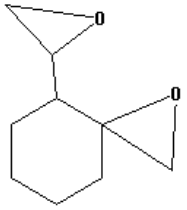
STN® Quick Reference Card

CASLINK for one-step structure searching in CAS REGISTRY℠, MARPAT®, and CAplus℠

Use the CASLINK database cluster for quick, easy, and cost-effective substance searching in REGISTRY, MARPAT, and CAplus. 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.



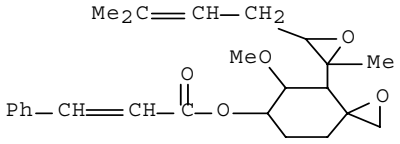
1 *Enter CASLINK. You are automatically connected to REGISTRY, MARPAT, and CAplus.*

2 *Upload the structure from STN Express® or STN® on the Web℠. 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
```



```
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).*

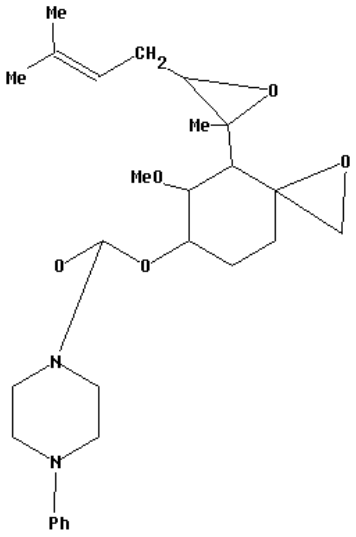
7 *Combine your structure search (L7) with text terms. The appropriate searches are automatically performed in the CASLINK databases. PATENT/DT limits the answers to patents.*

```
=> 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.

```
=> 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
```

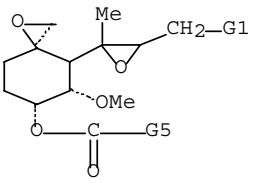
No hits were found for this specific structure in REGISTRY.

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

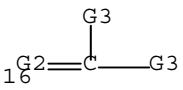
4 Display the desired bibliographic data (title) and first hit Markush structure (FHIT) to view the retrieved structure. The hit structure fragments are highlighted.

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

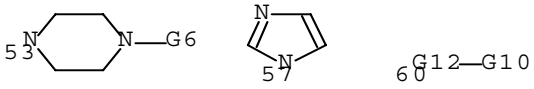
```
=> D TI FHIT

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 / COPh)
                    •
                    •
                    •
```

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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June 2008