

Supporting Information

Synthesis of thieno[2,3-*c*]acridine and furo[2,3-*c*]acridine derivatives *via* iodocyclization reaction, fluorescence properties and DFT mechanistic study

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List of the Content:

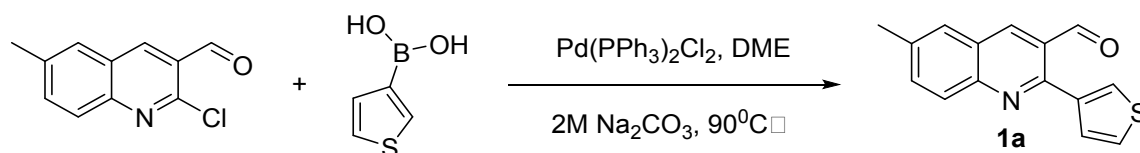
Experimental: General	3
General procedure and spectral data for Synthesis of 6-Methyl-2-(thiophen-3-yl)quinoline-3-carbaldehyde 1a-1h	3-6
General procedure for the synthesis of dibromo compounds	6
General procedure and spectral data for the synthesis of 3-(bromoethynyl)-6-methyl-2-(thiophen-3-yl)quinoline 2a-2h	7-9
General procedure and spectral data for the synthesis of 6-methyl-3-(phenylethynyl)-2-(thiophen-3-yl)quinoline 3a-3w	10-18
General procedure and spectral data for the synthesis of 5-iodo-8-methyl-4-phenylthieno[2,3- <i>c</i>]acridine 4a-4w	19-27
General procedure and spectral data for the synthesis of (E)-3-(2-Bromo-1,2-diiodovinyl)-2-(furan-3-yl)-6-methylquinoline 5a-5d	28-29
General procedure and spectral data for the synthesis of 8-Methyl-4,5-diphenylthieno[2,3- <i>c</i>]acridine 6a	30
General procedure and spectral data for the synthesis of 8-Methyl-4-phenylthieno[2,3- <i>c</i>]acridine 6b	30
General procedure and spectral data for the synthesis of Methyl (E)-3-(8-methyl-4-phenylthieno[2,3- <i>c</i>]acridin-5-yl)acrylate 6c	31
General procedure and spectral data for the synthesis of 11-Methyl-14,15-diphenylnaphtho[2,1- <i>a</i>]thieno[2,3- <i>c</i>]acridine 6d	32
Table S1. Crystal data and structure refinement for 5-iodo-8-methyl-4-phenylthieno[2,3- <i>c</i>]acridine 4a	33
Computational detail	34
Figure S1. Relative Gibbs free energy profiles at T = 298 K of the reactions leading to 4e-4h	35
Figure S2. Optimized structure of TS with some representative interatomic distances [Å]	36-38
Figure S3. Relative Gibbs free energy profiles at T = 298 K of the reactions leading to 4i-4l	39

Figure S4. Relative Gibbs free energy profiles at T = 298 K of the reactions leading to 4m-4p	39
Figure S5. Relative Gibbs free energy profiles at T = 298 K of the reactions leading to 4q-4s	40
Figure S6. Relative Gibbs free energy profiles at T = 298 K of the reactions leading to 4t-4w	40
TD DFT calculations on compounds 6a-6d	41
Table S2. Energy of excited states, coefficient of electronic configurations, and oscillator strength of 6a-6d at their S_0 equilibrium structures relative to those of the S_0 states.	42
Figure S7. Calculated absorption spectra of 6a-6d	43
Figure S8. Molecular orbitals of 6a	43
Figure S9. Molecular orbitals of 6b	44
Figure S10. Molecular orbitals of 6c	44
Figure S11. Molecular orbitals of 6d	45

Experimental: General

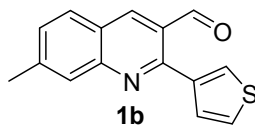
All solvents and reagents were purchased from the suppliers and used without further purification. Reactions were monitored by thin-layer chromatography (TLC) carried out on silica plates using UV-light or Iodine chamber for visualization. Column chromatography was performed on silica gel (60–120 mesh) using n-hexane and ethyl acetate as eluents. IR spectra were recorded on a JASCO FT/IR-460 Plus spectrophotometer. Evaporation and condensation was carried out *in vacuo*. NMR spectra were recorded with JEOL JNM-ECS 400 spectrometer with tetramethylsilane as an internal standard. Chemical shifts δ and coupling constants J are given in ppm (parts per million) and Hz (hertz), respectively. The following abbreviations were used as follows: s: singlet, d: doublet, t: triplet and m: multiplet. Additionally unknown compounds are characterized by HRMS analysis. All known compounds data are inconsistent with the given literature reports. Scale up reactions also performed as per the given general procedure without any deviation. Melting points were measured by a Yanaco micro melting point apparatus.

General procedure for Synthesis of 6-Methyl-2-(thiophen-3-yl)quinoline-3-carbaldehyde **1a-1h**:

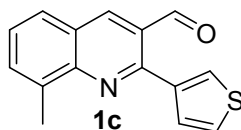


To a stirred solution of 2-chloro-6-methylquinoline-3-carbaldehyde¹ (prepared according to literature reports) (1 g, 4.86 mmol) in DME (8 mL) was added 3-thienylboronic acid (0.746 g, 5.84 mmol), Pd (PPh₃)₂Cl₂ (34.13 mg, 0.01 mmol) and 3 ml 2M Na₂CO₃. After completion of the reaction, the resulting mixture was washed with water (20 mL) and extracted with ethyl acetate (2 X 20 mL), further washed organic layer with brine. Purification was performed by column chromatography using n-hexane / ethyl acetate (97:3) as eluent to afford **1a** 1.04 g. Yield: 84%; Melting point: 121–122°C; IR (neat): 2867, 1683, 1620, 1576, 1557, 1403, 1359, 1132, 1039, 928, 903, 836, 797, 718, 459 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 10.30 (s, 1H), 8.68 (s, 1H), 8.06 (d, J = 8.5 Hz, 1H), 7.65–7.71 (m, 3H), 7.51 (dd, J = 8.5, 5.4 Hz, 2H), 2.56 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 191.70, 154.52, 148.41, 139.38, 137.67, 137.40, 135.23, 129.18, 129.13, 128.16, 127.87, 127.60, 126.70, 126.44, 21.70; HRMS (ESI): m/z = 254.0640 calcd. For C₁₅H₁₂NOS, found 254.0648 [M+H]⁺.

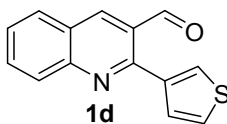
¹**Reference:** M. R. Herbert, D. L. Siegel, L. Staszewski, C. Cayan, U. Banerjee, S. Dhamija, J. Anderson, A. Fan, L. Wang, P. Rix, A. K. Shiao, T. S. Rao, S. A. Noble, R. A. Heyman, E. Bischoff, M. Guha, A. Kabakibi, A. B. Pinkerton, *Bioorg. Med. Chem. Lett.* **2010**, 20, 5718–5721.

7-Methyl-2-(thiophen-3-yl)quinoline-3-carbaldehyde (1b)

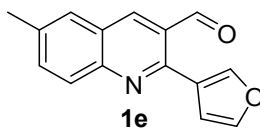
Yield: 91%; Melting point: 88-89°C; IR (neat): 2889, 1681, 1622, 1585, 143, 1360, 1120, 902, 869, 814, 804, 721, 470 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 10.31 (s, 1H), 8.75 (s, 1H), 7.95 (s, 1H), 7.87 (d, J = 8.5 Hz, 1H), 7.65 (t, J = 2.2 Hz, 1H), 7.52 (q, J = 2.4 Hz, 2H), 7.44 (dd, J = 8.5, 1.4 Hz, 1H), 2.60 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 191.65, 155.50, 150.10, 143.84, 139.53, 137.78, 129.94, 129.19, 128.56, 127.62, 127.29, 126.67, 124.51, 22.38; HRMS (ESI): m/z = 254.0640 calcd. For $\text{C}_{15}\text{H}_{12}\text{NOS}$, found 254.0640 $[\text{M}+\text{H}]^+$.

8-Methyl-2-(thiophen-3-yl)quinoline-3-carbaldehyde (1c)

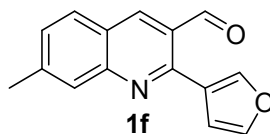
Yield: 89%; Melting point: 102-103°C; IR (neat): 2895, 1687, 1612, 1582, 1569, 1482, 1377, 1358, 1138, 903, 870, 760, 751, 652, 485 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 10.37 (s, 1H), 8.72 (s, 1H), 7.79 (d, J = 8.1 Hz, 1H), 7.61-7.68 (m, 3H), 7.45-7.51 (m, 2H), 2.83 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 191.93, 153.57, 148.81, 140.12, 138.39, 137.65, 132.68, 129.48, 127.85, 127.53, 127.41, 127.25, 126.42, 126.24, 17.96; HRMS (ESI): m/z = 254.0640 calcd. For $\text{C}_{15}\text{H}_{12}\text{NOS}$, found 254.0635 $[\text{M}+\text{H}]^+$.

2-(Thiophen-3-yl)quinoline-3-carbaldehyde (1d)

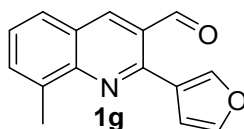
Yield: 86%; Melting point: 94-95°C; IR (neat): 3103, 1683, 1613, 1578, 1552, 1451, 1191, 1152, 901, 868, 786, 805, 744, 718, 487, 476 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 10.33 (s, 1H), 8.80 (s, 1H), 8.17 (d, J = 8.5 Hz, 1H), 7.98 (d, J = 8.1 Hz, 1H), 7.86 (t, J = 7.9 Hz, 1H), 7.67 (q, J = 1.3 Hz, 1H), 7.62 (t, J = 7.4 Hz, 1H), 7.51-7.55 (m, 2H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 191.61, 155.33, 149.82, 139.40, 138.18, 132.77, 129.57, 129.16, 127.90, 127.78, 127.56, 126.80, 126.39; HRMS (ESI): m/z = 240.0483 calcd. For $\text{C}_{14}\text{H}_{10}\text{NOS}$, found 240.0468 $[\text{M}+\text{H}]^+$.

2-(furan-3-yl)-6-methylquinoline-3-carbaldehyde (1e)

Yield: 88%; Melting point: 95-96°C; IR (neat): 3131, 1687, 1626, 1591, 1511, 1391, 1353, 1155, 1144, 1052, 1011, 937, 926, 875, 828, 803, 726, 592, 481 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 10.39 (s, 1H), 8.64 (s, 1H), 8.02 (d, J = 8.5 Hz, 1H), 7.87 (s, 1H), 7.60-7.68 (m, 3H), 6.93 (s, 1H), 2.55 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 191.45, 151.59, 148.63, 143.78, 143.42, 137.73, 137.59, 135.19, 129.06, 128.13, 127.81, 126.28, 124.43, 111.78, 21.66; HRMS (ESI): m/z = 238.0868 calcd. For $\text{C}_{15}\text{H}_{12}\text{NO}_2$, found 238.0854 $[\text{M}+\text{H}]^+$.

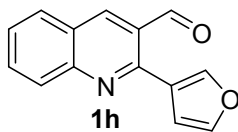
2-(Furan-3-yl)-7-methylquinoline-3-carbaldehyde (1f)

Yield: 82%; Melting point: 76-77°C; IR (neat): 3145, 1686, 1626, 1552, 1505, 1492, 1377, 1361, 1161, 1145, 1133, 1056, 1023, 925, 874, 855, 707, 599, 469 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 10.40 (s, 1H), 8.72 (s, 1H), 7.85-7.93 (m, 3H), 7.61 (t, J = 1.6 Hz, 1H), 7.44 (d, J = 6.7 Hz, 1H), 6.93 (s, 1H), 2.60 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 191.38, 152.57, 150.26, 143.89, 143.79, 143.50, 138.21, 129.90, 129.17, 128.44, 127.23, 124.49, 124.37, 111.79, 22.37; HRMS (ESI): m/z = 238.0868 calcd. For $\text{C}_{15}\text{H}_{12}\text{NO}_2$, found 238.0850 $[\text{M}+\text{H}]^+$.

2-(Furan-3-yl)-8-methylquinoline-3-carbaldehyde (1g)

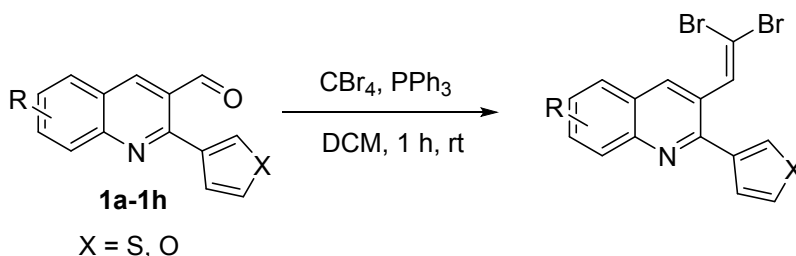
Yield: 76%; Melting point: 96-97°C; IR (neat): 2955, 1686, 1612, 1586, 1568, 1479, 1149, 1073, 1065, 1036, 934, 875, 770, 760, 726, 591, 485 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 10.41 (s, 1H), 8.63 (s, 1H), 7.90 (s, 1H), 7.72 (d, J = 8.1 Hz, 1H), 7.64 (d, J = 6.7 Hz, 1H), 7.58 (s, 1H), 7.43 (t, J = 7.6 Hz, 1H), 7.00 (s, 1H), 2.79 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 191.50, 150.62, 148.87, 143.74, 143.63, 138.95, 137.46, 132.68, 127.38, 127.33, 127.15, 126.01, 125.10, 111.85, 17.88; HRMS (ESI): m/z = 238.0868 calcd. For $\text{C}_{15}\text{H}_{12}\text{NO}_2$, found 238.0868 $[\text{M}+\text{H}]^+$.

2-(Furan-3-yl)quinoline-3-carbaldehyde (**1h**)



Yield: 86%; Melting point: 89-90°C; IR (neat): 3130, 1686, 1662, 1615, 1583, 1557, 1514, 1361, 1158, 1131, 1050, 1008, 936, 875, 787, 748, 720, 592, 490, 480 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 10.43 (s, 1H), 8.78 (s, 1H), 8.15 (d, J = 8.5 Hz, 1H), 7.98 (d, J = 8.1 Hz, 1H), 7.84-7.90 (m, 2H), 7.59-7.63 (m, 2H), 6.95 (q, J = 0.9 Hz, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 191.35, 152.44, 150.00, 143.87, 143.59, 138.61, 132.80, 129.54, 129.44, 127.86, 127.53, 126.27, 124.43, 111.76; HRMS (ESI): m/z = 224.0712 calcd. For $\text{C}_{14}\text{H}_{10}\text{NO}_2$, found 224.0687 $[\text{M}+\text{H}]^+$.

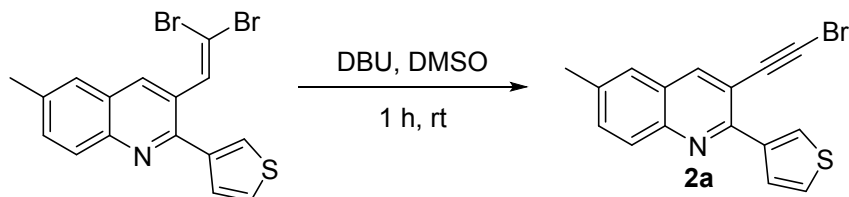
General procedure for the synthesis of dibromo compounds



To a stirred solution of **1a** (1 g, 3.95 mmol) and carbon tetrabromide (2.62 g, 7.9 mmol, 2 equiv.) in anhydrous dichloromethane (15 mL) was added triphenylphosphine (4.14 g, 15.79 mmol, 4 equiv) in portions over a period of 20 min at 0°C. The reaction mixture was turned brown that was allowed to stir at 0°C temperature for 2 h. After completion of reaction (monitored by TLC), reaction mixture was quenched with water (30 mL). The reaction mixture was extracted with dichloromethane (2 x 20 mL); organic layer was washed with brine (30 mL); dried over anhydrous sodium sulfate; solvent was evaporated under reduced pressure to afford a crude residue. After purification by column chromatography n-hexane / ethyl acetate (98:2), the isolated dibromo olefins were used for next step.² Yields 75-85%.

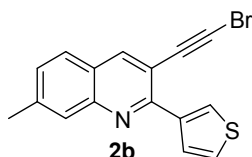
²**Reference:** a) E. J. Corey, P. L. Fuchs, *Tetrahedron Lett.* **1972**, 13, 3769-3772; b) A. K. Morri, Y. Thummala, V. R. Doddi, *Org. Lett.* **2015**, 17, 4640-4643; c) D. Nandini, M. Asthana, K. Mishra, R. P. Singh, R. M. Singh, *Tetrahedron Lett.* **2014**, 55, 6257-6262.

General procedure for the synthesis of 3-(bromoethynyl)-6-methyl-2-(thiophen-3-yl)quinoline 2a-2h:

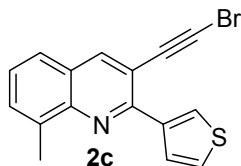


3-(Bromoethynyl)-6-methyl-2-(thiophen-3-yl)quinoline² (60 mg, 0.146 mmol, 1 equiv.) in DMSO (4 mL) was added DBU (61 mg, 0.440 mmol, 3 equiv.) drop wise over a period of 5 min at 15-20°C temperature. The reaction mixture was allowed to stir at the same temperature for 30 min. after completion; reaction mixture was quenched by drop wise addition of 5N aqueous HCl (3 mL) over a period of 10 min then continued stirring for 5 min. The reaction mixture was extracted with ethyl acetate (2 x 10 mL); organic layer was washed with water (10 mL). The organic layers was combined, dried over sodium sulfate and concentrated in vacuo; purified by column chromatography using n-hexanes/ethyl acetate (97:3) as eluent to afford **2a** 42 mg; Yield: 87%; Sticky; IR (KBr): 3011, 2957, 2193, 1625, 1586, 1552, 1435, 1253, 1215, 1171, 917, 882, 873, 805, 776, 727, 643 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 8.22 (t, *J* = 3.1 Hz, 2H), 7.91-7.96 (m, 2H), 7.51 (d, *J* = 9.0 Hz, 1H), 7.45 (s, 1H), 7.38-7.40 (m, 1H), 2.50 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 152.92, 145.66, 141.77, 141.11, 137.03, 133.09, 129.18, 128.93, 126.78, 125.95, 125.81, 125.02, 114.82, 79.03, 55.42, 21.71; HRMS (ESI): *m/z* = 327.9796 calcd. For C₁₆H₁₁NSBr, found 327.9816 [M+H]⁺.

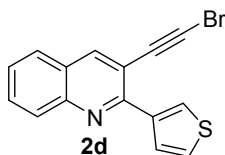
3-(Bromoethynyl)-7-methyl-2-(thiophen-3-yl)quinoline (2b)



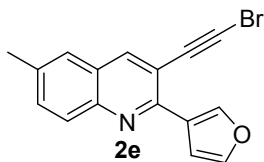
Yield: 79%; Sticky; IR (KBr): 3013, 2960, 2193, 1625, 1586, 1533, 1490, 1435, 1358, 1215, 917, 873, 805, 754, 644 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 8.25-8.28 (m, 2H), 7.93 (d, *J* = 4.9 Hz, 1H), 7.85 (s, 1H), 7.61 (d, *J* = 8.1 Hz, 1H), 7.40 (q, *J* = 2.7 Hz, 1H), 7.33 (d, *J* = 8.1 Hz, 1H), 2.54 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 153.70, 147.25, 142.18, 141.34, 141.14, 129.36, 128.95, 128.53, 126.96, 126.69, 125.02, 124.02, 114.00, 79.02, 55.15, 22.13; HRMS (ESI): *m/z* = 250.0690 calcd. For C₁₆H₁₂NS, found 250.0661 [M+H-Br]⁺.

3-(Bromoethynyl)-8-methyl-2-(thiophen-3-yl)quinoline (2c)

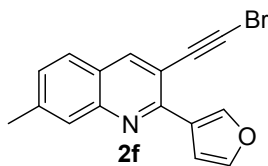
Yield: 75%; Melting point: 88-89°C; IR (neat): 3286, 3074, 2195, 1730, 1611, 1583, 1567, 1527, 1470, 1426, 1250, 1199, 1082, 928, 870, 808, 790, 762, 730, 638, 584 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.38 (s, 1H), 8.30 (s, 1H), 8.05 (d, J = 4.9 Hz, 1H), 7.54-7.57 (m, 2H), 7.39 (t, J = 7.2 Hz, 2H), 2.81 (s, 3H); $^{13}\text{C-NMR}$ (99 MHz, CHLOROFORM-D) δ 151.85, 145.94, 142.91, 141.60, 137.51, 130.84, 129.24, 126.91, 126.80, 125.79, 124.96, 124.86, 114.23, 79.18, 55.42, 17.83; HRMS (ESI): m/z = 250.0690 calcd. For $\text{C}_{16}\text{H}_{12}\text{NS}$, found 250.0660 $[\text{M}+\text{H}-\text{Br}]^+$.

3-(Bromoethynyl)-2-(thiophen-3-yl)quinoline (2d)

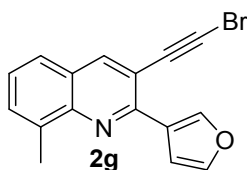
Yield: 77%; Melting point: 83-84°C; IR (neat): 3139, 2508, 2177, 1615, 1579, 1556, 1480, 1425, 1252, 1165, 1075, 906, 875, 855, 797, 744, 722, 614, 599 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.33 (s, 1H), 8.26 (q, J = 1.5 Hz, 1H), 8.06-8.09 (m, 1H), 7.93 (dd, J = 4.9, 0.9 Hz, 1H), 7.68-7.72 (m, 2H), 7.49 (t, J = 7.6 Hz, 1H), 7.40 (q, J = 2.7 Hz, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 153.71, 147.02, 142.51, 141.00, 130.76, 129.51, 128.95, 127.14, 127.06, 127.03, 125.93, 125.13, 114.94, 78.86, 55.74; HRMS (ESI): m/z = 236.0534 calcd. For $\text{C}_{15}\text{H}_{10}\text{NS}$, found 236.0507 $[\text{M}+\text{H}-\text{Br}]^+$.

3-(Bromoethynyl)-2-(furan-3-yl)-6-methylquinoline (2e)

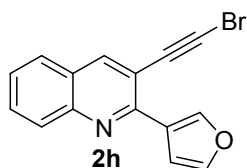
Yield: 75%; Sticky; IR (KBr): 3019, 2973, 1756, 1624, 1612, 1588, 1489, 1373, 1216, 1158, 1140, 1016, 827, 756, 667, 597 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.42 (s, 1H), 8.22 (s, 1H), 7.94 (d, J = 8.5 Hz, 1H), 7.52-7.54 (m, 2H), 7.48 (s, 1H), 7.27 (d, J = 8.5 Hz, 1H), 2.52 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 150.72, 145.72, 143.67, 142.86, 141.50, 136.88, 133.06, 129.05, 126.28, 125.84, 125.77, 114.54, 110.77, 78.92, 55.77, 21.68; HRMS (ESI): m/z = 312.0024 calcd. For $\text{C}_{16}\text{H}_{11}\text{NOBr}$, found 312.0037 $[\text{M}+\text{H}]^+$.

3-(Bromoethynyl)-2-(furan-3-yl)-7-methylquinoline (2f)

Yield: 85%; Melting point: 98-99°C; IR (neat): 3156, 3036, 2915, 2191, 1761, 1622, 1587, 1513, 1427, 1358, 1153, 1145, 1047, 999, 903, 873, 850, 774, 722, 586, 577, 467 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 8.43 (s, 1H), 8.25 (s, 1H), 7.83 (s, 1H), 7.61 (d, *J* = 8.5 Hz, 1H), 7.53 (t, *J* = 1.6 Hz, 1H), 7.26-7.34 (m, 2H), 2.55 (s, 3H); ¹³C-NMR (99 MHz, CHLOROFORM-D) δ 151.51, 147.31, 143.82, 142.86, 141.88, 141.30, 129.19, 128.40, 126.70, 126.34, 123.82, 113.70, 110.79, 78.92, 55.55, 22.10; HRMS (ESI): *m/z* = 234.0919 calcd. For C₁₆H₁₂NO, found 234.0890 [M+H-Br]⁺.

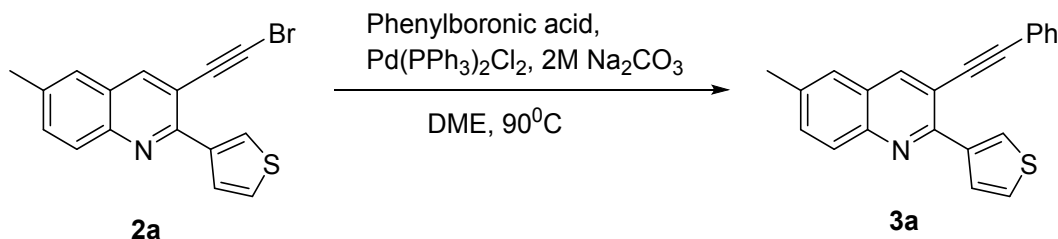
3-(Bromoethynyl)-2-(furan-3-yl)-8-methylquinoline (2g)

Yield: 83%; yellow liquid; IR (KBr): 3155, 3040, 1737, 1755, 1612, 1588, 1516, 1443, 1373, 1156, 1072, 1042, 1002, 929, 791, 741, 604, 588 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 8.47 (s, 1H), 8.23 (s, 1H), 7.52 (dd, *J* = 4.7, 3.4 Hz, 3H), 7.33-7.37 (m, 2H), 2.79 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 149.94, 145.93, 143.76, 142.79, 142.39, 137.33, 130.80, 126.81, 126.63, 125.57, 124.99, 114.00, 110.89, 78.99, 55.82, 17.77; HRMS (ESI): *m/z* = 234.0919 calcd. For C₁₆H₁₂NO, found 234.0938 [M+H-Br]⁺.

3-(Bromoethynyl)-2-(furan-3-yl)quinoline (2h)

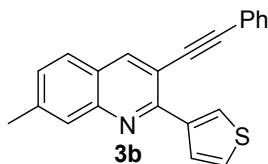
Yield: 78%; Melting point: 102-104°C; IR (neat): 3197, 2188, 1584, 1568, 1512, 1481, 1446, 1418, 1326, 1154, 1080, 1049, 1004, 934, 904, 871, 798, 778, 733, 587, 491, 470 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 8.45 (s, 1H), 8.30 (s, 1H), 8.04 (d, *J* = 9.0 Hz, 1H), 7.68-7.72 (m, 2H), 7.47-7.54 (m, 2H), 7.25-7.30 (m, 1H); ¹³C-NMR (100 MHz, CDCl₃) δ 151.53, 147.08, 143.92, 142.93, 142.19, 130.71, 129.37, 127.06, 126.90, 126.26, 125.73, 114.62, 110.80, 78.77, 56.07; HRMS (ESI): *m/z* = 297.9868 calcd. For C₁₅H₉NOBr, found 297.9855 [M+H]⁺.

General procedure for the synthesis of 6-methyl-3-(phenylethynyl)-2-(thiophen-3-yl)quinoline 3a-3w:

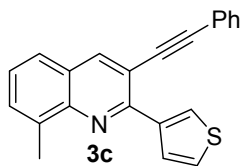


To the solution of 3-(bromoethynyl)-6-methyl-2-(thiophen-3-yl)quinoline **2a** (20 mg, 0.069 mmol, 1 equiv.) in DME (1 mL) was added phenyl boronic acid (9.66 mg, 0.0792 mmol, 1.3 equiv.); 2M Na₂CO₃ (0.3 ml) and Pd(PPh₃)₂Cl₂ (0.0427 mg, 0.1 equiv.); the reaction mixture was allowed to stir at 90°C for 1 h. The reaction mixture was extracted with ethyl acetate: brine (2 x 10 mL). The organic layer was dried over anhydrous sodium sulfate; the crude product was isolated by evaporating the solvent and purified by column chromatography using n-hexane/ ethyl acetate (97:3) as eluent to afford **3a** 16 mg; Yield: 81%; Melting point: 85-86 °C; IR (neat): 3055, 3121, 2197, 1596, 1578, 1570, 1485, 1444, 1434, 1354, 1260, 1074, 922, 874, 819, 802, 757, 689, 665, 626, 527, 480 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 8.35 (s, 1H), 8.31 (s, 1H), 7.97-8.01 (m, 2H), 7.53 (d, *J* = 7.6 Hz, 4H), 7.37-7.42 (m, 4H), 2.53 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 152.93, 145.63, 141.46, 140.53, 136.91, 132.80, 131.54, 129.18, 128.79, 128.61, 126.82, 126.22, 125.90, 124.77, 123.04, 115.52, 94.55, 88.53, 21.73; HRMS (ESI): *m/z* = 326.1003 calcd. For C₂₂H₁₆NS, found 326.0976 [M+H]⁺.

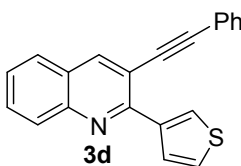
7-Methyl-3-(phenylethynyl)-2-(thiophen-3-yl)quinoline (3b)



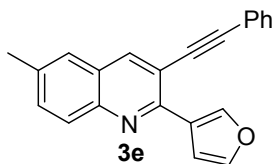
Yield: 73%; Sticky; IR (KBr): 3051, 3015, 1625, 1598, 1584, 1572, 1488, 1442, 1434, 1255, 1216, 851, 805, 754, 669, 642 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 8.36 (d, *J* = 4.9 Hz, 2H), 8.00-8.02 (m, 1H), 7.88 (s, 1H), 7.66 (d, *J* = 8.1 Hz, 1H), 7.51-7.53 (m, 2H), 7.34-7.42 (m, 5H), 2.56 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 153.69, 147.22, 141.50, 141.00, 140.95, 131.52, 129.27, 129.20, 128.76, 128.61, 128.55, 127.00, 126.79, 124.77, 124.27, 123.09, 114.68, 94.37, 88.54, 22.13; HRMS (ESI): *m/z* = 326.1003 calcd. For C₂₂H₁₆NS, found 326.1006 [M+H]⁺.

8-Methyl-3-(phenylethynyl)-2-(thiophen-3-yl)quinoline (3c)

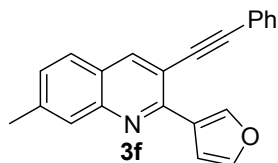
Yield: 75%; Melting point: 56-57°C; IR (neat): 3031, 2956, 2918, 1613, 1596, 1578, 1570, 1491, 1469, 1428, 1193, 1075, 918, 869, 789, 767, 753, 728, 688, 663, 635 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.51 (q, J = 1.3 Hz, 1H), 8.34 (s, 1H), 8.13 (dd, J = 4.9, 1.3 Hz, 1H), 7.51-7.58 (m, 4H), 7.35-7.40 (m, 5H), 2.82 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 151.74, 145.91, 142.00, 141.72, 137.49, 131.58, 130.58, 129.53, 128.83, 128.67, 126.99, 126.70, 126.02, 125.08, 124.64, 123.10, 114.87, 94.59, 88.74, 17.89; HRMS (ESI): m/z = 326.1003 calcd. For $\text{C}_{22}\text{H}_{16}\text{NS}$, found 326.1012 $[\text{M}+\text{H}]^+$.

3-(Phenylethynyl)-2-(thiophen-3-yl)quinoline (3d)

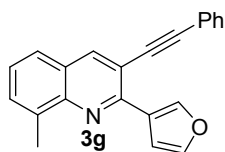
Yield: 77%; Sticky; IR (KBr): 3079, 3057, 1617, 1598, 1582, 1492, 1483, 1428, 1357, 1233, 1071, 916, 869, 729, 637, 546 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.38-8.41 (m, 2H), 8.10 (d, J = 8.5 Hz, 1H), 8.01-8.03 (m, 1H), 7.77 (d, J = 8.1 Hz, 1H), 7.68-7.72 (m, 1H), 7.50-7.54 (m, 3H), 7.42 (q, J = 2.7 Hz, 1H), 7.37-7.38 (m, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 153.71, 146.99, 141.36, 141.22, 131.57, 130.46, 129.52, 129.19, 128.88, 128.64, 127.15, 126.97, 126.20, 124.88, 122.97, 115.62, 94.74, 88.35; HRMS (ESI): m/z = 312.0847 calcd. For $\text{C}_{21}\text{H}_{14}\text{NS}$, found 312.0838 $[\text{M}+\text{H}]^+$.

2-(Furan-3-yl)-6-methyl-3-(phenylethynyl)quinoline (3e)

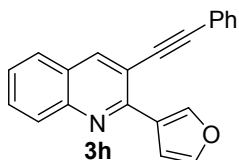
Yield: 74%; Melting point: 86-87°C; IR (neat): 3035, 2945, 1735, 1597, 1586, 1513, 1492, 1358, 1158, 1078, 1051, 1000, 918, 874, 755, 593 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.58 (s, 1H), 8.27 (s, 1H), 7.96 (d, J = 8.5 Hz, 1H), 7.57-7.60 (m, 2H), 7.49-7.54 (m, 3H), 7.40 (dd, J = 4.9, 1.8 Hz, 3H), 7.36 (d, J = 1.8 Hz, 1H), 2.51 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 150.53, 145.67, 143.83, 142.74, 140.47, 136.74, 132.78, 131.57, 129.05, 128.94, 128.70, 126.59, 126.00, 125.93, 122.89, 115.16, 110.98, 94.83, 88.32, 21.72; HRMS (ESI): m/z = 310.1232 calcd. For $\text{C}_{22}\text{H}_{16}\text{NO}$, found 310.1206 $[\text{M}+\text{H}]^+$.

2-(Furan-3-yl)-7-methyl-3-(phenylethynyl)quinoline (3f)

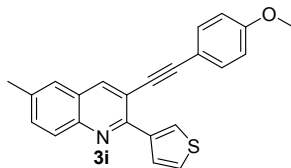
Yield: 78%; Sticky; IR (neat): 2958, 2924, 1758, 1725, 1625, 1588, 1572, 1513, 1443, 1166, 1155, 913, 873, 806, 509 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.60 (s, 1H), 8.30 (s, 1H), 7.85 (s, 1H), 7.54-7.63 (m, 4H), 7.30-7.39 (m, 5H), 2.54 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 151.31, 147.27, 144.00, 142.75, 140.96, 140.86, 131.55, 129.10, 128.89, 128.70, 128.41, 126.80, 126.67, 124.05, 122.95, 114.33, 111.01, 94.67, 88.34, 22.11; HRMS (ESI): m/z = 310.1232 calcd. For $\text{C}_{22}\text{H}_{16}\text{NO}$, found 310.1254 $[\text{M}+\text{H}]^+$.

2-(Furan-3-yl)-8-methyl-3-(phenylethynyl)quinoline (3g)

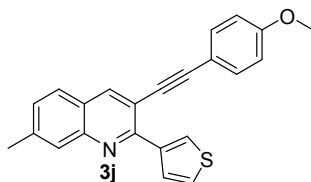
Yield: 77%; Sticky; IR (KBr): 3056, 2922, 1760, 1733, 1598, 1587, 1573, 1472, 1071, 1035, 926, 794, 594, 525 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.66 (s, 1H), 8.33 (s, 1H), 7.52-7.61 (m, 5H), 7.35-7.43 (m, 5H), 2.82 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 149.75, 145.92, 143.93, 142.69, 141.40, 137.33, 131.58, 130.54, 128.94, 128.72, 127.13, 126.54, 125.82, 125.09, 122.93, 114.66, 111.07, 94.90, 88.36, 17.81; HRMS (ESI): m/z = 310.1232 calcd. For $\text{C}_{22}\text{H}_{16}\text{NO}$, found 310.1232 $[\text{M}+\text{H}]^+$.

2-(Furan-3-yl)-3-(phenylethynyl)quinoline (3h)

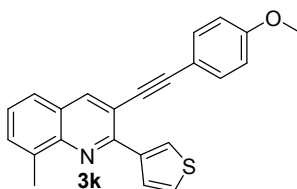
Yield: 81%; Sticky; IR (KBr): 3058, 2961, 1759, 1732, 1605, 1586, 1571, 1292, 1251, 1158, 1030, 873, 831, 683, 755, 736, 594 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.61 (d, J = 0.9 Hz, 1H), 8.36 (s, 1H), 8.06 (d, J = 8.5 Hz, 1H), 7.66-7.74 (m, 2H), 7.54-7.59 (m, 3H), 7.48 (t, J = 7.0 Hz, 1H), 7.37-7.40 (m, 4H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 151.34, 147.05, 144.08, 142.80, 141.13, 131.59, 130.42, 129.38, 128.99, 128.72, 127.14, 126.80, 126.59, 125.98, 122.82, 115.27, 111.02, 95.02, 88.15; HRMS (ESI): m/z = 296.1075 calcd. For $\text{C}_{21}\text{H}_{14}\text{NO}$, found 296.1104 $[\text{M}+\text{H}]^+$.

3-((4-Methoxyphenyl)ethynyl)-6-methyl-2-(thiophen-3-yl)quinoline (3i)

Yield: 72%; Melting point: 99-100°C; IR (neat): 2954, 2934, 1733, 1605, 1510, 1486, 1440, 1291, 1249, 1173, 1032, 918, 827, 802, 727 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.31 (d, $J = 23.3$ Hz, 2H), 7.98 (d, $J = 9.0$ Hz, 2H), 7.40-7.51 (m, 5H), 6.90 (d, $J = 9.0$ Hz, 2H), 3.83 (s, 3H), 2.53 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 160.05, 152.88, 145.44, 141.52, 140.10, 136.84, 133.04, 132.60, 129.20, 129.15, 126.77, 126.29, 125.86, 124.69, 115.88, 115.12, 114.28, 94.72, 87.30, 55.44, 21.74; HRMS (ESI): $m/z = 356.1109$ calcd. For $\text{C}_{23}\text{H}_{18}\text{NOS}$, found 356.1118 $[\text{M}+\text{H}]^+$.

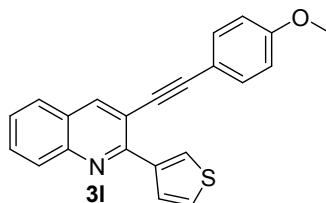
3-((4-Methoxyphenyl)ethynyl)-7-methyl-2-(thiophen-3-yl)quinoline (3j)

Yield: 77%; Sticky; IR (KBr): 2958, 2935, 1624, 1606, 1585, 1489, 1464, 1434, 1291, 1173, 1033, 831, 805, 755, 728 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.37 (s, 1H), 8.33 (s, 1H), 8.01 (d, $J = 4.9$ Hz, 1H), 7.87 (s, 1H), 7.65 (d, $J = 8.5$ Hz, 1H), 7.46 (d, $J = 8.5$ Hz, 2H), 7.41 (q, $J = 2.7$ Hz, 1H), 7.34 (d, $J = 8.1$ Hz, 1H), 6.90 (d, $J = 9.0$ Hz, 2H), 3.83 (s, 3H), 2.56 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 160.02, 153.62, 147.06, 141.58, 140.75, 140.52, 133.00, 129.23, 129.19, 128.52, 126.93, 126.72, 124.67, 124.34, 115.17, 115.04, 114.28, 94.52, 87.29, 55.44, 22.10; HRMS (ESI): $m/z = 356.1109$ calcd. For $\text{C}_{23}\text{H}_{18}\text{NOS}$, found 356.1098 $[\text{M}+\text{H}]^+$.

3-((4-Methoxyphenyl)ethynyl)-8-methyl-2-(thiophen-3-yl)quinoline (3k)

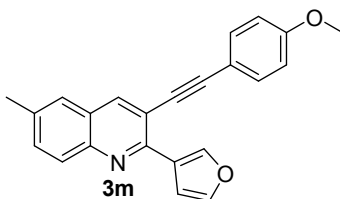
Yield: 74%; Sticky; IR (KBr): 3034, 3013, 1582, 1569, 1466, 1454, 1429, 1381, 1288, 1132, 1107, 1025, 1013, 861, 805, 667, 534 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.53 (d, $J = 2.7$ Hz, 1H), 8.34 (s, 1H), 8.13 (d, $J = 4.0$ Hz, 1H), 7.59 (d, $J = 8.1$ Hz, 1H), 7.48-7.54 (m, 3H), 7.36-7.41 (m, 2H), 6.91 (d, $J = 9.0$ Hz, 2H), 3.83 (s, 3H), 2.83 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 160.06, 151.68, 145.75, 142.07, 141.29, 137.45, 133.05, 130.38, 129.54, 127.83, 126.92, 126.64, 126.08, 125.01, 124.54, 115.24, 114.31, 94.73, 87.48, 55.45, 17.87; HRMS (ESI): $m/z = 356.1109$ calcd. For $\text{C}_{23}\text{H}_{18}\text{NOS}$, found 356.1106 $[\text{M}+\text{H}]^+$.

3-((4-Methoxyphenyl)ethynyl)-2-(thiophen-3-yl)quinoline (3l)



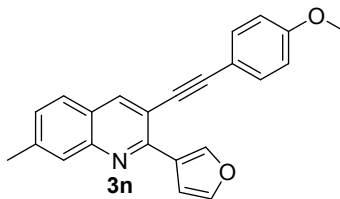
Yield: 70%; Yellow liquid syrup; IR (KBr): 3006, 2837, 1606, 1582, 1569, 1482, 1464, 1173, 1106, 916, 869, 805, 729, 628, 545 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.38-8.39 (m, 2H), 8.09 (d, J = 8.5 Hz, 1H), 8.02 (dd, J = 4.9, 1.3 Hz, 1H), 7.76 (d, J = 8.1 Hz, 1H), 7.67-7.71 (m, 1H), 7.40-7.53 (m, 4H), 6.89-6.91 (m, 2H), 3.83 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 160.10, 153.64, 146.81, 141.45, 140.76, 133.06, 130.25, 129.49, 129.23, 127.11, 127.08, 126.91, 126.27, 124.79, 115.98, 115.04, 114.30, 94.93, 87.14, 55.45; HRMS (ESI): m/z = 342.0953 calcd. For $\text{C}_{22}\text{H}_{16}\text{NOS}$, found 342.0955 $[\text{M}+\text{H}]^+$.

2-(Furan-3-yl)-3-((4-methoxyphenyl)ethynyl)-6-methylquinoline (3m)

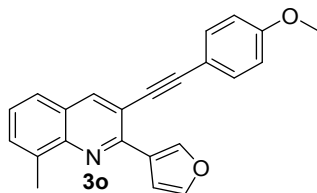


Yield: 74%; Melting point: 82-83°C; IR (neat): 2959, 2937, 1755, 1732, 1586, 1569, 1464, 1441, 1276, 1127, 1031, 874, 756, 594, 535 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.62-8.54 (1H), 8.28-8.18 (1H), 8.00-7.89 (1H), 7.59-7.43 (5H), 7.39-7.32 (1H), 6.96-6.86 (2H), 3.87-3.80 (3H), 2.56-2.47 (3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 160.14, 150.48, 145.50, 143.84, 142.68, 140.07, 136.65, 133.07, 132.57, 129.01, 126.63, 126.06, 125.88, 115.53, 114.96, 114.34, 111.00, 95.00, 87.10, 55.45, 21.71; HRMS (ESI): m/z = 340.1338 calcd. For $\text{C}_{23}\text{H}_{18}\text{NO}_2$, found 340.1318 $[\text{M}+\text{H}]^+$.

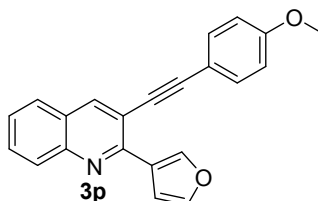
2-(Furan-3-yl)-3-((4-methoxyphenyl)ethynyl)-7-methylquinoline (3n)



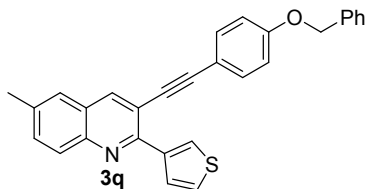
Yield: 76%; Sticky; IR (KBr): 3018, 2839, 1756, 1732, 1625, 1606, 1511, 1490, 1377, 1251, 1174, 1155, 959, 883, 756 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.60 (s, 1H), 8.30 (s, 1H), 7.85 (s, 1H), 7.64 (d, J = 8.5 Hz, 1H), 7.50-7.54 (m, 3H), 7.32-7.36 (m, 2H), 6.92 (d, J = 9.0 Hz, 2H), 3.84 (s, 3H), 2.56 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 160.11, 151.28, 147.11, 143.99, 142.68, 140.73, 140.48, 133.03, 129.04, 128.38, 126.73, 124.11, 115.01, 114.70, 114.33, 111.00, 94.81, 87.08, 55.46, 22.08; HRMS (ESI): m/z = 340.1338 calcd. For $\text{C}_{23}\text{H}_{18}\text{NO}_2$, found 340.1337 $[\text{M}+\text{H}]^+$.

2-(Furan-3-yl)-3-((4-methoxyphenyl)ethynyl)-8-methylquinoline (3o)

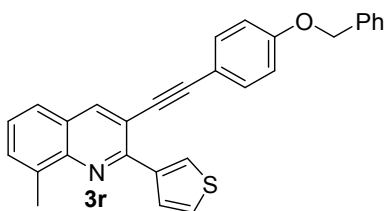
Yield: 70%; Sticky; IR (KBr): 2957, 2935, 1760, 1732, 1586, 1570, 1500, 1466, 1292, 1274, 1174, 874, 831, 767, 628, 594 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.67 (s, 1H), 8.31 (s, 1H), 7.58 (d, J = 8.1 Hz, 1H), 7.52-7.54 (m, 4H), 7.43 (d, J = 1.8 Hz, 1H), 7.37 (t, J = 7.4 Hz, 1H), 6.93 (d, J = 8.5 Hz, 2H), 3.84 (s, 3H), 2.83 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 160.15, 149.72, 145.77, 143.93, 142.63, 141.02, 137.29, 133.07, 130.35, 127.82, 127.17, 126.49, 125.88, 125.03, 114.99, 114.35, 111.08, 95.05, 87.12, 55.46, 17.80; HRMS (ESI): m/z = 340.1338 calcd. For $\text{C}_{23}\text{H}_{18}\text{NO}_2$, found 340.1346 $[\text{M}+\text{H}]^+$.

2-(Furan-3-yl)-3-((4-methoxyphenyl)ethynyl)quinoline (3p)

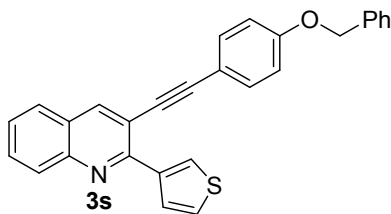
Yield: 77%; Sticky; IR (KBr): 2959, 2838, 1758, 1605, 1586, 1570, 1292, 1251, 1174, 1030, 873, 831, 783, 754, 734, 582 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.62 (s, 1H), 8.34 (s, 1H), 8.06 (d, J = 8.5 Hz, 1H), 7.66-7.74 (m, 2H), 7.47-7.54 (m, 4H), 7.38 (t, J = 0.9 Hz, 1H), 6.92 (d, J = 9.0 Hz, 2H), 3.83 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 160.20, 151.30, 146.88, 144.08, 142.75, 140.72, 133.08, 130.22, 129.35, 127.08, 126.73, 126.62, 126.04, 115.63, 114.88, 114.36, 111.02, 95.19, 86.94, 55.46; HRMS (ESI): m/z = 326.1181 calcd. For $\text{C}_{22}\text{H}_{16}\text{NO}_2$, found 326.1156 $[\text{M}+\text{H}]^+$.

3-((4-(Benzyloxy)phenyl)ethynyl)-6-methyl-2-(thiophen-3-yl)quinoline (3q)


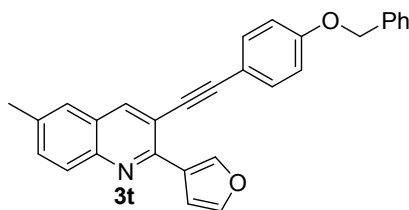
Yield: 74%; Melting point: 94-96°C; IR (neat): 3036, 2920, 1605, 1581, 1566, 1486, 1454, 1437, 1288, 1036, 1025, 1011, 871, 802, 728, 696, 626 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.34 (q, $J = 1.3$ Hz, 1H), 8.28 (s, 1H), 7.97-8.00 (m, 2H), 7.52 (d, $J = 7.2$ Hz, 2H), 7.36-7.47 (m, 8H), 6.97 (d, $J = 9.0$ Hz, 2H), 5.09 (s, 2H), 2.53 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 159.23, 152.89, 145.46, 141.52, 140.13, 136.85, 136.57, 133.06, 132.62, 129.19, 129.17, 128.76, 128.25, 127.58, 126.77, 126.29, 125.86, 124.71, 115.86, 115.39, 115.18, 94.67, 87.38, 70.16, 21.74; HRMS (ESI): $m/z = 432.1422$ calcd. For $\text{C}_{29}\text{H}_{22}\text{NOS}$, found 432.1401 $[\text{M}+\text{H}]^+$.

3-((4-(Benzyloxy)phenyl)ethynyl)-8-methyl-2-(thiophen-3-yl)quinoline (3r)


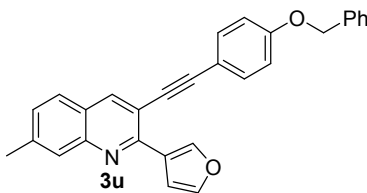
Yield: 72%; Melting point: 68-70°C; IR (neat): 3036, 2921, 1720, 1604, 1566, 1470, 1454, 1429, 1378, 1288, 1173, 1126, 1025, 830, 807, 696, 628, 573 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.52 (d, $J = 1.8$ Hz, 1H), 8.34 (s, 1H), 8.13 (d, $J = 4.0$ Hz, 1H), 7.36-7.60 (m, 11H), 6.98 (d, $J = 9.0$ Hz, 2H), 5.09 (s, 2H), 2.83 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 159.24, 151.69, 145.76, 142.06, 141.32, 137.46, 136.58, 133.07, 130.39, 129.53, 128.78, 128.26, 127.59, 126.92, 126.65, 126.08, 125.01, 124.55, 115.44, 115.20, 94.68, 87.56, 70.17, 17.87; HRMS (ESI): $m/z = 432.1422$ calcd. For $\text{C}_{29}\text{H}_{22}\text{NOS}$, found 432.1393 $[\text{M}+\text{H}]^+$.

3-((4-(Benzyloxy)phenyl)ethynyl)-2-(thiophen-3-yl)quinoline (3s)


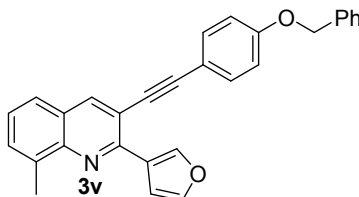
Yield: 78%; Melting point: 69-70°C; IR (neat): 3035, 3011, 1732, 1569, 1559, 1381, 1357, 1311, 1131, 1107, 916, 861, 637, 666, 582 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.37 (s, 2H), 8.09 (d, J = 8.5 Hz, 1H), 8.01 (d, J = 4.9 Hz, 1H), 7.75 (d, J = 8.1 Hz, 1H), 7.69 (t, J = 7.6 Hz, 1H), 7.34-7.52 (m, 9H), 6.97 (d, J = 8.5 Hz, 2H), 5.08 (s, 2H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 159.28, 153.65, 146.83, 141.45, 140.80, 136.56, 133.09, 130.27, 129.50, 129.23, 128.78, 128.27, 127.59, 127.11, 127.09, 126.91, 126.27, 124.81, 115.97, 115.32, 115.20, 94.88, 87.24, 70.16; HRMS (ESI): m/z = 418.1266 calcd. For $\text{C}_{28}\text{H}_{20}\text{NOS}$, found 418.1254 $[\text{M}+\text{H}]^+$.

3-((4-(Benzyloxy)phenyl)ethynyl)-2-(furan-3-yl)-6-methylquinoline (3t)


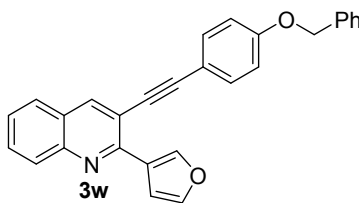
Yield: 90%; Melting point: 143-144°C; IR (neat): 3161, 2896, 2855, 2201, 1604, 1583, 1566, 1508, 1484, 1461, 1249, 1230, 1155, 1078, 1016, 924, 823, 799, 773, 737, 594, 534, 480 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.58 (s, 1H), 8.23 (s, 1H), 7.95 (d, J = 8.5 Hz, 1H), 7.33-7.53 (m, 11H), 6.98 (dt, J = 9.3, 2.4 Hz, 2H), 5.08 (s, 2H), 2.50 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 159.32, 150.49, 145.53, 143.85, 142.69, 140.10, 136.67, 136.56, 133.09, 132.59, 129.04, 128.78, 128.27, 127.60, 126.65, 126.07, 125.89, 115.52, 115.25, 111.01, 94.97, 87.21, 70.17, 21.72; HRMS (ESI): m/z = 416.1651 calcd. For $\text{C}_{29}\text{H}_{22}\text{NO}_2$, found 416.1676 $[\text{M}+\text{H}]^+$.

3-((4-(Benzyloxy)phenyl)ethynyl)-2-(furan-3-yl)-7-methylquinoline (3u)

Yield: 83%; Sticky; IR (KBr): 2919, 2865, 1758, 1624, 1604, 1588, 1509, 1454, 1287, 1245, 1174, 1009, 873, 880, 807, 780, 734, 696 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.59 (s, 1H), 8.26 (s, 1H), 7.84 (s, 1H), 7.61 (d, J = 8.5 Hz, 1H), 7.31-7.52 (m, 10H), 6.97 (d, J = 8.5 Hz, 2H), 5.06 (s, 2H), 2.53 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 159.28, 151.27, 147.12, 144.01, 142.70, 140.75, 140.51, 136.57, 133.06, 129.05, 128.78, 128.40, 128.28, 127.61, 126.76, 124.12, 115.24, 114.68, 111.03, 94.80, 87.21, 70.16, 22.10; HRMS (ESI): m/z = 416.1651 calcd. For $\text{C}_{29}\text{H}_{22}\text{NO}_2$, found 416.1629 $[\text{M}+\text{H}]^+$.

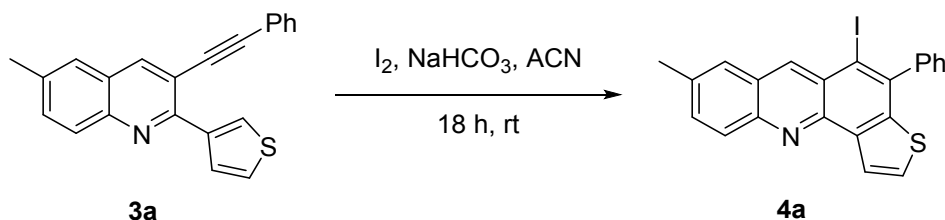
3-((4-(Benzyloxy)phenyl)ethynyl)-2-(furan-3-yl)-8-methylquinoline (3v)

Yield: 77%; Melting point: 84-85°C; IR (neat): 3018, 2923, 1605, 1587, 1571, 1509, 1455, 1470, 1379, 1289, 1245, 1231, 1216, 1174, 1158, 831, 668 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.66 (s, 1H), 8.30 (s, 1H), 7.51-7.58 (m, 5H), 7.34-7.44 (m, 7H), 6.99 (d, J = 9.0 Hz, 2H), 5.09 (s, 2H), 2.82 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 159.32, 149.72, 145.78, 143.93, 142.64, 141.05, 137.29, 136.56, 133.09, 130.37, 128.78, 128.28, 127.61, 127.18, 126.50, 125.88, 125.05, 115.26, 115.00, 111.09, 95.01, 87.22, 70.18, 17.81; HRMS (ESI): m/z = 416.1651 calcd. For $\text{C}_{29}\text{H}_{22}\text{NO}_2$, found 416.1664 $[\text{M}+\text{H}]^+$.

3-((4-(Benzyloxy)phenyl)ethynyl)-2-(furan-3-yl)quinoline (3w)

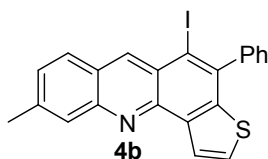
Yield: 74%; Melting point: 82-84°C; IR (neat): 3020, 2886, 1766, 1605, 1587, 1509, 1483, 1455, 1216, 1160, 1174, 1025, 874, 756, 669 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.61 (t, J = 0.9 Hz, 1H), 8.32 (s, 1H), 8.06 (d, J = 8.1 Hz, 1H), 7.64-7.73 (m, 2H), 7.43-7.53 (m, 5H), 7.32-7.42 (m, 5H), 6.97-7.00 (m, 2H), 5.07 (s, 2H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 159.38, 151.32, 146.91, 144.09, 142.77, 140.75, 136.56, 133.11, 130.24, 129.37, 128.78, 128.28, 127.60, 127.10, 126.74, 126.65, 126.05, 115.62, 115.28, 115.17, 111.04, 95.17, 87.06, 70.18; HRMS (ESI): m/z = 402.1494 calcd. For $\text{C}_{28}\text{H}_{20}\text{NO}_2$, found 402.1466 $[\text{M}+\text{H}]^+$.

General procedure for the synthesis of 5-iodo-8-methyl-4-phenylthieno[2,3-c]acridine 4a-4w:

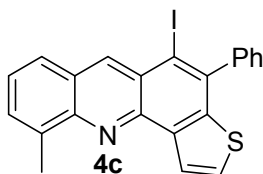


To a stirred solution of 6-methyl-3-(phenylethynyl)-2-(thiophen-3-yl)quinoline **3a** (27 mg, 0.083 mmol, 1 equiv.); iodine (126 mg, 0.498 mmol, 6 equiv.) and NaHCO₃ (41.82 mg, 0.497 mmol, 6 equiv.) in dry ACN (5 mL) was stirred for 18 h. After completion of reaction (monitored by TLC), reaction mixture was quenched by saturated sodium thiosulfate and extracted with ethyl acetate (15 mL). Solvent was evaporated under reduced pressure to afford a crude residue. The crude was purified by silica gel chromatography using hexane/ethyl acetate (97:3) as eluent to afford **4a**. Yield: 91%; Melting point: 228-230°C; IR (neat): 3052, 2915, 2182, 1585, 1551, 1491, 1353, 1314, 1139, 1029, 968, 913, 888, 815, 710, 694, 632, 532, 467 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.01 (s, 1H), 8.43 (d, *J* = 5.4 Hz, 1H), 8.16 (d, *J* = 9.0 Hz, 1H), 7.78 (s, 1H), 7.60 (dd, *J* = 8.8, 2.0 Hz, 1H), 7.46-7.50 (m, 4H), 7.39 (dd, *J* = 7.4, 2.0 Hz, 2H), 2.53 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 147.43, 144.02, 143.93, 142.36, 141.45, 141.20, 137.37, 135.97, 133.60, 129.40 (2C), 128.83, 128.76 (2C), 128.56, 127.53, 127.36, 126.91, 126.79, 124.54, 99.21, 21.94; HRMS (ESI): *m/z* = 451.9970 calcd. For C₂₂H₁₅NSI, found 451.9980 [M+H]⁺.

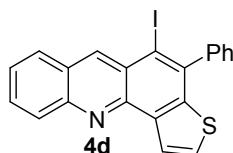
5-Iodo-9-methyl-4-phenylthieno[2,3-c]acridine (4b)



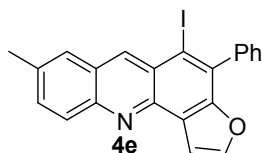
Yield: 89%; Melting point: 145-147°C; IR (neat): 3111, 3048, 2936, 1626, 1601, 1587, 1550, 1489, 1443, 1363, 1143, 1033, 907, 871, 748, 714, 702, 659, 632, 577 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.14 (s, 1H), 8.51 (d, *J* = 5.4 Hz, 1H), 8.11 (s, 1H), 8.00 (d, *J* = 8.5 Hz, 1H), 7.54-7.58 (m, 4H), 7.43-7.48 (m, 3H), 2.65 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 148.87, 144.62, 143.92, 142.65, 142.07, 141.41, 140.87, 137.29, 129.43 (2C), 128.86, 128.83, 128.77 (2C), 128.14, 127.43, 127.28, 126.38, 125.76, 124.59, 99.30, 22.42; HRMS (ESI): *m/z* = 451.9970 calcd. For C₂₂H₁₅NSI, found 451.9950 [M+H]⁺.

5-Iodo-10-methyl-4-phenylthieno[2,3-c]acridine (4c)

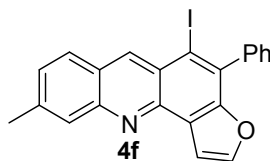
Yield: 84%; Melting point: 118-119°C; IR (neat): 3023, 2962, 2911, 2027, 1617, 1588, 1560, 1495, 1439, 1361, 1142, 1076, 1069, 892, 884, 810, 753, 712, 692, 637, 629, 528 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.05 (s, 1H), 8.49 (d, *J* = 5.4 Hz, 1H), 7.87 (d, *J* = 8.1 Hz, 1H), 7.51-7.62 (m, 5H), 7.41-7.46 (m, 3H), 2.97 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 147.69, 143.91, 143.41, 142.21, 141.06 (2 C), 137.84, 136.88, 130.14, 129.45 (2 C), 128.83, 128.76 (2 C), 127.34, 127.22, 126.52, 126.40, 125.90, 124.68, 99.07, 18.35; HRMS (ESI): *m/z* = 451.9970 calcd. For C₂₂H₁₅NSI, found 451.9949 [M+H]⁺.

5-Iodo-4-phenylthieno[2,3-c]acridine (4d)

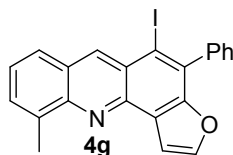
Yield: 86%; Melting point: 131-133°C; IR (neat): 3101, 3055, 2924, 1791, 1732, 1618, 1587, 1548, 1491, 1439, 1360, 1323, 1138, 1128, 1031, 897, 884, 776, 766, 755, 721, 628, 530, 469 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.20 (s, 1H), 8.53 (d, *J* = 5.4 Hz, 1H), 8.35 (d, *J* = 8.5 Hz, 1H), 8.11 (d, *J* = 7.6 Hz, 1H), 7.85 (t, *J* = 7.0 Hz, 1H), 7.56-7.63 (m, 5H), 7.47 (dd, *J* = 7.4, 2.0 Hz, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ 148.56, 144.59, 143.84, 142.77, 142.45, 141.37, 137.33, 130.79, 129.38 (2C), 128.94, 128.89, 128.79 (2C), 128.55, 127.47, 127.42, 126.85, 126.11, 124.65, 99.14; HRMS (ESI): *m/z* = 451.9813 calcd. For C₂₁H₁₃NSI, found 437.9796 [M+H]⁺.

5-Iodo-8-methyl-4-phenylfuro[2,3-c]acridine (4e)

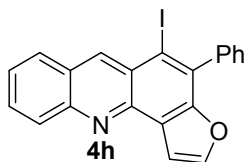
Yield: 87%; Melting point: 248-250°C; IR (neat): 3126, 3057, 1607, 1574, 1551, 1524, 1441, 1356, 1333, 1211, 1053, 905, 880, 812, 716, 701, 533 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.17 (s, 1H), 8.25 (d, *J* = 9.0 Hz, 1H), 7.88 (s, 1H), 7.68-7.73 (m, 3H), 7.55-7.60 (m, 3H), 7.49-7.51 (m, 2H), 2.61 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 152.99, 147.66, 144.88, 143.11, 142.22, 139.64, 135.75, 135.07, 133.87, 130.15 (2C), 128.78, 128.48 (2C), 128.23, 127.17, 126.98, 126.37, 123.99, 107.34, 99.53, 21.90; HRMS (ESI): *m/z* = 436.0198 calcd. For C₂₂H₁₅NOI, found 436.0186 [M+H]⁺.

5-Iodo-9-methyl-4-phenylfuro[2,3-c]acridine (4f)

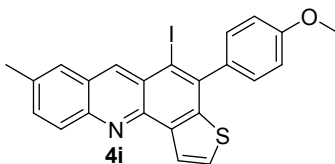
Yield: 80%; Melting point: 219-220°C; IR (neat): 3059, 3017, 1609, 1576, 1560, 1467, 1442, 1418, 1398, 1157, 1002, 890, 759, 719, 701, 643, 480 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 9.19 (s, 1H), 8.10 (s, 1H), 8.00 (d, J = 8.5 Hz, 1H), 7.71 (dd, J = 6.3, 1.8 Hz, 2H), 7.54-7.60 (m, 3H), 7.49-7.51 (m, 2H), 7.43 (d, J = 6.7 Hz, 1H), 2.65 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 153.16, 149.08, 144.83, 143.74, 142.79, 141.67, 139.64, 134.72, 130.18 (2C), 128.77, 128.66, 128.47 (2C), 128.37, 127.09, 125.84, 125.41, 123.92, 107.35, 99.67, 22.44; HRMS (ESI): m/z = 436.0198 calcd. For $\text{C}_{22}\text{H}_{15}\text{NOI}$, found 436.0190 $[\text{M}+\text{H}]^+$.

5-Iodo-10-methyl-4-phenylfuro[2,3-c]acridine (4g)

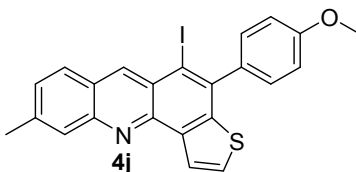
Yield: 85%; Melting point: 148-149°C; IR (neat) 3146, 2866, 1602, 1575, 1518, 1502, 1452, 1243, 1178, 1013, 999, 835, 821, 753, 740, 694, 619 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 9.19 (s, 1H), 7.95 (d, J = 8.5 Hz, 1H), 7.67-7.73 (m, 3H), 7.57 (dd, J = 9.0, 6.7 Hz, 3H), 7.47-7.52 (m, 3H), 3.01 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 152.97, 148.09, 144.78, 142.94, 142.68, 139.65, 136.73, 134.95, 130.31, 130.20 (2C), 128.76, 128.46 (2C), 127.06, 126.67, 126.08, 125.72, 124.50, 107.43, 99.32, 18.30; HRMS (ESI): m/z = 436.0198 calcd. For $\text{C}_{22}\text{H}_{15}\text{NOI}$, found 436.0178 $[\text{M}+\text{H}]^+$.

5-Iodo-4-phenylfuro[2,3-c]acridine (4h)

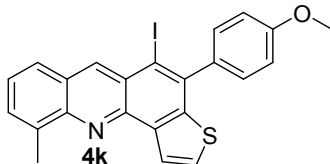
Yield: 81%; Melting point: 168-170°C; IR (neat): 3057, 3026, 1607, 1524, 1441, 1356, 1333, 1212, 1175, 1053, 905, 880, 812, 716, 701, 562 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 9.26 (s, 1H), 8.34 (d, J = 8.5 Hz, 1H), 8.11 (d, J = 8.1 Hz, 1H), 7.83-7.87 (m, 1H), 7.73 (q, J = 2.2 Hz, 2H), 7.49-7.62 (m, 6H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 153.19, 148.79, 144.93, 143.73, 143.19, 139.56, 135.27, 130.99, 130.15 (2C), 128.83, 128.77, 128.63, 128.49 (2C), 127.05, 126.30, 125.88, 124.01, 107.43, 99.53; HRMS (ESI): m/z = 422.0042 calcd. For $\text{C}_{21}\text{H}_{13}\text{NOI}$, found 422.0034 $[\text{M}+\text{H}]^+$.

5-Iodo-4-(4-methoxyphenyl)-8-methylthieno[2,3-c]acridine (4i)

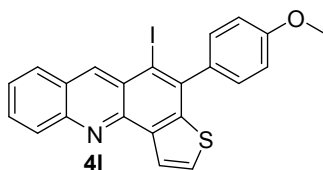
Yield: 89%; Melting point: 198-200°C; IR (neat): 3103, 2959, 2926, 1792, 1604, 1587, 1574, 1509, 1489, 1439, 1353, 1245, 1172, 1134, 1025, 894, 835, 821, 813, 720, 689, 470 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 9.10 (s, 1H), 8.51 (d, J = 5.4 Hz, 1H), 8.24 (d, J = 8.5 Hz, 1H), 7.87 (s, 1H), 7.69 (dd, J = 8.8, 2.0 Hz, 1H), 7.57 (d, J = 5.4 Hz, 1H), 7.41 (d, J = 8.5 Hz, 2H), 7.09 (d, J = 8.5 Hz, 2H), 3.93 (s, 3H), 2.61 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 159.85, 147.37, 144.03, 142.83, 141.47, 140.95, 137.23, 136.45, 135.95, 133.56, 130.71 (2C), 128.56, 127.53, 127.33, 127.03, 126.80, 124.58, 114.04 (2C), 99.88, 55.42, 21.94; HRMS (ESI): m/z = 482.0076 calcd. For $\text{C}_{23}\text{H}_{17}\text{NOI}$, found 482.0064 $[\text{M}+\text{H}]^+$.

5-Iodo-4-(4-methoxyphenyl)-9-methylthieno[2,3-c]acridine (4j)

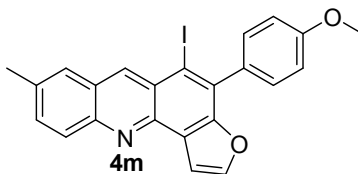
Yield: 86%; Melting point: 218-220°C; IR (neat): 3104, 3084, 2954, 1629, 1608, 1585, 1513, 1361, 1289, 1248, 1170, 1141, 1030, 903, 886, 831, 796, 725, 717, 578, 525 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 9.14 (s, 1H), 8.50 (d, J = 5.4 Hz, 1H), 8.11 (s, 1H), 8.00 (d, J = 8.5 Hz, 1H), 7.56 (d, J = 5.4 Hz, 1H), 7.42 (dd, J = 13.9, 8.5 Hz, 3H), 7.09 (d, J = 8.5 Hz, 2H), 3.93 (s, 3H), 2.65 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 159.84, 148.79, 144.61, 143.13, 142.08, 141.35, 140.62, 137.15, 136.43, 130.73 (2C), 128.83, 128.14, 127.40, 127.24, 126.50, 125.75, 124.63, 114.04 (2C), 99.96, 55.42, 22.40; HRMS (ESI): m/z = 482.0076 calcd. For $\text{C}_{23}\text{H}_{17}\text{NOI}$, found 482.0053 $[\text{M}+\text{H}]^+$.

5-Iodo-4-(4-methoxyphenyl)-10-methylthieno[2,3-c]acridine (4k)

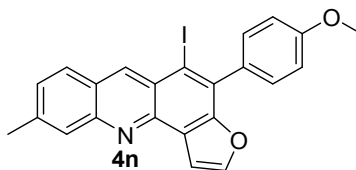
Yield: 78%; Melting point: 222-224^oC; IR (neat): 3098, 3084, 2929, 1607, 1587, 1572, 1511, 1460, 1275, 1244, 1173, 1026, 1013, 892, 831, 721, 544, 506 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.08 (s, 1H), 8.50 (d, *J* = 5.4 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.63 (d, *J* = 6.7 Hz, 1H), 7.53 (d, *J* = 4.9 Hz, 1H), 7.38-7.47 (m, 3H), 7.08 (d, *J* = 8.5 Hz, 2H), 3.92 (s, 3H), 2.99 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 159.84, 147.65, 143.45, 142.73, 142.24, 140.83, 137.72, 136.89, 136.43, 130.75 (2C), 130.10, 127.81, 127.36, 127.19, 126.42, 125.88, 124.72, 114.03 (2C), 99.70, 55.42, 18.33; HRMS (ESI): *m/z* = 482.0076 calcd. For C₂₃H₁₇NOSI, found 482.0057 [M+H]⁺.

5-Iodo-4-(4-methoxyphenyl)thieno[2,3-c]acridine (4l)

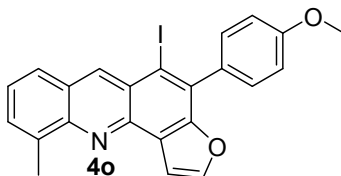
Yield: 88%; Melting point: 212-214^oC; IR (neat): 3086, 2926, 2851, 1605, 1586, 1573, 1510, 1492, 1452, 1362, 1288, 1247, 1172, 1030, 835, 748, 717, 698, 619, 469 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.20 (s, 1H), 8.52 (d, *J* = 5.4 Hz, 1H), 8.34 (d, *J* = 8.5 Hz, 1H), 8.11 (d, *J* = 8.5 Hz, 1H), 7.85 (t, *J* = 7.2 Hz, 1H), 7.57-7.63 (m, 2H), 7.41 (d, *J* = 8.5 Hz, 2H), 7.09 (d, *J* = 8.5 Hz, 2H), 3.93 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 159.89, 148.50, 144.59, 143.24, 142.45 (2C), 141.13, 137.20, 136.36, 130.70 (3C), 128.92, 128.54, 127.42 (2C), 126.95, 126.08, 124.68, 114.06, 99.80, 55.43; HRMS (ESI): *m/z* = 467.9919 calcd. For C₂₂H₁₅NOSI, found 467.9909 [M+H]⁺.

5-Iodo-4-(4-methoxyphenyl)-8-methylfuro[2,3-c]acridine (4m)

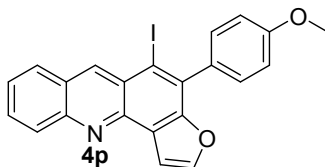
Yield: 81%; Melting point: 218-219^oC; IR (neat): 3048, 2970, 1633, 1578, 1472, 1395, 1363, 1219, 1084, 1010, 971, 923, 822, 772, 756, 561 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.16 (s, 1H), 8.23 (d, *J* = 8.5 Hz, 1H), 7.88 (s, 1H), 7.68-7.74 (m, 3H), 7.45 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.5 Hz, 2H), 3.93 (s, 3H), 2.61 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 159.87, 153.18, 147.61, 144.81, 143.13, 142.16, 135.69, 134.77, 133.77, 131.87, 131.48 (2C), 128.24, 127.16, 126.97, 126.48, 123.92, 113.85 (2C), 107.34, 100.02, 55.41, 21.90; HRMS (ESI): *m/z* = 466.0304 calcd. For C₂₃H₁₇NO₂I, found 466.0294 [M+H]⁺.

5-Iodo-4-(4-methoxyphenyl)-9-methylfuro[2,3-c]acridine (4n)

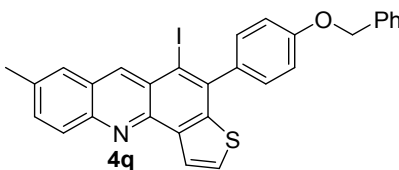
Yield: 77%; Melting point: 188-190°C; IR (neat): 3020, 2963, 1025, 1604, 1476, 1459, 1441, 1242, 1215, 1176, 1140, 958, 903, 756, 668 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.21 (s, 1H), 8.11 (s, 1H), 8.02 (d, *J* = 8.5 Hz, 1H), 7.72 (dd, *J* = 9.6, 2.0 Hz, 2H), 7.44-7.46 (m, 3H), 7.11 (d, *J* = 9.0 Hz, 2H), 3.93 (s, 3H), 2.66 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 159.86, 153.38, 149.01, 144.77, 143.75, 142.79, 141.60, 134.45, 131.86, 131.50 (2C), 128.64, 128.37, 127.08, 125.96, 125.42, 123.83, 113.86 (2C), 107.38, 100.17, 55.41, 22.44; HRMS (ESI): *m/z* = 466.0304 calcd. For C₂₃H₁₇NO₂I, found 466.0300 [M+H]⁺.

5-Iodo-4-(4-methoxyphenyl)-10-methylfuro[2,3-c]acridine (4o)

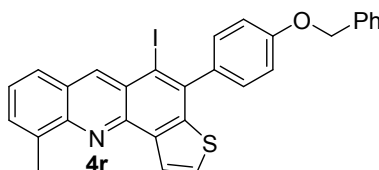
Yield: 73%; Melting point: 205-206°C; IR (neat): 3019, 2839, 1718, 1606, 1454, 1441, 1419, 1397, 1355, 1248, 1215, 1157, 1133, 1034, 913, 893, 833, 756, 651 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.17 (s, 1H), 7.94 (d, *J* = 8.5 Hz, 1H), 7.66-7.73 (m, 3H), 7.47 (t, *J* = 9.2 Hz, 3H), 7.10 (d, *J* = 9.0 Hz, 2H), 3.92 (s, 3H), 3.00 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 159.86, 153.17, 147.99, 144.69, 142.89, 142.66, 136.69, 134.64, 131.87, 131.53 (2C), 130.24, 127.03, 126.66, 126.16, 125.67, 124.41, 114.20, 113.84, 107.44, 99.81, 55.42, 18.30; HRMS (ESI): *m/z* = 466.0304 calcd. For C₂₃H₁₇NO₂I, found 466.0304 [M+H]⁺.

5-Iodo-4-(4-methoxyphenyl)furo[2,3-c]acridine (4p)

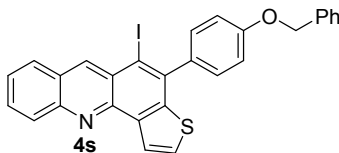
Yield: 68%; Melting point: 234-235°C; IR (neat): 2923, 2836, 1719, 1575, 1544, 1516, 1504, 1438, 1285, 1244, 1025, 881, 830, 792, 761, 748, 603 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.28 (s, 1H), 8.34 (d, *J* = 9.0 Hz, 1H), 8.13 (d, *J* = 8.5 Hz, 1H), 7.86 (t, *J* = 7.2 Hz, 1H), 7.74 (dd, *J* = 9.0, 1.8 Hz, 2H), 7.61 (t, *J* = 7.4 Hz, 1H), 7.46 (d, *J* = 8.5 Hz, 2H), 7.11 (d, *J* = 9.0 Hz, 2H), 3.93 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 159.91, 153.42, 148.73, 144.87, 143.76, 143.19, 134.99, 131.79, 131.48 (2C), 130.93, 128.77, 128.61, 127.06, 126.44, 125.87, 123.91, 113.88 (2C), 107.43, 100.01, 55.42; HRMS (ESI): *m/z* = 452.0148 calcd. For C₂₂H₁₅NO₂I, found 452.0175 [M+H]⁺.

4-(4-(Benzyloxy)phenyl)-5-iodo-8-methylthieno[2,3-c]acridine (4q)

Yield: 77%; Melting point: 220-221⁰C; IR (neat): 3116, 2896, 2922, 1733, 1605, 1582, 1550, 1509, 1453, 1376, 1244, 1172, 1022, 819, 795, 731, 696, 634, 492 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.12 (s, 1H), 8.52 (d, *J* = 5.4 Hz, 1H), 8.25 (d, *J* = 9.0 Hz, 1H), 7.89 (s, 1H), 7.70 (d, *J* = 9.0 Hz, 1H), 7.58 (d, *J* = 5.4 Hz, 1H), 7.52 (d, *J* = 7.2 Hz, 2H), 7.39-7.46 (m, 5H), 7.17 (d, *J* = 8.5 Hz, 2H), 5.18 (s, 2H), 2.62 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 159.17, 147.38, 144.04, 142.81, 141.50, 140.93, 137.25, 136.86, 136.70, 135.97, 133.58, 130.76 (2C), 128.76 (2C), 128.56, 128.24, 127.81 (2C), 127.54, 127.35, 127.04, 126.81, 124.59, 114.88 (2C), 99.85, 70.23, 21.94; HRMS (ESI): *m/z* = 558.0389 calcd. For C₂₉H₂₁NOSI, found 558.0405 [M+H]⁺.

4-(4-(Benzyloxy)phenyl)-5-iodo-10-methylthieno[2,3-c]acridine (4r)

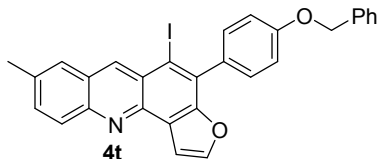
Yield: 75%; Melting point: 175-176⁰C; IR (neat): 3034, 2892, 2955, 1724, 1604, 1588, 1494, 1449, 1361, 1246, 1171, 1107, 1035, 1025, 760, 734, 716, 693, 621, 531, 499 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.11 (s, 1H), 8.53 (d, *J* = 5.4 Hz, 1H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.66 (d, *J* = 6.7 Hz, 1H), 7.37-7.56 (m, 9H), 7.16 (d, *J* = 8.5 Hz, 2H), 5.16 (s, 2H), 3.00 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 159.15, 147.70, 143.49, 142.72, 142.29, 140.81, 137.75, 136.91, 136.86, 136.67, 130.80 (2C), 130.14, 128.77 (2C), 128.25, 127.83 (2C), 127.40, 127.23, 126.70, 126.44, 125.92, 124.72, 114.86 (2C), 99.69, 70.22, 18.34; HRMS (ESI): *m/z* = 558.0389 calcd. For C₂₉H₂₁NOSI, found 558.0402 [M+H]⁺.

4-(4-(Benzyloxy)phenyl)-5-iodothiemo[2,3-c]acridine (4s)

Yield: 81%; Melting point: 169-171⁰C; IR (neat): 3034, 2920, 2214, 1620, 1603, 1583, 1549, 1508, 1453, 1360, 1240, 1175, 1009, 1001, 919, 910, 832, 734, 725, 715, 698, 632, 509 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.22 (s, 1H), 8.53 (d, *J* = 5.4 Hz, 1H), 8.35 (d, *J* = 8.5 Hz, 1H), 8.13 (d, *J* = 8.1 Hz, 1H), 7.86 (t, *J* = 7.2 Hz, 1H), 7.58-7.64 (m, 2H), 7.52 (d, *J* = 7.2 Hz, 2H), 7.37-7.46 (m, 5H), 7.18 (d, *J* = 8.5 Hz, 2H), 5.17 (s, 2H); ¹³C-NMR (100 MHz, CDCl₃) δ 159.20, 148.52, 144.62, 143.21, 142.49, 141.10, 137.22, 136.84, 136.61, 130.76 (3C), 128.93, 128.77 (2C), 128.56, 128.25, 127.82 (2C), 127.45 (2C), 126.97, 126.09,

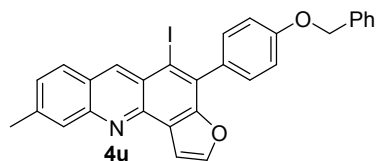
124.69, 114.89 (2C), 99.78, 70.23; HRMS (ESI): m/z = 544.0232 calcd. For $C_{28}H_{19}NO_2I$, found 544.0223 $[M+H]^+$.

4-(4-(Benzyloxy)phenyl)-5-iodo-8-methylfuro[2,3-c]acridine (4t)



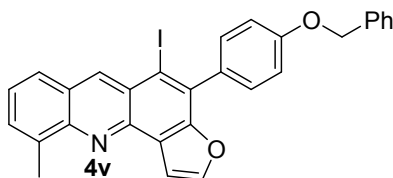
Yield: 71%; Melting point: 195-196°C; IR (neat): 3031, 3009, 2914, 2174, 1722, 1602, 1578, 1547, 1517, 1292, 1219, 1173, 1052, 1021, 912, 836, 819, 760, 747, 732, 694, 535 cm^{-1} ; 1H -NMR (400 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.23 (d, J = 8.5 Hz, 1H), 7.87 (s, 1H), 7.67-7.73 (m, 3H), 7.35-7.51 (m, 7H), 7.18 (d, J = 8.5 Hz, 2H), 5.16 (s, 2H), 2.60 (s, 3H); ^{13}C -NMR (100 MHz, $CDCl_3$) δ 159.18, 153.16, 147.60, 144.82, 143.13, 142.18, 136.89, 135.70, 134.73, 133.80, 132.12, 131.55 (2C), 128.77 (2C), 128.23 (2C), 127.78 (2C), 127.16, 126.98, 126.48, 123.92, 114.66 (2C), 107.35, 100.02, 70.20, 21.91; HRMS (ESI): m/z = 542.0617 calcd. For $C_{29}H_{21}NO_2I$, found 542.0626 $[M+H]^+$.

4-(4-(Benzyloxy)phenyl)-5-iodo-9-methylfuro[2,3-c]acridine (4u)



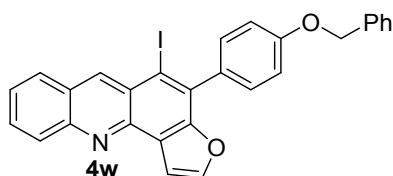
Yield: 70%; Melting point: 190-192°C; IR (neat): 3031, 2920, 2851, 1738, 1598, 1515, 1500, 1352, 1231, 1207, 997, 904, 830, 741, 689, 646, 587, 511, 473, 464 cm^{-1} ; 1H -NMR (400 MHz, $CDCl_3$) δ 9.22 (s, 1H), 8.11 (s, 1H), 8.03 (d, J = 8.5 Hz, 1H), 7.73 (dd, J = 9.9, 2.2 Hz, 2H), 7.37-7.52 (m, 8H), 7.19 (d, J = 9.0 Hz, 2H), 5.17 (s, 2H), 2.66 (s, 3H); ^{13}C -NMR (100 MHz, $CDCl_3$) δ 159.17, 153.37, 149.05, 144.78, 143.78, 142.80, 141.62, 136.90, 134.41, 132.12, 131.55 (2C), 128.76 (2C), 128.65, 128.38, 128.21, 127.77 (2C), 127.09, 125.97, 125.43, 123.86, 114.66 (2C), 107.37, 100.13, 70.20, 22.43; HRMS (ESI): m/z = 542.0617 calcd. For $C_{29}H_{21}NO_2I$, found 542.0620 $[M+H]^+$.

4-(4-(Benzyloxy)phenyl)-5-iodo-10-methylfuro[2,3-c]acridine (4v)



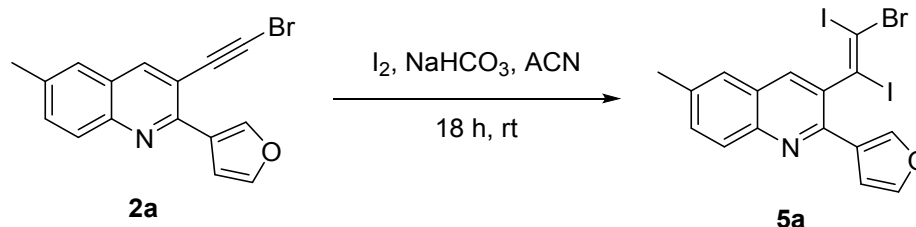
Yield: 73%; Melting point: 165-167°C; IR (neat): 3146, 2911, 2866, 1717, 1602, 1575, 1518, 1502, 1352, 1243, 1178, 1013, 999, 835, 821, 753, 740, 694, 619, 588 cm^{-1} ; ^1H -NMR (400 MHz, CDCl_3) δ 9.21 (s, 1H), 7.98 (d, J = 8.5 Hz, 1H), 7.69-7.75 (m, 3H), 7.47 (td, J = 16.5, 7.8 Hz, 8H), 7.19 (d, J = 9.0 Hz, 2H), 5.18 (s, 2H), 3.01 (s, 3H); ^{13}C -NMR (100 MHz, CDCl_3) δ 159.17, 153.18, 148.05, 144.72, 142.95, 142.71, 136.91, 136.72, 134.64, 132.13, 131.57 (2C), 130.27, 128.76 (2C), 128.21, 127.76 (2C), 126.68, 126.21, 125.70, 124.43, 115.18, 114.66 (2C), 107.45, 99.77, 70.21, 18.28; HRMS (ESI): m/z = 542.0617 calcd. For $\text{C}_{29}\text{H}_{21}\text{NO}_2\text{I}$, found 542.0613 $[\text{M}+\text{H}]^+$.

4-(4-(Benzyloxy)phenyl)-5-iodofuro[2,3-c]acridine (4w)



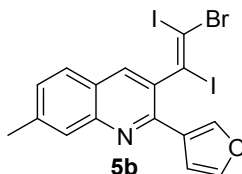
Yield: 69%; Melting point: 177-178°C; IR (neat): 3142, 2969, 1663, 1603, 1574, 1519, 1503, 1355, 1219, 1175, 1048, 1025, 1002, 831, 773, 739, 697, 591 cm^{-1} ; ^1H -NMR (400 MHz, CDCl_3) δ 9.25 (s, 1H), 8.33 (d, J = 9.0 Hz, 1H), 8.11 (d, J = 8.1 Hz, 1H), 7.82-7.86 (m, 1H), 7.72 (dd, J = 8.1, 1.8 Hz, 2H), 7.57-7.61 (m, 1H), 7.34-7.51 (m, 7H), 7.17-7.20 (m, 2H), 5.16 (s, 2H); ^{13}C -NMR (100 MHz, CDCl_3) δ 159.23, 153.38, 148.73, 144.87, 143.75, 143.17, 136.90, 134.94, 132.05, 131.56 (2C), 130.93, 128.77 (3C), 128.62, 128.23, 127.77 (2C), 127.05, 126.42, 125.87, 123.94, 114.70 (2C), 107.45, 100.01, 70.22; HRMS (ESI): m/z = 528.0461 calcd. For $\text{C}_{28}\text{H}_{19}\text{NO}_2\text{I}$, found 528.0455 $[\text{M}+\text{H}]^+$.

General procedure for the synthesis of (*E*)-3-(2-bromo-1,2-diiodovinyl)-2-(furan-3-yl)-6-methylquinoline **5a-5d**:

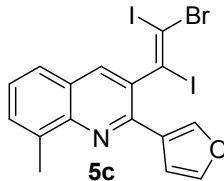


To a stirred solution of (*E*)-3-(2-bromo-1,2-diiodovinyl)-2-(furan-3-yl)-6-methylquinoline **2a** (20 mg, 0.064 mmol, 1 equiv.) and iodine (97.6 mg, 0.384 mmol, 6 equiv.); NaHCO₃ (32.3 mg, 0.384 mmol, 6 equiv.) in dry ACN (5 mL) was stirred for 18 h. After completion of reaction (monitored by TLC), reaction mixture was quenched by saturated sodium thiosulfate and extracted with ethyl acetate (20 mL). Solvent was evaporated under reduced pressure to afford a crude residue. The crude was purified by silica gel chromatography using n-hexane/ethyl acetate (97:3) as eluent to afford **5a**; Yield: 58%; Melting point: 103-105 °C; IR (neat): 3020, 2977, 1593, 1556, 1514, 1487, 1215, 1166, 1159, 1087, 931, 874, 826, 669, 622, 594 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 7.93-8.00 (m, 3H), 7.54-7.60 (m, 3H), 7.13 (d, *J* = 1.8 Hz, 1H), 2.55 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 146.99, 146.37, 143.41, 143.17, 138.85, 137.08, 135.78, 133.19, 129.12, 126.54, 126.34, 110.90, 110.77, 103.81, 61.30, 21.72; HRMS (ESI): *m/z* = 565.8114 calcd. For C₁₆H₁₁NOBrI₂, found 565.8138 [M+H]⁺.

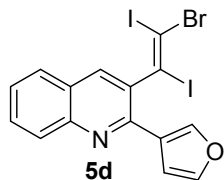
(*E*)-3-(2-Bromo-1,2-diiodovinyl)-2-(furan-3-yl)-7-methylquinoline (5b**)**



Yield: 43%; Sticky; IR (KBr): 2970, 2922, 1709, 1625, 1573, 1550, 1514, 1452, 1215, 1159, 1054, 1007, 874, 806, 756, 706, 667, 594 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 7.96-7.99 (m, 2H), 7.88 (s, 1H), 7.68-7.71 (m, 1H), 7.54 (d, *J* = 1.8 Hz, 1H), 7.38 (d, *J* = 8.5 Hz, 1H), 7.12 (d, *J* = 9.0 Hz, 1H), 2.56 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 147.95, 143.57, 143.18, 141.43, 138.10, 136.19, 135.49, 129.38, 128.43, 127.39, 125.70, 124.38, 110.94, 103.89, 61.42, 22.15; HRMS (ESI): *m/z* = 565.8114 calcd. For C₁₆H₁₁NOBrI₂, found 565.8123 [M+H]⁺.

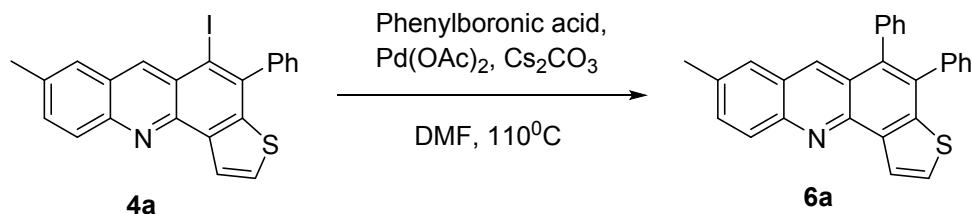
(E)-3-(2-Bromo-1,2-diiodovinyl)-2-(furan-3-yl)-8-methylquinoline (5c)

Yield: 59%; Melting point: 82-84°C; IR (neat): 2954, 2920, 1614, 1592, 1572, 1513, 1573, 1410, 1377, 1215, 1066, 1040, 1004, 932, 923, 874, 792, 710, 667, 593 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 7.97-8.01 (m, 2H), 7.54-7.65 (m, 3H), 7.42 (t, J = 7.6 Hz, 1H), 7.21-7.25 (m, 1H), 2.84 (s, 3H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 146.63, 146.15, 143.62, 143.11, 138.44, 137.47, 136.62, 135.93, 130.83, 126.85, 126.20, 125.68, 111.05, 103.92, 61.34, 17.85; HRMS (ESI): m/z = 565.8114 calcd. For $\text{C}_{16}\text{H}_{11}\text{NOBrI}_2$, found 565.8133 $[\text{M}+\text{H}]^+$.

(E)-3-(2-Bromo-1,2-diiodovinyl)-2-(furan-3-yl)quinoline (5d)

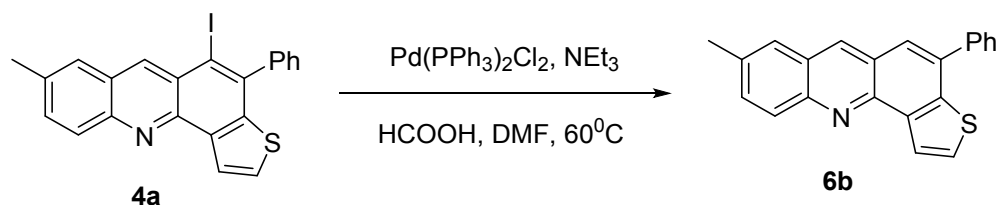
Yield: 51%; Sticky; IR (KBr): 2963, 2928, 1726, 1618, , 1591, 1545, 1513, 1484, 1418, 1215, 1158, 1053, 1005, 936, 873, 783, 667, 593 cm^{-1} ; $^1\text{H-NMR}$ (400 MHz, CDCl_3) δ 8.01-8.11 (m, 3H), 7.73-7.82 (m, 2H), 7.52-7.56 (m, 2H), 7.14 (d, J = 9.4 Hz, 1H); $^{13}\text{C-NMR}$ (100 MHz, CDCl_3) δ 147.90, 143.67, 143.24, 138.88, 136.48, 135.77, 130.83, 129.46, 127.76, 127.06, 126.32, 125.63, 110.81, 103.58, 61.53; HRMS (ESI): m/z = 551.7982 calcd. For $\text{C}_{15}\text{H}_9\text{NOBrI}_2$, found 551.7957 $[\text{M}+\text{H}]^+$.

General procedure for the synthesis of 8-Methyl-4,5-diphenylthieno[2,3-c]acridine (**6a**)



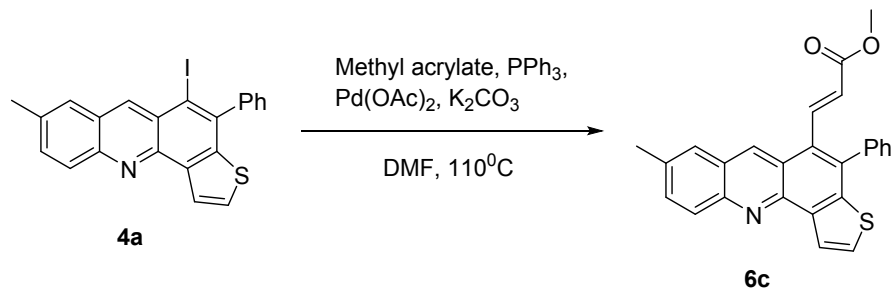
To a solution of 5-iodo-8-methyl-4-phenylthieno[2,3-c]acridine **4a** (30 mg, 0.075 mmol, 1 equiv.) the phenyl boronic acid (11.9 mg, 0.097 mmol, 1.3 equiv.) in 5 ml DMF, Pd(OAc)₂ (1.7 mg, 1 mol %), Cs₂CO₃ (73.08 mg, 0.224 mmol, 3 equiv.) were added. The resulting mixture was then heated at 110°C for 12 h. The solvent was removed under reduced pressure, the residue was extracted with ethyl acetate: brine; the crude was purified by silica gel chromatography using n-hexane/ethyl acetate (95:5) as eluents to afford 18 mg **6a**; Yield: 67%; Melting point: 257-259°C; IR (neat): 3054, 3022, 2979, 1738, 1601, 1586, 1574, 1550, 1439, 1373, 1310, 1123, 1027, 911, 894, 820, 808, 744, 696, 633, 536, 469 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 8.61 (d, *J* = 5.4 Hz, 1H), 8.41 (s, 1H), 8.24 (d, *J* = 8.5 Hz, 1H), 7.61-7.65 (m, 3H), 7.25-7.32 (m, 10H), 2.53 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 146.74, 144.88, 143.28, 139.37, 138.04, 136.71, 135.20, 134.93, 134.18, 133.64, 133.02, 131.68 (2C), 130.08 (2C), 128.88, 128.15 (2C), 128.01 (2C), 127.56, 127.17, 126.90, 126.47, 126.35, 125.75, 124.80, 21.79; HRMS (ESI): *m/z* = 402.1316 calcd. For C₂₈H₂₀NS, found 402.1344 [M+H]⁺.

General procedure for the synthesis of 8-Methyl-4-phenylthieno[2,3-c]acridine (**6b**)



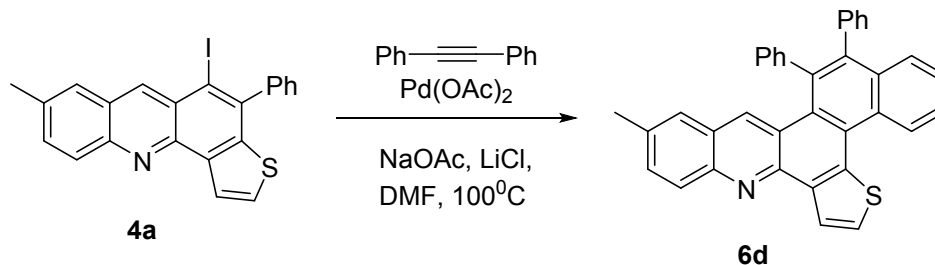
To a solution of the corresponding 5-iodo-8-methyl-4-phenylthieno[2,3-c]acridine **4a** (34 mg, 0.075 mmol, 1 equiv.) the formic acid (5.68 mmol, 0.150 mmol, 2 equiv.) in 5 ml DMF, Pd (PPh₃)₂Cl₂ (2.64 mg, 0.5 mol %), NEt₃ (31.54 mmol, 0.226 mmol, 3 equiv.) were added. The resulting mixture was then heated at 60 °C for 12 h. The solvent was removed under reduced pressure, the residue was extracted with ethyl acetate: brine and purified by silica gel column chromatography using n-hexane: ethyl acetate (95:5) as eluent to afford 21 mg **6b**, Yield: 86%; Melting point: 146-148 °C; IR (neat): 3098, 3048, 2970, 1633, 1600, 1578, 1547, 1472, 1395, 1363, 1219, 1084, 1010, 971, 957, 923, 822, 772, 756, 715, 694, 561 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 8.59-8.65 (m, 2H), 8.23 (d, *J* = 9.0 Hz, 1H), 7.83 (d, *J* = 7.2 Hz, 2H), 7.75 (d, *J* = 4.9 Hz, 2H), 7.64 (t, *J* = 4.9 Hz, 2H), 7.52 (dt, *J* = 26.0, 7.3 Hz, 3H), 2.58 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 147.19, 144.94, 140.93, 140.06, 137.89, 135.47, 135.42, 134.99, 132.88, 129.23, 128.97 (2C), 128.51 (3C), 126.80, 126.42, 126.14, 125.48, 124.78, 123.5, 21.90; HRMS (ESI): *m/z* = 326.1003 calcd. For C₂₂H₁₆NS, found 326.0984 [M+H]⁺.

General procedure for the synthesis of Methyl (E)-3-(8-methyl-4-phenylthieno[2,3-c]acridin-5-yl)acrylate (6c**)**



To a solution of the corresponding 5-iodo-8-methyl-4-phenylthieno[2,3-c]acridine **4a** (30 mg, 0.066 mmol, 1 equiv.) and the methyl acrylate (11.4 mg, 0.133 mmol, 2 equiv.) in 4 ml DMF; Pd (OAc)₂ (0.7 mg, 0.5 mol %), PPh₃ (17.4 mg, 0.066 mmol, 1 equiv.) and K₂CO₃ (18.4 mg, 0.133 mmol, 2 equiv.) were added. The resulting mixture was then heated under nitrogen atmosphere for 12 h. The solvent was removed under reduced pressure, the residue was extracted with ethyl acetate and purified by silica gel column chromatography using n-hexane: ethyl acetate (97:3) as eluent to afford 21 mg **6c**, Yield: 78%; Melting point: 170-172°C; IR (neat): 2948, 2916, 1712, 1702, 1633, 1587, 1503, 1428, 1375, 1315, 1288, 1258, 1170, 1160, 988, 898, 819, 738, 718, 703, 640, 467 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 8.99 (s, 1H), 8.55 (d, *J* = 5.4 Hz, 1H), 8.22 (d, *J* = 9.0 Hz, 1H), 8.05 (d, *J* = 16.6 Hz, 1H), 7.79 (s, 1H), 7.63-7.69 (m, 2H), 7.48-7.53 (m, 5H), 6.13 (d, *J* = 16.2 Hz, 1H), 3.79 (s, 3H), 2.60 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 166.97, 146.81, 144.78, 143.00, 141.87 (2C), 138.52, 137.70, 135.78, 135.21, 133.36, 133.20, 129.84 (2C), 128.88 (3C), 128.73, 128.04, 126.87, 126.48, 125.59, 124.98, 123.67, 51.89, 21.91; HRMS (ESI): *m/z* = 410.1215 calcd. For C₂₆H₂₀NO₂S, found 410.1245 [M+H]⁺.

General procedure for the synthesis of 11-Methyl-14,15-diphenylnaphtho[2,1-a]thieno[2,3-c]acridine (6d)



To a solution of 5-iodo-8-methyl-4-phenylthieno[2,3-c]acridine **4a** (30 mg, 0.067 mmol, 1 equiv.), Pd(OAc)₂ (0.3 mg, 5 mol %), NaOAc (11 mg, 0.133 mmol, 2 equiv.), LiCl (8.45 mg, 0.199 mmol, 3 equiv.), in 4 mL DMF; Diphenylacetylene (17 mg, 0.099 mmol, 1.5 equiv.) were added. The resulting mixture was heated at 100°C for 2 days. The mixture was allowed to cool to room temperature, diluted with ethyl acetate (15 mL); dried over sodium sulfate, and filtered. The solvent was removed under reduced pressure and the residue was purified by column chromatography using n-hexane: ethyl acetate (95:5) as eluent to afford 28 mg **6d**, Yield: 84%; Melting point: 274-276°C; IR (neat): 3052, 2917, 2850, 1582, 1548, 1515, 1473, 1388, 1293, 1081, 1071, 924, 821, 807, 752, 727, 716, 698, 656, 639, 551 cm⁻¹; ¹H-NMR (400 MHz, CDCl₃) δ 9.40 (d, *J* = 8.5 Hz, 1H), 8.67 (d, *J* = 5.4 Hz, 1H), 8.23 (s, 1H), 8.09 (d, *J* = 9.0 Hz, 1H), 7.71-7.81 (m, 3H), 7.52-7.58 (m, 2H), 7.26 (d, *J* = 8.5 Hz, 3H), 7.13-7.19 (m, 5H), 7.07 (d, *J* = 6.3 Hz, 2H), 6.95 (s, 1H), 2.44 (s, 3H); ¹³C-NMR (100 MHz, CDCl₃) δ 145.85, 145.79, 143.07, 139.59, 138.71, 138.28, 137.63 (2C), 137.57, 137.50, 134.98, 132.95, 132.42, 131.67 (2C), 131.40 (2C), 129.10, 128.40 (2C), 128.13, 127.95, 127.67 (2C), 127.16, 127.08 (2C), 126.90, 126.59 (2C), 126.35, 126.02, 125.03 (2C), 123.58, 21.76; HRMS (ESI): *m/z* = 502.1629 calcd. For C₃₆H₂₄NS, found 502.1611 [M+H]⁺.

Table S1. Crystal data and structure refinement for 5-iodo-8-methyl-4-phenylthieno[2,3-c]acridine (4a)

Empirical formula	C ₂₂ H ₁₄ INS
Formula weight	451.30
Temperature(K)	296(2)
Wavelength (Å)	0.71075
Crystal system	Orthorhombic
Space group	<i>Pbca</i>
Unit cell dimensions	
<i>a</i> (Å)	9.935(6)
<i>b</i> (Å)	20.797(12)
<i>c</i> (Å)	17.5203(10)
Volume (Å ³)	3620(3)
<i>Z</i>	8
Absorption coefficient (mm ⁻¹)	1.888
Density calculated (g/m ³)	1.656
<i>F</i> (000)	1776
Crystal size (mm)	1.0 x 0.1 x 0.1
θ range for data collection (°)	3.1-27.5
Limiting indices	-12 ≤ <i>h</i> ≤ 12, -27 ≤ <i>k</i> ≤ 15, -22 ≤ <i>l</i> ≤ 22
Reflection collected	31359
Independent reflections	4148 (<i>R</i> _{int} = 0.0530)
Completeness to θ = 25.245	99.8%
Refinement method	full-matrix least-squares on <i>F</i> ²
Goodness-of-fit on <i>F</i> ²	1.045
Final <i>R</i> indices [<i>I</i> > 2σ(<i>I</i>)]	<i>R</i> ₁ = 0.0497, <i>wR</i> ₂ = 0.1489
<i>R</i> indices (all data)	<i>R</i> ₁ = 0.0744, <i>wR</i> ₂ = 0.1688
Extinction coefficient	n/a
Largest difference peak and hole	0.677 and -0.607 (e Å ⁻³)

Computational Detail

All stationary point structures of the reactions were optimized B3LYP DFT method.¹ The 6-31G* electronic basis set was adopted for all atoms except for iodine. For iodine, Midi! electronic basis set was adopted.² Solvent effect (Acetonitrile) was taken into account by SCRF-PCM method,³ and ultrafine integration grid (specified by Int(Grid=Ultrafine) keyword in GAUSSIAN09 program⁴) was used for all DFT calculations to enhance the accuracy of calculations. Normal mode analyses were also performed to characterize the optimized structures and to obtained thermal correction to Gibbs free energy at $T = 298.15$ K. We have confirmed that all structures have the appropriate number of imaginary frequencies; 0 for minimum and 1 for transition state (TS) structures. Then we calculated B3LYP/6-311+G**+Midi! energies at the B3LYP/6-31G*+Midi! optimized geometries to obtained more reliable electronic energies.

To study experimental absorption spectra, we have performed time-dependent (TD) DFT calculations with B3LYP exchange-correlation density functional. For TD DFT calculations, the 6-31G* electronic basis set was adopted, and solvent effect (*n*-hexane) was taken into account. "Int(Grid=Ultrafine)" keyword was not used in TD DFT calculations, since these TD DFT calculations were carried out with GAUSSIAN16 program package,⁵ in which the ultrafine integration grid is the default setting. The excitation energies were calculated at S_0 equilibrium structure to study the experimental absorption spectra. The first 10 states were calculated using TD DFT method.

References for Computational detail

1. Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2006**, *120*, 215-241.
2. C. -C. Chen, M. -Y. Wu, H. -Y. Chen, M. -J. Wu, *J. Org. Chem.* **2017**, *82*, 6071-6081.
3. J. Tomasi, B. Mennucci, R. Cammi, *Chem. Rev.* **2005**, *105*, 2999-3093.
4. M. J. Frisch, et al. Gaussian 09, Revision B.01; Gaussian, Inc.: Wallingford CT, 2010.
5. M. J. Frisch, et al. Gaussian 16, Revision B.01; Gaussian, Inc.: Wallingford CT, 2016.

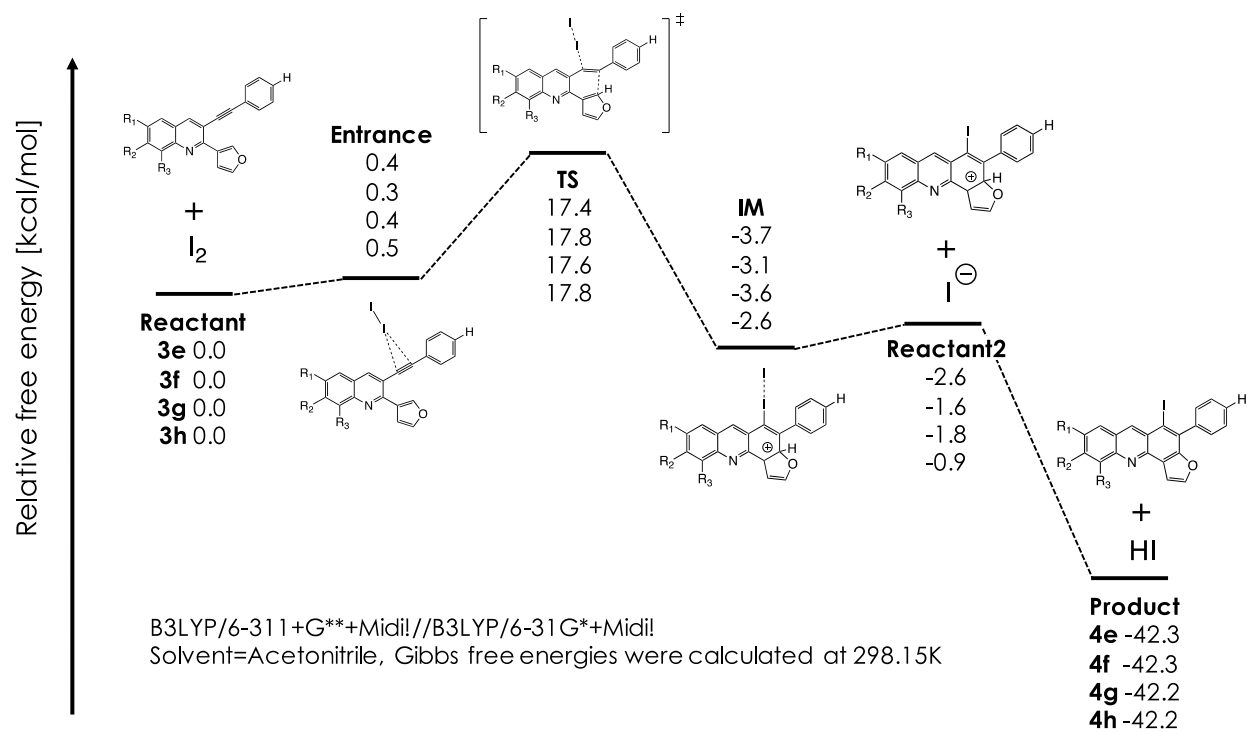


Figure S1. Relative Gibbs free energy profiles at T = 298 K of the reactions leading to **4e-4h**.

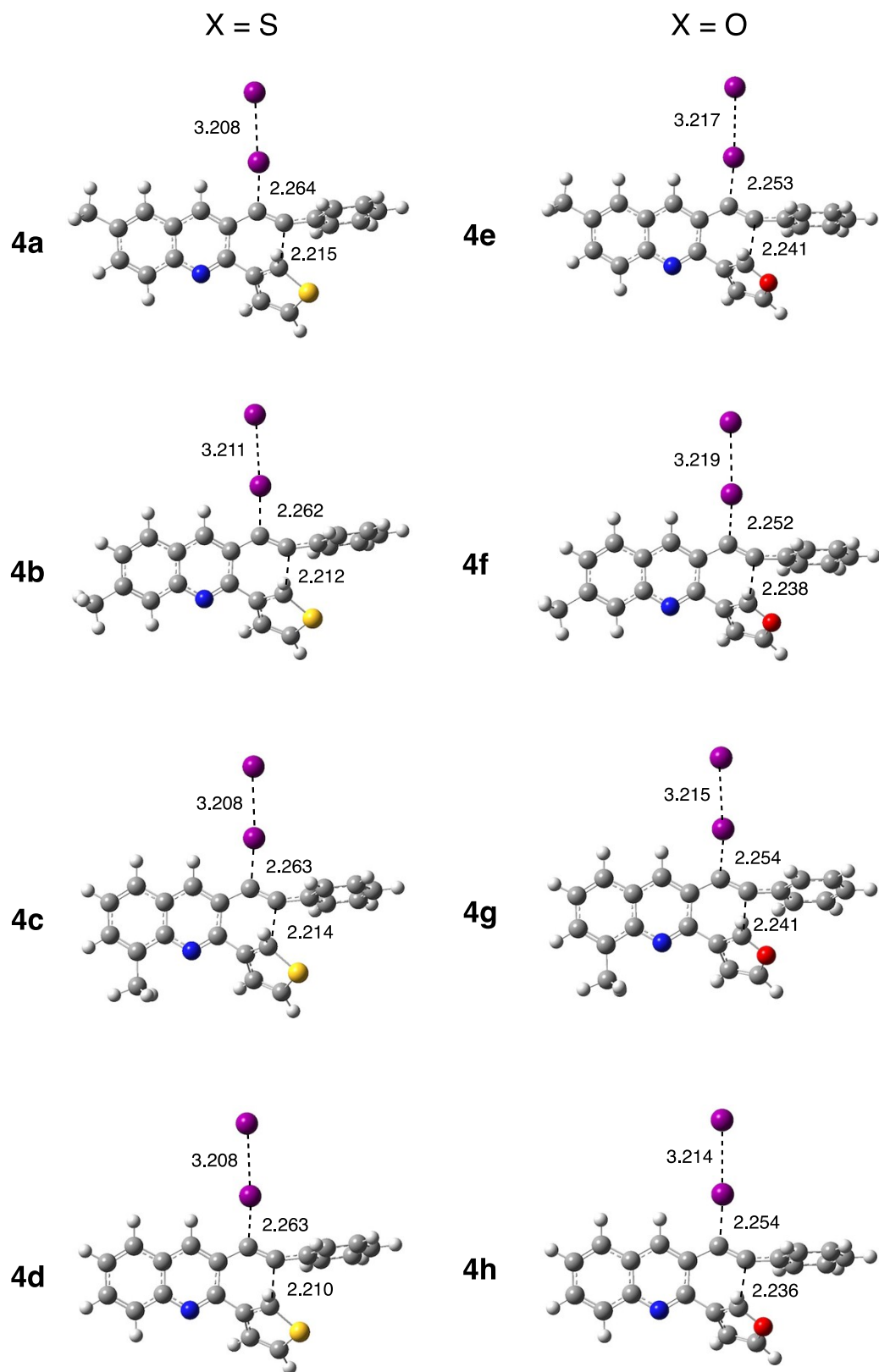


Figure S2. Optimized structure of TS with some representative interatomic distances [Å].

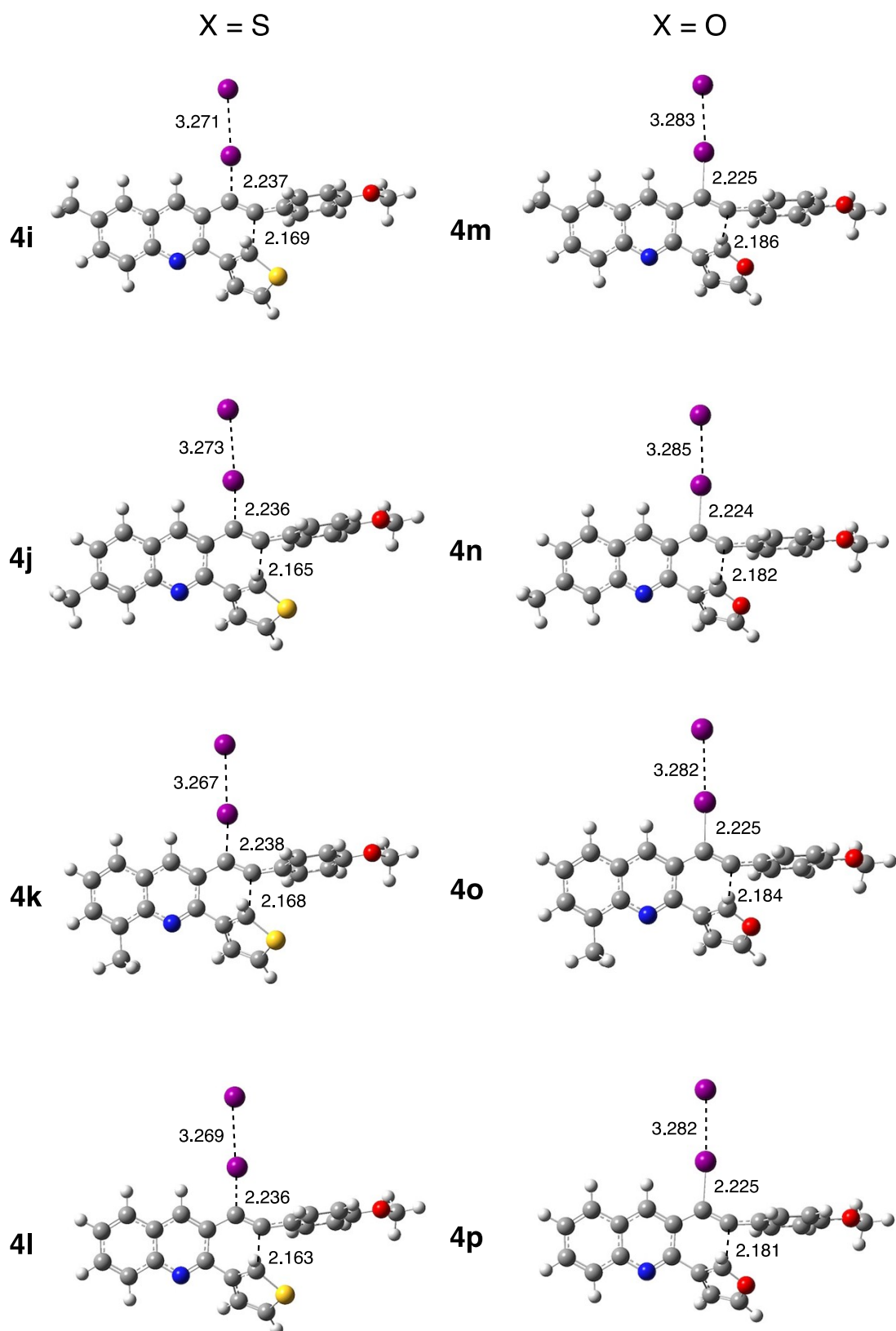


Figure S2. (cont.)

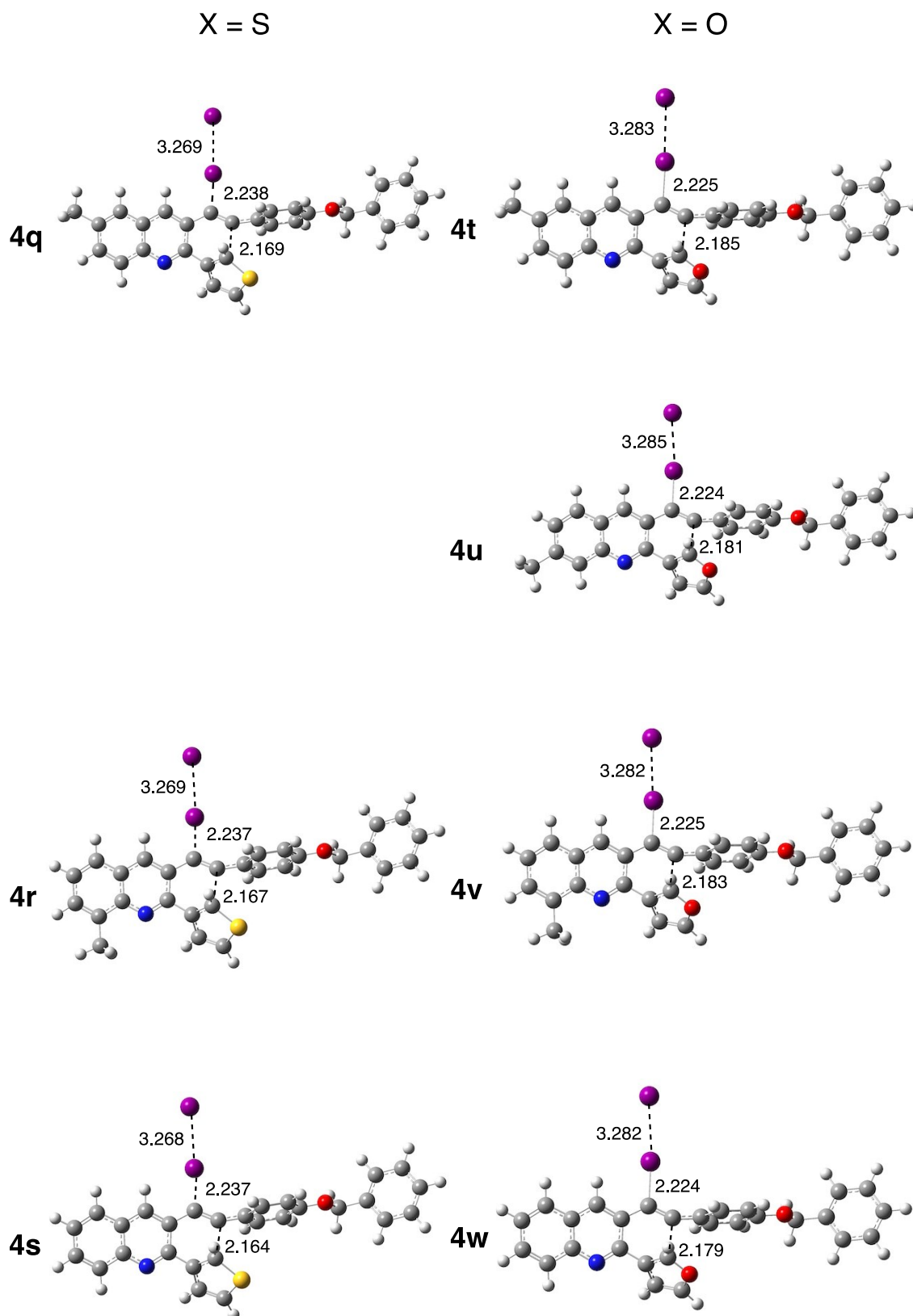


Figure S2. (cont.)

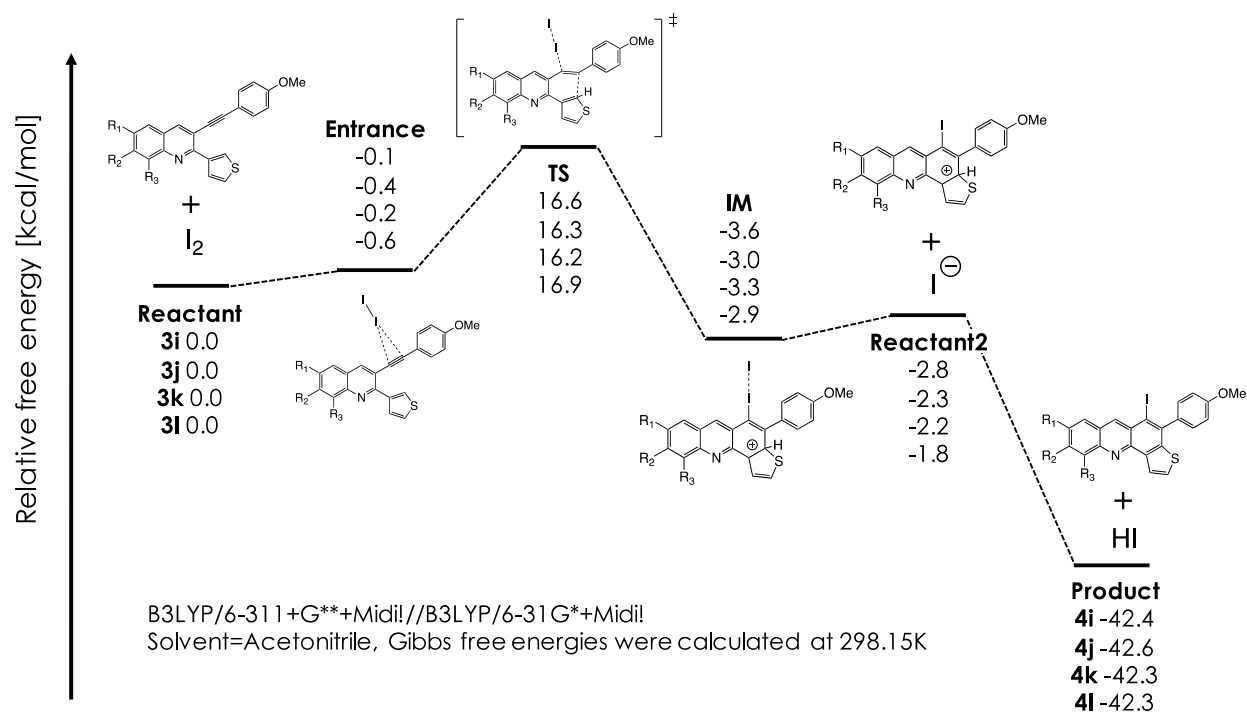


Figure S3. Relative Gibbs free energy profiles at T = 298 K of the reactions leading to **4i-4l**.

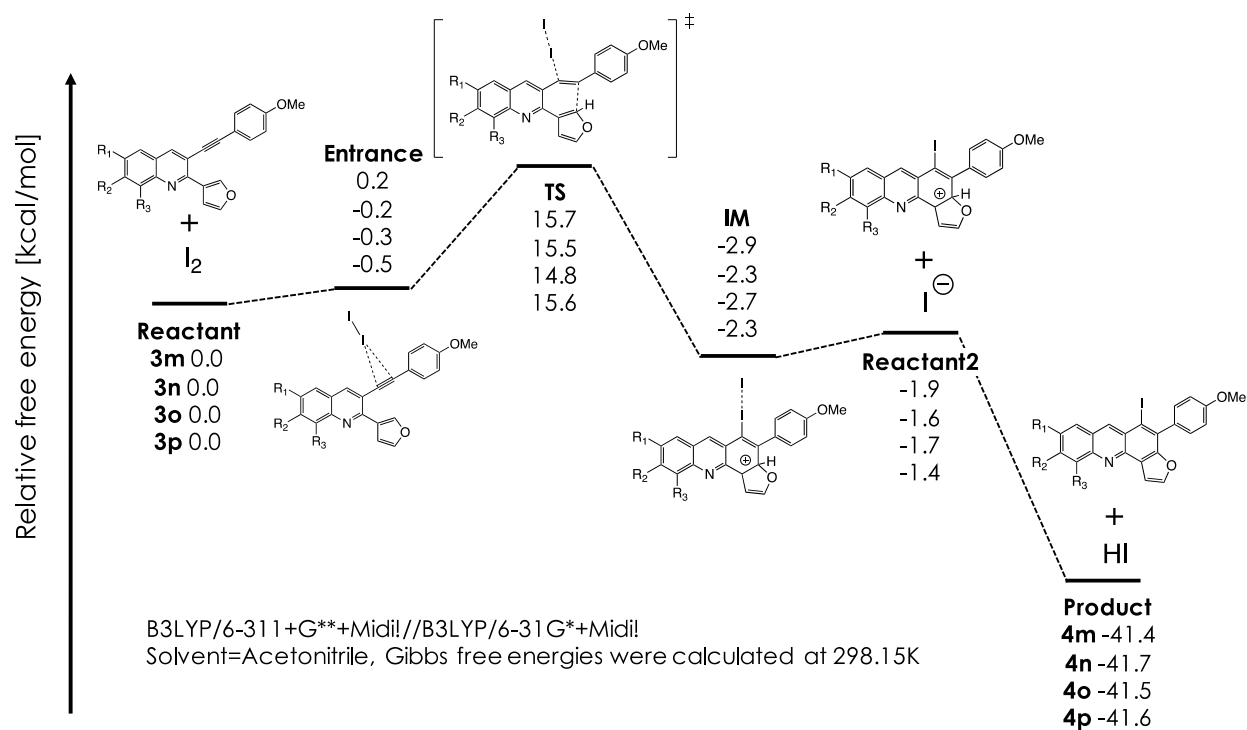


Figure S4. Relative Gibbs free energy profiles at T = 298 K of the reactions leading to **4m-4p**.

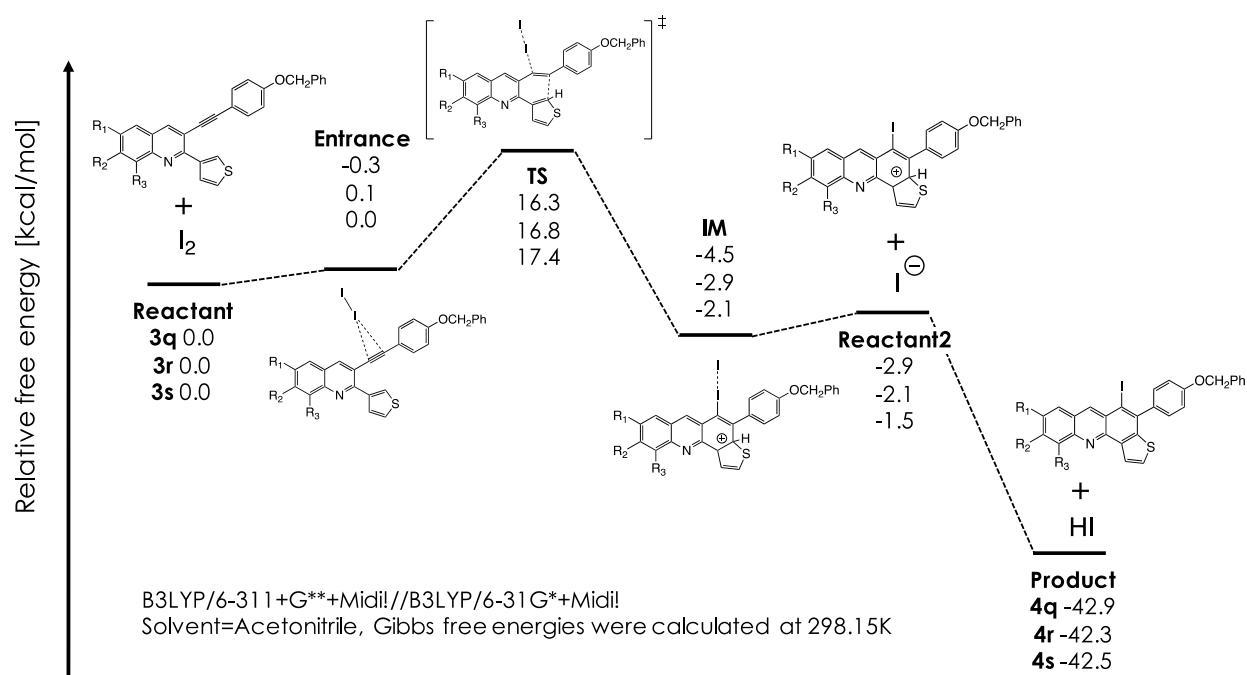


Figure S5. Relative Gibbs free energy profiles at T = 298 K of the reactions leading to **4q-4s**.

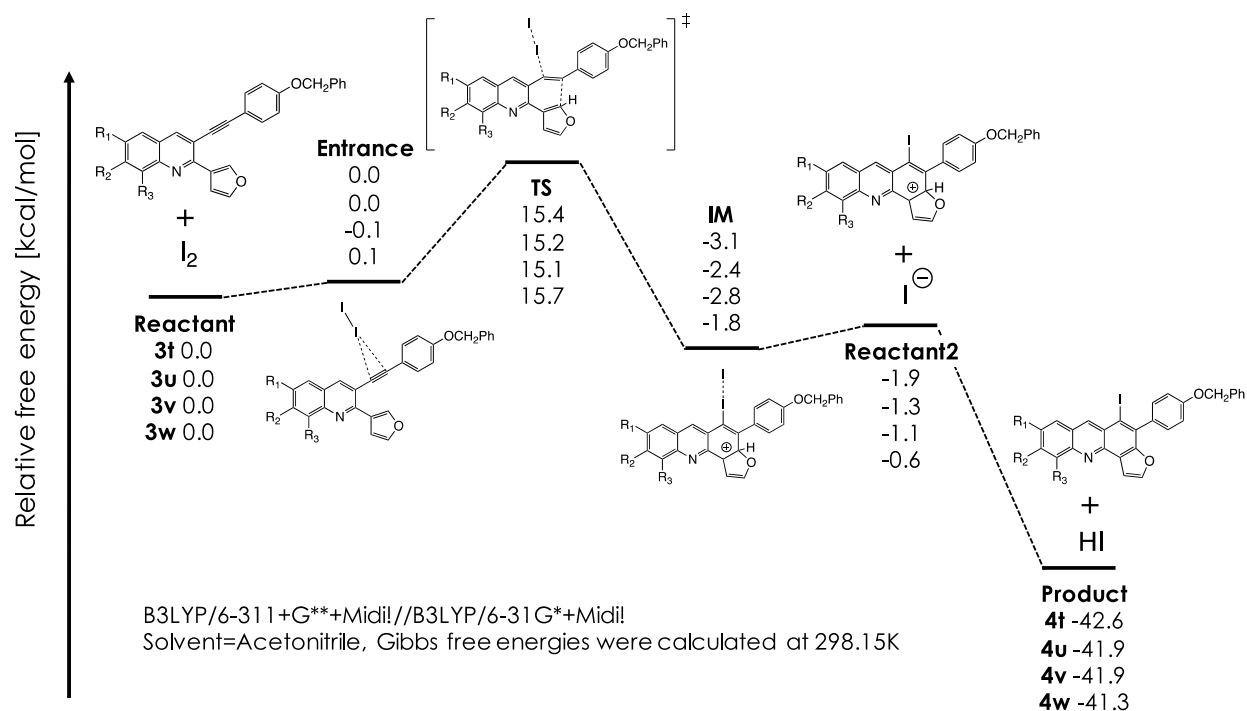


Figure S6. Relative Gibbs free energy profiles at T = 298 K of the reactions leading to **4t-4w**.

TD DFT calculations on compounds 6a-6d

Table S2 lists the energies of excited states of **6a-6d** at their ground state (S_0) equilibrium structures relative to those of the S_0 states. Only the transitions for the first excited state and with the largest (and the second largest) oscillator strength(s) are shown in Table S2. The contribution of the excitation configuration from HOMO to LUMO is 96%-98% (calculated from the coefficient of electronic configuration) in the first excited states of **6a-6d**. The lower wavelength of energies for excitation in **6c** and **6d** compared to those in **6a** and **6b** are attributed to the longer π -conjugation in frontier orbitals. On the other hand, the main contribution for the excitation with the largest oscillator strength in **6a** and **6b** is the transition from HOMO to LUMO+1. Since LUMO+1 orbital in **6a** and **6b** contain π -orbitals on a phenyl group, this transition can be regarded as an intramolecular charge transfer (ICT). Contrary to **6a** and **6b**, π -orbitals on phenyl groups are not involved in HOMO, LUMO, LUMO+1, and LUMO+2 orbitals in **6d**. In these MOs, π -orbitals are delocalized on all fused-rings. The excitations with the first and second largest oscillator strengths in **6d**, thus, did not show ICT character.

The excitations with the first and the second largest oscillator strengths in **6c** differ from those in **6d**. The main contributions in these excitations in **6c** are the transitions from HOMO-7 (100) to LUMO (108), and HOMO (107) to LUMO+2 (110). The HOMO-7 orbital in **6c** mainly consists of lone pair of oxygen atom and σ -orbital of C-C bond in methyl acetate. It should be noted here that Hiyama et al. reported similar type of transition in firefly luciferin.¹ In addition, only the LUMO+2 orbital in **6c** has π -lobe on a phenyl group. These transitions, thus, can be classified into ICT.

References for TD DFT calculations on compounds 6a-6d

1. M. Hiyama, H. Akiyama, K. Yamada, N. Koga, *Photochem. Photobiol.* **2012**, *88*, 889-898.

Table S2. Energy of excited states, coefficient of electronic configurations, and oscillator strength of **6a-6d** at their S_0 equilibrium structures relative to those of the S_0 states.

Entry ^a	Transition		Coefficient	Energy [nm]	Oscillator strength
	From ^b	To ^b			
6a (S_1)	105	106	0.699	399.25	0.139
6a (S_5) ^c	105	107	0.566	290.32	0.610
6b (S_1)	85	86	0.699	395.49	0.133
6b (S_5) ^c	85	87	0.566	289.34	1.062
6c (S_1)	107	108	0.701	419.32	0.226
6c (S_9) ^c	100	108	0.356	282.40	0.407
	101	108	-0.304		
	107	110	0.361		
6c (S_{10}) ^c	100	108	0.468	280.64	0.458
	107	110	-0.364		
6d (S_1)	131	132	0.694	419.70	0.166
6d (S_4) ^c	131	133	0.585	335.75	0.459
6d (S_6) ^c	131	134	0.553	313.02	0.453

^aOnly the excitations for the first excited state and with the largest (and the second largest oscillator strength(s) are shown. ^bHOMO/LUMO are 105/106 (**6a**), 85/86 (**6b**), 107/108 (**6c**), and 131/132 (**6d**).

^cOnly the transitions with the significant coefficient (> 0.4) are shown.

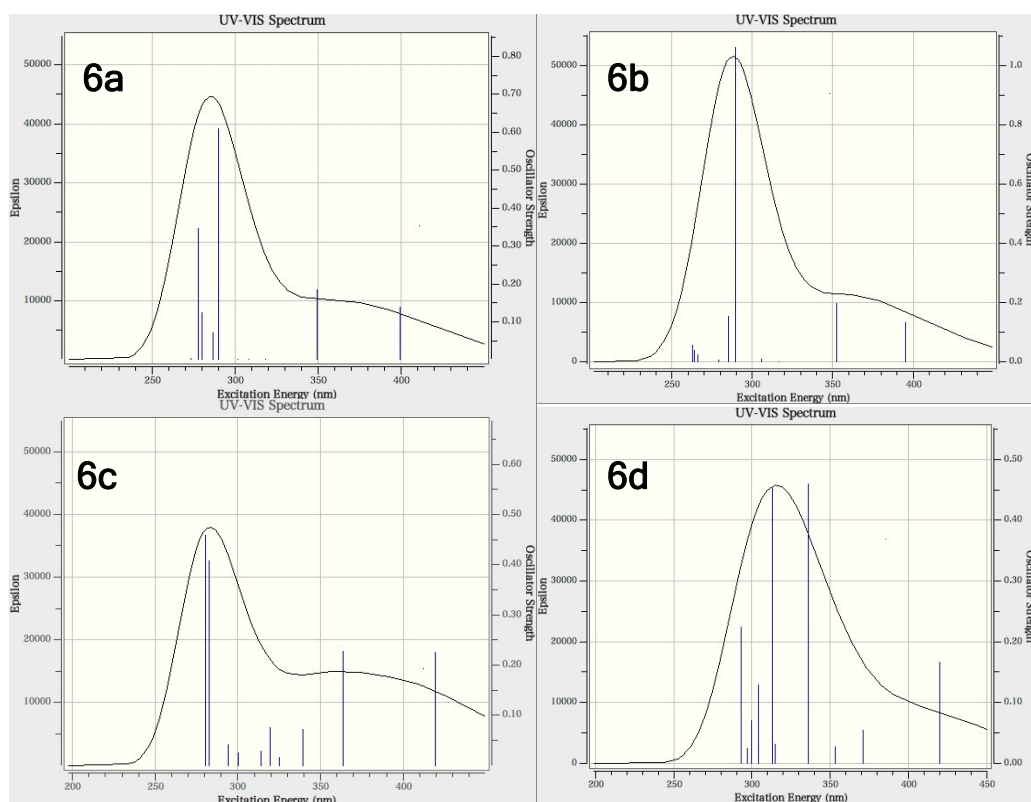


Figure S7. Calculated absorption spectra of **6a-6d**.

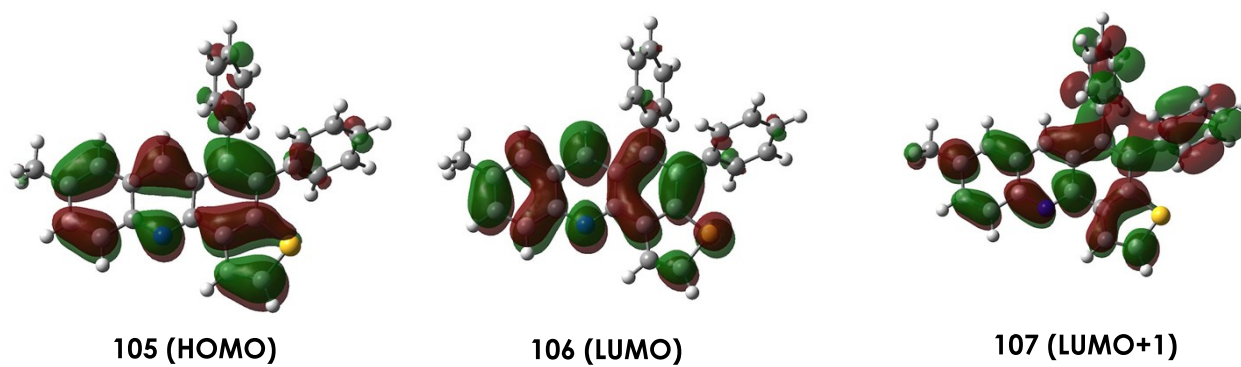


Figure S8. Molecular orbitals of **6a**.

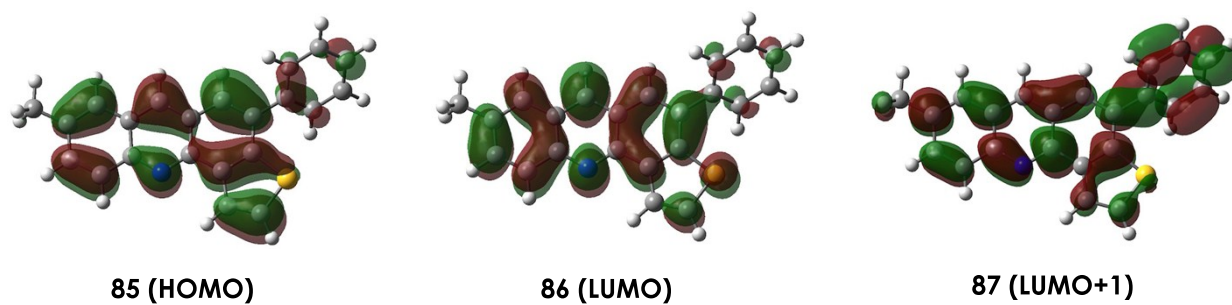


Figure S9. Molecular orbitals of 6b.

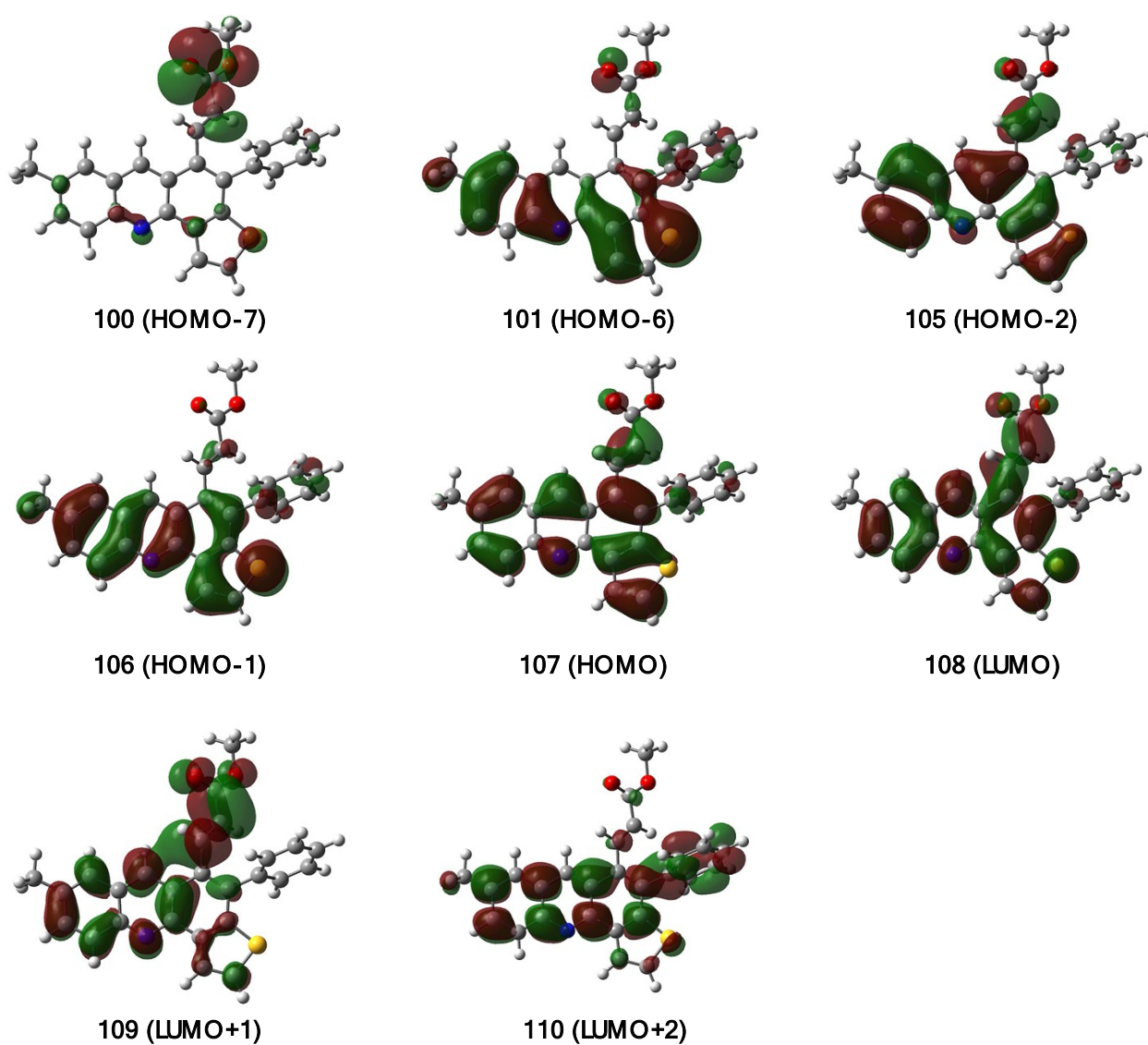


Figure S10. Molecular orbitals of 6c.

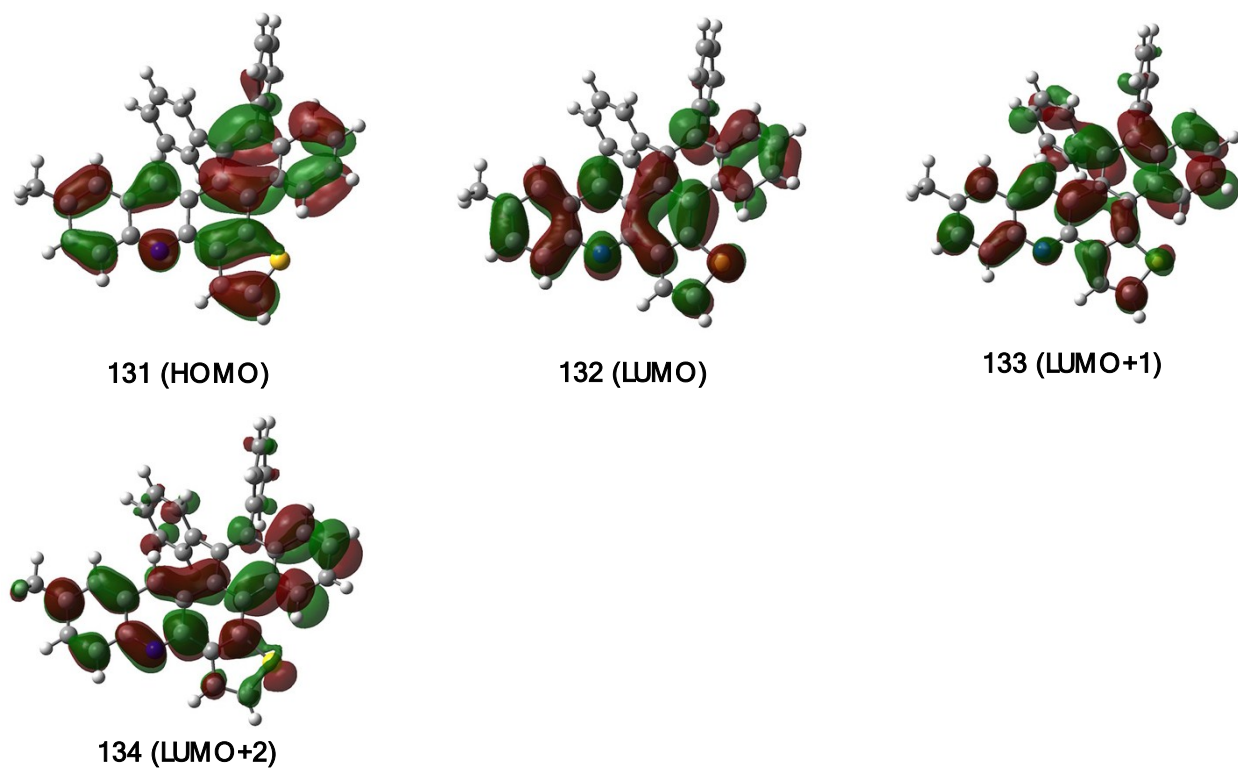


Figure S11. Molecular orbitals of **6d**.