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Supporting Information

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General Consideration

All experiments were performed in a screw capped reaction vial under conventional heating. Reactions were monitored by thin layer chromatography (TLC) on Merck gel 60 F_{254} plates. The ¹H and ¹³C NMR spectra (CDCl₃ and DMSO-d₆) were recorded on a JEOL ECX-400P NMR at 400 MHz and 100 MHz, respectively using TMS as internal standard. The high-resolution mass spectral data was obtained using an AGILENT 6520 Q-TOF spectrometer, Bruker ESI instrument-amaZon SL Dual Funnel Iontrap Bench Top and Waters QTOF mass spectrometer. Melting point were recorded on a Büchi M-560 melting point apparatus and are uncorrected. All the chemicals and reagents were purchased from commercial sources and used as received. TBHP 70% aqueous and 5-6 M in decane solution were used. 1-Methyl-3-phenylquinoxalin-2(1*H*)-one¹⁻³ derivatives were prepared according to the literature procedures.

General procedure for the synthesis of compounds 3(a-z)

An oven dried 10 mL screw capped reaction vial with a small stirring bar was charged with a mixture of 1-methyl-3-phenylquinoxalin-2(1H)-one **1** (1 mmol), Benzaldehyde **2** (1.5 mmol), Pd(OAc)₂(10 mol%), TBPB (6 mmol) and H₂O (3mL). The resulting mixture was stirred at 90 °C for 18 hours. The progress of the reaction was monitored by TLC. After Completion of the reaction, the reaction mixture was cooled up to ambient temperature, washed with 20 mL saturated solution of NaHCO₃ and extracted with ethyl acetate (3 X 15 mL). The organic layer was separated, dried over anhydrous Na₂SO₄ and concentrated on a rotary evaporator to obtained the crude product. The crude product thus obtained was further purified on a silica gel column using hexane/ethyl acetate (8:2) as eluent to afford the pure targeted products.

General procedure for the synthesis of compounds 5(a-g)

An oven dried 10 mL screw capped reaction vial with a small stirring bar was charged with a mixture of 1-methyl-3-phenylquinoxalin-2(1H)-one **1** (1 mmol), Benzyl Alcohols **4** (1.5 mmol), Pd(OAc)₂ (10 mol%), TBPB (6 mmol) and H₂O (3mL). The resulting mixture was stirred at 90 °C for 18 hours. The progress of the reaction was monitored by TLC. After Completion of the reaction, the reaction mixture was cooled up to ambient temperature, washed with 20 mL saturated solution of NaHCO₃ and extracted with ethyl acetate (3 X 15 mL). The organic layer was separated, dried over anhydrous Na₂SO₄ and concentrated on a rotary

evaporator to obtained the crude product. The crude product thus obtained was further purified on a silica gel column using hexane/ethyl acetate (8:2) as eluent to afford the pure targeted products.

General procedure for the synthesis of compounds 7a

An oven dried 10 mL screw capped reaction vial with a small stirring bar was charged with a mixture of 1-methyl-3-phenylquinoxalin-2(1H)-one **1** (0.423 mmol), Pd(OAc)₂ (10 mol%), Aqueous TBHP (12 mmol) and Toluene **6** (3mL) The resulting mixture was stirred at 90 °C for 18 hours. The progress of the reaction was monitored by TLC. After Completion of the reaction, the reaction mixture was cooled up to ambient temperature, washed with 20 mL saturated solution of NaHCO₃ and extracted with ethyl acetate (3 X 15 mL). The organic layer was separated, dried over anhydrous Na₂SO₄ and concentrated on a rotary evaporator to obtained the crude product. The crude product thus obtained was further purified on a silica gel column using hexane/ethyl acetate (8:2) as eluent to afford the pure targeted products.

General procedure for the synthesis of compound 18

An oven dried 10 mL screw capped reaction vial with a small stirring bar was charged with a mixture of 3-(2-(4-bromobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (1 mmol), Boronic acids (2.0 mmol), Pd(PPh_3)_4 (5 mol%), Cs₂CO₃ (1.5 mmol) and Toluene (2mL). The resulting mixture was heated at 110 °C for 16 hours. The progress of the reaction was monitored by TLC. After Completion of the reaction, the reaction mixture was cooled up to ambient temperature and then diluted with water and extracted with EtOAc (3×10 mL). The organic layer was separated, dried over anhydrous Na₂SO₄ and concentrated on a rotary evaporator to obtain the crude product. The crude product thus obtained was further purified on a silica gel column using hexane/ethyl acetate (8:2) as eluent to afford the pure targeted products.

General procedure for the synthesis of compounds 19

An oven dried 10 mL screw capped reaction vial with a small stirring bar was charged with a mixture of 3-(2-benzoyl-4-bromophenyl)-1-methylquinoxalin-2(1H)-one (1 mmol), Boronic acids (2.0 mmol), $Pd(PPh_3)_4$ (5 mol%), Cs_2CO_3 (1.5 mmol) and Toluene (2mL). The resulting mixture was heated at 110 °C for 16 hours. The progress of the reaction was monitored by TLC.

After Completion of the reaction, the reaction mixture was cooled up to ambient temperature and then diluted with water and extracted with EtOAc (3×10 mL). The organic layer was separated, dried over anhydrous Na₂SO₄ and concentrated on a rotary evaporator to obtain the crude product. The crude product thus obtained was further purified on a silica gel column using hexane/ethyl acetate (8:2) as eluent to afford the pure targeted products.

References

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3-(2-benzoylphenyl)-1-methylquinoxalin-2(1H)-one (3a)



It was obtained as yellow solid having melting point 166-168 $^{\rm o}{\rm C}$ with 81% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, J = 7.7 Hz, 1H), 7.84 (m, J = 7.0 Hz, 3H), 7.66 (td, J = 7.5, 1.6 Hz, 2H), 7.58 (d, J = 6.1 Hz, 1H), 7.55 – 7.50 (m, 2H), 7.48 (d, J = 7.4 Hz, 1H), 7.39 (t, J = 7.5 Hz, 2H), 7.35 – 7.30 (m, 1H), 7.24 (d, J = 7.2 Hz, 1H), 3.58 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 195.99, 155.31, 154.31,

138.54, 138.46, 137.31, 133.78, 133.61, 133.07, 132.74, 132.12, 130.95, 130.92, 130.50, 130.20, 128.35, 125.74, 123.99, 113.83,

29.46.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for $C_{22}H_{16}N_2O_2$:341.1290; found:341.1290.

3-(2-(4-bromobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3b)



It was obtained as yellow solid having melting point 180-182 $^{\rm o}{\rm C}$ with 75% yield.

¹H NMR (400 MHz, DMSO- d_6) δ 7.89 (d, J = 7.4 Hz, 1H), 7.75 (t, J = 8.2 Hz, 2H), 7.68 (d, J = 6.4 Hz, 2H), 7.65 (d, J = 6.0 Hz 2H), 7.62 (d, J = 6.0 Hz, 2H), 7.55 – 7.50 (m, 2H), 7.39 (t, J = 7.6 Hz, 1H), 3.51 (s, 3H). ¹³C NMR (100 MHz, DMSO- d_6) δ 194.93, 155.64, 153.73, 138.80, 136.12, 136.05, 133.16, 132.28, 131.66, 131.40, 131.09, 130.81, 130.77, 129.31, 128.61, 126.71, 123.75, 114.80, 29.21.

m/z

 $[M+H]^+$

calculated

for

HRMS (ESI⁺): C₂₂H₁₅BrN₂O₂:419.0395; found:419.0390

1-methyl-3-(2-(4-nitrobenzoyl)phenyl)quinoxalin-2(1H)-one (3c)



It was obtained as yellow solid having melting point 94-96 °C with 68% yield.

¹H NMR (400 MHz, DMSO- d_6) δ 8.30 (d, J = 8.8 Hz, 2H), 7.97 – 7.92 (m, 3H), 7.77 (d, J = 6.9 Hz, 2H), 7.69 – 7.62 (m, 2H), 7.54 (s, 1H), 7.52 (s, 1H), 7.43 – 7.38 (m, 1H), 3.51 (s, 3H).

¹³C NMR (100 MHz, DMSO- d_6) δ 194.58, 155.34, 153.79, 149.52, 142.18, 138.41, 135.92, 133.17, 132.27, 131.55, 130.99, 130.94, 130.90, 129.50, 129.36, 128.67, 123.86, 123.52, 114.88, 29.27.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₅N₃O₄:386.1141;

found:386.1124.

1-methyl-3-(2-(4-methylbenzoyl)phenyl)quinoxalin-2(1H)-one (3d)



It was obtained as yellow solid having melting point 188-190 $^{\rm o}{\rm C}$ with 79% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, J = 7.8 Hz, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.77 (s, 1H), 7.75 (s, 1H), 7.64 (t, J = 7.5 Hz, 1H), 7.57 (d, J = 7.7 Hz, 1H), 7.51 (t, J = 7.8 Hz, 2H), 7.34 – 7.28 (m, 1H), 7.24 (d, J = 9.6 Hz, 1H), 7.21 (s, 1H), 7.19 (s, 1H), 3.57 (s, 1H), 2.37 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 196.59, 156.89, 154.56,

143.22, 139.94, 136.87, 135.13, 133.63, 133.23, 131.03, 130.76, 130.44, 130.41, 130.38, 129.48, 129.06, 128.95, 123.72, 113.70,

29.38, 21.75. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₃H₁₈N₂O₂:355.1447; found:355.1434.

3-(2-(4-methoxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3e)



It was obtained as white solid having melting point 200-202 $^{\circ}$ C with 80% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, *J* = 6.6 Hz, 1H), 7.84 (dd, *J* = 8.3, 3.1 Hz, 3H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.57 (d, *J* = 7.7 Hz, 1H), 7.52 (dd, *J* = 7.9, 4.1 Hz, 2H), 7.34 – 7.29 (m, 1H), 7.24 (s, 1H), 6.90 (s, 1H), 6.87 (s, 1H), 3.83 (s, 3H), 3.58 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 195.65, 163.16, 156.87, 154.55, 140.05, 136.80, 133.61, 133.24, 132.58, 130.90, 130.76, 130.53, 130.42, 130.39, 129.35, 129.08, 123.75, 113.73, 113.53, 55.55, 29.40.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₃H₁₈N₂O₃:371.1396; found:371.1393.

3-(2-(4-hydroxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3f)



It was obtained as yellow solid having melting point 250-252 $^{\rm o}{\rm C}$ with 66% yield.

¹H NMR (400 MHz, DMSO- d_6) δ 10.31 (s, 1H), 7.83 (d, J = 6.4 Hz, 1H), 7.72 (d, J = 8.2 Hz, 1H), 7.67 (d, J = 7.6 Hz, 1H), 7.63 (d, J = 8.7 Hz, 1H), 7.61 (s, 2H), 7.59 (s, 1H), 7.54 – 7.49 (m, 2H), 7.38 (t, J = 7.5 Hz, 1H), 6.81 (s, 1H), 6.79 (s, 1H), 3.52 (s, 3H).

¹³C NMR (100 MHz, DMSO- d_6) δ 194.30, 161.70, 156.28, 153.69, 139.72, 136.27, 133.19, 132.35, 132.29, 130.62, 130.58, 130.36, 129.28, 129.04, 128.66, 128.28, 123.61, 114.91, 114.73,

29.14.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₆N₂O₃:357.1239; found:357.1235.

3-(2-(2-fluorobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3g)



It was obtained as yellow solid having melting point 160-162 $^{\circ}$ C with 72% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.89 (dd, J = 8.0, 1.5 Hz, 1H), 7.84 (dd, J = 7.7, 1.3 Hz, 1H), 7.68 (dtd, J = 15.0, 7.5, 1.7 Hz, 2H), 7.59 (d, J = 7.7 Hz, 1H), 7.56 – 7.53 (m, 1H), 7.51 (d, J = 6.5 Hz, 1H), 7.47 – 7.40 (m, 1H), 7.36 – 7.32 (m, 1H), 7.26 (d, J = 8.5 Hz, 1H), 7.17 (t, J = 7.6 Hz, 1H), 7.09 – 7.03 (m, 1H), 3.61 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 193.35, 161.20 (d, J = 257.1 Hz), 157.21, 154.62, 139.85, 136.65, 133.82, 133.72,

133.66, 133.25, 132.00 (d, J = 7.5 Hz), 130.75, 130.45 (d, J = 7.7 Hz), 129.46, 129.39, 128.60 (d, J = 26.0 Hz), 126.59, 126.47, 123.97 (d, J = 5.0 Hz), 123.78, 116.57 (d, J = 22.3 Hz), 113.73, 29.40.

¹⁹F NMR (377 MHz, Chloroform-*d*) δ -110.14 (dt, J = 12.3, 6.7 Hz). HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₅FN₂O₂:359.1196; found:359.1187.

1-methyl-3-(2-(3-nitrobenzoyl)phenyl)quinoxalin-2(1H)-one (3h)



It was obtained as yellow solid having melting point 164-166 $^{\circ}$ C with 61% yield.

¹H NMR (400 MHz, DMSO- d_6) δ 8.41 (d, J = 5.2 Hz, 2H), 8.13 (d, J = 7.7 Hz, 1H), 7.93 (d, J = 6.5 Hz, 1H), 7.80 (d, J = 2.9 Hz, 1H), 7.78 (d, J = 4.0 Hz, 1H), 7.76 (s, 1H), 7.68 (d, J = 9.1 Hz, 1H), 7.63 (d, J = 9.8 Hz, 1H), 7.58 (d, J = 7.7 Hz, 1H), 7.52 (d, J = 8.5 Hz, 1H), 7.40 (d, J = 7.2 Hz, 1H), 3.49 (s, 3H). ¹³C NMR (100 MHz, DMSO- d_6) δ 193.89, 155.33, 153.79, 147.50, 138.44, 138.18, 135.96, 135.64, 133.13, 132.27, 131.56, 130.99, 130.90, 130.28, 129.54, 129.36, 128.66, 126.96, 123.90,

123.84, 114.85, 29.25.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₅N₃O₄:386.1141; found:386.1133.

3-(2-(4-bromo-2-fluorobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3i)



It was obtained as yellow solid having melting point 188-190 °C with 63% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.88 (td, J = 8.0, 1.2 Hz, 2H), 7.69 – 7.65 (m, 1H), 7.60 (t, J = 7.9 Hz, 1H), 7.56 (dd, J = 7.2, 1.4 Hz, 1H), 7.53 (d, J = 5.1 Hz, 1H), 7.37 – 7.32 (m, 2H), 7.30 – 7.28 (m, 1H), 7.27 (s, 1H), 3.61 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 192.35, 160.99 (d, J = 262.0 Hz), 156.80, 154.56, 139.71, 136.51, 133.68, 133.26, 133.12 (d, J = 2.7 Hz), 132.06, 130.90, 130.54 (d, J = 17.7 Hz), 129.45, 129.01, 128.99, 127.55, 127.51, 127.10 (d, J = 9.5 Hz),

125.52 (d, J = 11.6 Hz), 123.90, 120.29 (d, J = 25.2 Hz), 113.80, 29.46. ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -107.29 (t, J = 8.6 Hz). HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₄BrFN₂O₂:437.0301; found:437.0293.

3-(2-(3-bromo-4-fluorobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3j)



It was obtained as yellow solid having melting point 194-196 $^{\circ}$ C with 70% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.11 (d, J = 6.7 Hz, 1H), 7.97 (d, J = 7.7 Hz, 1H), 7.84 (dd, J = 8.0, 1.5 Hz, 1H), 7.82 – 7.77 (m, 1H), 7.68 (td, J = 7.4, 1.7 Hz, 1H), 7.56 (d, J = 8.8 Hz, 1H), 7.54 – 7.50 (m, 2H), 7.35 (t, J = 7.0 Hz, 1H), 7.28 (d, J = 7.2Hz, 1H), 7.13 (t, J = 8.3 Hz, 1H), 3.60 (s, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 194.10, 161.61 (d, J =254.9 Hz), 156.10, 154.50, 138.97, 136.64, 135.74, 135.28 (d, J =

254.9 Hz, 156.10, 154.50, 138.97, 136.64, 135.74, 135.28 (d, J = 3.6 Hz), 133.53, 133.16, 131.48 (d, J = 7.9 Hz), 131.09, 130.73, 144, 129.01, 123.96, 116.30 (d, J = 23.2 Hz), 113.83, 109.39 (d, J = 21.4 Hz)

130.38, 130.16, 129.34, 129.01, 123.96, 116.30 (d, *J* = 23.2 Hz), 113.83, 109.39 (d, *J* = 21.4 Hz), 29.47.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -100.49. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₄BrFN₂O₂:437.0301; found:437.0297.

3-(2-(4-chloro-2-fluorobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3k)



It was obtained as yellow solid having melting point 202-204 $^{\rm o}{\rm C}$ with 83% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, J = 5.0 Hz, 1H), 7.87 (d, J = 4.5 Hz, 1H), 7.68 (t, J = 8.0 Hz, 2H), 7.57 (d, J = 8.6 Hz, 1H), 7.54 (s, 1H), 7.53 (s, 1H), 7.38 – 7.33 (m, 1H), 7.28 (d, J = 7.2 Hz, 1H), 7.17 (dd, J = 8.3, 2.0 Hz, 1H), 7.11 (dd, J = 9.8, 1.9 Hz, 1H), 3.62 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*)) δ 192.14, 161.09 (d, J = 261.0 Hz), 156.71, 154.47, 139.65, 139.08 (d, J = 10.3 Hz), 136.40, 133.58, 133.16, 132.91 (d, J = 2.9 Hz), 131.94, 130.80,

130.43 (d, J = 15.6 Hz), 129.34, 128.90, 128.88, 124.98 (d, J = 11.6 Hz), 124.52, 124.48, 123.80, 117.29 (d, J = 25.3 Hz), 113.69, 29.36.

¹⁹F NMR (377 MHz, Chloroform-*d*) δ -107.29.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for $C_{22}H_{14}BrClN_2O_2$:393.0806; found:393.0803.

3-(2-(3-chloro-4-fluorobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3l)



It was obtained as yellow solid having melting point 186-188 $^{\circ}$ C with 73% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, J = 6.3 Hz, 2H), 7.83 (d, J = 8.0 Hz, 1H), 7.75 (t, J = 7.8 Hz, 1H), 7.69 – 7.64 (m, 3H), 7.56 – 7.48 (m, 1H), 7.34 (d, J = 7.7 Hz, 1H), 7.26 (d, J = 8.8 Hz, 1H), 7.15 (t, J = 8.6 Hz, 1H), 3.58 (s, 3H).

¹³C NMR (101 MHz, Chloroform-*d*) δ 194.21, 160.68 (d, J = 256.0 Hz), 156.11, 154.51, 138.99, 136.65, 134.93 (d, J = 3.6 Hz), 133.55, 133.17, 132.85, 131.52, 131.11, 130.68 (d, J = 8.7 Hz), 130.39, 130.17, 129.33, 128.99, 128.52, 123.96, 121.50 (d, J = 8.7 Hz), 130.39, 130.17, 129.33, 128.99, 128.52, 123.96, 121.50 (d, J = 8.7 Hz), 130.39, 130.17, 129.33, 128.99, 128.52, 123.96, 121.50 (d, J = 8.7 Hz), 130.39, 130.17, 129.33, 128.99, 128.52, 123.96, 121.50 (d, J = 8.7 Hz), 130.39, 130.17, 129.33, 128.99, 128.52, 123.96, 121.50 (d, J = 8.7 Hz), 130.39, 130.17, 129.33, 128.99, 128.52, 123.96, 121.50 (d, J = 8.7 Hz), 130.39, 130.17, 129.33, 128.99, 128.52, 123.96, 121.50 (d, J = 8.7 Hz), 130.39, 130.17, 129.33, 128.99, 128.52, 123.96, 121.50 (d, J = 8.7 Hz), 130.39, 130.17, 129.33, 128.99, 128.52, 123.96, 121.50 (d, J = 8.7 Hz), 130.39, 130.17, 129.33, 128.99, 128.52, 123.96, 121.50 (d, J = 8.7 Hz), 120.50 (d, J

18.2 Hz), 116.48 (d, *J* = 21.6 Hz), 113.84, 29.48.

¹⁹F NMR (376 MHz, Chloroform-*d*) δ -108.52. HRMS (ESI⁺): m/z [M+H]⁺ calculated for $C_{22}H_{14}BrClN_2O_2$:393.0806; found:393.0799.

3-(2-(2,4-difluorobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3m)



It was obtained as yellow solid having melting point 178-180 $^{\rm o}{\rm C}$ with 81% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.89 (d, J = 2.3 Hz, 1H), 7.87 (s, 1H), 7.76 (dd, J = 15.9, 7.5 Hz, 1H), 7.67 (ddd, J = 7.9, 5.5, 3.3 Hz, 1H), 7.57 (d, J = 8.6 Hz, 1H), 7.53 (d, J = 3.2 Hz, 2H), 7.38 – 7.33 (m, 1H), 7.28 (d, J = 8.4 Hz, 1H), 6.91 (t, J = 8.3 Hz, 1H), 6.82 (td, J = 9.8, 9.1, 2.4 Hz, 1H), 3.62 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 192.14, 165.34 (dd, J = 10.2

255.7, 11.6 Hz), 162.15 (dd, J = 260.3, 12.6 Hz), 156.83, 154.57, 139.93, 136.47, 133.87 (dd, J = 10.2, 3.5 Hz), 131.92, 130.89,

130.57, 130.41, 130.18, 129.41, 128.95, 128.52, 123.87, 122.99 (d, J = 11.6 Hz), 113.78, 111.57 (dd, J = 21.7, 3.7 Hz), 104.91 (t, J = 25.5 Hz), 29.44.

¹⁹F NMR (377 MHz, Chloroform-*d*) δ -102.87 (dt, J = 15.4, 7.9 Hz), -104.87 (q, J = 10.3 Hz). HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₄F₂N₂O₂:377.1102; found:377.1088.

3-(2-benzoyl-4-chlorophenyl)-1-methylquinoxalin-2(1H)-one (3n)



It was obtained as white solid having melting point 128-130 $^{\circ}$ C with 74% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.96 (d, J = 8.3 Hz, 1H), 7.87 – 7.81 (m, 2H), 7.78 (dd, J = 8.0, 1.5 Hz, 1H), 7.62 (dd, J = 8.3, 2.2 Hz, 1H), 7.56 – 7.51 (m, 2H), 7.51 – 7.48 (m, 1H), 7.40 (t, J = 7.6 Hz, 2H), 7.31 (td, J = 7.8, 7.3, 1.2 Hz, 1H), 7.23 (d, J = 8.4 Hz, 1H), 3.56 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 195.48, 155.08, 154.39, 141.42, 137.13, 135.46, 134.98, 133.50, 133.02, 132.82, 132.27, 130.93, 130.79, 130.37, 130.12, 129.29, 128.39, 123.93, 113.77,

29.43.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₅ClN₂O₂:375.0900; found:375.0889.

3-(2-(2-bromobenzoyl)-4-chlorophenyl)-1-methylquinoxalin-2(1H)-one (30)



It was obtained as yellow solid having melting point 152-154 $^{\rm o}{\rm C}$ with 64% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, J = 8.1 Hz, 1H), 7.73 (d, J = 8.2 Hz, 1H), 7.69 (dd, J = 7.6, 1.8 Hz, 1H), 7.64 (dd, J = 8.1, 2.2 Hz, 1H), 7.62 – 7.58 (m, 1H), 7.56 (d, J = 7.0 Hz, 1H), 7.45 (d, J = 2.2 Hz, 1H), 7.36 (t, J = 7.6 Hz, 2H), 7.32 – 7.25 (m, 2H), 3.62 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 194.41, 156.73, 154.58,

140.19, 138.49, 135.79, 135.50, 134.01, 133.74, 133.30, 132.44,

132.30, 132.22, 131.74, 130.76, 130.60, 130.49, 127.09, 123.94, 121.24, 113.82, 29.48. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₄BrClN₂O₂:453.0005; found:453.0003. -(4-chloro-2-(3,4-dimethoxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3p)



It was obtained as yellow solid having melting point 196-198 $^{\circ}$ C with 86% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, J = 8.1 Hz, 1H), 7.78 (d, J = 8.1 Hz, 1H), 7.62 – 7.57 (m, 2H), 7.53 (t, J = 7.8 Hz, 1H), 7.39 (d, J = 6.5 Hz, 2H), 7.36 – 7.28 (m, 1H), 7.24 (d, J = 8.4 Hz, 1H), 6.80 (d, J = 8.9 Hz, 1H), 3.88 (s, 3H), 3.86 (s, 3H), 3.58 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 194.18, 155.17, 154.32, 153.03, 148.88, 141.56, 135.41, 134.98, 133.47, 133.02, 132.14, 130.78, 130.64, 130.36, 130.08, 129.30, 125.47, 123.91, 113.80,

111.48, 109.91, 56.14, 56.04, 29.43. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₄H₁₉ClN₂O₄:435.1112; found:435.1116.

3-(4-chloro-2-(4-fluorobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3q)



It was obtained as yellow solid having melting point 168-170 $^{\rm o}{\rm C}$ with 81% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, J = 8.3 Hz, 1H), 7.87 (dd, J = 8.6, 5.6 Hz, 2H), 7.77 (d, J = 8.0 Hz, 1H), 7.62 (dd, J = 8.3, 2.2 Hz, 1H), 7.55 (t, J = 7.9 Hz, 1H), 7.50 (d, J = 2.1 Hz, 1H), 7.35 – 7.30 (m, 1H), 7.26 (d, J = 8.5 Hz, 1H), 7.08 (t, J = 8.6Hz, 2H), 3.59 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 193.97, 165.57 (d, J = 254.6 Hz), 132.70 (d, J = 9.3 Hz), 141.27, 135.51, 134.83, 133.48, 133.00, 130.93 (d, J = 5.3 Hz), 132.39, 130.95, 130.90, 130.63,

130.35, 128.96, 125.89, 124.01, 115.60 (d, J = 21.8 Hz), 113.89, 113.83, 29.46. ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -105.40 – -105.52 (m). HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₄ClFN₂O₂:393.0806; found:393.0802.

3-(4-chloro-2-(3,4-dimethylbenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3r)



It was obtained as yellow solid having melting point 106-108 °C with 81% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.90 (d, J = 8.2 Hz, 1H), 7.80 (d, J = 8.0 Hz, 1H), 7.60 (d, J = 8.2 Hz, 2H), 7.57 (d, J = 7.7 Hz, 1H), 7.54 (d, J = 2.2 Hz, 1H), 7.51 (d, J = 7.1 Hz, 1H), 7.32 (t, J = 7.6 Hz, 1H), 7.23 (d, J = 8.4 Hz, 1H), 7.16 (d, J = 7.8 Hz, 1H), 3.56 (s, 3H), 2.27 (s, 3H), 2.24 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 195 31, 155 53, 154 36

¹³C NMR (100 MHz, Chloroform-*d*) δ 195.31, 155.53, 154.36, 142.45, 141.58, 136.79, 135.28, 135.06, 134.80, 133.53, 133.07,

132.16, 131.20, 130.81, 130.68, 130.38, 129.62, 129.35, 128.13, 123.86, 113.72, 29.42, 20.15, 19.83.

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HRMS (ESI<sup>+</sup>): m/z [M+H]^+ calculated for C_{24}H_{19}ClN_2O_2:403.1213; found:403.1209.
3-(2-benzoyl-4-bromophenyl)-1-methylquinoxalin-2(1H)-one (3s)
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It was obtained as yellow solid having melting point 224-226 $^{\rm o}{\rm C}$ with 70% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.06 (d, J = 1.9 Hz, 1H), 7.82 (ddd, J = 9.5, 8.2, 1.5 Hz, 3H), 7.65 (dd, J = 8.2, 2.0 Hz, 1H), 7.56 – 7.51 (m, 1H), 7.49 (t, J = 7.4 Hz, 1H), 7.42 (d, J = 8.2 Hz, 1H), 7.39 (t, J = 7.5 Hz, 2H), 7.33 (td, J = 7.8, 7.3, 1.2 Hz, 1H), 7.25 – 7.22 (m, 1H), 3.56 (s, 3H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 195.99, 155.32, 154.34, 138.57, 138.50, 137.37, 133.80, 133.65, 133.10, 132.73, 132.13, 130.96, 130.92, 130.54, 130.20, 128.36, 125.74, 123.99, 113.82,

29.46.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₅BrN₂O₂:419.0395; found:419.0390.

3-(4-bromo-2-(2,5-dimethoxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)one (3t)



It was obtained as yellow solid having melting point 178-180 $^{\circ}$ C with 65% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.83 – 7.78 (m, 2H), 7.73 (dd, J = 8.2, 2.0 Hz, 1H), 7.63 (d, J = 8.1 Hz, 1H), 7.57 – 7.47 (m, 1H), 7.30 (d, J = 8.1 Hz, 1H), 7.20 (d, J = 7.3 Hz, 1H), 7.07 (d, J = 3.2 Hz, 1H), 6.79 (dd, J = 9.0, 3.2 Hz, 1H), 6.63 (d, J = 9.0 Hz, 1H), 3.67 (s, 3H), 3.57 (s, 3H), 3.55 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 193.98, 156.42, 154.42,

153.04, 152.71, 142.17, 135.40, 134.07, 133.59, 133.06, 132.43, 131.67, 130.64, 130.33, 127.78, 123.74, 123.54, 119.71, 115.19,

113.66, 113.05, 56.31, 55.82, 29.23. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₄H₁₉BrN₂O₄:479.0606; found:479.0597.

3-(4-bromo-2-(4-methylbenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3u)



It was obtained as yellow solid having melting point 218-220 $^{\rm o}{\rm C}$ with 68% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, J = 8.2 Hz, 1H), 7.79 (d, J = 8.0 Hz, 1H), 7.77 (d, J = 2.1 Hz, 1H), 7.74 (d, J = 8.0 Hz, 2H), 7.67 (d, J = 2.1 Hz, 1H), 7.53 (td, J = 7.9, 7.3, 1.5 Hz, 1H), 7.32 (t, J = 7.7 Hz, 1H), 7.25 – 7.20 (m, 3H), 3.57 (s, 3H), 2.38 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 195.05, 155.38, 154.35, 143.72, 141.81, 135.47, 134.47, 133.79, 133.58, 133.11, 132.42, 132.06, 130.75, 130.38, 129.15, 123.92, 123.51, 113.77, 29.46,

21.83.

3-(4-bromo-2-(2-fluorobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3v)



It was obtained as yellow solid having melting point 186-188 $^{\rm o}{\rm C}$ with 56% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.84 (d, *J* = 7.7 Hz, 1H), 7.81 (d, *J* = 6.0 Hz, 1H), 7.78 (dd, *J* = 8.2, 1.9 Hz, 1H), 7.72 (td, *J* = 7.4, 1.8 Hz, 1H), 7.68 (s, 1H), 7.55 (td, *J* = 7.9, 7.3, 1.6 Hz, 1H), 7.45 (qd, *J* = 7.1, 1.8 Hz, 1H), 7.37 – 7.31 (m, 1H), 7.28 – 7.22 (m, 1H), 7.18 (t, *J* = 8.1 Hz, 1H), 7.08 – 7.03 (m, 1H), 3.60 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 191.78, 161.31 (d, J = 257.7 Hz), 155.55, 154.39, 141.88, 135.11, 134.54, 134.31 (d, J =

8.7 Hz), 133.60, 133.11, 132.41, 132.00, 131.74, 130.82, 130.46, 125.80 (d, J = 11.1 Hz), 124.16 (d, J = 3.6 Hz), 123.85 (d, J = 22.5 Hz), 116.77 (d, J = 21.7 Hz), 113.78, 29.47. ¹⁹F NMR (377 MHz, Chloroform-*d*) δ -109.48 (dd, J = 10.9, 6.2 Hz). HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₄ClFN₂O₂:437.0301; found:433.0298.

3-(4-bromo-2-(4-methoxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3w)



It was obtained as white solid having melting point 194-196 $^{\circ}$ C with 69% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.86 (d, J = 8.3 Hz, 1H), 7.83 (d, J = 8.8 Hz, 1H), 7.78 (dd, J = 8.0, 1.5 Hz, 1H), 7.75 (dd, J = 8.2, 2.0 Hz, 1H), 7.68 (d, J = 2.1 Hz, 1H), 7.53 (td, J = 8.0, 7.3, 1.6 Hz, 1H), 7.34 – 7.28 (m, 1H), 7.24 (d, J = 8.4 Hz, 1H), 6.89 (d, J = 8.8 Hz, 2H), 3.83 (s, 3H), 3.57 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 194.05, 163.39, 155.34, 154.32, 141.91, 135.40, 133.62, 133.53, 133.08, 132.52, 132.40, 131.93, 130.74, 130.39, 129.84, 123.91, 123.48, 113.79, 113.70,

55.58, 29.45. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₃H₁₇BrN₂O₃:449.0501; found:449.0500.

3-(4-bromo-2-(4-hydroxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3x)



It was obtained as yellow solid having melting point 260-262 °C with 58% yield.

¹H NMR (400 MHz, DMSO- d_6) δ 10.39 (s, 1H), 7.90 (d, J = 8.3 Hz, 1H), 7.83 (d, J = 8.3 Hz, 2H), 7.68 (d, J = 7.9 Hz, 1H), 7.63 (d, J = 7.8 Hz, 2H), 7.57 (d, J = 8.5 Hz, 2H), 7.52 (d, J = 8.3 Hz, 2H), 7.37 (t, J = 7.6 Hz, 2H), 6.80 (s, 2H), 6.78 (s, 2H), 3.51 (s, 6H).

¹³C NMR (100 MHz, DMSO- d_6) δ 192.73, 161.98, 154.80, 153.56, 141.78, 135.12, 133.20, 133.09, 132.73, 132.32, 132.19, 130.95, 129.33, 127.80, 123.77, 122.50, 115.07, 114.84, 29.23.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₅BrN₂O₃:435.0344; found:435.0342.

3-(4-chloro-2-(3-methoxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (3y)



It was obtained as yellow solid having melting point 178-180 $^{\rm o}{\rm C}$ with 68% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.71 (s, 1H), 8.37 (dd, J = 8.2, 2.4 Hz, 1H), 8.16 (d, J = 7.7 Hz, 1H), 7.98 (d, J = 8.3 Hz, 1H), 7.82 (dd, J = 8.3, 2.0 Hz, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.66 – 7.59 (m, 2H), 7.56 (td, J = 7.9, 7.3, 1.5 Hz, 1H), 7.34 (t, J = 7.7 Hz, 1H), 7.26 (d, J = 8.3 Hz, 1H), 3.57 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 192.94, 154.31, 154.21, 148.33, 140.53, 138.71, 135.66, 135.12, 134.55, 133.47, 132.98, 132.91, 131.36, 131.18, 130.38, 129.67, 127.09, 124.83, 124.23,

123.96, 113.92, 29.55. HRMS (ESI⁺): m/z [M+H]⁺ calculated for $C_{22}H_{14}BrN_3O_4$:464.0246; found:464.0246.

3-(2-benzoylphenyl)-6,7-dichloro-1-methylquinoxalin-2(1H)-one (3z)



It was obtained as yellow solid having melting point 164-166 $^{\circ}$ C with 80% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.89 (s, 1H), 7.87 (d, J = 7.7 Hz, 1H), 7.84 (s, 1H), 7.82 (s, 1H), 7.66 (t, J = 7.4 Hz, 1H), 7.58 (d, J = 6.0 Hz, 1H), 7.55 (d, J = 7.6 Hz, 1H), 7.51 (d, J = 7.7 Hz, 1H), 7.41 (t, J = 7.6 Hz, 2H), 7.33 (s, 1H), 3.52 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 196.82, 158.31, 154.08, 139.77, 137.65, 136.35, 134.50, 133.03, 132.66, 132.29, 131.31, 131.07, 130.81, 130.26, 129.77, 129.58, 128.33, 127.57, 115.26, 29.65.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₄Cl₂N₂O₂:409.0511; found:409.0511.

3-(2-benzoylphenyl)-1,6,7-trimethylquinoxalin-2(1H)-one (3aa)



It was obtained as yellow solid having melting point 218-220 °C with 47% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, J = 7.7 Hz, 1H), 7.82 (d, J = 6.9 Hz, 2H), 7.63 (td, J = 7.5, 1.5 Hz, 1H), 7.57 (s, 1H), 7.55 (s, 1H), 7.51 (d, J = 7.4 Hz, 1H), 7.49 – 7.43 (m, 1H), 7.36 (t, J = 7.6 Hz, 2H), 6.99 (s, 1H), 3.53 (s, 3H), 2.39 (s, 3H), 2.32 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 196.94, 155.18, 154.60, 140.43, 139.70, 137.94, 137.02, 132.64, 132.32, 131.64, 131.60, 131.02, 130.73, 130.37, 130.13, 129.45,

128.96, 128.13, 114.24, 29.25, 20.69, 19.27.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for $C_{24}H_{20}N_2O_2$:369.1598; found:369.1597.

1,6,7-trimethyl-3-(2-(4-methylbenzoyl)phenyl)quinoxalin-2(1H)-one (3ab)



It was obtained as yellow solid having melting point 216-218 $^{\rm o}{\rm C}$ with 37% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (d, J = 7.7 Hz, 1H), 7.74 (d, J = 8.2 Hz, 2H), 7.62 (td, J = 7.5, 1.6 Hz, 1H), 7.58 (s, 1H), 7.54 (dd, J = 7.7, 1.6 Hz, 1H), 7.49 (td, J = 7.4, 1.3 Hz, 1H), 7.18 (d, J = 8.0 Hz, 2H), 7.00 (s, 1H), 3.54 (s, 3H), 2.39 (s, 3H), 2.36 (s, 3H), 2.33 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 196.69, 155.42, 154.63, 143.11, 140.36, 139.92, 137.05, 135.25, 132.64, 131.72, 131.68,

130.92, 130.75, 130.42, 129.41, 128.93, 128.86, 114.26, 29.32, 21.76, 20.72, 19.30. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₅H₂₂N₂O₂:383.1754; found:383.1753.

6,7-dichloro-1-methyl-3-(2-(4-methylbenzoyl)phenyl)quinoxalin-2(1H)-one (3ac)



It was obtained as yellow solid having melting point 186-188 $^{\rm o}{\rm C}$ with 54% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.91 (s, 1H), 7.85 (d, J = 7.6 Hz, 1H), 7.75 (d, J = 8.2 Hz, 2H), 7.64 (td, J = 7.3, 1.8 Hz, 1H), 7.58 – 7.50 (m, 2H), 7.34 (s, 1H), 7.23 (d, J = 7.8 Hz, 2H), 3.52 (s, 3H), 2.40 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 196.51, 158.47, 154.03, 143.52, 139.91, 136.31, 134.85, 134.39, 133.03, 132.29, 131.19, 131.04, 130.77, 130.49, 129.67, 129.46, 129.07, 127.49, 115.25,

29.67, 21.81.

HRMS (ESI⁺): $m/z [M+H]^+$ calculated for $C_{23}H_{16}Cl_2N_2O_2$:423.0662; found:423.0656.

3-(2-(3-methoxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (5a)



It was obtained as yellow solid having melting point 144-146 °C with 75% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, J = 7.7 Hz, 1H), 7.83 (dd, J = 8.0, 1.5 Hz, 1H), 7.65 (td, J = 7.5, 1.5 Hz, 1H), 7.61 (d, J = 7.6 Hz, 1H), 7.54 (d, J = 7.5 Hz, 1H), 7.51 (d, J = 7.1 Hz, 1H), 7.38 (d, J = 7.5 Hz, 1H), 7.37 (s, 1H), 7.32 (t, J = 8.3 Hz, 1H), 7.27 (d, J = 7.9 Hz, 1H), 7.24 (d, J = 7.1 Hz, 1H), 7.01 (dd, J = 8.8, 2.2 Hz, 1H), 3.77 (s, 3H), 3.58 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 195.80, 158.39, 158.22, 154.72, 140.09, 137.12, 133.64, 133.21, 132.72, 131.79, 131.73,

130.31, 130.26, 130.18, 129.16, 127.87, 123.61, 119.98, 113.63, 111.36, 55.72, 29.30. HRMS (ESI⁺): m/z [M+H]⁺ calculated for $C_{23}H_{18}N_2O_3$:371.1396; found:371.1389.

3-(2-(2-methoxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (5b)



It was obtained as white solid having melting point 154-156 $^{\circ}$ C with 72% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.87 (dd, *J* = 8.0, 1.6 Hz, 1H), 7.72 (d, *J* = 7.0 Hz, 1H), 7.62 (d, *J* = 7.4 Hz, 2H), 7.56 (dd, *J* = 7.7, 1.9 Hz, 1H), 7.52 (d, *J* = 1.9 Hz, 1H), 7.49 (d, *J* = 8.9 Hz, 1H), 7.33 (d, *J* = 7.3 Hz, 1H), 7.30 (d, *J* = 5.9 Hz, 1H), 7.22 (d, *J* = 8.4 Hz, 1H), 6.89 (t, *J* = 7.5 Hz, 1H), 6.79 (d, *J* = 8.4 Hz, 1H), 3.68 (s, 3H), 3.58 (s, 3H).

 $\int_{-13C}^{13C} NMR (100 \text{ MHz, Chloroform-}d) \delta 195.80, 158.39, 158.22, 154.72, 140.09, 137.12, 133.64, 133.21, 132.72, 131.79, 131.73, 140.122,$

130.31, 130.26, 130.18, 129.16, 127.87, 123.61, 119.98, 113.63, 111.36, 55.72, 29.30. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₃H₁₈N₂O₃:371.1396; found:371.1392.

3-(2-(4-chlorobenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (5c)



It was obtained as yellow solid having melting point 146-148 $^{\rm o}{\rm C}$ with 65% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, J = 7.5 Hz, 1H), 7.83 (dd, J = 8.0, 1.5 Hz, 1H), 7.81 (d, J = 2.0 Hz, 1H), 7.79 (d, J= 1.8 Hz, 1H), 7.68 – 7.64 (m, 1H), 7.56 – 7.52 (m, 2H), 7.52 (s, 1H), 7.38 (d, J = 2.0 Hz, 1H), 7.37 (d, J = 1.9 Hz, 1H), 7.33 (td, J= 8.1, 7.7, 1.2 Hz, 1H), 7.26 (d, J = 8.5 Hz, 1H), 3.58 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 195.71, 156.35, 154.52, 139.40, 138.89, 136.70, 136.10, 133.56, 133.17, 131.63, 131.36, 130.95, 130.64, 130.37, 129.25, 129.17, 128.60, 123.90, 113.81,

29.44.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₂H₁₅ClN₂O₂:375.0900; found:375.0892.

3-(2-(4-methoxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (5d)



It was obtained as white solid having melting point 188-190 °C with 65% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.93 (d, J = 8.3 Hz, 1H), 7.84 (s, 1H), 7.82 (s, 1H), 7.78 (dd, J = 8.0, 1.5 Hz, 1H), 7.59 (dd, J = 8.3, 2.1 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.31 (td, J = 7.8, 1.2 Hz, 1H), 7.24 (d, J = 8.5 Hz, 1H), 6.91 (s, 1H), 6.88 (s, 1H), 3.83 (s, 3H), 3.57 (s, 3H).

¹³C NMR (100 MHz Chloroform-*d*) δ 194.18, 163.41, 155.30, 154.38, 141.78, 135.32, 134.96, 133.56, 133.10, 132.53, 132.25, 130.73, 130.64, 130.41, 129.89, 129.14, 123.91, 113.79, 113.71,

55.59, 29.46. HRMS (ESI⁺): m/z [M+H]⁺ calculated for $C_{23}H_{17}ClN_2O_3$:405.1006; found:405.1003.

3-(4-chloro-2-(3-methoxybenzoyl)phenyl)-1-methylquinoxalin-2(1H)-one (5e)



It was obtained as yellow solid having melting point 150-152 $^{\rm o}{\rm C}$ with 59% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.95 (d, J = 8.3 Hz, 1H), 7.78 (dd, J = 8.0, 1.6 Hz, 1H), 7.61 (dd, J = 8.3, 2.2 Hz, 1H), 7.57 (d, J = 2.2 Hz, 1H), 7.53 (td, J = 7.9, 7.2, 1.5 Hz, 1H), 7.37 – 7.31 (m, 3H), 7.30 – 7.27 (m, 1H), 7.25 – 7.22 (m, 1H), 7.02 (dd, J = 7.5, 2.1 Hz, 1H), 3.78 (s, 3H), 3.58 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 195.26, 159.57, 155.07, 154.38, 141.39, 138.56, 135.53, 135.02, 133.52, 133.02, 132.21,

 $\begin{array}{c} \hline \\ 130.94, 130.82, 130.39, 129.41, 129.37, 123.93, 123.06, 119.66, \\ 113.79, 113.63, 55.51, 29.43. \\ HRMS (ESI^+): m/z \ [M+H]^+ \ calculated \ for \ C_{23}H_{17}ClN_2O_3:405.1006; \ found:405.1003. \end{array}$

3-(2-(4-methoxybenzoyl)-4-methylphenyl)-1-methylquinoxalin-2(1H)-one (5f)



It was obtained as white solid having melting point 162-164 $^{\circ}$ C with 82% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.85 (d, J = 7.9 Hz, 1H), 7.83 (s, 1H), 7.81 (s, 1H), 7.78 (dd, J = 8.0, 1.5 Hz, 1H), 7.49 (td, J = 8.0, 7.3, 1.6 Hz, 1H), 7.43 (d, J = 9.8 Hz, 1H), 7.37 (d, J = 1.8 Hz, 1H), 7.31 – 7.26 (m, 1H), 7.21 (d, J = 8.4 Hz, 1H), 6.87 (s, 1H), 6.85 (s, 1H), 3.81 (s, 3H), 3.56 (s, 3H), 2.44 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 195.84, 163.03, 156.50, 154.59, 140.17, 139.42, 133.94, 133.51, 133.18, 132.43, 131.34, 130.75, 130.69, 130.26, 130.22, 129.92, 123.65, 113.64, 113.47,

55.51, 29.36, 21.51. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₄H₂₀N₂O₃:385.1552; found:385.1543.

1-methyl-3-(4-methyl-2-(3-nitrobenzoyl)phenyl)quinoxalin-2(1H)-one (5g)



It was obtained as white solid having melting point 184-186 °C with 67% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.70 (s, 1H), 8.33 (d, *J* = 8.3 Hz, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 7.97 (d, *J* = 7.9 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.58 (t, *J* = 7.9 Hz, 1H), 7.55 – 7.49 (m, 2H), 7.33 (d, *J* = 8.1 Hz, 1H), 7.30 (s, 1H), 7.24 (d, *J* = 8.4 Hz, 1H), 3.57 (s, 3H), 2.46 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 194.63, 155.43, 154.59, 148.28, 140.03, 139.59, 138.85, 135.62, 133.76, 133.44, 133.08, 132.29, 131.27, 130.66, 130.26, 129.43, 129.40, 126.65, 124.86,

123.99, 113.79, 29.47, 21.54.

HRMS (ESI⁺): $m/z [M+H]^+$ calculated for $C_{23}H_{17}N_3O_4$:400.1297; found:400.1291

3-(2-benzoyl-4-methylphenyl)-1-methylquinoxalin-2(1H)-one (7a)



It was obtained as yellow solid having melting point 144-146 $^{\rm o}{\rm C}$ with 80% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.87 (d, J = 7.8 Hz, 1H), 7.84 (s, 1H), 7.82 (s, 1H), 7.79 (dd, J = 8.0, 1.5 Hz, 1H), 7.53 – 7.48 (m, 1H), 7.46 (s, 1H), 7.45 (s, 1H), 7.37 (t, J = 7.7 Hz, 3H), 7.30 (t, J = 7.0 Hz, 1H), 7.22 (d, J = 8.4 Hz, 1H), 3.57 (s, 3H), 2.44 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 197.15, 156.36, 154.67,

¹³C NMR (100 MHz, Chloroform-*d*) δ 197.15, 156.36, 154.67, 139.91, 139.60, 138.10, 134.06, 133.53, 133.19, 132.31, 131.65, 130.76, 130.30, 130.16, 130.10, 128.17, 123.70, 113.64, 29.35,

21.50.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₃H₁₈N₂O₂:355.1447; found:355.1426.

3-(2-(1H-indole-3-carbonyl)phenyl)-1-methylquinoxalin-2(1H)-one (8)



It was obtained as white solid having melting point 266-268 $^{\circ}$ C with 64% yield.

¹H NMR (400 MHz, DMSO- d_6) δ 11.99 (s, 1H), 8.00 (d, J = 7.9 Hz, 1H), 7.90 (s, 1H), 7.79 – 7.72 (m, 2H), 7.68 (t, J = 7.3 Hz, 1H), 7.62 (q, J = 7.0 Hz, 2H), 7.49 (d, J = 11.2 Hz, 2H), 7.36 (t, J = 7.7 Hz, 1H), 7.21 (t, J = 7.6 Hz, 1H), 7.13 (t, J = 7.6 Hz, 1H), 3.46 (s, 3H).

¹³C NMR (101 MHz, DMSO- d_6) δ 189.93, 157.68, 153.67, 141.20, 136.61, 136.37, 135.55, 133.29, 132.43, 130.57, 130.36, 130.08, 129.31, 129.11, 128.74, 126.28, 123.52, 122.92, 121.66, 20.22

121.39, 115.44, 114.70, 112.20, 29.03. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₄H₁₇N₃O₂:380.1399; found:380.1391.

Ethyl 2-(3-(2-benzoylphenyl)-2-oxoquinoxalin-1(2H)-yl)acetate (9)



It was obtained as yellow solid having melting point 160-162 $^{\circ}$ C with 77% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, J = 7.6 Hz, 1H), 7.84 (d, J = 7.3 Hz, 3H), 7.66 (t, J = 8.3 Hz, 1H), 7.58 – 7.52 (m, 2H), 7.48 (td, J = 6.8, 5.2, 3.2 Hz, 2H), 7.39 (t, J = 7.6 Hz, 2H), 7.32 (t, J = 7.6 Hz, 1H), 7.02 (d, J = 8.4 Hz, 1H), 4.90 (s, 2H), 4.17 (q, J = 7.1 Hz, 2H), 1.20 (t, J = 7.1 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 196.88, 167.12, 156.49, 154.23, 139.67, 137.69, 136.51, 133.25, 132.69, 132.52, 131.23,

130.99, 130.71, 130.64, 130.25, 130.21, 129.60, 129.31, 128.26, 124.08, 113.17, 62.07, 43.80, 14.16.

HRMS (ESI⁺): m/z [M+Na]⁺ calculated for C₂₅H₂₀N₂O₄:435.1315; found:435.1314.

3-(2-benzoylphenyl)-1-(2-oxo-2-phenylethyl)quinoxalin-2(1H)-one (10)



It was obtained as yellow solid having melting point 150-152 $^{\rm o}{\rm C}$ with 69% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.98 (m, J = 7.8 Hz, 3H), 7.84 (d, J = 7.7 Hz, 3H), 7.68 – 7.62 (m, 1H), 7.59 (d, J = 7.4 Hz, 1H), 7.56 – 7.50 (m, 2H), 7.47 (m, J = 7.4 Hz, 3H), 7.38 (t, J = 7.5 Hz, 3H), 7.28 (m, J = 9.3 Hz, 1H), 6.87 (d, J = 8.2 Hz, 1H), 5.59 (s, 2H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 197.01, 191.15, 156.31, 154.38, 139.65, 137.77, 136.62, 134.60, 134.29, 133.36, 132.97,

132.50, 131.23, 131.11, 130.65, 130.52, 130.23, 129.58, 129.23, 129.06, 128.26, 123.91, 113.61, 48.74.

HRMS (ESI⁺): m/z [M+Na]⁺ calculated for $C_{29}H_{20}N_2O_3$:467.1366; found:467.1358.

2,2,6,6-tetramethylpiperidin-1-yl benzoate (11a)



It was obtained as white solid having melting point 88-90 °C with 30% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.09 (d, J = 7.2 Hz, 2H), 7.58 (t, J = 7.4 Hz, 1H), 7.47 (t, J = 7.6 Hz, 2H), 1.83 – 1.74 (m, 2H), 1.70 (d, J = 13.0 Hz, 1H), 1.59 (d, J = 12.5 Hz, 2H), 1.47 (d, J = 12.7 Hz, 1H), 1.28 (s, 6H), 1.13 (s, 6H). ¹³C NMR (101 MHz, Chloroform-*d*) δ 166.30, 132.76, 129.59, 129.46, 128.35, 60.29, 38.93, 31.85, 20.73, 16.88. HRMS (FSI[±]): m/z [M±H][±] calculated for C₁-H₂NO₂:262 1807:

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₆H₂₃NO₂:262.1807; found:262.1791.

3-(2-([1,1'-biphenyl]-4-carbonyl)phenyl)-1-methylquinoxalin-2(1H)-one (18)



It was obtained as White solid having melting point 198-200 °C with 55% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.94 (t, *J* = 7.6 Hz, 3H), 7.86 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.67 (td, *J* = 7.5, 1.4 Hz, 1H), 7.65 – 7.60 (m, 3H), 7.59 – 7.55 (m, 2H), 7.55 – 7.49 (m, 1H), 7.45 (t, *J* = 7.4 Hz, 2H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.36 – 7.31 (m, 1H), 7.23 (d, *J* = 8.5 Hz, 1H), 3.57 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 196.48, 156.78, 154.59, 145.17, 140.20, 139.80, 136.88, 136.53, 133.62, 133.25, 131.22, 130.84, 130.50, 130.41, 129.51, 129.20, 129.01, 128.19, 127.38, 126.93, 123.80, 113.75, 29.41.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for $C_{28}H_{20}N_2O_2$:417.1598; found: 417.1611.

3-(3-benzoyl-[1,1'-biphenyl]-4-yl)-1-methylquinoxalin-2(1H)-one (19)



It was obtained as yellow solid having melting point 206-208 $^{\rm o}{\rm C}$ with 60% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.07 (d, *J* = 8.0 Hz, 1H), 7.92 – 7.87 (m, 3H), 7.84 – 7.79 (m, 2H), 7.63 (d, *J* = 7.0 Hz, 2H), 7.56 – 7.48 (m, 2H), 7.48 – 7.43 (m, 2H), 7.42 – 7.36 (m, 3H), 7.33 (td, *J* = 7.6, 1.2 Hz, 1H), 7.25 (d, *J* = 9.4 Hz, 1H), 3.59 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 196.87, 156.10, 154.62, 142.24, 140.41, 139.89, 137.78, 135.59, 133.55, 133.20, 132.55,

131.38, 130.52, 130.36, 130.21, 129.53, 129.09, 128.31, 128.18, 128.16, 127.40, 123.82, 113.73, 29.42.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₈H₂₀N₂O₂:417.1598; found: 417.1611.

Important Crystal Data of Compound 3a

CCDC deposition number	2162471
Empirical Formula	$C_{22}H_{16}N_2O_2$
Formula weight	340.37
Temperature (K)	298
Crystal System	orthorhombic
Space Group	P n a 21
Unit Cell Dimension	a/Å = 24.354(3)
	b/Å = 8.7486(14)
	c/Å = 16.091(2)
	$\alpha/^{\circ} = 90$
	$\beta^{\circ} = 90$
	$\gamma/^{\circ} = 90$
Volume Å ³	3428.4(8)
Z	8
Density Calculated g/cm ³	1.319
Absorption coefficient (μ) mm ⁻¹	0.086
F (000)	1424.0
Radiation	MoK α ($\lambda = 0.71073$)
20 range for data collection/°	6.376 to 52.044
Index ranges	$-28 \le h \le 28$
	$-10 \le k \le 10$
	$-19 \le 1 \le 19$
Reflection Collected	40622
Independent Reflections	$6041 [R_{int} = 0.12, R_{sigma} = 0.1518]$
Data/Restraints/parameter s	6041/1/469
Goodness of fit on F ²	0.882
Final R indices	$R_1 = 0.0780, wR_2 = 0.1990$
[I>=2sigma(I)]	
R indices (all data)	$R_1 = 0.2110, wR_2 = 0.1990$
Largest difference peak	0.214/-0.175
and hole	
[e Å ⁻³]	

Copies of ¹H NMR, ¹³C NMR and ¹⁹F NMR Spectra



Figure 2: ¹³C NMR spectrum of compound **3a** (100 MHz, CDCl₃).



Figure 4: ¹³C NMR spectrum of compound **3b** (100 MHz, DMSO-d₆).



Figure 6: ¹³C NMR spectrum of compound **3c** (100 MHz, DMSO-d₆).



Figure 8: ¹³C NMR spectrum of compound 3d (100 MHz, CDCl₃).



Figure 10: ¹³C NMR spectrum of compound 3e (100 MHz, CDCl₃).



Figure 11: ¹H NMR spectrum of compound **3f** (400 MHz, DMSO-d₆).



Figure 12: ¹³C NMR spectrum of compound **3f** (100 MHz, DMSO-d₆).





Figure 14: ¹³C NMR spectrum of compound **3g** (100 MHz, CDCl₃).



Figure 15: ¹⁹F NMR spectrum of compound 3g (377 MHz, CDCl₃).





Figure 17: ¹³C NMR spectrum of compound **3h** (100 MHz, DMSO-d₆).



Figure 18: ¹H NMR spectrum of compound 3i (400 MHz, CDCl₃).



Figure 19: ¹³C NMR spectrum of compound 3i (100 MHz, CDCl₃).



Figure 20: ¹⁹F NMR spectrum of compound 3i (377 MHz, CDCl₃).



Figure 22: ¹³C NMR spectrum of compound 3j (100 MHz, CDCl₃).



Figure 23: ¹⁹F NMR spectrum of compound 3j (377 MHz, CDCl₃).



Figure 24: ¹H NMR spectrum of compound 3k (400 MHz, CDCl₃).



Figure 25: ¹³C NMR spectrum of compound 3k (100 MHz, CDCl₃).



Figure 26: ¹⁹F NMR spectrum of compound 3k (377 MHz, CDCl₃).



Figure 28: ¹³C NMR spectrum of compound 3l (100 MHz, CDCl₃).



Figure 29: ¹⁹F NMR spectrum of compound 3I (377 MHz, CDCl₃).



Figure 31: ¹³C NMR spectrum of compound 3m (100 MHz, CDCl₃).



Figure 32: ¹⁹F NMR spectrum of compound **3m** (377 MHz, CDCl₃).



Figure 34: ¹³C NMR spectrum of compound 3n (100 MHz, CDCl₃).



Figure 36: ¹³C NMR spectrum of compound **30** (100 MHz, CDCl₃).



Figure 38: ¹³C NMR spectrum of compound **3p** (100 MHz, CDCl₃).



f1 (ppm)

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Figure 40: ¹³C NMR spectrum of compound 3q (100 MHz, CDCl₃).



Figure 41: ¹⁹F NMR spectrum of compound 3q (377 MHz, CDCl₃).



Figure 43: ¹³C NMR spectrum of compound 3r (100 MHz, CDCl₃).



Figure 45: ¹³C NMR spectrum of compound 3s (100 MHz, CDCl₃).



Figure 47: ¹³C NMR spectrum of compound **3t** (100 MHz, CDCl₃).





Figure 49: ¹³C NMR spectrum of compound **3u** (100 MHz, CDCl₃).



Figure 51: ¹³C NMR spectrum of compound **3v** (100 MHz, CDCl₃).



Figure 52: ¹⁹F NMR spectrum of compound **3v** (377 MHz, CDCl₃).







Figure 55: ¹H NMR spectrum of compound **3x** (400 MHz, DMSO-d₆).



Figure 56: ¹³C NMR spectrum of compound 3x (100 MHz, DMSO-d₆).



Figure 58: ¹³C NMR spectrum of compound **3y** (100 MHz, CDCl₃).



Figure 60: ¹³C NMR spectrum of compound **3z** (100 MHz, CDCl₃).







Figure 62: ¹³C NMR spectrum of compound 3aa (100 MHz, CDCl₃).



Figure 63: ¹H NMR spectrum of compound 3ab (400 MHz, CDCl₃).



Figure 64: ¹³C NMR spectrum of compound **3ab** (100 MHz, CDCl₃).



Figure 66: ¹³C NMR spectrum of compound **3ac** (100 MHz, CDCl₃).



Figure 68: ¹³C NMR spectrum of compound 5a (100 MHz, CDCl₃).



Figure 70: ¹³C NMR spectrum of compound 5b (100 MHz, CDCl₃).



Figure 72: ¹³C NMR spectrum of compound 5c (100 MHz, CDCl₃).



Figure 74: ¹³C NMR spectrum of compound 5d (100 MHz, CDCl₃).



Figure 76: ¹³C NMR spectrum of compound 5e (100 MHz, CDCl₃).



Figure 78: ¹³C NMR spectrum of compound 5f (100 MHz, CDCl₃).



Figure 80: ¹³C NMR spectrum of compound 5g (100 MHz, CDCl₃).



Figure 82: ¹³C NMR spectrum of compound 7a (100 MHz, CDCl₃).



Figure 83: ¹H NMR spectrum of compound 8 (400 MHz, DMSO-d₆).



Figure 84: ¹³C NMR spectrum of compound 8 (100 MHz, DMSO-d₆).



Figure 86: ¹³C NMR spectrum of compound 9 (100 MHz, CDCl₃).



Figure 88: ¹³C NMR spectrum of compound 10 (100 MHz, CDCl₃).



Figure 90: ¹³C NMR spectrum of compound 11a (100 MHz, CDCl₃).





Figure 92: ¹³C NMR spectrum of compound 18 (100 MHz, CDCl₃)





Figure 94: ¹³C NMR spectrum of compound 19 (100 MHz, CDCl₃).