Supplementary Material

Competitive 1,3-dipolar cycloaddition reactions of an azomethine ylide with aromatic and carbonyl groups of nitro-substituted isatoic anhydrides

Asha M. D’Souza,† Daniel J. Rijinova,§ Roger Mulder, † Jonathan M. White,‡ Adam G. Meyer,† Christopher J. T. Hyland§ and John H. Ryan†*

† CSIRO Manufacturing, Ian Wark Laboratory, Bayview Avenue, Clayton, Vic. 3168, Australia
‡ School of Chemistry, Bio21 Institute, University of Melbourne, Parkville, Vic. 3010, Australia
§ School of Chemistry, University of Wollongong, Wollongong, NSW 2522, Australia

*E-mail: jack.ryan@csiro.au

1. Copies of $^1$H and $^{13}$C NMR spectra for new compounds (S2-S7).
2. X-ray crystallographic analysis of compound 16 (S8).
1. Copies of $^1$H and $^{13}$C NMR spectra for new compounds.

$^1$H NMR spectrum of 11 (200 MHz, CDCl$_3$)
$^{13}$C$^1$H NMR spectrum of 11 (50 MHz, CDCl$_3$)

$^1$H NMR spectrum of 13 (200 MHz, CDCl$_3$)
\[^{13}\text{C\{^1\text{H}\}}\text{ NMR spectrum of 13 (50 MHz, CDCl}_3)\]

\[^1\text{H}\text{ NMR spectrum of 14 (500 MHz, CDCl}_3)\]
$^{13}$C$\{^1$H$\}$ NMR spectrum of 14 (100 MHz, CDCl$_3$)

$^1$H NMR spectrum of 15 (500 MHz, CDCl$_3$)
$^{13}$C{\textsuperscript{1}H} NMR spectrum of 15 (126 MHz, CDCl₃)

$^{1}$H NMR spectrum of 16 (200 MHz, CDCl₃)
$^{13}\text{C} \{^1\text{H}\}$ NMR spectrum of 16 (50 MHz, CDCl$_3$)
2. X-ray crystallographic analysis of compound 16.

Crystallography. Intensity data were collected with an Oxford Diffraction XCalibur CCD diffractometer using Cu- Ka radiation, the temperature during data collection was maintained at 130.0(1) using an Oxford Cryosystems cooling device.

The structure was solved by direct methods and difference Fourier synthesis.\(^1\) Thermal ellipsoid plots were generated using the program ORTEP-3\(^2\) integrated within the WINGX\(^3\) suite of programs.

![Figure 1. Thermal ellipsoid plot of compound 16.](image)

Crystal data for 16. C\(_{27}\)H\(_{32}\)N\(_4\)O\(_4\), \(M = 476.56\) \(T = 130.0(2)\) K, \(l = 1.54184\) Å, Monoclinic, space group \(P2_1/c\) \(a = 17.6227(2)\) Å, \(b = 12.02730(10)\) Å, \(c = 11.40730(10)\) Å, \(V = 2416.41(4)\) Å\(^3\), \(Z = 4\), \(D_c = 1.310\) Mg \(M\(^{-3}\) \(m(Cu-Ka) = 0.721\) mm\(^{-1}\), \(F(000) = 1016\), crystal size 0.39 x 0.37 x 0.17 mm. \(q_{\text{max}} = 73.27^\circ\), 11361 reflections measured, 4724 independent reflections (\(R_{\text{int}} = 0.41\)) the final \(R = 0.0453\) [\(I > 2\sigma(I)\), 3801 data] and \(wR(F^2) = 0.125\) (all data) GOOF = 1.049.

References