Electronic Supplementary Information

Synthesis of 4-styrylcoumarins via FeCl₃-promoted cascade reactions of propargylamines with β-keto esters

Li-Qin Yan, Xiaoting Cai, Xinwei He,* Hui Wang, Mengqing Xie, Youpeng Zuo, Yongjia Shang*

Key Laboratory of Functional Molecular Solids, Ministry of Education, Anhui Laboratory of Molecule-Based Materials (State Key Laboratory Cultivation Base), College of Chemistry and Materials Science, Anhui Normal University, Wuhu 241000, P.R. China

* Corresponding author: shyj@mail.ahnu.edu.cn, xinweihe@mail.ahnu.edu.cn

Table of Contents

X-ray Crystallography Structures of Compounds 3ad-----------------------------S1

Copies of ¹H and ¹³C NMR Spectra for all Compounds---------------------------S2-S30
X-Ray Crystallography Structures of Compounds 3ad.

Figure S1. X-ray crystal structure of compound 3ad.

Crystal data for 3ad: C$_{19}$H$_{14}$O$_3$, $Mr = 290.30$, Monoclinic, $a = 8.5355$ (3) Å, $b = 9.9613$ (3) Å, $c = 17.9321$ (5) Å, $\alpha = 90^\circ$, $\beta = 100.199$ (2)$^\circ$, $\gamma = 90^\circ$, $V = 1500.58$ (8) Å$^3$, $T = 273(2)$ K, space group P2(1)/n, $Z = 4$, 15425 reflections collected, 3318 unique ($R_{int} = 0.0338$) which were used in all calculation. The ellipsoid contour probability level in the caption is 30%.

Crystallographic data for compound 3ad reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1868191.
\(^1\)H NMR Spectra of Compound 3aa

\(^{13}\)C NMR Spectra of Compound 3aa
$^1$H NMR and $^{13}$C NMR Spectra of Compound 3ab

$^{13}$C NMR Spectra of Compound 3ab
$^1$H NMR Spectra of Compound 3ac

$^{13}$C NMR Spectra of Compound 3ac
$^1$H NMR Spectra of Compound 3ad

$^{13}$C NMR Spectra of Compound 3ad
\( ^1H \) NMR Spectra of Compound 3ba

\( ^{13}C \) NMR Spectra of Compound 3ba
$^{1}H$ NMR Spectra of Compound 3bc

$^{13}C$ NMR Spectra of Compound 3bc
$^1$H NMR Spectra of Compound 3bd

$^{13}$C NMR Spectra of Compound 3bd
\(^1\)H NMR Spectra of Compound 3ca

\(^{13}\)C NMR Spectra of Compound 3ca
$^1$H NMR Spectra of Compound 3cb

$^{13}$C NMR Spectra of Compound 3cb
$^1$H NMR Spectra of Compound 3cc

$^{13}$C NMR Spectra of Compound 3cc
$^1$H NMR Spectra of Compound 3cd

$^{13}$C NMR Spectra of Compound 3cd
\(^1\)H NMR Spectra of Compound 3da

\[^{13}\]C NMR Spectra of Compound 3da
$^1$H NMR Spectra of Compound 3db

$^{13}$C NMR Spectra of Compound 3db
$^1$H NMR Spectra of Compound 3dc

$^{13}$C NMR Spectra of Compound 3dc
$^1$H NMR Spectra of Compound 3ea

$^{13}$C NMR Spectra of Compound 3ea
$^1$H NMR Spectra of Compound 3eb

$^{13}$C NMR Spectra of Compound 3eb
$^1$H NMR Spectra of Compound 3ec

$^{13}$C NMR Spectra of Compound 3ec

$^1$H NMR Spectra of Compound 3ed
\[ \text{13C NMR Spectra of Compound 3ed} \]

\[ \text{1H NMR Spectra of Compound 3fa} \]
$^{13}$C NMR Spectra of Compound 3fa

$^1$H NMR Spectra of Compound 3fb
$^{13}$C NMR Spectra of Compound 3fb
$^1$H NMR Spectra of Compound 3fc

$^{13}$C NMR Spectra of Compound 3fc
$^1$H NMR Spectra of Compound 3fd

![H NMR Spectra](image)

$^{13}$C NMR Spectra of Compound 3fd

![C NMR Spectra](image)
$^{1}$H NMR Spectra of Compound 3ga

$^{13}$C NMR Spectra of Compound 3ga
$^1$H NMR Spectra of Compound 3gb

$^{13}$C NMR Spectra of Compound 3gb
$^1$H NMR Spectra of Compound 3gc

$^{13}$C NMR Spectra of Compound 3gc
$^1$H NMR and $^{13}$C NMR Spectra of Compound 3gd

$^{13}$C NMR Spectra of Compound 3gd
$^1$H NMR Spectra of Compound 3ha

$^{13}$C NMR Spectra of Compound 3ha
$^1\text{H NMR Spectra of Compound 3hc}$

$^{13}\text{C NMR Spectra of Compound 3hc}$
$^1$H NMR Spectra of Compound 3ia

$^{13}$C NMR Spectra of Compound 3ia
$^1$H NMR Spectra of Compound 3ae

$^{13}$C NMR Spectra of Compound 3ae