Supporting Information

Preparation and anti-trypanosomal activity of a series of dipeptide-based vinyl sulfones

William Doherty, a Jinju James, a Paul Evans, a Laura Martin, b Nikoletta Adler, b Derek Nolan b and Andrew Knox b

a Centre for Synthesis and Chemical Biology, School of Chemistry and Chemical Biology, University College Dublin, Dublin 4, Ireland. Paul.evans@ucd.ie

b School of Biochemistry and Immunology, Trinity Biomedical Sciences Institute, Trinity College Dublin, Pearse Street, Dublin 2, Ireland. Aknox@tcd.ie
$^1\text{H} \ (400 \text{ MHz, CDCl}_3)$ and $^{13}\text{C} \ (100 \text{ MHz, CDCl}_3)$ NMR spectra of \textbf{6}. 

\begin{center}
\includegraphics[width=\textwidth]{nmr_spectra.png}
\end{center}
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) NMR spectra of 7
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) NMR spectra of 9
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) NMR spectra of 4
Reverse Phase HPLC trace of compound 4

HPLC analysis at 220 nm for compound 4: (C-18) MeCN-H$_2$O-0.1 M NH$_4$HCO$_3$(aq); 60:30:10 (0.4 mL/min): $t_r$ = 26.79 min. Purity: >95%.
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) NMR spectra of 1
Reverse Phase HPLC trace of compound 1

HPLC analysis at 220 nm for compound 1: (C-18), MeCN-H$_2$O-0.1 M NH$_4$HCO$_3$(aq); 60:30:10 (0.4 mL/min); $t_r = 31.19$ min. Purity: $>95\%$. 

![HPLC Trace of Compound 1](image)
$^1$H (500 MHz, CDCl$_3$) and $^{13}$C (125 MHz, CDCl$_3$) NMR spectra of 13
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) NMR spectra of 15
$^1$H (400 MHz, d$^6$-DMSO) and $^{13}$C (100 MHz, d$^6$-DMSO) NMR spectra of 17
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) NMR spectra of 18
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) NMR spectra of \textbf{19}
Reverse Phase HPLC trace of compound 19

HPLC analysis at 220 nm for compound 19: (C–18), MeCN-H2O-0.1 M NH4 HCO3(aq); 90:9:1 (0.4 mL/min); t_r = 9.66 min. Purity: >95%.
UV-Visible spectrum (CHCl$_3$) for compound 19 (conc = $1 \times 10^{-5}$ M).

Fluorescence emission spectrum (CHCl$_3$) of 19 (conc = $1 \times 10^{-6}$ M). Excitation at 340 nm.

Normalised UV–Vis absorbance (black) and fluorescence emission (blue) spectra for compound 19.
$^1$H (600 MHz, CDCl$_3$) and $^{13}$C (150 MHz, CDCl$_3$) NMR spectra of 20
600 MHz 2D NOE Spectrum of 20

Key Chemical Shifts

\[
\begin{align*}
\delta H_a &= 3.74-3.78 \text{ ppm} \\
\delta H_b &= 3.23 \text{ ppm} \\
\delta H_c &= 2.77 \text{ ppm} \\
\delta H_d &= 2.51-2.59 \text{ ppm}
\end{align*}
\]
$^1$H (500 MHz, CDCl$_3$) and $^{13}$C (125 MHz, CDCl$_3$) NMR spectra of 21
500 MHz 2D NOE Spectrum of 21

Key Chemical Shifts
\[ \delta H_b = 3.70 - 3.78 \text{ ppm} \]
\[ \delta H_d = 2.91 - 2.98 \text{ ppm} \]
\[ \delta H_b + \delta H_d = 3.11 - 3.20 \text{ ppm} \]
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) spectra of 22
$^{19}$F NMR (376 MHz, CDCl$_3$) spectrum of 22
$^1$H (400 MHz, d$_6$-DMSO) and $^{13}$C (100 MHz, d$_6$-DMSO) NMR spectra of 23
$^1$H (600 MHz, CDCl$_3$) and $^{13}$C (150 MHz, CDCl$_3$) NMR spectra of 24
600 MHz 2D NOE Spectrum of 24

Key Chemical Shifts

$\delta H_a = 3.02 - 3.05$ ppm
$\delta H_b = 3.42 - 3.47$ ppm
$\delta H_c = 3.68 - 3.74$ ppm
\(^1\text{H} (400 \text{ MHz, CDCl}_3) \text{ and } \^{13}\text{C} (100 \text{ MHz, CDCl}_3) \text{ NMR spectra of } 25
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) NMR spectra of 26
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) NMR spectra of 29
$^1$H (400 MHz, CDCl$_3$) and $^{13}$C (100 MHz, CDCl$_3$) NMR spectra of 31