CoRS

A Comprehensive Research Information System For Small Molecules

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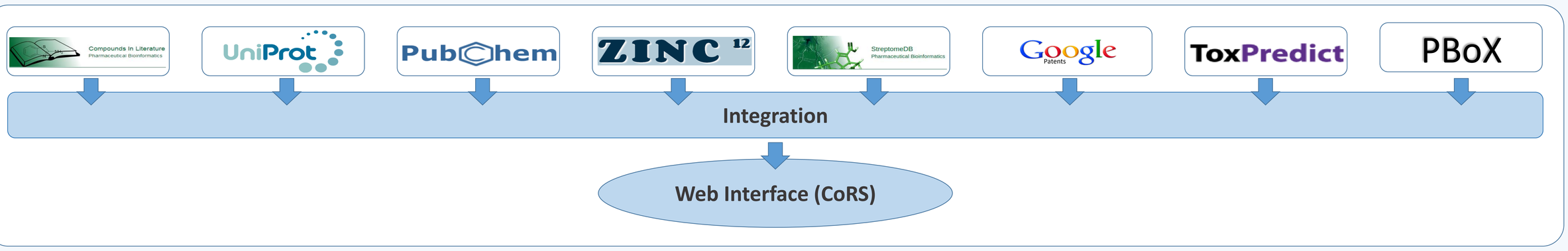
What is CoRS ?

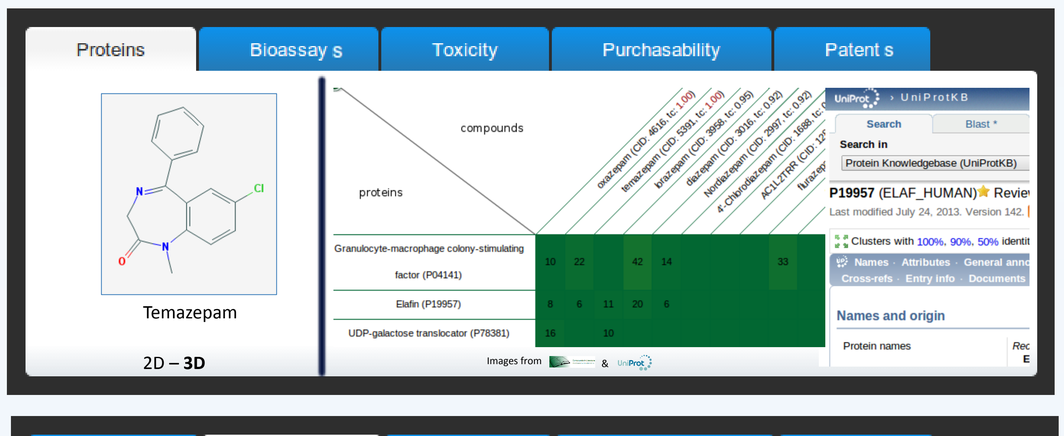
An important task in the field of pharmaceutical sciences is the analysis of the biological effects of small molecules[1]. To identify potential new similar drugs or to assess health risks from chemicals requires prior knowledge of compounds. The ongoing CoRS project is aiming at the **integration** of existing data resources of molecules that are combined with tools for the **prediction** of molecular effects. CoRS integrates databases such as PubChem, StreptomeDB[3], CIL[4], PBoX[6], ToxPredict and UniProt, and has the capability to search for compounds that can be easily **synthesized** via building blocks.

Aim

To have a system which gathers data from publicly available resources of compounds and **displays a digest of information** at one place useful for pharmaceutical researchers working in the field of drug discovery.



"Type in compound name or draw a chemical structure ..."

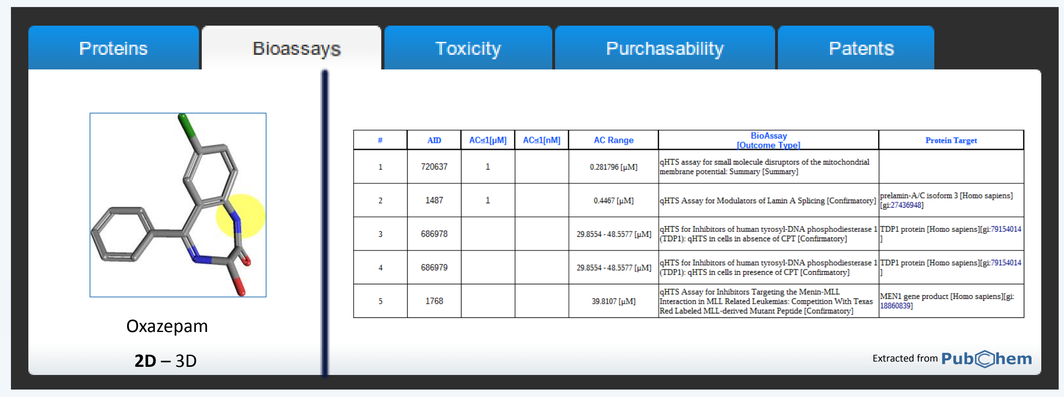


Which proteins co-occured with compounds in literature?

The tab **Proteins** displays information of CIL[4], which gives the related proteins of the given compound which are mentioned in the literature database PubMed. This information accelerates the time consuming process of literature research.

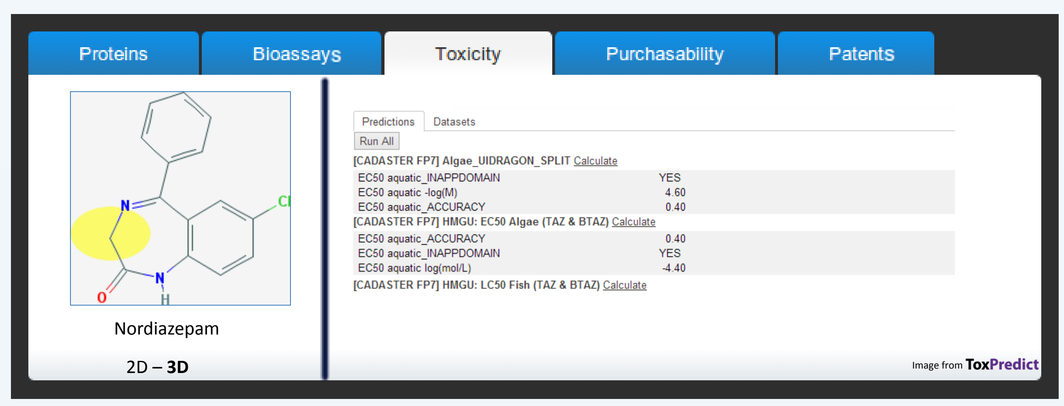
Has the compound been tested in bioassays ?

The tab **Bioassays** displays crucial information of various experiments useful in drug discovery. The data is extracted from the publicly available database PubChem, which consists of three interconnected databases: Substance, BioAssay and Compound[5]. Here the information is displayed with assay identifier and details of bioassays can be retrieved upon browsing.



Is the compound toxic?

For a queried compound and to similar compounds CoRS will indicate **Toxicity** prediction. This information is provided by the OpenTox community through ToxPredict web service.



Similar compounds difference is indicated by yellow color

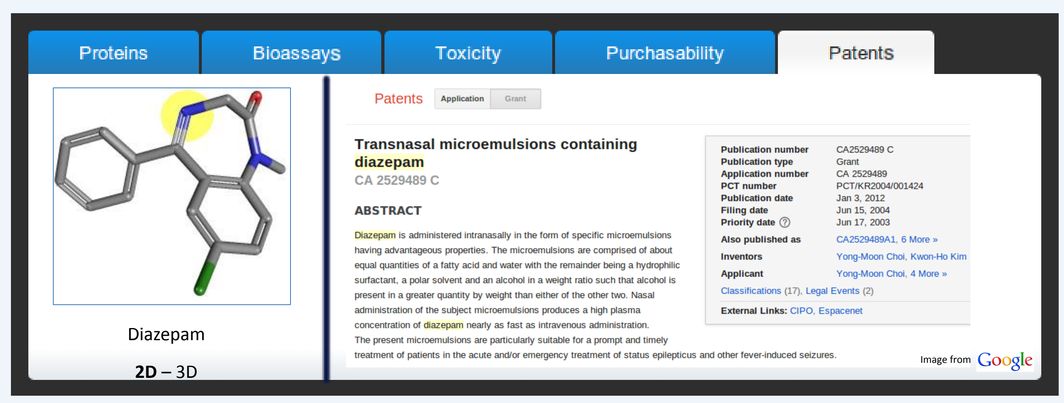
"Drug discovery made easy!"

Is the compound purchasable ?

Millions of molecules are commercially available. The **Purchasability** tab gives information about vendors. This information in CoRS is integrated from ZINC[2] and PBoX[6] sources and displayed in this tab.

Has the compound been patented ?

For a newly developed compound, patent information will be crucial. CoRS takes information from Google Patents and displays the **Patents** information in this tab. All the documents available through Google Patents originate from US Patent and Trademark office.



References

[1] Bolton E. et al.: **Integrated Platform of Small Molecules and Biological Activities**. *Annual Rep Comput Chem* 2008, 4: 217-241.
[2] Irwin JJ. et al.: **ZINC: A Free Tool to Discover Chemistry for Biology.** *J. Chem Inf Model* 2012, 52(7): 1757-1768.
[3] Lucas X, Senger C. et al.: **StreptomeDB: a resource for natural compounds isolated from Streptomyces species.** *Nucleic acids res* 2013, 41(D1): D1130-D1136.
[4] Grüning BA, Senger C. et al.: **Compounds In Literature (CIL): screening for compounds and relatives in PubMed.** *Bioinformatics* 2011, 27(9): 1341-2.
[5] Wang Y. et al.: **An overview of the PubChem BioAssay resource.** *Nucleic acids res.* 2012, 38: D255-D66.
[6] Lucas X,. et al.: **Manuscript under preparation.**

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