Supporting Information

IDENTIFICATION OF A NOVEL INDOLEAMINE 2,3-DIOXYGENASE INHIBITOR BEARING AN EIGHT-MEMBERED RING FUSED INDOLE SCAFFOLD AND ITS STRUCTURE ACTIVITY RELATIONSHIP

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**Table S1.** Structures and Biological Activities of 15 Hit Compounds

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<thead>
<tr>
<th>Structure</th>
<th>A431 cell % inhibition at 10 μM</th>
<th>A431 cell viability at 10 μM</th>
<th>rhIDO % inhibition at 30 μM</th>
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<td>96%</td>
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<tr>
<td>Structure</td>
<td>A431 cell % inhibition at 10 μM</td>
<td>A431 cell viability at 10 μM</td>
<td>rhIDO % inhibition at 30 μM</td>
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</table>
$^1$H NMR spectrum for compound 5a (500 MHz, CDCl₃)

$^1$H NMR spectrum for compound 5b (500 MHz, CDCl₃)
$^1$H NMR spectrum for compound 5c (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 5c (150 MHz, CDCl$_3$)
\(^1\)H NMR spectrum for compound 5d (500 MHz, CDCl\(_3\))

\(^{13}\)C NMR spectrum for compound 5d (150 MHz, CDCl\(_3\))
$^1$H NMR spectrum for compound 5e (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 5e (150 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 5f (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 5f (150 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 5g (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 5g (150 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 5h (500 MHz, DMSO-$d_6$, 100 °C)

$^{13}$C NMR spectrum for compound 5h (125 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 5i (500 MHz, DMSO-$d_6$, 100 °C)

$^{13}$C NMR spectrum for compound 5i (125 MHz, DMSO-$d_6$, 100 °C)
$^1$H NMR spectrum for compound 5j (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 5j (125 MHz, CDCl$_3$)
\textbf{\textsuperscript{1}H NMR spectrum for compound 5l (500 MHz, CDCl\textsubscript{3})}

\textbf{\textsuperscript{13}C NMR spectrum for compound 5l (125 MHz, CDCl\textsubscript{3})}

\[5l\]
$^1$H NMR spectrum for compound 5m (500 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 5n (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 5n (125 MHz, CDCl$_3$)

![NMR Spectra](image-url)
$^1$H NMR spectrum for compound 5o (500 MHz, DMSO-$d_6$, 100 °C)

$^{13}$C NMR spectrum for compound 5o (125 MHz, DMSO-$d_6$, 100 °C)

5o

Br
Me
N
N
Boc
Me
$^1$H NMR spectrum for compound 5p (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 5p (125 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 7a (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 7a (125 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 7b (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 7b (125 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 7c (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 7c (125 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 7d (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 7d (125 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 7e (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 7e (125 MHz, CDCl$_3$)

![1H NMR spectrum](image)

![13C NMR spectrum](image)
$^1$H NMR spectrum for compound 7f (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 7f (125 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 7g (500 MHz, CDCl₃)

$^{13}$C NMR spectrum for compound 7g (125 MHz, CDCl₃)
$^1$H NMR spectrum for compound 7h (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 7h (125 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 7i (500 MHz, CDCl$_3$)

$^{13}$C NMR spectrum for compound 7i (125 MHz, CDCl$_3$)
$^1$H NMR spectrum for compound 7j (500 MHz, DMSO-$_d^6$, 100 °C)

$^{13}$C NMR spectrum for compound 7j (125 MHz, DMSO-$_d^6$, 100 °C)