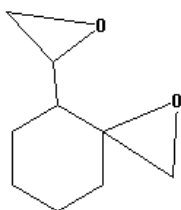


## CASLINK for one-step structure searching in CAS REGISTRY<sup>SM</sup>, MARPAT<sup>®</sup>, and CPlus<sup>SM</sup>

Use the CASLINK database cluster for quick, easy, and cost-effective substance searching in REGISTRY, MARPAT, and CPlus. Search an exact structure or a structure fragment, and you automatically get a single set of literature and patent references to specific substances or Markush structures that match the structure query.

(HCASLINK is available if you prefer to search HCAplus.)

Find patents and other references on substances that contain the following fragment of the known antitumor drug ovalicin.



- 1 Enter CASLINK. You are automatically connected to REGISTRY, MARPAT, and CPlus.
- 2 Upload the structure from STN Express<sup>®</sup> or STN<sup>®</sup> on the Web<sup>SM</sup>. An L-number is assigned for the structure.
- 3 Conduct a sample (default) substructure search (SSS) on the structure query (L1). Sample searches are automatically run in REGISTRY (L2) and MARPAT (L3).
- 4 Display a structure in the free SCAN format from one of the answer sets (L2) to verify that your query is retrieving appropriate answers.

```

=> FILE CASLINK
=>
L1      STRUCTURE UPLOADED

=> S L1 SSS

S L1 SSS SAM FILE=REGISTRY
      .
      .
      .
L2      38 SEA SSS SAM L1

S L2 SSS SAM FILE=MARPAT
      .
      .
      .
L3      3 SEA SSS SAM L1

=> D L2 SCAN STR

L2      38 ANSWERS      REGISTRY      COPYRIGHT 2008 ACS on STN

      Me2C=CH-CH2
      |
      O
      |
      MeO
      |
      Ph-CH=CH-C(=O)-O-
      |
      O
  
```

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1) : 0

**5** Conduct a full substructure search.

The following steps are automatically performed:

- Search the full **REGISTRY** database (L4).
- Search the full **MARPAT** database (L5).
- Search for references in **CAPLUS** (L6).
- Remove duplicates (L7).

**6** Display some answers, e.g., the title (TI) and corporate source (CS) from **MARPAT** (answer 1) and **CAPLUS** (answer 36).

**7** Combine your structure search (L7) with text terms. The appropriate searches are automatically performed in the **CASLINK** databases. **PATENT/DT** limits the answers to patents.

```
=> S L1 FULL
S L1 SSS FUL FILE=REGISTRY

L4          672 SEA SSS FUL L1

S L4 SSS FUL FILE=MARPAT

L5          35 SEA SSS FUL L1

S L4 FILE=CAPLUS
L6          973 FILE CAPLUS

DUP REM L5 L6
L7          971 DUP REM L5 L6 (37 DUPLICATES REMOVED)
           ANSWERS '1-35' FROM FILE MARPAT
           ANSWERS '36-971' FROM FILE CAPLUS

=> D TI CS 1 36

L7 ANSWER 1 OF 971 MARPAT COPYRIGHT 2008 ACS on STN
   DUPLICATE 1
TI Fumagillin-related compound inhibitors of methionine
   aminopeptidase 2 and use for the treatment of angiogenic
   and other conditions
PA Praecis Pharmaceuticals, Inc., USA

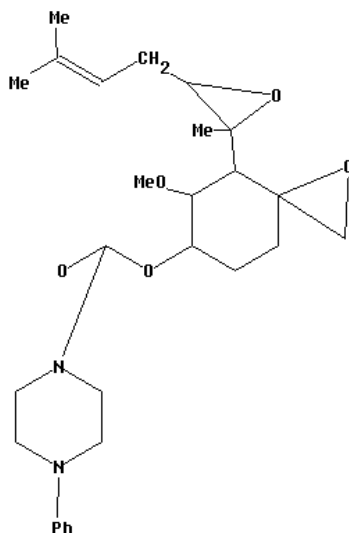
L7 ANSWER 36 OF 971 CAPLUS COPYRIGHT 2008 ACS on STN
   DUPLICATE 15
TI A concise synthesis of fumagillol
CS Skaggs Institute for Chemical Biology and Department of
   Chemistry, The Scripps Research Institute, La Jolla, CA,
   92037, USA

=> S L7 AND PATENT/DT
      .
      .
      .
L11 247 DUP REM L10 L8 (34 DUPLICATES REMOVED)
     ANSWERS '1-35' FROM FILE MARPAT
     ANSWERS '36-247' FROM FILE CAPLUS
```

Find published references, including patent claims, to the following phenyl piperidino analog of ovalicin.

1 Upload the structure.

=>  
Uploading...



L1 STRUCTURE UPLOADED

2 Conduct an exact sample (EXA SAM) structure search in CASLINK.

=> FILE CASLINK

=> S L1 EXA SAM

S L1 EXA SAM FILE=REGISTRY  
L2 0 SEA EXA SAM L1

S L2 CSS SAM FILE=MARPAT  
L3 0 SEA CSS SAM L1

3 Conduct an exact full structure search in CASLINK.

No hits were found for this specific structure in REGISTRY.

CASLINK automatically performs a closed structure search (CSS) in MARPAT. One answer is found.

=> S L1 EXA FULL

S L1 EXA FUL FILE=REGISTRY  
01  
L4 0 SEA EXA FUL L1

S L4 CSS FUL FILE=MARPAT  
L5 1 SEA CSS FUL L1

S L4 FILE=CAPLUS  
L6 0 FILE CAPLUS

DUP REM L5 L6  
L6 HAS NO ANSWERS  
L7 1 DUP REM L5 L6 (0 DUPLICATES REMOVED)  
ANSWER '1' FROM FILE MARPAT

4 Display the desired bibliographic data (title) and first hit Markush structure (FHIT) to view the retrieved structure. The hit structure fragments are highlighted.

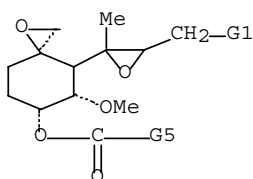
This relevant patent would not have been found if the exact search were conducted only in REGISTRY.

=> D TI FHIT

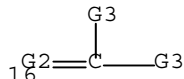
L7 ANSWER 1 OF 1 MARPAT COPYRIGHT 2008 ACS on STN

TI Preparation of O-acylfumagillol derivatives as angiogenesis inhibitors

MSTR 1B



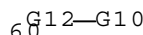
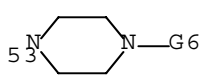
G1 = 16 / Bu-i (opt. substd. by 1 or more G7)



G2 = CH (opt. substd. by 1 or more G7)

G3 = Me (opt. substd. by 1 or more G7)

G5 = NH2 (opt. substd.) / 60 / heterocycle <containing 1 or more N, attached through 1 or more N> / (Examples: pyrrolidino / piperidino / morpholino / 53 / 57)



G6 = H / Me / Et / Ph

G7 = R / (Specifically claimed: halo / dialkylamino) / (Examples: OH / NH2 / alkylamino <containing 1-3 C> / heterocycle <containing 1 or more N, attached through 1 or more N, 5- to 6-membered monocyclic ring> (opt. substd.))

G10 = R / (Examples: alkyl <containing 1-6 C> / 42 / Ph / naphthyl / CPh)

•  
•  
•

### For more information

Enter HELP CASLINK at an arrow prompt in any of the CAS databases included in the CASLINK (or HCASLINK) cluster.



A division of the  
American Chemical Society

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