

CoRS

A Comprehensive Research Information System For Small Molecules

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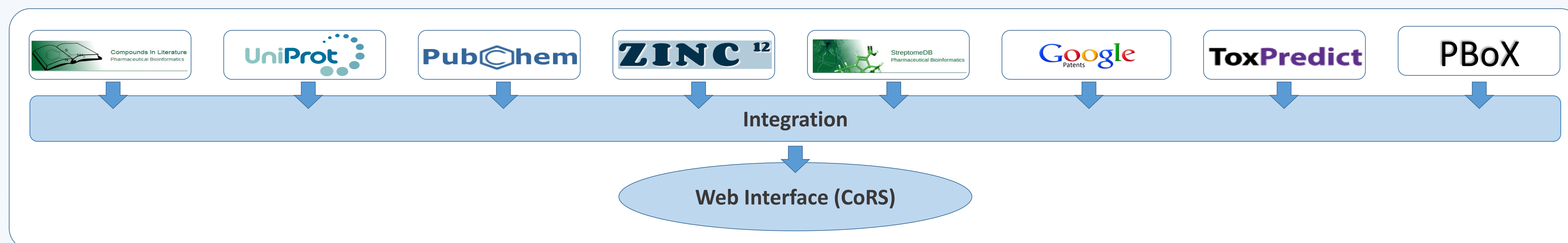


What is CoRS ?

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 ...”

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.

“Drug discovery made easy!”

Is the compound 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.

Similar compounds difference is indicated by yellow color

Proteins | Bioassays | Toxicity | Purchasability | Patents

Temazepam
2D - 3D

Protein	Score
Granulocyte-macrophage colony-stimulating factor (P04141)	15
Elafin (P19957)	1
UDP-galactose 4-epimerase (P78381)	1

Which proteins co-occurred 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.

Proteins | Bioassays | Toxicity | Purchasability | Patents

Oxazepam
2D - 3D

#	AB	AC1Q[M]	AC1Q[M]	AC Range	Bioassay (Bioactivity Target)	Protein Target
1	720637	1		0.36176 [µM]	qRTS assay for small molecule disruption of the astrocytoid membrane potential (Stimulatory)	
2	1487	1		0.4487 [µM]	qRTS Assay for Modulators of Lamin A Splicing (Constraining)	phospho-A-C coatomer 3 (Homo sapiens) [p174894]
3	686878			29.8254 - 48.3377 [µM]	qRTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TFPI) qRTS in cells in absence of CPT (Constraining)	TFPI protein (Homo sapiens) [p793404]
4	686879			29.8254 - 48.3377 [µM]	qRTS for Inhibitors of human tyrosyl-DNA phosphodiesterase 1 (TFPI) qRTS in cells in presence of CPT (Constraining)	TFPI protein (Homo sapiens) [p793404]
5	1768			38.8387 [µM]	qRTS Assay for Inhibitors Targeting the Mitotic Spindle Disruption in MEL-1 Related Leishmania. Competition With Test (Red Labelled MEL-derived Mitotic Peptide) (Constraining)	MED12 gene product (Homo sapiens) [p100000]

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.

Proteins | Bioassays | Toxicity | Purchasability | Patents

Nordiazepam
2D - 3D

Predictions	Datasets
[CADASTER FP7] Algae_UIDRAGON_SPLIT Calculate	
EC50 aquatic_INAPPODOMAIN	YES
EC50 aquatic_log[M]	4.60
EC50 aquatic_ACCURACY	0.40
[CADASTER FP7] HMGU: EC50 Algae (TAZ & BTAZ) Calculate	
EC50 aquatic_ACCURACY	0.40
EC50 aquatic_INAPPODOMAIN	YES
EC50 aquatic_log[mol/L]	-4.40
[CADASTER FP7] HMGU: LC50 Fish (TAZ & BTAZ) Calculate	

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.

Proteins | Bioassays | Toxicity | Purchasability | Patents

Lorazepam
2D - 3D

In ZINC since	Heavy atoms	Benign functionality
July 23 rd , 2004	21	Yes

Popular Name: Lorazepam
PubMed - Wikipedia - Google
CAS Numbers: 110032-65-0, 846-49-1, 907200-04-8

Vendors

Vendor	Count
Active BioPharma	696
Amadis Chemical	A840886
BePharm Building Blocks	B20025
ChiralBlock BioScience BB	736
Sesquia Research Products	188;8-17-6

Annotations: BindingDB.org, ChEMBL DrugSt, ChEMBL12, ChEMBL13

Proteins | Bioassays | Toxicity | Purchasability | Patents

Diazepam
2D - 3D

Patents | Application | Grant

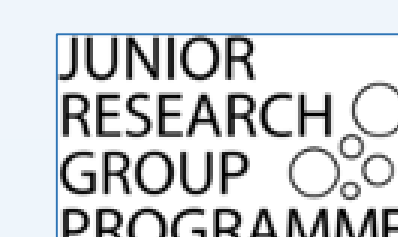
Transnasal microemulsions containing diazepam
CA 2529489 C

ABSTRACT
Diazepam is administered intranasally in the form of specific microemulsions having advantageous properties. The microemulsions are comprised of about equal quantities of a fatty acid and water with the remainder being a hydrophilic surfactant, a polar solvent and an alcohol in a weight ratio such that alcohol is present in a greater quantity by weight than either of the other two. Nasal administration of the subject microemulsions produces a high plasma concentration of diazepam nearly as fast as intravenous administration. The present microemulsions are particularly suitable for a prompt and timely treatment of patients in the acute and/or emergency treatment of status epilepticus and other fever-induced seizures.

Publication number: CA2529489 C
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Priority date: Jun 17, 2003
Also published as: CA2529489A1, 6 More >
Inventors: Yong-Moon Cho, Keon-Ho Kim
Applicant: Yong-Moon Cho, 4 More >
Classifications: (17), Legal Events (2)
External Links: CIPO, Espacenet

References

- [1] Bolton E. et al.: **Integrated Platform of Small Molecules and Biological Activities**. *Annual Rep Comput Chem* 2008, 4: 217-241.
- [2] Irwin J.J. 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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