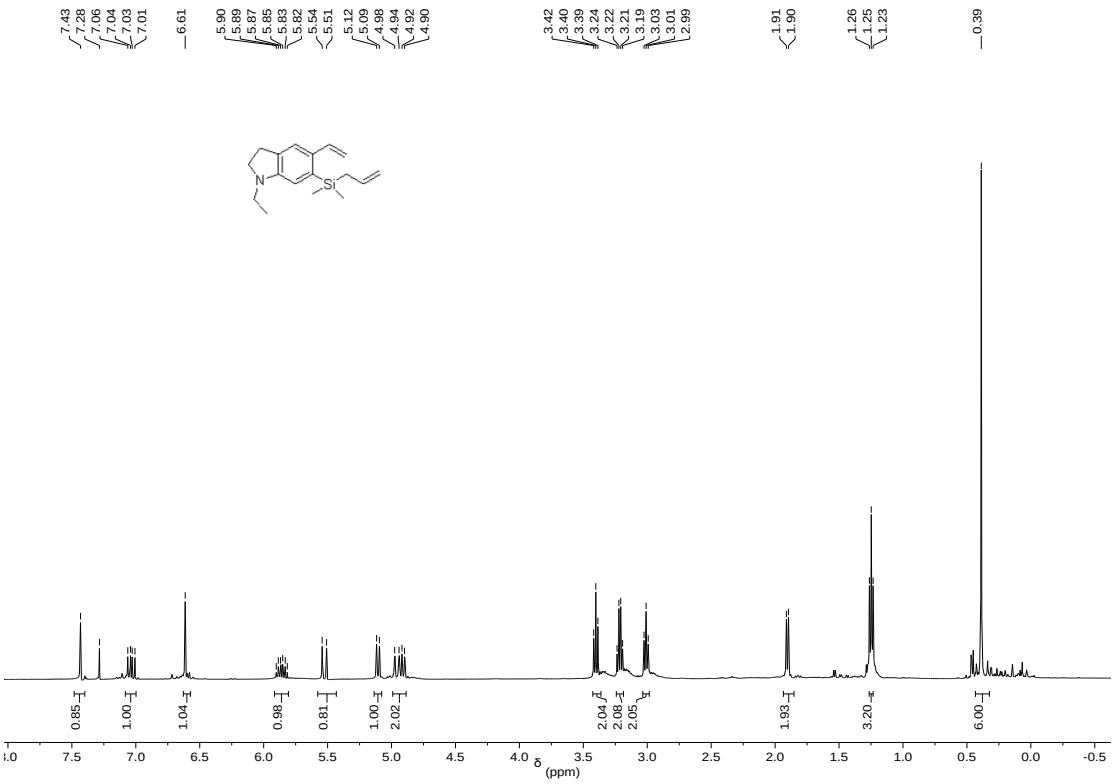

7.30
7.28
7.22
7.21
6.53
6.52
6.38
6.38
6.37
6.36
5.98
5.96
4.01
3.99
3.98
2.46
2.44
2.43
2.42
2.40
0.34
1.00
0.95
0.98
1.02
0.97
4.03
2.20
5.87
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
δ (ppm)

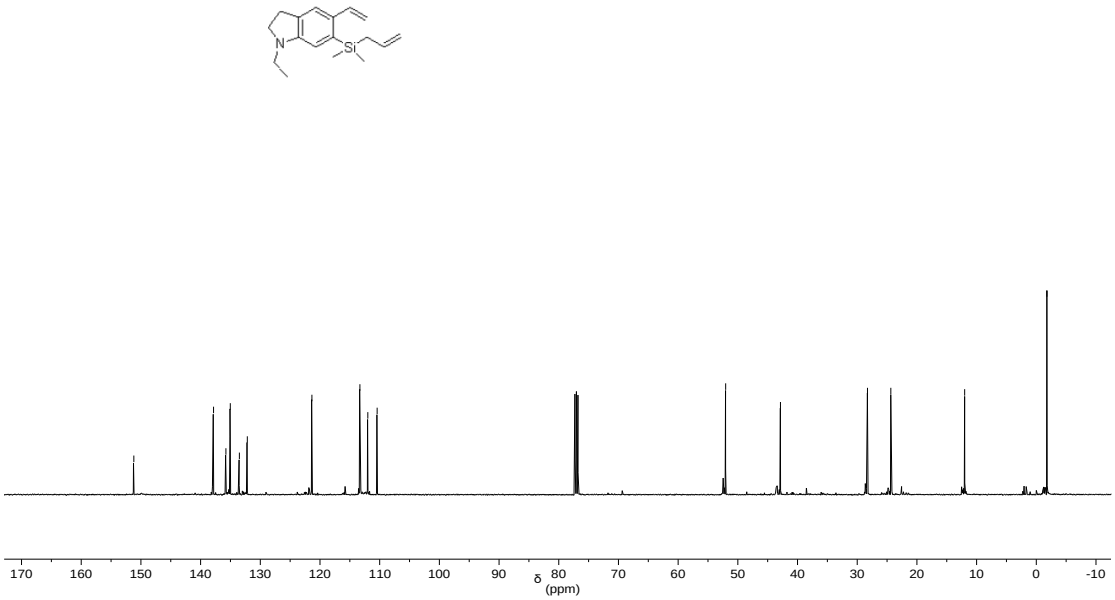

151.6
148.8
139.7
133.8
129.3
127.6
117.4
111.3
77.1
51.8
16.7
-4.1
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
δ (ppm)

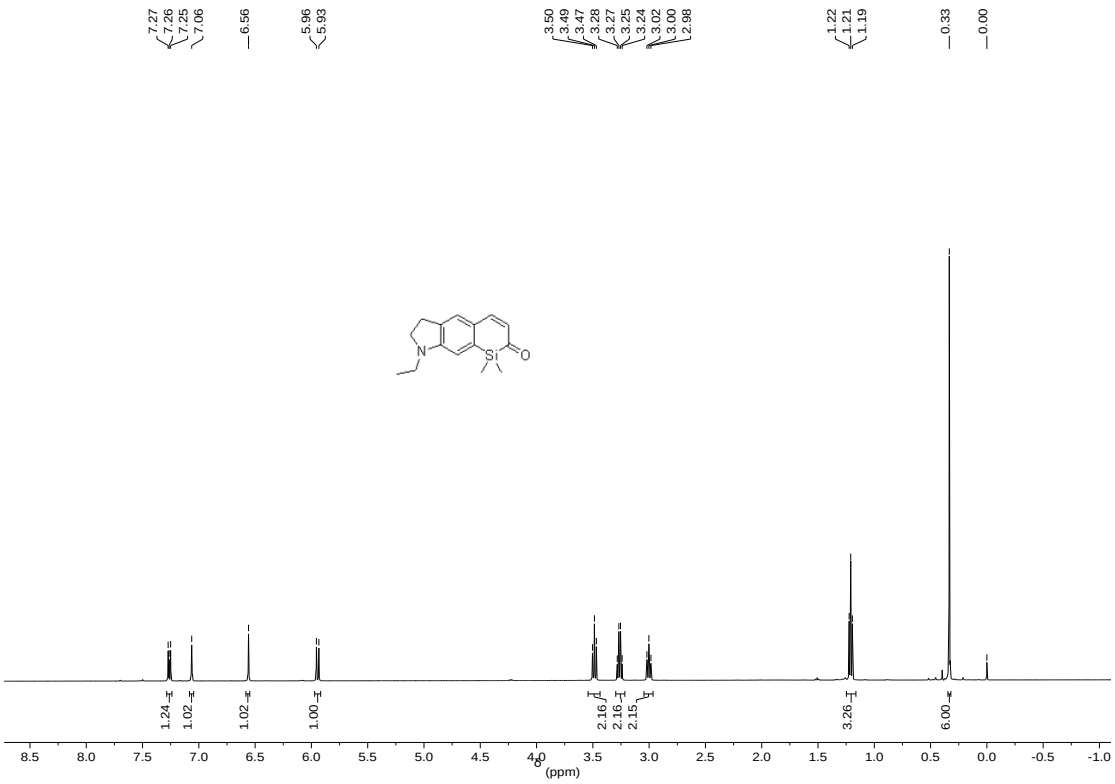
Compound 2e-5e:

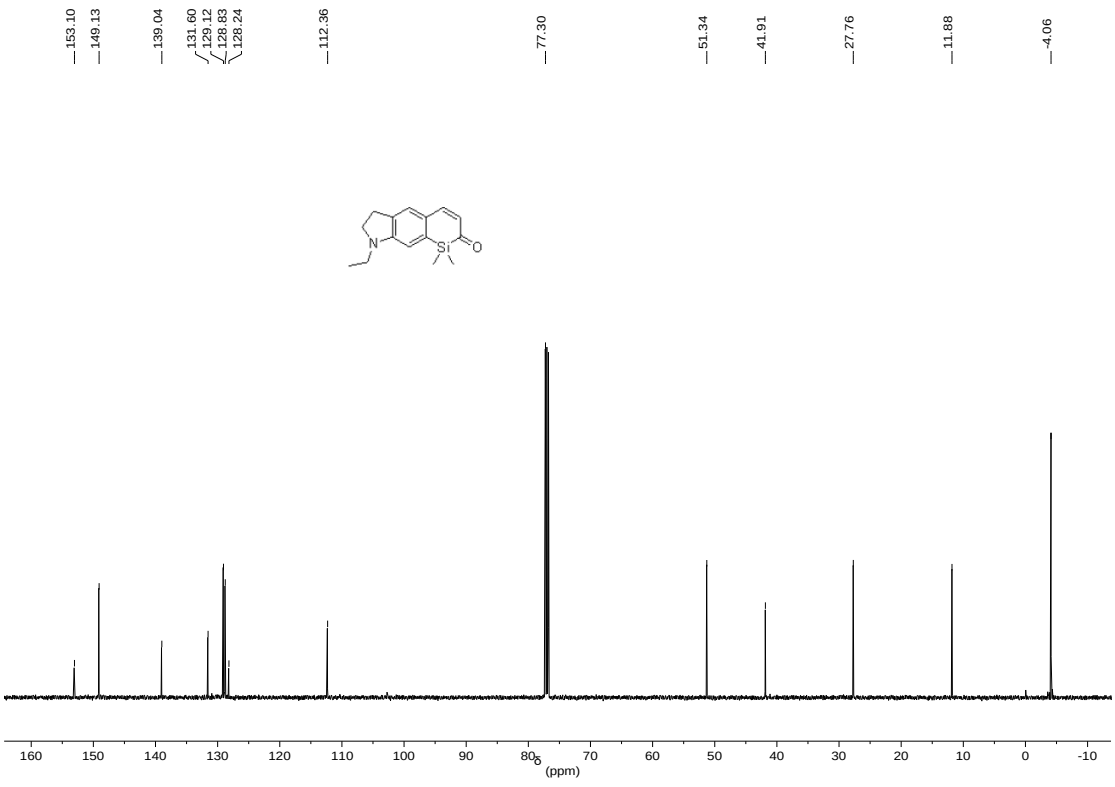




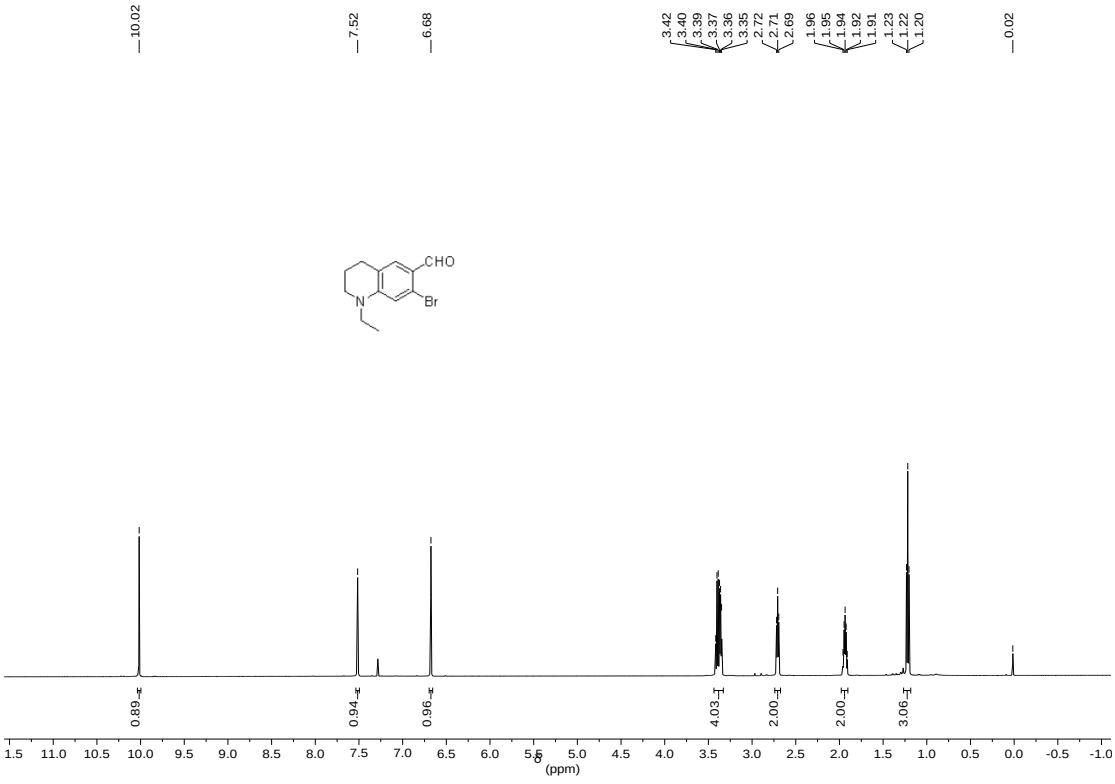

7.43
7.28
7.06
7.04
7.03
7.01
6.61
5.90
5.89
5.87
5.85
5.83
5.82
5.54
5.51
5.12
5.09
4.98
4.94
4.92
4.90
3.42
3.40
3.39
3.24
3.22
3.21
3.19
3.03
3.01
2.99
1.91
1.90
1.26
1.25
1.23
0.39
0.85
1.00
1.04
0.98
0.81
1.00
2.02
2.04
2.08
2.05
1.93
3.20
6.00
δ (ppm)

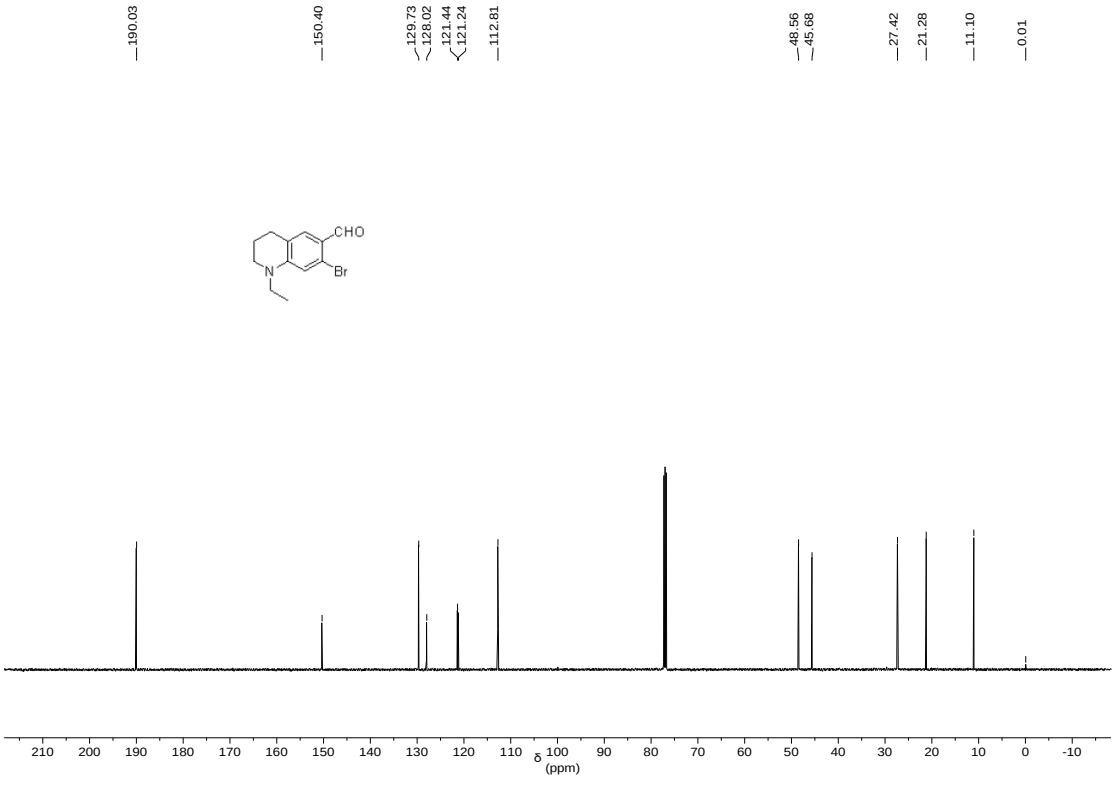

151.25
137.89
135.82
135.09
133.57
132.24
121.41
113.37
112.05
110.49
52.10
42.92
28.34
24.43
12.06
-1.72
δ (ppm)

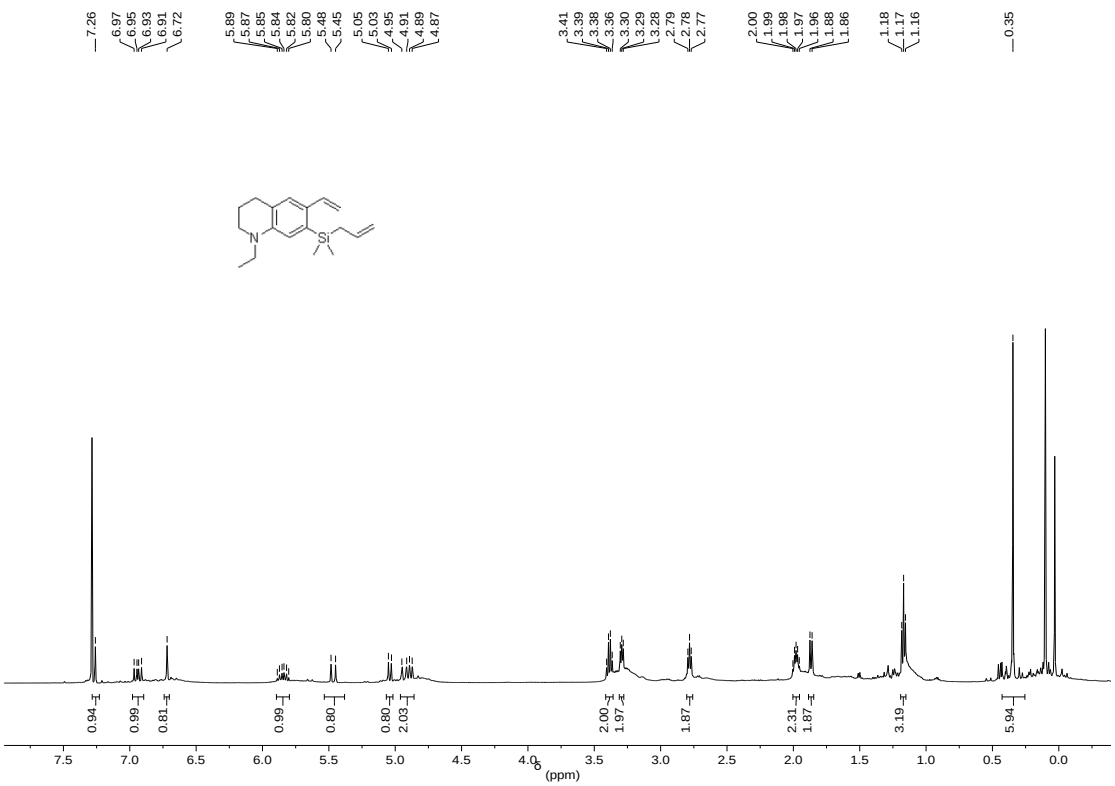

7.27
7.26
7.25
7.06
6.56
5.96
5.93
3.50
3.49
3.47
3.28
3.27
3.25
3.24
3.02
3.00
2.98
1.22
1.21
1.19
0.33
0.00
1.24
1.02
1.02
1.00
2.16
2.16
2.15
3.26
6.00
δ (ppm)

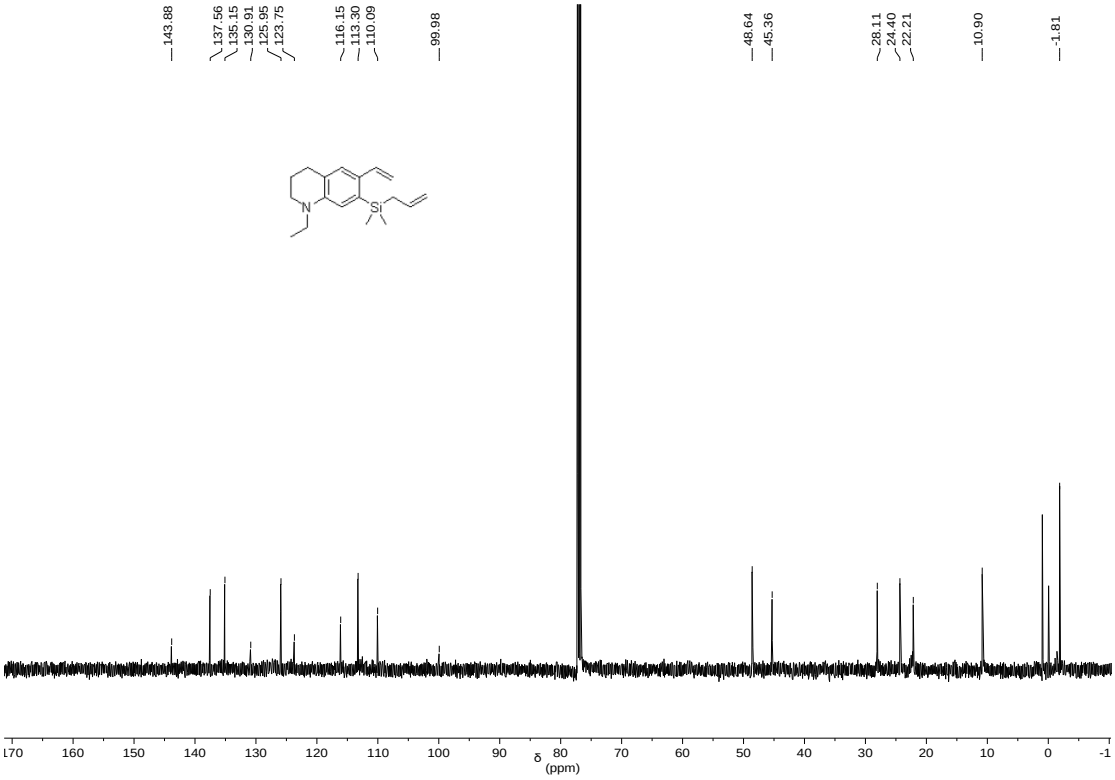

153.10
149.13
139.04
131.60
129.12
128.83
128.24
112.36
77.30
51.34
41.91
27.76
11.88
-4.06
δ (ppm)

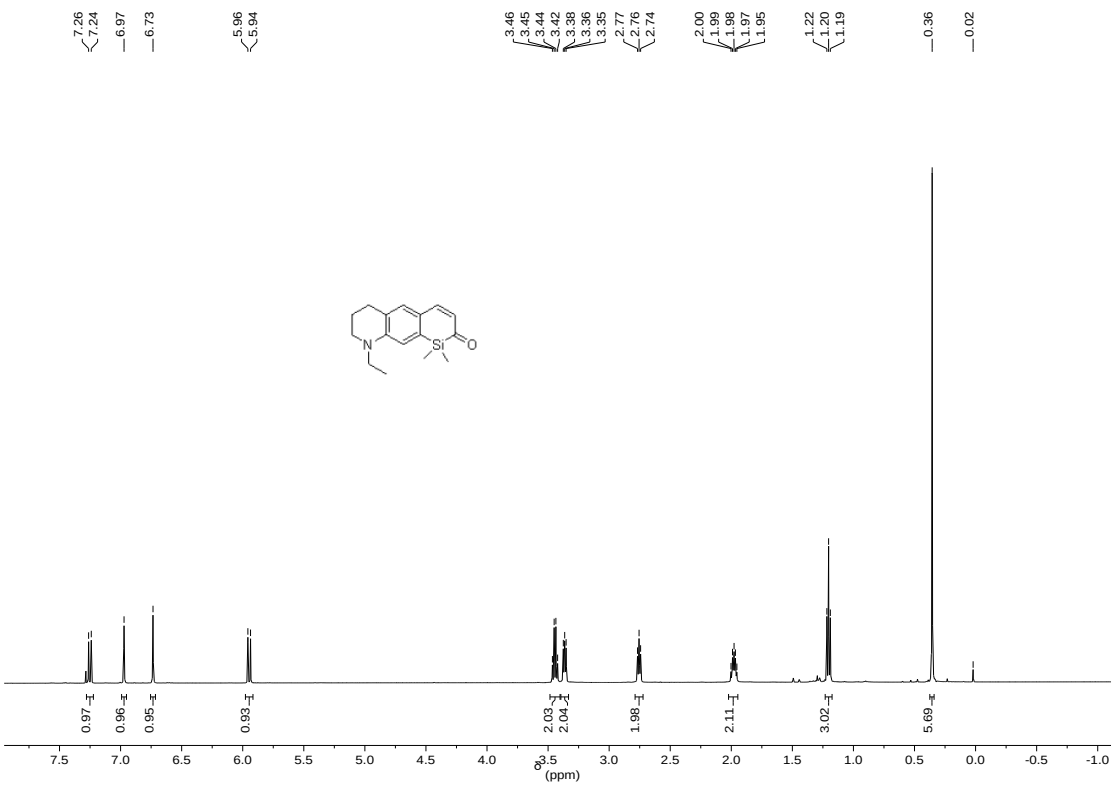
Compound 2f-5f:

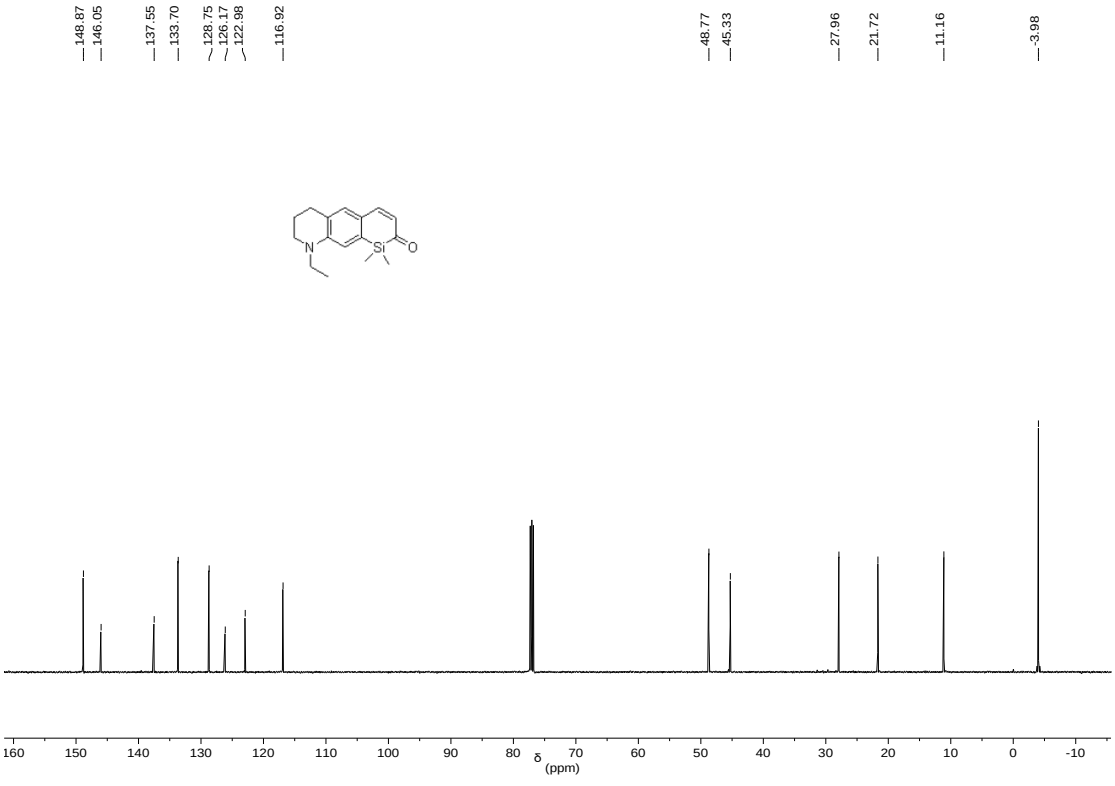





7.26
6.97
6.95
6.93
6.91
6.72
5.89
5.87
5.85
5.84
5.82
5.80
5.48
5.45
5.05
5.03
4.95
4.91
4.89
4.87
3.41
3.39
3.38
3.36
3.30
3.29
3.28
2.79
2.78
2.77
2.00
1.99
1.98
1.97
1.96
1.88
1.86
1.18
1.17
1.16
0.35
0.94
0.99
0.81
0.99
0.80
0.80
2.03
2.00
1.97
1.87
2.31
1.87
3.19
5.94
δ (ppm)


143.88
137.56
135.15
130.91
125.95
123.75
116.15
113.30
110.09
99.98
48.64
45.36
28.11
24.40
22.21
10.90
-1.81
δ (ppm)


7.26
7.24
6.97
6.73
5.96
5.94
3.46
3.45
3.44
3.42
3.38
3.36
3.35
2.77
2.76
2.74
2.00
1.99
1.98
1.97
1.95
1.22
1.20
1.19
0.36
0.02
Si
O
N
0.97
0.96
0.95
0.93
2.03
2.04
1.98
2.11
3.02
5.69
δ (ppm)


148.87
146.05
137.55
133.70
128.75
126.17
122.98
116.92
48.77
45.33
27.96
21.72
11.16
-3.98
Si
O
N
δ (ppm)

HRMS

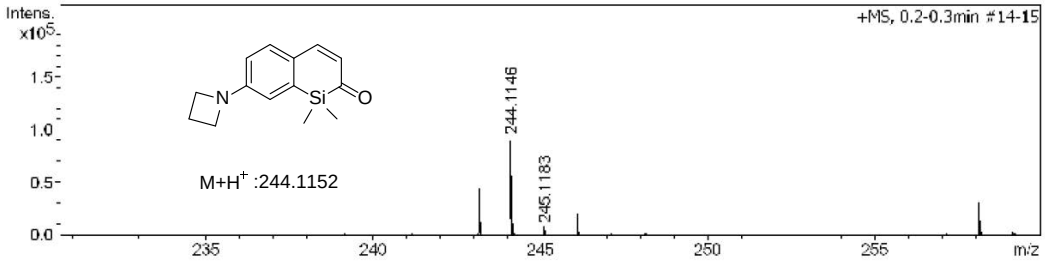
Mass Spectrum List Report

Analysis Info

Acquisition Date	6/8/2018 2:47:02 PM		
Analysis Name	D:\Data\chem. dep\cuixiaoyan\YJJ-0608-4_P1-C-4_01_9394.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	YJJ-0608-4	Instrument	maXis impact 282001.00122
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	244.1146	28485	1382.3	89926	100.0	0.0086
2	245.1183	17009	93.2	6077	6.8	0.0144

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e Conf	N-Rule
244.1146	1	C14H18NOSi	244.1152	2.5	75.7	1	100.00	7.5	even	ok

Mass Spectrum List Report

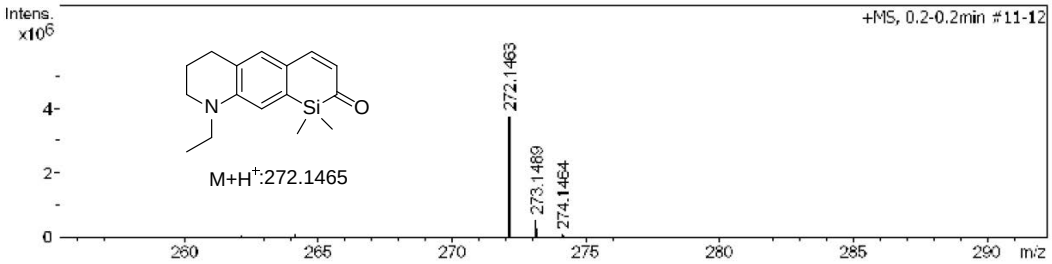
Analysis Info

Acquisition Date 1/24/2019 11:32:16 AM

Analysis Name	D:\Data\chem. dep\cuixiaoyan\LC-0123-1_P1-C-2_01_12534.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	LC-0123-1	Instrument	maXis impact 282001.00122
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	272.1463	48015	19589.2	3760468	100.0	0.0057
2	273.1489	30497	2874.0	552588	14.7	0.0090
3	274.1464	17710	392.9	75674	2.0	0.0155

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e Conf	N-Rule
272.1463	1	C16H22NOSi	272.1465	0.8	46.3	1	100.00	7.5	even	ok

Mass Spectrum List Report

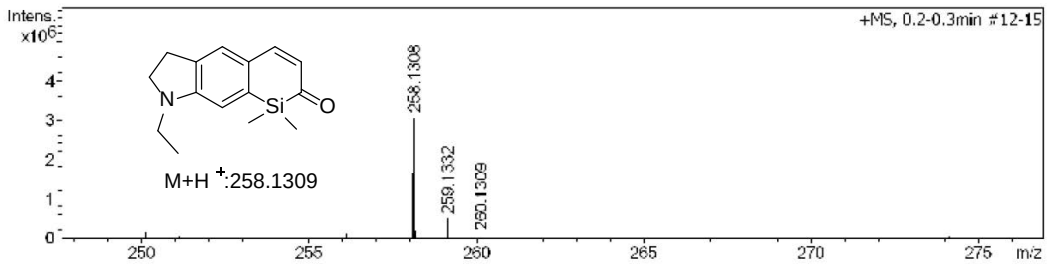
Analysis Info

Acquisition Date 1/24/2019 11:35:24 AM

Analysis Name	D:\Data\chem. dep\cuixiaoyan\LC-0123-2_P1-C-3_01_12535.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	LC-0123-2	Instrument	maXis impact 282001.00122
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	2.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	258.1308	40249	35298.9	3051851	100.0	0.0064
2	259.1332	29499	5668.7	490448	16.1	0.0088
3	260.1309	17639	757.7	65687	2.2	0.0147

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e Conf	N-Rule
258.1308	1	C15H20NOSi	258.1309	0.4	34.5	1	100.00	7.5	even	ok

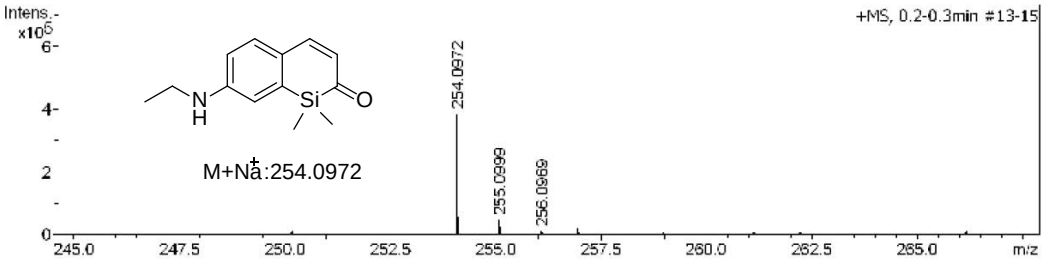
Analysis Info

Acquisition Date 3/1/2018 12:23:34 PM

Analysis Name	D:\Data\chem. dep\cuixiaoyan\LC-0301-3_P1-C-6_01_7973.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	LC-0301-3	Instrument	maXis impact 282001.00122
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	254.0972	30335	5189.8	382554	100.0	0.0084
2	255.0999	20839	607.6	44870	11.7	0.0122
3	256.0969	15232	107.6	7950	2.1	0.0168

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e Conf	N-Rule
254.0972	1	C13H17NNaOSi	254.0972	-0.2	43.2	1	100.00	6.5	even	ok

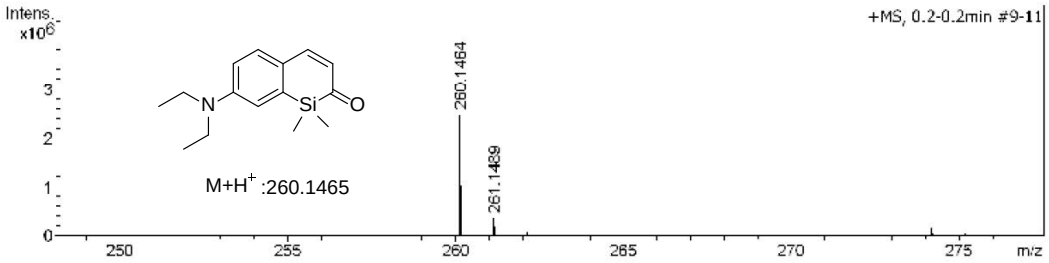
Analysis Info

Acquisition Date 3/9/2018 1:45:09 PM

Analysis Name	D:\Data\chem. dep\cuixiaoyan\LC-0309-1_P1-D-2_01_8053.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	LC-0309-1	Instrument	maXis impact 282001.00122
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	260.1464	50680	33937.7	2463023	100.0	0.0051
2	261.1489	32029	4793.9	348435	14.1	0.0082
3	262.1513	8202	531.1	38713	1.6	0.0320

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e Conf	N-Rule
260.1464	1	C15H22NOSi	260.1465	0.4	44.4	1	100.00	6.5	even	ok

Mass Spectrum List Report

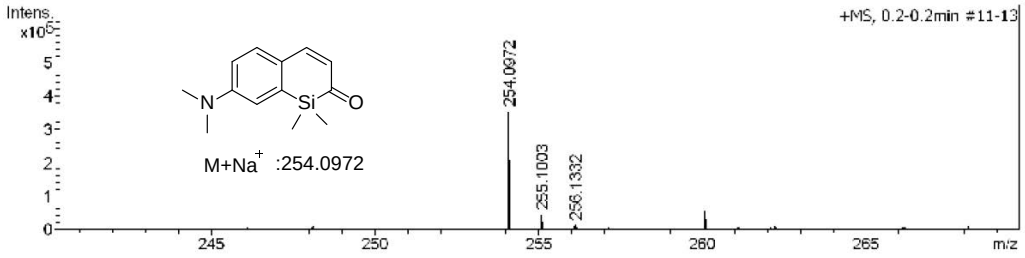
Analysis Info

Acquisition Date 2/28/2018 11:48:01 AM

Analysis Name	D:\Data\chem. dep\cuixiaoyan\LC-0228-1_P1-B-3_01_7965.d		
Method	Tune_pos_low_LC with calibration_2min.m	Operator	ECNU-Chem
Sample Name	LC-0228-1	Instrument	maXis impact 282001.00122
Comment			

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	1.5 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	6.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	500.0 Vpp	Set Divert Valve	Waste



#	m/z	Res.	S/N	I	I %	FWHM
1	254.0972	28939	4526.0	351402	100.0	0.0088
2	255.1003	18716	549.2	42716	12.2	0.0136
3	256.1332	13790	150.0	11689	3.3	0.0186

Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma		Score	rdb	e Conf	N-Rule
254.0972	1	C13H17NNaOSi	254.0972	0.0	40.4	1	100.00	6.5	even	ok