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Supporting Information

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General Consideration

All microwave assisted experiments were performed in a closed vial reaction vial applying a dedicated CEM-Discover monomode microwave apparatus operating at a frequency of 2.45 GHz with continuous irradiation power from 0 to 300 W (CEM Corporation, P.O. Box 200, Matthews, NC 28106). Reactions were monitored by thin layer chromatography (TLC) on Merck gel 60 F₂₅₄ plates. The ¹H and ¹³C NMR spectra (CDCl₃ and DMSO-d₆) were recorded on a JEOL ECX-400P NMR and Bruker NMR 400 MHz and 100 MHz, respectively using TMS as internal standard. The high-resolution mass spectral data were recorded on a 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. 3-phenyl-2*H*-benzo[*b*][1,4]oxazin-2-one derivatives were well known compounds and were prepared according to literature¹⁻³.

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



An oven dried 10 mL screw capped reaction vial with a small stirring bar was charged with a mixture of 3-phenyl-2*H*-benzo[*b*][1,4]oxazin-2-one 1 (1 mmol), NBS 2 (1.2 mmol), Pd(OAc)₂ (5 mol%), PTSA (0.25 mmol) and DCE (2mL). The resulting mixture was irradiated under microwave (150W) at 100 °C for 15 mins. 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 (9:1) as eluent to afford the pure targeted products.

General procedure for the synthesis of compounds 4(a-i)



An oven dried 10 mL screw capped reaction vial with a small stirring bar was charged with a mixture of 3-phenyl-2*H*-benzo[*b*][1,4]oxazin-2-one **1** (1 mmol), NIS **2** (1.25 mmol), Pd(OAc)₂ (5 mol%), PTSA (0.25 mmol) and DCE (2mL). The resulting mixture was irradiated under microwave (150W) at 80 °C for 5 mins. 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 (9:1) as eluent to afford the pure targeted products.

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



An oven dried 10 mL screw capped reaction vial with a small stirring bar was charged with a mixture of 3-phenyl-2*H*-benzo[*b*][1,4]oxazin-2-one 1 (1 mmol), NCS 2 (1.5 mmol), Pd(OAc)₂ (5 mol%), PTSA (0.5 mmol) and DCE (2mL). The resulting mixture was irradiated under microwave (150W) at 120 °C for 30 mins. 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 (9:1) as eluent to afford the pure targeted products.

General procedure for the synthesis of compounds 8-12



An oven dried 10 mL screw capped reaction vial with a small stirring bar was charged with a mixture of 3-(2-bromophenyl)-2*H*-benzo[b][1,4]oxazin-2-one (1 mmol), Boronic acids (2.0 mmol), Pd(PPh₃)₂ (5 mol%), Cs₂CO₃ (1.5 mmol) and Toluene (2mL). The resulting mixture was irradiated under microwave (150W) at 110 °C for 30 mins. 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 ($3 \times 10 \text{ mL}$). 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 (9:1) as eluent to afford the pure targeted products.

References

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Analytical Data

3-(2-bromophenyl)-2*H*-benzo[b][1,4]oxazin-2-one (3a)



It was obtained as **White solid** having melting point **130-132** °C with **84%** yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.86 (dd, J = 7.9, 1.6 Hz, 1H), 7.70 (dd, J = 8.1, 0.9 Hz, 1H), 7.61-7.56 (m, 1H), 7.53 (dd, J = 7.6, 1.8 Hz, 1H), 7.49-7.42 (m, 2H), 7.40 (d, J = 1.4 Hz, 1H), 7.38-7.35 (m, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 154.34, 151.76, 147.01, 135.91, 133.26, 132.09, 131.57, 131.28, 130.75, 129.83, 127.70, 125.90, 122.36, 116.74. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₈BrNO₂: 301.9811; found: 301.9811.

3-(2-bromophenyl)-6-methyl-2*H*-benzo[b][1,4]oxazin-2-one (3b)



It was obtained as White solid having melting point 128-130 °C with 80% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.69 (d, J = 9.2 Hz, 1H), 7.64 (s, 1H), 7.52 (dd, J = 7.6, 1.8 Hz, 1H), 7.45 (td, J = 7.5, 1.3 Hz, 1H), 7.40-7.33 (m, 2H), 7.27 (d, J = 8.4 Hz, 1H), 2.46 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 154.17, 151.98, 144.95, 136.05, 135.87, 133.23, 132.99, 131.45, 131.02, 130.75, 129.64, 127.64, 122.39, 116.28, 20.94. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₅H₁₀BrNO₂: 315.9968; found: 315.9972.

3-(2-bromophenyl)-7-methyl-2*H*-benzo[b][1,4]oxazin-2-one (3c)



It was obtained as White solid having melting point 133-135 °C with 82% yield.

¹**H** NMR (400 MHz, Chloroform-*d*) δ 7.72 (d, J = 8.1 Hz, 1H), 7.69 (d, J = 8.0 Hz, 1H), 7.52 (d, J = 7.6 Hz, 1H), 7.45 (t, J = 8.1 Hz, 1H), 7.36 (t, J = 8.6 Hz, 1H), 7.23 (d, J = 6.3 Hz, 1H), 7.19 (s, 1H), 2.51 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 153.11, 152.05, 147.02, 143.63, 136.14, 133.28, 131.44, 130.82, 129.43, 127.69, 127.02, 122.52, 116.83, 21.97. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₅H₁₀BrNO₂: 315.9968; found: 315.9978.

3-(2-bromophenyl)-6-chloro-2*H*-benzo[b][1,4]oxazin-2-one (3d)



It was obtained as White solid having melting point 115-117 °C with 76% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.84 (d, J = 2.5 Hz, 1H), 7.70 (dd, J = 8.0, 1.2 Hz, 1H), 7.54 (d, J = 7.4 Hz, 1H), 7.51 (dd, J = 6.0, 2.2 Hz, 1H), 7.47 (td, J = 7.5, 1.2 Hz, 1H), 7.41-7.35 (m, 1H), 7.33 (d, J = 8.8 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 155.43, 151.17, 145.59, 135.54, 133.34, 131.94, 131.80, 131.77, 131.03, 130.75, 129.27, 127.71, 122.28, 117.87. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇BrClNO₂: 335.9421; found: 335.9420.

3-(2-bromophenyl)-7-chloro-2*H*-benzo[b][1,4]oxazin-2-one (3e)



It was obtained as White solid having melting point 130-132 °C with 71% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.77 (d, J = 9.2 Hz, 1H), 7.69 (d, J = 7.9 Hz, 1H), 7.52 (d, J = 7.6 Hz, 1H), 7.46 (t, J = 7.5 Hz, 1H), 7.38 (d, J = 5.8 Hz, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 154.15, 150.99, 147.36, 137.90, 135.65, 133.32, 131.72, 130.76, 130.61, 129.96, 127.70,

126.45, 122.34, 117.04.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇BrClNO₂: 335.9421; found: 335.9424.

3-(2-bromophenyl)-6-fluoro-2*H*-benzo[b][1,4]oxazin-2-one (3f)



It was obtained as White solid having melting point 110-112 °C with 61% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.70 (d, J = 8.0 Hz, 1H), 7.58-7.52 (m, 1H), 7.51 (d, J = 1.9 Hz, 1H), 7.49-7.44 (m, 1H), 7.42-7.34 (m, 2H), 7.31 (td, J = 9.2, 8.5, 2.8 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 160.80, 158.36, 155.48, 151.39, 143.38, 135.61, 133.34, 131.78, 131.62, 130.74, 127.71, 122.27, 119.54, 119.29, 117.84, 117.75, 115.67, 115.43.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇BrFNO₂: 319.9717; found: 319.9713.



3-(2-bromo-4-chlorophenyl)-2*H*benzo[b][1,4]oxazin-2-one (3g)

It was obtained as White solid having melting point 138-140 °C with 77% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.85 (dd, J = 7.9, 1.6 Hz, 1H), 7.72 (d, J = 1.9 Hz, 1H), 7.60 (ddd, J = 8.2, 7.4, 1.6 Hz, 1H), 7.49 (d, J = 8.2 Hz, 1H), 7.46 (d, J = 1.9 Hz, 1H), 7.44-7.41 (m, 1H), 7.39 (dd, J = 8.2, 1.3 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 153.32, 151.66, 147.02, 136.98, 134.38, 133.11, 132.36, 131.70, 131.25, 129.91, 128.07, 126.03, 123.02, 116.81. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇BrClNO₂: 335.9421; found: 335.9438.



3-(2-bromo-6-methoxyphenyl)-2Hbenzo[b][1,4]oxazin-2-one (3h)

It was obtained as White solid having melting point 140-142 °C with 81% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.87 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.58 (ddd, *J* = 8.2, 7.5, 1.6 Hz, 1H), 7.46-7.40 (m, 1H), 7.38 (dd, *J* = 8.4, 1.4 Hz, 1H), 7.34-7.27 (m, 2H), 6.96 (dd, *J* = 7.6, 1.7 Hz, 1H), 3.79 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 158.98, 153.17, 151.79, 146.92, 131.92, 131.88, 131.41, 129.82, 125.73, 125.08, 123.01, 116.76, 110.32, 56.33. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₅H₁₀BrNO₃: 331.9917; found: 331.9882.



3-(2-bromo-6-methoxyphenyl)-2Hbenzo[b][1,4]oxazin-2-one (3i)

It was obtained as White solid having melting point 128-130 °C with 65% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.86 (dd, J = 8.0, 1.6 Hz, 1H), 7.61-7.53 (m, 2H), 7.42 (td, J = 7.6, 1.3 Hz, 1H), 7.38 (dd, J = 8.3, 1.3 Hz, 1H), 7.06 (d, J = 3.0 Hz, 1H), 6.92 (dd, J = 8.9, 3.0 Hz, 1H), 3.83 (s, 3H).

¹³C NMR (100 MHz, Chloroform-d) δ 159.12, 154.24, 151.67, 147.04, 136.49, 134.00, 132.13, 131.24, 129.84, 125.90, 117.79, 116.74, 116.06, 112.59, 55.79.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₅H₁₀BrNO₃: 331.9917; found: 331.9911.

3-(2-bromo-4-methoxyphenyl)-2*H*-benzo[b][1,4]oxazin-2-one (3j)



It was obtained as **White solid** having melting point **118-120** °C with **76%** yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.84 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.61-7.52 (m, 1H), 7.49 (d, *J* = 8.6 Hz, 1H), 7.41 (td, *J* = 7.8, 1.5 Hz, 1H), 7.38-7.34 (m, 1H), 7.24 (d, *J* = 2.5 Hz, 1H), 6.98 (dd, *J* = 8.6, 2.5 Hz, 1H), 3.86 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 161.55, 153.94, 152.07, 147.01, 131.86, 131.79, 131.44, 129.73, 128.18, 125.81, 123.21,

118.83, 116.67, 113.72, 55.88.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₅H₁₀BrNO₃: 331.9917; found: 331.9916.

3-(2-bromophenyl)-2*H*-naphtho[2,3-b][1,4]oxazin-2-one (3k)



It was obtained as **yellow solid** having melting point **204-206** °C with **63%** yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.36 (s, 1H), 8.00 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.92 (d, *J* = 8.3 Hz, 1H), 7.74 (s, 1H), 7.71 (dd, *J* = 8.0, 1.2 Hz, 1H), 7.63 (ddd, *J* = 8.4, 6.9, 1.3 Hz, 1H), 7.59 (d, *J* = 1.7 Hz, 1H), 7.57-7.52 (m, 1H), 7.48 (td, *J* = 7.6, 1.3 Hz,

1H), 7.42-7.35 (m, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 154.48, 151.69, 144.46, 136.04, 134.42, 133.31, 131.59, 130.99, 130.83, 130.41, 129.92, 129.15, 129.00, 127.69, 127.58, 126.40, 122.49, 112.96.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₈H₁₀BrNO₂: 351.9968; found: 351.9975.

3-(2-iodophenyl)-2H-benzo[b][1,4]oxazin-2-one (4a)



It was obtained as **White solid** having melting point **126-128** °C with **72%** yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.97 (d, *J* = 8.0 Hz, 1H), 7.87 (dd, *J* = 7.9, 1.7 Hz, 1H), 7.59 (td, *J* = 7.8, 1.7 Hz, 1H), 7.54-7.48 (m, 2H), 7.47-7.36 (m, 2H), 7.20 (ddd, *J* = 7.9, 5.4, 3.9 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 156.12, 151.59, 147.04, 139.69, 139.39, 132.07, 131.46, 131.24, 130.16, 129.81, 128.42, 125.94, 116.77, 96.02.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₈INO₂: 349.9672; found: 349.9673.

3-(2-iodophenyl)-6-methyl-2*H*-benzo[b][1,4]oxazin-2-one (4b)



It was obtained as White solid having melting point 120-122 °C with 78% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.93 (d, *J* = 8.0 Hz, 1H), 7.62 (d, *J* = 2.1 Hz, 1H), 7.47 (d, *J* = 4.5 Hz, 2H), 7.36 (dd, *J* = 8.4, 2.1 Hz, 1H), 7.23 (d, *J* = 3.5 Hz, 1H), 7.20-7.12 (m, 1H), 2.44 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 156.00, 151.87, 145.01, 139.71, 139.53, 135.96, 133.01, 131.39, 131.02, 130.16, 129.65, 128.39, 116.36, 96.10, 20.99. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₅H₁₀INO₂: 363.9829; found: 363.9823.

3-(2-iodophenyl)-7-methyl-2*H*-benzo[b][1,4]oxazin-2-one (4c)



It was obtained as White solid having melting point 148-150 °C with 82% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.99-7.92 (m, 1H), 7.73 (d, J = 8.1 Hz, 1H), 7.50 (d, J = 0.6 Hz, 1H), 7.49-7.48 (m, 1H), 7.23 (dd, J = 8.1, 1.8 Hz, 1H), 7.21-7.15 (m, 2H), 2.51 (s, 3H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 154.87, 151.85, 146.98, 142 (1, 120 55, 121 22, 120 18, 120 27, 120 21, 128 20)

143.61, 139.66, 139.55, 131.33, 130.18, 129.37, 129.31, 128.39, 127.05, 116.83, 96.20, 21.97. **HRMS (ESI⁺):** m/z [M+H]⁺ calculated for C₁₅H₁₀INO₂: 363.9829; found: 363.9828.

6-chloro-3-(2-iodophenyl)-2*H*-benzo[b][1,4]oxazin-2-one (4d)



It was obtained as White solid having melting point 98-100 °C with 66% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 2.5 Hz, 1H), 7.54 (dd, J = 8.9, 2.5 Hz, 1H), 7.50 (d, J = 2.9 Hz, 2H), 7.34 (d, J = 8.8 Hz, 1H), 7.24-7.18 (m, 1H).
¹³C NMR (100 MHz, Chloroform-*d*) δ 157.16, 151.03, 145.61, 139.79, 138.97, 131.94, 131.74, 131.70, 131.10, 130.17, 129.25,

128.44, 117.91, 95.84.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇ClINO₂: 383.9283; found: 383.9301.

7-chloro-3-(2-iodophenyl)-2H-benzo[b][1,4]oxazin-2-one (4e)



It was obtained as White solid having melting point 132-134 °C with 67% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, J = 8.0 Hz, 1H), 7.78 (d, J = 9.1 Hz, 1H), 7.50 (d, J = 3.8 Hz, 2H), 7.40 (q, J = 4.0, 3.3 Hz, 2H), 7.21 (ddd, J = 7.9, 5.5, 3.7 Hz, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 155.92, 150.87, 147.38, 139.77, 139.10, 137.91, 131.62, 130.60, 130.17, 129.92, 128.45, 126.52, 117.10, 95.95. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇ClINO₂: 383.9283; found: 383.9286.

6-fluoro-3-(2-iodophenyl)-2H-benzo[b][1,4]oxazin-2-one (4f)



It was obtained as White solid having melting point 118-120 °C with 59% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.97 (d, J = 8.0 Hz, 1H), 7.56 (dd, J = 8.1, 2.8 Hz, 1H), 7.50 (d, J = 3.4 Hz, 2H), 7.37 (dd, J = 9.1, 4.8 Hz, 1H), 7.32 (td, J = 9.2, 8.5, 2.8 Hz, 1H), 7.21 (ddd, J = 8.0, 5.7, 3.5 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 160.84, 158.40, 157.20, 151.24, 143.40, 143.37, 139.78, 139.05, 131.67, 130.16, 128.43, 119.52, 119.28, 117.87, 117.79, 115.65, 115.41, 95.82.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇FINO₂: 367.9578; found: 367.9576.

3-(4-chloro-2-iodophenyl)-2*H*-benzo[b][1,4]oxazin-2-one (4g)



126.05, 116.83, 96.28.

It was obtained as White solid having melting point 149-151 °C with 77% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.98 (d, J = 2.0 Hz, 1H), 7.86 (dd, J = 7.9, 1.6 Hz, 1H), 7.60 (td, J = 8.0, 1.6 Hz, 1H), 7.51-7.45 (m, 2H), 7.43 (d, J = 7.3 Hz, 1H), 7.40 (d, J = 8.3 Hz, 1H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 155.06, 151.50, 147.07,

139.29, 137.80, 136.63, 132.32, 131.21, 130.97, 129.88, 128.72,

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇ClINO₂: 383.9283; found: 383.9308.

3-(2-iodo-4-methoxyphenyl)-2*H*-benzo[b][1,4]oxazin-2-one (4h)



It was obtained as **White solid** having melting point **116-118** °C with **69%** yield.

¹**H** NMR (400 MHz, Chloroform-*d*) δ 7.85 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.57 (ddd, *J* = 8.2, 7.4, 1.6 Hz, 1H), 7.50 (d, *J* = 2.5 Hz, 1H), 7.47 (d, *J* = 8.6 Hz, 1H), 7.42 (td, *J* = 7.7, 1.4 Hz, 1H), 7.38 (dd, *J* = 8.2, 1.3 Hz, 1H), 7.02 (dd, *J* = 8.5, 2.5 Hz, 1H), 3.85 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 161.03, 155.46, 151.96, 147.01, 131.79, 131.53, 131.33, 131.14, 129.68, 125.87, 125.36, 116.69, 114.32, 96.57, 55.82. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₅H₁₀INO₃: 379.9778; found: 379.9785.

3-(2-iodophenyl)-2H-naphtho[2,3-b][1,4]oxazin-2-one (4i)



It was obtained as Yellow solid having melting point 198-200 °C with 60% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 8.38 (s, 1H), 8.00 (t, *J* = 8.7 Hz, 2H), 7.93 (d, *J* = 8.4 Hz, 1H), 7.76 (s, 1H), 7.64 (ddd, *J* = 8.3, 6.7, 1.3 Hz, 1H), 7.60-7.46 (m, 3H), 7.22 (td, *J* = 7.6, 2.0 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 156.28, 151.55, 144.53, 139.76, 139.50, 134.45, 131.50, 131.06, 130.39, 130.25, 129.91, 129.17, 129.02, 128.42, 127.62, 126.43, 113.03, 96.17. HRMS (ESI⁺): m/z [M+H]⁺ calculated for $C_{18}H_{10}INO_2$: 399.9829; found: 399.9820.

3-(2-chlorophenyl)-2*H*-benzo[b][1,4]oxazin-2-one (5a)



It was obtained as **White solid** having melting point **146-148** °C with **74%** yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.86 (dd, J = 7.9, 1.3 Hz, 1H), 7.61-7.54 (m, 2H), 7.53-7.50 (m, 1H), 7.48-7.44 (m, 1H), 7.42 (ddd, J = 8.5, 4.6, 2.8 Hz, 2H), 7.39 (d, J = 8.1 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 153.32, 151.87, 147.03, 134.06, 133.46, 132.09, 131.51, 131.39, 130.80, 130.17, 129.86, 127.12, 125.88, 116.73. **HRMS (ESI**⁺): m/z [M+H]⁺ calculated for C₁₄H₈ClNO₂: 258.0316; found: 258.0308.

3-(2-chlorophenyl)-6-methyl-2*H*-benzo[b][1,4]oxazin-2-one (5b)



It was obtained as White solid having melting point 114-116 °C with 77% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.64 (d, *J* = 2.1 Hz, 1H), 7.55 (dd, *J* = 7.2, 2.0 Hz, 1H), 7.51 (dd, *J* = 7.5, 1.6 Hz, 1H), 7.47-7.43 (m, 1H), 7.41 (dd, *J* = 7.2, 1.7 Hz, 1H), 7.38 (dd, *J* = 8.4, 2.2 Hz, 1H), 7.28 (s, 1H), 2.46 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 153.11, 152.12, 144.92, 135.87, 134.14, 133.43, 133.02, 131.41, 131.09, 130.78, 130.14, 129.65, 127.08, 116.27, 20.96. HRMS (ESI⁺): m/z [M+H]⁺ calculated for $C_{15}H_{10}CINO_2$: 272.0473; found: 272.0483.

3-(2-chlorophenyl)-7-methyl-2*H*-benzo[b][1,4]oxazin-2-one (5c)



It was obtained as White solid having melting point 148-150 °C with 82% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.72 (d, *J* = 8.1 Hz, 1H), 7.55 (dd, *J* = 7.2, 2.1 Hz, 1H), 7.50 (dd, *J* = 7.7, 1.6 Hz, 1H), 7.47-7.37 (m, 2H), 7.22 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.18 (s, 1H), 2.51 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 152.14, 152.02, 146.98, 143.63, 134.24, 133.52, 131.36, 130.84, 130.15, 129.49, 129.43, 127.09, 126.99, 116.79, 21.96. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₅H₁₀ClNO₂: 272.0473; found: 272.0489.

6-chloro-3-(2-chlorophenyl)-2*H*-benzo[b][1,4]oxazin-2-one (5d)



It was obtained as White solid having melting point 150-152 °C with 65% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.84 (d, J = 2.6 Hz, 1H), 7.58-7.52 (m, 2H), 7.51-7.48 (m, 1H), 7.48-7.43 (m, 1H), 7.41 (dd, J = 7.4, 1.6 Hz, 1H), 7.33 (d, J = 8.9 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 154.39, 151.28, 145.55, 133.62, 133.40, 131.96, 131.82, 131.77, 131.01, 130.79, 130.23, 129.28, 127.14, 117.85. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇Cl₂NO₂: 291.9927; found: 291.9935.

7-chloro-3-(2-chlorophenyl)-2*H*-benzo[b][1,4]oxazin-2-one (5e)



It was obtained as White solid having melting point 154-156 °C with 67% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.78 (d, J = 9.1 Hz, 1H), 7.55 (dd, J = 7.3, 1.9 Hz, 1H), 7.51 (dd, J = 7.9, 1.5 Hz, 1H), 7.48-7.44 (m, 1H), 7.42 (dd, J = 7.3, 1.6 Hz, 1H), 7.40-A7.37 (m, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 153.11, 151.11, 147.35,

137.92, 133.76, 133.46, 131.68, 130.80, 130.63, 130.23, 130.04, 127.13, 126.44, 117.02. **HRMS (ESI⁺):** m/z [M+H]⁺ calculated for C₁₄H₇Cl₂NO₂: 291.9927; found: 291.9962.

3-(2-chlorophenyl)-6-fluoro-2*H*-benzo[b][1,4]oxazin-2-one (5f)



It was obtained as **White solid** having melting point **95-97** °C with **59%** yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.46 (dd, J = 7.8, 2.4 Hz, 2H), 7.41 (td, J = 7.9, 1.7 Hz, 1H), 7.34 (dtd, J = 14.5, 7.6, 1.7 Hz, 2H), 7.27 (dd, J = 9.1, 4.8 Hz, 1H), 7.21 (ddd, J = 14.5, 8.0, 4.1 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 160.73, 158.29, 154.39, 151.44, 143.29, 133.67, 133.35, 131.70, 130.75, 130.18, 127.10, 119.51, 119.26, 117.78, 117.69, 115.62, 115.38. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇ClFNO₂: 276.0222; found: 276.0234.

3-(2,4-dichlorophenyl)-2*H*-benzo[b][1,4]oxazin-2-one (5g)



It was obtained as White solid having melting point 145-147 °C with 77% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.85 (dd, *J* = 7.9, 1.6 Hz, 1H), 7.60 (ddd, *J* = 9.0, 7.5, 1.6 Hz, 1H), 7.54 (d, *J* = 2.0 Hz, 1H), 7.51 (d, *J* = 8.3 Hz, 1H), 7.48-7.36 (m, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 152.24, 151.75, 146.98, 137.05, 134.44, 132.49, 132.37, 131.80, 131.31, 130.16, 129.91, 127.53, 126.01, 116.77.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₄H₇Cl₂NO₂: 291.9854; found: 291.9951.

3-(2-chloro-4-methoxyphenyl)-2*H*-benzo[b][1,4]oxazin-2-one (5h)



It was obtained as **White solid** having melting point **121-123** °C with **73%** yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.84 (dd, J = 8.0, 1.6 Hz, 1H), 7.56 (dd, J = 7.7, 1.6 Hz, 1H), 7.52 (d, J = 8.6 Hz, 1H), 7.40 (td, J = 7.7, 1.3 Hz, 1H), 7.36 (dd, J = 8.2, 1.3 Hz, 1H), 7.05 (d, J = 2.5 Hz, 1H), 6.93 (dd, J = 8.6, 2.5 Hz, 1H), 3.86 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 161.74, 152.88, 152.14, 146.94, 134.56, 131.96, 131.77, 131.48, 129.71, 126.30, 125.78, 116.63, 115.67, 113.19, 55.87. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₅H₁₀ClNO₃: 288.0442; found: 288.0431.

3-(2-chlorophenyl)-2H-naphtho[2,3-b][1,4]oxazin-2-one (5i)



It was obtained as **Yellow solid** having melting point **201-203** °C with **71%** yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 8.35 (s, 1H), 7.99 (d, J = 8.1 Hz, 1H), 7.91 (d, J = 8.3 Hz, 1H), 7.73 (s, 1H), 7.65-7.59 (m, 2H), 7.57-7.51 (m, 2H), 7.45 (dtd, J = 14.8, 7.3, 1.9 Hz, 2H). ¹³C NMR (100 MHz, Chloroform-*d*) δ 153.40, 151.78, 144.40,

134.40, 134.12, 133.51, 131.54, 130.86, 130.44, 130.19, 129.92, 129.14, 128.99, 127.56, 127.11, 126.37, 124.30, 112.91.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₈H₁₀ClNO₂: 308.0473; found: 308.0476.

3-(4'-methoxy-[1,1'-biphenyl]-2-yl)-2H-benzo[b][1,4]oxazin-2-one (8)



It was obtained as **White solid** having melting point **123-125** °C with 87% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.82 (dd, J = 8.0, 1.7 Hz, 1H), 7.67-7.63 (m, 1H), 7.60-7.54 (m, 1H), 7.53-7.45 (m, 3H), 7.39 (td, J = 7.7, 1.4 Hz, 1H), 7.27-7.20 (m, 3H), 6.83 (d, J = 8.7 Hz, 2H), 3.78 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 159.12, 156.42, 151.66, 146.89, 141.77, 133.97, 133.61, 131.54, 131.22, 130.61, 130.04, 129.95, 129.49, 127.28, 125.57, 116.57, 114.13, 55.31.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₁H₁₅NO₃: 330.1125; found: 330.1127.

3-(3'-methyl-[1,1'-biphenyl]-2-yl)-2*H*-benzo[b][1,4]oxazin-2-one (9)



It was obtained as **White solid** having melting point **132-134** °C with 85% yield.

¹H NMR (400 MHz, Chloroform-*d*) δ 7.81 (dd, J = 7.9, 1.6 Hz, 1H), 7.70-7.63 (m, 1H), 7.60-7.55 (m, 1H), 7.49 (ddt, J = 11.8, 8.0, 2.0 Hz, 3H), 7.37 (td, J = 7.7, 1.4 Hz, 1H), 7.24 (dd, J = 8.7, 1.5 Hz, 1H), 7.19-7.15 (m, 1H), 7.13 (d, J = 7.6 Hz, 1H), 7.09-7.06 (m, 1H), 7.03 (dd, J = 7.5, 1.6 Hz, 1H), 2.28 (s, 3H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 156.29, 151.71, 146.82, 142.17, 141.00, 138.41, 133.98, 131.49, 131.24, 130.60, 130.07, 129.94, 129.76, 129.46, 128.38, 128.34, 127.57, 126.02, 125.58, 116.49, 21.56.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₁H₁₅NO₂: 314.1176; found: 314.1196.

2'-(2-oxo-2H-benzo[b][1,4]oxazin-3-yl)-[1,1'-biphenyl]-4-carbaldehyde (10)



It was obtained as **White solid** having melting point **118-120** °C with 50% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 10.08 (s, 1H), 8.00 (d, *J* = 8.3 Hz, 3H), 7.81 (dd, *J* = 8.4, 6.9 Hz, 4H), 7.76-7.71 (m, 1H), 7.65-7.55 (m, 1H), 7.54-7.49 (m, 1H), 7.47 (d, *J* = 8.1 Hz, 1H), 7.39 (ddd, *J* = 7.7, 5.6, 2.2 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 192.03, 191.89, 155.15, 151.78, 147.47, 146.78, 145.69, 140.90, 136.10, 135.23, 133.89, 131.68, 131.44, 130.81, 130.51, 130.06, 129.58, 128.55, 128.17, 125.82, 116.63. HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₁H₁₃NO₃: 328.0968; found: 328.0976.

3-(2-(thiophen-3-yl)phenyl)-2*H*-benzo[b][1,4]oxazin-2-one (11)



It was obtained as **White solid** having melting point **148-150** °C with **80%** yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.83 (dd, J = 7.8, 1.7 Hz, 1H), 7.67-7.62 (m, 1H), 7.59-7.54 (m, 2H), 7.52 (dd, J = 1.6, 0.8 Hz, 1H), 7.51-7.46 (m, 1H), 7.43-7.37 (m, 1H), 7.31 (dd, J = 5.0, 3.0 Hz, 1H), 7.29-7.27 (m, 1H), 7.11 (dd, J = 4.9, 1.4 Hz, 1H), 7.07 (dd, J = 3.0,

1.3 Hz, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 156.25, 151.75, 146.90, 141.82, 136.70, 134.03, 131.47, 131.39, 130.66, 129.84, 129.58, 129.51, 128.39, 127.75, 126.53, 125.67, 123.12, 116.65.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₁₈H₁₁NO₂S: 306.0583; found: 306.0579.

3-([1,1'-biphenyl]-2-yl)-2*H*-benzo[b][1,4]oxazin-2-one (12)



It was obtained as White solid having melting point 138-140 °C with 91% yield.

¹**H NMR (400 MHz, Chloroform-***d***)** δ 7.78 (dd, J = 7.9, 1.6 Hz, 1H), 7.69-7.65 (m, 1H), 7.60-7.55 (m, 1H), 7.52-7.45 (m, 3H), 7.36 (td, J = 7.7, 1.4 Hz, 1H), 7.29 (d, J = 4.7 Hz, 5H), 7.25-7.21 (m, 1H).

¹³C NMR (100 MHz, Chloroform-*d*) δ 156.15, 151.71, 146.89, 142.19, 141.14, 134.04, 131.55, 131.27, 130.63, 130.17, 130.04, 129.51, 128.97, 128.64, 127.65, 127.55, 125.59, 116.56.

HRMS (ESI⁺): m/z [M+H]⁺ calculated for C₂₀H₁₃NO₂: 300.1019; found: 300.1020.

Copies of ¹H NMR and ¹³C NMR Spectra









--- 2.46

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







Figure 6: ¹³C NMR spectrum of compound **3c** (100 MHz, CDCl₃).





Figure 7: ¹H NMR spectrum of compound **3d** (400 MHz, CDCl₃).



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



Figure 9: ¹H NMR spectrum of compound 3e (400 MHz, CDCl₃).



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





Figure 12: ¹³C NMR spectrum of compound 3f (100 MHz, CDCl₃).

7.28 7.28 7.28 7.28 7.28 7.28 7.28 7.55





Figure 13: ¹H NMR spectrum of compound 3g (400 MHz, CDCl₃).



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



Figure 16: ¹³C NMR spectrum of compound **3h** (100 MHz, CDCl₃).

f1 (ppm)




Figure 18: ¹³C NMR spectrum of compound 3i (100 MHz, CDCl₃).





Figure 20: ¹³C NMR spectrum of compound 3j (100 MHz, CDCl₃).







Figure 21: ¹H NMR spectrum of compound 3k (400 MHz, CDCl₃).



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



Figure 23: ¹H NMR spectrum of compound 4a (400 MHz, CDCl₃).



Figure 24: ¹³C NMR spectrum of compound 4a (100 MHz, CDCl₃).



Figure 26: ¹³C NMR spectrum of compound 4b (100 MHz, CDCl₃).



- 2.51



Figure 28: ¹³C NMR spectrum of compound 4c (100 MHz, CDCl₃).







Figure 30: ¹³C NMR spectrum of compound 4d (100 MHz, CDCl₃).







Figure 31: ¹H NMR spectrum of compound 4e (400 MHz, CDCl₃).



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Figure 33: ¹H NMR spectrum of compound 4f (400 MHz, CDCl₃).



Figure 34: ¹³C NMR spectrum of compound 4f (400 MHz, CDCl₃).



Figure 35: ¹H NMR spectrum of compound 4g (400 MHz, CDCl₃).



Figure 36: ¹³C NMR spectrum of compound 4g (400 MHz, CDCl₃).



Figure 38: ¹³C NMR spectrum of compound 4h (400 MHz, CDCl₃).





Figure 39: ¹H NMR spectrum of compound 4i (400 MHz, CDCl₃).



Figure 40: ¹³C NMR spectrum of compound 4i (400 MHz, CDCl₃).



Figure 42: ¹³C NMR spectrum of compound 5a (400 MHz, CDCl₃).



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100 90 f1 (ppm) 00 190 180 150 140 130 120 170 160 110 80 70 60 50 40 30 20 10 0 Figure 44: ¹³C NMR spectrum of compound **5b** (400 MHz, CDCl₃).



- 2.51



Figure 47: ¹H NMR spectrum of compound 5d (400 MHz, CDCl₃).





Figure 50: ¹³C NMR spectrum of compound 5e (400 MHz, CDCl₃).







Figure 52: ¹³C NMR spectrum of compound 5f (400 MHz, CDCl₃).



Figure 53: ¹H NMR spectrum of compound 5g (400 MHz, CDCl₃).



Figure 54: ¹³C NMR spectrum of compound 5g (400 MHz, CDCl₃).



Figure 56: ¹³C NMR spectrum of compound 5h (400 MHz, CDCl₃).









Figure 58: ¹³C NMR spectrum of compound 5i (400 MHz, CDCl₃).



Figure 60: ¹³C NMR spectrum of compound 8 (400 MHz, CDCl₃).



— 2.28

Figure 62: ¹³C NMR spectrum of compound 9 (400 MHz, CDCl₃).



Figure 64: ¹³C NMR spectrum of compound 10 (400 MHz, CDCl₃).





Figure 68: ¹³C NMR spectrum of compound 12 (400 MHz, CDCl₃).