Special Issue

Deep Learning in Molecular Science and Technology

Message from the Guest Editors

We are witnessing a renaissance in molecular science and technology being driven by the application of deep learning technology to the increasingly available measured and computed data together with a rapidly growing body of literature. Breakthroughs in deep learning algorithms and hardware have greatly boosted the simulation and modelling of complex molecular systems at a level of accuracy necessary for quantitative analysis. This growing field offers unique opportunities in a wide spectrum of challenges. This Special Issue aims to present the current advances in methodology development and applications towards this “holy grail” of deep learning. We welcome the submission of both review and original research articles to this Special Issue.

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As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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