Supporting information

pH Sensitive Fluorescent Phototrigger based on benzo[b]acridine-12-yl) methanol (BAM): Synthesis, Photophysical, Photochemical and Biological Applications


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Supplementary Data

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\(^1\)H NMR spectrum of 12-methylbenzo[a]acridine (2) (CDCl\(_3\), 200 MHz)

\(^{13}\)C NMR spectrum of 12-methylbenzo[a]acridine (2) (CDCl\(_3\), 50 MHz).
$^1$H NMR spectrum of 12-(bromomethyl)benzo[a]acridine (3) (CDCl$_3$, 200 MHz)

$^{13}$C NMR spectrum of 12-(bromomethyl)benzo[a]acridine (3) (CDCl$_3$, 50 MHz)
$^1$H NMR spectrum of (benzo[a]acridin-12-yl)methyl 2-phenylacetate (5a) (CDCl$_3$, 200 MHz).

$^{13}$C NMR spectrum of (benzo[a]acridin-12-yl)methyl 2-phenylacetate (5a) (CDCl$_3$, 50 MHz).
H NMR spectrum of (benzo[a]acridin-12-yl)methyl benzoate (5b) (CDCl₃, 200 MHz).

C NMR spectrum of (benzo[a]acridin-12-yl)methyl benzoate (5b) (CDCl₃, 100 MHz).

H NMR spectrum of (benzo[a]acridin-12-yl)methyl benzoate (5b) (CDCl₃, 200 MHz).

C NMR spectrum of (benzo[a]acridin-12-yl)methyl benzoate (5b) (CDCl₃, 100 MHz).
$^1$H NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-methylbenzoate (5c) (CDCl$_3$, 200 MHz).

$^{13}$C NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-methylbenzoate (5c) (CDCl$_3$, 50 MHz).
H NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-methoxybenzoate (5d) (CDCl₃, 200 MHz)

¹³C NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-methoxybenzoate (5d) (CDCl₃, 100 MHz)
$^1$H NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-vinylbenzoate (5e) (CDCl$_3$, 200 MHz)

$^{13}$C NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-vinylbenzoate (5e) (CDCl$_3$, 100 MHz)
$^1$H NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-nitrobenzoate (5f) (CDCl$_3$, 200 MHz)

$^{13}$C NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-nitrobenzoate (5f) (CDCl$_3$, 50 MHz)
$^1$H NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-(pivalamido)butanoate (7a) (CDCl$_3$, 200 MHz)

$^{13}$C NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-(pivalamido)butanoate (7a) (CDCl$_3$, 100 MHz)
$^1$H NMR spectrum of (R)-benzo[a]acridin-12-ylmethyl 2-(tert-butoxycarbonylamino) propanoate (7b) (CDCl$_3$, 200 MHz)

$^{13}$C NMR spectrum of (R)-benzo[a]acridin-12-ylmethyl 2-(tert-butoxycarbonylamino) propanoate (7b) (CDCl$_3$, 100 MHz)
Figure-S1. UV-vis absorption spectra of representative esters (5c-5d) and (7a-b) in MeOH (2.0×10^{-4} M)

Figure-S2. Emission spectra of representative esters (5c-5d) and (7a-b) in MeOH (2.0×10^{-4} M)
Figure-S3. UV-vis spectral change of ester 5d (2x10^{-4} M) in ACN-H_2O (50-50 v/v) at regular intervals of irradiation (0-150 min).

Figure-S4.a. Normalized UV-vis absorption spectrum (black line) and emission spectrum (red line) of ester 5c in ACN:HEPES (30:70) b. Fluorescence spectra of the ester 5c in ACN and in increasing percentage of HEPES buffer in ACN (2.0 × 10^{-5} M).
Table-S1. Photolytic data of BAM esters (5c) on irradiation (≥410 nm) in acetonitrile-HEPES (30:70 v/v)

<table>
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<tr>
<th>Ester</th>
<th>Carboxylic acid</th>
<th>Time of photolysis (min)</th>
<th>% of acid generated</th>
<th>Quantum yield ( (\phi_p) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>5c</td>
<td>p-CH(_3)C(_6)H(_4)CO(_2)H</td>
<td>400</td>
<td>90</td>
<td>0.106</td>
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\( ^a \) % of carboxylic acid released as determined by HPLC, \( ^b \) photochemical quantum yield for the generated carboxylic acids (error limit within ± 5%).

Figure-S5. HPLC profile of BAM-Cbl stability in DMSO supplemented with 10% fetal bovine serum and incubated at 37 °C in the dark for a period of 10 days (X axis is offset by 10 s and the Y axis is offset by 10 mAU for better visualization).
$^1$H NMR spectrum of photo product (benzo[a]acridin-12-yl)methanol (8) (CDCl$_3$, 200 MHz)

$^{13}$C NMR spectrum of photo product (benzo[a]acridin-12-yl)methanol (8) (CDCl$_3$, 50 MHz)
$^1$H NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-(4-(bis(2-chloroethyl)amino)phenyl)butanoate (10) (CDCl$_3$, 200 MHz)

$^{13}$C NMR spectrum of (benzo[a]acridin-12-yl)methyl 4-(4-(bis(2-chloroethyl)amino)phenyl)butanoate (10) (CDCl$_3$, 100 MHz)