## Supporting information

# Visible light mediated synthesis of 1,3-diarylated imidazo[1,5a] pyridines via oxidative amination of C-H catalyzed by graphitic carbon nitride 

Nandishkumar Talpada ${ }^{a \neq}$, Anuj S. Sharma ${ }^{q \neq}$, Vinay S. Sharma ${ }^{* a}$, Rajender $S$ Varma ${ }^{b}$, Pranav S. Shrivastav*a, Rahul Ahmed ${ }^{c}$, Achalkumar Ammathnadu Sudhakar*cd<br>${ }^{\text {a }}$ Department of Chemistry, School of Sciences, Gujarat University, Ahmedabad, Gujarat 380009, India.<br>${ }^{\mathrm{b}}$ Centre of Excellence for Research in Sustainable Chemistry, Department of Chemistry, Federal University of São Carlos, 13565-905 São Carlos-SP, Brazil.<br>${ }^{\text {c Department }}$ of Chemistry, Indian Institute of Technology, Guwahati, 781039, Assam, India.<br>${ }^{\mathrm{d}}$ Centre for Sustainable Polymers, Indian Institute of Technology, Guwahati, 781039, Assam, India.<br>$\neq$ Both are equally contributed<br>*Corresponding Author<br>Vinay S Sharma-Email: vinaysharma3836@gmail.com<br>Pranav S Shrivastav-Email: pranavs@gujaratuniversity.ac.in<br>Achalkumar Ammathnadu Sudhakar-Email: achalkumar@iitg.ac.in

| Entry | Table of Contents | Page No. |
| :---: | :---: | :---: |
| Chemicals, reagents and instrumentation |  | S3 |
| Preparation of g-C ${ }_{3} \mathrm{~N}_{4}$ |  | S3 |
| Figure S1-S8 | SEM-EDX images of g-C ${ }_{3} \mathrm{~N}_{4}$ | S4-S11 |
| Figure S9 | TGA of g-C3 ${ }^{\text {N }}$ | S12 |
| Table S1 | Comparison table for the GCM (green chemistry matrics) for the synthesis of Compound 3a. | S13 |
| Calculation of Green chemistry metrics (GCM) for compound 3a |  | S13 |
| Calculation of Green chemistry metrics (GCM) for compound 3a by reported ones |  | S15 |
| Table S2 | Comparison table for the synthesis of 1,3-diarylated Imidazo $[1,5 \mathrm{a}$ ] pyridines compound (3a) by deploying reported catalysts. | S19 |
| Figure S10-S13 | SEM-EDX images of reused g-C ${ }_{3} \mathrm{~N}_{4}$ | S20-23 |
| Synthesis and structural characterization of compounds (3a to 3v) |  | S24 |
| Copies of LC-MS, ${ }^{1} \mathrm{H}$ NMR and ${ }^{13} \mathrm{C}$ NMR |  | S35 |
| References |  | S102 |

## Chemicals, reagents and instrumentation

All reagents and the chemicals used for the preparation of catalyst were purchased from commercial sources (Merck and Spectrochem). The crystalline or amorphous nature of graphitic carbon nitride $\left(\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}\right)$ was analysed by using powder X-ray diffractometer (PXRD) (Shimadzu, Maxima 7000 S ) using $\mathrm{CuK} \alpha(\lambda=1.5418 \AA$ at 40 kV and $40 \mathrm{~mA} .2 \theta$ range was from 5 to $80{ }^{\circ} \mathrm{C}$ (scanning speed $=5^{\circ} \mathrm{min}^{-1}$ ). Fourier-transform infrared spectroscopy (FTIR) studies were done for functional group analysis using Perkin Elmer, Frontier equipment. Morphology studies were analyzed using FESEM with OXFORD EDS, Zeiss, Sigma.. Thermogravimetric analysis was conducted from $25{ }^{\circ} \mathrm{C}$ to $700{ }^{\circ} \mathrm{C}$ (heating rate, $10^{\circ} \mathrm{C} / \mathrm{min}$ ) under nitrogen atmosphere using STAR system. ${ }^{1} \mathrm{H} \mathrm{NMR}(600 \mathrm{MHz})$ and ${ }^{13} \mathrm{C}$ NMR ( 151 MHz ) were recorded on Bruker NMR spectrometerusing TMS as internal standard in $\mathrm{CDCl}_{3}$.

## Preparation of g-C3N4

Synthesis of $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}$ was accomplished according to the method reported in our earlier report ${ }^{1}$. The graphitic carbon nitride support $\left(\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}\right)$ was synthesized by calcinations of urea at $550{ }^{\circ} \mathrm{C}$ for 3 h in Muffle furnace in an inert atmosphere.


Figure S1. SEM-EDX images of $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(\mathrm{C}=28.24 \%, \mathrm{~N}=53.14 \%$ and $\mathrm{O}=18.62 \%)$.


Figure S2. SEM-EDX images of $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(\mathrm{C}=31.97 \%, \mathrm{~N}=53.44 \%$ and $\mathrm{O}=14.59 \%)$.


Figure S3. SEM-EDX images of $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(\mathrm{C}=34.57 \%, \mathrm{~N}=47.17 \%$ and $\mathrm{O}=18.26 \%)$.


Figure S 4 . SEM-EDX images of $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(\mathrm{C}=34.27 \%, \mathrm{~N}=47.43 \%$ and $\mathrm{O}=18.30 \%)$.


Figure S5. SEM-EDX images of $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(\mathrm{C}=30.27 \%, \mathrm{~N}=48.43 \%$ and $\mathrm{O}=21.30 \%)$.


Figure S6. SEM-EDX images of $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(\mathrm{C}=32.44 \%, \mathrm{~N}=47.16 \%$ and $\mathrm{O}=20.41 \%)$.


Figure S7. SEM-EDX images of $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(\mathrm{C}=68.45 \%, \mathrm{~N}=15.74 \%$ and $\mathrm{O}=15.82 \%)$.


Figure S8. SEM-EDX images of $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(\mathrm{C}=29.62 \%, \mathrm{~N}=44.81 \%$ and $\mathrm{O}=25.57 \%)$.


Figure S9. TGA of g-C3 $\mathrm{N}_{4}$.

Table S1. Comparison table for the GCM (green chemistry metrics) for the synthesis of Compound 3a.

| Green Metrics | Catalyst |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | $\mathrm{Cu}(\mathrm{OAc})_{2} . \mathrm{H}_{2} \mathrm{O}$ | $\mathrm{I}_{2}$ | CuBr | $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}$ |
| Environmental impact factor (Ef) | 38.73 | 47.33 | 135 | 0.97 |
| Process mass intensity (PMI) | 39.73 | 48.33 | 136 | 1.96 |
| Reaction mass efficiency (RME) | 49.53 | 89.03 | 40.68 | 51.0 |
| Atom economy (AE) | 48 | 52.36 | 59 | 93.10 |
| Carbon efficiency (CE) | 53.23 | 95.48 | 43.6 | 54.46 |
| Chemical yield (CY) | 92.48 | 99.15 | 43.72 | 95.0 |
| Mass intensity (MI) | 2.13 | 1.69 | 2.67 | 1.96 |
| Mass productivity (MP) | 45.0 | 59.17 | 37.45 | 51.02 |
| Optimum efficiency (OE) | 103.18 | 170.03 | 69 | 55.0 |
| References | 2 | 3 | 4 | This Work |

Calculation of Green chemistry metrics (GCM) for compound (3a) ${ }^{5-6}$.


## Environmental impact factor (Ef):

$\boldsymbol{E}$-factor $=$ [Total mass of raw materials minus the total mass of product] / Mass of product
$\boldsymbol{E}$-factor $=[0.183 \mathrm{~g}+0.321 \mathrm{~g}-0.256 \mathrm{~g}] /[0.256 \mathrm{~g}]$
E-Factor $=0.97$

## Process mass intensity (PMI):

$\boldsymbol{P M I}=\sum($ Mass of stoichiometric reactants $) /[$ Mass of product $]$
$P M I=\sum[(0.183 \mathrm{~g}+0.321 \mathrm{~g}] /[0.256 \mathrm{~g}]$
PMI $=1.96$

## Reaction mass efficiency (RME):

$\boldsymbol{R M E}=$ Mass of product $/ \sum($ Mass of stoichiometric reactants $) \times 100$
$\boldsymbol{R M E}=[0.256] / \Sigma[0.183 \mathrm{~g}+0.321 \mathrm{~g}] \times 100$

```
RME = 51.0 %
```


## Atom economy (AE):

$\boldsymbol{A} \boldsymbol{E}=[$ MW of product $] \% \sum(\mathrm{MW}$ of stoichiometric reactants $) \times 100$
$\boldsymbol{A} \boldsymbol{E}=[270.33] \% \sum[183.21+107.15] \times 100$
$\mathrm{AE}=\mathbf{9 3 . 1 0 \%}$

## Carbon efficiency (CE):

$\boldsymbol{C E}=[$ Amount of carbon in product $] /[$ Total carbon present in reactants $] \times 100$
$\boldsymbol{C E}=[$ no. of moles of product $\times$ no. of carbons in product] $\times 100 /[$ no. of moles $\times$ no. of carbon + (no. of moles $\times$ no. of carbon atoms]
$\boldsymbol{C E}=[0.946 \times 19] \times 100 /[1 \times 12+3 \times 7]$
$\mathrm{CE}=\mathbf{5 4 . 4 6 \%}$

## Chemical yield (CY):

$\boldsymbol{C Y}=[$ Weight of product $\times$ MW of starting material $] \times 100 /$ [Weight of Starting material $\times$ MW of Product]
$\boldsymbol{C Y}=[0.256 \mathrm{~g} \times 183.21] \times 100 /[0.183 \times 270.33]$
$\mathrm{CY}=\mathbf{9 5 . 0}$ \%

## Mass intensity (MI):

$\boldsymbol{M I}=\sum W e i g h t($ Total materials input)/[Weight of Product $]$
$M I=\sum[(0.183 \mathrm{~g}+0.321 \mathrm{~g}] /[0.256 \mathrm{~g}]$
$\mathrm{MI}=\mathbf{1 . 9 6}$
Mass productivity (MP):
$M P=100 / M I$
$\mathrm{MP}=\mathbf{5 1 . 0 2}$ \%

## Optimum efficiency (OE):

$\boldsymbol{O} \boldsymbol{E}=[\mathrm{RME}] \times 100 / \mathrm{AE}$
$\mathrm{OE}=55.0 \%$
Note:-The Reaction was performed with $\mathrm{g}-\mathrm{C}_{3} \mathbf{N}_{4}$ catalyst that was recovered and recycled. Hence the mass of the catalyst is excluded.

Calculation of Green chemistry metrics (GCM) for compound (3a) by $\mathrm{Cu}(\mathrm{OAc})_{2} \mathbf{H}_{2} \mathrm{O}$ (reported ones).

$\boldsymbol{E}$-factor $=[$ Total mass of raw materials minus the total mass of product $] /$ mass of product
$\boldsymbol{E}$-factor $=[0.03664 \mathrm{~g}+0.06429 \mathrm{~g}+0.00598 \mathrm{~g}($ Catalyst $)+1.88 \mathrm{~g}(\mathrm{DMF})-0.050 \mathrm{~g}] /[0.050$ g]

E -Factor $=38.73$
$\boldsymbol{P M I}=\sum$ (mass of stoichiometric reactants)/[Mass of product]
$\boldsymbol{P M I}=\Sigma[(0.03664 \mathrm{~g}+0.06429 \mathrm{~g}+0.00598 \mathrm{~g}($ Catalyst $)+1.88 \mathrm{~g}(\mathrm{DMF})] /[0.050]$
PMI $=39.73$
$\boldsymbol{R M E}=$ mass of $\operatorname{product} / \sum($ mass of stoichiometric reactants $) \times 100$
$\boldsymbol{R M E}=[0.050] / \sum[0.03664 \mathrm{~g}+0.06429 \mathrm{~g}] \times 100$
RME $=49.53 \%$
$\boldsymbol{A} \boldsymbol{E}=[M W$ of product $] \% \sum($ MW of stoichiometric reactants $) \times 100$
$\boldsymbol{A} \boldsymbol{E}=[270.33] \% \sum[183.21+107.15+199.65($ Catalyst $)+73.09(\mathrm{DMF})] \times 100$
$A E=48 \%$
$\boldsymbol{C E}=[$ Amount of carbon in product $] /[$ Total carbon present in reactants] $\times 100$
$\boldsymbol{C E}=[$ no. of moles of product $\times$ no. of carbons in product] $\times 100 /[$ no. of moles $\times$ no. of carbon + (no. of moles $\times$ no. of carbon atoms + (no. of moles $\times$ no. of carbon atoms)]
$\boldsymbol{C E}=[0.1849 \times 19] \times 100 /[0.2 \times 12+0.6 \times 7]$
$C E=53.23$
$\boldsymbol{C Y}=[$ Weight of product $\times$ MW of starting material $] \times 100 /[$ Weight of Starting material $\times$ MW of Product]
$\boldsymbol{C Y}=[0.050 \mathrm{~g} \times 183.21] \times 100 /[0.03664 \times 270.33]$
CY $=92.48 \%$
$\boldsymbol{M I}=\sum W$ eight $($ Total materials input)/[Weight of Product $]$
$M \mathbf{I I}=\sum[(0.03664 \mathrm{~g}+0.06429 \mathrm{~g}+0.00598 \mathrm{~g}] /[0.050 \mathrm{~g}]$
$M I=2.13$
$\mathbf{M P}=100 / \mathrm{MI}$
MP $=45.0$
$\boldsymbol{O E}=[\mathrm{RME}] \times 100 / \mathrm{AE}$
$O E=103.18$
Calculation of Green chemistry metrics (GCM) for compound (3a) by $\mathbf{I}_{2}$ (reported ones).

$\boldsymbol{E}$-factor $=$ [Total mass of raw materials minus the total mass of product $] /$ mass of product
$\boldsymbol{E}$-factor $=\left[0.0916 \mathrm{~g}+0.0589 \mathrm{~g}+0.0761 \mathrm{~g}\left(\mathrm{I}_{2}\right)+6.25 \mathrm{~g}(\mathrm{DCE})-0.1340 \mathrm{~g}\right] /[0.1340 \mathrm{~g}]$
E-Factor $=47.33$
$\boldsymbol{P M I}=\sum($ mass of stoichiometric reactants $) /[$ Mass of product]
$\boldsymbol{P M I}=\sum[(0.0916 \mathrm{~g}+0.0589 \mathrm{~g}+0.0761 \mathrm{~g}(\mathrm{I} 2)+6.25 \mathrm{~g}(\mathrm{DCE})] /[0.1340]$
PMI $=48.33$
$\boldsymbol{R M E}=$ mass of product $/ \sum$ (mass of stoichiometric reactants) $\times 100$
$\boldsymbol{R M E}=[0.1340] / \Sigma[0.0916 \mathrm{~g}+0.0589 \mathrm{~g}] \times 100$
RME $=89.03$ \%
$\boldsymbol{A} \boldsymbol{E}=[M W$ of product $] \% \sum(\mathrm{MW}$ of stoichiometric reactants $) \times 100$
$\boldsymbol{A} \boldsymbol{E}=[270.33] \% \sum[183.21+107.15+126.9(\mathrm{I} 2)+98.95(\mathrm{DCE})] \times 100$
$A E=52.36 \%$
$\boldsymbol{C} \boldsymbol{E}=[$ Amount of carbon in product $] /$ Total carbon present in reactants] $\times 100$
$\boldsymbol{C E}=[$ no. of moles of product $\times$ no. of carbons in product] $\times 100 /[$ no. of moles $\times$ no. of carbon + (no. of moles $\times$ no. of carbon atoms)]
$\boldsymbol{C E}=[0.495 \times 19] \times 100 /[0.5 \times 12+0.55 \times 7]$
$C E=95.48 \%$

## Chemical yield (CY):

$\boldsymbol{C Y}=[$ Weight of product $\times$ MW of starting material $] \times 100 /[$ Weight of Starting material $\times$ MW of Product]
$\boldsymbol{C Y}=[0.1340 \mathrm{~g} \times 183.21] \times 100 /[0.0916 \times 270.33]$
CY = 99.15 \%

## Mass intensity (MI):

$\boldsymbol{M I}=\sum W$ eight $($ Total materials input)/[Weight of Product $]$
$M I=\Sigma[(0.0916 \mathrm{~g}+0.0589 \mathrm{~g}+0.0761 \mathrm{~g}] /[0.1340 \mathrm{~g}]$
$M I=1.69$

## Mass productivity (MP):

$\mathbf{M P}=100 / \mathrm{MI}$
MP $=59.17$

## Optimum efficiency (OE):

$\boldsymbol{O E}=[\mathrm{RME}] \times 100 / \mathrm{AE}$
OE = $170.03 \%$
Calculation of Green chemistry metrics (GCM) for compound (3a) by $\mathbf{C u B r}$ (reported ones).

$\boldsymbol{E}$-factor $=[$ Total mass of raw materials minus the total mass of product $] /$ mass of product
$\boldsymbol{E}$-factor $=\left[0.0183 \mathrm{~g}+0.0107 \mathrm{~g}+0.00253 \mathrm{~g}(\mathrm{CuBr})+1.572 \mathrm{~g}\left(\mathrm{CH}_{3} \mathrm{CN}\right)-0.0118 \mathrm{~g}\right] /[0.0118$ g]

```
E-Factor = 135
PMI = \(mass of stoichiometric reactants)/[Mass of product]
PMI = \sum[(0.0183 g + 0.0107 g + 0.00253g (CuBr) + 1.572 g (CH3CN)]/[0.0118 ]
PMI = 136
RME = mass of product / }\sum(\mathrm{ mass of stoichiometric reactants ) }\times10
RME = [0.0118]/ }[0.0183\textrm{g}+0.0107\textrm{g}]\times10
RME = 40.68%
AE}=[MW of product] % ((MW of stoichiometric reactants) > 100
AE}=[270.33]%\sum[183.21+107.15+126.9(CuBr)+41.05(CH3CN)]\times10
AE = 59 %
CE}=[\mathrm{ Amount of carbon in product] [Total carbon present in reactants] }\times10
CE}=[\mathrm{ no. of moles of product }\times\mathrm{ no. of carbons in product] }\times100/[no. of moles \times no. of
carbon + (no. of moles }\times\mathrm{ no. of carbon atoms)]
CE}=[0.0436\times19]\times100/[0.1\times12+0.10\times7
CE = 43.6 %
CY}=[W\mathrm{ Weight of product }\times\mathrm{ MW of starting material] }\times100/[Weight of Starting material \times
MW of Product]
CY}=[0.0118\textrm{g}\times183.21]\times100/[0.0183\times270.33
CY=43.72 %
MI = \sumWeight (Total materials input)/[Weight of Product]
MI= \sum[(0.0183 g + 0.0107 g + 0.00253 g ]/[0.0118g]
MI = 2.67
MP = 100/MI
MP = 37.45 %
OE=[RME] \times 100/AE
OE = 69 %
```

Table S2. Comparison table for the synthesis of 1,3-diarylated Imidazo[1,5a] pyridines compound $3 a$ by deploying other reported catalysts.

| Catalyst | $\mathrm{T}\left({ }^{\circ} \mathrm{C}\right)$ | Solvent | Time | Catalyst <br> Quantity | Base | Yield | Ref. |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{Cu}(\mathrm{OAc})_{2} \cdot \mathrm{H}_{2} \mathrm{O}$ | 110 | DMF | 8 h | 0.15 Eq | - | 93 | 2 |
| $\mathrm{I}_{2}$ | Reflux | DCE | 6 h | 0.0006 Eq | NaOAc <br> $(0.0015 \mathrm{Eq})$ | 99 | 3 |
| CuBr | 80 | $\mathrm{CH}_{3} \mathrm{CN}$ | 24 h | $20 \mathrm{~mol} \%$ | - | 42 | 4 |
| ${\mathrm{~g}-\mathrm{C}_{3} \mathrm{~N}_{4}}^{\mathrm{RT}}$ | - | 10 h | $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(50$ <br> $\mathrm{mg})$ | - | 95 | Present <br> work |  |


$9 \mu \mathrm{~m}$
Electron Image 1


Figure S10. SEM-EDX spectrum of reused g-C3 $\mathrm{N}_{4}(\mathrm{C}=31.72 \%, \mathrm{~N}=48.06 \%, \mathrm{O}=20.22$ \%).


Figure S11. SEM-EDX spectrum of reused $\mathrm{g}_{\mathrm{C}} \mathrm{C}_{3}(\mathrm{C}=56.16 \%, \mathrm{~N}=28.45 \%, \mathrm{O}=15.39$ \%).


Figure S12. SEM-EDX spectrum of reused $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(\mathrm{C}=27.04 \%, \mathrm{~N}=44.68 \%, \mathrm{O}=28.28$ \%).


Figure S13. SEM-EDX spectrum of reused $\mathrm{g}-\mathrm{C}_{3} \mathrm{~N}_{4}(\mathrm{C}=30.13 \%, \mathrm{~N}=51.71 \%, \mathrm{O}=18.15$ \%).

# Synthesis and Structural characterization of Compounds 3a to Compound 3v 



In a 20 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), benzyl amine ( $0.321,3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3a).
1,3-Diphenylimidazo[1,5-a]pyridine (Compound 3a) ${ }^{\mathbf{2}}$ : LCMS $97.98 \%(254 \mathrm{~nm})\left(\mathrm{ES}^{+}\right)$calcd for $\mathrm{C}_{19} \mathrm{H}_{14} \mathrm{~N}_{2}{ }^{+}$, 270.11; found, $271.2\left(\mathrm{MH}^{+}\right)$. ${ }^{\mathbf{1}} \mathbf{H}$ NMR ( $\mathbf{6 0 0} \mathbf{~ M H z , ~} \boldsymbol{C D C l}_{3}$ ) $\delta 8.21(\mathrm{~d}, \mathrm{~J}=7.2$ $H z, 1 \mathrm{H}), 7.94(\mathrm{~d}, J=7.8 \mathrm{~Hz}, 2 \mathrm{H}), 7.87(\mathrm{~d}, J=9.6 \mathrm{~Hz}, 1 \mathrm{H}), 7.81(\mathrm{~d}, J=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.53(\mathrm{~d}$, $J=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.49(\mathrm{t}, J=7.2 \mathrm{~Hz}, 2 \mathrm{H}), 7.33(\mathrm{t}, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 6.82-6.84(\mathrm{~m}, 1 \mathrm{H}), 6.63(\mathrm{t}$, $J=6.6 \mathrm{~Hz}, 1 \mathrm{H}$ ). ${ }^{13} \mathbf{C}$ NMR ( $\mathbf{1 5 1 ~ M H z}, \boldsymbol{C D C l}_{3}$ ) $\delta 138.14,134.97,132.02,130.18,129.03$, $128.83,128.73,128.34,126.85,126.55,121.78,119.71,119.18,113.24$.


In a 20 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 4-methoxy benzyl amine ( $0.411 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture ( RM ) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3b).
3-(4-Methoxyphenyl)-1-phenylimidazo[1,5-a]pyridine (Compound 3b) ${ }^{\mathbf{2}}$ : LCMS $93.66 \%(220 \mathrm{~nm})(E S+)$ calcd for $\mathrm{C}_{20} \mathrm{H}_{16} \mathrm{~N}_{2} \mathrm{O}^{+}, 300.12$; found, $301.2\left(\mathrm{MH}+\right.$ ). ${ }^{1} \mathrm{H}$ NMR ( 600 MHz, CDCl $_{3}$ ) $\delta 8.18(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.95(d, J=7.2 \mathrm{~Hz}, 2 H), 7.84(d, J=9 \mathrm{~Hz}, 1 \mathrm{H})$, $7.77(d, J=9.0 \mathrm{~Hz}, 2 H), 7.48(t, J=7.8 \mathrm{~Hz}, 2 H), 7.31(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.08(d, J=8.4$ $H z, 2 H), \quad 6.79-6.77(m, 1 H), 6.57(\mathrm{t}, \quad \mathrm{J}=6.6 \mathrm{~Hz}, 1 \mathrm{H}), 3.90(\mathrm{~s}, 3 \mathrm{H}) .{ }^{13} \mathrm{C}$ NMR(151MHz, CDCl $_{3}$ ) $8160.05,138.15,135.05,131.65,129.81,128.71,127.36,126.77,126.45,1$ 22.62,121.76,119.44,119.13,114.47,113 03, 55.43.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 4-methyl benzyl amine ( $0.363 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture ( RM ) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3c).
1-Phenyl-3-p-tolylimidazo[1,5-a]pyridine (Compound 3c) ${ }^{2}$. LCMS $97.14 \%$ (254 nm) (ES+) calcd for $\mathrm{C}_{20} \mathrm{H}_{16} \mathrm{~N}_{2}{ }^{+}, 284.13$; found, $285.2(\mathrm{MH}+) .{ }^{\mathbf{1}} \mathbf{H} \mathbf{N M R}\left(\mathbf{6 0 0} \mathbf{~ M H z}, \mathbf{C D C l}_{3}\right) \delta 8.22(d, J$ $=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.96(d, J=7.8 \mathrm{~Hz}, 2 H), 7.85(d, J=9 \mathrm{~Hz}, 1 \mathrm{H}), 7.75(d, J=7.8 \mathrm{~Hz}, 2 \mathrm{H}), 7.49$ $(t, J=7.8 \mathrm{~Hz}, 2 H), 7.36(d, J=7.8 \mathrm{~Hz}, 2 H), 7.32(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 6.77-6.80(\mathrm{~m}, 1 \mathrm{H}), 6.57$ $(t, J=6.6 \mathrm{~Hz}, \mathrm{lH}), 2.46(\mathrm{~s}, 3 \mathrm{H}) .{ }^{13} \boldsymbol{C}$ NMR (151 MHz, CDCl $\left._{3}\right) \delta$ 138.84, 138.32, 135.05, $131.82,129.70,128.72,128.25,127.55,127.28,126.81,126.48,121.85,119.56,119.12$, 113.09, 21.46.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 3-methyl benzyl amine ( $0.363 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture ( RM ) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3d).
1-Phenyl-3-m-tolylimidazo[1,5-a]pyridine (Compound 3d) ${ }^{\mathbf{2}}$. Mass LCMS 100\% (210 nm) (ES+) calcd for $\mathrm{C}_{20} \mathrm{H}_{16} \mathrm{~N}_{2}{ }^{+}, 284.13$; found, $285.2\left(\mathrm{MH}+\right.$ ). ${ }^{\mathbf{1}} \mathbf{H}$ NMR ( $\mathbf{6 0 0} \mathbf{~ M H z}, \boldsymbol{C D C l}_{3}$ ) $\delta 8.25$ $(d, J=7.2 \mathrm{~Hz}, l \mathrm{H}), 7.97(d, J=7.8 \mathrm{~Hz}, 2 H), 7.85(d, J=9 \mathrm{~Hz}, 1 \mathrm{H}), 7.70(\mathrm{~s}, 1 \mathrm{H}), 7.64(d, J=$ $7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.49(t, J=7.2 \mathrm{~Hz}, 2 \mathrm{H}), 7.44(t, J=7.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.33(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.28-$ $7.30(m, l H), 6.78-6.80(m, l H), 6.58(t, J=6.6 \mathrm{~Hz}, 1 \mathrm{H}), 2.48(s, 3 H) .{ }^{13} \mathbf{C}$ NMR ( 151 MHz , CDCl $_{3}$ ) $\delta 138.92,138.32,135.02,131.92,130.05,129.65,129.24,128.8,127.62,126.83$, 126.51, 125.11, 121.89, 119.64, 119.12, 113.14, 21.52.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone $(0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 4-chloro benzyl amine $(0.424 \mathrm{~g}, 3 \mathrm{mmol}), g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3e).
3-(4-Chlorophenyl)-1-phenylimidazo[1,5-a]pyridine (Compound 3e) ${ }^{\mathbf{2}}$. LCMS 100\% (210 $\mathrm{nm})\left(\mathrm{ES}^{+}\right)$calcd for $\mathrm{C}_{19} \mathrm{H}_{13} \mathrm{ClN}_{2}+, 304.07$; found, $305.2\left(\mathrm{MH}^{+}\right)$. ${ }^{\mathbf{1}} \mathbf{H}$ NMR ( 600 MHz, CDCl $_{3}$ ) $\delta 8.21(d, J=7.2 \mathrm{~Hz}, l \mathrm{H}), 7.94(d, J=7.8 \mathrm{~Hz}, 2 H), 7.87(d, J=9.6 \mathrm{~Hz}, l \mathrm{H}), 7.81(d, J=8.4$ $H z, 2 H), 7.53(d, J=8.4 \mathrm{~Hz}, 2 H), 7.49(t, J=7.2 \mathrm{~Hz}, 2 H), 7.33(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 6.82-$ $6.84(\mathrm{~m}, \mathrm{lH}), 6.63(t, J=6.6 \mathrm{~Hz}, \mathrm{lH}) .{ }^{13} \mathbf{C}$ NMR (151 MHz, $\left.\boldsymbol{C D C l}_{3}\right) \delta$ 136.93, 134.76, $132.33,129.4,129.18,128.72,128.47,127.90,126.80$, , $121.45,119.81,119.28,113.61$.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 4-bromo benzyl amine ( $0.558 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture ( RM ) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3f).
3-(4-Bromophenyl)-1-phenylimidazo[1,5-a]pyridine (Compound 3f) ${ }^{7}$. ${ }^{1} \mathrm{H}$ NMR ( 600 $\left.\mathbf{M H z}, \boldsymbol{C D C l}_{3}\right)^{\mathbf{1}} \mathbf{H}$ NMR ( $\mathbf{6 0 0} \mathbf{~ M H z}, \mathbf{C D C l}_{3}$ ) $\delta 8.21(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.94(d, J=7.8 \mathrm{~Hz}$, $2 H), 7.87(d, J=9 \mathrm{~Hz}, 1 \mathrm{H}), 7.75(d, J=8.4 \mathrm{~Hz}, 2 H), 7.69(d, J=9.0 H z, 2 H), 7.49(t, J=7.8$ $\mathrm{Hz}, 2 H), 7.33(t, J=7.2 \mathrm{~Hz}, l \mathrm{H}), 6.82-6.84(\mathrm{~m}, \mathrm{lH}), 6.63(t, J=7.2 \mathrm{~Hz}, l \mathrm{H}) .{ }^{13} \mathbf{C}$ NMR (151 $\mathrm{MHz}_{\mathbf{Z}} \boldsymbol{C D C l}_{3}$ ) $\delta 136.93,134.74,132.38,132.23,129.69,129.38,129.11,128.78,128.39$, $127.9,126.8,122.83,121.53,119.89,119.29,113.65$.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone $(0.183 \mathrm{~g}, 1 \mathrm{mmol})$, 4 -trifluoro methyl ( $0.525 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3g).
1-Phenyl-3-(4-(trifluoromethyl)phenyl)imidazo[1,5-a]pyridine (Compound $\quad \mathbf{3 g}$ ) ${ }^{\mathbf{2}}{ }^{1} \mathbf{H}$ NMR ( $\left.600 \mathrm{MHz}, \boldsymbol{C D C l}_{3}\right) \delta 8.28(d, J=7.8 \mathrm{~Hz}, 1 \mathrm{H}), 8.02(d, J=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.95(d, J=$ $7.2 \mathrm{~Hz}, 2 H), 7.90(d, J=9 \mathrm{~Hz}, 1 \mathrm{H}), 7.81(d, J=7.8 \mathrm{~Hz}, 2 H), 7.50(t, J=7.8 \mathrm{~Hz}, 2 \mathrm{H}), 7.35(t$, $J=7.8 \mathrm{~Hz}, 1 \mathrm{H}), 6.86(d d, J=9.6,6.6 \mathrm{~Hz}, 1 \mathrm{H}), 6.67(t, J=7.8 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathbf{C}$ NMR ( 151 MHz , CDCl $\left._{3}\right) \delta 136.48,134.64,133.71,132.86,130.37(q, J=32.6 \mathrm{~Hz}), 128.82,128.32,128.25$, 126.87, $126.00(q, J=3.7 \mathrm{~Hz}), 124.02(d, J=272.1 \mathrm{~Hz}), 121.49,120.21,119.37,122.15$, 119.65, 113.95.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 3-nitro benzyl amine ( $0.456 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture ( RM ) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow orange solid). (Compound 3h) ${ }^{7}$. 3-(3-nitrophenyl)-1-phenylimidazo[1,5-a]pyridine (Compound 3h). ${ }^{\mathbf{1}} \mathrm{H}$ NMR ( $\mathbf{6 0 0} \mathbf{~ M H z}$, $\left.\boldsymbol{C D C l}_{3}\right) \delta 8.75(\mathrm{~s}, 1 \mathrm{H}), 8.26-8.31(\mathrm{~m}, 3 \mathrm{H}), 7.91-7.95(\mathrm{~m}, 3 \mathrm{H}), 7.74(\mathrm{t}, \mathrm{J}=7.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.51(\mathrm{t}$, $J=6.6 \mathrm{~Hz}, 2 H), 7.36(t, J=6.6 \mathrm{~Hz}, 1 \mathrm{H}), 6.91(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 6.74(\mathrm{~s}, 1 \mathrm{H}) .{ }^{13} \mathbf{C}$ NMR ( 151 MHz, CDCl $_{3}$ ) $\delta$ 148.66, 133.96, 131.93, 130.21, 128.87, 127.03, 126.87, 123.17, 122.39, 121.25, 120.51, 119.51, 114.47.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 2, 4 dimethoxy benzyl amine ( $0.501 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10$ mL ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography (90$10 \%$ hexane:ethyl acetate) to afford the desired product (Pale yellow solid). (Compound 3i).
3-(3-nitrophenyl)-1-phenylimidazo[1,5-a]pyridine (Compound 3i). ${ }^{1} \mathrm{H}$ NMR ( 600 MHz , CDCl $\left._{3}\right) \delta 7.97(d, J=8.4 \mathrm{~Hz}, 2 H), 7.86(d, J=9 \mathrm{~Hz}, 1 \mathrm{H}), 7.60(t, J=7.2 \mathrm{~Hz}, 2 \mathrm{H}), 7.47(t, J=$ $7.8 \mathrm{~Hz}, 2 H), 7.29(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 6.79-6.83(\mathrm{~m}, 1 \mathrm{H}), 6.68(d d, J=1.8 \mathrm{~Hz}, 1 \mathrm{H}), 6.62(d, J$ $=2.4 \mathrm{~Hz}, 1 \mathrm{H}), 6.53(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 3.90(\mathrm{~s}, \mathrm{lH}), 3.81(\mathrm{~s}, \mathrm{lH}) .{ }^{13} \mathrm{C}$ NMR ( 151 MHz , CDCl $_{3}$ ) $\delta 162.18,158.64,136.19,135.27,133.57,131.16,128.63,127.24,126.72,126.19$, 123.46, 119.41, 118.61, 111.8, 105.30, 98.79, 55.58.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 3trifluoromethyl benzyl amine ( $0.525,3 \mathrm{mmol}$ ), $g-C_{3} N_{4}$ ( 50 mg ) were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation (60 W) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc $(3 \times 10 \mathrm{~mL})$ and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3j).
1-Phenyl-3-(3-(trifluoromethyl) phenyl) imidazo[1,5-a]pyridine (Compound $\mathbf{3 j})^{\mathbf{3}} .{ }^{\mathbf{1}} \mathbf{H}$ NMR ( $\left.600 \mathrm{MHz}, \boldsymbol{C D C l}_{3}\right) \delta 8.24(d, J=7.2 \mathrm{~Hz}, \mathrm{lH}), 8.16(\mathrm{~s}, \mathrm{lH}), 8.06(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H})$, $7.95(d, J=7.8 \mathrm{~Hz}, 2 H), 7.89(d, J=9 \mathrm{~Hz}, 1 \mathrm{H}), 7.72(d, J=7.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.68(t, J=7.8 \mathrm{~Hz}$, $1 H), 7.51(t, J=7.8 \mathrm{~Hz}, 2 H), 7.35(t, J=7.8 \mathrm{~Hz}, 1 \mathrm{H}), 6.85-6.87(\mathrm{~m}, ~ l \mathrm{H}), 6.67(t, J=6.6 \mathrm{~Hz}$, $1 H) .{ }^{13} \mathrm{C}$ NMR ( $\mathbf{1 5 1 ~ M H z}, \mathrm{CDCl}_{3}$ ) $\delta 136.45,134.64,132.66,131.68(t, J=32.7 \mathrm{~Hz})$, 131.24, 131.07, 129.59, 128.83, 128.14, 126.87, 126.84, 125.32 ( $q, J=3.9 \mathrm{~Hz}$ ), 125.07 ( $q, J$ $=3.7 \mathrm{~Hz}), 123.93(d, J=272.8 \mathrm{~Hz}), 121.33,121.23,120.15,119.36,113.97$.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 3-amino benzyl amine ( $0.366 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture ( RM ) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3k).
3-(1-phenylimidazo[1,5-a]pyridin-3-yl)aniline (Compound 3k). ${ }^{1} \mathrm{H}$ NMR ( 600 MHz , $\left.\mathbf{C D C l}_{3}\right) \delta 8.27(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.95(d, J=7.2 \mathrm{~Hz}, 2 H), 7.84(d, J=9.6 \mathrm{~Hz}, 1 \mathrm{H}), 7.48(t$, $J=7.8 \mathrm{~Hz}, 2 H), 7.31(t, J=7.8 \mathrm{~Hz}, 2 H), 7.18(t, J=7.2 \mathrm{~Hz}, 2 H), 6.76-6.80(\mathrm{~m}, 2 H), 6.56(t, J$ $=6.6 \mathrm{~Hz}, 1 \mathrm{H}), 3.85(\mathrm{~s}, 2 H) .{ }^{13} \mathrm{C}$ NMR ( 151 MHz, CDCl $_{3}$ ) $\delta 147.20,138.36,135.00,131.75$, 131.01, 129.81, 128.72, 127.61, 126.82, 126.49, 122.16, 119.65, 119.05, 117.98, 115.62. 115.13, 113.04.


In a 30 mL glass vial, (4-chlorophenyl)(pyridin-2-yl)methanone ( $0.217 \mathrm{~g}, 1 \mathrm{mmol}$ ), benzyl amine ( $0.321 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3l).
1-(4-Chlorophenyl)-3-phenylimidazo[1,5-a]pyridine (Compound 3l) ${ }^{\mathbf{3}}$. LCMS 98.26\% (254 $\mathrm{nm})\left(\mathrm{ES}^{+}\right)$calcd for $\mathrm{C}_{19} \mathrm{H}_{13} \mathrm{ClN}_{2}{ }^{+}, 304.07$; found, $305.2\left(\mathrm{MH}^{+}\right) .{ }^{\mathbf{1}} \mathbf{H}$ NMR ( $600 \mathbf{M H z}, \boldsymbol{C D C l}_{3}$ ) $\delta 8.26(s, l H), 7.89(d, J=5.4 \mathrm{~Hz}, 2 H), 7.82-7.84(m, 3 H), 7.56(s, 2 H), 7.45-7.48(\mathrm{~m}, 3 H)$, $6.83(s, l H), 6.61(s, l H) .{ }^{13} \mathbf{C}$ NMR (151 MHz, CDCl $\left._{3}\right) \delta$ 138.32, 133.52, 132.10, 130.77, 129.99, 129.07, 128.97, 128.86, 128.33, 127.86, 127.75, 121.91, 120.14, 118.87. 113.31.


In a 30 mL glass vial, (4-chlorophenyl)(pyridin-2-yl)methanone ( $0.217 \mathrm{~g}, 1 \mathrm{mmol}$ ), 4methoxy benzylamine ( $0.411 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10$ mL ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography (90$10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3m).
1-(4-chlorophenyl)-3-(4-methoxyphenyl)imidazo[1,5-a]pyridine (Compound 3m). LCMS $97.25 \%(210 \mathrm{~nm})\left(\mathrm{ES}^{+}\right)$calcd for $\mathrm{C}_{20} \mathrm{H}_{15} \mathrm{ClN}_{2} \mathrm{O}^{+}, 334.08$; found, $335.2\left(\mathrm{MH}^{+}\right) .{ }^{\mathbf{1}} \mathbf{H}$ NMR ( 600 MHz, CDCl $_{3}$ ) $\delta 8.18(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.89(d, J=8.4 \mathrm{~Hz}, 2 H), 7.75-7.79(\mathrm{~m}, 3 \mathrm{H}), 7.44(d$, $J=8.4 \mathrm{~Hz}, 2 H), 7.08(d, J=8.4 \mathrm{~Hz}, 2 H), 6.79-6.82(m, 1 H), 6.58(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 3.90(s$, 3H). ${ }^{13}$ C NMR ( $\mathbf{1 5 1 ~ M H z}, \boldsymbol{C D C l}_{3}$ ) $\delta 160.17,138.35,133.63,131.99,130.42,129.81$, $128.84,127.82,127.46,122.44,121.90,119.88,118.84,114.53,113.10,55.43$.


In a 30 mL glass vial, (4-chlorophenyl)(pyridin-2-yl)methanone ( $0.217 \mathrm{~g}, 1 \mathrm{mmol}$ ), 4methyl benzylamine ( $0.363 \mathrm{~g}, 3 \mathrm{mmol}$ ), g-C3 $N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10$ mL ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography (9010\% hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3n).
1-(4-chlorophenyl)-3-(p-tolyl)imidazo[1,5-a]pyridine (Compound 3n). LCMS 100\% (210 $\mathrm{nm})\left(\mathrm{ES}+\right.$ ) calcd for $\mathrm{C}_{20} \mathrm{H}_{15} \mathrm{ClN}_{2}{ }^{+}, 318.09$; found, $319.2\left(\mathrm{MH}+\right.$ ). ${ }^{\mathbf{1}} \mathbf{H} \mathbf{N M R}\left(\mathbf{6 0 0} \mathbf{~ M H z}, \boldsymbol{C D C l}_{3}\right)$ $\delta 8.22(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.89(d, J=8.4 \mathrm{~Hz}, 2 H), 7.78(d, J=9 \mathrm{~Hz}, 1 \mathrm{H}), 7.72(d, J=7.8$ $H z, 2 H), 7.44(d, J=8.4 \mathrm{~Hz}, 2 H), 7.36(d, J=7.8 \mathrm{~Hz}, 2 H), 6.79-6.82(m, l H), 6.58(t, J=$ $7.2 \mathrm{~Hz}, \mathrm{lH}), 2.46(\mathrm{~s}, 3 \mathrm{H}) .{ }^{13} \mathbf{C}$ NMR ( $\mathbf{1 5 1 ~ M H z , ~}$ CDCl $_{3}$ ) $\delta$ 139.01, 138.50, 133.61, 132.01, 130.57, 129.74, 128.84, 128.24, 127.85, 127.62, 127.10, 121.99, 119.99, 118.83, 113.15, 21.44.


In a 30 mL glass vial, (4-chlorophenyl)(pyridin-2-yl)methanone ( $0.217 \mathrm{~g}, 1 \mathrm{mmol}$ ), 3methyl benzyl amine ( $0.363 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10$ mL ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography (9010\% hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3o).
1-(4-chlorophenyl)-3-(m-tolyl)imidazo[1,5-a]pyridine (Compound 3o). LCMS 100\% (210 nm ) ( $\mathrm{ES}+$ ) calcd for $\mathrm{C}_{20} \mathrm{H}_{15} \mathrm{ClN}_{2}{ }^{+}$, 318.09; found, 319.2 (MH+). ${ }^{\mathbf{1}} \mathbf{H}$ NMR ( $\mathbf{6 0 0} \mathbf{~ M H z}$, CDCl $\left._{3}\right) \delta 8.25(d, J=6.6 \mathrm{~Hz}, 1 \mathrm{H}), 7.89(d, J=8.4 \mathrm{~Hz}, 2 H), 7.79(d, J=9.0 \mathrm{~Hz}, l \mathrm{H}), 7.67(\mathrm{~s}$, $1 H), 7.62(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.43-7.45(\mathrm{~m}, 3 \mathrm{H}), 7.29(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 6.81-6.84(\mathrm{~m}, \mathrm{lH})$, $6.60(t, J=6.6 \mathrm{~Hz}, \mathrm{lH}), 2.47(\mathrm{~s}, 3 \mathrm{H}) .{ }^{13} \mathbf{C}$ NMR (151 MHz, $\left.\boldsymbol{C D C l}_{3}\right) \delta$ 138.98, 138.51, $133.55,132.49,132.06,130.66,129.86,129.21,128.84,127.87,127.68,125.12,122.03$, 120.07, 118.83, 113.20, 21.50.


In a 30 mL glass vial, (4-chlorophenyl)(pyridin-2-yl)methanone ( $0.217 \mathrm{~g}, 1 \mathrm{mmol}$ ), 4chloro benzyl amine ( $0.424 \mathrm{~g}, 3 \mathrm{mmol}$ ), $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10$ mL ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography (90$10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3p).
1,3-bis(4-chlorophenyl)imidazo[1,5-a]pyridine (Compound 3p). LCMS 197.90\% (254 nm) (ES+) calcd for $\mathrm{C}_{19} \mathrm{H}_{12} \mathrm{C}_{12} \mathrm{~N}_{2}{ }^{+}, 338.03$; found, $339.2\left(\mathrm{MH}+\right.$ ). ${ }^{\mathbf{1}} \mathbf{H}$ NMR ( $600 \mathbf{M H z}, \boldsymbol{C D C l}_{3}$ ) $\delta$ $8.21(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.87(d, J=9.0 \mathrm{~Hz}, 2 \mathrm{H}), 7.79-7.82(\mathrm{~m}, 3 \mathrm{H}), 7.53(d, J=8.4 \mathrm{~Hz}$, $2 H), 7.45(d, J=8.4 \mathrm{~Hz}, 2 H), 6.85-6.87(m, l H), 6.65(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathbf{C}$ NMR (151 MHz, CDCl $_{3}$ ) $\delta 137.12,134.85,133.31,132.31,131.09,129.49,129.35,128.92,128.49$, 127.97, 127.88, 121.69, 120.30, 119.00, 113.68.


In a 30 mL glass vial, (4-chlorophenyl)(pyridin-2-yl)methanone ( $0.217 \mathrm{~g}, 1 \mathrm{mmol}$ ), 4bromo benzyl amine ( $0.558 \mathrm{~g}, 3 \mathrm{mmol}$ ) and $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10$ mL ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography (90$10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3q).
3-(4-bromophenyl)-1-(4-chlorophenyl)imidazo[1,5-a]pyridine (Compound $\mathbf{3 q}$ ). ${ }^{\mathbf{1}} \mathbf{H}$ NMR ( $600 \mathrm{MHz}, \boldsymbol{C D C l}_{3}$ ) $\delta 8.21(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 7.87(d, J=8.4 \mathrm{~Hz}, 2 H), 7.81(d, J=9.6 \mathrm{~Hz}$, $1 H), 7.73(d, J=8.4 \mathrm{~Hz}, 2 H), 7.69(d, J=7.8 \mathrm{~Hz}, 2 H), 7.45(d, J=7.8 \mathrm{~Hz}, 2 H), 6.86(t, J=7.2$ $\mathrm{Hz}, \mathrm{lH}), 6.64(t, J=6.6 \mathrm{~Hz}, \mathrm{lH}){ }^{13}{ }^{\mathbf{C}}$ NMR ( $\mathbf{1 5 1 ~ M H z}$, CDCl $_{3}$ ) $\delta$ 137.14, 133.29, 132.29, 131.14, 129.69, 128.92, 128.02, 127.88, 123.02, 121.68, 120.33, 119.01, 113.73.


In a 30 mL glass vial, (4-chlorophenyl)(pyridin-2-yl)methanone ( $0.217 \mathrm{~g}, 1 \mathrm{mmol}$ ), 4trifluoromethyl benzylamine ( $0.525 \mathrm{~g}, 3 \mathrm{mmol}$ ) and $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation (60 W) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc $(3 \times 10 \mathrm{~mL})$ and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3r).
1-(4-chlorophenyl)-3-(4-(trifluoromethyl)phenyl)imidazo[1,5-a]pyridine(Compound $\mathbf{3 r}$ ). ${ }^{1} \mathbf{H}$ NMR ( $600 \mathrm{MHz}, \boldsymbol{C D C l}_{3}$ ) $\delta 8.28(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 8.00(d, J=7.8 \mathrm{~Hz}, 2 \mathrm{H}), 7.88(d, J=$ $8.4 \mathrm{~Hz}, 2 H), 7.81-7.85(\mathrm{~m}, 3 \mathrm{H}), 7.46(d, J=7.8 \mathrm{~Hz}, 2 \mathrm{H}), 6.89(t, J=6.6 \mathrm{~Hz}, 1 \mathrm{H}), 6.69(t, J=$ $6.6 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathbf{C}$ NMR ( $\mathbf{1 5 1 ~ M H z}$, CDCl $_{3}$ ) $\delta 136.65,133.51,133.16,132.47,131.57,130.55$ $(q, J=33.2 \mathrm{~Hz}), 128.95,128.36,128.28,127.92,126.05(q, J=3.9 \mathrm{~Hz}), 123.97(\mathrm{~d}, J=272.1$ $\mathrm{Hz}), 121.62,120.64,119.08,114.03$.


In a 30 mL glass vial, (4-chlorophenyl)(pyridin-2-yl)methanone ( $0.217 \mathrm{~g}, 1 \mathrm{mmol}$ ), 2,4-dimethoxy benzylamine ( $0.501 \mathrm{~g}, 3 \mathrm{mmol}$ ) and $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation (60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc ( $3 \times 10 \mathrm{~mL}$ ) and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid) (Compound 3s).
1-(4-chlorophenyl)-3-(2,4-dimethoxyphenyl)imidazo[1,5-a]pyridine (Compound $3 s$ ). ${ }^{1} \mathrm{H}$ NMR ( $\left.600 \mathrm{MHz}, \boldsymbol{C D C l}_{3}\right) \delta 7.90(d, J=5.4 \mathrm{~Hz}, 2 \mathrm{H}), 7.80(d, J=7.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.59(\mathrm{~s}, 2 \mathrm{H})$, $7.43(s, 2 H), 6.83(s, l H), 6.68(d, J=5.4 \mathrm{~Hz}, 1 \mathrm{H}), 6.62(s, l H), 6.55(s, l H), 3.90(s, 3 H)$, $3.81(s, 3 H) .{ }^{13} \mathbf{C}$ NMR (151 MHz, CDCl $_{3}$ ) $\delta$ 162.28, 158.65, 136.42, 133.87, 133.48, 131.68, 129.97, 128.75, 127.75, 127.35, 123.58, 119.83, 118.30, 111.97, 105.36, 98.82, 55.58.


In a 30 mL glass vial, (4-chlorophenyl)(pyridin-2-yl)methanone ( $0.217 \mathrm{~g}, 1 \mathrm{mmol}$ ), 3trifluoromethyl benzyl amine ( $0.525 \mathrm{~g}, 3 \mathrm{mmol}$ ) and $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture (RM) was stirred under visible light irradiation (60 $\mathrm{W})$ for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc $(3 \times 10 \mathrm{~mL})$ and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography ( $90-10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3t).
1-(4-chlorophenyl)-3-(3-(trifluoromethyl)phenyl)imidazo[1,5-a]pyridine (Compound 3t). ${ }^{1} \mathbf{H}$ NMR ( $600 \mathrm{MHz}, \boldsymbol{C D C l}_{3}$ ) $\delta 8.24(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 8.14(s, l H), 8.05(d, J=7.2 \mathrm{~Hz}$, $1 H), 7.89(d, J=8.4 \mathrm{~Hz}, 2 H), 7.84(d, J=9 \mathrm{~Hz}, 1 \mathrm{H}), 7.73(d, J=7.8 \mathrm{~Hz}, 1 \mathrm{H}), 7.69(t, J=$ $7.2 \mathrm{~Hz}, l \mathrm{H}), 7.46(d, J=8.4 \mathrm{~Hz}, 2 \mathrm{H}), 6.88-6.90(\mathrm{~m}, l \mathrm{H}), 6.69(t, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}) .{ }^{13} \mathbf{C}$ NMR ( 151 MHz, CDCl $_{3}$ ) $\delta 136.63,133.19,132.44,131.54(t, J=32.6 \mathrm{~Hz}$ ), 131.24, 130.90, 129.63, $128.95,128.20,127.91,126.60,125.46(q, J=3.9 \mathrm{~Hz}), 125.07(q, J=3.7 \mathrm{~Hz}), 123.89(d, J=$ 272.7 Hz ), 121.47, 121.18, 120.55, 119.07, 114.02.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 3-methoxy benzylamine ( $0.411 \mathrm{~g}, 3 \mathrm{mmol}$ ) and $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture ( RM ) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc $(3 \times 10 \mathrm{~mL})$ and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography (90$10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3u).
3-(2-methoxyphenyl)-1-phenylimidazo[1,5-a]pyridine (Compound 3u) ${ }^{7}$. LCMS $96.47 \%(254 \mathrm{~nm})(\mathrm{ES}+)$ calcd for $\mathrm{C}_{20} \mathrm{H}_{16} \mathrm{~N}_{2} \mathrm{O}+, 300.12$; found, $301.2\left(\mathrm{MH}^{+}\right) .{ }^{1} \mathrm{H}$ NMR (400 $M H z, D M S O-d 6) \delta 8.49(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 8.01(d, J=9.6 \mathrm{~Hz}, 1 \mathrm{H}), 7.95(d, J=7.6 \mathrm{~Hz}$, $2 H), 7.51-7.44(m, 4 H), 7.39(s, l H), 7.30(t, J=7.6 \mathrm{~Hz}, 1 \mathrm{H}), 7.09(d, J=7.2 \mathrm{~Hz}, 1 \mathrm{H}), 6.98$ $(t, J=6.0 \mathrm{~Hz}, 1 \mathrm{H}), 6.79(d, J=6.8 \mathrm{~Hz}, 1 \mathrm{H}), 3.86(\mathrm{~s}, 3 \mathrm{H}) .{ }^{13} \mathbf{C}$ NMR ( $\left.100 \mathrm{MHz}, \boldsymbol{C D C l}_{3}\right) \delta$ 160.14137.96, 134.88, 131.93, 131.33, 130.04, 128.76, 127.76, 126.87, 126.62, 121.97, $120.42,119.81,119.18,114.98,113.78,113.32,55.51$.


In a 30 mL glass vial, phenyl(pyridin-2-yl)methanone ( $0.183 \mathrm{~g}, 1 \mathrm{mmol}$ ), 2-chloro benzylamine ( $0.424 \mathrm{~g}, 3 \mathrm{mmol}$ ) and $g-C_{3} N_{4}(50 \mathrm{mg})$ were added at room temperature (RT). The reaction mixture ( RM ) was stirred under visible light irradiation ( 60 W ) for 10 h . After the reaction completion, the resulting reaction mass was extracted with EtOAc $(3 \times 10 \mathrm{~mL})$ and dried with sodium sulphate. The obtained filtrate was concentrated under reduced pressure. The obtained crude material was further purified by column chromatography (90$10 \%$ hexane:ethyl acetate) to afford the desired product (Yellow solid). (Compound 3v).
3-(2-chlorophenyl)-1-phenylimidazo[1,5-a]pyridine (Compound 3v) ${ }^{\mathbf{7}}{ }^{1}{ }^{\mathbf{1}} \mathrm{H}$ NMR ( 600 $\mathbf{M H z}$, CDCl $\left._{3}\right) \delta 7.98(d, J=5.2 \mathrm{~Hz}, 2 H), 7.91(d, J=9 \mathrm{~Hz}, 1 \mathrm{H}), 7.70(d, J=6.6 \mathrm{~Hz}, 1 \mathrm{H})$, $7.62(d, J=7.2 \mathrm{~Hz}, l \mathrm{H}), 7.58(d, J=7.2 \mathrm{~Hz}, l \mathrm{H}), 7.44-7.50(m, 4 H), 7.32(t, J=7.2 \mathrm{~Hz}, l \mathrm{H})$, $6.87(t, J=7.2 \mathrm{~Hz}, \mathrm{lH}), 6.63(t, J=6.6 \mathrm{~Hz}, \mathrm{lH}) .{ }^{13} \mathbf{C}$ NMR (151 MHz, CDCl $\left.{ }_{3}\right) \delta$ 135.71, 134.92, 134.40, 133.40, 132.93, 131.65, 130.98, 130.86, 129.96, 129.35, 128.72, 128.17, 127.29, 127.27, 126.76, 126.53, 124.63, 122.62, 119.94, 118.89, 112.86.

## Copies of LC-MS, ${ }^{1} \mathrm{H}$ NMR and ${ }^{13} \mathrm{C}$ NMR



Compound (3a)
LC-MS of Compound 3a


Channel Name 210.0nm; Channel PDA Spectrum


Channel Name 254.Onm; Channel PDA Spectrum

Peak Results
Channel: PDA Spectrum

|  | RT |  |  |  |  |  |  |  | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | :--- | ---: | ---: | ---: | ---: | ---: | :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 1.331 |  | 1624 | 2266 | 0.61 | PDA Spectrum | 254.0 nm |  |  |  |  |  |  |  |
| 2 | 1.458 |  | 3019 | 5248 | 1.41 | PDA Spectrum | 254.0 nm |  |  |  |  |  |  |  |
| 3 | 1.865 |  | 653321 | 1419185 | 100.00 | PDA Spectrum | 210.0 nm |  |  |  |  |  |  |  |
| 4 | 1.865 |  | 176653 | 363634 | 97.98 | PDA Spectrum | 254.0 nm |  |  |  |  |  |  |  |



Base Peak 271.19 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG (1.6:1.7;2.2:3.8;0.2:1.2) x 20.000 Th: 0.010 Retention Time 1.889
${ }^{1} \mathrm{H}$ NMR of Compound 3a


${ }^{13} \mathrm{C}$ NMR of Compound 3a



Compound (3b)
LC-MS analysis of Compound 3b


Peak Results
Channel: PDA Spectrum

|  | RT | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | :--- | ---: | ---: | ---: | ---: | ---: | :--- |
| 1 | 1.380 |  | 4384 | 6113 | 6.34 | PDA Spectrum | 220.0 nm |
| 2 | 1.737 |  | 42212 | 90240 | 93.66 | PDA Spectrum | 220.0 nm |

Match Plot


Base Peak 301.18 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG $(0.1: 1.5 ; 1.9: 3.8) \times 20.000 \mathrm{Th}: 0.010$ Retention Time 1.766
${ }^{1}$ H NMR of Compound 3 b


${ }^{13} \mathrm{C}$ NMR of Compound 3 b






Compound (3c)

## LC-MS analysis of Compound 3c


__Channel Name 254.Onm; Channel PDA Spectrum
Peak Results
Channel: PDA Spectrum

|  | RT | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | :--- | ---: | ---: | ---: | ---: | ---: | :--- |
| 1 | 1.456 |  | 3931 | 7630 | 2.86 | PDA Spectrum | 254.0 nm |
| 2 | 1.960 |  | 424520 | 902743 | 100.00 | PDA Spectrum | 210.0 nm |
| 3 | 1.961 |  | 122448 | 259546 | 97.14 | PDA Spectrum | 254.0 nm |



Base Peak 285.21 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG (1.6:1.8;0.5:1.3;2.2:3.8) x 20.000 Th: 0.010 Retention Time 1.990
${ }^{1} \mathrm{H}$ NMR of Compound 3 c


${ }^{13} \mathrm{C}$ NMR of Compound 3c




Compound (3d)
LC-MS analysis of Compound 3d


Peak Results
Channel: PDA Spectrum

|  | RT | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :--- |
| 1 | 2.010 |  | 141643 | 302143 | 100.00 | PDA Spectrum | 210.0 nm |



Base Peak 285.18 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG (0.0:1.9;2.2:3.8) x $20.000 \mathrm{Th}: 0.010$ Retention Time 2.039


${ }^{13}$ C NMR of Compound 3d
$\stackrel{\text { N }}{\substack{\text { N } \\ 1}}$



ヘiNo $\stackrel{\text { ñ }}{\underset{\sim}{1}}$



Compound (3e)
LC-MS analysis of Compound 3e


Channel Name 210.0nm; Channel PDA Spectrum

__ Channel Name 254.0nm; Channel PDA Spectrum
Peak Results
Channel: PDA Spectrum

|  | RT | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | :--- | :--- | :--- | ---: | ---: | ---: | :--- |
| 1 | 2.176 |  | 257212 | 506509 | 100.00 | PDA Spectrum | 254.0 nm |
| 2 | 2.176 |  | 716419 | 1524302 | 100.00 | PDA Spectrum | 210.0 nm |

Match Plot


Base Peak 305.16 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG (0.1:2.1;2.5:3.8) x $20.000 \mathrm{Th}: 0.100$ Retention Time 2.207
${ }^{1} \mathrm{H}$ NMR of Compound 3 e

## 


${ }^{13}$ C NMR of Compound 3e



Compound (3f)
${ }^{1}$ H NMR of Compound 3 f

## 


${ }^{13}$ C NMR of Compound 3 f

##  <br> 




Compound (3g)
${ }^{1}$ H NMR of Compound 3 g

## 


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




Compound (3h)
${ }^{1} \mathrm{H}$ NMR of Compound 3h

${ }^{13}$ C NMR of Compound 3h



Compound (3i)
${ }^{1}$ H NMR of Compound 3 i





$\iiint j$
/ /J /



${ }^{13}$ C NMR of Compound 3i




Compound (3j)
${ }^{1}$ H NMR of Compound 3 j


${ }^{13}$ C NMR of Compound 3 j



$\begin{array}{llllllllllllllllllllllllllllllll}139 & 138 & 137 & 136 & 135 & 134 & 133 & 132 & 131 & 130 & 129 & 128 & 127 & 126 & 125 & 124 & 123 & 122 & 121 & 120 & 119 & 118 & 117 & 116 & 115 & 114 & 113\end{array}$


Compound (3k)
${ }^{1} \mathrm{H}$ NMR of Compound 3 k

${ }^{13} \mathrm{C}$ NMR of Compound 3 k



Compound (31)
LC-MS analysis of Compound 31



Peak Results
Channel: PDA Spectrum

|  | RT | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | :--- |
| 1 | 1.711 |  | 4749 | 7451 | 1.74 | PDA Spectrum | 254.0 nm |
| 2 | 2.221 |  | 208743 | 421874 | 98.26 | PDA Spectrum | 254.0 nm |
| 3 | 2.221 |  | 743355 | 1605691 | 100.00 | PDA Spectrum | 210.0 nm |



Base Peak 305.15 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG (1.8:2.1;0.1:1.3;2.4:3.9) $\times 20.000$ Th: 0.010 Retention Time 2.251
${ }^{1} \mathrm{H}$ NMR of Compound 31


|  |  |  |  |  |  |  |  |  |  | $\begin{aligned} & \text { Ti T O } \\ & \text { To } \\ & \hline \end{aligned}$ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 12.0 | 11.5 | 11.0 | 10.5 | 10.0 | 9.5 | 9.0 | 8.5 | 8.0 | 7.5 | 7.0 | 6.5 |  |  | 5.0 | 4.5 | 4.0 | 3.5 | 3.0 | 2.5 | 2.0 | 1.5 | 1.0 | 0.5 | 0.0 |
| 12.0 | 11.5 | 11.0 | 10.5 | 10.0 | 9.5 | 9.0 | 8.5 | 8.0 | 7.5 | . 0 | 6.5 | f1 (ppm |  | 5.0 | 4.5 | 4.0 | 3.5 | 3.0 | 2.5 | 2.0 | 1.5 | 1.0 | 0.5 | 0.0 |


${ }^{13}$ C NMR of Compound 31


``` ๗
```





$\stackrel{-}{m}$



Compound (3m)

## LC-MS analysis of Compound 3m




Peak Results
Channel: PDA Spectrum

|  | RT | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | :--- | :--- | ---: | ---: | ---: | ---: | :--- |
| 1 | 1.062 |  | 10211 | 13613 | 2.56 | PDA Spectrum | 254.0 nm |
| 2 | 1.716 |  | 8991 | 17321 | 3.26 | PDA Spectrum | 254.0 nm |
| 3 | 1.721 |  | 15545 | 33244 | 2.75 | PDA Spectrum | 210.0 nm |
| 4 | 2.145 |  | 533284 | 1177286 | 97.25 | PDA Spectrum | 210.0 nm |
| 5 | 2.145 |  | 234635 | 500175 | 94.18 | PDA Spectrum | 254.0 nm |

Match Plot


Base Peak 335.21 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG (0.1:1.8;2.4:3.9) x 20.000 Th: 0.010 Retention Time 2.177
${ }^{1}$ H NMR of Compound 3 m


${ }^{13} \mathrm{C}$ NMR of Compound 3 m


|  |  |  |  |  |  |  |  |  | 1 | 1 |  | T | 1 | 1 | 1 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 170 | 166 | 162 | 158 | 154 | 150 | 146 | 142 | $\begin{array}{r} 138 \\ \text { f1 (ppm) } \end{array}$ | 134 | 130 | 126 | 122 | 118 | 114 | 110 |



Compound (3n)
LC-MS analysis of Compound 3n


Peak Results
Channel: PDA Spectrum

|  | RT | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | :--- | :---: | :---: | :---: | :---: | :---: | :--- |
| 1 | 2.355 |  | 257651 | 531715 | 100.00 | PDA Spectrum | 210.0 nm |

Match Plot


Base Peak 319.20 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG (0.2:2.2;2.8:3.9) x 20.000 Th: 0.001 Retention Time 2.382
${ }^{1}$ H NMR of Compound $3 n$



${ }^{13}$ C NMR of Compound 3n




Compound (30)

## LC-MS of Compound 30



Peak Results
Channel: PDA Spectrum

|  | RT | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 2.379 |  | 275987 | 550076 | 100.00 | PDA Spectrum | 210.0 nm |

Match Plot


Base Peak 319.20 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG (1.0:2.2;2.7:3.9;0.1:1.5) x 20.000 Th: 0.010 Retention Time 2.407
${ }^{1} \mathrm{H}$ NMR of Compound 30



|  |  |  |  |
| :---: | :---: | :---: | :---: |
| J | $\iint$ |  | / |



${ }^{13} \mathrm{C}$ NMR of Compound 30




Compound (3p)

## LC-MS of Compound 3p




Channel Name 210.0nm; Channel PDA Spectrum

## Peak Results

Channel: PDA Spectrum

|  | RT | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | :--- | ---: | ---: | ---: | ---: | ---: | :--- |
| 1 | 1.707 |  | 4294 | 7433 | 2.10 | PDA Spectrum | 254.0 nm |
| 2 | 2.450 |  | 564323 | 1093627 | 100.00 | PDA Spectrum | 210.0 nm |
| 3 | 2.451 |  | 181645 | 345792 | 97.90 | PDA Spectrum | 254.0 nm |

Match Plot


Base Peak 339.18 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG $(1.8: 2.4 ; 0.0: 1.6 ; 2.7: 3.9) \times 20.000$ Retention Time 2.479
${ }^{1} \mathrm{H}$ NMR of Compound 3 p

## 



8.220
-8.208
(
葉管
$\int \pi$
$\underset{\sim}{\sim}$

No 0
0
0
0
0
0
0
$\left.\int\right)=($
$\int \quad /$






Compound (3q)
${ }^{1} \mathrm{H}$ NMR of Compound $3 q$

## 



$\left.\begin{array}{lllllllllllllllllllllllllllllll}12.0 & 11.5 & 11.0 & 10.5 & 10.0 & 9.5 & 9.0 & 8.5 & 8.0 & 7.5 & 7.0 & 6.5 & 6.0 & 5.5 & 5 & 1 & 1 & 1 & 1\end{array}\right)$

${ }^{13} \mathrm{C}$ NMR of Compound $3 q$

$\begin{array}{lllllllllllllllllllllllllllllllllllllllllll}140 & 139 & 138 & 137 & 136 & 135 & 134 & 133 & 132 & 131 & 130 & 129 & 128 & 127 & 126 & 125 & 124 & 123 & 122 & 121 & 120 & 119 & 118 & 117 & 116 & 115 & 114 & 113\end{array}$


Compound (3r)
${ }^{1} \mathrm{H}$ NMR of Compound 3 r

## 


${ }^{13}$ C NMR of Compound 3 r

##  






Compound (3s)
${ }^{1} \mathrm{H}$ NMR of Compound 3s




${ }^{13} \mathrm{C}$ NMR of Compound 3s





Compound (3t)

## ${ }^{1}$ H NMR of Compound 3 t


${ }^{13}$ C NMR of Compound $3 t$



Compound (3u)

## LC-MS of Compound 3u



Channel PDA Spectrum; Channel Name 254.0nm

## Peak Results

Channel: PDA Spectrum

|  | RT | Base <br> Peak <br> $(\mathrm{m} / \mathrm{z})$ | Height | Area | \% Area | Channel | Channel Name |
| :--- | :--- | :--- | ---: | ---: | ---: | ---: | :--- |
| 1 | 1.483 |  | 9020 | 11930 | 2.37 | PDA Spectrum | 254.0 nm |
| 2 | 1.788 |  | 2950 | 5060 | 1.00 | PDA Spectrum | 254.0 nm |
| 3 | 1.842 |  | 799 | 809 | 0.16 | PDA Spectrum | 254.0 nm |
| 4 | 1.946 |  | 294870 | 486016 | 96.47 | PDA Spectrum | 254.0 nm |
| 5 | 1.946 |  | 875637 | 1666342 | 100.00 | PDA Spectrum | 210.0 nm |



Base Peak 301.18 Channel Description 1: QDa Positive(+) Scan (60.00-1250.00)Da, Centroid, CV=10 - AVG (2.7:3.9) 20.000 Th: 0.010 Retention Time 1.966
${ }^{1} \mathrm{H}$ NMR of Compound 3 u


## 


$\underline{D}_{2} \mathrm{O}$ NMR of Compound 3 u


${ }^{13} \mathrm{C}$ NMR of Compound 3 u




Compound (3v)
${ }^{1} \mathrm{H}$ NMR of Compound 3 v

## 


${ }^{13} \mathrm{C}$ NMR of Compound 3 v

##  <br> 


$\begin{array}{lllllllllllllllllll}180 & 170 & 160 & 150 & 140 & 130 & 120 & 110 & 100_{f 1}(\mathrm{ppm}) & 90 & 80 & 70 & 60 & 50 & 40 & 30 & 20 & 10 & 0\end{array}$



## References

1. A. S. Sharma, V. S Sharma and H. Kaur, ACS Applied Nano Materials., 2020, 3, 1191-1202.
2. H. Wang, W. Xu, Z. Wang, L. Yu, K. Xu, J. Org. Chem., 2015, 80, 2431-2435.
3. Z. Hu, J. Hou, J. Liu, W. Yu, J. Chang, Org. Biomol. Chem., 2018, 16, 5653.
4. M. Li, Y. Xie, Y. Ye, Y. Zou, H. Jiang, W. Zeng, Org. Lett., 2014, 23, 6232-6235.
5. U. C. Rajesh, G. Purohit, D. S. Rawat, ACS Sustainable Chemistry \& Engineering .,2015, 10, 2397-2404
6. U. Gulati, U. C. Rajesh, D. S. Rawat, ACS Sustainable Chemistry \& Engineering., 2018, 6, 10039-10051.
7. A. Joshi, D. C. Mohan, S. Adimurthy, J. Org. Chem., 2016, 19, 9461-9469.
