

インターネットを利用した

3DMET: 生体内分子の三次元構造データベース

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インターネットで簡単な操作により、部分構造と物性値から類似分子を検索し、分子の立体構造と物性値を閲覧することができる。

- ホームページ上で天然分子の三次元構造、物性値を閲覧することができる「3DMET (生体内分子の三次元構造データベース)」を開発しました。
- 細胞内での分子認識においては三次元構造が重要であり、特に農業分野で利用できる(農薬の設計、食品の成分分析等)天然物を中心に構成されています。
- 簡易な入力操作で、構造や物性が類似している化合物を検索し、その構造と種々の物性値を表示します。2008年8月1日にリリース2を公開、現在5676件の立体構造を収録し、30件の物性値から検索が可能です。
- システムを一般に公開(利用無料)しており、毎月約50ヶ国からアクセスがあります。

3DMET
A three-dimensional-structure database
of natural metabolites

Home
Search Molecules
Substructure **new**
Universal param
2D param
3D param
Documents
What's new?
Contact us
Q&A

3DMET is a database collecting three-dimensional structures of natural metabolites.

Three-dimensional structure is an important factor for molecular recognition. This recognition is always performed in the living cell. As we know, atom chirality is also essential factor of the 3D-structure for molecular recognition. However, many programs of 2D-3D converters can not transform correctly about all of the natural metabolites. Thus, 3DMET (3D-structure database of natural metabolites) has been developed.

This database has not only 3D-structures but also some descriptors. Each structures are searchable these descriptors. This system also has a simple search system for substructure of the molecule. The search can be performed by three levels depending on the accuracy.
-> see "Search Molecules"

The benefits to use 3DMET are:

- we can view a minimized 3D-structure of the molecule
- the 3D-structures are verified.
- we can refer both of the 2D and 3D structures of a molecule.
- we can obtain many molecular descriptors for 2D and 3D structures.
- we can find any molecules related to both of descriptors and substructures.
-> see "Documents"

Today's molecule (B00020)

Jmol

To showing 3D-structures, Jmol is used in the each data page. If you cannot see the structure of the "Today's molecule", you may need to install the [Java Runtime Environment](#).

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Search molecule (Substructure search)

Search by
level 1 loose search
level 2 **strict search**
level 3 strict search

JME Editor courtesy of Peter Ertl, Novartis Help for JME editor

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Search Results

30 entries were detected.

met_id	cpd_id	name
B00020	B00020	Catechol, 1,2-Benzenediol, o-Benzenediol, 1,2-Dihydroxybenzene, Brenzcatechin, Pyrocatechol
B00046	B00046	Phenol, Benzenol, Hydroxybenzene, Phenic acid, Phenylic acid
B00128	B00128	Phenyl acetate, Acetylphenol, Acetic acid,phenyl ester
B00283	B00283	Anisole, Methoxybenzene, Methyl phenyl ether, Phenol methyl ether
B00284	B00284	Aspirin, Acetylsalicylic acid, 2-Acetoxybenzenecarboxylic acid, Acetylsalicylate
B00305	B00305	Flavonol
B00308	B00308	o-Methoxyphenol, Guaiacol, Catechol monomethyl ether
B00351	B00351	Benzenediol
B00383	B00383	2-Iodophenol
B00397	B00397	Phenol sulfate
B00452	B00452	2-Hydroxybiphenyl, 2-Biphenylol, 2-Phenylphenol
B00484	B00484	Phenolic phosphate, Phenylphosphate
B00604	B00604	2-Iodophenol methyl ether
B00648	B00648	Dibenz[1,4]dioxin-2,3-dione
B00919	B00919	Salicylaldehyde, o-Hydroxybenzaldehyde

3DMET
3DMET: B00023

Universal description

Entry	B00023
Name	Catechol, 1,2-Benzenediol, o-Benzenediol, 1,2-Dihydroxybenzene, Brenzcatechin, Pyrocatechol
Formula	C6H6O2
Weight	110.0968
Canonical SMILES	Oc1ccccc1O
InChI	1/C6H6O2/c7-5-3-1-2-4-6(5)/h1-4,7-8H
CASRN	120-80-9

2D and 3D structures/descriptors

2D Structure of KEGG

3D structure (visualized by Jmol)

計算資源:

大規模アプリケーションサーバ
MOE (分子モデリングアプリケーション)

分子の構造入力でわかりやすい部分構造検索ができる。ゲノムネットのCOMPOUNDと連携しており、二次元構造と三次元構造を対照して検討できる。