A series of novel blue emitting compounds, 2H-imidazo[5,1-a]isoquinolinium chloride derivatives were synthesized by the reaction of isoquinoline with trifluoroacetimidoyl chlorides and isocyanides in dry CH2Cl2 in excellent yields. Fluorescence data were collected which were found these compounds absorbs UV and emits blue light at about 481 nm, and having moderate to good fluorescence quantum yields. Also these compounds show high Stokes shifts that can be used to develop ultrasensitive fluorescent molecular probes to study a variety of biological events and processes.

**Keywords:** Blue emitting compounds, 2H-imidazo[5,1-a]isoquinolinium chloride derivatives, Trifluoroacetimidoyl chlorides, Isoquinoline

**Experimental section**

All chemicals and solvents were purchased from commercial sources and used without further purification unless otherwise stated. Melting points were determined on a Melt-Tem II melting point apparatus and are uncorrected. IR spectra were obtained on a Matson-1000 FT-IR spectrometer. Peaks are reported in wave numbers (cm$^{-1}$). All of the NMR spectra were recorded on a Bruker model DRX-400 AVANCE ($^1$H: 400, $^{13}$C: 100) NMR spectrometer. Chemical shifts of $^1$H and $^{13}$C-NMR are reported in parts per million (ppm) from tetramethylsilane (TMS) as an internal standard in DMSO-d$_6$ or CDCl$_3$ as a solvent. UV–visible (UV–vis) and photoluminescence (PL) spectra were measured using a Perkin Elmer and Avantes spectrometer (AvaSpec-2048 TEC) respectively.
General procedure for the synthesis of 3-(trifluoromethyl)-2H-imidazo[5,1-a]isoquinolinium chloride derivatives (4a-j)

To a magnetically stirred solution of isoquinoline (1 mmol) and the 2,2,2-trifluoroacetimidoyl chloride derivatives (1 mmol) in dichloromethane (10 mL) was added a 1 mmol of isocyanide derivatives at room temperature. Then the reaction mixture was allowed to stir for appropriate time to complete reaction. The solvent was removed under reduced pressure, and the residue was washed with hot EtOAc and a pure product obtained.

1-(cyclohexylamino)-2-(p-tolyl)-3-(trifluoromethyl)-2H-imidazo[5,1-a]isoquinolin-4-ium chloride (4a)

M.P = 231-232 °C, Yield = 431 mg, 94%, IR (KBr, cm⁻¹): 3417, 3074, 2925, 2850. \(^1\)H-NMR (400 MHz, DMSO-d₆) δ = 8.74 (d, 1H, J = 8.4 Hz), 8.55 (d, 1H, J = 7.6 Hz), 8.12 (d, 1H, J = 8.4 Hz), 7.94-7.81 (m, 3H), 7.60 (d, 2H, J = 8.4 Hz), 7.55 (d, 2H, J = 8.4 Hz), 7.58 (d, 1H, NH, J = 7.6), 2.74-2.68 (m, 1H, CH cyclohexyl), 2.49 (s, 3H, CH₃), 1.66-1.45 (m, 5H), 1.19-0.95 (m, 5H). \(^{13}\)C-NMR (100 MHz, DMSO-d₆) δ = 21.44 (Me), 25.20, 25.41, 33.87, 57.99, 117.41 (q, J = 270 Hz, CF₃), 118.40 (q, J = 41 Hz, C-CF₃), 120.32, 122.51, 122.88, 122.73, 127.12, 128.19, 128.96, 129.61, 130.26, 130.46, 130.90, 135.86, 142.0 1 ppm. Elemental analysis: Value calculated for C₂₅H₂₅ClF₃N₃: C, 65.28; H, 5.48; N, 9.14%, Value found: C, 65.22; H, 5.37; N, 9.15 %.

1-(cyclohexylamino)-3-(trifluoromethyl)-2-(2-(trifluoromethyl)phenyl)-2H-imidazo[5,1-a]isoquinolin-4-ium chloride (4b)

M.P = 231-232 °C, Yield = 431 mg, 94%, IR (KBr, cm⁻¹): 3417, 3074, 2925, 2850. \(^1\)H-NMR (400 MHz, DMSO-d₆) δ = 8.67 (d, 1H, J = 8.4 Hz), 8.59 (d, 1H, J = 7.2 Hz), 8.23-8.05 (m, 5H), 7.98-7.84 (m, 3H), 6.18 (d, 1H, NH, J = 8.8 Hz), 2.81-2.73 (m, 1H, CH cyclohexyl), 1.90-1.26 (m, 5H), 1.07-0.87 (m, 5H). \(^{13}\)C-NMR (100 MHz, DMSO-d₆) δ = 25.27, 25.38, 25.54, 34.14, 34.34, 58.76, 117.16 (q, J = 270 Hz, CF₃), 117.45 (q, J = 41 Hz, C-CF₃), 119.13, 120.10, 120.13, 120.23 (q, J = 272 Hz, CF₃), 122.50, 123.65, 123.90, 126.43 (q, J = 31 Hz, C-CF₃), 127.26, 128.71, 128.75, 128.87, 129.17, 130.61, 131.06, 131.55, 133.76, 134.72, 137.27 ppm. Elemental analysis: Value calculated for C₂₅H₂₂ClF₆N₃: C, 58.43; H, 4.31; N, 8.18 %. Value found: C, 58.34; H, 4.26; N, 8.14 %.

2-(2-cyanophenyl)-1-(cyclohexylamino)-3-(trifluoromethyl)-2H-imidazo[5,1-a]isoquinolin-4-ium chloride (4c)
M.P = 185-188 °C, Yield = 446 mg, 95%, IR (KBr, cm⁻¹): 3423, 3070, 2932, 2855, 2232. ¹H-NMR (400 MHz, DMSO-d₆) δ = 8.79 (d, 1H, J = 8.0 Hz), 8.70 (d, 1H, J = 6.4 Hz), 8.62 (d, 1H, J = 7.6 Hz), 8.56 (d, 1H, J = 8.4 Hz), 8.50 (d, 1H, J = 7.2 Hz), 8.46 (d, 1H, J = 8.0 Hz), 8.39 (d, 1H, J = 7.8 Hz), 8.34 (d, 1H, J = 8.4 Hz), 8.23-8.16 (m, 4H), 8.08-7.85 (m, 6H), 7.77 (t, 1H, J = 7.2 Hz), 7.65 (t, 1H, J = 7.2 Hz), 7.43 (d, 1H, NH, J = 7.6 Hz), 6.44 (d, 1H, NH, J = 8.8 Hz), 2.93-2.88 (m, 1H, CH cyclohexyl), 2.71-2.69 (m, 1H, CH cyclohexyl), 1.92-0.88 (m, 20H). ¹³C-NMR (100 MHz, DMSO-d₆) δ = 25.25, 25.34, 33.87, 34.36, 58.94, 11.82, 114.95, 117.22 (q, J = 270 Hz, CF₃), 117.66 (q, J = 41 Hz, C-CF₃), 120.03, 120.38, 120.41, 122.44, 123.58, 123.98, 125.53, 126.74, 127.63, 127.83, 129.12, 130.69, 130.92, 131.04, 132.22, 133.54, 133.58, 135.02, 135.53, 136.31, 136.49, 138.53, 147.44 ppm. Elemental analysis: Value calculated for C₂₅H₂₂ClF₃N₄: C, 63.76; H, 4.71; N, 11.90 %, Value found: C, 63.64; H, 4.65; N, 11.78 %.

1-(cyclohexylamino)-2-(2-fluorophenyl)-3-(trifluoromethyl)-2H-imidazo[5,1-a]isoquinolin-4-ium chloride (4d)
M.P = 159-161 °C. Yield = 430 mg, 93%, IR (KBr, cm⁻¹): 3476, 3134, 2930, 2856. ¹H-NMR (400 MHz, DMSO-d₆) δ = 8.75 (d, 1H, J = 8.4 Hz), 8.56 (d, 1H, J = 7.2 Hz), 8.14 (d, 1H, J = 7.2 Hz), 7.94-7.73 (m, 5H), 7.78-7.73 (m, 1H), 7.64-7.60 (m, 1H), 6.18 (d, 1H, NH, J = 8.0), 2.76-2.68 (m, 1H, CH cyclohexyl), 1.64-0.82 (m, 10H). ¹³C-NMR (100 MHz, DMSO-d₆) δ = 25.31, 33.96, 34.09, 55.50, 58.57, 117.48 (d, C-CF₂, J = 18 Hz), 117.91 (q, C-CF₃, J = 42 Hz), 117.27 (q, J = 271 Hz, CF₃), 119.94 (d, C-F, J = 280 Hz), 119.70 (d, J = 12 Hz), 120.42, 122.63, 123.08, 123.95, 126.12, 127.16, 128.95, 130.38, 130.96 (d, J = 21 Hz, C-CF), 135.08, 136.15, 155.63, 158.14 ppm. Elemental analysis: Value calculated for C₂₄H₂₂ClF₄N₃: C, 62.14; H, 4.78; N, 9.06 %, Value found: C, 62.11; H, 4.74; N, 9.01 %.

2-(4-chlorophenyl)-1-(cyclohexylamino)-3-(trifluoromethyl)-2H-imidazo[5,1-a]isoquinolin-4-ium chloride (4e)
M.P = 231-233 °C. Yield = 451 mg, 94%, IR (KBr, cm⁻¹): 3435, 3074, 2925, 2850. ¹H-NMR (400 MHz, DMSO-d₆) δ = 8.76 (d, 1H, J = 8.4 Hz), 8.55 (d, 1H, J = 7.6 Hz), 8.12 (d, 1H, J = 7.2 Hz), 7.93-7.80 (m, 3H), 7.68 (d, 2H, J = 8.4 Hz), 7.55 (d, 2H, J = 8.4 Hz), 5.81 (d, 1H, NH, J = 8.0 Hz), 2.73-2.70 (m, 1H, CH cyclohexyl), 1.65-1.44 (m, 5H), 1.20-0.95 (m, 5H). ¹³C-NMR (100 MHz, DMSO-d₆) δ = 21.43, 25.20, 25.40, 33.87, 57.99, 117.40 (q, J = 271 Hz, CF₃), 118.38 (q, J = 41 Hz, C-CF₃), 119.60, 120.29, 122.50, 122.86, 123.72, 127.10, 128.19, 128.94, 129.61, 130.23, 130.44, 130.87, 135.85, 1141.98, 151.27 ppm. Elemental
analysis: Value calculated for C24H22Cl2F3N3: C, 60.01; H, 4.62; N, 8.75 %, Value found: C, 60.04; H, 4.64; N, 8.69 %.

1-(cyclohexylamino)-2-(2,5-difluorophenyl)-3-(trifluoromethyl)-2H-imidazo[5,1-aj]isoquinolin-4-ium chloride (4f)

M.P = 225-226 °C, Yield = 461 mg, 96%, IR (KBr, cm\(^{-1}\)): 3423, 3171, 2928, 2855. \(^1\)H-NMR (400 MHz, DMSO-d\(_6\)) \(\delta = 8.69\) (d, 1H, J = 8.4 Hz), 8.58 (d, 1H, J = 7.6 Hz), 8.47 (d, 1H, J = 8.0 Hz), 8.17 (d, 1H, J = 7.6 Hz), 8.14 (d, 1H, J = 7.6 Hz), 7.94-7.84 (m, 10H), 7.78 (t, 1H, J = 7.2 Hz), 7.66 (t, 1H, J = 7.2 Hz), 7.43 (d, 1H, J = 7.6 Hz), 6.20 (d, 1H, NH, J = 8.0 Hz), 5.69 (d, 1H, NH, J = 7.2 Hz), 2.93-2.88 (m, 1H, CH cyclohexyl), 2.80-2.76 (m, 1H, CH cyclohexyl), 2.12-1.01 (m, 20H). \(^{13}\)C-NMR (100 MHz, DMSO-d\(_6\)) \(\delta = 25.25, 25.33, 33.87, 34.04, 58.53, 117.44\) (q, J = 42 Hz, C-CF\(_3\)), 114.46 (q, J = 271 Hz, CF\(_3\)), 118.06, 118.53, 119.03, 119.12, 119.24, 119.33, 120.22, 120.40, 122.18, 122.59, 123.27, 123.82, 127.20, 129.07, 130.56, 131.06, 136.03, 152.47, 154.96, 156.64, 159.06 ppm. Elemental analysis: Value calculated for C\(_{24}\)H\(_{21}\)ClF\(_5\)N\(_3\): C, 59.82; H, 4.39; N, 8.72%, Value found: C, 59.78; H, 4.36; N, 8.73 %.

1-(tert-butylamino)-2-(2,4-dimethylphenyl)-3-(trifluoromethyl)-2H-imidazo[5,1-aj]isoquinolin-4-ium chloride (4g)

M.P = 270-271 °C, Yield = 420 mg, 94%, IR (KBr, cm\(^{-1}\)): 3333, 3156, 2969, 2926. \(^1\)H-NMR (400 MHz, DMSO-d\(_6\)) \(\delta = 9.09\) (d, 1H, J = 8.0 Hz), 8.58 (d, 1H, J = 7.2 Hz), 8.13 (d, 1H, J = 7.6 Hz), 7.95-7.84 (m, 3H), 7.61 (d, 1H, J = 8.0 Hz), 7.40 (s, 1H), 7.34 (d, 1H, J = 7.6 Hz), 5.41 (s, 1H, NH), 2.43 (s, 3H, CH\(_3\)), 2.18 (s, 3H, CH\(_3\)), 0.97 (s, 9H, 3CH\(_3\)). \(^{13}\)C-NMR (100 MHz, DMSO-d\(_6\)) \(\delta = 17.67, 21.28, 30.73, 56.38, 117.26\) (q, J = 271 Hz, CF\(_3\)), 118.28, 119.34 (q, J = 41 Hz, C-CF\(_3\)), 121.08, 124.46, 127.46, 127.78, 128.81, 128.98, 129.62, 130.23, 130.65, 132.13, 133.28, 136.20, 142.02 ppm. Elemental analysis: Value calculated for C\(_{24}\)H\(_{22}\)ClF\(_3\)N\(_3\): C, 64.35; H, 5.63; N, 9.38 %, Value found: C, 64.31; H, 5.61; N, 9.28 %.

1-(tert-butylamino)-2-(2,5-difluorophenyl)-3-(trifluoromethyl)-2H-imidazo[5,1-aj]isoquinolin-4-ium chloride (4h)

M.P = 243-245 °C, Yield = 418 mg, 92%, IR (KBr, cm\(^{-1}\)): 3448, 3096, 2978, 2914. \(^1\)H-NMR (400 MHz, DMSO-d\(_6\)) \(\delta = 9.11\) (d, 1H, J = 8.0 Hz), 8.82 (d, 1H, J = 7.6 Hz), 8.60 (d, 1H, J = 7.2 Hz), 8.20 (d, 1H, J = 7.2 Hz), 8.15 (d, 1H, J = 7.6 Hz), 7.81-7.97 (m, 11H), 7.72-7.64 (m, 1H), 7.41 (d, 1H, J = 7.6 Hz), 5.73 (s, 1H, NH), 5.13 (s, 1H, NH), 1.22 (s, 9H, 3CH\(_3\)), 0.99 (s,
9H, 3CH3). 13C-NMR (100 MHz, DMSO-d6) δ = 30.23, 31.17, 56.89, 56.91, 116.97 (q, J = 271 Hz, CF3), 119.74 (q, J = 42 Hz, C-CF3), 118.33, 120.56, 121.92, 122.56, 122.92, 123.50, 124.46, 125.02, 125.67, 127.78, 127.90, 128.24, 128.35, 128.60, 129.03, 129.80, 129.91, 130.57, 131.18, 133.06, 152.38, 154.65, 156.46, 158.87 ppm. Elemental analysis: Value calculated for C22H19ClF5N3: C, 57.97; H, 4.20; N, 9.22 %, Value found: C, 57.93; H, 4.16; N, 9.18 %.

1-(tert-butylamino)-2-(p-tolyl)-3-(trifluoromethyl)-2H-imidazo[5,1-a]isoquinolin-4-ium chloride (4i)

M.P = 209-211 °C, Yield = 402 mg, 93%, IR (KBr, cm\(^{-1}\)): 3443, 3105, 2971, 2864. 1H-NMR (400 MHz, DMSO-d6) δ = 9.15 (d, 1H, J = 8.0 Hz), 8.59 (d, 1H, J = 6.8 Hz), 8.12 (d, 1H, J = 7.6 Hz), 7.95-7.83 (m, 3H), 7.69 (d, 2H, J = 8.4 Hz), 7.53 (d, 2H, J = 8.0 Hz), 7.50-7.40 (m, 4H), 7.13-7.11 (m, 1H), 7.04 (d, 2H, J = 8.0 Hz), 6.44 (d, 2H, J = 6.8 Hz), 6.10-6.08 (m, 1H), 5.42 (s, 1H, NH), 5.40 (s, 1H, NH) 2.47 (s, 3H, CH3), 2.30 (s, 3H, CH3), 1.59 (s, 9H, 3CH3), 0.92 (s, 9H, 3CH3). 13C-NMR (100 MHz, DMSO-d6) δ = 21.17, 21.36, 27.93, 30.34, 56.63, 58.04, 109.27, 115.79 (q, J = 286 Hz, CF3), 117.22 (q, J = 271 Hz, CF3), 119.93 (q, J = 42 Hz, C-CF3), 125.21 (q, J = 43 Hz, C-CF3), 120.18, 120.57, 127.07, 121.96, 124.11, 124.29, 125.94, 127.06, 127.66, 128.09, 128.59, 128.87, 128.90, 129.69, 130.06, 130.21, 130.41, 130.86, 132.93, 142.03 ppm. Elemental analysis: Value calculated for C23H23ClF3N3: C, 63.67; H, 5.34; N, 9.68 %, Value found: C, 63.61; H, 5.26; N, 9.58 %.

1-(tert-butylamino)-3-(trifluoromethyl)-2-(2-(trifluoromethyl)phenyl)-2H-imidazo[5,1-a]isoquinolin-4-ium chloride (4j)

M.P = 231-232 °C, Yield = 448 mg, 92%, IR (KBr, cm\(^{-1}\)): 3415, 3078, 2965, 2895. 1H-NMR (400 MHz, DMSO-d6) δ = 9.03 (d, 1H, J = 8.0), 8.63 (d, 1H, J = 7.2), 8.22-8.04 (m, 5H), 7.99-7.88 (m, 3H), 5.51 (s, 1H, NH), 1.0 (s, 9H, 3CH3). 13C-NMR (100 MHz, DMSO-d6) δ = 30.54, 57.01, 116.93 (q, J = 272 Hz, CF3), 118.34, 119.42 (q, J = 42 Hz, C-CF3), 126.85 (q, J = 31 Hz, C-CF3), 120.39 (q, J = 270 Hz, CF3), 121.93, 122.44, 123.25, 124.46, 125.32, 127.80, 129.11, 130.58, 131.24, 132.66, 134.32, 134.52, 136.36, 138.44 ppm. Elemental analysis: Value calculated for C23H20ClF6N3: C, 56.62; H, 4.13; N, 8.61 %, Value found: C, 56.59; H, 4.10; N, 8.56 %.