Supplementary information

Oxidative Radical Si-Incorporation: A Selective and Facile Entry to Si-Containing Heterocycles

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(A) General Information

\(^1\)H NMR, \(^{13}\)C NMR and \(^{19}\)F NMR spectra were recorded on a Bruker 400 MHz or 500 MHz advance spectrometer at room temperature in CDCl\(_3\) with tetramethylsilane as internal standard. Low-resolution mass spectra (LRMS) data were measured on GCMS-QP2010 Ultra. High-resolution mass spectra (HRMS) was recorded on an electrospray ionization (ESI) apparatus using time-of-flight (TOF) mass spectrometry. Melting Point were recorded on Hanon MP100 Apparatus. All products were identified by \(^1\)H and \(^{13}\)C NMR, HRMS. Unless otherwise noted, all reactions were carried out using standard Schlenk techniques, and all starting materials and solvents were commercially available and were used without further purification. Column chromatography was performed on silica gel (300-400 mesh) using petroleum ether (PE)/ethyl acetate (EA).

(a) Typical Experimental Procedure for Synthesis of Silino[3,4-c]quinolin-5(3\(H\))-ones (3):

To a Schlenk tube were added \(N\)-\(2\)-(Ethynyl)aryl)acrylamides 1 (0.2 mmol), silanes 2 (3 equiv), Cu(MeCN)\(_4\)PF\(_6\) (10 mol%), TBPB (4 equiv), and PhCF\(_3\) (2 mL). Then the tube is evacuated briefly under high vacuum and charged with argon through using standard Schlenk techniques; this process is repeated three times. Then the reaction mixture was stirred at 120 °C (oil bath temperature) for the indicated time (about 48 h) until complete consumption of starting material as monitored by TLC and/or GC-MS analysis. After the reaction was finished, the reaction mixture was filtered through Celite to give a light yellow solution, and concentrated in vacuum. The resulting residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate) to afford the desired products 3.
(b) Typical Experimental Procedure for Synthesis of Silolo[3,4-c]quinolin-4-ones (5):

To a Schlenk tube were added N-(2-(Ethynyl)aryl)acrylamides 1 (0.2 mmol), silanes 2 (2 equiv), TBPB (2 equiv), and PhCF₃ (2 mL). Then the tube is evacuated briefly under high vacuum and charged with argon through using standard Schlenk techniques; this process is repeated three times. Then the reaction mixture was stirred at 120 °C (oil bath temperature) for the indicated time (about 15 h) until complete consumption of starting material as monitored by TLC and/or GC-MS analysis. After the reaction was finished, the reaction mixture was filtered through Celite to give a light yellow solution, and concentrated in vacuum. The resulting residue was purified by silica gel column chromatography (petroleum ether/ethyl acetate) to afford the desired products 5.

(c) Optimization of the reaction conditions

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[a] Standard conditions: 1a (0.2 mmol), 2a (3 equiv), Cu(MeCN)₄PF₆ (10 mol%), TBPB (4 equiv), PhCF₃ (2 mL), 120 °C, argon and 48 h. [b] Yield is that of the isolated product. [c] 1a (1 mmol).
(d) NOE of product 3ad
(e) GC-MS analysis of trimethylsilyl benzoate

![Diagram of trimethylsilyl benzoate structure]

[MS Spectrum]

# of Peaks  197

Raw Spectrum 6.190 (scan : 539)  Base Peak  m/z 178.85 (Inten : 1,904,850)

Background  6.155 (scan : 532)

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(B) Analytical data

3,3-diisopropyl-2,2,4a,6-tetramethyl-1-phenyl-2,4,4a,6-
tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3aa): White solid, 
mp 136.6-138.4 °C (uncorrected); \(^1\)H NMR (400 MHz, CDCl\(\text{3}\)) \(\delta\): 
7.42 (d, \(J = 7.6\) Hz, 1H), 7.27 (d, \(J = 6.8\) Hz, 1H), 7.09 (t, \(J = 7.4\) Hz, 1H), 6.97-6.92 (m, 2H), 6.80 (d, \(J = 8.0\) Hz, 1H), 6.55 (d, \(J = 7.6\) Hz, 1H), 6.48 (t, \(J = 7.4\) Hz, 1H), 6.43 (d, \(J = 7.6\) Hz, 1H), 3.36 (s, 3H), 2.41 (d, \(J = 15.6\) Hz, 1H), 1.42 (s, 3H), 1.20-1.19 (m, 7H), 1.15 (s, 4H), 1.13 (s, 3H), 1.05-1.04 (m, 3H), 0.89 (d, \(J = \)
15.2 Hz, 1H), 0.83 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 174.6, 149.0, 141.0, 138.7, 132.8, 131.4, 130.8, 130.3, 129.1, 127.9, 126.4, 126.2, 125.9, 121.4, 112.9, 45.7, 30.7, 30.4, 28.9, 24.0, 23.3, 19.6, 19.5, 19.4, 18.9, 13.9, 11.5, 10.8; LRMS (EI, 70 eV) m/z (%): 431 (M$^+$, 1), 416 (100), 330 (7); HRMS m/z (ESI) calcd for C$_{28}$H$_{38}$NOSi [M+H]$^+$ 432.2717, found 432.2725.

6-benzyl-3,3-diisopropyl-2,2,4a-trimethyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ba): Colorless oil; $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.43 (d, $J = 7.6$ Hz, 1H), 7.31-7.25 (m, 3H), 7.23-7.19 (m, 3H), 7.08 (t, $J = 7.4$ Hz, 1H), 6.99 (t, $J = 7.6$ Hz, 1H), 6.81 (t, $J = 7.6$ Hz, 1H), 6.71 (d, $J = 8.0$ Hz, 1H), 6.57 (d, $J = 7.6$ Hz, 1H), 6.44 (t, $J = 7.6$ Hz, 1H), 6.40 (d, $J = 7.6$ Hz, 1H), 5.32 (d, $J = 16.0$ Hz, 1H), 5.02 (d, $J = 16.0$ Hz, 1H), 2.46 (d, $J = 15.6$ Hz, 1H), 1.41 (s, 3H), 1.27 (s, 3H), 1.21-1.20 (m, 7H), 1.15 (s, 4H), 1.08-1.07 (m, 3H), 0.93 (d, $J = 15.6$ Hz, 1H), 0.88 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 174.5, 149.6, 140.9, 137.9, 137.4, 132.6, 131.5, 130.8, 130.4, 129.4, 128.5, 127.9, 126.9, 126.4 (2C), 126.2, 125.9, 121.6, 114.1, 47.2, 45.8, 30.3, 28.8, 24.2, 23.5, 19.7, 19.5 (2C), 19.0, 13.7, 11.5, 11.0; LRMS (EI, 70 eV) m/z (%): 492 (M$^+$-15, 100), 386 (3), 91 (40); HRMS m/z (ESI) calcd for C$_{34}$H$_{42}$NOSi [M+H]$^+$ 508.3030, found 508.3041.

6-allyl-3,3-diisopropyl-2,2,4a-trimethyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ca): Colourless oil; $^1$H NMR (500 MHz, CDCl$_3$) δ: 7.43 (d, $J = 7.5$ Hz, 1H), 7.28 (td, $J = 7.5$, 1.0 Hz, 1H), 7.09 (t, $J = 7.5$ Hz, 1H), 6.96-6.89 (m, 2H), 6.80 (d, $J = 8.0$ Hz, 1H), 6.56 (dd, $J = 7.5$, 1.5 Hz, 1H), 6.48-6.45 (m, 1H), 6.43 (d, $J = 7.5$ Hz, 1H), 5.92-5.85 (m, 1H), 5.17 (dd, $J = 10.5$, 1.0 Hz, 1H), 5.11 (dd, $J = 17.5$, 1.5 Hz, 1H), 4.74-4.70 (m, 1H), 4.39-4.35 (m, 1H), 2.43 (d, $J = 15.5$ Hz, 1H), 1.42 (s,
3,3-diisopropyl-2,2,4a-trimethyl-1-phenyl-6-tosyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3da): Light yellow solid, mp 160.1-162.2 °C (uncorrected); \(^1\)H NMR (500 MHz, CDCl\(_3\)) δ: 8.04 (d, \(J = 8.5\) Hz, 2H), 7.58 (d, \(J = 8.0\) Hz, 1H), 7.41-7.38 (m, 3H), 7.32 (t, \(J = 7.3\) Hz, 1H), 7.18 (t, \(J = 7.5\) Hz, 1H), 7.11 (td, \(J = 7.5, 0.5\) Hz, 1H), 7.09-7.05 (m, 1H), 6.79-6.76 (m, 1H), 6.67 (dd, \(J = 7.5, 1.0\) Hz, 1H), 6.57 (d, \(J = 7.5\) Hz, 1H), 2.47 (s, 3H), 2.06 (d, \(J = 15.5\) Hz, 1H), 1.26 (s, 3H), 1.20-1.19 (m, 7H), 1.08 (s, 4H), 1.01 (s, 3H), 0.92-0.89 (m, 4H), 0.80 (s, 3H); \(^1\)C NMR (125 MHz, CDCl\(_3\)) δ: 174.6, 151.0, 144.8, 140.0, 136.7, 133.6, 132.8, 131.1, 130.9, 130.6, 130.1, 129.3, 129.0, 128.3, 126.3 (3C), 125.0, 122.1, 48.5, 29.1, 27.8, 25.0, 23.6, 21.6, 20.0, 19.6, 19.2, 17.7, 14.1, 11.1 (2C); LRMS (EI, 70 eV) \(m/z\) (%): 416 (M\(^+\)-155, 100), 386 (8), 131 (70), 91 (22); HRMS \(m/z\) (ESI) calcd for C\(_{39}\)H\(_{40}\)NO\(_3\)Si [M+H]\(^+\) 572.2649, found 572.2661.

3,3-diisopropyl-2,2,4a-trimethyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ea): White solid, mp 250.1-251.8 °C (uncorrected); \(^1\)H NMR (400 MHz, CDCl\(_3\)) δ: 8.21 (s, 1H), 7.43 (d, \(J = 6.8\) Hz, 1H), 7.28 (d, \(J = 9.6\) Hz, 1H), 7.11 (t, \(J = 6.4\) Hz, 1H), 6.94 (t, \(J = 7.0\) Hz, 1H), 6.89 (t, \(J = 7.2\) Hz, 1H), 6.62 (d, \(J = 7.2\) Hz, 1H), 6.52 (d, \(J = 7.2\) Hz, 1H), 6.45-6.38 (s, 2H), 2.40 (d, \(J = 15.2\) Hz, 1H),
1.44 (s, 3H), 1.24-1.09 (m, 17H), 0.89 (d, J = 15.6 Hz, 1H), 0.83 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 176.1, 150.2, 141.1, 135.3, 132.3, 131.7, 130.6, 130.2, 128.0, 127.2, 126.5, 126.3, 126.0, 121.4, 113.8, 45.4, 30.6, 29.1, 23.9, 23.5, 19.7 (2C), 19.5, 19.0, 12.8, 11.4, 10.8; LRMS (EI, 70 eV) m/z (%): 417 (M$^+$, 1), 402 (100), 316 (6); HRMS m/z (ESI) calcd for C$_{27}$H$_{36}$NOSi [M+H]$^+$ 418.2561, found 418.2567.

3,3-diisopropyl-2,2,4a,6-tetramethyl-1-(p-tolyl)-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3fa): White solid, mp 134.2-135.5 °C (uncorrected); $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.30 (d, J = 7.6 Hz, 1H), 7.08 (d, J = 8.0 Hz, 1H), 6.96 (t, J = 7.6 Hz, 1H), 6.80 (d, J = 8.0 Hz, 1H), 6.74 (d, J = 7.6 Hz, 1H), 6.57 (d, J = 7.6 Hz, 1H), 6.50 (t, J = 7.4 Hz, 1H), 6.30 (d, J = 8.0 Hz, 1H), 3.36 (s, 3H), 2.40 (d, J = 15.2 Hz, 1H), 2.25 (s, 3H), 1.40 (s, 3H), 1.19-1.18 (m, 7H), 1.14 (s, 4H), 1.11 (s, 3H), 1.03-1.02 (m, 3H), 0.88 (d, J = 15.2 Hz, 1H), 0.83 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 174.7, 149.0, 138.7, 137.9, 135.3, 132.6, 131.5, 130.7, 130.0, 129.3, 128.5, 127.0, 126.2, 121.5, 112.9, 45.7, 30.7, 30.4, 28.9, 24.0, 23.3, 21.1, 19.6, 19.5, 19.4, 18.9, 13.9, 11.5, 10.8; LRMS (EI, 70 eV) m/z (%): 445 (M$^+$, 1), 430 (100), 344 (6); HRMS m/z (ESI) calcd for C$_{29}$H$_{40}$NOSi [M+H]$^+$ 446.2874, found 446.2887.

3,3-diisopropyl-1-(4-methoxyphenyl)-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ga): White solid, mp 143.2-145.4 °C (uncorrected); $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.32 (d, J = 8.0 Hz, 1H), 6.96 (t, J = 7.6 Hz, 1H), 6.85-6.80 (m, 2H), 6.57-6.50 (m, 2H), 6.48 (dd, J = 8.4, 2.4 Hz, 1H), 6.33 (d, J = 8.4 Hz, 1H), 3.74 (s, 3H), 3.36 (s, 3H), 2.40 (d, J = 15.2 Hz, 1H), 1.40 (s, 3H), 1.19 (s, 7H), 1.14 (s, 4H), 1.11 (s, 3H), 1.03-1.02 (m, 3H), 0.88 (d, J = 15.2 Hz, 1H), 0.83 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 174.7, 157.7,
148.7, 138.7, 133.4, 132.8, 132.0, 131.5, 131.0, 129.3, 126.2, 121.6, 113.0, 112.9, 112.0, 55.0, 45.7, 30.7, 30.4, 28.9, 24.0, 23.4, 19.6, 19.5, 19.4, 18.9, 13.9, 11.5, 10.8;
LRMS (EI, 70 eV) m/z (%): 461 (M⁺, 1), 446 (100), 360 (3); HRMS m/z (ESI) calcd for C₂₉H₄₀NO₂Si [M+H]⁺ 462.2823, found 462.2835.

1-[[1,1'-biphenyl]-4-yl]-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ha): White solid, mp 150.6-152.3 °C (uncorrected); ¹H NMR (400 MHz, CDCl₃) δ: 7.57-7.54 (m, 3H), 7.49 (d, J = 7.6 Hz, 1H), 7.40 (t, J = 7.2 Hz, 2H), 7.30 (t, J = 7.2 Hz, 1H), 7.20 (d, J = 7.6 Hz, 1H), 6.96 (t, J = 7.4 Hz, 1H), 6.82 (d, J = 8.0 Hz, 1H), 6.60 (d, J = 7.6 Hz, 1H), 6.50-6.46 (m, 2H), 3.38 (s, 3H), 2.43 (d, J = 15.2 Hz, 1H), 1.46 (s, 3H), 1.21-1.14 (m, 14H), 1.05 (s, 3H), 0.93-0.88 (m, 4H); ¹³C NMR (100 MHz, CDCl₃) δ: 174.6, 148.7, 140.7, 140.2, 138.7, 138.3, 133.0, 131.5, 131.3, 130.6, 129.0, 128.7, 127.1, 126.8, 126.4 (2C), 124.8, 121.6, 113.0, 45.8, 30.4, 29.0, 24.0, 23.3, 19.6, 19.5 (2C), 18.9, 13.9, 11.5, 10.8; LRMS (EI, 70 eV) m/z (%): 492 (M⁺-15, 100), 406 (5), 246 (4); HRMS m/z (ESI) calcd for C₃₄H₄₂NOSi [M+H]⁺ 508.3030, found 508.3037.

1-(4-chlorophenyl)-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ia): White solid, mp 148.6-151.1 °C (uncorrected); ¹H NMR (400 MHz, CDCl₃) δ: 7.36 (dd, J = 8.5, 2.0 Hz, 1H), 7.27 (dd, J = 8.5, 2.0 Hz, 1H), 7.01-6.98 (m, 1H), 6.91 (dd, J = 8.0, 2.5 Hz, 1H), 6.82 (d, J = 8.0 Hz, 1H), 6.56-6.51 (m, 2H), 6.36 (dd, J = 8.5, 2.0 Hz, 1H), 3.36 (s, 3H), 2.41 (d, J = 15.5 Hz, 1H), 1.40 (s, 3H), 1.19-1.18 (m, 7H), 1.14-1.12 (m, 7H), 1.02-1.00 (m, 3H), 0.88 (d, J = 15.5 Hz, 1H), 0.81 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 174.4, 147.7, 139.5,
138.7, 133.6, 132.1, 131.7, 131.4, 131.3, 128.6, 128.1, 126.7, 126.5, 121.7, 113.1, 45.8, 30.7, 30.4, 28.9, 23.9, 23.2, 19.6, 19.4 (2C), 18.8, 13.8, 11.4, 10.7; LRMS (EI, 70 eV) m/z (%): 467 (M⁺+2, 0.4), 465 (M⁺, 1), 452 (38), 450 (100), 364 (7); HRMS m/z (ESI) calcd for C₃₈H₇₅ClNOSi [M+H]+ 466.2328, found 466.2341.

1-(4-fluorophenyl)-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ja):

White solid, mp 135.1-136.7 °C (uncorrected); ¹H NMR (400 MHz, CDCl₃) δ: 7.39-7.36 (m, 1H), 7.02-6.97 (m, 2H), 6.82 (d, J = 8.0 Hz, 1H), 6.64 (td, J = 8.6, 2.4 Hz, 1H), 6.55-6.50 (m, 2H), 6.40-6.36 (m, 1H), 3.36 (s, 3H), 2.40 (d, J = 15.2 Hz, 1H), 1.40 (s, 3H), 1.19-1.18 (m, 7H), 1.15 (s, 4H), 1.12 (s, 3H), 1.03-1.02 (m, 3H), 0.89 (d, J = 15.2 Hz, 1H), 0.82 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 174.5, 161.2 (d, J = 243.4 Hz), 147.9, 138.7, 136.9 (d, J = 3.6 Hz), 133.5, 132.4 (d, J = 7.5 Hz), 131.4, 131.3 (d, J = 7.7 Hz), 128.8, 126.5, 121.6, 114.8 (d, J = 20.6 Hz), 113.3 (d, J = 21.2 Hz), 113.1, 45.8, 30.7, 30.3, 28.9, 24.0, 23.3, 19.6, 19.5, 19.4, 18.8, 13.9, 11.5, 10.8; ¹⁹F NMR (375 MHz, CDCl₃) δ: -116.6; LRMS (EI, 70 eV) m/z (%): 449 (M⁺, 1), 434 (100), 348 (7); HRMS m/z (ESI) calcd for C₃₈H₇₅FNOSi [M+H]+ 450.2623, found 450.2631.

3,3-diisopropyl-2,2,4a,6-tetramethyl-1-(m-tolyl)-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ka):

White solid, mp 120.5-121.9 °C (uncorrected); ¹H NMR (400 MHz, CDCl₃) δ: 7.26-7.20 (m, 1H), 7.15 (t, J = 7.4 Hz, 0.47H), 6.98-6.90 (m, 2H), 6.84-6.79 (m, 1.53H), 6.58 (t, J = 7.2 Hz, 1H), 6.51-6.46 (m, 1H), 6.23-6.20 (m, 1H), 3.37 (s, 1.4H), 3.35 (s, 1.6H) 2.43-2.38 (m, 2.6H), 2.01 (s, 1.4H), 1.42 (s, 1.6H), 1.39 (s, 1.4H) 1.20-1.19 (m, 7H), 1.15 (s, 4H), 1.12 (s, 3H), 1.07-1.04 (m, 3H), 0.88 (d, J = 15.6 Hz, 1H), 0.84 (s, 1.4H), 0.83 (s, 1.6H); ¹³C NMR (100 MHz,
CDCl₃ δ: 174.7 (2C), 149.1 (2C), 140.9, 140.8, 138.6 (2C), 137.3, 135.5, 132.5 (2C), 131.4, 131.3, 131.2, 130.9, 129.2, 129.1, 127.9, 127.6, 127.5, 126.6, 126.5, 126.3, 126.0, 121.4 (2C), 112.9, 112.8, 45.7, 30.7, 30.4 (2C), 28.9, 28.8, 24.0, 23.9, 23.3 (2C), 21.7, 21.3, 19.7, 19.6, 19.5 (2C), 18.9 (2C), 14.0, 13.9, 11.5 (2C), 10.9, 10.8; LRMS (EI, 70 eV) m/z (%): 445 (M⁺, 1), 430 (100), 344 (6); HRMS m/z (ESI) calcd for C₂₉H₄₀NOSi [M+H]⁺ 446.2874, found 446.2883.

1-(3-chlorophenyl)-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3la):

White solid, mp 138.5-140.2 °C (uncorrected); ¹H NMR (400 MHz, CDCl₃) δ: 7.44 (s, 0.55H), 7.32 (d, J = 7.6 Hz, 0.45H), 7.22 (t, J = 7.6 Hz, 0.45H), 7.09 (d, J = 8.0 Hz, 1H), 7.05-6.94 (m, 1H), 6.89-6.81 (m, 1H), 6.56-6.52 (m, 2H), 6.41 (s, 0.45H), 6.32 (d, J = 7.2 Hz, 0.55H), 3.37 (s, 1.35H), 3.36 (s, 1.65H), 2.41 (d, J = 15.2 Hz, 1H), 1.43 (s, 1.65H), 1.40 (s, 1.35H), 1.19-1.13 (m, 14H), 1.02 (s, 3H), 0.88 (d, J = 15.2 Hz, 1H), 0.83 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 174.3 (2C), 147.5, 147.4, 142.9 (2C), 138.7, 138.6, 133.8 (2C), 133.6, 132.5, 131.4, 131.1, 130.4, 129.9, 129.0, 128.5 (2C), 128.3, 127.5, 126.9, 126.7, 126.1, 121.7, 121.5, 113.2, 113.0, 45.8 (2C), 30.7 (2C), 30.4, 29.0, 28.8, 23.9, 23.8, 23.3, 23.2, 19.6, 19.5, 19.4 (2C), 18.9, 18.8, 13.8, 11.4, 10.8, 10.7; LRMS (EI, 70 eV) m/z (%): 467 (M⁺+2, 0.4), 465 (M⁺, 1), 452 (37), 450 (100), 364 (3); HRMS m/z (ESI) calcd for C₂₉H₃₅ClNOSi [M+H]⁺ 466.2328, found 466.2332.

3,3-diisopropyl-2,2,4a,6-tetramethyl-1-(thiophen-2-yl)-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ma):

White solid, mp 133.5-134.8 °C (uncorrected); ¹H NMR (400 MHz, CDCl₃) δ: 7.09-7.02 (m, 2H), 6.84 (d, J = 8.0 Hz, 4H), 6.62 (t, J = 7.6 Hz, 1H), 3.35 (s, 3H), 2.42 (d, J = 15.2 Hz, 1H), 1.39 (s, 3H), 1.17-1.12 (m,
14H), 0.97 (s, 3H), 0.90 (s, 3H), 0.83 (d, J = 15.6 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 174.0, 138.5, 136.5, 129.8, 126.8, 125.8, 121.8, 113.1, 46.2, 30.7, 28.4, 19.4, 19.3, 19.2, 18.4, 13.6, 11.5, 10.5; LRMS (EI, 70 eV) m/z (%): 437 (M$^+$, 1), 422 (100), 336 (6); HRMS m/z (ESI) calcd for C$_{26}$H$_{36}$NOSSi [M+H]$^+$ 438.2281, found 438.2293.

3,3-diisopropyl-2,2,4a,6-tetramethyl-1-pentyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3na): Colourless oil;

$^1$H NMR (400 MHz, CDCl$_3$) δ: 7.29 (d, J = 7.6 Hz, 1H), 7.23 (t, J = 7.6 Hz, 1H), 7.02 (t, J = 7.2 Hz, 1H), 6.92 (d, J = 8.0 Hz, 1H), 3.31 (s, 3H), 2.27 (d, J = 15.2 Hz, 1H), 2.20-2.18 (m, 2H), 1.78-1.67 (m, 1H), 1.55-1.48 (s, 1H), 1.32-1.06 (m, 21H), 1.02 (s, 3H), 0.88-0.85 (m, 6H), 0.77 (d, J = 15.6 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 175.3, 148.1, 138.8, 130.6, 130.1, 128.9, 127.1, 121.9, 113.6, 45.8, 32.3, 31.9, 30.6, 30.3, 28.6, 23.5, 22.5, 22.2, 19.8, 19.5, 19.1, 18.6, 14.1, 13.7, 11.0, 10.5; LRMS (EI, 70 eV) m/z (%): 425 (M$^+$, 1), 410 (100), 324 (3); HRMS m/z (ESI) calcd for C$_{27}$H$_{44}$NOSi [M+H]$^+$ 426.3187, found 426.3195.

3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3oa): Colourless oil;

$^1$H NMR (400 MHz, CDCl$_3$) δ: 7.38 (d, J = 7.6 Hz, 1H), 7.26 (d, J = 7.8 Hz, 1H), 7.04 (t, J = 7.4 Hz, 1H), 6.93 (d, J = 8.0 Hz, 1H), 5.77 (s, 1H), 3.36 (s, 3H), 2.19 (d, J = 15.6 Hz, 1H), 1.17-1.14 (m, 14H), 1.09-1.07 (m, 6H), 0.93-0.91 (m, 3H), 0.86 (d, J = 15.6 Hz, 1H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 174.6, 142.5, 138.0, 134.8, 128.5, 127.8, 125.4, 122.9, 113.6, 44.4, 30.5, 30.3, 28.3, 27.2, 20.8, 19.7, 19.3, 19.0, 18.4, 13.4, 11.8, 11.0; LRMS (EI, 70 eV) m/z (%): 355 (M$^+$, 1), 340 (100), 254 (9); HRMS m/z (ESI) calcd for C$_{22}$H$_{34}$NOSi [M+H]$^+$ 356.2404, found 356.2413.
3,3-diisopropyl-2,2,4a,6-tetramethyl-1-phenyl-8-(trifluoromethyl)-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3pa): White solid, mp 115.6-117.4 °C (uncorrected); ¹H NMR (400 MHz, CDCl₃) δ: 7.43 (d, J = 7.2 Hz, 1H), 7.30 (t, J = 7.2 Hz, 1H), 7.13 (t, J = 7.0 Hz, 1H), 7.02 (s, 1H), 6.95 (t, J = 7.4 Hz, 1H), 6.73 (d, J = 8.0 Hz, 1H), 6.65 (d, J = 7.6 Hz, 1H), 6.39 (d, J = 7.6 Hz, 1H), 3.40 (s, 3H), 2.42 (d, J = 15.2 Hz, 1H), 1.44 (s, 3H), 1.20-1.12 (m, 14H), 1.03 (s, 3H), 0.91 (d, J = 15.6 Hz, 1H), 0.83 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 174.5, 151.2, 140.3, 139.1, 132.6, 131.6, 130.5, 130.0, 128.4 (q, J = 32.2 Hz), 128.2, 126.5, 126.4, 123.9 (q, J = 270.4 Hz), 118.0 (q, J = 3.6 Hz), 109.8 (q, J = 3.6 Hz), 45.6, 30.8, 30.4, 28.8, 23.8, 23.6, 19.6, 19.4 (2C), 18.8, 13.9, 11.4, 10.7; ¹⁹F NMR (375 MHz, CDCl₃) δ: -62.5; LRMS (EI, 70 eV) m/z (%): 499 (M⁺, 1), 484 (100), 398 (7); HRMS m/z (ESI) calcd for C₂₉H₃₇F₃NOSi [M+H]⁺ 500.2591, found 500.2603.

3,3-diisopropyl-2,2,4a,6,9-pentamethyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3qa): White solid, mp 117.9-118.7 °C (uncorrected); ¹H NMR (400 MHz, CDCl₃) δ: 7.44 (d, J = 8.0 Hz, 1H), 7.28 (d, J = 8.0 Hz, 1H), 7.09 (t, J = 7.5 Hz, 1H), 6.94 (td, J = 7.5, 1.0 Hz, 1H), 6.74 (dd, J = 8.0, 1.0 Hz, 1H), 6.67 (d, J = 8.0 Hz, 1H), 6.42 (d, J = 7.5 Hz, 1H), 6.35 (d, J = 1.5 Hz, 1H), 3.34 (s, 3H), 2.40 (d, J = 15.0 Hz, 1H), 1.85 (s, 3H), 1.42 (s, 3H), 1.20-1.19 (m, 7H), 1.15-1.13 (m, 7H), 1.04-1.03 (m, 3H), 0.88 (d, J = 15.5 Hz, 1H), 0.84 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ: 174.5, 148.8, 141.2, 136.3, 133.0, 132.3, 130.7 (2C), 130.5, 128.8, 127.9, 126.8, 126.0, 125.8, 112.6, 45.7, 30.7, 30.5, 28.9, 24.0, 23.3, 20.2, 19.6, 19.5 (2C), 18.9, 13.9, 11.5, 10.8; LRMS (EI, 70 eV) m/z (%): 445 (M⁺, 1), 430 (100), 344 (6); HRMS m/z (ESI) calcd for C₂₉H₄₀NOSi [M+H]⁺ 446.2874, found 446.2880.
9-chloro-3,3-diisopropyl-2,2,4a,6-tetramethyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ra):

White solid, mp 121.0-122.5 °C (uncorrected); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\): 7.43 (d, \(J = 7.6\) Hz, 1H), 7.33 (t, \(J = 7.6\) Hz, 1H), 6.99 (t, \(J = 7.4\) Hz, 1H), 6.92 (dd, \(J = 8.8, 1.6\) Hz, 1H), 6.72 (d, \(J = 8.8\) Hz, 1H), 6.53 (s, 1H), 6.42 (d, \(J = 7.6\) Hz, 1H), 3.34 (s, 3H), 2.39 (d, \(J = 15.2\) Hz, 1H), 1.42 (s, 3H), 1.19 (s, 7H), 1.14 (s, 7H), 1.04-1.03 (m, 3H), 0.90 (d, \(J = 15.2\) Hz, 1H), 0.85 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\): 174.4, 150.6, 140.4, 137.3, 131.8, 131.2, 130.6, 130.4, 130.2, 128.1, 126.8, 126.5, 126.4, 126.2, 114.0, 45.6, 30.8, 30.4, 28.8, 23.9, 23.5, 19.6, 19.5, 19.4, 18.9, 13.9, 11.5, 10.8; LRMS (EI, 70 eV) \(m/z\) (%): 467 (M\(^{+}\)+2, 0.3), 465 (M\(^{+}\), 1), 452 (42), 450 (100), 364 (2); HRMS \(m/z\) (ESI) calcd for C\(_{28}\)H\(_{37}\)ClNOSi [M+H]\(^{+}\) 466.2328, found 466.2335.

3-isopropyl-2,2,4a,6-tetramethyl-1-phenyl-3-(p-tolyl)-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ab): dr = 1:1;

Colorless oil; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\): 7.52 (d, \(J = 7.2\) Hz, 2H), 7.43 (d, \(J = 7.6\) Hz, 1H), 7.29 (t, \(J = 7.6\) Hz, 1H), 7.21 (d, \(J = 7.6\) Hz, 2H), 7.11 (t, \(J = 7.2\) Hz, 1H), 7.00-6.95 (m, 2H), 6.84 (d, \(J = 8.0\) Hz, 1H), 6.57-6.49 (m, 3H), 3.39 (s, 3H), 2.68 (d, \(J = 15.2\) Hz, 1H), 2.37 (s, 3H), 1.34 (d, \(J = 15.6\) Hz, 1H), 1.28 (s, 3H), 1.21 (s, 3H), 1.07-1.03 (m, 7H), 0.81 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\): 174.3, 148.8, 141.4, 138.9, 138.8, 135.0, 132.8, 131.6, 131.3, 130.7, 130.0, 129.0, 128.6, 128.0, 126.5 (2C), 125.9, 121.5, 113.0, 46.1, 30.9, 30.8, 29.9, 22.5, 22.4, 21.5, 18.3, 17.8, 12.8, 10.9; LRMS (EI, 70 eV) \(m/z\) (%): 479 (M\(^{+}\), 1), 464 (100), 304 (2); HRMS \(m/z\) (ESI) calcd for C\(_{32}\)H\(_{38}\)NOSi [M+H]\(^{+}\) 480.2717, found 480.2730.
$^1$H NMR (400 MHz, CDCl$_3$) δ: 7.55 (d, $J = 7.2$ Hz, 2H), 7.38 (d, $J = 7.6$ Hz, 1H), 7.28 (d, $J = 7.6$ Hz, 1H), 7.16 (d, $J = 7.2$ Hz, 2H), 7.09 (d, $J = 7.4$ Hz, 1H), 6.98-6.91 (m, 2H), 6.81 (d, $J = 8.0$ Hz, 1H), 6.64 (d, $J = 7.6$ Hz, 1H), 6.51 (t, $J = 7.4$ Hz, 1H), 6.33 (d, $J = 7.6$ Hz, 1H), 3.32 (s, 3H), 2.58 (d, $J = 15.6$ Hz, 1H), 2.34 (s, 3H), 1.29-1.24 (m, 5H), 1.21-1.17 (m, 5H), 1.15-1.14 (m, 4H), 0.86 (s, 3H);

$^{13}$C NMR (100 MHz, CDCl$_3$) δ: 175.4, 149.1, 140.1, 138.8, 138.6, 135.4, 134.2, 131.1, 130.9, 130.5, 130.3, 129.0, 128.3, 127.8, 126.5, 126.0, 125.9, 121.5, 113.1, 45.5, 30.8, 29.0, 26.4, 25.7, 22.8, 21.4, 19.5, 19.0, 13.4, 11.1; LRMS (EI, 70 eV) m/z (%): 479 (M$^+$, 1), 464 (100), 304 (6);

HRMS m/z (ESI) calcd for C$_{32}$H$_{38}$NOSi [M+H]$^+$ 480.2717, found 480.2725.

(2R,4aS)-3,3-dihexyl-4a,6-dimethyl-2-pentyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ac): dr > 20:1; Colorless oil; $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.26-7.00 (m, 6H), 6.85 (d, $J = 8.0$ Hz, 1H), 6.66 (d, $J = 7.2$ Hz, 1H), 6.55 (t, $J = 7.2$ Hz, 1H), 3.39 (s, 3H), 2.35 (d, $J = 15.2$ Hz, 1H), 2.00-1.79 (m, 2H), 1.59 (s, 3H), 1.37-1.08 (m, 26H), 0.94-0.79 (s, 7H), 0.64-0.45 (m, 4H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 173.9, 147.6, 144.5, 138.9, 133.3, 131.8, 128.7, 127.8 (2C), 126.8, 125.9, 121.7, 113.1, 46.4, 34.4, 33.6, 33.4, 32.5, 31.5, 31.3, 31.2, 30.8, 30.4, 30.0, 29.7, 23.8, 23.7, 22.6 (2C), 22.5, 15.0, 14.1 (2C), 11.7, 11.0; HRMS m/z (ESI) calcd for C$_{32}$H$_{38}$NOSi [M+H]$^+$ 558.4126, found 558.4135.

(2R,4aS)-3,3-diethyl-2,4a,6-trimethyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ad): dr > 20:1; Colorless oil; $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.26-7.00 (m, 6H), 6.85 (d, $J = 8.4$ Hz, 1H), 6.65 (d, $J = 7.6$ Hz, 1H), 6.55 (d, $J = 7.4$ Hz, 1H), 3.39 (s, 3H), 2.30 (d, $J = 15.2$ Hz, 1H), 1.69-1.64 (m, 1H), 1.48 (d, $J = 7.2$ Hz, 3H), 1.15 (s, 3H), 1.01 (t, $J = 8.0$ Hz, 3H), 0.87 (t, $J = 7.8$ Hz, 3H), 0.81 (d, $J =
15.2 Hz, 1H), 0.71-0.49 (m, 4H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 173.9, 147.5, 145.3, 138.9, 133.0, 131.5, 128.6, 127.8 (2C), 126.8, 125.9, 121.7, 113.2, 46.2, 30.8, 30.1, 23.8, 18.7, 13.9, 7.5, 7.2, 2.2, 2.0; LRMS (EI, 70 eV) m/z (%): 389 (M$^+$, 1), 374 (100), 344 (16), 87 (40); HRMS $m/z$ (ESI) calcd for C$_{25}$H$_{32}$NOSi [M+H]$^+$ 390.2248, found 390.2263.

**5-methyl-11-phenyl-6a-((triethylsilyl)methyl)-5,6a-dihydro-6H-indeno[1,2-c]quinolin-6-one (4sd):** Yellow solid, mp 57.6-58.8 °C (uncorrected); $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.94-7.92 (m, 1H), 7.40-7.30 (m, 5H), 7.26-7.24 (m, 2H), 7.20 (d, J = 8.0 Hz, 1H), 7.14-7.11 (m, 1H), 7.09-7.03 (m, 2H), 6.82 (t, J = 7.6 Hz, 1H), 3.37 (s, 3H), 1.64 (d, J = 14.4 Hz, 1H), 1.24 (d, J = 14.4 Hz, 1H), 0.52 (t, J = 7.8 Hz, 9H), 0.05-0.06 (m, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 172.0, 145.0, 144.4, 140.1, 138.9, 138.5, 134.3, 129.0, 128.8, 128.4, 127.8, 127.7, 127.4, 126.3, 125.7, 122.4, 121.5, 120.4, 115.0, 57.8, 30.4, 22.0, 7.2, 3.6; LRMS (EI, 70 eV) m/z (%): 451 (M$^+$, 50), 436 (34), 374 (100), 87 (46); HRMS $m/z$ (ESI) calcd for C$_{30}$H$_{34}$NOSi [M+H]$^+$ 452.2404, found 452.2415.

**5-methyl-12-phenyl-6a-((triethylsilyl)methyl)-6a,7-dihydrobenzo[j]phenanthridin-6(5H)-one (4td):** yellow solid, mp 68.5-70.2 °C (uncorrected); $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.40-7.31 (m, 3H), 7.28-7.16 (m, 4H), 7.11-7.05 (m, 3H), 6.92 (d, J = 8.0 Hz, 1H), 6.79 (d, J = 8.0 Hz, 1H), 6.59 (t, J = 7.6 Hz, 1H), 3.52 (d, J = 16.4 Hz, 1H), 3.39-3.35 (m, 4H), 1.06-1.00 (m, 2H), 0.76 (t, J = 7.8 Hz, 9H), 0.44-0.34 (m, 6H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 174.0, 139.6, 139.0, 135.1, 134.3, 133.4, 133.0, 131.1, 130.8, 128.6 (2C), 128.0, 127.6, 127.1, 126.4, 125.9, 123.5, 121.9, 114.1, 45.2, 38.6, 30.3, 18.9, 7.3, 3.8; LRMS (EI, 70 eV) m/z (%): 465 (M$^+$, 10), 436 (100), 388
(35), 336 (56); HRMS m/z (ESI) calcd for C_{31}H_{36}NOSi [M+H]^+ 466.2561, found 466.2573.

2,2-diethyl-3a,5-dimethyl-1-phenyl-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5ae): Light yellow oil; \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\): 7.24 (t, \(J = 7.4\) Hz, 2H), 7.20-7.14 (m, 2H), 6.99 (t, \(J = 8.2\) Hz, 3H), 6.88 (d, \(J = 7.6\) Hz, 1H), 6.69 (t, \(J = 7.4\) Hz, 1H), 3.44 (s, 3H), 1.77 (d, \(J = 16.0\) Hz, 1H), 1.27 (s, 3H), 1.15 (t, \(J = 7.6\) Hz, 3H), 1.04 (d, \(J = 15.6\) Hz, 1H), 0.98-0.87 (m, 2H), 0.76 (t, \(J = 7.6\) Hz, 3H), 0.62-0.47 (m, 2H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\): 176.1, 150.9, 142.1, 141.1, 139.6, 129.5, 128.6, 128.5, 127.4, 125.6, 123.1, 121.8, 114.5, 53.6, 30.5, 28.7, 16.7, 8.1, 7.2, 6.2, 4.4; LRMS (EI, 70 eV) m/z (%): 361 (M\(^+\), 100), 346 (52), 284 (26), 151 (29); HRMS m/z (ESI) calcd for C_{23}H_{28}NOSi [M+H]^+ 362.1935, found 362.1943.

3a,5-dimethyl-1,2,2-triphenyl-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5af): Light yellow solid, mp 175.1-176.6 °C (uncorrected); \(^1\)H NMR (400 MHz, CDCl\(_3\)) \(\delta\): 7.68 (d, \(J = 6.4\) Hz, 2H), 7.64-7.58 (m, 1H), 7.49-7.42 (m, 2H), 7.36 (d, \(J = 7.2\) Hz, 2H), 7.30 (d, \(J = 7.0\) Hz, 1H), 7.22 (t, \(J = 7.8\) Hz, 3H), 7.15-7.09 (m, 3H), 7.03 (d, \(J = 8.0\) Hz, 1H), 6.98 (d, \(J = 7.2\) Hz, 3H), 6.72 (t, \(J = 7.4\) Hz, 1H), 3.44 (s, 3H), 2.32 (d, \(J = 16.0\) Hz, 1H), 1.55 (d, \(J = 16.0\) Hz, 1H), 1.40 (s, 3H); \(^{13}\)C NMR (100 MHz, CDCl\(_3\)) \(\delta\): 175.5, 153.1, 140.2, 139.9, 139.7, 135.6, 135.0, 133.9, 133.9, 129.8, 129.7, 129.5, 129.0, 128.5, 128.1 (2C), 127.8, 126.0, 123.0, 122.0, 114.7, 53.8, 30.5, 28.5, 19.9; LRMS (EI, 70 eV) m/z (%): 457 (M\(^+\), 56), 379 (89), 339 (100); HRMS m/z (ESI) calcd for C_{31}H_{28}NOSi [M+H]^+ 458.1935, found 458.1946.

3a,5-dimethyl-1-phenyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5ag): White solid,
mp 178.8-180.7 °C (uncorrected); 1H NMR (400 MHz, CDCl3) δ: 7.22 (t, J = 7.4 Hz, 2H), 7.18-7.11 (m, 2H), 6.98 (t, J = 7.4 Hz, 3H), 6.91 (d, J = 8.0 Hz, 1H), 6.68 (t, J = 7.6 Hz, 1H), 3.43 (s, 3H), 2.02 (d, J = 15.2 Hz, 1H), 1.27 (s, 3H), 1.22 (d, J = 15.6 Hz, 1H), 0.31 (s, 9H), -0.12 (s, 9H); 13C NMR (100 MHz, CDCl3) δ: 176.4, 147.2, 142.6, 141.8, 139.5, 129.5, 128.5, 128.3, 127.7, 125.7, 123.3, 121.8, 114.5, 56.3, 30.4, 27.7, 16.6, 0.0, -1.4; LRMS (EI, 70 eV) m/z (%): 449 (M+, 52), 434 (100), 376 (63), 246 (47), 73 (55); HRMS m/z (ESI) calcd for C25H36NOSi3 [M+H]+ 450.2099, found 450.2104.

5-benzyl-3a-methyl-1-phenyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5bg): Light yellow solid, mp 125.6-127.8 °C (uncorrected); 1H NMR (400 MHz, CDCl3) δ: 7.32 (t, J = 7.4 Hz, 2H), 7.26-7.21 (m, 5H), 7.14 (t, J = 7.2 Hz, 1H), 7.03-6.97 (m, 3H), 6.91-6.88 (m, 2H), 6.64 (t, J = 7.6 Hz, 1H), 5.48 (d, J = 16.4 Hz, 1H), 5.02 (d, J = 16.4 Hz, 1H), 2.18 (d, J = 15.6 Hz, 1H), 1.41 (s, 3H), 1.22 (d, J = 15.6 Hz, 1H), 0.33 (s, 9H), -0.09 (s, 9H); 13C NMR (100 MHz, CDCl3) δ: 176.3, 147.2, 143.0, 141.8, 138.7, 137.3, 129.6, 128.7, 128.5, 128.2, 127.8, 127.0, 126.2, 125.8, 123.7, 122.0, 115.5, 56.5, 46.8, 27.9, 16.0, -0.1, -1.4; LRMS (EI, 70 eV) m/z (%): 452 (M+, 73), 361 (33), 91 (100), 73 (35); HRMS m/z (ESI) calcd for C31H40NOSi3 [M+H]+ 526.2412, found 526.2424.

3a-methyl-1-phenyl-5-tosyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5dg): White solid, mp 200.2-202.3 °C (uncorrected); 1H NMR (400 MHz, CDCl3) δ: 7.92 (d, J = 8.0 Hz, 2H), 7.77 (d, J = 8.0 Hz, 1H), 7.33-7.28 (m, 5H), 7.22 (t, J = 7.2 Hz, 1H), 7.03 (d, J = 7.2 Hz, 2H), 6.97 (t, J = 7.6 Hz, 1H), 6.88 (d, J = 7.6 Hz, 1H), 2.42 (s, 3H), 1.72 (d, J = 15.6 Hz, 1H), 1.17 (s, 3H), 1.05 (d, J =
15.6 Hz, 1H), 0.30 (s, 9H), -0.25 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 176.2, 145.7, 144.7, 144.0, 140.5, 136.6, 134.9, 129.3, 129.1, 128.7, 128.5, 128.0, 127.6 (2C), 126.4, 125.7, 123.9, 59.3, 26.3, 21.6, 16.2, -0.3, -1.5; LRMS (EI, 70 eV) m/z (%): 434 (M$^-$-155, 37), 346 (41), 73 (100); HRMS m/z (ESI) calcd for C$_{31}$H$_{40}$NO$_3$Si$_3$ [M+H]$^+$ 590.2031, found 590.2045.

3a-methyl-1-phenyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5eg): Light yellow solid, mp 208.2-210.1 ºC (uncorrected); $^1$H NMR (400 MHz, CDCl$_3$) δ: 8.19 (s, 1H), 7.24 (t, J = 7.6 Hz, 2H), 7.15 (t, J = 7.2 Hz, 1H), 7.09 (t, J = 7.6 Hz, 1H), 6.97 (d, J = 7.6 Hz, 2H), 6.87 (d, J = 8.0 Hz, 1H), 6.79 (d, J = 8.0 Hz, 1H), 6.64 (t, J = 7.6 Hz, 1H), 1.97 (d, J = 15.2 Hz, 1H), 1.37 (s, 3H), 1.21 (d, J = 15.2 Hz, 1H), 0.31 (s, 9H), -0.11 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 177.53, 147.0, 143.7, 141.9, 136.3, 129.6, 128.6, 128.4, 127.5, 125.8, 122.0, 121.6, 115.2, 56.2, 28.0, 15.5, 0.0, -1.4; LRMS (EI, 70 eV) m/z (%): 435 (M$^+$, 60), 420 (100), 362 (100), 232 (75), 73 (95); HRMS m/z (ESI) calcd for C$_{24}$H$_{34}$NOSi$_3$ [M+H]$^+$ 436.1943, found 436.1954.

3a,5-dimethyl-1-(thiophen-2-yl)-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5mg): Light yellow solid, mp 168.7-170.4 ºC (uncorrected); $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.29 (d, J = 7.6 Hz, 1H), 7.22 (t, J = 7.8 Hz, 1H), 7.14 (d, J = 5.2 Hz, 1H), 7.01 (d, J = 8.4 Hz, 1H), 6.89 (t, J = 4.0 Hz, 1H), 6.81 (t, J = 7.6 Hz, 1H), 6.64 (d, J = 3.6 Hz, 1H), 3.42 (s, 3H), 2.04 (d, J = 15.2 Hz, 1H), 1.23 (s, 3H), 1.18 (d, J = 15.6 Hz, 1H), 0.32 (s, 9H), -0.05 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 176.0, 148.6, 143.2, 139.6, 133.7, 129.2, 128.8, 127.1, 124.7, 124.3, 123.2, 121.9, 114.7, 56.4, 30.4, 27.4, 16.7, -0.1, -1.4; LRMS (EI, 70 eV) m/z (%): 455
(M⁺, 56), 440 (89), 382 (67), 246 (55), 73 (100); HRMS m/z (ESI) calcd for C$_{23}$H$_{34}$NOSSi$_3$ [M+H]$^+$ 456.1663, found 456.1673.

3a,5-dimethyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5og): yellow oil liquid; $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.47 (d, J = 7.6 Hz, 1H), 7.18 (t, J = 7.8 Hz, 1H), 6.93 (t, J = 7.4 Hz, 1H), 6.88 (d, J = 8.4 Hz, 1H), 6.13 (s, 1H), 3.28 (s, 3H), 1.79 (d, J = 15.2 Hz, 1H), 1.15 (d, J = 15.2 Hz, 1H), 1.12 (s, 3H), 0.09 (s, 9H), 0.00 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 176.3, 157.0, 138.4, 129.0, 126.1, 124.1, 124.0, 122.6, 114.5, 55.1, 30.1, 28.8, 17.4, -0.2, -1.1; LRMS (EI, 70 eV) m/z (%): 373 (M⁺, 45), 358 (100), 260 (90), 212 (45), 73 (47); HRMS m/z (ESI) calcd for C$_{19}$H$_{32}$NOSi$_3$ [M+H]$^+$ 374.1786, found 374.1799.

3a,5-dimethyl-1-phenyl-7-(trifluoromethyl)-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5pg): Light yellow solid, mp 114.5-116.2 °C (uncorrected); $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.24 (t, J = 7.6 Hz, 2H), 7.20 (s, 1H), 7.16 (t, J = 7.4 Hz, 1H), 7.00-6.92 (m, 4H), 3.47 (s, 3H), 2.05 (d, J = 15.6 Hz, 1H), 1.26 (s, 3H), 1.22 (d, J = 15.6 Hz, 1H), 0.31 (s, 9H), -0.11 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 176.1, 146.3, 145.5, 141.2, 139.9, 130.0 (q, J = 32.4 Hz), 129.8, 128.7, 127.5, 126.5 (d, J = 1.2 Hz), 126.2, 123.9 (q, J = 270.5 Hz), 118.5 (q, J = 3.7 Hz), 111.3 (q, J = 3.9 Hz), 56.1, 30.5, 27.7, 16.5, -0.1, -1.4; $^{19}$F NMR (375 MHz, CDCl$_3$) δ: -62.7; LRMS (EI, 70 eV) m/z (%): 444 (M⁺-73, 74), 354 (52), 314 (60), 73 (100); HRMS m/z (ESI) calcd for C$_{26}$H$_{35}$F$_3$NOSi$_3$ [M+H]$^+$ 518.1973, found 518.1981.

5-methyl-1,3a-diphenyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5sg): White solid, mp 184.5-186.5 °C (uncorrected); $^1$H NMR (400 MHz, CDCl$_3$) δ:
7.14 (t, $J = 6.8$ Hz, 4H), 7.07-6.99 (m, 3H), 6.97-6.91 (m, 3H), 6.90-6.83 (m, 2H), 6.66 (d, $J = 8.0$ Hz, 1H), 6.50 (t, $J = 7.6$ Hz, 1H), 3.31 (s, 3H), 2.49 (d, $J = 15.6$ Hz, 1H), 1.21 (d, $J = 15.6$ Hz, 1H), 0.00 (s, 9H), -0.21 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 173.2, 147.5, 144.9, 144.6, 141.4, 139.2, 129.1, 128.5, 128.2, 128.0 (2C), 126.4, 126.3, 126.0, 124.9, 121.9, 114.7, 65.0, 30.8, 19.6, -0.1, -1.3; LRMS (EI, 70 eV) m/z (%): 496 (M$^+$-15, 17), 438 (100), 246 (19), 73 (41); HRMS m/z (ESI) calcd for C$_{30}$H$_{38}$NOSi$_3$ [M+H]$^+$ 512.2256, found 512.2263.

6a-((1,1,1,3,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-5-methyl-12-phenyl-6a,7-dihydrobenzo[j]phenanthridin-6(5H)-one (4tg): Light yellow solid, mp 176.1-177.1 °C (uncorrected); $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.20-7.18 (m, 3H), 7.16 (s, 1H), 7.07 (d, $J = 7.4$ Hz, 1H), 7.02-6.91 (m, 4H), 6.83 (d, $J = 8.0$ Hz, 1H), 6.70 (d, $J = 7.6$ Hz, 1H), 6.56-6.51 (m, 2H), 3.68 (d, $J = 16.4$ Hz, 1H), 3.27 (s, 3H), 3.15 (d, $J = 16.4$ Hz, 1H), 1.34 (d, $J = 14.8$ Hz, 1H), 1.19 (d, $J = 14.8$ Hz, 1H), 0.00 (s, 27H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 173.2, 139.0, 138.5, 136.3, 133.7, 133.1, 132.5, 130.7, 129.8, 128.3, 128.0 (2C), 127.4, 127.0, 126.3, 126.2, 125.7, 121.9, 113.9, 45.8, 36.6, 30.6, 19.3, 1.4; HRMS m/z (ESI) calcd for C$_{34}$H$_{48}$NOSi$_4$ [M+H]$^+$ 598.2807, found 598.2815.

3a,5-dimethyl-1-octyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5ug): Colourless oil liquid; $^1$H NMR (400 MHz, CDCl$_3$) δ: 7.29 (d, $J = 7.6$ Hz, 1H), 7.23 (d, $J = 8.4$ Hz, 1H), 7.03 (t, $J = 7.4$ Hz, 1H), 6.98 (d, $J = 8.0$ Hz, 1H), 3.33 (s, 3H), 2.53-2.45 (m, 1H), 2.31-2.23 (m, 1H), 1.98 (d, $J = 15.6$ Hz, 1H), 1.48-1.40 (m, 2H), 1.33-1.21 (m, 10H), 1.08 (s, 3H), 0.95 (d, $J = 15.6$ Hz, 1H), 0.84 (t, $J = 6.4$ Hz, 3H), 0.17 (s, 9H), 0.08 (s, 9H); $^{13}$C NMR (100 MHz, CDCl$_3$) δ: 176.7, 146.2, 143.3,
139.3, 128.1, 127.9, 124.8, 122.0, 114.5, 56.0, 32.1, 31.8 (2C), 30.4, 30.2, 29.4, 29.3, 27.7, 22.7, 15.1, 14.1, -0.3, -0.8; LRMS (EI, 70 eV) m/z (%): 412 (M⁺-73, 42), 386 (100), 246 (72), 73 (51); HRMS m/z (ESI) calcd for C_{27}H_{48}NOSi_3 [M+H]^+ 486.3038, found 486.3053.
(C) Spectra

3,3-diisopropyl-2,2,4a,6-tetramethyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3aa)
6-benzyl-3,3-diisopropyl-2,2,4a-trimethyl-1-phenyl-2,4,4a,6-tetrahydropyrrolo[3,4-c]quinolin-5(3H)-one (3ba)
6-allyl-3,3-diisopropyl-2,2,4a-trimethyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ca)
3,3-diisopropyl-2,2,4a-trimethyl-1-phenyl-6-tosyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3da)
3,3-diisopropyl-2,2,4a-trimethyl-1-phenyl-2,4,4a,6-tetrahydro[3,4-c]quinolin-5(3H)-one (3ea)
3,3-diisopropyl-2,2,4a,6-tetramethyl-1-(p-tolyl)-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3fa)
3,3-diisopropyl-1-(4-methoxyphenyl)-2,2a,4,6-tetramethyl-2,4a,6-
tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ga)
1-((1,1'-biphenyl)-4-yl)-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-
tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ha):
1-(4-chlorophenyl)-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydropyrrolo[3,4-c]quinolin-5(3H)-one (3ia)
1-(4-fluorophenyl)-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-
tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ja)
3,3-diisopropyl-2,2,4a,6-tetramethyl-1-(m-tolyl)-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ka)
1-(3-chlorophenyl)-3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3a)
3,3-diisopropyl-2,2,4a,6-tetramethyl-1-(thiophen-2-yl)-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ma)
3,3-diisopropyl-2,2,4a,6-tetramethyl-1-penty-2,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3na)
3,3-diisopropyl-2,2,4a,6-tetramethyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3oa)
3,3-diisopropyl-2,2,4a,6-tetramethyl-1-phenyl-8-(trifluoromethyl)-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3pa)
3,3-diisopropyl-2,2a,6,9-pentamethyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3qa)
9-chloro-3,3-diisopropyl-2,2,4a,6-tetramethyl-1-phenyl-2,4,4a,6-
tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ra)
3-isopropyl-2,2a,6-tetramethyl-1-phenyl-3-(p-tolyl)-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ab)
(2R,4aS)-3,3-dihexyl-4a,6-dimethyl-2-pentyl-1-phenyl-2,4,4a,6-
tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ac)
(2R,4aS)-3,3-diethyl-2,4a,6-trimethyl-1-phenyl-2,4,4a,6-tetrahydrosilino[3,4-c]quinolin-5(3H)-one (3ad)
5-methyl-11-phenyl-6a-((triethylsilyl)methyl)-5,6a-dihydro-6\textit{H}-inden\text-[1,2-c]\textit{quinolin}-6-one (4sd)
5-methyl-12-phenyl-6a-((triethylsilyl)methyl)-6a,7-dihydrobenzo[j]phenanthridin-6(5H)-one (4td)
2,2-diethyl-3a,5-dimethyl-1-phenyl-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5ae)
3a,5-dimethyl-1,2,2-triphenyl-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one

(5af)
3a,5-dimethyl-1-phenyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5ag)
5-benzyl-3a-methyl-1-phenyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5bg)
3a-methyl-1-phenyl-5-tosyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5dg)
3a-methyl-1-phenyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5eg)
3a,5-dimethyl-1-(thiophen-2-yl)-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5mg)
3a,5-dimethyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5og)
3a,5-dimethyl-1-phenyl-7-(trifluoromethyl)-2,2-bis(trimethylsilyl)-2,3,3a,5-
tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5pg)
5-methyl-1,3a-diphenyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5sg)
6a-((1,1,3,3-hexamethyl-2-(trimethylsilyl)trisilan-2-yl)methyl)-5-methyl-12-phenyl-6a,7-dihydrobenzo[j]phenanthridin-6(5H)-one (4tg)
3a,5-dimethyl-1-octyl-2,2-bis(trimethylsilyl)-2,3,3a,5-tetrahydro-4H-silolo[3,4-c]quinolin-4-one (5ug)
(D) The X-ray Single-Crystal Diffraction Analysis of 3fa, 5ag, and 5sg

Table S2. Crystal data and structure refinement for ljh052.

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<th>Identification code</th>
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<td>Temperature</td>
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<td>Wavelength</td>
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<td>Crystal system, space group</td>
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<td>Unit cell dimensions</td>
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b = 10.946(6) Å  beta = 104.243(8) deg.
c = 13.488(7) Å  gamma = 97.077(9) deg.

Volume 1328.9(18) Å³
Z, Calculated density 2, 1.114 Mg/m³
Absorption coefficient 0.108 mm⁻¹
F(000) 484
Crystal size 0.20 x 0.19 x 0.15 mm
Theta range for data collection 2.25 to 27.98 deg.
Limiting indices -13<=h<=13, -14<=k<=14, -16<=l<=17
Reflections collected / unique 16176 / 6232 [R(int) = 0.0606]
Completeness to theta = 27.98 97.0 %
Absorption correction Semi-empirical from equivalents
Max. and min. transmission 0.9839 and 0.9787
Refinement method Full-matrix least-squares on F²
Data / restraints / parameters 6232 / 0 / 300
Goodness-of-fit on F² 1.036
Final R indices [I>2sigma(I)] R1 = 0.0610, wR2 = 0.1592
R indices (all data) R1 = 0.0876, wR2 = 0.1819
Largest diff. peak and hole 0.303 and -0.375 e.Å⁻³
Table S3. Crystal data and structure refinement for ljh046.

<table>
<thead>
<tr>
<th>Identification code</th>
<th>ljh046</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical formula</td>
<td>C23 H33 N O S Si3</td>
</tr>
<tr>
<td>Formula weight</td>
<td>455.83</td>
</tr>
<tr>
<td>Temperature</td>
<td>296(2) K</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Crystal system, space group</td>
<td>Monoclinic, P2(1)/c</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>$a = 15.2467(12)$ Å, $\alpha = 90$ deg. $b = 12.7713(10)$ Å, $\beta = $</td>
</tr>
</tbody>
</table>
111.9210(10) deg.

\[ c = 14.1931(11) \text{ Å} \quad \text{gamma} = 90 \text{ deg.} \]

Volume \quad 2563.9(3) \text{ Å}^3

Z, Calculated density \quad 4, \quad 1.181 \text{ Mg/m}^3

Absorption coefficient \quad 0.281 \text{ mm}^{-1}

\( F(000) \) \quad 976

Crystal size \quad 0.24 \times 0.23 \times 0.20 \text{ mm}

Theta range for data collection \quad 1.44 \text{ to } 27.63 \text{ deg.}

Limiting indices \quad -19 \leq h \leq 19, \quad -16 \leq k \leq 12, \quad -16 \leq l \leq 18

Reflections collected / unique \quad 15319 / 5887 \quad [R(int) = 0.0173]

Completeness to theta = 27.63 \quad 98.7 \%

Absorption correction \quad \text{Semi-empirical from equivalents}

Max. and min. transmission \quad 0.9460 \text{ and } 0.9357

Refinement method \quad \text{Full-matrix least-squares on } F^2

Data / restraints / parameters \quad 5887 / 12 / 263

Goodness-of-fit on \( F^2 \) \quad 1.053

Final \( R \) indices \([I>2\sigma(I)]\) \quad R1 = 0.0555, \quad wR2 = 0.1431

R indices (all data) \quad R1 = 0.0650, \quad wR2 = 0.1519

Largest diff. peak and hole \quad 1.244 \text{ and } -0.960 \text{ e.Å}^{-3}
Table S4. Crystal data and structure refinement for ljh047_0m.

<table>
<thead>
<tr>
<th>Identification code</th>
<th>ljh047_0m</th>
</tr>
</thead>
<tbody>
<tr>
<td>Empirical formula</td>
<td>C_{30} H_{37} N O Si_3</td>
</tr>
<tr>
<td>Formula weight</td>
<td>511.88</td>
</tr>
<tr>
<td>Temperature</td>
<td>296(2) K</td>
</tr>
<tr>
<td>Wavelength</td>
<td>0.71073 Å</td>
</tr>
<tr>
<td>Crystal system, space group</td>
<td>Triclinic, P-1</td>
</tr>
<tr>
<td>Unit cell dimensions</td>
<td>a = 10.4692(7) Å</td>
</tr>
<tr>
<td></td>
<td>alpha = 109.3200(10) deg.</td>
</tr>
<tr>
<td></td>
<td>b = 11.8609(8) Å</td>
</tr>
<tr>
<td></td>
<td>beta =</td>
</tr>
</tbody>
</table>
90.0710(10) deg.

\[ c = 12.6888(9) \text{ Å} \]
\[ \gamma = 92.8340(10) \text{ deg.} \]

Volume \[ 1484.81(18) \text{ Å}^3 \]
Z, Calculated density \[ 2, 1.145 \text{ Mg/m}^3 \]
Absorption coefficient \[ 0.182 \text{ mm}^{-1} \]
\[ F(000) = 548 \]
Crystal size \[ 0.23 \times 0.21 \times 0.20 \text{ Å} \]
Theta range for data collection \[ 2.56 \text{ to } 27.49 \text{ deg.} \]
Limiting indices \[ -13 \leq h \leq 13, -15 \leq k \leq 15, -16 \leq l \leq 16 \]
Reflections collected / unique \[ 18340 / 6738 \] [\( R \text{(int)} = 0.0145 \)]
Completeness to theta = 27.49 \[ 98.8\% \]
Absorption correction \[ \text{Semi-empirical from equivalents} \]
Max. and min. transmission \[ 0.9645 \text{ and } 0.9594 \]
Refinement method \[ \text{Full-matrix least-squares on } F^2 \]
Data / restraints / parameters \[ 6738 / 24 / 323 \]
Goodness-of-fit on \( F^2 \) \[ 1.039 \]
Final R indices [\( I > 2\sigma(I) \)] \[ R_1 = 0.0424, wR_2 = 0.1141 \]
R indices (all data) \[ R_1 = 0.0501, wR_2 = 0.1212 \]
Largest diff. peak and hole \[ 0.527 \text{ and } -0.694 \text{ e.Å}^{-3} \]