Supporting Information

Protecting-Group-Free Synthesis of a Dual CCK1/CCK2 Receptor Antagonist

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Supporting information

1) $^1$H and $^{13}$C NMR spectra

2) Chiral HPLC chromatogram of compound 8

3) Chiral HPLC chromatogram of compound 1
Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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1H, 600 MHz, d6-DMSO

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![Chemical structure and NMR spectrum](image)

(°H, 600 MHz, MeOD)
$\text{Br} - \text{C} - \text{O} - \text{HAc}$

(90% ee)

$\text{Br} - \text{C} - \text{O} - \text{HAc}$

(99% ee)

(R)-isomer

(S)-isomer

DAD1 A, Sig=220,16 Ref=off (HMM1480148-TEST.D)

DAD1 B, Sig=254,16 Ref=off (HMM1480148-TEST.D)
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\[
\text{Br} \quad \text{F}
\]
\[
\begin{array}{c}
\text{NH}_2 \\
\text{OH}
\end{array}
\]

\((1^H, 600 \text{ MHz, } d_4-\text{AcOH})\)
(13C, 151 MHz, d4-AcOH)
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The figure shows a 1H NMR spectrum of a compound in D2O. The spectrum contains peaks at various chemical shifts, indicated by f1 (ppm) and f2 (g). The compound structure is also shown, labeled as (1H, 600 MHz, D2O).
(13C, 151 MHz, D2O)
$\text{H NMR, DMSO-$d_6$, 500 MHz}$
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13C NMR, DMSO-d6, 500 MHz
1H NMR, DMSO-d6, 600 MHz
13C NMR, DMSO-d6, 600 MHz
$^1$H NMR, DMSO-$d_6$, 500 MHz
13C NMR, DMSO-d6, 500 MHz
1H NMR, 600 MHz, DMSO-d6
Chiral Hewlett Packard HPLC
Chiralpak OD-H, 4.6 x 250 mm column
100% EtOH, with 0.2% trifluoroacetic acid in ethanol
Flow rate 0.3 mL/min, pressure 39 bar
Retention time: 17.0 (another enantiomers 15.0 minutes)