MedeA COD GUI

Gateway to the Open-Access Collection of Crystal Structures

With the *MedeA* ®[1] *COD GUI*, you have rapid access to atomic structures of the Crystallography Open Database (*COD*), the fastest growing collection of organic, inorganic, metal-organics compounds, and mineral compounds.

At-a-Glance

The *MedeA COD GUI* is fully integrated with *MedeA InfoMaticA* to provide crystal structure data from COD

Key Benefits

- Quick and efficient structure search and retrieval
- Full integration with all *MedeA* modules

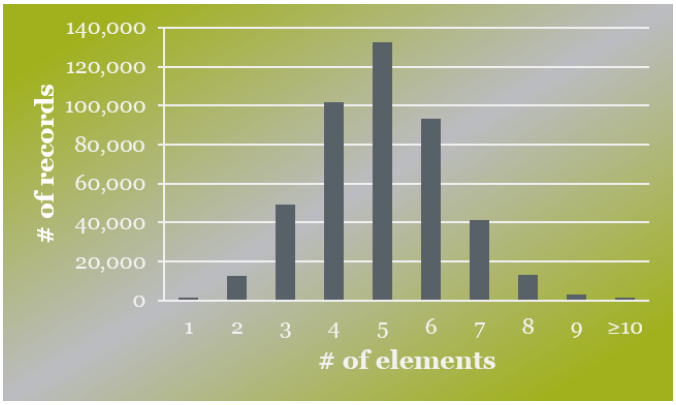

Fig. 1: Number of records by constituent count that can be accessed via the MedeA COD GUI

COD started in March 2003, and already encompassed around 10,000 structures in 2004. In 2014, within 11 years, COD accumulated over 250,000 structures. Since then, more than 35,000 have been added to COD each year. COD is recommended by scientific journals to deposit crystallographic data.

With the *MedeA COD GUI*, you have full access to all COD structure data records and can fully leverage the rich COD content to perform atomistic simulations with *MedeA*.

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

Specifications

- 4.4 GB database file stored on disk
- Access to more than 450,000 structure records
- Regular COD updates, along with *MedeA* updates

Key Features

- Largest open access collection of crystal structures of organic molecules
- Fully compatible with all *MedeA* compute engines and *MedeA* property modules
- Ideally suited for materials properties screening and optimization

Properties

- Detailed information of lattice parameters, symmetry (space group), and bibliographic reference
- Atomic coordinates, and interatomic distances and angles
- Atomic coordination
- Pair correlation function
- X-ray diffraction (XRD) powder pattern (radiation source dependent)

Required Modules

- *MedeA Environment* (includes *MedeA InfoMaticA*)

Recommended Modules

- *MedeA Pearson*
- *MedeA ICSD*
- *MedeA VASP*
- *MedeA HT-Launchpad*

Find Out More

Learn more about *MedeA InfoMaticA* in the video tutorial: How to Calculate Elastic Constants with MedeA VASP 5 on the Materials Design Youtube Channel.

COD is an academic project managed by the Vilnius University Institute of Biotechnology in Lithuania. The primary citation of COD is S. Gražulis, *et al.*, *Nucleic Acids Res.* **40**, D420 (2012).

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