Supporting Information

Highly Regioselective Synthesis of Fused Seven-Membered Ring through Copper-Catalyzed Cross-Coupling

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General experimental procedures

Unless otherwise stated, all reactions were carried out under N₂. 2-halophenols and solvents were obtained from commercial sources and used without any further purification. ¹H NMR spectra were recorded at 400 MHz or 500 MHz using TMS as internal standard. ¹³C NMR spectra were recorded at 100 MHz or 125MHz using TMS as internal standard. The multiplicities are reported as follows: singlet (s), doublet (d), doublet of doublets (dd), triplet (t), quartet (q), multiplet (m). Coupling constants are reported in Hertz (Hz). Mass spectroscopy data were collected on HRMS-EI and HRMS-ESI instrument.

General procedure for synthesis of substrates

2a-g were prepared according to the method of reference 1, and 2h was prepared according to the method of reference 2.

Characterization data of compounds 2a-h

2a

2-(2-Bromophenyl)-1H-indole (2a). ¹H NMR (CDCl₃, 500 MHz) δ 8.63 (s, 1H), 7.66-7.79 (m, 2H), 7.61 (dd, 1H, J = 7.5 Hz, 1.5Hz), 7.42 (d, 1H, J = 8.5 Hz), 7.38 (td, 1H, J = 7.5 Hz, 1.0Hz), 7.19-7.23 (m, 2H), 7.14 (t, 1H, J = 7.0 Hz), 6.82 (d, 1H, , J = 1.0 Hz). ¹³C NMR (CDCl₃, 125 MHz) δ 131.0, 131.0, 128.8, 128.2, 126.2, 124.0, 122.9, 122.5, 117.4, 116.1, 115.6, 115.0, 105.8, 98.4.

2b

2-(2-Iodophenyl)-1H-indole (2b). ³¹H NMR (DMSO-ｄ₆, 500 MHz) δ 11.38 (s, 1H), 8.04 (t, 1H, J = 7.0 Hz), 7.60 (d, 1H, J = 8.0 Hz), 7.50-7.55 (m, 2H), 7.42 (d, 1H, J = 8.0 Hz), 7.13-7.18 (m, 2H), 7.03-7.06 (m, 1H), 6.70 (d, 1H, J = 1.5 Hz). ¹³C NMR
(DMSO-$d_6$, 125 MHz) $\delta$ 139.9, 139.0, 137.9, 136.2, 130.9, 129.7, 128.3, 127.7, 121.5, 120.2, 119.2, 111.4, 102.0, 98.5.

2c

2-(2-Chlorophenyl)-1H-indole (2c). $^1$H NMR (DMSO-$d_6$, 500 MHz) $\delta$ 11.45 (s, 1H), 7.74 (dd, 1H, $J = 7.5$ Hz, 1.0 Hz), 7.60 (t, 2H, $J = 7.0$ Hz), 7.43-7.49 (m, 2H), 7.39 (t, 1H, $J = 7.5$ Hz), 7.13-7.16 (m, 1H), 7.03 (t, 1H, $J = 7.0$ Hz), 6.89 (d, 1H, $J = 1.0$ Hz). $^{13}$C NMR (DMSO-$d_6$, 125 MHz) $\delta$ 136.5, 134.2, 131.3, 131.0, 130.6, 130.6, 129.0, 127.9, 127.5, 121.9, 120.3, 119.3, 111.4, 103.0.

2d

2-(2-Bromophenyl)-5-methyl-1H-indole (2d). $^1$H NMR (CDCl$_3$, 500 MHz) $\delta$ 8.55 (s, 1H), 7.67 (d, 1H, $J = 8.0$ Hz), 7.59 (dd, 1H, $J = 7.5$ Hz, 1.0Hz), 7.44 (s, 1H), 7.35-7.38 (m, 1H), 7.31 (d, 1H, $J = 8.5$ Hz), 7.19 (td, 1H, $J = 8.0$ Hz, 1.5Hz), 7.05 (d, 1H, $J = 8.0$ Hz), 6.73 (d, 1H, $J = 1.5$ Hz), 2.46 (s, 3H). $^{13}$C NMR (CDCl$_3$, 125 MHz) $\delta$ 136.3, 134.6, 134.0, 133.6, 131.4, 129.4, 129.1, 128.5, 127.7, 124.3, 121.3, 120.4, 110.7, 103.2, 21.5.

2e

2-(2-Bromophenyl)-5-fluoro-1H-indole (2e). $^1$H NMR (CDCl$_3$, 500 MHz) $\delta$ 8.61 (s, 1H), 7.67 (d, 1H, $J = 8.0$ Hz), 7.57 (d, 1H, $J = 7.5$ Hz), 7.37 (t, 1H, $J = 7.5$ Hz), 7.28-7.32 (m, 2H), 7.19-7.22 (m, 1H), 6.96 (td, 1H, $J = 9.5$ Hz, 2.5Hz), 6.76 (s, 1H). $^{13}$C
NMR (CDCl$_3$, 125 MHz) $\delta$ 158.1 ($J_{CF} = 233.1$ Hz), 138.0, 134.1, 133.1, 132.8, 131.4, 129.5, 128.5 ($J_{CF} = 9.1$ Hz), 127.8, 121.3, 111.5 ($J_{CF} = 72.8$ Hz), 111.3 ($J_{CF} = 90.4$ Hz), 105.5 ($J_{CF} = 23.6$ Hz), 103.7 ($J_{CF} = 4.4$ Hz). (EI): m/z (%) = 291 ([M$^+$/H], 97), 290 ([M$^+$], 17), 209 (33), 183 (100), 149 (31), 104 (38).

![Structure 2f]

2f

2-(2-Bromophenyl)-5-chloro-1H-indole (2f). $^1$H NMR (CDCl$_3$, 500 MHz) $\delta$ 8.61 (s, 1H), 7.66 (d, 1H, $J = 8.0$ Hz), 7.60 (s, 1H), 7.55 (d, 1H, $J = 8.0$ Hz), 7.34-7.37 (m, 1H), 7.29 (d, 1H, $J = 8.5$ Hz), 7.18-7.21 (m, 1H), 7.14-7.16 (m, 1H), 6.72 (s, 1H). $^{13}$C NMR (CDCl$_3$, 125 MHz) $\delta$ 137.7, 134.6, 134.1, 133.0, 131.4, 129.6, 129.2, 127.8, 125.8, 122.9, 121.3, 120.2, 112.1, 103.2. (EI): m/z (%) = 307 ([M$^+$], 40), 305 (31), 165 (100), 65 (21), 51 (23).

![Structure 2g]

2g

5-Bromo-2-(2-bromophenyl)-1H-indole (2g). $^1$H NMR (CDCl$_3$, 500 MHz) $\delta$ 8.68 (s, 1H), 7.77 (s, 1H), 7.68 (d, 1H, $J = 8.0$ Hz), 7.58 (dd, 1H, $J = 8.0$ Hz, 1.5 Hz), 7.36-7.39 (m, 1H), 7.29 (s, 2H), 7.22 (td, 1H, $J = 8.0$ Hz, 1.5 Hz), 6.73 (d, 1H, $J = 2.0$ Hz). $^{13}$C NMR (CDCl$_3$, 125 MHz) $\delta$ 137.5, 134.8, 134.1, 132.9, 131.5, 129.9, 129.6, 127.8, 125.4, 123.3, 121.3, 113.4, 112.5, 103.1. (EI): m/z (%) = 351 ([M$^+$], 1), 250 (100), 206 (23), 172 (16), 71 (23).

![Structure 2h]
2-(2-Bromophenyl)-1H-benzo[d]imidazole (2h). $^1$H NMR (DMSO-$d_6$, 400 MHz) δ 12.79 (s, 1H), 7.82 (d, 1H, $J = 7.6$ Hz), 7.76 (d, 1H, $J = 7.2$ Hz), 7.70 (d, 1H, $J = 6.4$ Hz), 7.55 (t, 2H, $J = 6.8$ Hz), 7.46 (t, 1H, $J = 7.2$ Hz), 7.24 (s, 2H). $^{13}$C NMR (DMSO-$d_6$, 100 MHz) δ 150.8, 143.5, 134.5, 133.8, 132.7, 132.6, 131.8, 128.2, 123.1, 122.0, 121.9, 119.5, 112.0.

General procedure for synthesis of indole-fused dibenzo[b,f][1,4]oxazepines
A sealable tube (20 mL) was charged with CuI (3.8 mg, 0.02 mmol), dibenzoylmethane (4.5 mg, 0.02 mmol), tripotassium phosphate (127.4 mg, 0.6 mmol), the 2-halophenol (1, 0.24 mmol) and the 2-(2-halophenyl)-1H-indole (2, 0.20 mmol). DMF (2 mL) was added and the tube sealed. The mixture was allowed to stir under N$_2$ at 120 °C for 12 h. Saturated aqueous NaCl (25 mL), and EtOAc (25 mL) were added to the cooled reaction mixture successively. The organic phase was separated, and the aqueous phase was further extracted with EtOAc (2 × 25 mL). The combined organic layers were dried over anhydrous Na$_2$SO$_4$ and concentrated. The residue was purified by column chromatography on silica gel using petroleum ether as eluent to provide the desired products (3).

Characterization data of compounds 3a-l

8-Chlorodibenzo[b,f]indolo[1,2-d][1,4]oxazepine (3a) [New compound]. Eluent: petroleum ether. White solid, mp = 133-135 °C (uncorrected). $^1$H NMR (DMSO-$d_6$, 400 MHz) δ 7.75-7.79 (m, 3H), 7.69 (t, 2H, $J = 7.2$ Hz), 7.49 (d, 1H, $J = 8.0$ Hz), 7.38-7.44 (m, 2H), 7.19-7.33 (m, 3H), 7.05 (s, 1H). $^{13}$C NMR (DMSO-$d_6$, 100 MHz) δ 157.3, 153.6, 136.4, 136.3, 131.0, 130.8, 130.4, 129.7, 129.0, 126.8, 126.6, 125.9,
124.3, 123.6, 123.2, 122.0, 121.5, 121.4, 111.7, 104.1. HRMS (El) Calcd for C$_{20}$H$_{12}$NOCl (M)$^+$ 317.0607; Found, 317.0604.

![3b]

**Indolo[1,2-\textit{d}][\textit{b,f}]\[1,4\]oxazepine (3b) [New compound].** Eluent: petroleum ether. White solid, mp = 135-137 °C (uncorrected). $^1$H NMR (DMSO-$d_6$, 400 MHz) δ 7.75-7.79 (m, 2H), 7.70 (d, 2H, $J = 8.8$ Hz), 7.54-7.57 (m, 1H), 7.37-7.44 (m, 2H), 7.31-7.35 (m, 2H), 7.18-7.29 (m, 3H), 7.02 (s, 1H). $^{13}$C NMR (DMSO-$d_6$, 100 MHz) δ 157.7, 153.3, 136.7, 136.4, 131.3, 130.7, 129.7, 129.0, 128.0, 126.6, 126.5, 124.8, 124.5, 123.5, 123.0, 121.9, 121.5, 121.3, 111.7, 103.7. HRMS (El) Calcd for C$_{20}$H$_{13}$NO (M)$^+$ 283.0997; Found, 283.0996.

![3c]

**8-Bromodibenzo[\textit{b,f}]indolo[1,2-\textit{d}][1,4]oxazepine (3c) [New compound].** Eluent: petroleum ether. White solid, mp = 133-135 °C (uncorrected). $^1$H NMR (DMSO-$d_6$, 500 MHz) δ 7.91 (d, 1H, $J = 2.0$ Hz), 7.82 (dd, 1H, $J = 8.0$ Hz, 1.5 Hz), 7.72-7.77 (m, 3H), 7.56 (dd, 1H, $J = 8.0$ Hz, 2.0 Hz), 7.52 (dd, 1H, $J = 8.5$ Hz, 1.0 Hz), 7.46 (td, 1H, $J = 7.5$ Hz, 1.5 Hz), 7.35 (td, 1H, $J = 7.5$ Hz, 1.0 Hz), 7.30 (td, 1H, $J = 7.0$ Hz, 1.0 Hz), 7.23-7.26 (m, 1H), 7.08 (s, 1H). $^{13}$C NMR (DMSO-$d_6$, 125 MHz) δ 162.2, 158.6, 141.2, 135.8, 135.7, 134.6, 134.5, 133.9, 131.6, 131.2, 130.9, 129.2, 128.5, 126.9, 126.4, 126.3, 123.7, 116.5, 109.1, 109.0. HRMS (El) Calcd for C$_{20}$H$_{12}$NOBr (M)$^+$ 361.0102; Found, 361.0107.
9-Chlorodibenzob,f]indolo[1,2-d][1,4]oxazepine (3d) [New compound]. Eluent: petroleum ether. White solid, mp = 133-135 °C (uncorrected). $^1$H NMR (DMSO-d$_6$, 500 MHz) δ 7.83 (d, 1H, $J = 7.5$ Hz), 7.71-7.75 (m, 3H), 7.51-7.55 (m, 2H), 7.44-7.47 (m, 1H), 7.35 (t, 2H, $J = 8.5$ Hz), 7.29 (t, 1H, $J = 7.0$ Hz), 7.24 (t, 1H, $J = 7.5$ Hz), 7.08 (s, 1H). $^{13}$C NMR (DMSO-d$_6$, 125 MHz) δ 156.5, 148.3, 136.2, 135.9, 132.7, 130.3, 129.4, 128.6, 127.5, 126.9, 126.7, 126.6, 124.1, 123.3, 121.8, 121.3, 121.2, 111.5, 104.0. HRMS (EI) Calcd for C$_{20}$H$_{12}$ClNO (M)$^+$ 317.0607; Found, 317.0608.

6-Chlorodibenzob,f]indolo[1,2-d][1,4]oxazepine (3e) [New compound]. Eluent: petroleum ether. White solid, mp = 151-153 °C (uncorrected). $^1$H NMR (CDCl$_3$, 500 MHz) δ 7.69-7.73 (m, 2H), 7.33-7.36 (m, 2H), 7.26-7.32 (m, 4H), 7.21-7.24 (m, 3H), 6.84 (s, 1H). $^{13}$C NMR (CDCl$_3$, 125 MHz) δ 158.9, 157.8, 136.6, 136.3, 130.0, 129.8, 129.6, 128.8, 128.3, 128.0, 127.7, 126.1, 125.3, 122.2, 121.2, 120.9, 120.8, 120.5, 113.8, 104.4. HRMS (EI) Calcd for C$_{20}$H$_{12}$ClNO (M)$^+$ 317.0607; Found, 317.0606.
Dibenzo[b,f]indolo[1,2-d][1,4]oxazepine-8-carbonitrile (3f) [New compound]. 
Eluent: petroleum ether. White solid, mp = 173-175 °C (uncorrected). 
$^1$H NMR (CDCl$_3$, 500 MHz) $\delta$ 7.87 (d, 1H, $J = 8.0$ Hz), 7.68-7.73 (m, 4H), 7.57 (dd, 1H, $J = 8.5$ Hz, 2.0 Hz), 7.36-7.39 (m, 1H), 7.32-7.34 (m, 1H), 7.27-7.30 (m, 3H), 6.93 (s, 1H). $^{13}$C NMR (CDCl$_3$, 125 MHz) $\delta$ 157.2, 153.3, 136.7, 136.6, 136.6, 130.3, 129.6, 129.4, 128.7, 126.7, 126.3, 125.2, 124.3, 123.6, 122.4, 121.5, 120.9, 117.7, 111.4, 109.9, 104.8. HRMS (EI) Calcd for C$_{21}$H$_{12}$N$_2$O (M) $^+$ 308.0950; Found, 308.0955.

Benzo[f]naphtho[1,2-b]indolo[1,2-d][1,4]oxazepine (3g) [New compound]. Eluent: petroleum ether. White solid, mp = 166-168 °C (uncorrected). 
$^1$H NMR (CDCl$_3$, 500 MHz) $\delta$ 8.63 (d, 1H, $J = 8.0$ Hz), 7.89 (t, 2H, $J = 9.0$ Hz), 7.79 (d, 1H, $J = 8.0$ Hz), 7.73-7.76 (m, 3H), 7.65 (t, 1H, $J = 8.0$ Hz), 7.53 (t, 2H, $J = 8.5$ Hz), 7.31-7.34 (m, 1H), 7.26-7.28 (m, 2H), 7.21-7.24 (m, 1H), 6.93 (s, 1H). $^{13}$C NMR (CDCl$_3$, 125 MHz) $\delta$ 158.5, 148.3, 137.3, 136.9, 132.7, 129.6, 129.3, 129.1, 128.2, 128.0, 127.7, 127.1, 126.4, 125.7, 125.5, 125.2, 122.8, 122.6, 121.9, 121.5, 121.2, 111.6, 103.3. HRMS (EI) Calcd for C$_{24}$H$_{15}$NO (M) $^+$ 333.1154; Found, 333.1156.
2-Methyl-8-chlorodibenzo[b,f]indolo[1,2-d][1,4]oxazepine (3h) [New compound].

Eluent: petroleum ether. White solid, mp = 143-145 °C (uncorrected). \(^1\)H NMR (CDCl\(_3\), 500 MHz) \(\delta\) 7.71 (dd, 1H, \(J = 8.0\) Hz, 1.5Hz), 7.67 (d, 1H, \(J = 8.5\) Hz), 7.57 (d, 1H, \(J = 8.5\) Hz), 7.49 (s, 1H), 7.45 (d, 1H, \(J = 2.5\) Hz), 7.30-7.34 (m, 2H), 7.26 (t, 1H, \(J = 1.0\) Hz), 7.23-7.25 (m, 1H), 7.10 (dd, 1H, \(J = 8.0\) Hz, 1.0Hz), 6.80 (s, 1H), 2.48 (s, 3H). \(^1^3\)C NMR (CDCl\(_3\), 125 MHz) \(\delta\) 152.3, 148.5, 131.5, 129.8, 126.1, 125.8, 125.7, 124.6, 124.2, 124.0, 120.7, 120.5, 119.7, 119.6, 119.4, 117.9, 115.7, 115.6, 105.8, 98.0, 16.2. HRMS (EI) Calcd for C\(_{21}\)H\(_{14}\)NOCl (M) \(^+\) 331.0764; Found, 331.0768.

2-Fluoro-8-chlorodibenzo[b,f]indolo[1,2-d][1,4]oxazepine (3i) [New compound].

Eluent: petroleum ether. White solid, mp = 162-164 °C (uncorrected). \(^1\)H NMR (CDCl\(_3\), 500 MHz) \(\delta\) 7.70 (d, 1H, \(J = 8.0\) Hz), 7.64 (d, 1H, \(J = 8.0\) Hz), 7.59-7.61 (m, 1H), 7.46 (d, 1H, \(J = 2.0\) Hz), 7.31-7.38 (m, 3H), 7.26-7.28 (m, 2H), 7.00 (td, 1H, \(J = 9.0\) Hz, 2.5 Hz), 6.83 (s, 1H). \(^1^3\)C NMR (CDCl\(_3\), 125 MHz) \(\delta\) 158.7 \((J_{CF} = 235\) Hz), 155.8 \((J_{CF} = 463.1\) Hz), 138.3, 133.2, 131.8, 130.6, 130.3, 129.8, 129.7, 129.3, 126.1, 125.9, 124.9, 124.4, 123.3, 121.0, 111.8 \((J_{CF} = 100.1\) Hz), 111.7 \((J_{CF} = 116.4\) Hz).
106.0 \( (J_C = 23.9 \text{ Hz}) \), 103.3 \( (J_C = 5.0 \text{ Hz}) \). HRMS (EI) Calcd for C\textsubscript{20}H\textsubscript{11}NOFCl (M) + 335.0513; Found, 335.0512.

\[
\begin{align*}
\text{3j} & \\
\text{2-Chloro-8-chlorodibenzo[b,f]indolo[1,2-d][1,4]oxazepine (3j) [New compound].} \\
\text{Eluent: petroleum ether. White solid, mp = 165-167 °C (uncorrected).} \\
\text{\textsuperscript{1}H NMR (CDCl}_3, 500 MHz) \delta 7.64 (dd, 1H, \textit{J} = 8.0 \text{ Hz, 1.5 Hz}), 7.61 (d, 1H, \textit{J} = 2.0 \text{ Hz}), 7.52-7.54 (m, 2H), 7.42 (d, 1H, \textit{J} = 2.5 \text{ Hz}), 7.27-7.34 (m, 2H), 7.19-7.23 (m, 2H), 7.16 (dd, 1H, \textit{J} = 9.0 \text{ Hz, 2.0 Hz}), 6.75 (s, 1H).} \\
\text{\textsuperscript{13}C NMR (CDCl}_3, 125 MHz) \delta 157.6, 153.9, 138.1, 135.0, 132.0, 130.4, 130.3, 129.4, 127.2, 126.1, 125.9, 124.9, 124.3, 123.3, 123.2, 121.1, 120.6, 112.4, 103.0. HRMS (EI) Calcd for C\textsubscript{20}H\textsubscript{11}NOCl\textsubscript{2} (M) + 351.0218; Found, 351.0219.
\end{align*}
\]

\[
\begin{align*}
\text{3k} & \\
\text{2-Bromo-8-chlorodibenzo[b,f]indolo[1,2-d][1,4]oxazepine (3k) [New compound].} \\
\text{Eluent: petroleum ether. White solid, mp = 174-176 °C (uncorrected).} \\
\text{\textsuperscript{1}H NMR (CDCl}_3, 500 MHz) \delta 7.79 (d, 1H, \textit{J} = 1.5 \text{ Hz}), 7.67 (d, 1H, \textit{J} = 8.0 \text{ Hz}), 7.57 (d, 1H, \textit{J} = 8.5 \text{ Hz}), 7.51 (d, 1H, \textit{J} = 9.0 \text{ Hz}), 7.44 (d, 1H, \textit{J} = 2.0 \text{ Hz}), 7.29-7.37 (m, 3H), 7.23-
\end{align*}
\]
7.26 (m, 2H), 6.78 (s, 1H). $^{13}$C NMR (CDCl$_3$, 125 MHz) δ 157.7, 154.0, 137.9, 135.3, 132.0, 130.9, 130.4, 130.3, 129.4, 126.1, 125.9, 125.8, 125.0, 124.3, 123.7, 123.3, 121.0, 114.7, 112.7, 102.8. HRMS (EI) Calcd for C$_{20}$H$_{11}$NOBrCl (M)$^+$ 394.9713; Found, 394.9712.

![Chemical Structure](image)

**3l**

8-Chlorodibenzo[b,f]benzimidazo[1,2-d][1,4]oxazepine (3l) [New compound].

Eluent: petroleum ether / ethyl acetate (20:1). White solid, mp = 199-201 °C (uncorrected). $^1$H NMR (CDCl$_3$, 500 MHz) δ 8.22 (dd, 1H, $J$ = 7.5 Hz, 2.0Hz), 7.94 (dd, 1H, $J$ = 7.0 Hz, 1.0Hz), 7.68-7.71 (m, 2H), 7.50-7.53 (m, 2H), 7.31-7.43 (m, 5H). $^{13}$C NMR (CDCl$_3$, 125 MHz) δ 158.9, 153.4, 149.5, 143.8, 134.1, 133.1, 132.5, 130.7, 128.8, 126.3, 126.2, 124.0, 123.9, 123.8, 123.5, 122.7, 121.0, 120.7, 111.2. HRMS (EI) Calcd for C$_{19}$H$_{11}$N$_2$OCl (M)$^+$ 318.0560; Found, 318.0561.
Characterization data of intermediates 6a and 7a in control experiments

**6a**

2-(2-(4-chlorophenoxy)phenyl)-1H-indole (6a) [New compound]. $^1$H NMR (CDCl$_3$, 400 MHz) $\delta$ 9.31 (s, 1H), 7.88–7.90 (m, 1H), 7.63 (d, 1H, $J$ = 8.0 Hz), 7.36 (d, 1H , $J$ = 7.6 Hz), 7.31–7.33 (m, 2H), 7.21–7.24 (m, 2H), 7.17 (t, 1H, $J$ = 7.6 Hz), 7.10 (t, 1H, $J$ = 7.2 Hz), 7.02 (d, 2H, $J$ = 9.2 Hz), 6.95 (d, 1H, $J$ = 1.2 Hz), 6.89–6.92 (m, 1H). $^{13}$C NMR (CDCl$_3$, 100 MHz) $\delta$ 155.0, 153.2, 136.3, 134.5, 130.0, 129.1, 128.6, 128.5, 128.0, 124.4, 123.3, 122.2, 120.4, 120.4, 120.0, 119.6, 110.9, 101.1. HRMS (EI) Calcd for C$_{20}$H$_{14}$NOCl (M)$^+$ 319.0764; Found, 319.0770.

**7a**

2-(1-(4-chlorophenyl)-1H-indol-2-yl)phenol (7a) [New compound]. $^1$H NMR (CDCl$_3$, 400 MHz) $\delta$ 7.68–7.70 (m, 1H), 7.29–7.32 (m, 3H), 7.21–7.23 (m, 2H), 7.18 (d, 1H , $J$ = 8.0 Hz), 7.12 (d, 2H, $J$ = 8.4 Hz), 6.93 (d, 1H, $J$ = 8.0 Hz), 6.88 (d, 1H, $J$ = 7.2 Hz), 6.81 (s, 1H), 6.75 (t, 1H, $J$ = 7.2 Hz), 5.84 (s, 1H). $^{13}$C NMR (CDCl$_3$, 100 MHz) $\delta$ 153.8, 138.4, 136.1, 134.5, 133.0, 131.0, 129.4, 128.7, 128.0, 123.1, 121.2, 120.8, 120.1, 118.1, 115.6, 110.6, 104.5. HRMS (EI) Calcd for C$_{20}$H$_{14}$NOCl (M)$^+$ 319.0764; Found, 319.0763.
Representation of the X-ray crystal structure of 3d (CCDC 890740)
References


H NMR of substrate 2a

$^{13}$C NMR of substrate 2a

$^1$H NMR of substrate 2b
\(^{13}\text{C}\) NMR of substrate 2b

\(^{1}\text{H}\) NMR of substrate 2c
$^{13}$C NMR of substrate 2c

$^1$H NMR of substrate 2d

$^{13}$C NMR of substrate 2d
$^1$H NMR of substrate 2e

$^{13}$C NMR of substrate 2e
$^1$H NMR of substrate 2f

$^{13}$C NMR of substrate 2f

$^1$H NMR of substrate 2g
\[ ^{13}\text{C NMR of substrate } 2g \]

\[ ^{1}\text{H NMR of substrate } 2h \]

\[ ^{13}\text{C NMR of substrate } 2h \]
$^{1}$H NMR of product 3a

$^{13}$C NMR of product 3a
$^1$H NMR of product 3b

$^{13}$C NMR of product 3b

$^1$H NMR of product 3c
$^{13}$C NMR of product 3c

$^1$H NMR of product 3d
$\textbf{13}^\text{C} \text{NMR of product 3d}$

$\textbf{1}^\text{H} \text{NMR of product 3e}$

$\textbf{13}^\text{C} \text{NMR of product 3e}$
$^1$H NMR of product 3g

$^{13}$C NMR of product 3g

$^1$H NMR of product 3h
$^{13}$C NMR of product 3h

$^1$H NMR of product 3i
$^{13}$C NMR of product 3i

$^1$H NMR of product 3j

$^{13}$C NMR of product 3j
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$^1$H NMR of product 3k

$^1$H NMR of product 3l

$^{13}$C NMR of product 3k
$^{13}$C NMR of product 3l

$^1$H NMR of intermediate 6a
$^{13}\text{C NMR of intermediate } 6\text{a}$

$^{1}\text{H NMR of intermediate } 7\text{a}$

$^{13}\text{C NMR of intermediate } 7\text{a}$