

Resource Summary Report

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National Cancer Institute 3D Structure Database

RRID:SCR_008211

Type: Tool

Proper Citation

National Cancer Institute 3D Structure Database (RRID:SCR_008211)

Resource Information

URL: http://dtp.nci.nih.gov/docs/3d_database/dis3d.html

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Description: The NCI DIS 3D database is a collection of 3D structures for over 400,000 drugs. The database is an extension of the NCI Drug Information System. The structural information stored in the DIS is only the connection table for each drug. The connection table is just a list of which atoms are connected and how they are connected. It is essentially a searchable database of three-dimensional structures has been developed from the chemistry database of the NCI Drug Information System (DIS), a file of about 450,000 primarily organic compounds which have been tested by NCI for anticancer activity. The DIS database is very similar in size and content to the proprietary databases used in the pharmaceutical industry; its development began in the 1950s; and this history led to a number of problems in the generation of 3D structures. This information can be searched to find drugs that share similar patterns of connections, which can correlate with similar biological activity. But the cellular targets for drug action, as well as the drugs themselves, are 3 dimensional objects and advances in computer hardware and software have reached the point where they can be represented as such. In many cases the important points of interaction between a drug and its target can be represented by a 3D arrangement of a small number of atoms. Such a group of atoms is called a pharmacophore. The pharmacophore can be used to search 3D databases and drugs that match the pharmacophore could have similar biological activity, but have very different patterns of atomic connections. Having a diverse set of lead compounds increases the chances of finding an active compound with acceptable properties for clinical development. Sponsor: The ICBG are supported by the Cooperative Agreement mechanism, with funds from nine components of the NIH, the National Science Foundation, and the Foreign Agricultural Service of the USDA.

Synonyms: NCI DIS 3D Database

Resource Type: data or information resource, database

Keywords: drug, 3d, 3d molecular structures, anticancer, atom, atomic, biological, cellular, chemistry, clinical, compound, development, interaction, lead, organic, pattern, pharmaceutical, pharmacophore, structural, structure

Resource Name: National Cancer Institute 3D Structure Database

Resource ID: SCR_008211

Alternate IDs: nif-0000-21279

Record Creation Time: 20220129T080246+0000

Record Last Update: 20260729T044205+0000

Ratings and Alerts

No rating or validation information has been found for National Cancer Institute 3D Structure Database.

No alerts have been found for National Cancer Institute 3D Structure Database.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We have not found any literature mentions for this resource.