MS30.O06

Using the Knowledge from Every Organic Crystal Structure Ever Published

C. Groom[1], S. Ward[1], N. Feeder[1], E. Pidcock[1], P. Wood[1], P. Galek[1]
[1]*Cambridge Crystallographic Data Centre, Cambridge, UK*

The crystallographic community has done something remarkable and almost unique in science. It has operated in such a way that the data generated in virtually every experiment reported in a publication is available to all. This data, in the form of individual crystal structures, is valuable not just in itself, but as a collection. To fully exploit the results of a new structure determination, we never analyse a single structure, we analyse it in the context of every previous crystal structure. Our knowledge of molecular geometry and molecular interactions derived from these structural databases is put to routine use in almost every field of chemistry. This presentation will specifically highlight what we can learn from the world's database of small molecule crystal structures and demonstrate how we can apply that knowledge not just to increase our understanding in structural chemistry, but in structural biology too.

Keywords: Database, Structure