Supplementary Material

Electrochemical synthesis of 4-quinazolinone derivatives mediated by acetic acid

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1. Electrochemical Reactor set up

The electrochemical reactor was set up starting with a 5v mobile charger and a multiple USB port. A mobile phone charger was attached to a multiple USB port to divert the current to different reaction vessels. The wire from USB port was attached to electrodes through alligator clips, the electrodes were mainly carbon (0.5 mm diameter) and wire of aluminium (0.5 mm diameter) (Figure 1). Constant electric current of 0.35A cm\(^{-2}\) was passed through the reaction mixture for required time at room temperature for complete conversion. This was helpful in carrying out multiple reactions at a time.

![Figure 1. Multiple reaction assembly.](image)

Scale up assembly to keep reaction in bigger scale. 5g batches were done. (Figure 2)

![Figure 2. Electrochemical batch of a 5g reaction.](image)
2. Analytical data of Compound 3a to 3q, 4 and 5.

$^1$H NMR of Compound 3a

Molecular Weight: 222.25

$^{13}$C NMR of Compound 3a
LCMS of Compound 3a

$\text{Molecular Weight: 222.25}$

$\text{Peak Results}$

<table>
<thead>
<tr>
<th>Retention Time (min)</th>
<th>Base Peak (m/z)</th>
<th>Height (a.u.)</th>
<th>Area (\text{f.u.})</th>
<th>% Area</th>
<th>Channel</th>
<th>Channel Name</th>
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$\text{1H NMR of Compound 3b}$

$\text{Molecular Weight: 252.27}$

$\text{Current Data Parameters}$

$\text{F1 - Acquisition parameters}$

$\text{Current Data Parameters}$

$\text{F2 - Processing parameters}$
$^{13}$C NMR of Compound 3b
LCMS of Compound 3b

![LCMS Graphs]

### Peak Results

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<tr>
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<tr>
<td>3</td>
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<tr>
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### Molecular Weight

Molecular Weight: 252.27
$^{1}H$ NMR of Compound 3c

Molecular Weight: 282.30

$^{13}C$ NMR of Compound 3c
LCMS of Compound 3c

\[
\text{Molecular Weight: } 2030
\]

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<td>720.0</td>
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\[^1H\) NMR of Compound 3d

Exact Mass: 229.03

16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 1 ppm
$^{13}$C NMR of Compound 3d

LCMS of Compound 3d

Exact Mass: 229.03
$^1$H NMR of Compound 3e

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

![LCMS Graph]

Exact Mass: 212.0688

$^1$H NMR of Compound 3f

![NMR Spectrum]
**13C NMR of Compound 3f**

![NMR Spectrum Image]

**LCMS of Compound 3f**

![LCMS Image]

**Molecular Weight:** 292.27
$^1$H NMR of Compound 3g

Molecular Weight: 252.27

$^{13}$C NMR of Compound 3g
LCMS of Compound 3g
$^1$H NMR of Compound 3h

Molecular Weight: 282.30

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

![LCMS Graph]

**Peak Results**

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**Molecular Weight**: 262.36

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$^1$H NMR of Compound 3i

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

Exact Mass: 146.05
\(^1\)H NMR of Compound 3j

\(^{13}\)C NMR of Compound 3j
LCMS of Compound 3j

![LCMS Graph]

Peak Results

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<th>Height (pF)</th>
<th>Area (pA/sec)</th>
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Peak Results

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<th>Area (pA/sec)</th>
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Exact Mass: 160.06

$^1$H NMR of Compound 3k

![NMR Spectrum]
$^{13}$C NMR of Compound 3k

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LCMS of Compound 3k

Molecular Weight: 176.18
$^1$H NMR of Compound 3l

Molecular Weight: 272.05

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

Molecular Weight: 272.05
LCMS of Compound 3l

<table>
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<th>Retention Time (min)</th>
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<th>% Area</th>
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Molecular Weight: 272.05

$^1$H NMR of Compound 3m

Molecular Weight: 160.2
$^{13}$C NMR of Compound 3m

Molecular Weight: 160.2

LCMS of Compound 3m

Molecular Weight: 160.2
$^1$H NMR of Compound 3n

Chemical Formula: C$_8$H$_6$N$_2$O
Molecular Weight: 174.20

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

Chemical Formula: C$_8$H$_4$N$_2$O
Molecular Weight: 174.20
LCMS of Compound 3n

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<th>Base Peak (m/z)</th>
<th>Height (µl)</th>
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Chemical Formula: C_{12}H_{10}N_{2}O
Molecular Weight: 174.20
$^1$H NMR of Compound 3o

6-Chloro-2-methylquinazolin-4(3H)-one
Chemical Formula: C$_7$H$_5$ClN$_2$O$_2$
Molecular Weight: 191.6

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

6-Chloro-2-methylquinazolin-4(3H)-one
Chemical Formula: C$_7$H$_5$ClN$_2$O$_2$
Molecular Weight: 191.6
LCMS of Compound 3o

Peak Results
Channel 1 PDA Spectrum

<table>
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<th>Base Peak (m/z)</th>
<th>Height (a.u.)</th>
<th>Area (a.u. / sec)</th>
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<th>Channel Name</th>
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<tbody>
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<td>PDA Spectrum</td>
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Chemical Formula: C16H15N2
Molecular Weight: 244.56

NMR Data

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$^1$H NMR of Compound 3p

$^{13}$C NMR of Compound 3p
LCMS of Compound 3p

![LCMS Graphs]

### Peak Results

#### Channel 1: ESI Spectrum

<table>
<thead>
<tr>
<th>Retention Time (min)</th>
<th>Base Peak (m/z)</th>
<th>Height (mAU)</th>
<th>Area (µA-s)</th>
<th>% Area</th>
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<tbody>
<tr>
<td>1.051</td>
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<tr>
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<td>ESI Spectrum</td>
<td>275.3m/z</td>
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<tr>
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#### Channel 2: ESI Spectrum

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### Peak Results

#### Channel 1: MS Scan

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<td>S1: MS Scan</td>
<td>MS TIC</td>
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Chemical Formula: C14H13NO
Molecular Weight: 210.6
$^1$H NMR of Compound 3q

Molecular Weight: 206.20

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

Molecular Weight: 206.20
$^1$H NMR of Compound 4

![$^1$H NMR spectrum of Compound 4]

Exact Mass: 303.06

$^{13}$C NMR of Compound 4

![$^{13}$C NMR spectrum of Compound 4]

Exact Mass: 303.06
\(^1\)H NMR of Compound 5

Molecular Weight: 378.20

\(^{13}\)H NMR of Compound 5

Molecular Weight: 378.20