



# MedeA COD GUI

Gateway to the Open-Access Collection of Crystal Structures

With the MedeA<sup>®1</sup> 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

## 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

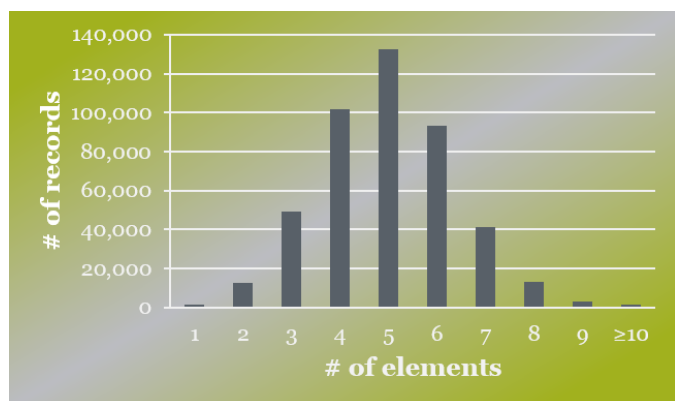


Figure 1: Number of records by constituent count that can be accessed via the MedeA COD GUI

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.

<sup>1</sup> MedeA and Materials Design are registered trademarks of Materials Design, Inc.

## Find Out More

*al.*, *Nucleic Acids Res.* **40**, D420 (2012).

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*