Synthesis of non-natural cyanthiwigin–gagunin hybrids through late-stage diversification of the cyanthiwigin natural product core

Kelly E. Kim, Yuka Sakazaki, and Brian M. Stoltz*

The Warren and Katharine Schlinger Laboratory for Chemistry and Chemical Engineering, Division of Chemistry and Chemical Engineering, California Institute of Technology, 1200 E. California Blvd, MC 101-20, Pasadena, CA 91125 (USA)

Table of Contents

Experimental Spectra (\(^1\)H NMR, \(^{13}\)C NMR, 2-D NMR, IR) S2
$^1$H NMR (500 MHz, CDCl$_3$) of compound 17.
Infrared spectrum (Thin Film, KBr) of compound 17.

$^{13}$C NMR (126 MHz, CDCl$_3$) of compound 17.
HSQC (500, 126 MHz, CDCl₃) of compound 17.

NOESY (500 MHz, CDCl₃) of compound 17.
$^1$H NMR (600 MHz, CDCl$_3$) of compound 18.
Infrared spectrum (Thin Film, KBr) of compound 18.

\(^{13}\)C NMR (126 MHz, CDCl\(_3\)) of compound 18.
HSQC (600, 126 MHz, CDCl₃) of compound 18.

NOESY (600 MHz, CDCl₃) of compound 18.
$^1$H NMR (400 MHz, CDCl$_3$) of compound 19.
Infrared spectrum (Thin Film, KBr) of compound 19.

$^{13}$C NMR (101 MHz, CDCl$_3$) of compound 19.
HSQC (400, 101 MHz, CDCl₃) of compound 19.

NOESY (400 MHz, CDCl₃) of compound 19.
$^1$H NMR (500 MHz, CDCl$_3$) of compound 20.
Infrared spectrum (Thin Film, KBr) of compound 20.

$^{13}$C NMR (126 MHz, CDCl$_3$) of compound 20.
$^1$H NMR (400 MHz, CDCl$_3$) of compound 21.
Infrared spectrum (Thin Film, KBr) of compound 21.

$^{13}$C NMR (101 MHz, CDCl$_3$) of compound 21.
HSQC (400, 101 MHz, CDCl₃) of compound 21.

NOESY (400 MHz, CDCl₃) of compound 21.
\(^1\)H NMR (400 MHz, CDCl\(_3\)) of compound 22.
Infrared spectrum (Thin Film, KBr) of compound 22.

$^{13}$C NMR (101 MHz, CDCl$_3$) of compound 22.
HSQC (400, 101 MHz, CDCl₃) of compound 22.

NOESY (400 MHz, CDCl₃) of compound 22.
\(^{1}H\) NMR (400 MHz, CDCl\(_3\)) of compound 23.
Infrared spectrum (Thin Film, KBr) of compound 23.

$^\text{13}C$ NMR (101 MHz, CDCl$_3$) of compound 23.
HSQC (400, 101 MHz, CDCl₃) of compound 23.

NOESY (400 MHz, CDCl₃) of compound 23.
$^1$H NMR (500 MHz, CDCl$_3$) of compound 15.
Infrared spectrum (Thin Film, KBr) of compound 15.

$^{13}$C NMR (126 MHz, CDCl$_3$) of compound 15.
HSQC (400, 101 MHz, CDCl₃) of compound 15.

NOESY (400 MHz, CDCl₃) of compound 15.
$^{1}$H NMR (500 MHz, CDCl$_3$) of compound 24.
Infrared spectrum (Thin Film, KBr) of compound 24.

$^{13}$C NMR (126 MHz, CDCl$_3$) of compound 24.
HSQC (500, 126 MHz, CDCl₃) of compound 24.

NOESY (500 MHz, CDCl₃) of compound 24.
$^{1}H$ NMR (500 MHz, CDCl$_3$) of compound 16.
Infrared spectrum (Thin Film, KBr) of compound 16.

$^{13}$C NMR (126 MHz, CDCl$_3$) of compound 16.
HSQC (500, 126 MHz, CDCl₃) of compound 16.

NOESY (500 MHz, CDCl₃) of compound 16.
$^1$H NMR (400 MHz, CDCl$_3$) of compound 25.
Infrared spectrum (Thin Film, KBr) of compound 25.

$^1$H NMR (101 MHz, CDCl$_3$) of compound 25.

$^{13}$C NMR (101 MHz, CDCl$_3$) of compound 25.
HSQC (400, 101 MHz, CDCl₃) of compound 25.

COSY (400 MHz, CDCl₃) of compound 25.
HMBC (400, 101 MHz, CDCl$_3$) of compound 25.

NOESY (400 MHz, CDCl$_3$) of compound 25.
"1H NMR (400 MHz, CDCl₃) of compound 27."
Infrared spectrum (Thin Film, KBr) of compound 27.

$^{13}$C NMR (101 MHz, CDCl$_3$) of compound 27.
HSQC (400, 101 MHz, CDCl₃) of compound 27.

HMBC (400, 101 MHz, CDCl₃) of compound 27.
$^1$H NMR (500 MHz, CDCl$_3$) of compound 14a.
Infrared spectrum (Thin Film, KBr) of compound 14a.

$^{13}$C NMR (126 MHz, CDCl$_3$) of compound 14a.
HSQC (500, 126 MHz, CDCl₃) of compound 14a.

COSY (500 MHz, CDCl₃) of compound 14a.
$^1$H NMR (500 MHz, CDCl$_3$) of compound 14b.
Infrared spectrum (Thin Film, KBr) of compound 14b.

$^{13}$C NMR (126 MHz, CDCl$_3$) of compound 14b.
HSQC (400, 126 MHz, CDCl₃) of compound 14b.

NOESY (400 MHz, CDCl₃) of compound 14b.
$^1$H NMR (500 MHz, CDCl$_3$) of compound 14c.
Infrared spectrum (Thin Film, KBr) of compound \textbf{14c}.

\textsuperscript{\textit{13}}C NMR (126 MHz, CDCl\textsubscript{3}) of compound \textbf{14c}.
HSQC (500, 126 MHz, CDCl₃) of compound 14c.

COSY (500 MHz, CDCl₃) of compound 14c.