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## **Supporting information**

For

## Oxidative annulation of L-phenylalanine using I<sub>2</sub>/DMSO: An easy approach for chemoselective syntheses of 2,3,5-trisubstituted pyridines and 2,5-disubstituted oxazoles

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- 1. Crystallographic data and molecular structure:
- 1.1 (3,5-diphenylpyridin-2-yl)(9H-fluoren-2-yl)methanone (3ae)



Figure 1: X-ray crystal structure of compound 3ae



Figure 2: Crystal packing of compound 3ae along b-axis



Figure 3: The molecular structure of 3ae (Displacement ellipsoid are drawn at the 50% probability level)

Table 1.	Cry	ystal	Data	and	structure	refine	ement	for	com	pound	3a	e

CCDC No.	2349633
Identification code	AKASPGNAP160201_0m_a
Empirical formula	$C_{31}H_{21}NO$
Formula weight	423.49
Temperature/K	298(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.5417(11)
b/Å	11.2513(12)
c/Å	11.7206(13)
$\alpha/^{\circ}$	63.057(3)
β/°	66.650(3)
$\gamma/^{\circ}$	78.851(3)
Volume/Å <sup>3</sup>	1137.6(2)
Z	2

$\rho_{calc}g/cm^3$	1.236
$\mu/\text{mm}^{-1}$	0.074
F(000)	444.0
Crystal size/mm <sup>3</sup>	$0.21\times0.18\times0.16$
Radiation	MoKa ( $\lambda = 0.71073$ )
$2\Theta$ range for data collection/	° 4.21 to 49.992
Index ranges	$-12 \le h \le 12, -13 \le k \le 13, -13 \le l \le 13$
Reflections collected	26455
Independent reflections	$3964 [R_{int} = 0.0218, R_{sigma} = 0.0140]$
Data/restraints/parameters	3964/0/298
Goodness-of-fit on F <sup>2</sup>	1.020
Final R indexes [I>= $2\sigma$ (I)]	$R_1 = 0.0448, wR_2 = 0.1387$
Final R indexes [all data]	$R_1 = 0.0523, wR_2 = 0.1552$
Largest diff. peak/hole / e Å-	3 0.28/-0.18

## 1.2 (3, 5-diphenylpyridin-2-yl)(furan-2-yl)methanone (3an)



Figure 4: X-ray crystal structure of compound 3an



Figure 5: Crystal packing of compound 3an along b-axis



Figure 6: The molecular structure of **3an** (Displacement ellipsoid are drawn at the 50% probability level)

Table 2.	Cry	stal	Data	and	structure	refinement	for	comp	oound	<u>3an</u>
	_									

CCDC No.	2271607
Identification code	AP1502
Empirical formula	$C_{22}H_{15}NO_2$
Formula weight	325.35
Temperature/K	297.15
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	9.5905(13)
b/Å	9.8247(13)
c/Å	17.961(2)
$\alpha/^{\circ}$	90
β/°	105.033(5)
γ/°	90
Volume/Å <sup>3</sup>	1634.4(4)
Z	4
$ ho_{calc}g/cm^3$	1.322
$\mu/mm^{-1}$	0.678
F(000)	680.0
Crystal size/mm <sup>3</sup>	$0.271 \times 0.266 \times 0.094$
Radiation	$CuK\alpha (\lambda = 1.54178)$
$2\Theta$ range for data collection/	° 9.588 to 144.614
Index ranges	$-11 \le h \le 11, -12 \le k \le 12, -22 \le l \le 22$

 $\begin{array}{ll} \mbox{Reflections collected} & 25224 \\ \mbox{Independent reflections} & 3215 \ [R_{int} = 0.0983, R_{sigma} = 0.0662] \\ \mbox{Data/restraints/parameters} & 3215/0/227 \\ \mbox{Goodness-of-fit on } F^2 & 1.055 \\ \mbox{Final R indexes [I>=2$\sigma$ (I)]} & R_1 = 0.0598, wR_2 = 0.1772 \\ \mbox{Final R indexes [all data]} & R_1 = 0.0898, wR_2 = 0.1913 \\ \mbox{Largest diff. peak/hole / e $$A$^-3} & 0.25/-0.20 \\ \end{array}$ 

## 1.3 (5-(3,4-dimethoxyphenyl)oxazol-2-yl)(phenyl)methanone (4ac)



Figure 7: X-ray crystal structure of compound 4ac



Figure 8: Crystal packing of compound 4ac along b-axis



Figure 9: The molecular structure of 4ac (Displacement ellipsoid are drawn at the 50% probability level)

 Table 3. Crystal Data and structure refinement for compound 4ac

CCDC No.	2349642
Identification code	AKASPGNOX08_0ma_a
Empirical formula	$C_{18}H_{15}NO_4$
Formula weight	309.31
Temperature/K	298(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	8.048(2)
b/Å	8.244(2)
c/Å	23.019(7)
α/°	90
β/°	96.925(7)
γ/°	90
Volume/Å <sup>3</sup>	1516.2(7)
Ζ	4
$\rho_{calc}g/cm^3$	1.355
µ/mm <sup>-1</sup>	0.097
F(000)	648.0
Crystal size/mm <sup>3</sup>	0.22  imes 0.18  imes 0.15
Radiation	MoKa ( $\lambda = 0.71073$ )
$2\Theta$ range for data collection/°	5.098 to 49.996
Index ranges	$-9 \le h \le 9, -9 \le k \le 9, -27 \le l \le 27$
Reflections collected	31025
Independent reflections	2644 [ $R_{int} = 0.0422, R_{sigma} = 0.0191$ ]
Data/restraints/parameters	2644/0/210
Goodness-of-fit on F <sup>2</sup>	1.132
Final R indexes $[I \ge 2\sigma(I)]$	$R_1 = 0.0996, wR_2 = 0.2551$
Final R indexes [all data]	$R_1 = 0.1037, wR_2 = 0.2573$
Largest diff. peak/hole / e Å-3	0.50/-0.31



2. Experimental procedure for the synthesis of 2, 3, 5-trisubstituted pyridine derivatives:

A well-dried round-bottomed flask was suspended with substituted acetophenone (**2a**, 1.0 mmol), Iodine (1.0 mmol) and DMSO (10 mL) heated at 90 °C for 3h. Then L-Phenylalanine (**1a**, 2.0 mmol) was added and continued the heating at the same temperature for 7h. The reaction completion was confirmed by TLC followed by the reaction mixture was quenched with saturated sodium thiosulfate solution and extracted the reaction mixture twice by using ethyl acetate. After the solvent evaporation by using a rotary evaporator, the obtained crude product was purified by column chromatography by using silica gel (60-120 mesh size) (eluting solvent hexane: ethyl acetate; 10:2).

#### Experimental procedure for the synthesis of 2,5-disubstituted oxazole derivatives



To a clean and dried round-bottomed flask was charged with substituted acetophenone (2a, 1.0 mmol), Iodine (1.2 mmol) and DMSO heated at 110 °C for 3h. Then L-Phenylalanine (1a, 1.0 mmol) was added and continued the heating at 110 °C for 9h. The reaction completion was confirmed by TLC followed by the reaction mixture was quenched with water and extracted twice by using ethyl acetate. After the solvent evaporation using a rotary evaporator, the obtained crude product was purified by column chromatography using silica gel (60-120 mesh size) (eluting solvent hexane: ethyl acetate; 10:1).

3. Table 4. Optimization of Reaction Conditions for synthesis of 2,5-disubstituted



Sl No	Iodine Source	Additives	1a:2f	Temp in °C	% yield
	( equiv)	(equiv)	(equiv)		(4f)
1	-	-	1:1	110(10h)	-
2	$I_2(0.5)$	-	1:1	110(10h)	48
3	PIDA(1.0)	-	1:1	110(10h)	-
4	KI (1.0)	-	1:1	110(10h)	-
5	$KI(1.0)+K_2S_2O_8(2.0)$	-	1:1	110(10h)	-
6	NH <sub>4</sub> I (1.0)	-	1:1	110(10h)	>30
7	TBAI (1.0)	-	1:1	110(10h)	-
8	$I_2(1.0)$	-	1:1	110 (10h)	78
9	$I_2(1.2)$	-	1:1	110 (10h)	80
10	$I_2(1.5)$	-	1:1	110 (10h)	63
11	$I_2(1.2)$	AcOH(0.5)	1:1	110 (10h)	35
12	$I_2(1.2)$	TFA (0.5)	1:1	110 (10h)	41
13	$I_2(1.2)$	Sulfanilic acid (0.5)	1:1	110 (10h)	38
14	$I_2(1.2)$	_	1:1	110 (12h)	90
15	$I_2(1.2)$	-	1:1	110 (14h)	73
16	$I_2(1.2)$	-	1:1	90 (12h)	53
17	$I_2(1.2)$	-	1:1	140 (12h)	38
18	$I_2(1.2)$	-	Only 1a	110(12h)	63 (5a)
19	$I_2(1.2)$	-	1.5:1	110(12h)	43

<sup>a</sup>Reaction conditions: 1a (1.0 mmol), 2a (1.0 mol),  $I_2$  (1.2 equiv) in DMSO (10 mL) were added to the flask and heated for 12 h at 110°C. AcOH= Acetic acid, TFA= trifluoroacetic acid

We started the reaction of 3,4-dimethoxy acetophenone(2c)(1.0 equiv) and L-phenylalanine (1a)(1.0 equiv) in DMSO (10mL)without an iodine source, and we couldn't achieve the desired product 4ac(Table 4, entry 1). But we got a good amount of 4ac in the presence of iodine (0.5 equiv) in DMSO(10mL) (Table 4, entry 2). It confirms the essential role of the iodine/DMSO in this strategy. Other iodine sources like PIDA, KI, KI+K<sub>2</sub>S<sub>2</sub>O<sub>8</sub>, NH<sub>4</sub>I, and TBAI were failed to produce 4ac (Table 4, entries 3-7). By varying the iodine loading, we found that 1.2 equiv was sufficient for the conversion (Table 4 entries 8-10). Acid additives like AcOH, TFA, and sulfanilic acid did not help to increase the yield (Table 4, entries 11-13). Reaction time increased to 12h led to an increase in the

yield of up to 90%(Table 4, entry 14). But further increase of temperature to 14h led to decrease in the yield(Table 4, entry 15). Reaction temperature screening revealed that 110 °C is good for better yield (Table 4, entries 14,16,17). Further increase in temperature led to unwanted products, which could be due to the recycling of iodine by coproduct HI and DMSO. Reaction without the addition of acetophenone produced 3,5-disubstituted pyridine(5a,63%) might be due to homoconstruction of phenylalanine (Table-4, entry 18). Increasing the amount of phenylalanine up to 1.5 equiv produced 4ac with less yield(43%) than 1.0 equiv (Table-4, entry 18). The optimised conditions involve 1a(1.0 equiv), 2c(1.0 equiv),  $I_2(1.2 \text{ equiv})$  and DMSO (10mL), heated at 110 °C for 12h (Table-4, entry 14).

## 5(a) Spectral data of 2,3,5-trisubstituted pyridine derivatives

## i) [1,1'-biphenyl]-4-yl(3,5-diphenylpyridin-2-yl)methanone (3aa)

Yield: 365 mg, 89%; Colourless solid; m.p =132-136 °C;

<sup>1</sup>**H-NMR** (400 MHz, DMSO-d<sub>6</sub>) δ 9.02 (d, J = 2.1 Hz, 1H), 8.28 (d, J = 2.1 Hz, 1H), 7.95-7.91 (m, 4H), 7.83 (d, J = 8.6 Hz, 2H), 7.77-7.75 (m, 2H), 7.59-7.36 (m, 11H); <sup>13</sup>**C-NMR** (101 MHz, DMSO-d<sub>6</sub>) δ 194.1, 153.4, 145.4, 145.1, 138.7, 137.2, 136.7, 136.1, 134.8, 130.7, 130.1, 129.2, 129.1, 128.8, 128.6, 128.5, 128.1, 127.4, 127.1, 127.0, 126.6; **FT-IR** (KBr cm<sup>-1</sup>): 3110 (=C-H), 1666 (C=O), 1633 (C=N), 1554 (C=C);



HRMS (ESI) Calcd for  $C_{30}H_{21}NO [M+H]^+$ , 412.1696; found, 412.1537.

## ii) (3,5-diphenylpyridin-2-yl)(4-hydroxyphenyl)methanone(3ab)

Yield: 270 mg, 77%; Colourless solid; m.p =128-132 °C;

<sup>1</sup>**H-NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  10.60 (s, 1H), 9.00 (d, J = 2.1 Hz, 1H), 8.25 (d, J = 2.0 Hz, 1H), 7.95 (d, J = 5.5 Hz, 2H), 7.70 (d, J = 8.7 Hz, 2H), 7.62-7.53 (m, 3H), 7.47-7.37 (m, 5H), 6.89 (d, J = 8.9 Hz, 2H);

<sup>13</sup>C-NMR (101 MHz, DMSO-d<sub>6</sub>) δ 193.1, 162.7, 154.2, 145.4, 137.3, 136.3, 135.9, 135.5, 132.6, 129.2, 128.7, 128.6, 128.0, 127.6, 127.3, 115.5; **FT-IR** (KBr cm<sup>-1</sup>): 3379 (O-H), 3070 (=C-H), 1697 (C=O), 1608 (C=N), 1550 (C=C),1253 (C-O);



HRMS (ESI) Calcd for C<sub>24</sub>H<sub>17</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 352.1332; found, 352.1335.

## iii) (3,4-dimethoxyphenyl)(3,5-diphenylpyridin-2-yl)methanone (3ac)

Yield: 359 mg, 91%; Colourless solid; m.p =138-140 °C;

<sup>1</sup>**H-NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.98 (s, 1H), 8.23 (s, 1H), 7.92 (d, J = 7.5 Hz, 2H), 7.58-7.30 (m, 10H), 7.03 (d, J = 8.4 Hz, 1H), 3.84 (s, 3H), 3.78 (s, 3H);<sup>13</sup>**C NMR** (100 MHz, DMSO-d<sub>6</sub>)  $\delta$  193.2, 153.8,



153.6, 148.7, 145.2, 136.2, 136.1, 135.8, 129.1, 128.8, 128.6, 128.5, 127.9, 127.2, 126.1, 110.8, 55.7,

55.4; **FT-IR** (KBr, cm-1): 3062(=C-H), 1639(C=O), 1552(C=N), 1502(C=C), 1245(C-O);

HRMS (ESI) Calcd for C<sub>26</sub>H<sub>21</sub>NO<sub>3</sub> [M+H]<sup>+</sup>, 396.1594; found, 396.1535.

iv) (3,5-diphenylpyridin-2-yl)(naphthalen-2-yl)methanone (3ad)

Yield: 319 mg, 83%; Colourless solid; m.p =172-174 °C;

<sup>1</sup>**H-NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.07 (d, J = 2.1 Hz, 1H), 8.45 (s, 1H),

8.32 (d, J = 2.0 Hz, 1H), 8.12-7.93 (m, 6H), 7.73-7.68 (m, 1H), 7.64-7.58

(m, 3H), 7.54-7.48 (m, 3H), 7.38-7.32 (m, 3H);

<sup>13</sup>C-NMR (101 MHz, DMSO-d<sub>6</sub>) δ 194.5, 153.4, 145.4, 137.1, 136.5, 136.0, 136.0, 135.9, 135.1, 133.2, 132.7, 131.8, 129.7, 129.1, 129.0, 128.6, 128.5, 128.4, 127.9, 127.6, 127.2, 126.9, 124.2;

FT-IR (KBr cm<sup>-1</sup>): 3136 (=C-H), 1701 (C=O), 1625 (C=N), 1562 (C=C), 1211 (C-O);

HRMS (ESI): Calcd for C<sub>28</sub>H<sub>19</sub>NO [M+H]<sup>+</sup>, 386.1540; found, 386.1551.

## v) (3,5-diphenylpyridin-2-yl)(9H-fluoren-2-yl)methanone (3ae)

Yield: 376 mg, 89%; Colourless solid; m.p=186-188 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.04 (d, J = 2.1 Hz, 1H), 8.29 (d, J = 2.1 Hz, 1H), 8.05-7.86 (m, 7H), 7.69-7.36 (m, 10H), 4.01 (s, 2H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ 194.7, 154.1, 146.6, 145.6, 144.8, 143.4, 139.9, 137.4, 136.7, 136.3, 136.2, 134.6, 129.6, 129.5, 128.9, 128.8, 128.6, 128.3, 127.5, 127.3, 126.8, 125.6, 121.5, 120.2, 36.6;

FT-IR (KBr cm<sup>-1</sup>): 3110 (=C-H), 2952 (C-H), 1701 (C=O), 1658 (C=N), 1544 (C=C), 1357(-CH<sub>2</sub> bending), 1238 (C-O);

HRMS (ESI) Calcd for C<sub>31</sub>H<sub>21</sub>NO [M+H]<sup>+</sup>, 424.1696; found, 424.1641.

## vi) (3,5-diphenylpyridin-2-yl)(naphthalen-1-yl)methanone (3af)

Yield: 304 mg, 79%; Colourless solid;  $\text{mp} = 136-140 \text{ }^{\circ}\text{C}$ ; <sup>1</sup>**H** NMR (400 MHz, DMSO- $d_6$ )  $\delta$  8.95 (d, J = 2.0 Hz, 1H), 8.67 (d, J =8.1 Hz, 1H), 8.23 (d, J = 2.1 Hz, 1H), 8.15 (d, J = 8.1 Hz, 1H), 8.01 (d, J = 7.9 Hz, 1H), 7.90 (d, J = 7.2 Hz, 2H), 7.75 (d, J = 7.2 Hz, 1H), 7.66-7.43 (m, 9H), 7.31-7.22 (m, 2H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>)  $\delta$ 196.9, 154.6, 145.7, 137.5, 137.0, 136.6, 136.4, 136.2, 134.0, 133.3, 132.9, 130.5, 129.4, 129.0, 128.8, 128.7, 128.1, 127.5, 126.8, 125.3, 124.8; FT-IR (KBr cm<sup>-1</sup>): 3120 (=C-H), 1712 (C=O), 1562 (C=N), 1485 (C=C), 1184 (C-O);







## vii) (4-chlorophenyl)(3,5-diphenylpyridin-2-yl)methanone (3ag)

Yield: 236 mg, 64%; Colourless solid; mp =168-172 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.97 (d, J = 2.1 Hz, 1H), 8.23 (d, J = 2.1 Hz, 1H), 7.89 (d, J = 7.2 Hz, 2H), 7.81 (d, J = 8.6 Hz, 2H), 7.57-7.32 (m, 10H);<sup>13</sup>**C NMR** (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  193.6, 152.9, 145.6, 138.9, 137.1, 136.9, 136.4, 136.2, 136.1, 134.7, 131.9, 129.3, 129.0, 128.9, 128.8, 128.7, 128.2, 127.4; **FT-IR** (KBr, cm<sup>-1</sup>): 3035(=C-H), 1668(C=O),

1589(C=N), 1421(C=C), 1299(C-O), 829(C-H out of plane bending), 717(C-Cl); HRMS (ESI) Calcd for C<sub>24</sub>H<sub>16</sub>ClNO [M+H]<sup>+</sup>, 370.0993; found, 370.099.



viii) (4-bromophenyl)(3,5-diphenylpyridin-2-yl)methanone (3ah)

Yield: 289 mg, 70%; Colourless solid; mp =164-168 °C

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.94 (d, J = 2.0 Hz, 1H), 8.19 (d, J = 2.1 Hz, 1H), 7.85 (d, J = 7.3 Hz, 2H), 7.69 (dd, J = 17.9, 8.6 Hz, 4H), 7.52-7.31 (m, 8H);<sup>13</sup>**C NMR** (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  193.8, 152.9, 145.6, 137.2, 137.0, 136.5, 136.2, 136.1, 135.1, 132.0, 129.4, 128.8, 128.8, 128.3, 127.4; **FT-IR** (KBr, cm<sup>-1</sup>): 3124(=C-H), 1645(C=O), 1573(C=N), 1490(C=C), 1157(C-O), 808(C-H out of plane bending), 673(C-Br); HRMS (ESI) Calcd for C<sub>24</sub>H<sub>16</sub>BrNO [M+H]<sup>+</sup>, 414.0488; found, 414.0495.

## ix) (3,5-diphenylpyridin-2-yl)(4-fluorophenyl)methanone(3ai)

Yield: 215 mg, 61%; Colourless solid; mp =112-116 °C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.98 (d, J = 2.1 Hz, 1H), 8.23 (d, J = Hz, 1H), 7.91-7.87 (m, 4H), 7.56-7.30 (m, 10H);<sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  193.2, 166.6, 164.1, 153.1, 145.5, 137.2, 136.8, 136.3, 136.2, 136.1, 133.1, 133.0, 132.8, 129.3, 129.2, 128.8, 128.7, 128.2, 127.4, 116.1, 115.9; **FT-IR** (KBr, cm<sup>-1</sup>): 3095(=C-H), 1664(C=O), 1575(C=N), 1506(C=C), 1255 (C-F), 1236 (C-O);



3ah

HRMS (ESI) Calcd for C<sub>24</sub>H<sub>16</sub>FNO [M+H]<sup>+</sup>, 354.1289; found, 354.1299.

x) (2,4-dichlorophenyl)(3,5-diphenylpyridin-2-yl)methanone (3aj) Yield: 242 mg, 60%; Colourless solid; mp =156-158 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.95 (d, J = 2.0 Hz, 1H), 8.18 (d, J =

Hz, 1H), 7.87 (d, J = 7.2 Hz, 2H), 7.65-7.61 (m, 2H), 7.51-7.35 (m, 9H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  193.1, 151.4, 145.6, 137.7, 137.6, 137.4, 136.9, 136.8, 136.5, 135.7, 132.7, 132.7, 129.8, 129.3, 129.0, 128.9, 128.5, 128.0, 127.6, 127.4; FT-IR (KBr, cm<sup>-1</sup>): 3058(=C-H), 1691(C=O), 1604(C=N), 1458(C=C), 1191(C-O), 754, 725(C-Cl);

HRMS (ESI) Calcd for  $C_{24}H_{15}Cl_2NO \ [M+H]^+$ , 404.0604; found, 404.0610.

## xi) (3,5-diphenylpyridin-2-yl)(4-nitrophenyl)methanone (3ak)

Yield: 258 mg, 68%; Colourless solid; mp=156-158 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-  $d_6$ )  $\delta$  9.02 (d, J = 2.1 Hz, 1H), 8.28 (d, J = 2.1 Hz, 1H), 7.92 (d, J = 8.6 Hz, 2H), 7.83 (d, J = 8.6 Hz, 2H), 7.75 (d, J = 5.3 Hz, 1H), 7.60-7.36 (m, 9H); <sup>13</sup>**C NMR** (101 MHz, DMSO- $d_6$ )  $\delta$  193.2, 152.0, 150.0, 146.5, 145.5, 140.8, 137.3, 137.0, 136.4, 135.9, 131.3, 129.3, 128.8, 128.7, 128.2, 127.4, 127.2, 123.8; **FT-IR** (KBr, cm<sup>-1</sup>): 3141(=C-H), 1691(C=O), 1627(C=N),1568 (asymmetric NO<sub>2</sub>), 1471(C=C), 1301(symmetric NO<sub>2</sub>),1238(C-O);

xii) (3,5-diphenylpyridin-2-yl)(4-(methylsulfonyl)phenyl)methanone (3al)

HRMS (ESI) Calcd for C<sub>24</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub> [M+H]<sup>+</sup>, 381.1254; found, 381.1252.

Yield: 293 mg, 71%; Colourless solid; mp =138-140 °C;

<sup>1</sup>**H** NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.04 (d, J = 2.0 Hz, 1H), 8.33 (d, J = 2.1 Hz, 1H), 8.12 (s, 2H), 7.97 (d, J = 7.0 Hz, 2H), 7.62-7.38 (m, 10H), 3.34 (s, 3H); <sup>13</sup>**C** NMR (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  193.7, 152.3, 145.5, 144.6, 139.9, 137.2, 137.1, 137.0, 136.4, 135.9, 130.9, 129.3, 128.9, 128.9, 128.7, 128.2, 127.4, 127.4, 43.2; **FT-IR** (KBr, cm<sup>-1</sup>): 3110(=C-H), 2923(-C-H), 1683(C=O), 1558(C=N), 1417(C=C), 1342 (asymmetric SO<sub>2</sub>), 1253(C-O), 1193(symmetric SO<sub>2</sub>);

HRMS (ESI) Calcd for C<sub>25</sub>H<sub>19</sub>NO<sub>3</sub>S [M+H]<sup>+</sup>, 414.1159; found, 414.1161.

xiii) (3,5-diphenylpyridin-2-yl)(thiophen-2-yl)methanone (3am)

Yield: 232 mg, 68%; Colourless solid; mp =128-130 °C;

<sup>1</sup>**H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.88 (d, J = 2.1 Hz, 1H), 7.98 (d, J = 2.1 Hz, 1H), 7.72 (dd, J = 3.8, 1.2 Hz, 1H), 7.69-7.66 (m, 3H), 7.53-7.42 (m, 3H), 7.38-7.32 (m, 5H), 7.10 (dd, J = 4.9, 3.8 Hz, 1H); <sup>13</sup>**C NMR** (101 MHz, CDCl<sub>3</sub>) δ 186.4, 152.7, 145.6, 143.0, 137.9, 137.8, 137.4, 136.9, 136.7, 135.9, 135.4, 129.3, 128.8, 128.7, 128.6, 128.1, 128.1,







127.3; **FT-IR** (KBr, cm<sup>-1</sup>): 3147(=C-H), 1627(C=O), 1587(C=N), 1483(C=C), 1259(C-O), 823(C-S); HRMS (ESI) Calcd for C<sub>22</sub>H<sub>15</sub>NOS [M+H]<sup>+</sup>, 342.0947; found, 342.0952.

#### xiv) (3,5-diphenylpyridin-2-yl)(furan-2-yl)methanone (3an)

Yield: 201 mg, 62 %; Colourless solid; m.p =110-112 °C;

<sup>1</sup>**H-NMR** (400 MHz, DMSO-d<sub>6</sub>) δ 9.00 (d, *J* = 2.0 Hz, 1H), 8.22 (d, *J* = 2.0 Hz, 1H), 8.06 (d, *J* = 0.9 Hz, 1H), 7.92 (d, *J* = 7.2 Hz, 2H), 7.60-7.52 (m, 3H), 7.44 (d, *J* = 3.4 Hz, 5H), 7.32 (d, *J* = 3.5 Hz, 1H), 6.75 (q, *J* = 1.7 Hz, 1H);<sup>13</sup>**C-NMR** (101 MHz, DMSO-d<sub>6</sub>) δ 181.9, 152.4, 151.7, 149.3, 145.7, 137.3, 137.2, 136.4, 136.3, 136.2, 129.5, 129.0, 128.8, 128.3, 127.5, 123.0,

113.2; **FT-IR** (KBr, cm<sup>-1</sup>): 3186(=C-H), 1668(C=O), 1625(C=N), 1404(C=C), 1217(C-O); HRMS (ESI) Calcd for C<sub>22</sub>H<sub>15</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 326.1176; found, 326.1166.

## xv)(3,5-diphenylpyridin-2-yl)(pyridin-3-yl)methanone (3ao)

Yield: 174 mg, 52%; Colourless solid; mp =132-134 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.89 (s, 1H), 8.83 (s, 1H), 8.67 (d, J = 3.8 Hz, 1H), 8.13 (d, J = 9.0 Hz, 1H), 7.80 (d, J = 7.3 Hz, 2H), 7.49-7.22 (m, 10H); <sup>13</sup>**C NMR** (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  193.7, 153.7, 150.9, 146.2, 145.6, 137.3, 137.2, 136.9, 136.4, 134.1, 132.5, 130.5, 129.3, 128.9, 128.7, 128.6, 128.2, 127.5, 123.9; **FT-IR** (KBr, cm<sup>-1</sup>): 3097, 3035(=C-H), 1704(C=O), 1558(C=N), 1469(C=C), 1369(C-N), 1261(C-O);

HRMS (ESI) Calcd for  $C_{23}H_{16}N_2O$  [M+H]<sup>+</sup>, 337.1336; found, 337.1344.

## xvi) (3,5-diphenylpyridin-2-yl)(phenyl)methanone (3ap)<sup>1</sup>

Yield: 214 mg, 64%; Colourless solid; mp =124-126 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.98 (d, J = 2.1 Hz, 1H), 8.23 (d, J = 2.0 Hz, 1H), 7.90 (d, J = 7.2

Hz, 2H), 7.80 (d, J = 7.2 Hz, 2H), 7.65 (t, J = 7.4 Hz, 1H), 7.56-7.32 (m, 10H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  194.8, 153.5, 145.5, 137.2, 136.7, 136.2, 136.1, 136.1, 133.9, 130.0, 129.3, 129.2, 128.8, 128.7, 128.2, 127.4, 127.2; **FT-IR** (KBr, cm<sup>-1</sup>): 3110(=C-H), 1689(C=O), 1591(C=N), 1494(C=C), 1244(C-O); HRMS (ESI) Calcd for C<sub>24</sub>H<sub>17</sub>NO [M+H]<sup>+</sup>, 336.1383; found, 336.1390.

## xvii) (3,5-diphenylpyridin-2-yl)(p-tolyl)methanone (3aq)

Yield: 279 mg, 80%; Colourless solid; mp =160-164  $^{\circ}$ C;



3an



<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.95 (d, J = 2.1 Hz, 1H), 8.21 (d, J = 2.0 Hz, 1H), 7.89 (d, J =

7.2 Hz, 2H), 7.67 (d, J = 8.1 Hz, 2H), 7.55-7.52 (m, 2H), 7.48 (d, J = 7.3 Hz, 1H), 7.40-7.29 (m, 7H), 2.35 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>)
194.3, 153.7, 145.5, 144.5, 137.2, 136.5, 136.2, 136.0, 135.9, 133.5, 130.1,
129.4, 129.3, 128.7, 128.7, 128.1, 127.4, 21.3; FT-IR (KBr, cm<sup>-1</sup>):
3164(=C-H), 2923(-C-H), 1662(C=O), 1604(C=N), 1469(C=C), 1298(C-O); HRMS (ESI) Calcd for C<sub>25</sub>H<sub>19</sub>NO [M+H]<sup>+</sup>, 350.1540; found, 350.1542.

δ 3aq CH<sub>3</sub>
δ

## xviii) (3,5-diphenylpyridin-2-yl)(4-methoxy-3-nitrophenyl)methanone(3ar)

Yield: 291 mg, 71%; yellow solid; mp =176-180 °C;

<sup>1</sup>**H-NMR** (400 MHz, DMSO-d<sub>6</sub>) δ 8.97 (d, *J* = 2.1 Hz, 1H), 8.29 (d, *J* = 2.1 Hz, 1H), 8.22 (d, *J* = 2.1 Hz, 1H), 8.09 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.88 (d, *J* = 7.2 Hz, 1H), 7.57-7.34 (m, 10H), 3.99 (s, 3H);

<sup>13</sup>**C-NMR** (101 MHz, DMSO-d<sub>6</sub>) δ 191.8, 156.0, 152.5, 145.6, 139.1, 137.3, 137.2, 136.9, 136.5, 136.3, 136.1, 129.5, 129.1, 128.9, 128.9, 128.7, 128.4,

127.5, 127.1, 114.7, 57.6; **FT-IR** (KBr, cm<sup>-1</sup>): 3035(=C-H), 2968(-C-H), 1668(C=O), 1589(C=N), 1548 (asymmetre NO<sub>2</sub>), 1421(C=C), 1299( symmetric NO<sub>2</sub>), 1217(C-O); MS (ESI) Calcd for C<sub>25</sub>H<sub>19</sub>NO [M+H]<sup>+</sup>, 411.134; found, 411.100.

## xix) (3,5-diphenylpyridin-2-yl)(3-hydroxyphenyl)methanone(3as)

Yield: 287 mg, 82%; yellow solid; mp =200-204 °C ;

<sup>1</sup>**H-NMR** (400 MHz, DMSO-d<sub>6</sub>) δ 9.88 (s, 1H), 8.95 (d, *J* = 2.1 Hz, 1H), 8.20 (d, *J* = 2.1 Hz, 1H), 7.88 (d, *J* = 7.2 Hz, 2H), 7.57-7.27 (m, 10H), 7.14 (d, *J* = 2.1 Hz, 1H);

<sup>13</sup>**C-NMR** (101 MHz, DMSO-d<sub>6</sub>) δ 194.8, 157.6, 145.5, 137.4, 137.2, 136.7, 136.2, 136.1, 135.9, 130.1, 129.4, 128.8, 128.8, 128.3, 127.5, 121.2, 116.0; **FT-IR** (KBr cm<sup>-1</sup>): 3401 (O-H), 3053 (=C-H), 1668 (C=O), 1582 (C=N), 1493 (C=C), 1008 (C-O); MS (ESI) Calcd for C<sub>24</sub>H<sub>17</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 352.1332; found, 352.15.



## xx) (3,4-dichlorophenyl)(3,5-diphenylpyridin-2-yl)methanone(3at)

Yield: 315 mg, 78%; yellow solid; mp =172-176 °C ; <sup>1</sup>H-NMR (400 MHz, DMSO-d<sub>6</sub>) δ 9.00 (d, *J* = 2.1 Hz, 1H), 8.25 (d, *J* 2.0 Hz, 1H), 7.97-7.94 (m, 2H), 7.71-7.37 (m, 11H); <sup>13</sup>C-NMR (101 MHz, DMSO-d<sub>6</sub>) δ 193.7, 145.5, 144.6, 139.9, 137.2, 137.1, 137.0, 136.4, 135.9, 130.9, 129.3, 128.9, 128.9, 128.7, 128.2,





127.4, 127.4; FT-IR (KBr, cm<sup>-1</sup>): 3213, 3001(=C-H), 1667(C=O), 1607(C=N), 1581(C=C), 1132(C-O), 851(C-Cl); MS (ESI) Calcd for C<sub>24</sub>H<sub>15</sub>Cl<sub>2</sub>NO [M+H]<sup>+</sup>, 404.0604; found, 404.10.

## xxi) (2,4-dimethoxyphenyl)(3,5-diphenylpyridin-2-yl)methanone (3au)

Yield: 186 mg, 51%; yellow solid; mp =156-158 °C ; <sup>1</sup>**H-NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.98 (d, J = 2.1 Hz, 1H), 8.23 (d, J =2.0 Hz, 1H), 7.90 (d, J = 7.2 Hz, 1H), 7.80 (d, J = 7.2 Hz, 2H), 7.66-7.33 (m, 8H), 6.82-6.80 (m, 2H), 3.92 (s, 3H), 3.80 (s, 3H); 3au <sup>13</sup>C-NMR (101 MHz, DMSO-d<sub>6</sub>) δ 181.9, 166.4, 159.1, 145.7, 141.1, 140.3, 139.9, 137.3, 137.2, 136.4, 136.3, 136.2, 129.5, 129.0, 128.8, 128.3, 127.5, 108.2, 105.6, 98.4, 55.9, 55.3; FT-IR (KBr, cm<sup>-1</sup>): 3062(=C-H), 2954(-C-H), 1678(C=O), 1571(C=N), 1610, 1444(C=C), 1239(C-O); MS (ESI) Calcd for C<sub>26</sub>H<sub>21</sub>NO<sub>3</sub> [M+H]<sup>+</sup>, 396.1594; found, 395.12.

## xxii) (2-bromophenyl)(3,5-diphenylpyridin-2-yl)methanone(3av)

Yield: 231 mg, 56%; yellow solid; mp =126-130 °C;

<sup>1</sup>**H-NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.95 (d, J = 2.0 Hz, 1H), 8.18 (d, J =1.8 Hz, 1H), 7.87 (d, J = 7.2 Hz, 1H), 7.65-7.61 (m, 2H), 7.51-7.35 (m, 11H); <sup>13</sup>C-NMR (101 MHz, DMSO-d<sub>6</sub>) δ 193.6, 152.9, 145.6, 138.9, 137.1, 136.9, 136.4, 136.2, 136.1, 134.7, 131.9, 129.3, 129.0, 128.9, 128.8, 128.7, 128.2, 127.4, 121.6; **FT-IR** (KBr, cm<sup>-1</sup>): 3093(=C-H), 1694(C=O), 1580(C=N), 1551(C=C), 1263(C-O), 575(C-Br), ; MS (ESI) Calcd for C<sub>24</sub>H<sub>16</sub>BrNO [M+H]<sup>+</sup>, 414.0488; found, 414.10.



## xxiii) [1,1'-biphenyl]-4-yl(3,5-bis(4-chlorophenyl)pyridin-2-yl)methanone (3ba)

Yield: 232 mg, 83%; Colourless solid; mp =188-192 °C <sup>1</sup>**H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.79 (d, J = 2.1 Hz, 1H), 7.88-7.86 (m, 3H), 7.58 (d, J = 8.3 Hz, 2H), 7.53 (d, J = 8.4 Hz, 4H), 7.43-7.17 (m, 9H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 194.1, 153.9, 146.4, 145.8, 139.8, 136.5, 136.2, 135.9, 135.2, 135.1, 134.9, 134.6, 131.0, 130.0, 129.5, 129.0, 128.9, 128.5, 128.3, 127.3, 127.2; **FT-IR** (KBr, cm<sup>-1</sup>): 3110(=C-H), 1701(C=O), 1544(C=N), 1483(C=C), 1236(C-O), 742(C-Cl); HRMS (ESI) Calcd for C<sub>30</sub>H<sub>19</sub>Cl<sub>2</sub>NO [M+H]<sup>+</sup>, 480.0922; found, 480.0927.





## xxiv) (3,5-bis(4-chlorophenyl)pyridin-2-yl)(naphthalen-2-yl)methanone (3bb) Yield: 339 mg, 75%; Colourless solid; mp =152-156 °C

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.00 (d, J = 2.0 Hz, 1H), 8.40 (s, 1H), 8.26 (d, J = 2.1 Hz, 1H), 8.03-7.87 (m, 6H), 7.67-7.63 (m, 1H), 7.56 (d, J = 8.4 Hz, 3H), 7.43 (d, J = 8.6 Hz, 2H), 7.35 (d, J = 8.4 Hz, 2H);<sup>13</sup>**C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  194.5, 171.1, 154.0, 145.8, 136.4, 136.1, 135.8, 135.1, 135.0, 134.5, 133.5, 133.2, 132.3, 130.2, 129.9, 129.7, 129.5, 129.1, 128.9, 128.9, 128.5, 127.8, 126.7, 124.9; **FT-IR** (KBr, cm<sup>-1</sup>): 3039(=C-H), 1652(C=O), 1533(C=N), 1492(C=C), 1298(C-O), 750( C-Cl); HRMS (ESI) Calcd for C<sub>28</sub>H<sub>17</sub>Cl<sub>2</sub>NO [M+H]<sup>+</sup>, 454.076; found, 454.0766.

## xxv) (3,5-bis(4-chlorophenyl)pyridin-2-yl)(4-chlorophenyl)methanone (3bc)

Yield: 297 mg, 68%; Colourless solid; mp =172-174 °C

<sup>1</sup>**H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.77 (d, J = 2.0 Hz, 1H), 7.87 (d, J = 2.1 Hz, 1H), 7.74 (d, J = 8.7 Hz, 2H), 7.53 (d, J = 8.6 Hz, 2H), 7.42 (d, J = 8.6 Hz, 2H), 7.33 (d, J = 6.7 Hz, 2H), 7.21 (dd, J = 8.6 Hz, 4H);<sup>13</sup>**C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  193.2, 153.3, 145.8, 140.2, 136.7, 136.3, 136.2, 135.7, 135.3, 134.9, 134.7, 134.5, 131.7, 130.0, 129.5, 129.0, 128.9,

128.5; **FT-IR** (KBr, cm<sup>-1</sup>): 3120(=C-H), 1712(C=O), 1562(C=N), 1485(C=C), 1184(C-O), 844(out of plane C-H bending for *p*-substituted), 748(C-Cl);

HRMS (ESI) Calcd for  $C_{24}H_{14}Cl_3NO [M+H]^+$ , 438.0214; found, 438.0223.

## xxvi) (3,5-bis(4-chlorophenyl)pyridin-2-yl)(phenyl)methanone (3bd)

Yield: 232 mg, 68%; Colourless solid; mp =156-158 °C

129.5, 129.4, 128.9, 128.5;

<sup>1</sup>**H NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.77 (d, J = 2.0 Hz, 1H), 7.85 (d, J = 2.1

Hz, 1H), 7.77 (d, *J* = 7.0 Hz, 2H), 7.52-7.46 (m, 3H), 7.41-7.32 (m,

4H), 7.23-7.16 (m, 4H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>) δ 194.5, 153.8,

145.7, 136.4, 136.1, 135.8, 135.1, 135.0, 134.5, 133.6, 130.3, 130.0,

**FT-IR** (KBr, cm-1): 3110, 3012 (=C-H), 1666(C=O), 1633(C=N), 1554(C=C), 1218(C-O), 844(out of plane C-H bending for *p*-substituted), 744( C-Cl);

HRMS (ESI) Calcd for  $C_{24}H_{15}Cl_2NO \ [M+H]^+$ , 404.0604; found, 404.0609.







## xxvii)2-phenylacetaldehyde(7)

Yield: 65 mg, 54%; Colourless liquid

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  9.49 (d, J = 3.5 Hz, 1H), 7.29 (t, J = 7.9

Hz, 2H), 7.19-7.13 (m, 3H), 3.61 (d, J = 3.5 Hz, 2H); <sup>13</sup>C-NMR (101

MHz, DMSO-d<sub>6</sub>) δ 199.3, 133.6, 129.0, 127.7, 125.9, 52.0; **FT-IR** (KBr,

cm<sup>-1</sup>): 3030(=C-H), 2922(-C-H), 2824, 2733(d, CHO), 1700(C=O),

1603(C=C), 1576 (CH<sub>2</sub> bending vibration), 1167(C-O); MS (ESI) Calcd for C<sub>8</sub>H<sub>8</sub>O [M+H]<sup>+</sup>, 121.0648; found, 121.00.

## xxviii)2-oxo-2-phenylacetaldehyde(8)

Yield: 121 mg, 91%; lightish yellow liquid;

<sup>1</sup>**H-NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  9.88 (s, 1H), 7.80 (dd, J = 4.5, 1.6 Hz, 2H), 7.52-7.50 (m, 1H), 7.33-7.24 (m, 2H); <sup>13</sup>**C-NMR** (101 MHz, DMSO-d<sub>6</sub>)  $\delta$ 198.3, 186.0, 138.2, 133.3, 129.5, 128.9; **FT-IR** (KBr, cm<sup>-1</sup>): 3106(=C-H), 2639(d, -CHO), 1727(aldehydic C=O),1657(ketone C=O), 1449(C=C), 1089(C-O), 1500-400( finger print region); MS (ESI) Calcd for C<sub>8</sub>H<sub>6</sub>O<sub>2</sub> [M+H]<sup>+</sup>, 135.0441; found, 135.10.

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## 5(b) Spectral data of 2,5-disubstituted oxazole derivatives

## i) (5-([1,1'-biphenyl]-4-yl)oxazol-2-yl)(phenyl)methanone(4aa)

Yield: 266 mg, 82%; Colourless solid; mp =150-154 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.37 (d, J = 7.2 Hz, 2H), 8.16 (s, 1H), 7.96 (d, J = 8.6 Hz, 2H), 7.86 (d, J = 8.6 Hz, 2H), 7.75-7.71 (m, 3H), 7.60 (t, J = 7.7 Hz, 2H), 7.49 (t, J = 7.6 Hz, 2H), 7.40 (t, J = 7.3 Hz, 1H);<sup>13</sup>**C NMR** (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  178.0, 156.6, 153.1, 141.4,

138.9, 135.0, 133.8, 131.4, 131.1, 130.4, 129.8, 129.6, 129.0, 128.5, 127.5, 126.7, 125.7, 125.3, 125.1; **FT-IR** (KBr, cm-1): 3137(=C-H), 1685(C=O), 1575(C=N), 1475(C=C), 1186(C-O); HRMS (ESI) Calcd for C<sub>22</sub>H<sub>15</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 326.1176; found, 326.1173.

## ii) (5-(4-hydroxyphenyl)oxazol-2-yl)(phenyl)methanone(4ab)

Yield: 193 mg, 73%; Colourless solid; mp =182-186 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>) δ 10.31 (s, 1H), 8.41 (d, *J* = 7.3 Hz, 2H), 7.94 (s, 1H), 7.80-7.78 (m, 3H), 7.66 (t, *J* = 7.6 Hz, 2H), 7.00 (d, *J* = 8.6 Hz, 2H);







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<sup>13</sup>C NMR (101 MHz, DMSO- d<sub>6</sub>) δ 177.8, 159.3, 155.9, 154.2, 135.2, 133.7, 130.3, 128.5, 127.1, 122.9, 117.3, 116.2; FT-IR (KBr, cm<sup>-1</sup>): 3388(=C-H), 1614(C=O), 1560(C=N), 1485(C=C), 1245(C-O);

HRMS (ESI) Calcd for C<sub>16</sub>H<sub>11</sub>NO<sub>3</sub> [M+H]<sup>+</sup>, 266.0812; found, 266.0809.

#### iii) (5-(3,4-dimethoxyphenyl)oxazol-2-yl)(phenyl)methanone(4ac)

Yield: 278 mg, 90%; Colourless solid; mp =134-136 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.42 (d, J = 7.3 Hz, 2H), 8.09 (s, 1H), 7.78 (t, J = 7.3 Hz, 1H), 7.66 (t, J = 7.6 Hz, 2H), 7.52-7.47 (m, 2H), 7.18 (d, J = 8.4 Hz, 1H), 3.92 (s, 3H), 3.88 (s, 3H) ; <sup>13</sup>**C NMR** (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  178.1, 156.3, 154.0, 150.6, 149.4, 135.3,

134.0, 130.5, 128.7, 124.0, 119.0, 118.6, 112.4, 108.5, 55.9, 55.8; **FT-IR** (KBr, cm<sup>-1</sup>): 3066(=C-H), 2964(-C-H) 1649(C=O), 1614(C=N), 1564(C=C), 1485( CH<sub>3</sub> bending), 1261(C-O); HRMS (ESI) Calcd for C<sub>18</sub>H<sub>15</sub>NO<sub>4</sub> [M+H]<sup>+</sup>, 310.1074; found, 310.1079.

#### ix) (5-(2,4-dimethoxyphenyl)oxazol-2-yl)(phenyl)methanone (4ad)

Yield: 250 mg, 81%; Colourless solid; mp =180-182 °C;

<sup>1</sup>**H-NMR** (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.40-8.38 (m, 2H), 8.25 (s, 1H), 7.60-7.55 (m, 2H), 7.43 (m, 3H), 6.42 (s, 1H), 3.95 (s, 3H), 3.88 (s, 3H);<sup>13</sup>**C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.6, 159.1, 157.4, 154.7, 148.8, 135.8, 134.5, 132.6, 129.7, 127.4, 125.7, 109.8, 94.2, 55.5, 54.9; **FT-IR** (KBr, cm-1): 3118(=C-H), 2829(-C-H), 1714(C=O), 1664(C=N), 1562(C=C), 1485(CH<sub>3</sub> bending), 1184(C-O);

HRMS (ESI) Calcd for C<sub>18</sub>H<sub>15</sub>NO<sub>4</sub> [M+H]<sup>+</sup>, 310.1074; found, 310.1072.

## v) (5-(2-fluoro-4-methoxyphenyl)oxazol-2-yl)(phenyl)methanone(4ae)

Yield: 198 mg, 67%; Colourless solid; mp =140-142 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-  $d_6$ )  $\delta$  8.27 (d, J = 8.6 Hz, 2H), 7.77-

7.65 (m, 3H), 7.55-7.52 (m, 2H), 7.02-6.92 (m, 2H), 3.77 (s, 3H);<sup>13</sup>C

**NMR** (101 MHz, DMSO-d<sub>6</sub>) δ 178.5, 162.5, 161.5, 158.9, 156.2,

148.8, 135.3, 134.4, 130.7, 129.0, 128.4, 128.3, 126.5, 126.4, 112.1,

107.4, 107.3, 102.9, 102.6, 56.4; **FT-IR** (KBr, cm<sup>-1</sup>): 3093, 3053(=C-H), 2954(-C-H), 1668(C=O), 1571(C=N), 1481( CH<sub>3</sub> bending), 1425(C=C), 1253(C-O), 1018( C-F);



OCH<sub>3</sub>





HRMS (ESI) Calcd for  $C_{17}H_{12}FNO_3$  [M+H]<sup>+</sup>, 298.0874; found, 298.0871.

## vi) phenyl(5-(thiophen-2-yl)oxazol-2-yl)methanone(4af)

Yield: 173 mg, 68%; Colourless solid; mp =114-116 °C;

<sup>1</sup>**H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.40-8.36 (m, 2H), 7.75-7.72 (m, 1H), 7.57-7.52 (m, 2H), 7.47-7.42 (m, 4H), 7.35-7.35 (m, 1H), 7.04 (dd, *J* = 5.0, 3.7 Hz, 1H); <sup>13</sup>**C NMR** (101 MHz, CDCl<sub>3</sub>) δ 173.7, 151.7, 145.1, 130.6, 129.1, 126.1, 125.3, 124.4, 123.8, 123.6, 123.2, 122.2, 120.7, 118.8; **FT-IR** (KBr, cm-1): 3099, 3049(=C-H), 1716(C=O), 1658(C=N), 1514(C=C), 1236(C-

O), 850(C-S); HRMS (ESI) Calcd for C<sub>14</sub>H<sub>9</sub>NO<sub>2</sub>S [M+H]<sup>+</sup>, 256.0444; found, 256.0441.

#### vii) (5-(furan-2-yl)oxazol-2-yl)(phenyl)methanone (4ag)

Yield: 143 mg, 60%; Colourless solid; mp =162-166 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>) δ 8.25 (d, J = 7.3 Hz, 2H), 7.86 (s, 1H), 7.76 (d, J = 6.1 Hz, 1H), 7.62 (t, J = 7.2 Hz, 1H), 7.51-7.45 (m, 2H), 7.03 (d, J = 3.2 Hz, 1H), 6.64 (s, 1H);<sup>13</sup>**C NMR** (101 MHz, DMSO-d<sub>6</sub>) δ 177.8, 156.0, 145.6, 141.7, 134.9, 134.0, 130.5, 129.4, 128.6, 125.2, 125.0, 124.1, 112.7, 111.1; **FT-IR** (KBr, cm-1): 3062(=C-H), 1733(C=O), 1577(C=N),

1436(C=C), 1234(C-O); HRMS (ESI) Calcd for C<sub>14</sub>H<sub>9</sub>NO<sub>3</sub> [M+H]<sup>+</sup>, 240.0645; found, 240.0662.

## viii) (5-(naphthalen-2-yl)oxazol-2-yl)(phenyl)methanone(4ah)

Yield: 218 mg, 73%; Colourless solid; mp =156-158 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>) δ 8.42-8.40 (m, 3H), 8.20 (s, 1H), 8.09-8.06 (m, 2H), 7.98-7.96 (m, 2H), 7.78-7.74 (m, 1H), 7.65-7.59 (m, 4H); <sup>13</sup>**C NMR** (101 MHz, DMSO-d<sub>6</sub>) δ 178.1, 156.7, 153.6, 135.0, 134.0, 133.3, 132.9, 130.5, 129.1, 128.6, 127.9, 127.6, 127.5,

127.2, 125.5, 124.5, 123.7, 122.4; **FT-IR** (KBr, cm<sup>-1</sup>): 3267, 3110 (=C-H), 1699(C=O), 1579(C=N), 1461(C=C), 1213(C-O); HRMS (ESI) Calcd for C<sub>20</sub>H<sub>13</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 300.1019; found, 300.1017.

## ix) (5-(naphthalen-1-yl)oxazol-2-yl)(phenyl)methanone(4ai)

Yield: 209 mg, 70%; Colourless solid; mp =172-174 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>) δ 8.47-8.44 (m, 3H), 8.16-8.10 (m, 3H), 8.02 (d, *J* = 7.3 Hz, 1H), 7.81-7.65 (m, 6H); <sup>13</sup>**C NMR** (101 MHz, DMSOd<sub>6</sub>) δ 178.3, 157.0, 153.0, 135.0, 134.0, 133.5, 131.0, 130.5, 129.3, 129.0, 128.6, 127.9, 127.7, 126.7, 125.6, 124.6, 123.5;









**FT-IR** (KBr, cm<sup>-1</sup>): 3109(=C-H), 1703(C=O), 1546(C=N), 1481(C=C), 1234(C-O); HRMS (ESI) Calcd for C<sub>20</sub>H<sub>13</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 300.1019; found, 300.1025.

## x) phenyl(5-phenyloxazol-2-yl)methanone(4aj)<sup>5</sup>

Yield: 161 mg, 65%; Colourless solid; mp =132-134 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.40 (dd, J = 8.4, 1.2 Hz, 2H), 8.12 (s, 1H), 7.91-7.89 (m, 2H), 7.77-7.73 (m, 1H), 7.64-7.48 (m, 5H); <sup>13</sup>**C NMR** (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  178.0, 156.5, 153.4, 135.0, 133.9, 130.4, 130.0, 129.3, 128.5, 126.3, 125.1, 125.0; **FT-IR** (KBr, cm<sup>-1</sup>): 3035(=C-H), 1737(C=O), 1502(C=N), 1425(C=C), 1249(C-O);



HRMS (ESI) Calcd for  $C_{16}H_{11}NO_2$  [M+H]<sup>+</sup>, 250.0863; found, 250.0860.

## xi) (5-(benzo[d][1,3]dioxol-5-yl)oxazol-2-yl)(phenyl)methanone(4ak)

Yield: 184 mg, 63%; Colourless solid; mp =120-124 °C;

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ 8.36 (d, *J* = 7.2 Hz, 2H), 8.00 (s, 1H),
7.80-7.90 (1H), 7.69-7.78 (1H), 7.63-7.41 (m, 3H), 7.10 (d, *J* = 8.1 Hz,
1H), 6.14 (s, 2H);<sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ 177.9, 156.1, 153.5,
148.9, 148.2, 135.1, 133.8, 130.4, 128.5, 127.2, 124.0, 119.8, 109.2,

105.3, 101.8, 40.1; **FT-IR** (KBr, cm-1): 3068(=C-H), 2979 (-C-H), 1693(C=O), 1483(C=N), 1454(C=C), 1402(CH<sub>2</sub> bending) 1290(C-O);

HRMS (ESI) Calcd for C<sub>17</sub>H<sub>11</sub>NO<sub>4</sub> [M+H]<sup>+</sup>, 294.0761; found, 294.0759.

## xii) phenyl(5-phenyl-4-propyloxazol-2-yl)methanone (4al)

238 mg, 82% yield; colourless solid; mp 132-134 °C; <sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>): δ 8.40 (dd, J

= 8.4, 1.2 Hz, 2H), 7.91-7.89 (m, 2H), 7.77-7.73 (m, 1H), 7.64-7.48 (m, 4H), 7.52-7.48 (t, *J* = 7.2 Hz, 1H);<sup>13</sup>**C NMR** (101 MHz, DMSO-d<sub>6</sub>): δ 178.0, 156.5, 153.3, 134.9, 133.8, 130.4, 130.0, 129.3, 128.5, 126.3, 125.1, 31.2, 22.1, 14.0; **FT-IR** (KBr, cm<sup>-1</sup>): 3099(=C-H), 2993, 2848 (-C-H), 1716(C=O),

1658(C=N), 1514( C=C), 1446(CH<sub>2</sub> bending), 1236(C-O);

HRMS (ESI) *m/z*: [M+H]<sup>+</sup> Calcd for C<sub>19</sub>H<sub>17</sub>NO<sub>2</sub>, 292.1332; found, 292.1331.

## xiii) (4-chlorophenyl)(5-(p-tolyl)oxazol-2-yl)methanone (4ba)

Yield: 207 mg, 70%; Colourless solid; mp =142-144 °C;

<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ 8.38 (d, J = 8.6 Hz, 2H), 7.96 (s, 1H),
7.75 (d, J = 7.9 Hz, 2H), 7.64 (d, J = 8.4 Hz, 2H), 7.35 (d, J = 7.9 Hz,
2H), 2.37 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ 177.5, 156.2,
153.5, 144.7, 140.0, 132.5, 130.6, 130.0, 129.2, 125.1, 124.3, 123.7,



4al



21.3; **FT-IR** (KBr, cm<sup>-1</sup>): 3051(=C-H), 2920(-C-H), 1672(C=O), 1606(C=N), 1500(C=C), 1450 (CH<sub>3</sub> bending), 1249(C-O), 767(C-C1); HRMS (ESI) Calcd for  $C_{17}H_{12}CINO_2$  [M+H]<sup>+</sup>, 298.0620; found, 298.0878.

#### xiv) (4-chlorophenyl)(5-(4-methoxyphenyl)oxazol-2-yl)methanone (4bb)

Yield: 197 mg, 63%; Colourless solid; mp =166-170 °C;

<sup>1</sup>**H NMR** (400 MHz, CDCl<sub>3</sub>) δ 8.39 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.6 Hz, 2H), 7.43 (d, *J* = 7.8 Hz, 3H), 6.92 (d, *J* = 8.7 Hz, 2H), 3.79 (s, 3H); <sup>13</sup>**C NMR** (101 MHz, CDCl<sub>3</sub>) δ 176.6, 160.8, 155.9, 154.3, 139.8, 133.4, 131.8, 128.4, 126.7, 122.4, 118.8, 114.3; **FT-IR** (KBr,

cm<sup>-1</sup>): 3018(=C-H), 2914(-C-H), 1697(C=O), 1650(C=N), 1593(C=C), 1492 (CH<sub>3</sub> bending), 1217(C-O), 811(C-Cl); HRMS (ESI) Calcd for C<sub>17</sub>H<sub>12</sub>ClNO<sub>3</sub> [M+H]<sup>+</sup>, 314.0569; found, 314.0580.

#### xv)(4-chlorophenyl)(5-(4-chlorophenyl)oxazol-2-yl)methanone (4bc)<sup>5</sup>

Yield: 215 mg, 68%; Colourless solid; mp =148-150 °C;

<sup>1</sup>**H NM**R (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.41 (d, J = 8.7 Hz, 2H), 7.69 (d, J = 8.7 Hz, 2H), 7.53 (s, 1H), 7.44 (d, J = 8.7 Hz, 2H), 7.39 (d, J = 8.6 Hz, 2H); <sup>13</sup>**C NMR** (101 MHz, CDCl<sub>3</sub>)  $\delta$  177.1, 156.8, 153.4, 140.6, 136.2, 133.5, 132.2, 129.5, 128.9, 126.7, 125.0, 124.2; **FT-IR** (KBr, cm<sup>-1</sup>): 3137(=C-H), 1685(C=O), 1575(C=N), 1475(C=C), 1186(C-

O), 759( C-Cl); HRMS (ESI) Calcd for C<sub>16</sub>H<sub>9</sub>Cl<sub>2</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 318.0073; found, 318.0084.

## xvi) p-tolyl(5-(p-tolyl)oxazol-2-yl)methanone (4ca)<sup>5</sup>

Yield: 200 mg, 72%; Colourless solid; mp =136-140 °C;

<sup>1</sup>**H** NMR (400 MHz, DMSO-d<sub>6</sub>)  $\delta$  8.24 (d, J = 8.3 Hz, 2H), 7.98 (s, 1H), 7.71 (d, J = 8.1 Hz, 2H),

7.35 (d, J = 8.1 Hz, 2H), 7.30 (d, J = 7.9 Hz, 2H), 2.36 (s, 3H), 2.31 (s, 3H); <sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>)  $\delta$  177.5, 153.5, 144.7, 140.0, 132.5, 130.6, 130.0, 129.2, 125.1, 124.3, 123.7, 21.3, 21.1; **FT-IR** (KBr, cm<sup>-1</sup>): 3062(=C-H), 2914, 2885(-C-H), 1716(C=O), 1568(C=N), 1467(CH<sub>3</sub> bending), 1427(C=C), 1238(C-O); HRMS (ESI) Calcd for C<sub>18</sub>H<sub>15</sub>NO<sub>2</sub> [M+H]<sup>+</sup>, 278.1166; found, 278.1185.

#### xvii) **3,5-diphenylpyridine** (5a)<sup>1</sup>

Yield: 145 mg, 63%; Colourless solid; mp =137-138 °C;





N

4bb

H<sub>3</sub>CO



<sup>1</sup>H NMR (400 MHz, DMSO-d<sub>6</sub>) δ 8.94 (d, J = 2.1 Hz, 2H), 8.35 (t, J = 2.1 Hz, 1H), 7.91 (d, J = 7.3 Hz, 4H), 7.61-7.49 (m, 6H);
<sup>13</sup>C NMR (101 MHz, DMSO-d<sub>6</sub>) δ 146.1, 136.7, 135.6, 132.0, 128.9, 128.0, 126.9; FT-IR (KBr, cm<sup>-1</sup>): 3109, 3058(=C-H), 1579(C=N), 1406(C=C), 1217(C-O); HRMS (ESI) Calcd for C<sub>17</sub>H<sub>13</sub>N [M+H]<sup>+</sup>, 232.1121; found, 232.1126.

#### xviii) 3,5-bis(4-chlorophenyl)pyridine (5b)

Yield: 179 mg, 60%; Colourless solid; mp =162-166 °C; <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>)  $\delta$  8.55 (d, *J* = 2.0 Hz, 2H), 7.78 (t, *J* = 2.1 Hz, 1H), 7.36 (d, *J* = 8.4 Hz, 4H), 7.26-7.23 (m, 4H); <sup>13</sup>C NMR (101 MHz, CDCl<sub>3</sub>)  $\delta$  135.3, 134.9, 133.8, 131.9, 128.7, 127.9; FT-IR (KBr, cm<sup>-1</sup>): 3112(=C-H), 1596 (C=N), 1508 (C=C), 1242(C-O), 790( C-Cl); HRMS (ESI) Calcd for C<sub>17</sub>H<sub>11</sub>Cl<sub>2</sub>N [M+H]<sup>+</sup>, 300.0342; found, 300.0349.



## xix) 2-benzyl-5-(1H-indol-3-yl)oxazole (6a)

Yield: 198 mg, 72%; Colourless solid; mp =148-150 °C;

<sup>1</sup>**H NMR** (400 MHz, DMSO-d<sub>6</sub>) δ 11.54 (s, 1H), 7.82 (d, *J* = 7.8 Hz, 1H), 7.73 (d, *J* = 2.8 Hz, 1H), 7.47 (d, *J* = 8.1 Hz, 1H), 7.37-7.32 (m, 5H), 7.26-7.11 (m, 3H), 4.19 (s, 2H);<sup>13</sup>**C NMR** (101 MHz, DMSO-d<sub>6</sub>) δ 160.1, 147.9, 136.4, 136.3, 128.8, 128.7, 126.9, 123.6, 123.2, 122.2, 120.2, 119.5, 119.4, 112.2, 33.8;



**FT-IR** (KBr, cm<sup>-1</sup>): 3338(-N-H), 3062(=C-H), 2914, 2829(-C-H), 1637(C=N), 1552(C=C), 1458(CH<sub>2</sub> bending), 1155(C-O); **HRMS** (ESI) Calcd for C<sub>17</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub> [M+H]<sup>+</sup>, 275.1179; found, 275.1179.



## 6. Copies of <sup>1</sup>H NMR, <sup>13</sup>C NMR and IR spectra of 2, 3, 5- trisubstituted pyridines and 2,5-

disubstituted oxazoles

## <sup>1</sup>H-NMR spectrum of compound 3aa



<sup>13</sup>C-NMR spectrum of compound 3aa



<sup>1</sup>H-NMR spectrum of compound 3ab



<sup>13</sup>C-NMR spectrum of compound 3ab









<sup>13</sup>C-NMR spectrum of compound 3ac



FT-IR spectrum of compound 3ac



<sup>1</sup>H-NMR spectrum of compound 3ad



<sup>13</sup>C-NMR spectrum of compound 3ad



FT-IR spectrum of compound 3ad



<sup>1</sup>H-NMR spectrum of compound 3ae



<sup>13</sup>C-NMR spectrum of compound 3ae



<sup>1</sup>H-NMR spectrum of compound 3af



<sup>13</sup>C-NMR spectrum of compound 3af







<sup>1</sup>H-NMR spectrum of compound 3ag



<sup>13</sup>C-NMR spectrum of compound 3ag



<sup>1</sup>H-NMR spectrum of compound 3ah



<sup>13</sup>C-NMR spectrum of compound 3ah



FT-IR spectrum of compound 3ah



<sup>1</sup>H-NMR spectrum of compound 3ai



<sup>13</sup>C-NMR spectrum of compound 3ai


<sup>1</sup>H-NMR spectrum of compound 3aj



<sup>13</sup>C-NMR spectrum of compound 3aj



FT-IR spectrum of compound 3aj







<sup>13</sup>C-NMR spectrum of compound 3ak



FT-IR spectrum of compound 3ak



<sup>1</sup>H-NMR spectrum of compound 3al



<sup>13</sup>C-NMR spectrum of compound 3al







<sup>1</sup>H-NMR spectrum of compound 3am



<sup>13</sup>C-NMR spectrum of compound 3am



<sup>1</sup>H-NMR spectrum of compound 3an



<sup>13</sup>C-NMR spectrum of compound 3an







<sup>1</sup>H-NMR spectrum of compound 3ao



<sup>13</sup>C-NMR spectrum of compound 3ao



<sup>1</sup>H-NMR spectrum of compound 3ap



<sup>13</sup>C-NMR spectrum of compound 3ap



FT-IR spectrum of compound 3ap



<sup>1</sup>H-NMR spectrum of compound 3aq



<sup>13</sup>C-NMR spectrum of compound 3aq



FT-IR spectrum of compound 3aq



<sup>1</sup>H-NMR spectrum of compound 3ar



<sup>13</sup>C-NMR spectrum of compound 3ar



FT-IR spectrum of compound 3ar



<sup>1</sup>H-NMR spectrum of compound 3as



<sup>13</sup>C-NMR spectrum of compound 3as





## <sup>1</sup>H-NMR spectrum of compound 3at



<sup>13</sup>C-NMR spectrum of compound 3at



FT-IR spectrum of compound 3at



<sup>1</sup>H-NMR spectrum of compound 3au



<sup>13</sup>C-NMR spectrum of compound 3au



FT-IR spectrum of compound 3au



<sup>1</sup>H-NMR spectrum of compound 3av



<sup>13</sup>C-NMR spectrum of compound 3av



FT-IR spectrum of compound 3av



<sup>1</sup>H-NMR spectrum of compound 3ba



<sup>13</sup>C-NMR spectrum of compound 3ba



FT-IR spectrum of compound 3ba



<sup>1</sup>H-NMR spectrum of compound 3bb



<sup>13</sup>C-NMR spectrum of compound 3bb







<sup>1</sup>H-NMR spectrum of compound 3bc



<sup>13</sup>C-NMR spectrum of compound 3bc



<sup>1</sup>H-NMR spectrum of compound 3bd



<sup>13</sup>C-NMR spectrum of compound 3bd







<sup>1</sup>H-NMR spectrum of intermediate [7]



<sup>13</sup>C-NMR spectrum of intermediate [7]







<sup>1</sup>H-NMR spectrum of intermediate [8]



<sup>13</sup>C-NMR spectrum of intermediate [8]



FT-IR spectrum of compound [8]



<sup>1</sup>H-NMR spectrum of compound 4aa



<sup>13</sup>C-NMR spectrum of compound 4aa



FT-IR spectrum of compound 4aa



<sup>1</sup>H-NMR spectrum of compound 4ab



<sup>13</sup>C-NMR spectrum of compound 4ab







<sup>1</sup>H-NMR spectrum of compound 4ac



<sup>13</sup>C-NMR spectrum of compound 4ac



<sup>1</sup>H-NMR spectrum of compound 4ad



<sup>13</sup>C-NMR spectrum of compound 4ad



FT-IR spectrum of compound 4ad



<sup>1</sup>H-NMR spectrum of compound 4ae



<sup>13</sup>C-NMR spectrum of compound 4ae


<sup>1</sup>H-NMR spectrum of compound 4af



<sup>13</sup>C-NMR spectrum of compound 4af







<sup>1</sup>H-NMR spectrum of compound 4ag



<sup>13</sup>C-NMR spectrum of compound 4ag



FT-IR spectrum of compound 4ag



<sup>1</sup>H-NMR spectrum of compound 4ah



<sup>13</sup>C-NMR spectrum of compound 4ah







### <sup>1</sup>H-NMR spectrum of compound 4ai



<sup>13</sup>C-NMR spectrum of compound 4ai







<sup>1</sup>H-NMR spectrum of compound 4aj



<sup>13</sup>C-NMR spectrum of compound 4aj



FT-IR spectrum of compound 4aj



## <sup>1</sup>H-NMR spectrum of compound 4ak







FT-IR spectrum of compound 4ak







<sup>13</sup>C-NMR spectrum of compound 4al





#### <sup>1</sup>H-NMR spectrum of compound 4ba







<sup>1</sup>H-NMR spectrum of compound 4bb



<sup>13</sup>C-NMR spectrum of compound 4bb



FT-IR spectrum of compound 4bb



### <sup>1</sup>H-NMR spectrum of compound 4bc



<sup>13</sup>C-NMR spectrum of compound 4bc







<sup>1</sup>H-NMR spectrum of compound 4ca











<sup>1</sup>H-NMR spectrum of compound 5a



<sup>13</sup>C-NMR spectrum of compound 5a



<sup>1</sup>H-NMR spectrum of compound 5b



<sup>13</sup>C-NMR spectrum of compound 5b







# <sup>1</sup>H-NMR spectrum of compound 6a







FT-IR spectrum of compound 6a

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