ACCOUNTS
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GUEST EDITORIAL

Aromatic Interactions

In 2011, Ken Houk and I organized a workshop entitled "Aromatic Interactions in Chemistry and Biology" in Mesilla, New Mexico. This workshop brought together about 30 chemists whose research interests encompass aromatic interactions, spanning fields from host–guest and supramolecular systems to protein and DNA research to computational chemistry and topics ranging from π–π stacking and edge–face interactions to cation–π interactions, sulfur–π interactions, carbohydrate–π interactions, and anion–π interactions, among others. This workshop generated lively discussion on the topic, even including criticism of the term "aromatic interactions", since, as one participant pointed out, it is the π system that matters—these interactions do not require that the π system is aromatic (a good point, but no one suggested a better all-encompassing term). This workshop lead to the suggestion of this special issue, and many of the "lively discussions" are recorded here in the following 17 Accounts. Importantly, a primary theme that arises from these Accounts is that although chemists and biologists are now well aware of aromatic interactions, particularly π–π and cation–π interactions, ongoing research has continued to refine our understanding of these interactions. Thus, these Accounts provide some important new insights into these interactions that will be useful to researchers in a wide range of fields.

Accounts by Schneider, Rebek, and Klärner and Schrader highlight a wide range of supramolecular systems in which aromatic interactions play a key role and that have aided in defining aromatic interactions. Three Accounts by Ballester, Dunbar, and Johnson describe supramolecular approaches to studying anion–π interactions, providing new insight into this intriguing area. Accounts by Dougherty and Hof focus on the cation–π interaction, with Dougherty's article giving a lovely description of the discovery of the cation–π interaction and both Accounts highlighting the role of cation–π interactions in protein–protein and protein–small molecule recognition. A number of other Accounts focus on the role of aromatic interactions in biomolecules as well. Gao's Account focuses on the fine-tuning of π–π and edge–face interactions in proteins through introduction of specifically fluorinated aromatic amino acids. Zondlo describes the influence of prolyl–π interactions in proteins, while Rotello describes the role of aromatic interactions in tuning flavin reactivity. Jimenez-Barbero provides insights into the importance of carbohydrate–π interactions in carbohydrate recognition.

Lastly, five Accounts focus on computational modeling of aromatic interactions. Sherrill, Grimme, and Hobza provide excellent insight into the requirements for properly modeling aromatic interactions. Accounts by Sherrill and Wheeler also provide keen new perspectives into the balance of forces that give rise to aromatic interactions and how they are influenced by substituents. The Account by Hobza describes computational studies of aromatic interactions in proteins and DNA. Finally, Krenske and Houk demonstrate the critical role that aromatic interactions play in controlling stereoselectivity in a wide range of asymmetric reactions.

In summary, anyone who has intentionally or accidentally utilized an aromatic interaction in the course of their research will find this issue extremely useful in understanding what these interactions are and why they are important in so many fields.

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