

API-Surrogate search: About

Current search algorithm accepts either **text** or **SMILES**

- 1) **Text** can be name of API or inactive ingredient
- 2) **SMILES** can be *canonical* or *isomeric* (it provide extra information like stereochemistry of molecule)
 - (a) If user provide SMILES of novel molecule, code calculate the Tanimoto similarity and shows output of similar molecule

API-Surrogate search: Homepage

User can search by name of API / SMILES

The screenshot shows the homepage of the API surrogate search tool. At the top, the Aganitha logo is visible. The main heading is "API surrogate search". Below it is a search bar with the placeholder text "Search by API names, SMILES, properties or Draw structures to derive SMILES". A suggestion "Try: Ritonavir C1=CC=C(C=C1)C=O" is shown below the search bar. An "Advanced search" section contains two sliders: "M.W" with a range from 0 to 1000 g/mol, and "LogD" with a range from -3 to 5. Below the sliders are "Search" and "Draw" buttons. A callout box on the right shows a "Draw molecule" interface with a SMILES string input field containing CC(=O)Oc1ccccc1C(=O)O and a chemical structure editor displaying the structure of aspirin. A callout box at the bottom left explains the advanced search features.

Search by API names, SMILES, properties or Draw structures to derive SMILES

Try: Ritonavir C1=CC=C(C=C1)C=O

Advanced search

M.W
Min: 0 g/mol Max: 1000 g/mol

LogD
Min: -3 Max: 5

Search Draw

Advanced search to prioritize / sort results based on properties such as M.W., LogD
To be added: A comprehensive list of physicochemical properties for searching

Draw molecule

SMILES string
CC(=O)Oc1ccccc1C(=O)O

This value is automatically generated from your drawing

Home Search with structure

User can draw / edit structure

API-Surrogate search: Text-based search

api-surrogate.demos.aganitha.ai/results?query=Ritonavir&advanced=true&mw_min=0&mw_max=1000&logd_min=-3&logd_max=5

similar APIs found for input API i.e., Ritonavir

Download all results in a spreadsheet

Search Results for : Ritonavir

25 Approved formulations found for 1 API(s)

Home Columns Download

Brand Name	API	All active ingredients	Inactive Ingredients	Dosage Form	Dosage & Administration
Kaletra	RITONAVIR	LOPINAVIR (200 mg/1 1); ...	COPOVIDONE; SORBITA...	TABLET, FILM COATED	KALETRA tablets may be ...
Kaletra	RITONAVIR	Lopinavir (200 mg/1 1); Ri...	COPOVIDONE K25-31; S...	TABLET, FILM COATED	KALETRA tablets may be ...
Kaletra	RITONAVIR	LOPINAVIR (200 mg/1 1); ...	COPOVIDONE K25-31; S...	TABLET, FILM COATED	KALETRA tablets may be ...
Kaletra	RITONAVIR	LOPINAVIR (200 mg/1 1); ...	SORBITAN MONOLAURA...	TABLET, FILM COATED	KALETRA tablets may be ...
Kaletra	RITONAVIR	LOPINAVIR (200 mg/1 1); ...	SORBITAN MONOLAURA...	TABLET, FILM COATED	KALETRA tablets may be ...
Kaletra	RITONAVIR	LOPINAVIR (200 mg/1 1); ...	SORBITAN MONOLAURA...	TABLET, FILM COATED	KALETRA tablets may be ...
Paxlovid	RITONAVIR	NIRMATRELVIR (150 mg/...	SILICON DIOXIDE; CROS...	KIT	PAXLOVID is nirmatrelvir ...
Lopinavir and Ritonavir	RITONAVIR	LOPINAVIR (100 mg/1 1); ...	CALCIUM PHOSPHATE, ...	TABLET, FILM COATED	Tablets: May be taken wit...
Norvir	RITONAVIR	RITONAVIR (100 mg/1 1)	COPOVIDONE K25-31; A...	TABLET, FILM COATED	1. Adult patients: 600 mg...
Kaletra	RITONAVIR	LOPINAVIR (200 mg/1 1); ...	COPOVIDONE K25-31; S...	TABLET, FILM COATED	Tablets: May be taken wit...

Page Size: 1 to 10 of 25 Page 1 of 3

Contains

Contains

Does not contain

Begins with

Ends with

Equals

Does not equal

Each column can be filtered

Toggle Columns

- ✓ Brand Name
- ✓ API
- ✓ All active ingredients
- ✓ Inactive Ingredients
- SMILES
- Molecular Weight
- Molecular Formula
- CAS ID
- PubChem CID
- TPSA
- XLogP
- IUPAC Name
- InChIKey
- ✓ Dosage Form
- ✓ Dosage & Administration

Add / remove columns

3

Confidential and Proprietary. © 2017-24 Aganitha

aganitha

API-Surrogate search: Text-based search output

The screenshot displays the Aganitha API-Surrogate search interface. The browser address bar shows the URL `api-surrogate.demos.aganitha.ai/drug/50980`. The page title is "Search Results for : Ritonavir" with a subtitle "25 Approved formulations found for 1 API".

Search Results Table:

Brand Name	API
Kaletra	RITONAVIR
Kaletra	RITONAVIR
Kaletra	RITONAVIR
Kaletra	RITONAVIR
Kaletra	RITONAVIR
Kaletra	RITONAVIR
Paxlovid	RITONAVIR
Lopinavir and Ritonavir	RITONAVIR
Norvir	RITONAVIR
Kaletra	RITONAVIR

Brand name: Ritonavir
Generic name: Ritonavir

General Information

Manufacturer American Health Packaging	Dosage Form TABLET, FILM COATED
Administration Route ORAL	

Active ingredients with strength

1. RITONAVIR (100 mg/1 1)

Inactive Ingredients

1. COPOVIDONE K25-31
2. STARCH, CORN
3. ANHYDROUS DIBASIC CALCIUM PHOSPHATE
4. DIBASIC CALCIUM PHOSPHATE DIHYDRATE
5. HYPROMELLOSE 2910 (6 MPA.S)
6. MANNITOL
7. MICROCRYSTALLINE CELLULOSE
8. MICROCRYSTALLINE CELLULOSE 102
9. POLYETHYLENE GLYCOL 400
10. POLYETHYLENE GLYCOL 6000

Active Ingredients

RITONAVIR
Formula:
 $C_{37}H_{48}N_6O_5S_2$
MW: 720.90 g/mol
Canonical SMILES:
CC(C)C1=NC(=CS1)CN(C)C(=O)NC(C(C)C)C(=O)NC(C2=CC=CC=C2)CC(C(C3=CC=CC=C3)NC(=O)OCC4=CN=CS4)O
Inchi Key: NCDNCNXCDXHOMX-XGKFQTDJSA-N
IUPAC Name: 1,3-thiazol-5-ylmethyl N-[(2S,3S,5S)-3-hydroxy-5-[[[(2S)-3-methyl-2-[[methyl-[(2-propan-2-yl-1,3-thiazol-4-yl)methyl]carbamoyl]amino]butanoyl]amino]-1,6-diphenylhexan-2-yl]]carbamate

Page Size: 1 to 10 of 25 Page 1 of 3

API-Surrogate search: SMILES-based search output

Calculates Tanimoto similarity and shows results for top 10 APIs
To be added: Similarity search based on physicochemical properties"

api-surrogate.demos.aganitha.ai/results?query=C1%3DCC%3DC%28C%3DC1%29C%3DO

aganitha

Search Results for : C1=CC=C(C=C1)C=O
Top-10 similar APIs (Tanimoto similarity range: 0.52-0.32) found
395 Approved formulations found for 10 API(s)

Home Columns Download

Brand Name	API	All active ingredients	Inactive Ingredients	Dosage Form	Dosage & Administration
T.R.U.E. Test	CINNAMALDEHYDE	NICKEL SULFATE HEXAH...	HYDROXYPROPYL CELL...	KIT	Apply the three adhesive...
Safe OPA	O-PHTHALALDEHYDE	O-PHTHALALDEHYDE (2...	WATER; MONOBASIC PO...	LIQUID	■ Rinse thoroughly for m...
Ultimate Phenolics	CINNAMIC ACID	ACETYLCHOLINE CHLOR...	WATER; ALCOHOL; GLYC...	SOLUTION/ DROPS	• One full dropper 2x dail...
BioPhenolics	CINNAMIC ACID	Acetylcholine chloride (1...	Water; ALCOHOL; GLYCE...	SPRAY	Adults 4 sprays 3 times a...
BACT COMBINATION	CINNAMIC ACID	ADENOSINE PHOSPHAT...	WATER; ALCOHOL	LIQUID	1-10 drops under the ton...
Sugar and Food Additive ...	CINNAMIC ACID	CINNAMIC ACID (6 [hp_...	WATER; ALCOHOL	LIQUID	3 to 10 drops under the t...
Respiratory Plus	CINNAMIC ACID	ARSENIC TRIIODIDE (8 [...	WATER; ALCOHOL	LIQUID	1-10 drops under the ton...
Multi-Phenolic	CINNAMIC ACID	MANNOSE, D- (12 [hp_X...	WATER; ALCOHOL	LIQUID	Adults and children 5 to 1...
Sugar Cravings	CINNAMIC ACID	CINNAMIC ACID (6 [hp_...	WATER; ALCOHOL	LIQUID	10 drops under the tongu...
Respiratory Plus	CINNAMIC ACID	RIBES NIGRUM LEAF (3 [...	WATER; ALCOHOL	LIQUID	1-10 drops under the ton...

Page Size: 1 to 10 of 395 Page 1 of 40