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EDITORIAL

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Data-Driven High-Throughput Prediction of the 3-D Structure of Small Molecules: Review and Progress. A Response from The Cambridge Crystallographic Data Centre

Sentiments expressed in the paper "Data-Driven High-Throughput Prediction of the 3-D Structure of Small Molecules: Review and Progress", recently published in the *Journal of Chemical Information and Modeling*[1] may give readers a misleading impression of important scientific resources.

The authors state that "*One obstacle in this area may be the closed nature of the CSD, which unlike the PDB cannot be used without severe restrictions, even for academic research purposes.*" The only substantive restrictions placed on the use of the Cambridge Structural Database are that licensees will not redistribute derived data without prior permission of the CCDC and that use of the system is acknowledged appropriately. The authors do not explain how this presents an obstacle to research in this area. It seems rather ironic that the authors criticize the very resource that has made their research possible, in this way. In as much as the service described in this article uses data from the Cambridge Structural Database, express permission was immediately granted by the Cambridge Crystallographic Data Centre.

The authors continue "*This is yet another example of the unfortunate state of affairs in chemoinformatics, where an overly zealous culture of closeness and secrecy, sometimes related to short-term profits, have greatly hampered scientific progress.*" The Cambridge Structural Database is maintained and distributed by the Cambridge Crystallographic Data Centre (CCDC). This is a not-for-profit organization, which has charitable status, conferred and overseen by a U.K. Government Commission. This is in recognition of the scientific objectives of the organization and ensures that all income earned is applied for the benefit of science. The CSD is licensed at below cost to academic organizations in 70 countries throughout the world. However, in cases where scientists are not able to source the modest funding for the database, access is never denied. The activities of Cambridge Crystallographic Data Centre Software Limited, an organization that develops and licenses other software in the area of drug discovery, provides the additional income to the CCDC that make this possible.

This self-funding mechanism has been discussed elsewhere[2] and has allowed this comprehensive and accurate resource, which requires much effort, to be developed and maintained.

In addition, the CCDC provides a completely free service whereby data associated with any specific experiment can be obtained from our Web site. The CCDC prides itself on its openness and willingness to collaborate with scientists internationally and has a strong track record in this regard. Far from hampering scientific progress, our culture does much to advance science, as evidenced from the research our tools and products have enabled[3] and the scientific output of the organization itself.[4]

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REFERENCES

(1) Andronico, A.; Randall, A.; Benz, R. W.; Baldi, P. Data-Driven High-Throughput Prediction of the 3-D Structure of Small Molecules: Review and Progress. *J. Chem. Inf. Model.* **2011**, *51*, 760–776, DOI: 10.1021/ci100223t.

(2) Allen, F. H.; Taylor, R. Librarians, crystal structures and drug design. *Chem. Commun.* **2005**, *41*, 5135–5140.

(3) Wong, R.; Allen, F. H.; Willett, P. The scientific impact of the Cambridge Structural Database: A citation-based study. *J. Appl. Crystallogr.* **2010**, *43*, 811–824.

(4) Cambridge Crystallographic Data Centre Publications. http://www.ccdc.cam.ac.uk/about_ccdc/company_information/ccdc_publications/papers/ (accessed August 30, 2011).

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