

Sourcing data for knowledge base

Access to databases and models:

Wombat, MDLCrossFire, Integrity, Prous, Genego/ GVK MCD, Molsoft ICM /PDB view, ChemoSoft, Smart Mining, Cerius2, Discovery Studio, NeuroSolution, AutoDock, Surflex

Experimental data:

- Broad collaborations with NIH, FMP, CNIO and other screening centers
- Grant and non-profit contracts

WOMBAT

Structure: CCCCCCCCOc1ccc(cc1)C(=O)N2C=NC(=N2)C3=CC=CC=C3

act#	receptor	act_type	act_val	act_val	act_val	keywords
1	LTC4	IC50	9.300	9.300	9.300	receptor Inhibition IC50 GPCR G-protein G-protein receptor Inhibition IC50

MDLCrossFire Commander

Query Builder: Search in: Beliner(2005/04)

Search Field Name in Hierarchy: impl. free sites

Chemical Structure: O=C(N)c1nc(C2=CC=CC=C2)ncn1

Similarity Analysis

Select Histogram Entries of interest:

Similarity Score

- ≥ 99 (most similar)
- 95-98
- 90-94
- 85-89
- 80-84
- 75-79
- 70-74
- 65-69
- 60-64 (least similar)

Get Substances

Histogram Entries 1-9 of 9

Integrity

Select another Knowledge Area

Records Retrieved: 1 in Drugs & Biologics

Drugs & Biologics Search Results

Query > Entry Number = 411850

Entry Number: 411850 **UPDATED**

CAS Registry No. 256414-75-2

Molecular Formula C20H10F6N2OS

Molecular Weight 440.3627

Highest Phase Preclinical

Chemical Structure: Cc1ccc(cc1)C2=CC(=C(C=C2)S(=O)(=O)N3C=NC(=N3)C(F)(F)F)C(F)(F)F

SEW-2871

Chemical Name/Description: 5-[4-Phenyl-5-(trifluoromethyl)thien-2-yl]-3-[3-(trifluoromethyl)phenyl]-1,2,4-oxadiazole

Code Name: SEW-2871

Generic Name: Brand Name

Therapeutic Group: Cellular / Molecular Mechanism

Pharmacological Tools: Lymphospholipid edg1 (S1P1) Receptor Agonists

Renal Failure, Agents for

Organization: Maybridge University of Arizona

Product Summary: REPORT

Related Information: Targets 1 Literature 7