API-Surrogate search: About
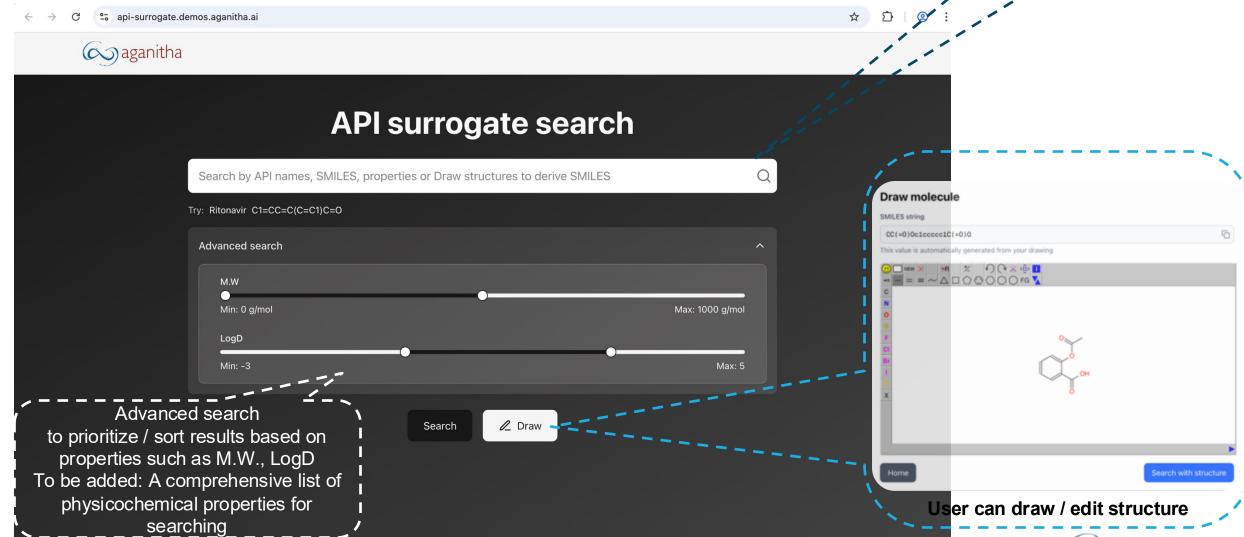
Current search algorithm accepts either *text* or **SMILES**

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

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API-Surrogate search: Homepage

User can search by name of API / SMILES

User can draw / edit structure

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

API-Surrogate search: Text-based search

Contains ▼

Contains
Does not contain
Begins with
Ends with
Equals
Does not equal

Each column can be filtered

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

Download all results in a spreadsheet

api-surrogate.demos.aganitha.ai/results?query=Ritonavir&advanced=true&mw_min=0&mw_max=1000&logd_min=-3&logd_max=5
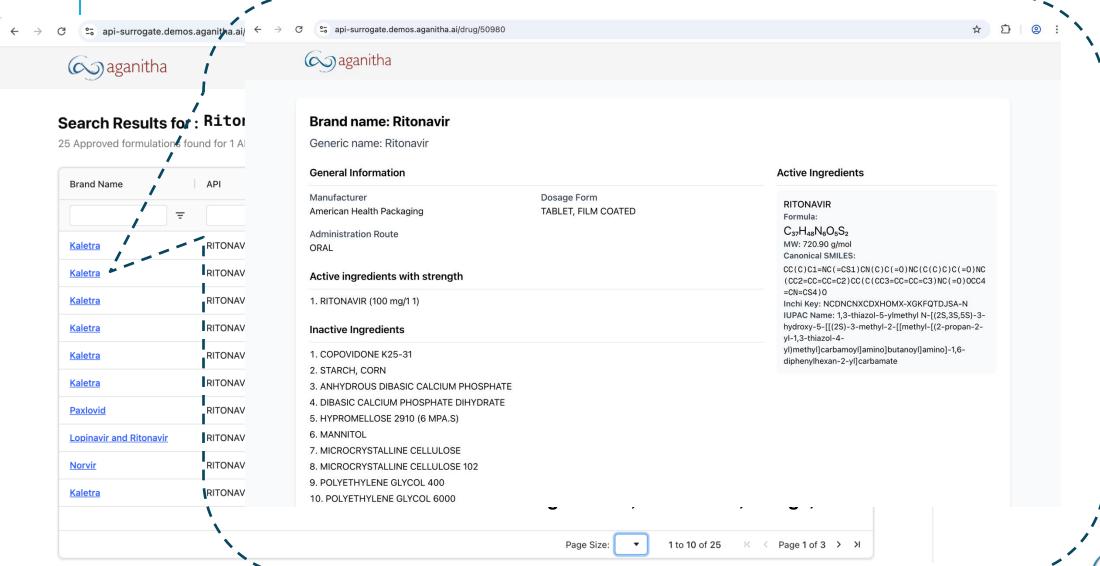
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Search Results for : `Ritonavir`
25 Approved formulations found for 1 API(s)

🏠 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 ⟩ ⟩⟩

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

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API-Surrogate search: Text-based search output

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

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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 > >|

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