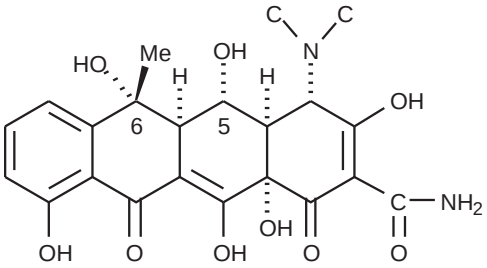
STN® Quick Reference Card

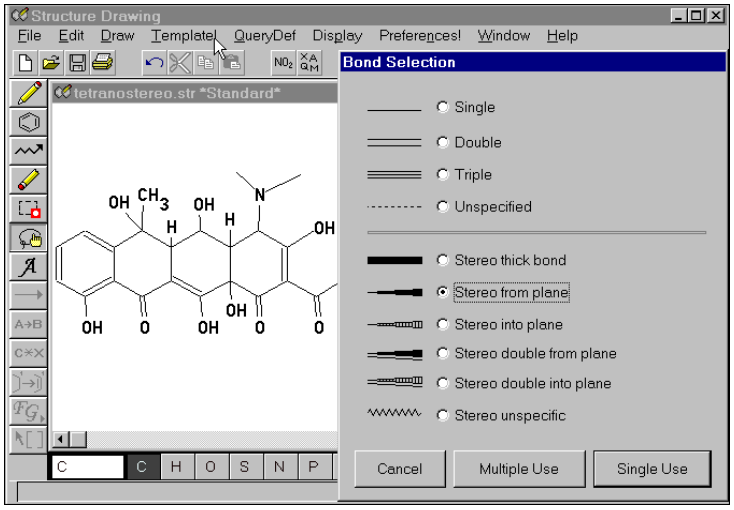
CAS REGISTRY℠: Stereoisomer searching

With StereoSearch, you can refine structure search results in REGISTRY to find just the isomers you need.

What 5-OH derivatives of the following stereoisomer of tetracycline exist?



*1 Build a stereo structure query and the equivalent flat structure. To create stereospecific bonds, select **Draw > Bond**. In the Bond Selection dialog box, select **Stereo from plane** or **Stereo into plane**. Click the appropriate bond.*



2 Log on to STN, enter REGISTRY, and upload the stereo structure (L1) and the equivalent flat structure query (L2).

3 Search the flat query (L2). Answers include all substances matching the query, including the stereospecific substances.

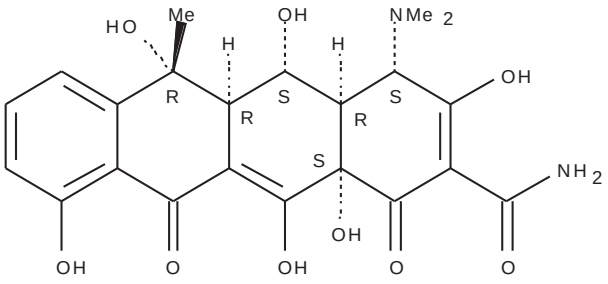
```
=> FILE REGISTRY
                •
                •
                •
L1    STRUCTURE UPLOADED

                •
                •
                •
L2    STRUCTURE UPLOADED

=> S L2 FULL
FULL SEARCH INITIATED  15:57:32   FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   2025 TO ITERATE
100.0% PROCESSED    2025 ITERATIONS
SEARCH TIME: 00.00.01

L3          341 SEA SSS FUL L2
```

4 *Search the stereo query (L1) using the answer set L3 from the search of the flat query as the subset. Answers include only the substances with the stereochemistry required.*

5 *Display one of the answers. The structure diagram includes stereo bonds and labels, as well as the statement that this is absolute stereochemistry.*

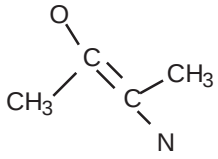
6 *Create another answer set that may have relevant stereoisomers that have not yet been converted for StereoSearch. Scan the answers for isomers of interest.*

```
=> S L1 SUBSET=L3 FUL
FULL SUBSET SEARCH INITIATED  15:59:18
FULL SUBSET SCREEN SEARCH COMPLETED -    341 TO ITERATE
100.0% PROCESSED     341 ITERATIONS
SEARCH TIME: 00.00.01

L4            2 SEA SUB=L3 SSS FUL L1

=> D
L4  ANSWER 1 OF 2  COPYRIGHT 2008 ACS
RN  65309-81-1  REGISTRY
CN  2-Naphthacenecarboxamide, 4-(dimethylamino)-1,4,4a,
    5,5a,6,11,12a-octahydro-3,5,6,10,12,12a-hexahydroxy-
    6-methyl-1,11-dioxo-,[4S-(4α, 4aα, 5α, 5aα,
    6α,12aα)]-
    (9CI)  (CA INDEX NAME)
FS  STEREOSEARCH
MF  C22 H24 N2 O9
LC  STN Files:   CA, CAplus, REAXYSFILE
    (*File contains numerically searchable property
    data)
Absolute stereochemistry.
```

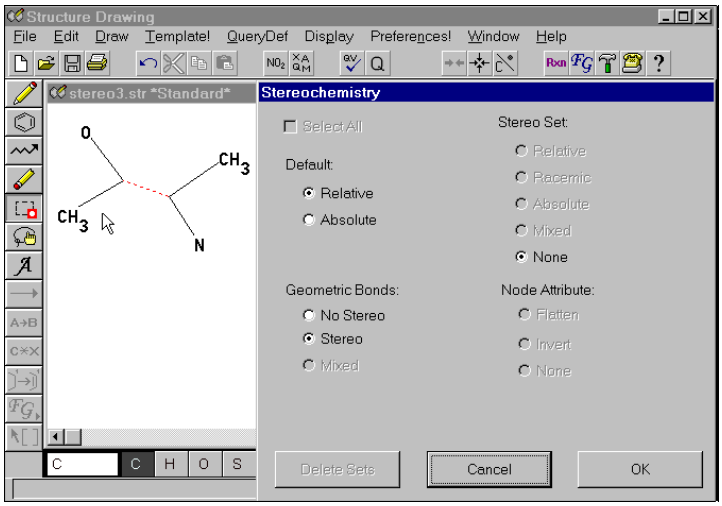



```
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> S L3 NOT STEREOSEARCH/FS
          3921626 STEREOSEARCH/FS
L5              61 L3 NOT STEREOSEARCH/FS

=> D SCAN
             .
             .
             .
```

How can I make substances with this substructure, including the stereospecific double bond?



1 *Build the stereo query. Draw the double bond with the geometry you want. Highlight the double bond with the* ***Selection Tool****. Select* ***QueryDef*** *>* ***Stereochemistry****. Under* ***Geometric Bonds****, select* ***Stereo****. Also build the equivalent flat structure.*



2 *Upload the stereo structure (L1) and the flat structure (L2).*

3 *Seach the flat structure (L2).*

4 *Search the stereo query using the answer set (L3) as the subset.*

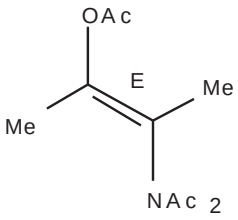
```
                •
                •
                •
L1    STRUCTURE UPLOADED

                •
                •
                •
L2    STRUCTURE UPLOADED

=> S L2 FUL
FULL SEARCH INITIATED  8:26:39
FULL SCREEN SEARCH COMPLETED -   72136 TO ITERATE
100.0% PROCESSED   72136 ITERATIONS
SEARCH TIME: 00.00.03

L3       34 SEA SSS FUL L2

=> S L1 SUB=L3 FUL
FULL SUBSET SEARCH INITIATED  8:27:03
FULL SUBSET SCREEN SEARCH COMPLETED -   34 TO ITERATE
100.0% PROCESSED   34 ITERATIONS    4 ANSWERS
SEARCH TIME: 00.00.01

L4       4 SEA SUB=L3 SSS FUL L1
```

5 *Enter CAplus[SM].*

6 *Search the REGISTRY answer set with /PREP to find preparative papers.*

7 *Display the title and the hit CAS Registry Numbers® with structures and CA index names.*

```
=> FIL CAPLUS

=> S L4/PREP
L5      2 L4/PREP

=> D TI HITSTR 2

L5  ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS
TI  Dakin-West reaction
IT  110788-53-9P
    RL: RCT (Reactant); SPN (Synthetic preparation);
        PREP (Preparation)
        (prepn. and hydrolysis of)
RN  110788-53-9 CAPLUS
CN  Acetamide, N-acetyl-N-[2-(acetyloxy)-1-methyl-1-
    propenyl]-, (E)-  (9CI) (CA INDEX NAME)

Double bond geometry as shown.
```



For more information

Refer to the STN Express® User Guide, available at www.cas.org.

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American Chemical Society

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