Supporting information

for

Photodynamic Anticancer and Antibacterial Activities of Sn(IV) N-Confused *Meso*-tetra(methylthiophenyl)porphyrin

Somila Dingiswayo [1], Balaji Babu [1,2], Kristen Burgess [1], John Mack [1,*] and Tebello Nyokong [1]

[1] Institute for Nanotechnology Innovation, Rhodes University, Makhanda 6140, South Africa; j.mack@ru.ac.za
[1,2] Department of Chemistry, SRM University - AP, Amaravati, Andhra Pradesh, 522502, India
***** Correspondence: j.mack@ru.ac.za

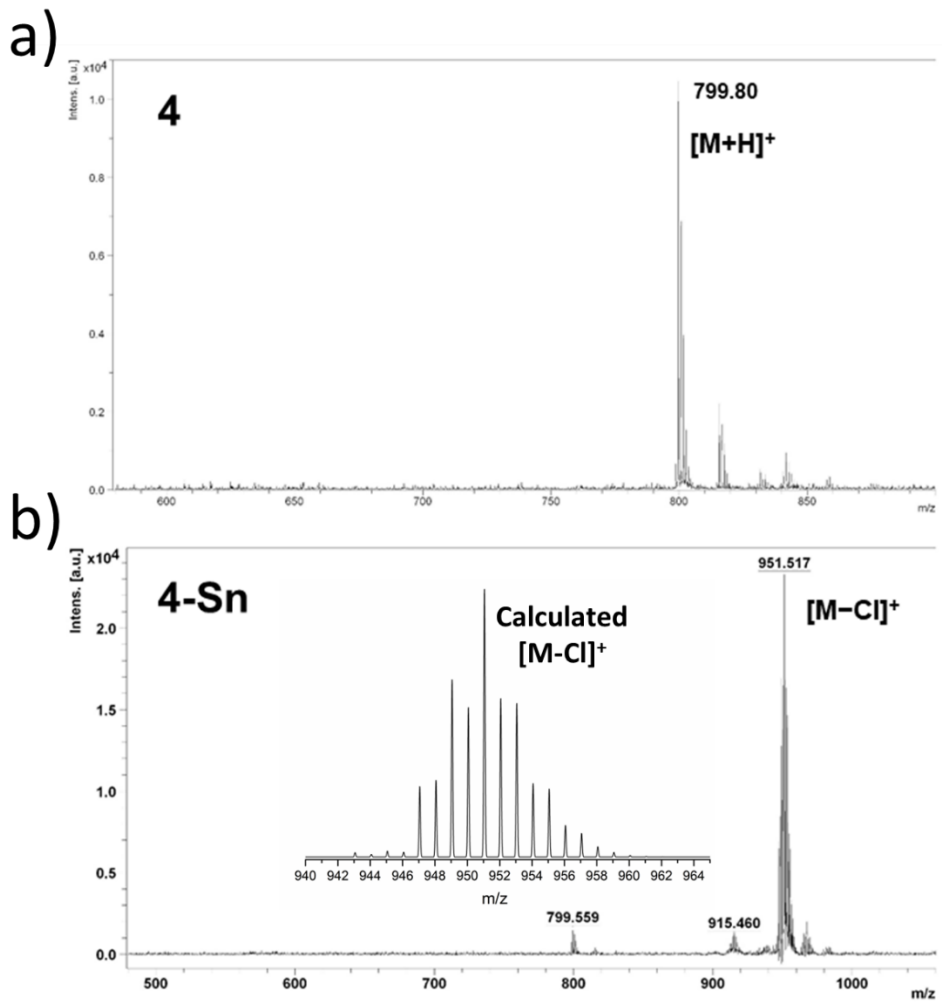

Figure S1. MALDI-TOF MS data for (a) **4** and (b) **4-Sn** (inset: calculated isotopic distribution pattern for $[M-Cl]^+$.

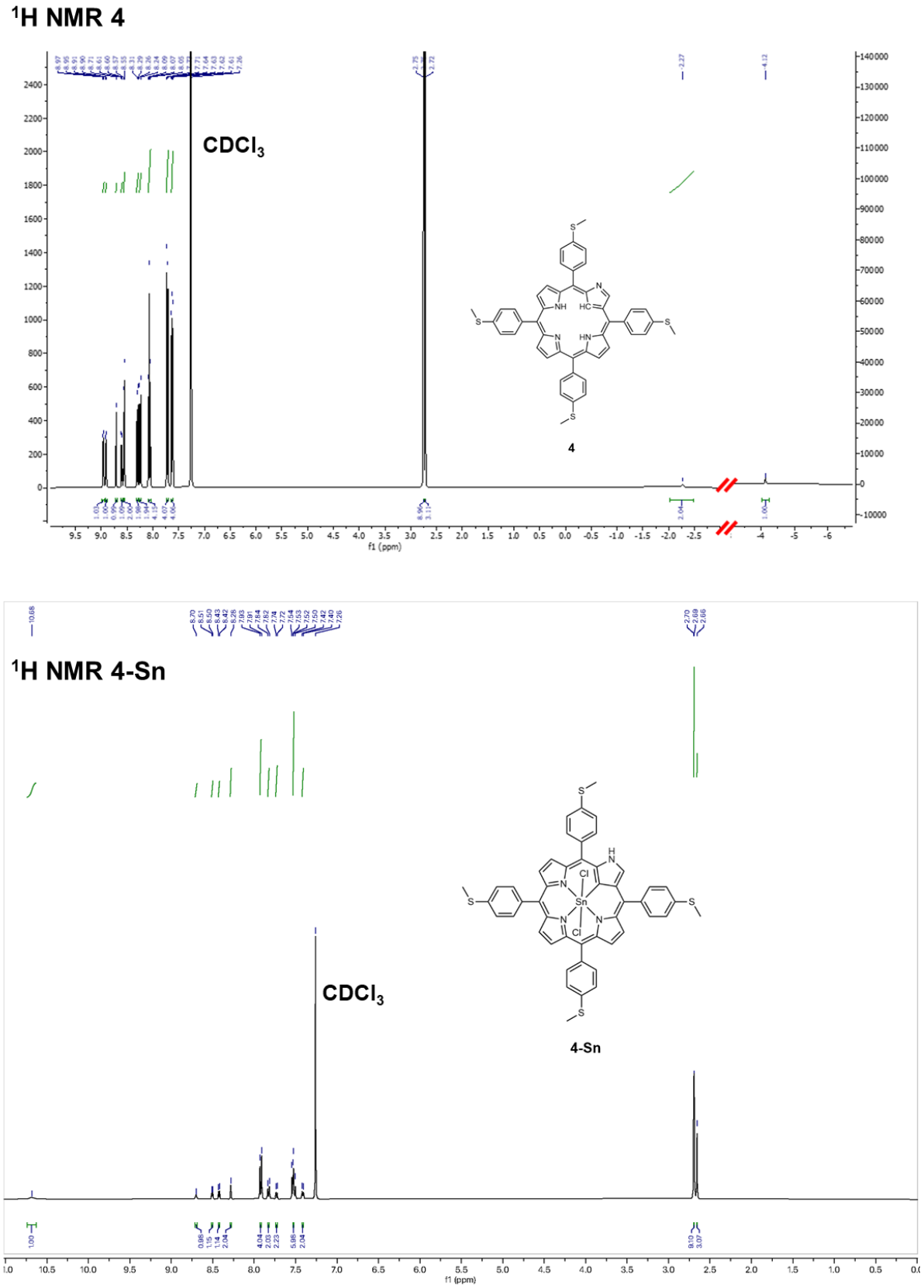

Figure S2. ^{1}H NMR spectra of (a) **4** and (b) **4-Sn** in $CDCl_3$.

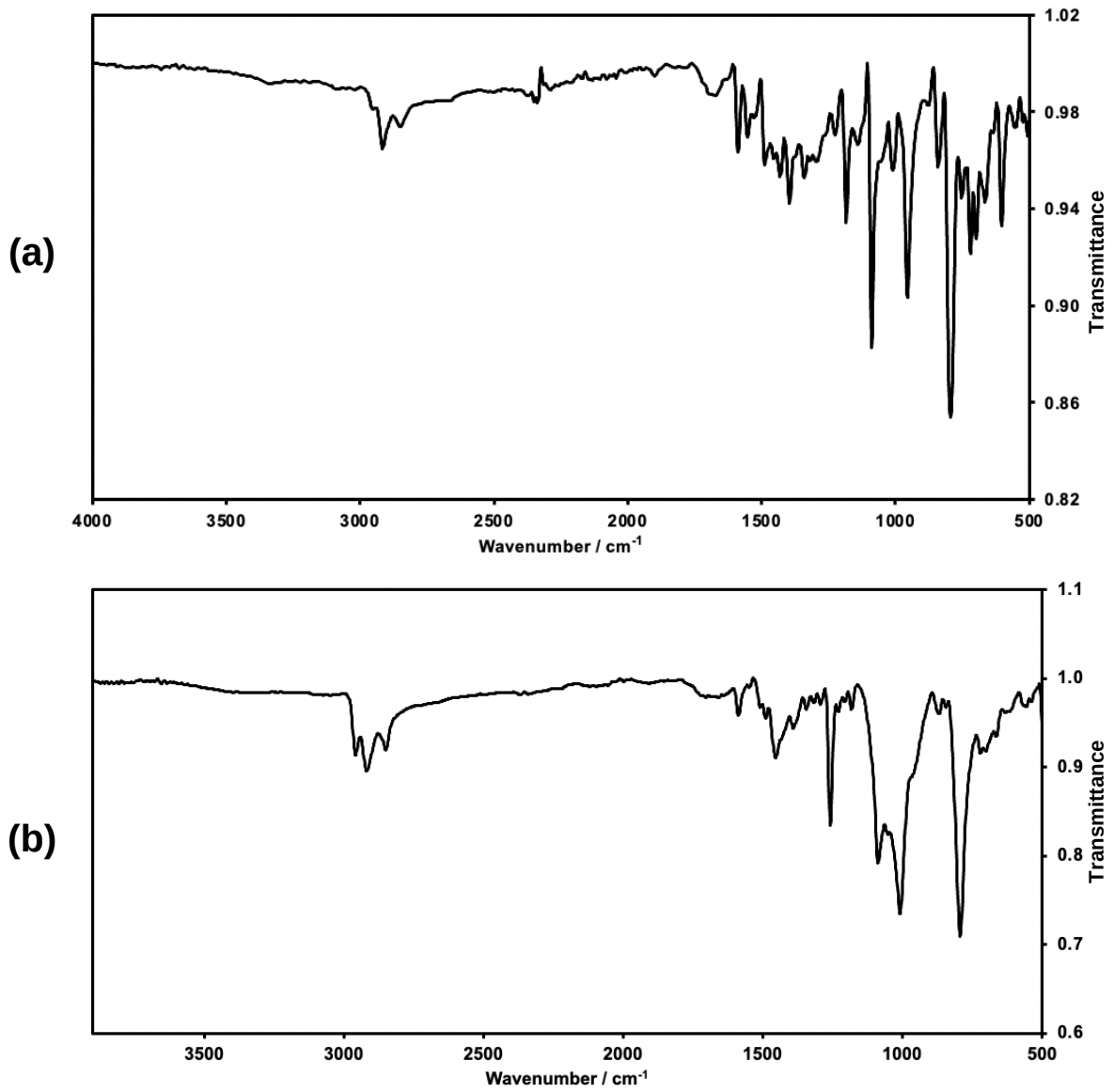

Figure S3. FTIR spectra of (a) **4** and (b) **4-Sn**.

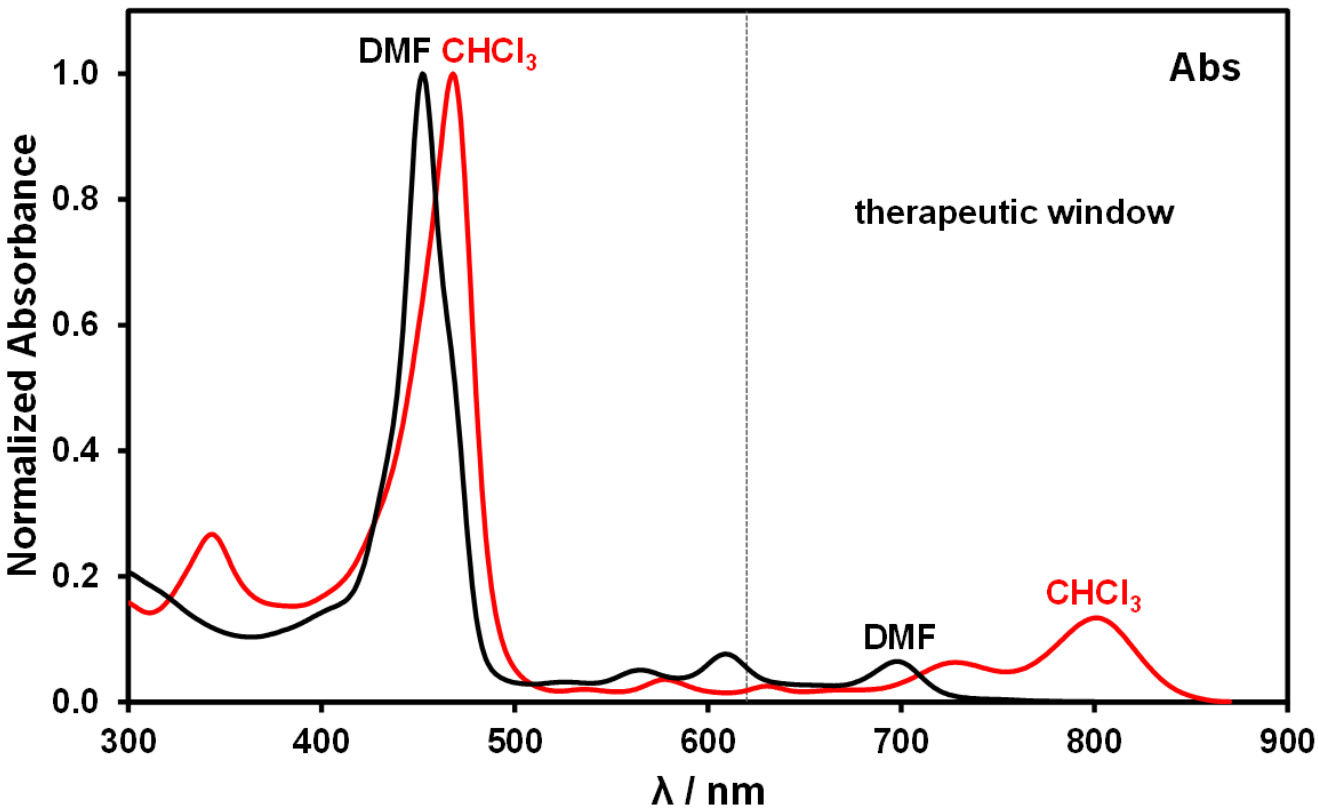

Figure S4. Normalised UV-visible absorption spectra of **4-Sn** in DMF and $CHCl_3$.

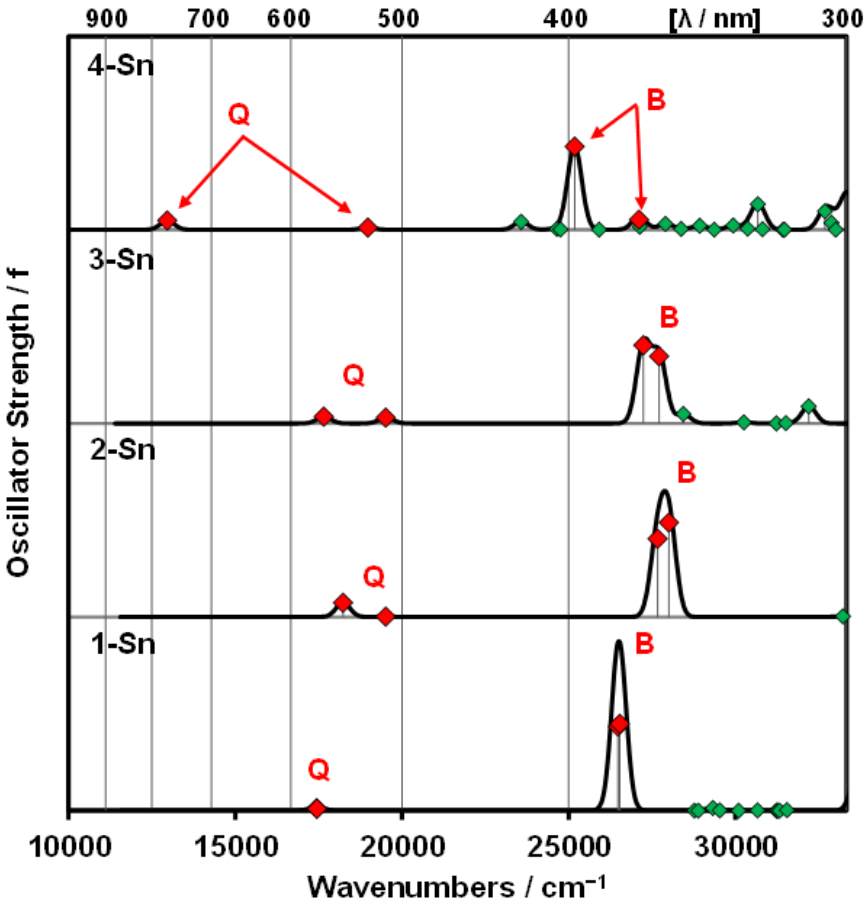

Figure S5. Calculated TD-DFT spectra for the B3LYP optimized geometries of **1-Sn**, **2-Sn**, **3-Sn** and **4-Sn** at the CAM-B3LYP/SDD level of theory. Red diamonds highlight the Q and B bands. Chemcraft was used to generate the simulated spectra at a bandwidth of 500 cm^{-1}. Calculation details are provided in Table S1.

Table S1. TD-DFT spectra for the B3LYP/SDD optimised geometries of **1-Sn**, **2-Sn**, **3-Sn** and **4-Sn** calculated with the CAM-B3LYP functional and SDD basis sets.

1-Sn

Band[a]	#[b]	Exp[c]	Calc[d]	Wavefunction[e]
Q	1	611	573 (0.04)	**36% s** → **-a; 27% s** →**-s; 20% a** → **-s; 16% a** → **-a;** …
	2		572 (0.04)	**36% s** → **-s; 27% s** → **-a; 20% a** → **-a; 15% a**→ **-s;** …
B	3	434	375 (1.43)	**46% a** → **-a; 26% s** →**-s; 15% a** → **-s; 8% s** → **-a;** …
	4		374 (1.46)	**47% a** → **-s; 26% s** → **-a; 15% a** → **-a; 8% s** → **-s;** …

2-Sn

Band[a]	#[b]	Exp[c]	Calc[d]	Wavefunction[e]
$\mathbf{Q_x}$	1	619	549 (0.21)	**75% s** → **-a; 24% a** → **-s;** …
$\mathbf{Q_y}$	2	568	513 (0.00)	**59% a** → **-a; 39% s** → **-s;** …
B	3	431	362 (1.29)	**60% s** → **-s; 38% a** →**-a;** …
	4		357 (1.45)	**73% a** → **-a; 23% s** → **-a;** …

3-Sn

Band[a]	#[b]	Exp[c]	Calc[d]	Wavefunction[e]
$\mathbf{Q_x}$	1	633	588 (0.06)	**68% a** → **-s; 32% s** → **-a;** …
$\mathbf{Q_y}$	2	605	504 (0.08)	**67% s** → **-s; 31% a** → **-a;** …
B	3	436	360 (1.38)	**63% s** → **-a; 31% a** →**-s;** …
	4		355 (1.73)	**66% a** → **-a; 29% s** → **-s;** …

4-Sn

Band[a]	#[b]	Exp[c]	Calc[d]	Wavefunction[e]
$\mathbf{Q_x}$	1	697	771 (0.14)	**92% s** → **-a; 5% a** → **-s;** …
$\mathbf{Q_y}$	2	609	527 (0.03)	**67% s** → **-s; 31% a** → **-s;** …
B	6	452	397 (1.29)	**59% a** → **-s; 27% s** →**-a;** 10% H−6 → -s; …
	8		370 (0.19)	**69% a** → **-s;** …

[a]Band assignment is rationalized in the main text. [b]The number of the state in ascending energy terms. [c]Experimental wavelengths of the bands (nm) in DMF from Table 1 in the main text for **1-Sn**, **2-Sn**, **3-Sn**, **4-Sn**. (f). [d]Calculated band energies (nm) with the oscillator strength (f) values in round brackets. [e]Wavefunctions derived from the eigenvectors predicted in the TD-DFT calculations. Bold face is used to highlight contributions from one-electron transitions between the **s**, **a**, **-s** and **-a** MOs. H and L denote the HOMO and LUMO, respectively. Only one-electron contributions > 10% are consistently provided.

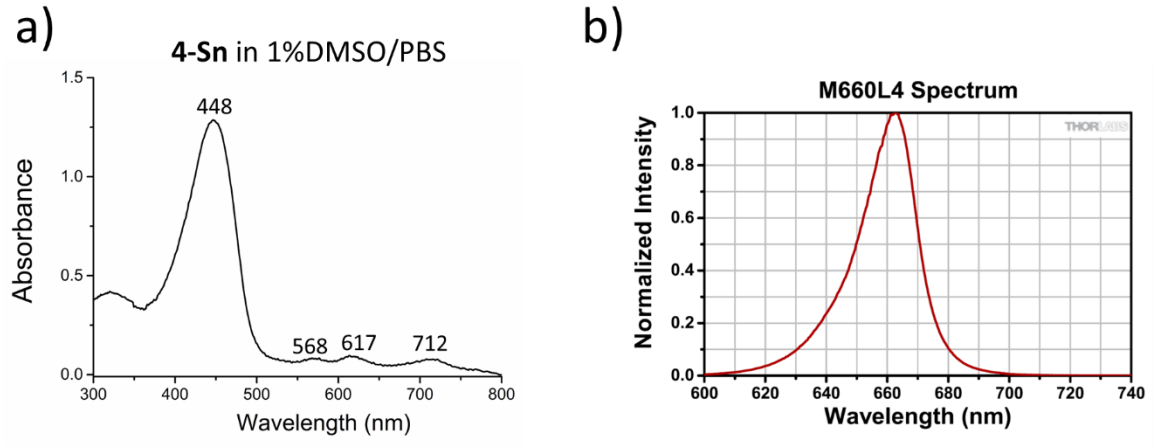

Figure S6. (a) Absorption spectra of **4-Sn** in 1% DMSO/PBS, (b) the emission profile of the Thorlabs M660L4 LED.