

Special issue on “Molecular Sensors and Molecular Logic Gates”

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This issue of *Frontiers of Chemical Science and Engineering* highlights recent progress toward fluorescent probes that was originally conceived to coincide with 7th Conference on Molecular Sensors and Molecular Logic Gates (MSMLG 2020) to celebrate the career of Seiji Shinkai and hosted by Anthony Czarnik at the University of Nevada in Reno. Sadly, that meeting was cancelled due to the pandemic associated with COVID-19. However, this collection of research and review papers will now serve as an introduction to MSMLG 2022 which will be in Dublin, Ireland on 7–10 June 2022, where Thorfinnur Gunnlaugsson will be the local host. The collection of papers contained in this special issue covers *in vitro* and *in vivo* applications and illustrates the potential for practical sensing and imaging of disease-related species.

Within this collection of papers Zhu et al. reported a molecular probe BDMP for the detection of UDP-glucuronosyltransferase 1A8 [1]. When boron-dipyrromethene derivative BDMP was converted to the glucuronidated metabolite, a significant increase in emission at 580 nm was observed. While Zhou et al. summarized recent developments of reaction-based fluorescent probes for the detection of hydrogen sulphide (H₂S) [2]. The probes were grouped based on their fluorescent response when reduced, attacked by nucleophiles or by the precipitation of metal sulphides. Shi et al. used quinolone-indole as a scaffold to develop a H₂S selective probe [3]. Using this system, H₂S can be detected via ratiometric fluorescence signals since the nucleophilic addition by HS⁻ interrupts the conjugated system. Sodium nitroprusside dehydrate was used as a stimulus to induce endogenous H₂S in HeLa cells, the increase of which was imaged using the probe. The probe also exhibited good capacity to image exogenous H₂S in mice. Mitochondrial DNA (mtDNA) is associated with many diseases including cancers. Since damage of mtDNA can cause the surrounding microenvironment to become hydrophobic. Feng et al. developed the molecular tool MBI-CN which can be converted to MBI-CHO under hydrophobic conditions [4]. The fluorescence intensity ratio (i.e., I₅₅₃/I₄₃₇) decreased when MBI-CHO was bound to mtDNA. Chen et al. replaced *N*-mustard with fatty *N*-mustard to develop three lysosome-targeted anticancer fluorescent drugs (CXL118, CXL121, and CXL122) [5], where intramolecular cyclization was more likely to occur due to increased basicity of the nitrogen atom in fatty *N*-mustard [6]. De Moliner et al. established a library of nitrobenzodiazole derivatives [7]. Screening indicated that compound 3i was a suitable fluorescent sensor able to discriminate Fe²⁺ and Fe³⁺ ions. Fe²⁺ led to a fluorescence “turn-on”, while reduced emission was observed upon addition of Fe³⁺. Sasaki et al. focused on two polythiophene-based fluorescent probes which were able to detect eight kinds of metal ions in aqueous solution [8]. The carboxyl units of the probes bound to the metal ions. While the lengths of the alkyl chains were responsible for the different fluorescence response modes. Zhao et al. developed Azo-2C5 and Azo-2C6 transporters [9]. These carriers were capable of transporting Cl⁻ due to good affinity with the thiourea groups. Azo-2C5 exhibited enhanced ability for the transport of Na⁺ over Azo-2C6. Since the benzo-15-crown-5 in Azo-2C5 was a better match for Na⁺. Dual-function optical probes have received significant recent interest [10]. As such, Zhou et al. have clarified the recent advances of such probes for sensing and the imaging of two species in cells and *in vivo* [11]. Last but not least, Xie et al. have developed probe KTLip for exploring lysine delipoylation via fluorescence protein labeling and “off-on” signaling [12].

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Guest Editors

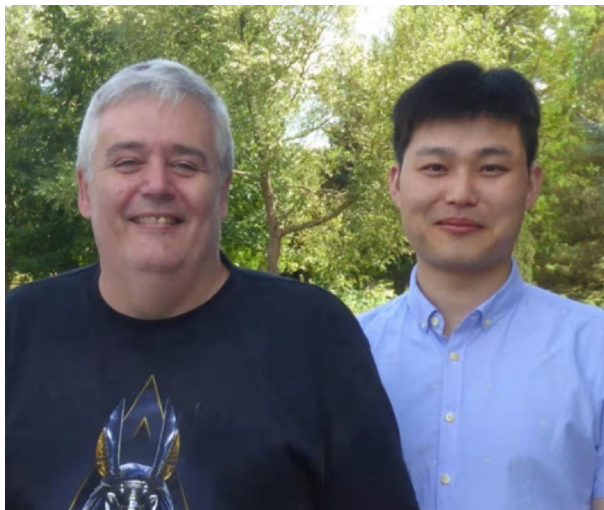


Photo taken by Adam C. Sedgwick. Tony D. James (Left) and Luling Wu (Right) at the University of Bath (July 2018). “*It does not matter how slowly you go as long as you do not stop.*” —Confucius

Luling Wu was awarded scholarships by the China Scholarship Council and University of Bath to carry out a PhD under supervision of Professor Tony D. James at the University of Bath. He is a referee for peer-reviewed journals including *JACS Au*, *Chemical Science* and *CCS Chemistry*. He is a Member of the Royal Society of Chemistry (MRSC). He is an editor for “Fluorescent Chemosensors”, part of the *Monographs in Supramolecular Chemistry* published by the RSC.

Tony D. James is a Professor at the University of Bath, Fellow of the Royal Society of Chemistry and holds a prestigious Royal Society Wolfson Research Merit Award (2017–2022). He obtained his BSc from the University of East Anglia (1986), PhD from the University of Victoria with Thomas M. Fyles (1991) and carried out Postdoctoral Research with Seiji Shinkai (1991–1995). He was a Royal Society University Research Fellow at the University of Birmingham (1995–2000) before moving to the University of Bath in 2001. In 2013 he was awarded the Daiwa-Adrian Prize, in 2015 the inaugural CASE Prize, 2018 the MSMLG Czarnik Award and 2020 Frontiers in Chemistry Diversity Award. His research interests include many aspects of supramolecular chemistry, including molecular recognition, molecular self-assembly and sensor design. He is the author of over 376 papers and has an h-index of 74.