Editorial

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From the Editor

So you have a robust assay. So you have a diverse or focus set of compounds to test with your assay. Now here comes the data tsunami leaving you with only 2 options: swim or drown.

For any research project generating data is key to getting cause–effect information when testing a hypothesis or looking for a solution to a defined problem. However, generating large amounts of data alone does not translate data directly into knowledge. The challenge is to navigate through all the data and, more importantly, make sense of all the data to then be in a position to make an educated and logical conclusion as to what the data indicates and what the next step should be.

For this, SAR (structure–activity relationship) approaches have been and continue to be extremely useful in analyzing data and making direct correlations to chemical structures. QSAR allows going a step further by measuring and quantifying cause–effect information to chemical structures. Both SAR and QSAR relationships provide the basis to make extrapolations and educated guesses or predictions. Some relationships are based on 2D chemical structure representations and others on 3D representations.

In this issue of *Molecular Diversity* we present several articles in QSAR approaches and their utility. We have a review on HQSAR (Hologram QSAR), a modern 2D fragment-based QSAR approach and its impact in drug design;

four independent articles on QSAR approaches to classify, identify and predict hERG blockers, HDAC inhibitors, organochlorine pollutants, and carcinogens; and we also present a computational chemistry article on the prediction of enzyme–small molecule interactions via the AdaBoost classifier.

In addition to the QSAR approaches, we also present ten research articles in the area of organic chemistry, two of them also in the area of medicinal chemistry.

One of the two medchem articles is on the solid-phase synthesis of RNA conjugates carrying nuclear localization peptide sequences for iRNA. The authors' approach consisted of using AKKKKLDK as the nuclear localization sequence and polyethylene-glycol-polystyrene (PEG-PS) as solid support. Using TNF- α inhibition in transfected HeLa cells as measurement for iRNA efficacy it was determined that the AKKKKLDK peptide sequence inhibited 80–90% TNF- α production.

From the ten organic chemistry research articles four are in the area of multi-component reactions (MCRs):

- 1) A three-component reaction for the synthesis of oxazine amines:

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2) A four-component reaction for the synthesis of thiazoles:

3) A pseudo five-component reaction:

4) A three-component reaction in water:

The popularity of MCRs and the power they offer to generate quickly and efficiently new chemotypes with a broad range of chemical diversity is reflected in the increasing number of articles and research we are receiving and bringing to you.

The search for knowledge and deeper understanding of science is a never ending process, and the more that is being discovered the more we realize there is to learn.

Where will all this take us? One can never know, but you can be certain of one thing... *Molecular Diversity* will be there with you along the way. Enjoy!