### Invited Lecture Inter-Disciplinary Explorations in Chemistry (I-DEC 2018)

### Reversible Chemical Probes for In Vivo Molecular Tracking

Ankona Datta\*

Department of Chemical Science Institute/University: Tata Institute of Fundamental Research (E-mail: ankona@tifr.res.in)

**Abstract**: Small molecules and ions are key players in biological regulation and signaling processes. Dynamic changes in molecular and ionic distributions are functionally relevant and hence essential for driving life. Chemical probes that can track small molecules and ions in living systems will help us record 'molecular motion pictures' revealing essential life processes. Changes in molecular distributions under pathophysiological conditions can also be tracked by using these probes. The major challenges in small molecule detection are: How do we detect dynamic concentration changes? How do we distinguish between chemically similar species that might have very distinct biological functions? And finally, what strategies can allow efficient translation of *in vitro* detection assays into living systems?

In our group, we use coordination chemistry and molecular recognition insights to build designer probes that can address these challenges. Optical imaging is our modality of choice because of its high sensitivity and spatiotemporal resolution for live imaging. By engineering molecular motifs spanning the range from proteins to small peptides and synthetic macrocycles we have developed reversible sensing strategies for *in vivo* molecular sensing.<sup>1-3</sup> Our forays into sensor development have not only led to sensitive chemical probes but have also enhanced our understanding of chemical selectivity principles. Using insights obtained from our fundamental sensor design endeavors we have therefore also initiated applied directions in the development of strategies for early disease diagnosis and routes for targeted chelation therapy.<sup>4</sup> In this talk, I will highlight our probe design principles and recent results on sensing signaling lipids and developing selective binders for metal ions in living systems.

#### **References:**

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## **Bio-Sketch of Speaker**

Dr. Ankona Datta

Designation Reader

Department: Department of Chemical Sciences Institute: Tata Institute of Fundamental Research Address: 1 Homi Bhaha Road, Colaba, Mumbai, 400005 Contact Number: +91-22-2278-2078 e-Mail: ankona@tifr.res.in



Ankona received her B.Sc. and M.Sc. degrees in chemistry from the Indian Institute of Technology, Kharagpur in 2000. She did her graduate work on chiral water soluble porphyrins for catalysis and recognition with Prof. John T. Groves at Princeton University (Ph.D., 2006). After graduating from Princeton she joined as a postdoctoral scholar in the laboratory of Prof. Ken Raymond at the University of California, Berkeley, where she worked on macromolecular MRI contrast agents.

Since 2010 she is a faculty in the Department of Chemical Science at the Tata Institute of Fundamental Research, India. She and her team of vibrant students are excited by the plethora of possibilities that coordination chemistry offers in developing sensors for bio-molecular imaging. The group applies the concepts of bio-mimetic chemistry and metal-protein interactions to develop chemical probes with the aim of tracking signaling molecules and ions in living systems.