Biological database Project

Drugs repurposing

Criteria of selection:

- Permability Blood Brain barrier
- Neuro degenerative disease drugs
- Failed clinical test in phase 1

Use of the database of the web site

DRUGBANK

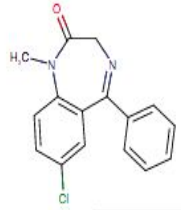
Diazepam

Targets (19) | Enzymes (10) | Carriers (1) | Transporters (1) | Biointeractions (32)

IDENTIFICATION

Name	Diazepam
Accession Number	DB00829 (APRD00642, DB07699)
Type	Small Molecule
Groups	Approved, Illicit, Investigational, Vet approved
Description	A benzodiazepine with anticonvulsant, anxiolytic, sedative, muscle relaxant, and amnesic properties and a long duration of action. Its actions are mediated by enhancement of gamma-aminobutyric acid activity. It is used in the treatment of severe anxiety disorders, as a hypnotic in the short-term management of insomnia, as a sedative and premedicant, as an anticonvulsant, and in the management of alcohol withdrawal syndrome. (From Martindale, The Extra

Structure



3D | Download | Similar Structures

- MOL
- SDF
- 3D-SDF
- PDB
- SMILES
- InChI

Synonyms

7-chloro-1,3 … nyl-2H-1,4-benzodiazepin-2-one

Diazepam

Methyl diaz

External IDs NSC-169897 … 7 / RO-5-2807 / WY-3467

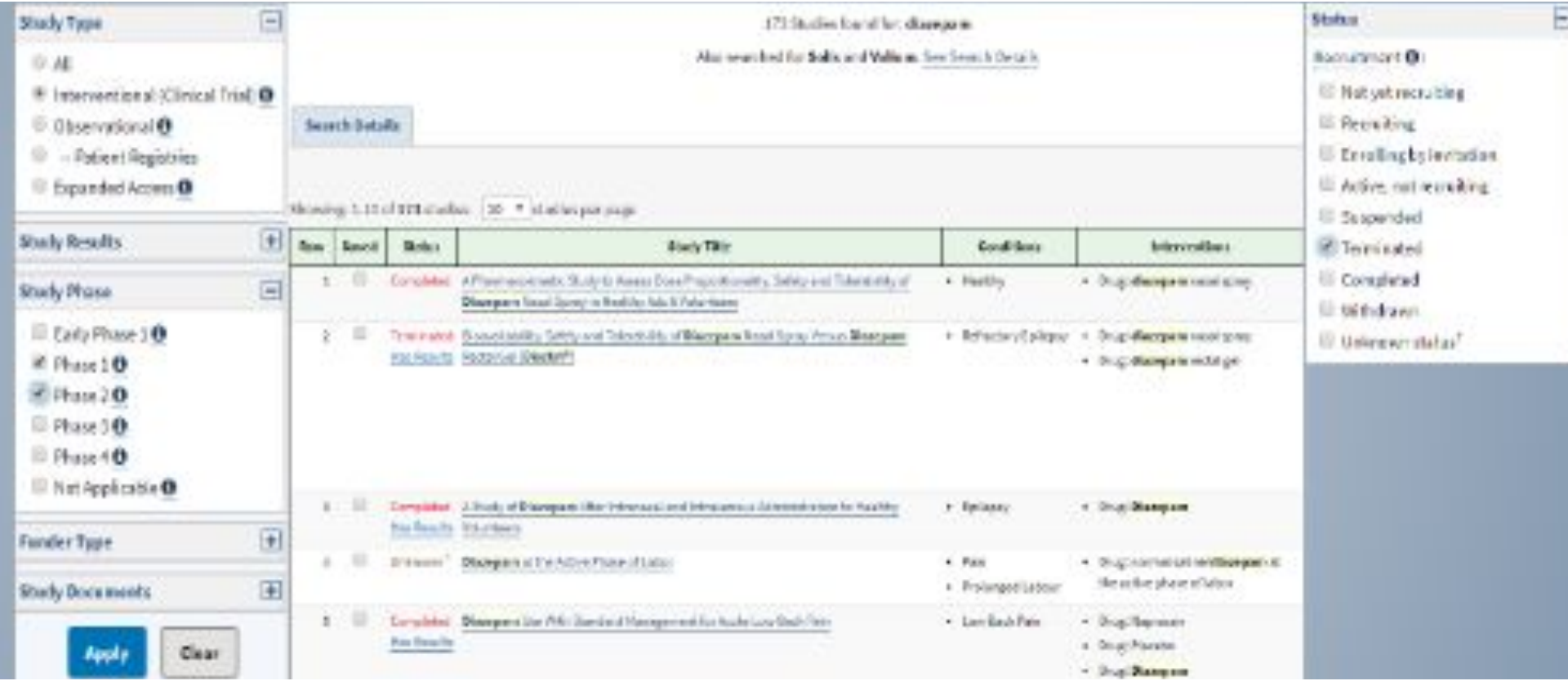
Product Ingredients

INGREDIENT	UNII	C

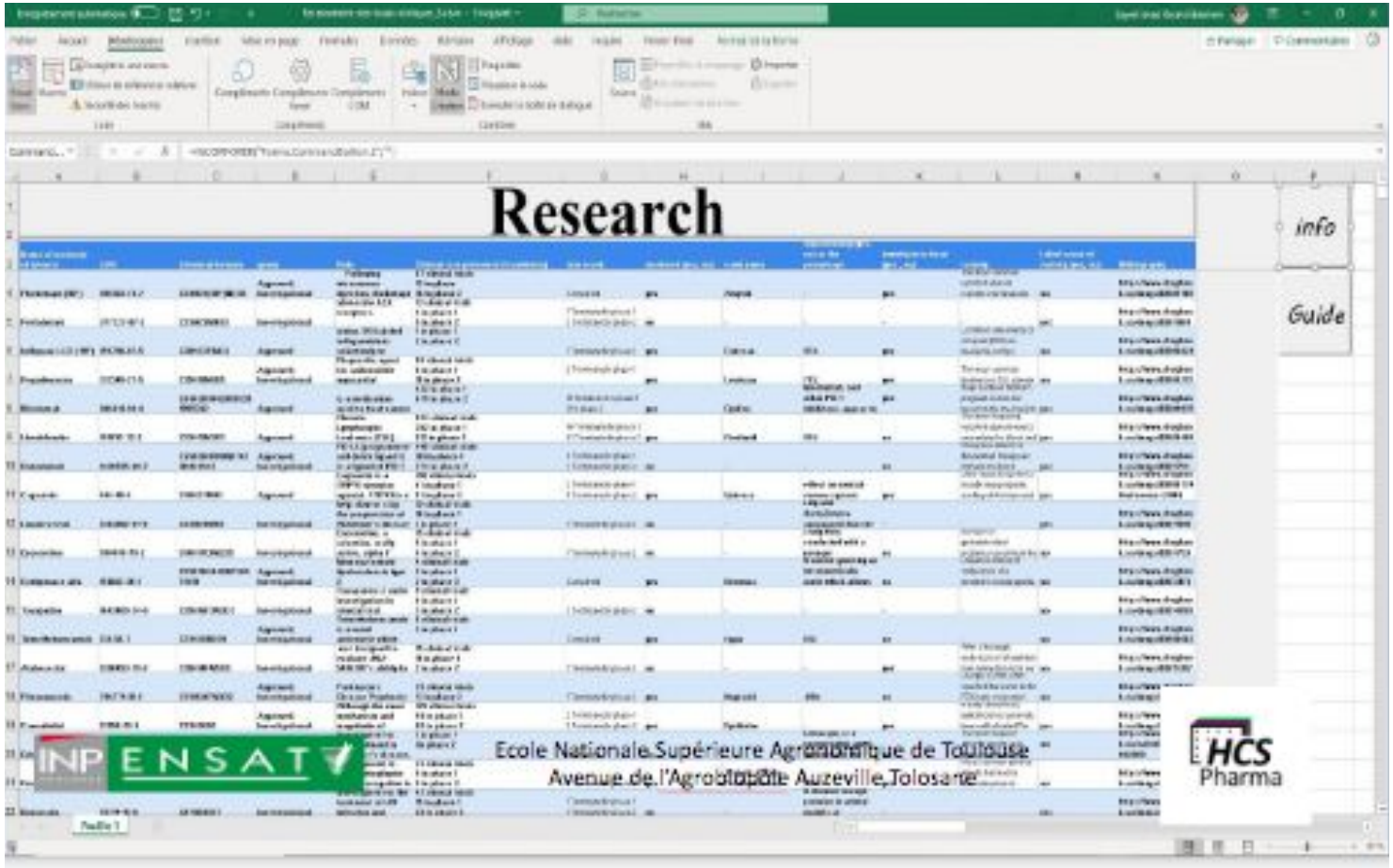
Predicted ADMET features

PROPERTY	VALUE	PROBABILITY
Human Intestinal Absorption	+	0.9948
Blood Brain Barrier	+	0.9934
Caco-2 permeable	+	0.8867

Use of the database of web site ClinicalTrials.gov



Use our own database stored on excel



Use of SMILES ?

Basics of SMILES

- SMILES specifically represents a valence model of a molecule, not a computer data structure, a mathematical abstraction, or an "actual substance".
- There are six generic SMILES encoding rules, corresponding to specification of atoms, bonds, branches, ring closures, and disconnections and isomerism.
- The function of SMILES is to clearly represent a particular valence model, not dictate which one should be used. For example one chemist might represent nitromethane as C[N+](=O)[O-] with a nitrogen of valence 4 in a charge-separated structure whereas another might represent it as CN(=O)=O with a neutral five-valent nitrogen. Both of them are correct.
- SMILES represents a chemist's model of molecules, not a computer scientist's model of a chemical data structures. SMILES grammar is such that it may be canonicalized, i.e., among all possible valid SMILES for a given molecule or reaction, a single, canonical (unique)