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Integrating Chemical Crystallography into Advanced Undergraduate Laboratories

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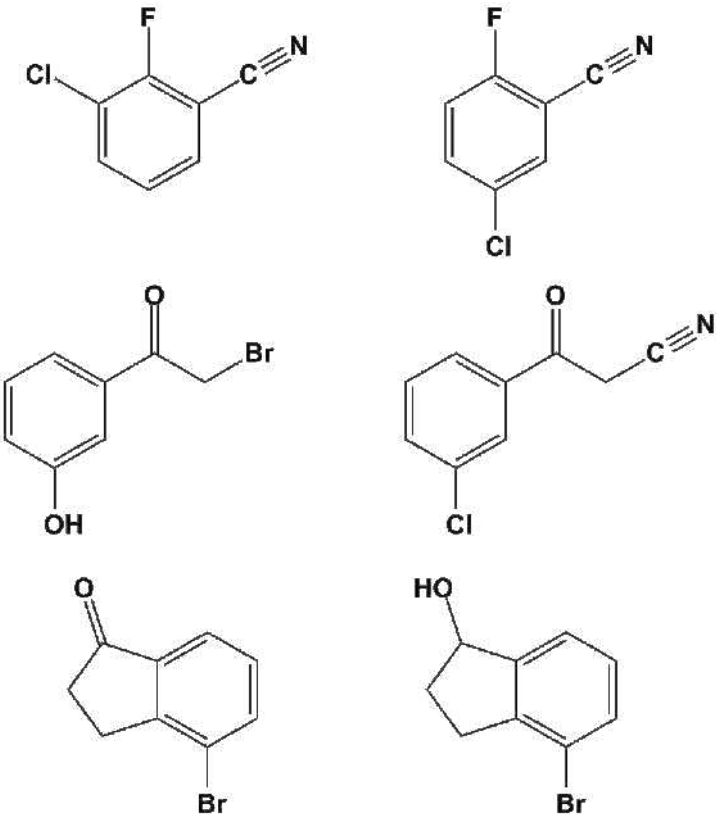
As scientific educators, it is important to mentor students in using state-of-the-art instrumentation and in the communication of new knowledge. Just as chemical crystallography and complimentary spectroscopic techniques such as NMR can be fast, effective tools to experimentally determine the structure of molecules and enhance students learning of molecular structure, they can also provide an inspiring opportunity for students to write short, scientific journal style reports that can be edited and published in collaboration with a mentor. This contribution will focus on incorporating X-ray crystallography into an advanced undergraduate integrated laboratory class as part of a discovery based exercise where the students do not know the identity of their small molecule organic compound, and the publication of the resulting crystal structures. The structures of some recently published examples are shown below. With examples of past student projects and published structures, topics will include: sample choice, the discovery based molecular structure determination lab module, structure validation, analysis and discussion of intermolecular interactions such as hydrogen bonding, π-stacking, halogen-halogen interactions, and C-H•••X (X = O, N, halogen) interactions, and the writing of descriptions of crystal and molecular structures for publication in collaboration with undergraduate students. This work was supported by grants from the U.S. National Science Foundation, No. 0521237 & 0911324.

[1] *H. Aldeborgh, K. George, M. Howe et al., J. Chem. Cryst., 2014, 44, 70-81*



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