Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

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

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Supporting Information

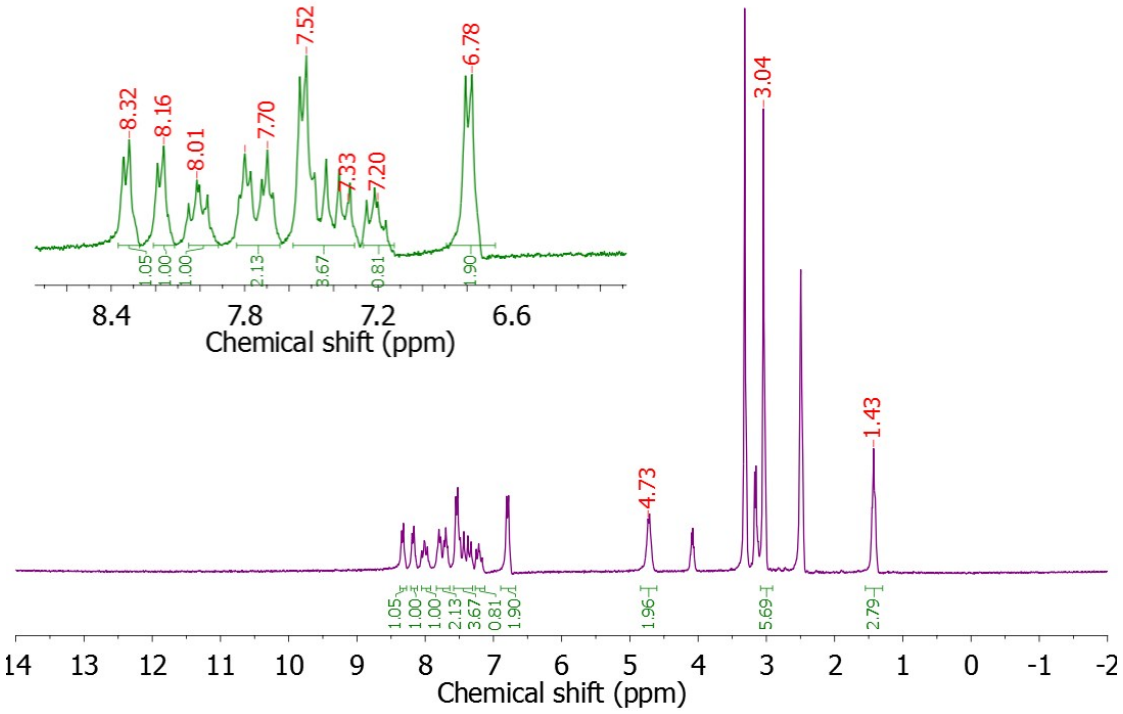


Figure S1.1 [1]H NMR spectra of **3a** (300 MHz in DMSO: MeOH 95:5)

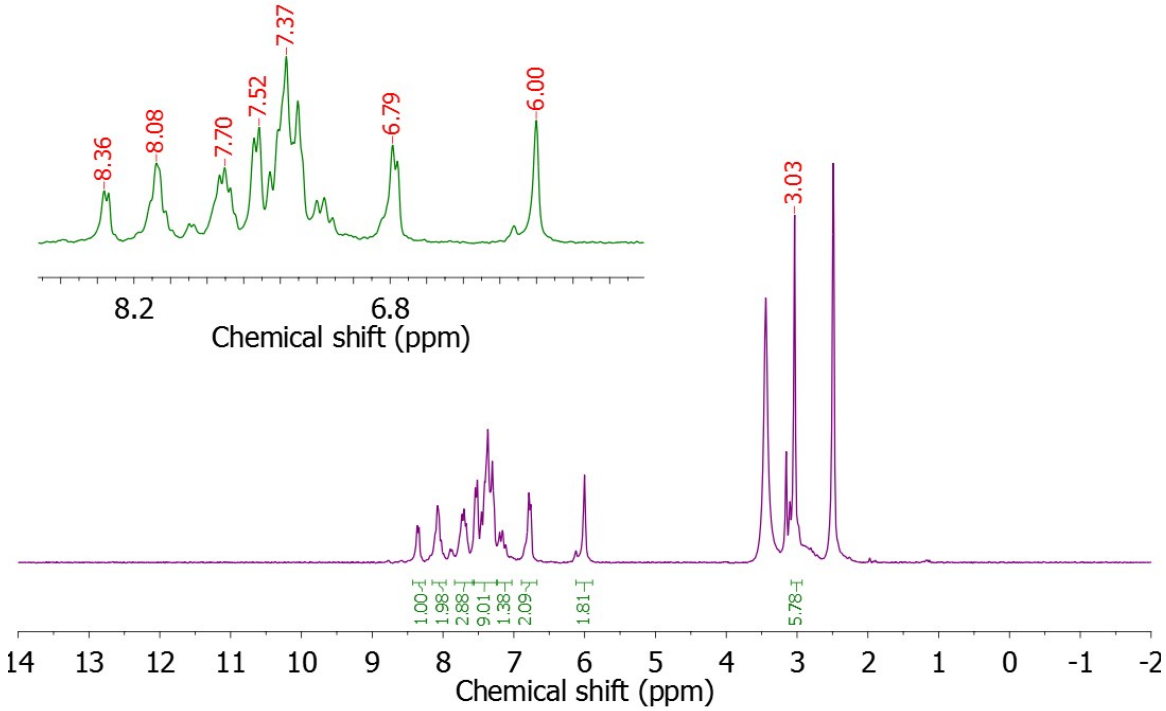


Figure S1.2 [1]H NMR spectra of **3b** (300 MHz in DMSO: MeOH 95:5)

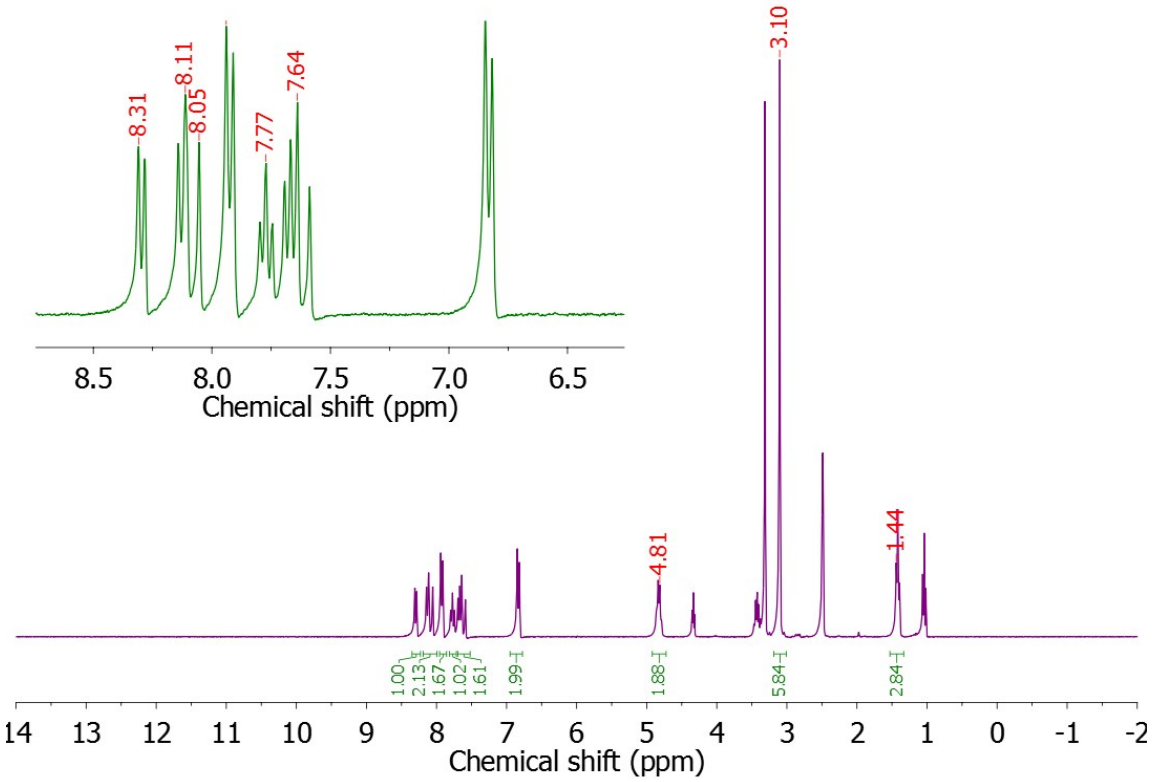


Figure S1.3 [1]H NMR spectra of **3c** (300 MHz in DMSO: EtOH 95:5)

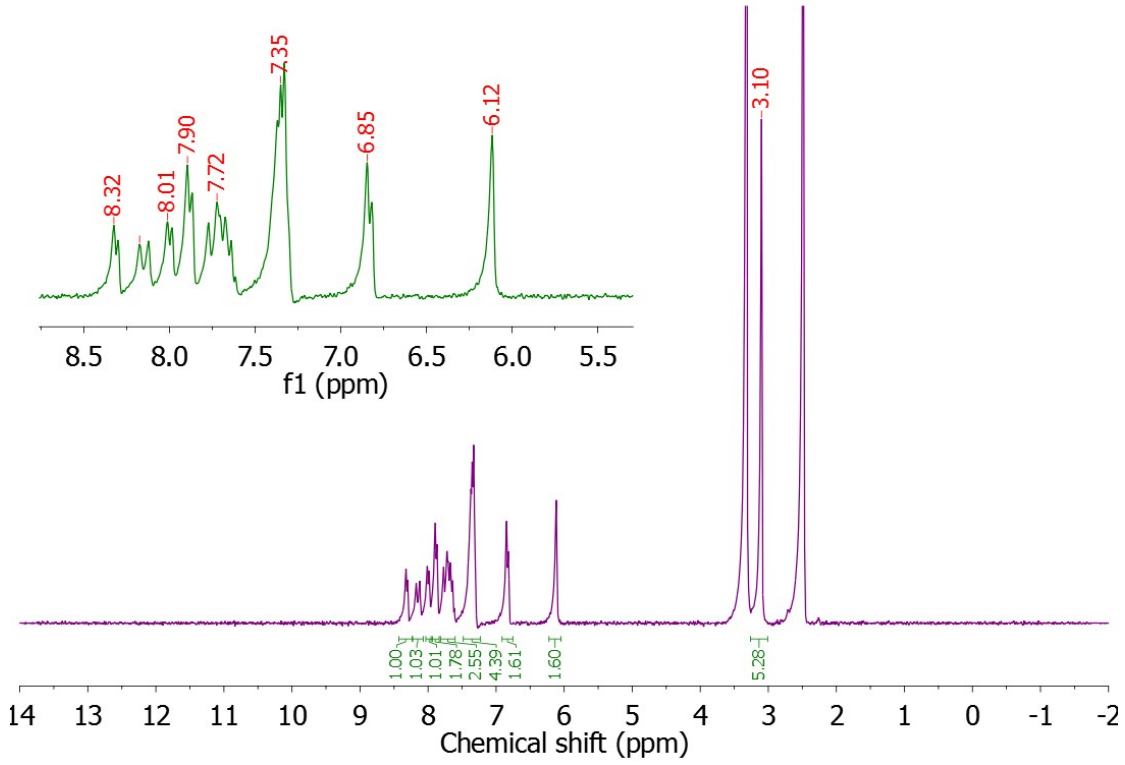


Figure S1.4 [1]H NMR spectra of **3d** (300 MHz in DMSO)

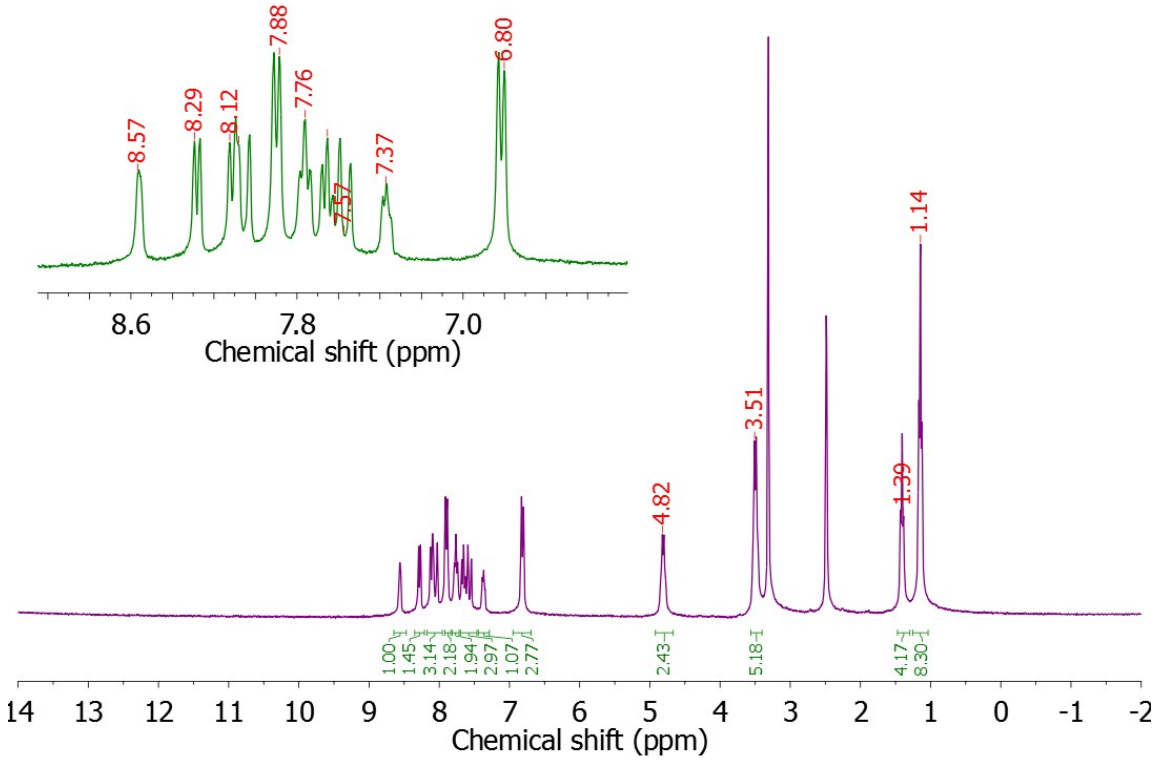


Figure S1.5 ^{1}H NMR spectra of **3e** (300 MHz in DMSO)

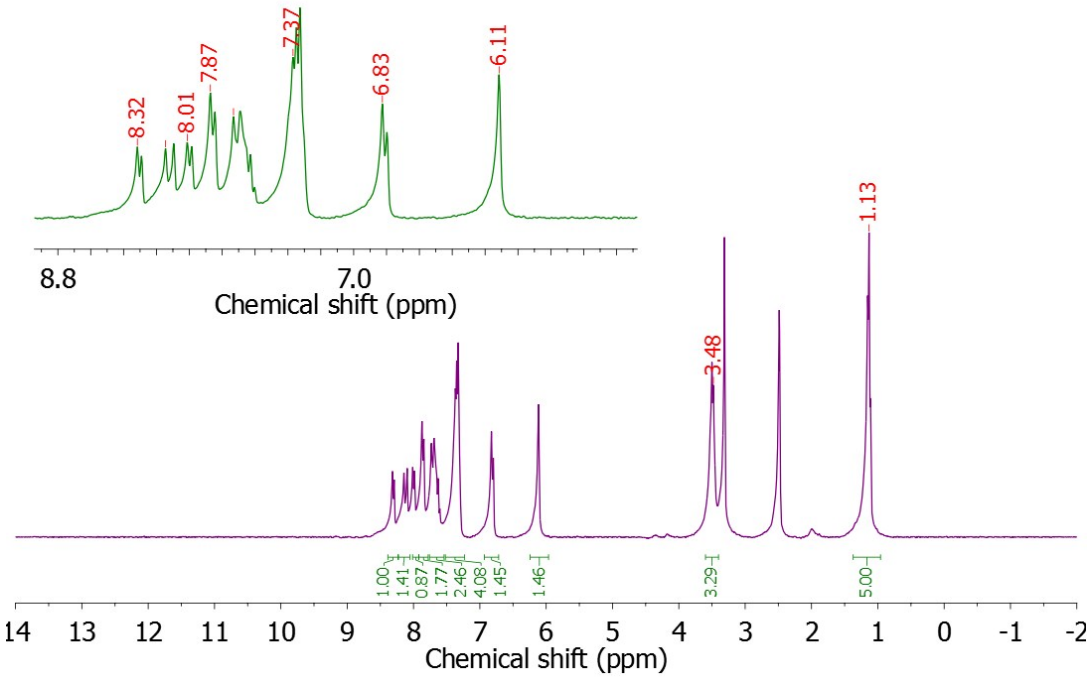


Figure S1.6 ^{1}H NMR spectra of **3f** (300 MHz in DMSO)

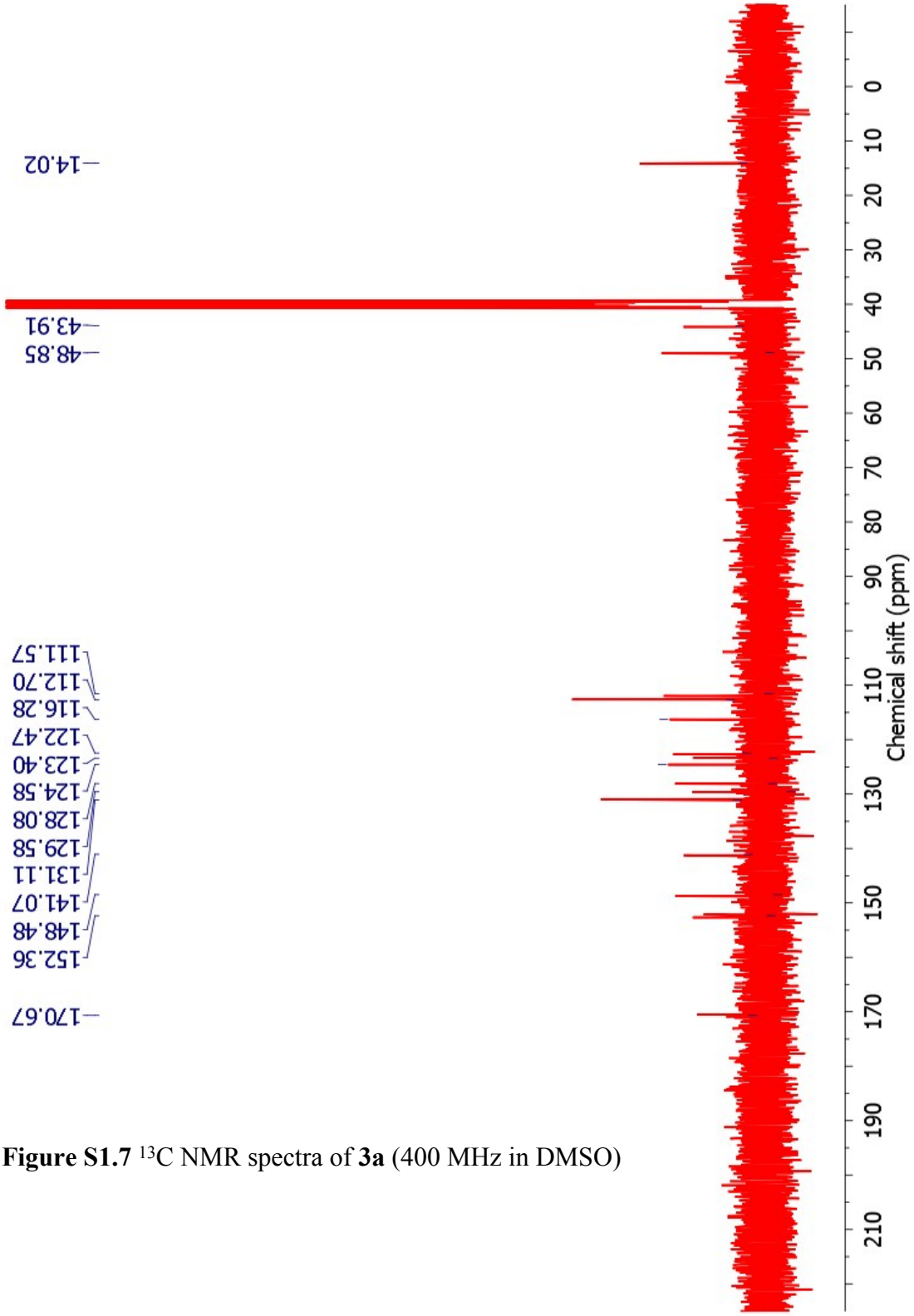


Figure S1.7 ^{13}C NMR spectra of **3a** (400 MHz in DMSO)

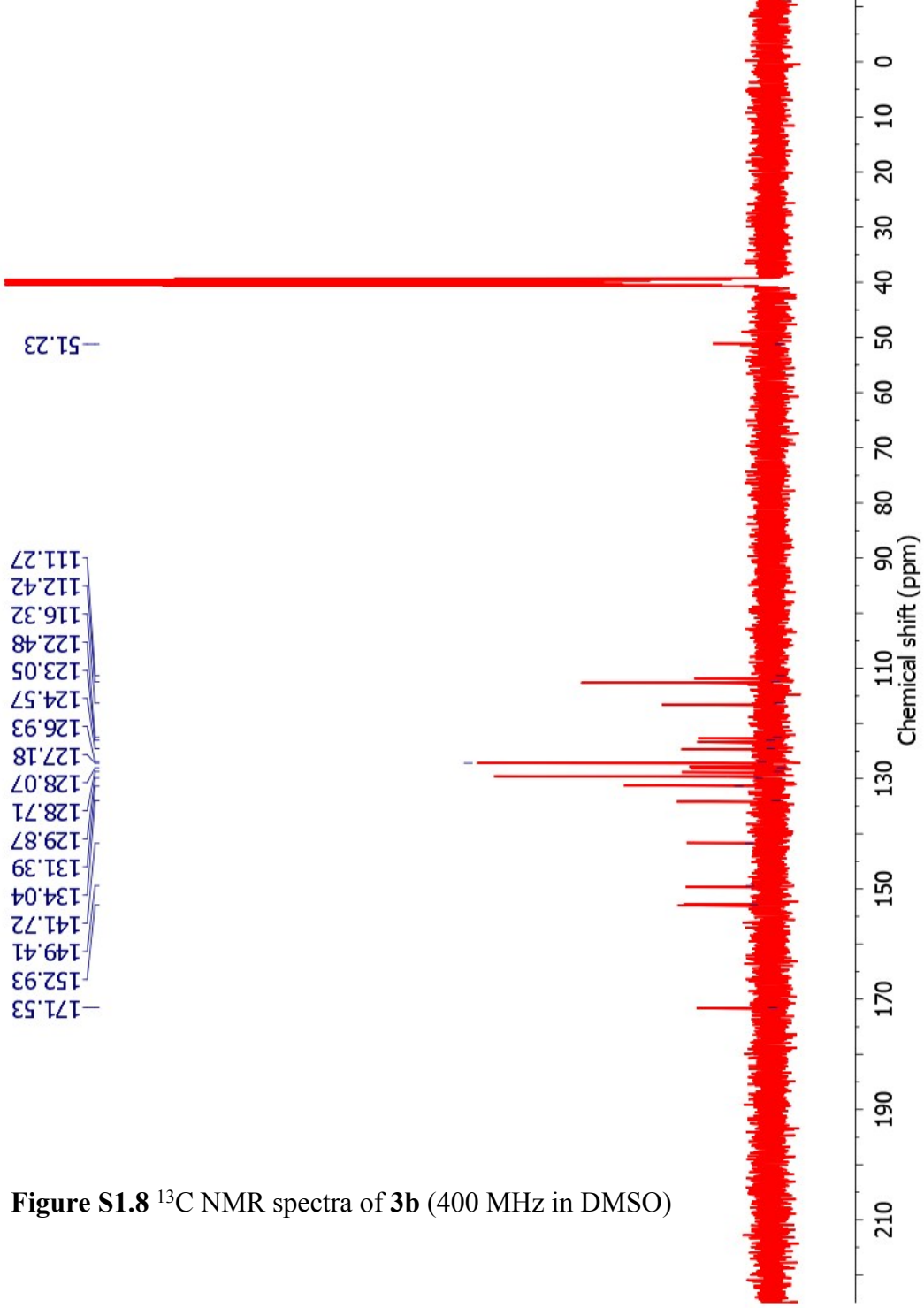


Figure S1.8 ^{13}C NMR spectra of **3b** (400 MHz in DMSO)

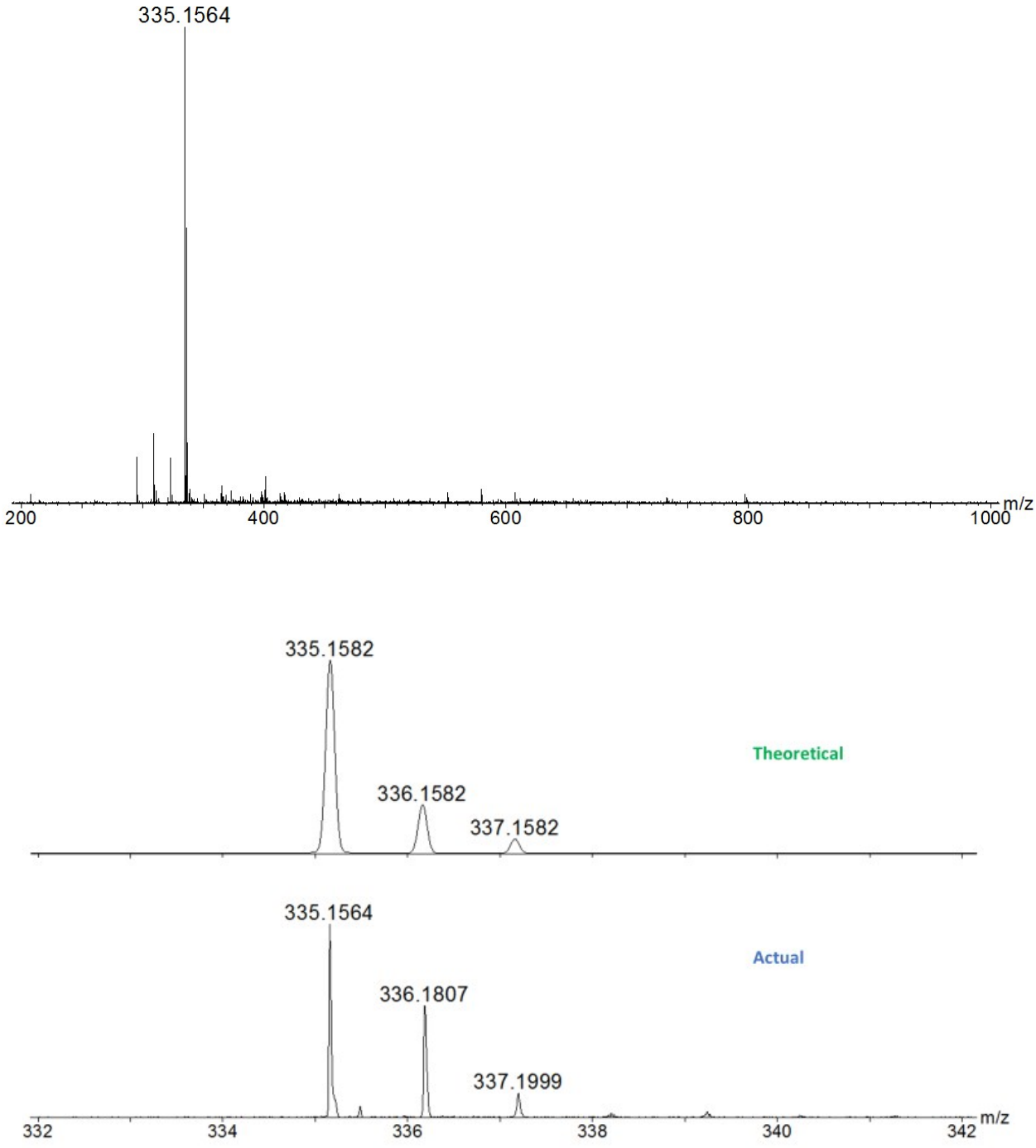


Figure S2.1 Mass spectra of **3a**

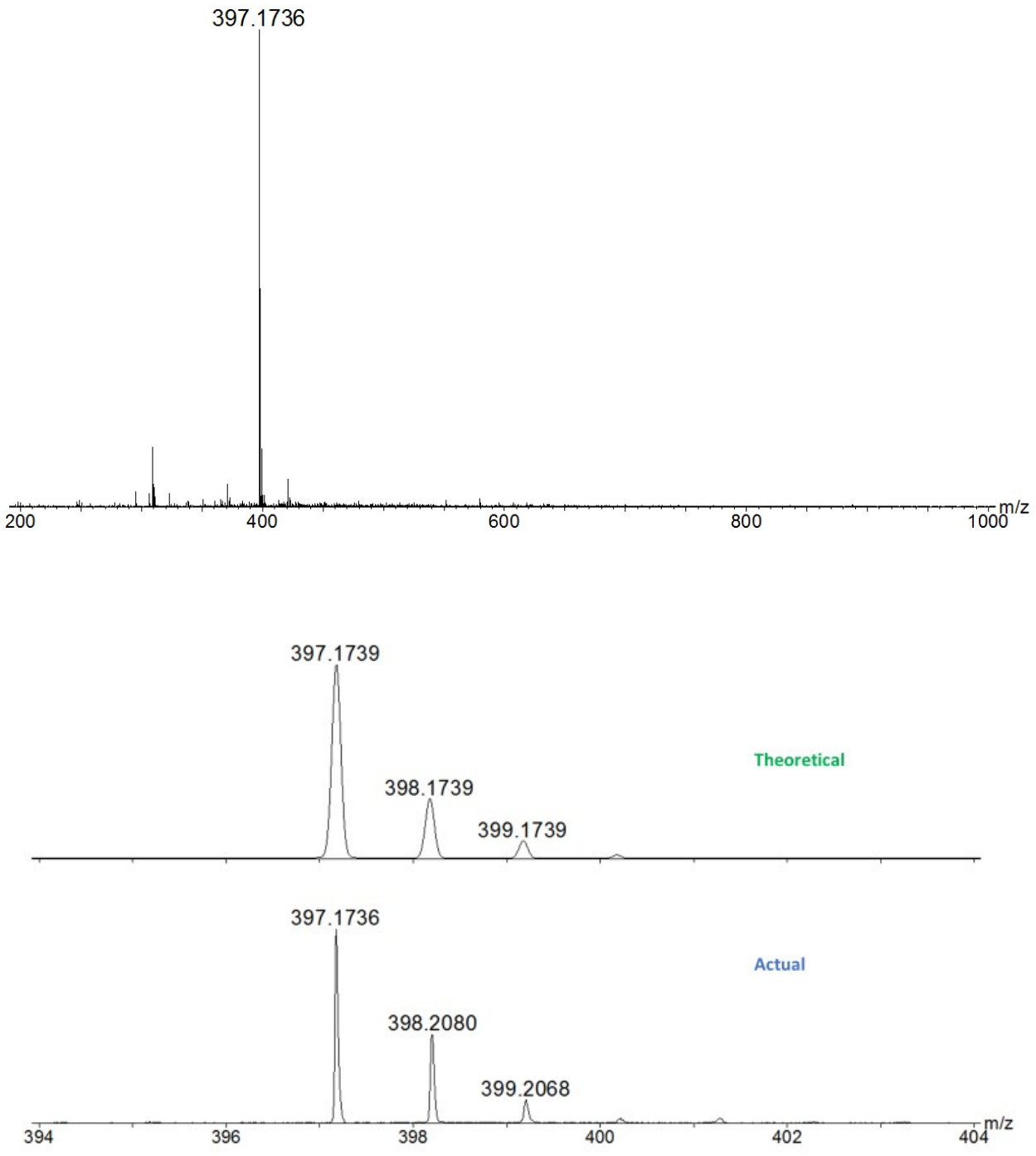


Figure S2.2 Mass spectra of **3b**

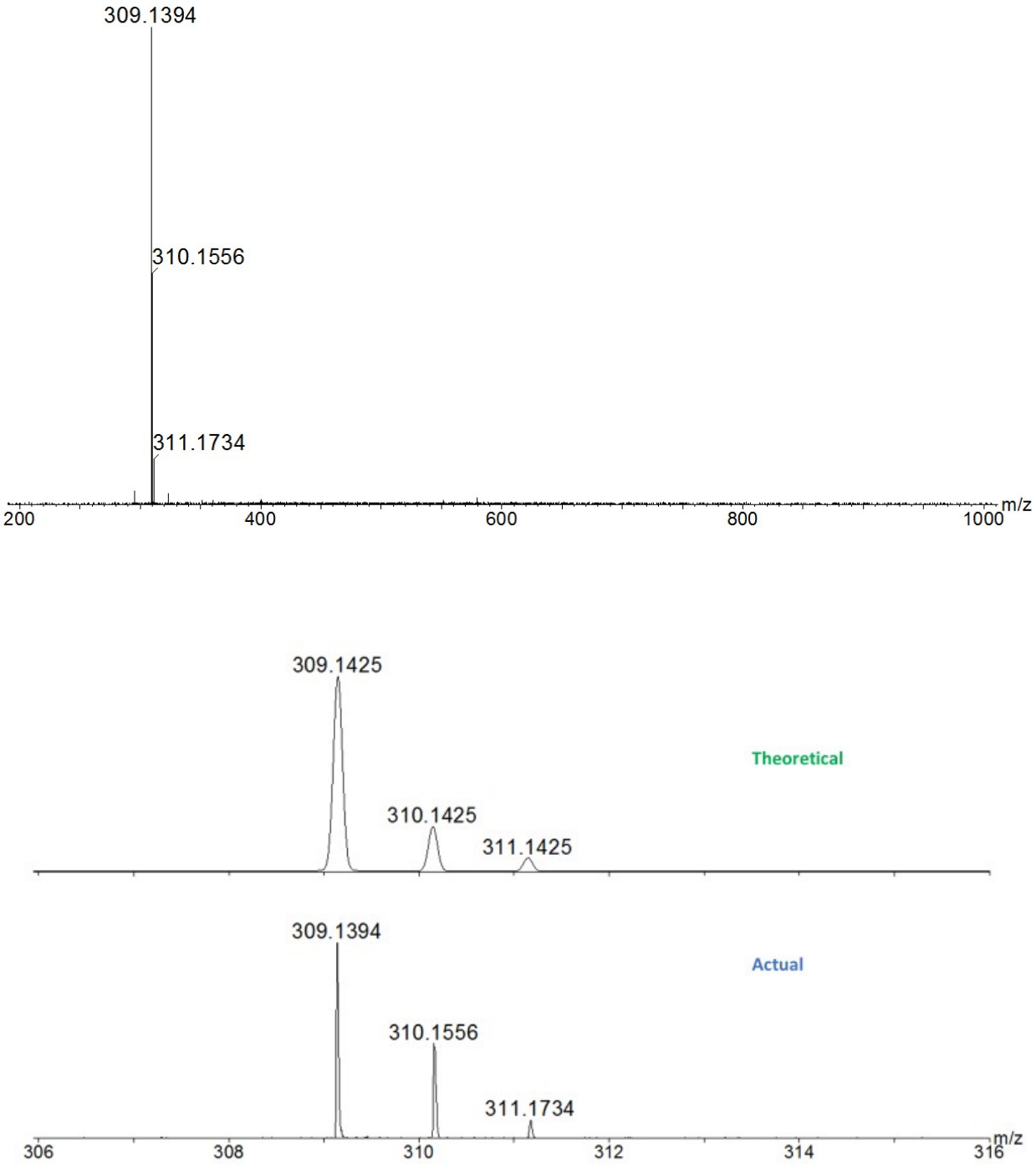


Figure S2.3 Mass spectra of **3c**

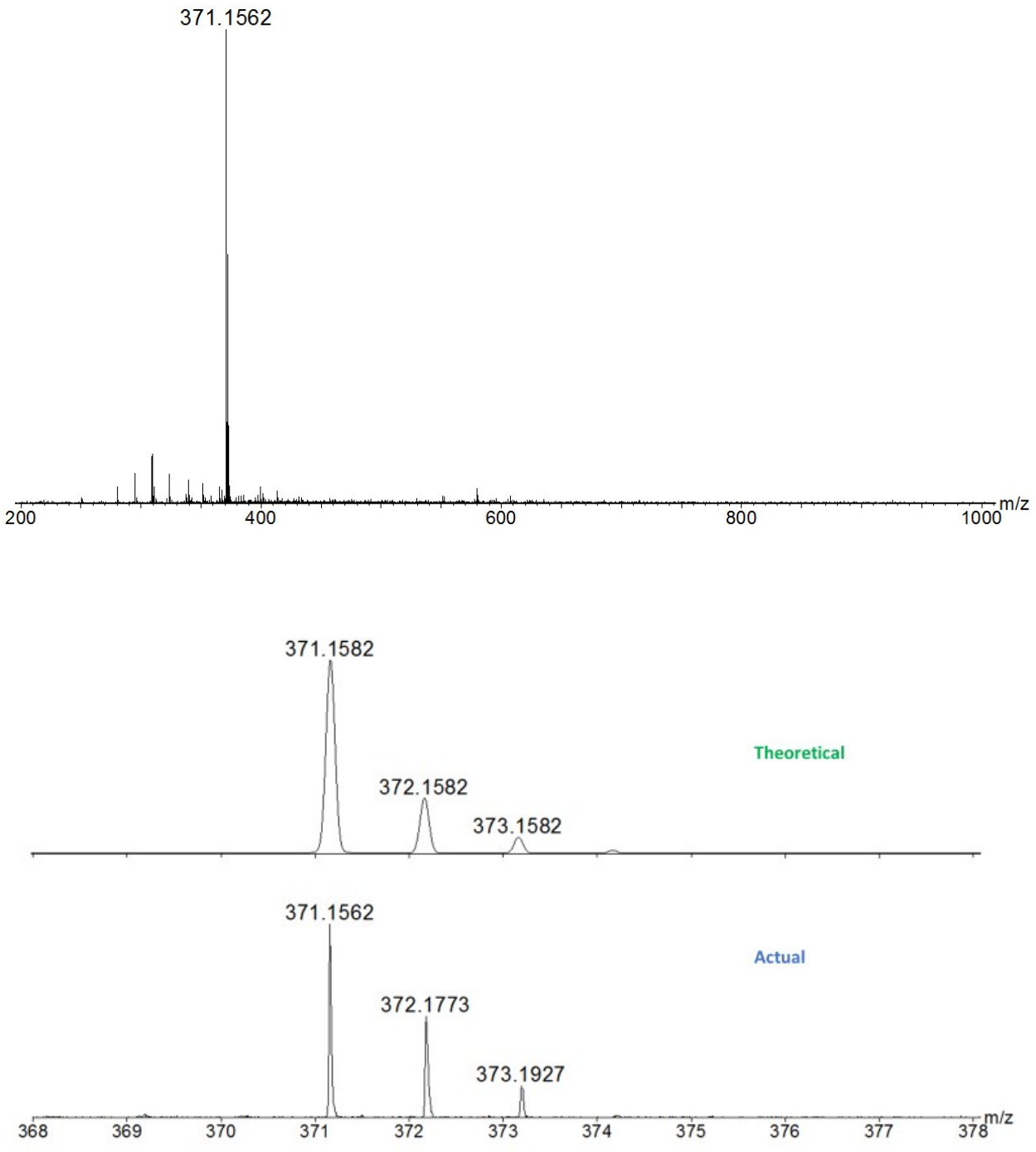


Figure S2.4 Mass spectra of **3d**

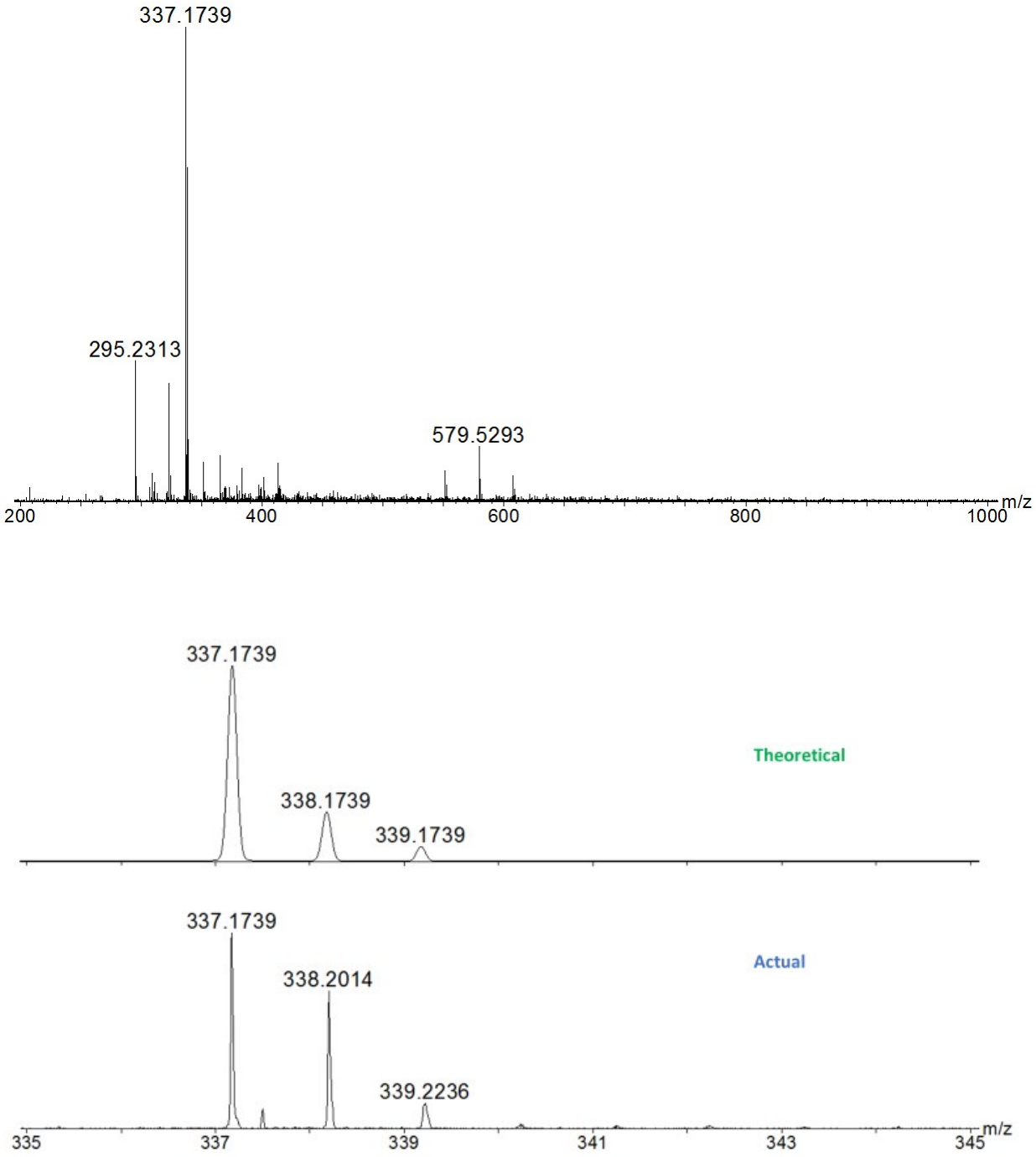


Figure S2.5 Mass spectra of **3e**

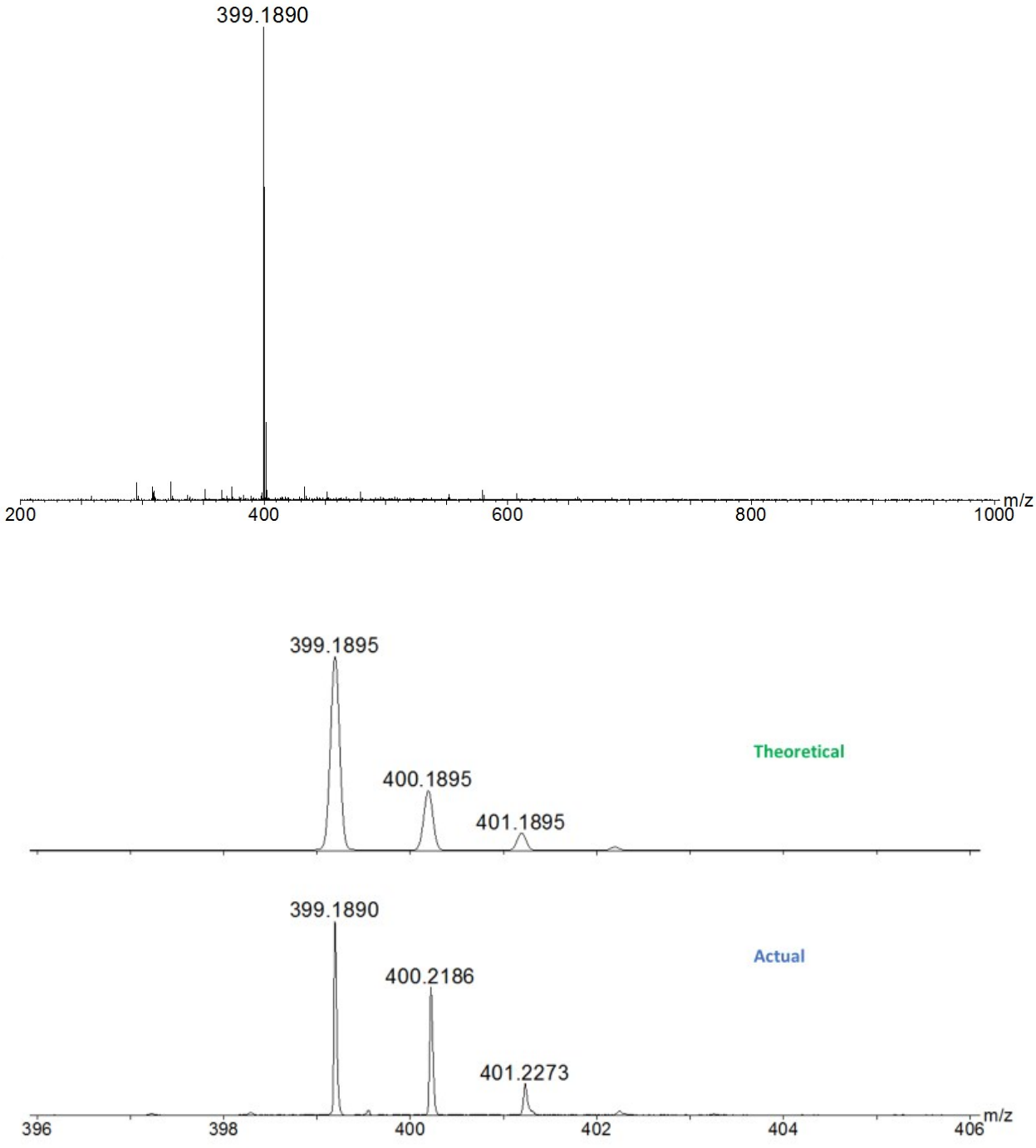


Figure S2.6 Mass spectra of **3f**

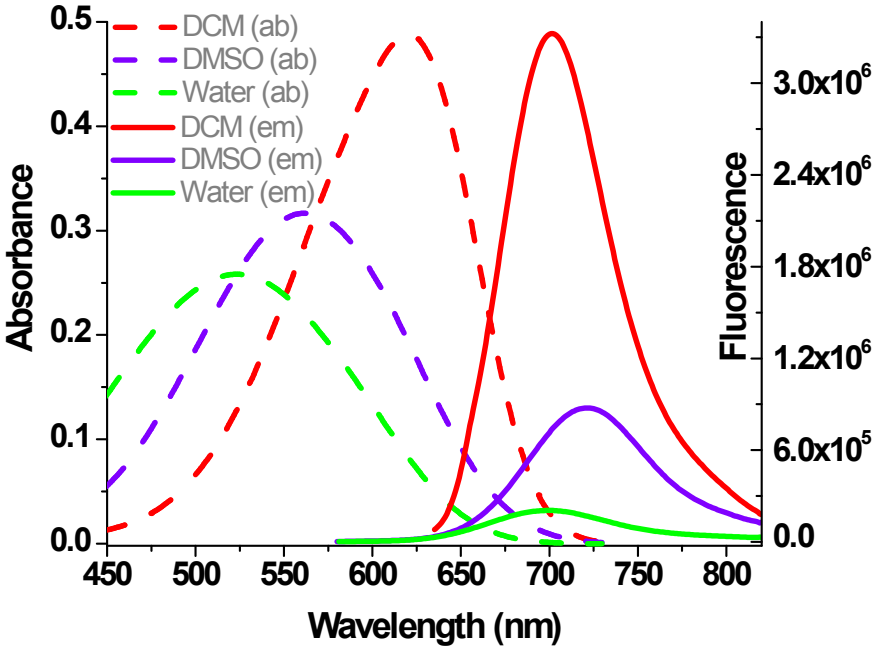


Figure S3.1 Absorbance and fluorescence emission spectra obtained for **3a** ($1x10^{-5}$ M) in different solvents at room temperature.

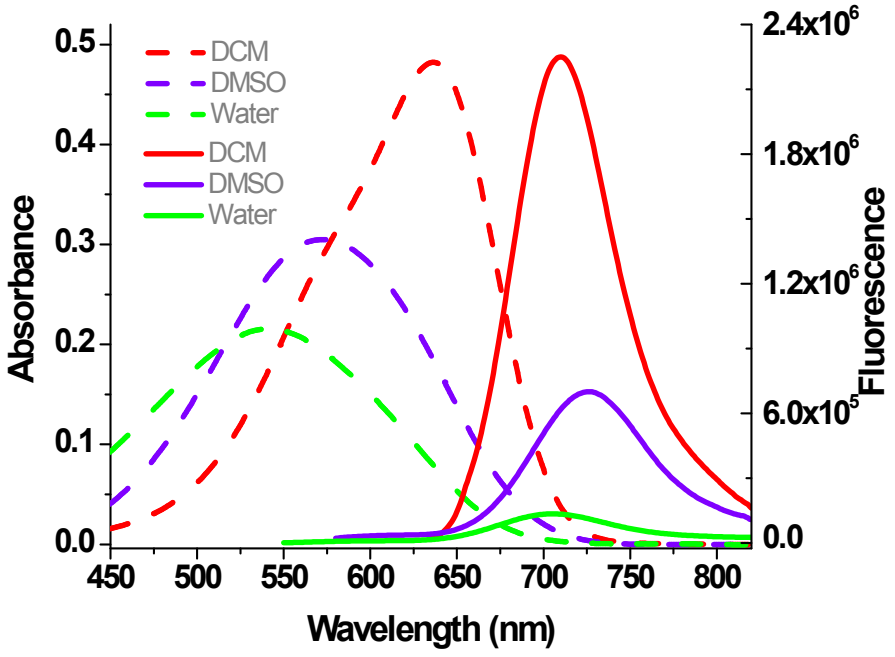


Figure S3.2 Absorbance and fluorescence emission spectra obtained for **3b** ($1x10^{-5}$ M) in different solvents at room temperature.

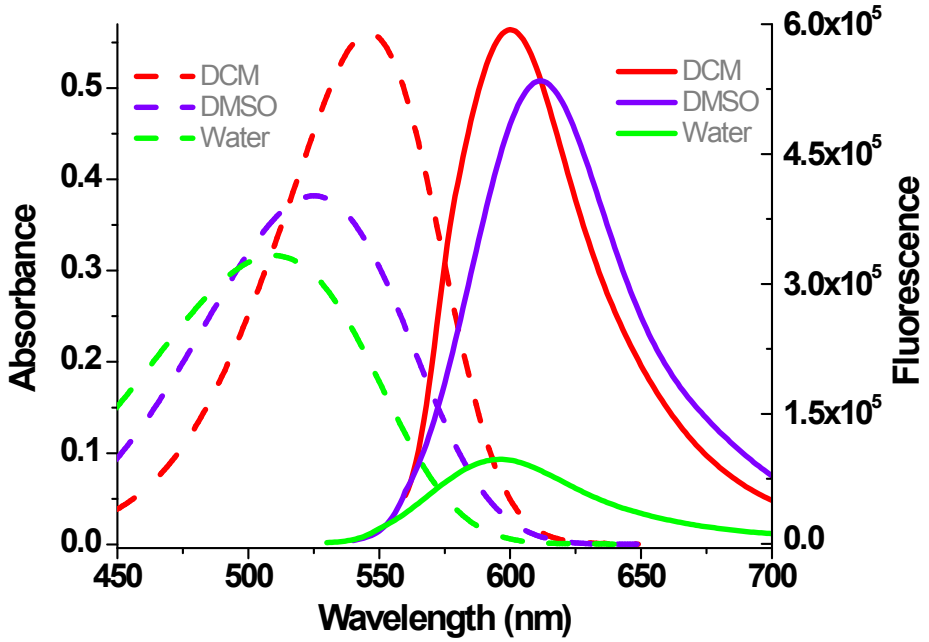


Figure S3.3 Absorbance and fluorescence emission spectra obtained for **3c** ($1x10^{-5}$ M) in different solvents at room temperature.

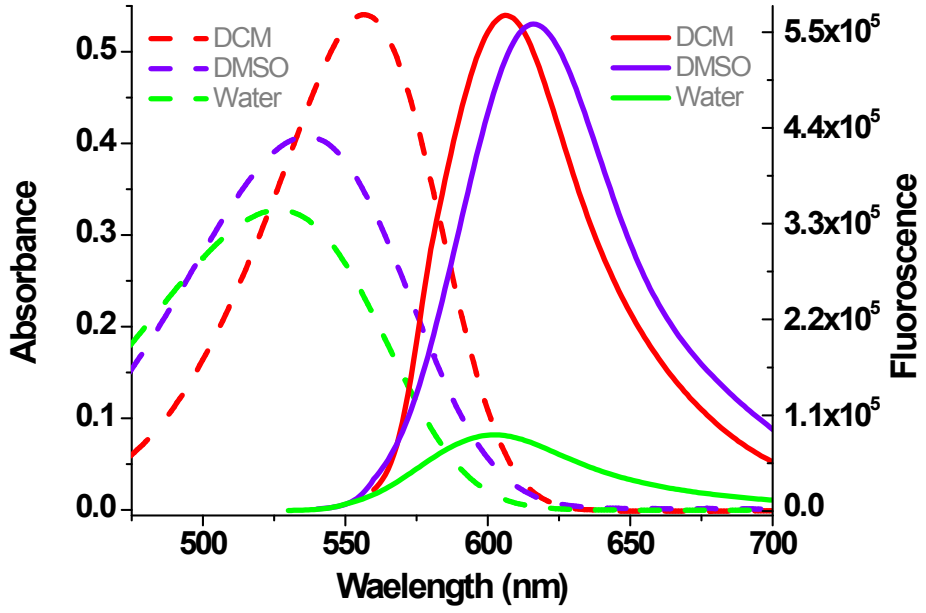


Figure S3.4 Absorbance and fluorescence emission spectra obtained for **3d** ($1x10^{-5}$ M) in different solvents at room temperature.

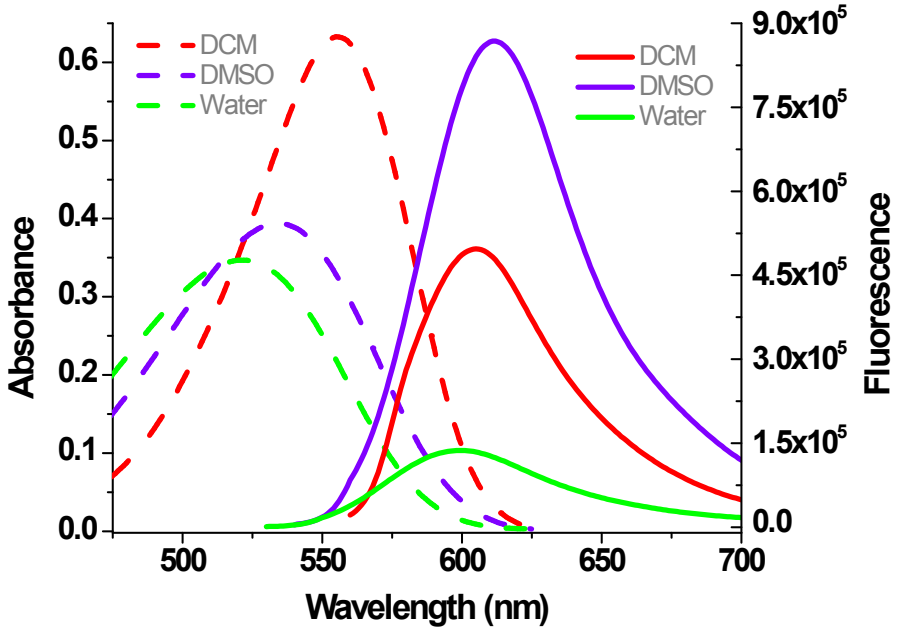


Figure S3.5 Absorbance and fluorescence emission spectra obtained for **3e** ($1x10^{-5}$ M) in different solvents at room temperature.

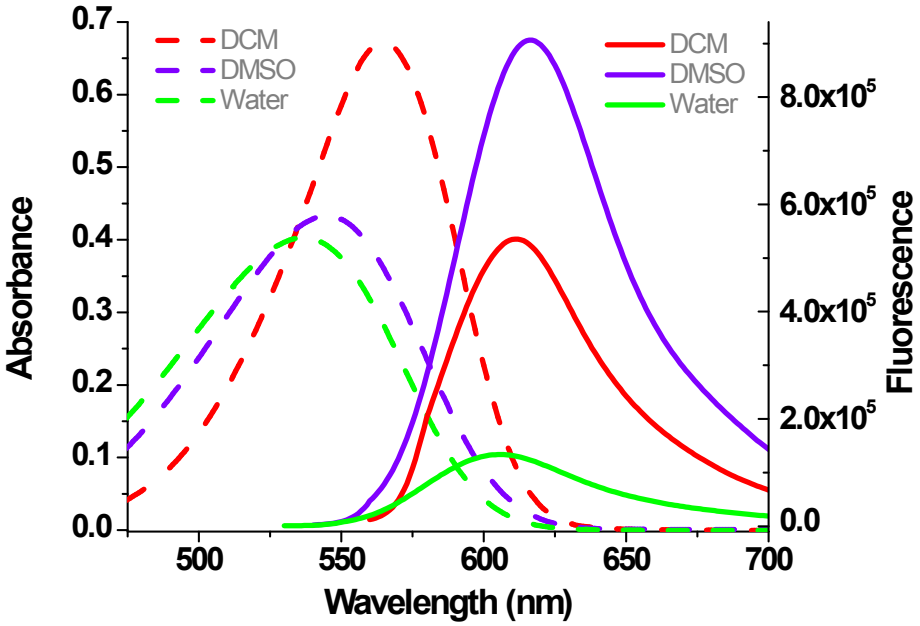


Figure S3.6 Absorbance and fluorescence emission spectra obtained for **3f** ($1x10^{-5}$ M) in different solvents at room temperature.

	DCM			DMSO			Water		
Entry	λ_{abs} (nm)	λ_{em} (Φ_{fl}) (nm)	$\Delta\lambda$ (nm)	λ_{abs} (nm)	λ_{em} (Φ_{fl}) (nm)	$\Delta\lambda$ (nm)	λ_{abs} (nm)	λ_{em} (Φ_{fl}) (nm)	$\Delta\lambda$ (nm)
3a	620	702 (**0.077**)	**82**	562	712	**150**	521	699 (**0.0046**)	**178**
3b	636	712 (**0.044**)	**76**	572	726	**154**	541	706 (**0.0035**)	**165**
3c	546	601 (**0.011**)	**55**	528	612	**84**	513	598 (**0.0025**)	**85**
3d	556	608 (**0.014**)	**52**	537	616	**79**	528	603 (**0.0017**)	**75**
3e	554	607 (**0.021**)	**53**	538	612	**74**	523	601 (**0.0024**)	**73**
3f	564	612 (**0.012**)	**43**	546	616	**70**	538	609 (**0.0024**)	**71**

Table S1. Optical properties obtained for **3a** – **3f**.

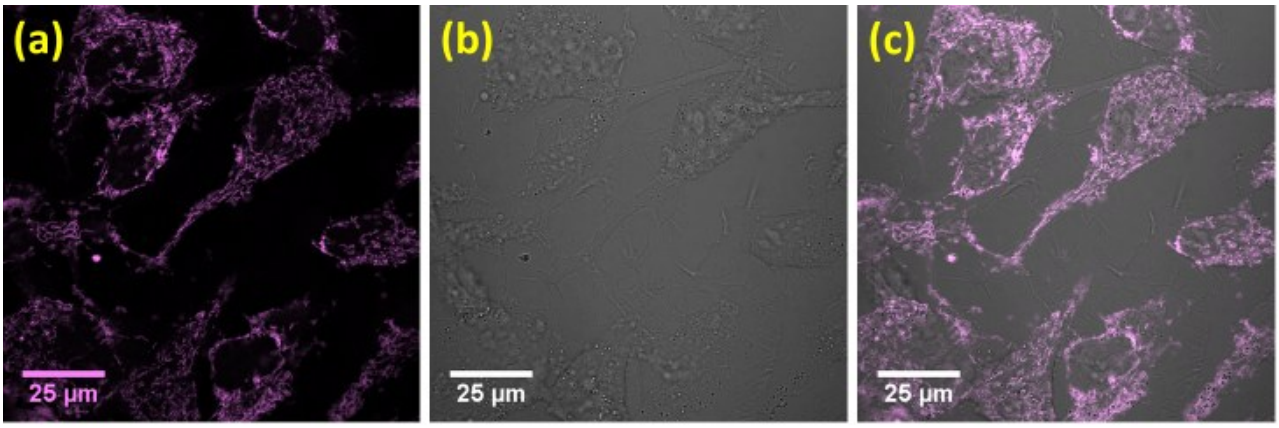


Figure S4.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3a** (200 nM) for 1 hour. From left to right images show the fluorescence **3a** (a), bright field (b) and overlapped image (c) respectively. 640 nm laser was used for excitation.

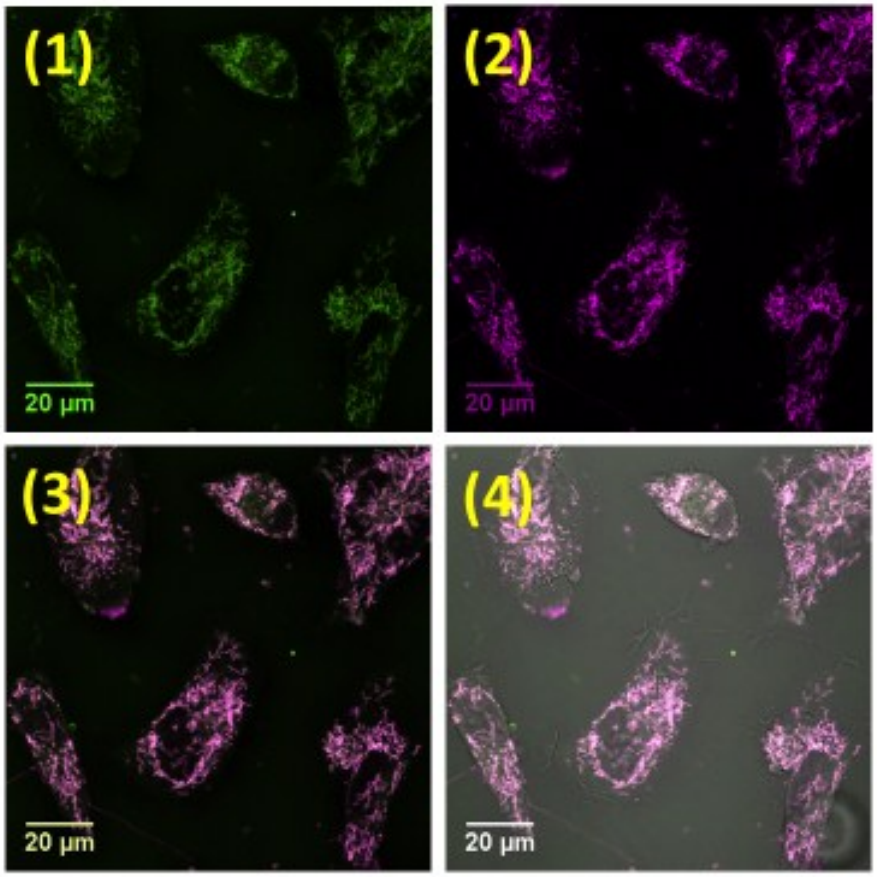


Figure S4.2 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3a** (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence **3a** (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/640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

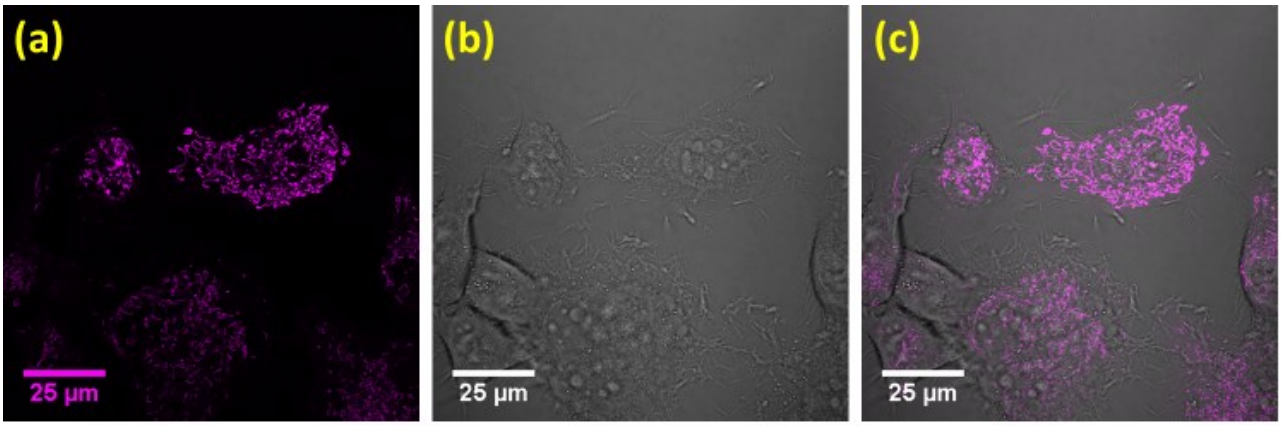


Figure S5.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3b** (200 nM) for 1 hour. From left to right images show the fluorescence **3b** (a), bright field (b) and overlapped image (c) respectively. 640 nm laser was used for excitation.

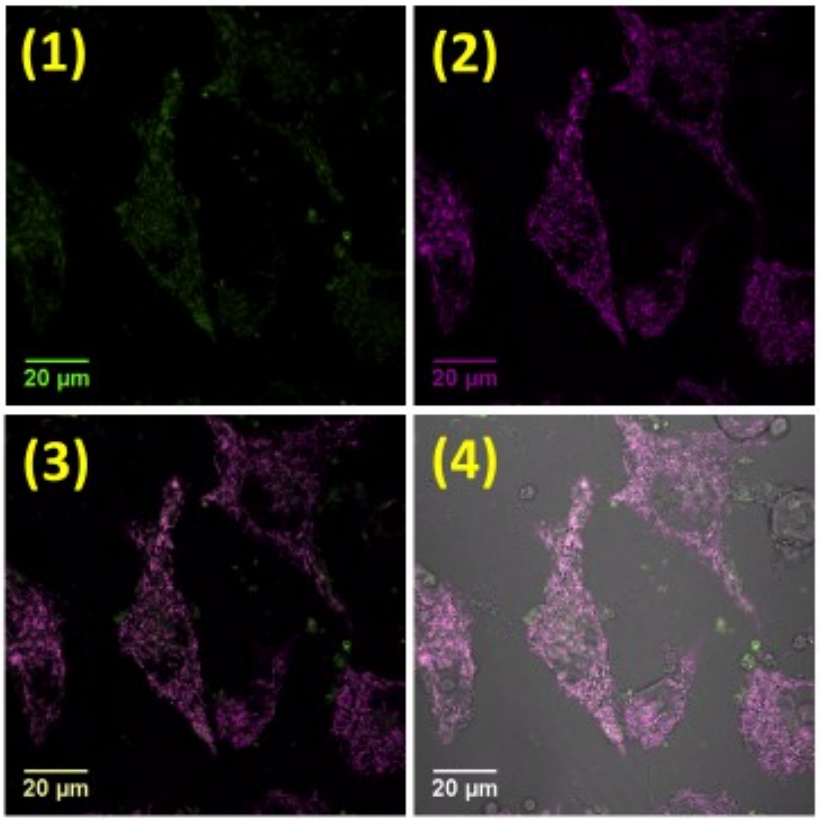


Figure S5.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3b** (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence **3b** (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/640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

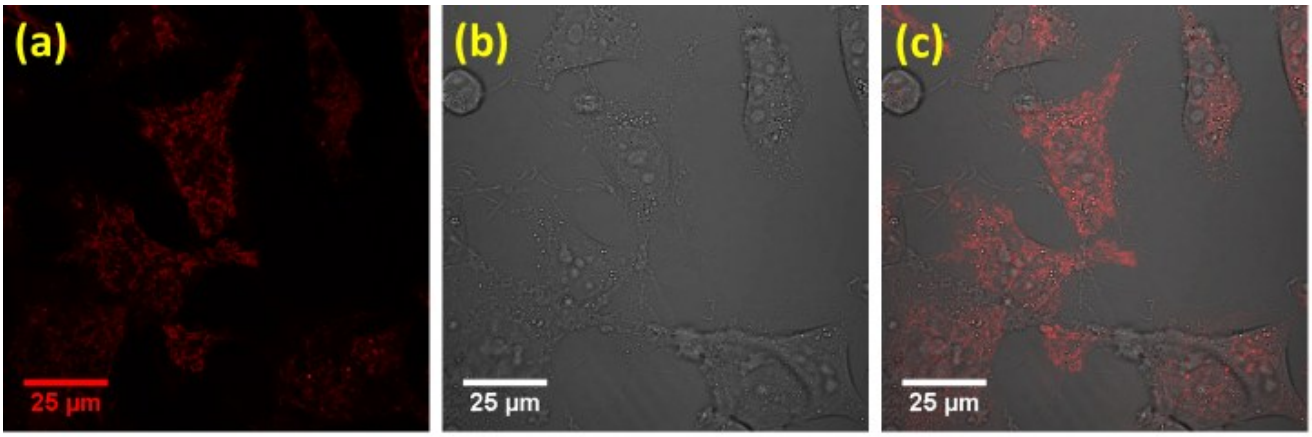


Figure S6.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3c** (200 nM) for 1 hour. From left to right images show the fluorescence **3c** (a), bright field (b) and overlapped image (c) respectively. 561 nm laser was used for excitation.

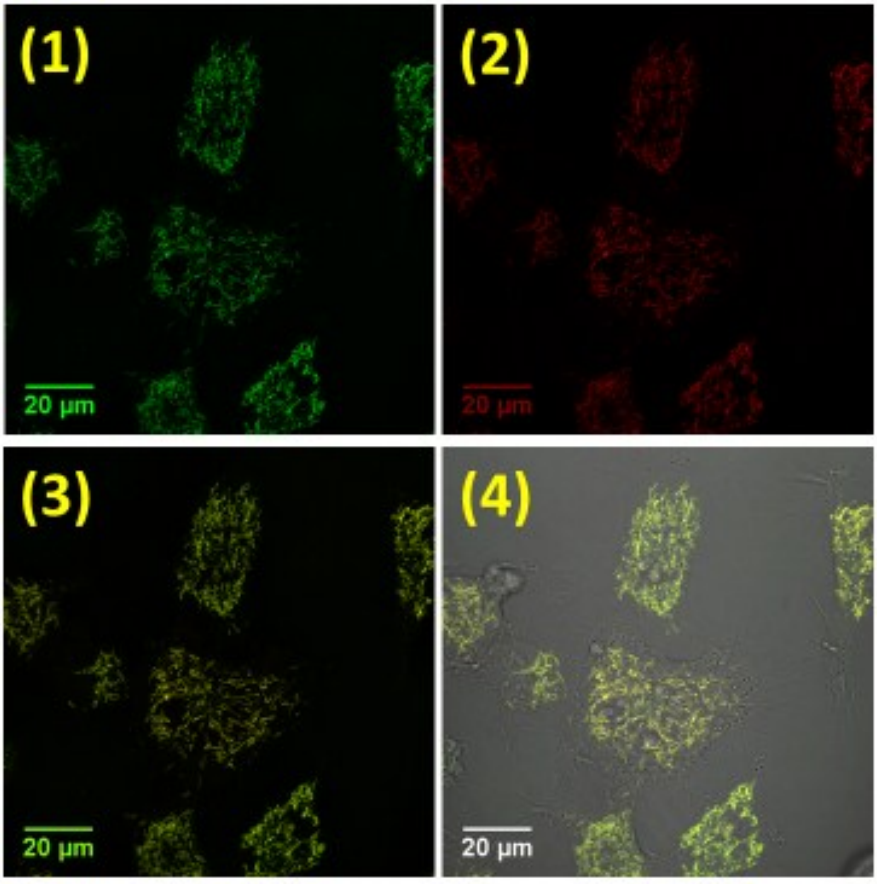


Figure S6.2 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3c** (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence **3c** (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/561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

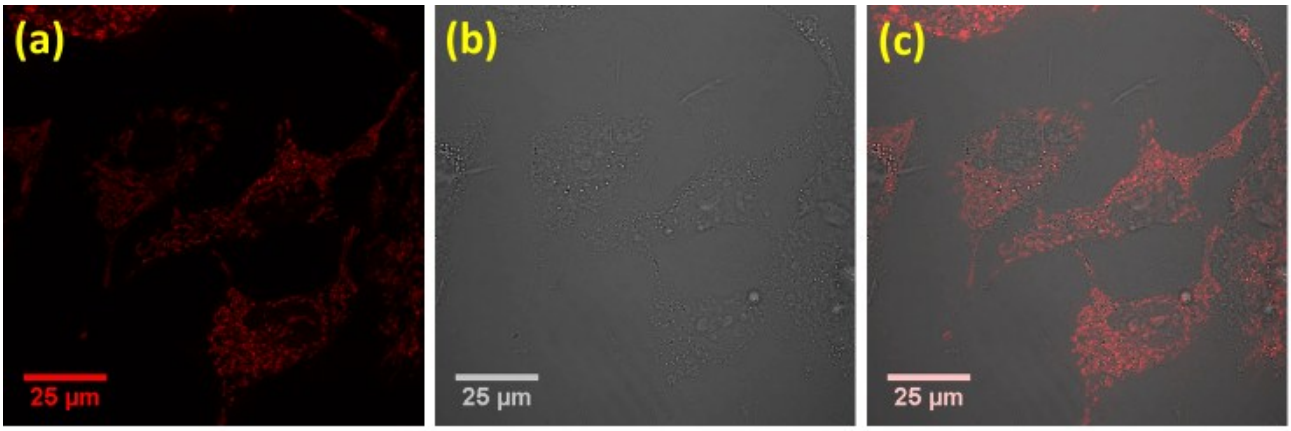


Figure S7.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3d** (200 nM) for 1 hour. From left to right images show the fluorescence **3d** (a), bright field (b) and overlapped image (c) respectively. 561 nm laser was used for excitation.

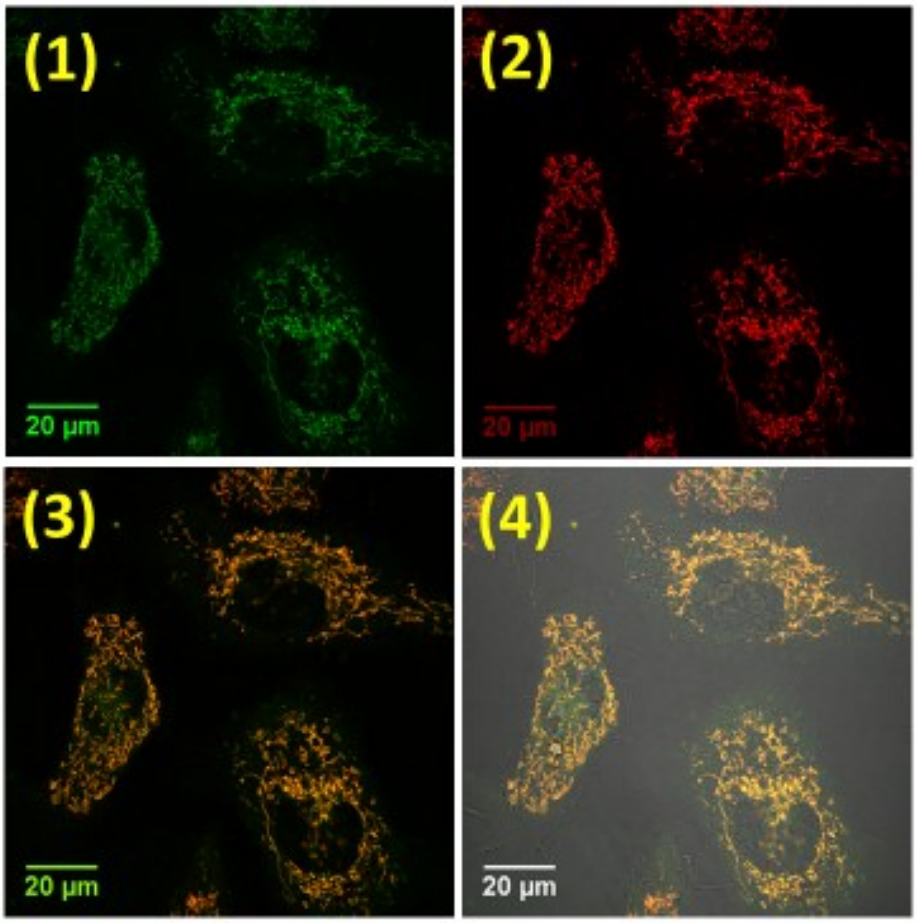


Figure S7.2 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3d** (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence **3d** (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/561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

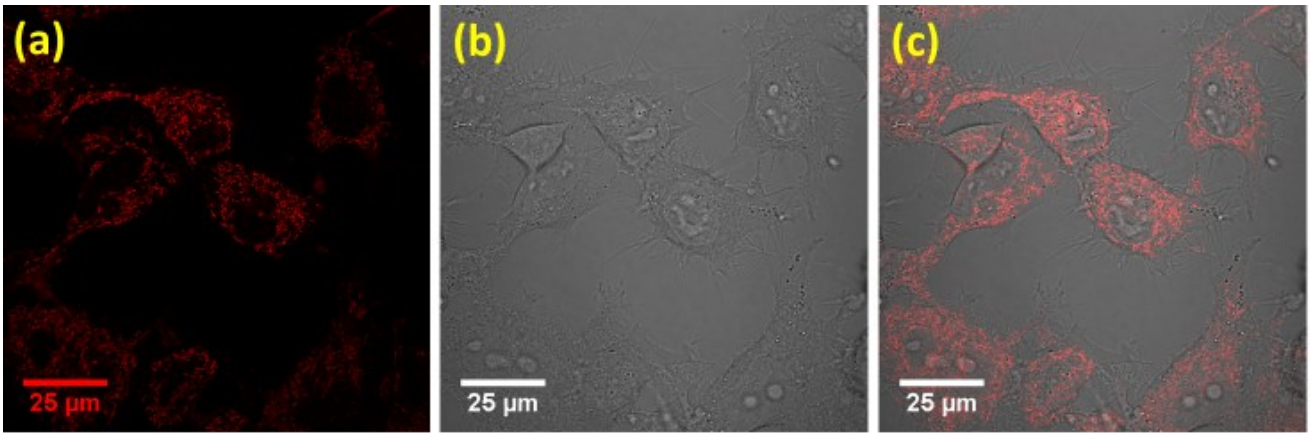


Figure S8.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3e** (200 nM) for 1 hour. From left to right images show the fluorescence **3e** (a), bright field (b) and overlapped image (c) respectively. 561 nm laser was used for excitation.

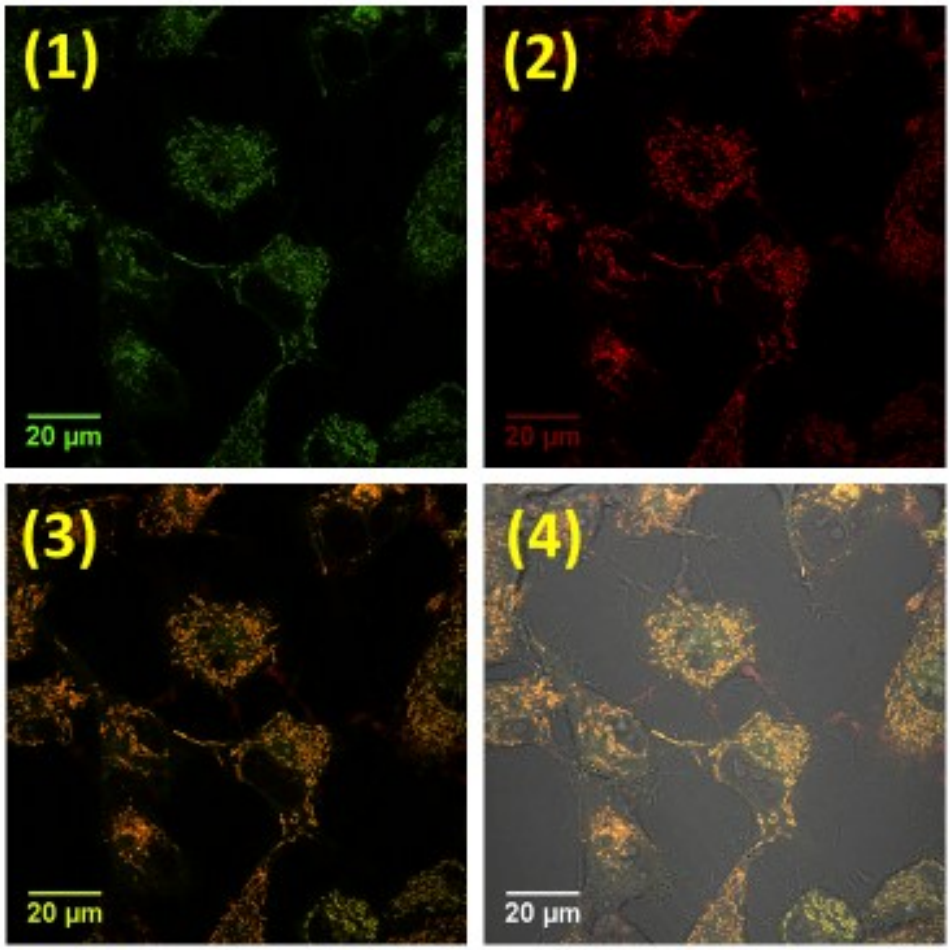


Figure S8.2 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3e** (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence **3e** (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/561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

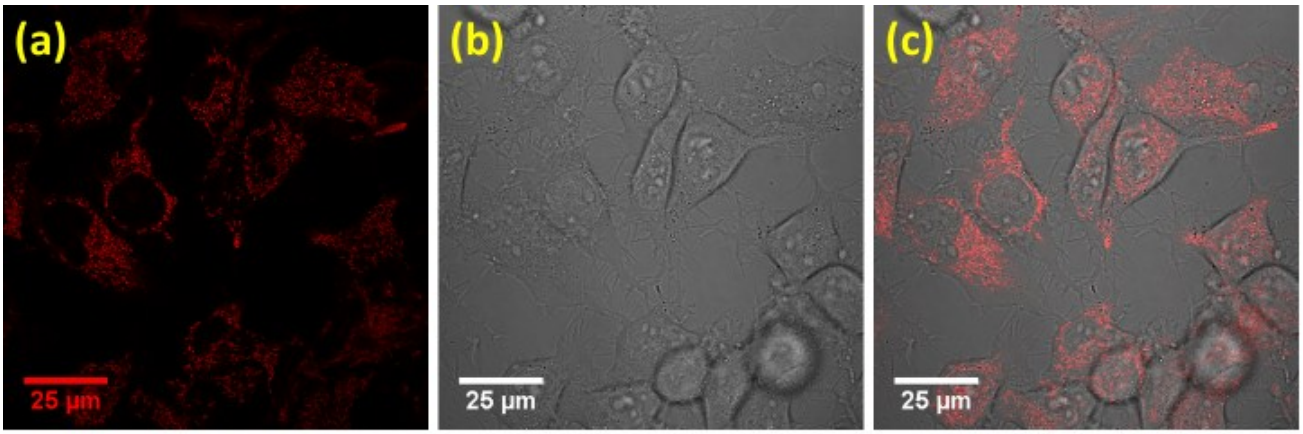


Figure S9.1 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3f** (200 nM) for 1 hour. From left to right images show the fluorescence **3f** (a), bright field (b) and overlapped image (c) respectively. 561 nm laser was used for excitation.

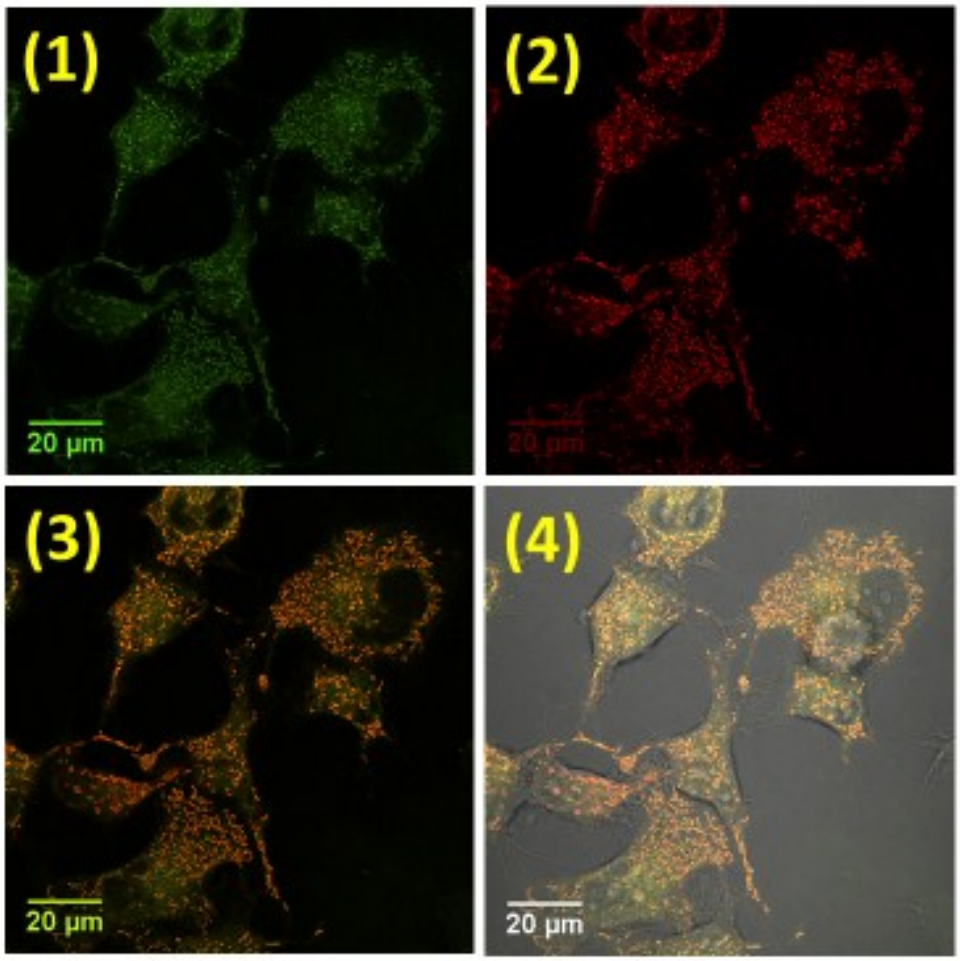


Figure S9.2 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3f** (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence **3f** (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/561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

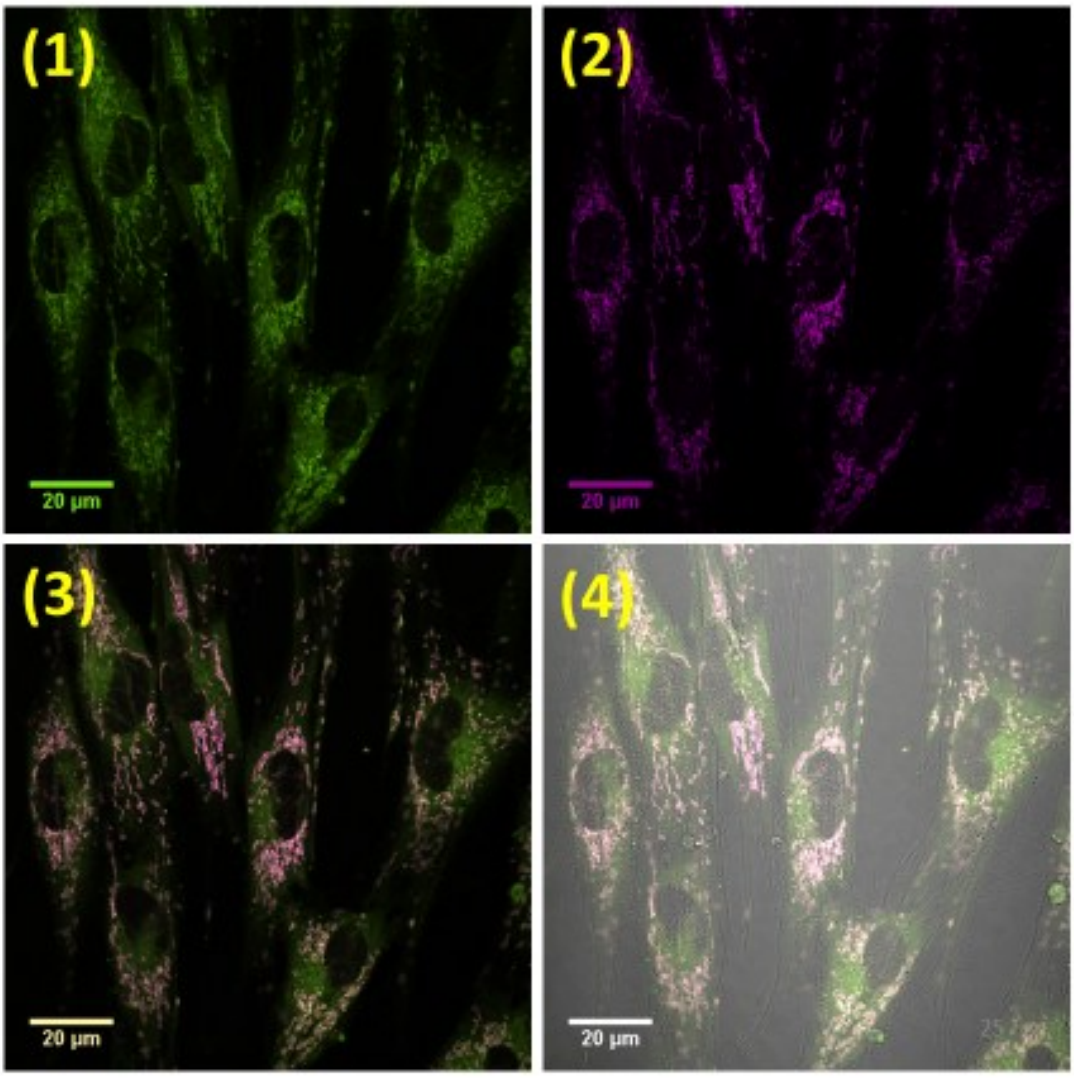


Figure S10 Fluorescent confocal microscopy images of human ovarian fibroblast cells (HOF) cells treated with **3a** (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence **3a** (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/640 nm lasers were used for excitation.

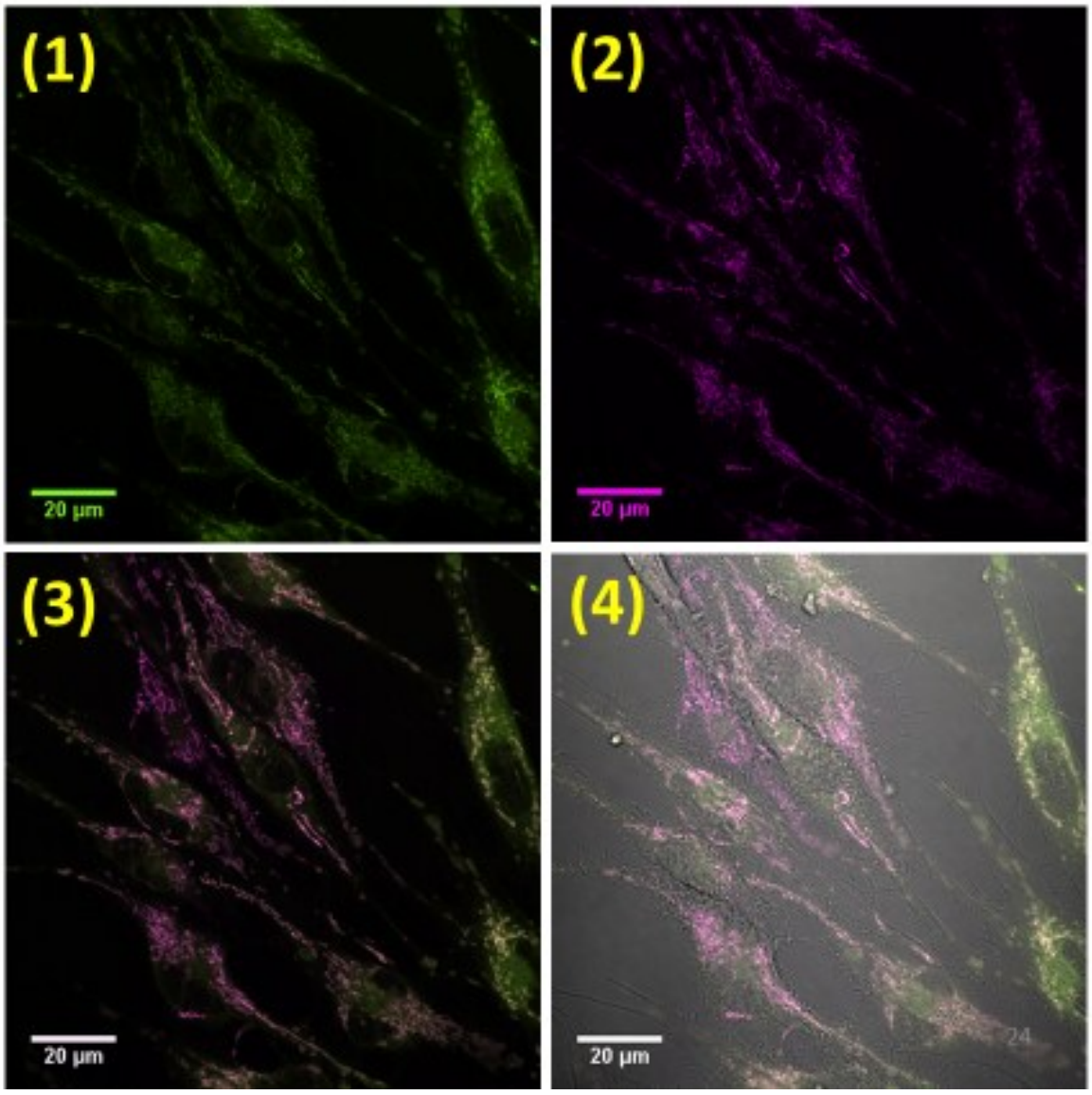


Figure S11 Fluorescent confocal microscopy images of human ovarian fibroblast cells (HOF) cells treated with **3b** (200 nM) for 1 hour. From left to right images show the fluorescence of mito-tracker green (1), fluorescence **3b** (2), overlapped image (3) and overlapped image with bright field (4) respectively. 488/640 nm lasers were used for excitation.

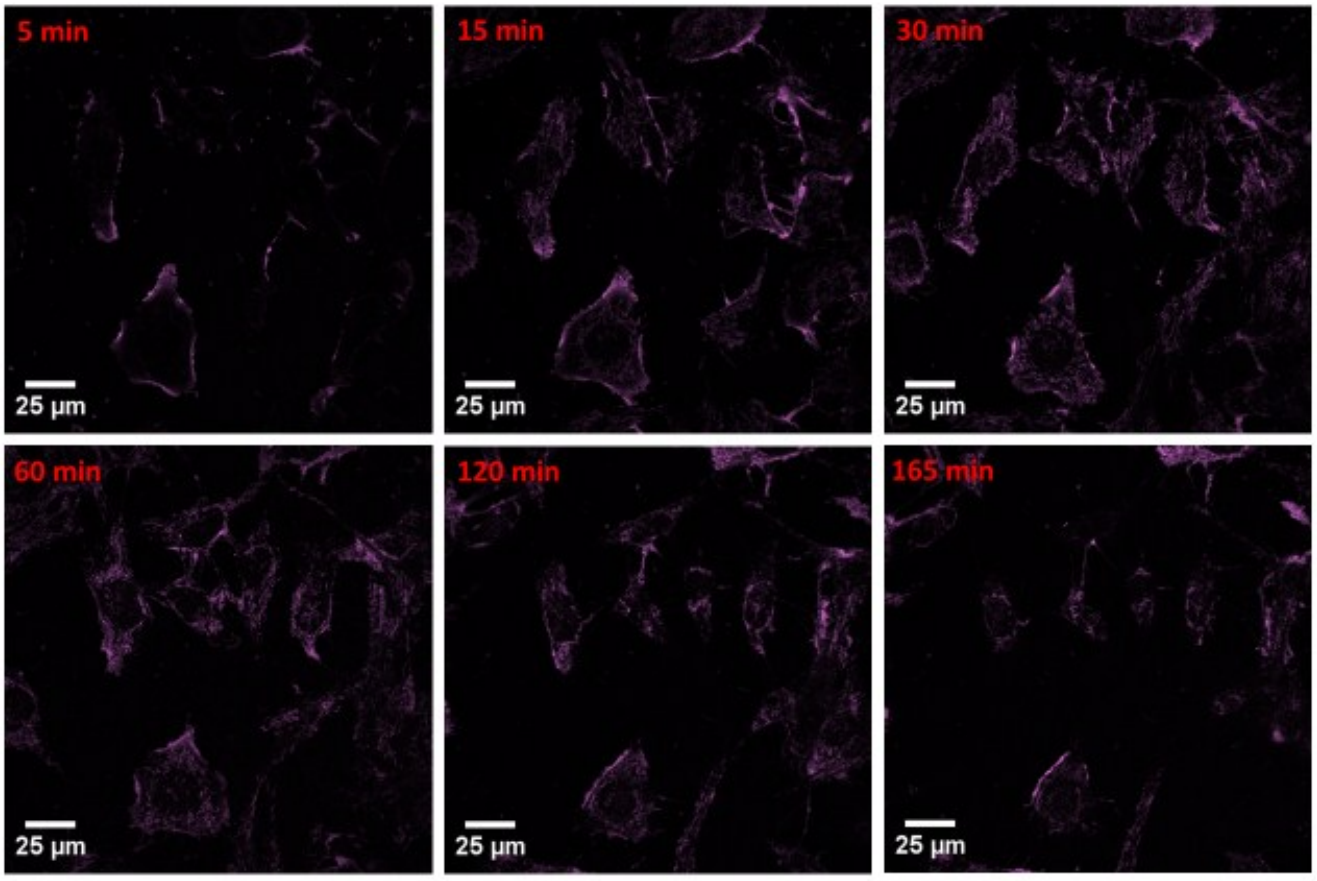


Figure S12 Fluorescent confocal microscopy images of MO3.13 cells (x100) treated with **3a** (200 nM) for a period of 2.5 hour. 640 nm laser was used for excitation.

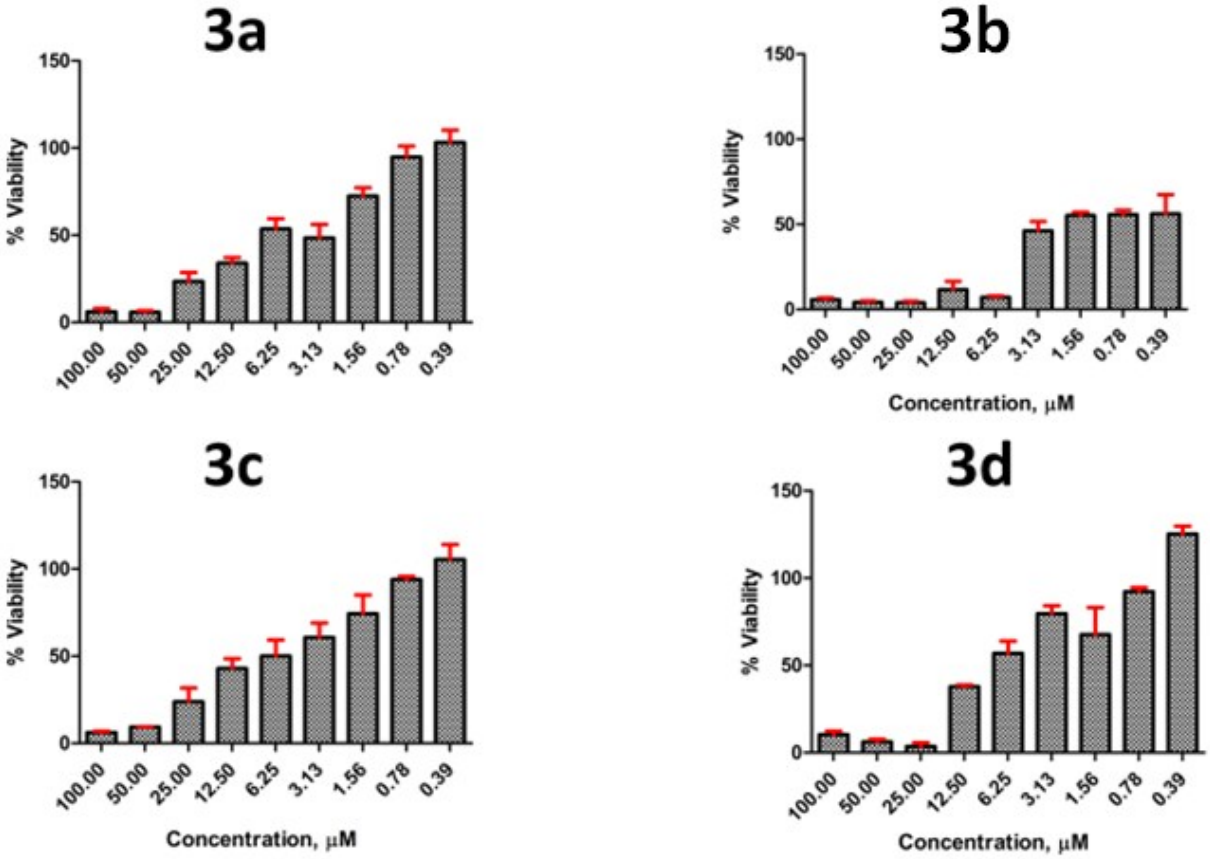


Figure S13 Cell viability results (bar-chart) obtained for **3a**, **3b**, **3c** and **3d** by MTT cell viability assay.

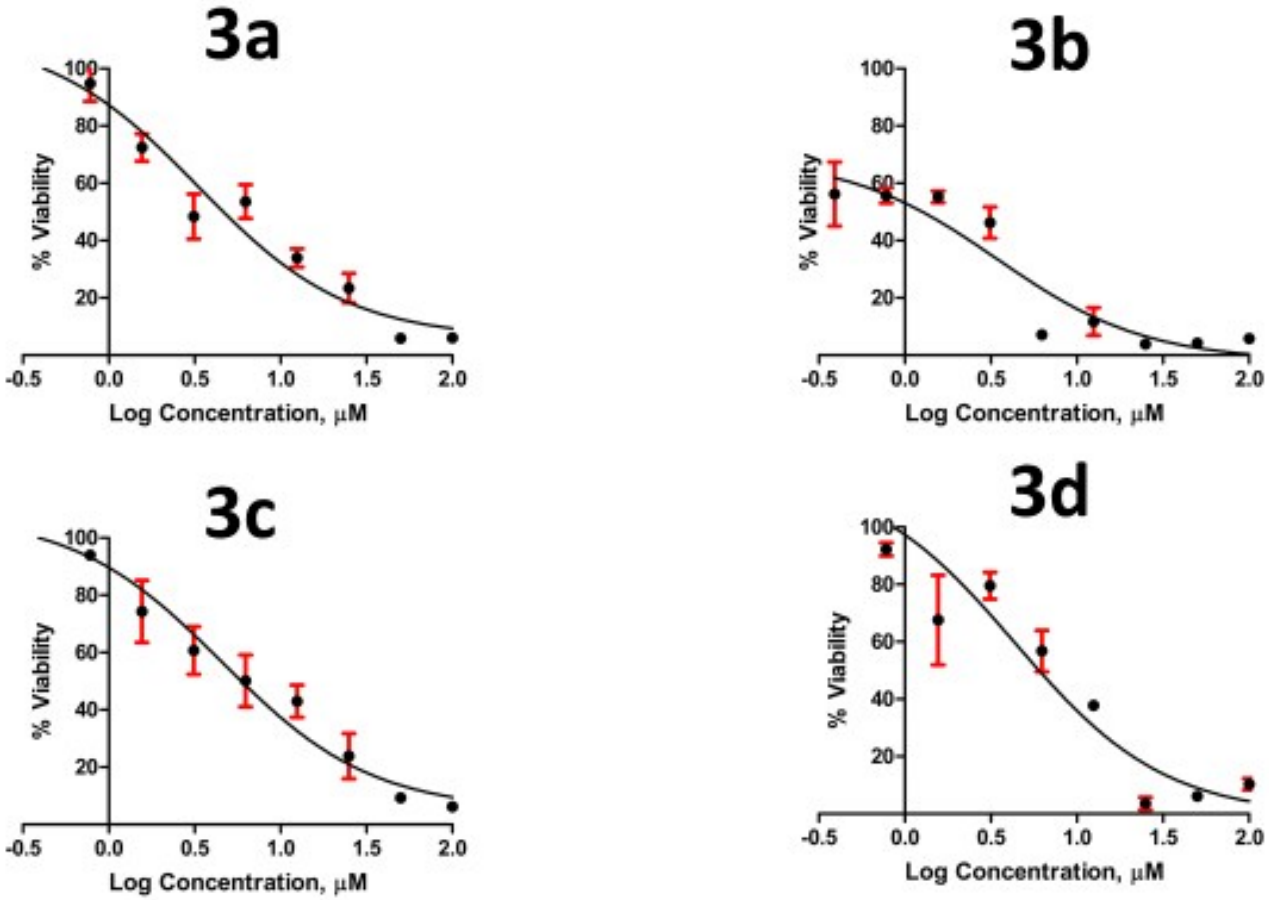
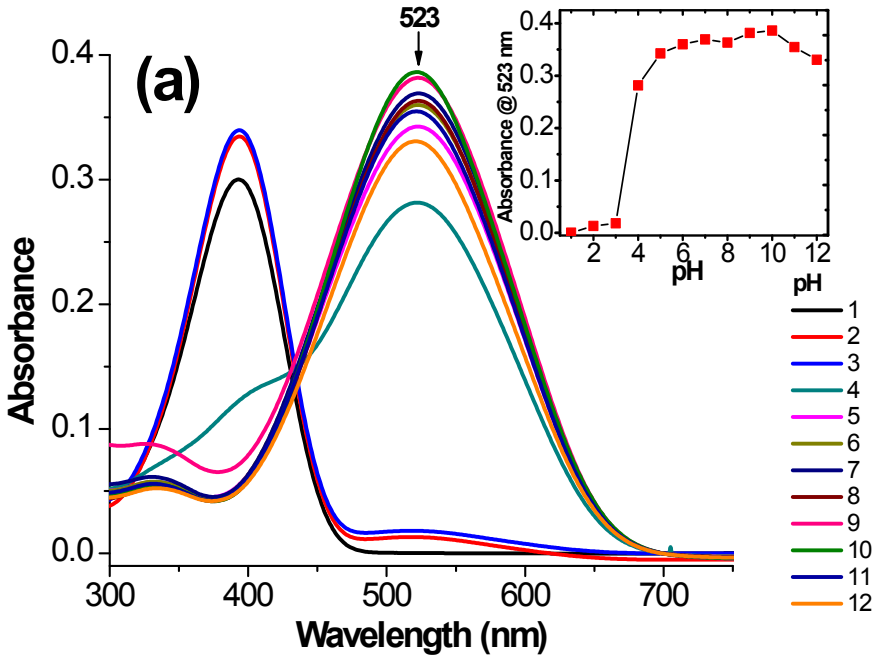


Figure S14 Cell viability results (cell viability curve) obtained for **3a**, **3b**, **3c** and **3d** by MTT cell viability assay.



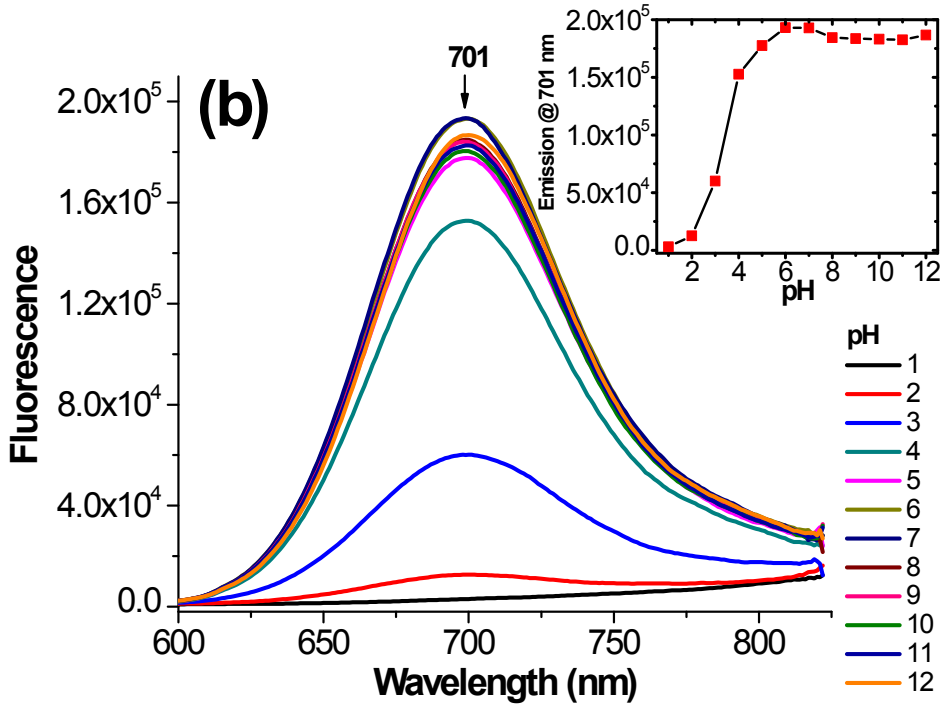


Figure S15 Absorbance (a) and fluorescence emission (b) spectra obtained for **3a** ($1x10^{-5}$ M) in different pH conditions at room temperature.

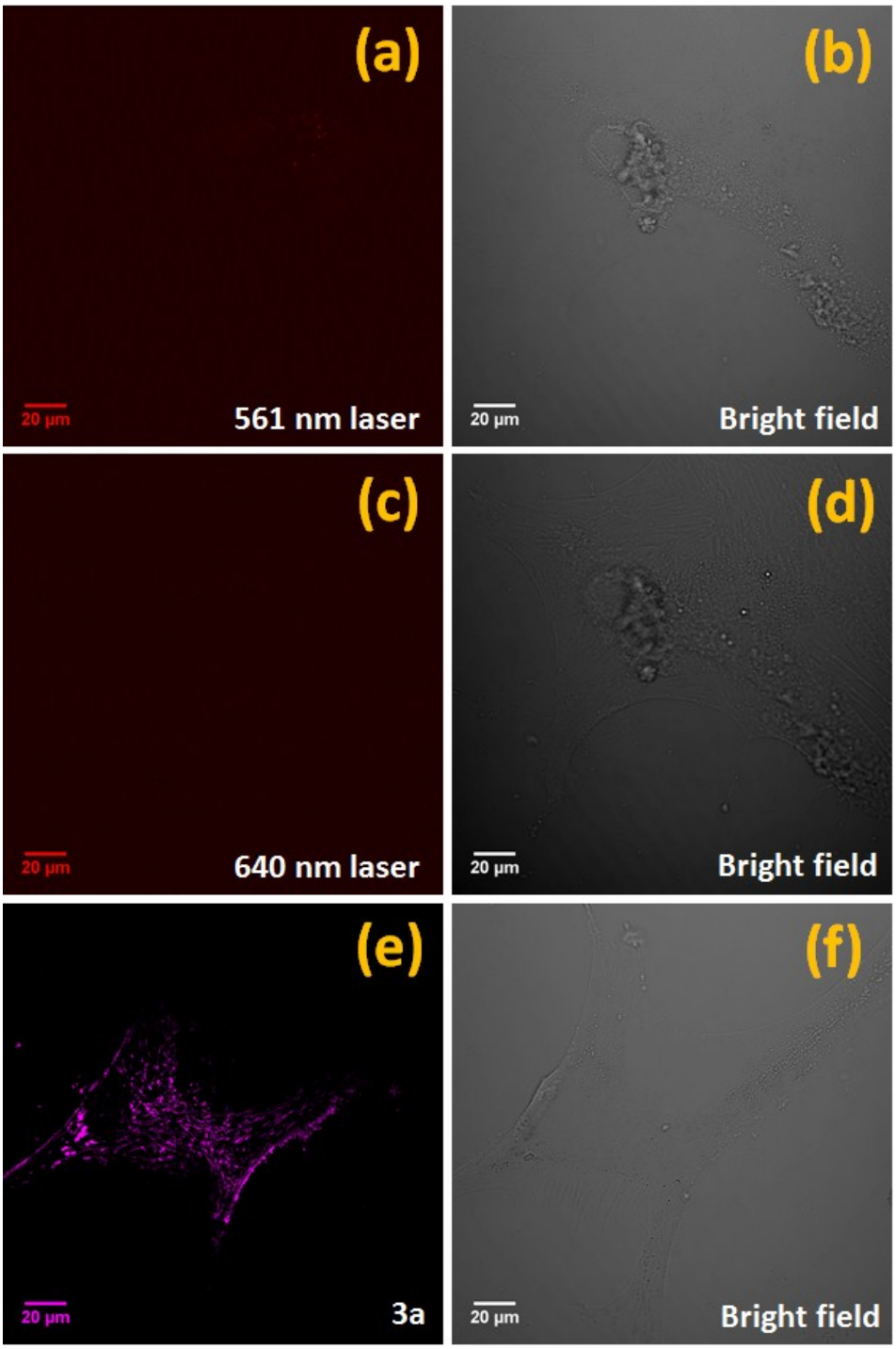


Figure S16 Fluorescent confocal microscopy images of MO3.13 cells (x100) obtained in the absence of any probe with 561 nm laser (a – b) and 640 nm laser (c – d) and treated with **3a** (200 nM) for 30 minutes. 640 nm laser was used for **3a** excitation.