BIOVIA MATERIALS STUDIO MOTIF

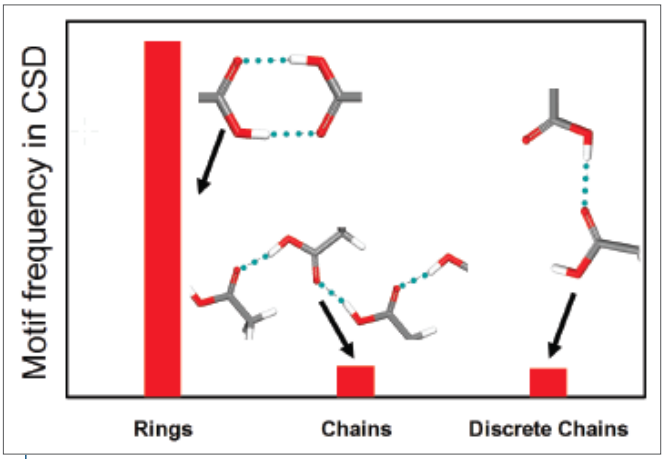
DATASHEET

BIOVIA Materials Studio Motif expands BIOVIA's toolset for crystal engineering efforts. It is a tool designed to analyze connectivity information in molecular crystals, providing a qualitative and quantitative analysis method of hydrogen bond topologies. Combined with the predictive capabilities of Polymorph, BIOVIA Materials Studio Motif helps categorizing proposed packing arrangements and introduces a similarity measure to related structures available in the Cambridge Structural Database (CSD), allowing for a statistical scoring of proposed structures

Polymorphism affects a wide array of materials properties, including solubility, bioavailability, mechanical stability, and manufacturability. For researchers dealing with solidification processes, selecting an optimal form introduces both challenges and opportunities. BIOVIA Materials Studio Motif supports these scientific efforts by generating knowledge about hydrogen bond topologies. This knowledge can help categorizing the tremendously complex design space, spanned not only by often numerous polymorphs, but also by salts, solvents, and co-crystals.

WHAT DOES BIOVIA MATERIALS STUDIO MOTIF DO?

BIOVIA Materials Studio Motif interfaces with the Cambridge Structural Database (CSD)[1] exploiting Cambridge Crystallographic Data Centre's (CCDC) Mercury functionality[2]. BIOVIA Materials Studio Motif answers the important question: Do molecules with comparable architecture crystallize in similar bonding configurations as the proposed new structure?



Hydrogen bond motifs of carboxyl groups together with their statistical occurrence

BIOVIA Materials Studio Motif supports two primary workflows: To extract connectivity information of molecular crystals and to compare this connectivity information to experimentally know structures.

The first workflow uses previously defined contact points – typically hydrogen bond acceptors/ donors or ionic contacts – to search for bonding motifs: Rings, infinite and finite chains, discrete motifs, and intermolecular contacts.

The second workflow queries the Cambridge Structural Database (CSD) for similar or related structures and their bonding motifs. BIOVIA Materials Studio Motif uses a similarity measure – based on Tanimoto coefficients – to gauge whether the bonding motifs of comparable CSD structures match those of the analyzed structure. As a result a similarity score is assigned to the analyzed structure. This allows for a statistical comparison of a proposed new polymorph and previously known structures with similar molecular architecture.

HOW DOES BIOVIA MATERIALS STUDIO MOTIF BENEFIT YOU?

BIOVIA Materials Studio Motif is a tool designed to support crystal engineering efforts. BIOVIA Materials Studio Motif adds an additional level of analysis and ranking capability when used together with Polymorph, BIOVIA's predictive crystal packing tool. Statistical ranking/scoring of packing results from Polymorph can add an additional layer of confidence to the results. In addition, classification of motifs gives valuable knowledge that can be used in the context of crystal engineering efforts, e.g. selective crystallization strategies[3].

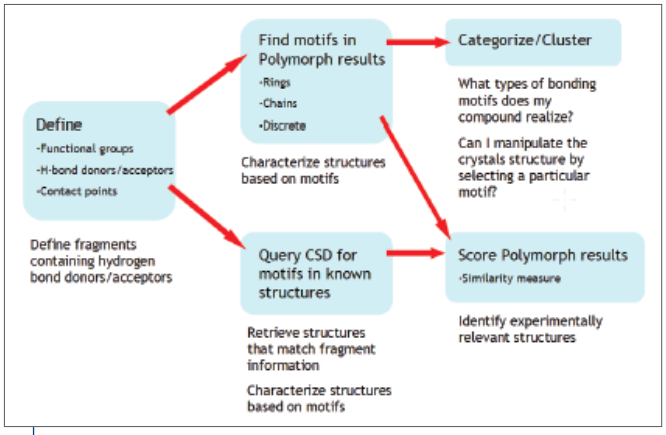
FEATURES

BIOVIA Materials Studio Motif searches are driven by an interactive setup step in which chemical knowledge of functional groups involved in hydrogen bonding, donor and acceptor sites, and classes of potential bonding motifs, is translated into a database query that can be sent to the CSD. BIOVIA Materials Studio Motif simplifies this setup by:

- Interactive definition of functional groups using the BIOVIA Materials Studio "Set" concept
- Creation of contact points via manual selection or automatic processing using fully configurable lists of donor/acceptor atoms
- Support for ionic contact points for salt selection studies

BIOVIA Materials Studio Motif allows for:

- Simple selection of motifs for query building
- Scoring function based on Taminoto coefficients
- Scoring against CSD entries or against input list, i.e. Polymorph output
- Reuse of previous CSD search results
- Client-server architecture for CSD access across your organization



BIOVIA Materials Studio Motif workflows

THE BIOVIA MATERIALS STUDIO ADVANTAGE

BIOVIA Materials Studio Motif is available through BIOVIA Material Studio's modeling and simulation suite that runs as a Windows® client on your PC, and provides a comprehensive range of software tools. Flexible client/server computing harnesses the power of a range of server technologies, to access leading methods in computational chemistry and materials science, delivering results direct to your desktop.

Results generated by BIOVIA Materials Studio Motif can be analyzed using BIOVIA Materials Studio's spreadsheet-like study table environment. The study table allows for a condensed representation of the results, associating crystal structures with motif formulas, number of motifs found, scoring information, as well as collecting related structures retrieved from the CSD. The resulting structural information can be further enriched as BIOVIA Materials Studio gives integrated access to related modeling and simulation functionality including morphology prediction, lattice energy evaluations based on molecular and quantum mechanics, advanced visualization, prediction of powder X-ray pattern, and statistical analysis.

To learn more about BIOVIA Materials Studio, go to **accelrys.com/materials-studio**

REFERENCES:

1. F. H. Allen, Acta Cryst., 2002, B58, 380-388.

2. C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler and J. van de Streek, J. Appl. Cryst., 2006, 39, 453-457.

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