Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B.

Synthesis of highly selective cyanine based lysosome markers by coupling 2-(2'-hydroxyphenyl)benzothiazole (HBT) : The impact of substituents towards selectivity and optical properties.

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Supporting Information

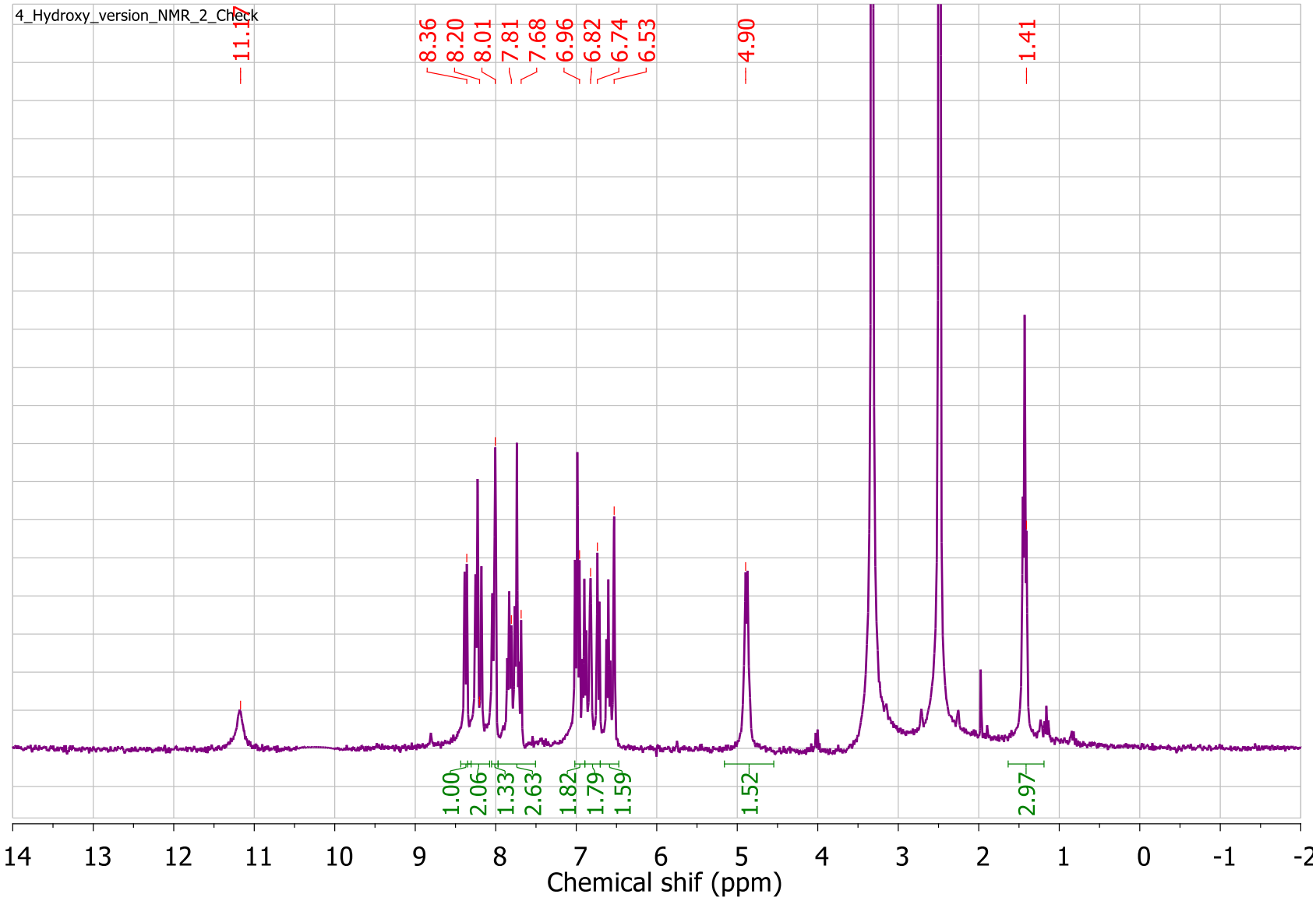


Figure S2.1 ^{1}H NMR spectra of **2a** (300 MHz in DMSO-d6)

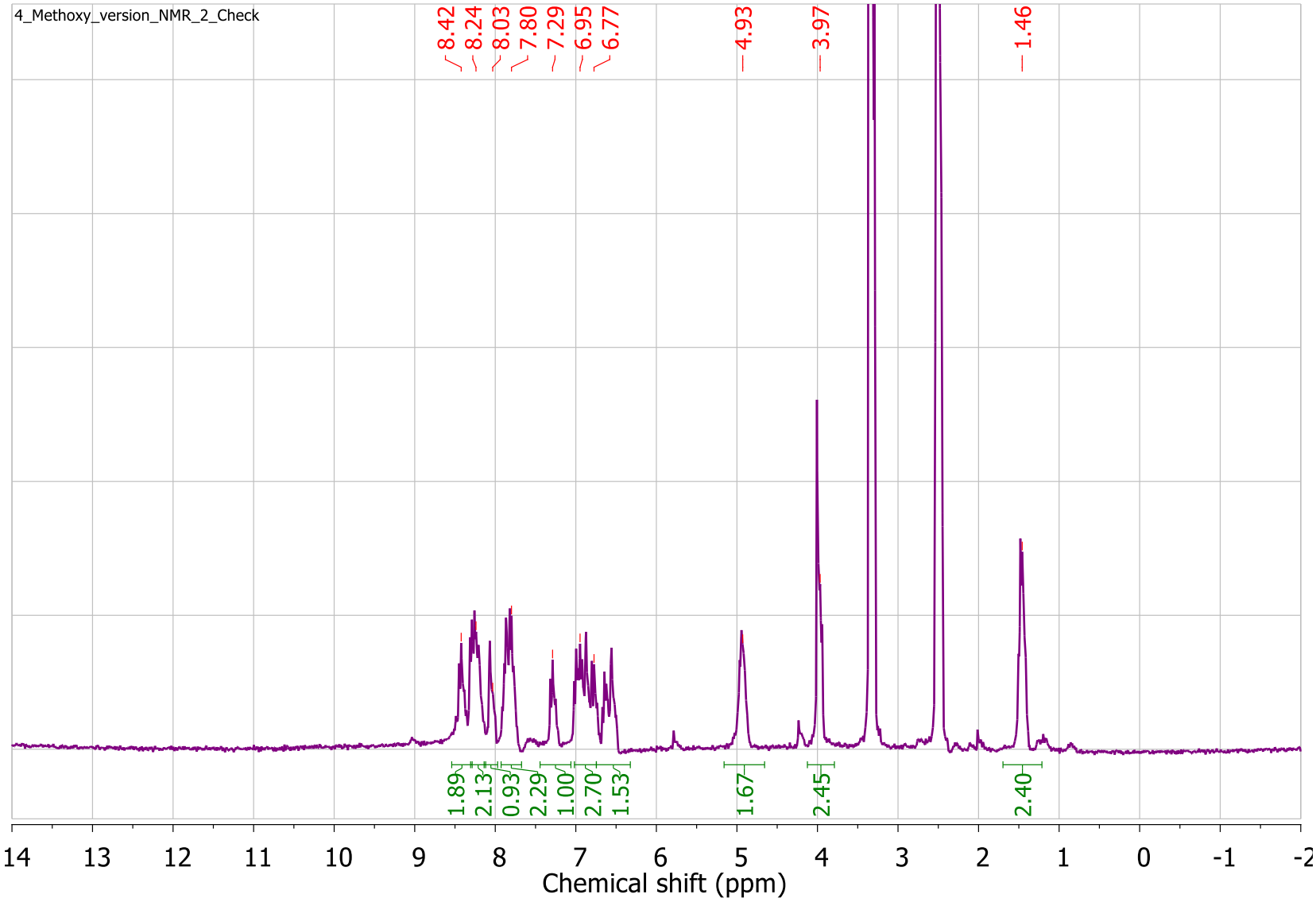


Figure S2.2 ^{1}H NMR spectra of **2b** (300 MHz in DMSO-d6)

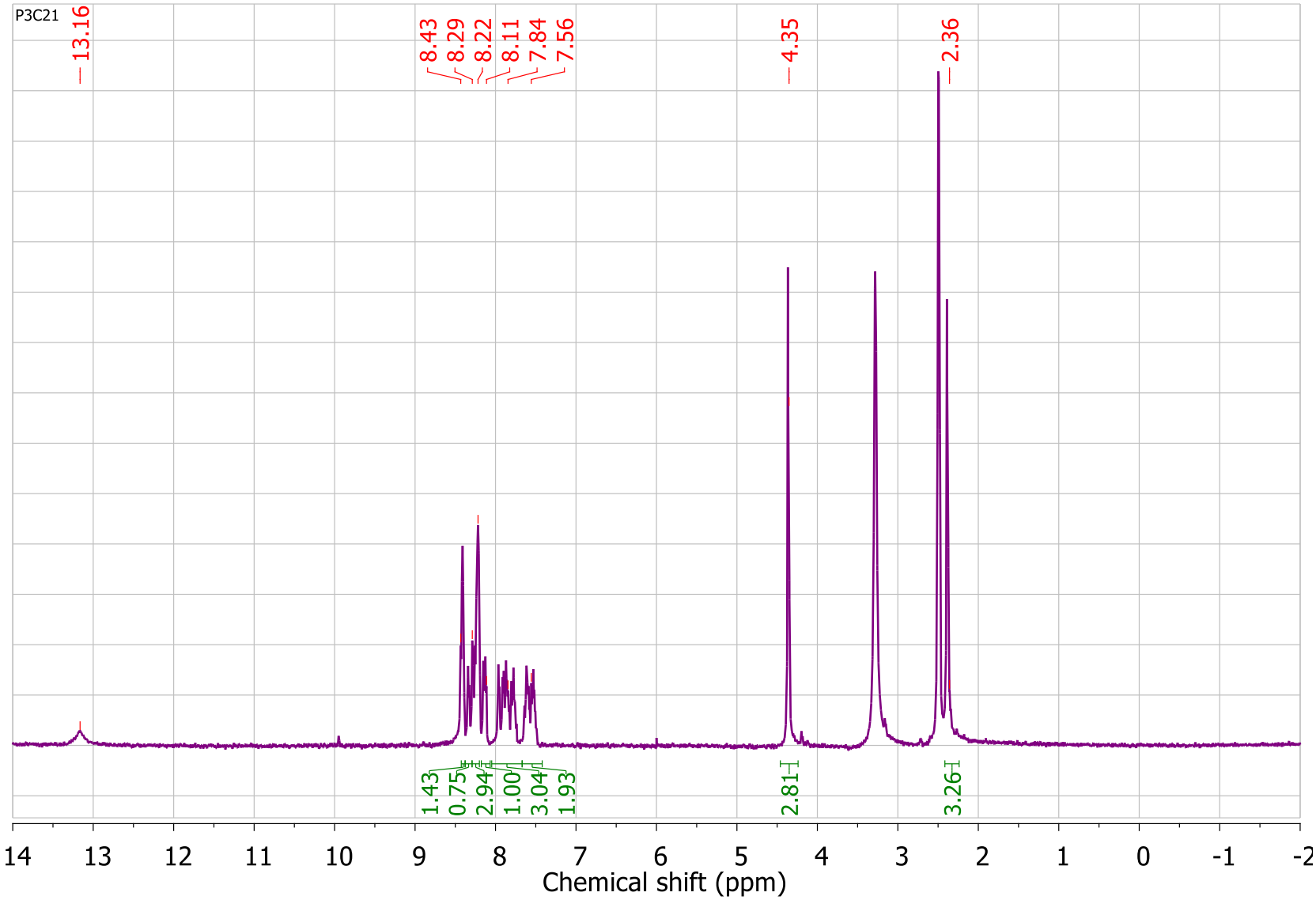


Figure S2.3 ^{1}H NMR spectra of **3a** (300 MHz in DMSO-d6)

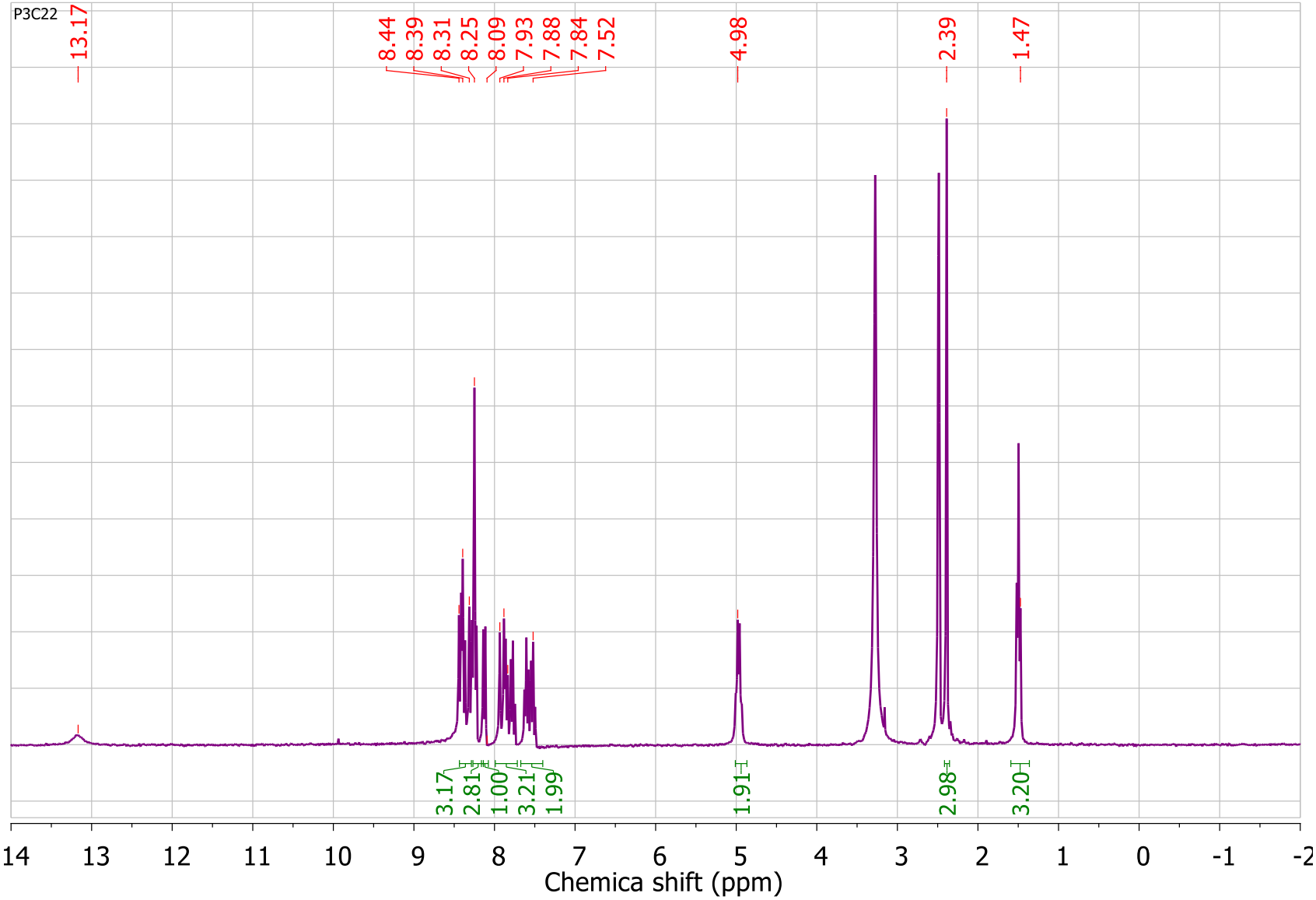


Figure S2.4 ^{1}H NMR spectra of **3b** (300 MHz in DMSO-d6)

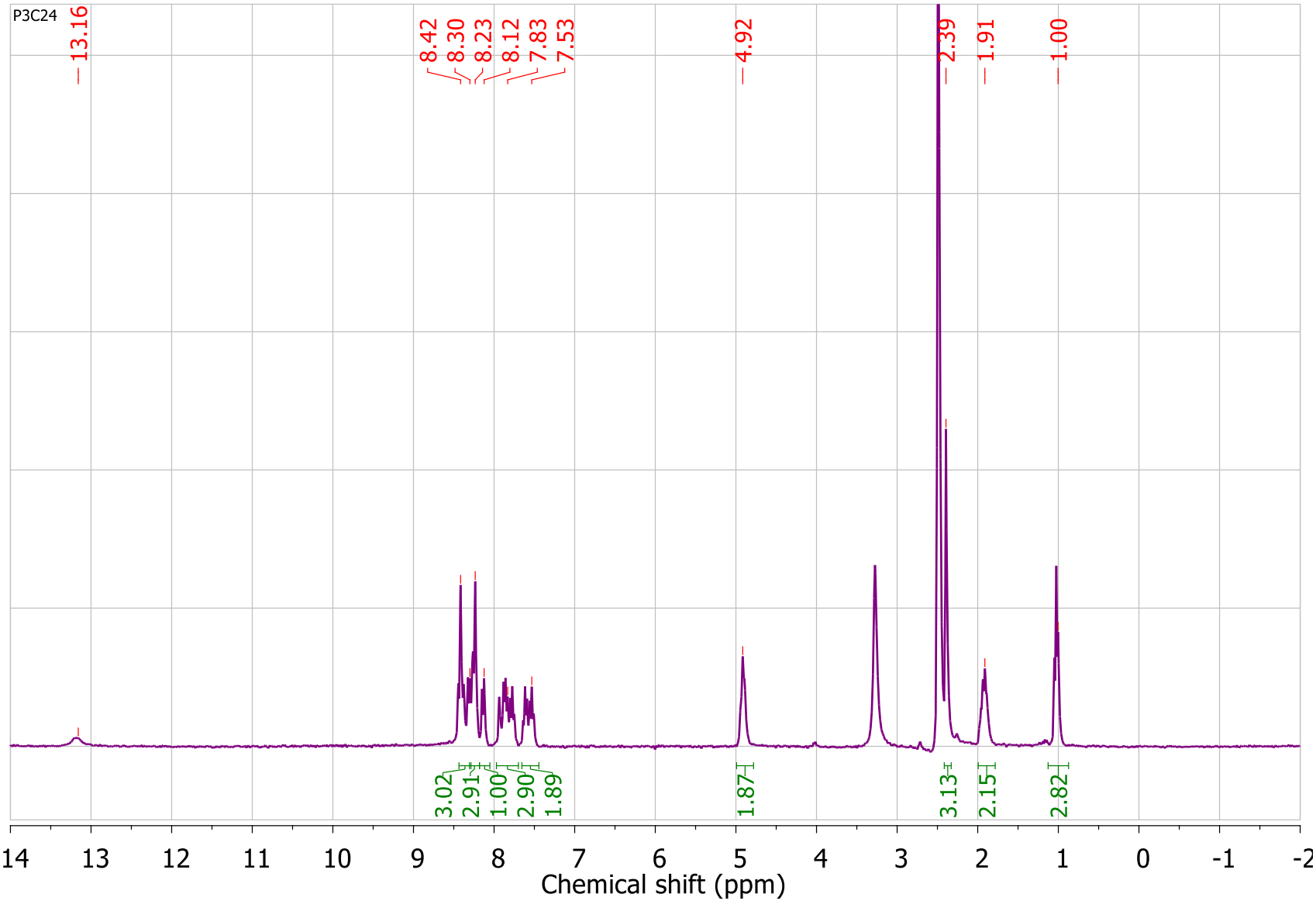


Figure S2.5 ^{1}H NMR spectra of **3c** (300 MHz in DMSO-d6)

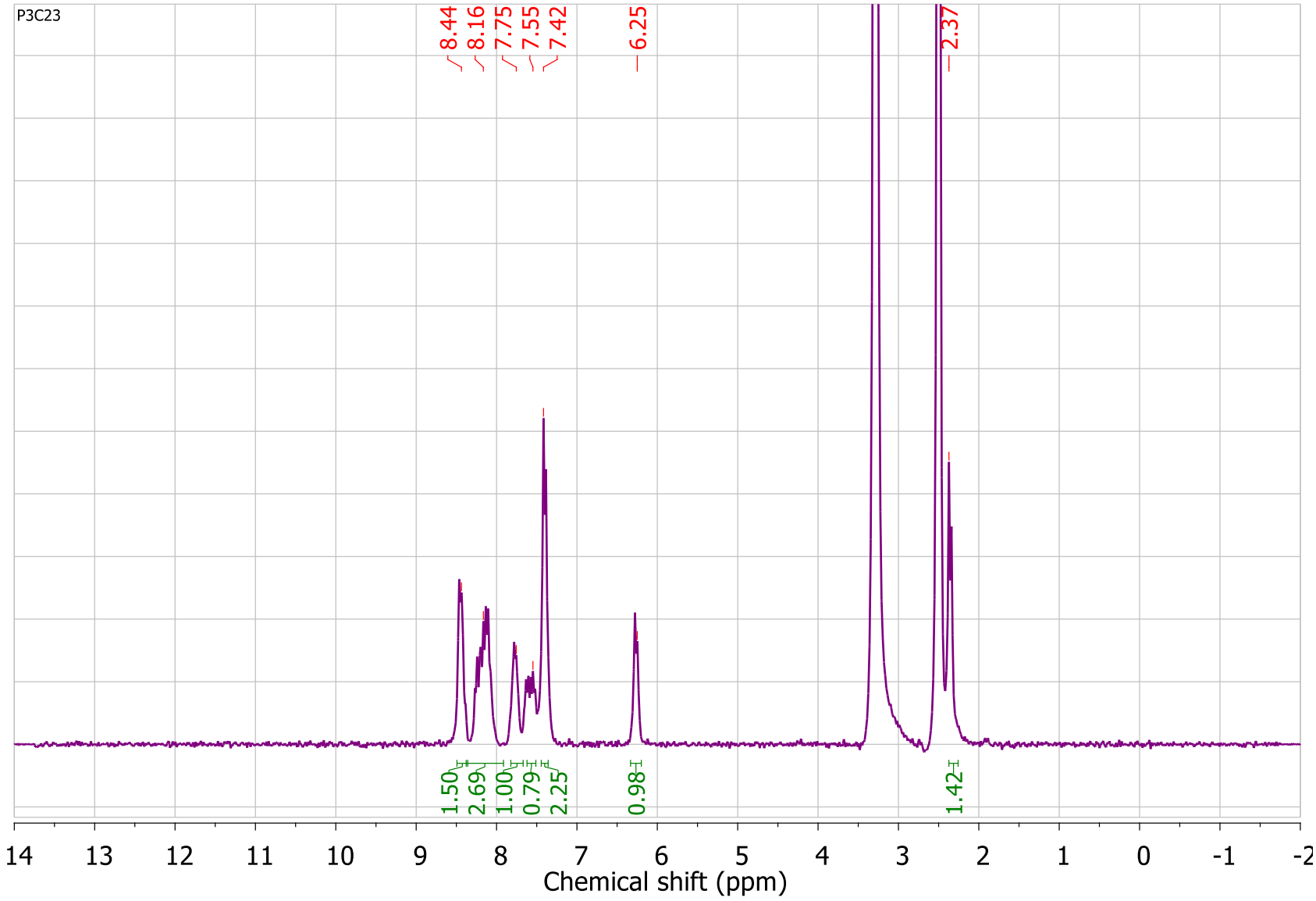


Figure S2.6 ^{1}H NMR spectra of **3d** (300 MHz in DMSO-d6)

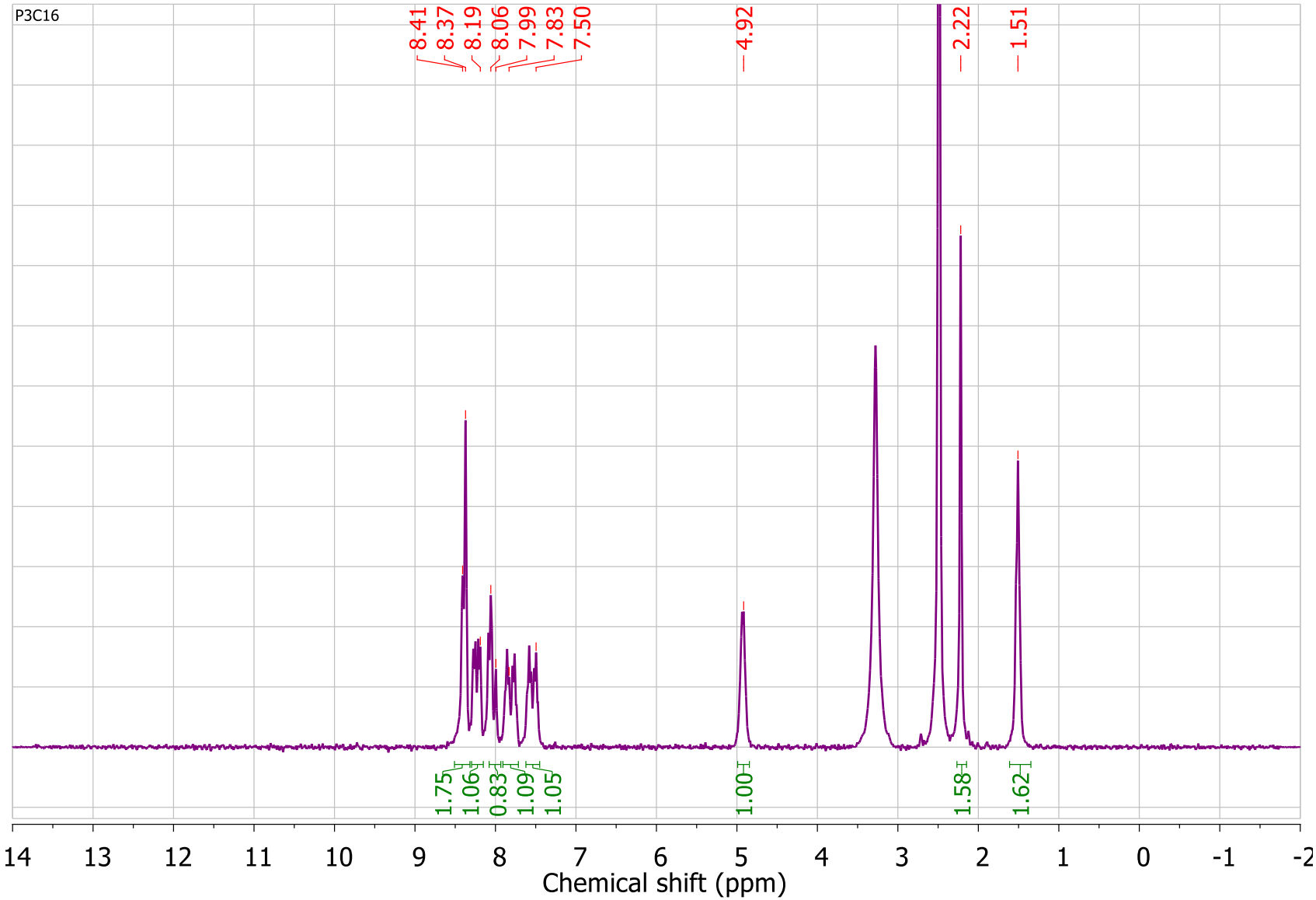


Figure S2.7 ^{1}H NMR spectra of **4a** (300 MHz in DMSO-d6)

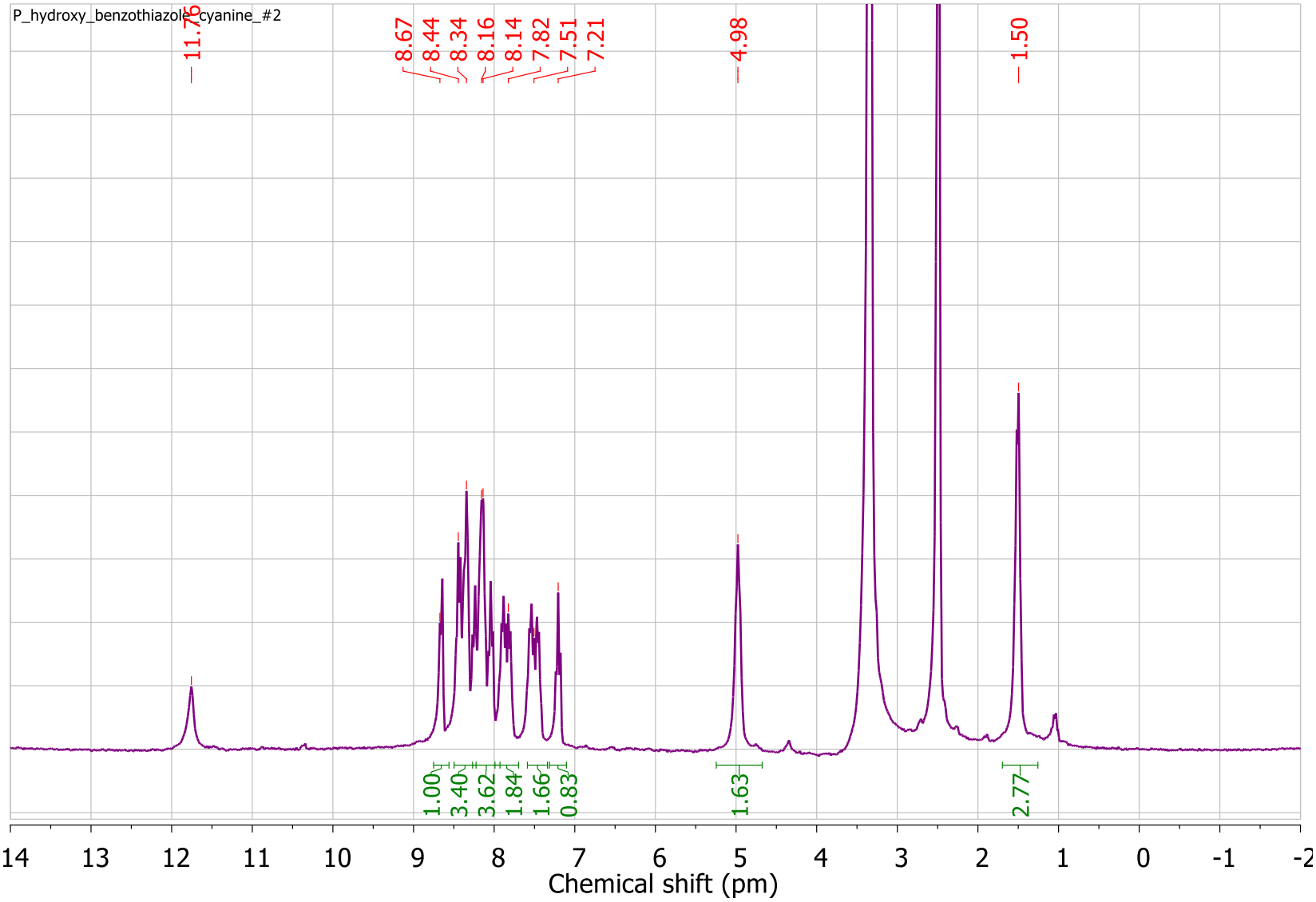


Figure S2.8 ^{1}H NMR spectra of **5a** (300 MHz in DMSO-d6)

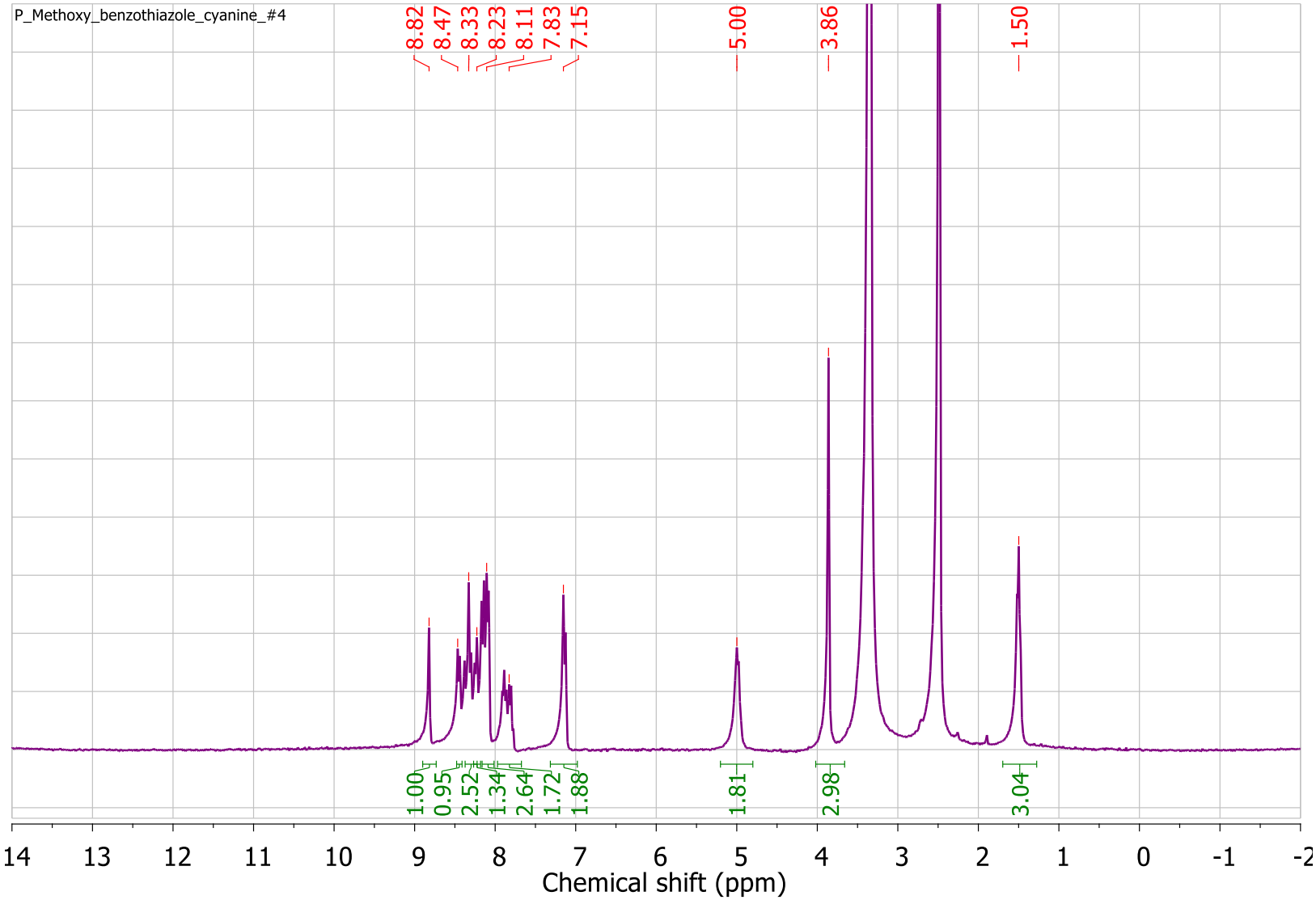


Figure S2.9 ^{1}H NMR spectra of **5b** (300 MHz in DMSO-d6)

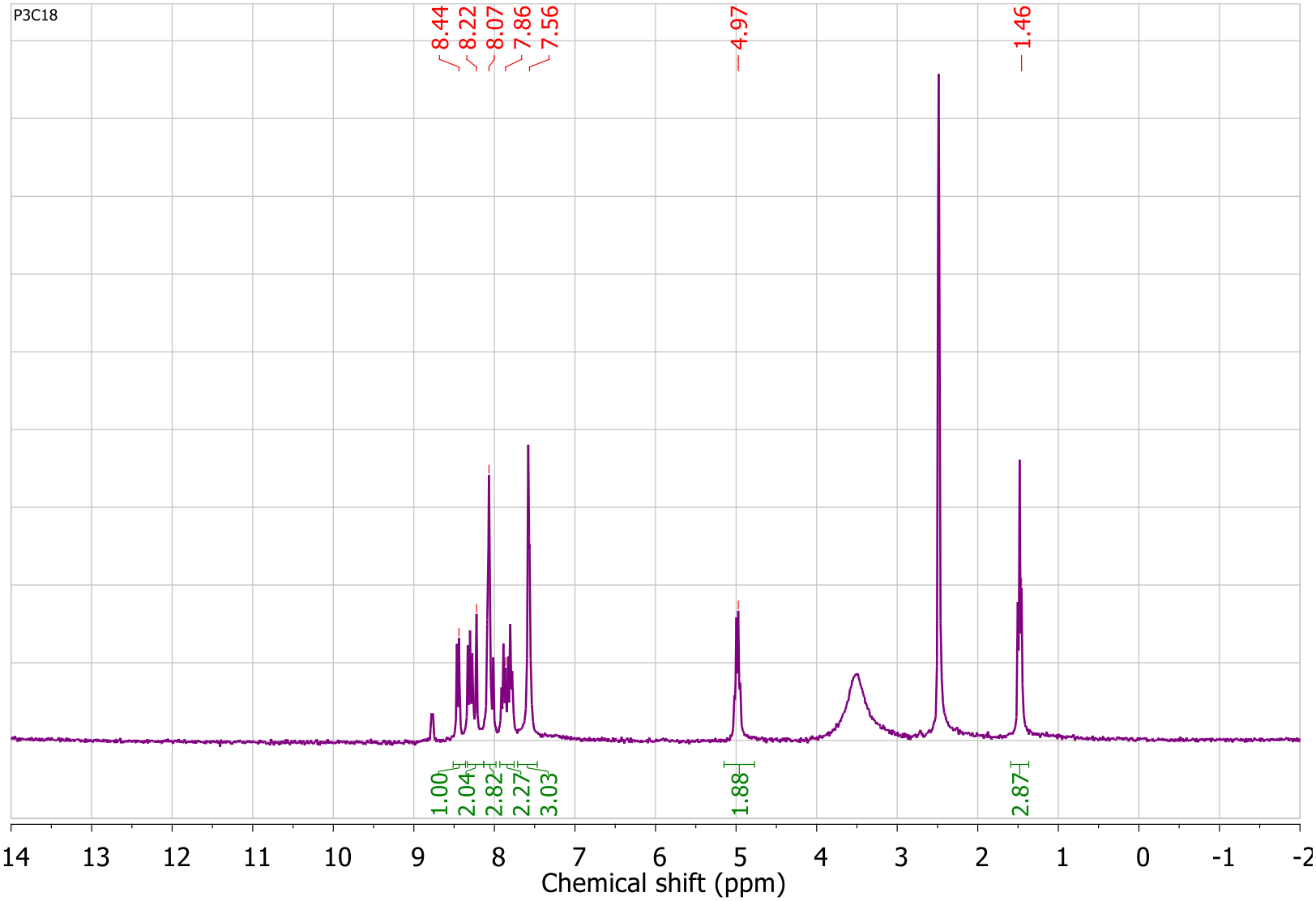


Figure S2.10 ^{1}H NMR spectra of **6a** (300 MHz in DMSO-d6)

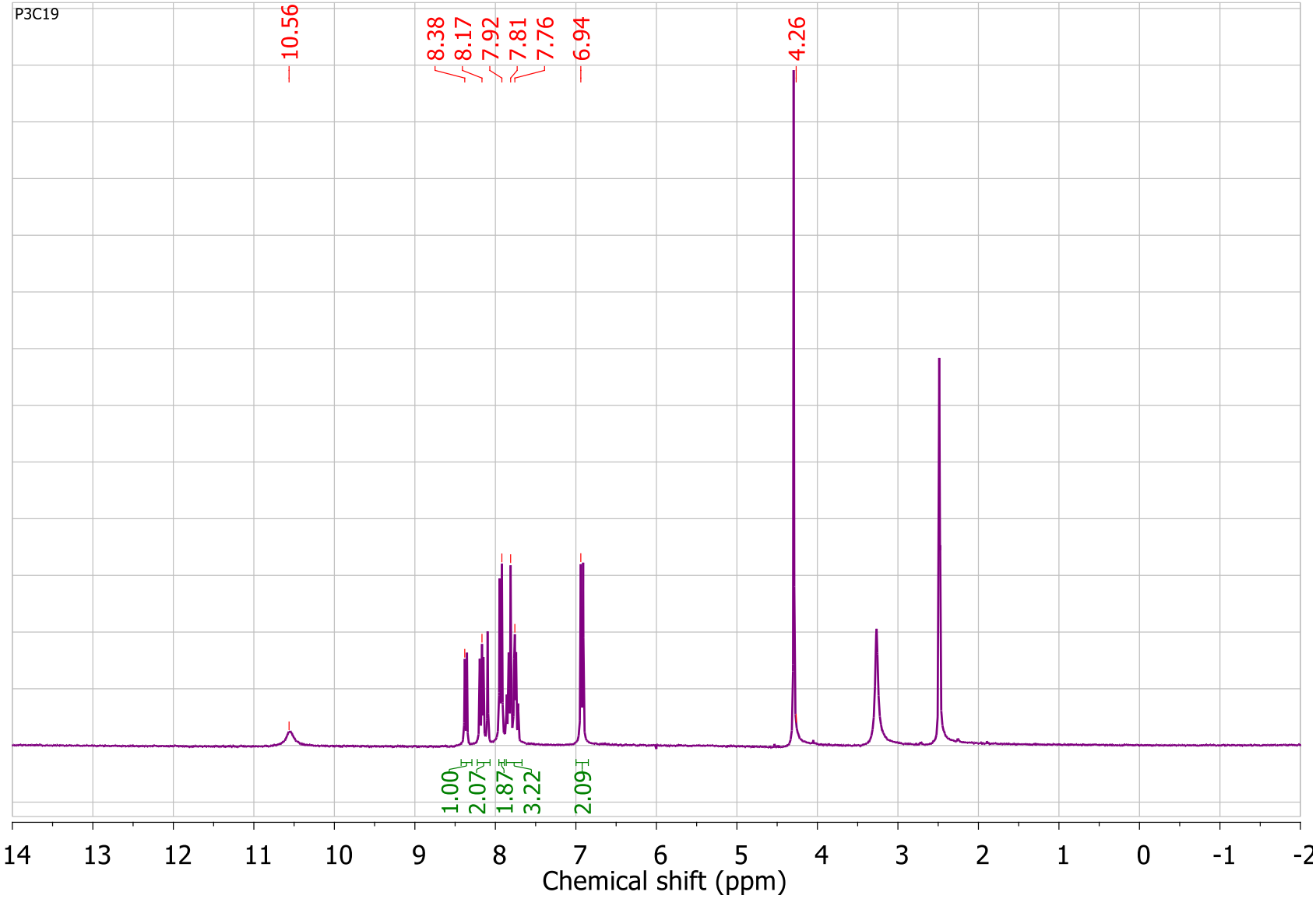


Figure S2.11 ^{1}H NMR spectra of **6b** (300 MHz in DMSO-d6)

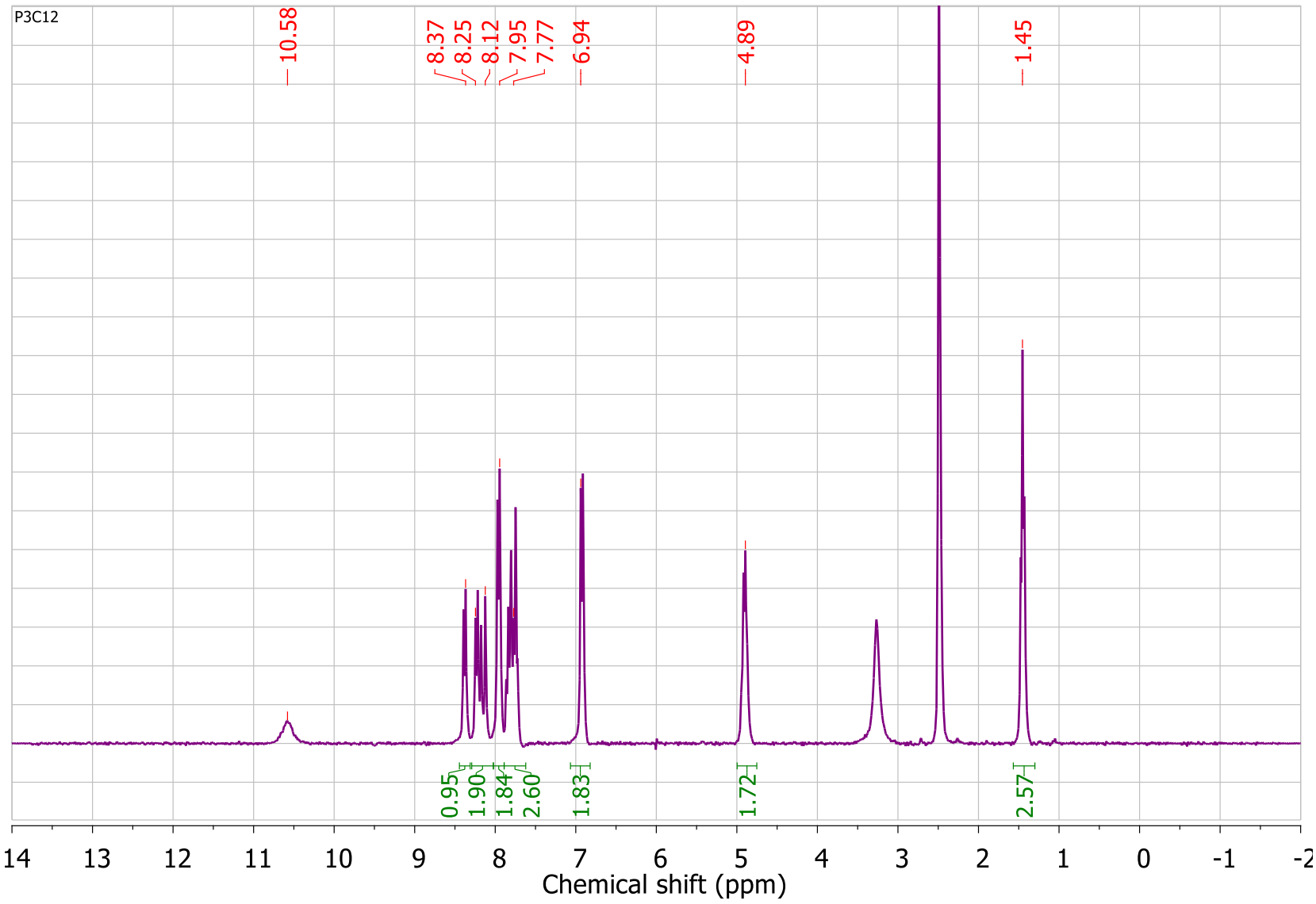


Figure S2.12 ^{1}H NMR spectra of **6c** (300 MHz in DMSO-d6)

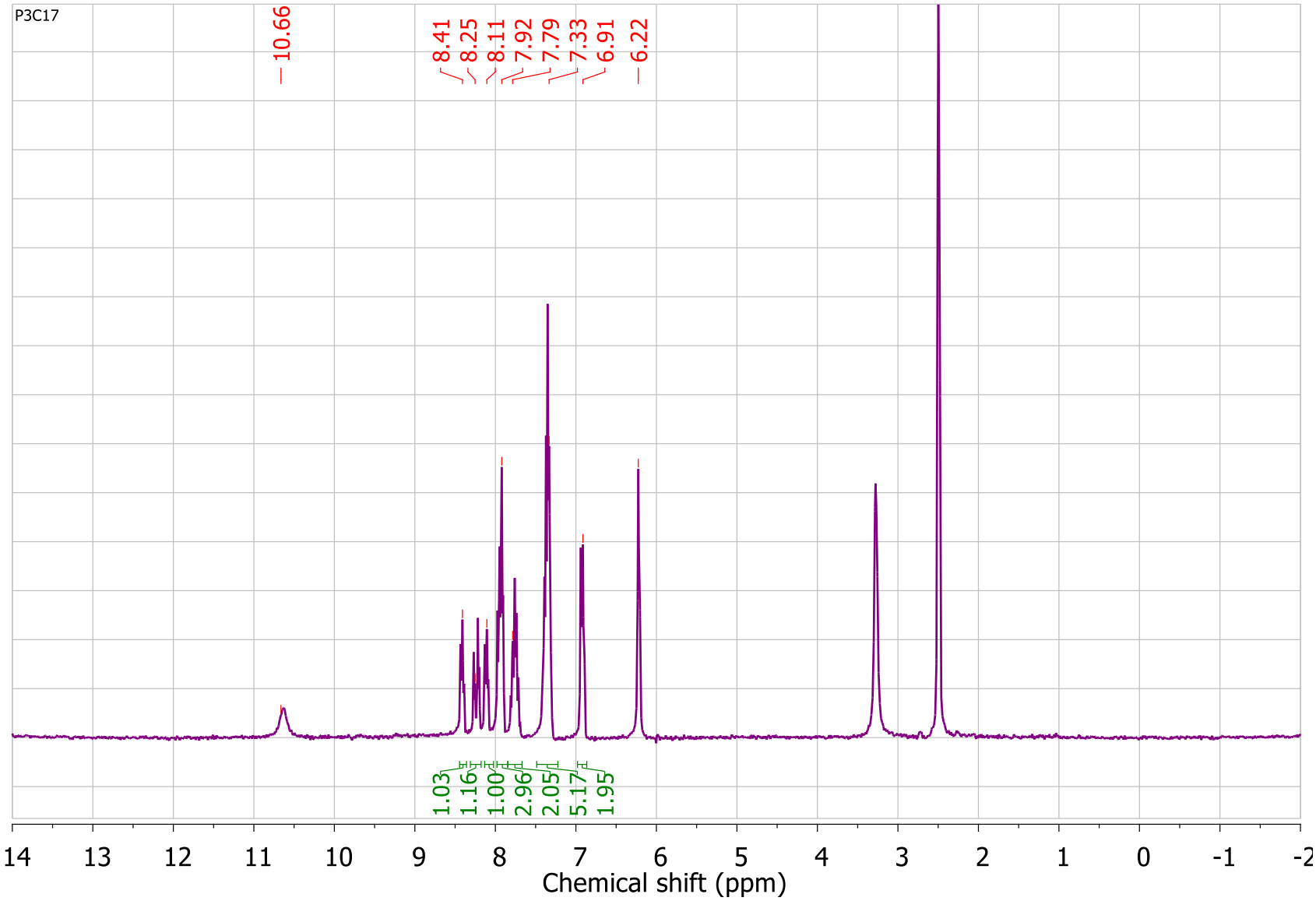


Figure S2.13 ^{1}H NMR spectra of **6d** (300 MHz in DMSO-d6)

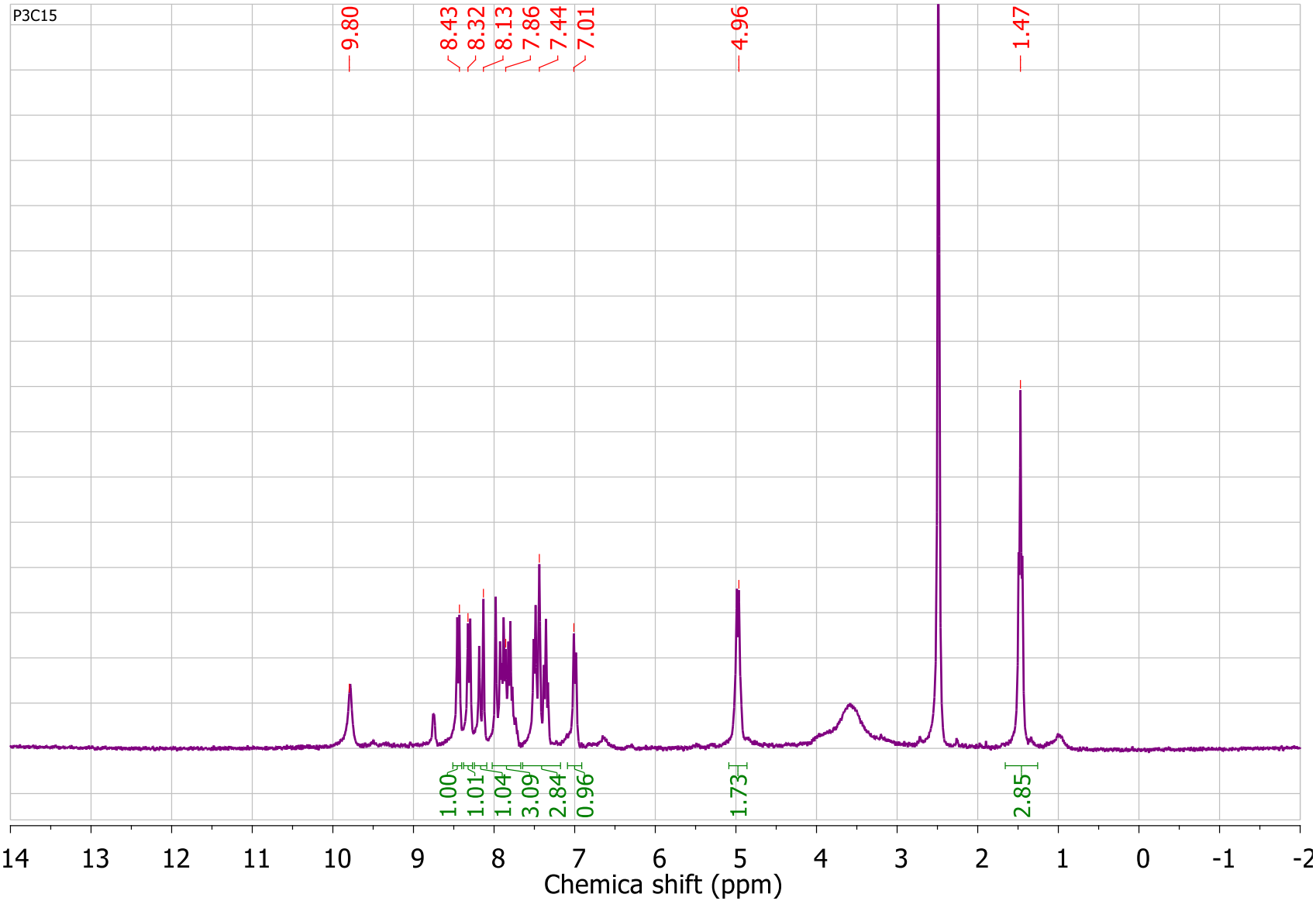


Figure S2.14 ^{1}H NMR spectra of **6e** (300 MHz in DMSO-d6)

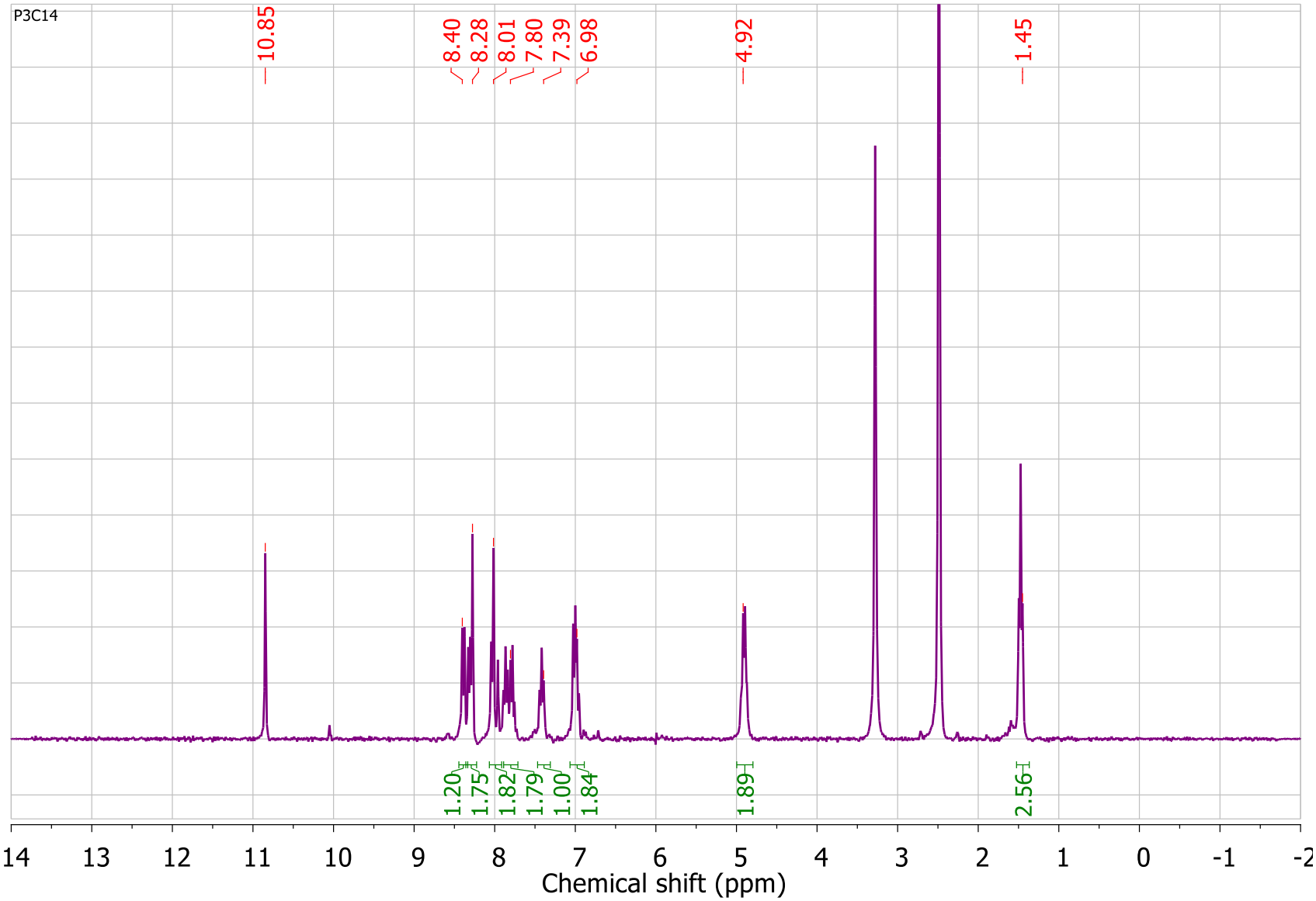


Figure S2.15 ^{1}H NMR spectra of **6f** (300 MHz in DMSO-d6)

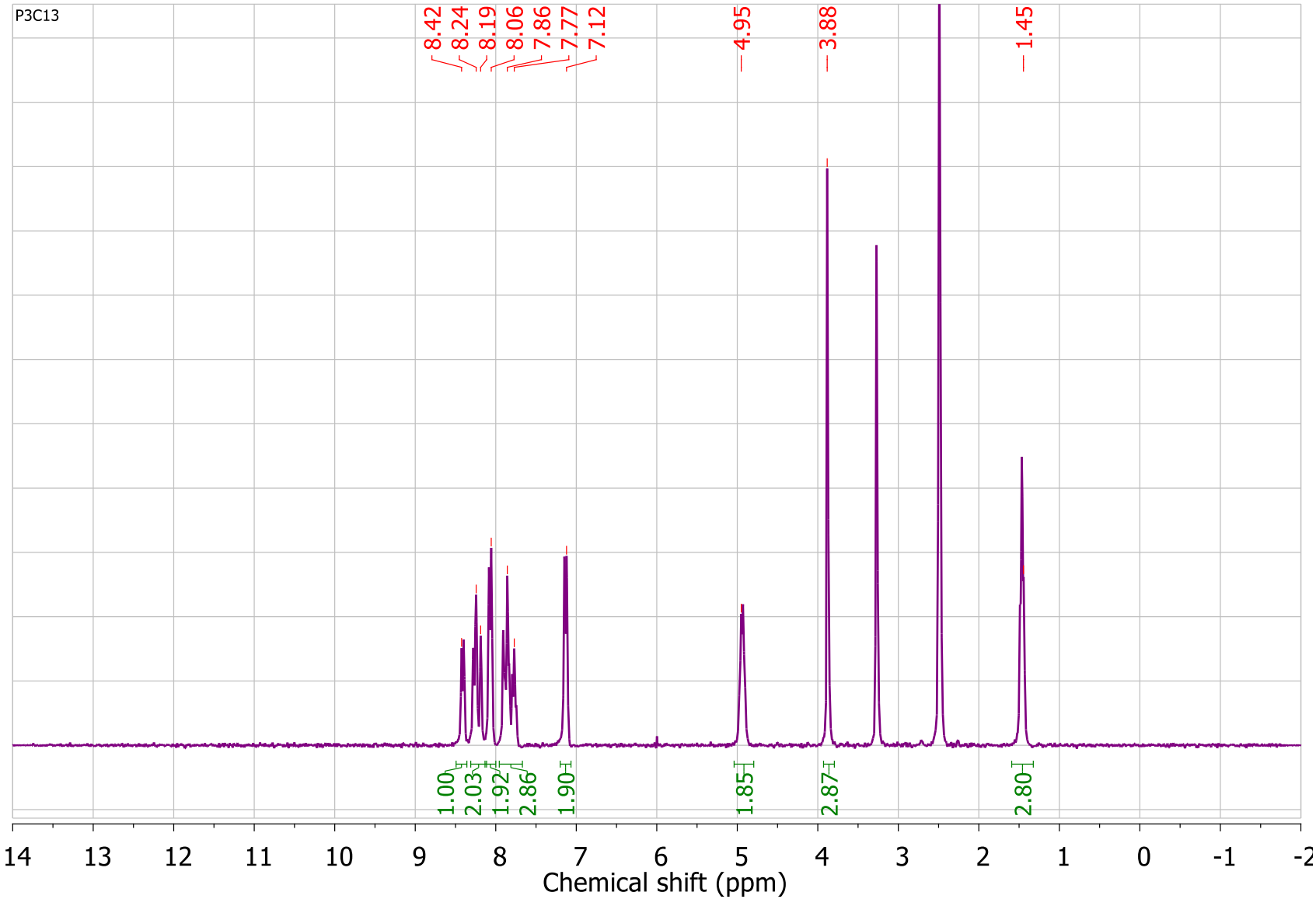


Figure S2.16 ^{1}H NMR spectra of **6g** (300 MHz in DMSO-d6)

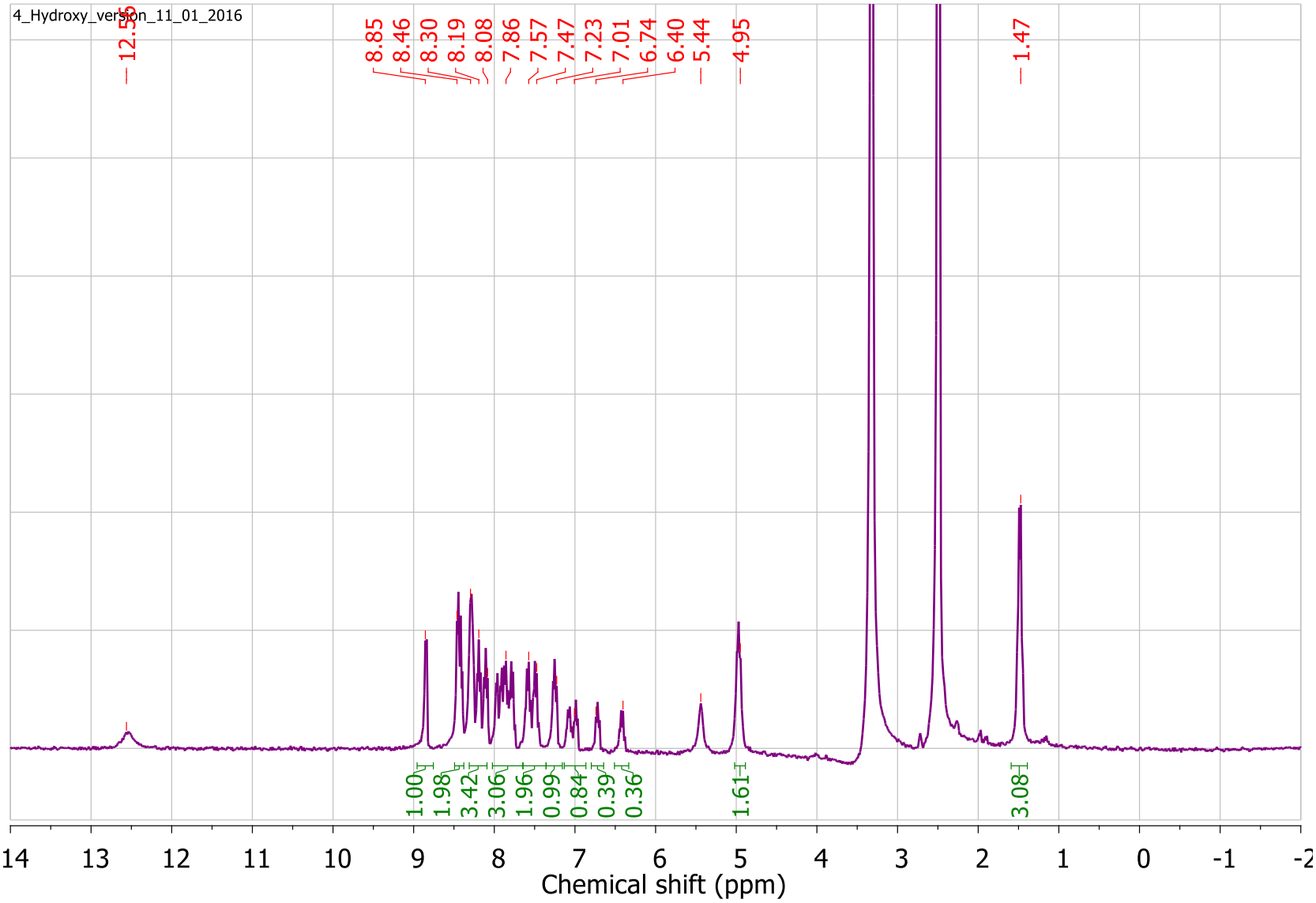


Figure S2.17 ^{1}H NMR spectra of **2c** (300 MHz in DMSO-d6)

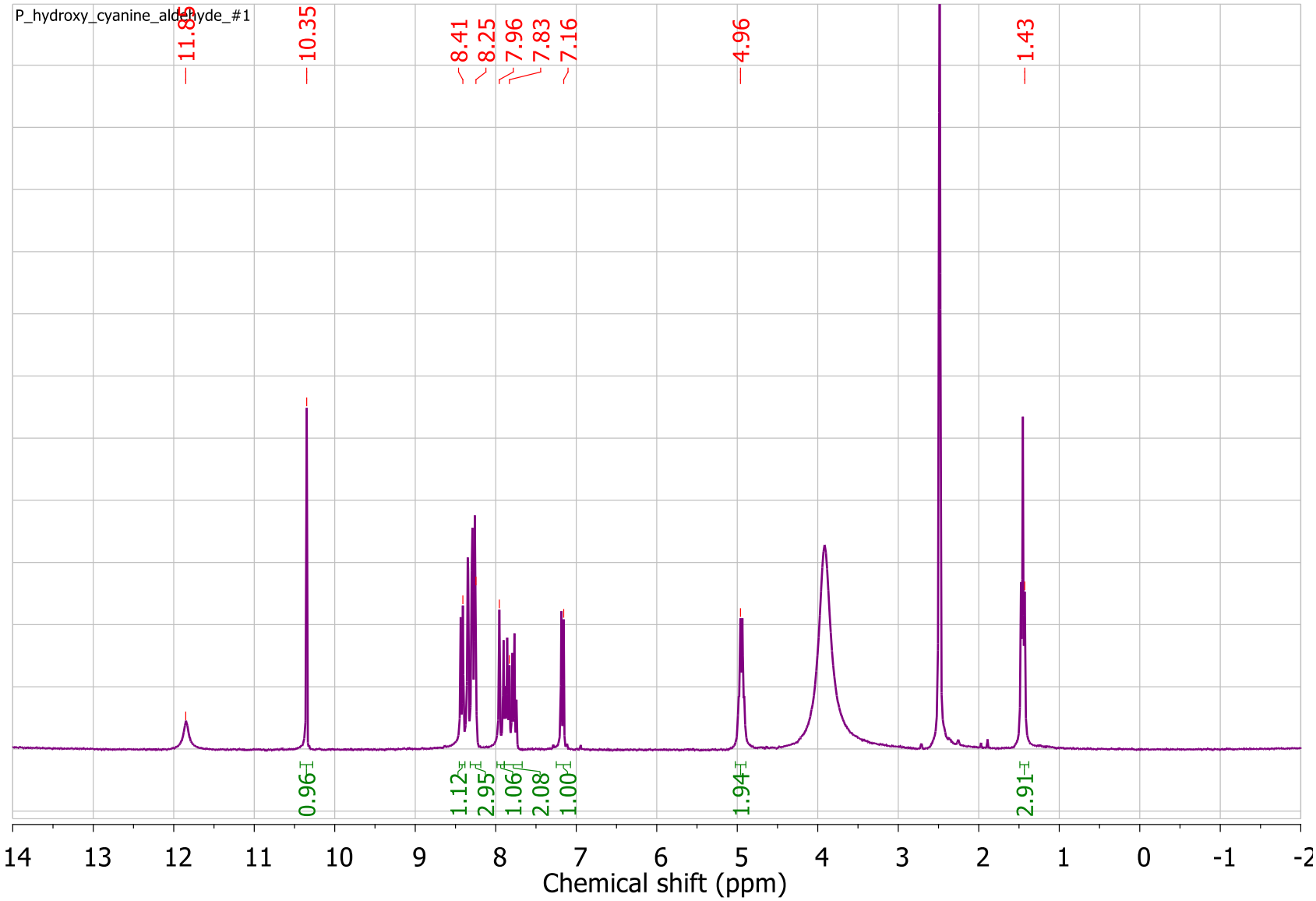


Figure S2.18 ^{1}H NMR spectra of **8a** (300 MHz in DMSO-d6)

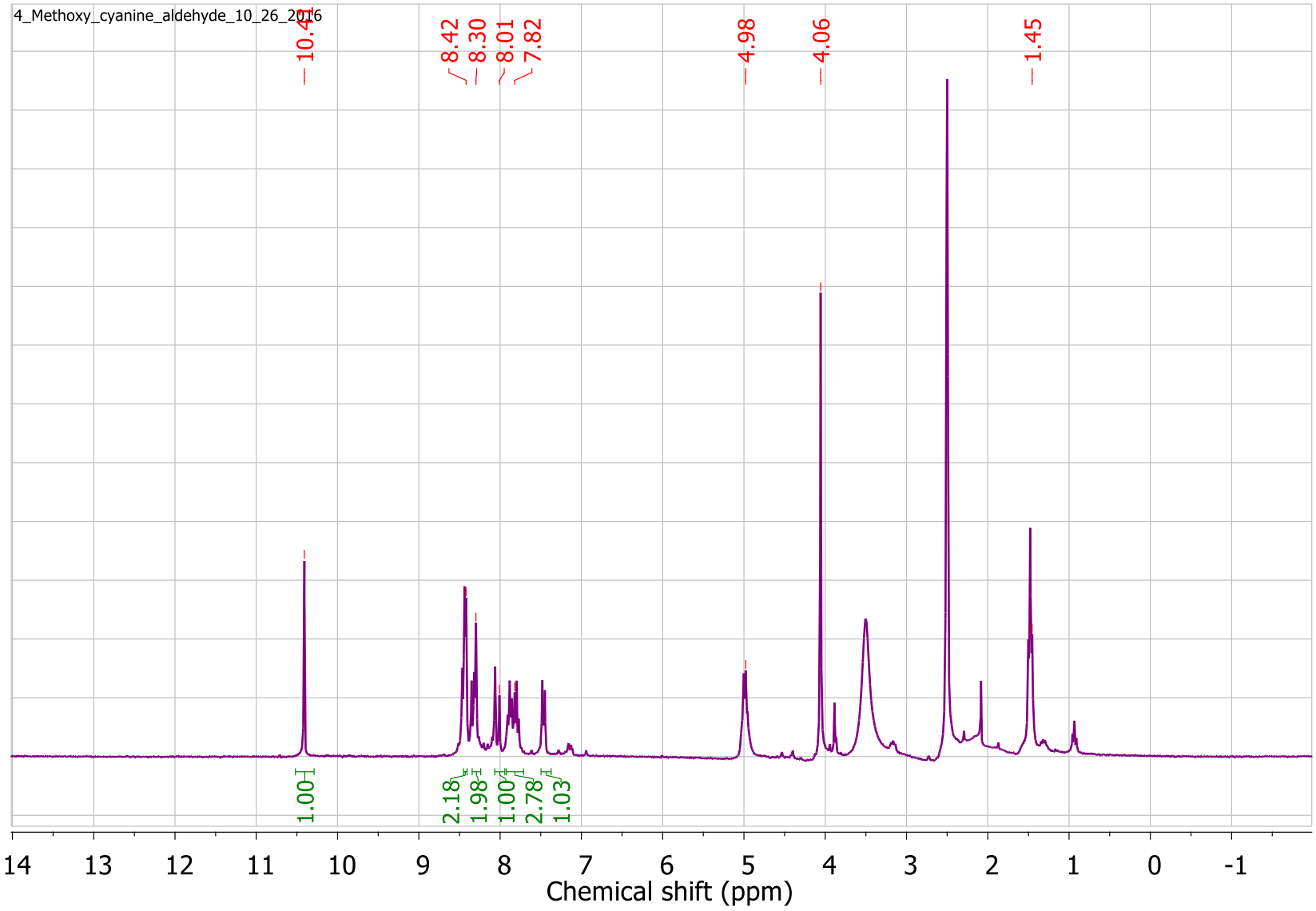


Figure S2.19 ^{1}H NMR spectra of **8b** (300 MHz in DMSO-d6)

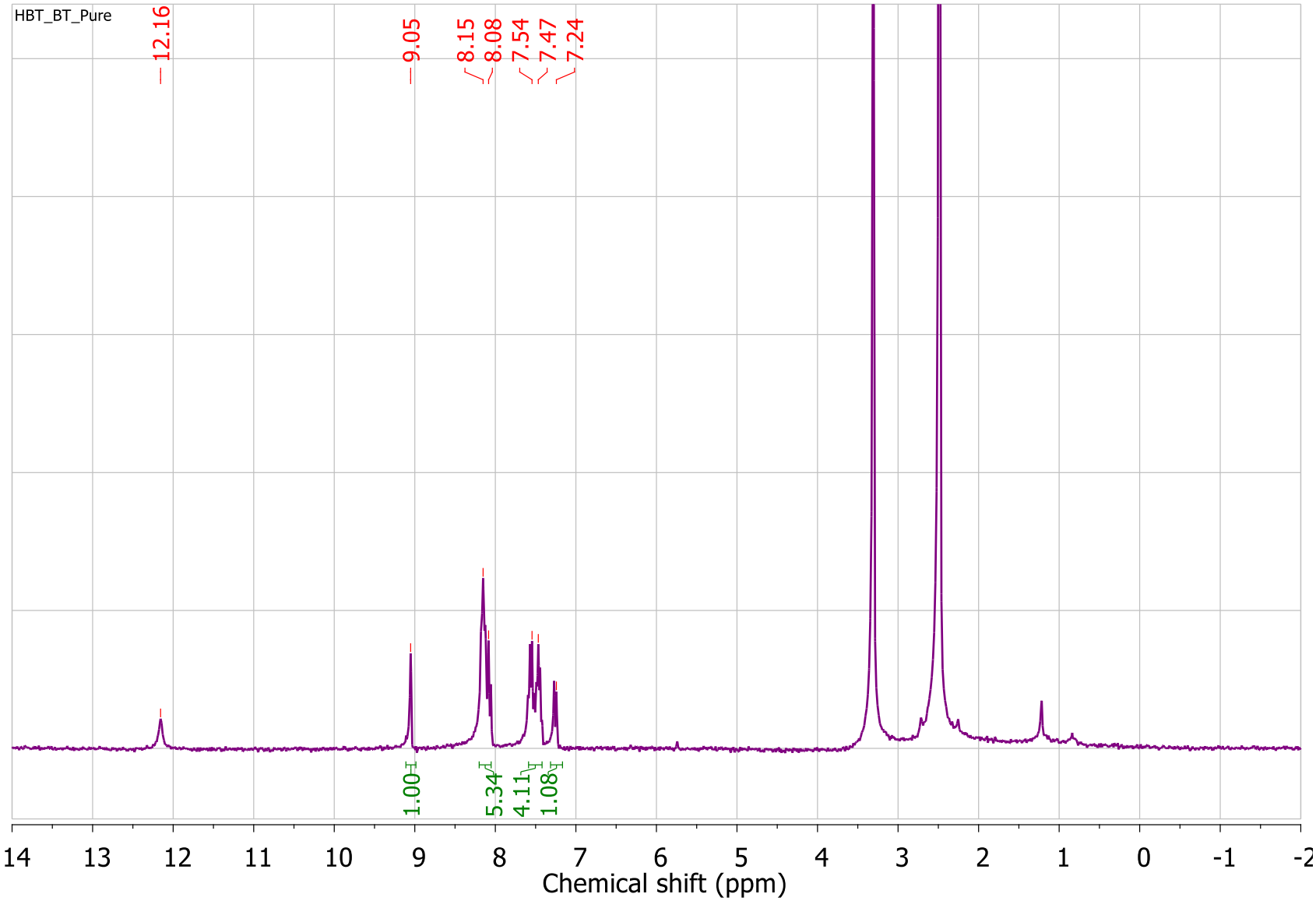


Figure S2.20 ^{1}H NMR spectra of **7** (300 MHz in DMSO-d6)

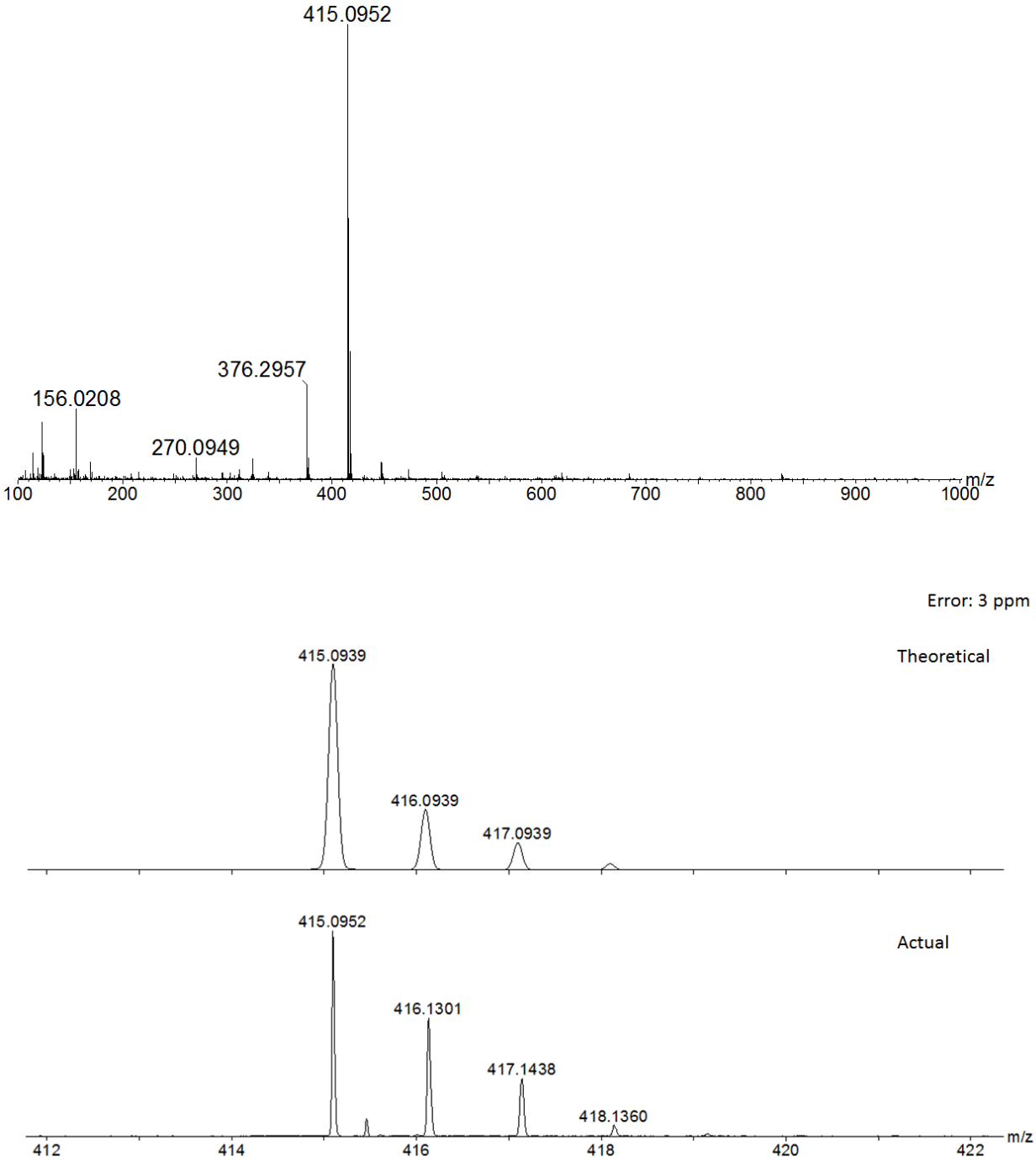


Figure S3.1 Mass spectra and isotope pattern (calculated vs experimental) of **2a** [$C_{24}H_{19}N_2OS_2^+$]

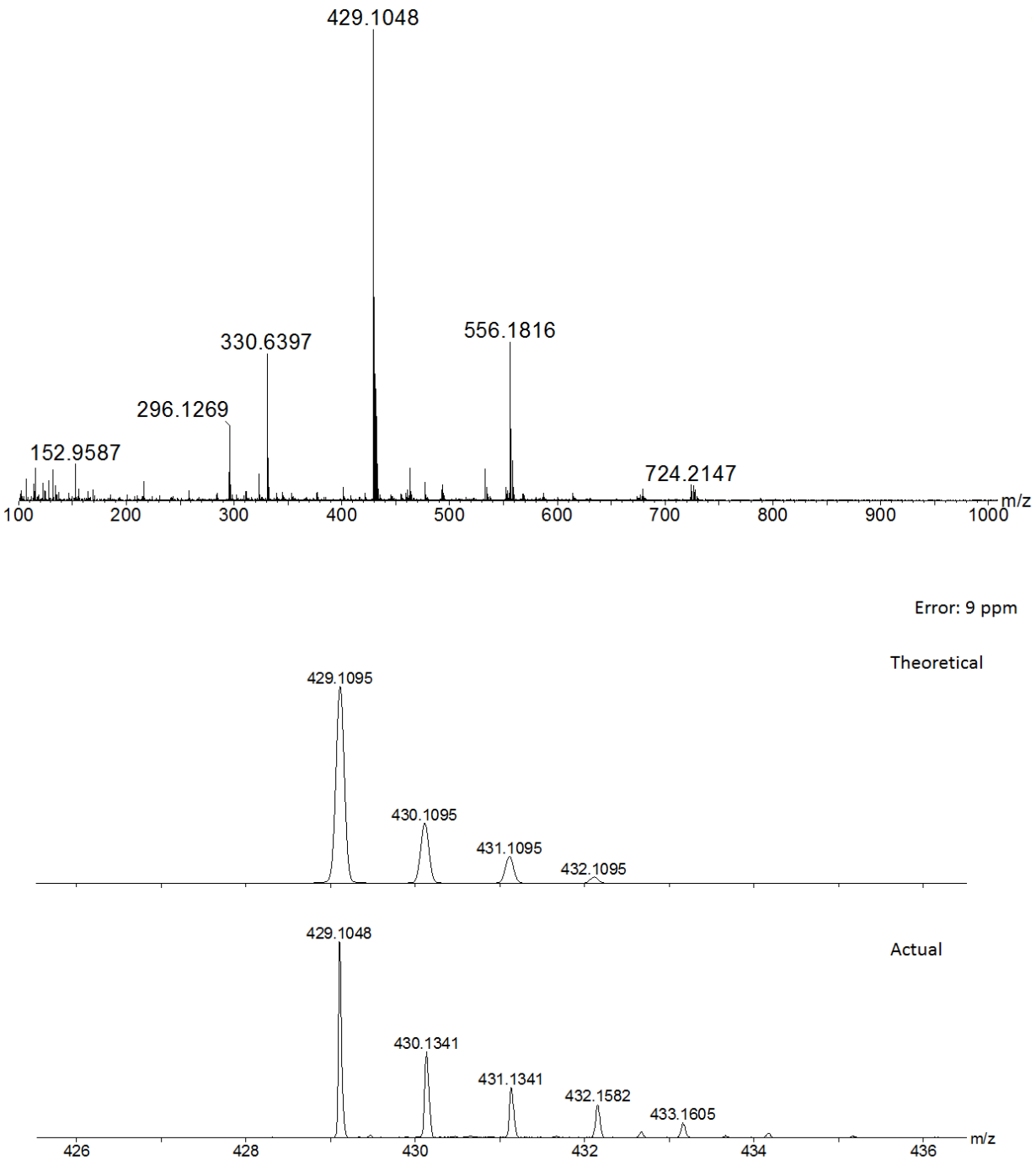


Figure S3.2 Mass spectra and isotope pattern (calculated vs experimental) of **2b** [$C_{25}H_{21}N_2OS_2^+$]

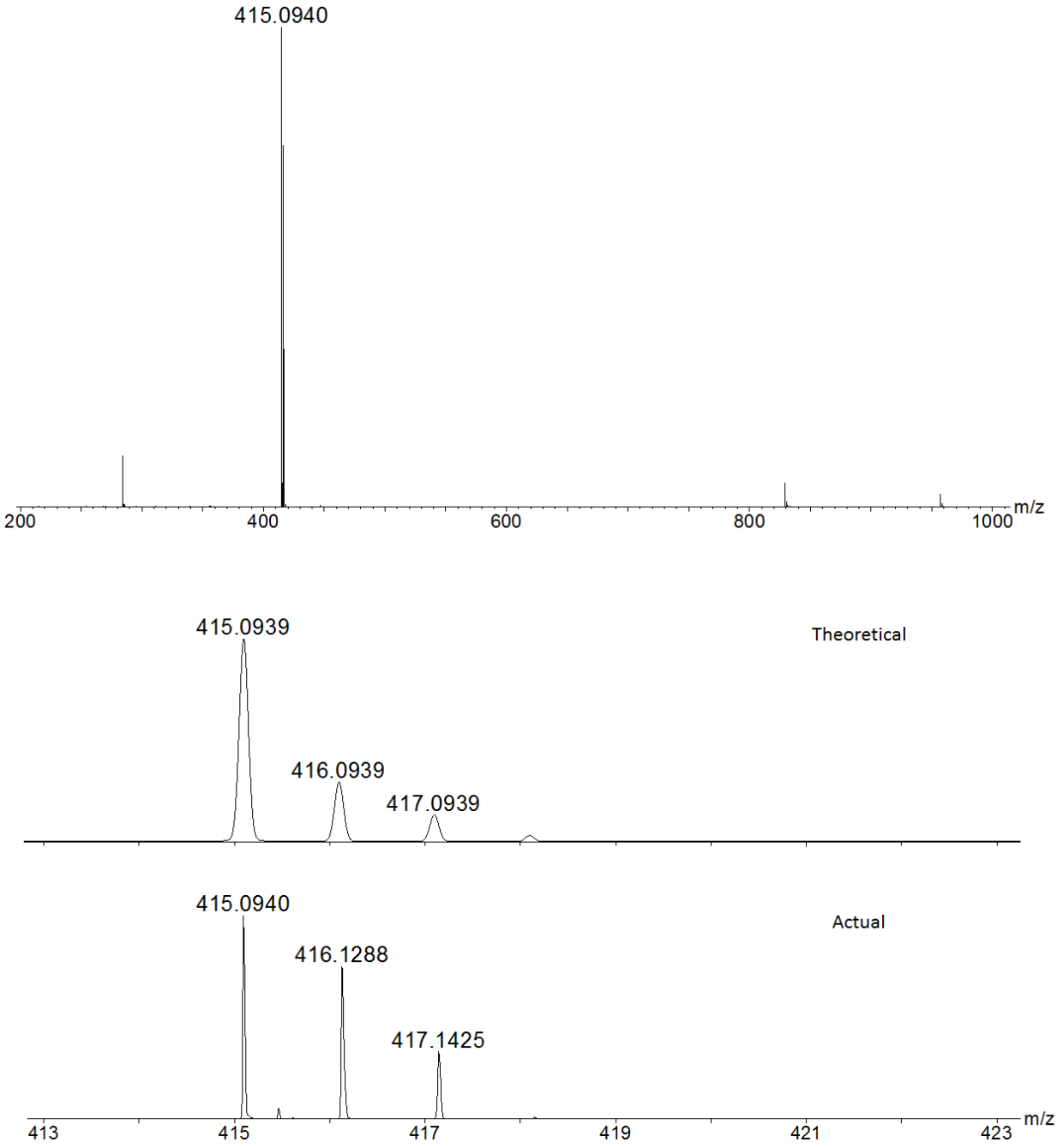


Figure S3.3 Mass spectra and isotope pattern (calculated vs experimental) of **3a** [$C_{24}H_{19}N_2OS_2^+$]

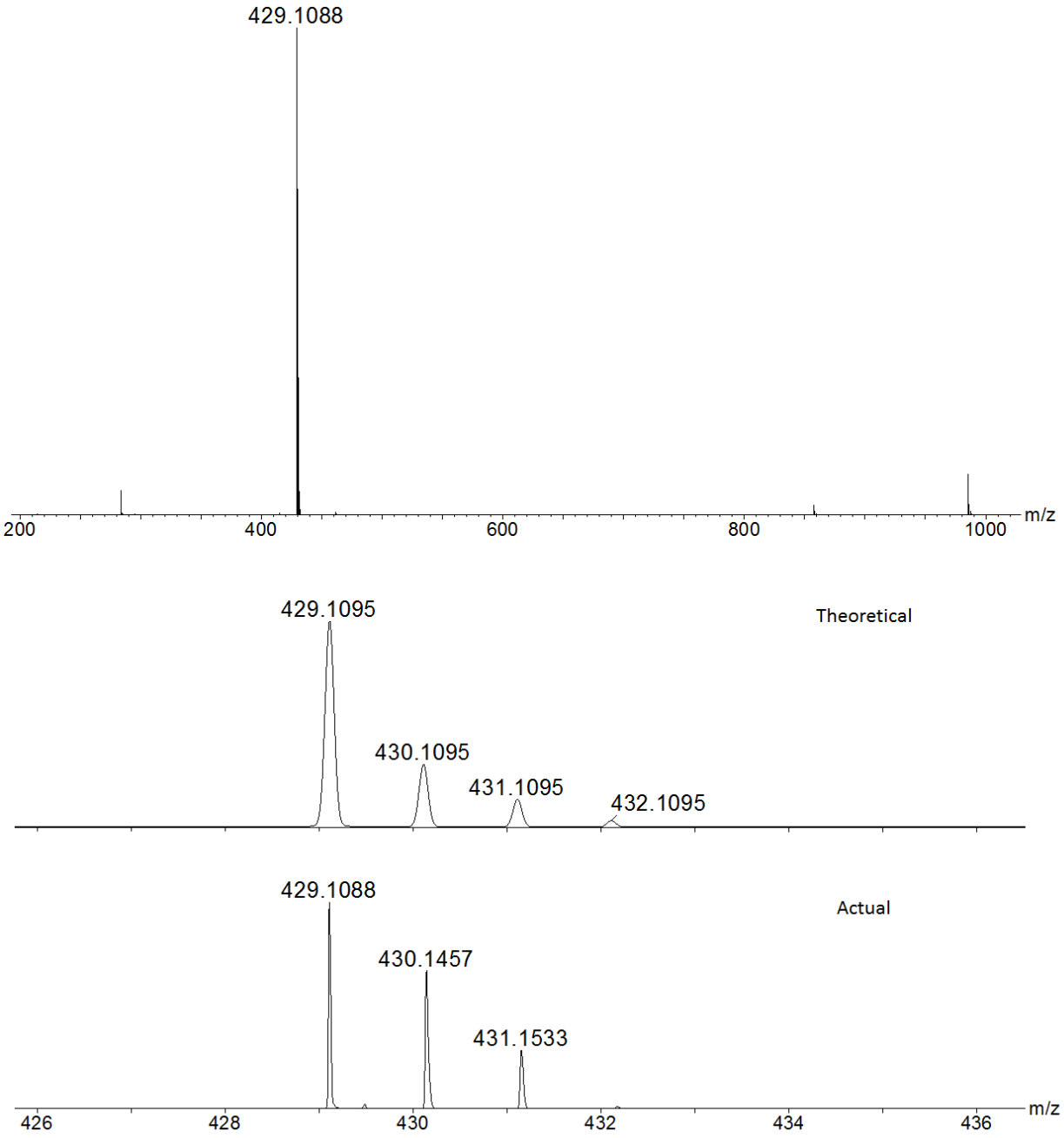


Figure S3.4 Mass spectra and isotope pattern (calculated vs experimental) of **3b** [$C_{25}H_{21}N_2OS_2^+$]

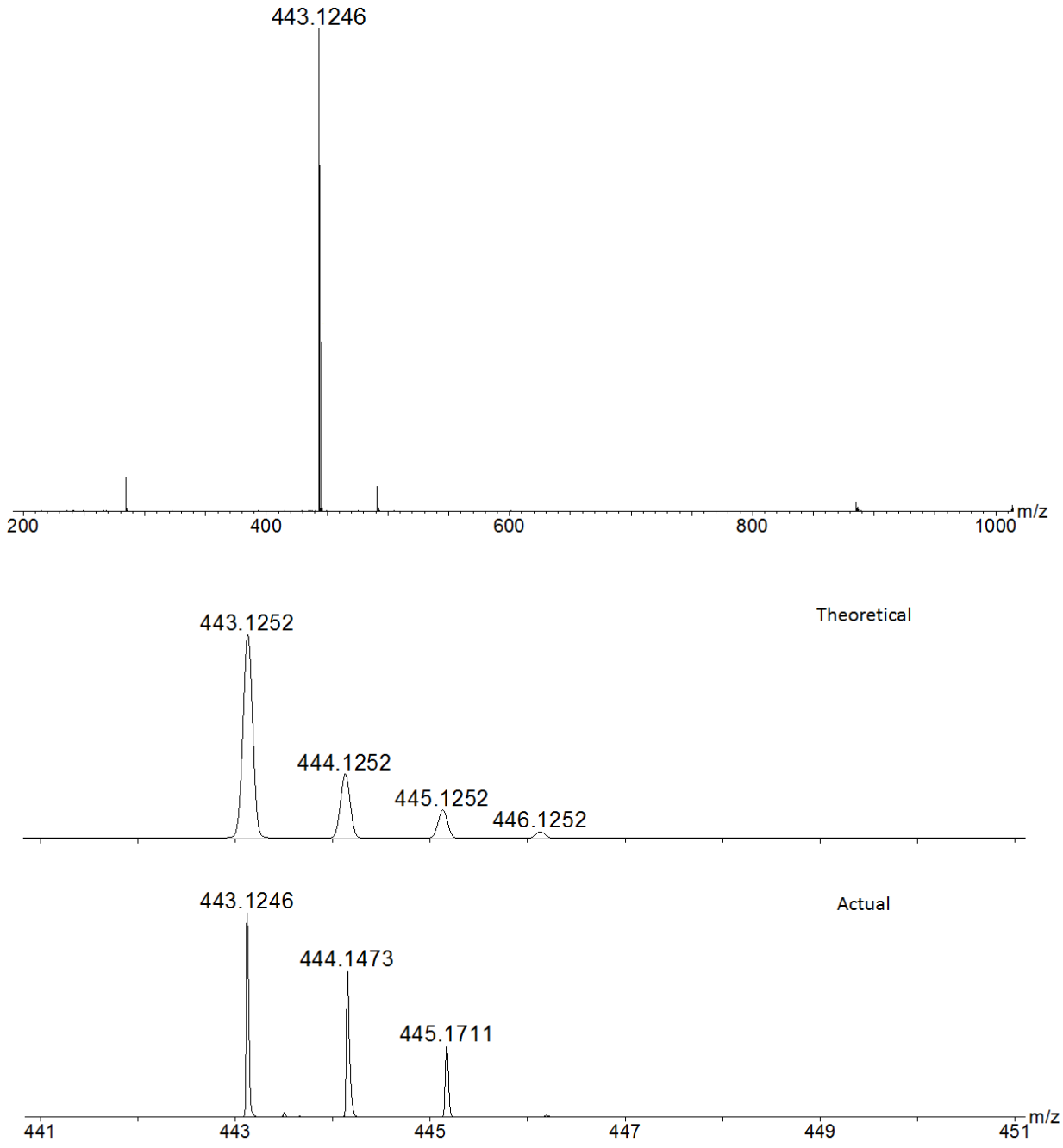


Figure S3.5 Mass spectra and isotope pattern (calculated vs experimental) of **3c** [$C_{26}H_{23}N_2OS_2^+$]

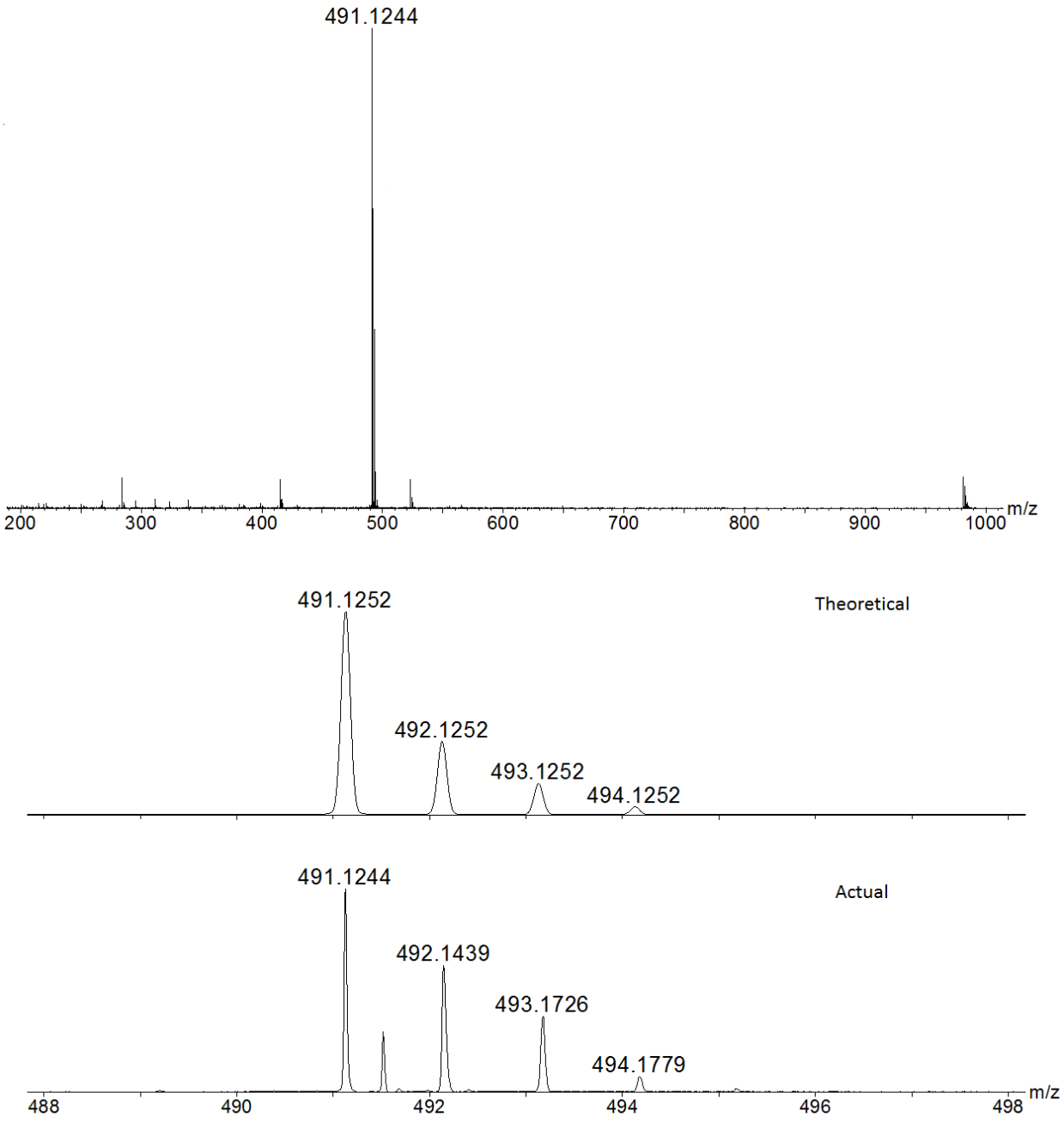


Figure S3.6 Mass spectra and isotope pattern (calculated vs experimental) of **3d** [$C_{30}H_{23}N_2OS_2^+$]

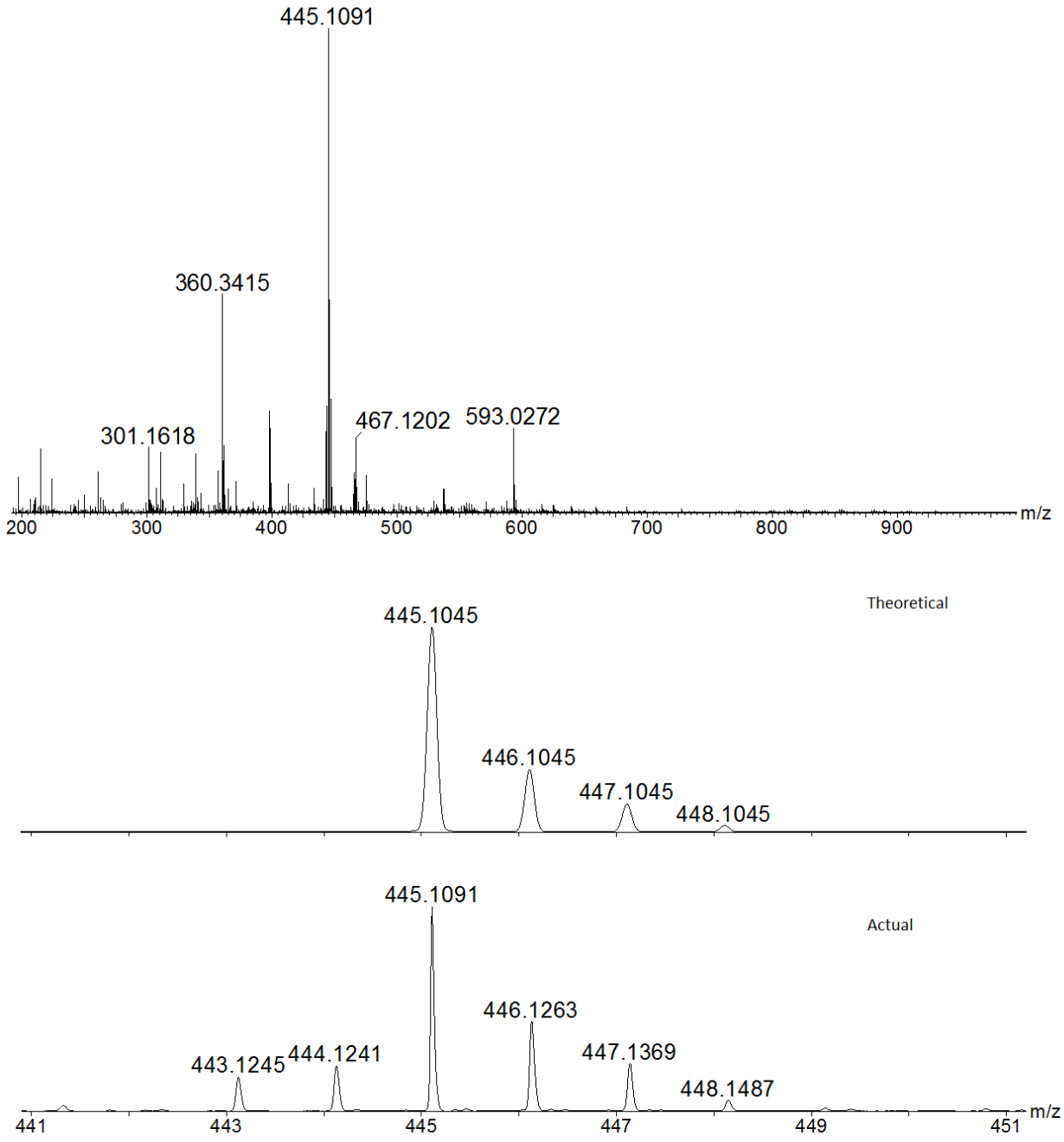


Figure S3.7 Mass spectra and isotope pattern (calculated vs experimental) of **4a** [$C_{25}H_{21}N_2O_2S_2^+$]

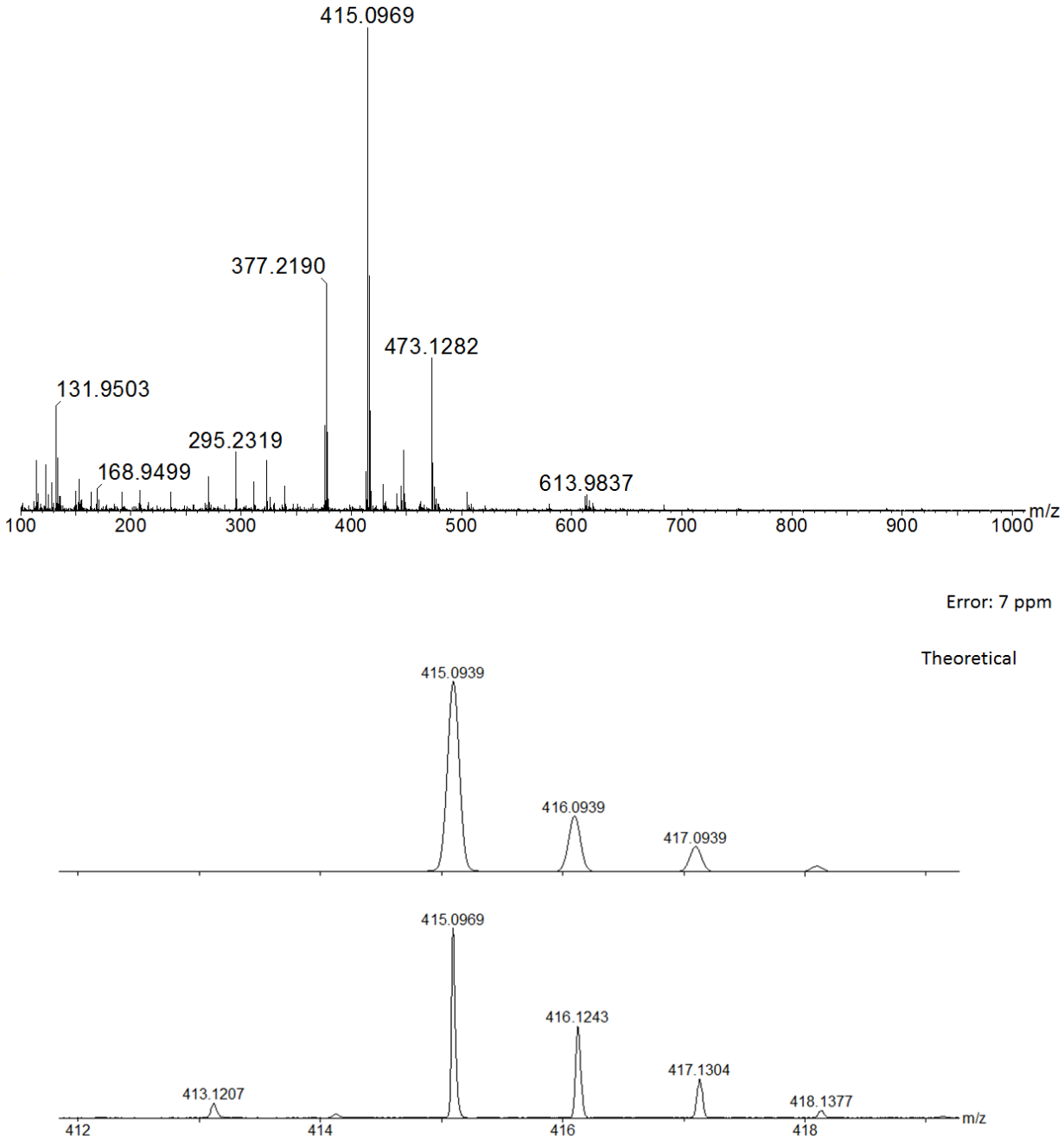


Figure S3.8 Mass spectra and isotope pattern (calculated vs experimental) of **5a** [$C_{24}H_{19}N_2OS_2^+$]

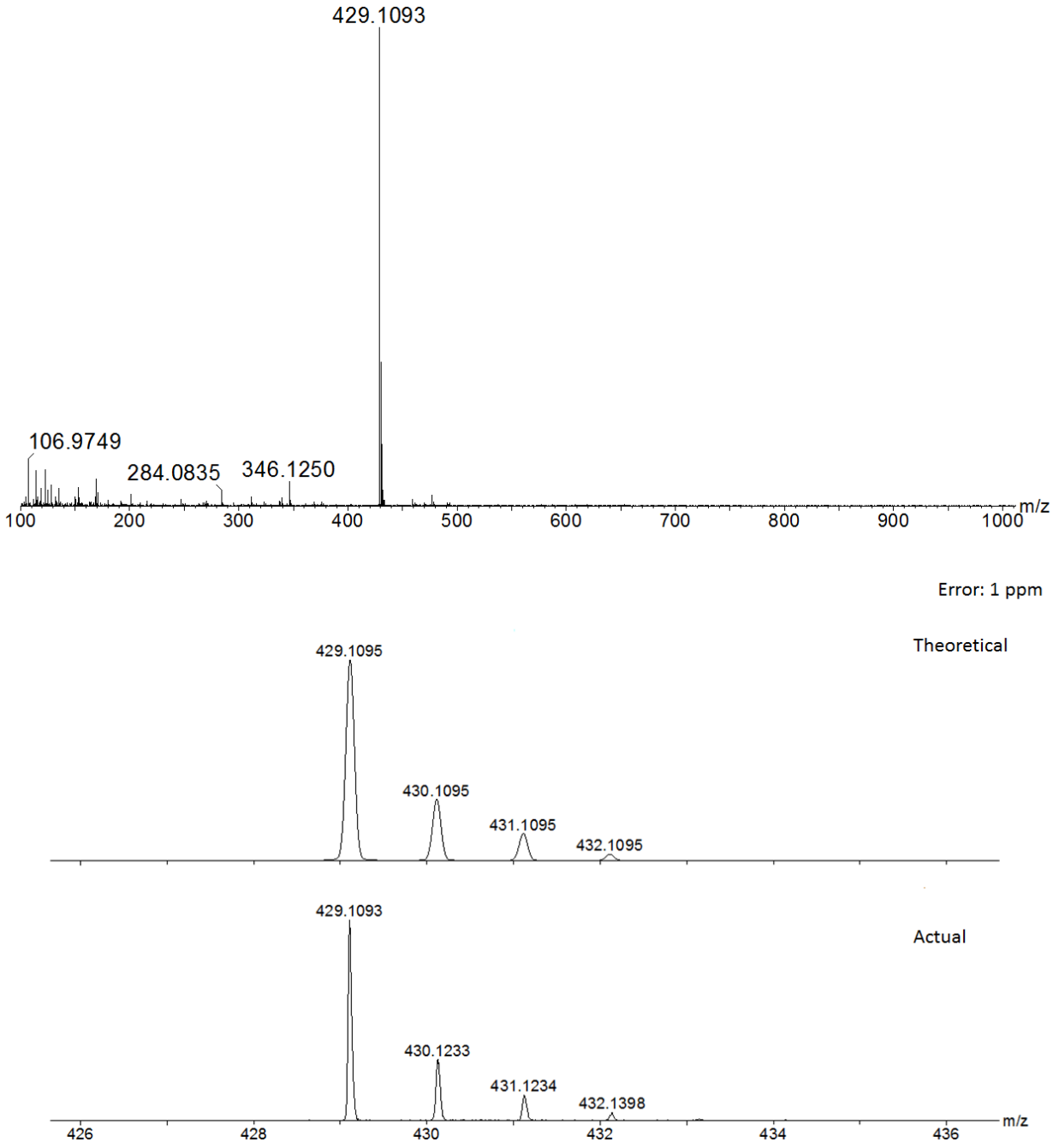


Figure S3.9 Mass spectra and isotope pattern (calculated vs experimental) of **5b** [$C_{25}H_{21}N_2OS_2^+$]

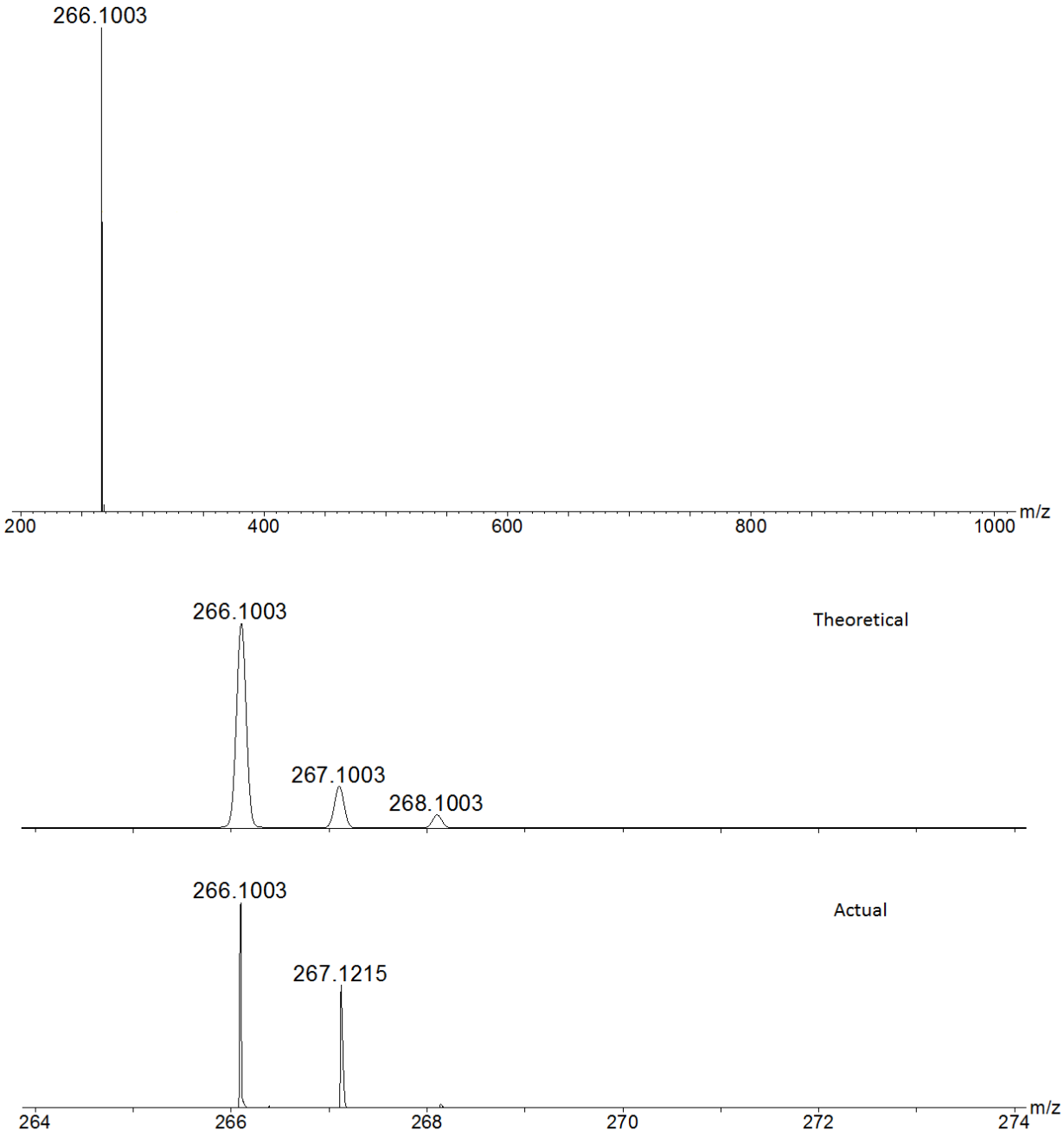


Figure S3.10 Mass spectra and isotope pattern (calculated vs experimental) of **6a** [$C_{17}H_{16}NS^{+}$]

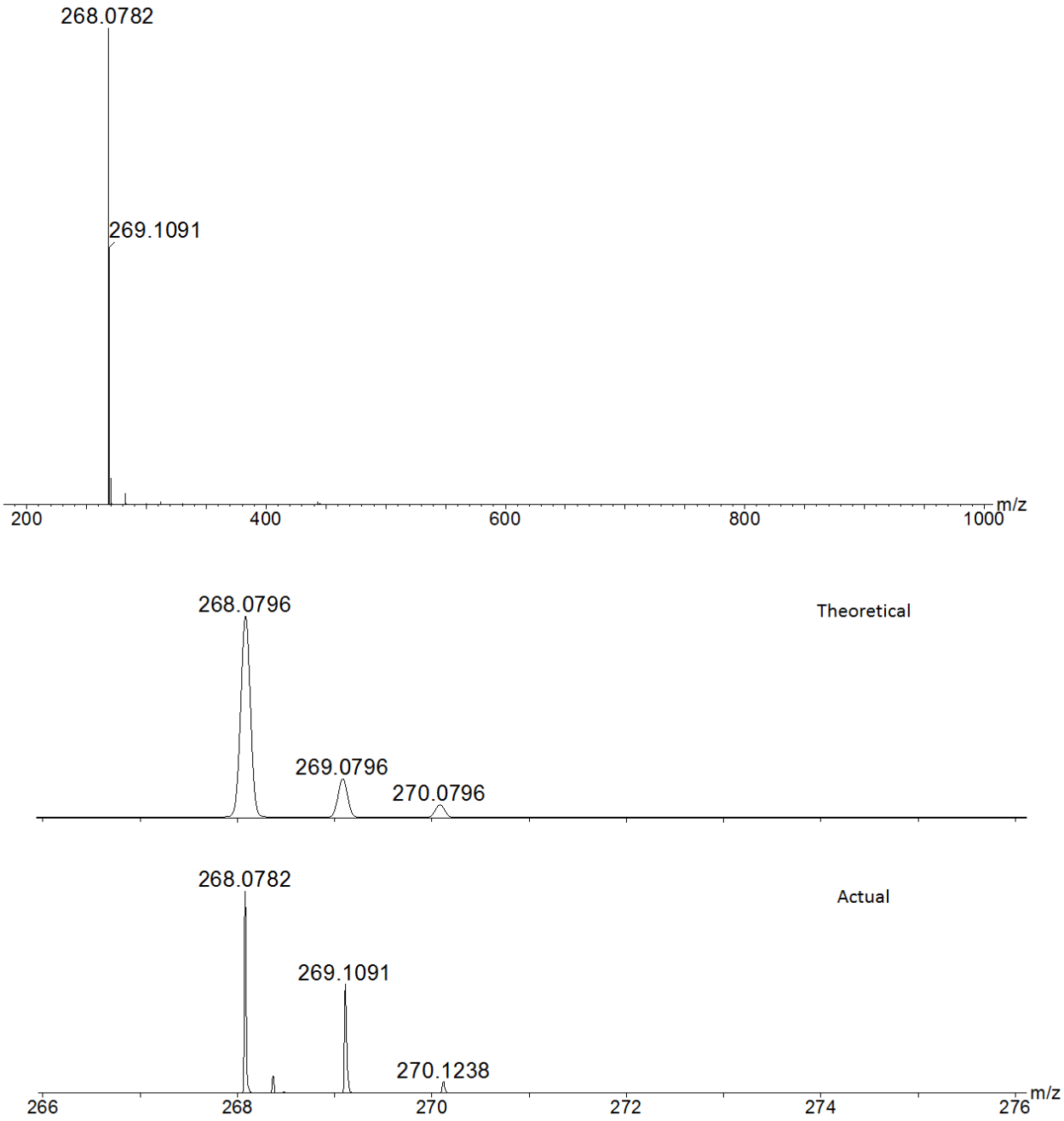


Figure S3.11 Mass spectra and isotope pattern (calculated vs experimental) of **6b** [$C_{16}H_{14}NOS^{+}$]

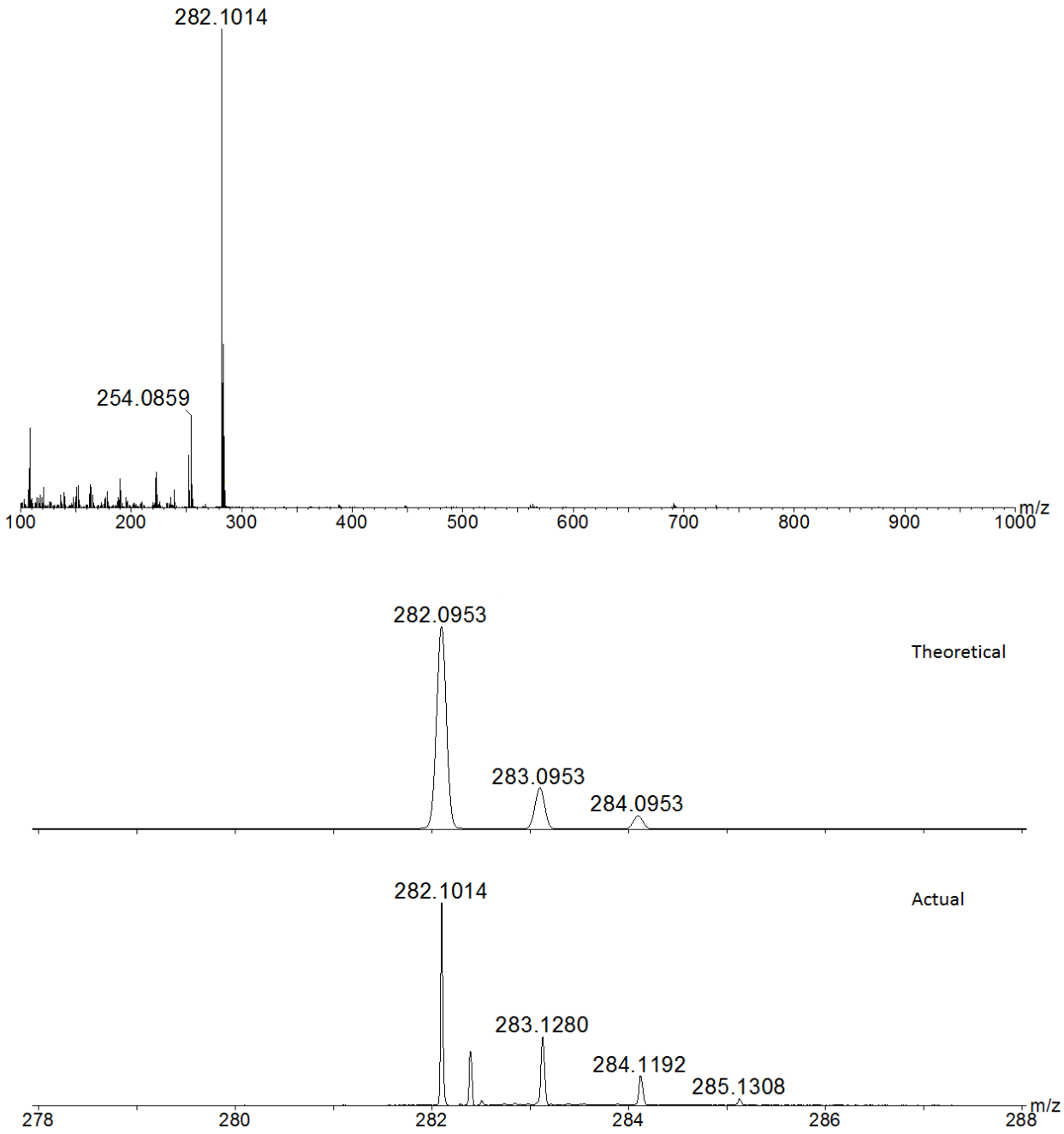


Figure S3.12 Mass spectra and isotope pattern (calculated vs experimental) of **6c** [$C_{17}H_{16}NOS^{+}$]

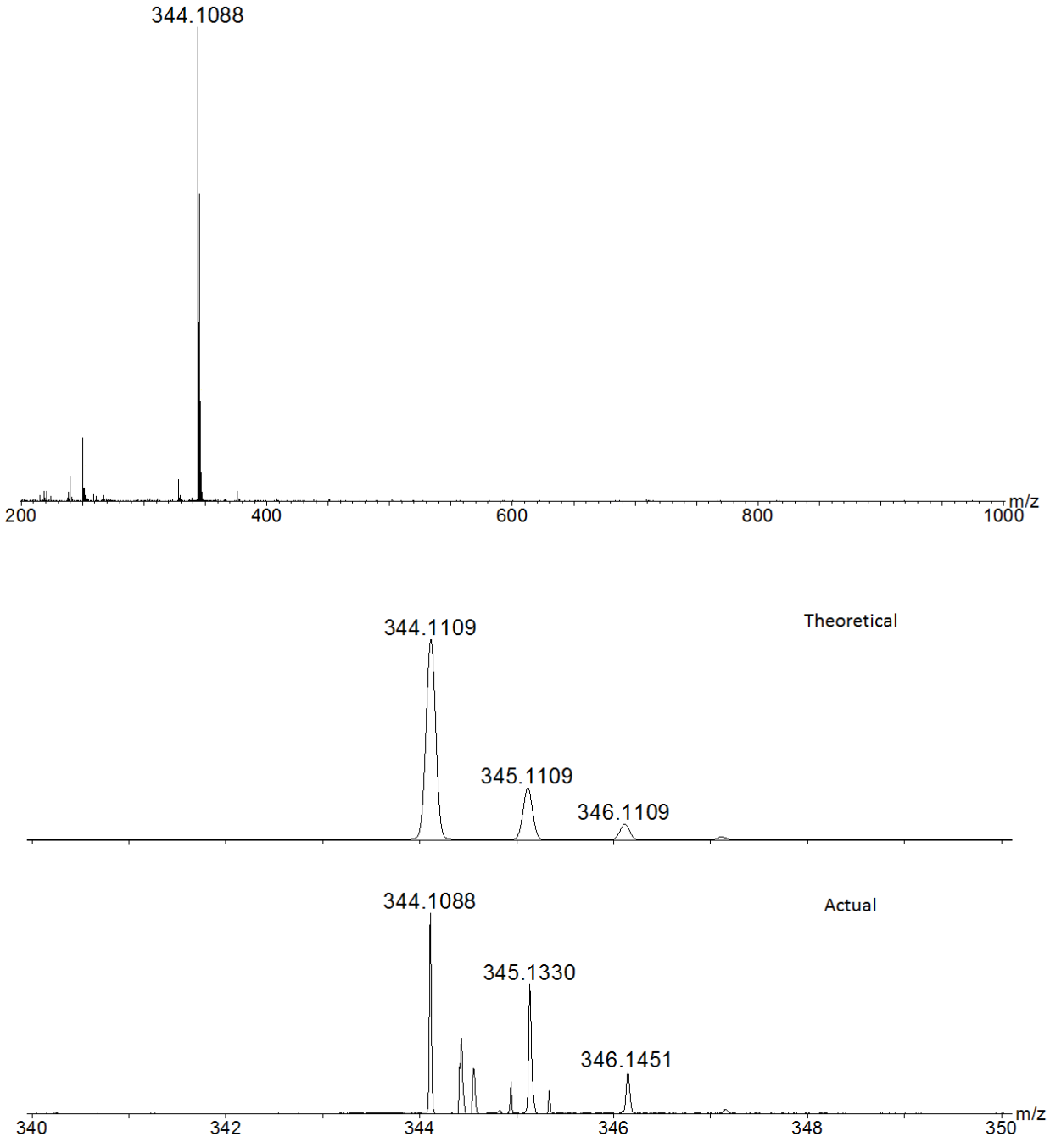


Figure S3.13 Mass spectra and isotope pattern (calculated vs experimental) of **6d** [$C_{22}H_{18}NOS^{+}$]

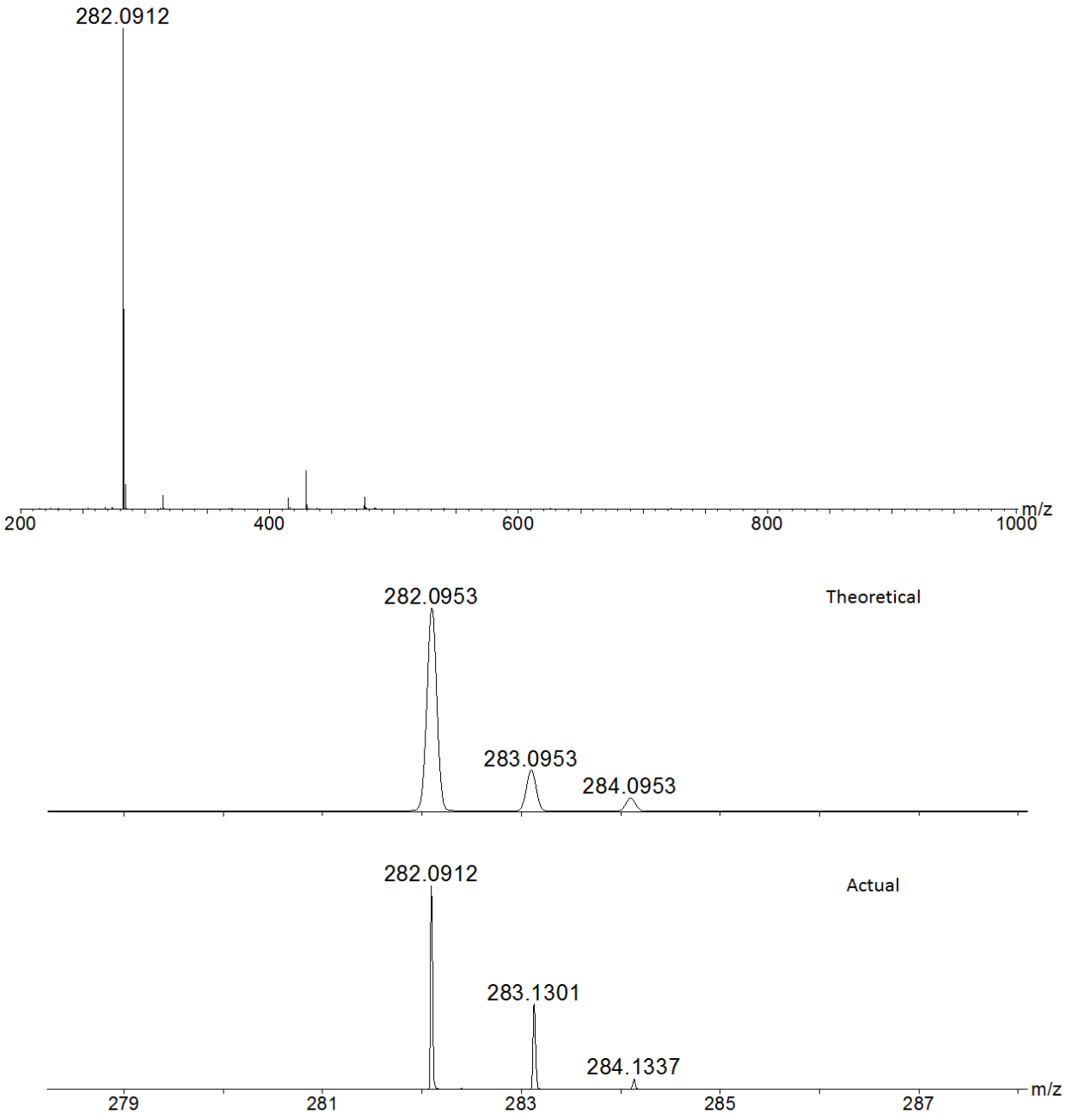


Figure S3.14 Mass spectra and isotope pattern (calculated vs experimental) of **6e** [$C_{17}H_{16}NOS^{+}$]

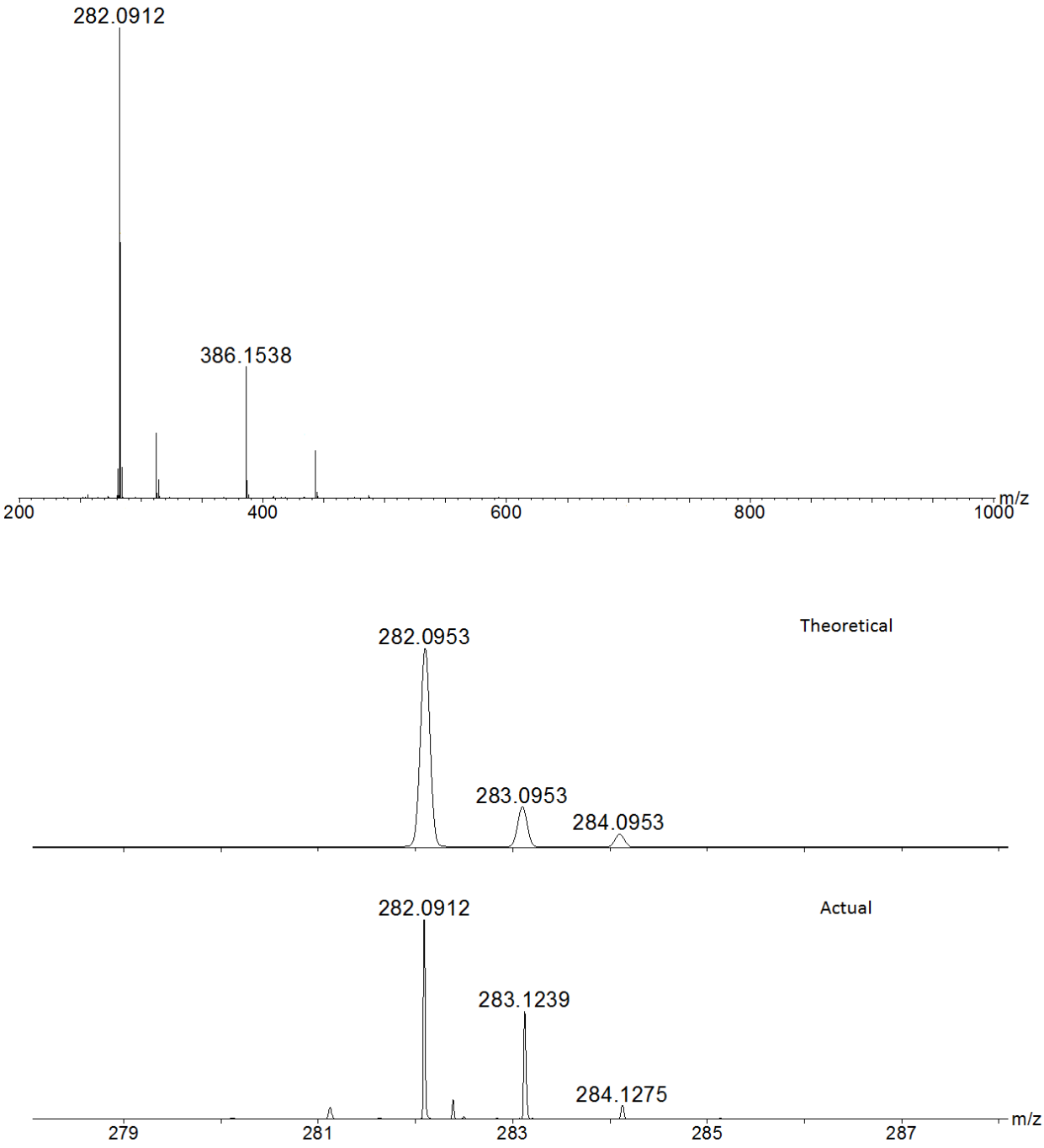


Figure S3.15 Mass spectra and isotope pattern (calculated vs experimental) of **6f** [$C_{17}H_{16}NOS^{+}$]

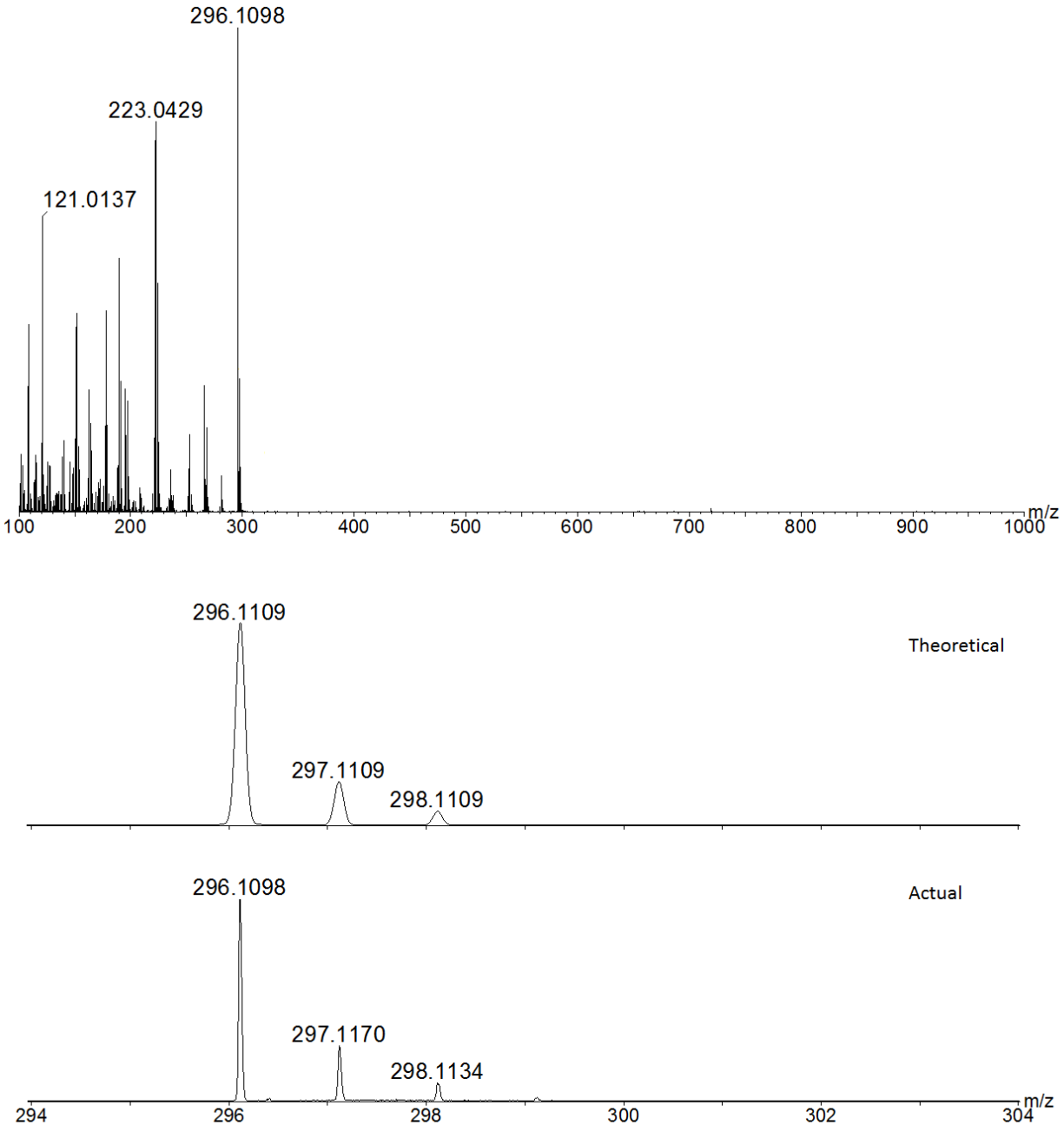


Figure S3.16 Mass spectra and isotope pattern (calculated vs experimental) of **6g** [$C_{18}H_{18}NOS^{+}$]

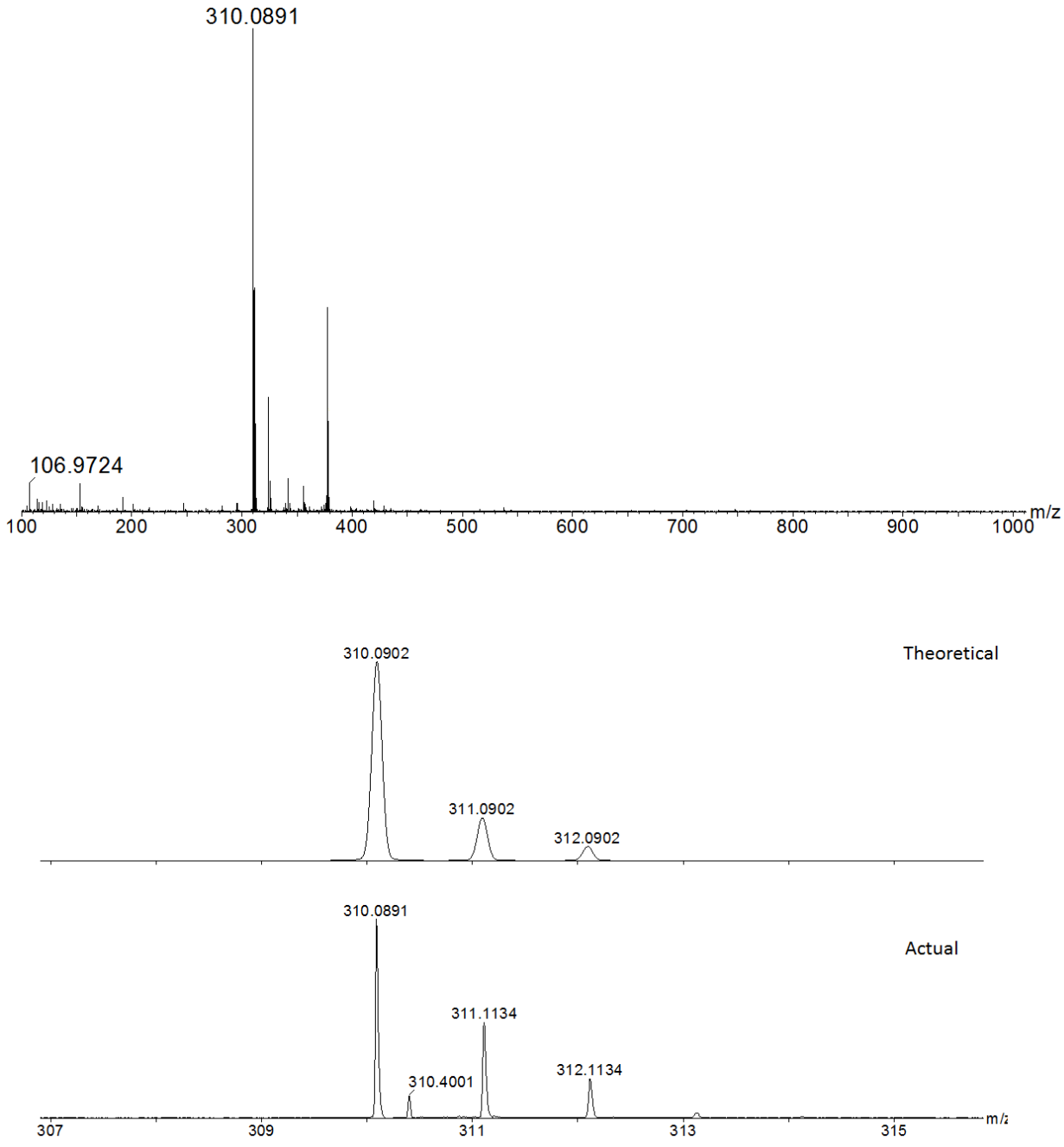


Figure S3.17 Mass spectra and isotope pattern (calculated vs experimental) of **8a** [$C_{18}H_{16}NO_2S^+$]

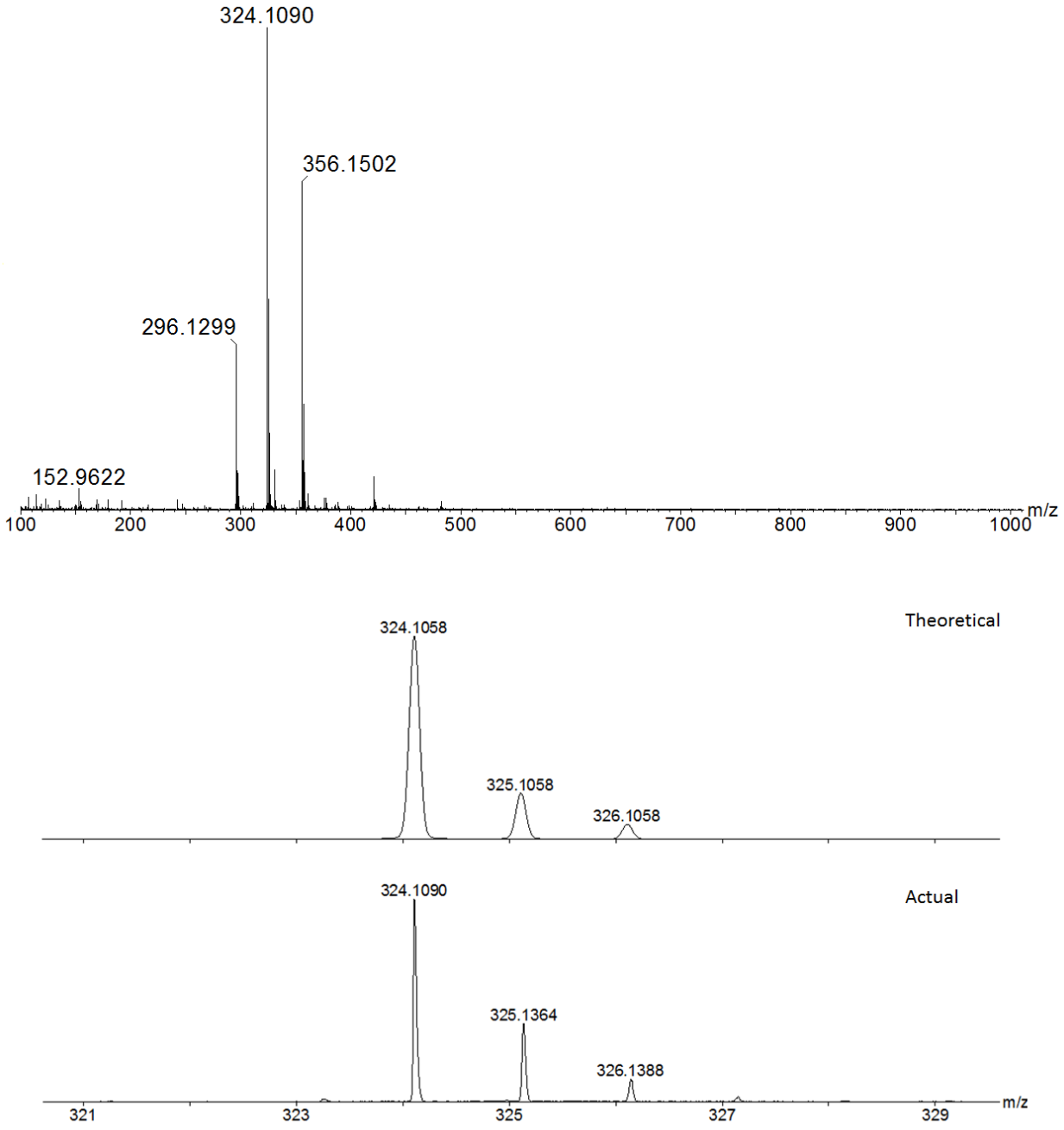


Figure S3.18 Mass spectra and isotope pattern (calculated vs experimental) of **8b** [$C_{19}H_{18}NO_2S^+$]

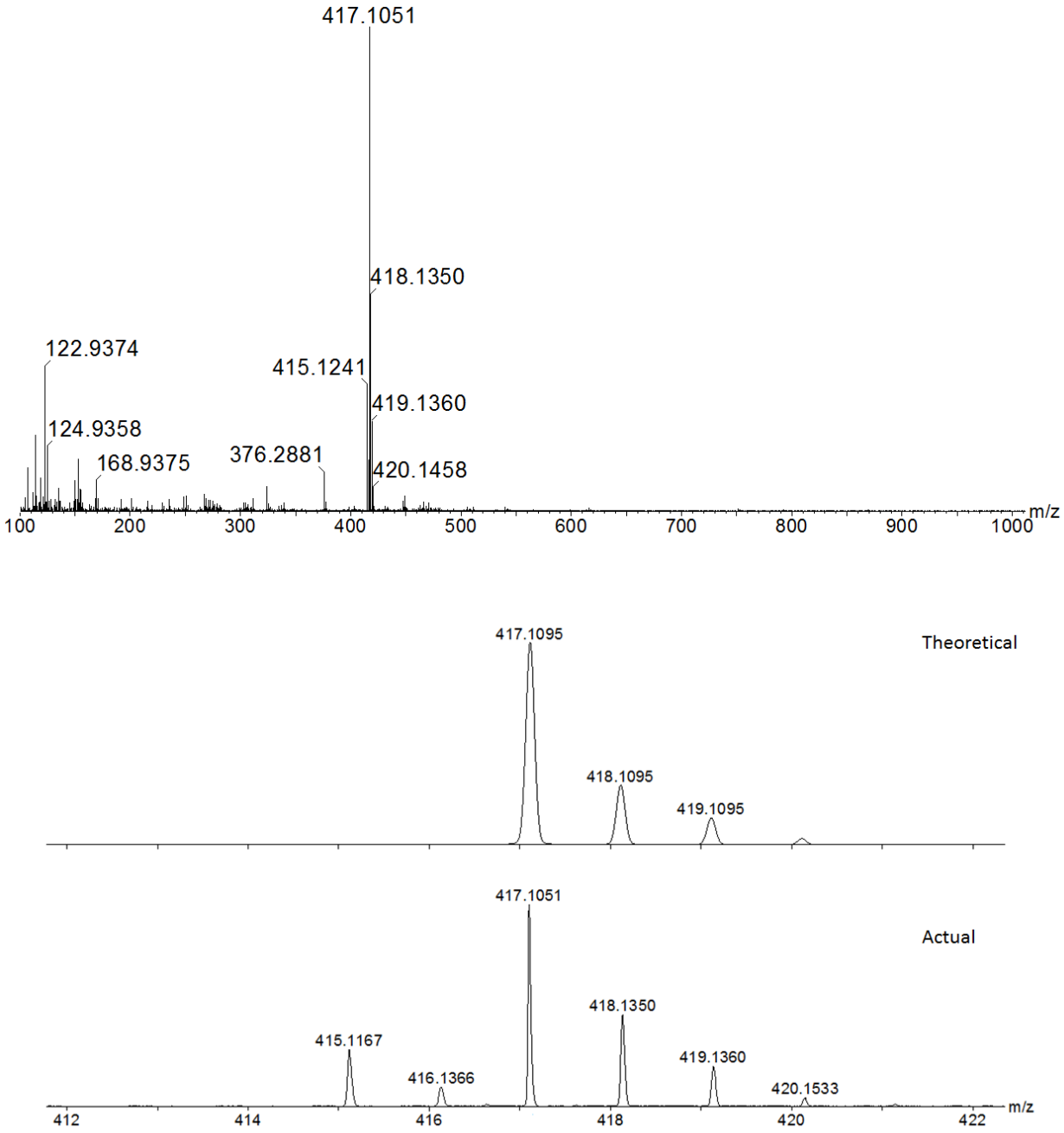


Figure S3.19 Mass spectra and isotope pattern (calculated vs experimental) of **2c** [$C_{24}H_{21}N_2OS_2^+$]

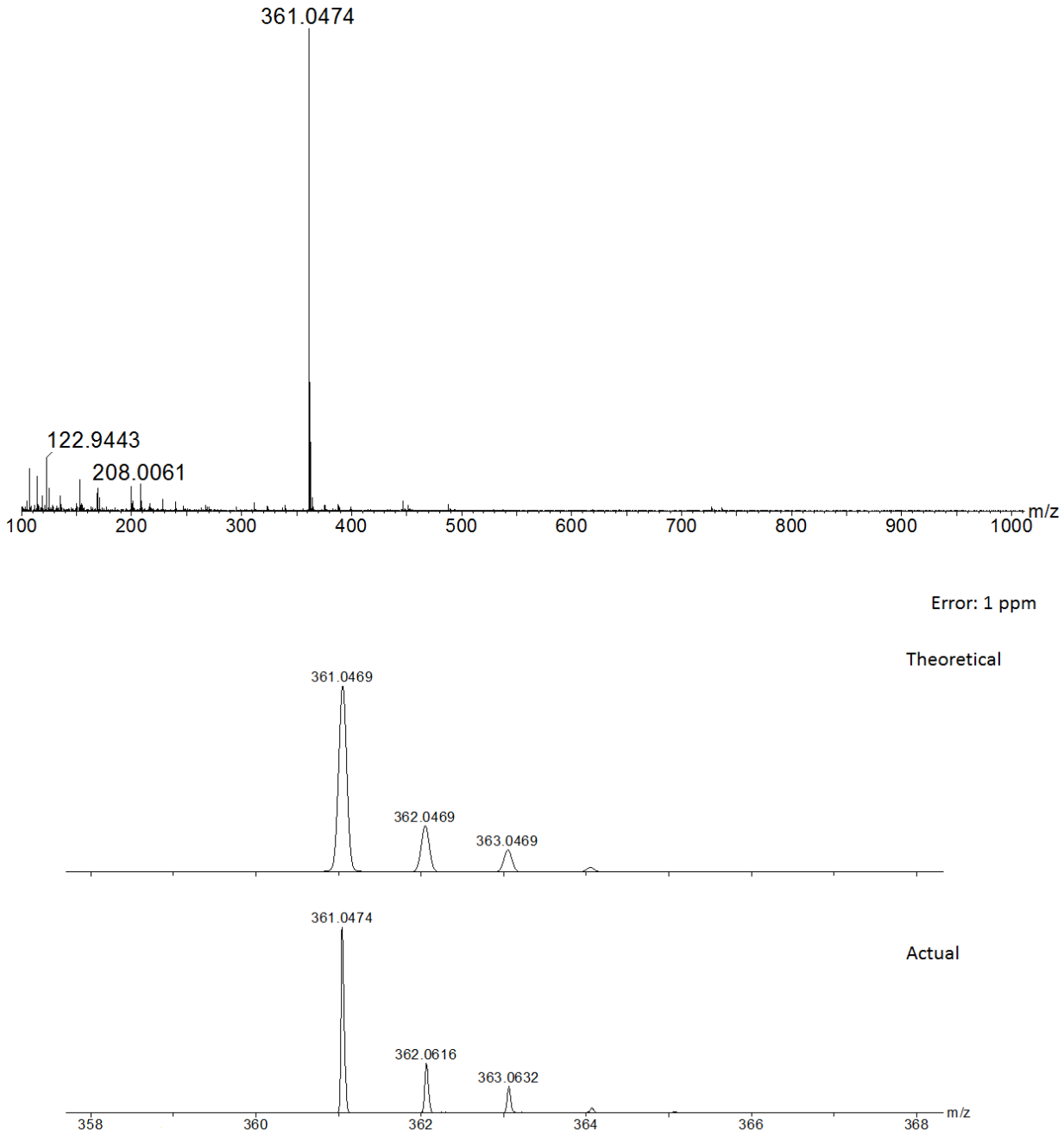


Figure S3.20 Mass spectra and isotope pattern (calculated vs experimental) of **7** [$C_{20}H_{13}N_2OS_2^+$]

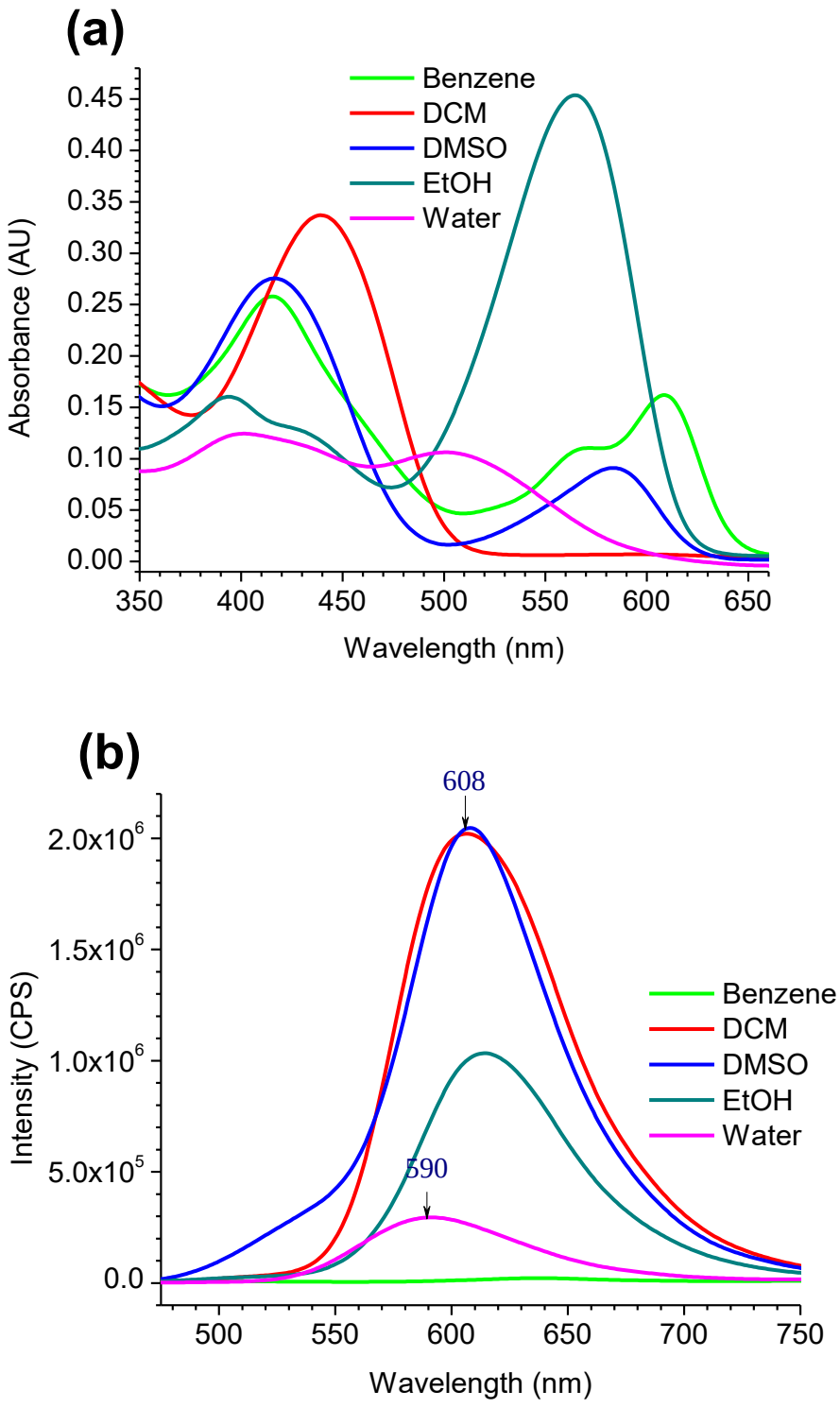


Figure S4.1 Absorbance (a) and emission (b) of probe **2a** (1 x 10^{-5} M) in different solvents at room temperature.

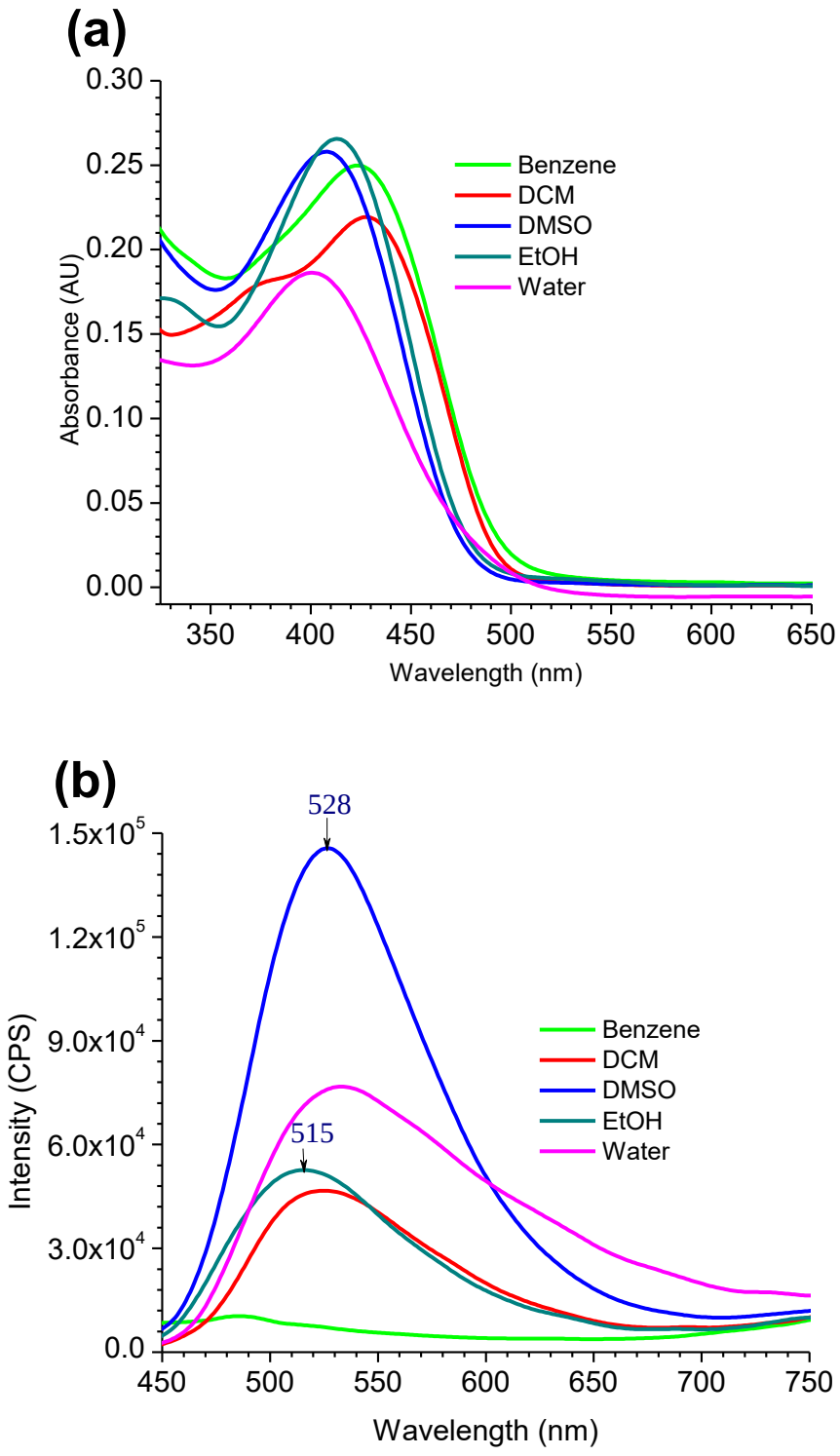


Figure S4.2 Absorbance (a) and emission (b) of probe **2b** (1 x 10^{-5} M) in different solvents at room temperature.

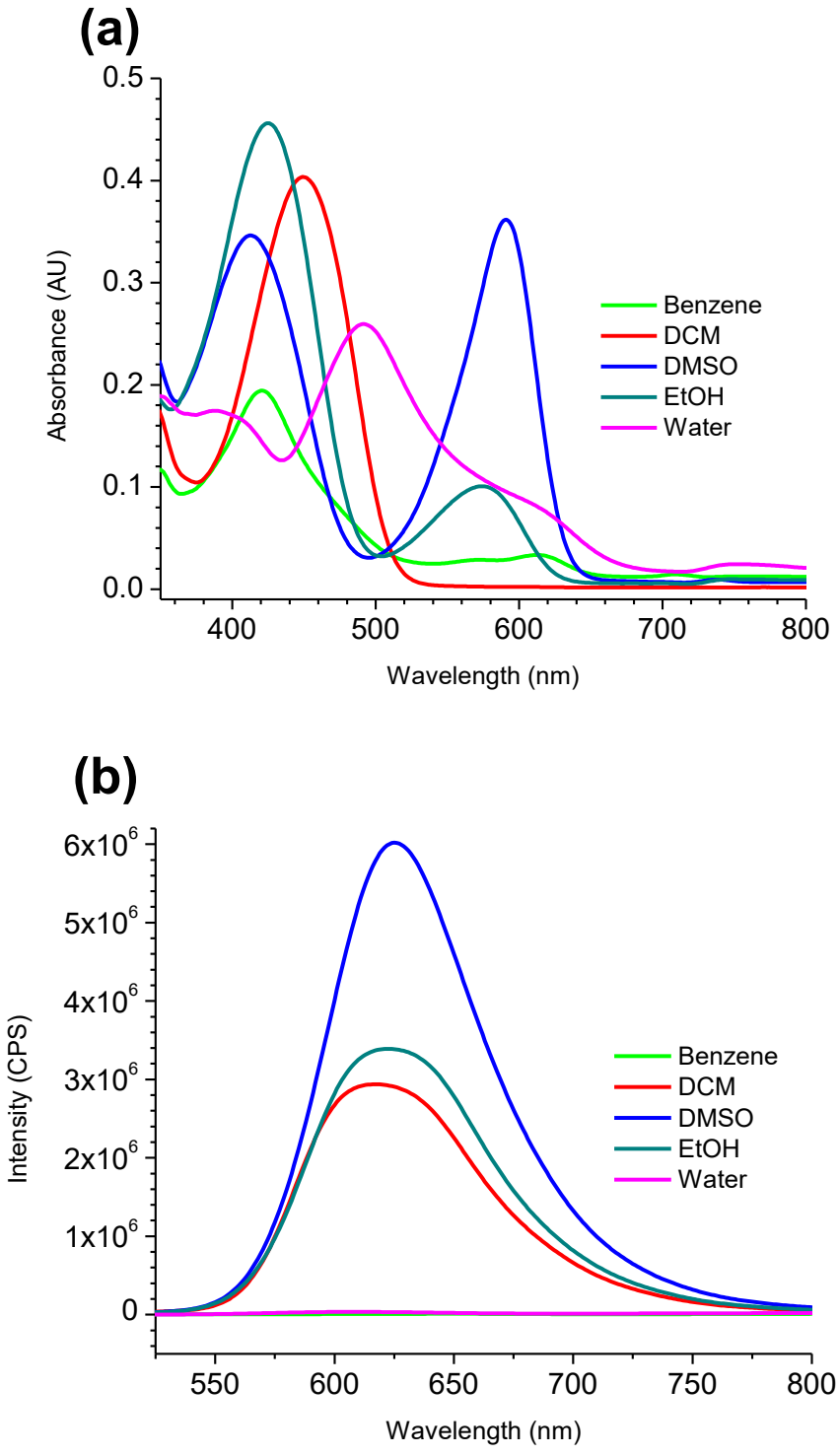


Figure S4.3 Absorbance (a) and emission (b) of probe **3a** (1 x 10^{-5} M) in different solvents at room temperature.

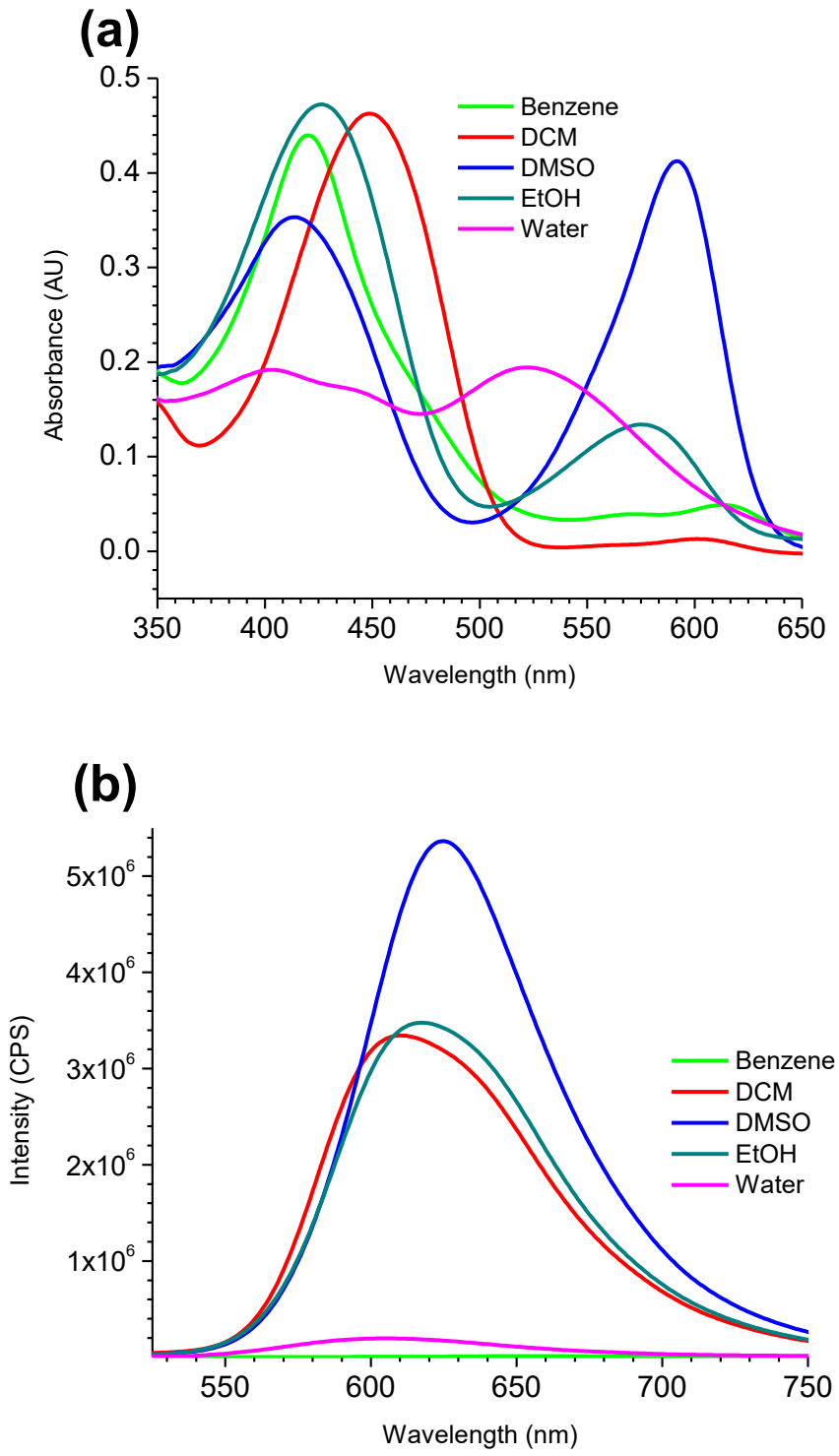


Figure S4.4 Absorbance (a) and emission (b) of probe **3b** (1 x 10^{-5} M) in different solvents at room temperature.

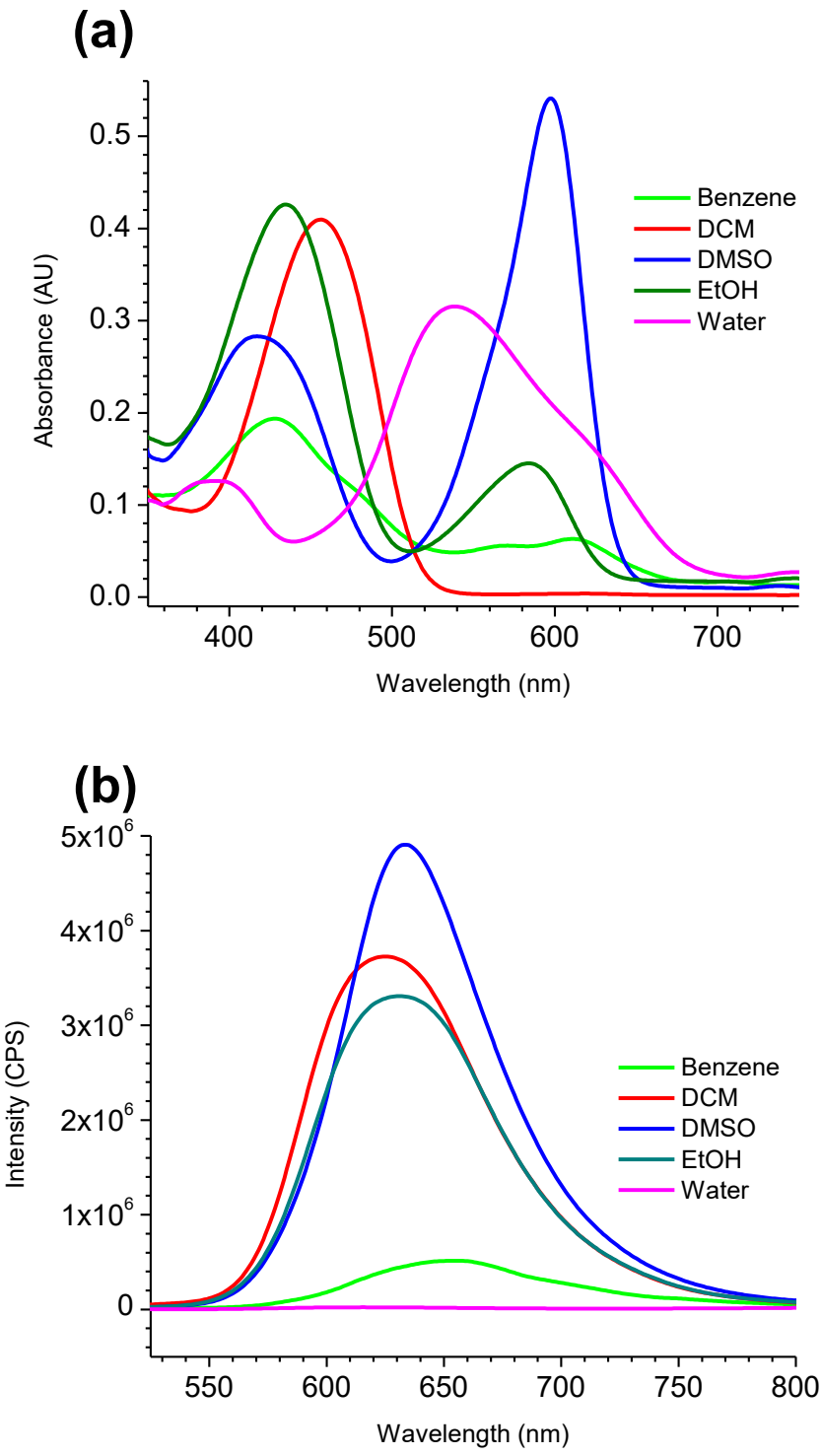


Figure S4.5 Absorbance (a) and emission (b) of probe **3c** (1 x 10^{-5} M) in different solvents at room temperature.

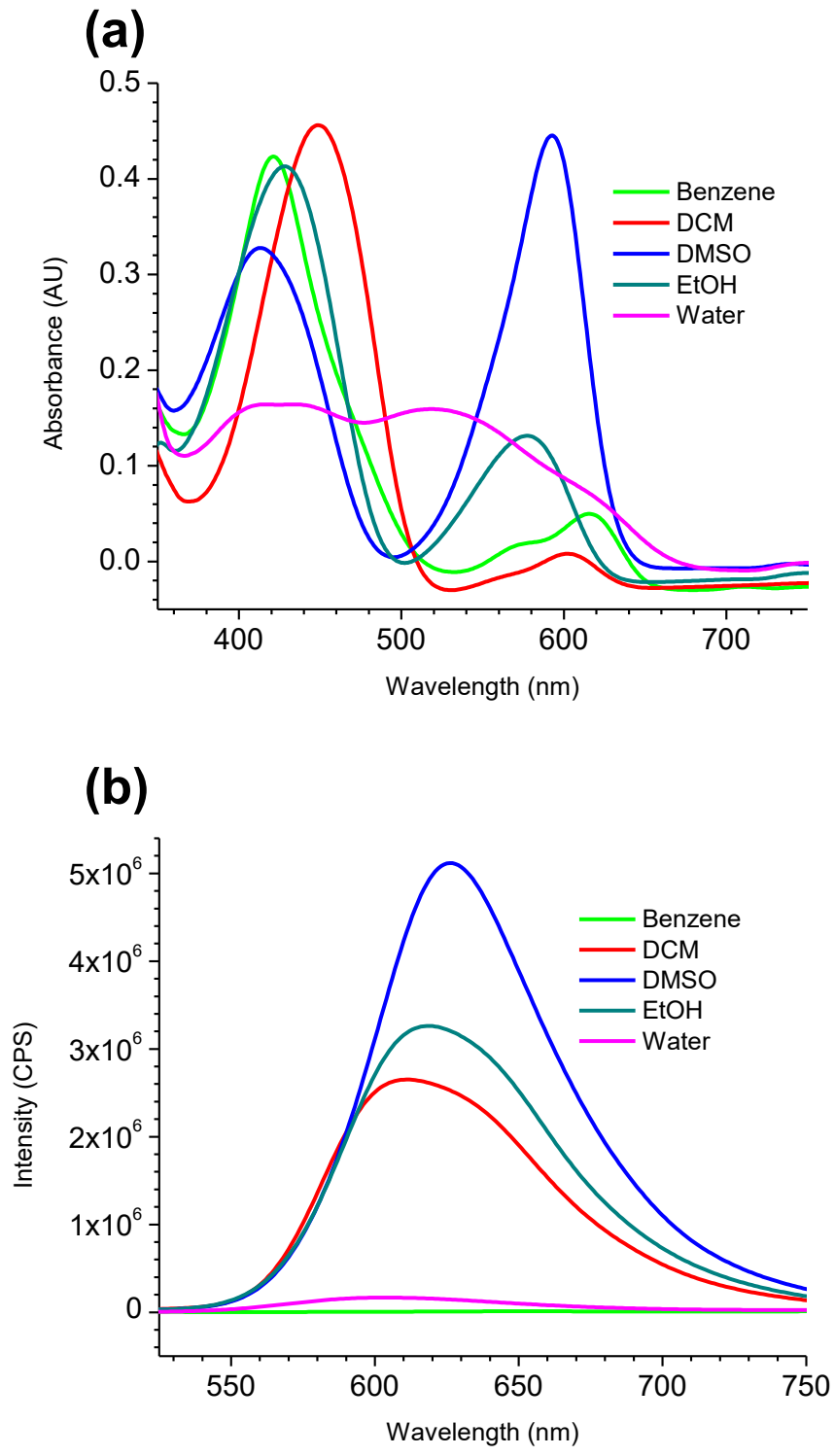


Figure S4.6 Absorbance (a) and emission (b) of probe **3d** (1 x 10^{-5} M) in different solvents at room temperature.

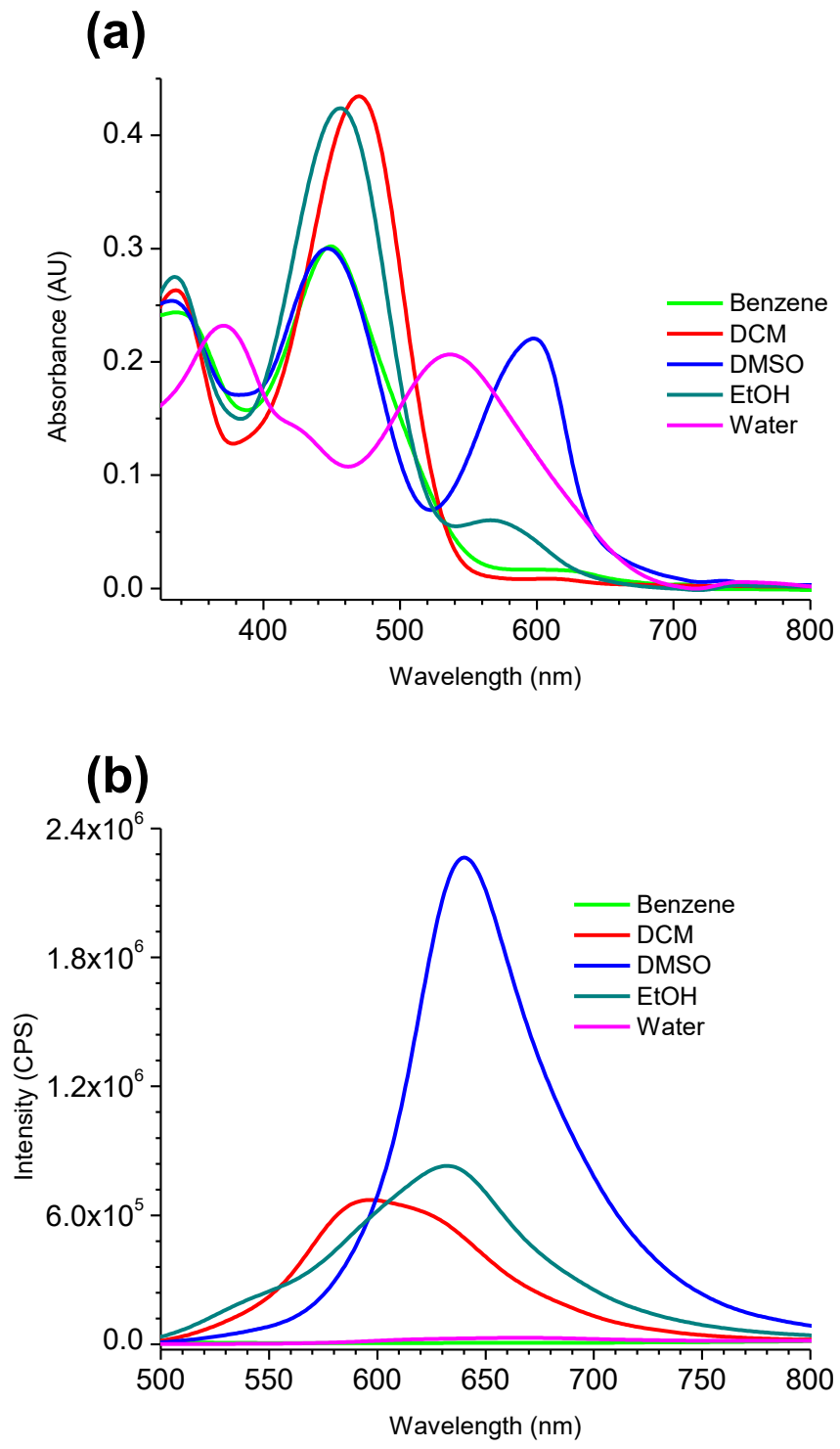


Figure S4.7 Absorbance (a) and emission (b) of probe **4a** (1 x 10^{-5} M) in different solvents at room temperature.

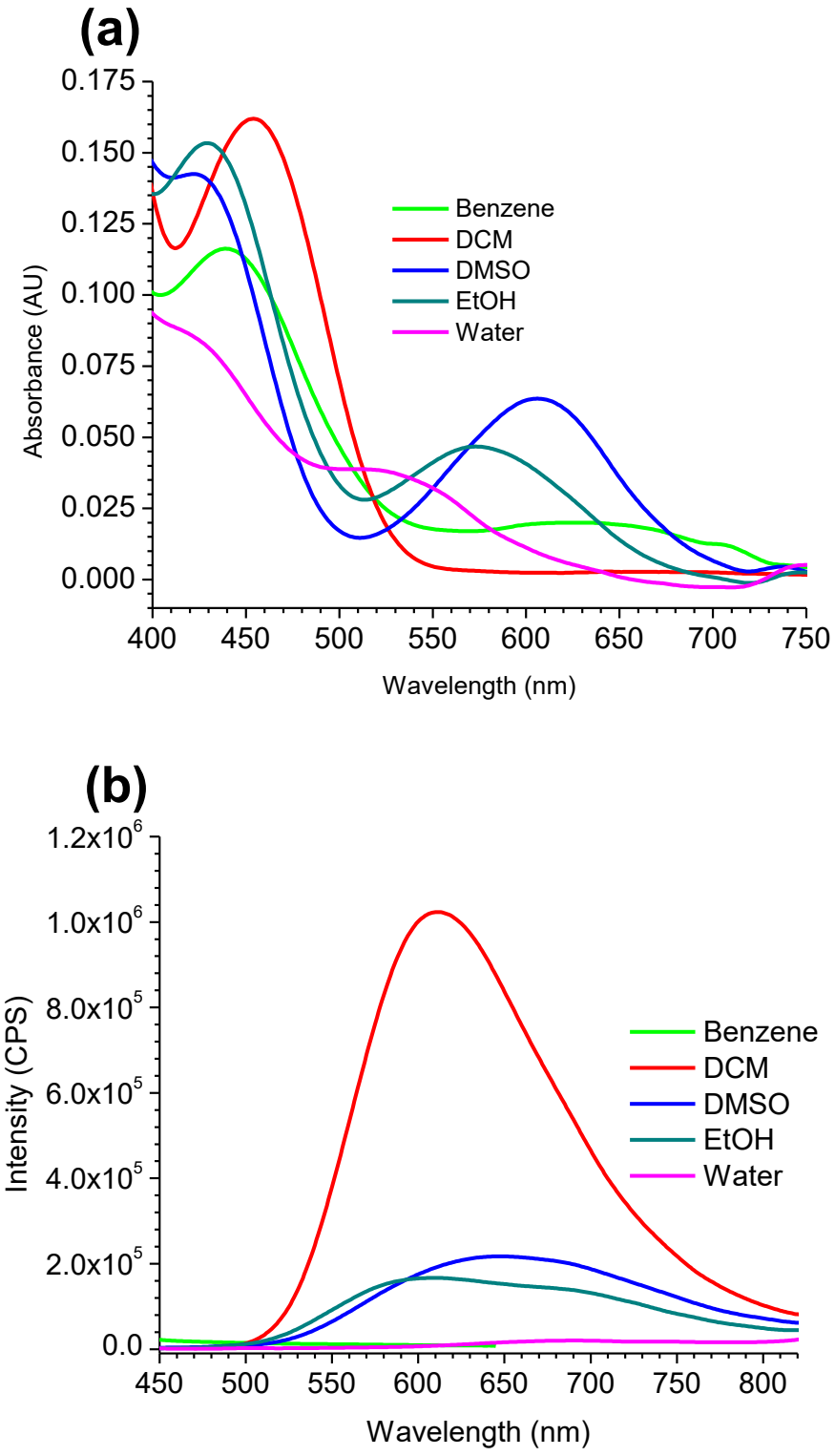


Figure S4.8 Absorbance (a) and emission (b) of probe **5a** (1 x 10^{-5} M) in different solvents at room temperature.

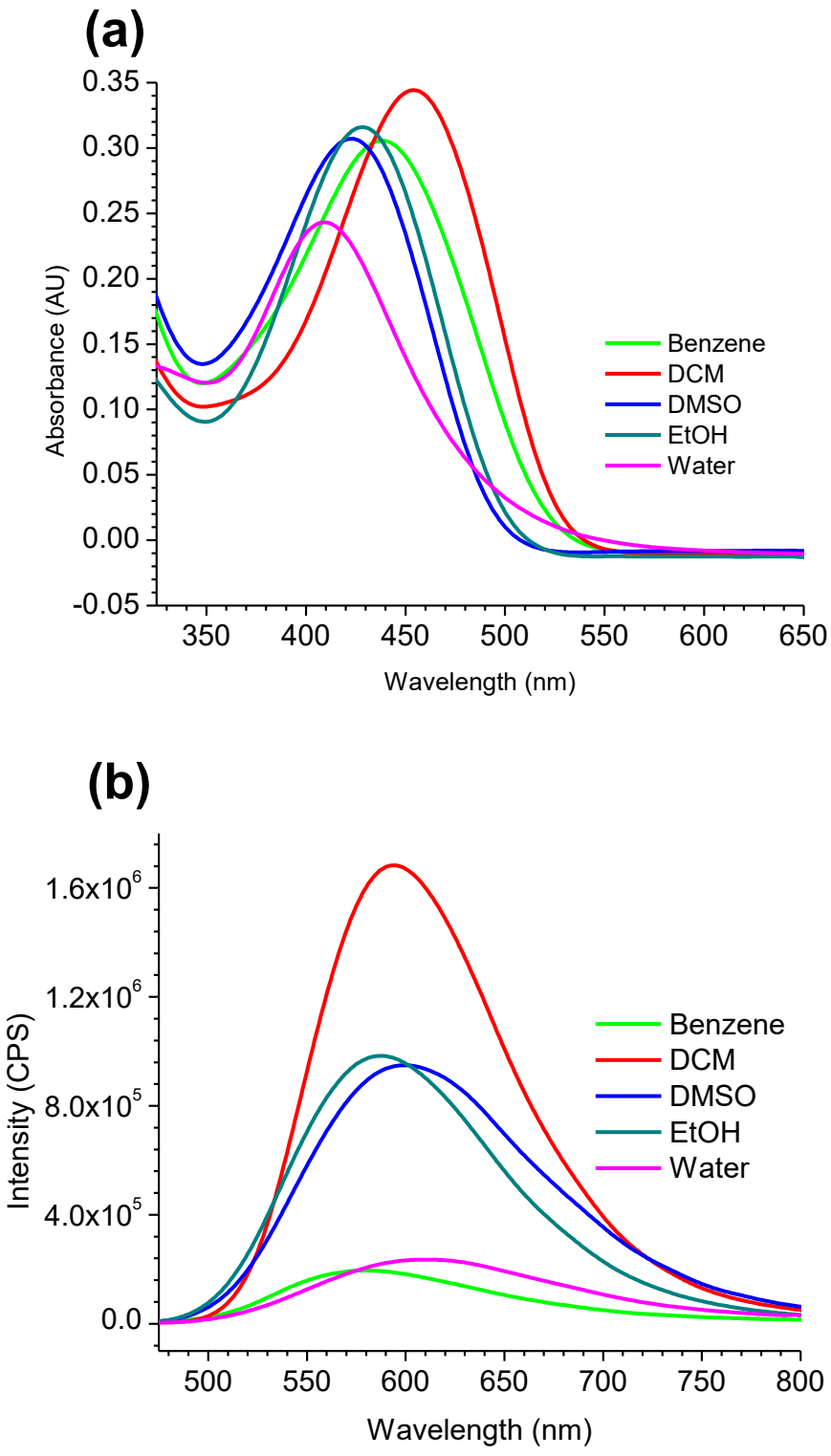


Figure S4.9 Absorbance (a) and emission (b) of probe **5b** (1 x 10^{-5} M) in different solvents at room temperature.

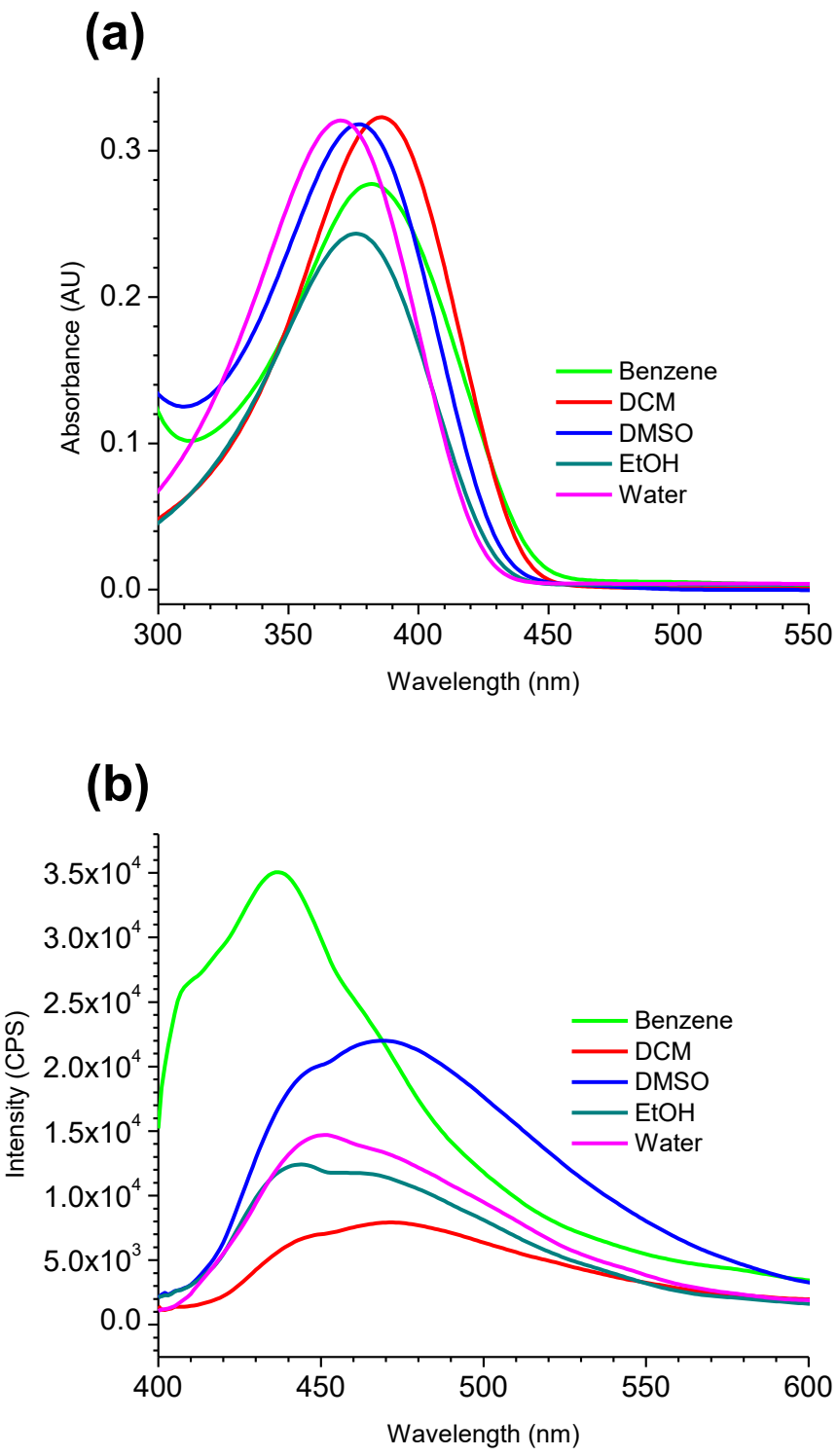


Figure S4.10 Absorbance (a) and emission (b) of probe **6a** (1 x 10^{-5} M) in different solvents at room temperature.

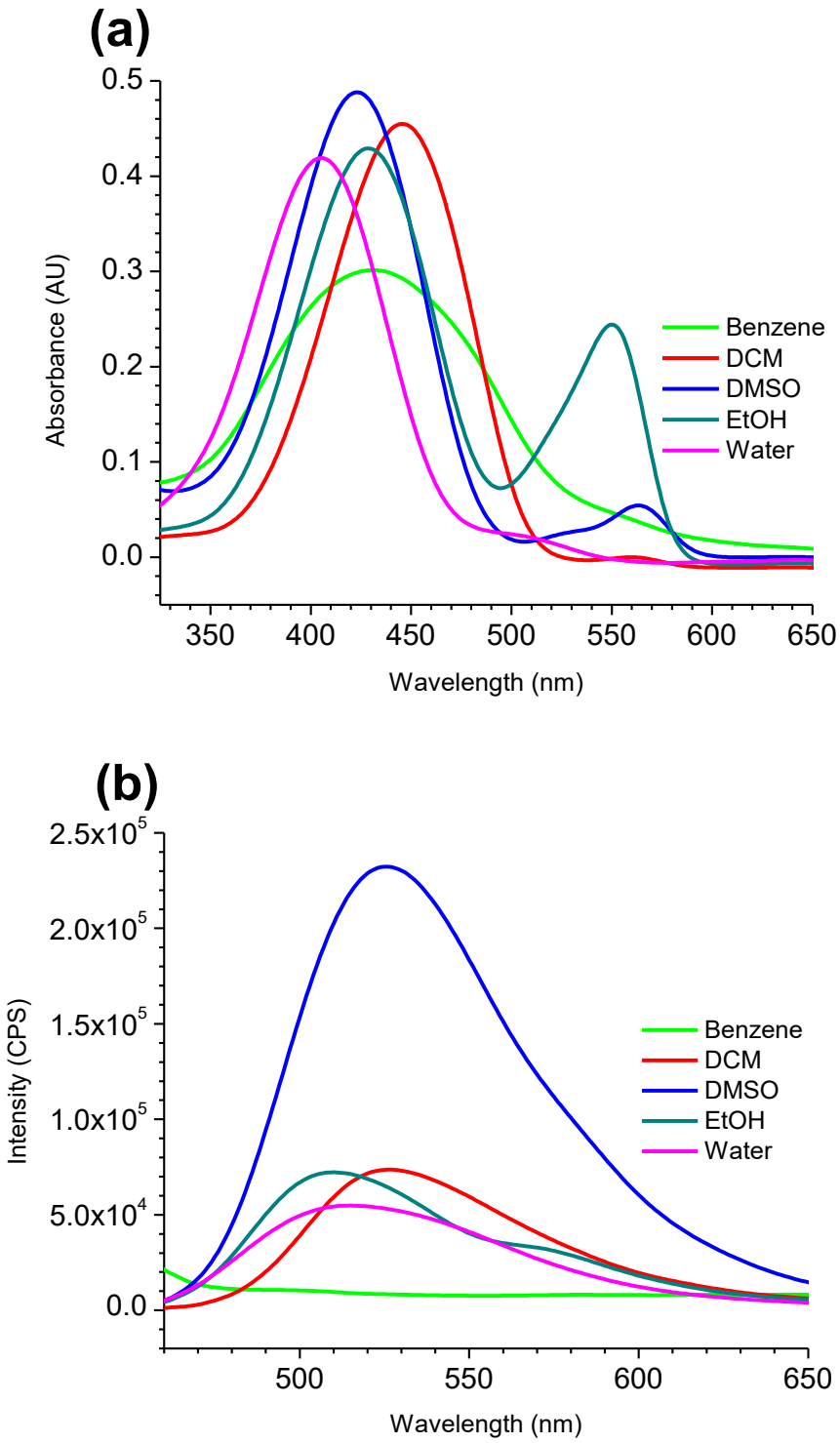


Figure S4.11 Absorbance (a) and emission (b) of probe **6b** (1×10^{-5} M) in different solvents at room temperature.

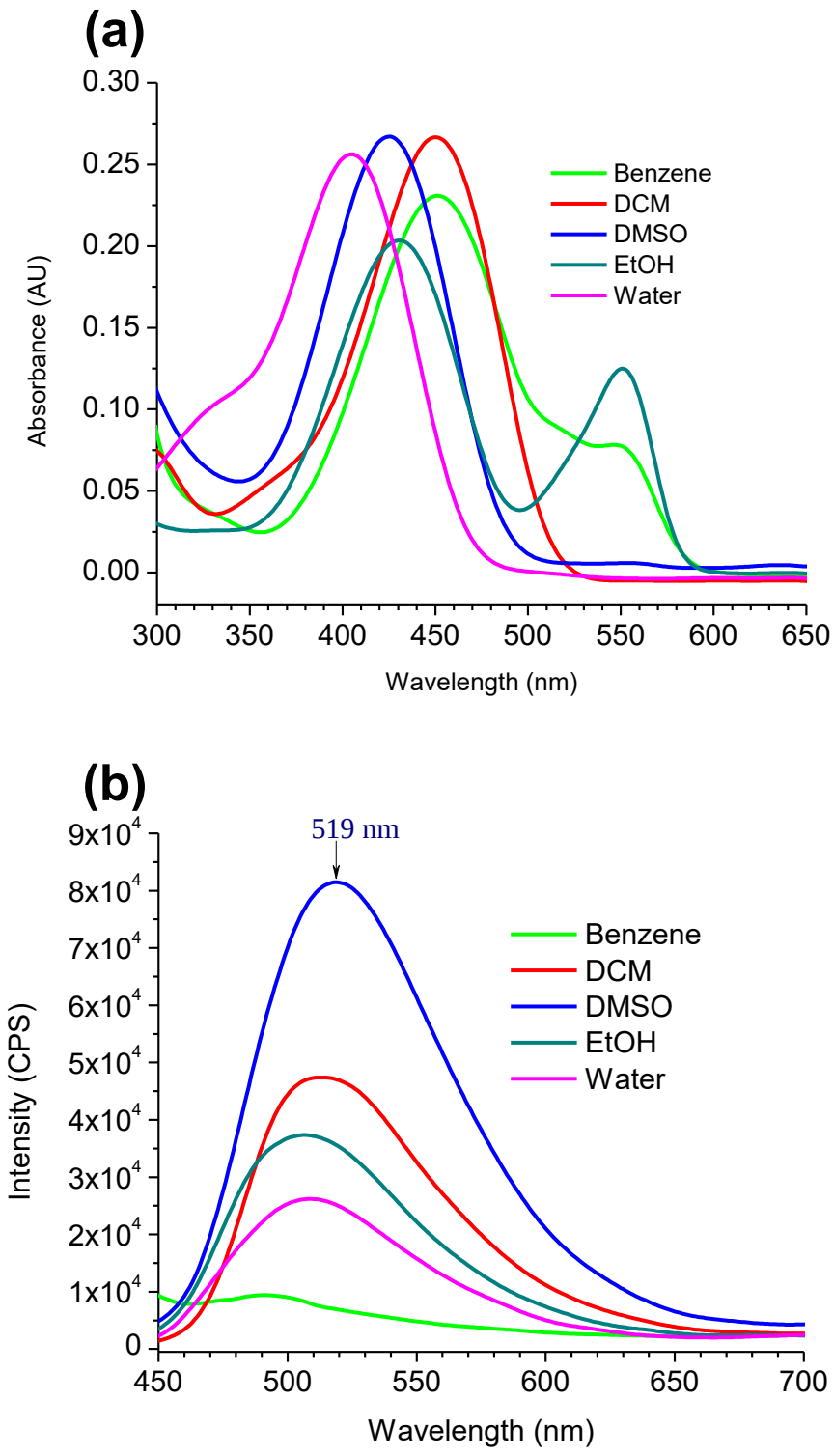


Figure S4.12 Absorbance (a) and emission (b) of probe **6c** (1 x 10^{-5} M) in different solvents at room temperature.

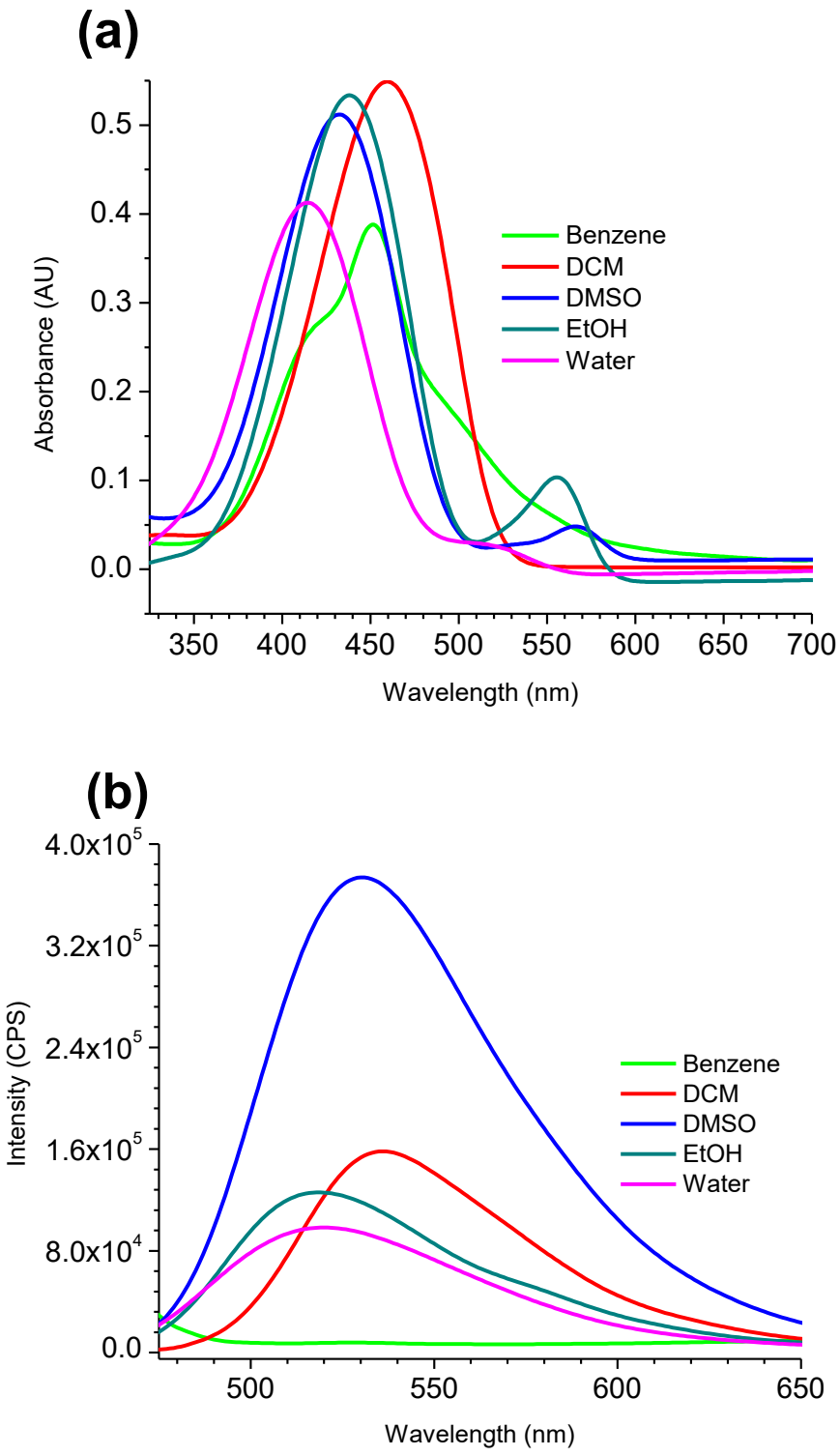


Figure S4.13 Absorbance (a) and emission (b) of probe **6d** (1 x 10^{-5} M) in different solvents at room temperature.

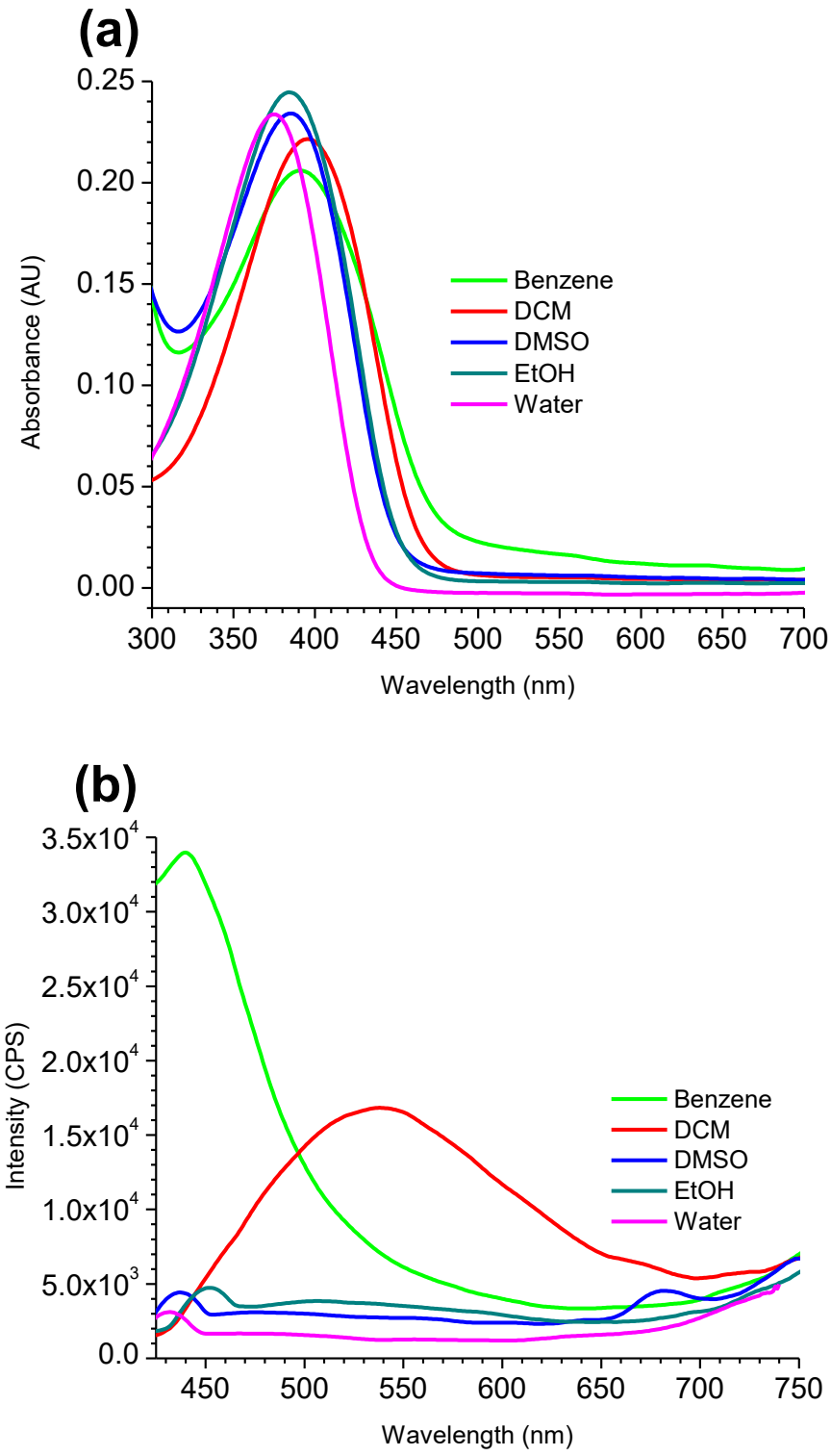


Figure S4.14 Absorbance (a) and emission (b) of probe **6e** (1 x 10^{-5} M) in different solvents at room temperature.

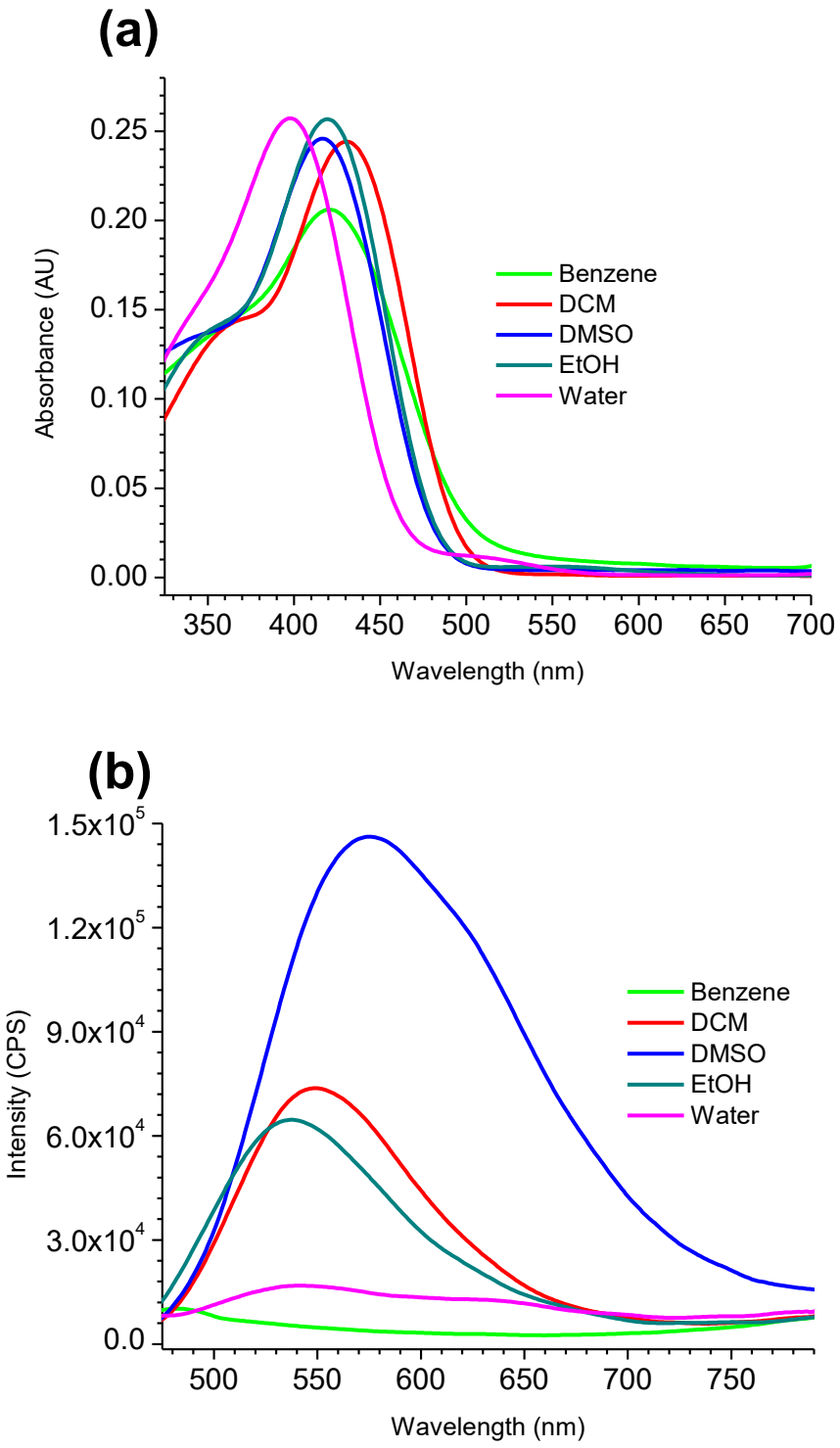


Figure S4.15 Absorbance (a) and emission (b) of probe **6f** (1 x 10^{-5} M) in different solvents at room temperature.

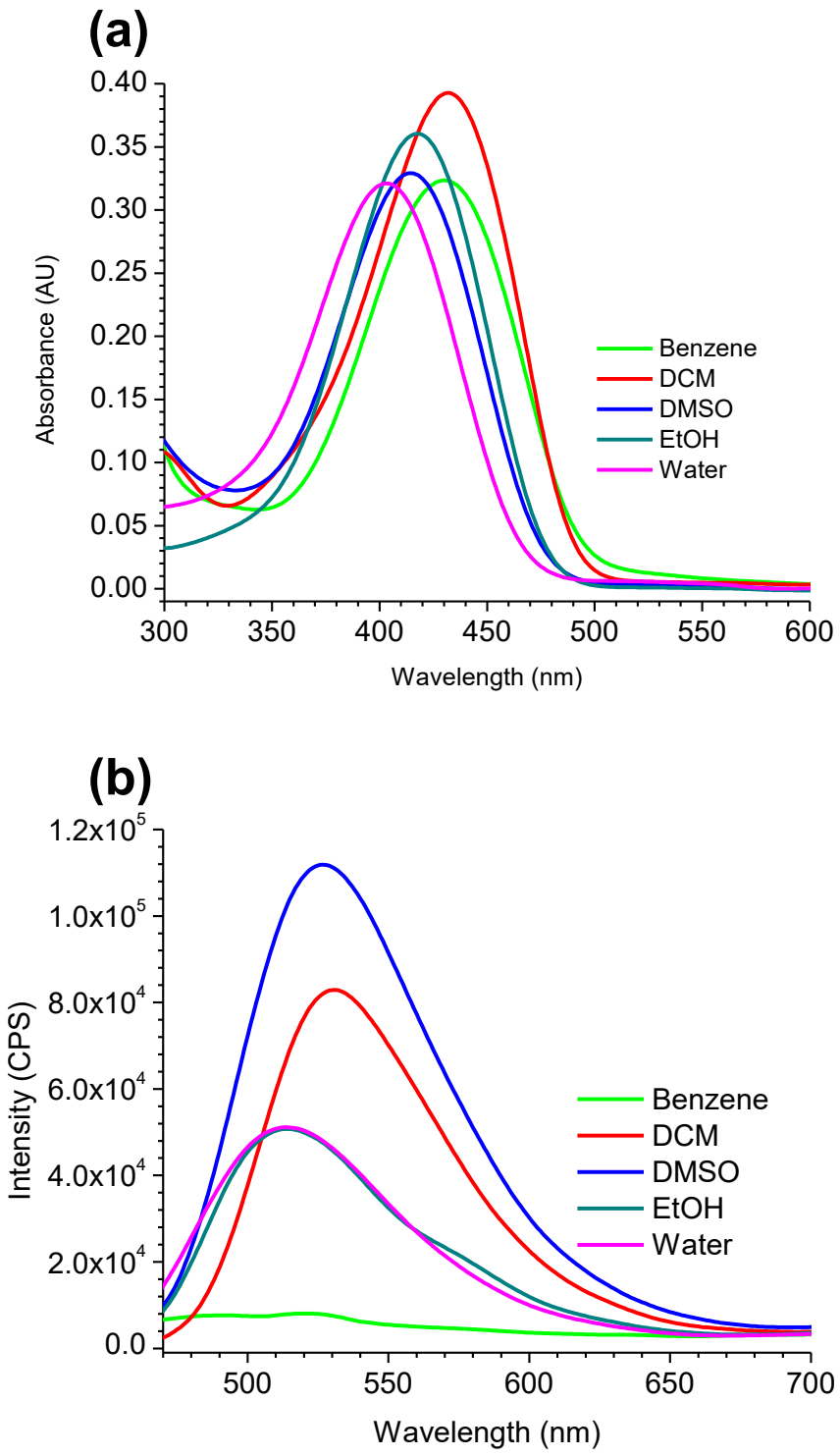


Figure S4.16 Absorbance (a) and emission (b) of probe **6g** (1 x 10^{-5} M) in different solvents at room temperature.

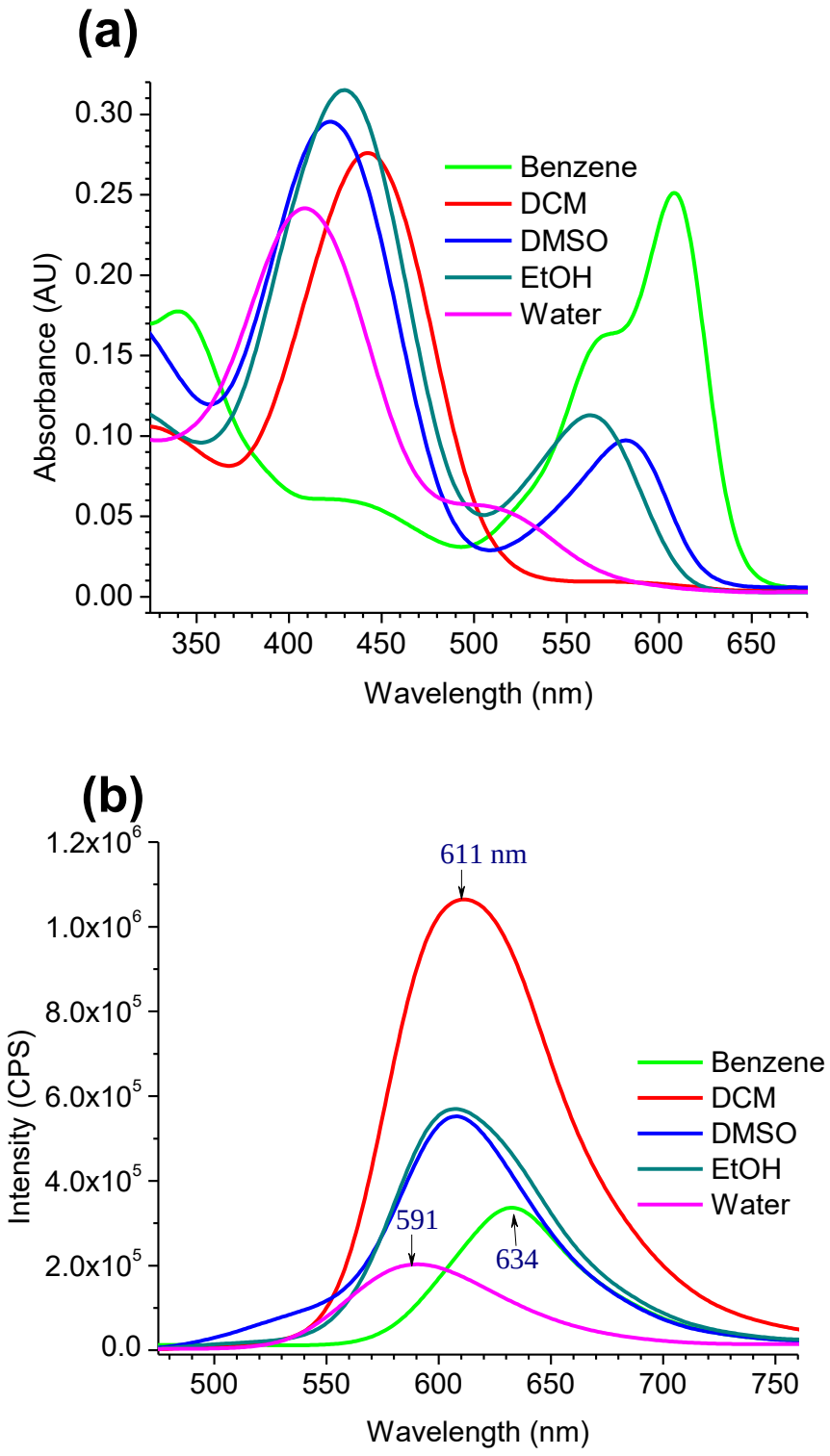


Figure S4.17 Absorbance (a) and emission (b) of probe **2c** (1 x 10^{-5} M) in different solvents at room temperature.

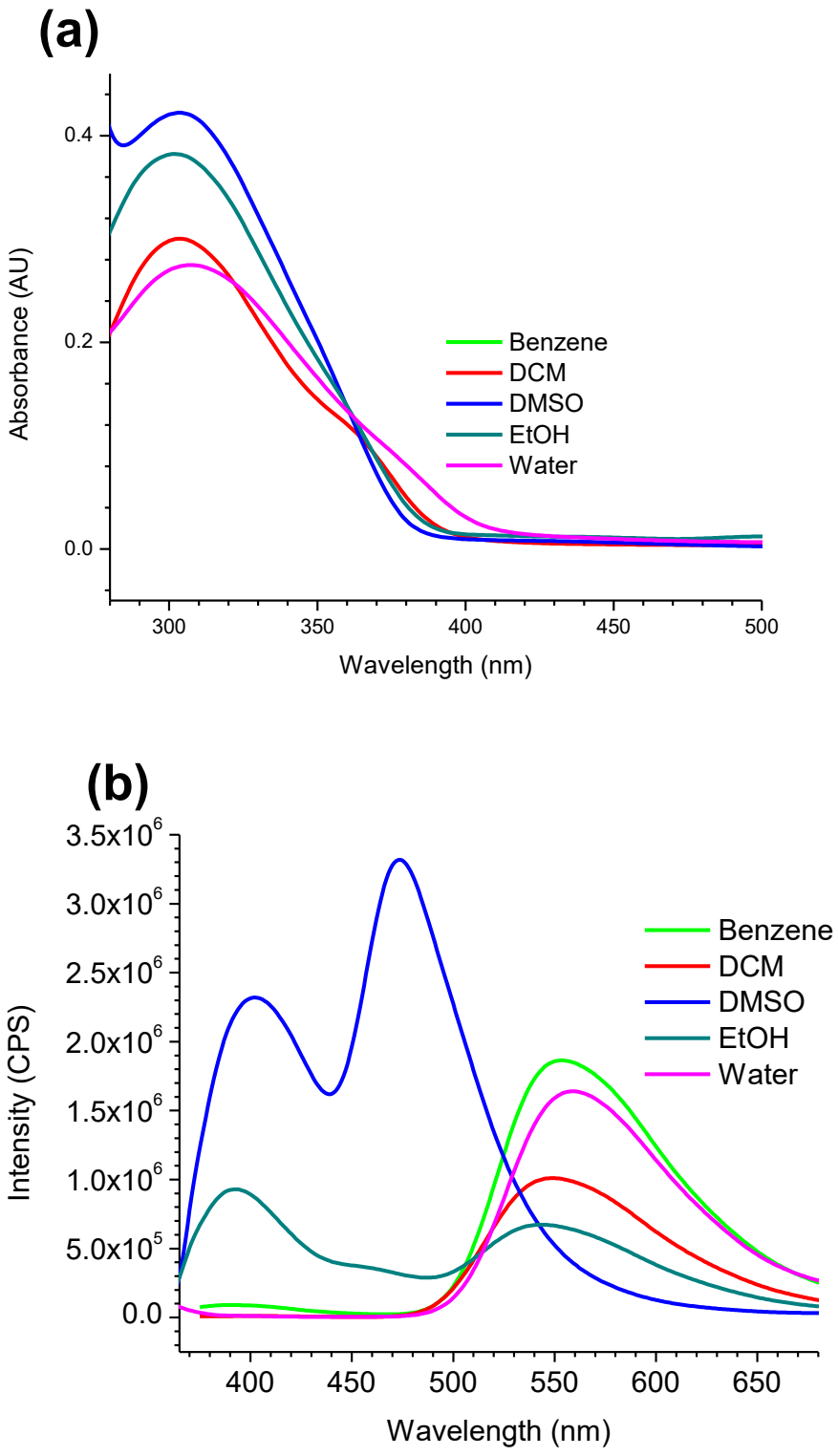


Figure S4.18 Absorbance (a) and emission (b) of probe **7** (1 x 10^{-5} M) in different solvents at room temperature.

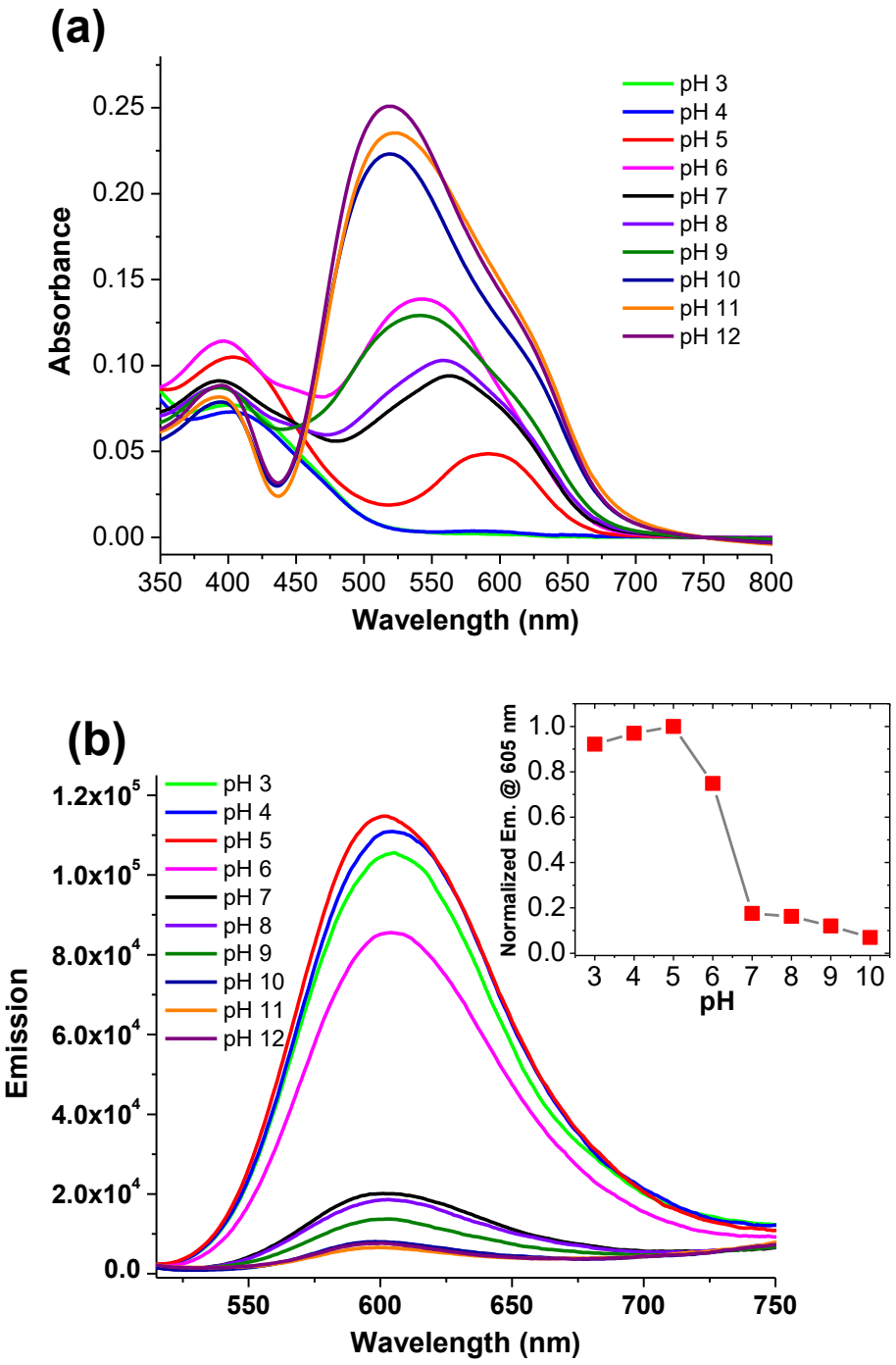


Figure S5 Absorbance (a) and emission (b) of probe **3b** (1 x 10^{-5} M) in different aqueous pH solutions at room temperature.

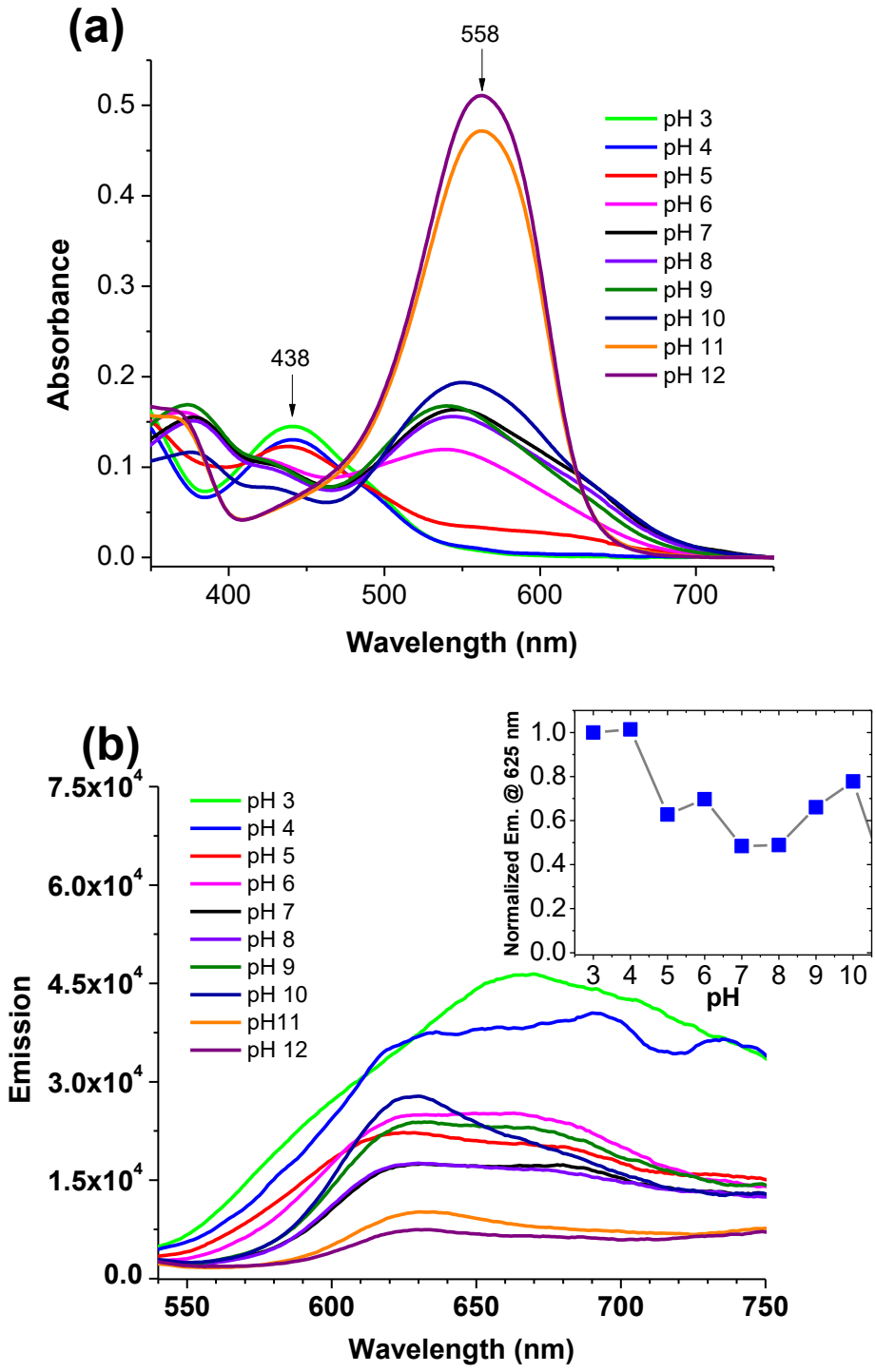


Figure S6 Absorbance (a) and emission (b) of probe **4a** (1 x 10^{-5} M) in different aqueous pH solutions at room temperature.

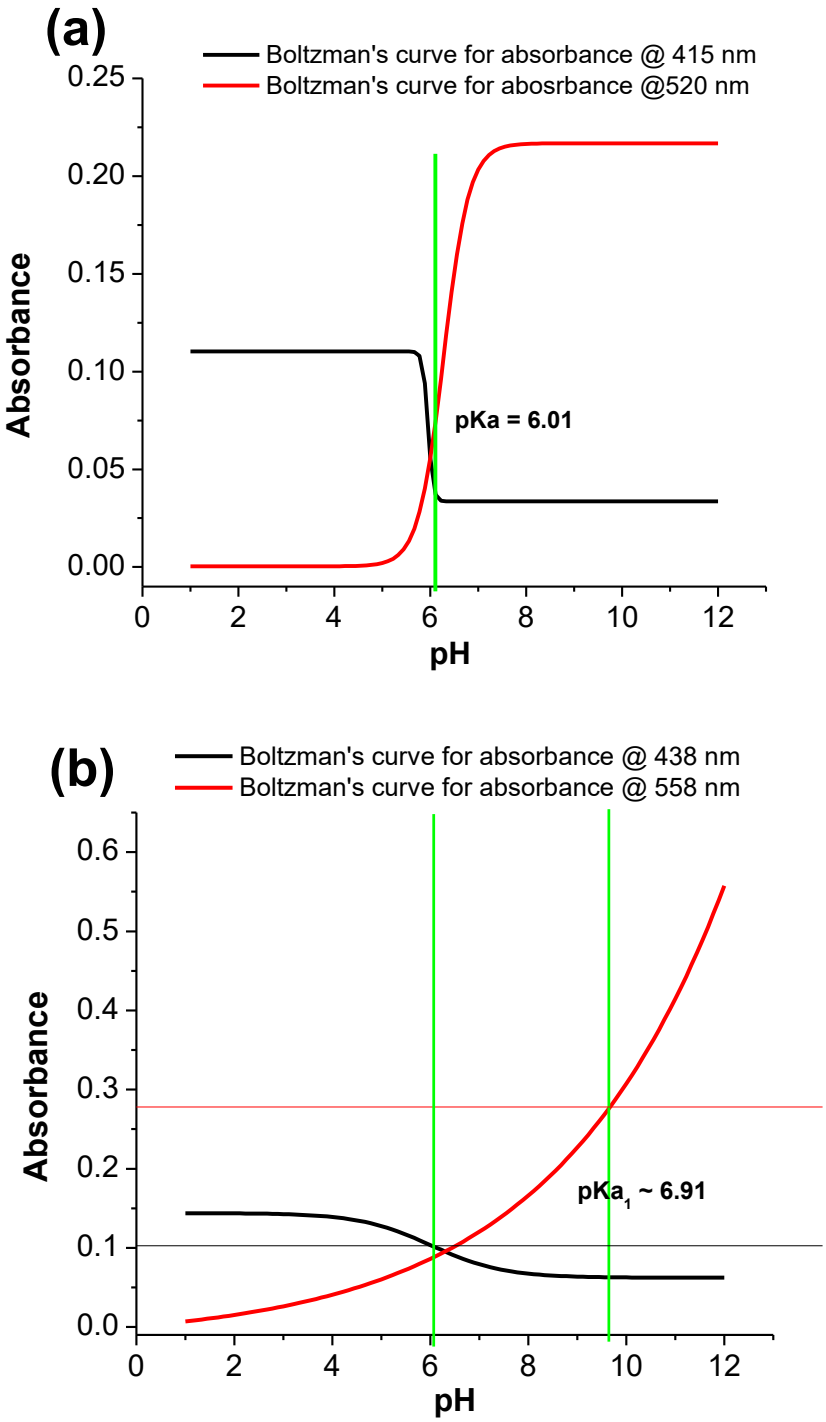


Figure S7 pKa determination for **3b** (a) and **4a** (b) by Boltzman's method.

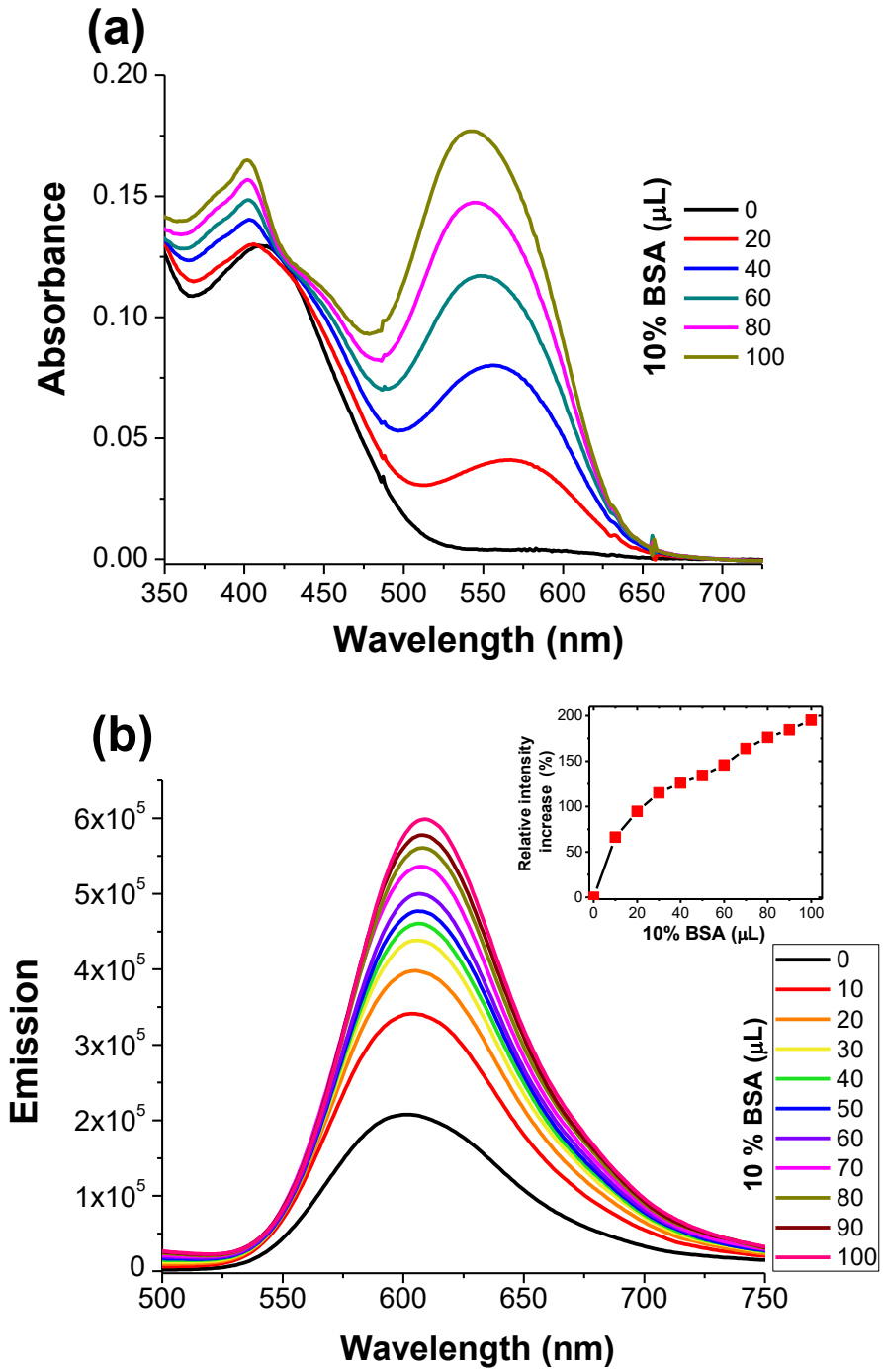


Figure S8 Absorption (a) and emission (b) recorded for probe **3b** (1 x 10^{-5} M) in aqueous acid (pH = 4.5) upon sequential addition of 10% BSA at room temperature.

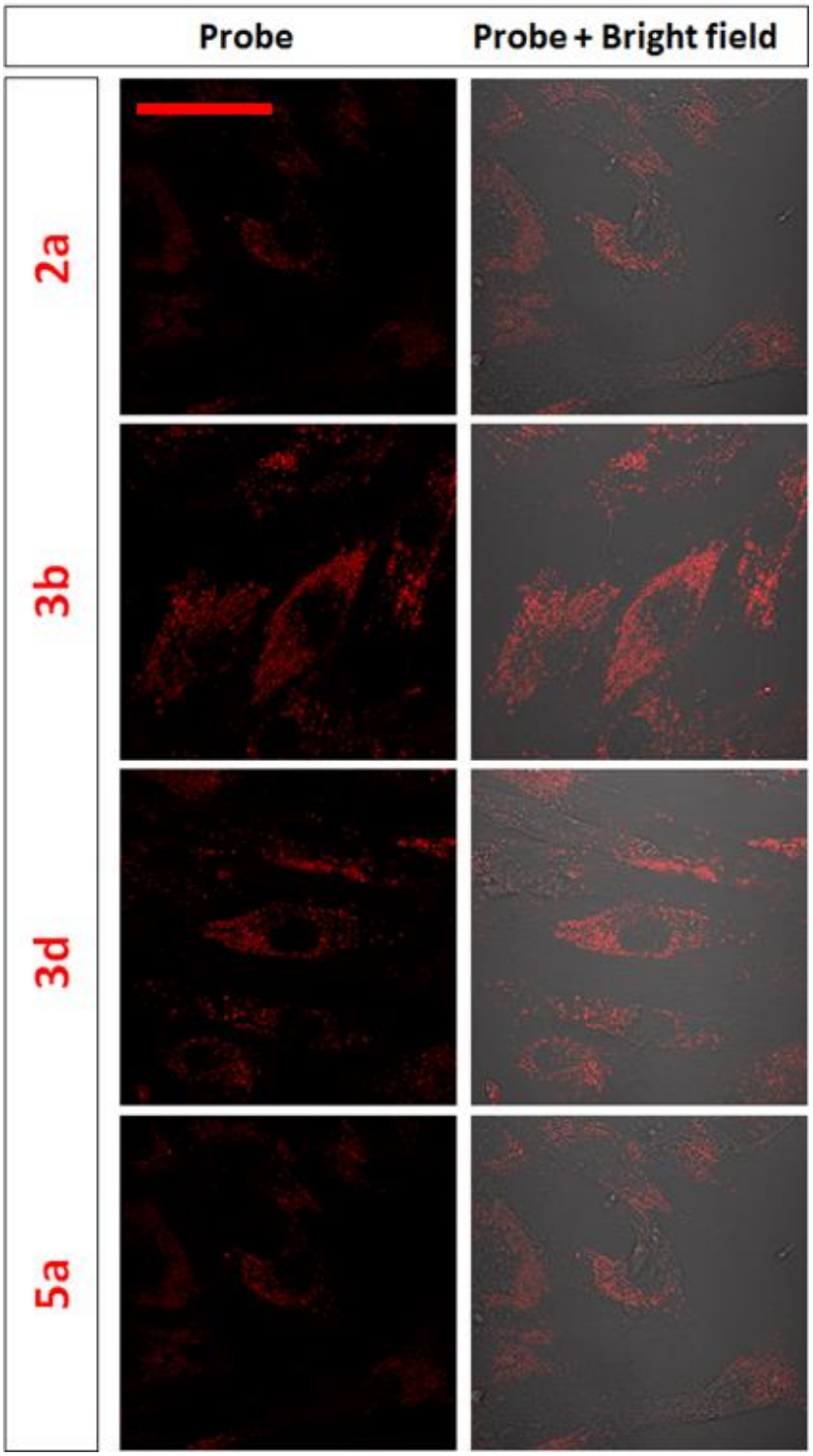


Figure S9 Fluorescence confocal microscopy images obtained for NHLF cells incubated for 30 minutes with probes **2** -**5** (500 nM). Probes were excited with 405 nm laser. Scale bar represents 25 microns.

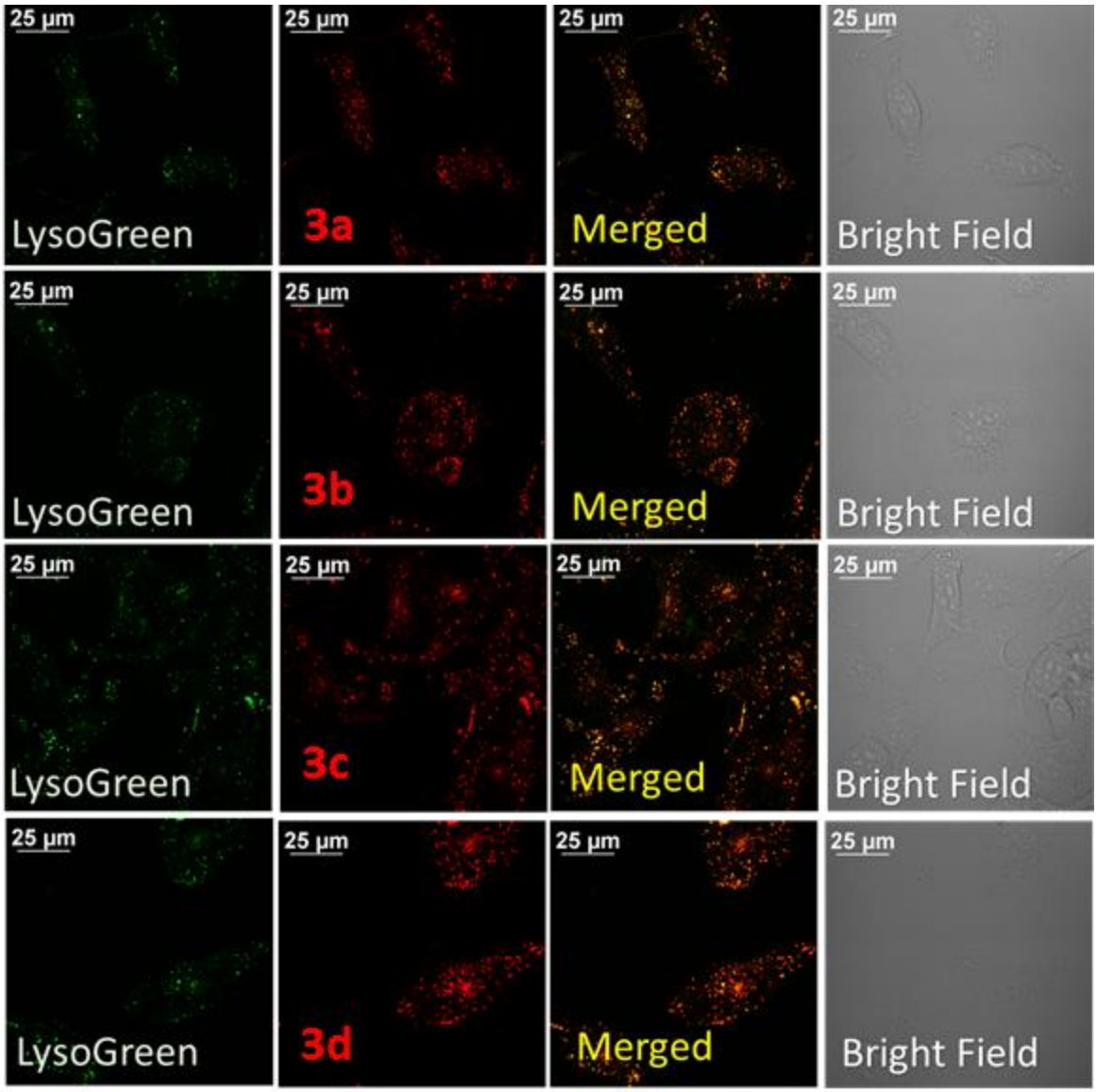


Figure S10 Fluorescence confocal microscopy images obtained for MO3.13 cells incubated for 30 minutes with probes **3a** -**3b** (500 nM) and LysoTracker® Green (70 nm). Probes were excited with 405/561 nm laser and LysoTracker® Green was excited with 488 nm laser line. Images from right to left represents the staining of the commercial LysoTracker®, Staining of the probe **3a** - **3d**, overlapped image, and the bright filed.

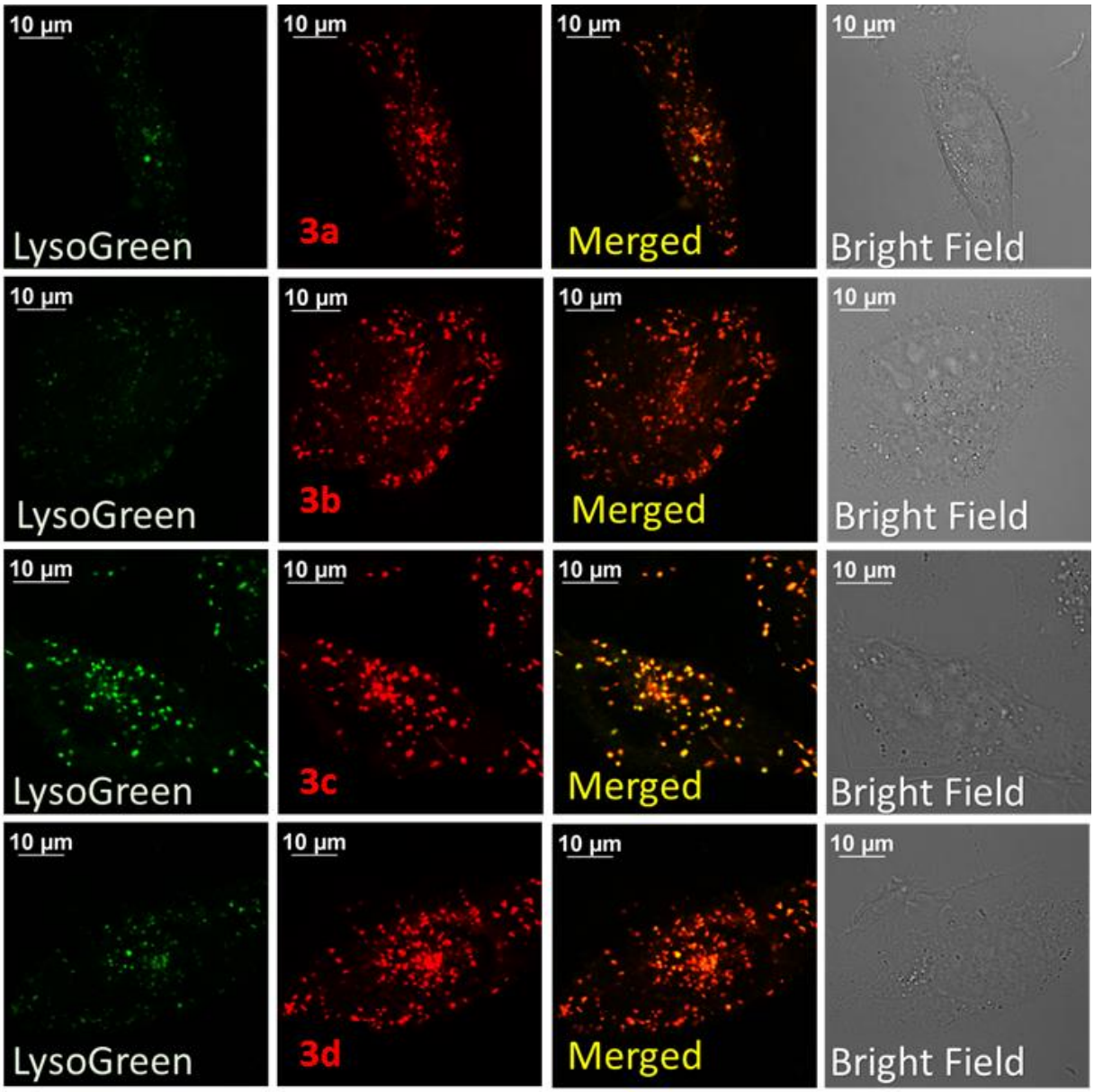


Figure S11 Fluorescence confocal microscopy images (digitally zoomed-in) obtained for MO3.13 cells incubated for 30 minutes with probes **3a** -**3b** (500 nM) and LysoTracker® Green (70 nm). Probes were excited with 405/561 nm laser and LysoTracker® Green was excited with 488 nm laser line. Images from right to left represents the staining of the commercial LysoTracker®, Staining of the probe **3a** -**3d**, overlapped image, and the bright filed.

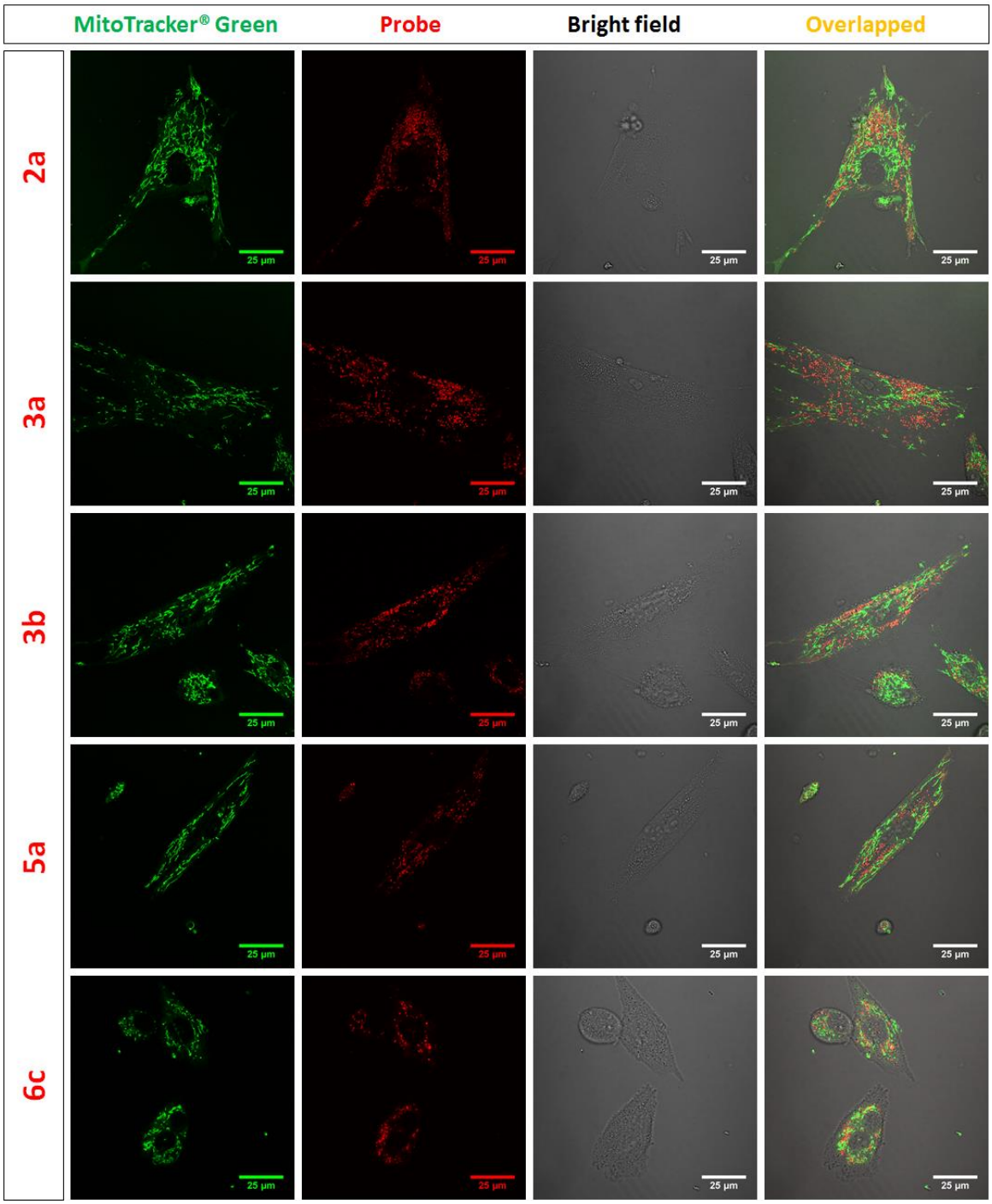


Figure S12 Fluorescence confocal microscopy images obtained for NHLF cells incubated for 30 minutes with probes **2** - **6** (500 nM) and MitoTracker® Green (200 nm). Probes were excited with 405/561 nm laser and MitoTracker® Green was excited with 488 nm laser line. Images from right to left represents the staining of the commercial MitoTracker®, Staining of the probe **2** -**6**, brightfield image, and the overlapped images. Calculated Mander's overlap coefficients were found to be 0.31 (**2a**), 0.28 (**3a**), 0.33 (**3b**), 0.29 (**5a**) and 0.35 (**6c**) respectively (n = 30)

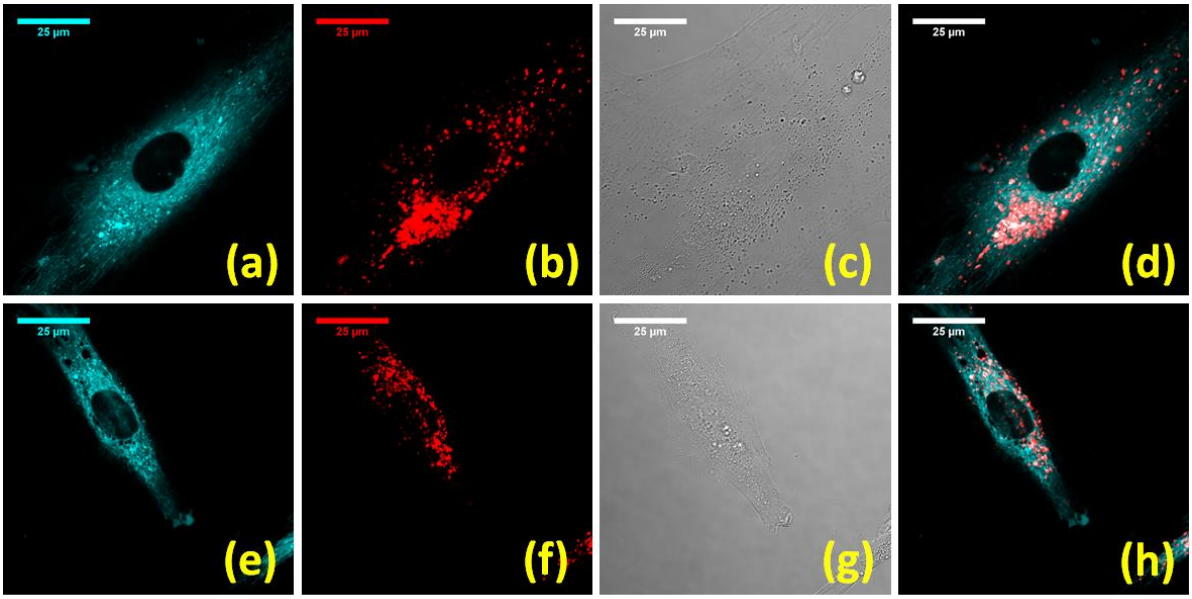


Figure S13 Fluorescence confocal microscopy images obtained for NHLF cells incubated for 30 minutes with probes **3b** and **3d** (500 nM) in the presence of ERTracker® Red (500 nm). Probes were excited with 405 nm laser and ERTracker® Red was excited with 561 nm laser line. Images from right to left represents the staining of the commercial ERTracker® (a,e), Staining of the probe (b,f), brightfield image (c,g), and the overlapped images (d,h). Calculated Mander's overlap coefficients found to be 0.26 (**3b**) and 0.29 (**3d**) respectively (n = 30).

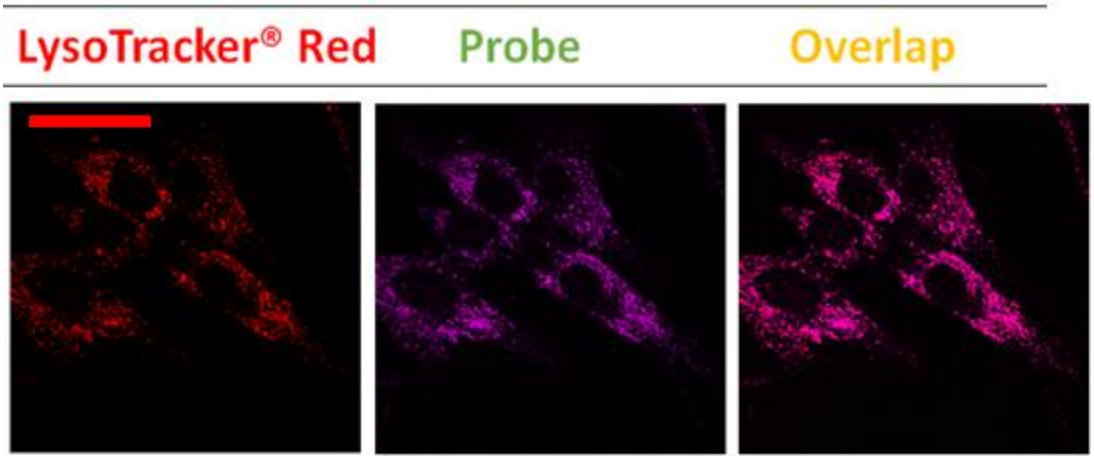


Figure S14 Fluorescence confocal microscopy images obtained for NHLF cells incubated for 30 minutes with probes **2c** (500 nM) and LysoTracker® Red (70 nm). Probes were excited with 405/561 nm laser and LysoTracker® Red was excited with 561 nm laser line. Images from right to left represents the staining of the commercial LysoTracker®, Staining of the probe, and overlapped images. The scale bar represents 25 microns.

Probe	Calculated Mander's overlap coefficient
2a	0.9213 (+/- 0.0013)
2b	0.8716 (+/- 0.0023)
2c	0.9012 (+/- 0.0011)
3a	0.9007 (+/- 0.0017)
3b	0.9134 (+/- 0.0014)
3c	0.9176 (+/- 0.0022)
3d	0.9207 (+/- 0.0013)
4a	0.3476 (+/- 0.0023)
5a	0.9104 (+/- 0.0019)
5b	0.9067 (+/- 0.0015)
6a	0.7615 (+/- 0.0033)
6b	0.7305 (+/- 0.0053)
6c	0.7891 (+/- 0.0073)
6d	0.7691 (+/- 0.0053)
6e	0.7406 (+/- 0.0093)
6f	0.7486 (+/- 0.0033)
6g	0.7523 (+/- 0.0073)

Table S15.1 Calculated Mander's overlap coefficient for probes **2** – **6** in the presence of commercial LysoTracker® probes in NHLF cells. (n=40)

Probe	Calculated Mander's overlap coefficient
2a	0.3714 (+/- 0.0053)
3a	0.3318 (+/- 0.0013)
3b	0.3452 (+/- 0.0031)
5a	0.3696 (+/- 0.0042)
6c	0.4317 (+/- 0.0028)

Table S15.2 Calculated Mander's overlap coefficient for probes **2** – **6** in the presence of commercial MitoTracker® probes in NHLF cells. (n=40)

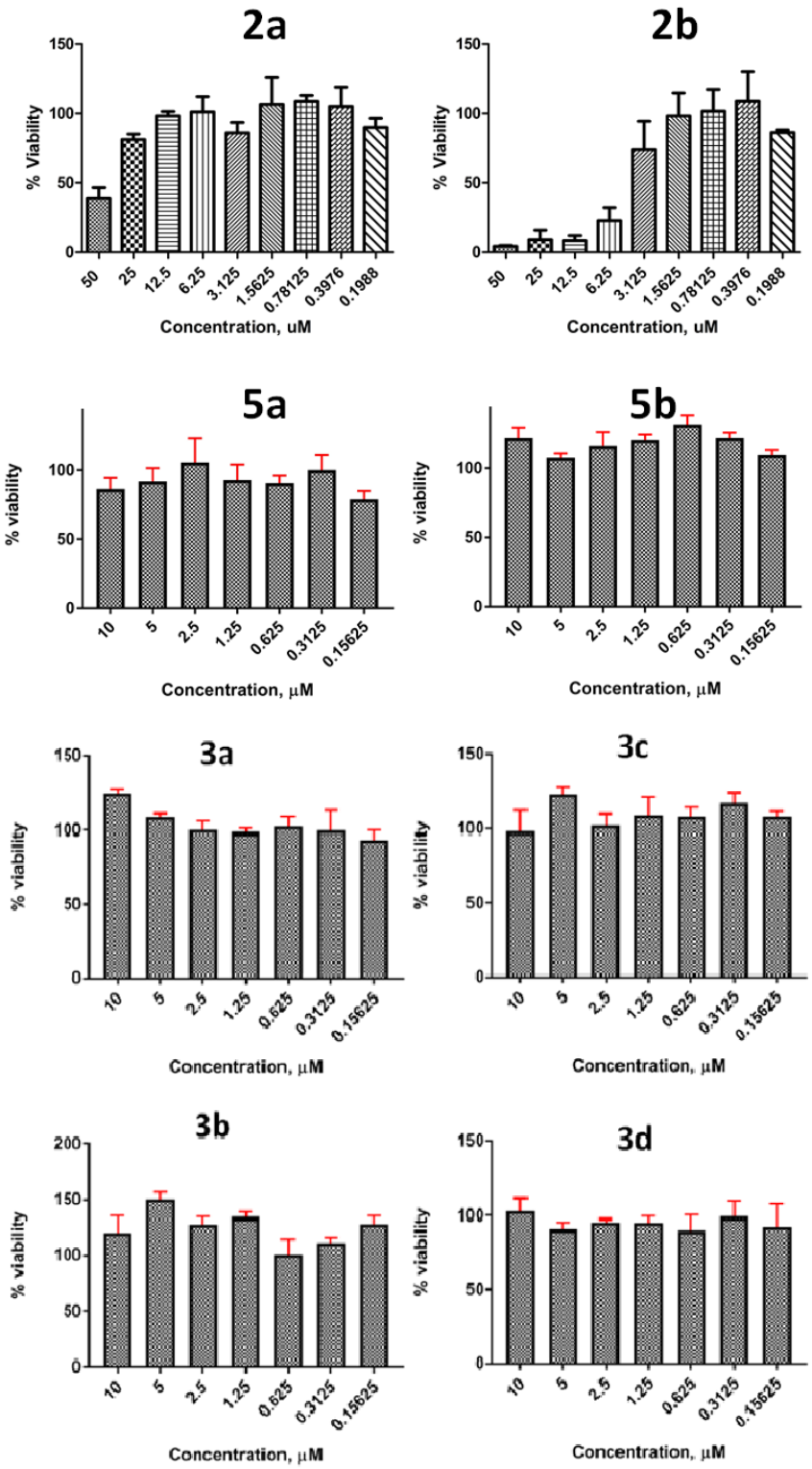


Figure S16 MTT cell proliferation viability assay results for probes **2** – **5**.

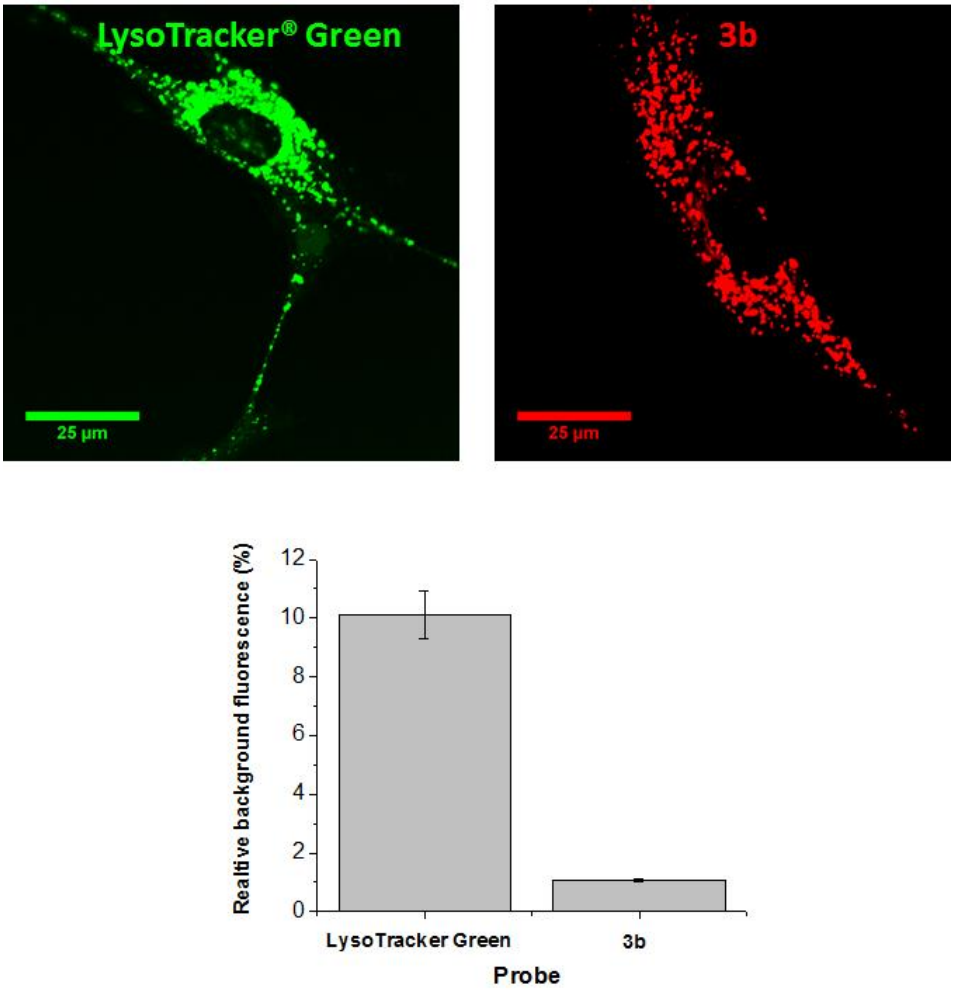


Figure S17 Relative background fluorescence intensity calculated for Lysotracker® Green DND-26 and Probe **3b** in NHLF cells. Lysotracker® Green was excited with 488 nm laser line and the probe 3b was excited with 405 laser line. Fluorescence confocal microscopy images were analyzed by ImageJ (NIH) software to calculate relative background florescence percentage (n =30).

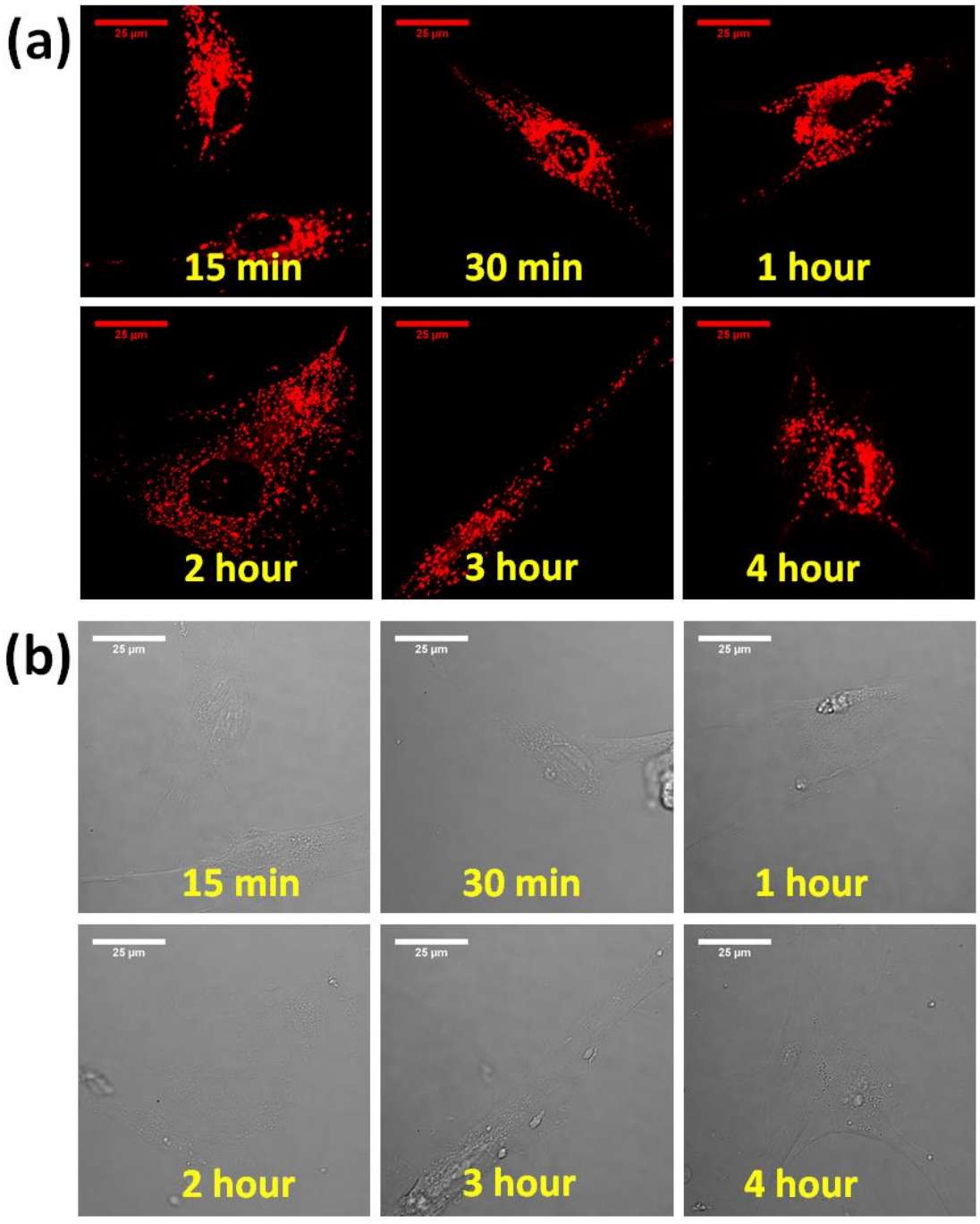


Figure S18 (a) Long-term imaging ability assessment for probe **3d** in for NHLF cells. Cells were incubated with **3d** (500 nM) for 30 minutes and confocal microscopy images were obtained at different time intervals intervals under consistent parameters of the microscope. Probe **3d** was excited with 405 nm laser and the emissions were collected in the 570 nm to 700 nm range. Figures (a) and (b) represents the emission of **3d** and the bright field imaging respectively.

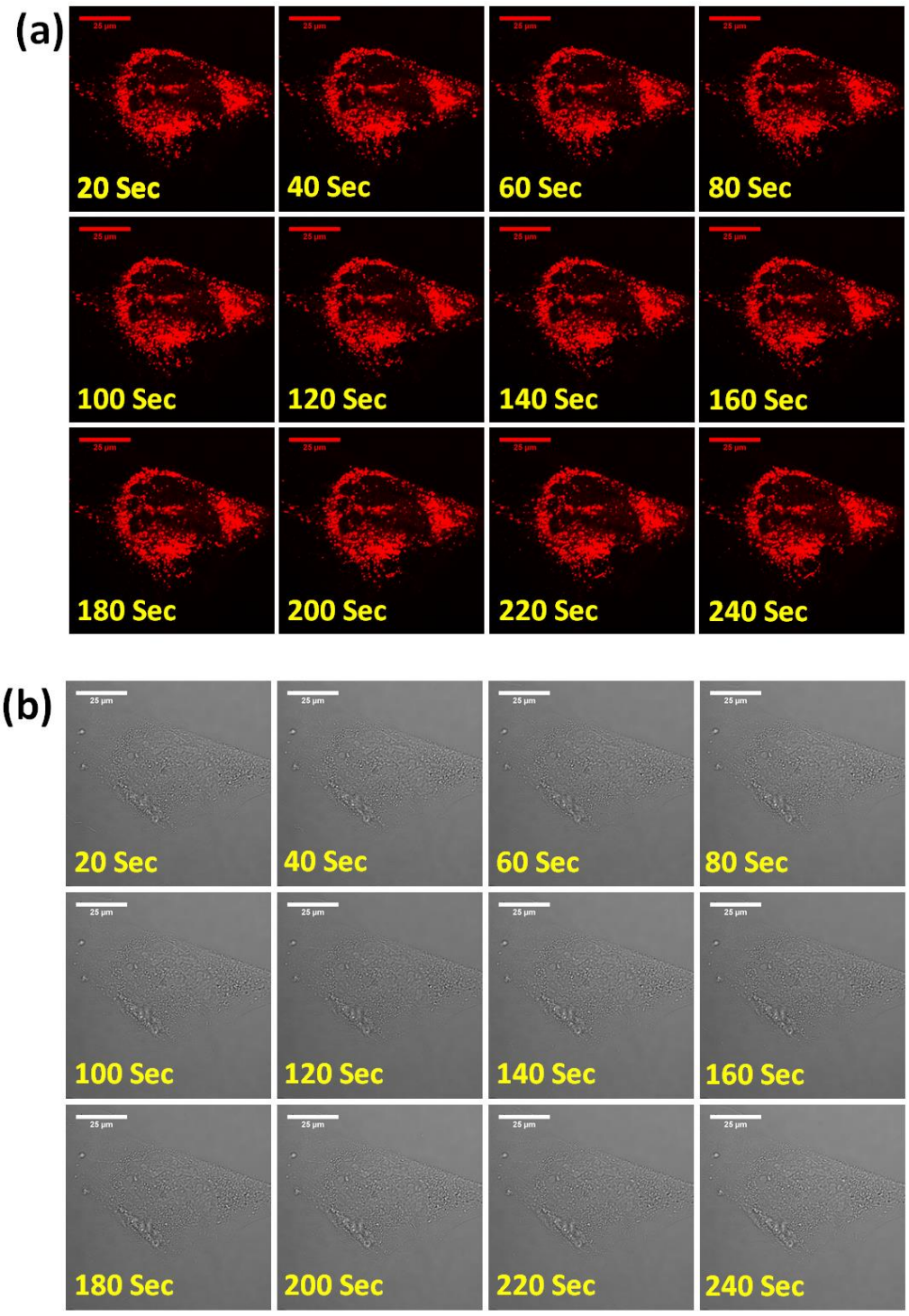


Figure S19 (a) - Fluorescence confocal microscopy images obtained for probe **3d** (500 nM) in NHLF cells upon continuous irradiation with 405 nm laser line (Laser power percentage 3.0; Digital zoom = 1; Pinhole = 1AU; Master Gain = 150; Digital offset = 0.) Fluorescence confocal microscopy images were obtained at 20 sec time intervals. Figures (a) and (b) represents the emission of **3d** and the bright field imaging respectively.

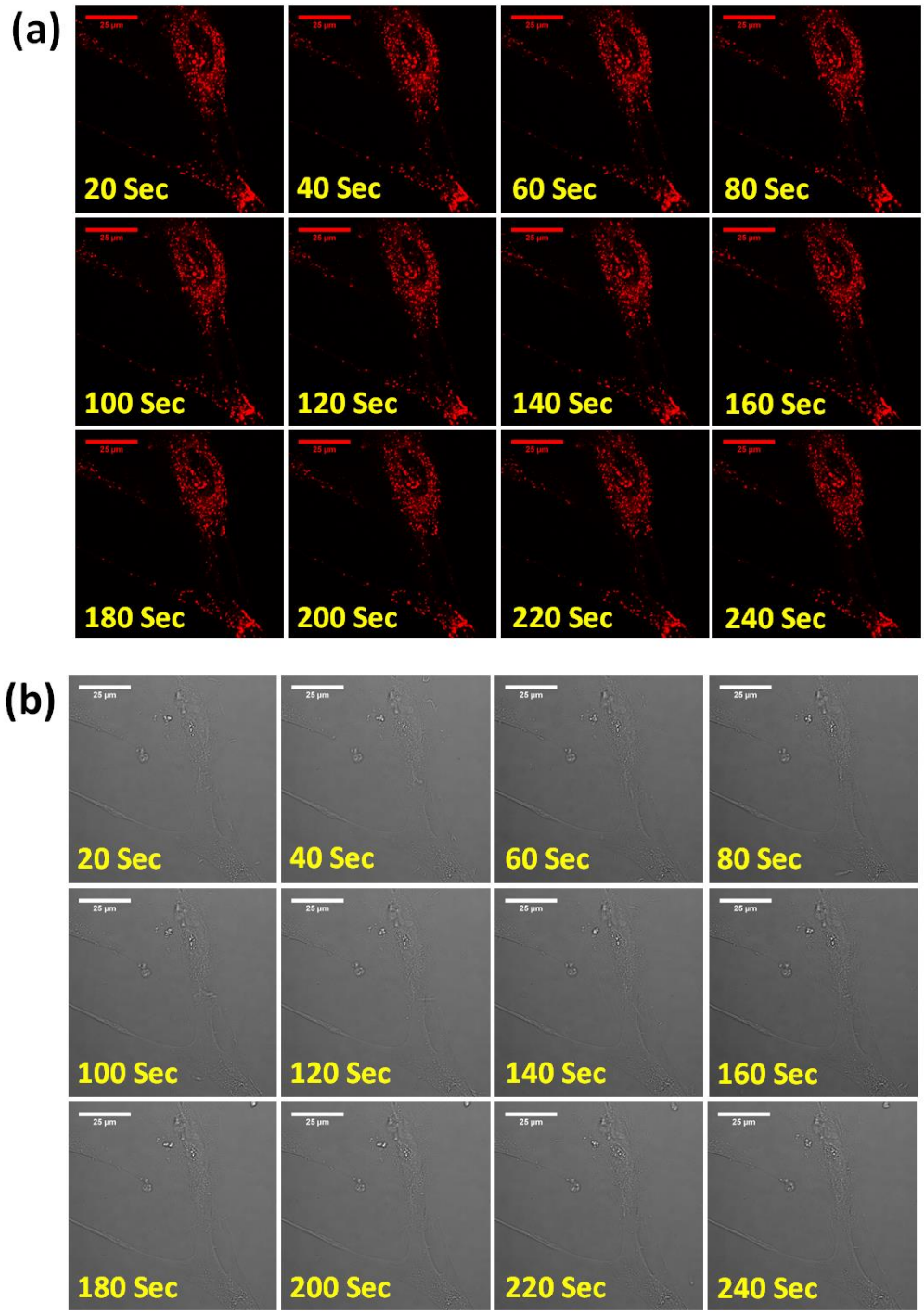


Figure S20 (a) - Fluorescence confocal microscopy images obtained for probe **3b** (500 nM) in NHLF cells upon continuous irradiation with 405 nm laser line (Laser power percentage 3.0; Digital zoom = 1; Pinhole = 1AU; Master Gain = 150; Digital offset = 0.) Fluorescence confocal microscopy images were obtained at 20 sec time intervals. Figures (a) and (b) represents the emission of **3b** and the bright field imaging respectively.

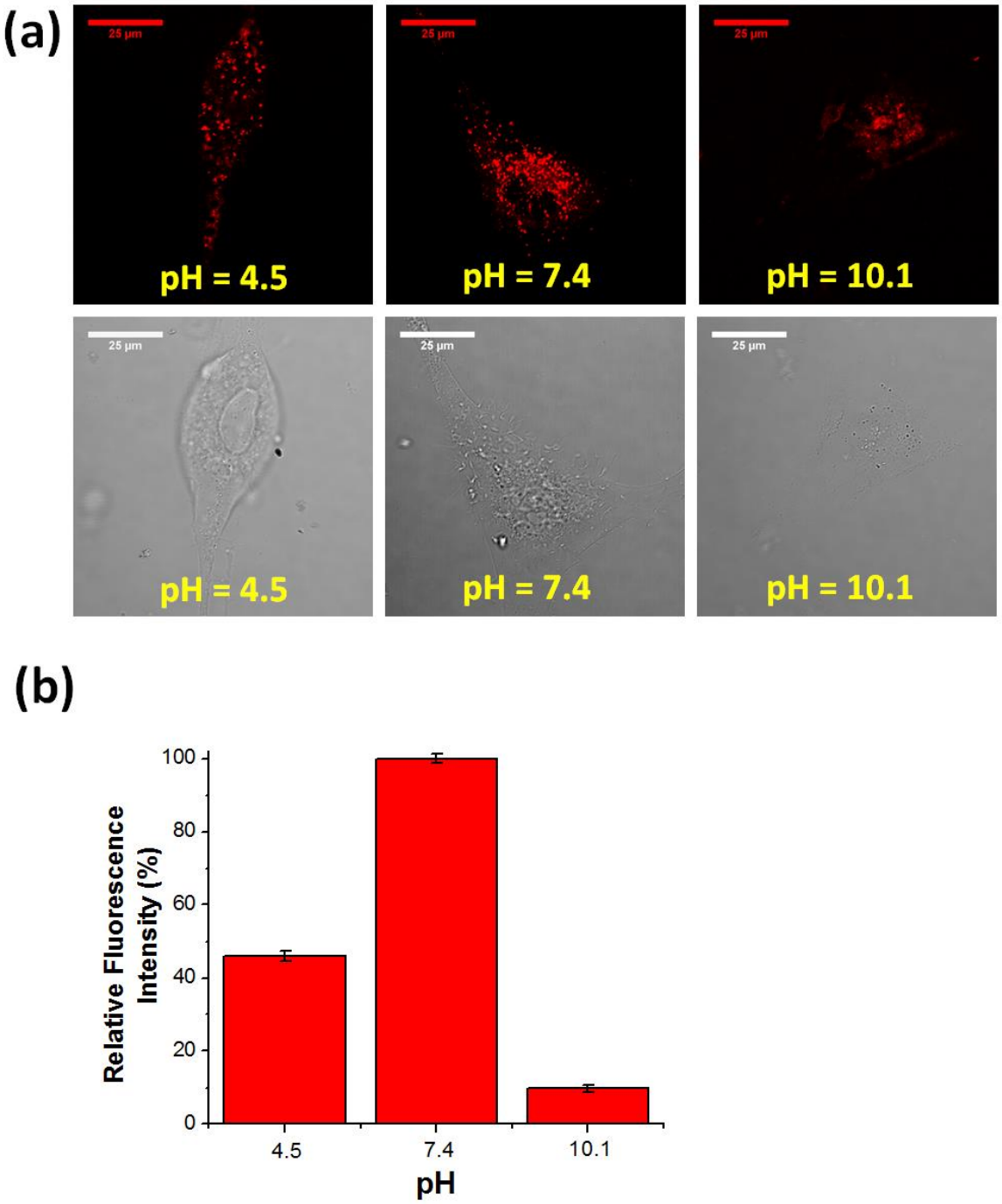


Figure S21.1 (a)- Fluorescence confocal microscopy images of NHLF cells incubated with probe **3d** (500 nM) for 30 minutes under different pH conditions. Figure (b) represents the relative fluorescence intensity (averaged) obtained under different pH conditions. Probe **3d** was excited with 405 nm laser line and the emission were collected from 750 nm to 700 nm range.

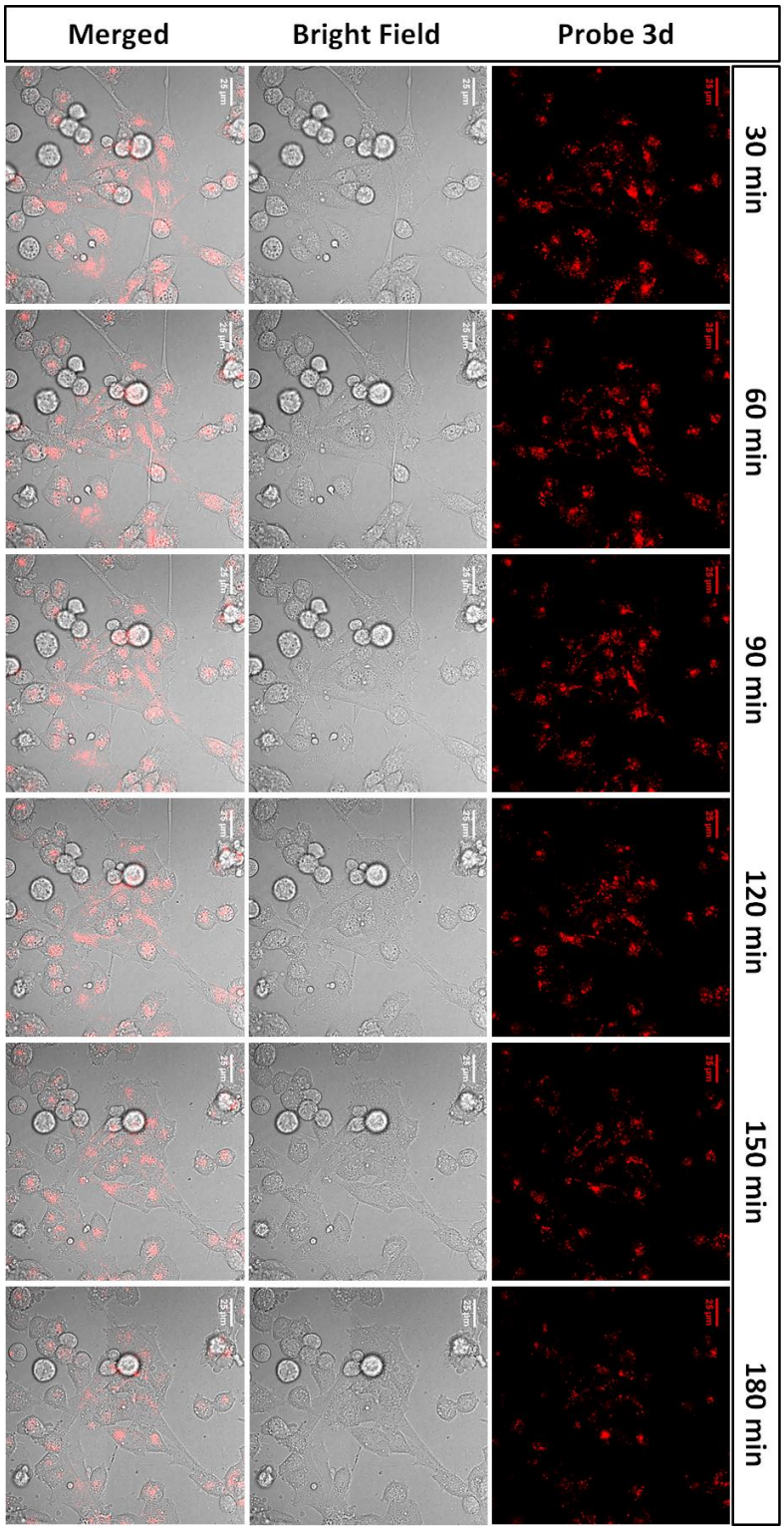


Figure S21.2 (a)- Fluorescence confocal microscopy images of NHLF cells incubated with probe **3d** (500 nM) for 30 minutes in the presence of 3 mM NH_4Cl. Images were taken under different time intervals and averaged fluorescence intensities (normalized) were analyzed. Probe **3d** was excited with 405 nm laser line and the emission were collected from 750 nm to 700 nm range.

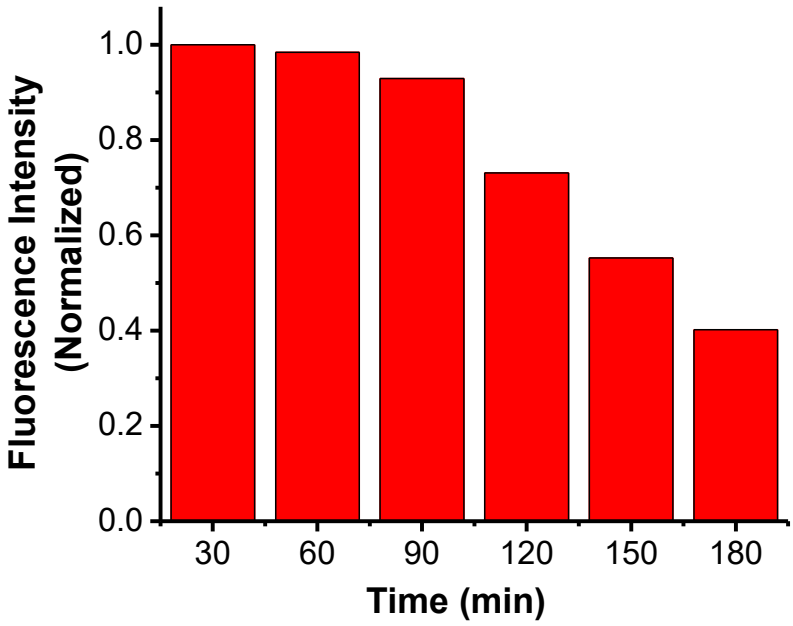


Figure S21.3 (a)- Fluorescence confocal microscopy images of NHLF cells incubated with probe **3d** (500 nM) for 30 minutes in the presence of 3 mM NH_4Cl. Images were taken under different time intervals and averaged fluorescence intensities (normalized) were analyzed by ImageJ (NIH) software. Probe **3d** was excited with 405 nm laser line and the emission were collected from 750 nm to 700 nm range.

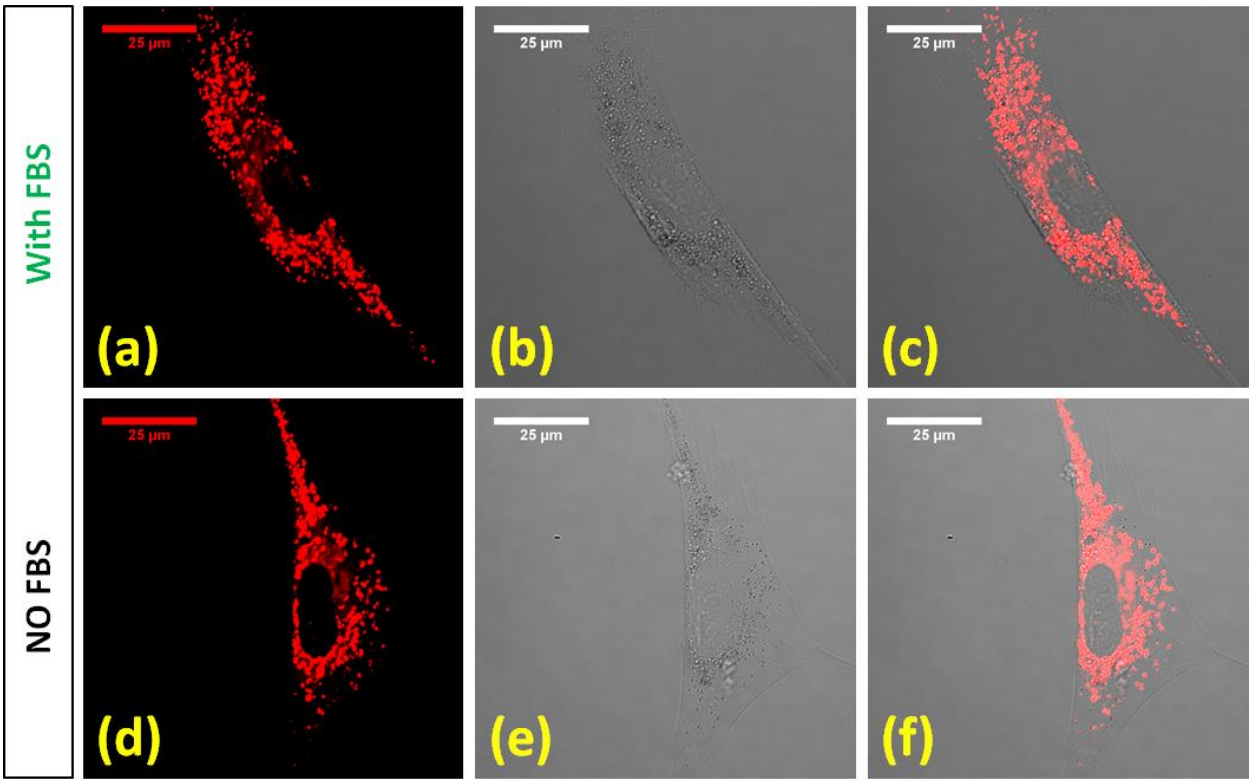


Figure S22 Fluorescence confocal microscopy images of NHLF cells incubated with probe **3d** (500 nM) for 30 minutes under with FBS (top row) without FBS (bottom row) conditions. Images from left to right represents the staining of the probe **3d**, bright filed and the merged image. Probe 3b was excited with 405 nm laser line and the emission was collected from 570 nm to 700 nm range.

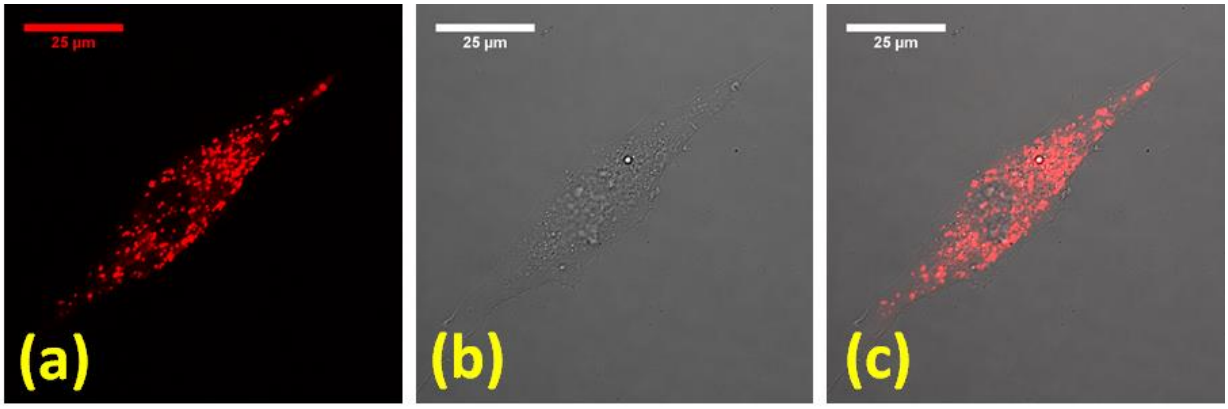


Figure S23.1 NHLF cells were incubated with FCCP (1 µM) for 1 hours. The cells were further incubated with probe **3d** (500 nM) for 30 minutes. Fluorescence confocal images were obtained by exciting cells with 405 nm laser line and the emission were collected from 570 nm to 700 nm range. Images from left to right represents the staining of the probe **3d** (a), bright filed (b) and the merged image (c).

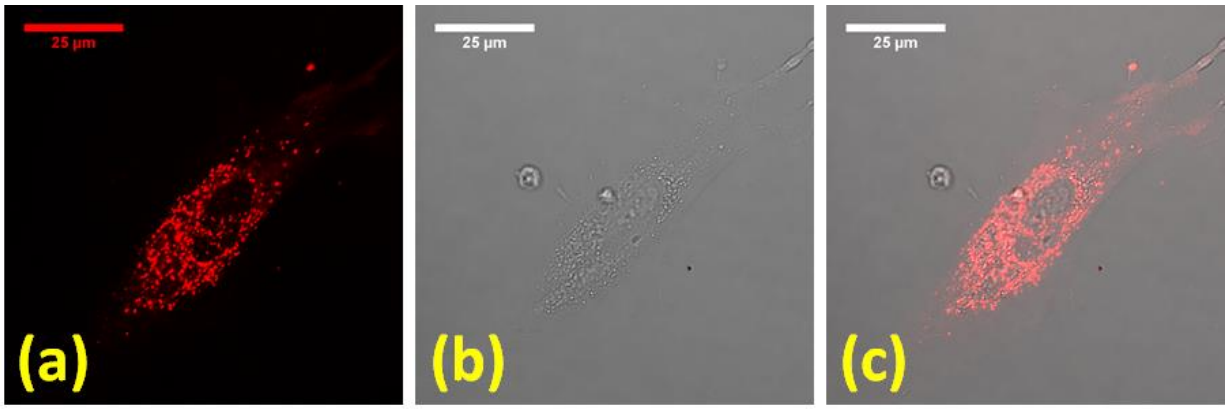


Figure S23.2 NHLF cells were incubated with probe **3d** (500 nM) for 30 minutes. Then FCCP (1 µM) was added to the solution. Fluorescence confocal images were obtained by exciting cells with 405 nm laser line and the emission were collected from 570 nm to 700 nm range. Images from left to right represents the staining of the probe **3d** (a), bright filed (b) and the merged image (c).

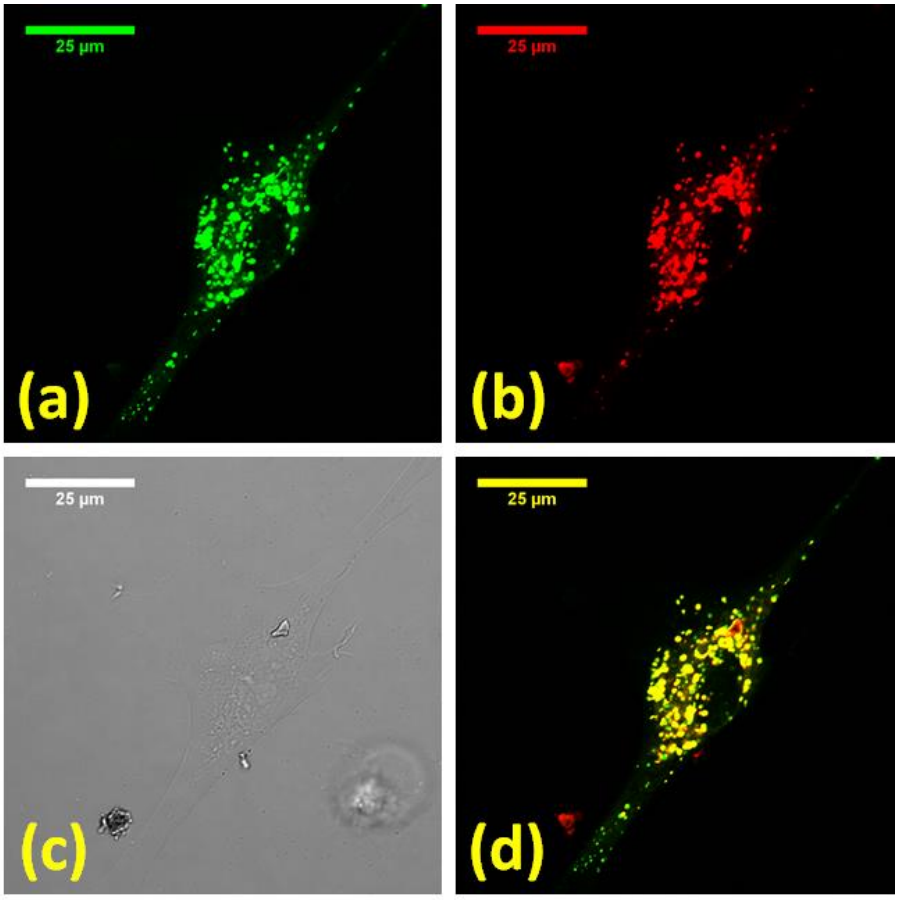


Figure S24.1 NHLF cells were incubated with FCCP (1 µM) for 1 hour. The cells were further incubated with probe **3d** (500 nM) for 30 minutes. Then LysoTracker® Green DND-26 (70 nM) was introduced into the cells and co-localization images were obtained. Images from left to right represents the staining of the LysoTracker® Green (a), probe **3d** (b), bright filed (c) and the merged image (d). Fluorescence confocal images were obtained by exciting cells with 405 nm laser line and the emission were collected from 570 nm to 700 nm range. LysoTracker® Green was excited with 488 nm laser line and the emission was collected from 495 to 550 nm range.

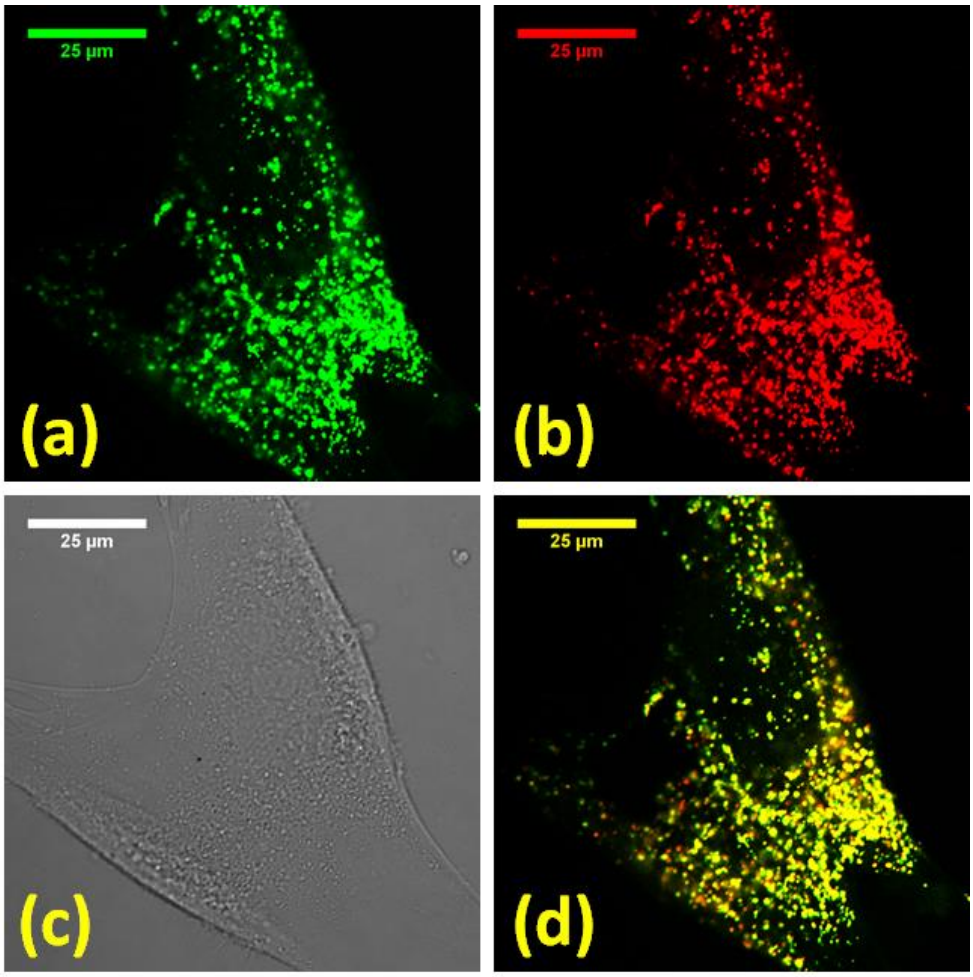


Figure S24.2 NHLF cells were incubated with probe **3d** (500 nM) nd LysoTracker® Green DND-26 (70 nM) for 30 minutes. Then FCCP (1 µM) was added to the solution. Images from left to right represents the staining of the LysoTracker® Green (a), probe **3d** (b), bright filed (c) and the merged image (d). Fluorescence confocal images were obtained by exciting cells with 405 nm laser line and the emission were collected from 570 nm to 700 nm range. LysoTracker® Green was excited with 488 nm laser line and the emission was collected from 495 to 550 nm range.

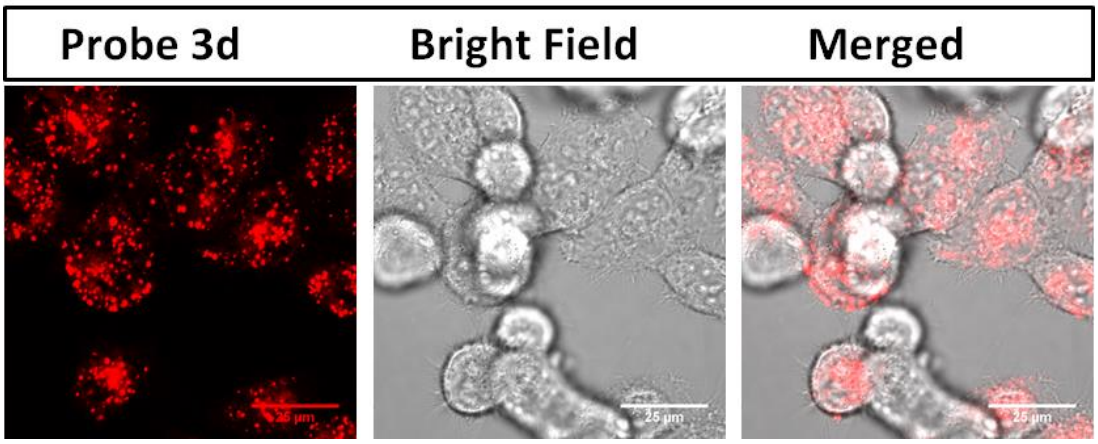


Figure S24.3 NHLF cells were first incubated with 0.75% H_2O_2 (v/v) for 30 minutes and probe **3d** (500 nM) was added and incubated for further 30 minutes. Fluorescence confocal images were obtained by exciting cells with 405 nm laser line and the emission were collected from 570 nm to 700 nm range.

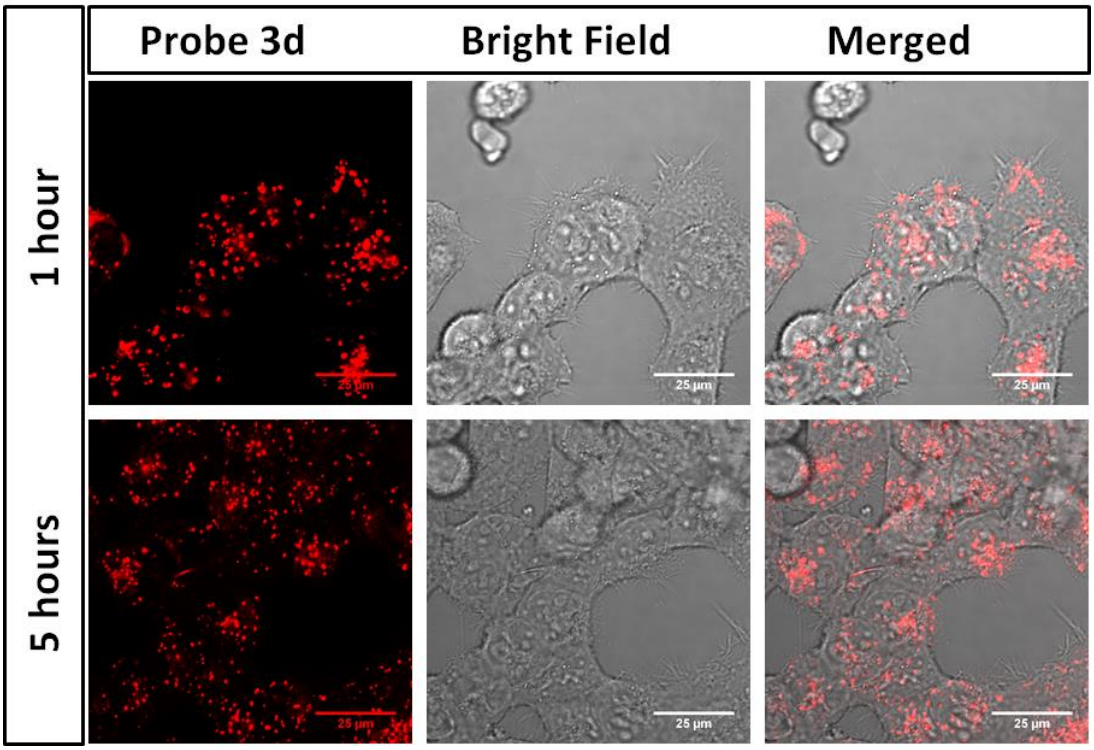


Figure S24.4 NHLF cells were first incubated with 3% H_2O_2 (v/v) for 30 minutes and probe **3d** (500 nM) was added and incubated for further 30 minutes. Images were obtained at 1 hour and 5 hour intervals. Fluorescence confocal images were obtained by exciting cells with 405 nm laser line and the emission were collected from 570 nm to 700 nm range.

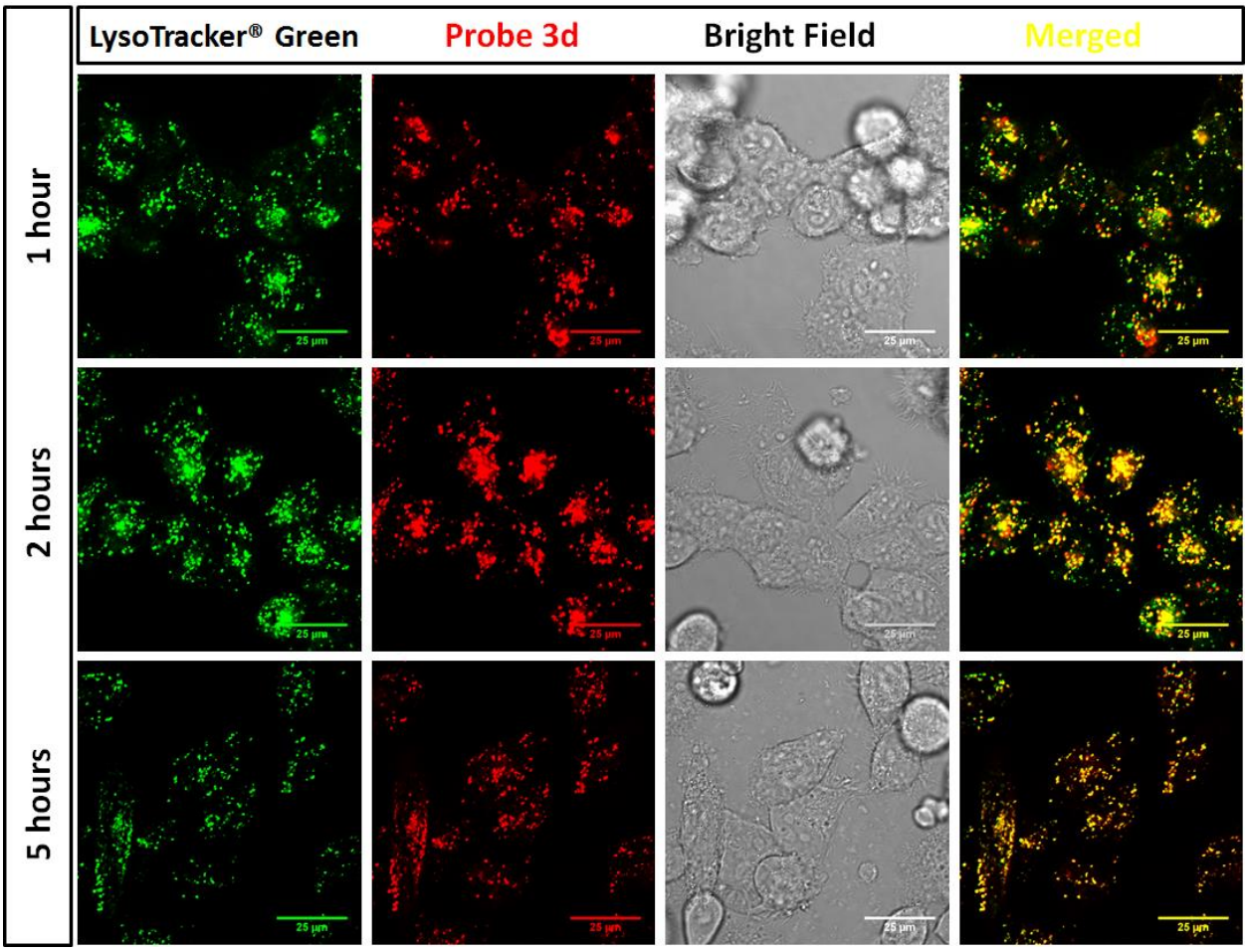


Figure S24.4 NHLF cells were first incubated with 3% H_2O_2 (v/v) for 30 minutes and probe **3d** (500 nM) and LysoTracker® Green (70 nM) were added and incubated for further 30 minutes. Images were obtained at 1 hour, 2 hour and 5 hour intervals. Fluorescence confocal images were obtained by exciting Probe **3d** with 405 nm laser line and the emission were collected from 570 nm to 700 nm range. LysoTracker® Green was excited with 488 nm laser line and the emission was collected from 495 to 550 nm range.

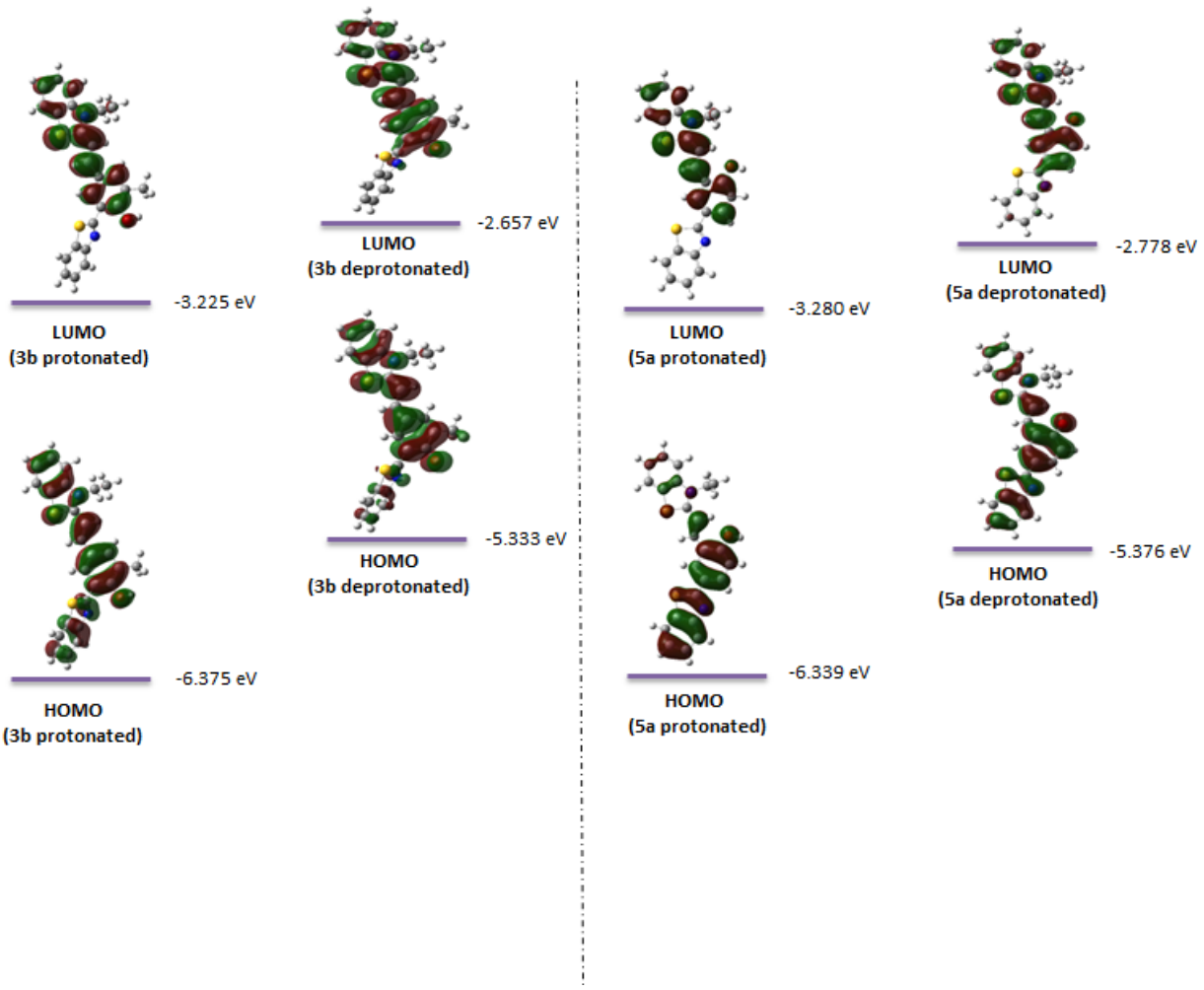


Figure S25 Quantum mechanical HOMO/LUMO orbitals energy calculated for probes **3b** and **5a** by using DFT/B3LYP method with the 6-311G+(2d,p) basis set under protonated and de-protonated conditions in water.

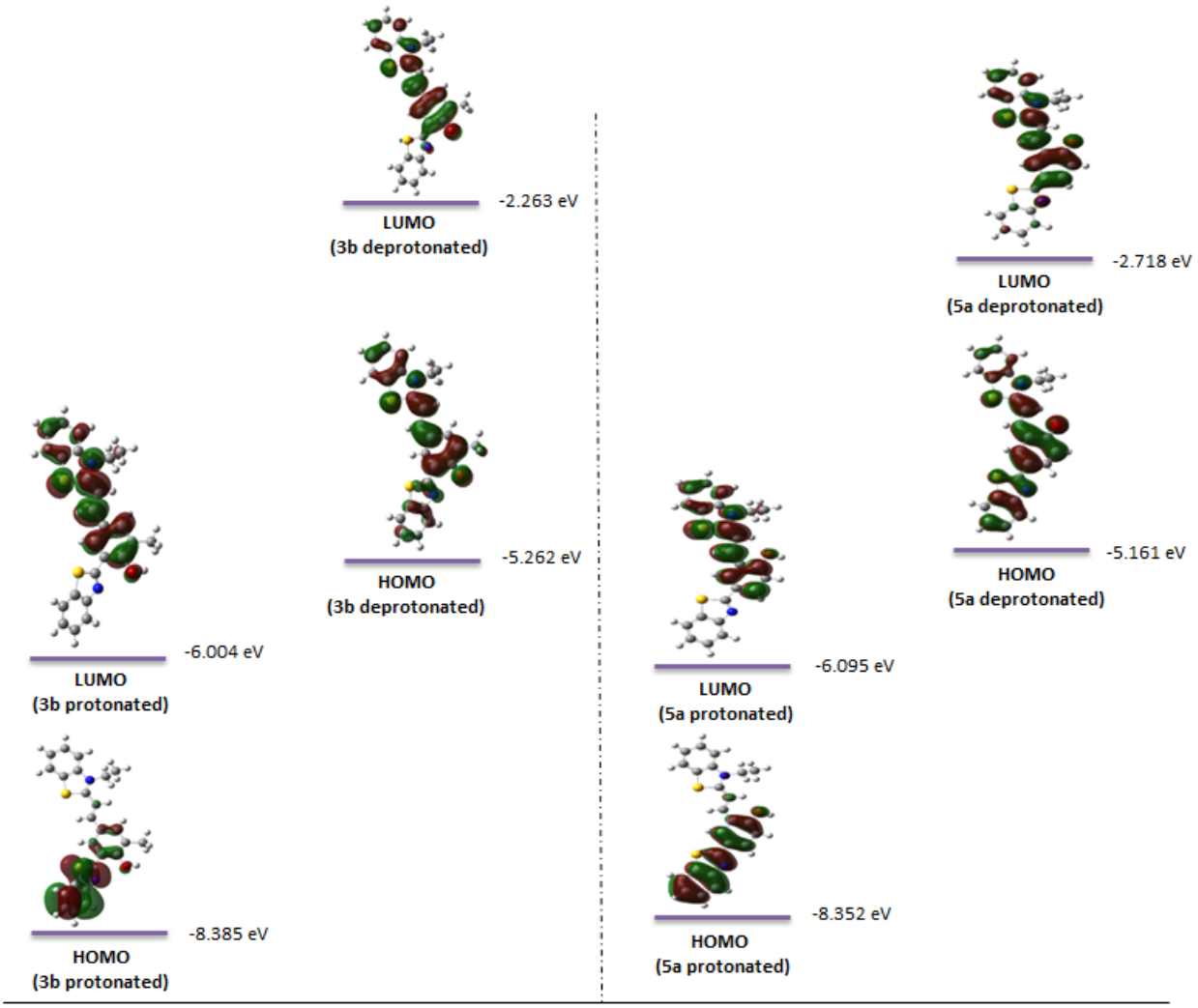


Figure S26 Quantum mechanical HOMO/LUMO orbitals energy calculated for probes **3b** and **5a** by using DFT/B3LYP method with the 6-311G+(2d,p) basis set under protonated and de-protonated conditions in gas phase.

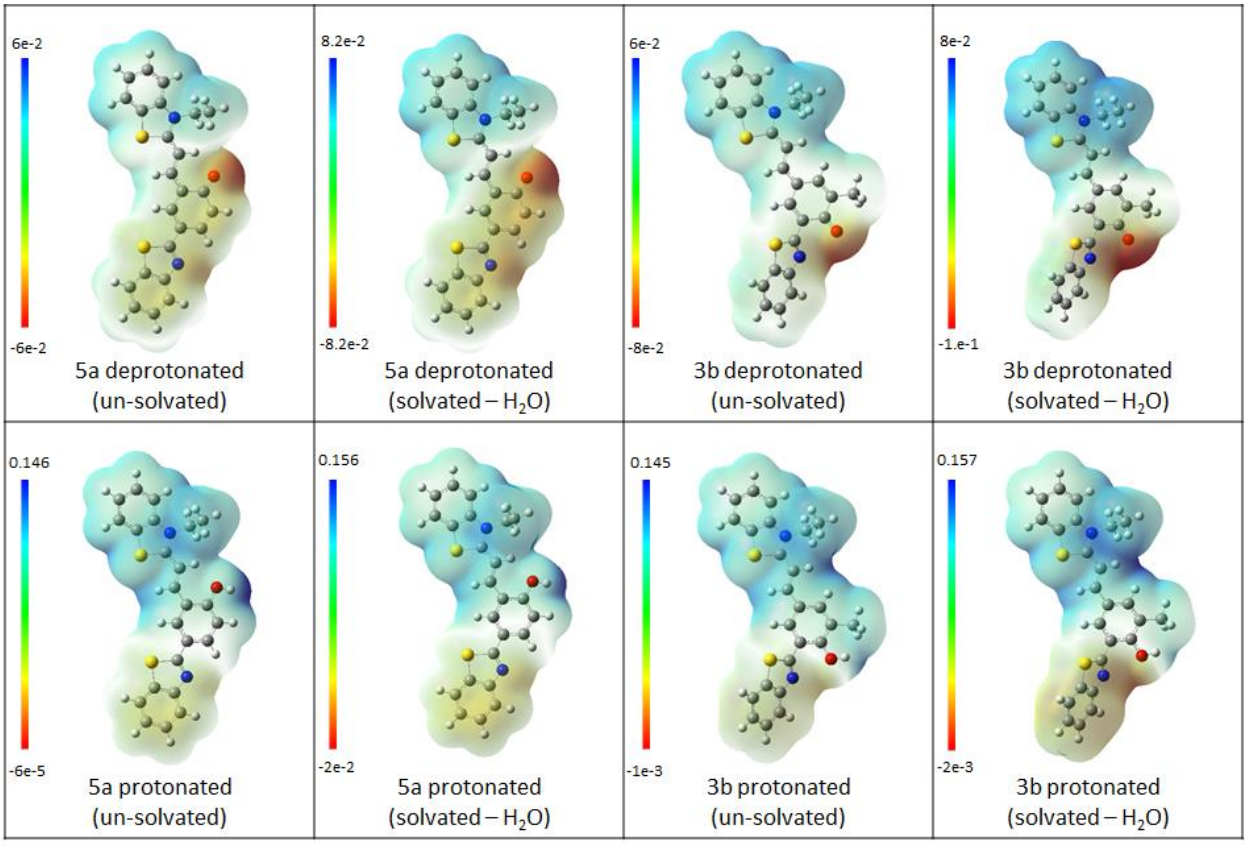


Figure S27 The molecular electrostatic potential mapped onto total SCF electron density for the protonated and deprotonated forms in un-solvated vs. solvated environments including the color codes for the range of potentials.

Computational Methods:

All calculations were carried out using the Gaussian16 suite of programs through the Ohio Super Computer Center in Columbus, Ohio.[1] Geometry optimizations were performed without symmetry constraints and the resulting optimized geometries were identified as true energy minima through frequency calculation (i.e. no imaginary frequencies were found). The density functional theory method (DFT) utilizing the B3LYP hybrid functional with the 6311G+(2d,p) basis set was used for all calculations. To calculate molecular

properties such as partial atomic charges, orbital interaction, and hybridization, NBO analysis was performed on all structures using the NBO program in the Gaussian16 package (NBO Version 3.1)[2,3]. Atomic electrostatic potential surfaces (Merz-Kollman ESP)[4,5] were also generated for each structure. The polarizable continuum model (PCM) which is a solvent model that has been widely developed to study solvent effects on molecular properties was used to study the molecules in a solvated environment.[6]

References:

1) a) J. Frisch, et al. GaussianInc., Gaussian 16 Rev. B.01, Wallingford CT, 2016 b) GaussView, Version 6, Dennington, Roy; Keith, Todd A.; Millam, John M. Semichem Inc., Shawnee Mission, KS, 2016

c) Ohio Supercomputer Center. Columbus OH: Ohio Supercomputer Center. http://osc.edu/ark:/19495/f5s1ph73

2) Alan E. Reed, Frank Weinhold, J. Chem. Phys. 78, 4066 (1983)

3) J.E. Carpenter, F. Weinhold, Journal of Molecular Structure (Theochem), 169 (1988) 41-62

4) U.C. Singh. P.A. Kollman, J. Comput. Chem., 5, (1984) 129-145

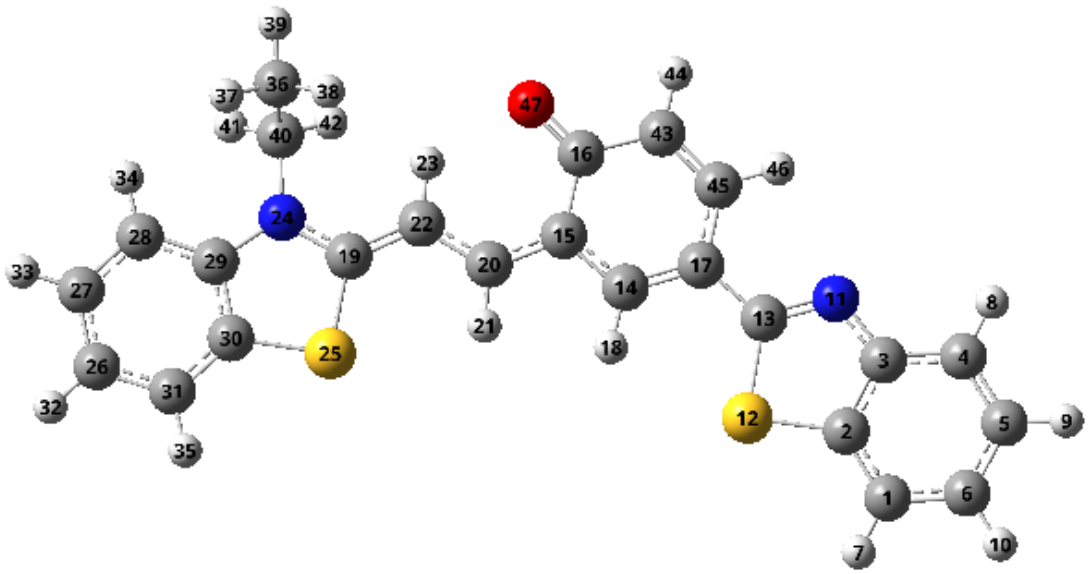
5) B. H. Besler, K.M. Merz, Jr., P.A.Kollman, J. Comput. Chem., 11 (1990), 431-439

6) Mennucci, B.; Cancès, E.; Tomasi, J. (1997) J. Phys. Chem. B. 101, (49), 10506–10517

Supplemental:

Bond length, Dihedral angle, and x,y,z coordinates for the geometry optimizations performed without symmetry constraints and the resulting optimized geometries were identified as true energy minima through frequency calculation. The density functional theory method (DFT) utilizing the B3LYP hybrid functional with the 6311G+(2d,p) basis set was used for all calculations.

5a Deprotonated (No solvent)



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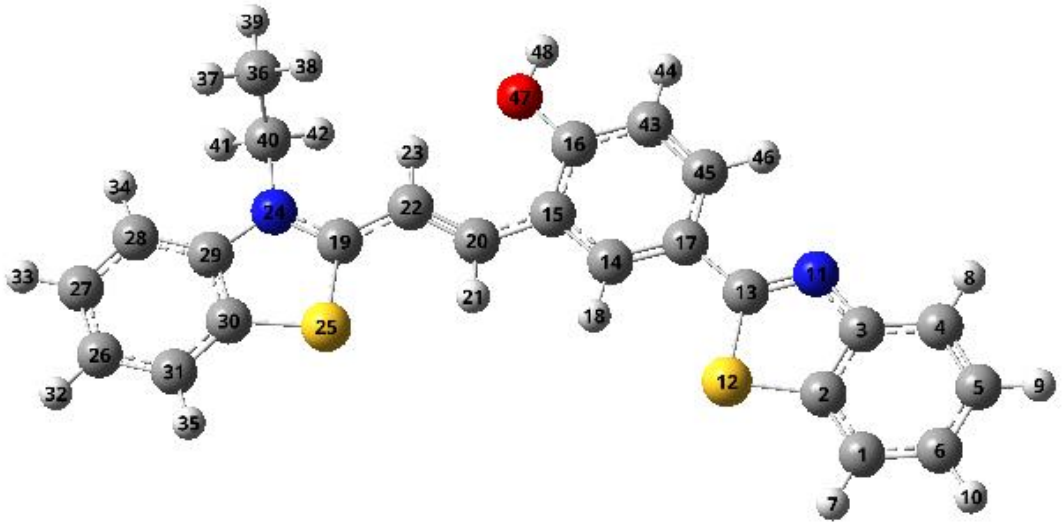
3	C	2	1		1.411688	121.5439		6.207175	-0.02701	0.016555
4	C	3	2	1	1.398617	119.3576	-0.00102	7.568808	0.292443	0.022447
5	C	4	3	2	1.385508	119.1134	0.003436	8.501238	-0.73141	0.06644
6	C	1	2	3	1.388897	118.2044	-0.00154	8.096877	-2.07204	0.10482
7	H	1	6	5	1.082873	120.6202	-180	6.441599	-3.44798	0.129532
8	H	4	3	2	1.082748	119.3217	179.9996	7.869655	1.332125	-0.00748
9	H	5	4	3	1.083322	119.642	179.9972	9.558149	-0.49371	0.071297
10	H	6	1	2	1.083242	119.4299	-179.997	8.842648	-2.85695	0.138905
11	N	3	2	1	1.378078	115.4071	179.9967	5.176347	0.886636	-0.02518
12	S	2	1	6	1.74702	129.3333	179.998	4.069505	-1.47294	0.037747
13	C	11	3	2	1.297038	112.3024	0.007676	4.011863	0.315442	-0.0205
14	C	13	11	3	2.481784	151.8021	179.9216	1.531864	0.404434	-0.05112
15	C	14	13	11	1.422842	152.4595	0.123476	0.295005	1.106773	-0.08827
16	C	15	14	13	1.483274	119.0072	-0.13955	0.310775	2.589251	-0.13422
17	C	14	13	11	1.370723	29.49209	0.112842	2.748573	1.03566	-0.05841
18	H	14	13	11	1.086021	90.32431	-179.914	1.486366	-0.68007	-0.01628

19	C	15	14	13	3.762736	134.2459	179.7265	-3.31911	0.059856	-0.10664
20	C	15	14	13	1.395172	118.3043	179.7402	-0.88702	0.365633	-0.08238
21	H	20	15	14	1.08957	115.1875	0.118181	-0.75629	-0.71548	-0.04691
22	C	19	15	14	1.382876	19.1474	-179.422	-2.19034	0.858649	-0.11921
23	H	22	19	15	1.080003	119.5638	-179.322	-2.29801	1.932786	-0.15151
24	N	19	15	14	1.368291	144.0145	-177.342	-4.60527	0.52177	-0.17476
25	S	19	15	14	1.764817	105.5951	2.107164	-3.30351	-1.70121	0.007348
26	C	25	19	15	4.075565	103.4372	179.3973	-7.25864	-2.68461	0.018568
27	C	26	25	19	1.393841	98.65291	-0.2636	-7.79424	-1.4005	-0.06513
28	C	27	26	25	1.390934	121.1909	0.239707	-6.97257	-0.27994	-0.12754
29	C	28	27	26	1.393789	118.6479	0.187446	-5.59093	-0.46256	-0.10888
30	C	29	28	27	1.400315	119.8363	-0.5509	-5.06021	-1.75514	-0.01691
31	C	30	29	28	1.386024	121.4678	0.593086	-5.87986	-2.87114	0.044686
32	H	26	25	19	1.082413	141.3308	-179.871	-7.91584	-3.54331	0.066883
33	H	27	26	25	1.082749	119.7118	-179.567	-8.86864	-1.26703	-0.07905
34	H	28	27	26	1.08136	120.0946	-179.396	-7.40717	0.708733	-0.18229
35	H	31	30	29	1.082649	120.7392	179.8133	-5.45679	-3.86539	0.112595
36	C	24	19	15	2.500064	115.4236	-38.2772	-5.048	2.650391	1.059452
37	H	36	24	19	1.091577	92.8703	-122.595	-5.83208	2.197875	1.669361
38	H	36	24	19	1.090442	93.50874	-13.7879	-4.10871	2.604101	1.611405
39	H	36	24	19	1.091664	142.3037	111.9708	-5.29658	3.70223	0.905927
40	C	24	19	15	1.469972	122.4261	0.151943	-4.92396	1.95198	-0.29204
41	H	40	24	19	1.089911	107.003	149.0303	-5.85152	2.026336	-0.8595
42	H	40	24	19	1.088937	107.6885	34.64232	-4.14772	2.415222	-0.8992
43	C	16	15	14	1.454239	115.5434	0.247848	1.629425	3.202359	-0.1427
44	H	43	16	15	1.08328	116.1506	179.8699	1.652439	4.284807	-0.17837
45	C	43	16	15	1.353481	122.5219	-0.22705	2.770306	2.475046	-0.1064
46	H	45	43	16	1.082686	120.773	-179.911	3.737645	2.961285	-0.11244
47	O	16	15	14	1.242433	123.2423	-179.686	-0.72102	3.280784	-0.16281

5a Protonated (No solvent)



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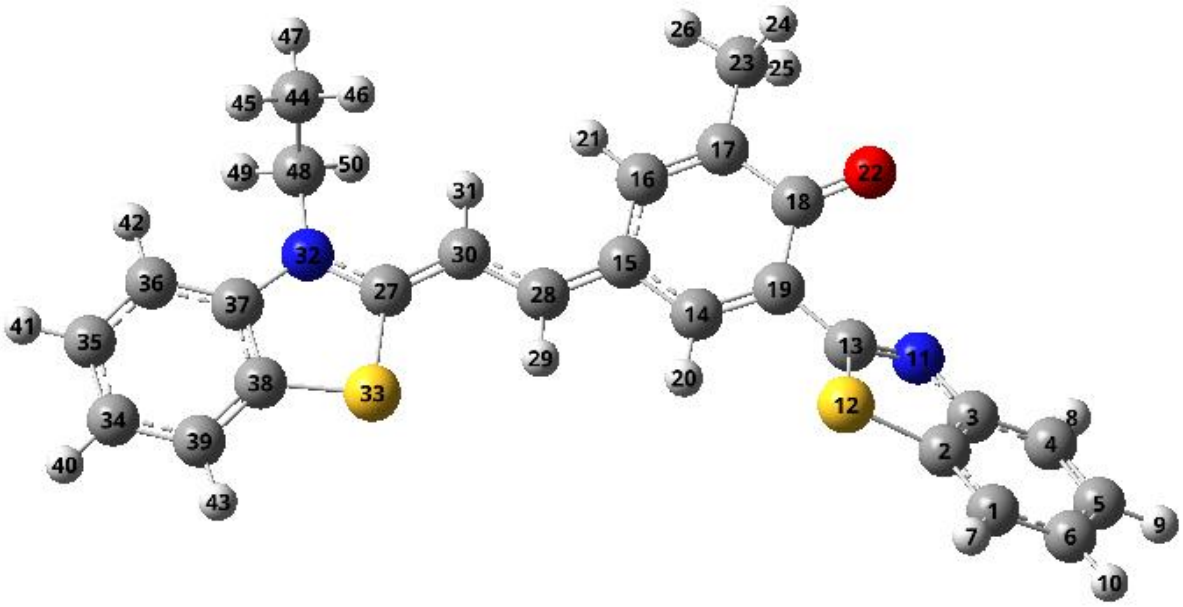
4	C	3	2	1	1.399061	119.5851	-0.00195	7.558347	0.208734	0.023139
5	C	4	3	2	1.383214	118.812	0.002138	8.462348	-0.83773	0.054308
6	C	1	2	3	1.38691	117.8379	0.00104	8.024027	-2.16989	0.077074
7	H	1	6	5	1.082358	120.7396	179.9974	6.341618	-3.51116	0.086731
8	H	4	3	2	1.082436	119.5335	-179.999	7.884413	1.240738	0.005367
9	H	5	4	3	1.082758	119.6754	179.9979	9.524655	-0.6284	0.061294
10	H	6	1	2	1.082863	119.3082	-179.997	8.752072	-2.97111	0.101279
11	N	3	2	1	1.379041	115.132	179.9978	5.176789	0.852676	-0.01555
12	S	2	1	6	1.747305	129.2265	179.9948	4.017055	-1.47524	0.019968
13	C	11	3	2	1.292984	111.9497	-0.00139	4.008219	0.299278	-0.01665
14	C	13	11	3	2.50606	150.4882	179.9454	1.508949	0.481289	-0.04594
15	C	14	13	11	1.411894	152.2372	0.118156	0.310892	1.227813	-0.07434
16	C	15	14	13	1.416031	117.4616	0.009194	0.421493	2.639203	-0.10418
17	C	14	13	11	1.385079	29.42128	0.127589	2.761703	1.072094	-0.04623
18	H	14	13	11	1.083809	90.25573	-179.876	1.425156	-0.59904	-0.02314
19	C	15	14	13	3.82264	130.5275	179.9861	-3.33401	0.075801	-0.08688
20	C	15	14	13	1.436646	117.2355	179.957	-0.92276	0.491575	-0.07176
21	H	20	15	14	1.087462	112.9494	0.03121	-0.7738	-0.58535	-0.04687
22	C	20	15	14	1.361652	129.6995	-179.717	-2.20636	0.945083	-0.10004
23	H	22	20	15	1.077016	119.6022	-0.12069	-2.39565	2.004979	-0.12746
24	N	19	15	14	1.344215	144.4541	-174.327	-4.61031	0.48582	-0.1861
25	S	19	15	14	1.7394	103.9239	4.161113	-3.22717	-1.65284	0.074066
26	C	25	19	15	4.061405	103.2399	-179.289	-7.11211	-2.83513	0.007257

27	C	26	25	19	1.39901	98.55433	-0.47257	-7.71031	-1.57705	-0.12167
28	C	27	26	25	1.38626	121.3224	0.226512	-6.94892	-0.42058	-0.18946
29	C	28	27	26	1.39469	118.1013	0.053077	-5.56105	-0.54316	-0.12661
30	C	29	28	27	1.398272	120.2897	-0.28384	-4.96967	-1.80314	0.00711
31	C	26	25	19	1.386599	22.25975	179.2538	-5.73296	-2.96242	0.073518
32	H	26	25	19	1.0822	141.7455	179.8128	-7.73183	-3.7209	0.057385
33	H	27	26	25	1.082248	119.5236	-179.7	-8.78891	-1.50166	-0.16852
34	H	28	27	26	1.081054	120.1847	-179.632	-7.43068	0.542654	-0.28306
35	H	31	26	25	1.082132	121.0031	179.6216	-5.26706	-3.93391	0.174265
36	C	24	19	15	2.501368	117.4875	-41.0899	-5.24425	2.587629	1.012806
37	H	36	24	19	1.090673	92.61844	-122.642	-6.02372	2.084649	1.586385
38	H	36	24	19	1.090895	93.86681	-14.0576	-4.33412	2.606799	1.613929
39	H	36	24	19	1.091153	142.3379	112.7503	-5.5608	3.617742	0.84171
40	C	24	19	15	1.480177	123.7685	-1.7285	-5.01014	1.903679	-0.3301
41	H	40	24	19	1.088588	106.5245	147.2878	-5.91029	1.910902	-0.94223
42	H	40	24	19	1.087703	107.7029	33.37928	-4.23933	2.407536	-0.90897
43	C	16	15	14	1.391648	120.0902	0.01167	1.676357	3.240866	-0.10501
44	H	43	16	15	1.085119	119.4206	-180	1.748463	4.323342	-0.12801
45	C	43	16	15	1.381363	120.7741	-0.01784	2.826656	2.476557	-0.07657
46	H	45	43	16	1.081911	120.4255	-179.985	3.799362	2.950239	-0.07713
47	O	16	15	14	1.358817	118.7057	-179.974	-0.71565	3.38254	-0.13136
48	H	47	16	15	0.966108	109.8327	-179.877	-0.49252	4.322307	-0.15174

3b Deprotonated (No solvent)



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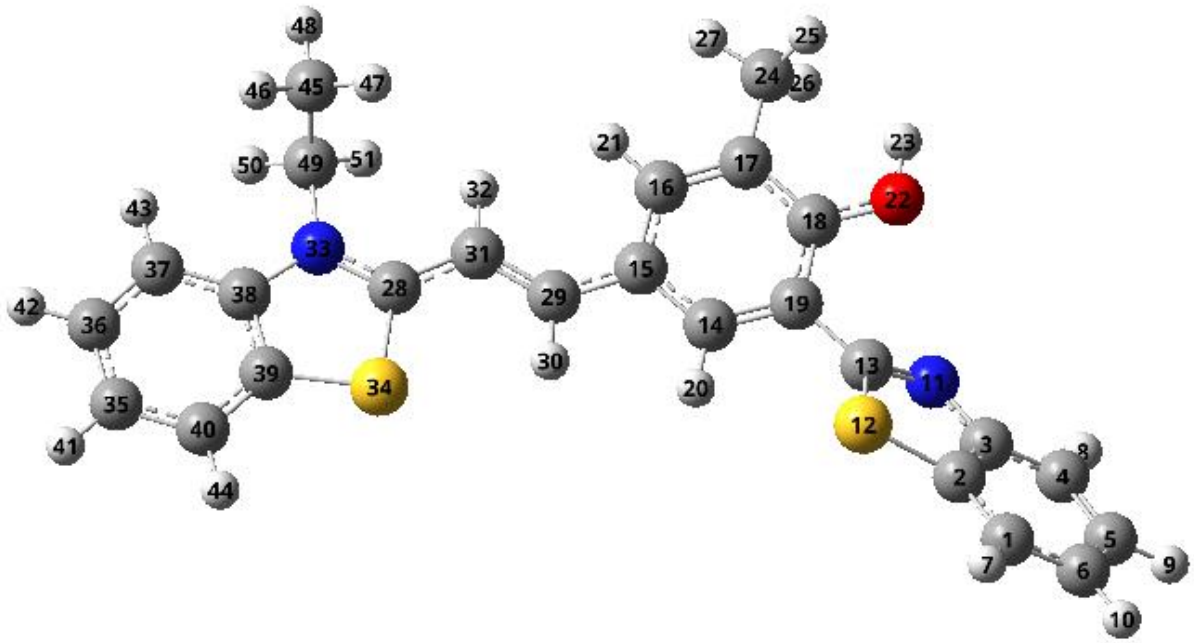
4	C	3	2	1	1.398718	119.4803	0.081874	7.112246	-0.61854	-1.11773
5	C	4	3	2	1.384437	119.0866	-0.08618	8.008131	-1.63071	-0.81845
6	C	1	2	3	1.387371	118.2271	-0.0179	7.677674	-2.63602	0.101289
7	H	1	6	5	1.082881	120.625	-179.93	6.194642	-3.423	1.446413
8	H	4	3	2	1.082617	119.1942	-179.89	7.354538	0.165736	-1.82361
9	H	5	4	3	1.083348	119.6813	-179.845	8.979057	-1.64709	-1.29874
10	H	6	1	2	1.083385	119.4101	179.8783	8.394949	-3.41743	0.321838
11	N	3	2	1	1.379398	115.536	179.8479	4.880432	0.337238	-0.69698
12	S	2	1	6	1.743553	129.6031	-179.466	3.937936	-1.34429	1.058902
13	C	11	3	2	1.288677	112.0644	-0.07879	3.826954	0.103904	0.007596
14	C	13	11	3	2.456885	142.6063	-145.855	1.377309	0.289808	-0.0234
15	C	14	13	11	1.43215	153.9694	-65.2737	0.141944	1.013729	-0.05279
16	C	15	14	13	1.44009	117.1609	-0.94617	0.222609	2.451527	-0.06216
17	C	16	15	14	1.352539	122.6309	-1.10174	1.399882	3.116222	-0.02253
18	C	17	16	15	1.481364	120.6561	-0.74436	2.682087	2.377882	0.049885
19	C	14	13	11	1.36115	30.90206	-67.4354	2.594541	0.898392	0.003064
20	H	14	13	11	1.085704	88.43744	112.2096	1.325035	-0.79436	-0.04795
21	H	16	15	14	1.085069	118.7634	179.0486	-0.69722	3.025846	-0.10012
22	O	18	17	16	1.226747	120.5834	-175.199	3.743287	2.980667	0.174035
23	C	17	16	15	1.498784	122.9308	-179.535	1.491288	4.612216	-0.02178

24	H	23	17	16	1.092769	110.6862	120.3276	1.999286	4.967466	0.878149
25	H	23	17	16	1.09292	110.7196	-122.473	2.092156	4.963315	-0.8645
26	H	23	17	16	1.091382	111.2219	-1.10118	0.501376	5.068523	-0.07631
27	C	15	14	13	3.76067	134.4626	178.3946	-3.4864	0.029359	-0.14639
28	C	15	14	13	1.384142	118.8158	178.3141	-1.04626	0.30456	-0.08605
29	H	28	15	14	1.087579	115.2731	0.378024	-0.94123	-0.77792	-0.08068
30	C	27	15	14	1.375392	19.6766	-179.076	-2.3579	0.815272	-0.12363
31	H	30	27	15	1.080749	117.4254	-179.004	-2.49752	1.886962	-0.12525
32	N	27	15	14	1.376468	145.6124	-177.568	-4.7848	0.481737	-0.211
33	S	27	15	14	1.769261	104.2674	1.962948	-3.46005	-1.73884	-0.09109
34	C	33	27	15	4.077861	103.5728	179.1397	-7.40861	-2.75664	-0.13501
35	C	34	33	27	1.39256	98.69476	-0.19036	-7.95542	-1.47674	-0.18054
36	C	35	34	33	1.392174	121.1754	0.215423	-7.14309	-0.34633	-0.20156
37	C	36	35	34	1.393412	118.7324	0.23509	-5.76006	-0.51486	-0.18115
38	C	37	36	35	1.400099	119.74	-0.61909	-5.21829	-1.80476	-0.12716
39	C	38	37	36	1.385023	121.5022	0.639121	-6.02688	-2.92905	-0.10631
40	H	34	33	27	1.082376	141.2231	-179.805	-8.05685	-3.62326	-0.11823
41	H	35	34	33	1.082795	119.7507	-179.566	-9.03091	-1.35218	-0.19653
42	H	36	35	34	1.081533	119.9695	-179.349	-7.58872	0.638822	-0.22633
43	H	39	38	37	1.08271	120.7029	179.7981	-5.59398	-3.9207	-0.06775
44	C	32	27	15	2.499889	115.4826	-37.8097	-5.26112	2.571108	1.076282
45	H	44	32	27	1.091307	93.16772	-123.185	-6.05226	2.101351	1.663114
46	H	44	32	27	1.090911	93.19209	-14.8211	-4.33235	2.50528	1.644749
47	H	44	32	27	1.092034	142.3994	111.0351	-5.51054	3.62683	0.950673
48	C	32	27	15	1.464381	122.5557	0.594336	-5.12036	1.904904	-0.29105
49	H	48	32	27	1.090106	107.254	149.1862	-6.04676	1.987189	-0.85968
50	H	48	32	27	1.090028	107.7666	35.18356	-4.3516	2.394795	-0.88868

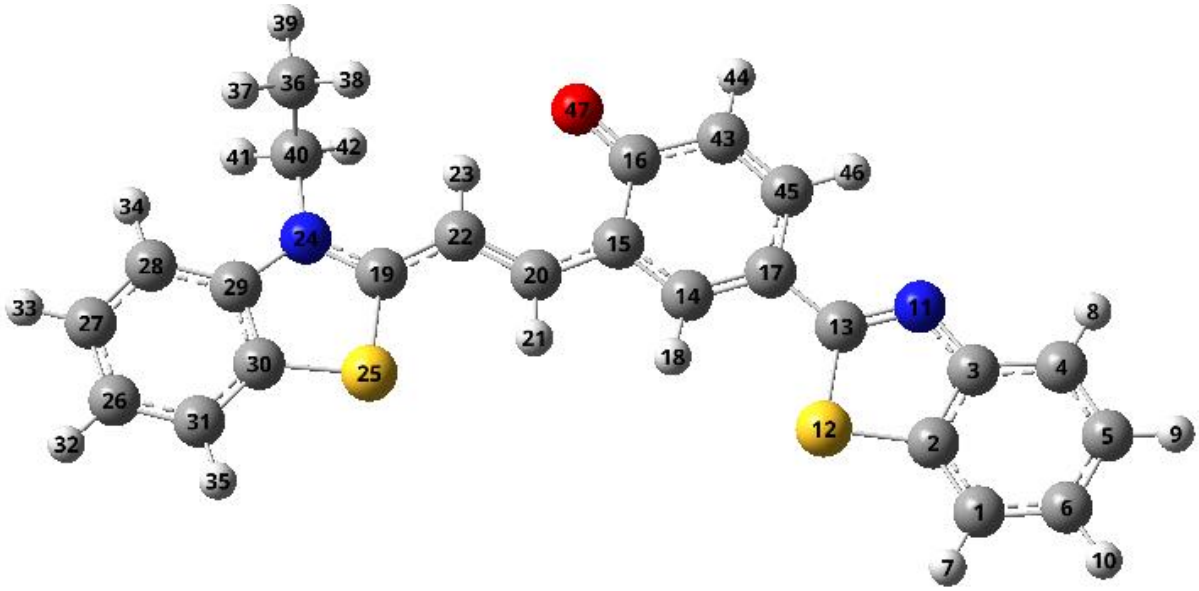
3b Protonated (No solvent)



Label	Symbol	NA	NB	NC	Bond Å	Angle	Dihedral	X	Y	Z
1	C							6.394407	-2.70044	0.707708
2	C	1			1.392698			5.505382	-1.66823	0.418283
3	C	2	1		1.411922	121.5117		5.839827	-0.63864	-0.48815
4	C	3	2	1	1.399094	119.6339	0.296758	7.088457	-0.65112	-1.11921
5	C	4	3	2	1.382879	118.831	-0.2081	7.970192	-1.6772	-0.83275
6	C	1	2	3	1.386203	117.8985	-0.20111	7.626646	-2.69229	0.072823
7	H	1	6	5	1.082388	120.7298	-179.953	6.137029	-3.48667	1.405681
8	H	4	3	2	1.082411	119.4517	179.8626	7.340908	0.13843	-1.81526
9	H	5	4	3	1.082803	119.6935	-179.899	8.940927	-1.6997	-1.31195
10	H	6	1	2	1.082929	119.3081	-179.989	8.335443	-3.48414	0.28093
11	N	3	2	1	1.38046	115.283	-179.83	4.864999	0.32041	-0.67685
12	S	2	1	6	1.745326	129.3239	-179.599	3.901279	-1.38216	1.043729
13	C	11	3	2	1.288968	111.7054	-0.18147	3.813748	0.076736	0.028085
14	C	13	11	3	2.482146	142.2142	-145.979	1.340728	0.287508	-0.00013
15	C	14	13	11	1.406356	153.1451	-64.2245	0.144713	1.026961	-0.02451
16	C	15	14	13	1.410794	117.917	-0.89297	0.238409	2.434636	-0.02782
17	C	16	15	14	1.37749	121.8595	-0.46465	1.453674	3.082519	0.001446
18	C	17	16	15	1.417117	118.6684	0.15249	2.63804	2.304999	0.032439
19	C	14	13	11	1.385641	30.76244	-65.6739	2.587133	0.892544	0.020054
20	H	14	13	11	1.083599	87.78181	113.9203	1.290778	-0.7948	-0.01749
21	H	16	15	14	1.08331	120.0498	179.7199	-0.66095	3.038116	-0.0509
22	O	18	17	16	1.338015	121.0127	-178.007	3.841845	2.88498	0.101421
23	H	22	18	17	0.965698	111.1668	-0.39594	3.764754	3.847451	0.118114

24	C	17	16	15	1.506478	121.6746	-179.344	1.548527	4.585968	0.012451
25	H	24	17	16	1.09532	111.8349	118.2611	2.035838	4.956783	0.920609
26	H	24	17	16	1.094997	111.7976	-120.583	2.108543	4.964366	-0.84907
27	H	24	17	16	1.0891	110.8628	-1.10961	0.558098	5.037375	-0.02523
28	C	15	14	13	3.809388	132.7984	178.3456	-3.52514	0.010329	-0.12473
29	C	15	14	13	1.430558	118.241	178.4865	-1.09328	0.310898	-0.0581
30	H	29	15	14	1.087335	114.177	0.602777	-0.98243	-0.77075	-0.05113
31	C	29	15	14	1.365339	128.1446	-179.217	-2.36012	0.818341	-0.10015
32	H	31	29	15	1.080586	119.691	-0.12108	-2.50791	1.888733	-0.10932
33	N	28	15	14	1.34699	144.1539	-175.09	-4.78514	0.476849	-0.22036
34	S	28	15	14	1.742203	104.3556	3.878418	-3.49457	-1.72865	-0.02322
35	C	34	28	15	4.062822	103.2819	-179.718	-7.42715	-2.7406	-0.15458
36	C	35	34	28	1.398262	98.57027	-0.41731	-7.97017	-1.45523	-0.2446
37	C	36	35	34	1.386915	121.3067	0.217726	-7.15926	-0.33034	-0.26824
38	C	37	36	35	1.394283	118.1467	0.073486	-5.77865	-0.51325	-0.20113
39	C	38	37	36	1.397889	120.2525	-0.32781	-5.24261	-1.80076	-0.10591
40	C	35	34	28	1.387156	22.1968	179.3465	-6.0545	-2.92765	-0.08365
41	H	35	34	28	1.082181	141.6927	179.8577	-8.08366	-3.60074	-0.13842
42	H	36	35	34	1.082256	119.5498	-179.697	-9.04417	-1.33191	-0.29564
43	H	37	36	35	1.081116	120.1351	-179.604	-7.59963	0.654974	-0.33179
44	H	40	35	34	1.08216	120.9796	179.6569	-5.63059	-3.9208	-0.01274
45	C	33	28	15	2.501608	117.2991	-40.3802	-5.33421	2.565421	1.042352
46	H	45	33	28	1.090642	92.72922	-122.666	-6.13956	2.081214	1.595943
47	H	45	33	28	1.091064	93.76085	-14.2219	-4.42901	2.52179	1.649912
48	H	45	33	28	1.091204	142.3642	112.526	-5.60154	3.614203	0.903355
49	C	33	28	15	1.478092	123.7701	-1.13595	-5.12456	1.911992	-0.31995
50	H	49	33	28	1.088624	106.6193	147.6643	-6.02192	1.977915	-0.93273
51	H	49	33	28	1.088082	107.7573	33.92623	-4.33352	2.401699	-0.88419

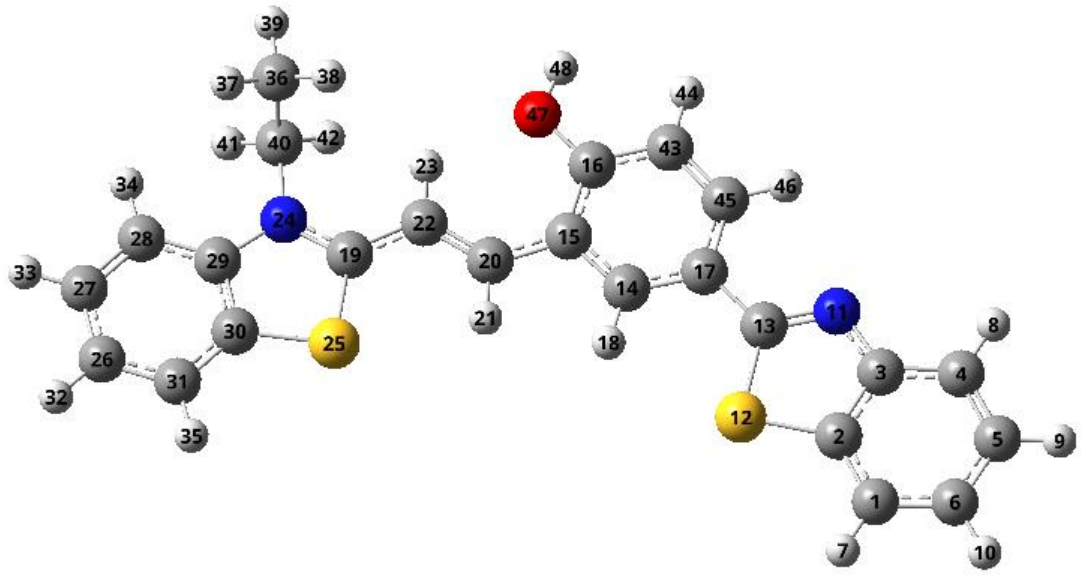
5a deprotonated (H_2O solvent)



Label	Symbol	NA	NB	NC	Bond Å	Angle	Dihedral	X	Y	Z
1	C							6.660467	-2.46128	0.103727
2	C	1			1.391312			5.75798	-1.40337	0.058017
3	C	2	1		1.411283	121.6552		6.191723	-0.06094	0.019795
4	C	3	2	1	1.399455	119.3172	-0.0089	7.563377	0.216496	0.028147
5	C	4	3	2	1.386972	119.0983	-0.00118	8.464349	-0.837	0.073903
6	C	1	2	3	1.390094	118.1563	0.005933	8.018605	-2.16503	0.111235
7	H	1	6	5	1.082696	120.6518	179.9961	6.319396	-3.48845	0.132584
8	H	4	3	2	1.083163	119.6595	-179.995	7.902426	1.244815	-0.00097
9	H	5	4	3	1.083234	119.5968	-179.997	9.527889	-0.63149	0.08074
10	H	6	1	2	1.083069	119.4282	-179.998	8.73927	-2.97277	0.146501
11	N	3	2	1	1.380717	115.3839	179.993	5.186697	0.884795	-0.02371
12	S	2	1	6	1.748675	129.2371	-179.996	4.009831	-1.44091	0.037295
13	C	11	3	2	1.301032	112.298	0.00582	4.002127	0.34677	-0.02105
14	C	13	11	3	2.487416	152.3657	179.8225	1.518784	0.485366	-0.05322
15	C	14	13	11	1.413359	152.657	0.413937	0.301846	1.203043	-0.09305
16	C	15	14	13	1.468065	119.2648	-0.10833	0.33506	2.669827	-0.14458
17	C	14	13	11	1.381124	29.463	0.360057	2.757464	1.096187	-0.06171
18	H	14	13	11	1.085601	90.22964	-179.622	1.453485	-0.59758	-0.01452
19	C	15	14	13	3.791071	132.2855	179.7375	-3.32025	0.083878	-0.10392
20	C	15	14	13	1.416297	117.5602	179.7659	-0.90071	0.454938	-0.08358
21	H	20	15	14	1.088435	114.2967	-0.00606	-0.75709	-0.62331	-0.04569
22	C	20	15	14	1.376062	128.0705	-179.892	-2.19324	0.925804	-0.11815
23	H	22	20	15	1.078648	117.8263	-0.36677	-2.33925	1.994001	-0.15158
24	N	19	15	14	1.351436	144.3	-177.615	-4.60076	0.511173	-0.16782
25	S	19	15	14	1.751429	104.5276	1.743925	-3.24089	-1.66226	0.006525

26	C	25	19	15	4.067183	103.2372	179.8126	-7.15303	-2.7745	0.001758
27	C	26	25	19	1.397614	98.5807	-0.22748	-7.73073	-1.50469	-0.08291
28	C	27	26	25	1.388745	121.2756	0.198014	-6.9481	-0.35891	-0.14013
29	C	28	27	26	1.394343	118.2733	0.095432	-5.5616	-0.5041	-0.11307
30	C	29	28	27	1.398679	120.1734	-0.35342	-4.98971	-1.77732	-0.0228
31	C	30	29	28	1.388532	121.5571	0.421263	-5.77211	-2.92306	0.033264
32	H	26	25	19	1.082362	141.5615	-179.924	-7.78495	-3.65216	0.045424
33	H	27	26	25	1.082447	119.6514	-179.674	-8.80858	-1.40696	-0.10253
34	H	28	27	26	1.08087	120.1738	-179.603	-7.41379	0.614722	-0.1989
35	H	31	30	29	1.081946	120.8907	179.8706	-5.31823	-3.90287	0.1009
36	C	24	19	15	2.49852	116.666	-39.8616	-5.15351	2.591003	1.101577
37	H	36	24	19	1.090867	92.80057	-122.974	-5.93275	2.094182	1.681179
38	H	36	24	19	1.090756	93.46816	-14.21	-4.2261	2.566625	1.675223
39	H	36	24	19	1.091141	142.1554	111.9759	-5.44298	3.633858	0.962837
40	C	24	19	15	1.476399	123.2866	-0.80509	-4.9757	1.935926	-0.26401
41	H	40	24	19	1.088128	106.8255	148.0876	-5.89393	1.981373	-0.84609
42	H	40	24	19	1.087326	107.6767	33.90222	-4.21097	2.439731	-0.85022
43	C	16	15	14	1.446567	115.5945	0.154113	1.653431	3.26512	-0.15354
44	H	43	16	15	1.08409	116.7025	179.9039	1.698925	4.347536	-0.193
45	C	43	16	15	1.361089	122.6756	-0.15105	2.794518	2.524235	-0.11388
46	H	45	43	16	1.082846	120.1646	-179.955	3.760927	3.012649	-0.12168
47	O	16	15	14	1.257242	123.2403	-179.83	-0.70057	3.381831	-0.17895

5a protonated (H_2O solvent)



Label	Symbol	NA	NB	NC	Bond Å	Angle	Dihedral	X	Y	Z
1	C							6.630089	-2.49849	0.080658
2	C	1			1.392394			5.738674	-1.42946	0.044185
3	C	2	1		1.41085	121.6198		6.187675	-0.09201	0.032948
4	C	3	2	1	1.399555	119.5071	0.000643	7.561439	0.174167	0.058939
5	C	4	3	2	1.385429	118.9288	-0.00433	8.449427	-0.88864	0.095317
6	C	1	2	3	1.388412	117.9925	-0.00126	7.988703	-2.21351	0.106006
7	H	1	6	5	1.082462	120.7541	179.9888	6.279049	-3.52241	0.088847
8	H	4	3	2	1.08295	119.7069	-179.997	7.909663	1.199569	0.050465
9	H	5	4	3	1.083033	119.6322	-179.997	9.514944	-0.69573	0.115737
10	H	6	1	2	1.082999	119.3663	-179.999	8.701781	-3.02812	0.134533
11	N	3	2	1	1.381033	115.1889	-179.99	5.190313	0.862537	-0.00383
12	S	2	1	6	1.74655	129.236	179.9933	3.992639	-1.44783	0.005954
13	C	11	3	2	1.296591	112.0308	0.013625	4.008115	0.330313	-0.02097
14	C	13	11	3	2.500369	151.7556	179.0529	1.514143	0.505141	-0.0582
15	C	14	13	11	1.406752	152.4952	1.692898	0.31528	1.240166	-0.09582
16	C	15	14	13	1.415915	117.4627	-0.01195	0.415902	2.651899	-0.13706
17	C	14	13	11	1.388676	29.69829	1.711498	2.765717	1.106786	-0.06063
18	H	14	13	11	1.083452	90.22943	-178.234	1.433595	-0.57481	-0.02511
19	C	15	14	13	3.828741	130.628	-179.891	-3.32926	0.066889	-0.10138
20	C	15	14	13	1.444871	117.1689	179.9813	-0.91929	0.489537	-0.0893
21	H	20	15	14	1.08633	112.9777	-0.15806	-0.76217	-0.58491	-0.05776
22	C	20	15	14	1.355893	129.2388	179.9104	-2.19758	0.940782	-0.11779
23	H	22	20	15	1.076695	119.9883	-0.17559	-2.3942	1.998949	-0.14768
24	N	19	15	14	1.34011	143.9218	-177.046	-4.6011	0.483476	-0.17039
25	S	19	15	14	1.736005	104.1161	2.304652	-3.21795	-1.66108	0.022857

26	C	25	19	15	4.057919	103.0771	-179.955	-7.10241	-2.83476	0.008406
27	C	26	25	19	1.400413	98.55697	-0.24712	-7.70109	-1.57254	-0.08927
28	C	27	26	25	1.385799	121.3565	0.191122	-6.93985	-0.41623	-0.15166
29	C	28	27	26	1.395328	118.0089	0.03748	-5.55081	-0.54342	-0.11514
30	C	29	28	27	1.398698	120.3831	-0.23871	-4.9585	-1.80641	-0.01329
31	C	26	25	19	1.386345	22.29544	179.5191	-5.72286	-2.96618	0.047647
32	H	26	25	19	1.082242	141.7544	-179.988	-7.72297	-3.72017	0.055294
33	H	27	26	25	1.082204	119.5496	-179.726	-8.78014	-1.49423	-0.11551
34	H	28	27	26	1.080598	120.2709	-179.691	-7.42033	0.549127	-0.22178
35	H	31	26	25	1.081579	121.1799	179.6405	-5.25493	-3.93826	0.12448
36	C	24	19	15	2.49929	117.2939	-40.5827	-5.19914	2.55404	1.095146
37	H	36	24	19	1.090503	92.50336	-122.146	-5.9657	2.03685	1.673154
38	H	36	24	19	1.09068	93.82624	-13.3557	-4.27311	2.557165	1.671373
39	H	36	24	19	1.090851	142.0364	113.3435	-5.51736	3.587605	0.952196
40	C	24	19	15	1.482159	123.9518	-1.22483	-5.00161	1.906969	-0.27066
41	H	40	24	19	1.087365	106.5026	147.9542	-5.91642	1.929811	-0.85801
42	H	40	24	19	1.086542	107.7466	33.98184	-4.24563	2.423279	-0.85589
43	C	16	15	14	1.395061	120.1453	0.040384	1.668935	3.265164	-0.14021
44	H	43	16	15	1.084009	119.2284	-179.978	1.728654	4.347069	-0.17167
45	C	43	16	15	1.380248	120.7418	-0.03743	2.823935	2.510415	-0.10263
46	H	45	43	16	1.081351	119.9009	-179.997	3.788117	2.99997	-0.10554
47	O	16	15	14	1.351465	118.5629	-179.963	-0.72207	3.380042	-0.17293
48	H	47	16	15	0.967309	110.5599	179.8636	-0.5197	4.325646	-0.19673

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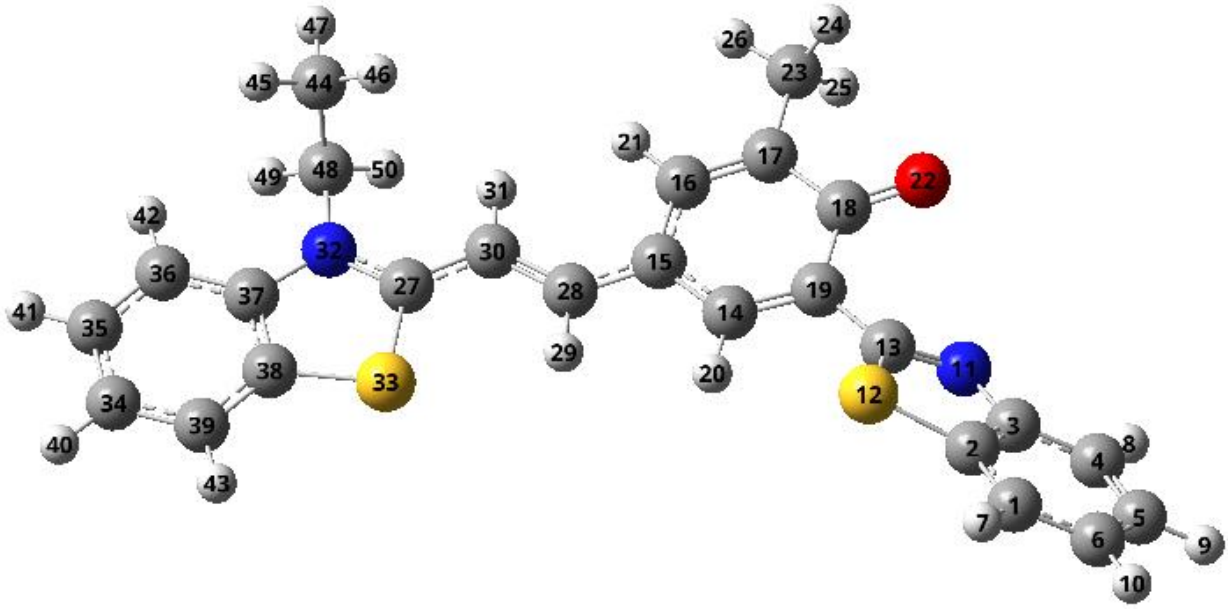
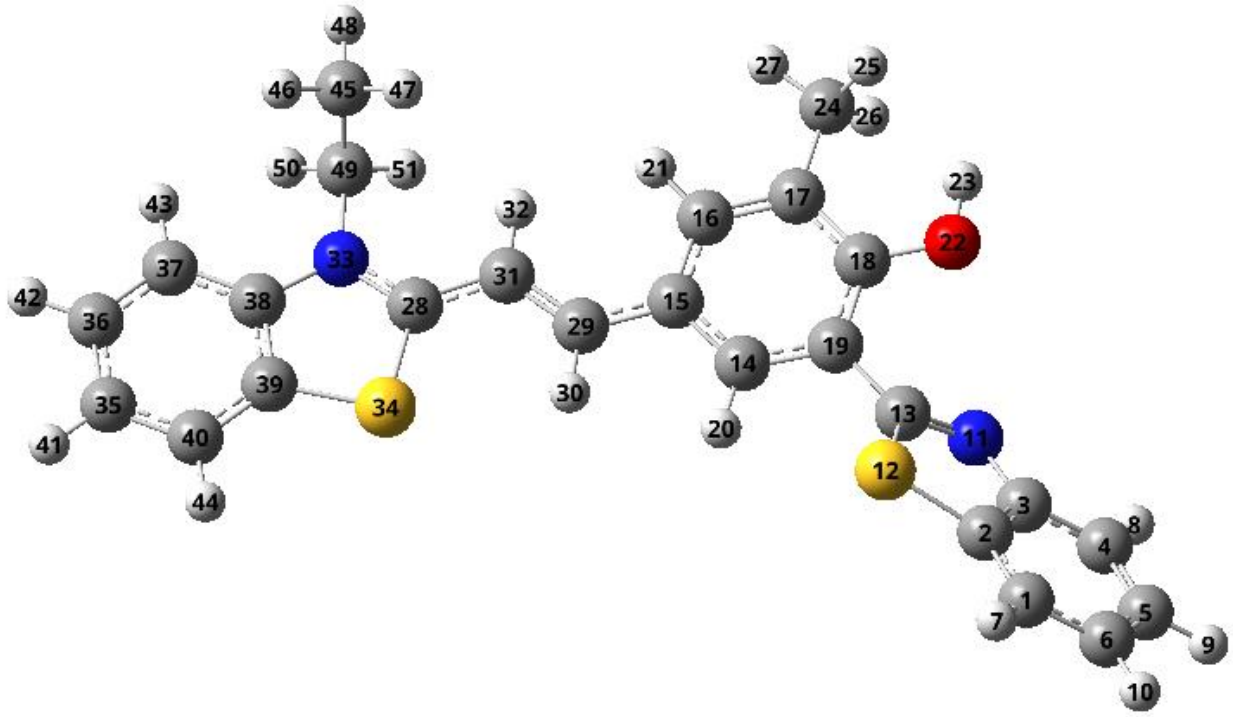
3b deprotonated (H_2O solvent)



Label	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	C							6.355562	-2.70669	0.715937
2	C	1			1.393057			5.492285	-1.65355	0.422262
3	C	2	1		1.412035	121.4854		5.867863	-0.6158	-0.45857
4	C	3	2	1	1.39973	119.4321	0.03963	7.134977	-0.64275	-1.05265
5	C	4	3	2	1.385876	119.0785	-0.12311	7.9944	-1.68957	-0.75906
6	C	1	2	3	1.388501	118.1877	0.094234	7.608959	-2.71342	0.118539
7	H	1	6	5	1.082571	120.6637	179.9237	6.061809	-3.49973	1.391781
8	H	4	3	2	1.083149	119.6417	179.8518	7.425693	0.150293	-1.73073
9	H	5	4	3	1.083194	119.6434	-179.933	8.977531	-1.71897	-1.21282
10	H	6	1	2	1.083126	119.417	179.8588	8.296959	-3.52157	0.334646
11	N	3	2	1	1.382451	115.4523	179.6217	4.912401	0.361307	-0.66721
12	S	2	1	6	1.744288	129.5195	-179.601	3.87674	-1.34731	1.004306
13	C	11	3	2	1.295187	112.2363	-0.11138	3.825282	0.134019	-0.00086
14	C	13	11	3	2.455011	144.8146	-145.136	1.378252	0.330185	-0.02621
15	C	14	13	11	1.415764	154.2591	-64.2238	0.156354	1.044896	-0.04949
16	C	15	14	13	1.430177	117.1887	-1.00449	0.234511	2.472935	-0.05111
17	C	16	15	14	1.360999	122.5591	-0.58201	1.419475	3.141661	-0.01974
18	C	17	16	15	1.467215	120.8153	-0.18403	2.692574	2.413507	0.021865
19	C	14	13	11	1.376171	31.28225	-65.4682	2.607593	0.9485	-0.01031
20	H	14	13	11	1.085206	87.92068	113.7127	1.331073	-0.7538	-0.047
21	H	16	15	14	1.084576	119.0139	179.6365	-0.68351	3.049983	-0.07471
22	O	18	17	16	1.248061	120.4536	-176.914	3.772832	3.032554	0.108355
23	C	17	16	15	1.501851	121.8873	-179.41	1.483635	4.642101	-0.00879
24	H	23	17	16	1.093405	111.0679	120.149	1.992072	5.007239	0.887705

25	H	23	17	16	1.093522	111.1528	-121.675	2.055265	5.018855	-0.86148
26	H	23	17	16	1.090776	110.968	-0.74785	0.483354	5.075816	-0.04226
27	C	15	14	13	3.78137	133.9524	178.4092	-3.48233	0.01995	-0.14006
28	C	15	14	13	1.406161	118.7898	178.3901	-1.04991	0.323008	-0.0825
29	H	28	15	14	1.087424	114.7001	0.501172	-0.93274	-0.75808	-0.07873
30	C	28	15	14	1.384939	127.866	-179.53	-2.34025	0.824851	-0.11785
31	H	30	28	15	1.080274	119.3722	-0.02853	-2.49292	1.894275	-0.12159
32	N	27	15	14	1.357384	144.705	-177.034	-4.75984	0.473818	-0.20698
33	S	27	15	14	1.756567	104.3514	2.506179	-3.44205	-1.73501	-0.07651
34	C	33	27	15	4.070457	103.3007	179.5754	-7.37931	-2.76528	-0.14791
35	C	34	33	27	1.396479	98.59265	-0.26291	-7.92959	-1.48294	-0.2023
36	C	35	34	33	1.389934	121.26	0.222861	-7.12211	-0.35177	-0.22092
37	C	36	35	34	1.394027	118.3806	0.124163	-5.73922	-0.52417	-0.18655
38	C	37	36	35	1.398742	120.0534	-0.42078	-5.19505	-1.81129	-0.12584
39	C	38	37	36	1.387654	121.5965	0.485504	-6.00054	-2.94109	-0.10826
40	H	34	33	27	1.082381	141.4703	-179.914	-8.0283	-3.6314	-0.13389
41	H	35	34	33	1.082526	119.6879	-179.627	-9.00498	-1.36164	-0.22822
42	H	36	35	34	1.080942	120.1275	-179.546	-7.56774	0.632427	-0.25577
43	H	39	38	37	1.082077	120.8613	179.8449	-5.56675	-3.93141	-0.06364
44	C	32	27	15	2.499502	116.466	-39.2291	-5.27827	2.539051	1.102045
45	H	44	32	27	1.090907	92.84344	-122.926	-6.07149	2.047363	1.666957
46	H	44	32	27	1.090898	93.50398	-14.2367	-4.35605	2.483569	1.682127
47	H	44	32	27	1.091241	142.1376	111.9755	-5.54482	3.590481	0.982668
48	C	32	27	15	1.473998	123.2386	-0.32231	-5.10631	1.904918	-0.27463
49	H	48	32	27	1.088347	106.9152	148.4264	-6.02113	1.981957	-0.85917
50	H	48	32	27	1.087957	107.7884	34.4397	-4.3319	2.407533	-0.85023

3b protonated (H_2O solvent)



Label	Symbol	NA	NB	NC	Bond	Angle	Dihedral	X	Y	Z
1	C							6.404866	-2.67244	0.749257
2	C	1			1.393483			5.517703	-1.64398	0.437802
3	C	2	1		1.411397	121.4939		5.848034	-0.64486	-0.50277
4	C	3	2	1	1.399664	119.5841	0.122156	7.092073	-0.68279	-1.14307
5	C	4	3	2	1.384809	118.9212	-0.14519	7.97392	-1.70454	-0.83314
6	C	1	2	3	1.387457	118.0314	-0.01335	7.633717	-2.69089	0.105345
7	H	1	6	5	1.082329	120.7498	179.9329	6.147036	-3.43622	1.47148
8	H	4	3	2	1.082951	119.6902	179.8579	7.346399	0.081655	-1.86676
9	H	5	4	3	1.083027	119.657	-179.939	8.940132	-1.74485	-1.32075
10	H	6	1	2	1.083028	119.3613	179.9584	8.340012	-3.48012	0.331639
11	N	3	2	1	1.382844	115.2659	179.821	4.871628	0.310832	-0.71618
12	S	2	1	6	1.744286	129.3986	-179.729	3.919774	-1.33266	1.064087
13	C	11	3	2	1.293187	111.8111	-0.05995	3.821051	0.093993	0.006041
14	C	13	11	3	2.478589	142.4486	-144.666	1.349221	0.275506	-0.01656
15	C	14	13	11	1.400509	153.0746	-67.7766	0.150419	0.999423	-0.0322
16	C	15	14	13	1.407854	117.9646	-0.77723	0.227922	2.405124	-0.02501
17	C	16	15	14	1.380659	122.0207	-0.22174	1.436826	3.071519	0.001235
18	C	17	16	15	1.412416	118.6294	0.25448	2.627837	2.312443	0.015862
19	C	14	13	11	1.391204	31.0371	-68.4805	2.590495	0.903571	-0.00169
20	H	14	13	11	1.08313	87.89779	110.7734	1.309771	-0.80673	-0.03632
21	H	16	15	14	1.082665	120.0405	179.9656	-0.67793	2.997955	-0.03719

22	O	18	17	16	1.348735	120.9279	-178.419	3.83316	2.914908	0.073467
23	H	22	18	17	0.966666	110.5683	1.597591	3.730934	3.874749	0.125408
24	C	17	16	15	1.50644	121.3433	-179.36	1.501731	4.576403	0.022945
25	H	24	17	16	1.094837	111.7975	118.9399	1.998113	4.948946	0.924879
26	H	24	17	16	1.094451	111.7615	-120.078	2.040502	4.971849	-0.84376
27	H	24	17	16	1.088788	110.5035	-0.46474	0.499546	5.001623	0.006426
28	C	15	14	13	3.81476	133.405	178.5905	-3.52505	-0.01785	-0.12451
29	C	15	14	13	1.442036	118.3676	178.7864	-1.09161	0.267444	-0.06437
30	H	29	15	14	1.086432	114.3762	0.595667	-0.97562	-0.81278	-0.06345
31	C	29	15	14	1.356795	127.1745	-179.199	-2.34628	0.782755	-0.09846
32	H	31	29	15	1.079979	119.9618	-0.08471	-2.48982	1.853146	-0.10226
33	N	28	15	14	1.341571	143.1643	-174.875	-4.77186	0.46881	-0.21629
34	S	28	15	14	1.737709	104.9379	4.079642	-3.51216	-1.75285	-0.02852
35	C	34	28	15	4.059928	103.0775	-179.673	-7.4557	-2.70934	-0.15763
36	C	35	34	28	1.399969	98.54787	-0.34311	-7.9811	-1.41463	-0.24471
37	C	36	35	34	1.386296	121.3362	0.229252	-7.15521	-0.30143	-0.26728
38	C	37	36	35	1.39491	118.0439	0.046679	-5.77695	-0.50594	-0.2015
39	C	38	37	36	1.398442	120.3731	-0.27635	-5.25789	-1.80124	-0.10979
40	C	35	34	28	1.386869	22.27892	179.3715	-6.08626	-2.91745	-0.08887
41	H	35	34	28	1.082248	141.7301	179.9642	-8.12465	-3.55994	-0.14211
42	H	36	35	34	1.082203	119.5687	-179.676	-9.0532	-1.27556	-0.29408
43	H	37	36	35	1.080622	120.3043	-179.648	-7.57894	0.69073	-0.32913
44	H	40	35	34	1.081694	121.1711	179.588	-5.67435	-3.91528	-0.02011
45	C	33	28	15	2.499181	117.5032	-40.9085	-5.29609	2.549099	1.065696
46	H	45	33	28	1.090534	92.49406	-122.454	-6.10668	2.065335	1.611751
47	H	45	33	28	1.09073	93.82507	-13.6952	-4.38954	2.492813	1.669586
48	H	45	33	28	1.090871	142.0595	113.0269	-5.55367	3.600569	0.931289
49	C	33	28	15	1.481241	123.9649	-1.46823	-5.09242	1.912277	-0.30415
50	H	49	33	28	1.087574	106.5252	147.6054	-5.98715	1.993718	-0.91705
51	H	49	33	28	1.08682	107.7965	33.70801	-4.29391	2.396641	-0.85998

Thermochemical data for the geometry optimizations performed without symmetry constraints and the resulting optimized geometries were identified as true energy minima through frequency calculation. The density functional theory method (DFT) utilizing the B3LYP hybrid functional with the 6311G+(2d,p) basis set was used for all calculations.

Molecule		Dipole Moment (Debye)	Polarizability α (a.u.)	E (Thermal) kcal/mol	Heat Capacity (Cv) cal/mol K
3b (protonated)	Non-solvated	13.6139	463.206	267.16	102.66
3b (protonated)	Solvated	18.4949	622.678	267.15	102.63
3b (deprotonated)	Non-solvated	12.9565	499.468	258.50	101.69
3b (deprotonated)	Solvated	23.9422	743.268	258.49	101.33
5a (protonated)	Non-solvated	13.1672	440.093	248.99	96.63
5a (protonated)	Solvated	17.7017	597.655	248.94	96.61
5a (deprotonated)	Non-solvated	9.5578	497.978	240.33	95.34
5a (deprotonated)	Solvated	17.3083	703.243	240.28	95.19

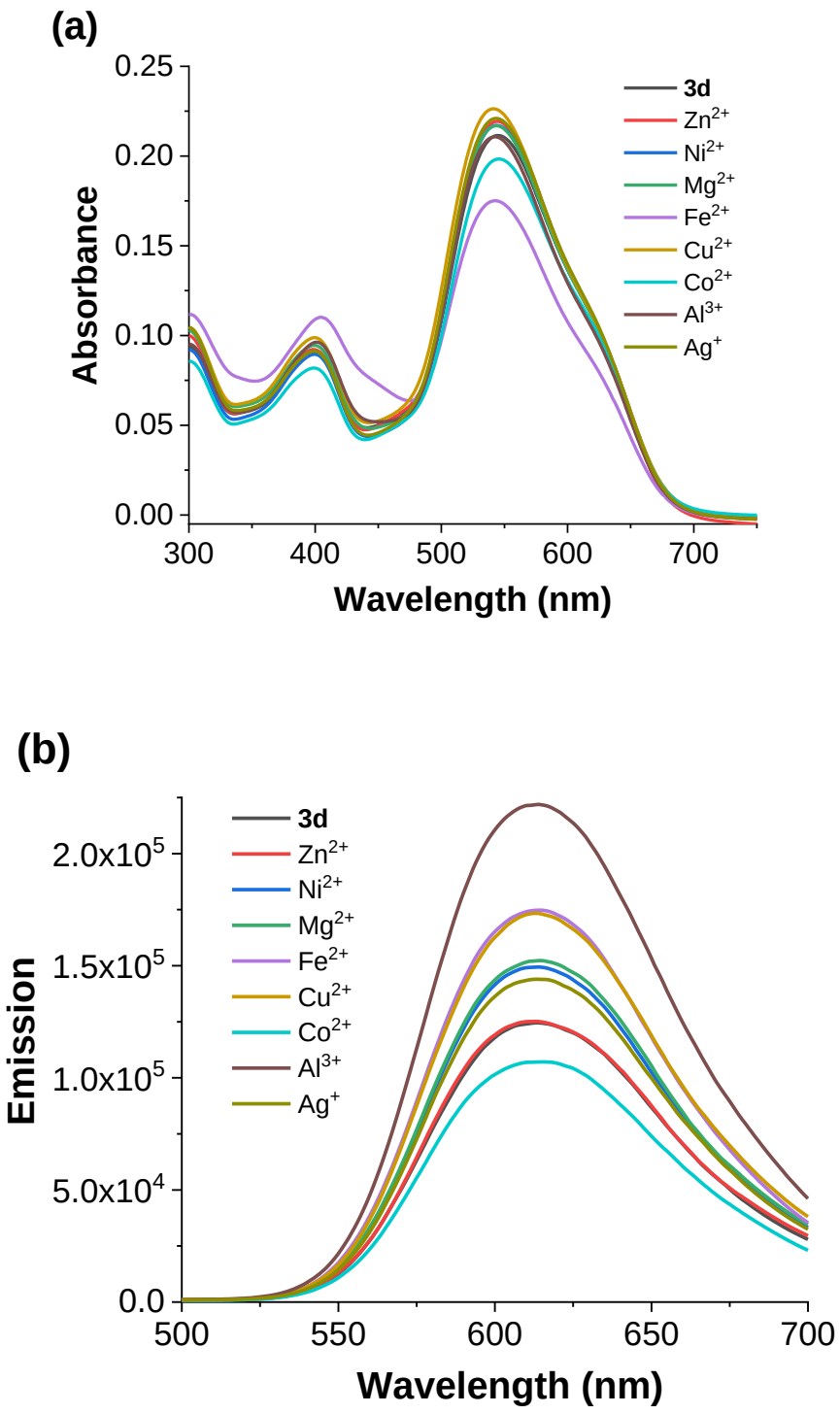


Figure S28.1 Absorbance (a) and emission (b) of probe **3d** (1 x 10^{-5} M in water) upon addition of 10 eq. of different metal ions species at room temperature.

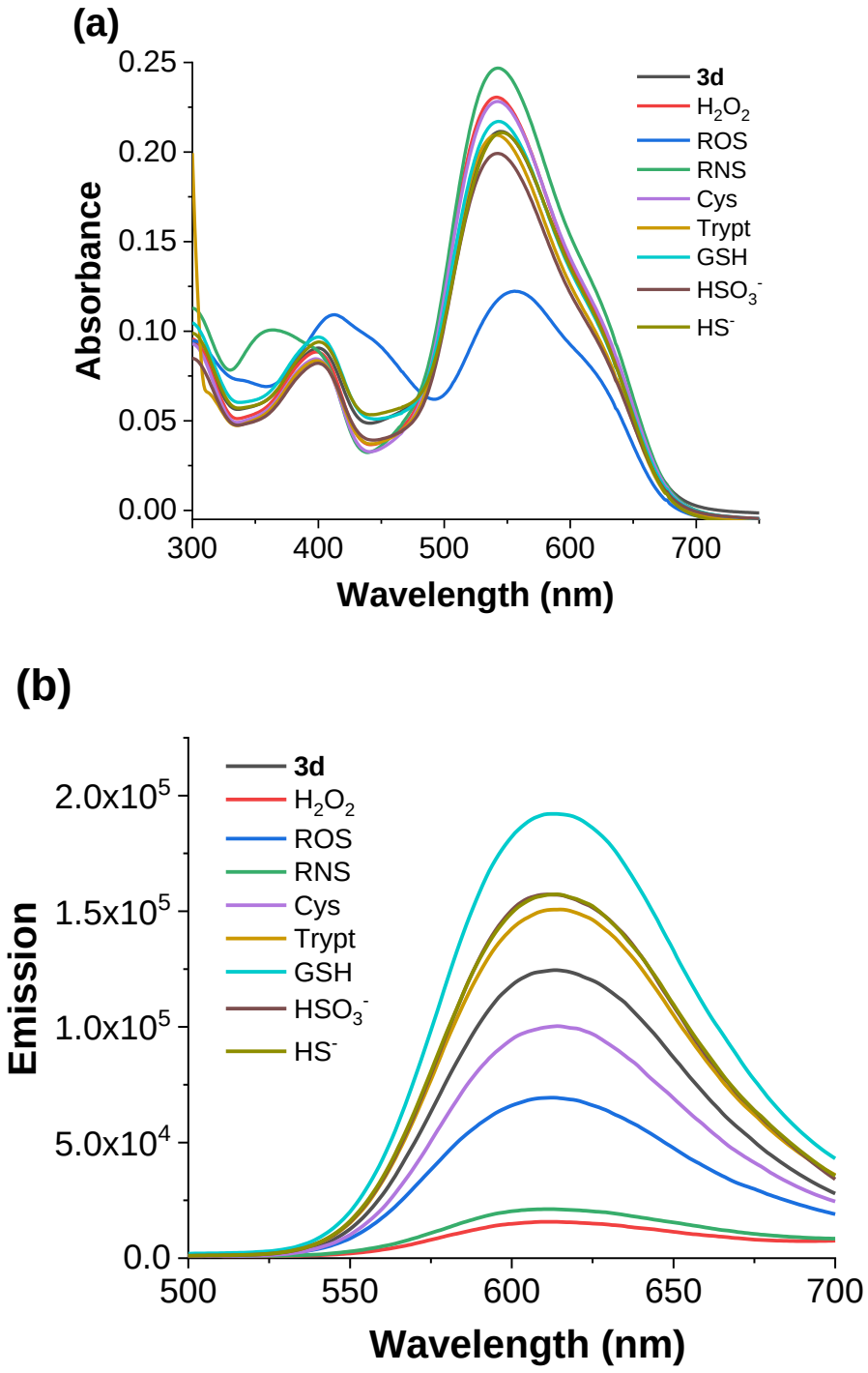


Figure S28.2 Absorbance (a) and emission (b) of probe **3d** (1 x 10^{-5} M in water) upon addition of 10 eq. of different reactive species at room temperature.