Supporting Information

Ammonium chloride catalyzed three-component reaction for the synthesis of fused 4H-chromene derivatives in aqueous medium

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Experimental General

Melting points were determined on a Büchi melting point apparatus and are uncorrected. IR spectra were recorded on Perkin-Elmer 281 IR spectrophotometer. $^1$H and $^{13}$C NMR spectra were recorded on Varian 400 spectrometer TMS as internal reference; chemical shifts ($\delta$ scale) are reported in parts per million (ppm). $^1$H NMR Spectra are reported in the order: multiplicity, coupling constant (J value) in hertz (Hz) and no of protons; signals were characterized as s (singlet), d (doublet), t (triplet), m (multiplet), br s (broad singlet) and dt (doublet of triplet). Elemental analyses were carried out using Perkin-Elmer 2400 Series II CHNS/O analyzer at the Department of Chemistry, Indian Institute of Technology, Guwahati. The X-ray crystal structures were determined with a Siemen P-4 diffractometer. Complete crystallographic data of 4k (CCDC no. is 926004) for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, Copies of this information may be obtained free of charge from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44-1223-336033, e-mail: deposit@ccdc.cam.ac.uk or via: www.ccdc.cam.ac.uk).

Crystallographic Description

Crystal data were collected with Bruker Smart Apex-II CCD diffractometer using graphite monochromated MoK$\alpha$ radiation ($\lambda = 0.71073$ Å) at 298 K. Cell parameters were retrieved using SMART software and refined with SAINT on all observed reflections. Data reduction was performed with the SAINT software and corrected for Lorentz and polarization effects. Absorption corrections were applied with the program SADABS. The structure was solved by direct methods implemented in SHELX-97 program and refined by full-matrix least-squares methods on F2. All non-hydrogen atomic positions were located in difference Fourier maps and refined anisotropically. The hydrogen atoms were placed in their geometrically generated positions. Compound 4k empirical formula C$_{26}$H$_{19}$NO$_3$, colorless crystal, formula wt 400.90, Orthorhombic, C2/c, a = 11.6732(9) Å, b = 9.2582(7) Å, c = 37.329(3) Å, V = 4034.3(5) Å$^3$, Z = 8, F (0 0 0) = 1680, GOF(S) = 1.007. Final indices $R_{\text{obs}} = 0.0476$, $wR_{\text{obs}} = 0.0889$ with $I > 2\sigma(I)$; $R_{\text{all}} = 0.0616$, $wR_{\text{all}} = 0.0938$ for all data.
Complete crystallographic data of **4k** for the structural analysis have been deposited with the Cambridge Crystallographic Data Centre, as supplementary publication with CCDC no. 926004. Copies of this information may be obtained free of charge from the Director, Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK, (fax: +44-1223-336033, e-mail: deposit@ccdc.cam.ac.uk or via: www.ccdc.cam.ac.uk).

**Table S1.** Crystal data and structure refinement for **4k**. For atomic coordinates and equivalent isotropic displacement parameters and bond angles, please check the CIF.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Compound 4k</th>
<th>Parameters</th>
<th>Compound 4k</th>
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<td>Z</td>
<td>8</td>
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<td>Empirical formula</td>
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<td>Unit cell dimensions</td>
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<td>a</td>
<td>11.6732(9) Å</td>
<td>Completeness to θ°</td>
<td>99% (θ = 25.23 °)</td>
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</tr>
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<td>b</td>
<td>9.2582(7) Å</td>
<td>Refinement method</td>
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<td>α</td>
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<td>β</td>
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<td>Final R indices [&gt;2sigma(I)]</td>
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<td>γ</td>
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<td>R indices (all data)</td>
<td>R&lt;sub&gt;all&lt;/sub&gt; = 0.0616, wR&lt;sub&gt;all&lt;/sub&gt; = 0.0938</td>
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<td>Volume</td>
<td>4034.3(5) Å&lt;sup&gt;3&lt;/sup&gt;</td>
<td>Largest diff. peak and hole</td>
<td>0.157 and -0.190e.Å&lt;sup&gt;-3&lt;/sup&gt;</td>
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$^1$H NMR spectra of compound (5)
$^1$H NMR spectra of compound (6)
$^1$H NMR spectra of compound (4a)
$^{13}$C NMR spectra of (4a)
MS spectra of (4a)
$^1$H NMR spectra of compound (4b)
$^13$C NMR spectra of (4b)
MS spectra of (4b)
$^1$H NMR spectra of compound (4c)
$^{13}$C NMR spectra of (4c)
$^1$H NMR spectra of compound (4d)
\(^{13}\)C NMR spectra of (4d)
MS spectra of (4d)
$^1$H NMR spectra of compound (4e)
$^{13}$C NMR spectra of (4e)
MS spectra of (4e)
$^1$H NMR spectra of compound (4f)
$^{13}$C NMR spectra of (4f)
MS spectra of (4f)
$^1$H NMR spectra of compound (4g)
$^{13}$C NMR spectra of (4g)
MS spectra of (4g)
$^1$H NMR spectra of compound (4h)
$^{13}$C NMR spectra of (4h)
MS spectra of (4h)

![Graph showing mass spectra of (4h)](image_url)
H NMR spectra of compound (4i)
$^{13}$C NMR spectra of (4i)
MS spectra of (4i)

+ESI Scan (7.0 sec) Frag=175.0V SB-SH–6.d

[Graph of MS spectra showing a peak at m/z 425.0139]

4i
$^1$H NMR spectra of compound (4j)
$^{13}$C NMR spectra of (4j)
MS spectra of (4j)
\textsuperscript{1} H NMR spectra of compound (4k)
$^{13}$C NMR spectra of (4k)
$^1$H NMR spectra of compound (4l)
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MS spectra of (4l)

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![Graph of MS spectra with peak at m/z 355.1335](image)

4l
$^1$H NMR spectra of compound (4m)
$^{13}$C NMR spectra of (4m)

![C NMR spectra of (4m)](image_url)
MS spectra of (4m)
$^1$H NMR spectra of compound (4n)
\(^{13}\)C NMR spectra of (4n)
MS spectra of (4n)
$^1$H NMR spectra of compound (4o)
$^{13}$C NMR spectra of (4o)
MS spectra of (4o)
$^1$H NMR spectra of compound (4p)
$^{13}$C NMR spectra of (4p)
MS spectra of (4p)

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![Molecular Structure](image)

4p
$^1$H NMR spectra of compound (8a)
$^{13}$C NMR spectra of (8a)
MS spectra of (8a)
$^1$H NMR spectra of compound (8b)
$^{13}$C NMR spectra of (8b)
MS spectra of (8b)