

**ELECTRONIC SUPPLEMENTARY INFORMATION**

for

**Axial Ligand Modified High Valent Tin(IV) Porphyrins: Synthesis, Structure, Photophysical Studies and Photodynamic Antimicrobial Activities on *Candida Albicans***

**Rahul Soman<sup>a</sup>, Darpan Raghav<sup>b</sup>, Subramaniam Sujatha<sup>a</sup>, Krishnan Rathinasamy<sup>b\*</sup> and Chellaiah Arunkumar<sup>a\*</sup>**

<sup>a</sup>Bioinorganic Materials Research Laboratory, Department of Chemistry, National Institute of Technology Calicut, Kozhikode, Kerala, India – 673 601.

<sup>b</sup>School of Biotechnology, National Institute of Technology Calicut, Kozhikode, Kerala, India – 673 601.

Email: arunkumarc@nitc.ac.in, rathin@nitc.ac.in

**CONTENTS**

**Fig. S1** Optical absorption spectra of tin(IV) porphyrins, **1–3** in acetone at 298 K.

**Fig. S2** <sup>1</sup>H NMR spectrum of H<sub>2</sub>T(4-CMP)P in CDCl<sub>3</sub> at 298 K.

**Fig. S3** <sup>1</sup>H NMR spectrum of Sn<sup>IV</sup>(Cl)<sub>2</sub>T(4-CMP)P in CDCl<sub>3</sub> at 298 K.

**Fig. S4** <sup>1</sup>H NMR spectrum of **1** in CDCl<sub>3</sub> at 298 K.

**Fig. S5** <sup>1</sup>H NMR spectrum of **2** in DMSO-d6 at 298 K.

**Fig. S6** <sup>1</sup>H NMR spectrum of **3** in CDCl<sub>3</sub> at 298 K.

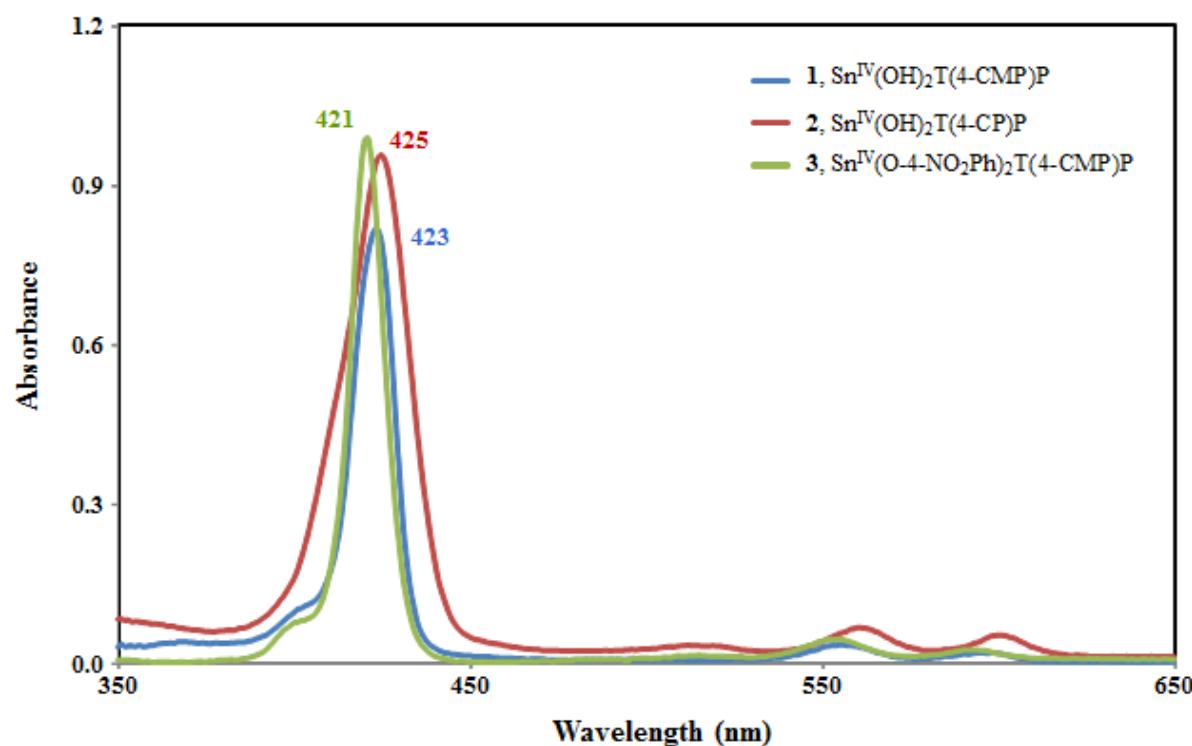
**Fig. S7** ESI-mass spectrum of **2**.

**Fig. S8** Fluorescence decay curves of freebase and tin(IV) porphyrins observed at 600 nm along with IRF measured in toluene and THF respectively. ( $\lambda_{\text{exc}} = 460$  nm).

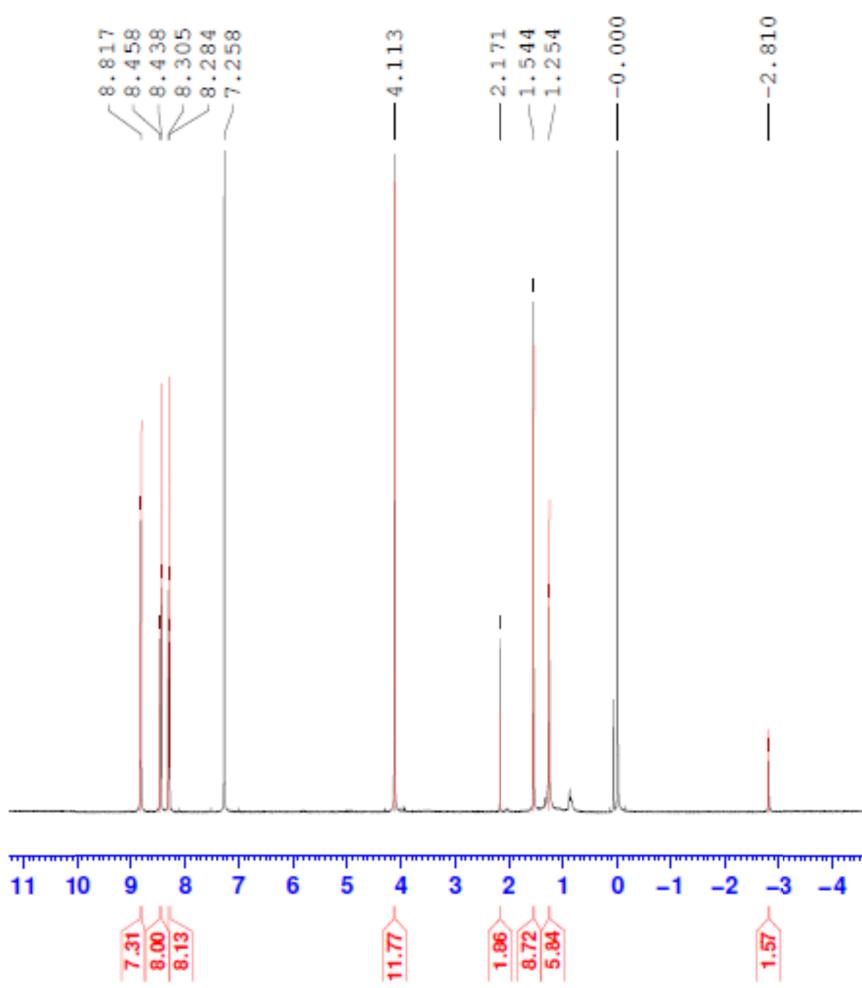
**Fig. S9** Important molecular orbitals of Sn<sup>IV</sup>(Cl)<sub>2</sub>T(4-CMP)P at the BP86/def2-SVP level of theory. Orbital energies (in eV) are given in parenthesis.

**Fig. S10** Important molecular orbitals of **1** at the BP86/def2-SVP level of theory. Orbital energies (in eV) are given in parenthesis.

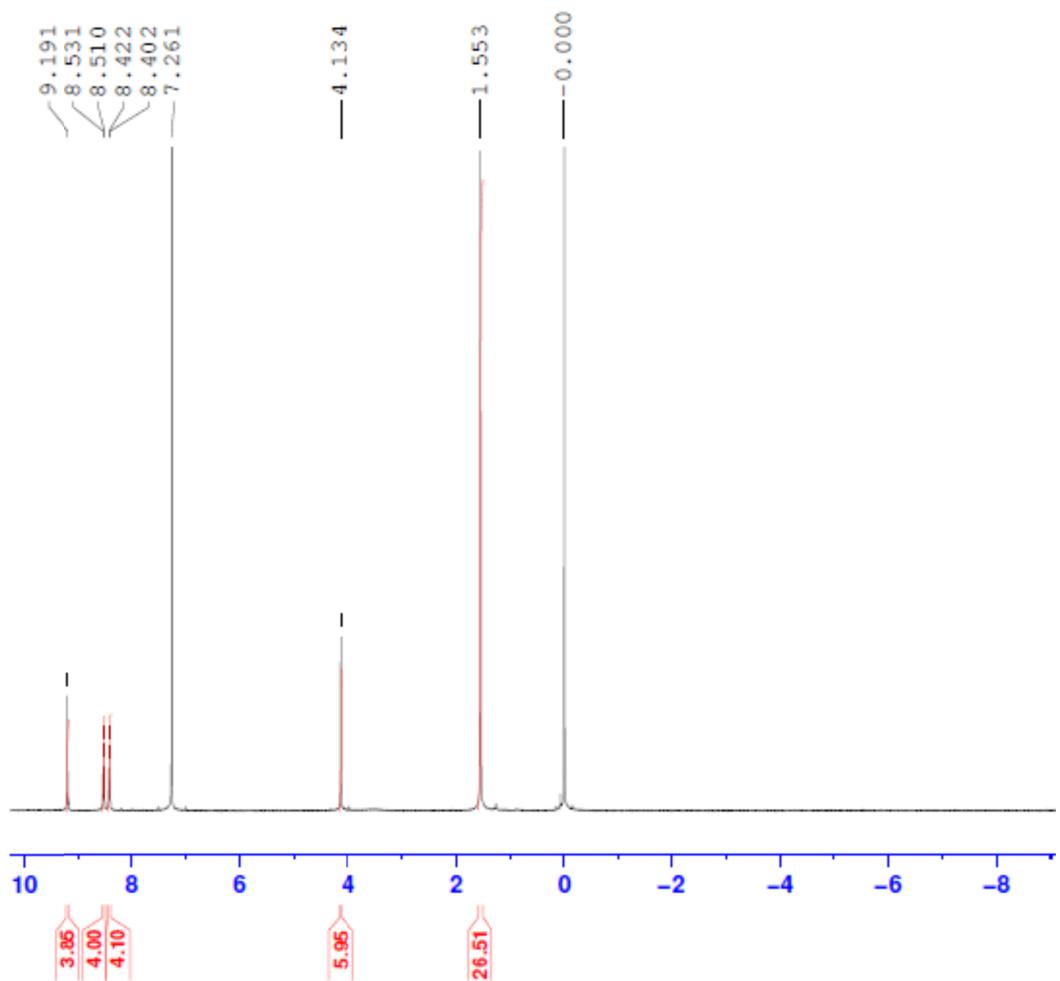
**Fig. S11** Important molecular orbitals of **3** at the BP86/def2-SVP level of theory. Orbital energies (in eV) are given in parenthesis.



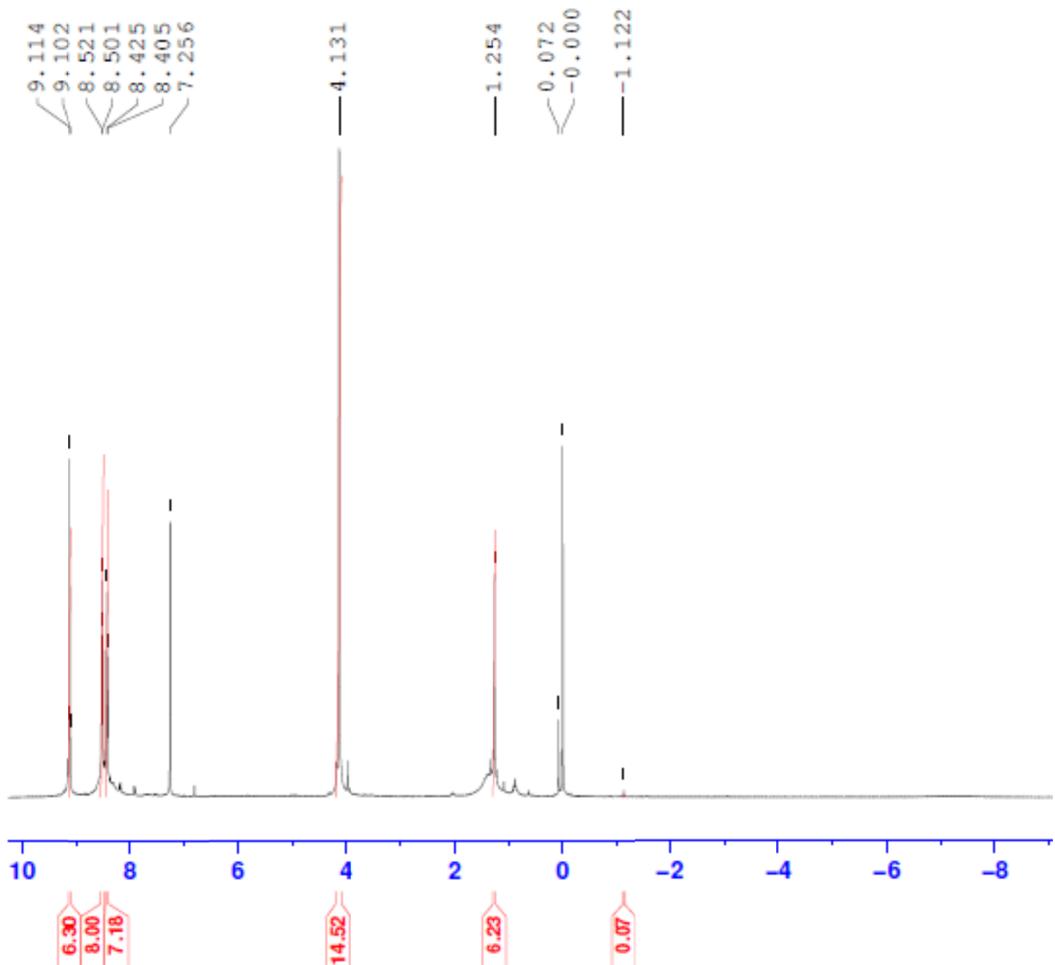
**Fig. S1** Optical absorption spectra of tin(IV) porphyrins, **1–3** in acetone at 298 K.



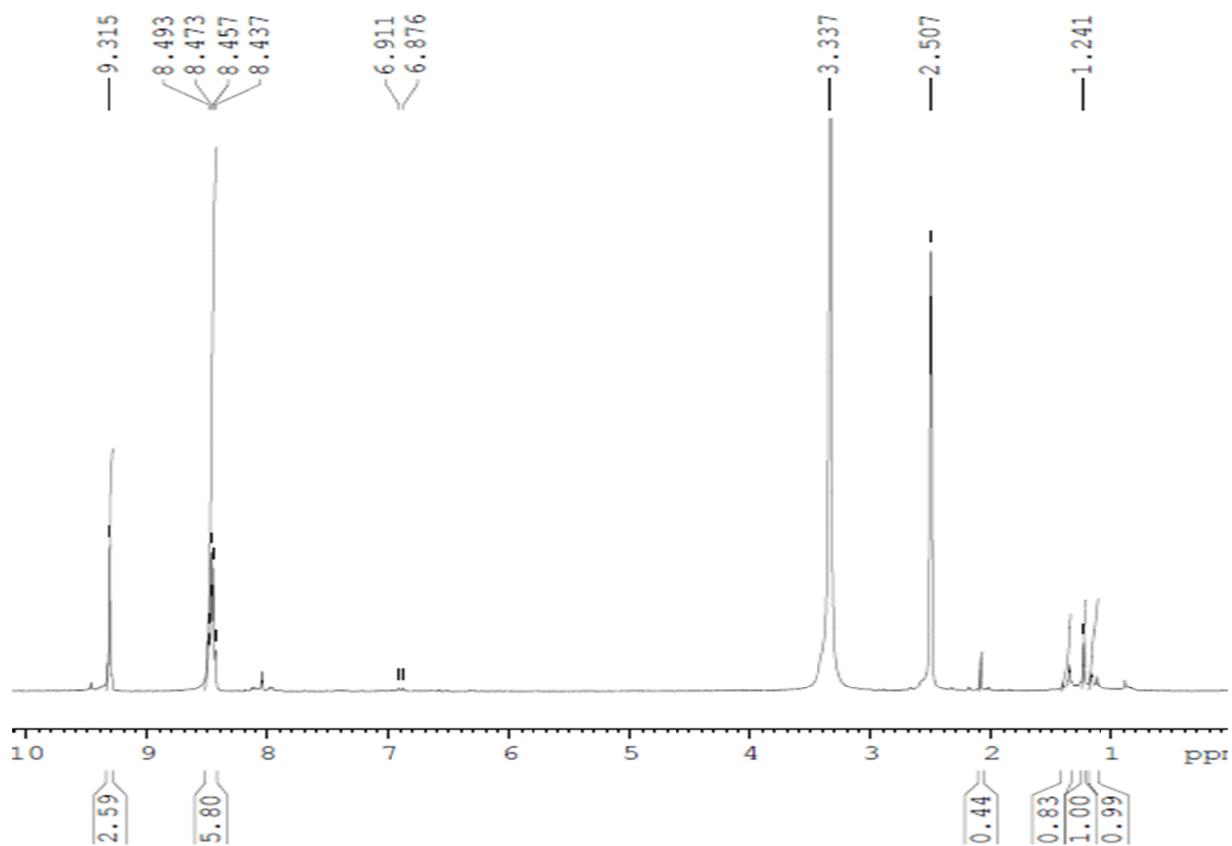
**Fig. S2**  ${}^1\text{H}$  NMR spectrum of  $\text{H}_2\text{T}(4\text{-CMP})\text{P}$  in  $\text{CDCl}_3$  at 298 K.



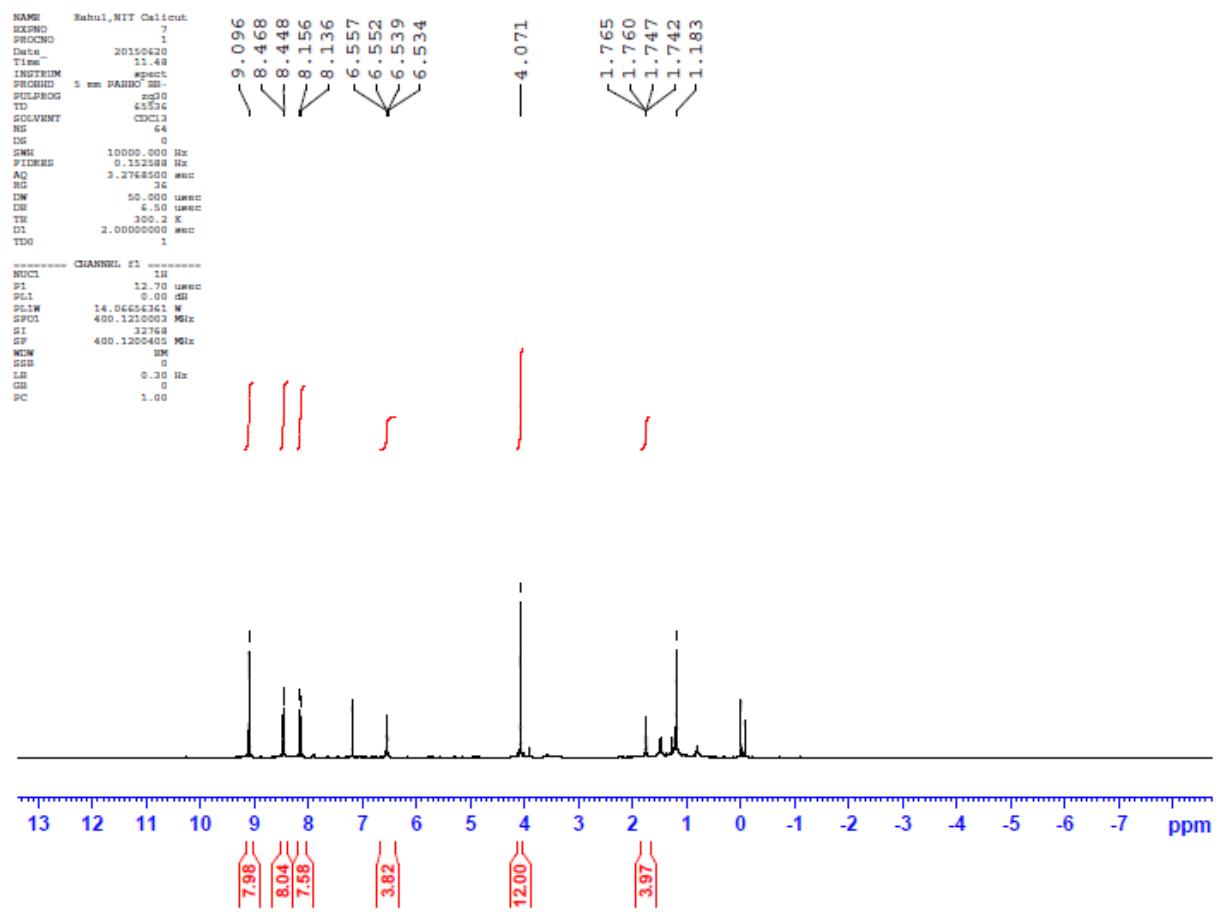
**Fig. S3**  ${}^1\text{H}$  NMR spectrum of  $\text{Sn}^{\text{IV}}(\text{Cl})_2\text{T}(4\text{-CMP})\text{P}$  in  $\text{CDCl}_3$  at 298 K.



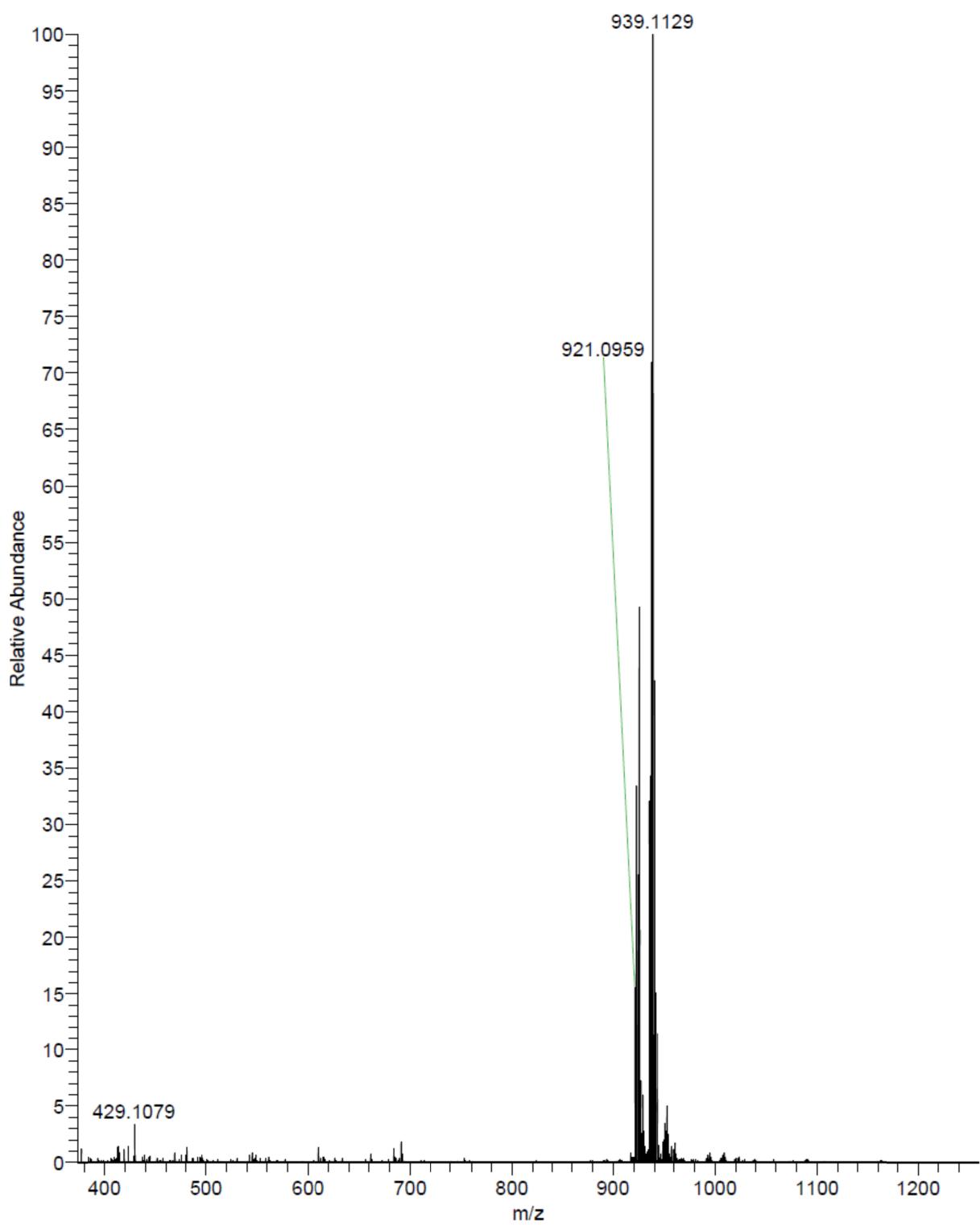
**Fig. S4** <sup>1</sup>H NMR spectrum of **1** in  $\text{CDCl}_3$  at 298 K.



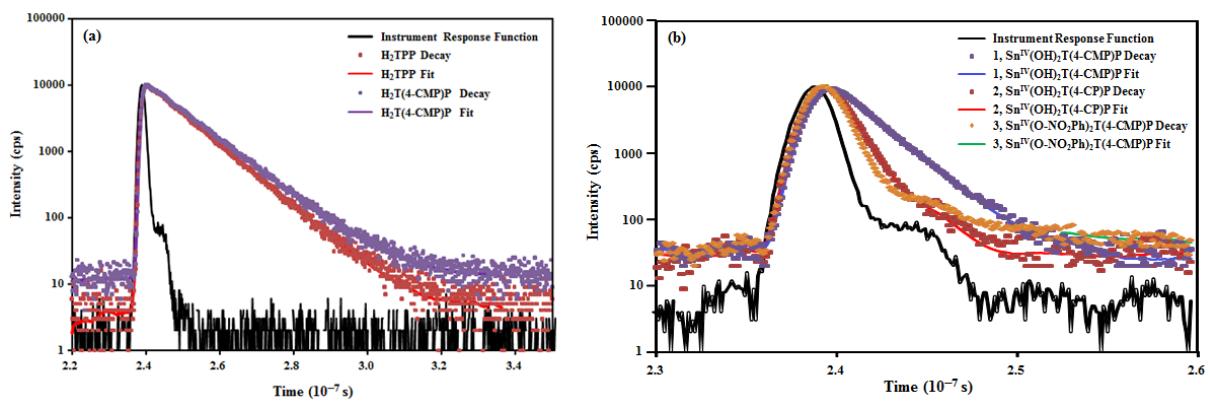
**Fig. S5**  ${}^1\text{H}$  NMR spectrum of **2** in  $\text{DMSO-d}_6$  at 298 K.



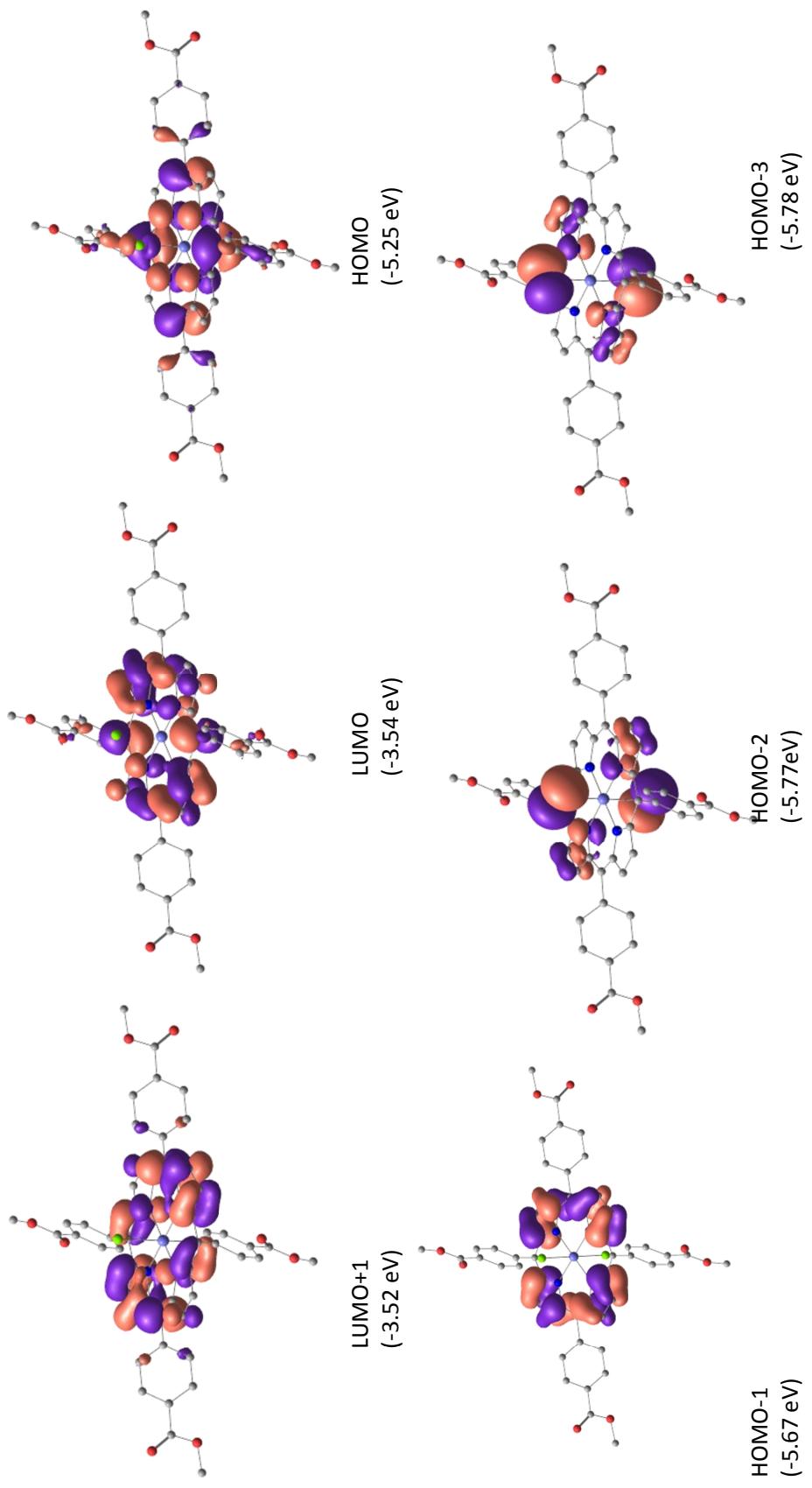
**Fig. S6**  $^1\text{H}$  NMR spectrum of **3** in  $\text{CDCl}_3$  at 298 K.



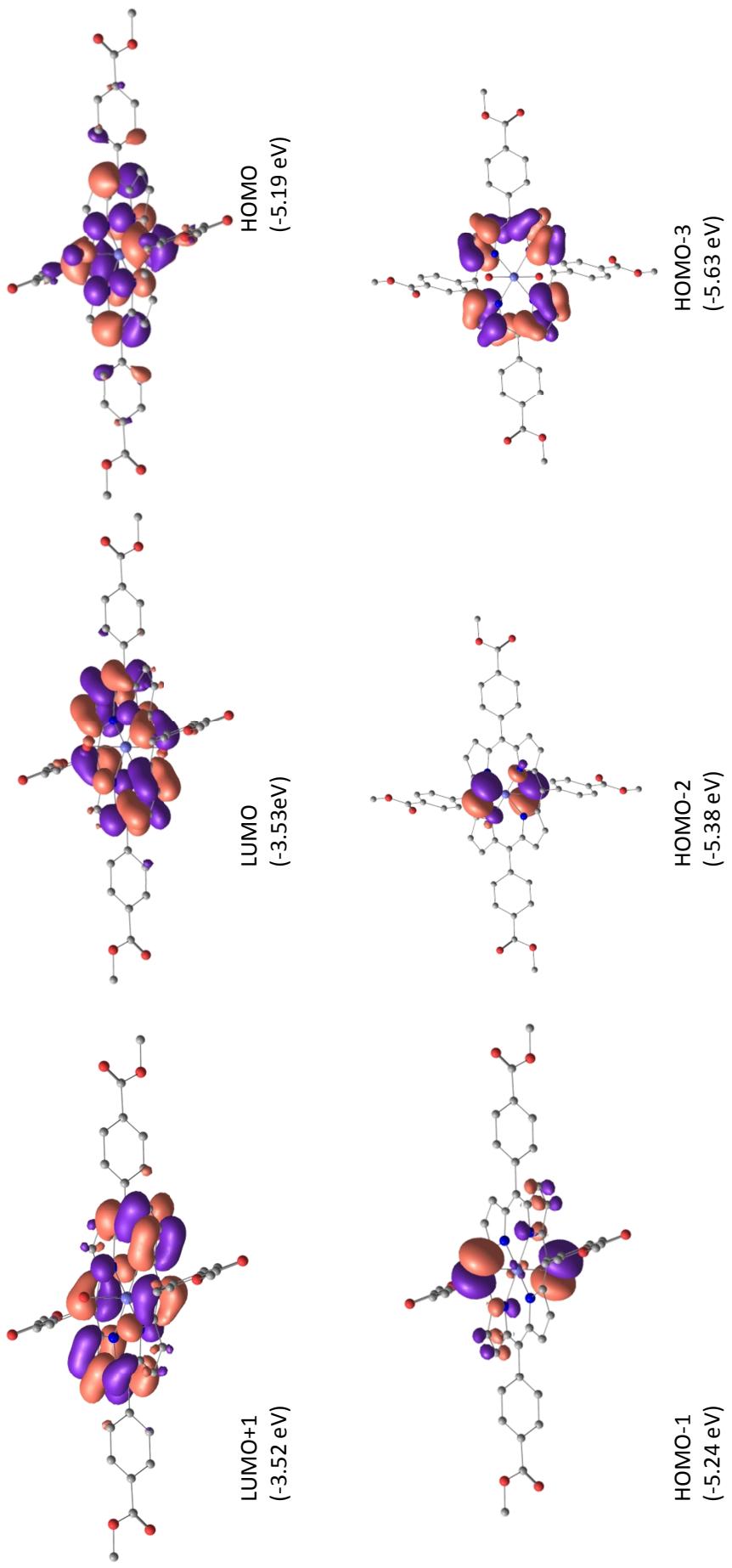
**Fig. S7** ESI-mass spectrum of **2**.



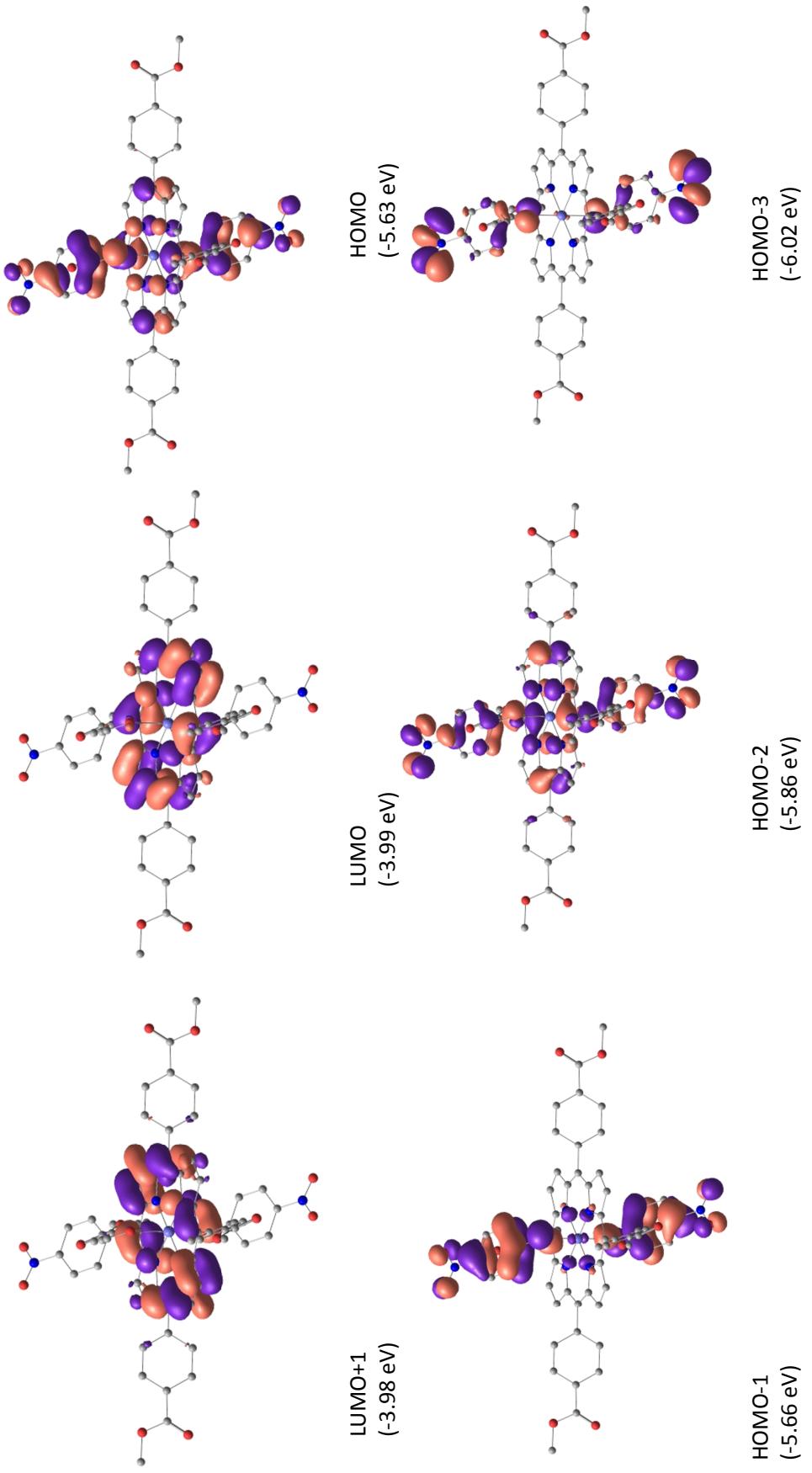
**Fig. S8** Fluorescence decay curves of freebase and tin(IV) porphyrins observed at 600 nm along with IRF measured in toluene and THF respectively. ( $\lambda_{\text{exc}} = 460 \text{ nm}$ ).



**Fig. S9** Important molecular orbitals of  $\text{Sn}^{\text{IV}}(\text{Cl})_2\text{T}(4\text{-CMP})\text{P}$  at the BP86/def2-SVP level of theory. Orbital energies (in eV) are given in parenthesis.



**Fig. S10** Important molecular orbitals of **1** at the BP86/def2-SVP level of theory. Orbital energies (in eV) are given in parenthesis.



**Fig. S11** Important molecular orbitals of **3** at the BP86/def2-SVP level of theory. Orbital energies (in eV) are given in parenthesis.