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 ¹³C NMR spectra were recorded using a Bruker DRX-500 spectrometer employing CDCl₃ 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 roundbottom flask were heated at 120 °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 (3×20 mL) and dried to give quinazoline-4(3H)-one derivatives (**B**). These intermediates were used for the next step without further purification. To a solution of quinazoline-4(3H)- 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), CoBr₂ (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 MgSO₄, 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), $CoBr_2$ (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 H_2 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 H_2 detector under standard conditions. Just as shown in Figure S2, as the reaction proceeded, the H_2 was observed clearly and the concentration increased gradually.



Figure S2. H_2 detection experiment by a H_2 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 H_2 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 H_2 detector under standard conditions. Just as shown in Figure S3, as the reaction proceeded, the H_2 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.

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.

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(1H)-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(1H)-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(1H)-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(1H)-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)-2,3dihydropyrrolo[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, 5.7Hz, 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-**

11*H*-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-11*H*-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-11*H*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-

11*H*-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-11*H*-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-11*H*-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-6,8,9,11tetrahydro-7*H*-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-11*H*-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 C23H45N2OSi4 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-((triphenylsily1)methy1)-2,3-dihydropyrrolo[2,1-***b***]quinazolin-9(1***H***)-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(1H)-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-11H-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(1H)-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(1H)-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(1H)-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, JC-F = 251.3 Hz), 163.76, 160.30, 151.6 (d, JC-F = 13.8 Hz), 128.9 (d, JC-F = 10.0 Hz), 117.4 (d, JC-F = 2.5 Hz), 114.9 (d, JC-F = 23.8 Hz), 112.4 (d, JC-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(1H)-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(1H)-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, JC-F = 14.3 Hz), 164.5 (q, JC-F = 8.8 Hz), 163.57 (d, JC-F = 15.0 Hz), 161.44 (d, JC-F = 14.9 Hz), 157.50 (d, JC-F = 3.6 Hz), 153.03 (d, JC-F = 14.4 Hz), 108.77 (dd, JC-F = 21.8, 4.5 Hz), 102.56 (dd, JC-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 ¹³C NMR spectra

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

0 Si-Si. Si. T Ч T Ч Ч Ч ٣ Ч Ч -00 00. 00. 8. 8. 00. 00. 00.3 8. 00. -2.5 7.5 5.0 4.5 f1 (ppm) 0.5 8.5 8.0 7.0 5.5 4.0 3.5 3.0 2.0 1.0 9.0 6.5 6.0 1.5 0. ¹³C{¹H} NMR spectrum of 3a (125 MHz, CDCl₃) _162.74 ~161.08 -149.52126.07 44.27 43.46 -29.49 -10.84133.95 -1.36Śi 180 100 90 f1 (ppm) 170 160 150 130 120 110 80 70 60 30 20 10 0 140 50 40



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





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







7.1.6 7.

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











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





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



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

-101.27-101.27-101.31-101.33-106.23-106.25



20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22 fl (ppm)



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





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



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



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





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



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



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



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



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



4.5 4.0 f1 (ppm)

3.5

3.0

2.5

2.0

1.0

1.5

0.5

0.0

5.0

5.5

8.0

8.5

7.5

7.0

6.5

6.0

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



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



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



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





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



¹⁹F NMR spectrum of 4d (125 MHz, CDCl₃)



20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22 fl (ppm)





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

¹⁹F NMR spectrum of 4e (125 MHz, CDCl₃)



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



S41

4.5 f1 (ppm)

4.0

3.5

5.0

5.5

6.0

8.5

8.0

7.5

7.0

6.5

3.0

2.5

2.0

1.5

1.0

0.5

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



¹⁹F NMR spectrum of 4g (125 MHz, CDCl₃)



20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22 fl (ppm)

88.88.20 88.20 88.20 88.20 98.20 98.20 98.20 98.20 96.20 96.20 97.79 96.20 96.20 96.20 96.20 96.20 96.20 96.20 96.20 96.20 96.20 96.20 97.79 96.20 96.

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)

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

S45

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

88.828 88.829 88.829 88.829 88.827 88.827 88.827 88.829 88

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

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

8,829 8,339 8,4239 8,349 8,349

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

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

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

8.8.16 8.8.14 8.8.14 7.7.55 7.7.75 8.8.14 7.7.75 7.75 7.7

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

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

S53

¹⁹F NMR spectrum of 6c (125 MHz, CDCl₃)

-104.07 -104.09 -104.11 -104.12 0 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22 f1 (ppm) 20 10 -10 -20 -30 -50 -60 0 -40 ¹H NMR spectrum of 6d (500 MHz, CDCl₃) CI 1.00-1 1.00-1 1.00-1 1.00-1 1.00-1 3.00H 1.00-1 1.004 $1.00 \pm$

5.5 5.0 f1 (ppm)

6.0

6.5

8.5 8.0 7.5 7.0

9.0

10.0 9.5

4.5 4.0

3.5

3.0 2.5 2.0

1.5

1.0 0.5

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

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

7.15 6.88 7.87 7.87

¹⁹F NMR spectrum of 6e (125 MHz, CDCl₃)

-101.02 -101.04 -101.06 -101.08 -106.09 -106.11

20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -22 fl (ppm)

M. Copies of HRMS Spectra

HRMS spectra of 3a: [M+H]⁺ Calcd for C₂₁H₃₉N₂OSi₄ 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+
447.2139	6.12e+005
% 448.2155 0 282.9097 301.1447 360.3237 373.1590 431.1869 469.1957 485.1787 559.5223 591.5062 616.8511	685.4485 m/z
240 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 580 600 620 640 6	60 680
Minimum: -1.5 Maximum: 5.0 20.0 50.0	
Mass Calc. Mass mDa PPM DBE i=F1T Norm Conf(%) Formula 447.2139 447.2139 0.0 0.0 7.5 89.5 n/a n/a C21 H39 N2 0 Si4	

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

Elemental Compo	osition Report	Page 1
Single Mass Anal Tolerance = 20.0 PP Element prediction: (Number of isotope p	alysis PM / DBE: min = -1.5, max = 50.0 Off peaks used for i-FIT = 3	
Monoisotopic Mass, Ev 2501 formula(e) evalua Elements Used: C: 22-22 H: 41-41 7	Even Electron lons Jated with 1 results within limits (up to 50 closest results for each mass) 1 N: 0-100 O: 0-100 Na: 0-1 Si: 1-4	
230519-7-359-3-X-25 16	6 (0.187)	1: TOF MS ES+ 9.04e+006
100	461,2299	
%-	462.2309	
	463.2288	
0 125.9846	214.9176271.1268 387.1735 4453.2110 559.5190 613.1828 685.4489 820).5547 891.7269 m/z
100 150	200 250 300 350 400 450 500 550 600 650 700 750 800	850 900
Minimum: Maximum:	5.0 20.0 5.0 5.0	
Mass Calc. Mas: 461.2299 461.2296	ss mDa PPM DBE i-FIT Norm Conf(%) Formula 0.3 0.7 7.5 214.2 n/a n/a C22 H41 N2 0 Si4	

HRMS spectra of 3c: [M+H]⁺ Calcd for C₂₂H₄₁N₂O₂Si₄ 477.2240; Found 477.2248.

Element	al Compos	sition	Repor	t									Page 1
Single N Tolerance Element p Number o	lass Analy = 20.0 PPM prediction: O of isotope per	r sis A / E ff aks us)BE: mii ed for i-	n = -1.5 FIT = 3	, max =	50.0							
Monoisoto 2674 form Elements 0 C: 22-22 7 230519-7-3	pic Mass, Eve ula(e) evaluat Jsed: H: 41-41 59-3-X-21 14 (0	en Elec ed with N: 0-1 0.169)	tron lons 1 result: 100 O:	s within I : 0-100	imits (up Na: 0-	to 50 cl -1 Si:	osest n 1-4	esults for	each mass)			1: TC	OF MS ES+
		,					477 00.	10					1.51e+006
100-							411.22	10					
%-				152,5909	101.0		4	78.2263	499.2066		531.4835		548.8295
0 410	422.2972	430	440	450	461.1	470	45	400.2255	0 500	510 5	20 530	540.2479	550 m/z
Minimun: Maximun:		5.0	20.0	-1, 5 50, 0	400	470			5 500	515 5	20 330	540	
Mass 477.2248	Calc. Mass 477.2245	mDa 0, 3	PPM 0, 6	DBE 7,5	i-FIT 123.2	Norm n/a	Conf (n/a	8) Formul C22 14	.a 11 N2 O2 S14				

HRMS spectra of 3d: [M+H]⁺ Calcd for C₂₃H₄₃N₂O₃Si₄ 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) 1: 1: 1:	TOF MS ES+									
100 507.2359	1.71e+006									
%- 301.1447 338.3448 360.3243 376.3039 433.1803 491.2076 529.2177 545.1965 587.5657 649.6773 685.4514 725.314	38 761.2920									
275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725	750 m/z									
Minimum: -1.5 Maximum: 5.0 20.0 50.0										
Mass Calc. Mass mDa PPM DBE i-FIT Norm Conf (%) Formula 507.2359 507.2351 0.8 1.6 7.5 168.0 n/a n/a C23 H43 N2 03 Si4										

HRMS spectra of 3e: [M+H]⁺ Calcd for C₂₁H₃₇FN₂OSi₄ 465.2040; Found 465.2044.

Eleme	ental Compo	sition Repo	rt							Page 1
Single Tolerar Elemer Numbe	e Mass Analy nce = 20.0 PP nt prediction: C er of isotope pe	/sis M / DBE: m Off eaks used for	in = -1.5, max = 5 i-FIT = 3	0.0						
Monoiso 2305 for Element C: 21-2	otopic Mass, Ev rmula(e) evalua ts Used: 1 H: 38-38 N	en Electron Ion ted with 1 resul I: 0-100 O: 0-	s ts within limits (up t 100 Na: 0-1 Si:	o 50 closes 1-4 F: 1-	t results for each	n mass)				
7 230519-	7-359-3-X-17 15 (0.178)							1:	TOF MS ES+
100				465.2	2044					4.258+000
%	93.1494 406.3	²⁹⁸ 422.3028	438.2561 449.172	9 453.1921	466.2061 467.2038 468.2034 48	7.1862	503.1624	515.1829	528.2134	535.2566
0	400 410	420 43	80 440 450	460	470 480	490	500 5	510 520	530	540
Minimum Maximum	1:	5.0 20.0	-1.5 50.0							
Mass 465.204	Calc. Mass 4 465.2045	mDa PPM -0.1 -0.2	DBE i-F1T 7.5 152.7	Norm Con n/a n/a	f(%) Formula C21 H38 N2	2 0 Si4 F				

HRMS spectra of 3f: [M+H]⁺ Calcd for C₂₁H₃₇F₂N₂OSi₄ 483.1946; Found 483.1945.

Eleme	ental Compo	sition Re	port						Page 1
Single Toleran Elemen Number	e Mass Analy nce = 20.0 PPI nt prediction: C er of isotope pe	/sis M / DBE off eaks used f	: min = -1.5, for i-FIT = 3	max = 50.0					
Monois 2299 fo Elemen C: 21-2 7 230519-	otopic Mass, Ev rmula(e) evalua ts Used: 21 H: 37-37	en Electron ted with 1 re N: 0-100	lons sults within lin O: 0-100	nits (up to 50 clos F: 2-2 Na: 0-	sest results fo 1 Si: 1-4	r each mass)			1: TOE MS ES+
200010-	1-000-0-7-20 14 (0.103)		402	1045				3.87e+006
					484 1959	505.1765			
-						50E 1770			
0	422.2967 43	37.2442446.8	016,451.1469	467.1631	485.1938	507.17	56 521.15	542.2692.546	3.2075 559.5217
0 -	420 430	440	450 460	470 480	490	500 510	520	530 540	550 560
Minimum Maximum	12	5.0 20	-1.5 0.0 50.0						
Mass 483.194	Calc. Mass 5 483,1951	mDa Pl -0.6 -1	M DBE 1,2 7,5	i-F1T Norm (141.0 n/a n	Conf(%) Form n/a C21	ula H37 X2 0 F2 Si4			

HRMS spectra of 3g: [M+H]⁺ Calcd for C₂₁H₃₈ClN₂OSi₄ 481.1744; Found 481.1745.

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 CI: 0-4 $\frac{5}{230519-7:359-3\times-13} = 20.254)$ 1: TOF MS ES+ 1.656+005 1: TOF MS ES+ 1.650+005 1: TOF MS ES+

Page 1

HRMS spectra of 3h: [M+H]⁺ Calcd for C₂₂H₃₈F₃N₂OSi₄ 515.2008; Found 515.2009.

Elemen	tal Compo	sition	Repor	t										Page 1
Single I Tolerance Element Number o	Mass Analy e = 20.0 PPI prediction: C of isotope pe	ysis M / D Off eaks use	BE: mir ed for i-	n = -1.5, FIT = 3	max =	50.0								
Monoisoto 2470 form Elements C: 22-22 7 230519-7-3	opic Mass, Ev iula(e) evalua Used: H: 38-38 359-3-X-27 13 (en Electr ted with N: 0-10	ron lons 1 result: 00 O:	s within li 0-100	mits (up F: 3-3	to 50 o Na:	closest r 0-1 S	esults for ea ii: 1-4	ach ma	ss)			1: 1	OF MS ES+
20001011							515	2009						6.31e+006
100 %								516.2019						
-								517.2030						
0	457.1441	474.8448	480.85	01	499.	1689		518.2047	5	37.1822	547.1967	559.5176.56	3.1951	578.2103
450	460	470	480	490	5	00	510	520	530	540	550	560	570	580
Minimum: Maximum:		5.0	20.0	$^{-1.5}_{50.0}$										
Mass 515,2009	Calc. Mass 515,2013	mDa -0.4	PPM -0.8	DBE	i-FIT 181.7	Norm n/a	Conf (%) Formula C22 H38	N2 0 I	3 Si4				

HRMS spectra of 3i: [M+H]⁺ Calcd for C₂₃H₄₁N₂O₃Si₄ 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 Elements Used: C: 23-23 H: 41-41 N: 0-100 O: 0-100 Si: 1-4	mass)
2 230525-1-362-1-X20 13 (0.161)	1: TOF MS ES+
100 505,2192	Suberood
% 506.2209	
- 437.2456 458.9177 474.8321 489.1877 507.2191 508.2195 527.2010 520.529.2012 440 450 450 460 470 480 490 500 510 510 520 530 54	2 543.1780 568.2326 581.2926 595.2002 m/z 0 550 570 580 590 600
Mininum: -1.5 Maxinum: 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 N	2 03 Si4

HRMS spectra of 3j: [M+H]⁺ Calcd for C₂₇H₅₁N₂O₅Si₄ 595.2870; Found 595.2882.

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+006 595.2882 100 596.2897 617.2699 % 597.2888 618.2716
 523.2311
 537.5392
 559.5159
 579.2560
 598.2902
 619.2714
 643.2731
 663.4527

 530
 540
 550
 560
 570
 580
 590
 600
 610
 620
 630
 640
 650
 660
 670
 680
 688.5240, m/z Minimum: Maximum: 5.0 20.0 -1.550.0 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 05 Si4

Page 1

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	
230519-7-359-3-L-1 13 (0.161)	1: TOF MS ES+ 6.65e+006
100 461.2298	
%	
463.2287	
0 406.3325 412.8734 430.2673 445.1986 ^{459.2176} 404.2200 483.2110 499.1830	508.0012 524.2401 532.8604 m/z
400 410 420 430 440 450 460 470 480 490 500	510 520 530
Minimum: -1.5 Maximum: 5.0 20.0 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 C221H41 N2 0 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+
100 475.2448	6.16e+005
%- 476.2463	
282.9116 301.1404 360.3270 412.8711 474.8528 477.4243 513.2057 559.5215 587.5421 616.8358 260 280 300 320 340 360 380 400 420 440 460 480 500 520 540 560 620 640 6	685.4372 m/z 60 680 700
Minimum: -1.5 Maximum: 5.0 20.0 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 0 Si4	

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

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) 1: TOF MS ES+ 6.67e+006 521.2510 100 522.2520 % 523.2499 543.2322 685.4310 803.3365 880.5626 933.5334 214.9178 301.1469 381.2974 447.1947 0 m/z 600 1000 200 300 400 500 700 800 900 Minimum: Maximum: 5.0 20.0 ^{-1.5} 5.0 20.0
 Mass
 Calc. Mass
 mDa
 PPM
 DBE
 i=F1T
 Norm
 Conf (%)
 Formula

 521.2510
 521.2507
 0.3
 0.6
 7.5
 238.4
 n/a
 n/a
 C24 H45 N2 03 Si4

Page 1

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

Eleme	ntal Compo	sition R	eport									P	age 1
Single Toleran Elemen Numbe	Mass Analy ce = 20.0 PPI t prediction: C r of isotope pe	/sis M / DBI off eaks used	E: min = -1.4	5, max = 50.0 3									
Monoiso 2490 for Element C: 22-22	topic Mass, Ev mula(e) evaluat s Used: P. H: 40-40 N	en Electro ted with 1 I: 0-100	n lons results within O: 0-100 N	limits (up to 50 a: 0-1 Si: 1-4) closest re F: 1-1	esults for	each mass)						
5 230519-7	7-359-3-L-15 21 (I	0.246)										1: TOF	MS ES+
100					479.2	2204							
%	282.9079 301	.1428	360.3261	405.1648 418.8	3907	480.2219 481.2199 482.2211	559.5	5309	587.5673	643.2528	685.4	304 72	1.1242 .
0	250 275 3	300 325	350 375	400 425	450 475	500	525 550	575	600 6	25 650	675	700	725
Minimum Maximum		5.0	-1.5 20.0 50.0										
Mass 479.220	Calc. Mass 4 479.2202	mDa 1 0.2	PPM DBE 0.4 7.5	i-FIT Nor 120.8 n/a	m Conf(n/a	6) Formul C22 H4	a 0 N2 0 Si4	F					

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)	1: TOF MS ES+
497.2104	1.172-000
% 520.1937 521.1915 559.5148 610.8058 685.4452 7	773 2413 789 2404
250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700 725	750 775 800
Minimum: -1.5 Maximum: 5.0 20.0 50.0	
Mass Calc. Mass mDa PPM DBE i-F1T Norm Conf(%) Formula 497,2104 497,2108 -0.4 -0.8 7.5 104.9 n/a n/a C22 H39 N2 0 Si4 F2	

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

Element	al Composition F	Report			
Single N	ass Analysis		50.0		
Flomont	= 5.0 mDa / DBt	$=: \min = -1.5, r$	nax = 50.0		
Number of	isotope peaks use	d for i-FIT = 3			
Monoisoto 501 formul	ic Mass, Even Electr a(e) evaluated with 1	on lons results within lir	nits (up to 5	best isotopic matches for each mass)	
Elements I	sed:			,	
C: 22-22	H: 40-40 N: 0-20	00 O: 0-200	Si: 4-4	: 1-2	
3 230904-1-4	7-2-1-12 27 (0 265)				
20000114	1 2 2 12 21 (0.200)				
100			495	09	
1				497 1876	
-					
0/					
/0				498 1879	
				100.1010	

Page 1

1: TOF MS ES+ 1.25e+007

 432.2763.437.2452
 463.7565
 479.1573.483.1604
 490.1858

 0
 430.450
 440
 450.1753.483.1604
 450.501.1854
 532.4432.537.5253
 559.5308.564.3655
 578.3791

 Minimum:
 -1.5
 -1.5
 -1.5
 -1.5
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HRMS spectra of 4g: [M+H]⁺ Calcd for C₂₃H₄₀F₃N₂OSi₄ 529.2170; Found 529.2170.

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

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

Elemental Composition Report	Elemental	Composition	Report
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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 cl Elements Used: C: 28-28 H: 53-53 N: 0-100 O: 0-100 Si: 1-4	osest results for each mass)
230704-4-386-3-I-22- 30 (0.339)	1: TOF MS ES+
100 - 609	9.3037
	631.2855
% 344.2271 388.2518 424 3600 512.4127 535.2471 559.5186	632.2874 633.2858 634.2861 679.2707 775 3178 803.5692 851.7923 909 3897
350 375 400 425 450 475 500 525 550 575 60	0 625 650 675 700 725 750 775 800 825 850 875 900
Minimum: -1.5 Maximum: 5.0 20.0 50.0	
Mass Calc. Mass mDa PPM DBE i-FIT Norm 609.3037 609.3032 0.5 0.8 7.5 447.2 n/a	Conf (%) Formula n/a C28 1153 N2 05 Si4

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HRMS spectra of 1'j-A: [M+H]⁺ Calcd for C₂₃H₄₅N₂OSi₄ 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)	1: TOF MS ES+
100 477.2608	1.97e+005
%- 282.9048301.1449 360.3261 406.3273 474.8393 500.2444 559.5182 587.5515 621.7825 685.4429	747.8171784.5114
225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650 675 700	725 750 775
Minimum: -1.5 Maximum: 5.0 20.0 50.0	
Mass Calc. Mass mDa PPM DBE i-F1T Norm Conf(%) Formula 477.2608 477.2609 -0.1 -0.2 6.5 94.3 n/a n/a C23 H45 N2 0 Si4	

HRMS spectra of 1'k-A: [M+H]⁺ Calcd for C₂₄H₄₇N₂OSi₄ 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)	1: TOF MS ES+ 2 66e+005
100 491.2768	
% 492.2785 492.2785 513.2889 544.2603 559.5172 616.8369	685.4344_701.4221
225 250 275 300 325 350 375 400 425 450 475 500 525 550 575 600 625 650	675 700 725
Minimum: -1.5 Maximum: 5.0 20.0 50.0	
Mass Calc. Mass mDa PPM DBE i=ElT Norm Conf(%) Formula 491.2768 491.2765 0.3 0.6 6.5 79.7 n/a n/a C24.147 N2 0 Si4	

HRMS spectra of 5a: [M+H]⁺ Calcd for C₃₀H₂₇N₂OSi 459.1893; Found 459.1888.

Elemen	tal Compo	sition	Repo	rt								<u>_</u>	Page 1
Single I Tolerance Element Number o	lass Analy e = 20.0 PP prediction: C of isotope pe	ysis M / D Off eaks us	BE: m	in = -1.5 i-FIT = 3	, max =	50.0							
Monoisoto 1545 form Elements	pic Mass, Ev ula(e) evalua Used:	en Elect ted with	ron lon 1 resul	s ts within	imits (up	to 50 c	losest res	ults for ea	ach mass)				
C: 30-30	H: 27-27	N: 0-1	00 C	0: 0-100	Na: 0	-1 Si:	1-2						
5 230519-7-3	59-3-X-1 9 (0.	118)										1: TO	F MS ES+
100-						459	9.1888						5.176.00
100-													
-													
%-													
							460.191	В					
							lf -	401	1709				
- 384.	1523 395.1674	415.2	381	437.	1920 4	57.1777	461.19	18 401.	482.1730	497.1523	512.5049	535.2123	543.1549
3	90 400	410	420	430	440	450	460 4	70 48	0 490	500 5	10 520	530 540	- Tr + 11/2
Minimum:				-1.5									
Maximum;		5.0	20.0	50.0									
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Norm	Conf (%)	Formula					
459.1888	459.1893	-0.5	-1.1	19.5	186.0	n/a	n/a	C30 H27	N2 0 Si				

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

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

Elemental Composition	Report	Page 1
Single Mass Analysis Tolerance = 20.0 PPM / D Element prediction: Off Number of isotope peaks use	BE: min = -1.5, max = 50.0 ed for i-FIT = 3	
Monoisotopic Mass, Even Elect 648 formula(e) evaluated with 1 Elements Used: C: 18-18 H: 27-27 N: 0-100	on lons results within limits (up to 50 closes O: 0-100 Na: 0-1 Si: 1-2	t results for each mass)
5 230519-7-359-3-X-0 9 (0.119)		1: TOF MS ES+
100	3	15.1887
%		
	285.1417	316.1911 337.1706
214.9179 227.0711	269.1213 282.2827 286.1440	317.1895 338.1726353.2670 381.2984406.3355 413.2659 431.2913,
200 210 220 230 240	250 260 270 280 290 300 3 ⁻	0 320 330 340 350 360 370 380 390 400 410 420 430
Minimum: Maximum: 5.0	$ \begin{array}{ccc} -1.5 \\ 20.0 & 50.0 \end{array} $	
Mass Calc. Mass mDa	PPM DBE i-FIT Norm Co	nf(%) Formula a C18 H27 N2 O Si

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

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)

100							329.204	4					3.10e+004
%													
0	327.2773 327.	5912	32	8.2013	328.5361	329	.1669 3	29.2586	329.860	7 330.2182	330.6839	331.1933	m/z
327.00	327.5	D	328.00		328.50	329	9.00	329.50	33	0.00	330.50	331.00	331.50
Minimum: Maximum:		5.0	20.0	-1.5 50.0									
Mass 329.2044	Calc. Mass 329.2049	mDa -0.5	PPM −1.5	DBE 7.5	i-FIT 180.7	Norm n/a	Conf (% n/a) Formula C19 H29	N2 O Si				

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1: TOF MS ES+

S65