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Foreword

Celebrating RACI and Academy of Science Awards 2020–2021

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In spite of a very difficult year with numerous disruptions caused by the COVID-19 pandemic, Australian chemists have continued to perform, and it is a pleasure to present this year's special issue featuring the recipients of awards and medals issued by the Royal Australian Chemical Institute (RACI) and the Australian Academy of Science (AAS).

Michael Kassiou (The University of Sydney) received the RACI's 2020 Applied Research Award and contributes an Account describing the work of his group on the secondary target for the benzodiazepine drug diazepam, the 18 kDa translocator protein (TSPO), which is a transmembrane protein linked to inflammatory conditions in the central and peripheral nervous systems. It has become a key biomarker for assessing microglial activation using PET imaging in patients with diseases ranging from atherosclerosis to Alzheimer's disease.[1]

Danielle Skropeta (University of Wollongong) received the RACI's 2020 Margaret Sheil Leadership Award. Together with associates at the University of Wollongong and the Illawarra Health and Medical Research Institute, she contributes an Account on sialyltransferase (ST) inhibitors as potential anticancer agents. Sialic acid residues mediate numerous critical interactions in cell–cell communication including cell recognition, invasion, migration, receptor binding, and immunological responses. The ST enzymes involved in biosynthesis of sialylated glycans are highly upregulated up to 40–60 % in a range of cancers, with tumour hypersialylation strongly correlated with both tumour progression and treatment resistance. The group has produced a leading series of ST inhibitors found to be non-toxic in a range of cell studies with improved synthetic accessibility.[2]

Debbie S. Silvester (Curtin University) was awarded the 2021 Le Fèvre Medal from the AAS. Together with colleagues in Portugal and Spain, she highlights in a mini-review the use of ionic polymers as catalysts to convert CO_2 into cyclic carbonates. Emerging ionic polymers reported for this purpose include materials such as poly(ionic liquid)s (PILs), ionic porous organic polymers (iPOPs) or ionic covalent organic frameworks (iCOFs) among others, which share ionic moieties including cations such as imidazolium, pyridinium, viologen, ammonium, phosphonium, and guanidinium, and anions such as halides, BF_4^-, PF_6^-, and Tf_2N^-. The mechanistic aspects and efficiency of the CO_2 conversion reaction and the polymer design including functional groups and porosity are discussed in detail. This review is intended to aid the design of new polymer catalysts.[3]

Paul R. Haddad (University of Tasmania) won the 2021 Leighton Memorial Medal of the RACI. In a paper with Maryam Taraji, he describes a quality by design (QbD) optimisation workflow capable of discovering the optimal chromatographic conditions for separation of new compounds in hydrophilic interaction liquid chromatography (HILIC). This workflow features the application of quantitative structure−retention relationship (QSRR) methodology in conjunction with design of experiments (DoE) principles and was used to carry out a two-level full factorial DoE optimisation for a mixture of pharmaceutical analytes. A dual-filtering approach which considers both retention time (*tR*) and structural similarity filtering was used to identify the optimal set of analytes to train the QSRR in order to maximise prediction accuracy. Experimental separations of pharmaceutical test compounds were in good agreement with theoretical predictions.[4]

Nicholas G. White (Australian National University) was the joint winner of the 2020 RACI Rennie Memorial Medal. In a paper with C. M. Thomas, É. M. Foyle, and S. E. Walker he reports the assembly of hydrogen bonded cages using amidinium⋯carboxylate hydrogen bonding interactions, where a tris-amidinium hydrogen bond donor tecton based on a tetraphenylmethane scaffold was prepared, its self–assembly with terephthalate anion was studied, a new tricarboxylate hydrogen bond acceptor tecton was synthesised, and its assembly with

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a 1,3-benzenebis(amidinium) hydrogen bond donor was explored. Molecular modelling and ^{1}H NMR spectroscopy were consistent with interactions between the components in d_6-DMSO solvent mixtures. DOSY NMR spectroscopy was consistent with diffusion of the components resulting in cage formation in DMSO solution, but an X-ray crystal structure showed that one assembly did not have the desired cage structure in the solid state.[5]

Lars Goerick (The University of Melbourne) was the other joint winner of the 2020 RACI Rennie Memorial Medal. In a paper with N. Mehta, he describes a proof-of-concept study of the suitability of Kruse and Grimme's geometric counterpoise correction (gCP) for basis set superposition errors (BSSEs) in double-hybrid density functional calculations with a double-ζ basis set. As the gCP only requires geometrical information, it is essentially free of additional cost. Assessment of its suitability for the B2PLYP/def2-SVP level of theory revealed error compensation effects — missing London dispersion and the BSSE correction. B2PLYP-gCP-D3(BJ)/def2-SVP with the re-parametrised DFT-D3(BJ) and gCP corrections is proposed as a better alternative. The gCP-correction represents a significant improvement over B2PLYP-D3(BJ), particularly for intramolecular noncovalent interactions.[6]

Paul Low (University of Western Australia) was the 2020 recipient of the H. G. Smith Memorial Award of the RACI. In a paper with co-workers from UWA, Curtin University, and the Liverpool and Lancaster Universities in the UK, he reports an experimental verification of the so-called molecular circuit law, which states that 'the conductance *GXBY* of an asymmetric molecule X-B-Y is the geometric mean *GXBXGYBY* of the conductance of the two symmetric molecules derived from it, *GXBX* and *GYBY*'. A series of diarylacetylene derivatives of the general form X-B-X, Y-B-Y, and X-B-Y where X and Y represent anchor groups and B a molecular bridge was prepared. The single-molecule conductance values determined by the scanning tunnelling microscope break-junction method were found to be in excellent agreement with the predictions made on the basis of this law.[7]

Thomas Maschmeyer (The University of Sydney) was the 2021 recipient of the David Craig Medal of the AAS. He contributes a paper with J. Strachan, L. Chen, T. Ellis, and A. Masters on the influence of crystal disorder in MoS_2 cathodes for secondary hybrid Mg-Li batteries. Noting that the full extent to which the electrochemical properties of MoS_2 electrodes are influenced by their morphological characteristics, such as crystalline disorder, remains unclear, the paper reports that disorder introduced by ball-milling decreases the Faradaic component of cell capacity and leads to increasingly pseudo-capacitive behaviour. After high-temperature annealing, a more battery-like character of the cell is restored, consistent with a decrease in disorder. These findings aid the optimisation of MoS_2 electrodes, which show promise in several battery technologies.[8]

Conflicts of Interest

The author declares no conflicts of interest.

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