# Supporting information

# Regioselective Switching Approach for the Synthesis of $\alpha$ and $\delta$ Carboline Derivatives

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	HN N HN N 1a	Acid cata  Solvent , ⊺	alyst Femp	H N A	+ H	N J 3a
Entry	a Acid catalyst	Solvent	Tmep. ( <sup>o</sup> C)	Time (min)	Yield <b>2a</b> (%) <sup>b</sup>	Yield <b>3a</b> (%) <sup>b</sup>
1	FeCl <sub>3</sub> 20 mol%	$CH_2CI_2$	r.t.	25	29	36
2	ZrCl <sub>4</sub> 1eq	$CH_2CI_2$	r.t.	overnight	19	21
3	l <sub>2</sub> 20 mol%	$CH_2CI_2$	r.t.	60	24	38
4	TFA 20 mol%	$CH_2CI_2$	r.t.	30	24	26
5	Sc(OTf) <sub>3</sub> 10 mol%	$CH_2CI_2$	r.t.	overnight	15	8
6	FeCl <sub>3</sub> 20 mol%	1,2-DCE	80	15	34	29
7	InCl <sub>3</sub> 20 mol%	1,2-DCE	60	30	21	19
8	l <sub>2</sub> 20 mol%	1,2-DCE	80	25	35	41
9	l <sub>2</sub> 20 mol%	CH <sub>3</sub> CN	60	120	5	42
10	l <sub>2</sub> 20 mol%	CH <sub>3</sub> CN	80	120	n.	d.
11	l <sub>2</sub> 20 mol%	1,2-DME	60	15	10	50
12	l <sub>2</sub> 20 mol%	1,2-DME	80	15	9	52
13	l <sub>2</sub> 20 mol%	EtOH	60	30	6	41
14	l <sub>2</sub> 20 mol%	PEG-400	80	overnight	N.	R.
15	l <sub>2</sub> 20 mol%	DMSO	80	overnight	N.	R.
16	NbCl <sub>5</sub> 20 mol%	CH <sub>3</sub> CN	60	60	18	36
17	NbCl <sub>5</sub> 20 mol%	1,2-DME	60	60	19	19
18	NbCl <sub>5</sub> 20 mol%	DMSO	80	overnight	N.	R.

Table S1: Optimization studies of  $\delta$ -carboline on acid catalyst and solvent.

<sup>a</sup>All of reactions were carried out with 1 mmol **1a**, 2 mL solvent and acid catalyst.

<sup>b</sup>All of yields were determined from crude 1H NMR spectrum with dibromomethane as internal standard.



# Table S2: Optimization studies of $\delta$ -carboline on I<sub>2</sub> and solvent

Entry <sup>a</sup>	X (mol%)	Y (mL)	Temp. ( <sup>o</sup> C)	Time (min)	Yield <b>2a</b> (%) <sup>b</sup>	Yield <b>3a</b> (%) <sup>b</sup>
1	20	2	60	15	10	50
2	20	2	80	15	9	52
3	30	2	80	15	8	57
4	40	2	80	15	9	60
5	50	2	80	60	3	32
6	40	5	80	15	10	60
7	40	2	100	15	10	60
8	40	5	100	15	10	70
9	40	1	100	15	10	60
10	40	10	100	20	11	57

<sup>a</sup>All of reaction were carried out with 1mmol **1a**.

<sup>b</sup>All of yields were determined from crude 1H NMR spectrum with dibromomethane as internal standard.



# Table S3: Optimization studies of α-carboline

<sup>a</sup>The reactions were carried out with 1 mmol **1a**, 1 eq. DDQ and solvent, followed by addition of iodine as acid catalyst.

<sup>b</sup>All of yields were determined from crude 1H NMR spectrum with dibromomethane as internal standard.

#### **General information**

Reagents and solvents were purchased from various commercial sources and were used directly without any further purification, unless otherwise stated. Column chromatography was performed with 63–200 mesh silica gel. <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded at 400 and 100 MHz, or 500 and 125 MHz, respectively. Chemical shifts are reported in parts per million (d) using TMS and chloroform as internal standards and coupling constants are expressed in Hertz. Melting points were recorded using an electro thermal capillary melting point apparatus and are uncorrected. HRMS spectra were recorded using ESI-TOF or EI+ mode. The starting material indolyl carbonyl compound derivatives I were synthesized from various indole and chalcone derivatives followed by reported literatures.<sup>1</sup>

# Preparation of indoyloxime esters 1a-1u



#### **General procedures:**

A suspension of indolyl carbonyl compound I (5 mmol), hydroxylamine hydrochloride (0.52g, 7.5 mmol) in pyridine (1.25 mL) and EtOH (10 mL) was heated to 60 °C for 1 h. After completion of the reaction, the mixture was concentrated under reduced pressure. The residue was diluted with ethyl acetate (50 mL), and the organic layer was washed with aq. 3M HCI (20 mL) for two times, and then aq. NaHCO<sub>3</sub> (10 mL) for two times. The organic layer was dried over MgSO<sub>4</sub> and concentrated under reduced pressure to afford the crude indolyloxime II. Further, acetic anhydride (0.56g, 6 mmol) was added slowly to a solution of indolyloxime II (crude) in pyridine (2.5 mL) and CH<sub>2</sub>Cl<sub>2</sub>

<sup>&</sup>lt;sup>1</sup> F. Portela-Cubillo, B. A. Surgenor, R. A. Aitken, J.C. Walton J. Org. Chem. 2008, 73, 8125

(2.5 mL). The reaction mixture was stirred at ambient temperature for 3 h. After completion of the reaction, the mixture was diluted with ethyl acetate (50 mL), and the organic layer was washed with with aq. 3M HCl (20 mL) for three times, and then aq. NaHCO<sub>3</sub> (20 mL) for three times. The organic layer was dried over MgSO<sub>4</sub> and concentrated under reduced pressure. the residue was purified by column chromatography on silica gel (eluent: hexane/ethyl acetate = 5:1) to afford the pure indolyloxime ester **1a-1u**.

# (Z)-3-(1H-indol-3-yl)-1,3-diphenylpropan-1-one O-acetyl oxime (1a)



Brown solid, 76% yield; mp 117-118 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.10 (brs, 1H), 7.54-7.52 (m, 2H), 7.42-7.38 (m, 1H), 7.35-7.29 (m, 3H), 7.25-7.09 (m, 7H), 7.05 (d, J = 2.1 Hz, 1H), 6.97-6.93 (m, 1H), 4.44 (t, J = 7.8 Hz, 1H), 3.73 (dd, J = 12.9, 6.9 Hz, 1H), 3.64 (dd, J = 12.9, 8.7 Hz, 1H), 1.95 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

$$\begin{split} &\delta \ 169.0, \ 165.2, \ 143.1, \ 136.8, \ 134.3, \ 130.5, \ 128.8, \ 128.5, \ 128.0, \ 127.7, \ 126.8, \\ &126.7, \ 122.3, \ 121.6, \ 119.7, \ 119.6, \ 118.4, \ 111.4, \ 40.6, \ 34.7, \ 19.7,; \ HRMS \ (EI) \\ &m/z \ calcd. \ For \ C_{25}H_{22}N_2O_2 \ (M^+) \ 382.1681, \ found \ 382.1689. \end{split}$$

(Z)-3-(2-fluorophenyl)-3-(1H-indol-3-yl)-1-phenylpropan-1-one O-acetyl oxime (1b)



Pink solid, 99% yield; mp 124-126 °C; <sup>1</sup>H NMR (400 MHz, CDCl3)  $\delta$  8.20 (brs, 1H), 7.55 (d, *J* = 7.2 Hz, 2H), 7.42-7.38 (m, 1H), 7.39-7.35 (m, 4H), 7.21-7.17 (m, 1H), 7.15-7.09 (m, 3H), 7.00-6.93 (m, 3H), 4.83 (t, *J* = 7.86 Hz, 1H), 3.78-3.67 (m, 2H), 2.03 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl3)  $\delta$ 169.0, 165.3, 160.9 (d, *J*<sub>C-F</sub> = 245.8 Hz), 136.6,

134.1, 130.1 (d,  $J_{C-F} = 13.9 \text{ Hz}$ ), 129.9 (d,  $J_{C-F} = 4.3 \text{ Hz}$ ), 129.6, 128.5 (d,  $J_{C-F} = 8.4 \text{ Hz}$ ), 128.3, 127.5, 126.5, 124.2 (d,  $J_{C-F} = 3.3 \text{ Hz}$ ), 122.3, 121.9, 119.6, 119.2, 116.9, 115.7 (d,  $J_{C-F} = 22.4 \text{ Hz}$ ), 111.4, 34.0, 33.7, 19.8; HRMS (ESI) m/z calcd. For C<sub>25</sub>H<sub>21</sub>FN<sub>2</sub>O<sub>2</sub>Na (M+23) 423.1485, found 423.1483.

(Z)-3-(2-chlorophenyl)-3-(1H-indol-3-yl)-1-phenylpropan-1-one O-acetyl oxime (1c)



Brown solid, 99% yield; mp 137-139 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.35 (brs, 1H), 7.53 (d, *J* = 7.6 Hz, 2H), 7.37 (t, *J* = 7.28 Hz, 1H), 7.31-7.28 (m, 6H), 7.13-7.05 (m, 4H), 6.97 (t, *J* = 7.5 Hz, 1H), 5.12 (t, *J* = 7.9 Hz, 1H), 3.77 (dd, *J* = 13.4, 7.6 Hz, 1H), 3.58 (dd, *J* = 13.4, 8.3 Hz, 1H), 2.14 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  169.1, 165.2, 140.7,

136.5, 133.9, 133.5, 130.3, 129.5, 128.5, 127.9, 127.5, 126.9, 126.6, 122.2, 121.8, 119.4, 119.2, 117.2, 111.3, 36.4, 33.9, 19.8; HRMS (EI) m/z calcd. For  $C_{25}H_{21}CIN_2O_2$  (M<sup>+</sup>) 416.1292, found 416.1292.

(Z)-3-(2-bromophenyl)-3-(1H-indol-3-yl)-1-phenylpropan-1-one O-acetyl oxime (1d)



Brown solid, 70% yield; mp 138-139 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.24 (brs, 1H), 7.53-7.47 (m, 3H), 7.39-7.27 (m, 6H), 7.14-7.07 (m, 3H), 7.00-6.95 (m, 2H), 5.10 (t, *J* = 7.9 Hz, 1H), 3.77 (dd, *J* = 13.5, 7.7 Hz, 1H), 3.50 (dd, *J* = 13.5, 8.2 Hz, 1H), 2.15 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  169.3, 165.2, 142.5, 136.6, 134.1, 133.0, 130.4,

129.8, 128.6, 128.3, 127.7, 127.6, 126.7, 124.4, 122.4, 121.8, 119.7, 119.5, 117.7, 111.4, 39.2, 34.2, 20.0; HRMS (ESI) m/z calcd. For  $C_{25}H_{21}BrN_2O_2Na$  (M+23) 483.0684, found 483.0694.

(Z)-3-(1H-indol-3-yl)-3-(naphthalen-1-yl)-1-phenylpropan-1-one O-acetyl oxime (1e)



White solid, 66% yield; mp 141-143 °C, two isomers; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.08 (brs, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.82 (d, *J* =8.0 Hz, 1H), 7.71 (d, *J* = 8.2 Hz, 1H), 7.53 (d, *J* = 7.1 Hz, 1H), 7.46-7.26 (m, 9H), 7.09 (t, *J* = 7.7 Hz, 1H), 7.01 (d, *J* = 1.4 Hz, 1H), 6.91 (t, *J* = 7.5 Hz, 1H), 5.30 (1H, t, *J* = 7.7 Hz, CH), 3.96 (dd, *J* = 13.1, 8.1

Hz, 1H), 3.73 (dd, J = 13.1, 7.4 Hz, 1H), 1.91 (s, 3H); <sup>13</sup>C NMR (100 MHz,

CDCl<sub>3</sub>)  $\delta$  169.1, 165.6, 139.1, 136.7, 134.4, 134.2, 131.8, 130.4, 129.0, 128.7, 127.7, 127.6, 126.8, 126.1, 125.6, 125.5, 125.2, 123.5, 122.3, 122.2, 119.5, 118.5, 111.4, 36.1, 34.9, 19.6; HRMS (ESI) m/z calcd. For C<sub>29</sub>H<sub>24</sub>N<sub>2</sub>O<sub>2</sub>Na (M+23) 455.1736, found 455.1746.

(Z)-3-(1H-indol-3-yl)-3-(2-nitrophenyl)-1-phenylpropan-1-one O-acetyl oxime (1f)



Yellow solid, 74% yield; mp 85-86 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.18 (brs, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.48-7.45 (m, 3H), 7.39-7.34 (m, 2H), 7.30-7.22 (m, 5H), 7.13-7.09 (m, 2H), 6.94 (t, *J* = 7.5 Hz, 1H), 5.29 (t, *J* = 7.9 Hz, 1H), 3.83 (dd, *J* = 13.4, 8.1 Hz, 1H), 3.61 (dd, *J* = 13.4, 8.0 Hz, 1H), 2.12 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  169.2,

164.6, 150.0, 137.6, 136.6, 133.8, 132.6, 130.6, 130.4, 128.7, 127.8, 127.6, 126.5, 124.4, 122.7, 122.3, 119.9, 119.3, 116.5, 111.4, 34.9, 34.4, 19.9; HRMS (ESI) m/z calcd. For  $C_{25}H_{21}N_3O_4Na$  (M+23) 450.1430, found 450.1442.

(Z)-3-(1H-indol-3-yl)-3-(3-methoxyphenyl)-1-phenylpropan-1-one O-acetyl oxime (1g)



Red oil, 90% yield; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$ 8.06 (brs, 1H,), 7.55-7.53 (m, 2H), 7.42-7.28 (m, 5H), 7.15-7.11 (m, 2H), 7.07 (d, J = 1.7 Hz, 1H), 6.96 (d, J = 7.5 Hz, 1H), 6.82 (d, J = 7.7 Hz, 1H), 6.76 (s, 1H), 6.69 (dd, J = 8.2, 1.8 Hz, 1H), 4.42 (t, J = 7.8 Hz, 1H), 3.73 (dd, J = 12.9, 7.0 Hz, 1H), 3.7 (s, 3H), 3.64 (dd, J = 13.0, 8.7 Hz, 1H), 1.98 (s,

3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  169.0, 165.3, 159.7, 144.7, 136.8, 134.3, 130.5, 129.4, 128.7, 126.7, 122.3, 121.7, 120.5, 119.6, 119.5, 118.1, 114.2, 111.8, 111.4, 55.3, 40.6, 34.6, 19.7; HRMS (ESI) m/z calcd. For C<sub>26</sub>H<sub>24</sub>rN<sub>2</sub>O<sub>3</sub>Na (M+23) 435.1679, found 435.1668.

# (Z)-3-(benzo[d][1,3]dioxol-5-yl)-3-(1H-indol-3-yl)-1-phenylpropan-1-one O-acetyl oxime (1h)



White solid, 76% yield; mp 140-141 °C, <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.17 (brs, 1H,), 7.54-7.97 (m, 2H,), 7.43-7.39 (m, 1H), 7.36-7.27 (m, 4H), 7.15-7.11 (m, 1H), 7.06 (d, J = 2.2 Hz, 1H), 6.99-6.95 (m, 1H), 6.68-6.63 (m, 3H), 5.85 (dd, J = 4.5, 1.3 Hz, 2H), 4.38 (dd, J = 8.8, 6.8 Hz, 1H), 3.68 (dd, J = 12.9, 6.7 Hz, 1H), 3.61 (dd, J = 12.9, 9.1 Hz, 1H), 2.04 (s, 3H); <sup>13</sup>C NMR (100 MHz,

CDCl<sub>3</sub>)  $\delta$  168.9, 165.3, 147.7, 146.3, 137.0, 136.8, 134.2, 130.5, 128.7, 127.7, 126.6, 122.2, 121.4, 121.0, 119.4, 118.2, 111.5, 108.4, 107.9, 100.9, 40.4, 34.8, 19.7; 119.52, HRMS (EI) m/z calcd. For C<sub>26</sub>H<sub>22</sub>N<sub>2</sub>O<sub>4</sub> (M<sup>+</sup>) 426.1580, found 426.1575.

(Z)-3-(1H-indol-3-yl)-1-phenyl-3-(thiophen-2-yl)propan-1-one O-acetyl oxime (1i)



Pink solid, 60% yield; two isomers 6:1; mp 146-147 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.20 (brs, 1H), 7.57 (d, J = 7.2 Hz, 2H), 7.43-7.30 (m, 6H), 7.16-7.09 (m, 3H), 7.03-6.99 (m, 2H), 6.90-6.86 (m, 2H), 4.71 (t, J = 7.7 Hz, 1H), 3.86 (dd, J = 13.0, 8.2 Hz, 1H), 3.68 (dd, J = 12.9, 7.3 Hz, 1H), 1.91 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)

δ 168.8, 164.8, 147.8, 136.8, 134.0, 130.6, 128.8, 127.6, 126.7, 126.4, 124.6, 124.1, 122.3, 122.0, 119.7, 119.6, 117.5, 111.6, 36.3, 35.6, 19.5; HRMS (ESI) m/z calcd. For  $C_{23}H_{20}N_2O_2NaS$  (M+23) 411.1143, found 411.1143.

(Z)-1-(4-chlorophenyl)-3-(1H-indol-3-yl)-3-phenylpropan-1-one O-acetyl oxime (1j)



White solid, 66% yield; mp 191-192 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.22 (brs, 1H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.31-7.21 (m, 8H), 7.19-7.11 (m, 2H), 7.03 (s, 1H), 6.97 (1H, t, *J* = 7.5 Hz, CH), 4.46 (t, *J* = 7.8 Hz, 1H), 3.71 (dd, *J* = 13.0, 6.9 Hz, 1H), 3.62 (dd, *J* = 12.9, 8.8 Hz, 1H), 2.00 (s, 3H); <sup>13</sup>C NMR

(Z)-1-(4-bromophenyl)-3-(1H-indol-3-yl)-3-phenylpropan-1-one O-acetyl oxime (1k)



White solid, 82% yield; mp 175-176 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.18 (brs, 1H), 7.45 (d, *J* = 8.5 Hz, 2H), 7.31-7.25 (m, 4H), 7.19-7.17 (m, 6H), 7.03 (d, *J* = 1.6 Hz, 1H), 6.97 (t, *J* = 7.48 Hz, 1H), 4.46 (t, *J* = 7.8 Hz, 1H), 3.71 (dd, *J* = 12.9, 6.9 Hz, 1H), 3.62 (dd, *J* = 12.9, 8.8 Hz, 1H), 2.00 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  168.8, 164.3, 142.9,

136.8, 136.6, 132.7, 128.9, 128.5, 127.9, 126.9, 126.6, 122.4, 121.6, 119.6, 118.1, 118.1, 111.5, 40.6, 34.7, 19.6; HRMS (ESI) m/z calcd. For  $C_{25}H_{21}BrN_2O_2Na$  (M+23) 483.0684, found 483.0697.

(Z)-3-(1H-indol-3-yl)-1-(4-nitrophenyl)-3-phenylpropan-1-one O-acetyl oxime (1I)



White solid, 50% yield; mp 113 -114 °C; <sup>1</sup>H NMR (400 MHz, CDCI<sub>3</sub>)  $\delta$  8.12 (brs, 1H), 8.09 (d, *J* = 8.7 Hz, 2H), 7.58 (d, *J* = 8.7 Hz, 2H), 7.31-7.11 (m, 8H), 7.05 (d, *J* = 1.4 Hz, 1H), 6.97 (t, *J* = 7.5 Hz, 1H), 4.49 (t, *J* = 7.9 Hz, 1H), 3.8 (dd, *J* = 13.0, 7.1 Hz, 1H), 3.65 (dd, *J* = 12.9, 8.8 Hz, 1H,), 2.09 (s, 3H); <sup>13</sup>C NMR (100 MHz,

CDCl<sub>3</sub>)  $\delta$  168.4, 163.8, 148.8, 142.6, 140.6, 136.8, 128.7, 128.6, 127.9, 127.1, 126.5, 123.7, 122.6, 121.6, 119.8, 119.6, 117.9, 111.5, 40.6, 35.1, 19.7; HRMS (ESI) m/z calcd. For C<sub>25</sub>H<sub>21</sub>N<sub>3</sub>O<sub>4</sub>Na (M+23) 450.1430, found 450.1442.

# (Z)-3-(1H-indol-3-yl)-1-(4-isopropylphenyl)-3-phenylpropan-1-one O-acetyl oxime (1m)



White solid, 65% yield; two isomers; mp 135-137 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.10 (brs, 1H), 7.31 (d, *J* = 8.4 Hz, 1H), 7.26-7.10 (m ,10H), 6.95 (t, *J* = 7.2 Hz, 1H), 4.46 (t, *J* = 7.7 Hz, 1H), 3.73 (dd, *J* = 12.9, 6.9 Hz, 1H), 3.65 (dd, *J* = 12.9, 8.7 Hz, 1H), 2.92 (sep, *J* = 6.9 Hz, 1H), 1.93 (s, 3H), 1.25 (d, *J* = 7.0 Hz, 6H); <sup>13</sup>C NMR (100 MHz,

CDCl<sub>3</sub>)  $\delta$  169.1, 165.0, 151.6, 143.2, 136.8, 131.7, 128.5, 128.0, 127.7, 126.9, 126.8, 122.3, 121.7, 119.8, 119.5, 118.5, 111.4, 40.7, 34.6, 34.2, 24.0, 24.0, 19.7; HRMS (ESI) m/z calcd. For C<sub>28</sub>H<sub>28</sub>N<sub>2</sub>O<sub>2</sub>Na (M+23) 447.2048, found 447.2048.

(Z)-3-(1H-indol-3-yl)-1-(4-isobutylphenyl)-3-phenylpropan-1-one O-acetyl oxime (1n)



White solid, 66% yield; mp 119-120 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.33 (brs, 1H), 7.51 (d, *J* = 8.1 Hz, 2H), 7.31-7.12 (m, 10H), 7.06 (d, *J* = 2.2 Hz, 1H), 6.99 (t, *J* =7.5 Hz, 1H), 4.51 (t, *J* = 7.7 Hz, 1H), 3.76 (dd, *J* = 12.9, 6.7 Hz, 1H), 3.68 (dd, *J* = 12.9, 8.9 Hz, 1H), 2.52 (d, *J* = 7.2 Hz, 2H), 1.99 (s, 3H), 1.9 (n, *J* = 6.74 Hz, 1H), 0.94

(d, J = 6.64 Hz, 6H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  169.1, 165.3, 144.5, 143.1, 136.8, 131.5, 129.5, 128.4, 127.9, 127.4, 126.7, 126.7, 122.1, 121.7, 119.6, 119.6, 119.3, 118.1, 111.4, 45.3, 40.7, 34.6, 30.3, 22.5, 19.6; HRMS (ESI) m/z calcd. For C<sub>29</sub>H<sub>30</sub>N<sub>2</sub>O<sub>2</sub>Na (M+23) 461.2205, found 461.2224.

(Z)-1-(4-(tert-butyl)phenyl)-3-(1H-indol-3-yl)-3-phenylpropan-1-one O-acetyl oxime (10)



White solid, 70% yield; mp 110-112 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.15 (brs, 1H), 7.52-7.50 (m, 2H), 7.36 (d, *J* = 8.5 Hz, 2H), 7.3 (d, *J* = 8.2 Hz, 1H), 7.26-7.20 (m, 5H), 7.17-7.10 (m, 3H), 6.95 (t, *J* =7.5 Hz, 1H), 4.47 (t, *J* = 7.7 Hz, 1H), 3.73 (dd, *J* = 12.9, 6.9 Hz, 1H), 3.65 (dd, *J* = 12.9, 8.6

Hz, 1H), 1.92 (s, 3H), 1.32 (s, 9H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  169.1, 165.0, 153.9, 143.2, 136.8, 131.2, 128.4, 128.0, 127.4, 126.8, 125.7, 122.3, 121.7, 119.8, 119.5, 118.4, 111.4, 40.7, 34.9, 34.6, 31.4, 19.7; HRMS (ESI) m/z calcd. For C<sub>29</sub>H<sub>30</sub>N<sub>2</sub>O<sub>2</sub>Na (M+23) 461.2205, found 461.2208.

(Z)-3-(1H-indol-3-yl)-3-phenyl-1-(p-tolyl)propan-1-one O-acetyl oxime (5p)



White solid, 52% yield; mp 135-137 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.25 (brs, 1H), 7.49 (d, *J* = 8.2 Hz, 2H), 7.30-7.22 (m, 4H), 7.20-7.10 (m, 6H), 7.05 (d, *J* = 2.1 Hz, 1H), 6.96 (t, *J* = 7.4 Hz, 1H), 4.46 (t, *J* = 7.7 Hz, 1H), 3.73-3.62 (m, 2H), 2.37 (s, 3H), 1.95 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  169.1, 165.1, 143.2, 140.8, 136.8, 131.3, 129.5,

128.4, 128.0, 127.6, 126.7, 122.2, 121.7, 119.7, 119.4, 118.2, 111.4, 40.7, 34.5, 19.7, 21.5; HRMS (ESI) m/z calcd. For  $C_{26}H_{24}N_2O_2Na$  (M+23) 419.1736, found 419.1748.

(Z)-3-(1H-indol-3-yl)-1-(naphthalen-2-yl)-3-phenylpropan-1-one O-acetyl oxime (1q)



White solid, 73% yield; mp 161-163 °C, two isomers; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.14 (brs, 1H), 7.92 (s, 1H), 7.83-7.73 (m, 4H), 7.50 (p, *J* = 7.6 Hz, 2H), 7.31 (d, *J* = 8.2 Hz, 1H), 7.27-7.19 (m, 5H), 7.16-7.00 (m, 3H), 6.95 (1H, t, *J* = 7.48 Hz, CH), 4.54 (1H, t, *J* = 7.74 Hz, CH), 3.82 (1H, dd, *J* = 12.94, 7.0 Hz, CH<sub>2</sub>), 3.75 (1H, dd, *J* = 12.9, 8.62

Hz, CH<sub>2</sub>), 1.99 (3H, s, CH<sub>3</sub>); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) δ 168.8, 164.8, 142.9, 136.7, 134.2, 132.9, 131.4, 128.8, 128.3, 127.8, 127.6, 127.2, 126.7, 126.6, 126.5, 124.3, 122.2, 121.6, 119.6, 119.4, 118.1, 111.2, 40.7, 34.4, 19.5; HRMS (ESI) m/z calcd. For C<sub>29</sub>H<sub>24</sub>N<sub>2</sub>O<sub>2</sub>Na (M+23) 455.1736, found 455.1752.

(Z)-3-(1H-indol-3-yl)-1-(4-methoxyphenyl)-3-phenylpropan-1-one O-acetyl oxime (1r)



White solid, 80% yield; mp 138-139 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.06 (brs, 1H), 7.52 (d, *J* = 8.7 Hz, 2H), 7.31 (d, *J* = 8.1 Hz, 1H), 7.25-7.10 (m, 8H), 6.94 (d, *J* = 7.5 Hz, 1H), 6.84 (d, *J* = 8.7 Hz, 2H), 4.45 (t, *J* = 7.7 Hz, 1H), 3.81 (s, 3H), 3.69 (dd, *J* = 12.9, 7.0 Hz, 1H), 3.62 (dd, *J* = 13.0, 8.7 Hz, 1H), 1.91 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$ 

169.1, 164.5, 161.6, 143.2, 143.2, 136.8, 129.2, 128.5, 128.0, 126.8, 126.5, 122.3, 121.6, 119.8, 119.5, 118.4, 114.2, 111.4, 55.5, 40.8, 34.4, 19.7; HRMS (ESI) m/z calcd. For C<sub>26</sub>H<sub>24</sub>N<sub>2</sub>O<sub>3</sub>Na (M+23) 435.1685, found 435.1694.

(Z)-3-(5-bromo-1H-indol-3-yl)-1,3-diphenylpropan-1-one O-acetyl oxime (1s)



White solid, 73% yield; mp 125-127°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.39 (brs, 1H), 7.50 (d, *J* = 7.4 Hz, 2H), 7.43-7.31 (m, 4H), 7.25-7.11 (m, 7H), 6.98 (d, *J* = 1.9 Hz, 1H,), 4.37 (t, *J* = 7.8 Hz, 1H), 3.73 (dd, *J* = 13.0, 7.3 Hz, 1H), 3.59 (dd, *J* = 13.0, 8.5 Hz, 1H), 2.01 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  169.1, 165.3, 142.6, 135.4, 134.1, 130.6,

128.8, 128.6, 128.4, 127.8, 127.6, 127.0, 125.1, 123.1, 122.1, 117.7, 112.9, 112.7, 40.4, 34.7, 19.8; HRMS (ESI) m/z calcd. For C<sub>25</sub>H<sub>21</sub>BrN<sub>2</sub>O<sub>2</sub>Na (M+23) 483.0684, found 483.0697.

(Z)-3-(5-nitro-1H-indol-3-yl)-1,3-diphenylpropan-1-one O-acetyl oxime (1t)



Yellow solid, 66% yield; mp 174-177 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.74 (brs, 1H), 8.09 (d, J = 2.2 Hz, 1H), 7.92 (dd, J = 9.0, 2.2 Hz, 1H), 7.65 (d, J = 2.1 Hz, 1H), 7.55-7.53 (m, 2H), 7.48 (d, J = 9.0 Hz, 1H), 7.45-7.43 (m, 1H), 7.38 (t, J = 7.4 Hz, 2H), 7.28 (d, J = 7.2 Hz, 2H), 7.22 (t, J = 7.5 Hz, 2H), 7.14 (t, J = 7.16 Hz, 1H), 4.49 (t, J = 7.9 Hz,

1H), 3.79-3.68 (m, 2H), 2.05 (s, 3H);  $^{13}\text{C}$  NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  168.4, 165.1, 143.4, 140.6, 139.9, 134.4, 130.8, 128.9, 128.7, 128.1, 127.7, 127.0,

126.9, 125.9, 119.9, 117.0, 116.1, 112.4, 39.9, 34.3, 19.8; HRMS (ESI) m/z calcd. For  $C_{25}H_{21}N_3O_4Na$  (M+23) 450.1430, found 450.1431.

# (Z)-3-(5-methoxy-1H-indol-3-yl)-1,3-diphenylpropan-1-one O-acetyl oxime (1u)



White solid, 80% yield; mp 144-146 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.27 (brs, 1H), 7.56 (d, *J* = 7.4 Hz, 2H), 7.42 (t, *J* = 7.3 Hz, 1H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.26-7.15 (m, 6H), 7.00 (d, *J* = 2.2 Hz, 1H), 6.78 (dd, *J* = 8.8, 2.3 Hz, 1H), 6.66 (d, *J* = 2.2 Hz, 1H), 4.41 (t, *J* = 7.8 Hz, 1H), 3.74-3.60 (m, 5H), 2.00 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  169.0,

165.3, 153.8, 142.9, 134.1, 131.9, 130.5, 128.7, 128.4, 127.9, 127.6, 127.0, 126.8, 122.5, 117.7, 112.1, 101.7, 55.9, 40.6, 34.7, 19.7; HRMS (ESI) m/z calcd. For  $C_{26}H_{24}N_2O_3Na$  (M+23) 435.1685, found 435.1678.

# Synthesis of $\delta$ -carbolines 3a-3u

#### **General procedure:**

A mixture of indolyloxime esters **1a-1u** (1 mmol) and iodine (0.102g, 0.4 eq.) in 1,2-dimethoxyethane (1,2-DME, 5 mL) was heated to 100 °C. After completion of the reaction, the mixture was allowed to cool to ambient temperature and worked up with aq. Na<sub>2</sub>S<sub>2</sub>O<sub>3</sub> (1 mL) and aq. NaHCO<sub>3</sub> (1 mL). The reaction mixture was extracted with ethyl acetate (20 mL) for three times. The combined organic layer was dried over MgSO<sub>4</sub> and concentrated under reduce pressure. The residue was purified by column chromatography on silica gel (eluent: hexane/ethyl acetate = 12:1) to afford  $\delta$ -carbolines **3a-3u** and minor mixture of  $\alpha$ -carbolines **2a-2u**.

# 2,4-diphenyl-δ-carboline (3a)



White solid, 70% yield; mp 232-234 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.49 (d, *J* = 7.8 Hz, 1H), 8.41 (brs, 1H,), 8.17 (d, *J* = 7.5 Hz, 2H), 7.8 (brs, 1H), 7.76 (d, *J* = 7.3 Hz, 2H), 7.59 (t, *J* = 7.5 Hz, 2H), 7.51 (t, *J* = 7.3 Hz, 4H), 7.46-7.39 (m, 2H,, 7.33 (t, *J* = 7.4 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  151.4,

143.1, 141.0, 140.7, 137.2, 132.4, 130.2, 129.7, 128.9, 128.9, 128.4, 128.3, 128.1, 127.4, 123.3, 121.6, 120.6, 117.4, 111.4. HRMS (EI) m/z calcd. For

C<sub>23</sub>H<sub>16</sub>N<sub>2</sub> (M<sup>+</sup>) 320.1313, found 320.1317.

# 4-(2-fluorophenyl)-2-phenyl-δ-carboline (3b)



White solid, 66% yield; mp 258-259 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.42 (brs, 1H), 8.31 (1H, d, J = 7.8 Hz, CH), 8.27-8.25 (m, 2H), 7.97 (s, 1H), 7.80 (td, J = 7.6, 1.7 Hz, 1H), 7.66-7.61 (m, 1H), 7.58-7.39 (m, 7H), 7.31-7.24 (m, 1H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  159.9 (d,  $J_{C-F} = 247.3$  Hz), 148.9, 142.2, 141.9, 140.1, 132.1, 132.1, 131.5 (d,  $J_{C-F} = 247.3$  Hz)

8.3 Hz), 130.7, 129.2, 128.4 (d,  $J_{C-F} = 24.3$  Hz), 127.0, 126.9, 125.6 (d,  $J_{C-F} = 3.1$  Hz), 124.4 (d,  $J_{C-F} = 15.3$  Hz), 124.4, 122.0, 120.8, 120.1, 118.3, 116.8 (d,  $J_{C-F} = 21.5$  Hz), 112.5. HRMS (ESI) m/z calcd. For C<sub>23</sub>H<sub>16</sub>FN<sub>2</sub> (M+1) 339.1292, found 339.1299.

# 4-(2-chlorophenyl)-2-phenyl-δ-carboline (3c)



White solid, 63% yield; mp 253-255 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.37 (brs, 1H), 8.32 (d, *J* = 7.8 Hz, 1H), 8.27-8.25 (m, 2H), 7.9 (s, 1H), 7.75-7.71 (m, 1H), 7.70-7.65 (m, 1H), 7.61-7.48 (m, 6H), 7.41-7.38 (m, 1H), 7.31-7.27 (m, 1H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  148.6, 142.1, 141.9, 140.1, 135.8, 132.9, 132.3, 130.9, 130.8, 130.4, 129.2, 128.5,

128.2, 127.0, 122.1, 121.8, 120.1, 118.2, 112.6. HRMS (EI) m/z calcd. For  $C_{23}H_{16}\text{CIN}_2$  (M+1) 355.1002, found 355.1009.

# 4-(2-bromophenyl)-2-phenyl-δ-carboline (3d)



White solid, 46% yield; mp 266-267°C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.30 (brs, 1H), 8.28 (d, *J* = 7.8 Hz, 1H), 8.44-8.22 (m, 2H), 7.88-7.86 (m, 1H), 7.85 (s, 1H), 7.64-7.57 (m, 2H), 7.52-7.46 (m, 5H), 7.40-7.35 (m, 1H), 7.28-7.24 (m, 1H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  148.6, 142.2, 141.9, 140.1, 137.8, 133.5, 132.2, 132.1, 131.0, 130.6, 129.2, 128.7,

128.5, 128.2, 126.9, 123.1, 122.2, 120.7, 120.1, 118.1, 112.6. HRMS (EI) m/z calcd. For  $C_{23}H_{16}BrN_2$  (M+1) 399.0491, found 399.0493.

# 4-(naphthalen-1-yl)-2-phenyl-δ-carboline (3e)



White solid, 59% yield; mp 242-243 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.53 (d, *J* = 7.84 Hz, 1H), 8.18 (d, *J* = 7.4 Hz, 2H), 8.00-7.99 (m, 3H), 7.87 (s, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.66-7.60 (m, 2H), 7.43-7.38 (m, 2H), 7.57-7.46 (m, 4H), 7.35-7.29 (m, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  151.0, 142.7, 140.9, 140.6, 134.5, 134.1, 131.4, 131.1, 129.4,

128.9, 128.9, 128.3, 128.1, 127.7, 127.4, 127.2, 126.7, 125.9, 125.7, 123.2, 121.6, 120.6, 119.3, 111.4. HRMS (EI) m/z calcd. For  $C_{27}H_{19}N_2$  (M+1) 371.1548, found 371.1556.

## 4-(2-nitrophenyl)-2-phenyl-δ-carboline (3f)



Yellow solid; mp 280-281 °C; <sup>1</sup>H NMR (400 MHz,  $(CD_3)_2SO)$   $\delta$  11.40 (s, 1H), 8.31-8.28 (m, 2H), 8.23-8.21 (m, 2H), 7.93 (td, J = 7.5, 1.1 Hz, 1H), 7.88 (s, 1H), 7.84-7.77 (m, 2H), 7.52-7.47 (m, 4H), 7.38 (t, *J* = 7.3 Hz, 1H), 7.29-7.26 (m, 1H); <sup>13</sup>C NMR (100 MHz,  $(CD_3)_2SO)$   $\delta$  148.8, 148.7, 141.9, 141.9, 139.9, 134.6, 133.2, 131.6, 130.8, 130.6, 129.9,

129.2, 128.5, 128.2, 126.9, 125.4, 122.2, 120.8, 120.3, 116.9, 112.5. HRMS (EI) m/z calcd. For  $C_{23}H_{15}N_3O_2$  (M<sup>+</sup>) 365.3841.

# 4-(3-methoxyphenyl)-2-phenyl-δ-carboline (3g)



White solid, 70% yield; mp 179-181 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.49 (d, *J* = 7.8 Hz, 1H), 8.41 (s, 1H), 8.17 (d, *J* = 7.6 Hz, 2H), 7.8 (s, 1H), 7.59 (t, *J* = 7.5 Hz, 2H), 7.53-7.38 (m, 6H), 7.35-7.27 (m, 3H), 7.04 (dd, *J* = 8.1, 1.9 Hz, 1H), 3.89 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  160.6, 151.4, 143.1, 141.0, 140.7, 138.6, 132.2, 130.8, 130.2, 128.9, 128.2,

128.1, 127.4, 123.3, 121.6, 120.6, 120.6, 117.3, 114.2, 111.4, 55.7. HRMS (EI) m/z calcd. For C<sub>24</sub>H<sub>19</sub>N<sub>2</sub>O (M+1) 351.1492, found 351.1498.

# 4-(benzo[d][1,3]dioxol-5-yl)-2-phenyl-δ-carboline (3h)



White solid, 68% yield; mp 221-222 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.47 (d, *J* = 7.8 Hz, 1H), 8.34 (brs, 1H), 8.15 (d, *J* = 7.7 Hz, 2H), 7.52-7.44 (m, 4H), 7.74 (s, 1H), 7.39 (t, *J* = 7.26 Hz, 1H), 7.33 (t, *J* = 7.4 Hz, 1H), 7.24 (d, *J* = 8.8 Hz, 2H), 7.01 (d, *J* = 7.8 Hz, 1H), 6.08 (s, 2H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  151.5, 148.9, 148.4, 143.1, 141.0, 140.8,

132.1, 130.2, 128.9, 128.2, 128.1, 127.4, 123.4, 122.1, 121.6, 120.6, 117.2, 111.4, 109.5, 108.7, 101.8. HRMS (ESI) m/z calcd. For  $C_{24}H_{17}N_2O_2$  (M+1) 365.1290, found 365.1288.

# 2-phenyl-4-(thiophen-2-yl)-δ-carboline (3i)



White solid, 73% yield; mp 249-250 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.52 (brs, 1H,), 8.46 (d, *J* = 7.8 Hz, 1H), 8.15 (d, *J* = 7.4 Hz, 2H), 7.88 (s, 1H), 7.59 (d, *J* = 7.8 Hz, 1H), 7.52-7.46 (m, 5H), 7.40 (t, *J* = 7.4 Hz, 1H), 7.34-7.31 (m, 1H), 7.25-7.24 (m, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  151.3, 143.6, 141.1, 140.5, 138.9, 129.2, 128.9, 128.6, 128.3, 128.3,

127.4, 126.9, 126.5, 125.2, 123.3, 121.6, 120.9, 116.2, 111.6; HRMS (ESI) m/z calcd. For  $C_{21}H_{15}N_2S$  (M+1) 327.0596, found 327.0597.

# 2-(4-chlorophenyl)-4-phenyl-δ-carboline (3j)



White solid, 63% yield; mp 310-311 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.49 (brs, 1H), 8.32-8.26 (m, 3H), 8.41 (s, 1H), 8.17 (d, *J* = 7.5 Hz, 2H), 8.00 (s, 1H), 7.91-7.89 (m, 2H), 7.65-7.49 (m, 7H), 7.27 (t, *J* = 7.5 Hz, 1H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  148.0, 142.7, 142.2, 139.1, 136.8, 133.2, 132.4, 130.3, 129.7, 129.2, 129.1, 129.1, 128.7, 128.19,

122.2, 120.7, 120.2, 116.9, 112.8. HRMS (EI) m/z calcd. For C<sub>23</sub>H<sub>16</sub>ClN<sub>2</sub> (M+1) 355.1002, found 355.1010.

## 2-(4-bromophenyl)-4-phenyl-δ-carboline (3k)



White solid, 68% yield; mp 315-317 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.52 (brs, 1H), 8.30-8.25 (m, 3H), 8.00 (s, 1H), 7.93-7.91 (m, 2H), 7.77-7.51 (m, 7H), 7.29 (t, *J* = 7.5 Hz, 1H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  148.0, 142.7, 142.2, 139.4, 136.8, 132.4, 131.9, 130.3, 129.7, 129.2, 129.1, 129.1, 128.2, 122.2, 121.9, 120.8, 120.2, 116.9,

112.8. HRMS (EI) m/z calcd. For C<sub>23</sub>H<sub>15</sub>BrN<sub>2</sub> (M<sup>+</sup>) 398.0419, found 398.0418.

# 2-(4-nitrophenyl)-4-phenyl-δ-carboline (3l)



Yellow solid, 66% yield; mp 315-316 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.64 (brs, 1H), 8.59-8.55 (m, 2H), 8.35-8.31 (m, 3H), 8.16 (s, 1H), 7.94-7.92 (m, 2H), 7.68-7.54 (m, 5H), 7.32 (t, *J* = 7.0 Hz, 1H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  147.3, 146.6, 146.4, 143.1, 142.4, 132.4, 136.5, 130.7, 129.7, 129.3, 129.2, 128.5,

127.8, 124.3, 122.1, 120.9, 120.5, 118.0, 112.9. HRMS (EI) m/z calcd. For  $C_{23}H_{15}N_3O_2\ (M^+)\ 365.3841$ 

# 2-(4-isopropylphenyl)-4-phenyl-δ-carboline (3m)



White solid, mp 245-247 °C; <sup>1</sup>H NMR (400 MHz,  $(CD_3)_2SO$ )  $\delta$  11.45 (brs, 1H), 8.29 (d, J = 7.8 Hz, 1H), 8.18 (d, J = 8.2 Hz, 2H), 7.95 (s, 1H), 7.92 (d, J = 7.3 Hz, 2H), 7.65 (t, J = 7.5 Hz, 2H), 7.62-7.50 (m, 3H), 7.38 (2H, d, J = 8.2 Hz, CH), 7.28 (t, J = 7.5 Hz, 1H), 2.95 (sep, J = 6.9 Hz, 1H), 1.26 (d, J = 6.8 Hz, 6H): <sup>13</sup>C NMR (100 MHz,

 $(CD_3)_2SO) \ \delta \ 149.6, \ 148.7, \ 142.6, \ 142.1, \ 138.0, \ 136.9, \ 132.4, \ 130.0, \ 129.7, \\ 129.1, \ 129.1, \ 128.0, \ 127.1, \ 127.0, \ 122.3, \ 120.7, \ 120.1, \ 116.8, \ 112.8, \ 33.7, \\ 24.3. \ HRMS (ESI) \ m/z \ calcd. \ For \ C_{26}H_{23}N_2 \ (M+1) \ 363.1861, \ found \ 363.1859.$ 

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# 2-(4-isobutylphenyl)-4-phenyl-δ-carboline (3n)



White solid, 68% yield; mp 254-255 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.50 (d, *J* = 7.8 Hz, 1H), 8.29 (brs, 1H), 8.08 (d, *J* = 8.1 Hz, 2H), 7.80 (s, 1H), 7.77 (d, *J* = 7.4 Hz, 2H), 7.61 (t, *J* = 7.54 Hz, 2H), 7.54-7.50 (m, 2H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.34 (t, *J* = 7.44 Hz, 1H), 7.29 (d, *J* = 8.0 Hz, 2H), 2.56 (d, *J* = 7.2 Hz, 2H), 1.94 (sep, *J* = 6.7 Hz, 1H),

0.95 (d, J = 6.6 Hz, 1H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  151.5, 142.9, 141.8, 140.8, 138.1, 137.1, 132.2, 129.8, 129.5, 129.5, 128.8, 128.2, 127.8, 126.9, 123.2, 121.4, 120.4, 117.1, 111.1, 45.2, 30.3, 22.4; HRMS (ESI) m/z calcd. For C<sub>27</sub>H<sub>25</sub>N<sub>2</sub> (M+1) 377.2018, found 377.2015.

# 2-(4-(tert-butyl)phenyl)-4-phenyl-δ-carboline (30)



White solid, 63% yield; mp 284-285 °C; <sup>1</sup>H NMR (400 MHz, CDCI<sub>3</sub>)  $\delta$  8.49 (d, *J* = 7.8 Hz, 1H), 8.36 (brs, 1H,), 8.09 (d, *J* = 8.4 Hz, 2H), 7.79 (brs, 1H), 7.77-7.75 (m , 2H), 7.6 (t, *J* = 7.5 Hz, 2H), 7.55-7.49 (m, 4H), 7.45 (d, *J* = 8.0 Hz, 1H), 7.34 (t, *J* = 7.4 Hz, 1H), 1.40 (s, 9H); <sup>13</sup>C NMR (100 MHz, CDCI<sub>3</sub>)  $\delta$  151.6, 151.3, 143.1, 140.9, 138.0,

137.3, 132.3, 130.1, 129.7, 128.9, 128.4, 127.9, 127.1, 125.9, 123.4, 121.6, 120.6, 117.3, 111.4, 34.8, 31.6; HRMS (ESI) m/z calcd. For  $C_{27}H_{25}N_2$  (M+1) 377.2018, found 377.2019.

## 4-phenyl-2-(p-tolyl)-δ-carboline (3p)



White solid, 67% yield; mp 304-305 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.45 (brs, 1H), 8.30 (d, *J* = 7.8 Hz, 1H), 8.19 (d, *J* = 8.0 Hz, 2H), 7.96 (s, 1H), 7.92 (d, *J* = 7.3 Hz, 2H), 7.68-7.50 (m, 5H), 7.77-7.51 (m, 7H), 7.33-7.20 (m, 3H), 2.38 (s, 3H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  149.5, 142.6, 142.1, 137.7, 137.5, 136.9, 132.4, 130.01, 129.7,

129.7, 129.1, 129.1, 127.9, 126.9, 122.3, 120.7, 120.1, 116.7, 112.7, 21.3. HRMS (ESI) m/z calcd. For  $C_{24}H_{19}N_2$  (M+1) 335.1548 found 335.1556.

# 2-(naphthalen-2-yl)-4-phenyl-δ-carboline (3q)



Yellow solid, 65% yield; mp 286-287 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.53 (brs, 1H), 8.84 (s, 1H), 8.56 (dd, *J* = 8.6, 1.6 Hz, 1H), 8.37 (d, *J* = 7.8Hz, 1H), 8.21 (s, 1H), 8.08 (t, *J* = 8.6 Hz, 2H), 7.98 (d, *J* = 7.6 Hz, 3H), 7.71-7.52 (m, 7H), 7.32 (t, *J* = 7.4 Hz, 1H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$ 149.2, 142.8, 142.2, 137.7, 136.9, 133.8, 133.3,

132.5, 130.3, 129.7, 129.2, 129.2, 128.9, 128.5, 128.1, 128.1, 128.0, 126.8, 126.6, 125.8, 125.4, 122.4, 120.8, 120.2, 117.4, 112.8,. HRMS (EI) m/z calcd. For  $C_{27}H_{18}N_2$  (M<sup>+</sup>) 370.1470, found 370.1468.

## 2-(4-methoxyphenyl)-4-phenyl-δ-carboline (3r)



White solid, 80% yield; mp 288-290 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.38 (brs, 1H), 8.29-8.19 (m, 3H), 7.90-7.88 (s, 2H), 7.65-7.47 (m5H), 7.25 (t, *J* = 7.4 Hz, 1H), 7.05 (d, *J* = 8.6 Hz, 2H), 3.81 (s, 3H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  159.9, 149.4, 142.5, 142.1, 137.0, 132.9, 132.4, 129.8, 129.7, 129.1, 129.1, 128.3, 127.9, 122.3, 120.7,

120.0, 116.4, 114.5, 112.7, 55.7. HRMS (EI) m/z calcd. For  $C_{24}H_{18}N_2O$  (M<sup>+</sup>) 350.1419, found 350.1422.

#### 8-bromo-2,4-diphenyl-δ-carboline (3s)



White solid, 70% yield; mp 219-222 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.63 (brs, 1H), 8.38 (d, *J* = 1.9 Hz, 1H), 8.29-8.27 (m, 2H), 8.02 (s, 1H), 7.91-7.89 (m, 2H), 7.66-7.62 (m, 3H), 7.58-7.54 (m, 2H), 7.50 (t, *J* = 7.6 Hz, 2H), 7.40 (t, *J* = 7.3 Hz, 1H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  150.0, 141.3, 140.7, 139.9, 136.6, 133.0, 130.7, 130.4,

129.7, 129.3, 129.1, 129.1, 128.6, 127.1, 124.1, 122.9, 117.7, 114.9, 112.3; HRMS (ESI) m/z calcd. For C<sub>23</sub>H<sub>16</sub>BrN<sub>2</sub> (M+1) 399.0491, found 399.0484.

# 8-nitro-2,4-diphenyl-δ-carboline (3t)



Yellow solid, 60% yield; mp 254-256 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  12.18 (brs, 1H), 9.07 (d, *J* = 1.6 Hz, 1H), 8.36 (dd, *J* = 8.8, 1.9 Hz, 1H), 8.30 (d, *J* = 7.5 Hz, 2H), 8.08 (s, 1H), 7.89 (d, *J* = 7.3 Hz, 1H), 7.72-7.51 (m, 6H), 7.44 (t, *J* = 7.1 Hz, 1H), <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  151.1, 144.9, 142.3, 139.6, 136.1, 133.9, 131.8, 129.8,

129.6, 129.2, 128.9, 127.3, 123.2, 121.9, 118.5, 117.2, 113.2; HRMS (ESI) m/z calcd. For  $C_{23}H_{16}N_3O_2$  (M+1) 366.1243, found 366.1243.

#### 8-methoxy-2,4-diphenyl-δ-carboline (3u)



White solid, 76% yield; mp 259-260 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  11.27 (brs, 1H), 8.27 (d, *J* = 7.5 Hz, 2H), 7.95 (brs, 1H), 7.90 (d, *J* = 7.3 Hz, 2H), 7.73 (d, *J* = 2.0 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 2H), 7.56-7.48 (m, 4H), 7.38 (t, *J* = 7.2 Hz, 2H), 7.14 (dd, *J* = 8.7, 2.3 Hz, 1H), 3.89 (s, 3H); <sup>13</sup>C NMR (100 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  154.2, 149.0, 142.5,

140.3, 137.0, 136.9, 132.4, 130.7, 129.7, 129.1, 129.1, 129.0, 128.4, 127.1, 122.6, 118.1, 116.8, 113.7, 102.2, 56.0. HRMS (ESI) m/z calcd. For C<sub>24</sub>H<sub>19</sub>N<sub>2</sub>O (M+1) 351.1492, found 351.1493.

#### Synthesis of α-carbolines 2a-2u

#### **General procedure:**

А mixture of indolyloxime esters 1a-1u (1 mmol) and 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ, 0.227q. 1 eq.) in 1,2-dichloroethane (1,2-DCE, 10 mL) was stirred at ambient temperature for 30 min, followed by addition of iodine (0.508g, 20 mol%) and the reaction mixture was heated to 60 °C. After completion of the reaction, the mixture was allowed to cool to ambient temperature and diluted with ethyl acetate (50 mL). The reaction mixture was washed with aq. 1M NaOH (10 mL) for two times. The combined water layer was extracted with ethyl acetate (20 mL) for three times. The combined organic layer was dried over MgSO4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (eluent: hexane/ethyl acetate = 12:1) to afford  $\alpha$ -carbolines **2a-2u**.

# 2,4-diphenyl-α-carboline (2a)



White solid, 70% yield; mp 216.5-217.5°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>),  $\delta$  11.81 (brs, 1H), 8.24 (td , J = 6.2, 1.2 Hz, 2H), 7.78-7.77 (m, 2H), 7.49-7.46 (m, 8H), 7.22 (td, J = 7.8, 0.8 Hz, 1H), 6.96 (td, J = 7.7, 0.6 Hz , 1H), 6.55 (d, J = 8.2 Hz, 1H); <sup>13</sup>C NMR  $\delta$  154.5, 153.5, 146.4, 140.4, 139.6, 139.5, 129.3, 129.0, 128.9, 128.9, 128.8, 128.0, 126.6, 122.5,

120.8, 119.7, 114.6, 113.1, 111.6; HRMS (EI) m/z calcd. For  $C_{23}H_{16}N_2$  (M<sup>+</sup>) 320.1313, found 320.1313.

#### 4-(2-fluorophenyl)-2-phenyl-α-carboline (2b)



White solid, 77% yield; mp 250-251 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  11.79 (brs, 1H), 8.21 (d, *J* = 7.3 Hz, 2H), 7.65-7.47 (m, 6H), 7.41-7.30 (m, 3H), 7.18 (t, *J* = 7.58 Hz, 1H), 6.98 (t, *J* = 7.5 Hz, 1H), 6.55 (d, *J* = 8.1 Hz, 1H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  160.9, 158.5, 154.2, 153.0, 140.1, 139.4, 131.2, 131.2, 130.6, 130.6, 129.1, 128.8, 127.8, 126.8, 126.6,

126.5, 124.5, 122.0, 120.6, 119.8, 116.3, 116.1, 114.9, 113.7, 111.3; HRMS (ESI) m/z calcd. For  $C_{23}H_{16}N_2F$  (M+1) 339.1298, found 339.1300.

#### 4-(2-chlorophenyl)-2-phenyl-α-carboline (2c)



White solid, 90% yield; mp 243-244 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  11.42 (brs, 1H), 8.22 (d, *J* = 7.4 Hz, 2H), 7.66-7.64 (m, 1H), 7.58-7.45 (m, 7H), 7.21 (7, *J* = 7.7 Hz, 1H), 7.15 (d, *J* = 7.8 Hz, 1H), 6.98 (t, *J* = 7.5 Hz, 1H), 6.67 (d, *J* = 8.1 Hz, 1H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  154.3, 153.2, 142.9, 140.3, 139.6, 138.0, 133.2, 130.9, 130.2, 130.1, 129.4,

129.0, 128.1, 127.3, 126.7, 122.2, 120.7, 119.9, 114.7, 113.9, 111.6; HRMS (ESI) m/z calcd. For C<sub>23</sub>H<sub>16</sub>N<sub>2</sub>Cl (M+1) 355.1002, found 355.1002.

# 4-(2-bromophenyl)-2-phenyl-α-carboline (2d)



Brown solid, 85% yield; mp 254-255 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  11.73 (brs, 1H), 8.24 (d, *J* = 7.2 Hz, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.58-7.49 (m, 6H), 7.45-7.40 (m, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.11 (d, *J* = 7.9 Hz, 1H), 6.97 (t, *J* = 7.6 Hz, 1H), 6.58 (d, *J* = 8.2 Hz, 1H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  154.3, 153.1, 144.5, 140.3, 140.0, 139.5, 133.4, 130.9,

130.2, 129.3, 129.0, 128.0, 127.9, 126.7, 122.8, 122.3, 120.7, 120.0, 114.5, 113.7, 111.5; HRMS (ESI) m/z calcd. For  $C_{23}H_{16}N_2Br$  (M+1) 399.0497, found 399.0497.

#### 4-(naphthalen-1-yl)-2-phenyl-α-carboline (2e)



White solid, 57% yield; mp 247-248 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  12.07 (brs, 1H), 8.29 (d, *J* = 7.3 Hz, 2H), 8.07 (dd, *J* = 6.9, 2.0 Hz, 1H), 8.03 (d, *J* = 8.2 Hz, 1H), 7.75-7.67 (m, 4H), 7.59-7.49 (m, 4H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.13-7.09 (m, 1H), 6.79-6.73 (m, 2H), 6.53 (d, *J* = 8.1 Hz, 1H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  154.1, 153.1, 144.3, 140.1,

139.4, 136.8, 133.6, 131.1, 129.2, 128.8, 128.8, 128.4, 127.8, 126.6, 126.5, 126.3, 126.2, 125.9, 125.5, 122.4, 120.6, 119.6, 115.4, 114.6, 111.2; HRMS (ESI) m/z calcd. For  $C_{27}H_{19}N_2$  (M+1) 371.1548, found 371.1549.

#### 4-(2-nitrophenyl)-2-phenyl-α-carboline (2f)



Yellow solid, 93% yield; mp 238-239 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  11.83 (brs, 1H), 8.26 (d, *J* = 8.2 Hz, 1H), 8.20 (d, *J* = 7.4 Hz, 2H), 7.81 (t, *J* = 7.5 Hz, 1H), 7.73 (t, *J* = 7.8 Hz, 1H), 7.66 (d, *J* = 7.5 Hz, 1H), 7.57-7.50 (m, 4H), 7.17 (t, *J* = 7.6 Hz, 1H), 7.02 (d, *J* = 7.9 Hz, 1H), 6.93 (t, *J* = 7.5 Hz, 1H), 6.54 (d, *J* = 8.2 Hz, 1H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  154.6,

153.0, 148.7, 141.6, 140.1, 139.6, 134.3, 133.6, 132.0, 129.8, 129.4, 129.1, 128.1, 126.9, 125.1, 121.5, 120.3, 120.1, 113.3, 111.8; HRMS (ESI) m/z calcd. For  $C_{23}H_{16}N_3O_2$  (M+1) 366.1243, found 366.1242.

# 4-(3-methoxyphenyl)-2-phenyl-α-carboline (2g)



Yellow solid, 71% yield; mp 194-195 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  11.91 (brs, 1H), 8.25-8.23 (m, 2H), 7.69 (d, *J* = 7.9 Hz, 1H), 7.61 (s, 1H), 7.59-7.49 (m, 4H,), 7.36 (d, *J* = 7.6 Hz, 1H), 7.31-7.30 (m, 1H), 7.21-7.17 (m, 1H), 7.11 (dd, *J* = 8.2, 2.5 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 6.54 (d, *J* = 8.2 Hz, 1H), 3.90 (3H, s, CH<sub>3</sub>); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  159.9,

154.3, 153.1, 145.9, 140.6, 140.1, 139.3, 129.9, 129.1, 128.8, 127.7, 126.4, 122.5, 121.1, 120.6, 119.6, 114.5, 114.3, 114.0, 112.7, 111.2, 55.4; HRMS (ESI) m/z calcd. For  $C_{24}H_{19}N_2O$  (M+1) 351.1497, found 351.1500.

# 4-(benzo[d][1,3]dioxol-5-yl)-2-phenyl-α-carboline (2h)



White solid, 82% yield; mp 242-243 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  11.41 (brs, 1H), 8.19 (d, *J* = 7.2 Hz, 2H), 7.74 (d, *J* = 8.0 Hz, 1H), 7.56-7.48 (m, 4H), 7.25-7.19 (m, 3H), 7.04-7.01 (m, 2H), 6.66 (d, *J* = 8.6 Hz, 1H), 6.10 (s, 1H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  154.5, 153.5, 148.3, 148.2, 146.0, 140.4, 139.5, 133.3, 129.3, 129.0, 127.9, 126.6, 122.7, 122.6,

120.8, 119.7, 114.6, 113.0, 111.5, 109.5, 108.9, 101.6; HRMS (ESI) m/z calcd. For  $C_{24}H_{17}N_2O_2$  (M+1) 365.1290, found 365.1290.

# 2-phenyl-4-(thiophen-2-yl)-α-carboline (2i)



White solid, 73% yield; mp 249-250 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  11.37 (brs, 1H), 8.20 (d, *J* = 7.1 Hz, 2H), 8.00 (d, *J* = 8.06 Hz, 1H), 7.66 (s, 1H), 7.62 (dd, *J* = 3.5, 0.7 Hz, 1,), 7.57-7.48 (m, 4H), 7.29 (dd, *J* = 5.0, 3.6 Hz, 1H), 7.23 (d, *J* = 7.1 Hz, 1,), 7.06 (t, *J* = 7.6 Hz, 1H), 6.66 (d, *J* = 8.1 Hz, 1H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  154.2, 153.4, 140.3, 139.9,

139.3, 138.7, 129.1, 128.9, 127.8, 127.7, 127.7, 126.6, 122.3, 120.5, 119.6, 115.1, 112.9, 111.4; HRMS (ESI) m/z calcd. For  $C_{21}H_{15}N_2S$  (M+1) 327.0956, found 327.0955.

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# 2-(4-chlorophenyl)-4-phenyl-α-carboline (2j)



White solid, 96% yield; mp 271-273 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  12.11 (brs, 1H), 8.23 (d, *J* = 7.4 Hz, 2H), 7.80 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 8.4 Hz, 2H), 7.54-7.50 (m, 4H), 7.46-7.40 (m, 2H), 7.06 (t, *J* = 7.8 Hz, 1H); <sup>13</sup>C NMR (100MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  153.6, 153.1, 144.2, 140.1, 139.6, 137.9, 134.1, 131.0, 129.4, 129.3, 129.2, 127.4,

127.0, 122.2, 120.1, 119.9, 113.3, 111.9, 111.7; HRMS (ESI) m/z calcd. For  $C_{23}H_{16}N_2CI$  (M+1) 355.1002, found 355.0999.

#### 2-(4-bromophenyl)-4-phenyl-α-carboline (2k)



White solid, 80% yield; mp 287-288 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  12.11 (brs, 1H), 8.20 (d, *J* = 8.5 Hz, 2H), 7.78-7.76 (m, 2H), 7.70-7.68 (m, 2H), 7.65-7.59 (m, 3H), 7.53 (d, *J* = 8.8 Hz, 2H), 7.41 (t, *J* = 7.7 Hz, 1H); <sup>13</sup>C NMR (100MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  152.4, 151.6, 145.1, 139.6, 138.4, 138.3, 131.5, 1288, 128.7, 128.7, 128.5, 126.5,

122.2, 121.7, 119.7, 119.2, 112.7, 111.6, 111.3; HRMS (ESI) m/z calcd. For  $C_{23}H_{16}N_2Br$  (M+1) 399.0497, found 399.0498.

2-(4-nitrophenyl)-4-phenyl-α-carboline (2l)



Yellow solid, 96% yield; mp 296-297 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  12.19 (brs, 1H), 8.49 (d, *J* = 8.9 Hz, 2H), 8.31 (d, *J* = 9.0 Hz, 2H), 7.81 (s, 1H), 7.78-7.75 (m, 2H), 7.66-7.58 (m, 3H), 7.55-7.53 (m, 2H), 7.43 (t, *J* = 8.9 Hz, 1H), 7.04 (t, *J* = 7.5 Hz, 1H); <sup>13</sup>C NMR (100MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  152.9, 150.6, 147.8, 145.7, 145.6,

140.5, 138.7, 129.4, 129.3, 129.3, 129.1, 128.3, 127.6, 124.3, 122.5, 120.0, 119.9, 114.4, 113.1, 111.9; HRMS (ESI) m/z calcd. For  $C_{23}H_{16}N_3O_2$  (M+1) 366.1243, found 366.1241.

# 2-(4-isopropylphenyl)-4-phenyl-α-carboline (2m)



White solid, 52% yield; mp 272-273 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  12.55 (brs, 1H), 8.18 (d, *J* = 8.0 Hz, 2H), 7.78 (d, *J* = 7.0 Hz, 2H), 7.63-7.54 (m, 5H), 7.44 (d, *J* = 8.1 Hz, 2H), 7.11 (t, *J* = 7.7 Hz, 1H), 6.96 (t, *J* = 7.6 Hz, 1H), 6.29 (d, *J* = 8.0 Hz, 1H,), 3.05 (sep, *J* = 6.9 Hz, 1H), 1.37 (d, *J* = 6.9 Hz, 6H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  154.7,

153.7, 150.0, 146.4, 139.7, 139.6, 138.2, 128.9, 128.8, 128.2, 127.5, 126.3, 122.3, 120.7, 119.5, 114.4, 112.9, 111.7, 34.31, 24.3; HRMS (ESI) m/z calcd. For  $C_{26}H_{23}N_2$  (M+1) 363.1861, found 363.1858.

# 2-(4-isobutylphenyl)-4-phenyl-α-carboline (2n)



White solid, 61% yield; mp 241.5-242.2°C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  11.47 (brs, 1H), 8.13 (d , *J* = 8.0 Hz, 2H), 7.75 (d , *J* = 7.0 Hz, 2H), 7.62-7.54 (m, 5H,, 7.32 (d, *J* = 7.9 Hz, 2H), 7.17 (t, *J* = 7.5 Hz 1H), 6.90 (t, *J* = 7.6 Hz, 1H), 6.70 (1H, d, *J* = 8.0 Hz ,CH), 2.58 (2H, d, J = 7.1 Hz, 2H), 1.96 (n, *J* = 6.7 Hz, 1H), 0.98 (d, *J* = 6.5 Hz,

6H),; <sup>13</sup>C NMR  $\delta$  154.6, 153.5, 146.3, 142.9, 139.5, 137.8, 130.1, 128.9, 128.8, 127.7, 126.4, 122.4, 120.8, 119.6, 114.4, 112.8, 111.6, 45.4, 30.5, 22.7,; HRMS (ESI) m/z calcd. For C<sub>27</sub>H<sub>25</sub>N<sub>2</sub> (M+1) 377.2012, found 377.2018.

# 2-(4-(tert-butyl)phenyl)-4-phenyl-α-carboline (20)



White solid, 60% yield; mp 237-238 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  12.45 (brs, 1H), 8.18 (d, *J* = 8.4 Hz, 2H), 7.77 (d, *J* = 6.7 Hz, 2H), 7.63-7.56 (m, 7H), 7.10 (t, *J* = 7.6 Hz, 1H), 6.96 (t, *J* = 7.5 Hz, 1H), 6.30 (d, *J* = 8.1 Hz, 2H), 1.43 (s, 9H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  154.7, 153.6, 152.2, 146.3, 139.6, 139.6, 137.7, 128.9, 128.8, 127.9,

126.3, 122.3, 120.7, 119.5, 114.5, 112.9, 111.7, 34.9, 31.6; HRMS (ESI) m/z calcd. For  $C_{27}H_{25}N_2$  (M+1) 377.2018, found 377.2021.

# 4-phenyl-2-(p-tolyl)-α-carboline (2p)



White solid, 60% yield; mp 252-254 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  12.05 (brs, 1H), 8.12 (d, *J* = 8.2 Hz, 2H), 7.77-7.75 (m, 2H), 7.65-7.56 (m, 4H), 7.54-7.51 (m, 2H), 7.39 (t, *J* = 7.7 Hz, 1H), 7.30 (d, *J* = 8.2 Hz, 2H), 7.02 (t, *J* = 7.5 Hz, 1H), 2.36 (s, 3H); <sup>13</sup>C NMR (100MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  153.6, 153.1, 145.5, 139.9, 139.2, 138.7, 136.9,

129.8, 129.3, 129.2, 129.1, 127.2, 126.8, 122.1, 120.4, 119.7, 113.0, 111.8, 111.6, 21.1; HRMS (ESI) m/z calcd. For  $C_{24}H_{19}N_2$  (M+1) 335.1548, found 355.1548.

# 2-(naphthalen-2-yl)-4-phenyl-α-carboline (2q)



White solid, 73% yield; mp 276-277 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  12.14 (brs, 1H), 8.22 (s, 1H), 8.45 (dd, *J* = 8.6, 1.6 Hz, 1H), 8.08-8.04 (m, 2H), 7.97-7.95 (m, 1H), 7.87 (s, 1H), 7.83-7.81 (m, 2H), 7.68-7.53 (m, 7H), 7.42 (t, *J* = 7.7 Hz, 1H), 7.05 (t, *J* = 7.6 Hz, 1H); <sup>13</sup>C NMR (100MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  153.3, 153.2, 145.7, 140.1, 139.2,

137.1, 133.7, 133.6, 129.3, 129.3, 129.1, 129.1, 128.6, 128.0, 127.0, 127.0, 126.9, 126.5, 125.2, 122.2, 120.4, 119.8, 113.7, 112.0, 111.9; HRMS (ESI) m/z calcd. For  $C_{27}H_{19}N_2$  (M+1) 371.1548, found 371.1548.

# 2-(4-methoxyphenyl)-4-phenyl-α-carboline (2r)



White solid, 54% yield; mp 236-237 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  11.63 (brs, 1H), 8.18 (d, *J* = 8.8 Hz, 2H), 7.78-7.75 (m, 2H), 7.62-7.54 (m, 5H), 7.23-7.19 (m, 1H), 7.07 (d, *J* = 8.8 Hz, 2H,), 6.99 (t, *J* = 7.2 Hz, 1H), 6.72 (d, *J* = 8.1 Hz, 2H), 3.89 (s, 3H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  160.7, 154.4, 153.4, 146.3, 139.6, 139.4, 133.0, 129.1, 128.9,

128.8, 126.4, 122.5, 121.1, 119.8, 114.7, 114.0, 112.5, 111.5, 55.7; HRMS (ESI) m/z calcd. For  $C_{24}H_{19}N_2O$  (M+1) 351.1497, found 351.1497.

## 6-bromo-2,4-diphenyl-α-carboline (2s)



White solid, 82% yield; mp 259-260 °C; <sup>1</sup>H NMR (400 MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  12.28 (brs, 1H), 8.24 (d, *J* = 7.3 Hz, 2H), 7.77 (d, *J* = 6.7 Hz, 2H), 7.70-7.59 (m, 5H), 7.55-7.43 (m, 5H); <sup>13</sup>C NMR (100MHz, (CD<sub>3</sub>)<sub>2</sub>SO)  $\delta$  154.5, 153.2, 146.1, 139.5, 138.7, 138.7, 129.5, 129.5, 129.4, 129.4, 129.2, 129.0, 127.5, 124.3, 122.2, 113.9, 113.7, 111.6, 110.9;

HRMS (ESI) m/z calcd. For C<sub>23</sub>H<sub>16</sub>N<sub>2</sub>Br (M+1) 399.0497, found 399.0497.

# 6-nitro-2,4-diphenyl-α-carboline (2t)



Pale yellow solid, 77% yield; mp 272-273 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  12.78 (brs, 1H), 8.60 (d, J = 2.1 Hz, 1H), 8.22-8.20 (m, 2H), 8.06 (dd, J =9.0, 2.2 Hz, 1H), 7.78-7.76 (m, 2H), 7.69-7.59 (m, 7H), 6.28 (d, J = 9.0 Hz, 1H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  156.4, 154.6, 147.9, 143.0, 141.4, 139.8, 137.9, 129.9, 129.8, 129.7, 129.5, 128.6, 128.3,

122.3, 120.4, 119.2, 116.2, 113.3, 111.3; HRMS (ESI) m/z calcd. For  $C_{23}H_{16}N_3O_2\ (M+1)\ 366.1243,$  found 366.1241.

# 6-methoxy-2,4-diphenyl-α-carboline (2u)



While solid, 65% yield; mp 201-202 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  12.06 (brs, 1H), 8.24 (d, *J* = 7.1 Hz, 2H), 7.77 (d, *J* = 7.0 Hz, 2H), 7.62-7.49 (m, 7H), 7.11 (d, *J* = 2.3 Hz, 1H), 6.83 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.37 (d, *J* = 8.8 Hz, 1H), 3.66 (s, 3H); <sup>13</sup>C NMR (100MHz, CDCl<sub>3</sub>)  $\delta$  154.4, 153.9, 153.6, 146.4, 140.4, 139.3, 134.5, 129.3, 128.9, 128.9, 128.9,

128.9, 128.3, 121.1, 115.4, 114.1, 113.1, 112.2, 105.7, 55.8; HRMS (ESI) m/z calcd. For  $C_{24}H_{19}N_2O$  (M+1) 351.1497, found 351.1500.

Synthesis of alkenyl oxime ester 4



mixture indolyloxime А of ester 1a (1 mmol) and 0.227g, 2,3-Dichloro-5,6-dicyano-1,4-benzoquinone (DDQ, 1 eq.) in 1,2-dichloroethane (1,2-DCE, 10 mL) was stirred at ambient temperature for 30 min. After completion of reaction, the mixture was diluted with CH<sub>2</sub>Cl<sub>2</sub> (20 mL). The organic layer was washed with aq. 1M NaOH (10 mL) for two times. The combined water layer was extracted with CH<sub>2</sub>Cl<sub>2</sub> (20 mL) for three times. The combined organic layer was dried over MgSO<sub>4</sub> and concentrated under reduced pressure. The residue was purified by recrystallation from CH<sub>2</sub>Cl<sub>2</sub>/hexane as solvent to afford alkenyl oxime ester 4.

(1Z,2Z)-3-(1H-indol-3-yl)-1,3-diphenylprop-2-en-1-one O-acetyl oxime (4)



Brown solid, 90% yield; two isomers 10:1; mp 106-108 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.64 (brs, 1H), 7.78 (d, *J* = 7.9 Hz, 1H), 7.49 (d, *J* = 7.2 Hz, 2H), 7.44 (d, *J* = 7.9 Hz, 1H), 7.28-7.26 (m, 1H), 7.22 (t, *J* = 7.5 Hz, 2H), 7.17-7.03 (m, 9H), 6.96 (d, *J* = 2.7 Hz, 1H), 2.17 (s, 3H); <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>)  $\delta$  169.3, 164.1, 146.7, 140.2,

137.2, 134.6, 130.1, 129.8, 128.9, 128.5, 127.9, 127.9, 127.6, 125.9, 123.1, 121.2, 120.7, 118.8, 114.9, 112.1, 77.5; HRMS (ESI) m/z calcd. For  $C_{25}H_{20}N_2O_2Na$  (M+23) 403.1422, found 403.1423.

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# Control experiment of $\alpha$ -carboline



General procedure:

A mixture of alkenyl oxime ester **4** (0.5 mmol) and iodine (0.025g, 20 mol%) in 1,2-DCE (5 mL) was heated to 60 °C for 1 h. After completion of the reaction, the mixture was allowed to cool to ambient temperature and diluted with ethyl acetate (25 mL). The organic layer was washed with aq. NaS<sub>2</sub>O<sub>3</sub> (5 mL) and aq. NaHCO<sub>3</sub> (5 mL) for two times. The organic layer was dried over MgSO<sub>4</sub> and concentrated under reduced pressure to afford  $\alpha$ -carboline **2a** in 65% yield which were determined from crude 1H NMR spectrum with dibromomethane 10(µL) as internal standard.

# X-ray data of carbolines 2r/3g and intermediate 4

Table S4. Crystal data and structure refinement for 2r (CCDC number: 1515102)





Identification code	d18452	d18452			
Empirical formula	$C_{24}H_{18}N_2O$	$C_{24}H_{18}N_2O$			
Formula weight	350.40	350.40			
Temperature	200(2) K	200(2) K			
Wavelength	0.71073 Å				
Crystal system	Triclinic				
Space group	P -1				
Unit cell dimensions	a = 9.4800(12) Å	$\alpha = 88.685(4)^{\circ}.$			
	b = 13.2295(16) Å	$\beta = 73.346(4)^{\circ}.$			
	c = 15.0067(19) Å	$\gamma = 86.478(4)^{\circ}.$			
Volume	1799.7(4) Å <sup>3</sup>				
Z	4				
Density (calculated)	1.293 Mg/m <sup>3</sup>				
Absorption coefficient	$0.080 \text{ mm}^{-1}$				
F(000)	736				
Crystal size	0.47 x 0.25 x 0.06 mm <sup>3</sup>				
Theta range for data collection	2.25 to 25.03°.	2.25 to 25.03°.			
Index ranges	-11<=h<=11, -15<=k<=1	-11<=h<=11, -15<=k<=15, -17<=l<=17			
Reflections collected	62260	62260			
Independent reflections	6332 [R(int) = 0.0483]	6332 [R(int) = 0.0483]			
Completeness to theta = $25.03^{\circ}$	99.5 %	99.5 %			
Absorption correction	multi-scan	multi-scan			
Max. and min. transmission	0.9952 and 0.9635	0.9952 and 0.9635			
Refinement method	Full-matrix least-squares	on F <sup>2</sup>			
Data / restraints / parameters	6332 / 0 / 489	6332 / 0 / 489			
Goodness-of-fit on F <sup>2</sup>	1.084				
Final R indices $[I>2sigma(I)]$ R1 = 0.0374, wR2 = 0.0892					
R indices (all data)	R1 = 0.0530, wR2 = 0.10	R1 = 0.0530, wR2 = 0.1040			
Largest diff. peak and hole	0.169 and -0.190 e.Å <sup>-3</sup>	0.169 and -0.190 e.Å <sup>-3</sup>			

# Table S5. Crystal data and structure refinement for **3g** (CCDC number: 1515101)





Identification code	ch15606a	ch15606a		
Empirical formula	$C_{24}H_{18}N_2O$	$C_{24}H_{18}N_2O$		
Formula weight	350.40			
Temperature	200(2) K			
Wavelength	0.71073 Å			
Crystal system	Monoclinic			
Space group	P 21/n			
Unit cell dimensions	a = 13.365(2) Å	$\alpha = 90^{\circ}$ .		
	b = 17.037(3) Å	$\beta = 98.932(3)^{\circ}.$		
	c = 16.781(3)  Å	$\gamma = 90^{\circ}$ .		
Volume	3774.6(10) Å <sup>3</sup>			
Z	8			
Density (calculated)	$1.233 \text{ Mg/m}^3$			
Absorption coefficient	0.076 mm <sup>-1</sup>			
F(000)	1472	1472		
Crystal size	0.34 x 0.26 x 0.21 mm <sup>3</sup>	0.34 x 0.26 x 0.21 mm <sup>3</sup>		
Theta range for data collection	1.71 to 25.09°.	1.71 to 25.09°.		
Index ranges	-15<=h<=15, -20<=k<=	-15<=h<=15, -20<=k<=19, -19<=l<=19		
Reflections collected	23348	23348		
Independent reflections	6606 [R(int) = 0.0456]	6606 [R(int) = 0.0456]		
Completeness to theta = $25.09^{\circ}$	98.6 %	98.6 %		
Absorption correction	multi-scan	multi-scan		
Max. and min. transmission	0.9842 and 0.9746	0.9842 and 0.9746		
Refinement method	Full-matrix least-square	Full-matrix least-squares on F <sup>2</sup>		
Data / restraints / parameters	6606 / 0 / 487			
Goodness-of-fit on F <sup>2</sup>	1.058			
Final R indices [I>2sigma(I)] $R1 = 0.0505$ , wR2 = 0.1344				
R indices (all data)	R1 = 0.0789, wR2 = 0.1	R1 = 0.0789, wR2 = 0.1512		
Largest diff. peak and hole	0.368 and -0.379 e.Å <sup>-3</sup>	0.368 and -0.379 e.Å <sup>-3</sup>		



O-N HN K

Identification code	ch18179			
Empirical formula	C25 H20 C10 N2 O2			
Formula weight	380.43			
Temperature	200(2) K			
Wavelength	0.71073 Å			
Crystal system	Triclinic			
Space group	P -1			
Unit cell dimensions	a = 8.2571(7) Å	$\alpha = 66.416(5)^{\circ}.$		
	b = 16.8590(15) Å	$\beta = 86.395(5)^{\circ}.$		
	c = 17.1654(15) Å	$\gamma = 89.790(5)^{\circ}.$		
Volume	2185.0(3) Å <sup>3</sup>			
Z	4			
Density (calculated)	1.156 Mg/m <sup>3</sup>			
Absorption coefficient	0.074 mm <sup>-1</sup>			
F(000)	800			
Crystal size	al size $0.39 \ge 0.35 \ge 0.11 \text{ mm}^3$			
Theta range for data collection	1.32 to 25.46°.			
Index ranges	-9<=h<=9, -20<=k<=19, -20<=l<=18			
Reflections collected	19218			
Independent reflections	7965 [R(int) = 0.0512]			
Completeness to theta = $25.46^{\circ}$	98.4 %			
Absorption correction	multi-scan			
Max. and min. transmission	0.9919 and 0.9717			
Refinement method	Full-matrix least-squares on F <sup>2</sup>			
Data / restraints / parameters	7965 / 0 / 523			
Goodness-of-fit on F <sup>2</sup>	1.064			
Final R indices [I>2sigma(I)]	R1 = 0.0921, $wR2 = 0.2654$			
R indices (all data)	R1 = 0.1235, $wR2 = 0.2855$			
Largest diff. peak and hole	0.495 and -0.379 e.Å <sup>-3</sup>			

Table S6. Crystal data and structure refinement for **4** (CCDC number: 1515742)

#### (Z)-3-(1H-indol-3-yl)-1,3-diphenylpropan-1-one O-acetyl oxime Current Data Parameters NAME 20161224 EXPNO 1 PROCNO 1 F2 - Acquisi Date Time INSTRUM PROBHD PROBHD PROBHD PROBHD SOLVENT NS SOLVENT NS SWH FIDRES AQ 2 RG 2 DW DE TE DI 2. TD0 tion Parameters 20161224 19.17 2010/22+ 19:17 spect 5 mm PABBO BB/ G 22630 10 20079 Hz 0.220079 Hz 0.220079 Hz 0.220079 Hz 0.22079 Hz 0.22079 Hz 0.22079 Hz 0.22079 Hz 0.22079 Hz 0.22079 Hz 0.22078 Hz 0. Q Q 298.0 K 2.00000000 sec SFO1 NUC1 P1 PLW1 CHANNEL f1 ===== 400.1324008 MHz 1H 12.90 usec 15.00000000 W F2- Processing parameters 16384 SF 400.1300160 MHz WDW EM SSB 0 LB 0 Hz GB 0 PC 1.00 1a 9 5 10 8 7 6 2 0 ppm 4 1 $\mathbb{N}$ Д .004 1.019 3.006 . 931

#### (Z)-3-(1H-indol-3-yl)-1,3-diphenylpropan-1-one O-acetyl oxime



(Z)-3-(2-fluorophenyl)-3-(1H-indol-3-yl)-1-phenylpropan-1-one O-acetyl oxime



(Z)-3-(2-fluorophenyl)-3-(1H-indol-3-yl)-1-phenylpropan-1-one O-acetyl oxime



(Z)-3-(2-chlorophenyl)-3-(1H-indol-3-yl)-1-phenylpropan-1-one O-acetyl oxime



(Z)-3-(2-chlorophenyl)-3-(1H-indol-3-yl)-1-phenylpropan-1-one O-acetyl oxime


(Z)-3-(2-bromophenyl)-3-(1H-indol-3-yl)-1-phenylpropan-1-one O-acetyl oxime



(Z)-3-(2-bromophenyl)-3-(1H-indol-3-yl)-1-phenylpropan-1-one O-acetyl oxime







(Z)-3-(1H-indol-3-yl)-3-(naphthalen-1-yl)-1-phenylpropan-1-one O-acetyl oxime



## (Z)-3-(1H-indol-3-yl)-3-(2-nitrophenyl)-1-phenylpropan-1-one O-acetyl oxime





ppm

80 70 60 50 40 30 20 10

210 200 190 180 170 160 150 140 130 120 110 100 90

#### (Z)-3-(1H-indol-3-yl)-3-(3-methoxyphenyl)-1-phenylpropan-1-one O-acetyl oxime



(Z)-3-(1H-indol-3-yl)-3-(3-methoxyphenyl)-1-phenylpropan-1-one O-acetyl oxime









(Z)-1-(4-chlorophenyl)-3-(1H-indol-3-yl)-3-phenylpropan-1-one O-acetyl oxime



(Z)-1-(4-chlorophenyl)-3-(1H-indol-3-yl)-3-phenylpropan-1-one O-acetyl oxime



(Z)-1-(4-bromophenyl)-3-(1H-indol-3-yl)-3-phenylpropan-1-one O-acetyl oxime



(Z)-1-(4-bromophenyl)-3-(1H-indol-3-yl)-3-phenylpropan-1-one O-acetyl oxime







(Z)-3-(1H-indol-3-yl)-1-(4-nitrophenyl)-3-phenylpropan-1-one O-acetyl oxime



(Z)-3-(1H-indol-3-yl)-1-(4-isopropylphenyl)-3-phenylpropan-1-one O-acetyl oxime



(Z)-3-(1H-indol-3-yl)-1-(4-isobutylphenyl)-3-phenylpropan-1-one O-acetyl oxime



(Z)-3-(1H-indol-3-yl)-1-(4-isobutylphenyl)-3-phenylpropan-1-one O-acetyl oxime





(Z)-1-(4-(tert-butyl)phenyl)-3-(1H-indol-3-yl)-3-phenylpropan-1-one O-acetyl oxime



ition Parame 20140422 23.23

CHANNEL f1 ===== 400.1324008 MHz 1H 12.80 usec 15.00000000 W

(Z)-1-(4-(tert-butyl)phenyl)-3-(1H-indol-3-yl)-3-phenylpropan-1-one O-acetyl oxime

(Z)-3-(1H-indol-3-yl)-3-phenyl-1-(p-tolyl)propan-1-one O-acetyl oxime



(Z)-3-(1H-indol-3-yl)-3-phenyl-1-(p-tolyl)propan-1-one O-acetyl oxime



## (Z)-3-(1H-indol-3-yl)-1-(naphthalen-2-yl)-3-phenylpropan-1-one O-acetyl oxime



(Z)-3-(1H-indol-3-yl)-1-(naphthalen-2-yl)-3-phenylpropan-1-one O-acetyl oxime



(Z)-3-(1H-indol-3-yl)-1-(4-methoxyphenyl)-3-phenylpropan-1-one O-acetyl oxime



(Z)-3-(1H-indol-3-yl)-1-(4-methoxyphenyl)-3-phenylpropan-1-one O-acetyl oxime



(Z)-3-(5-bromo-1H-indol-3-yl)-1,3-diphenylpropan-1-one O-acetyl oxime



## (Z)-3-(5-bromo-1H-indol-3-yl)-1,3-diphenylpropan-1-one O-acetyl oxime



(Z)-3-(5-nitro-1H-indol-3-yl)-1,3-diphenylpropan-1-one O-acetyl oxime







(Z)-3-(5-methoxy-1H-indol-3-yl)-1,3-diphenylpropan-1-one O-acetyl oxime



2,4-diphenyl-α-carboline



## 2,4-diphenyl-α-carboline



4-(2-fluorophenyl)-2-phenyl-α-carboline



4-(2-fluorophenyl)-2-phenyl-α-carboline



4-(2-chlorophenyl)-2-phenyl-α-carboline



4-(2-chlorophenyl)-2-phenyl-α-carboline



4-(2-bromophenyl)-2-phenyl- $\alpha$ -carboline



4-(2-bromophenyl)-2-phenyl-α-carboline



4-(naphthalen-1-yl)-2-phenyl-α-carboline



4-(naphthalen-1-yl)-2-phenyl-α-carboline



# 4-(2-nitrophenyl)-2-phenyl-α-carboline



4-(2-nitrophenyl)-2-phenyl-α-carboline



4-(3-methoxyphenyl)-2-phenyl-α-carboline



#### 4-(3-methoxyphenyl)-2-phenyl-α-carboline





Current Data Parameters NAME H(piperonyl chalcone) EXPNO 61 PROCNO 1

ition Parameters 20161021 16.43

4-(benzo[d][1,3]dioxol-5-yl)-2-phenyl-α-carboline

111399 11281 11281 11281 11282

2-phenyl-4-(thiophen-2-yl)-α-carboline



2-phenyl-4-(thiophen-2-yl)-α-carboline



2-(4-chlorophenyl)-4-phenyl-α-carboline



2-(4-chlorophenyl)-4-phenyl-α-carboline



2-(4-bromophenyl)-4-phenyl-α-carboline



2-(4-bromophenyl)-4-phenyl-α-carboline



# 2-(4-nitrophenyl)-4-phenyl-α-carboline



2-(4-nitrophenyl)-4-phenyl-α-carboline



2-(4-isopropylphenyl)-4-phenyl-α-carboline



## 2-(4-isopropylphenyl)-4-phenyl-α-carboline



 $2\-(4\-isobutylphenyl)\-4\-phenyl\-\alpha\-carboline$ 



### 2-(4-isobutylphenyl)-4-phenyl-α-carboline



2-(4-(tert-butyl)phenyl)-4-phenyl-α-carboline



## 2-(4-(tert-butyl)phenyl)-4-phenyl-α-carboline



4-phenyl-2-(p-tolyl)-α-carboline



2-(naphthalen-2-yl)-4-phenyl-α-carboline



2-(naphthalen-2-yl)-4-phenyl-α-carboline



 $2-(4-methoxyphenyl)-4-phenyl-\alpha-carboline$ 



## $2-(4-methoxyphenyl)-4-phenyl-\alpha-carboline$



-bromo-2,4-diphenyl- $\alpha$ -carboline



6-bromo-2,4-diphenyl-α-carboline


6-nitro-2,4-diphenyl-α-carboline



#### 6-nitro-2,4-diphenyl-α-carboline



6-methoxy-2,4-diphenyl-α-carboline



6-methoxy-2,4-diphenyl-α-carboline



# 2,4-diphenyl-δ-carboline



2,4-diphenyl-δ-carboline



4-(2-fluorophenyl)-2-phenyl-δ-carboline



4-(2-fluorophenyl)-2-phenyl-δ-carboline



4-(2-chlorophenyl)-2-phenyl-δ-carboline



4-(2-chlorophenyl)-2-phenyl-δ-carboline





## 4-(2-bromophenyl)-2-phenyl-δ-carboline



### 4-(naphthalen-1-yl)-2-phenyl-δ-carboline



 $4\-(naphthalen-1-yl)\-2\-phenyl\-\delta\-carboline$ 



4-(2-nitrophenyl)-2-phenyl-δ-carboline



4-(2-nitrophenyl)-2-phenyl-δ-carboline



4-(3-methoxyphenyl)-2-phenyl-δ-carboline



#### 4-(3-methoxyphenyl)-2-phenyl-δ-carboline





### 4-(benzo[d][1,3]dioxol-5-yl)-2-phenyl-δ-carboline



2-phenyl-4-(thiophen-2-yl)-δ-carboline



2-phenyl-4-(thiophen-2-yl)-δ-carboline



 $2-(4-chlorophenyl)-4-phenyl-\delta-carboline$ 



2-(4-chlorophenyl)-4-phenyl-δ-carboline



2-(4-bromophenyl)-4-phenyl-δ-carboline



2-(4-bromophenyl)-4-phenyl-δ-carboline



2-(4-nitrophenyl)-4-phenyl-δ-carboline



2-(4-nitrophenyl)-4-phenyl-δ-carboline



2-(4-isopropylphenyl)-4-phenyl-δ-carboline



2-(4-isopropylphenyl)-4-phenyl-δ-carboline



2-(4-isobutylphenyl)-4-phenyl-δ-carboline



2-(4-isobutylphenyl)-4-phenyl-δ-carboline



2-(4-(tert-butyl)phenyl)-4-phenyl-δ-carboline





4-phenyl-2-(p-tolyl)-δ-carboline



2-(naphthalen-2-yl)-4-phenyl-δ-carboline



2-(naphthalen-2-yl)-4-phenyl-δ-carboline



# 2-(4-methoxyphenyl)-4-phenyl-δ-carboline



#### 2-(4-methoxyphenyl)-4-phenyl-δ-carboline



8-bromo-2,4-diphenyl-δ-carboline



8-bromo-2,4-diphenyl-δ-carboline



8-nitro-2,4-diphenyl-δ-carboline



8-nitro-2,4-diphenyl-δ-carboline



8-methoxy-2,4-diphenyl-δ-carboline



8-methoxy-2,4-diphenyl-δ-carboline





(1Z,2Z)-3-(1H-indol-3-yl)-1,3-diphenylprop-2-en-1-one O-acetyl oxime



(1Z,2Z)-3-(1H-indol-3-yl)-1,3-diphenylprop-2-en-1-one O-acetyl oxime