

Supporting Information

Visible-light-induced selective hydrolipocyclization and silylation of alkenes: Access to ring-fused quinazolin-4(3*H*)-ones and its silicon-substituted derivatives

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A. General Information

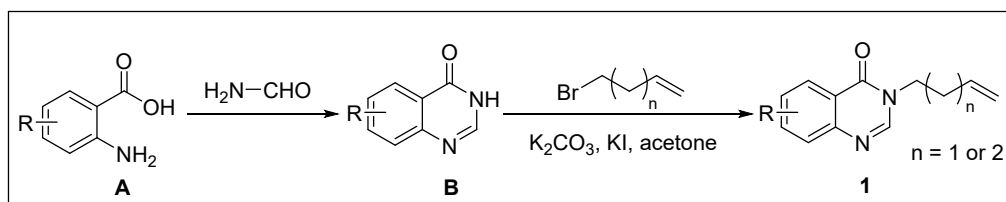
All purchased reagents and solvents were used without further purification unless otherwise noted. ^1H and ^{13}C NMR spectra were recorded using a Bruker DRX-500 spectrometer employing CDCl_3 as solvent. The chemical shifts are referenced to signals at 7.26 and 77.0 ppm, respectively. The data of HRMS was carried out on a high-resolution mass spectrometer (LCMS-IT-TOF). Melting points were determined with a Büchi Melting Point B-545 instrument. TLC was performed by using commercially prepared 100-400 mesh silica gel plates and visualization was effected at 254 nm. The blue light source (460-465 nm) was provided by Shanghai 3S Technology Co., LtdSSSTECH-AL2 parallel reactor (Figure S1)



Figure S1. Photoreactor used in this study.

B. Experimental Procedure¹⁻³

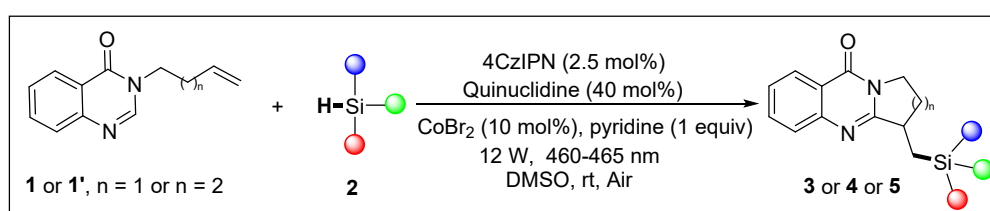
B1. General Procedure for the Synthesis of 1



The mixtures of anthranilic acid (**A**) (1 mmol) and an excess of formamide (10 mmol) in a round-bottom flask were heated at $120\text{ }^\circ\text{C}$ with stirring for 3-5 h. The reaction was checked by TLC. After the starting materials completely disappeared, the resulting mixtures were cooled to room temperature and then poured into ice-cold water. The light or dark brown precipitates were formed. The precipitates were filtered, washed with water ($3 \times 20\text{ mL}$) and dried to give quinazoline-4(3*H*)-one derivatives (**B**). These intermediates were used for the next step without further purification. To a solution of quinazoline-4(3*H*)-

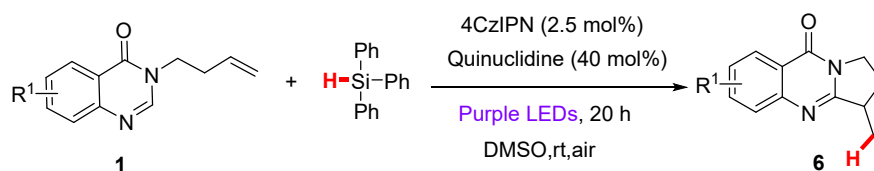
ones (**B**) (1 mmol) in acetone (10 mL) was added K_2CO_3 (207 mg, 1.5 mmol). The resulting mixture was heated at 60 °C with stirring for 30 min. KI (16.6 mg, 0.1 mmol) was added and after stirring for further 15 min, brominated olefins (0.13 mL, 1.2 mmol) diluted with acetone (1 mL) was dropwise added into the mixture. The reaction mixture was further stirred at 60 °C for 3 h. After the reaction completed, the resulting mixture was cooled and poured into ice-cold water. The solids were formed, filtered and dried to give the corresponding crude products **1**, which is purified by column chromatography on silica gel with a mixture of petroleum ether and ethyl acetate.

B2. General Procedure for the Synthesis of 3, 4 or 5



To a 10 mL Schlenk tube equipped with a magnetic stir bar was added 4CzIPN (0.0025 mmol), $CoBr_2$ (0.01 mmol), and quinuclidine (0.04 mmol). Then dry dimethyl sulfoxide (2.0 mL) was added in Schlenk tube, after which the alkenes (0.1 mmol), silanes (0.5 mmol) and pyridine (0.1 mmol) were added respectively at room temperature, then placed in the irradiation apparatus equipped with a 12 W blue light-emitting diode (LED). The resulting mixture was stirred at 25 °C until the starting material was completely consumed as monitored by TLC. After the reaction was completed, the resulting mixture was extracted with ethyl acetate, dried over anhydrous $MgSO_4$, filtered and evaporated in vacuo. The desired products were obtained in 35-81% yields after being purified by column chromatography on silica gel with a mixture of petroleum ether and ethyl acetate.

B3. General Procedure for the Synthesis of 6



To a 10 mL Schlenk tube equipped with a magnetic stir bar was added 4CzIPN (0.0025 mmol), quinuclidine (0.04 mmol). Then dry dimethyl sulfoxide (2.0 mL) was added, after which the alkenes (0.1 mmol), triphenylsilane (0.3 mmol) were added respectively at room temperature, then placed in the irradiation apparatus equipped with a 12 W purple light-emitting diode (LED). The resulting mixture

was stirred at 25 °C until the starting material was completely consumed as monitored by TLC. After the reaction was completed, the resulting mixture was extracted with ethyl acetate, dried over anhydrous MgSO₄, filtered and evaporated in vacuo. The desired products were obtained in 47-64% yields after being purified by column chromatography on silica gel with a mixture of petroleum ether and ethyl acetate.

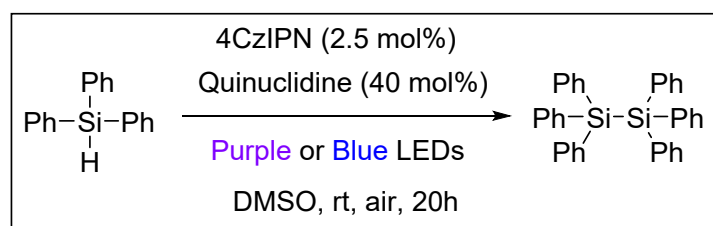
C. Gram Scale Reaction

To a 250 mL round-bottom flask equipped with a magnetic stir bar was added 4CzIPN (0.15 mmol), CoBr₂ (0.6 mmol), and quinuclidine (2.4 mmol). Then dry dimethyl sulfoxide (100 mL) was added, after which **1a** (6 mmol), **2a** (30 mmol) and pyridine (6 mmol) were added to the mixture at room temperature, respectively, then placed in the irradiation apparatus equipped with a 25 W blue light-emitting diode (LED). The resulting mixture was stirred at 25 °C until the starting material was completely consumed as monitored by TLC. After the reaction was completed, the resulting mixture was extracted with ethyl acetate, dried over anhydrous MgSO₄, filtered and evaporated in vacuo. The desired product **3a** was obtained in 60% yield after being purified by column chromatography on silica gel with a mixture of petroleum ether and ethyl acetate (volume ratio 10:1).

D. Light On-off Experiment

To a 10 mL Schlenk tube equipped with a magnetic stir bar was added 4CzIPN (0.0025 mmol), CoBr₂ (0.01 mmol), and quinuclidine (0.04 mmol). Then dry dimethyl sulfoxide (2.0 mL) was added, after which the **1a** (0.1 mmol), **2a** (0.5 mmol) and pyridine (0.1 mmol) were added respectively at room temperature, then placed in the irradiation apparatus equipped with a 25 W blue light-emitting diode (LED). The reaction mixture was stirred for 3, 7, 11, and 15 hours respectively. Meanwhile, the setting time span for 1 hours, and only stirred without light. The yield of the product **3a** was determined by GC and dodecane as internal standard.

E. Comparative Experiment for the Synthesis of Disilane



In order to find out why different products were obtained under different light source irradiation, a comparative experiment was conducted for the synthesis of disilane. The mixture of 0.5 mmol of triphenylsilane, 2.5 mol% of 4CzIPN and 40 mol% of quinuclidine was irradiated by different light source systems under standard conditions. After 1h, the disilane yield can reach 84 % under purple light, but only 34 % under blue light. The results disclosed that purple LEDs is more favorable for the synthesis of disilane, which provided important evidences for the selective silylation and hydroarylation process.

F. H₂ Detection Experiment

F1. H₂ Detection Experiment for the Synthesis of 3a

In order to demonstrate the release of H₂ during this procedure for the synthesis of **3a**, the model reaction of 3-(but-3-en-1-yl)quinazolin-4(3*H*)-one (**1a**) and 1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilane (**2a**) was monitored by a H₂ detector under standard conditions. Just as shown in Figure S2, as the reaction proceeded, the H₂ was observed clearly and the concentration increased gradually.



Figure S2. H₂ detection experiment by a H₂ detector for the synthesis of **3a** after 3 hours.

F2. H₂ Detection Experiment for the Synthesis of 6a

In order to demonstrate the release of H₂ during this photoreaction procedure for the synthesis of **6a**, the model reaction of 3-(but-3-en-1-yl)quinazolin-4(3*H*)-one (**1a**) and triphenylsilane was monitored by a H₂ detector under standard conditions. Just as shown in Figure S3, as the reaction proceeded, the H₂ was observed clearly and the concentration increased gradually.



Figure S3. H₂ detection experiment by a H₂ detector for the synthesis of **6a** after 3 hours.

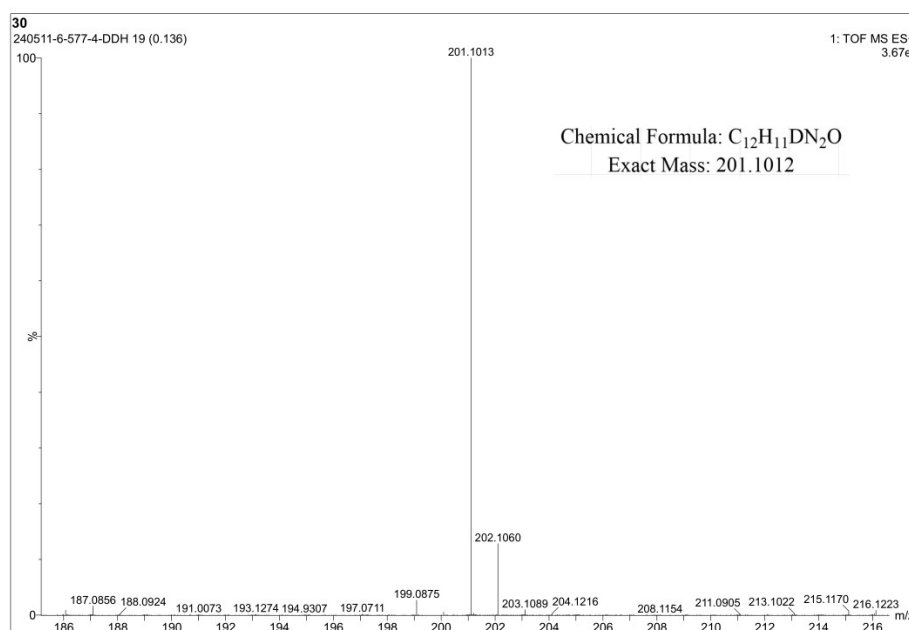
G. Labeling Experiment

G1. Typical Procedure for Preparation of Ph₃Si-D

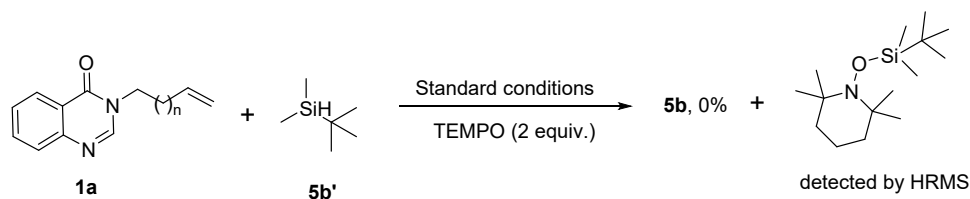
ⁿBuLi (2 equiv., 2 mmol) was added dropwise to a stirred solution of triphenylsilane (1 equiv., 1 mmol, 260 mg) in THF (5 mL) at -78 °C. Then the mixture was warmed to room temperature and stirred for 3 h. Afterwards, 1 mL of D₂O was added dropwise. The mixture was quenched by diethyl ether (3×5 mL), The combined organic layers was washed with brine (5 mL), dried and filtered over anhydrous sodium sulfate. The solvent was removed under reduce pressure, and the residue was purified by column chromatography (peteroleum ether) to get Ph₃SiD (213 mg, yield 82%) as a white solid.

G2. Experimental Procedure for Labeling Experiment

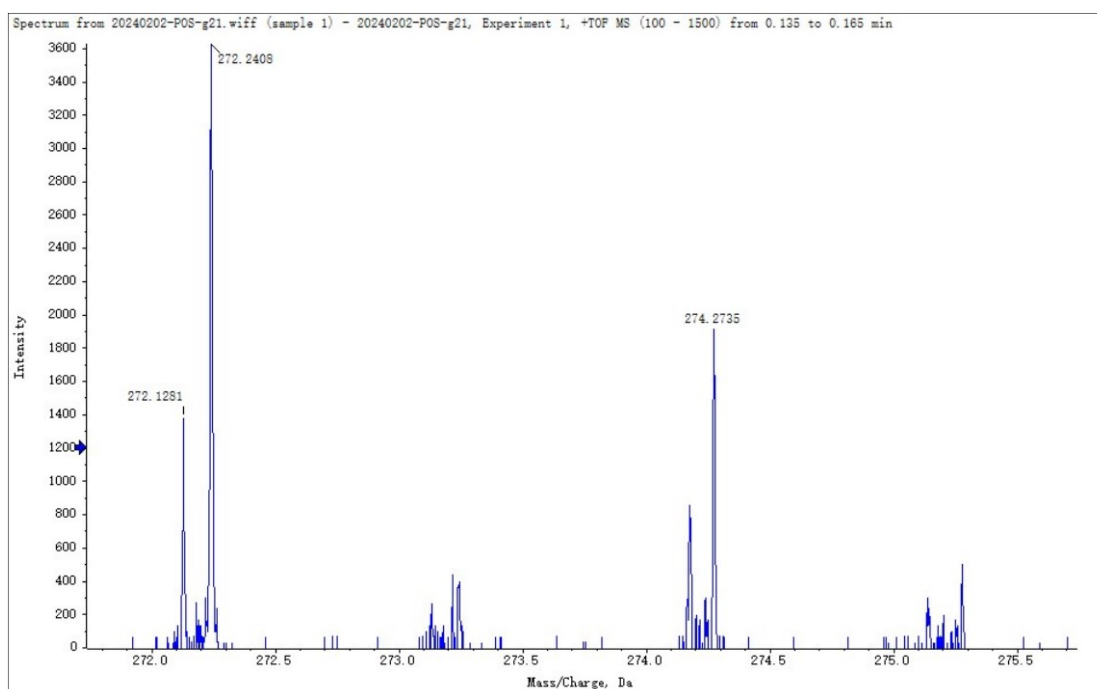
To a 10 mL Schlenk tube equipped with a magnetic stir bar was added 4CzIPN (0.0025 mmol), quinuclidine (0.04 mmol). Then dry dimethyl sulfoxide (2.0 mL) was added, after which the alkene (0.1 mmol) and Ph₃Si-D (0.3 mmol) were added respectively at room temperature, then placed in the irradiation apparatus equipped with a 12 W purple light-emitting diode (LED). The resulting mixture was stirred at 25 °C until the starting material was completely consumed as monitored by TLC. After the reaction was completed, the resulting mixture was extracted with ethyl acetate, dried over anhydrous MgSO₄, filtered and evaporated in vacuo. The desired deuterium-labeled product was obtained only in trace yield (detected by HRMS).



H. Trapping experiment of silicon free radicals



Under standard conditions, 2 equivalent of TEMPO was added to the system and no target product was obtained, fortunately the silicon radical was captured by HRMS as shown in the figure below.

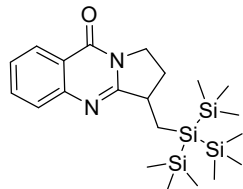


I. Supplementary References

1. L. Liu, W. Zhang, C. Xu, J. He, Z. Xu, Z. Yang, F. Ling, W. Zhong. *Adv. Synth. Catal.* **2022**, *364*, 1319-1325.
2. B. Mu, L. Zhang, G. Lv, K. Chen, T. Wang, J. Chen, T. Huang, L. Guo, Z. Yang, Y. Wu. *J. Org. Chem.* **2022**, *87*, 10146-10157.
3. B. Sun, R. Shi, K. Zhang, X. Tang, X. Shi, J. Xu, J. Yang, C. Jin. *Chem. Commun.* **2021**, *57*, 6050-6053.

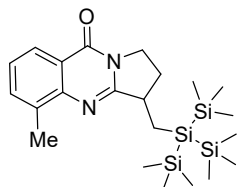
J. Characterization Data of Products

3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (3a)



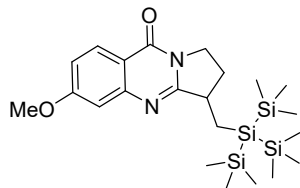
Yield 36.1 mg (81%, white solid); Melting point: 95.5-97.4 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.28 (d, *J* = 7.9 Hz, 1H), 7.72 (d, *J* = 4.0 Hz, 2H), 7.43 (dt, *J* = 8.2, 4.1 Hz, 1H), 4.25 (ddd, *J* = 12.5, 8.4, 3.7 Hz, 1H), 4.08-3.94 (m, 1H), 3.23 (dtd, *J* = 11.5, 8.4, 3.1 Hz, 1H), 2.50 (dtd, *J* = 12.3, 7.6, 3.8 Hz, 1H), 1.92-1.78 (m, 2H), 1.09-0.98 (m, 1H), 0.24 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 162.7, 161.1, 149.5, 134.0, 127.2, 126.3, 126.1, 120.7, 44.3, 43.5, 29.5, 10.8, 1.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₁H₃₉N₂OSi₄ 447.2134; Found 447.2139.

3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-5-methyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (3b)



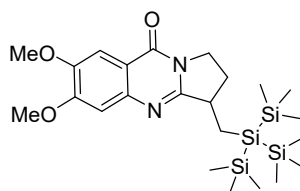
Yield 36.3 mg (79%, white solid); Melting point: 125.2-127.7 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.19-8.10 (m, 1H), 7.58 (d, *J* = 7.4 Hz, 1H), 7.33 (td, *J* = 7.6, 2.4 Hz, 1H), 4.31-4.22 (m, 1H), 4.02 (dtd, *J* = 14.9, 7.6, 2.4 Hz, 1H), 3.29-3.18 (m, 1H), 2.63 (d, *J* = 2.6 Hz, 3H), 2.56-2.48 (m, 1H), 1.93 (ddd, *J* = 14.7, 4.0, 1.9 Hz, 2H), 1.02 (ddd, *J* = 15.0, 10.6, 2.6 Hz, 1H), 0.45-0.20 (m, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 161.6, 161.5, 148.1, 135.7, 134.6, 125.5, 124.0, 120.5, 44.3, 43.4, 29.6, 17.4, 11.2, 1.2. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₂H₄₁N₂OSi₄ 461.2290; Found 461.2299.

3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-6-methoxy-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (3c)



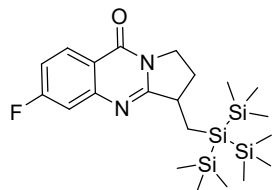
Yield 32.4 mg (68%, white solid); Melting point: 94.8-97.5 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.18 (dd, *J* = 8.9, 1.8 Hz, 1H), 7.12 (s, 1H), 7.02 (dt, *J* = 8.9, 2.2 Hz, 1H), 4.23 (td, *J* = 10.4, 8.6, 4.4 Hz, 1H), 4.00 (q, *J* = 6.3, 4.7 Hz, 1H), 3.94 (d, *J* = 1.8 Hz, 3H), 3.21 (q, *J* = 9.5 Hz, 1H), 2.50 (qd, *J* = 12.5, 10.3, 6.0 Hz, 1H), 1.89-1.81 (m, 2H), 1.07-0.98 (m, 1H), 0.25 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 164.4, 163.5, 160.7, 151.9, 127.8, 116.2, 114.2, 107.9, 55.6, 44.2, 43.6, 29.4, 10.9, 1.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₂H₄₁N₂O₂Si₄ 477.2240; Found 477.2248.

3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-6,7-dimethoxy-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (3d)



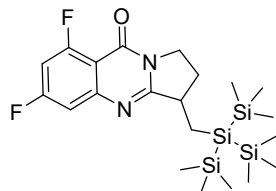
Yield 32.4 mg (64%, white solid); Melting point: 169.3-177.1 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.61 (s, 1H), 7.14 (s, 1H), 4.25 (ddd, *J* = 12.4, 8.5, 4.1 Hz, 1H), 4.02 (d, *J* = 8.4 Hz, 7H), 3.27-3.15 (m, 1H), 2.50 (dtd, *J* = 12.1, 7.6, 4.0 Hz, 1H), 1.85 (ddd, *J* = 12.4, 10.2, 5.8 Hz, 2H), 1.02 (dd, *J* = 14.6, 11.4 Hz, 1H), 0.25 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 161.6, 160.5, 154.6, 148.5, 145.8, 113.9, 107.7, 105.3, 56.3, 56.2, 44.3, 43.5, 29.6, 10.9, 1.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₃H₄₃N₂O₃Si₄ 507.2345; Found 507.2359.

6-fluoro-3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (3e)



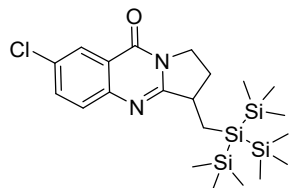
Yield 28.8 mg (62%, colorless liquid); ¹H NMR (500 MHz, Chloroform-*d*) δ 8.29 (dd, *J* = 8.7, 6.1 Hz, 1H), 7.37 (dd, *J* = 9.9, 2.5 Hz, 1H), 7.16 (td, *J* = 8.5, 2.4 Hz, 1H), 4.25 (ddd, *J* = 12.5, 8.5, 4.1 Hz, 1H), 4.00 (dt, *J* = 12.3, 7.8 Hz, 1H), 3.31-3.13 (m, 1H), 2.52 (dtd, *J* = 12.2, 7.8, 4.0 Hz, 1H), 1.92-1.77 (m, 2H), 1.02 (dd, *J* = 14.6, 11.0 Hz, 1H), 0.25 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 166.3 (d, *J*_{C-F} = 251.3 Hz), 164.15, 160.37, 151.8 (d, *J*_{C-F} = 13.8 Hz), 128.9 (d, *J*_{C-F} = 10.0 Hz), 117.4 (d, *J*_{C-F} = 2.5 Hz), 114.8 (d, *J*_{C-F} = 2.5 Hz), 112.5 (d, *J*_{C-F} = 22.5 Hz), 44.34, 43.57, 29.49, 10.86, 1.33. ¹⁹F NMR (471 MHz, Chloroform-*d*) δ -104.30, -104.31. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₁H₃₇FN₂OSi₄ 465.2040; Found 465.2044.

6,8-difluoro-3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (3f)



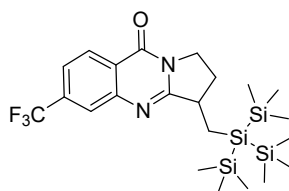
Yield 32.3 mg (67%, colorless liquid); ¹H NMR (500 MHz, Chloroform-*d*) δ 7.18 (dt, *J* = 9.7, 2.0 Hz, 1H), 6.84 (ddd, *J* = 11.0, 8.8, 2.5 Hz, 1H), 4.23 (ddd, *J* = 12.6, 8.6, 4.1 Hz, 1H), 3.97 (dt, *J* = 12.4, 7.9 Hz, 1H), 3.20 (dtd, *J* = 11.3, 8.3, 3.2 Hz, 1H), 2.51 (dtd, *J* = 12.3, 7.9, 4.1 Hz, 1H), 1.84 (ddd, *J* = 20.4, 16.5, 10.7 Hz, 2H), 1.00 (dd, *J* = 14.6, 10.9 Hz, 1H), 0.25 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 166.5 (d, *J*_{C-F} = 15.0 Hz), 164.92, 164.5 (d, *J*_{C-F} = 13.8 Hz), 163.5 (d, *J*_{C-F} = 15.0 Hz), 161.4 (d, *J*_{C-F} = 15.0 Hz), 157.63, 153.3 (d, *J*_{C-F} = 15.0 Hz), 109.1 (d, *J*_{C-F} = 5.0 Hz), 108.9 (d, *J*_{C-F} = 3.8 Hz), 107.5 (d, *J*_{C-F} = 10.0 Hz), 102.5 (d, *J*_{C-F} = 2.5 Hz), 102.4 (d, *J*_{C-F} = 51.3 Hz), 44.39, 43.62, 29.21, 10.82, 1.31. ¹⁹F NMR (471 MHz, Chloroform-*d*) δ -101.27, -101.29, -101.31, -101.33, -106.23, -106.25, -106.27. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₁H₃₇F₂N₂OSi₄ 483.1946; Found 483.1945.

7-chloro-3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (3g)



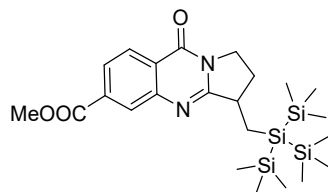
Yield 19.7 mg (41%, colorless liquid); ¹H NMR (500 MHz, Chloroform-*d*) δ 8.25 (s, 1H), 7.67 (s, 2H), 4.26 (ddd, *J* = 12.5, 8.6, 4.0 Hz, 1H), 4.00 (dt, *J* = 11.9, 7.8 Hz, 1H), 3.22 (dtd, *J* = 11.6, 8.5, 3.4 Hz, 1H), 2.52 (dtd, *J* = 12.1, 8.1, 4.0 Hz, 1H), 1.86 (ddd, *J* = 21.7, 11.5, 4.2 Hz, 2H), 1.03 (td, *J* = 12.4, 10.9, 3.0 Hz, 1H), 0.25 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 163.1, 160.1, 148.1, 134.3, 131.8, 128.9, 125.7, 121.8, 44.4, 43.5, 29.5, 10.8, 1.3. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₁H₃₈ClN₂OSi₄ 481.1744; Found 481.1745.

3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-6-(trifluoromethyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (3h)



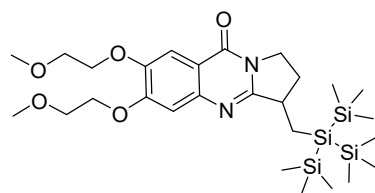
Yield 37 mg (72%, white solid); Melting point: 110.5-112.1 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.40 (d, *J* = 8.3 Hz, 1H), 8.07-7.96 (m, 1H), 7.64 (dd, *J* = 8.3, 1.8 Hz, 1H), 4.29 (ddd, *J* = 12.2, 8.3, 3.9 Hz, 1H), 4.03 (dt, *J* = 12.4, 7.9 Hz, 1H), 3.25 (dtd, *J* = 11.5, 8.3, 3.0 Hz, 1H), 2.55 (dtd, *J* = 12.1, 7.8, 4.0 Hz, 1H), 1.95-1.83 (m, 2H), 1.02 (dd, *J* = 14.6, 11.1 Hz, 1H), 0.26 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 164.25, 160.25, 149.57, 135.5 (q, *J*_{C-F} = 32.5 Hz), 127.44, 124.9 (q, *J*_{C-F} = 3.8 Hz), 123.6 (d, *J*_{C-F} = 271.3 Hz), 123.02, 122.0 (q, *J*_{C-F} = 3.8 Hz), 44.51, 43.59, 29.45, 10.93, 1.32. ¹⁹F NMR (471 MHz, Chloroform-*d*) δ -63.07, -63.08, -63.10, -63.12. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₂H₃₈F₃N₂OSi₄ 515.2008; Found 515.2009.

3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-9-oxo-1,2,3,9-tetrahydropyrrolo[2,1-*b*]quinazolin-6-yl acetate (3i)



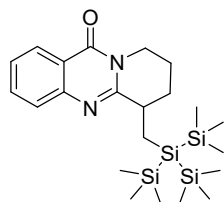
Yield 36.8 mg (73%, white solid); Melting point: 167.9-169.2 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.39 (d, *J* = 1.6 Hz, 1H), 8.32 (d, *J* = 8.3 Hz, 1H), 8.04 (dd, *J* = 8.3, 1.7 Hz, 1H), 4.26 (ddd, *J* = 12.4, 8.5, 4.0 Hz, 1H), 3.98 (s, 3H), 3.23 (dtd, *J* = 11.1, 7.8, 2.7 Hz, 1H), 2.53 (dtd, *J* = 12.0, 7.7, 4.0 Hz, 1H), 1.96-1.79 (m, 2H), 1.01 (dd, *J* = 14.6, 11.1 Hz, 1H), 0.39 (d, *J* = 17.6 Hz, 1H), 0.25 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 166.3, 163.6, 160.5, 149.4, 135.0, 129.2, 126.6, 126.1, 123.7, 52.5, 44.4, 43.5, 29.5, 10.9, 1.3. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₃H₄₁N₂O₃Si₄ 505.2189; Found 505.2192.

3-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-6,7-bis(2-methoxyethoxy)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (3j)



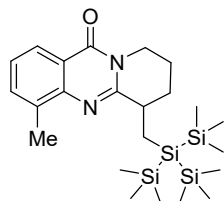
Yield 42.2 mg (71%, white solid); Melting point: 171.2-174.1 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.62 (s, 1H), 7.14 (s, 1H), 4.39-4.26 (m, 4H), 3.99 (dt, *J* = 12.4, 7.7 Hz, 1H), 3.92-3.76 (m, 4H), 3.50 (d, *J* = 2.9 Hz, 6H), 3.21 (d, *J* = 11.1 Hz, 1H), 2.49 (ddq, *J* = 12.5, 8.3, 5.0, 4.4 Hz, 1H), 1.84 (dt, *J* = 12.8, 3.7 Hz, 3H), 1.03 (dd, *J* = 14.6, 11.3 Hz, 1H), 0.25 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 161.5, 160.4, 154.3, 148.0, 145.8, 114.0, 109.0, 107.2, 70.8, 70.6, 68.6, 68.4, 59.3, 59.3, 44.3, 43.4, 29.6, 10.9, 1.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₇H₅₁N₂O₅Si₄ 595.2870; Found 595.2882.

6-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-one (4a)



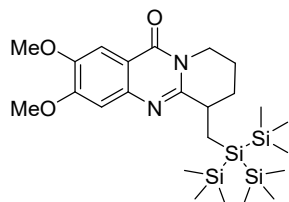
Yield 34 mg (74%, white solid); Melting point: 171.4-173.2 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.32-8.22 (m, 1H), 7.75-7.70 (m, 1H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.47-7.40 (m, 1H), 4.40 (dt, *J* = 14.0, 5.7 Hz, 1H), 3.86 (ddd, *J* = 14.1, 8.0, 6.1 Hz, 1H), 2.99 (d, *J* = 10.4 Hz, 1H), 2.19 (dq, *J* = 13.1, 6.5 Hz, 1H), 2.07-1.97 (m, 2H), 1.83-1.57 (m, 2H), 1.09 (dd, *J* = 14.6, 9.0 Hz, 1H), 0.24 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 162.3, 159.1, 147.6, 133.9, 127.1, 126.6, 126.0, 120.2, 41.4, 40.0, 27.8, 20.2, 12.0, 1.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₂H₄₁N₂OSi₄ 461.2290; Found 461.2298.

6-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-4-methyl-6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-one (4b)



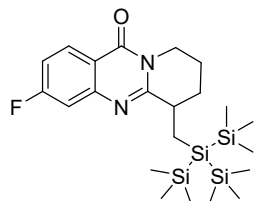
Yield 37.5 mg (79%, white solid); Melting point: 166.5-168.2 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.26-7.98 (m, 1H), 7.58 (d, *J* = 7.2 Hz, 1H), 7.32 (t, *J* = 7.6 Hz, 1H), 4.24 (dt, *J* = 14.1, 6.1 Hz, 1H), 3.97 (ddd, *J* = 13.7, 7.8, 5.4 Hz, 1H), 3.18-3.00 (m, 1H), 2.63 (s, 3H), 2.24-2.16 (m, 2H), 2.07 (dtd, *J* = 13.2, 7.7, 3.8 Hz, 1H), 2.02-1.94 (m, 1H), 1.67 (dtd, *J* = 13.3, 8.2, 5.4 Hz, 1H), 1.09 (dd, *J* = 14.6, 10.8 Hz, 1H), 0.25 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 162.0, 159.8, 144.2, 135.2, 134.5, 126.2, 124.4, 119.6, 42.4, 39.3, 26.8, 19.9, 17.9, 13.9, 1.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₃H₄₃N₂OSi₄ 475.2447; Found 475.2448.

6-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-2,3-dimethoxy-6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-one (4c)



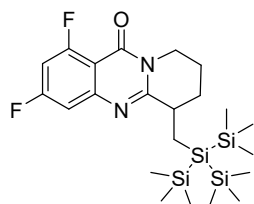
Yield 34.9 mg (67%, white solid); Melting point: 169.7-172.1 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.59 (s, 1H), 7.06 (s, 1H), 4.42 (dt, *J* = 14.0, 5.7 Hz, 1H), 4.02 (d, *J* = 9.0 Hz, 6H), 3.84 (dt, *J* = 14.1, 7.1 Hz, 1H), 2.96 (ddq, *J* = 13.1, 9.0, 4.2 Hz, 1H), 2.18 (dq, *J* = 13.1, 6.6 Hz, 1H), 1.99 (td, *J* = 8.4, 7.4, 3.6 Hz, 3H), 1.75-1.55 (m, 1H), 1.09 (dd, *J* = 14.5, 9.2 Hz, 1H), 0.23 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 161.5, 157.9, 154.8, 148.6, 143.8, 113.5, 107.4, 105.5, 56.3, 56.2, 41.3, 39.8, 27.9, 20.3, 11.9, 1.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₄H₄₅N₂O₃Si₄ 521.2502; Found 521.2510.

3-fluoro-6-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-one (4d)



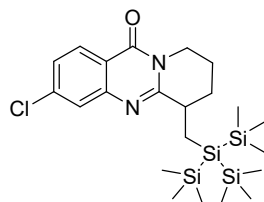
Yield 26.3 mg (55%, white solid); Melting point: 161.3-163.2 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.27 (dd, *J* = 8.8, 6.1 Hz, 1H), 7.36-7.29 (m, 1H), 7.14 (td, *J* = 8.6, 2.5 Hz, 1H), 4.36 (dt, *J* = 14.0, 5.6 Hz, 1H), 3.85 (ddd, *J* = 14.2, 8.1, 5.8 Hz, 1H), 2.98 (dh, *J* = 13.1, 3.7 Hz, 1H), 2.18 (dq, *J* = 13.2, 6.6 Hz, 1H), 2.01 (ddt, *J* = 14.5, 7.8, 4.9 Hz, 3H), 1.66 (dq, *J* = 14.3, 7.2 Hz, 1H), 1.07 (dd, *J* = 14.5, 9.2 Hz, 1H), 0.24 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 167.3, 165.3, 161.1 (d, *J*_{C-F} = 127.5 Hz), 149.7 (d, *J*_{C-F} = 13.8 Hz), 129.3 (d, *J*_{C-F} = 11.3 Hz), 116.9 (d, *J*_{C-F} = 2.5 Hz), 114.9 (d, *J*_{C-F} = 22.5 Hz), 112.1 (d, *J*_{C-F} = 22.5 Hz), 41.6, 40.1, 27.7, 20.1, 12.2, 1.4. ¹⁹F NMR (471 MHz, Chloroform-*d*) δ -104.39. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₂H₄₀FN₂OSi₄ 479.2202; Found 479.2204.

1,3-difluoro-6-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-one (4e)



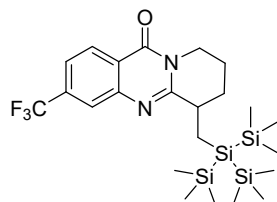
Yield 30.4 mg (63%, white solid); Melting point: 178.8-180.5 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.23 (d, *J* = 9.3 Hz, 1H), 6.83 (ddd, *J* = 11.2, 9.0, 2.4 Hz, 1H), 4.27 (dt, *J* = 14.2, 5.6 Hz, 1H), 3.82 (ddd, *J* = 14.0, 8.0, 5.7 Hz, 1H), 3.06 (d, *J* = 9.5 Hz, 1H), 2.14 (dq, *J* = 13.3, 7.0, 6.5 Hz, 1H), 2.05-1.92 (m, 3H), 1.70 (dq, *J* = 13.3, 6.5 Hz, 1H), 1.09 (dd, *J* = 14.5, 9.9 Hz, 1H), 0.23 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 166.7 (d, *J*_{C-F} = 15.0 Hz), 164.7 (d, *J*_{C-F} = 13.8 Hz), 163.3 (d, *J*_{C-F} = 15.0 Hz), 162.4, 161.2 (d, *J*_{C-F} = 13.8 Hz), 158.1, 149.2, 107.7 (d, *J*_{C-F} = 21.3 Hz), 106.6 (d, *J*_{C-F} = 6.3 Hz), 102.8 (t, *J*_{C-F} = 26.3 Hz), 41.9, 39.4, 26.9, 19.6, 13.1, 1.4. ¹⁹F NMR (471 MHz, Chloroform-*d*) δ -100.09, -106.12, -106.24, -106.28, -106.35, -106.36. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₂H₃₉F₂N₂OSi₄ 497.2108; Found 497.2104.

3-chloro-6-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-one (4f)



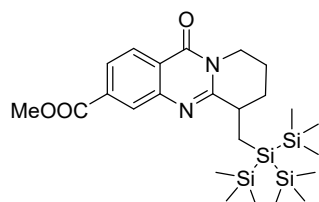
Yield 24.2 mg (49%, white solid); Melting point: 170.2-172.8 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.19 (d, *J* = 8.6 Hz, 1H), 7.77-7.60 (m, 1H), 7.38 (dd, *J* = 8.5, 2.0 Hz, 1H), 4.35 (dt, *J* = 14.1, 5.8 Hz, 1H), 3.86 (ddd, *J* = 14.1, 8.2, 5.8 Hz, 1H), 3.05-2.92 (m, 1H), 2.18 (dq, *J* = 13.1, 6.5 Hz, 1H), 2.01 (ddtd, *J* = 14.1, 11.4, 8.1, 4.0 Hz, 3H), 1.67 (dq, *J* = 13.9, 7.1 Hz, 1H), 1.07 (dd, *J* = 14.6, 9.5 Hz, 1H), 0.24 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 161.6, 160.7, 140.1, 128.1, 128.1, 126.7, 126.4, 118.5, 41.7, 40.0, 27.5, 20.0, 12.4, 1.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₂H₄₀ClN₂OSi₄ 495.1901; Found 495.1909.

6-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-3-(trifluoromethyl)-6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-one (4g)



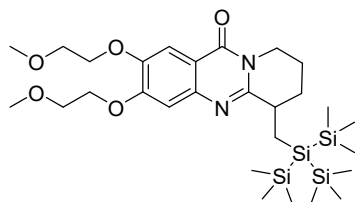
Yield 33.8 mg (64%, colorless liquid); ¹H NMR (500 MHz, Chloroform-*d*) δ 8.38 (d, *J* = 8.3 Hz, 1H), 7.93 (s, 1H), 7.63 (dd, *J* = 8.4, 1.8 Hz, 1H), 4.38 (dt, *J* = 14.1, 5.8 Hz, 1H), 3.88 (ddd, *J* = 14.1, 8.2, 6.0 Hz, 1H), 3.00 (tdd, *J* = 9.2, 6.1, 3.5 Hz, 1H), 2.21 (dq, *J* = 13.2, 6.6 Hz, 1H), 2.02 (ddt, *J* = 12.5, 8.5, 4.9 Hz, 3H), 1.74-1.62 (m, 1H), 1.08 (dd, *J* = 14.6, 9.6 Hz, 1H), 0.25 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 161.5, 160.8, 147.5, 135.5 (d, *J*_{C-F} = 32.5 Hz), 127.8, 124.7 (q, *J*_{C-F} = 2.5 Hz), 122.5, 122.3, 121.9 (q, *J*_{C-F} = 2.5 Hz), 41.8, 40.1, 27.5, 20.0, 12.3, 1.4. ¹⁹F NMR (471 MHz, CDCl₃) δ -63.13. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₃H₄₀F₃N₂OSi₄ 529.2170; Found 529.2170.

methyl 6-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-11-oxo-6,8,9,11-tetrahydro-7H-pyrido[2,1-b]quinazoline-3-carboxylate (4h)



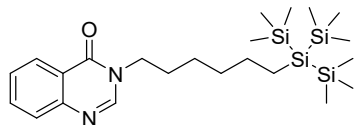
Yield 39.4 mg (76%, white solid); Melting point: 155.6-157.3 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.44-8.14 (m, 2H), 8.00 (dd, *J* = 8.3, 1.6 Hz, 1H), 4.34 (dt, *J* = 14.1, 5.8 Hz, 1H), 3.97 (s, 3H), 3.85 (ddd, *J* = 14.0, 8.1, 5.8 Hz, 1H), 2.96 (tdd, *J* = 9.7, 6.1, 3.5 Hz, 1H), 2.17 (dq, *J* = 13.4, 6.6 Hz, 2H), 2.05-1.96 (m, 2H), 1.73-1.57 (m, 1H), 1.06 (dd, *J* = 14.6, 9.6 Hz, 1H), 0.21 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 166.4, 161.8, 160.0, 147.4, 135.0, 129.1, 126.9, 125.9, 123.0, 52.5, 41.8, 40.1, 27.5, 20.0, 12.2, 1.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₄H₄₃N₂O₃Si₄ 519.2351; Found 519.2347.

6-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-2,3-bis(2-methoxyethoxy)-6,7,8,9-tetrahydro-11H-pyrido[2,1-b]quinazolin-11-one (4i)



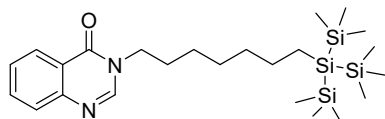
Yield 40.1 mg (67%, white solid); Melting point: 123.6-125.4 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.60 (s, 1H), 7.05 (s, 1H), 4.40 (dt, *J* = 14.0, 5.7 Hz, 1H), 4.28 (dt, *J* = 9.6, 4.7 Hz, 4H), 3.86 (dt, *J* = 12.0, 4.8 Hz, 4H), 3.50 (d, *J* = 5.0 Hz, 6H), 2.94 (s, 1H), 2.16 (dq, *J* = 13.1, 6.5 Hz, 1H), 1.99 (p, *J* = 6.5, 5.8 Hz, 3H), 1.88 (s, 1H), 1.63 (s, 1H), 1.09 (dd, *J* = 14.5, 9.0 Hz, 1H), 0.23 (s, 27H). ¹³C NMR (125 MHz, DMSO-*d*₆) δ 156.7, 153.0, 149.7, 143.4, 139.2, 108.8, 104.0, 102.6, 66.0, 65.8, 63.8, 63.6, 54.6, 54.5, 36.5, 35.0, 23.1, 15.5, 7.1, -3.4. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₈H₅₃N₂O₅Si₄ 609.3032; Found 609.3037.

3-(6-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)hexyl)quinazolin-4(3H)-one (1'j-A)



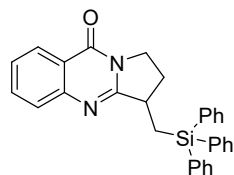
Yield 29.0 mg (61%, white solid); Melting point: 123.6-125.4 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.34 (dd, *J* = 8.0, 1.6 Hz, 1H), 8.05 (s, 1H), 7.77 (ddd, *J* = 8.5, 6.8, 1.5 Hz, 1H), 7.74-7.70 (m, 1H), 7.55-7.49 (m, 1H), 4.01 (t, *J* = 7.4 Hz, 2H), 1.80 (p, *J* = 6.9 Hz, 2H), 1.40 (d, *J* = 4.3 Hz, 6H), 0.77 (dd, *J* = 11.1, 4.9 Hz, 2H), 0.16 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 161.0, 148.1, 146.6, 134.1, 127.4, 127.2, 126.7, 122.2, 47.1, 33.8, 29.5, 29.1, 26.3, 7.6, 1.2. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₃H₄₅N₂O₅Si₄ 477.2603; Found 477.2608.

3-(7-(1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)heptyl)quinazolin-4(3H)-one (1'k-A)



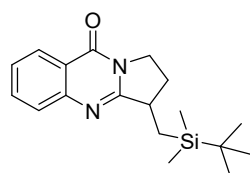
Yield 27.4 mg (56%, colorless liquid); ¹H NMR (500 MHz, Chloroform-*d*) δ 8.37-8.31 (m, 1H), 8.05 (s, 1H), 7.77 (td, *J* = 7.6, 7.0, 1.6 Hz, 1H), 7.75-7.70 (m, 1H), 7.56-7.50 (m, 1H), 4.02 (t, *J* = 7.4 Hz, 2H), 1.81 (q, *J* = 6.9 Hz, 2H), 1.44-1.31 (m, 8H), 0.81-0.68 (m, 2H), 0.16 (s, 27H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 161.1, 148.1, 146.6, 134.1, 127.4, 127.2, 126.7, 122.2, 47.1, 34.1, 29.4, 29.1, 28.8, 26.7, 7.5, 1.2. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₂₄H₄₇N₂OSi₄ 491.2760; Found 491.2768.

3-((triphenylsilyl)methyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (5a)



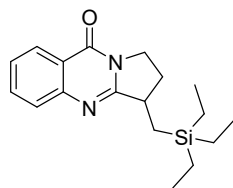
Yield 16 mg (35%, colorless liquid); ¹H NMR (500 MHz, Chloroform-*d*) δ 8.37-8.17 (m, 1H), 7.74 (td, *J* = 7.6, 6.9, 1.6 Hz, 1H), 7.71-7.60 (m, 7H), 7.49-7.36 (m, 10H), 4.15 (ddt, *J* = 8.9, 7.1, 3.0 Hz, 1H), 3.79 (ddd, *J* = 12.3, 9.2, 7.3 Hz, 1H), 3.53-3.34 (m, 1H), 2.58 (dd, *J* = 15.1, 3.1 Hz, 1H), 1.77-1.59 (m, 2H), 1.36-1.19 (m, 1H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 162.8, 161.0, 149.4, 135.7, 134.4, 134.0, 129.8, 128.1, 127.1, 126.4, 126.1, 120.7, 44.5, 40.4, 29.0, 16.0. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₃₀H₂₇N₂OSi 459.1893; Found 459.1888.

3-((tert-butyldimethylsilyl)methyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1H)-one (5b)



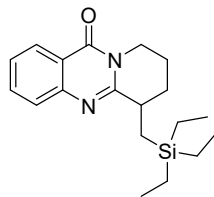
Yield 15.1 mg (48%, white solid); Melting point: 86.2-89.3 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.30 (d, *J* = 7.9 Hz, 1H), 7.73 (d, *J* = 6.7 Hz, 2H), 7.46 (tt, *J* = 7.7, 1.9 Hz, 1H), 4.37-4.24 (m, 1H), 3.98 (dt, *J* = 13.2, 8.4 Hz, 1H), 3.37-3.19 (m, 1H), 2.62-2.43 (m, 1H), 1.90-1.78 (m, 1H), 1.64 (dt, *J* = 14.7, 2.3 Hz, 1H), 0.96 (d, *J* = 1.8 Hz, 9H), 0.86-0.73 (m, 1H), 0.26-0.04 (m, 6H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 163.3, 161.1, 149.4, 134.1, 127.0, 126.4, 126.1, 120.6, 44.5, 40.7, 29.2, 26.5, 16.7, 15.3, -4.6, -5.8. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₁₈H₂₇N₂OSi 315.1893; Found 315.1894.

3-((triethylsilyl)methyl)-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (5c)



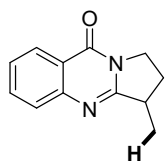
Yield 21.4 mg (68%, white solid); Melting point: 145.6-148.3 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.30 (d, *J* = 8.0 Hz, 1H), 7.77-7.68 (m, 2H), 7.45 (ddd, *J* = 8.1, 6.0, 2.2 Hz, 1H), 4.30 (ddd, *J* = 12.1, 8.6, 3.2 Hz, 1H), 4.01-3.92 (m, 1H), 3.26 (ddt, *J* = 11.5, 8.3, 4.3 Hz, 1H), 2.51 (dtd, *J* = 11.3, 7.7, 3.2 Hz, 1H), 1.85 (dq, *J* = 12.6, 9.0 Hz, 1H), 1.59 (dd, *J* = 14.8, 3.6 Hz, 1H), 1.01 (t, *J* = 8.0 Hz, 9H), 0.83 (dd, *J* = 14.9, 11.5 Hz, 1H), 0.66 (qd, *J* = 7.9, 2.6 Hz, 6H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 163.3, 161.1, 149.5, 134.0, 127.0, 126.4, 126.1, 120.6, 44.5, 40.5, 29.3, 14.5, 7.5, 3.9. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₁₈H₂₇N₂OSi 315.1893; Found 315.1887.

6-((triethylsilyl)methyl)-6,7,8,9-tetrahydro-11*H*-pyrido[2,1-*b*]quinazolin-11-one (5d)



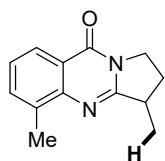
Yield 21.3 mg (65%, colorless liquid); ¹H NMR (500 MHz, Chloroform-*d*) δ 8.28 (d, *J* = 8.0 Hz, 1H), 7.73 (t, *J* = 7.5 Hz, 1H), 7.68 (s, 1H), 7.44 (t, *J* = 7.5 Hz, 1H), 4.32 (dt, *J* = 14.0, 5.9 Hz, 1H), 3.96 (ddd, *J* = 14.0, 8.2, 5.5 Hz, 1H), 3.08 (s, 1H), 2.16 (dq, *J* = 13.1, 6.5 Hz, 1H), 2.02 (ddp, *J* = 26.3, 12.9, 6.5, 6.1 Hz, 2H), 1.68 (dq, *J* = 14.6, 7.5 Hz, 1H), 1.56 (dd, *J* = 14.9, 5.1 Hz, 1H), 1.28 (s, 1H), 1.00 (t, *J* = 7.9 Hz, 9H), 0.64 (tp, *J* = 14.6, 7.2 Hz, 6H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 163.3, 161.1, 149.5, 134.0, 127.0, 126.4, 126.1, 120.6, 44.5, 40.5, 29.7, 29.2, 14.5, 7.5, 3.9. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₁₉H₂₉N₂OSi 329.2049; Found 329.2044.

3-methyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (6a)



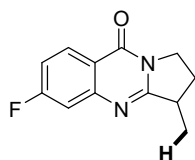
Yield 12.8 mg (64%, white solid); Melting point: 87-89 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.33 (dt, *J* = 22.9, 6.0 Hz, 1H), 7.74 (tt, *J* = 14.0, 8.1 Hz, 2H), 7.47 (dq, *J* = 14.2, 7.3 Hz, 1H), 4.40-4.22 (m, 1H), 4.04 (tt, *J* = 15.5, 6.0 Hz, 1H), 3.35 (dh, *J* = 15.1, 7.8 Hz, 1H), 2.63-2.37 (m, 1H), 2.02-1.82 (m, 1H), 1.69-1.38 (m, 3H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 162.4, 161.0, 149.3, 134.1, 127.0, 126.4, 126.2, 120.7, 44.6, 38.8, 28.6, 17.2.

3,5-dimethyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (6b)



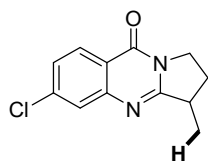
Yield 13.1 mg (61%, white solid); Melting point: 46-49 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.15 (d, *J* = 8.0 Hz, 1H), 7.58 (d, *J* = 7.3 Hz, 1H), 7.33 (td, *J* = 7.7, 2.2 Hz, 1H), 4.28 (ddt, *J* = 12.2, 8.8, 2.9 Hz, 1H), 4.01 (ddd, *J* = 12.3, 9.2, 7.0 Hz, 1H), 3.35 (h, *J* = 7.4 Hz, 1H), 2.64 (s, 3H), 2.50 (tdd, *J* = 12.2, 6.7, 3.3 Hz, 1H), 1.95-1.80 (m, 1H), 1.50 (dd, *J* = 7.0, 2.3 Hz, 3H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 161.4, 161.0, 147.9, 135.5, 134.7, 125.6, 124.0, 120.6, 44.5, 38.8, 28.7, 17.5, 17.3.

6-fluoro-3-methyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (6c)



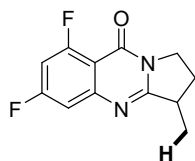
Yield 11.8 mg (54%, white solid); Melting point: 95-97 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.29 (dd, *J* = 8.9, 6.2 Hz, 1H), 7.34 (dd, *J* = 9.9, 2.5 Hz, 1H), 7.16 (td, *J* = 8.5, 2.5 Hz, 1H), 4.28 (ddd, *J* = 12.4, 8.7, 3.7 Hz, 1H), 4.01 (dt, *J* = 11.9, 8.0 Hz, 1H), 3.33 (h, *J* = 7.7 Hz, 1H), 2.51 (dtd, *J* = 12.3, 8.0, 3.7 Hz, 1H), 1.90 (dq, *J* = 12.6, 8.7 Hz, 1H), 1.49 (d, *J* = 7.0 Hz, 3H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 166.4 (d, *J*_{C-F} = 251.3 Hz), 163.76, 160.30, 151.6 (d, *J*_{C-F} = 13.8 Hz), 128.9 (d, *J*_{C-F} = 10.0 Hz), 117.4 (d, *J*_{C-F} = 2.5 Hz), 114.9 (d, *J*_{C-F} = 23.8 Hz), 112.4 (d, *J*_{C-F} = 22.5 Hz), 44.62, 38.91, 28.58, 17.10. ¹⁹F NMR (471 MHz, Chloroform-*d*) δ -104.11 (t, *J* = 8.2 Hz).

6-chloro-3-methyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (6d)



Yield 12.4mg (53%, white solid); Melting point: 89-91 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 8.41 (d, *J* = 8.4 Hz, 1H), 8.02 (s, 1H), 7.66 (d, *J* = 8.3 Hz, 1H), 4.32 (ddd, *J* = 12.3, 8.7, 3.5 Hz, 1H), 4.04 (dt, *J* = 12.6, 8.2 Hz, 1H), 3.38 (h, *J* = 7.6 Hz, 1H), 2.55 (dtd, *J* = 12.1, 7.9, 3.5 Hz, 1H), 1.93 (dtd, *J* = 12.5, 10.0, 9.6, 7.5 Hz, 1H), 1.52 (dd, *J* = 7.1, 2.0 Hz, 3H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 163.9, 160.1, 149.2, 135.8, 127.5, 124.6, 123.0, 122.2, 44.9, 38.9, 28.6, 17.0.

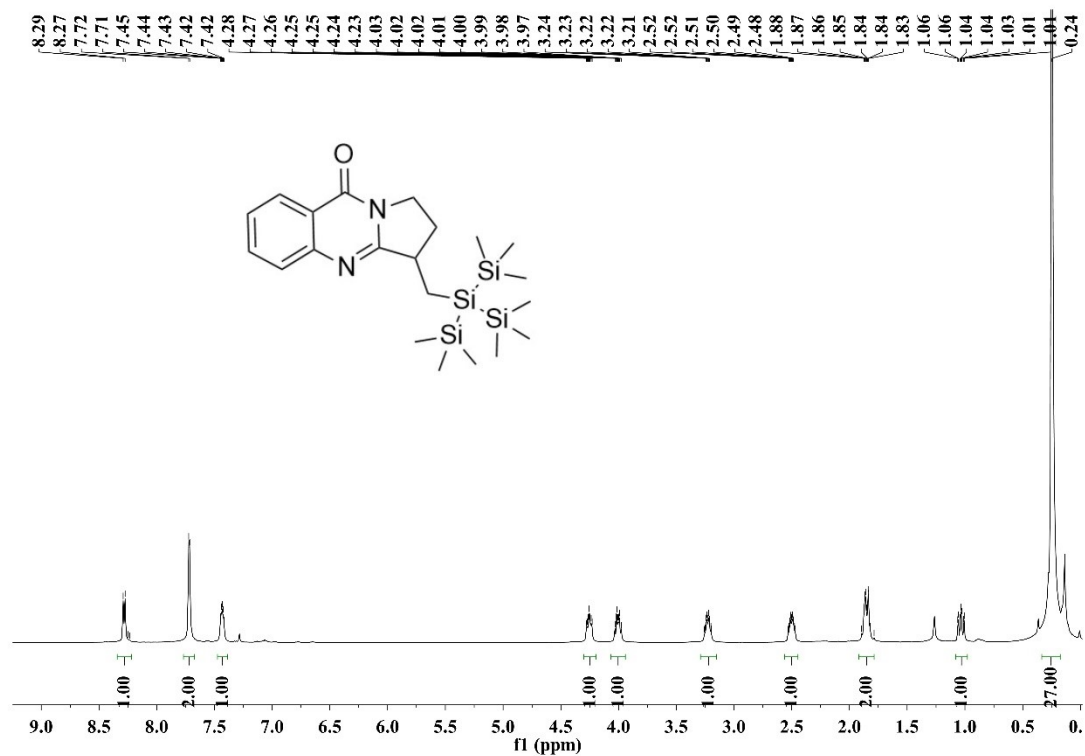
6,8-difluoro-3-methyl-2,3-dihydropyrrolo[2,1-*b*]quinazolin-9(1*H*)-one (6e)



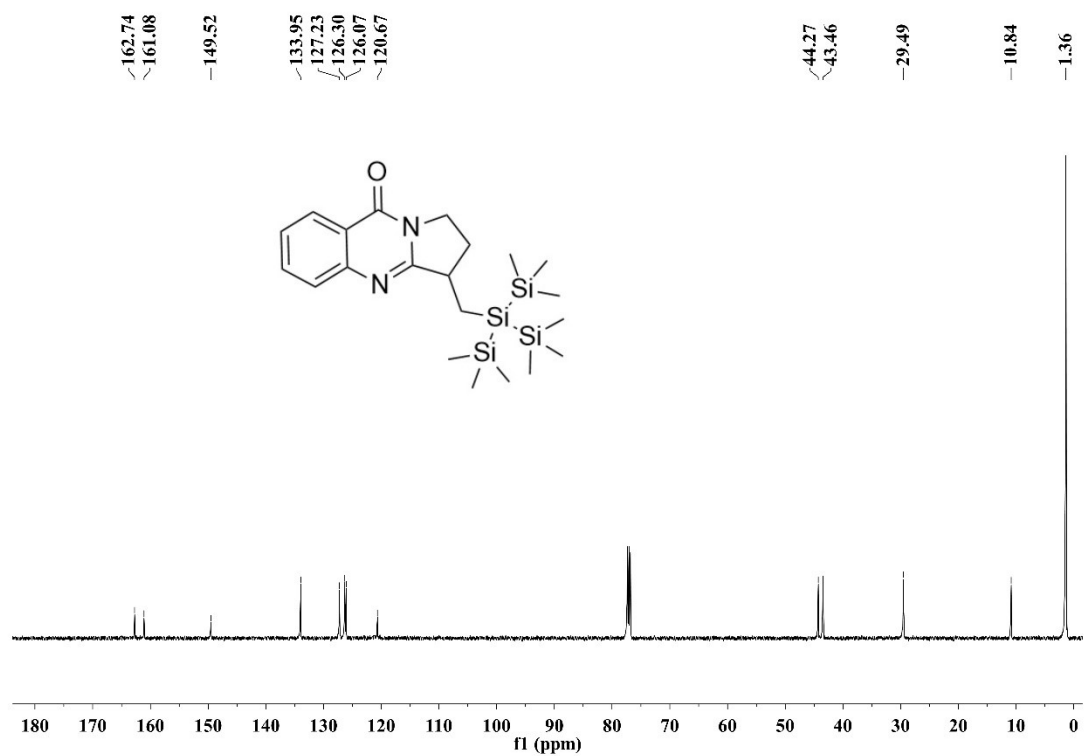
Yield 11.1 mg (47%, white solid); Melting point: 139-141 °C. ¹H NMR (500 MHz, Chloroform-*d*) δ 7.14 (d, *J* = 9.6 Hz, 1H), 6.95-6.69 (m, 1H), 4.24 (ddd, *J* = 12.6, 8.8, 3.7 Hz, 1H), 4.08-3.91 (m, 1H), 3.31 (h, *J* = 7.5 Hz, 1H), 2.50 (dtd, *J* = 12.3, 8.0, 3.5 Hz, 1H), 1.87 (dq, *J* = 12.5, 8.8 Hz, 1H), 1.46 (d, *J* = 7.0 Hz, 3H). ¹³C NMR (125 MHz, Chloroform-*d*) δ 166.56 (d, *J*_{C-F} = 14.3 Hz), 164.5 (q, *J*_{C-F} = 8.8 Hz), 163.57 (d, *J*_{C-F} = 15.0 Hz), 161.44 (d, *J*_{C-F} = 14.9 Hz), 157.50 (d, *J*_{C-F} = 3.6 Hz), 153.03 (d, *J*_{C-F} = 14.4 Hz), 108.77 (dd, *J*_{C-F} = 21.8, 4.5 Hz), 102.56 (dd, *J*_{C-F} = 26.9, 24.6 Hz), 44.67, 38.96, 28.27, 16.95. ¹⁹F NMR (471 MHz, CDCl₃) δ -101.02, -101.04, -101.06, -101.08, -106.09, -106.11, -106.14. HRMS (ESI-TOF) *m/z*: [M+H]⁺ Calcd for C₁₂H₁₁F₂N₂O 237.0834, Found 237.0839.

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

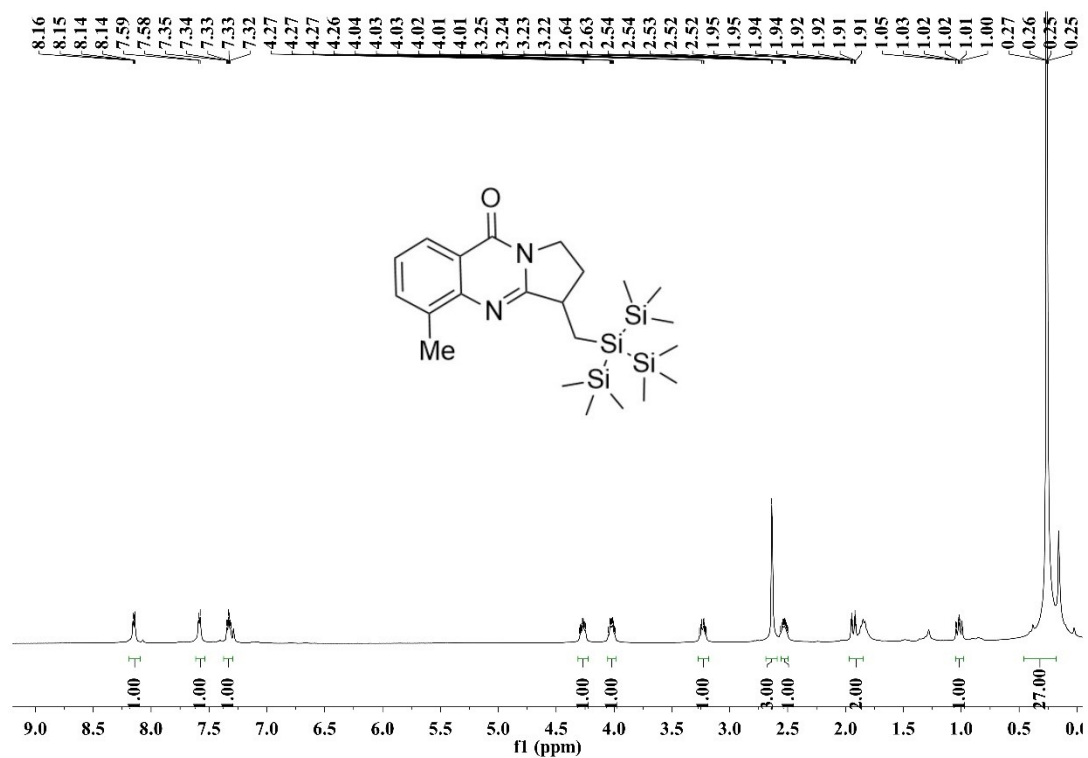
^1H NMR spectrum of 3a (500 MHz, CDCl_3)



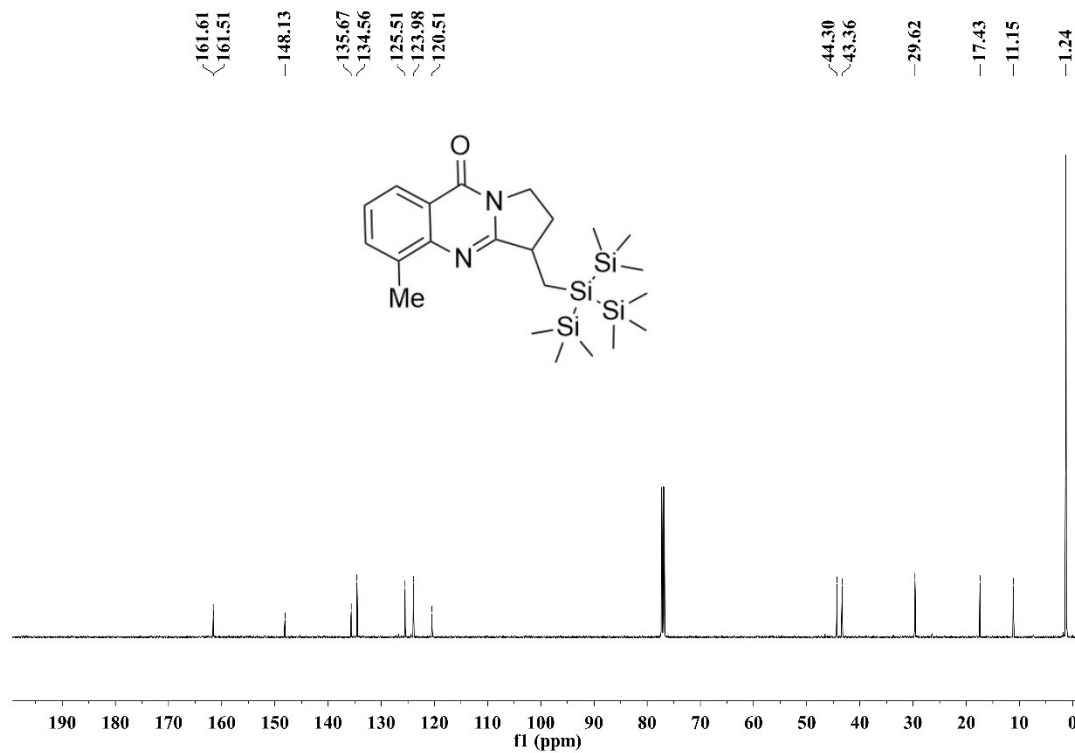
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 3a (125 MHz, CDCl_3)



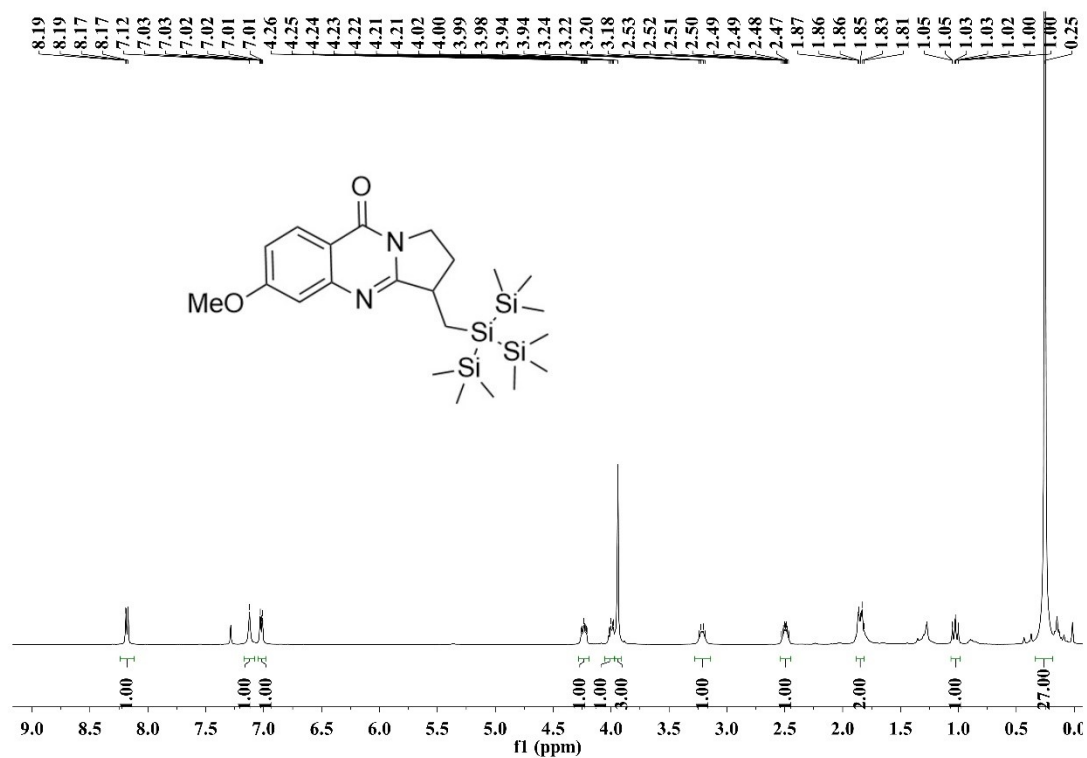
¹H NMR spectrum of 3b (500 MHz, CDCl₃)



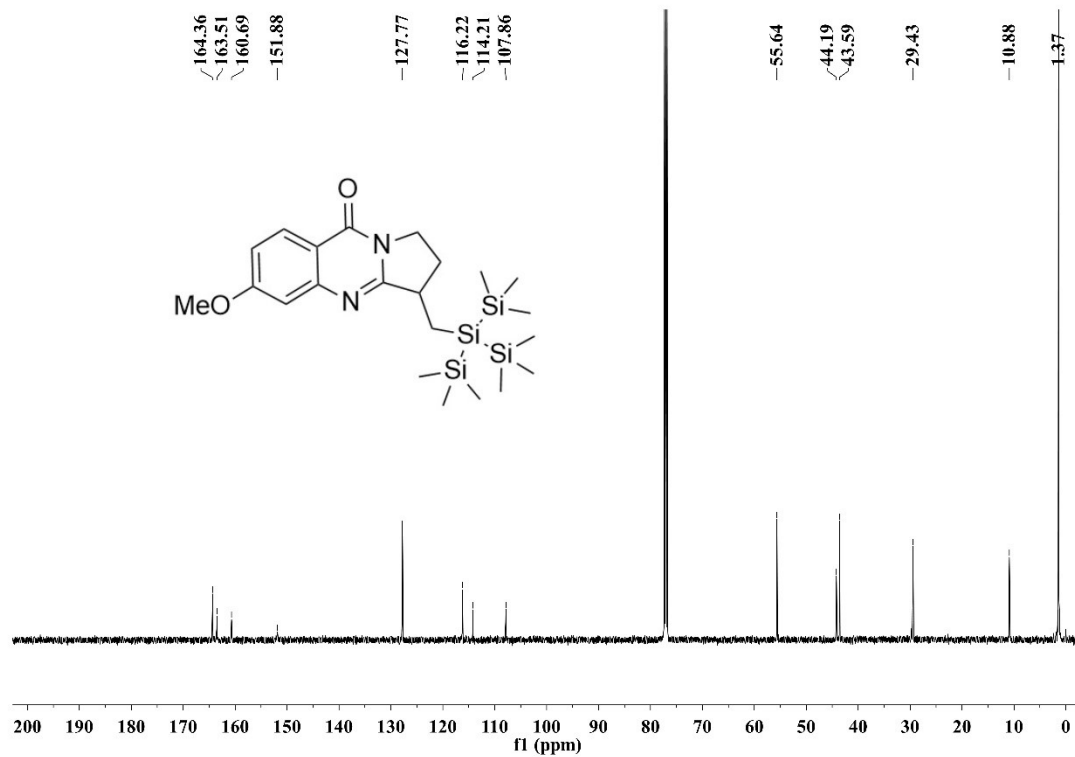
¹³C{¹H} NMR spectrum of 3b (125 MHz, CDCl₃)



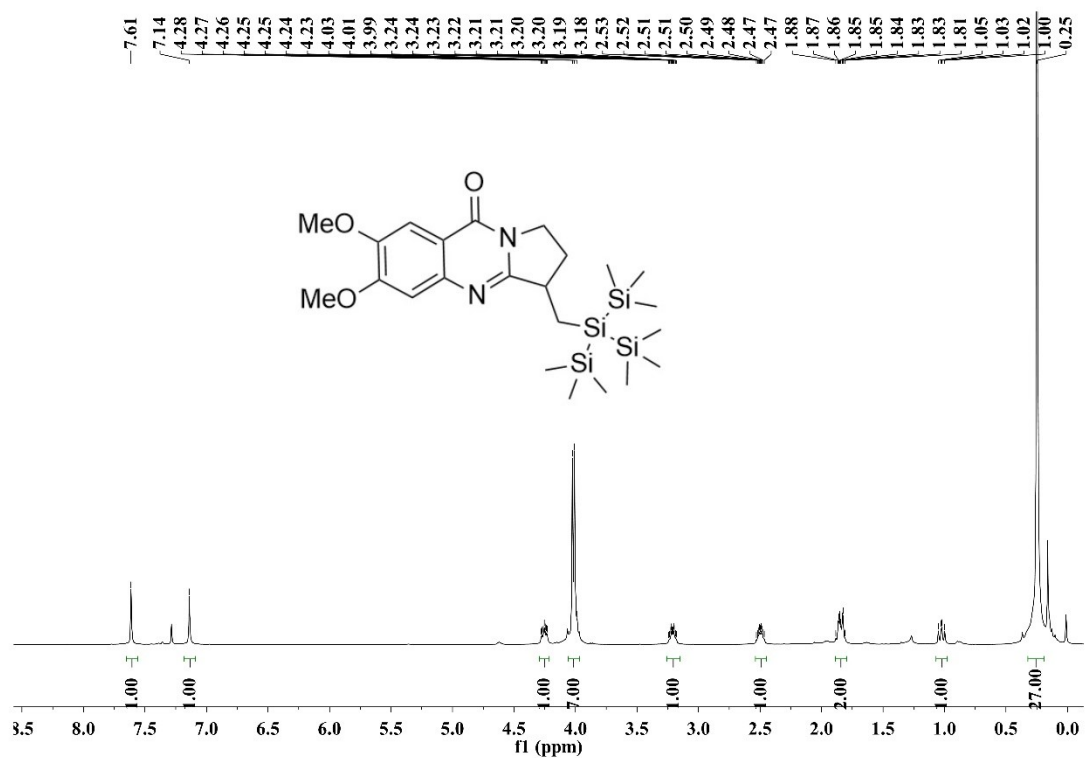
¹H NMR spectrum of 3c (500 MHz, CDCl₃)



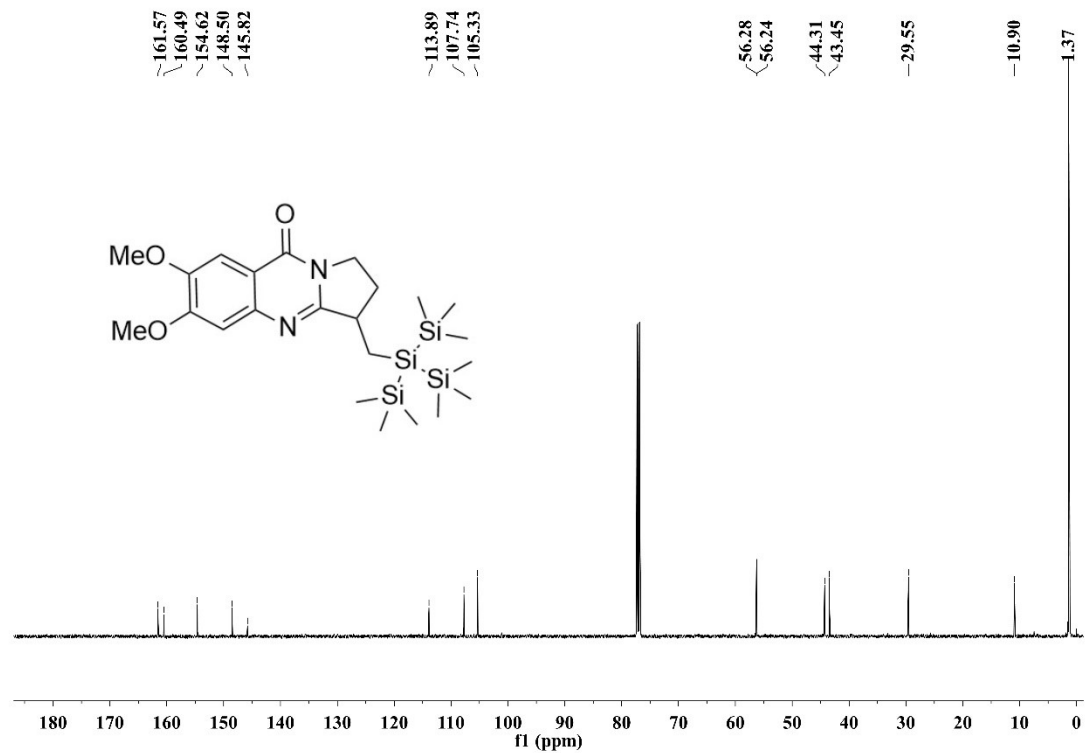
¹³C{¹H} NMR spectrum of 3c (125 MHz, CDCl₃)



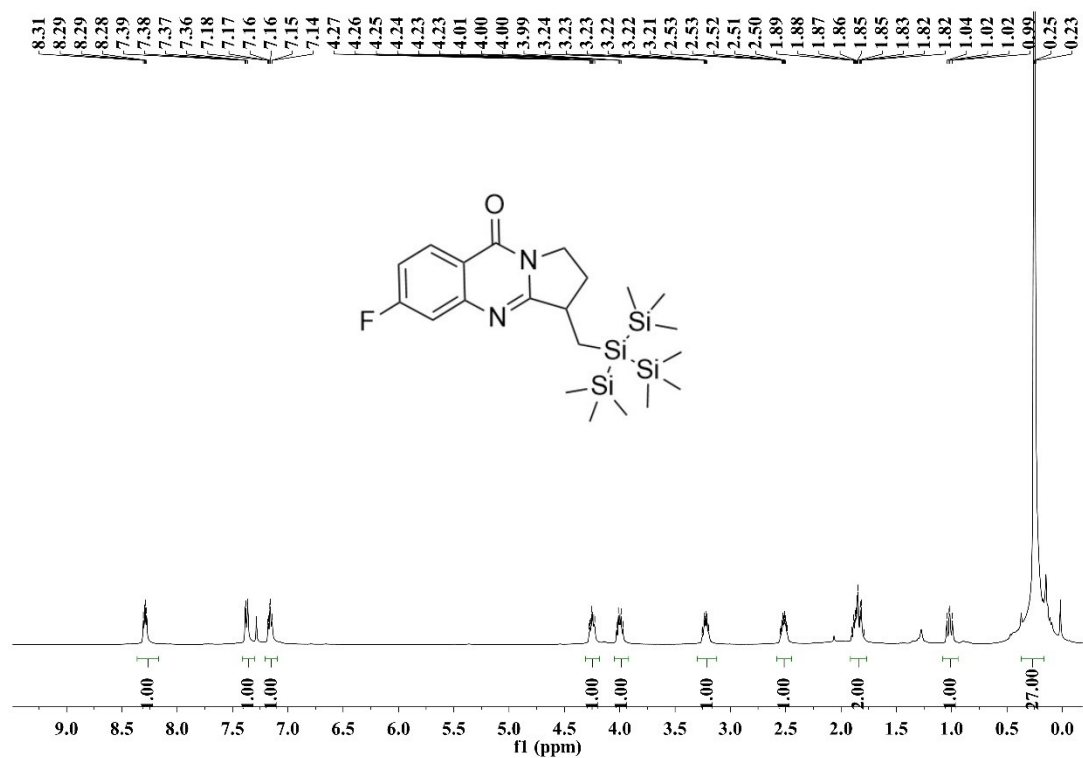
¹H NMR spectrum of 3d (500 MHz, CDCl₃)



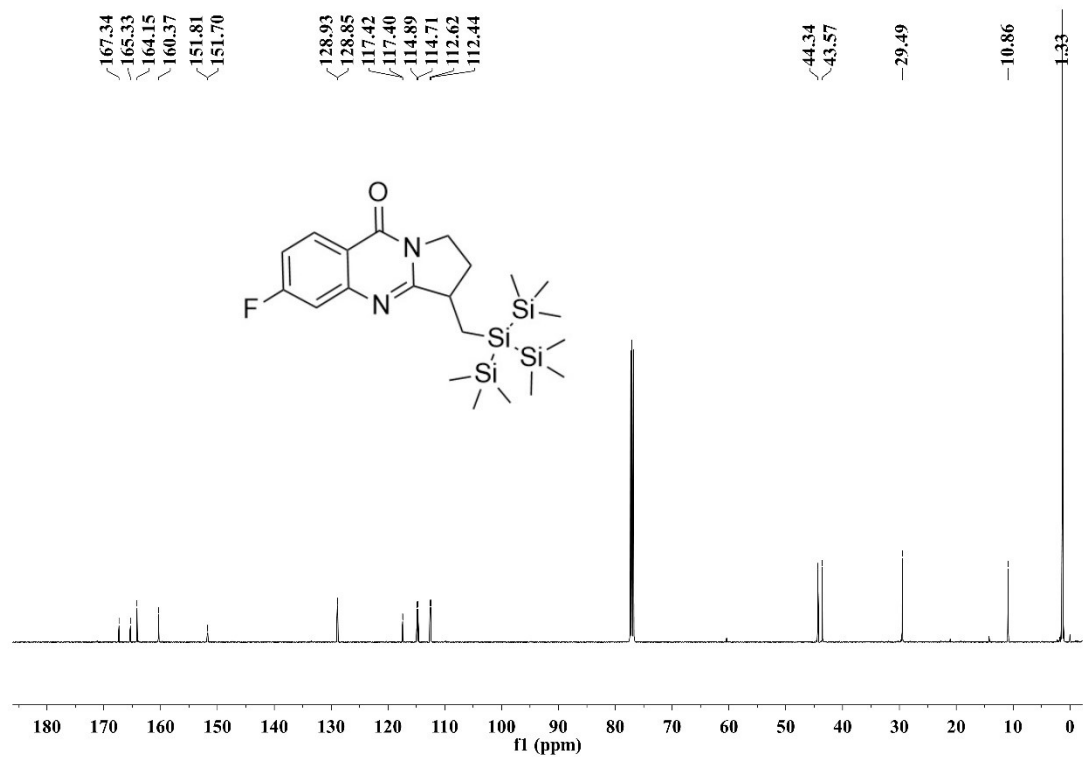
¹³C{¹H} NMR spectrum of 3d (125 MHz, CDCl₃)



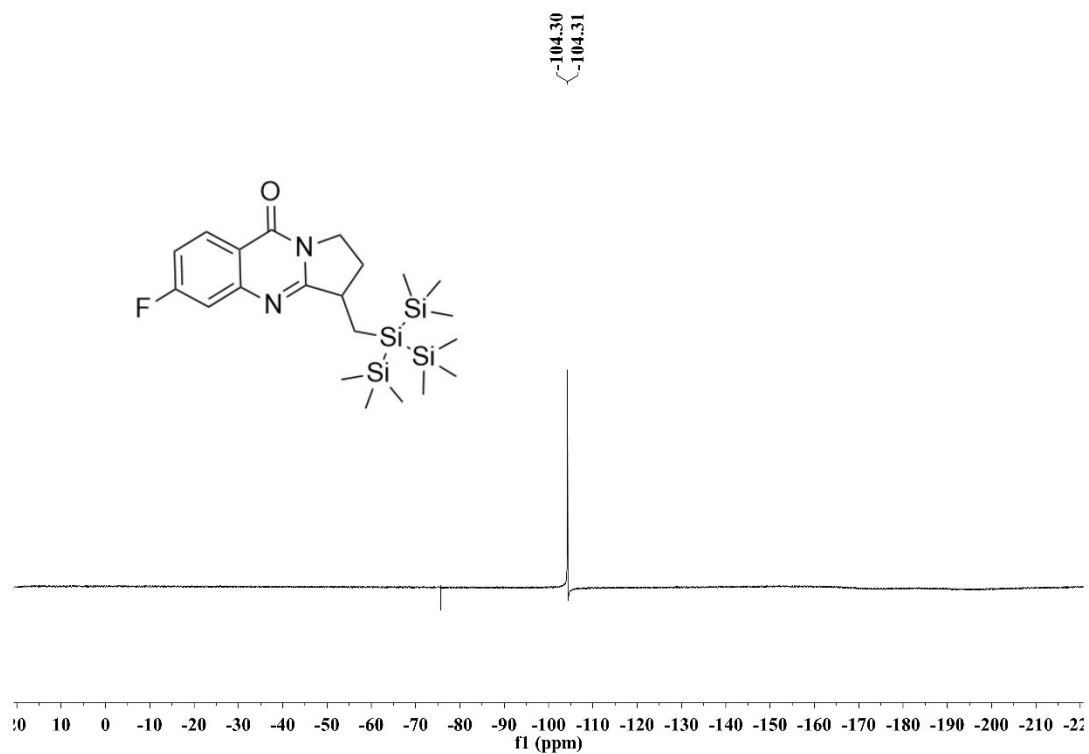
¹H NMR spectrum of 3e (500 MHz, CDCl₃)



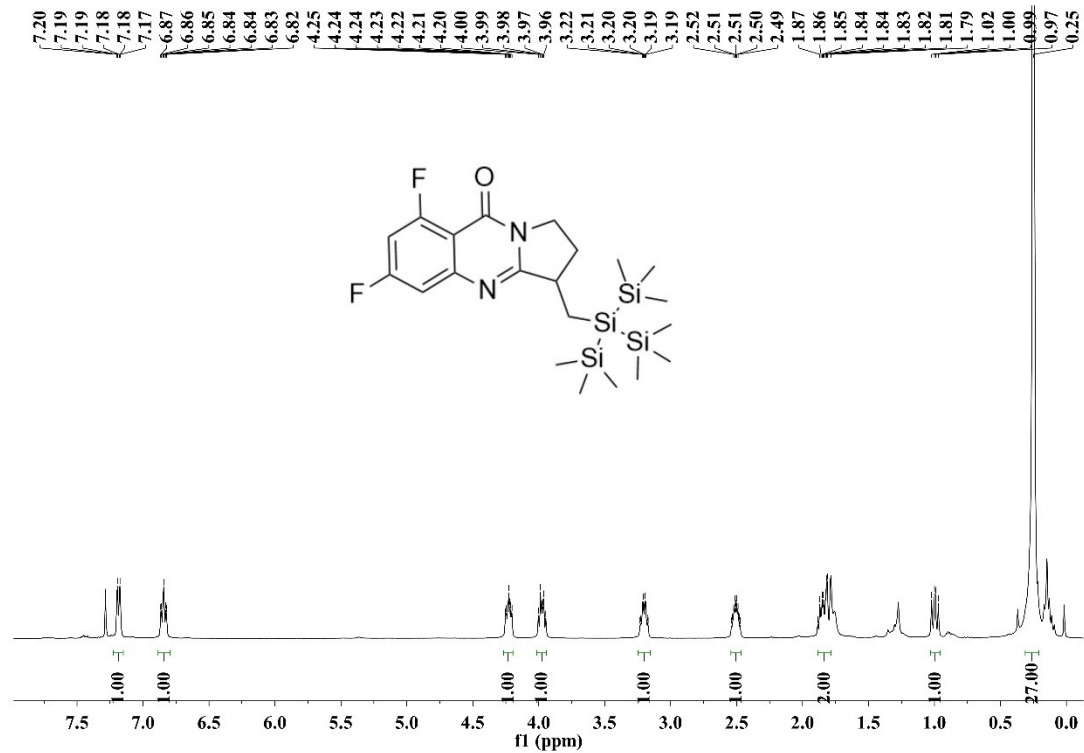
¹³C{¹H} NMR spectrum of 3e (125 MHz, CDCl₃)



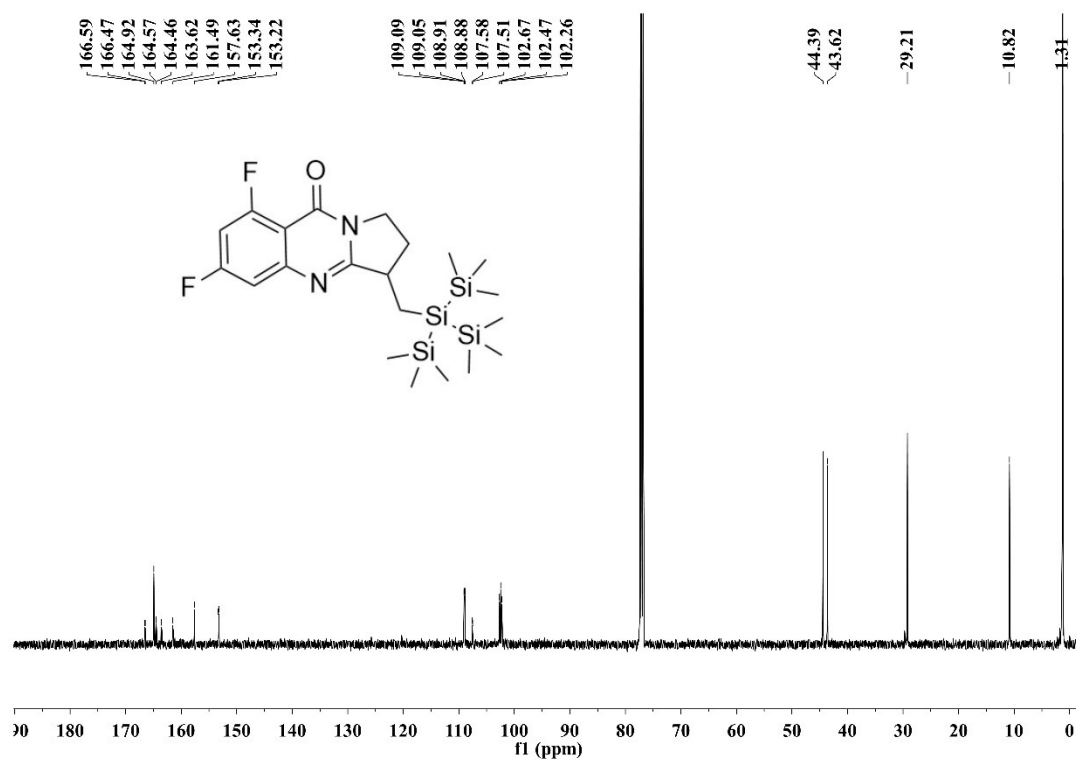
^{19}F NMR spectrum of 3e (125 MHz, CDCl_3)



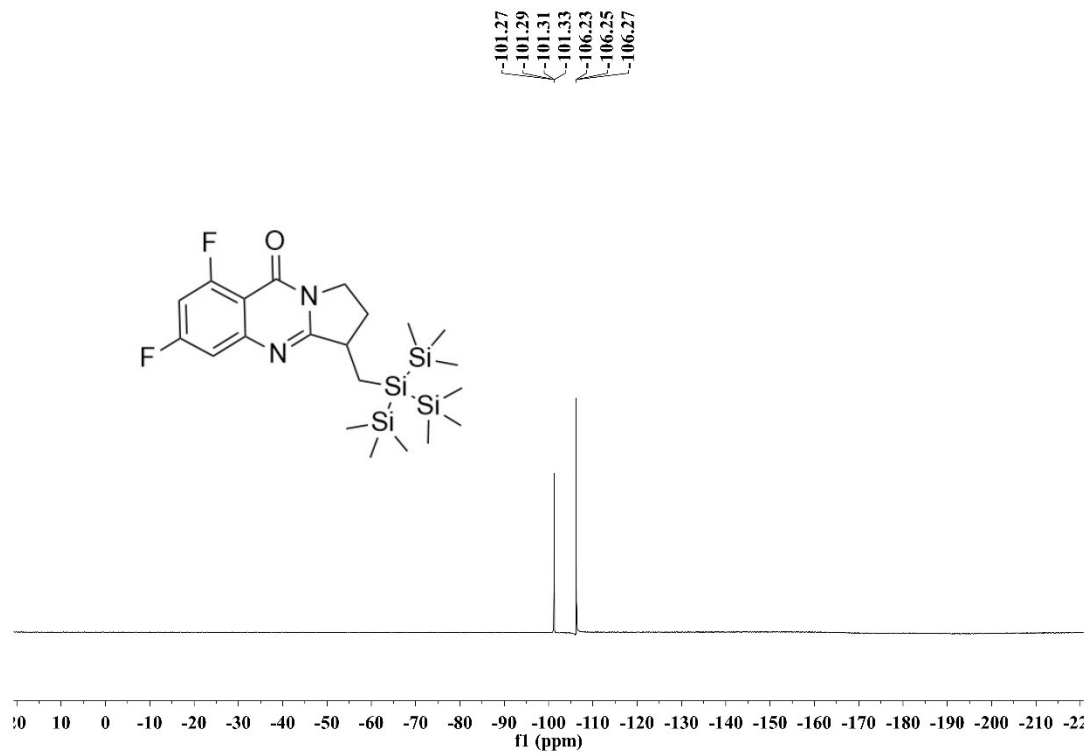
^1H NMR spectrum of 3f (500 MHz, CDCl_3)



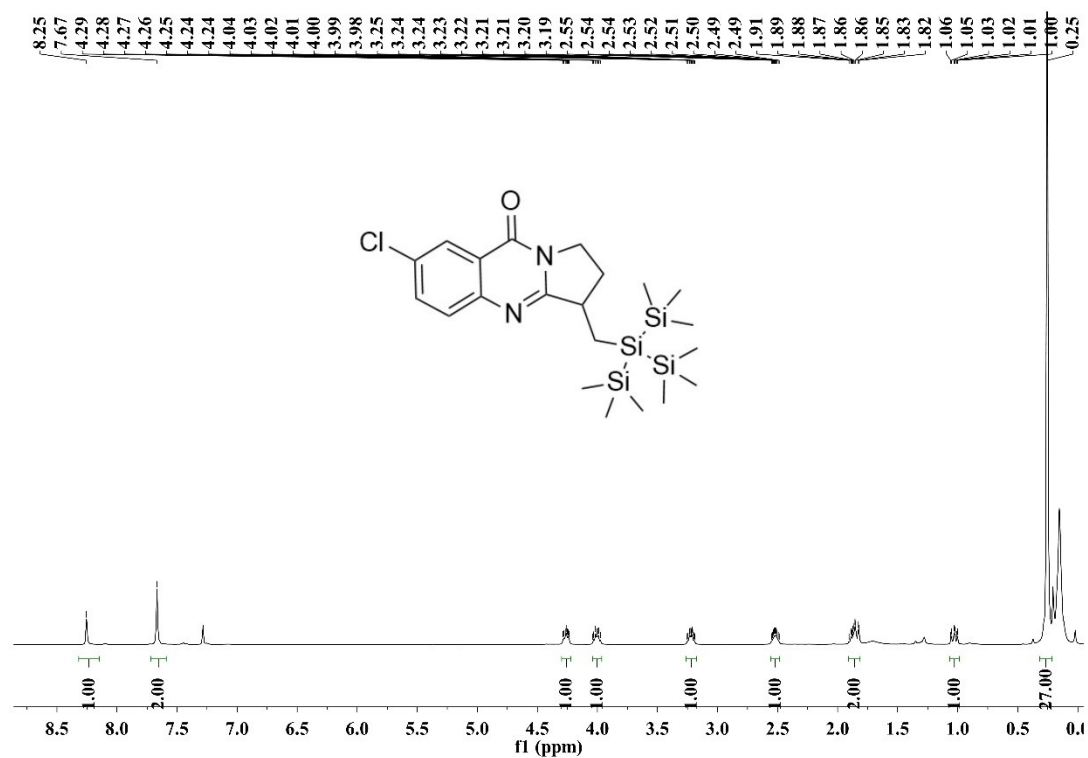
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 3f (125 MHz, CDCl_3)



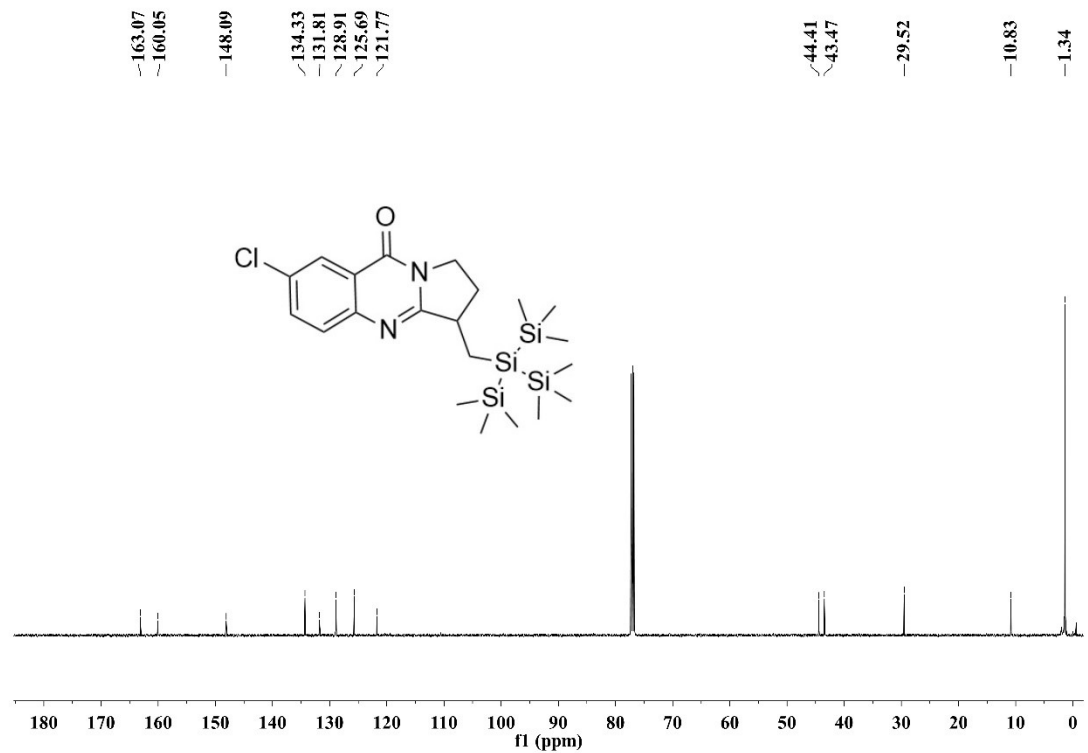
^{19}F NMR spectrum of 3f (125 MHz, CDCl_3)



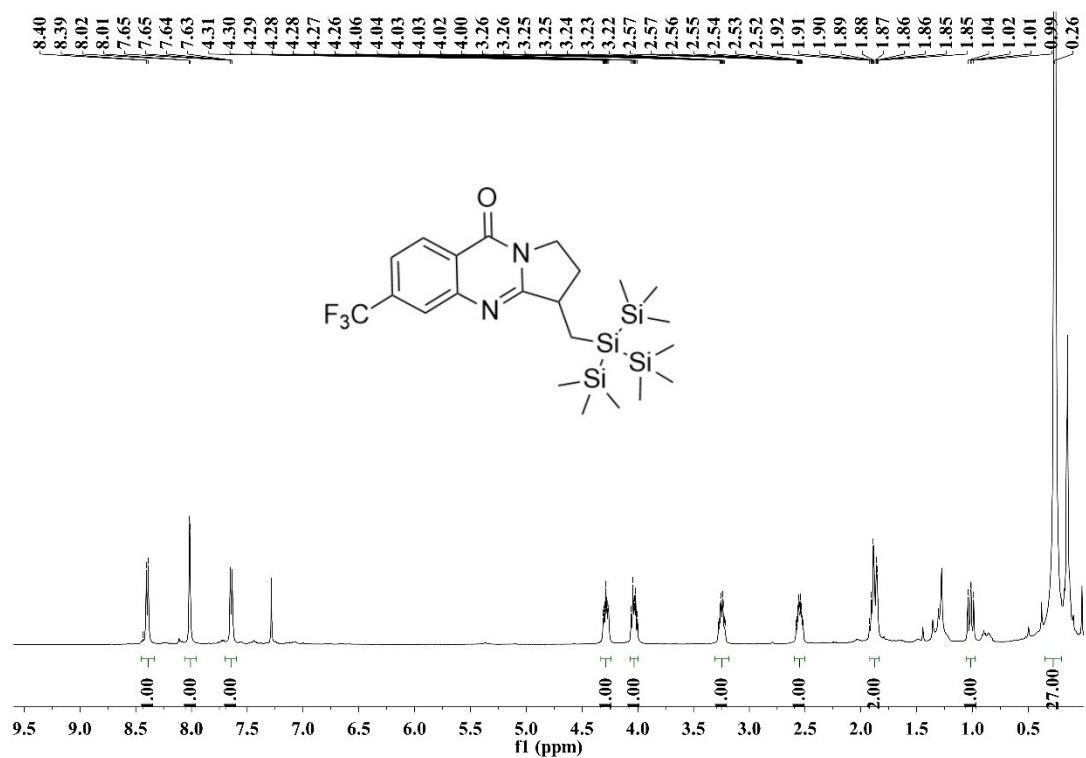
¹H NMR spectrum of 3g (500 MHz, CDCl₃)



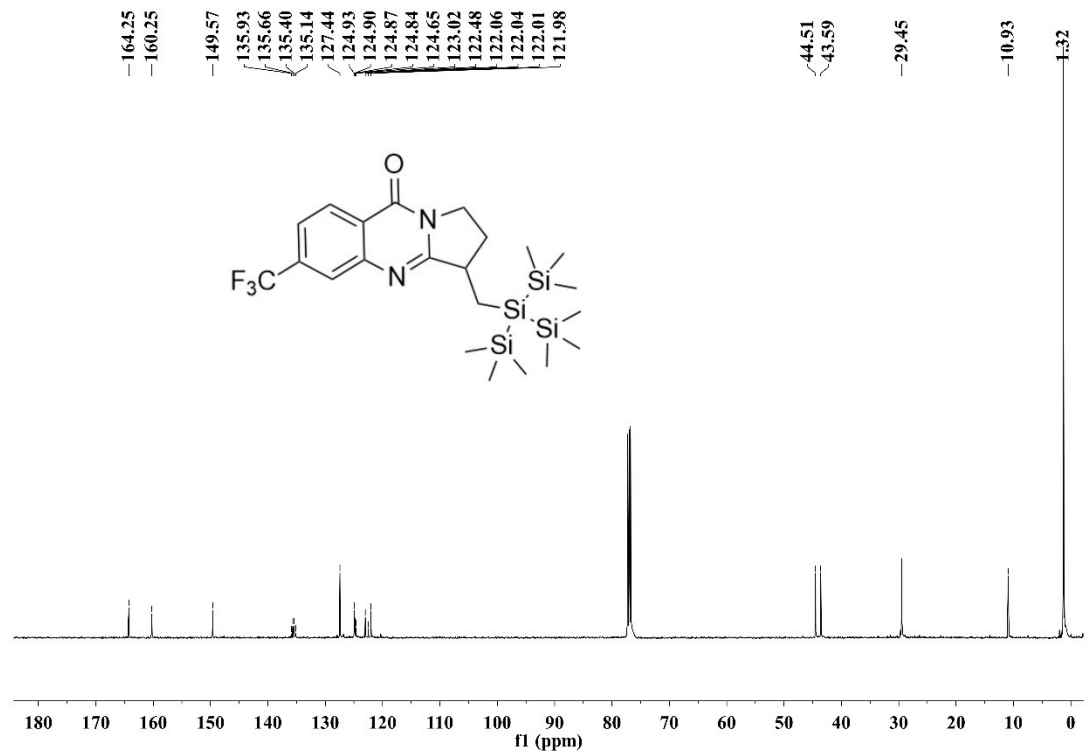
¹³C{¹H} NMR spectrum of 3g (125 MHz, CDCl₃)



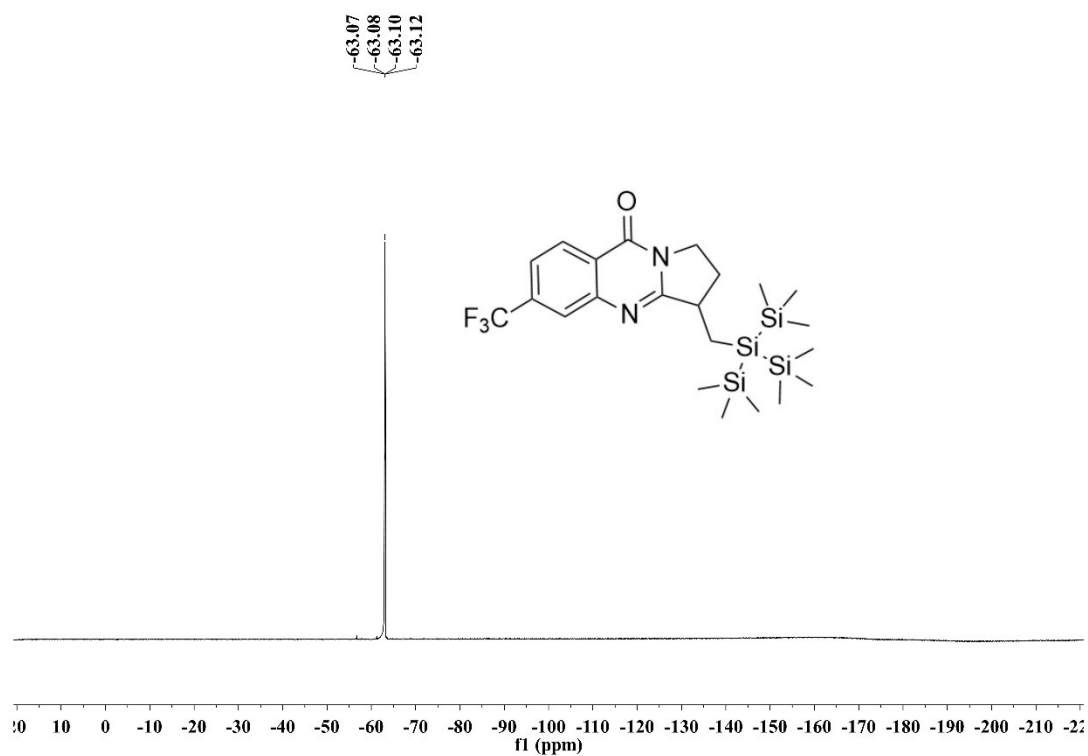
¹H NMR spectrum of 3h (500 MHz, CDCl₃)



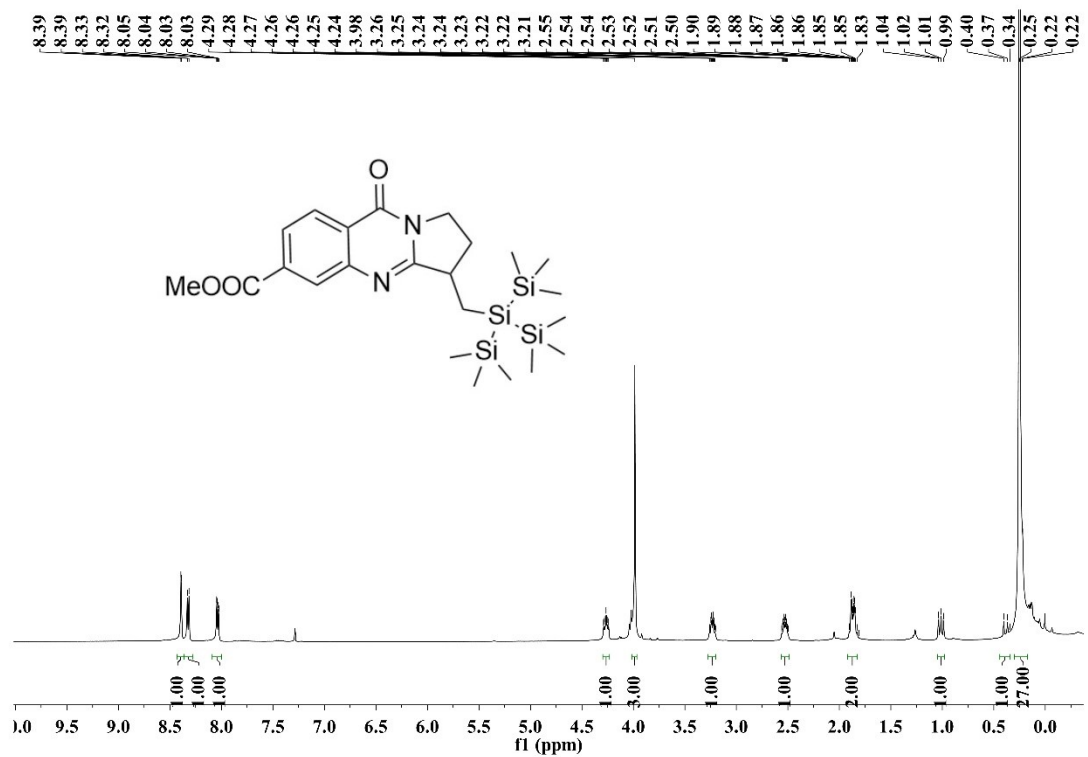
¹³C{¹H} NMR spectrum of 3h (125 MHz, CDCl₃)



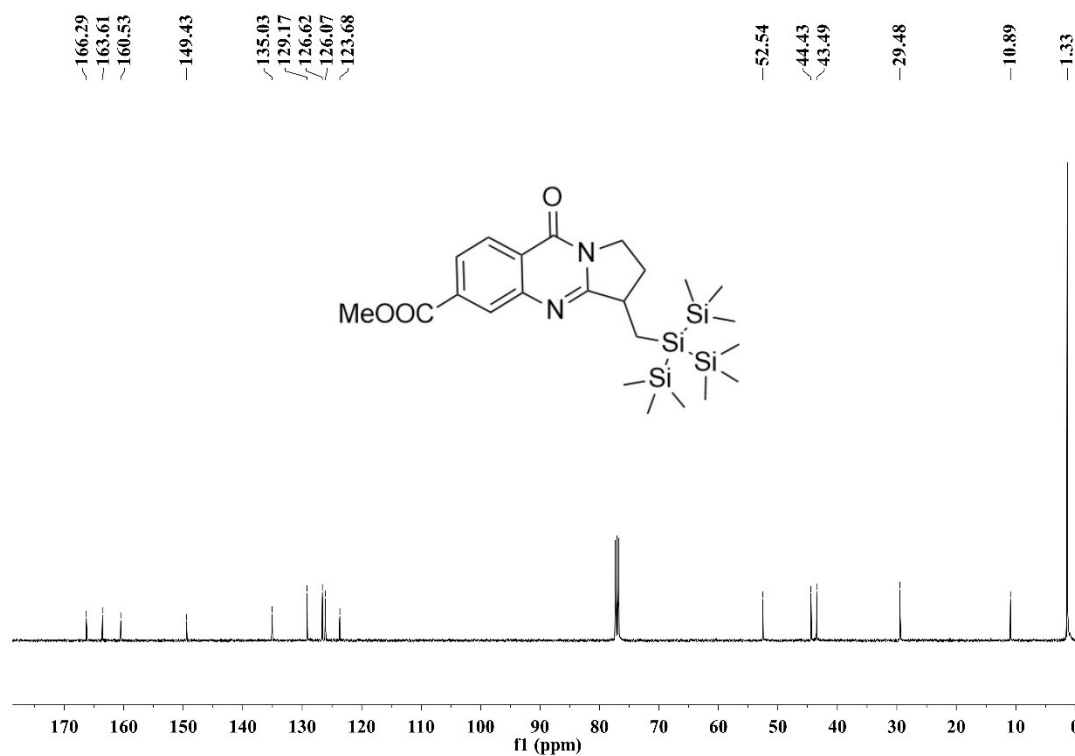
¹⁹F NMR spectrum of 3h (125 MHz, CDCl₃)



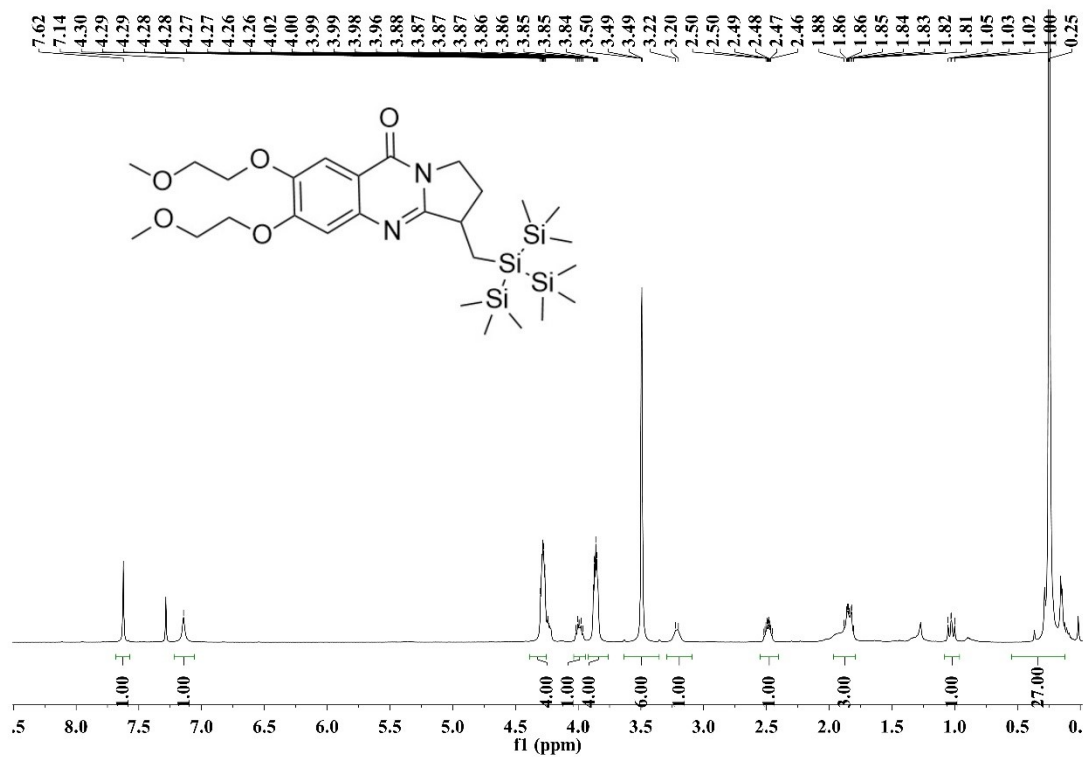
¹H NMR spectrum of 3i (500 MHz, CDCl₃)



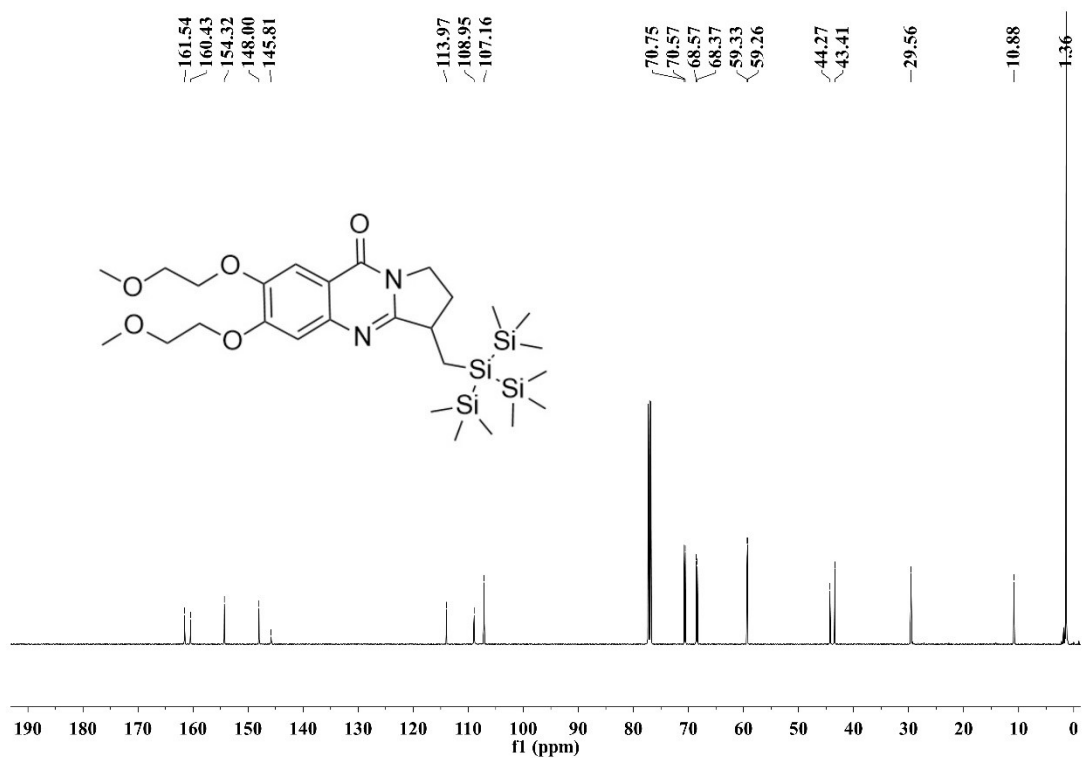
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 3i (125 MHz, CDCl_3)



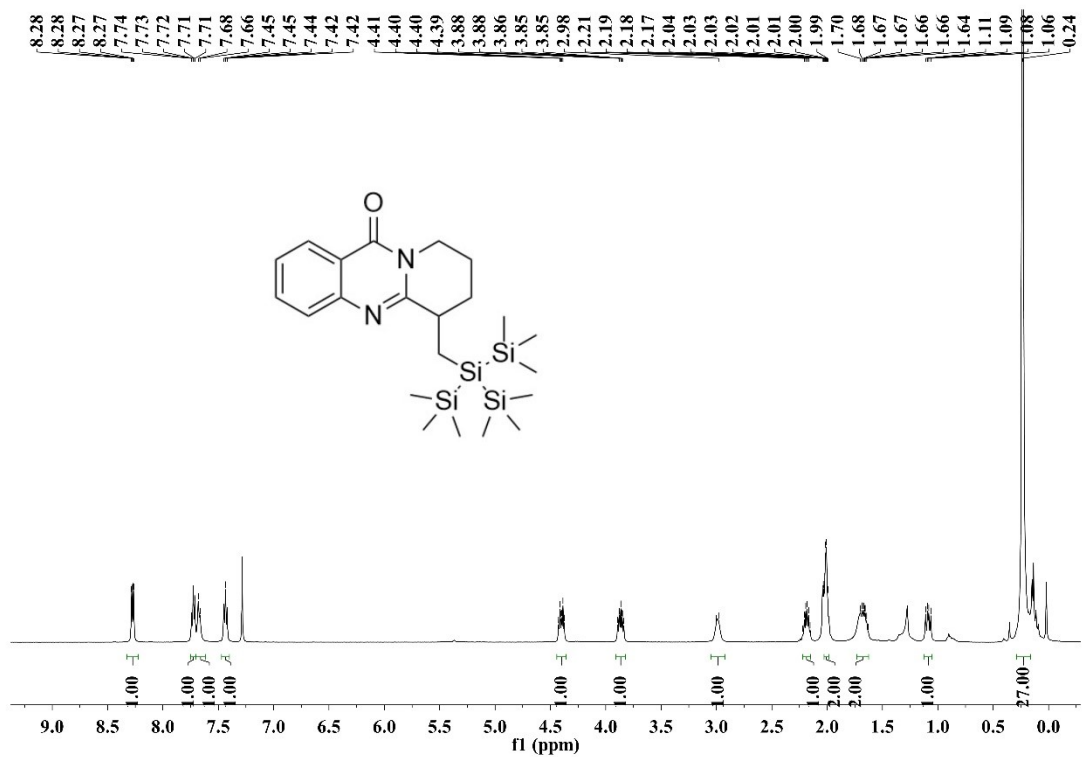
^1H NMR spectrum of 3j (500 MHz, CDCl_3)



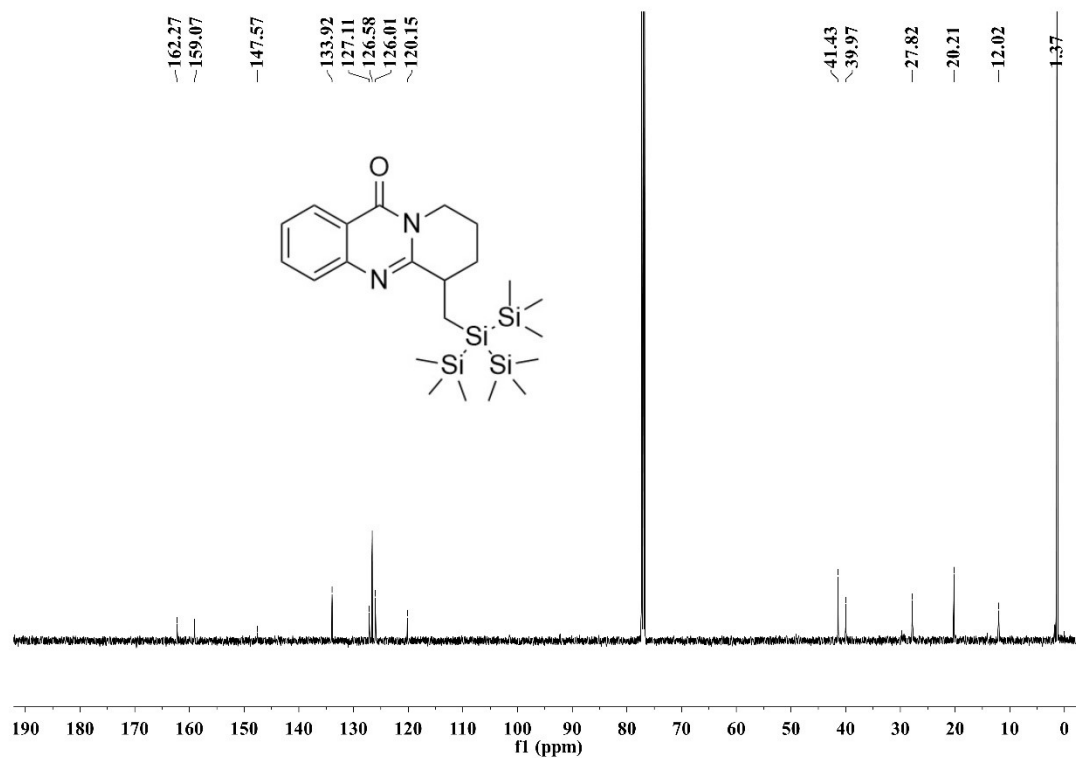
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 3j (125 MHz, CDCl_3)



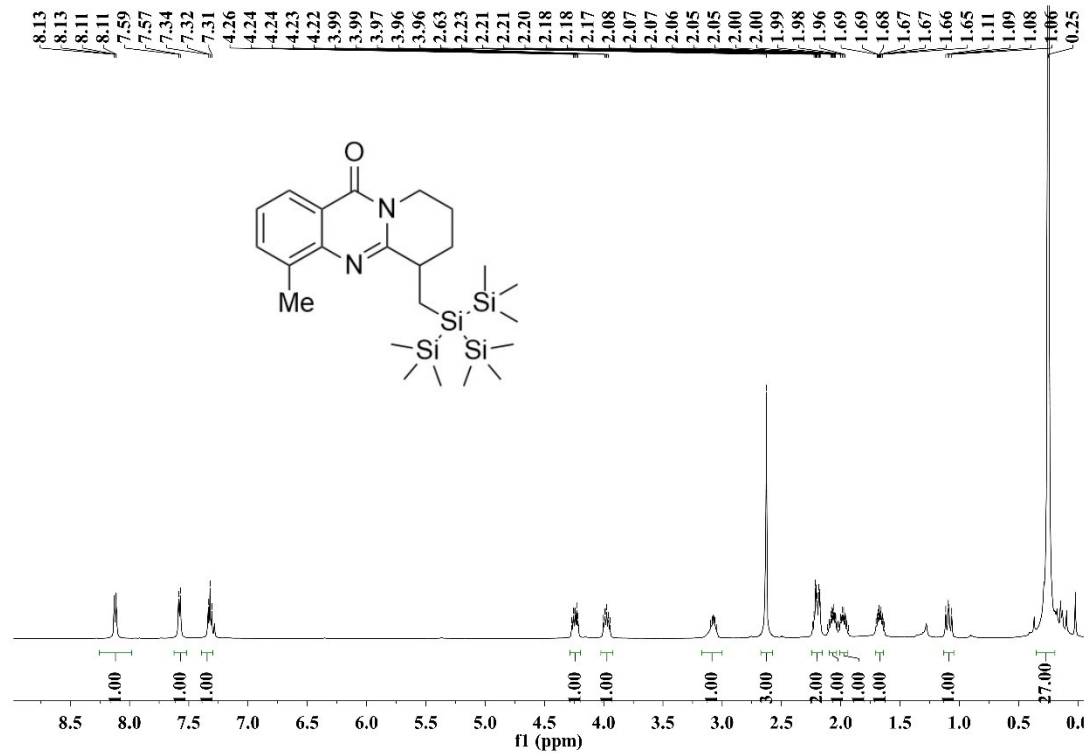
^1H NMR spectrum of 4a (500 MHz, CDCl_3)



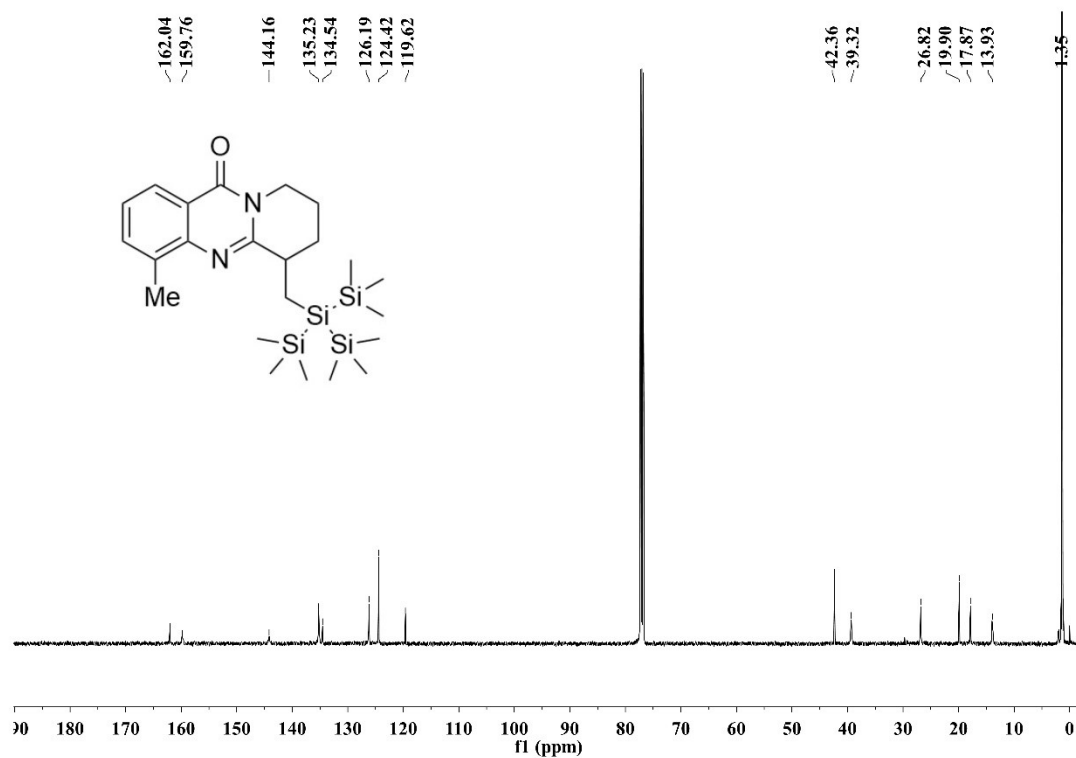
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4a (125 MHz, CDCl_3)



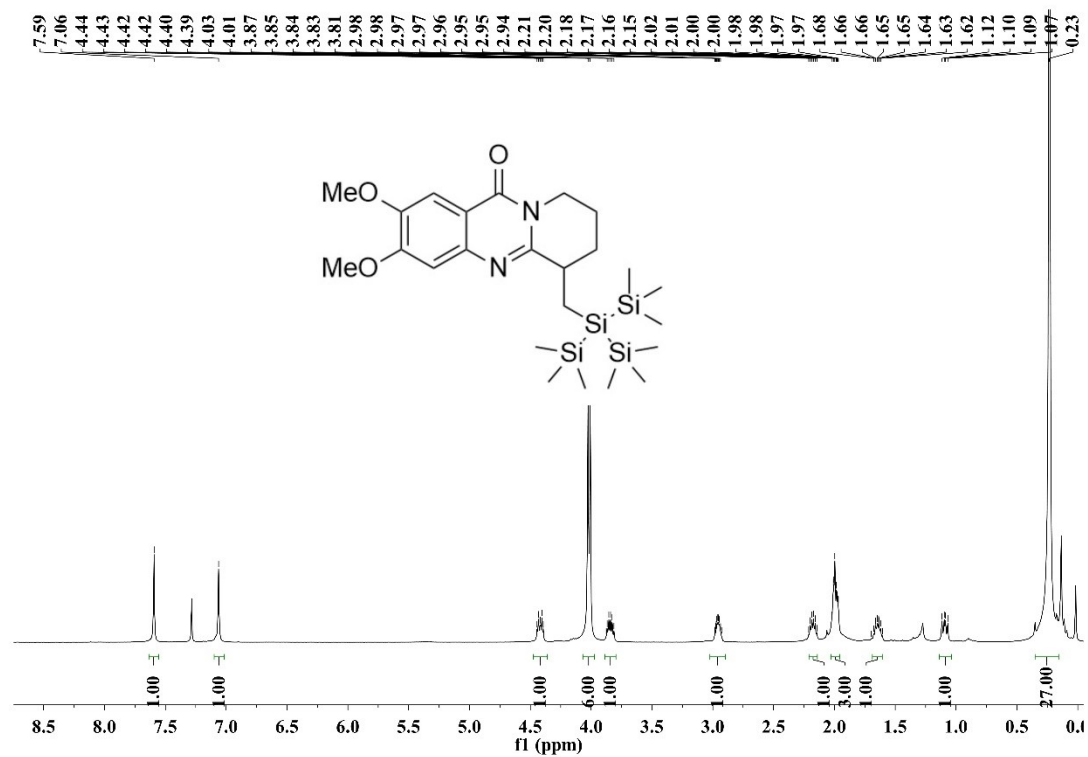
^1H NMR spectrum of 4b (500 MHz, CDCl_3)



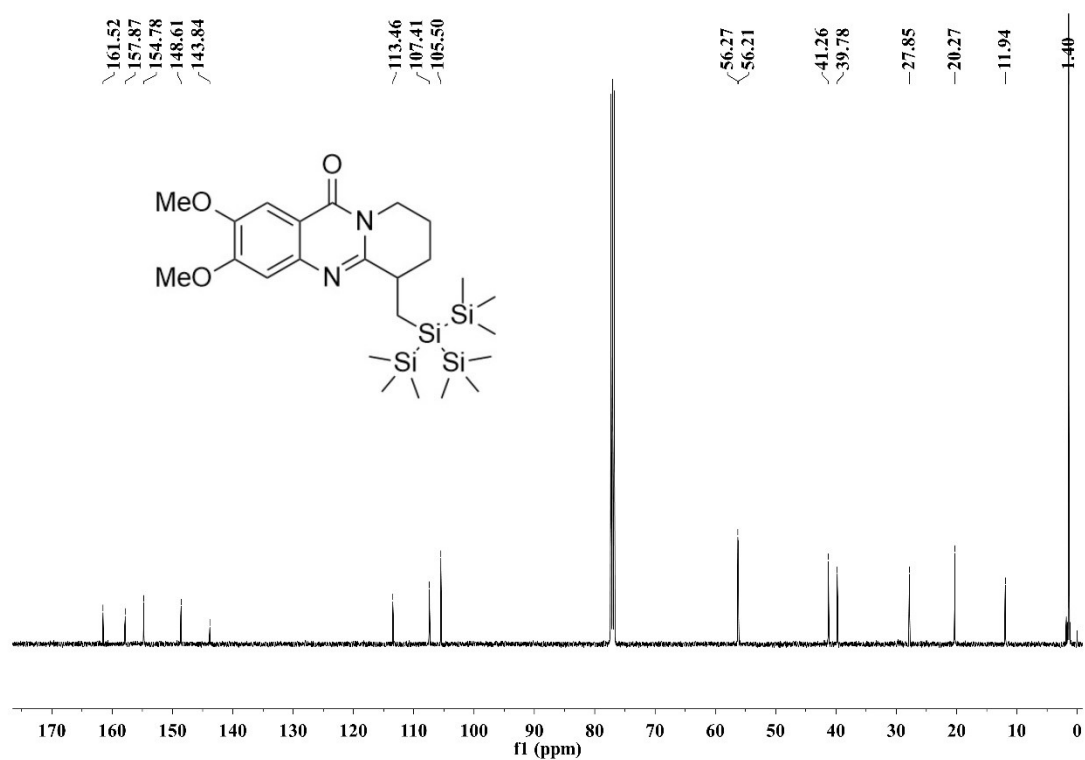
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4b (125 MHz, CDCl_3)



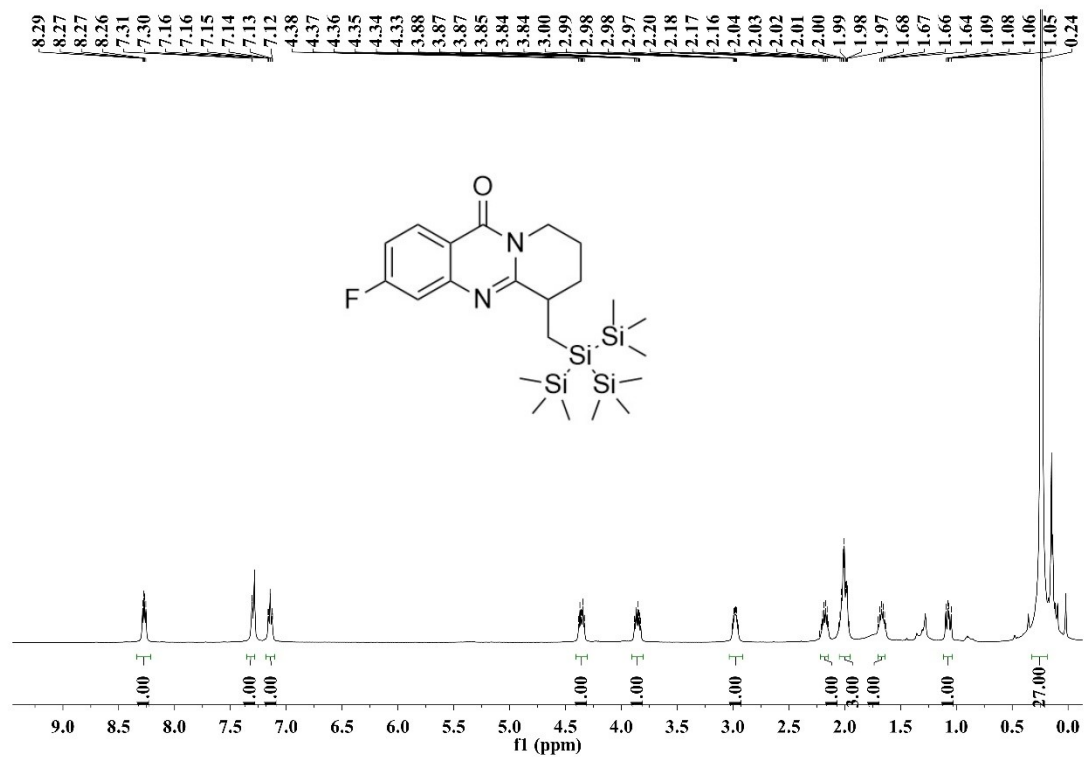
^1H NMR spectrum of 4c (500 MHz, CDCl_3)



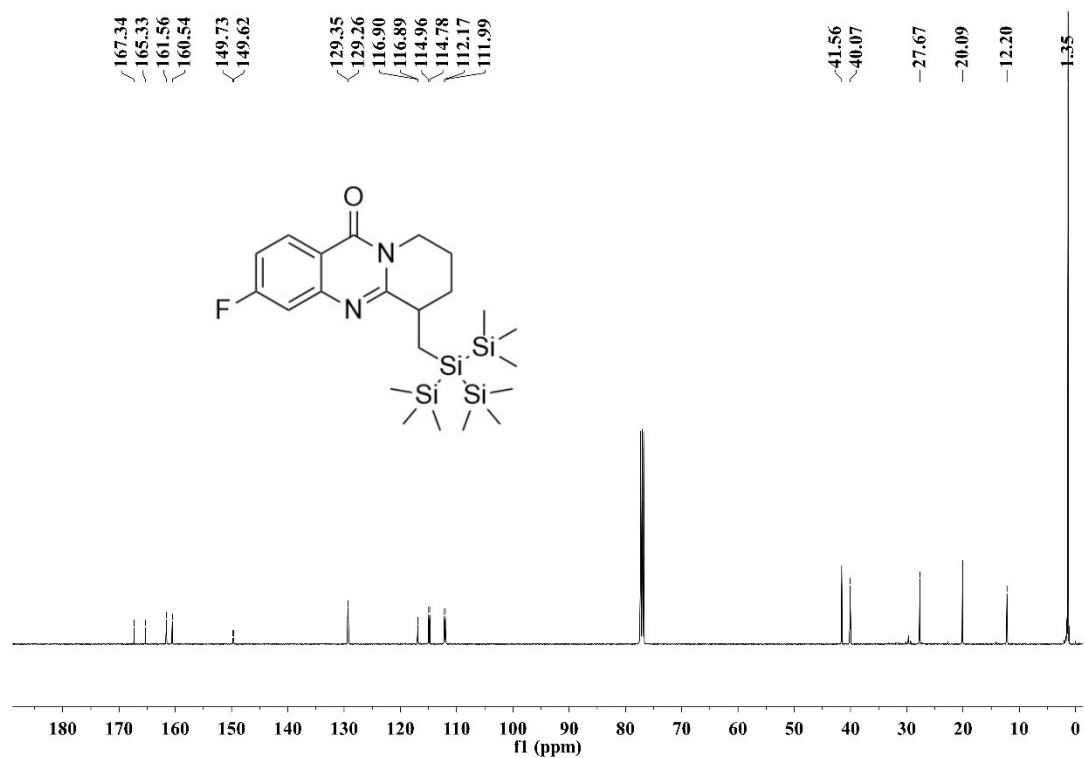
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4c (125 MHz, CDCl_3)



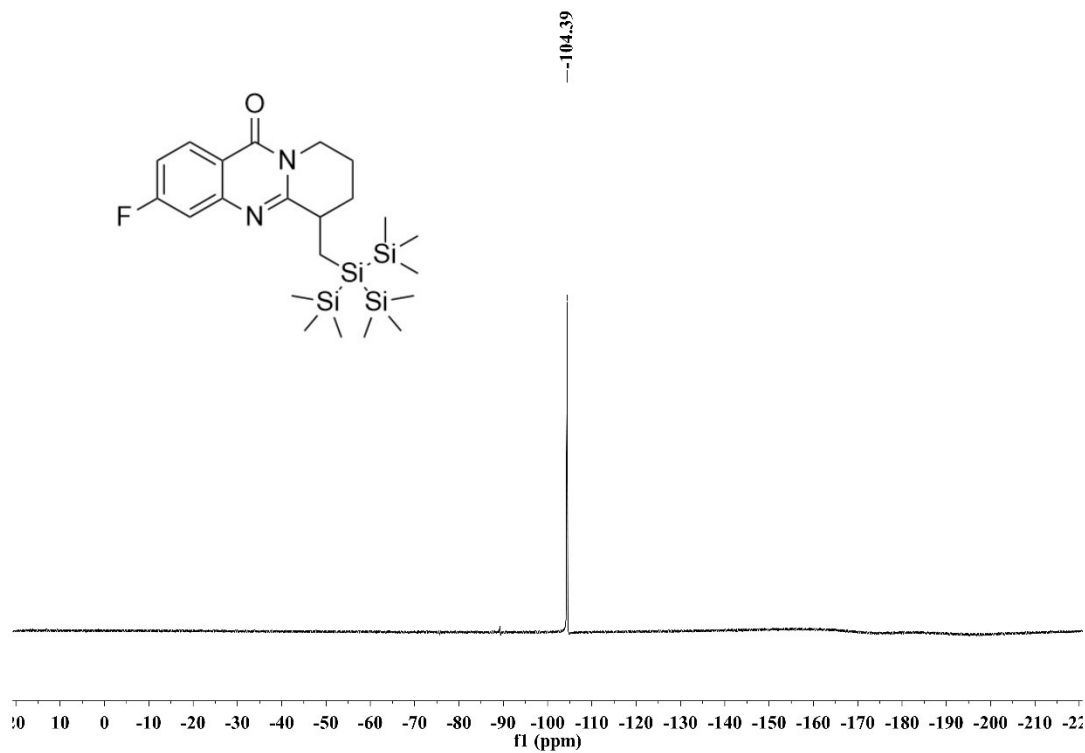
^1H NMR spectrum of 4d (500 MHz, CDCl_3)



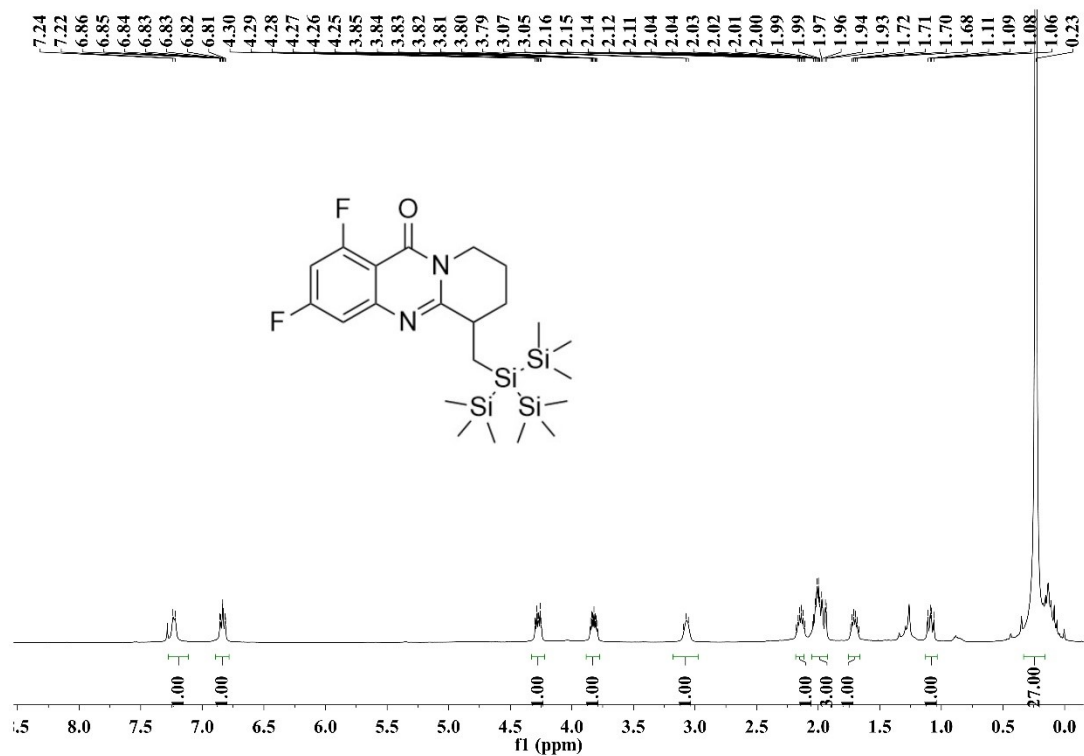
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4d (125 MHz, CDCl_3)



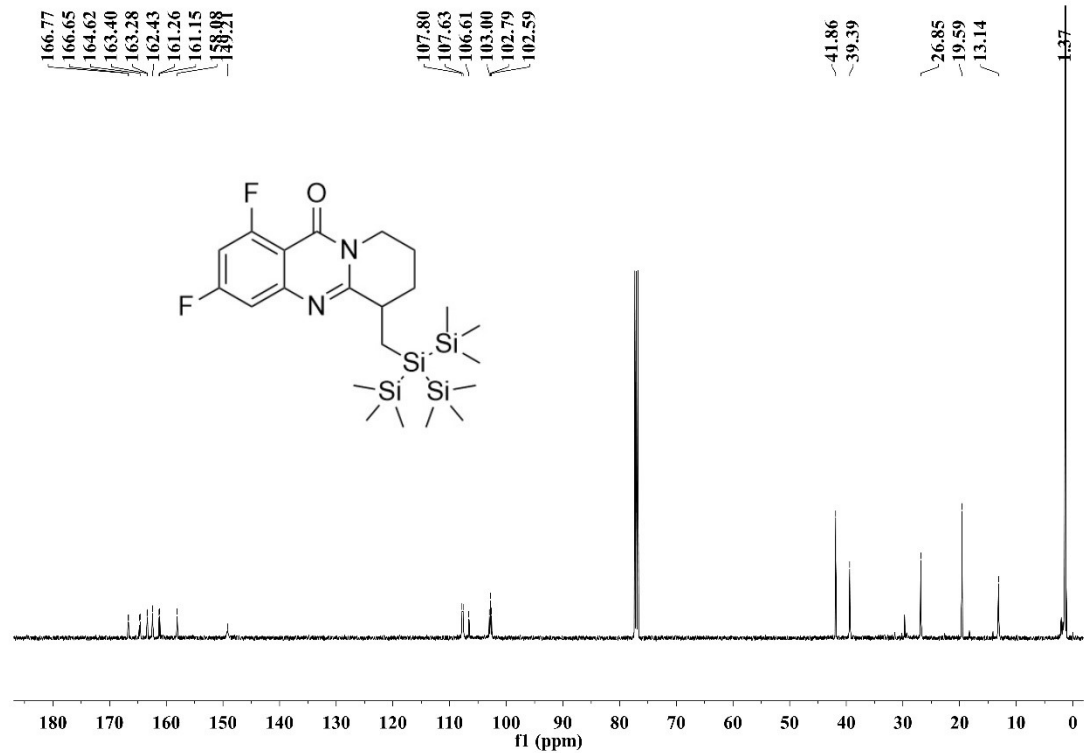
^{19}F NMR spectrum of 4d (125 MHz, CDCl_3)



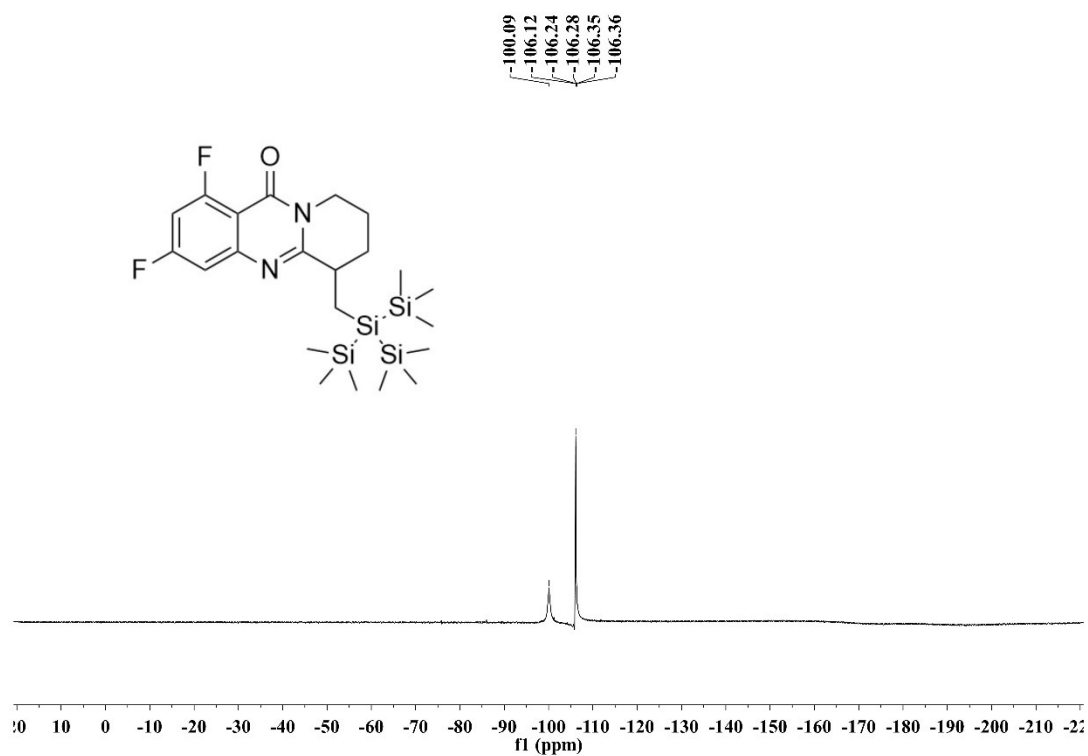
^1H NMR spectrum of 4e (500 MHz, CDCl_3)



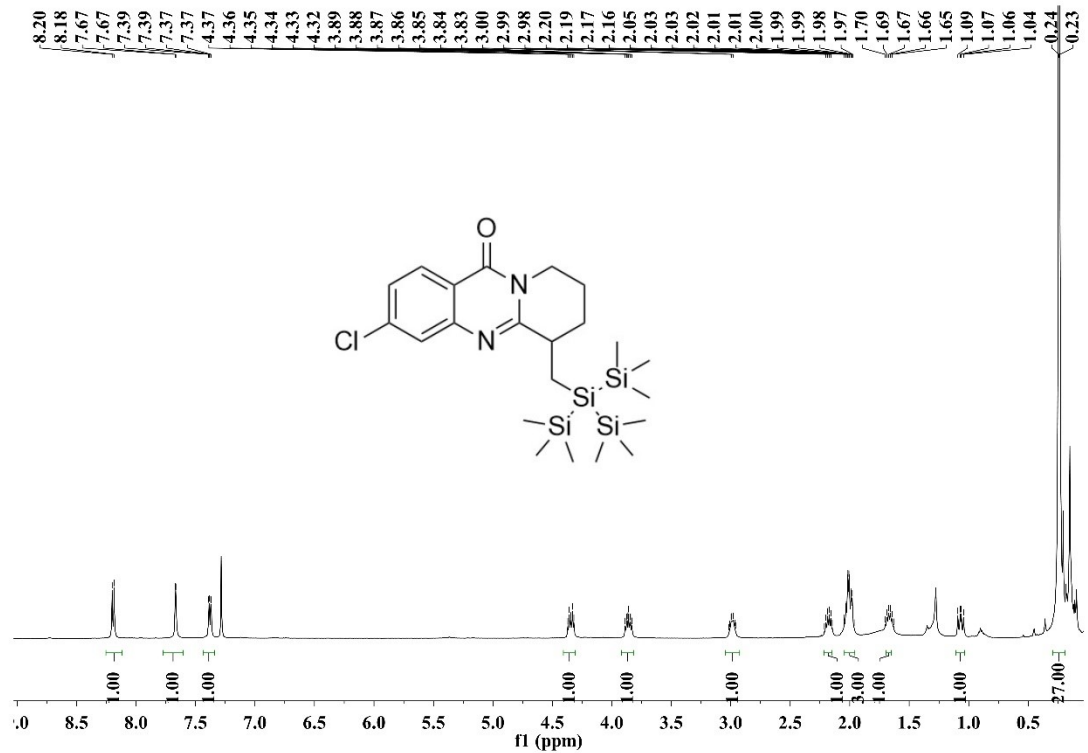
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4e (125 MHz, CDCl_3)



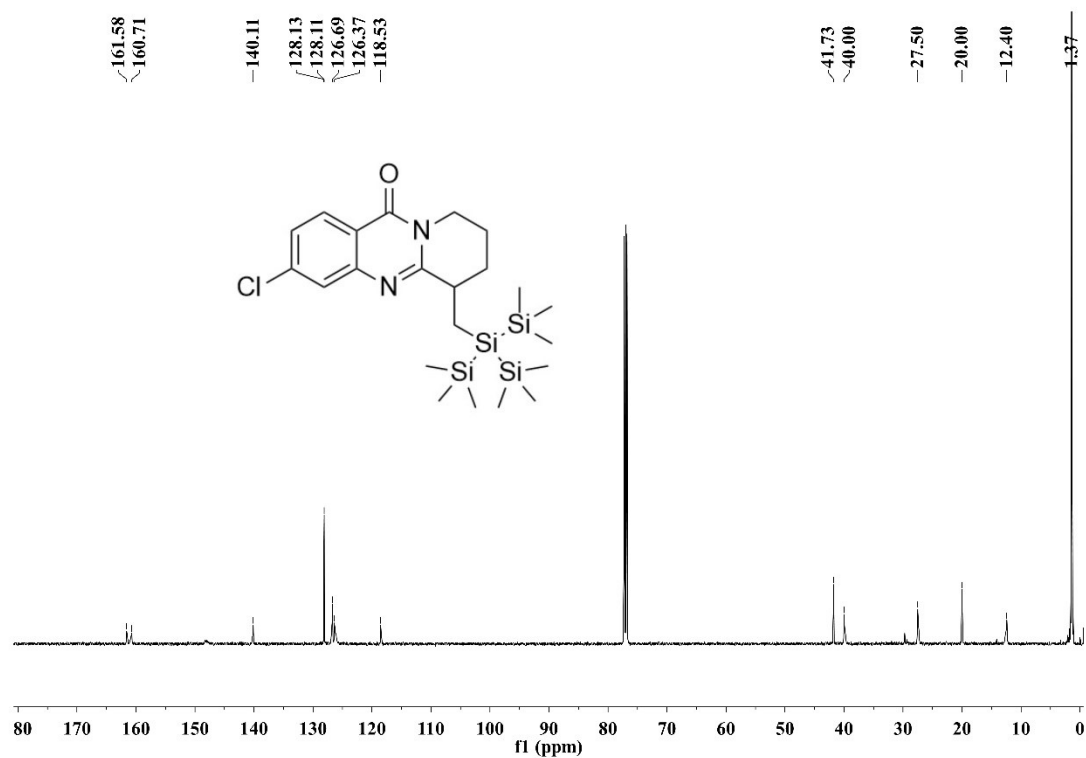
^{19}F NMR spectrum of 4e (125 MHz, CDCl_3)



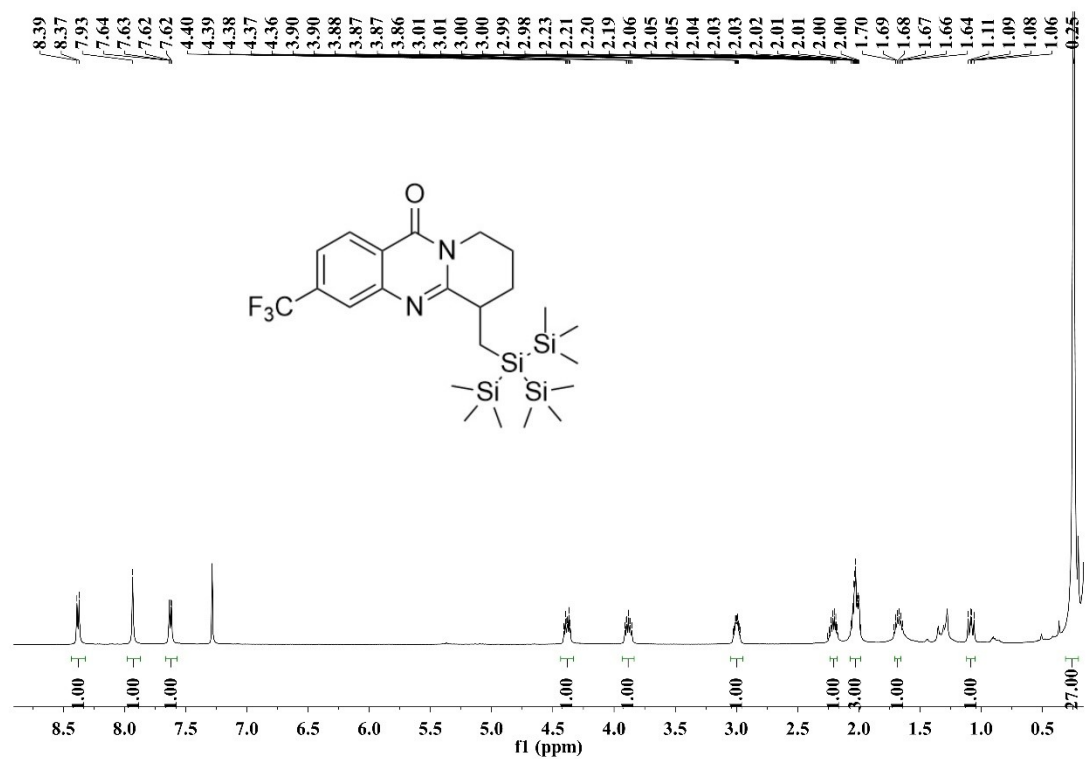
^1H NMR spectrum of 4f (500 MHz, CDCl_3)



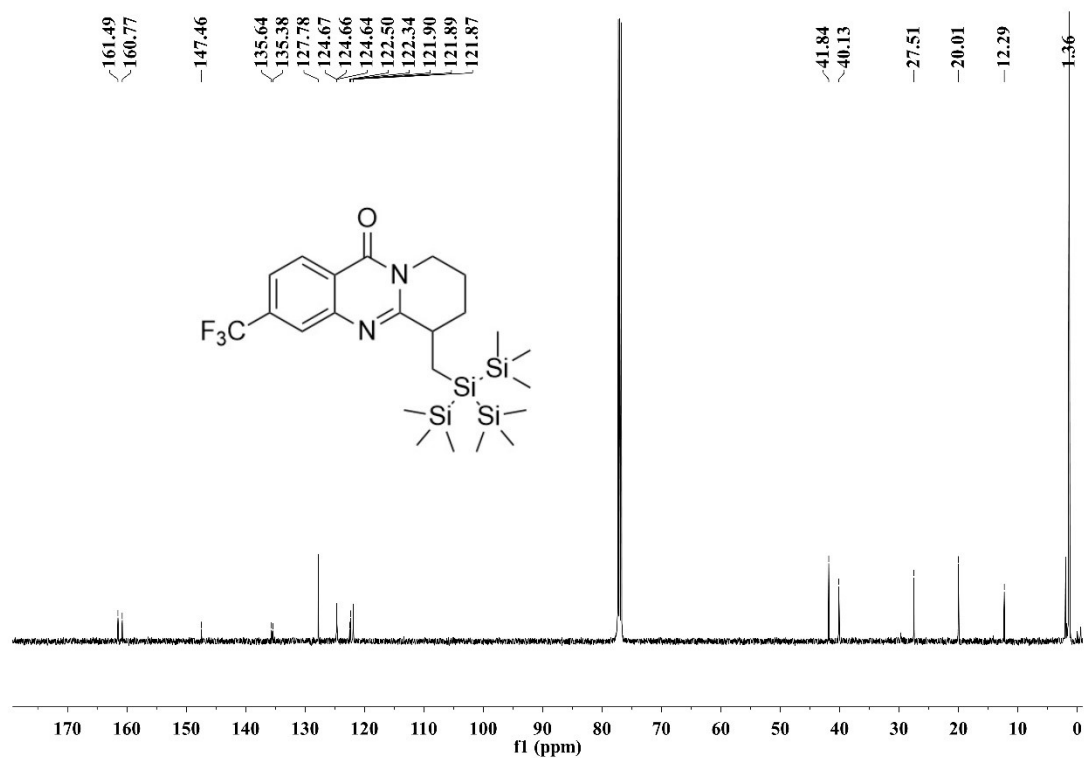
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4f (125 MHz, CDCl_3)



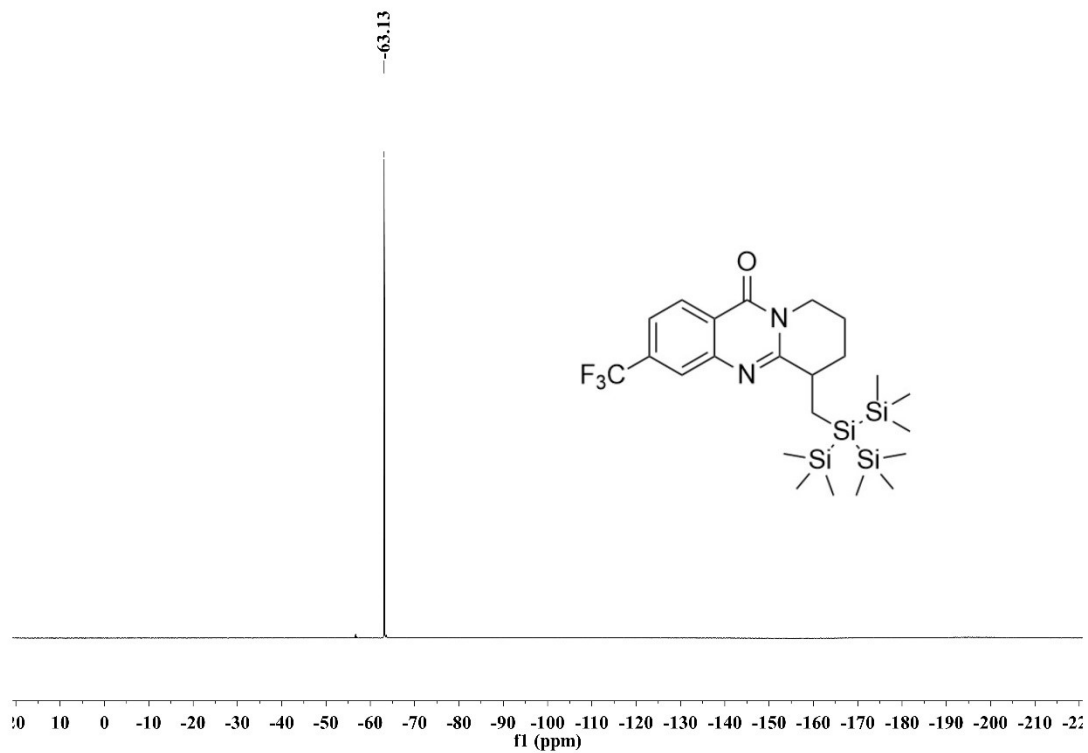
^1H NMR spectrum of 4g (500 MHz, CDCl_3)



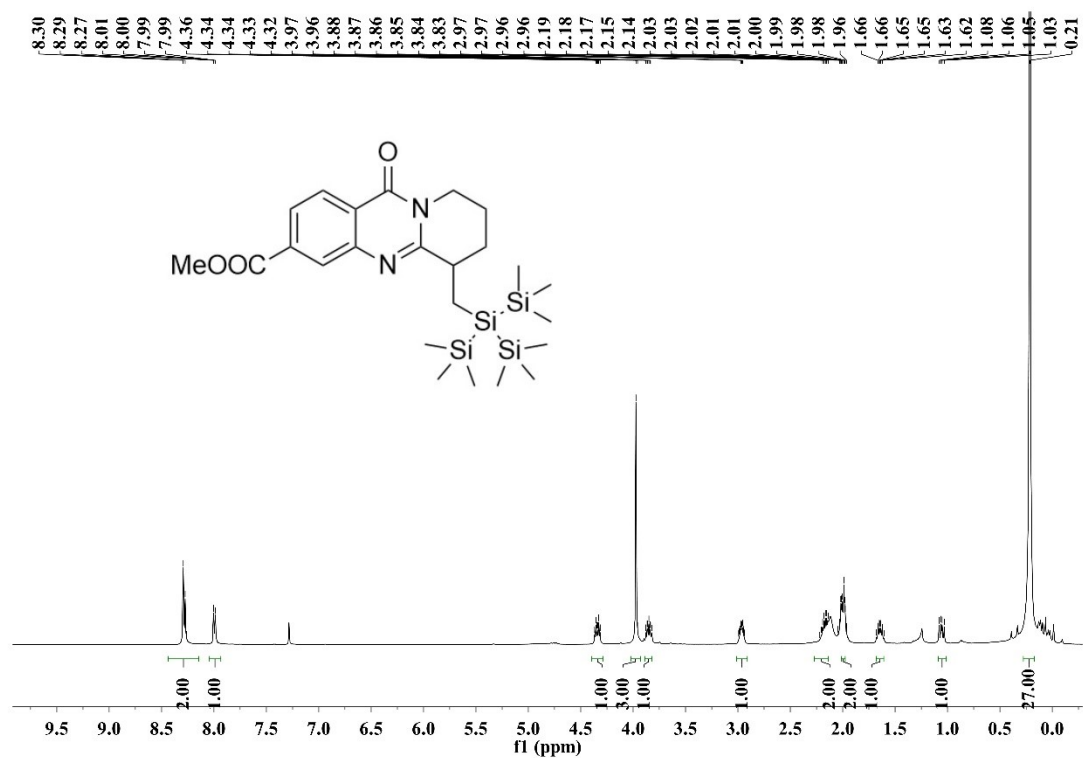
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 4g (125 MHz, CDCl_3)



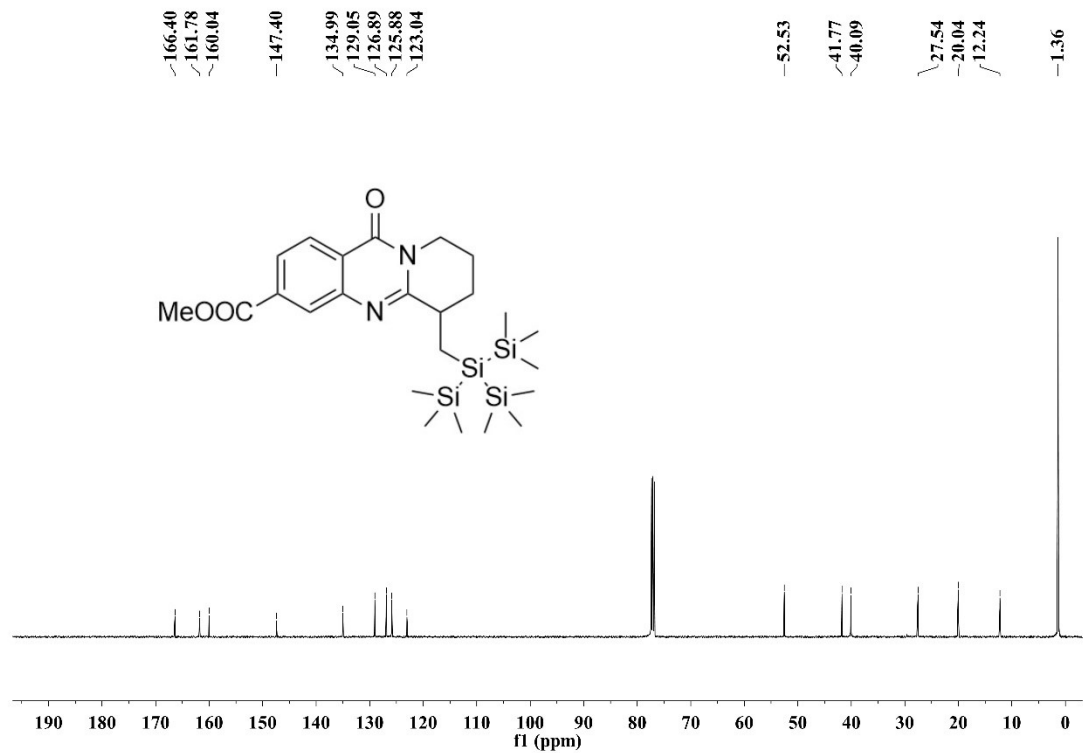
^{19}F NMR spectrum of 4g (125 MHz, CDCl_3)



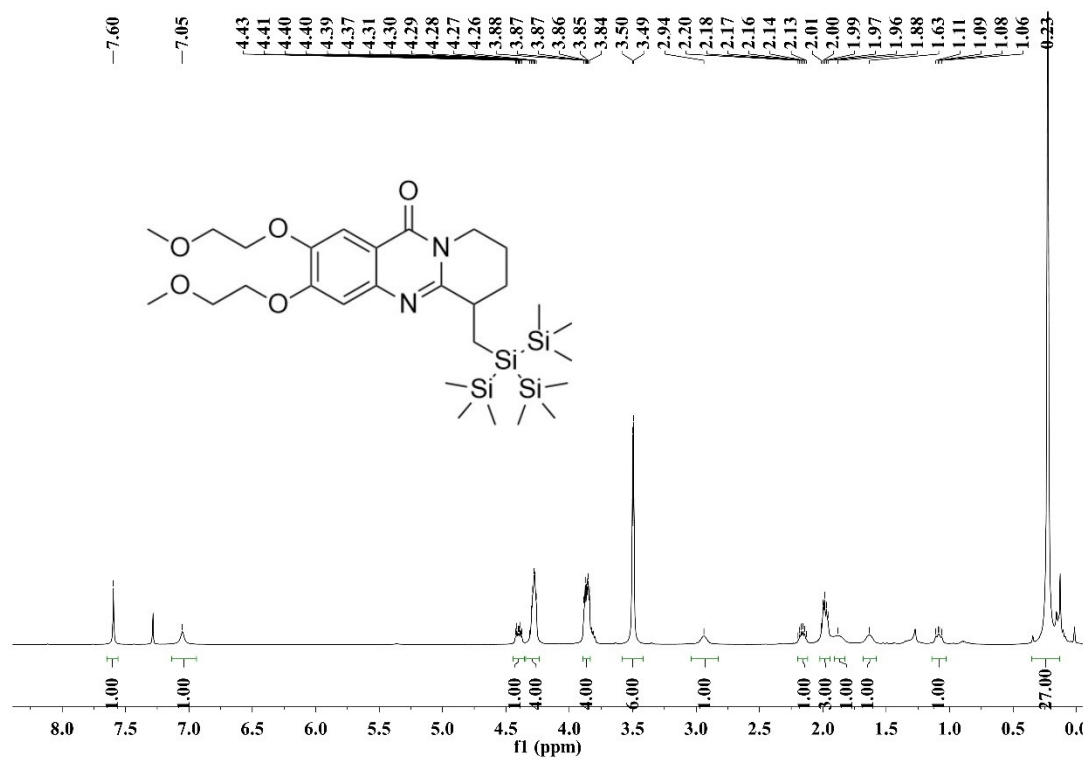
¹H NMR spectrum of 4h (500 MHz, CDCl₃)



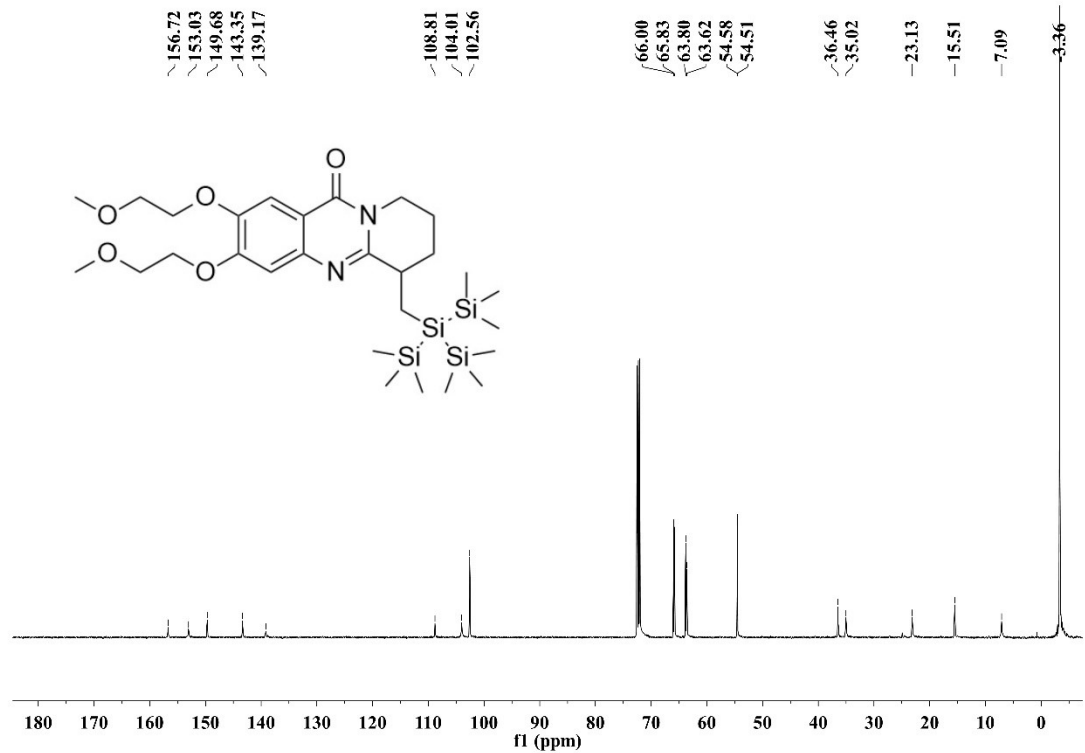
¹³C{¹H} NMR spectrum of 4h (125 MHz, CDCl₃)



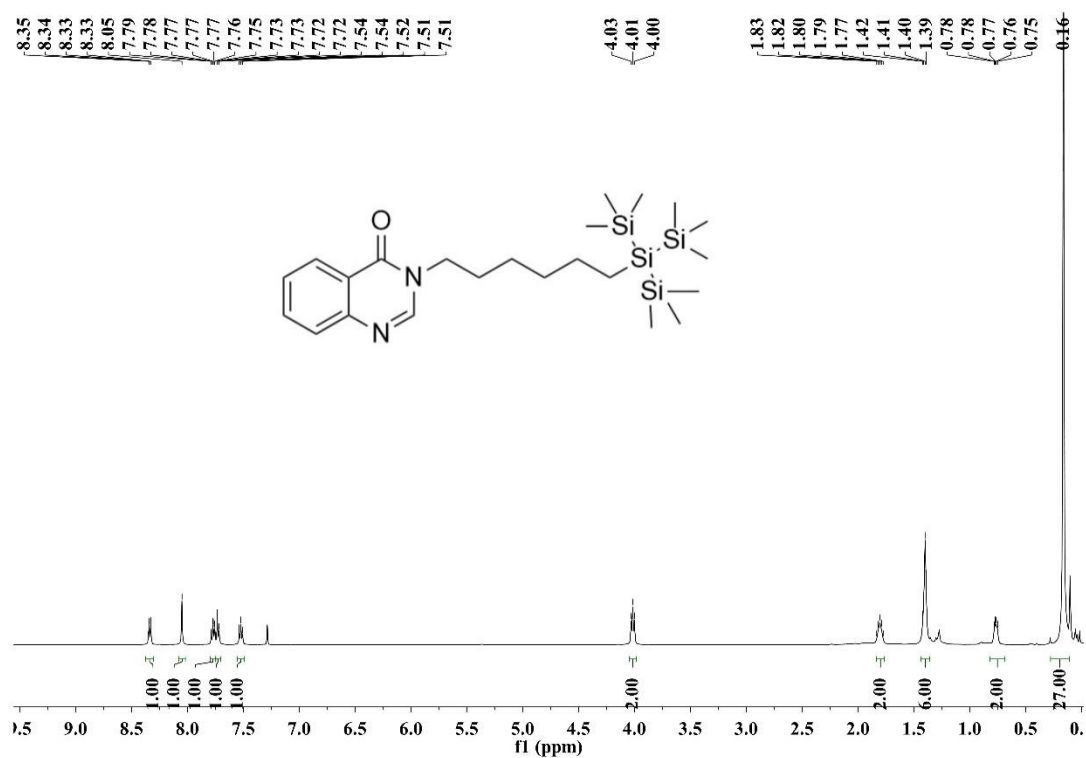
¹H NMR spectrum of 4i (500 MHz, CDCl₃)



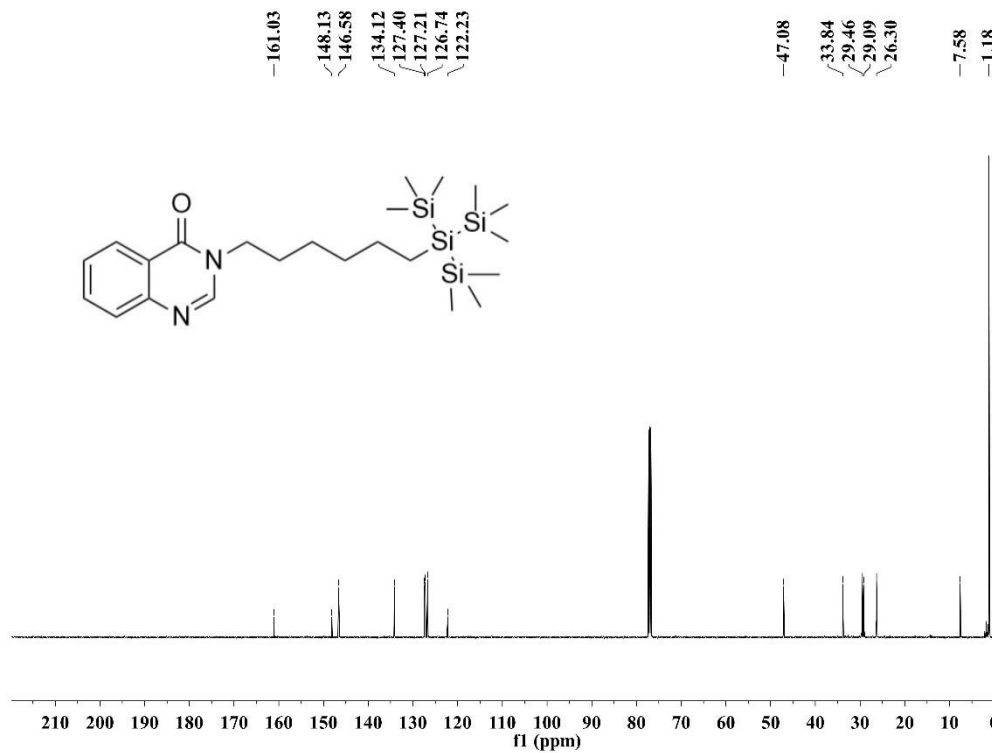
¹³C{¹H} NMR spectrum of 4i (125 MHz, CDCl₃)



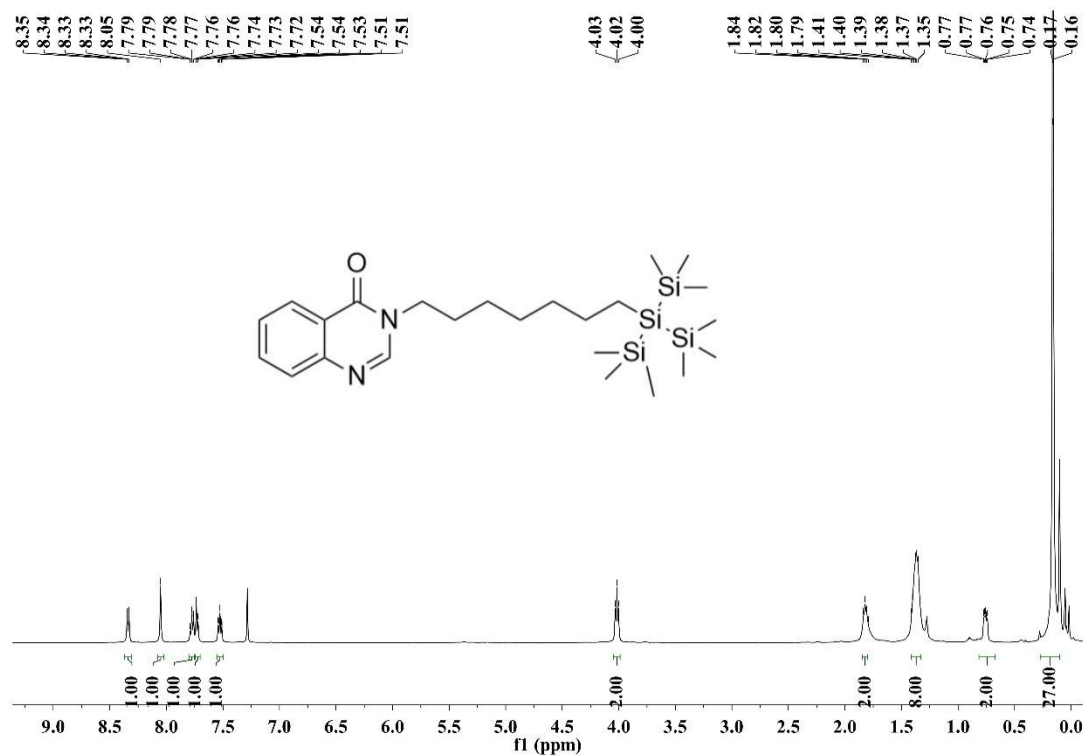
¹H NMR spectrum of 1'j-A (500 MHz, CDCl₃)



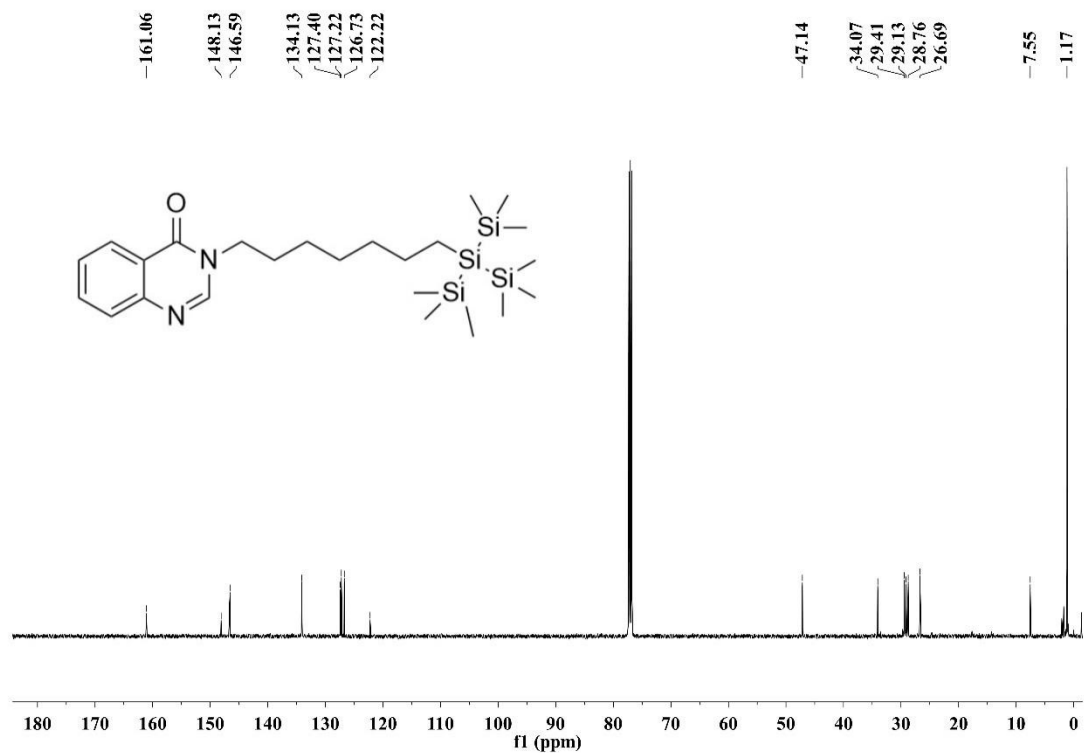
¹³C{¹H} NMR spectrum of 1'j-A (125 MHz, CDCl₃)



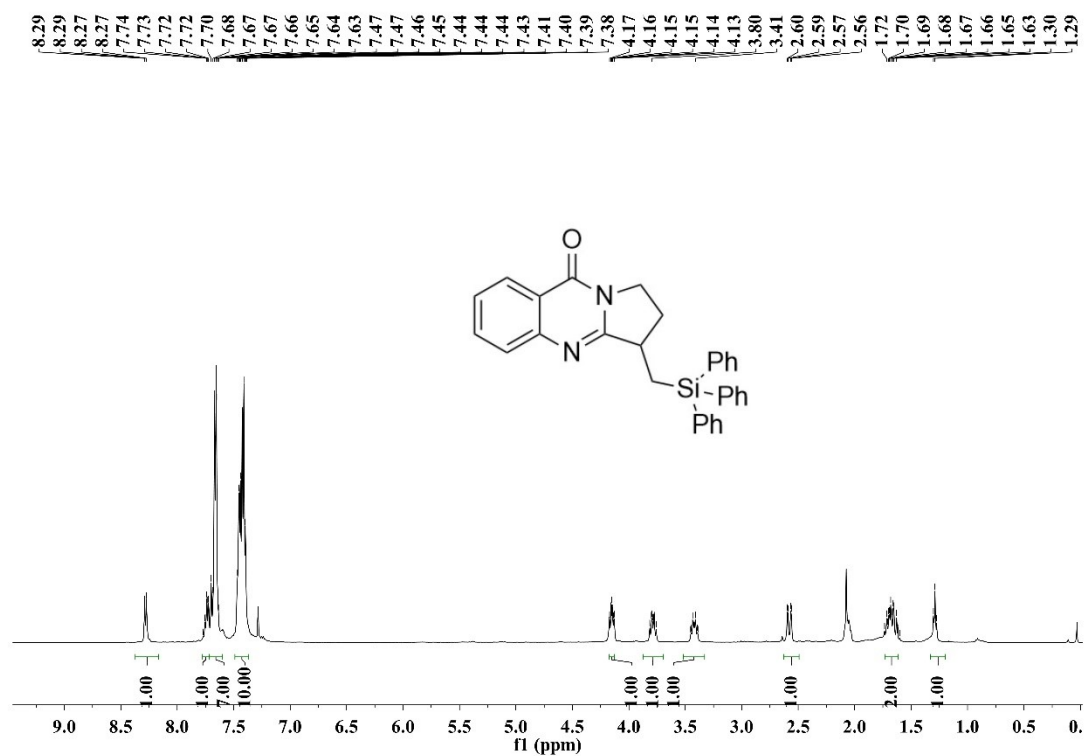
¹H NMR spectrum of 1'k-A (500 MHz, CDCl₃)



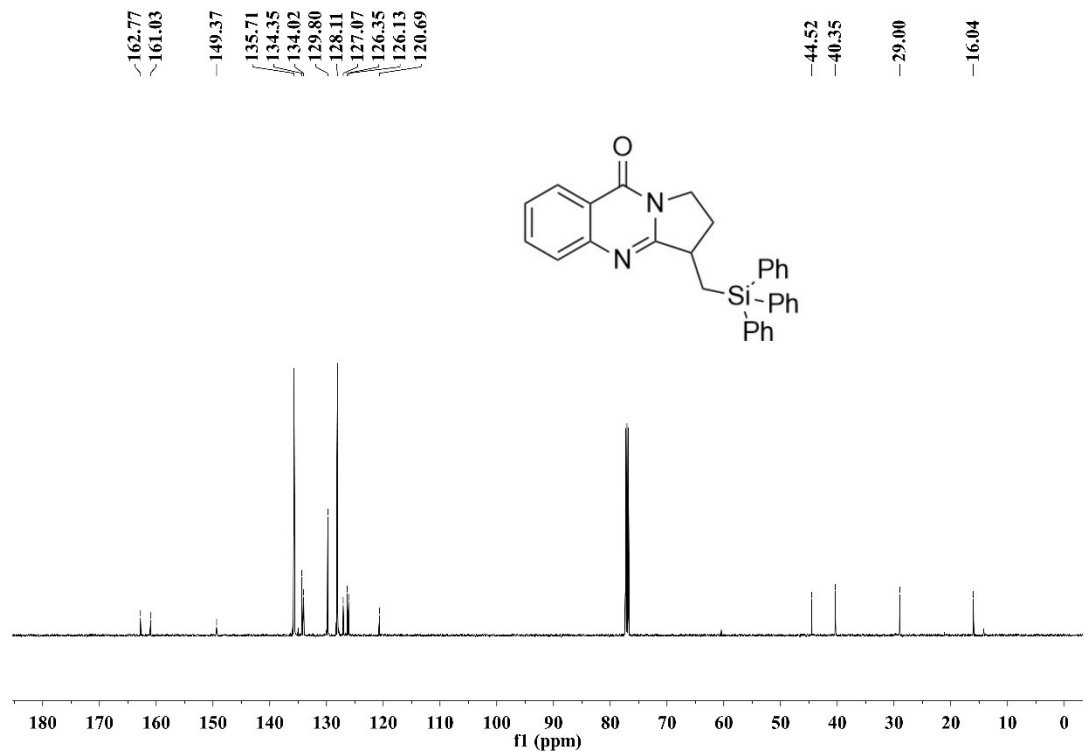
¹³C{¹H} NMR spectrum of 1'k-A (125 MHz, CDCl₃)



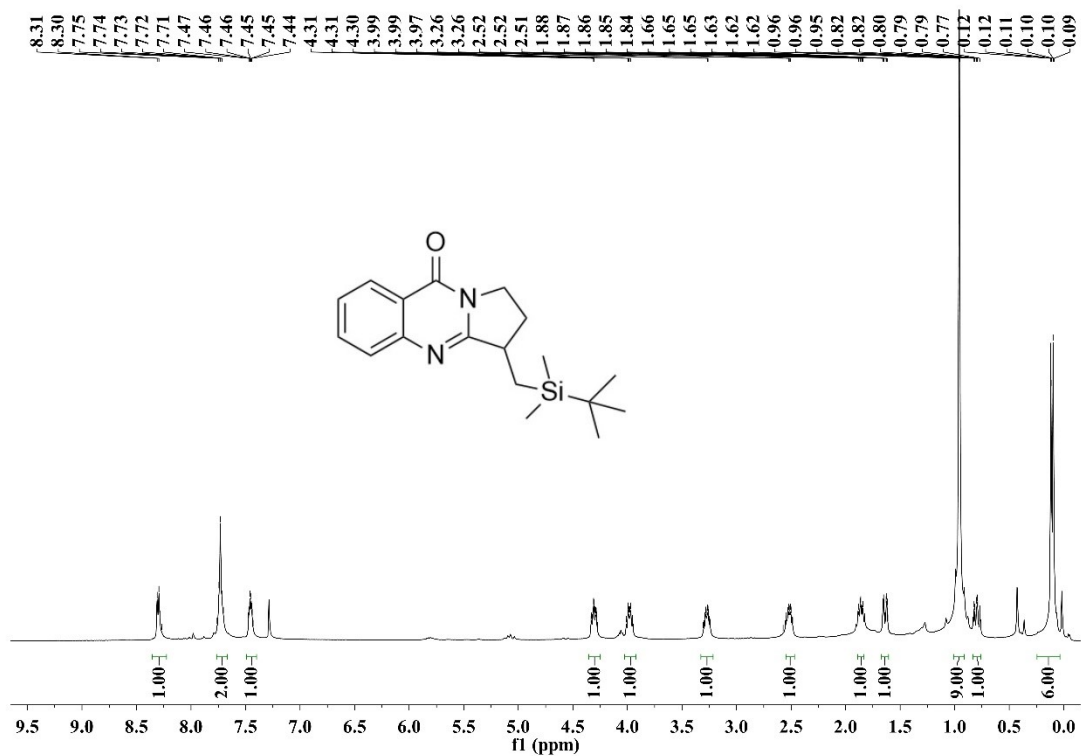
¹H NMR spectrum of 5a (500 MHz, CDCl₃)



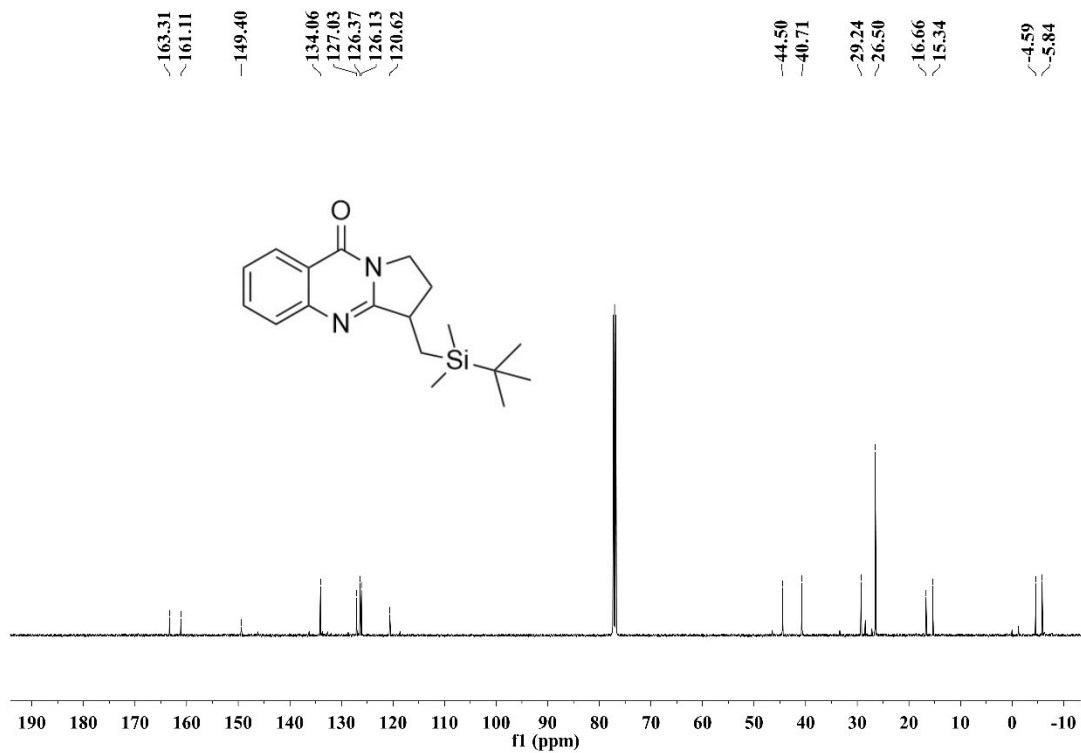
¹³C{¹H} NMR spectrum of 5a (125 MHz, CDCl₃)



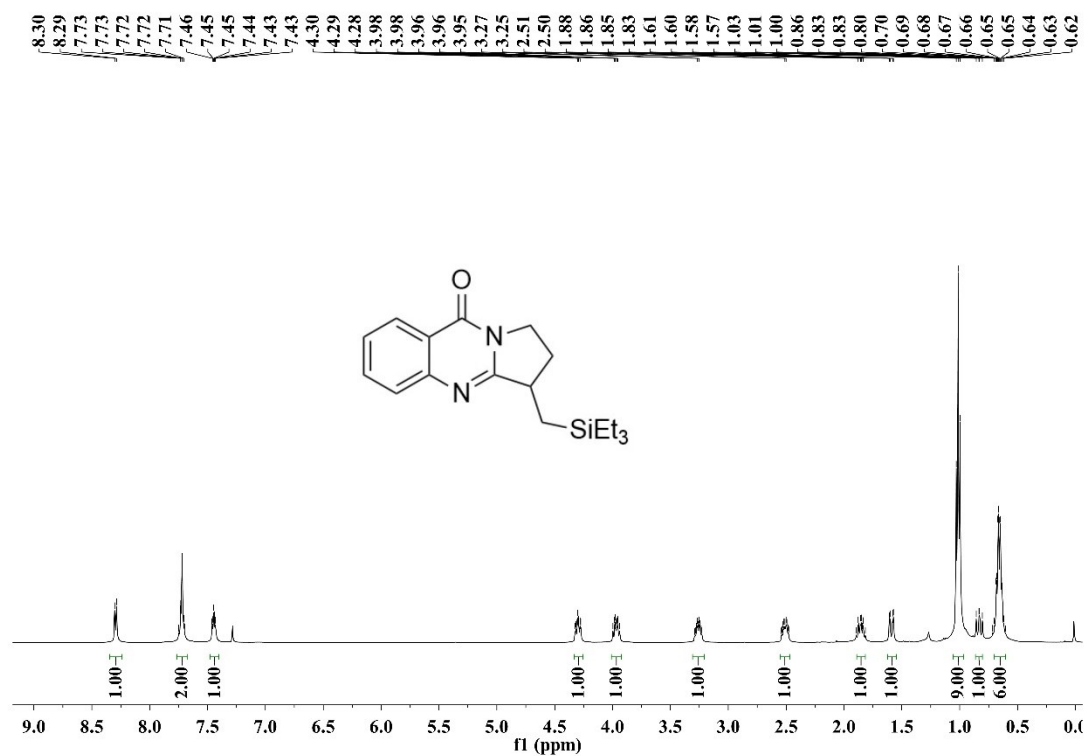
¹H NMR spectrum of 5b (500 MHz, CDCl₃)



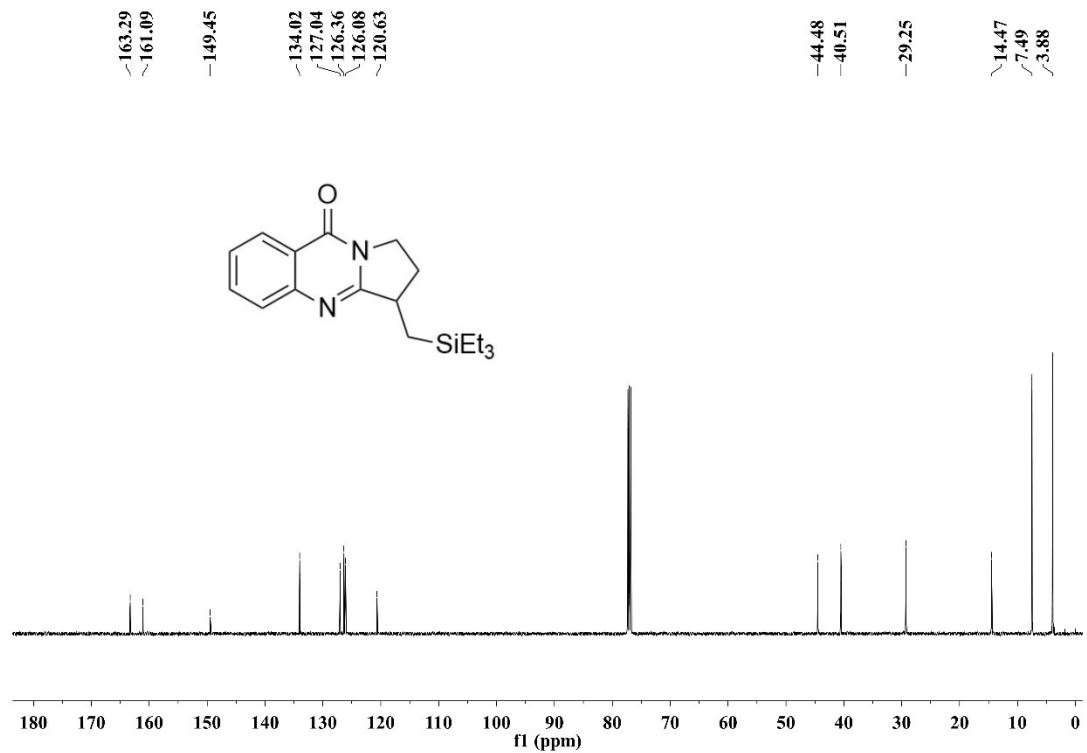
¹³C{¹H} NMR spectrum of 5b (125 MHz, CDCl₃)



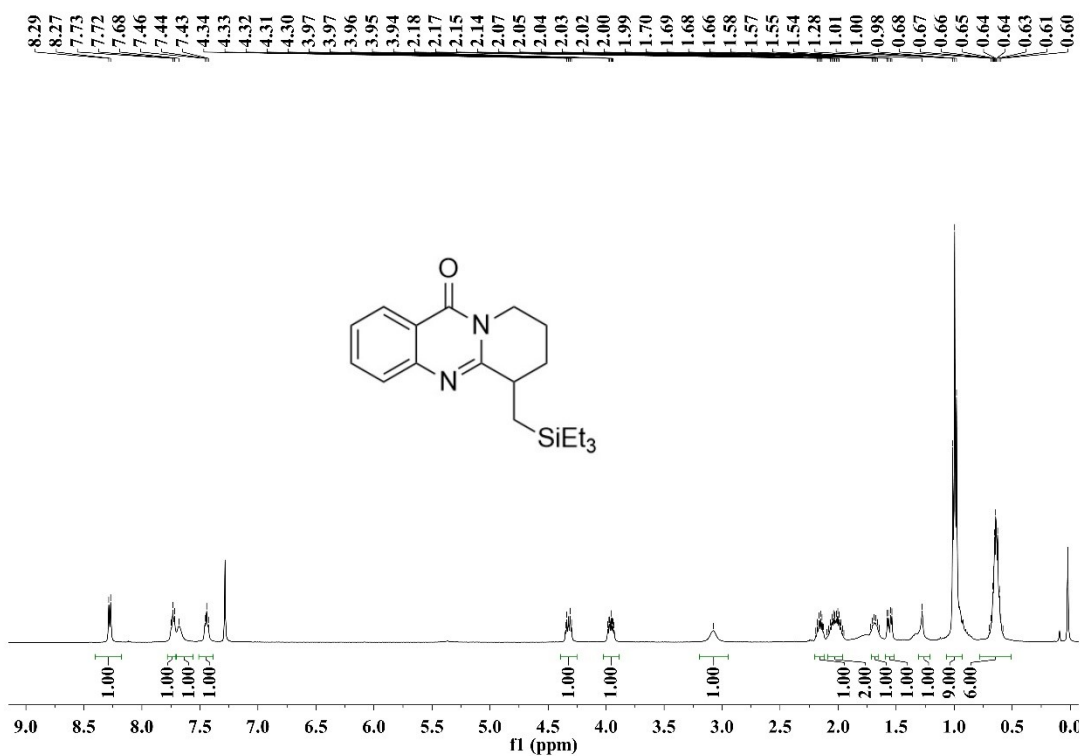
¹H NMR spectrum of 5c (500 MHz, CDCl₃)



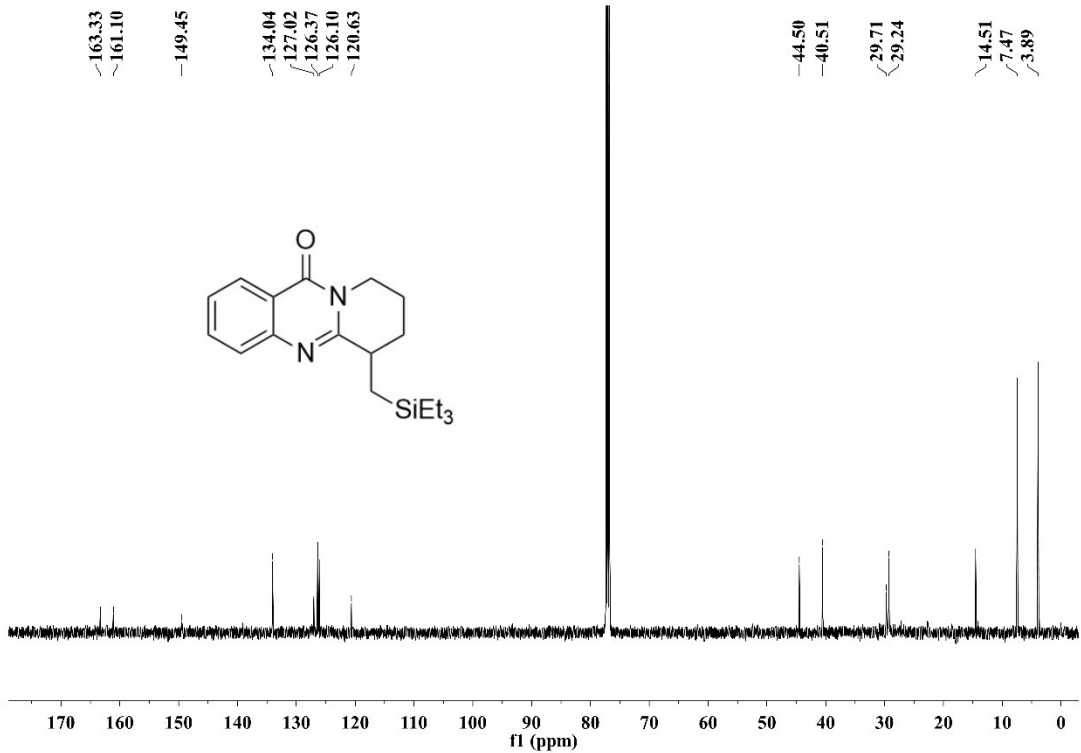
¹³C{¹H} NMR spectrum of 5c (125 MHz, CDCl₃)



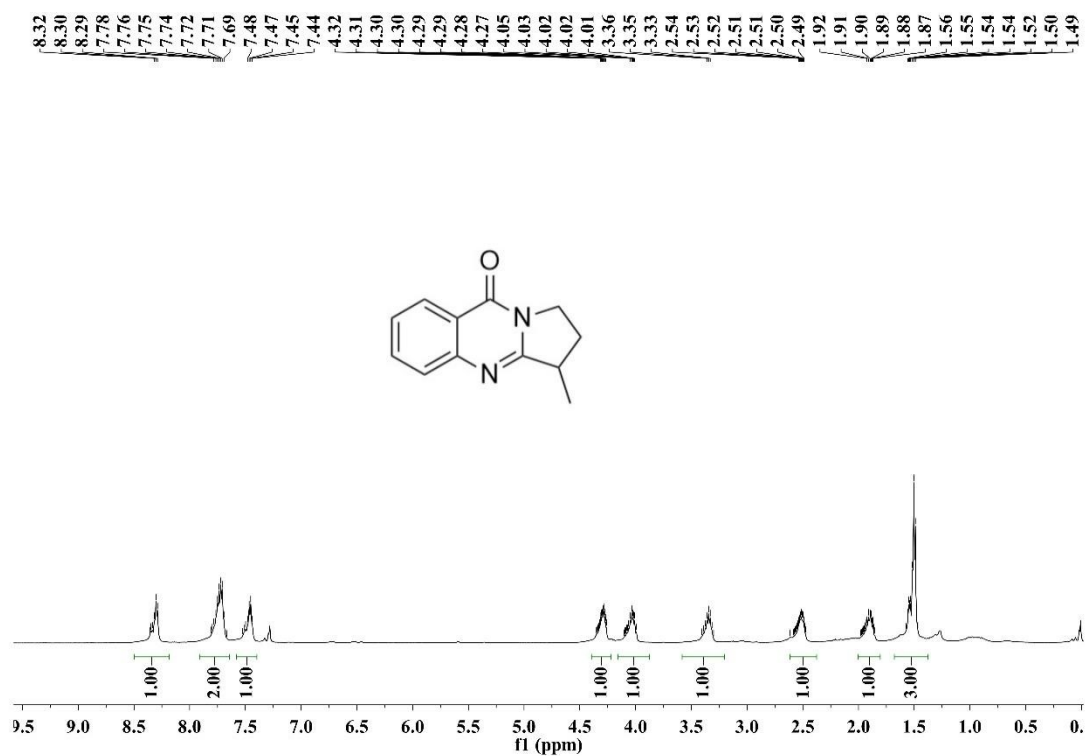
¹H NMR spectrum of 5d (500 MHz, CDCl₃)



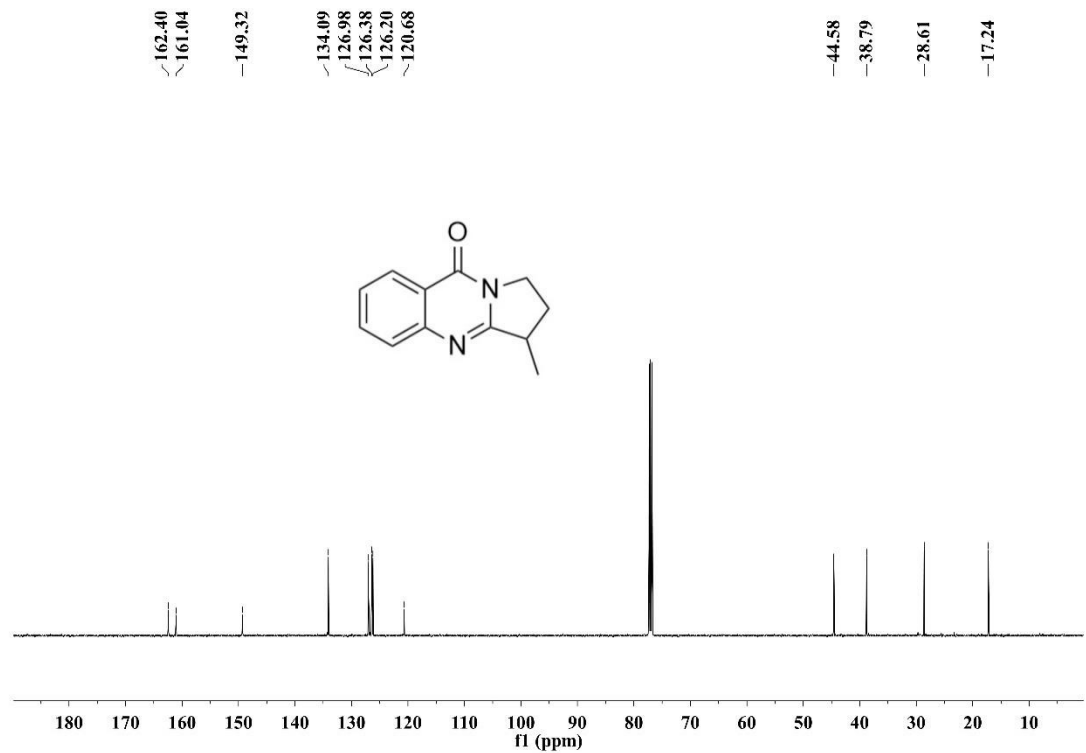
¹³C{¹H} NMR spectrum of 5d (125 MHz, CDCl₃)



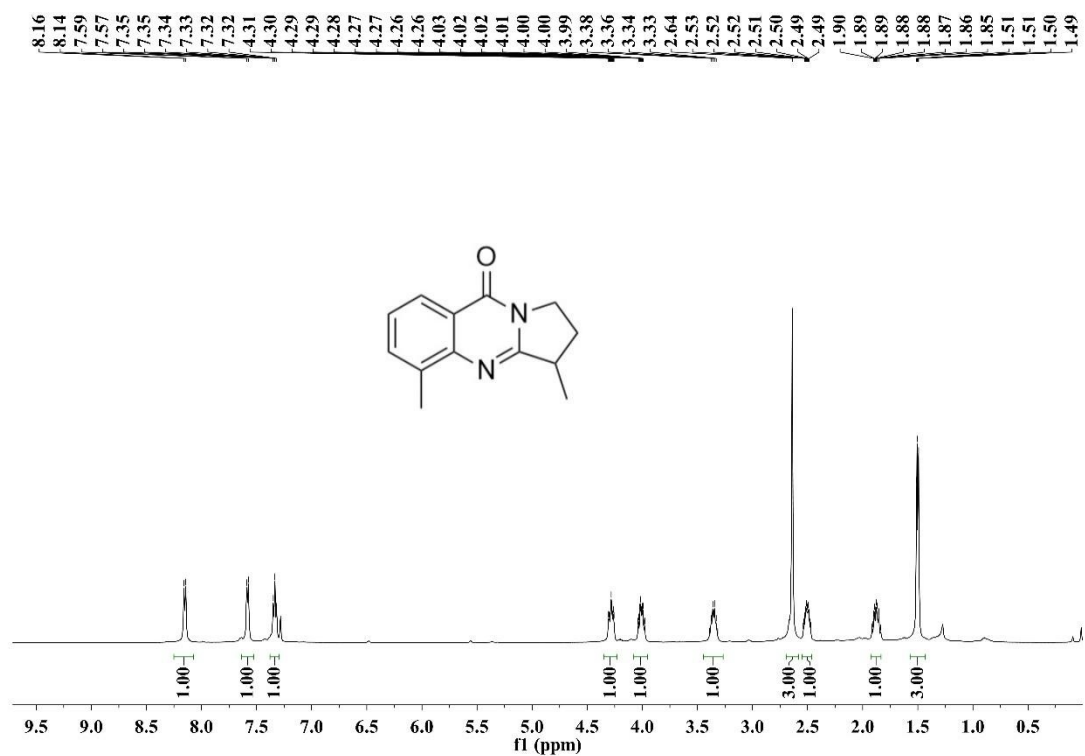
¹H NMR spectrum of 6a (500 MHz, CDCl₃)



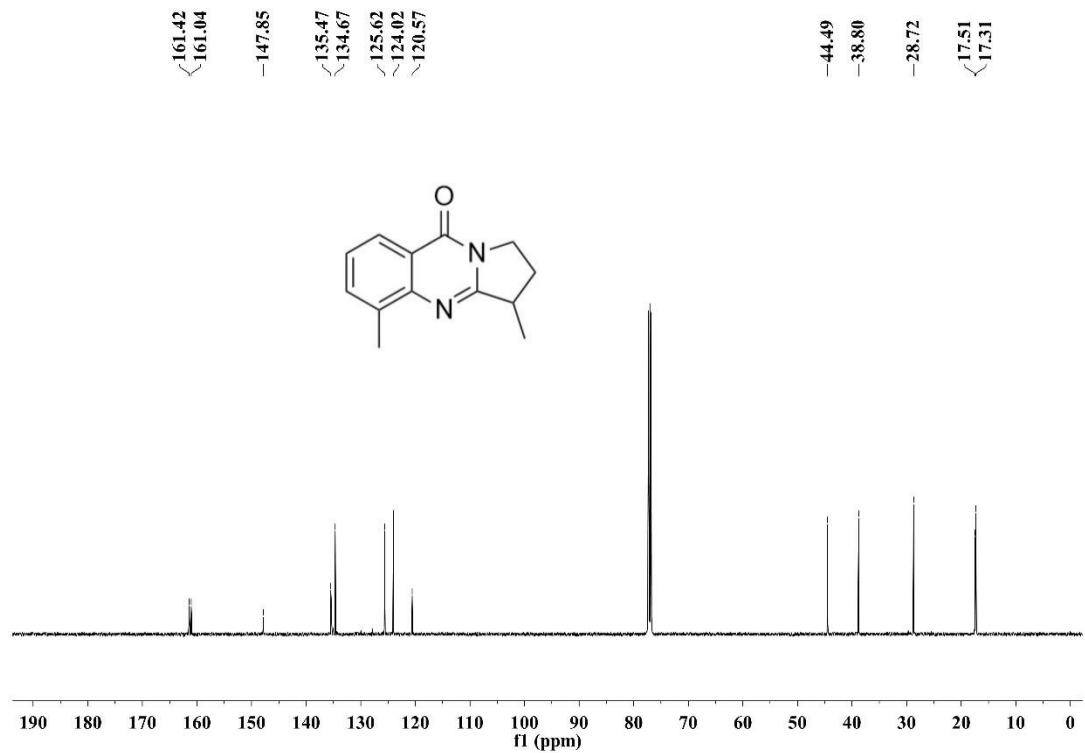
¹³C{¹H} NMR spectrum of 6a (125 MHz, CDCl₃)



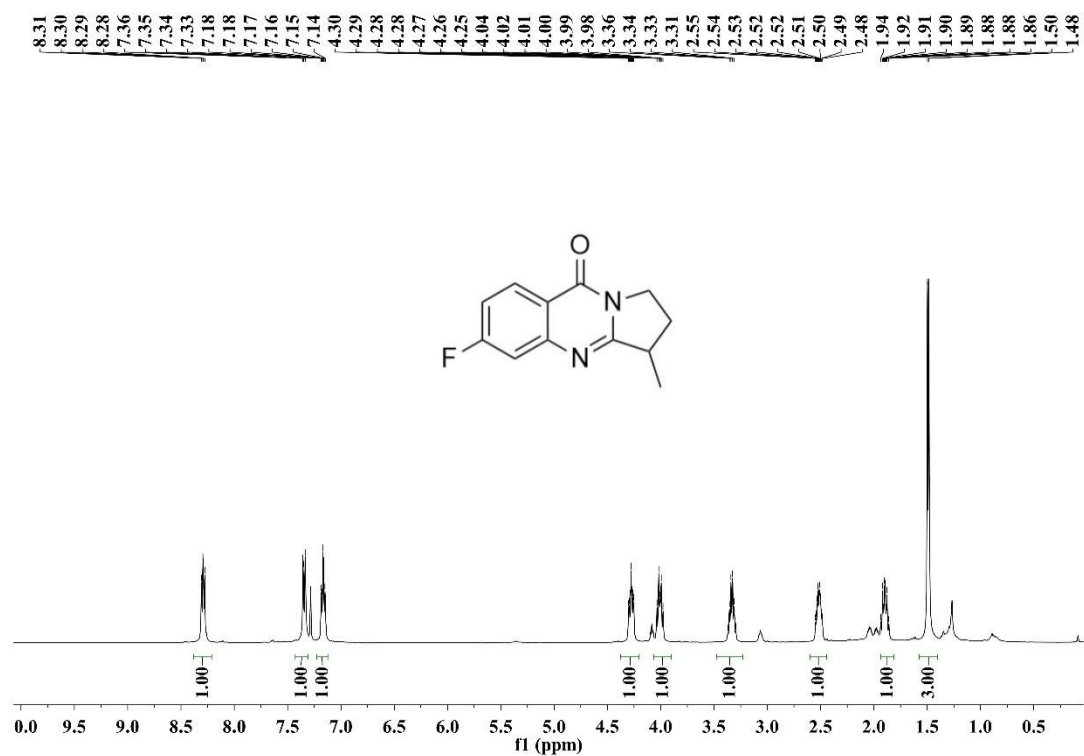
¹H NMR spectrum of 6b (500 MHz, CDCl₃)



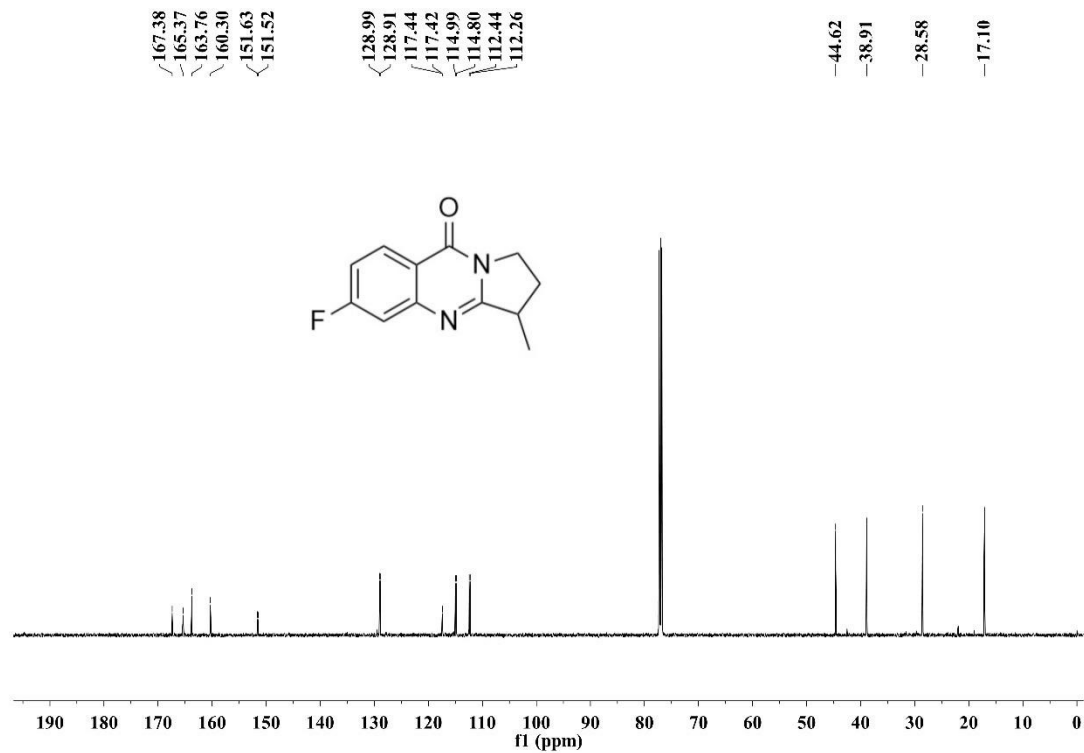
¹³C{¹H} NMR spectrum of 6b (125 MHz, CDCl₃)



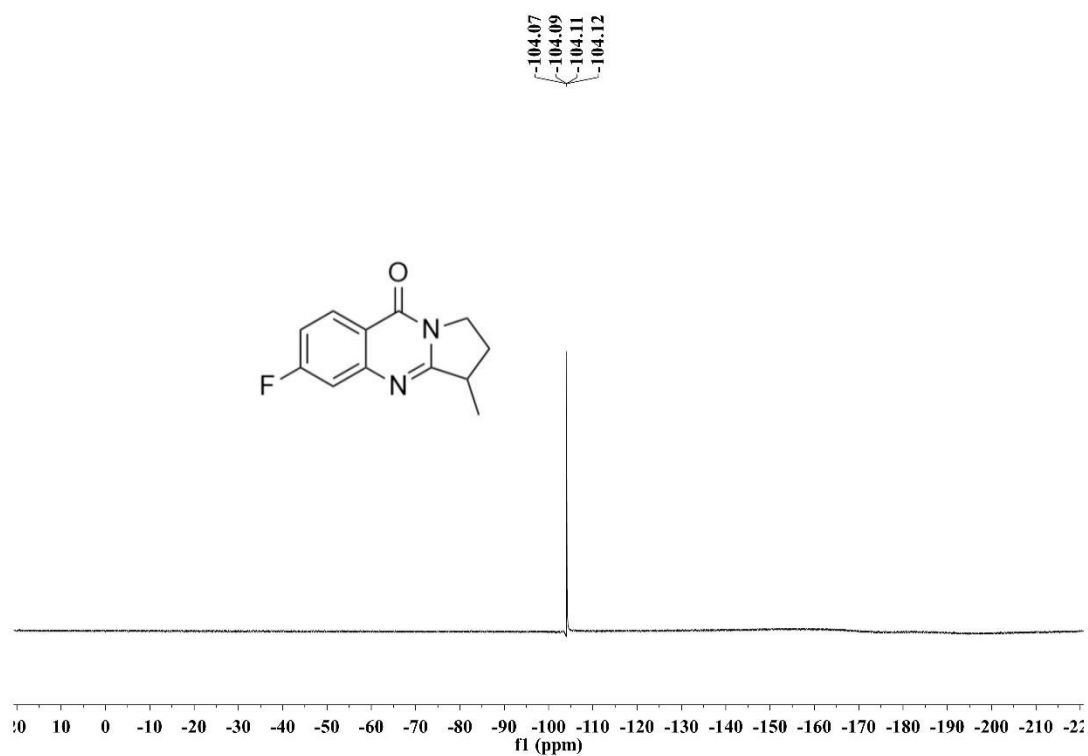
^1H NMR spectrum of 6c (500 MHz, CDCl_3)



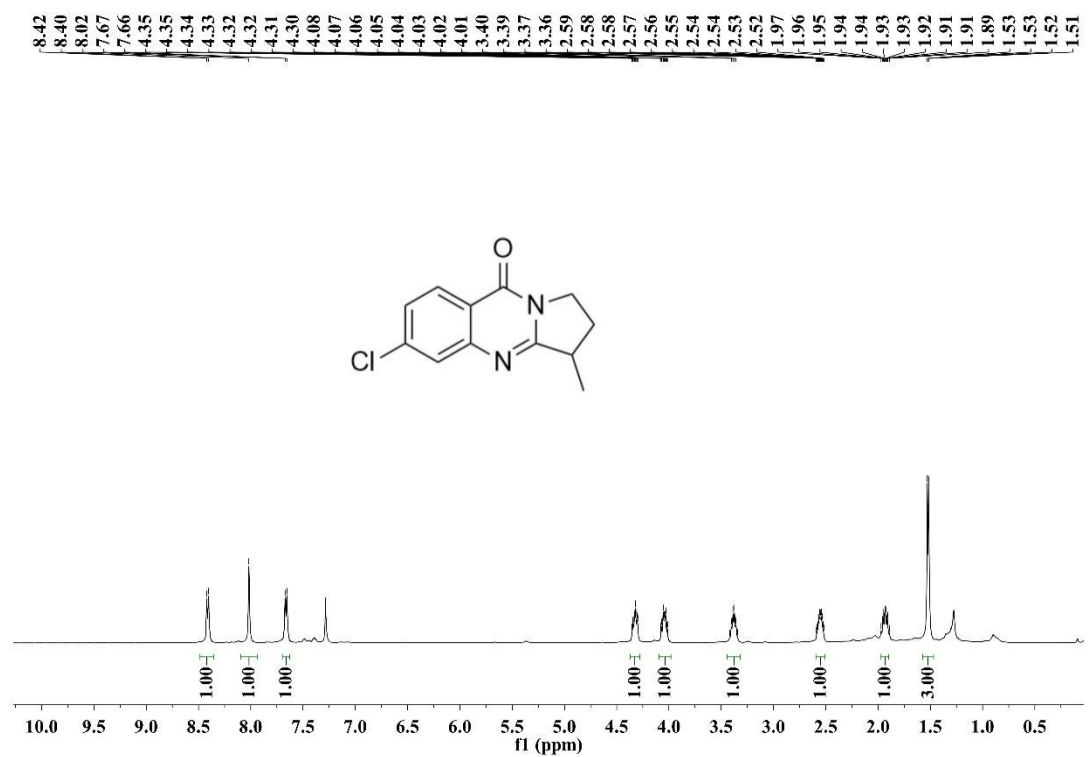
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 6c (125 MHz, CDCl_3)



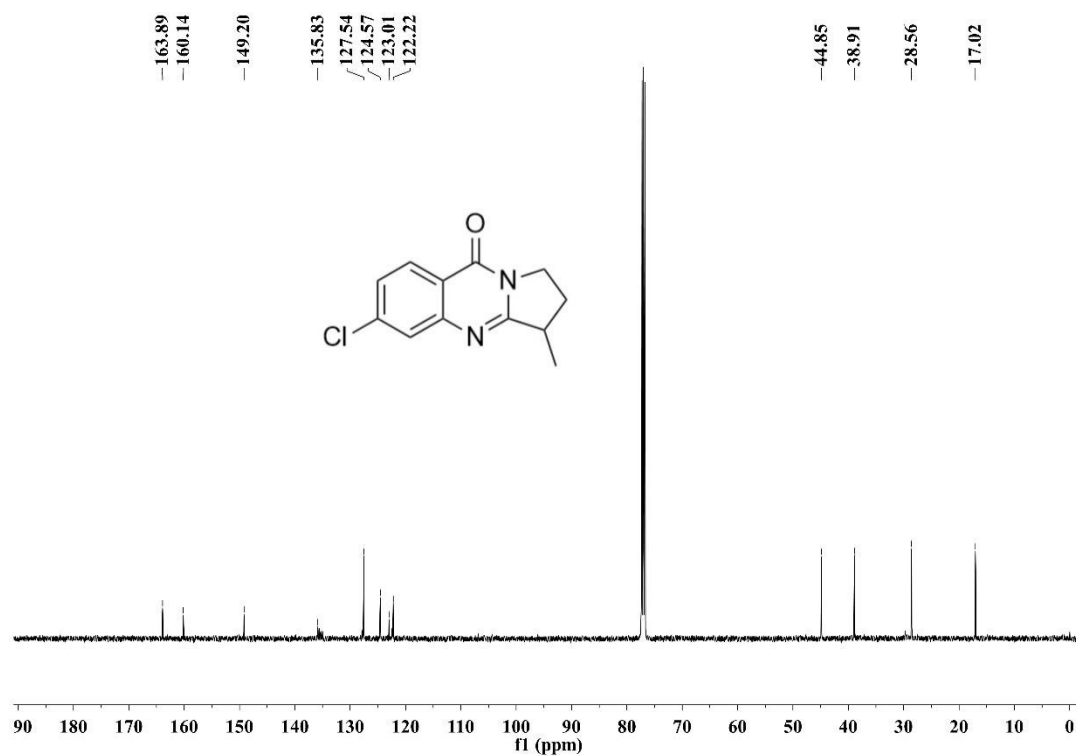
^{19}F NMR spectrum of 6c (125 MHz, CDCl_3)



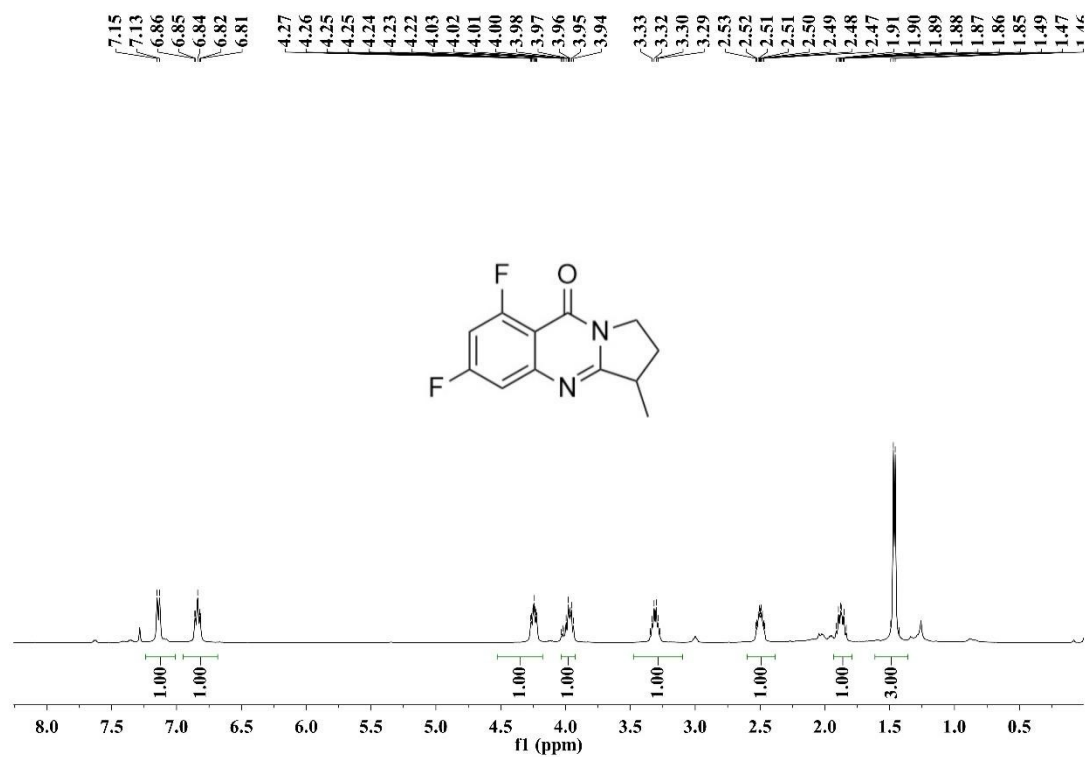
^1H NMR spectrum of 6d (500 MHz, CDCl_3)



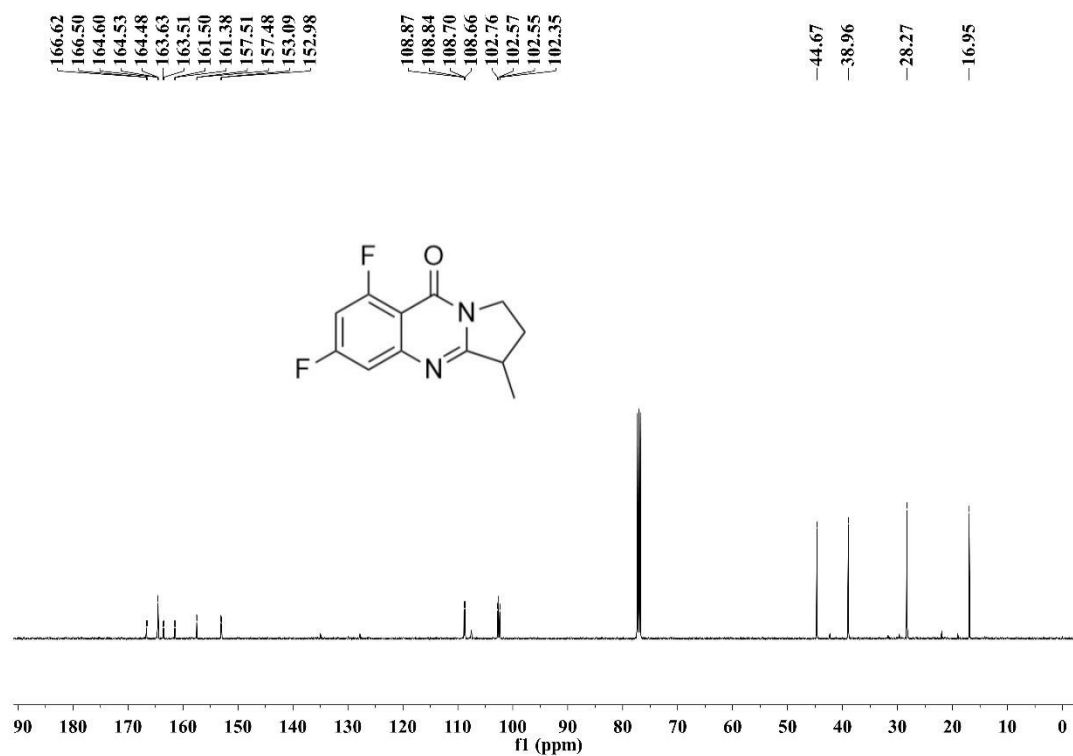
$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 6d (125 MHz, CDCl_3)



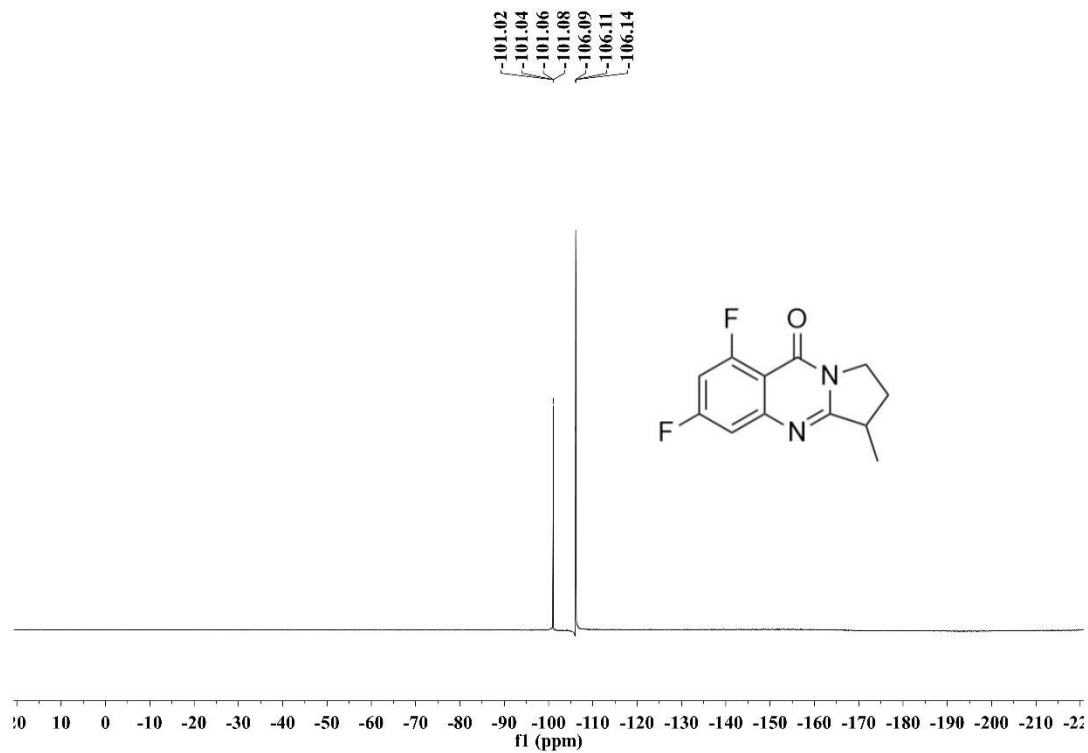
^1H NMR spectrum of 6e (500 MHz, CDCl_3)



$^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of 6e (125 MHz, CDCl_3)



^{19}F NMR spectrum of 6e (125 MHz, CDCl_3)



M. Copies of HRMS Spectra

HRMS spectra of 3a: $[M+H]^+$ Calcd for $C_{21}H_{39}N_2OSi_4$ 447.2134; Found 447.2139.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2316 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

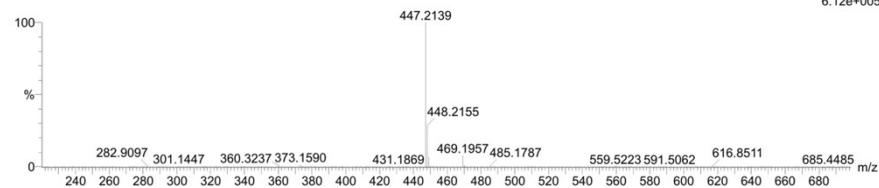
Elements Used:

C: 21-21 H: 39-39 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4

5

230519-7-359-3-X-2 16 (0.187)

1: TOF MS ES+
6.12e+005



Minimum: -1.5
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
447.2139	447.2139	0.0	0.0	7.5	89.5	n/a	n/a	C ₂₁ H ₃₉ N ₂ O Si ₄

HRMS spectra of 3b: $[M+H]^+$ Calcd for $C_{22}H_{41}N_2OSi_4$ 461.2290; Found 461.2299.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2501 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

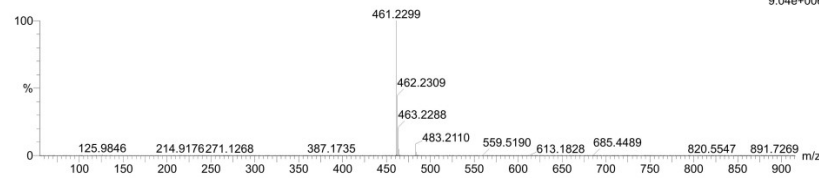
Elements Used:

C: 22-22 H: 41-41 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4

7

230519-7-359-3-X-25 16 (0.187)

1: TOF MS ES+
9.04e+006



Minimum: -1.5
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
461.2299	461.2296	0.3	0.7	7.5	214.2	n/a	n/a	C ₂₂ H ₄₁ N ₂ O Si ₄

HRMS spectra of 3c: $[M+H]^+$ Calcd for $C_{22}H_{41}N_2O_2Si_4$ 477.2240; Found 477.2248.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

2674 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

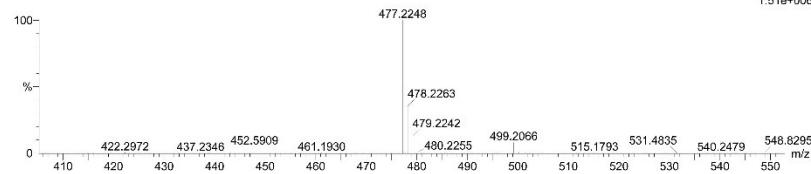
Elements Used:

C: 22-22 H: 41-41 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4

7

230519-7-359-3-X-21 14 (0.169)

1: TOF MS ES+
1.51e+006



Minimum: -1.5
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
477.2248	477.2245	0.3	0.6	7.5	123.2	n/a	n/a	C ₂₂ H ₄₁ N ₂ O ₂ Si ₄

HRMS spectra of 3d: $[M+H]^+$ Calcd for $C_{23}H_{43}N_2O_3Si_4$ 507.2345; Found 507.2359.

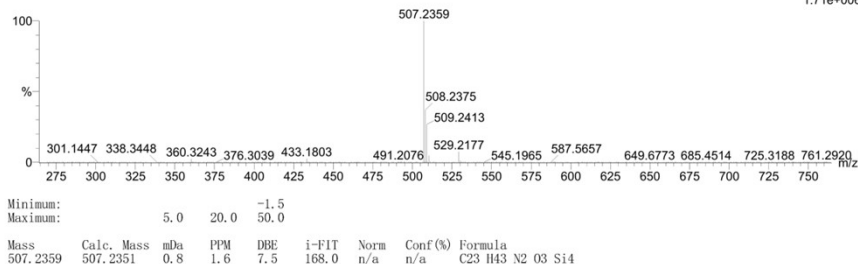
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
3058 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 23-23 H: 43-43 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4
5
230519-7-359-3-X-15 13 (0.161)



HRMS spectra of 3e: $[M+H]^+$ Calcd for $C_{21}H_{37}FN_2OSi_4$ 465.2040; Found 465.2044.

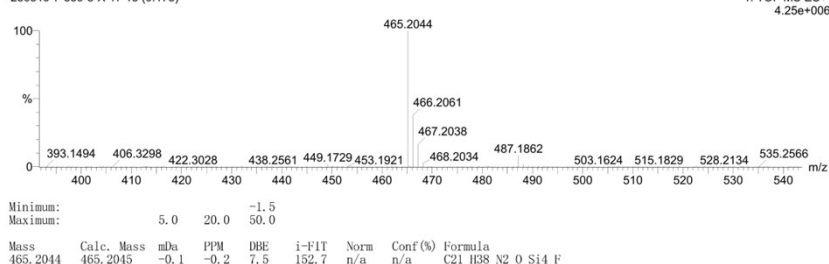
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2305 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 21-21 H: 38-38 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4 F: 1-1
7
230519-7-359-3-X-17 15 (0.178)



HRMS spectra of 3f: $[M+H]^+$ Calcd for $C_{21}H_{37}F_2N_2OSi_4$ 483.1946; Found 483.1945.

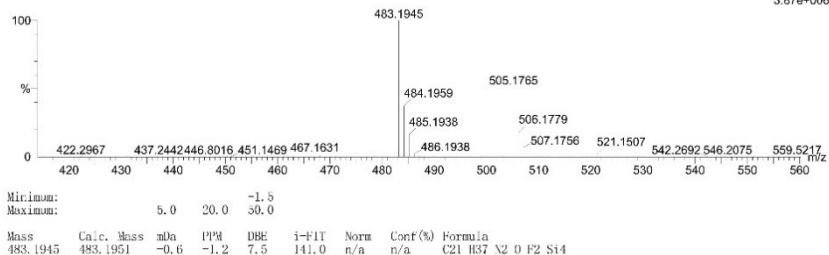
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
2299 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
Elements Used:
C: 21-21 H: 37-37 N: 0-100 O: 0-100 F: 2-2 Na: 0-1 Si: 1-4
7
230519-7-359-3-X-26 14 (0.169)



HRMS spectra of 3g: $[M+H]^+$ Calcd for $C_{21}H_{38}ClN_2OSi_4$ 481.1744; Found 481.1745.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

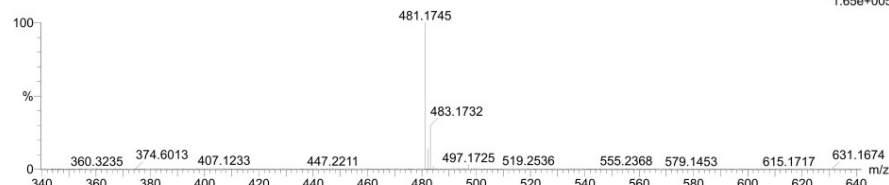
9944 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 21-21 H: 38-38 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4 Cl: 0-4

5

230519-7-359-3-X-13 22 (0.254)

1: TOF MS ES+
1.65e+005Minimum: -1.5
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
481.1745	481.1750	-0.5	-1.0	7.5	148.7	n/a	n/a	C21 H38 N2 O Si4 Cl

HRMS spectra of 3h: $[M+H]^+$ Calcd for $C_{22}H_{38}F_3N_2OSi_4$ 515.2008; Found 515.2009.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

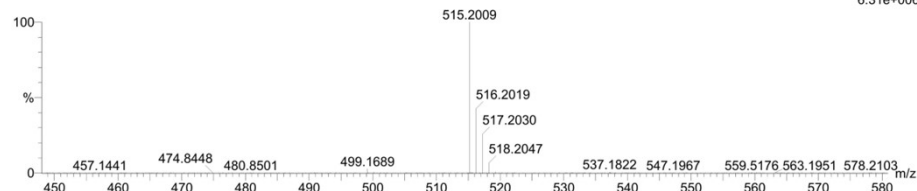
2470 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 22-22 H: 38-38 N: 0-100 O: 0-100 F: 3-3 Na: 0-1 Si: 1-4

7

230519-7-359-3-X-27 13 (0.161)

1: TOF MS ES+
6.31e+006Minimum: -1.5
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
515.2009	515.2013	-0.4	-0.8	7.5	181.7	n/a	n/a	C22 H38 N2 O F3 Si4

HRMS spectra of 3i: $[M+H]^+$ Calcd for $C_{23}H_{41}N_2O_3Si_4$ 505.2189; Found 505.2192.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

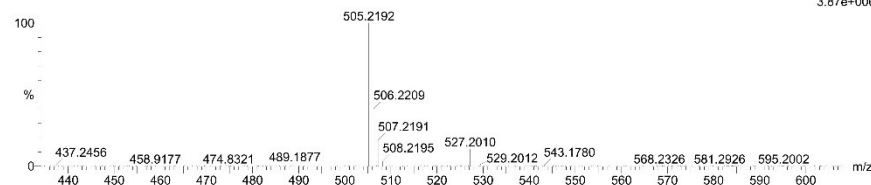
1590 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 23-23 H: 41-41 N: 0-100 O: 0-100 Si: 1-4

2

230525-1-362-1-X20 13 (0.161)

1: TOF MS ES+
3.87e+006Minimum: -1.5
Maximum: 5.0 20.0 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
505.2192	505.2194	-0.2	-0.4	8.5	116.8	n/a	n/a	C23 H41 N2 O3 Si4

HRMS spectra of 3j: $[M+H]^+$ Calcd for $C_{27}H_{51}N_2O_5Si_4$ 595.2870; Found 595.2882.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

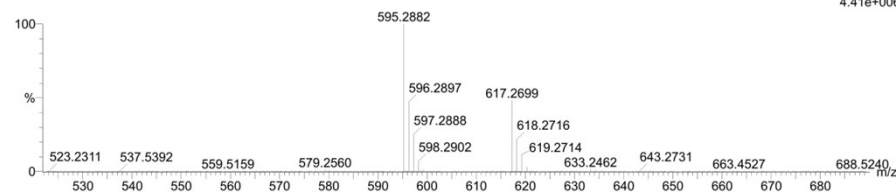
2276 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 27-27 H: 51-51 N: 0-100 O: 0-100 Si: 1-4

13

230704-4-386-3-x-28- 19 (0.220)

1: TOF MS ES+
4.41e+006Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
595.2882	595.2875	0.7	1.2	7.5	516.5	n/a	n/a	C27 H51 N2 O5 Si4

HRMS spectra of 4a: [M+H]⁺ Calcd for C₂₂H₄₁N₂OSi₄ 461.2290; Found 461.2298.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

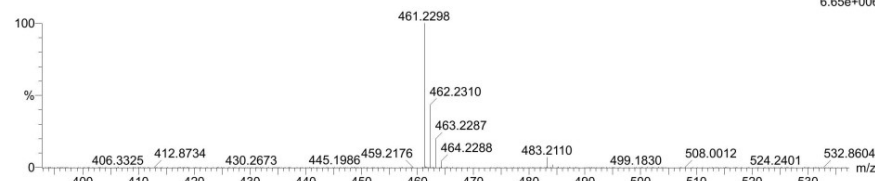
2501 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 22-22 H: 41-41 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4

7

230519-7-359-3-L-1 13 (0.161)

1: TOF MS ES+
6.65e+006Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
461.2298	461.2296	0.2	0.4	7.5	191.8	n/a	n/a	C22 H41 N2 O Si4

HRMS spectra of 4b: [M+H]⁺ Calcd for C₂₃H₄₃N₂OSi₄ 475.2447; Found 475.2448.

Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

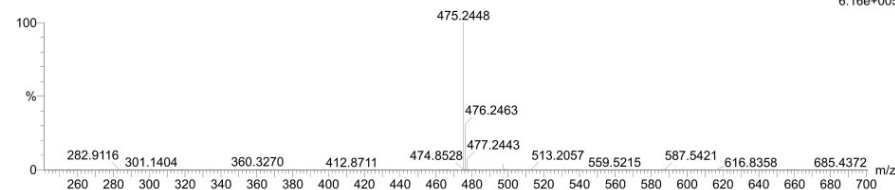
2689 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 23-23 H: 43-43 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4

7

230519-7-359-3-L-18 26 (0.297)

1: TOF MS ES+
6.16e+005Minimum: -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
475.2448	475.2452	-0.4	-0.8	7.5	115.9	n/a	n/a	C23 H43 N2 O3 Si4

HRMS spectra of 4c: [M+H]⁺ Calcd for C₂₄H₄₅N₂O₃Si₄ 521.2502; Found 521.2510.

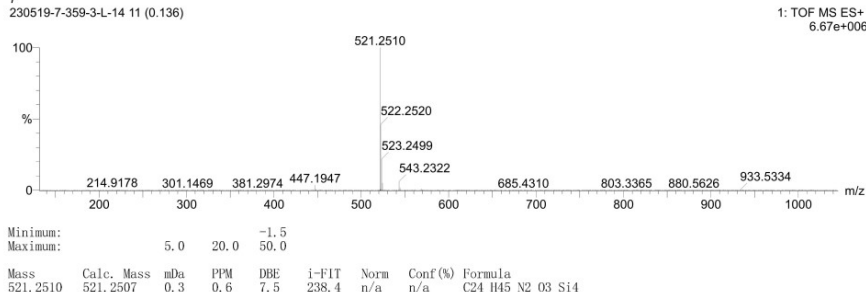
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 3266 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 24-24 H: 45-45 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4
 7
 230519-7-359-3-L-14 11 (0.136)



HRMS spectra of 4d: [M+H]⁺ Calcd for C₂₂H₄₀FN₂OSi₄ 479.2202; Found 479.2204.

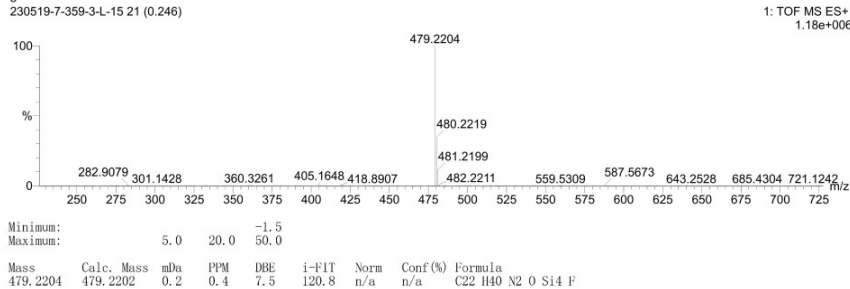
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 2490 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 22-22 H: 40-40 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4 F: 1-1
 5
 230519-7-359-3-L-15 21 (0.246)



HRMS spectra of 4e: [M+H]⁺ Calcd for C₂₂H₃₉F₂N₂OSi₄ 497.2108; Found 497.2104.

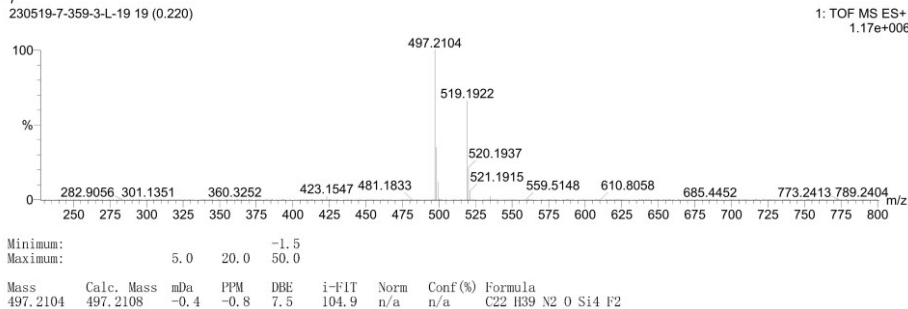
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 2482 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 22-22 H: 39-39 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4 F: 2-2
 7
 230519-7-359-3-L-19 19 (0.220)



HRMS spectra of 4f: [M+H]⁺ Calcd for C₂₂H₄₀ClN₂OSi₄ 495.1901; Found 495.1909.

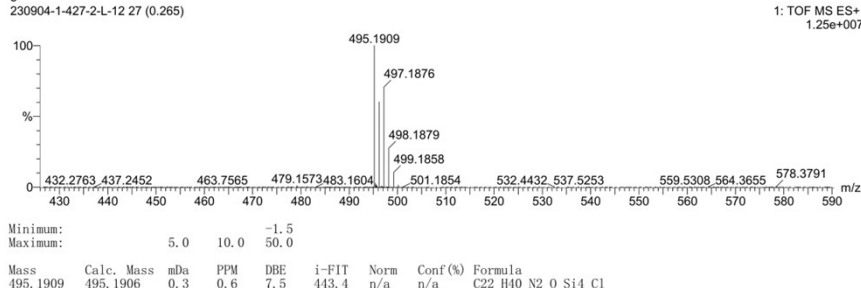
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 501 formula(e) evaluated with 1 results within limits (up to 50 best isotopic matches for each mass)
 Elements Used:
 C: 22-22 H: 40-40 N: 0-200 O: 0-200 Si: 4-4 Cl: 1-2
 3
 230904-1-427-2-L-12 27 (0.265)



HRMS spectra of 4g: [M+H]⁺ Calcd for C₂₃H₄₀F₃N₂OSi₄ 529.2170; Found 529.2170.

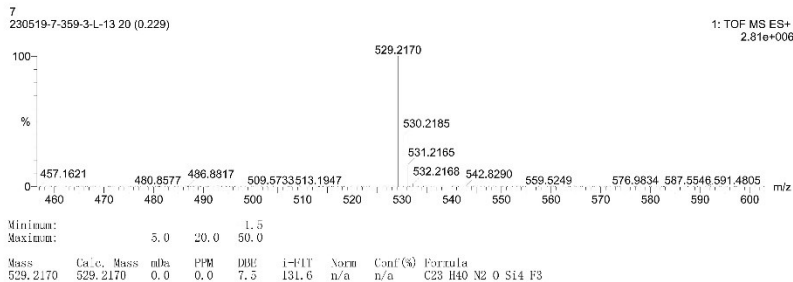
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 2660 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 23-23 H: 40-40 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4 F: 3-3
 7
 230519-7-359-3-L-13 20 (0.229)



HRMS spectra of 4h: [M+H]⁺ Calcd for C₂₄H₄₃N₂O₃Si₄ 519.2351; Found 519.2347.

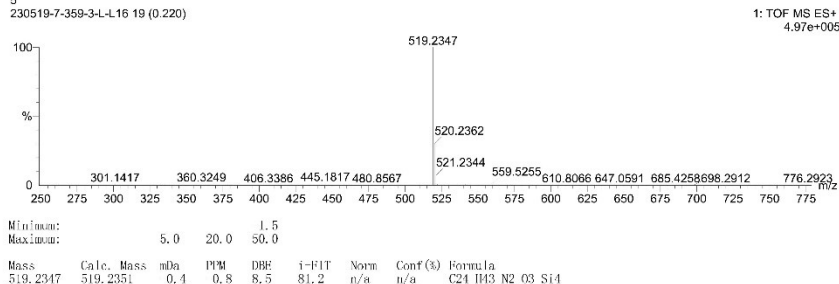
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 3247 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 24-24 H: 43-43 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4
 5
 230519-7-359-3-L-16 19 (0.220)



HRMS spectra of 4i: [M+H]⁺ Calcd for C₂₈H₅₃N₂O₅Si₄ 609.3032; Found 609.3037.

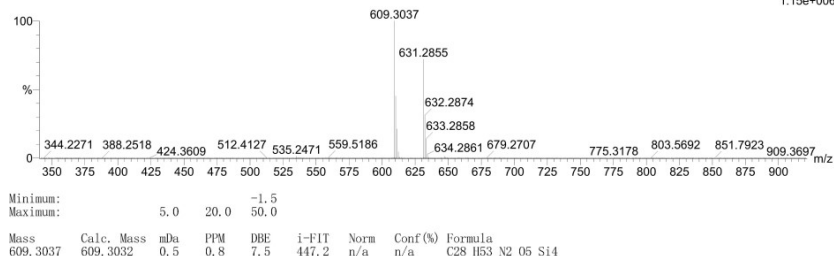
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 2403 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 28-28 H: 53-53 N: 0-100 O: 0-100 Si: 1-4
 13
 230704-4-386-3-22-30 (0.339)



HRMS spectra of 1'j-A: $[M+H]^+$ Calcd for $C_{23}H_{45}N_2OSi_4$ 477.2603; Found 477.2608.

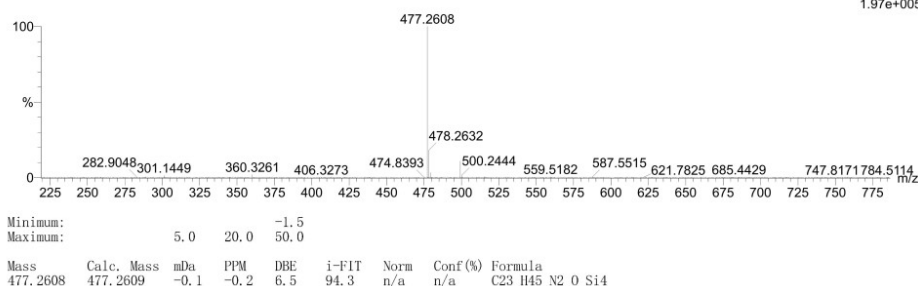
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 2710 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 23-23 H: 45-45 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4
 7
 230519-7-359-3-L-20 19 (0.220)



HRMS spectra of 1'k-A: $[M+H]^+$ Calcd for $C_{24}H_{47}N_2OSi_4$ 491.2760; Found 491.2768.

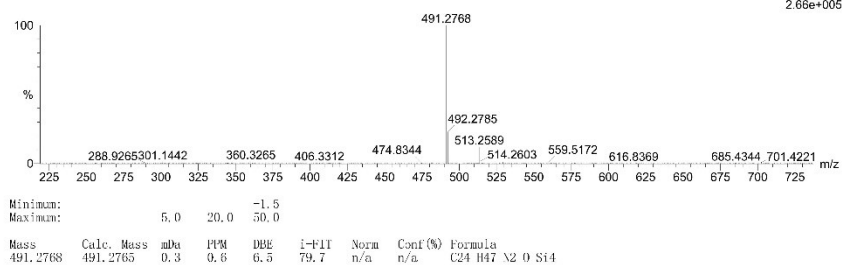
Elemental Composition Report

Page 1

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 2908 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 24-24 H: 47-47 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4
 7
 230519-7-359-3-L-21 24 (0.271)



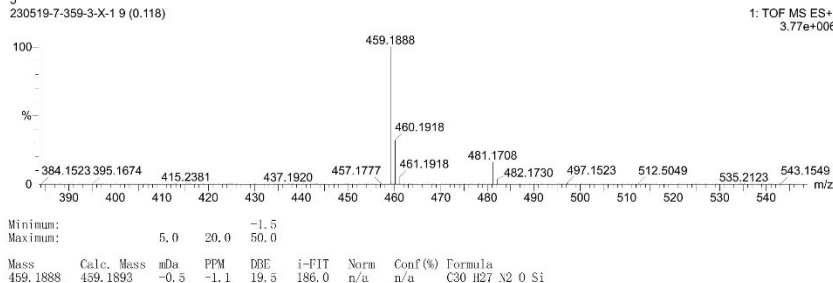
HRMS spectra of 5a: $[M+H]^+$ Calcd for $C_{30}H_{27}N_2OSi$ 459.1893; Found 459.1888.

Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 1545 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 30-30 H: 27-27 N: 0-100 O: 0-100 Na: 0-1 Si: 1-2
 5
 230519-7-359-3-X-1 9 (0.118)



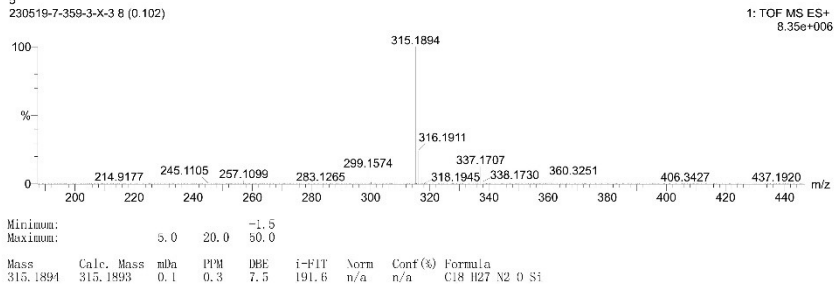
HRMS spectra of 5b: [M+H]⁺ Calcd for C₁₈H₂₇N₂OSi 315.1893; Found 315.1894.

Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 1083 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 18-18 H: 27-27 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4
 5
 230519-7-359-3-X-3 8 (0.102)



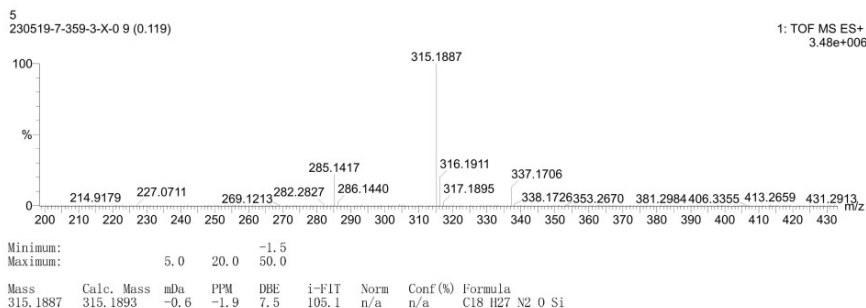
HRMS spectra of 5c: [M+H]⁺ Calcd for C₁₈H₂₇N₂OSi 315.1893; Found 315.1887.

Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0
 Element prediction: Off
 Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
 648 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)
 Elements Used:
 C: 18-18 H: 27-27 N: 0-100 O: 0-100 Na: 0-1 Si: 1-2



HRMS spectra of 5d: [M+H]⁺ Calcd for C₁₉H₂₉N₂OSi 329.2049; Found 329.2044.

Elemental Composition Report

Single Mass Analysis

Tolerance = 20.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

1206 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

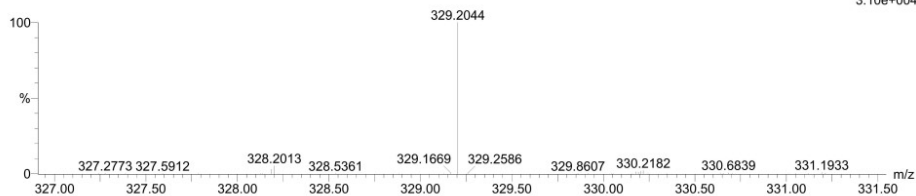
Elements Used:

C: 19-19 H: 29-29 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4

5

230519-7-359-3-X-12 10 (0.127)

1: TOF MS ES+
3.10e+004



Minimum: 5.0 20.0 -1.5
Maximum: 50.0

Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula
329.2044	329.2049	-0.5	-1.5	7.5	180.7	n/a	n/a	C19 H29 N2 O Si