## **'Aggregation Induced Emission' Active Iridium(III) Complexes** with Applications in Mitochondrial Staining

Parvej Alam<sup>a</sup>, Subhra Dash<sup>b</sup>, Claudia Climent<sup>c</sup>, Gurpreet Kaur<sup>d</sup>, Angshuman Roy Choudhury<sup>d</sup>, David Casanova<sup>e</sup>, Pere Alemany<sup>c</sup>, Rajdeep Chowdhury<sup>\*b</sup>, Inamur Rahaman Laskar<sup>\*a</sup>

<sup>a</sup>Department of Chemistry, Birla Institute of Technology and Science, Pilani Campus, Pilani, Rajasthan, India, <u>ir laskar@bits-pilani.ac.in</u>; <sup>b</sup>Department of Biology, Birla Institute of Technology and Science, Pilani Campus, Pilani, Rajasthan, India, rajdeep.chowdhury@pilani.bits-pilani.ac.in; <sup>c</sup>Departament de Ciència de Materials i Química Física and Institut de Química Teòrica i Computacional (IQTCUB), Universitat de Barcelona, Martí i Franquès 1-11, Barcelona 08028, Spain, <u>p.alemany@ub.edu</u>; <sup>d</sup>Department of Chemical Sciences, Indian Institute of Science Education and Research (IISER), Mohali, Sector 81, S. A. S. Nagar, Manauli PO, Mohali, Punjab, 140306, India, <u>angshurc@iisermohali.ac.in</u>; <sup>e</sup>Kimika Fakultatea, Euskal Herriko Unibertsitatea (UPV/EHU), Donostia International Physics Center, Paseo Manuel de Lardiazabal, 4, Donostia 20018, Euskadi, Spain.



(a)



(b)

Fig.S1: <sup>1</sup>H, NMR spectra and HRMS (a and b), respectively for L.









(c)

Fig.S2: (<sup>1</sup>H, <sup>19</sup>F) NMR spectra and HRMS (a, b and c), respectively for 1.



<sup>(</sup>a)



(b)

Fig.S3: <sup>1</sup>H NMR spectra and HRMS (a and b), respectively for 2.



Fig.S4: Solid state absorption spectra of the complexes  ${\bf 1}$  and  ${\bf 2}$  .



Fig.S5: Absorption spectra of the complex **2** in different organic solvents;  $c=1x10^{-5}M$ .



Fig.S6: Normalized emission spectra of the complex **2** in different organic solvents;  $c=1x10^{-5}M$ .



Fig.S7: Solid state emission of the complexes  ${\bf 1}$  and  ${\bf 2}$  .



(a)



Fig.S8: Particle size distribution of nano-aggregates of (a) complex **1** and (b) complex **2** formed in a MeOH / water mixture with a 90% water fraction.



Fig.S9: Absorption spectra of the complex **2** in different water fractions ( $f_w$ ); c=1x10<sup>-5</sup>M.



Fig.S10: Excitation spectra of the complex **2** in different water fractions ( $f_w$ ); c=1x10<sup>-5</sup>M.