NIR-Emitting Benzothiazolium Cyanines with Enhanced Stokes Shift for Mitochondria Imaging in Live Cells

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Supporting Information
**Figure S1.1** $^1$H NMR spectra of 3a (300 MHz in DMSO: MeOH 95:5)

**Figure S1.2** $^1$H NMR spectra of 3b (300 MHz in DMSO: MeOH 95:5)
Figure S1.3 $^1$H NMR spectra of 3c (300 MHz in DMSO: EtOH 95:5)

Figure S1.4 $^1$H NMR spectra of 3d (300 MHz in DMSO)
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Figure S3.2 Absorbance and fluorescence emission spectra obtained for 3b (1x10⁻⁵ M) in different solvents at room temperature.
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**Figure S3.4** Absorbance and fluorescence emission spectra obtained for 3d (1x10^{-5} M) in different solvents at room temperature.
Figure S3.5 Absorbance and fluorescence emission spectra obtained for 3e (1x10^{-5} M) in different solvents at room temperature.

Figure S3.6 Absorbance and fluorescence emission spectra obtained for 3f (1x10^{-5} M) in different solvents at room temperature.
<table>
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<td>521</td>
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<td>528</td>
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<tr>
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<td>528</td>
<td>603 (0.0017)</td>
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<tr>
<td>3e</td>
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<td>607 (0.021)</td>
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<td>612</td>
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<td>612 (0.012)</td>
<td>43</td>
<td>546</td>
<td>616</td>
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<td>538</td>
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**Table S1.** Optical properties obtained for 3a – 3f.
Figure S4.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3a (200 nM) for 1 hour. From left to right images show the fluorescence 3a (a), bright field (b) and overlapped image (c) respectively. 640 nm laser was used for excitation.

Figure S4.2 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3a (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence 3a (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/640 nm lasers were used for excitation.
Figure S5.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3b (200 nM) for 1 hour. From left to right images show the fluorescence 3b (a), bright field (b) and overlapped image (c) respectively. 640 nm laser was used for excitation.

Figure S5.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3b (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence 3b (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/640 nm lasers were used for excitation.
Figure S6.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3c (200 nM) for 1 hour. From left to right images show the fluorescence 3c (a), bright field (b) and overlapped image (c) respectively. 561 nm laser was used for excitation.

Figure S6.2 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3c (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence 3c (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/561 nm lasers were used for excitation.
Figure S7.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3d (200 nM) for 1 hour. From left to right images show the fluorescence 3d (a), bright field (b) and overlapped image (c) respectively. 561 nm laser was used for excitation.

Figure S7.2 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3d (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence 3d (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/561 nm lasers were used for excitation.
Figure S8.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3e (200 nM) for 1 hour. From left to right images show the fluorescence 3e (a), bright field (b) and overlapped image (c) respectively. 561 nm laser was used for excitation.

Figure S8.2 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3e (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence 3e (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/561 nm lasers were used for excitation.
Figure S9.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3f (200 nM) for 1 hour. From left to right images show the fluorescence 3f (a), bright field (b) and overlapped image (c) respectively. 561 nm laser was used for excitation.

Figure S9.2 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3f (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence 3f (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/561 nm lasers were used for excitation.
**Figure S10** Fluorescent confocal microscopy images of human ovarian fibroblast cells (HOF) cells treated with \(3a\) (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence \(3a\) (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/640 nm lasers were used for excitation.
Figure S11 Fluorescent confocal microscopy images of human ovarian fibroblast cells (HOF) cells treated with 3b (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence 3b (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/640 nm lasers were used for excitation.
Figure S12 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with 3a (200 nM) for a period of 2.5 hour. 640 nm laser was used for excitation.
Figure S13 Cell viability results (bar-chart) obtained for 3a, 3b, 3c and 3d by MTT cell viability assay.
Figure S14  Cell viability results (cell viability curve) obtained for 3a, 3b, 3c and 3d by MTT cell viability assay.
Figure S15 Absorbance (a) and fluorescence emission (b) spectra obtained for 3a (1x10^-5 M) in different pH conditions at room temperature.
Figure S16 Fluorescent confocal microscopy images of MO3.13 cells (x100) obtained in the absence of any probe with 561 nm laser (a – b) and 640 nm laser (c – d) and treated with 3a (200 nM) for 30 minutes. 640 nm laser was used for 3a excitation.