The first comparative study of the ability of different hydrophilic groups to water-solubilise fluorescent BODIPY dyes

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**Electronic Supplementary Material (ESI) for New Journal of Chemistry**

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(ESI+) mass spectrum of BODIPY carboxylic acid, N-hydroxysuccinimidyyl ester 2.
$^1$H NMR spectrum of *meso* pseudo-PEG BODIPY dye 4 recorded in DMSO-$d_6$ at 300 MHz.

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(ESI+) mass spectrum (low resolution) of meso dimethylalkylamino BODIPY dye 5.

(ESI+) mass spectrum (high resolution) of meso dimethylalkylamino BODIPY dye 5.
RP-HPLC elution profile (system A) of \textit{meso} dimethylalkylamino BODIPY dye 5.

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(ESI-) mass spectrum of meso sulfobetain BODIPY dye 6.
RP-HPLC elution profile (system A) of *meso* sulfobetain BODIPY dye 6.

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$^{13}$C NMR spectrum of *meso* trimethylalkylammonium BODIPY dye 7 recorded in DMSO-$d_6$ at 75.5 MHz.
$^{19}$F NMR spectrum of $meso$ trimethylalkylammonium BODIPY dye 7 recorded in DMSO-$d_6$ at 282.5 MHz.

(ESI+) mass spectrum of $meso$ trimethylalkylammonium BODIPY dye 7.
(ESI-) mass spectrum of meso trimethylalkylammonium BODIPY dye 7.

RP-HPLC elution profile (system A) of meso trimethylalkylammonium BODIPY dye 7.
Normalised absorption (—), emission (—) and excitation (—) spectra of *meso* trimethylalkylammonium BODIPY dye 7 in PBS at 25 °C.

$^1$H NMR spectrum of *meso* $\alpha$-sulfo-$\beta$-alanine BODIPY dye 8 (TBA$^+$ salt) recorded in DMSO-$d_6$ at 300 MHz.$^a$

$^a$Downfield displacement of the NMR signal of water was observed and was due to the presence of TBA$^+$ trifluoroacetate salt.
$^{13}$C NMR spectrum of meso $\alpha$-sulfo-$\beta$-alanine BODIPY dye 8 (TBA$^+$ salt) recorded in DMSO-$d_6$ at 75.5 MHz.

(ESI+) mass spectrum of meso $\alpha$-sulfo-$\beta$-alanine BODIPY dye 8.
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$^1$H NMR spectrum of meso disulfonated BODIPY dye 9 (TBA$^+$ salt) recorded in DMSO-$d_6$ at 300 MHz.$^a$

$^a$Downfield displacement of the NMR signal of water was observed and was due to the presence of TBA$^+$ trifluoroacetate salt.
$^{13}$C NMR spectrum of *meso* disulfonated BODIPY dye 9 (TBA$^+$ salt) recorded in DMSO-$d_6$ at 75.5 MHz.

(ESI+) mass spectrum of *meso* disulfonated BODIPY dye 9.
(ESI-) mass spectrum of *meso* disulfonated BODIPY dye 9.

RP-HPLC elution profile of *meso* disulfonated BODIPY dye 9.
Normalised absorption (—), emission (—) and excitation (—) spectra of meso disulfonated BODIPY dye 9 in PBS at 25 °C.

\[\text{Wavelength (nm)}\]

\[\text{Normalised Absorbance or Fluorescence intensity}\]

\(^1\text{H NMR spectrum of meso phosphonated BODIPY dye 10 (TBA}^+\text{ salt) recorded in DMSO-}d_6\text{ at 300 MHz.}^a\]

\(^a\text{Downfield displacement of the NMR signal of water was observed and was due to the presence of TBA}^+\text{ trifluoroacetate salt.}
$^{31}$P NMR spectrum of *meso* phosphonated BODIPY dye 10 (TBA$^+$ salt) recorded in DMSO-$d_6$ at 121.4 MHz.

(ESI+) mass spectrum of *meso* phosphonated BODIPY dye 10.
(ESI-) mass spectrum (low resolution) of \textit{meso} phosphonated BODIPY dye 10.

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Normalised absorption (—), emission (—) and excitation (—) spectra of \textit{meso} phosphonated BODIPY dye 10 in PBS at 25 °C.
\( ^1\)H NMR spectrum of \( N \)-benzoyloxy succinamic acid derivative 11 recorded in CDCl\(_3\) at 300 MHz.

\( ^{13}\)C NMR spectrum of \( N \)-benzoyloxy succinamic acid derivative 11 recorded in CDCl\(_3\) at 75.5 MHz.\(^a\)

\(^a\) this compound was isolated in a too small amount for visualisation of quaternary carbons C=O (3C).
(ESI+) mass spectrum of $N$-benzoyloxy succinamic acid derivative 11.

(ESI-) mass spectrum (low resolution) of $N$-benzoyloxy succinamic acid derivative 11.
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RP-HPLC elution profile (system A) of N-benzoyloxy succinamic acid derivative 11.
Normalised absorption (—), emission (—) and excitation (—) spectra of N-benzoyloxy succinamic acid derivative 11 in PBS at 25 °C.

$^1$H NMR spectrum of *meso* glyphosate BODIPY dye 12 (TBA$^+$ salt) recorded in DMSO-$d_6$ at 300 MHz.
$^{13}$C NMR spectrum of *meso* glyphosate BODIPY dye 12 (TBA$^+$ salt) recorded in DMSO-$d_6$ at 75.5 MHz.

$^{31}$P NMR spectrum of *meso* glyphosate BODIPY dye 12 (TBA$^+$ salt) recorded in DMSO-$d_6$ at 121.4 MHz.
(ESI+) mass spectrum of *meso* glyphosate BODIPY dye 12.

(ESI-) mass spectrum (low resolution) of *meso* glyphosate BODIPY dye 12.
(ESI-) mass spectrum (high resolution) of *meso* glyphosate BODIPY dye 12.

RP-HPLC elution profile (system A) of *meso* glyphosate BODIPY dye 12.