Supporting Information

Metal-Free C(sp3)–H Bond Activation: First Synthesis of Diarylpyridinium-azaarene-butenolate Zwitterionic salts on Chalcones

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General: All the reagents and solvents were purchased from Sigma-Aldrich or Merck chemical Co. and were used directly without any further purification. Organic solutions were concentrated under reduced pressure on a Büchi rotary evaporator. The progress of reaction was checked by thin-layer chromatography. The plates were visualized first with UV illumination followed by iodine. ¹HNMR spectra were recorded at 200 or 300 MHz using Brucker DRX-200 or 300 spectrometer and are reported in parts per million (ppm) on the δ scale relative to tetramethylsilane as an internal standard. Coupling constants (J) reported in Hz. ¹³CNMR spectra were recorded at 50 or 75 MHz. Mass spectra were obtained using JEOL SX-102 (ESI) instrument. Elemental analysis was performed using a Perkin-Elmer autosystem XL analyzer.

General procedure for the synthesis of zwitterionic salts via one pot multicomponent reaction of quinaldine, pyridine and chalcones: A mixture of quinaldine 1a–1c (1.0
mmol), pyridine 2 (4.0 mmol) and I₂ (1.0 mmol) were stirred at 100 °C for 2 h. To this mixture aromatic/hetero-aromatic chalcones 3a-m/5a-d (1.0 mmol) and NEt₃ (1.5 mmol) in ethanol (5.0 mL) were added and further stirred the reaction at room temperature for additional 22 h. After completion of the reaction as evidenced by TLC, solvent was removed in vacuo. It was diluted with a 50 mL of ethyl acetate and washed with water. The aqueous part was further extracted with ethyl acetate. The combined organic part was washed with brine and dried over Na₂SO₄. The solvent was evaporated to yield a crude product, which purified through silica gel column chromatography using MeOH/CHCl₃ (5:95) afforded desired products (4a-o/6a-d).

Characterization data of all the synthesized compounds:

1-(4-methoxyphenyl)-3-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4a)

Pale red solid, Yield 81%, ESIMS (m/z) = 459 (M+H)+. IR (KBr) max 3019, 2400, 1598, 1514, 1405, 1099, 1045, 928, 770, 669. ¹H NMR (300 MHz; CDCl₃) δ H 10.01 (d, J = 5.70 Hz, 2H), 8.83 (d, J = 8.28 Hz, 1H), 8.31 (t, J = 8.25 Hz, 2H), 8.21 (d, J = 8.25 Hz, 2H), 7.89 (d, J = 7.89 Hz, 1H), 7.79 (t, J = 7.08 Hz, 4H) 7.66 (t, J = 5.64 Hz, 3H), 7.48 (t, J = 7.38 Hz, 1H), 7.35 (d, J = 7.59 Hz, 2H), 6.74 (d, J = 8.31 Hz, 2H), 4.91 (t, J = 10.53 Hz, 1H) 4.16-4.07 (m, 1H), 3.67 (s, 3H), 2.97 (d, J = 15.12 Hz, 1H). Analysis hgc calculated for C₃₁H₂₆N₂O₂ C, 81.20; H, 5.72; N, 6.11; Found: C, 81.16; H, 5.68; N, 6.12. ¹³C NMR (75 MHz; CDCl₃) δC 196.6, 158.8, 153.5, 147.9, 145.5, 144.2, 138.2, 136.1, 133.2, 130.5, 129.9, 129.8, 129.5, 128.5, 128.0, 128.4, 123.8, 114.4, 114.0, 77.6, 75.1, 55.3, 55.1, 47.4, 41.6.

3-(4-fluorophenyl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4b)
Pale red solid, Yield 72%, ESIMS (m/z) = 447 (M+H)+. IR (KBr) max 3435, 3013, 2400, 1587, 1401, 1072, 772, 669. 1H NMR (300 MHz; CDCl3) δH 10.04 (d, J = 5.67 Hz, 2H), 8.81 (d, J = 8.22 Hz, 1H), 8.38-8.18 (m, 4H), 7.90 (d, J = 7.89 Hz, 1H), 7.79 (d, J = 6.96, 6H), 7.66 (t, J = 7.38 Hz, 1H) 7.50 (t, J = 7.26 Hz, 1H) 7.36 (t, J = 7.68 Hz, 2H) 6.92 (t, J = 8.25 Hz, 2H) 4.99 (t, J = 10.59 Hz, 1H) 4.20-4.11 (m, 1H), 2.99 (d, J = 15.15 Hz, 1H). Analysis calculated for C30H23FN2O C, 80.70; H, 5.19; N, 6.27; Found: C, 80.72; H, 5.23; N, 6.23. 13C NMR (50 MHz; DMSO-d6) δC 196.7, 153.5, 147.2, 146.6, 144.2, 138.5, 136.0, 134.6, 133.3, 130.7, 130.4, 129.0, 128.6, 128.2, 127.9, 122.5, 115.5, 115.1, 77.0, 45.0, 41.4.

3-(4-nitrophenyl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4c)

Pale yellow solid, Yield 80%, ESIMS (m/z) = 474 (M+H)+. IR (KBr) max 3410, 1681, 1597, 1404, 1346, 1217, 1109, 769, 669. 1H NMR (300 MHz; CDCl3) δH 10.10 (d, J = 5.73 Hz, 2H), 8.83 (d, J = 8.28 Hz, 1H), 8.36-8.06 (m, 6H), 8.01-7.96 (m, 3H), 7.93 (t, J = 8.04 Hz, 1H), 7.75-7.66 (m, 5H), 7.37 (d, J = 8.31 Hz, 2H), 7.50 (t, J = 7.14 Hz, 1H) 7.36 (t, J = 7.71 Hz, 2H), 5.19 (t, J = 10.11 Hz, 1H) 4.32-4.22 (m, 1H), 3.22 (s, 3H). Analysis calculated for C30H23N3O3 C, 76.09; H, 4.90; N, 8.87; Found: C, 76.07; H, 4.92; N, 8.84. 13C NMR (75 MHz; DMSO-d6) δC 196.9, 153.6, 147.7, 147.3, 147.1, 144.7, 139.1, 136.4, 134.0, 131.2, 130.4, 129.5, 129.2, 129.1, 128.9, 128.6, 128.4, 128.3, 123.9, 123.0, 76.9, 45.8, 41.7.

1-(4-bromophenyl)-3-(4-methoxyphenyl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4d)

Pale yellow solid, Yield 80%, ESIMS (m/z) = 537 (M+H)+. IR (KBr) max 3435, 3019, 2400, 1686, 1586, 1486, 1401, 1045, 761, 669. 1H NMR (300 MHz; CDCl3) δH 9.38 (d, J = 5.55 Hz, 2H), 8.39 (d, J = 8.28 Hz, 1H), 8.47 (t, J = 7.59 Hz, 1H), 8.19 (d, J = 8.28 Hz, 1H), 8.08 (d, J = 8.28 Hz, 1H), 8.01-7.96 (m, 3H), 7.93 (t, J = 8.04 Hz, 1H), 7.75-7.66 (m, 5H), 7.37 (d, J = 8.31 Hz, 2H), 6.73 (d, J = 8.46 Hz, 2H), 4.82 (t, J = 9.03 Hz, 1H) 3.79-3.70 (m, 1H), 3.62 (s, 3H), 3.19 (d, J = 14.46 Hz, 1H). Analysis calculated for C31H25BrN2O2 C, 69.28; H, 4.69; N, 5.21; Found: C, 69.27; H, 4.64; N, 5.23. 13C NMR (50 MHz;
DMSO-d₆ δC 196.2, 158.1, 153.5, 147.1, 146.4, 144.1, 138.4, 135.0, 131.6, 130.7, 129.8, 129.3, 129.0, 128.0, 127.8, 127.4, 122.5, 113.8, 77.2, 54.9, 45.2, 41.5.

3-(2,4-dichlorophenyl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4e)

Pale red solid, Yield 78%, ESIMS (m/z) = 497 (M+H)+. IR (KBr) max 3435, 3019, 2400, 1597, 1476, 1405, 1045, 759, 669. ¹H NMR (300 MHz; CDCl₃) δH 10.05 (d, J = 6.03 Hz, 2H), 8.80 (d, J = 8.37 Hz, 1H), 8.58 (br, 1H), 8.35-8.12 (m, 4H), 7.92-7.78 (m, 7H), 7.68 (t, J = 7.80 Hz, 1H), 7.37 (d, J = 7.17 Hz, 2H), 7.16 (s, 1H), 5.67 (t, J = 8.73 Hz, 1H) 4.29-4.00 (m, 1H), 3.11 (d, J = 14.40 Hz, 1H). Analysis calculated for C₃₀H₂₂Cl₂N₂O C, 72.44; H, 4.46; N, 5.63; Found: C, 72.42; H, 4.49; N, 5.63. ¹³C NMR (75 MHz; DMSO-d₆) δC 196.9, 153.4, 147.5, 145.2, 144.4, 139.1, 136.3, 135.7, 133.9, 133.3, 132.8, 131.2, 129.7, 129.4, 129.1, 128.8, 128.6, 128.5, 128.4, 127.8, 123.5, 122.1, 76.7, 42.1.

1-(4-bromophenyl)-3-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4f)

Pale yellow solid, Yield 72%, ESIMS (m/z) = 507 (M+H)+. IR (KBr) max 3435, 3019, 2400, 1631, 1587, 1401, 1072, 767, 669. ¹H NMR (300 MHz; CDCl₃) δH 10.01 (d, J = 5.88 Hz, 2H), 8.88 (d, J = 8.31 Hz, 1H), 8.36 (d, J = 9.09 Hz, 2H), 8.25 (t, J = 8.37 Hz, 2H), 7.94-7.74 (m, 5H), 7.69 (d, J = 8.49 Hz, 3H), 7.50 (d, J = 8.46 Hz, 2H), 7.26 (t, J = 7.65 Hz, 2H), 7.13 (t, J = 7.41 Hz, 1H), 4.99 (t, J = 9.54 Hz, 1H) 4.21-4.12 (m, 1H), 3.04 (d, J = 14.40 Hz, 1H). Analysis calculated for C₃₀H₂₃BrN₂O C, 71.01; H, 4.57; N, 5.52; Found: C, 71.00; H, 4.59; N, 5.53. ¹³C NMR (75 MHz; DMSO-d₆) δC 196.6, 154.0, 147.7, 147.0, 144.7, 139.0, 138.8, 135.5, 132.1, 131.2, 130.4, 129.5, 129.0, 128.8, 128.6, 128.4, 127.9, 123.0, 77.5, 46.3, 41.9.
1-(4-bromophenyl)-3-(4-chlorophenyl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4g)

Pale yellow solid, Yield 84%, ESIMS (m/z) = 541 (M+H)+. IR (KBr) max 3436, 2951, 2143, 1681, 1628, 1585, 1430, 1094, 771, 682, 572. 1H NMR (300 MHz; CDCl3) δH 10.04 (d, J = 5.88 Hz, 2H), 8.83 (d, J = 8.34 Hz, 1H), 8.44-8.22 (m, 4H), 7.88-7.78 (m, 4H), 7.70-7.57 (m, 4H), 7.52 (d, J = 8.40 Hz, 2H), 7.24 (d, J = 8.31 Hz, 2H), 5.01 (t, J = 10.17 Hz, 1H) 4.21-4.12 (m, 1H), 3.02 (d, J = 14.67 Hz, 1H). Analysis calculated for C30H22BrClN2O: C, 66.50; H, 4.09; N, 5.17; Found: C, 66.52; H, 4.06; N, 5.15. 13C NMR (75 MHz; DMSO-d6) δC 196.6, 153.9, 147.8, 147.3, 145.0, 144.8, 139.1, 138.6, 138.2, 138.0, 135.5, 132.6, 132.2, 131.3, 131.2, 130.8, 130.5, 129.6, 129.3, 129.1, 128.8, 128.5, 128.1, 123.1, 122.5, 77.3, 45.7, 41.9, 39.3.

3-(2-nitrophenyl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4h)

Pale yellow solid, Yield 88%, ESIMS (m/z) = 474 (M+H)+. IR (KBr) max 3436, 2143, 1628, 1596, 1530, 1350, 1218, 771, 688. 1H NMR (300 MHz; CDCl3) δH 10.10 (d, J = 5.55 Hz, 2H), 8.83 (t, J = 9.30 Hz, 2H), 8.61 (d, J = 11.73 Hz, 1H), 8.34 (d, J = 8.04 Hz, 1H), 8.26-8.21 (s, br, 2H), 7.95-7.76 (m, 7H), 7.66 (t, J = 7.26 Hz, 1H), 7.59 (t, J = 8.10 Hz, 1H), 7.49 (t, J = 7.35 Hz, 1H), 7.35 (t, J = 7.83 Hz, 2H), 5.16 (t, J = 11.55 Hz, 1H), 4.31-4.22 (m, 1H), 3.08 (d, J = 17.79 Hz, 1H). Analysis calculated for C30H23N3O3: C, 76.09; H, 4.90; N, 8.87; Found: C, 76.04; H, 4.91; N, 8.84. 13C NMR (75 MHz; DMSO-d6) δC 197.1, 153.7, 148.3, 147.7, 147.3, 144.8, 141.5, 139.1, 136.4, 135.9, 134.0, 131.3, 130.5, 129.6, 129.2, 128.9, 128.7, 128.4, 123.7, 123.1, 123.0, 77.0, 45.7, 41.7.
3-(2-chlorophenyl)-1-(3-methoxyphenyl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4i)

Pale brown solid, Yield 86%, ESIMS (m/z) = 493 (M+H)\(^+\). IR (KBr) max 3444, 2937, 2143, 1681, 1628, 1485, 1261, 771, 684. \(^1\)H NMR (300 MHz; CDCl\(_3\)) \(\delta\)H 10.04 (d, \(J = 5.88\) Hz, 2H), 8.82 (d, \(J = 8.28\) Hz, 1H), 8.54 (d, \(J = 7.74\) Hz, 1H), 8.36 (d, \(J = 8.25\) Hz, 1H), 8.27-8.24 (m, 3H), 7.94-7.77 (m, 4H), 7.58 (t, \(J = 7.20\) Hz, 1H), 7.46-7.38 (m, 2H), 7.28 (d, \(J = 7.80\) Hz, 1H), 7.17 (d, \(J = 7.83\) Hz, 1H), 7.09-7.02 (m, 2H), 5.72 (t, \(J = 9.99\) Hz, 1H), 4.25-4.15 (m, 1H), 3.78 (s, 3H), 3.15 (d, \(J = 14.22\) Hz, 1H). Analysis calculated for C\(_{31}\)H\(_{25}\)ClN\(_2\)O\(_2\): C, 75.52; H, 5.11; N, 5.68; Found: C, 75.50; H, 5.09; N, 5.63. \(^{13}\)C NMR (75 MHz; DMSO-d\(_6\)) \(\delta\)C 196.8, 159.8, 153.6, 147.7, 147.4, 139.1, 137.8, 136.4, 134.2, 131.2, 130.3, 130.1, 129.8, 128.6, 128.5, 128.4, 123.5, 121.0, 119.8, 113.1, 79.7, 55.9, 42.3.

3-(naphthalen-2-yl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4j)

Pale green solid, Yield 74%, ESIMS (m/z) = 479 (M+H)\(^+\). IR (KBr) max 3436, 2953, 2143, 1628, 1596, 1483, 1003, 772, 687. \(^1\)H NMR (300 MHz; CDCl\(_3\)) \(\delta\)H 9.93 (d, \(J = 4.26\) Hz, 2H), 8.86 (d, \(J = 7.53\) Hz, 1H), 8.70 (d, \(J = 8.16\) Hz, 1H), 8.61 (d, \(J = 4.65\) Hz, 1H), 8.38-8.27 (m, 3H), 7.98-7.82 (m, 6H), 7.75-7.66 (m, 5H), 7.51-7.46 (m, 4H), 6.15 (t, \(J = 10.11\) Hz, 1H), 4.45-4.36 (m, 1H), 3.35 (d, \(J = 15.72\) Hz, 1H). Analysis calculated for C\(_{34}\)H\(_{26}\)N\(_2\)O: C, 85.33; H, 5.48; N, 5.85; Found: C, 85.31; H, 5.45; N, 5.86. \(^{13}\)C NMR (75 MHz; DMSO-d\(_6\)) \(\delta\)C 197.6, 154.5, 154.3, 147.9, 146.7, 144.9, 139.1, 136.6, 136.1, 134.0, 133.7, 132.1, 131.3, 129.9, 129.5, 129.2, 128.8, 128.6, 128.5, 128.3, 127.7, 126.8, 126.4, 126.1, 125.7, 123.9, 123.5, 78.5, 43.2, 35.0, 32.2, 30.1.
1-(3-methoxyphenyl)-3-(naphthalen-2-yl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4k)

Pale yellow solid, Yield 89%, ESIMS (m/z) = 509 (M+H)+. IR (KBr) max 3436, 2944, 2143, 1682, 1628, 1484, 1261, 772, 683, 669. ¹H NMR (300 MHz; CDCl₃) δ H 9.92 (d, J = 5.76 Hz, 2H), 8.90 (d, J = 8.28 Hz, 1H), 8.67 (d, J = 8.73 Hz, 2H), 8.39-8.33 (m, 3H), 7.98-7.87 (m, 3H), 7.74-7.62 (m, 5H), 7.47-7.43 (m, 3H), 7.29 (d, J = 8.58 Hz, 2H), 7.06 (d, J = 7.83 Hz, 1H), 6.13 (t, J = 9.42 Hz, 1H), 4.45-4.36 (m, 1H), 3.78 (s, 3H), 3.35 (d, J = 14.64 Hz, 1H). Analysis calculated for C₃₅H₂₈N₂O₂ C, 82.65; H, 5.55; N, 5.51; Found: C, 82.62; H, 5.53; N, 5.53. ¹³C NMR (75 MHz; DMSO-d₆) δ C 197.4, 159.9, 154.2, 147.8, 146.7, 144.9, 139.1, 138.0, 136.0, 133.7, 132.0, 131.3, 130.4, 130.0, 129.0, 128.8, 128.6, 128.3, 126.9, 126.4, 126.1, 125.7, 123.9, 123.4, 121.2, 120.0, 113.0, 78.6, 55.9, 43.2.

1-(4-fluorophenyl)-3-(naphthalen-2-yl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4l)

Pale brown solid, Yield 89%, ESIMS (m/z) = 497 (M+H)+. IR (KBr) max 3435, 2927, 2143, 1678, 1627, 1483, 1430, 1004, 772, 683, 663. ¹H NMR (300 MHz; CDCl₃) δ H 9.88 (d, J = 5.97 Hz, 2H), 8.86 (d, J = 8.34 Hz, 1H), 8.65 (d, J = 7.98 Hz, 2H), 8.37-8.33 (m, 2H), 7.95-7.81 (m, 5H), 7.72-7.59 (m, 5H), 7.48-7.41 (m, 3H), 7.02 (t, J = 8.58 Hz, 2H), 6.11 (t, J = 9.21 Hz, 1H), 4.43-4.34 (m, 1H), 3.30 (d, J = 14.01 Hz, 1H). Analysis calculated for C₃₄H₂₅FN₂O C, 82.24; H, 5.07; N, 5.64; Found: C, 82.19; H, 5.04; N, 5.65. ¹³C NMR (75 MHz; DMSO-d₆) δ C 195.6, 153.6, 147.2, 146.1, 144.2, 138.5, 135.4, 133.1, 132.8, 132.7, 131.4, 131.0, 130.8, 130.7, 129.3, 128.4, 128.1, 128.0, 127.6, 126.2, 125.8, 125.4, 123.2, 122.8, 115.7, 115.4, 77.9, 42.5, 34.4, 33.8, 31.5.
3-(4-chlorophenyl)-1-phenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (4m)

Pale red solid, Yield 74%, ESIMS (m/z) = 463 (M+H)<sup>+</sup>. IR (KBr) max 3470, 3019, 2400, 1683, 1596, 1486, 1046, 759, 669. <sup>1</sup>H NMR (300 MHz; CDCl<sub>3</sub>) <sup>6</sup>H 10.04 (d, <i>J</i> = 5.52 Hz, 2H), 8.82 (d, <i>J</i> = 8.34 Hz, 1H), 8.41-8.18 (m, 4H), 7.89 (d, <i>J</i> = 7.89 Hz, 1H), 7.83-7.75 (m, 7H), 7.66 (t, <i>J</i> = 7.56 Hz, 1H) 7.49 (t, <i>J</i> = 7.53 Hz, 1H) 7.36 (d, <i>J</i> = 7.53 Hz, 1H) 7.19 (d, <i>J</i> = 8.07 Hz, 2H) 5.00 (d, <i>J</i> = 15.60 Hz, 1H). Analysis calculated for C<sub>30</sub>H<sub>23</sub>ClN<sub>2</sub>O C, 77.83; H, 5.01; N, 6.05; Found: C, 77.82; H, 4.99; N, 6.07. <sup>13</sup>C NMR (75 MHz; CDCl<sub>3</sub>) <sup>5</sup>C 196.2, 153.3, 147.9, 145.3, 144.4, 138.4, 136.7, 136.0, 133.6, 133.4, 130.9, 130.8, 130.6, 130.4, 129.4, 129.3, 128.8, 128.6, 128.4, 128.1, 127.4, 123.9, 74.3, 47.5, 41.4.

3-(4-chlorophenyl)-4-(6-fluoroquinolin-2-yl)-1-phenyl-4-(pyridin-1-ium-1-yl)but-1-en-1-olate (4 n)

Pale red solid, Yield 62%, ESIMS (m/z) = 481 (M+H)<sup>+</sup>. IR (KBr) max 3425, 3019, 2400, 1620, 1587, 1401, 1070, 772, 667. <sup>1</sup>H NMR (300 MHz; CDCl<sub>3</sub>) <sup>6</sup>H 10.02 (d, <i>J</i> = 5.70 Hz, 2H), 8.87 (d, <i>J</i> = 8.31 Hz, 1H), 8.44 (d, <i>J</i> = 11.85 Hz, 1H), 8.28-8.18 (m, 3H), 7.84-7.74 (m, 5H), 7.62 (t, <i>J</i> = 8.91 Hz, 1H), 7.52-7.46 (m, 2H), 7.37 (t, <i>J</i> = 7.74 Hz, 2H), 7.20 (d, <i>J</i> = 8.07 Hz, 2H), 4.98 (d, <i>J</i> = 10.44 Hz, 1H), 4.19-4.10 (m, 1H), 3.00 (d, <i>J</i> = 17.22 Hz, 1H). Analysis calculated for C<sub>30</sub>H<sub>22</sub>ClFNO C, 74.92; H, 4.61; N, 5.82; Found: C, 74.97; H, 4.55; N, 5.77. <sup>13</sup>C NMR (75 MHz; CDCl<sub>3</sub>) <sup>5</sup>C 196.2, 162.8, 159.5, 152.7, 145.5, 145.1, 144.3, 137.8, 137.3, 136.6, 135.9, 133.7, 133.5, 132.2, 132.1, 130.4, 129.3, 128.6, 128.1, 127.6, 124.5, 121.3, 121.0, 111.1, 110.8, 74.3, 47.3, 41.5.

3-(4-chlorophenyl)-4-(6-chloroquinolin-2-yl)-1-phenyl-4-(pyridin-1-ium-1-yl)but-1-en-1-olate (4 o)
Solid, Yield 58%, ESIMS (m/z) = 497 (M+H)+. IR (KBr) max 3464, 3013, 2400, 1673, 1587, 1483, 1072, 772, 669. $^1$H NMR (300 MHz; CDCl$_3$) $^6$H 9.95 (d, $J$ = 5.22 Hz, 2H), 8.71 (d, $J$ = 8.04 Hz, 1H), 8.29-8.10 (m, 4H), 7.81-7.67 (m, 7H), 7.57-7.50 (m, 1H), 7.41-7.32 (m, 1H) 7.27 (t, $J$ = 7.47 Hz, 1H), 7.10 (t, $J$ = 8.04 Hz, 2H), 4.90 (t, $J$ = 10.38 Hz, 1H), 4.11-4.02 (m, 1H), 2.91 (d, $J$ = 17.7 Hz, 1H). Analysis calculated for C$_{30}$H$_{22}$Cl$_2$N$_2$O C, 72.44; H, 4.46; N, 5.63; Found: C, 72.38; H, 4.49; N, 5.57. 13C NMR (75 MHz; CDCl$_3$) $^6$C 196.3, 153.3, 148.0, 145.3, 144.4, 138.5, 136.7, 136.0, 133.7, 133.5, 130.6, 130.5, 129.5, 129.3, 128.6, 128.1, 127.5, 123.9, 74.3, 47.5, 41.5.

1-(4-bromophenyl)-3-(1H-indol-3-yl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (6a)

Pale yellow solid, Yield 72%, ESIMS (m/z) = 546 (M+H)+. IR (KBr) max 3468, 3013, 4.46; N, 5.63; Found: C, 72.38; H, 4.49; N, 5.57. 13C NMR (75 MHz; CDCl$_3$) $^6$C 196.3, 153.3, 148.0, 145.3, 144.4, 138.5, 136.7, 136.0, 133.7, 133.5, 130.6, 130.5, 129.5, 129.3, 128.6, 128.1, 127.5, 123.9, 74.3, 47.5, 41.5.

1-(4-fluorophenyl)-3-(1H-indol-3-yl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl)but-1-en-1-olate (6b)

Pale yellow solid, Yield 79%, ESIMS (m/z) = 486 (M+H)+. IR (KBr) max 3470, 3019, 2400, 1683, 1596, 1486, 759, 669. $^1$H NMR (300 MHz; DMSO-d$_6$) $^6$H 10.98 (s, 1H), 9.44 (d, $J$ = 5.97 Hz, 2H), 8.60 (d, $J$ = 8.28 Hz, 1H), 8.33 (t, $J$ = 7.74 Hz, 1H), 8.21 (d, $J$ = 8.43 Hz, 1H), 8.13-8.02 (m, 3H), 7.88-7.83 (m, 3H), 7.74-7.58 (m, 7H), 7.24 (t, $J$ = 7.32 Hz, 2H), 5.17 (t, $J$ = 9.27 Hz, 1H), 3.88-3.80 (m, 1H), 3.26 (d, $J$ = 14.64 Hz, 1H). Analysis calculated for C$_{32}$H$_{24}$BrN$_3$O C, 70.33; H, 4.43; N, 7.69; Found: C, 70.30; H, 4.43; N, 7.65. 13C NMR (75 MHz; DMSO-d$_6$) $^6$C 197.1, 154.6, 147.8, 146.8, 145.0, 140.9, 139.0, 136.7, 135.8, 132.2, 131.3, 130.5, 129.7, 128.8, 128.5, 128.3, 127.9, 126.0, 123.8, 123.3, 121.9, 119.4, 119.2, 112.2, 111.6, 78.0, 42.0, 38.9.

Electronic Supplementary Material (ESI) for RSC Advances
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3-(4-chlorophenyl)-1-ferrocenyl-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl) but-1-en-1-olate (6c)

Pale red solid, Yield 83%, ESIMS (m/z) = 571 (M+H)\(^+\). IR (KBr) max 3435, 3019, 1663, 1485, 1096, 1045, 757, 669. \(^1\)H NMR (300 MHz; CDCl\(_3\)) \(\delta\)H 10.13 (d, \(J = 5.19\) Hz, 2H), 8.89 (d, \(J = 7.89\) Hz, 1H), 8.42 (t, \(J = 7.47\) Hz, 2H), 8.29 (t, \(J = 9.72\) Hz, 2H), 7.97-7.87 (m, 6H), 7.71 (t, \(J = 7.74\)Hz, 1H), 7.30 (s, 1H), 5.04 (t, \(J = 11.01\) Hz, 1H), 4.74 (d, \(J = 7.68\) Hz, 2H), 4.74 (s, 2H), 4.00-3.89 (m, 1H), 3.84 (s, 5H), 2.79 (d, \(J = 16.68\) Hz, 1H). Analysis calculated for C\(_{34}\)H\(_{27}\)ClFeN\(_2\)O C, 71.53; H, 4.77; N, 4.91; Found: C, 71.49; H, 4.76; N, 4.92. \(^{13}\)C NMR (75 MHz; DMSO-d\(_6\)) \(\delta\)C 199.9, 154.2, 147.8, 147.3, 144.8, 139.1, 138.4, 132.6, 131.3, 131.2, 129.0, 128.8, 128.5, 123.2, 78.8, 77.0, 72.8, 69.8, 69.7, 69.4, 45.3, 42.9.

1-ferrocenyl-3-(4-nitrophenyl)-4-(pyridin-1-ium-1-yl)-4-(quinolin-2-yl) but-1-en-1-olate (6d)

Pale red solid, Yield 84%, ESIMS (m/z) = 582 (M+H)\(^+\). IR (KBr) max 3435, 3019, 2400, 1630, 1405, 1215, 1046, 758, 669. \(^1\)H NMR (300 MHz; CDCl\(_3\)) \(\delta\)H 10.13 (d, \(J = 5.16\) Hz, 2H), 8.88 (d, \(J = 8.22\) Hz, 1H), 8.64 (d, \(J = 11.73\) Hz, 1H), 8.44 (d, \(J = 8.16\) Hz, 1H), 8.33-8.17 (m, 6H), 7.97-7.83 (m, 3H), 7.71 (t, \(J = 7.86\)Hz, 1H), 5.20 (t, \(J = 11.82\) Hz, 1H), 4.72 (d, \(J = 13.62\) Hz, 2H), 4.45 (s, 2H), 4.04-3.94 (m, 1H), 3.81 (s, 5H), 2.89 (d, \(J = 17.58\) Hz, 1H). Analysis calculated for C\(_{34}\)H\(_{27}\)FeN\(_3\)O\(_3\) C, 70.23; H, 4.68; N, 7.23; Found: C, 70.19; H, 4.62; N, 7.21. \(^{13}\)C NMR (75 MHz; DMSO-d\(_6\)) \(\delta\)C 199.9, 154.0, 147.9, 147.7, 147.5, 144.8, 139.3, 131.5, 130.9, 129.7, 129.1, 128.9, 128.7, 124.1, 123.4, 78.6, 76.8, 73.0, 70.0, 69.6, 45.7, 42.9.
Spectral data for all the synthesized compounds

$^1$H spectrum of 4a

$^{13}$C Spectrum of 4a
$^1$H spectrum of 4b

LALIT-311

$^{13}$C spectrum of 4b

LALIT-311
$^1$H spectrum of 4c

$^{13}$C spectrum of 4c
$^1$H spectrum of 4d

$^{13}$C spectrum of 4d
$^1$H spectrum of 4e

$^{13}$C spectrum of 4e
$^1$H spectrum of 4f

$^{13}$C spectrum of 4f
$^1\text{H}$ spectrum of 4g

$^{13}\text{C}$ spectrum of 4g
$^1$H spectrum of 4h

$^{13}$C spectrum of 4h
$^1$H spectrum of 4i

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$^1$H spectrum of 4j

$^1$C spectrum of 4j
$^1$H spectrum of 4k

$^{13}$C spectrum of 4k
$^1$H spectrum of 4l

$^{13}$C spectrum of 4l
$^1$H spectrum of 4m

$^{13}$C spectrum of 4m
$^1$H spectrum of 4n

$^{13}$C spectrum of 4n
$^1$H spectrum of 4o

$I_{\text{LALIT-C}}$

$^{13}$C spectrum of 4o

$I_{\text{LALIT-2}}$
$^1$H spectrum of 6a

$^{13}$C spectrum of 6a
$^1$H spectrum of 6b

$^{13}$C spectrum of 6b
$^1$H spectrum of 6c

$^{13}$C spectrum of 6c
$^{1}H$ spectrum of 6d

$^{13}C$ spectrum of 6d