

In response to customer requests for more detailed information on new and enhanced system features, we have created STNotes. STNotes give you the in-depth technical details you need for efficient use of STN. We hope you find this information useful. Please let us know how we can continue to improve in meeting your technical information needs.

EXTEND Option in Structure Searching

The EXTEND option in structure searching provides easy access to the candidate structures that pass preliminary screening.

The EXTEND option in structure searching provides easy access to the candidate structure search results of the preliminary screening process.

This option may be especially useful when zero answers are retrieved in the final set of results.

Structure Searching with EXTEND

Structure searches on STN are conducted in two steps. In the screening step, the query structure is analyzed for the presence of various structural fragments and other structural characteristics associated with screens. Those screens are then used to identify candidate structures. In the iteration step, the candidate structures are examined, atom-by-atom and bond-by-bond, to ensure exact match of the query structure and the final structure search results.

With the EXTEND option, you can extend your structure search results to the candidate structures that passed the



screening part of the search. When EXTEND is active, an L-number is assigned not only to the final answers but also to the candidate search results. You can then easily view the candidate search results in the same way as you would view other search results.

To apply EXTEND to all subsequent structure searches in an online session, enter SET EXTEND ON at an arrow prompt. To permanently retain the ON setting, enter SET EXTEND ON PERM. When you SET EXTEND ON, the system automatically creates an L-number for the candidate search results.

You can also enter EXTEND in the SEARCH command. However, there is no prompt for this option. If you decide to use EXTEND after performing a search, that search has to be conducted again with the EXTEND option.

This enhancement is available in the structure-searchable files on STN.

Using the EXTEND option to view candidates from the screening portion of a structure search.

```
=> FILE REGISTRY

=> SET EXTEND ON PERM
SET COMMAND COMPLETED

=>
Uploading extend3.str

L1          STRUCTURE UPLOADED

=> D SDA
L1 HAS NO ANSWERS
L1          STR

      4 N
     / \
    3 C  5 C
   / \ / \
  8 F 2 C 1 C 6 C
   / \ / \
  9 F 7 C 1 C 10 C
           \
           O 12
           |
           S 11

NODE ATTRIBUTES:
NSPEC  IS R      AT  1
.
.
.

*****CONNECTIONS*****
NOD SYM  ROL  NOD/BON/SIT/STE  NOD/BON/SIT/STE  NOD/
                                     BON/SIT/STE
1 C          6 RN          2 RN
.
.
.

=> S L1
'EXTEND' DOES NOT APPLY TO SAMPLE SEARCHES

SAMPLE SEARCH INITIATED 16:17:18
SAMPLE SCREEN SEARCH COMPLETED -      1 TO ITERATE

100.0% PROCESSED          1 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                       BATCH   **COMPLETE**
PROJECTED ITERATIONS:   1 TO      80
PROJECTED ANSWERS:     0 TO      0

L2          0 SEA SSS SAM L1

=> S L1 FULL
FULL SEARCH INITIATED 16:17:31
L3          60 SEA SSS FUL L1 EXTEND

CANDIDATE STRUCTURE SEARCH COMPLETED - 60 TO ITERATE

100.0% PROCESSED          60 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01

L4          0 SEA SSS FUL L1
```

Enter REGISTRY.

Enter SET EXTEND ON PERM to always have an L-number assigned to the candidate search results.

Upload a structure. Select the option "Modifiable Queries" if you want to modify the structure online or view the complete structure data.

Display SDA to view all the structure data.

Conduct a sample search. EXTEND does not apply.

Conduct a full structure search. An L-number (L3) is assigned to the candidate search results.

When you enter DISPLAY HISTORY, EXTEND is included in the description of any L-number answer set created by EXTEND.

You may use any of the standard display formats, e.g., IDE, to view EXTEND-created L-numbers with candidate answers. In addition, the DISPLAY SCAN option is available for scanning the CA index name, structure, and the molecular formula of randomly selected answers.

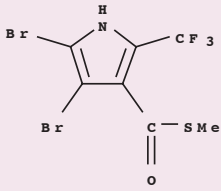
```

=> D HIS
FILE REGISTRY ENTERED...
                SET EXTEND ON PERM
L1              STRUCTURE UPLOADED
L2              0 S L1
L3              60 S L1 FULL EXTEND
L4              0 S L1 FULL

=> D SCAN L3

L3 60 ANSWERS  REGISTRY  COPYRIGHT 2004 ACS on STN
IN 1H-Pyrrole-3-carbothioic acid, 4,5-dibromo-2-
   (trifluoromethyl)-, S-methylester (9CI)
MF C7 H4 Br2 F3 N O S

```



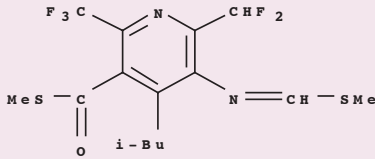
```

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

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

L3 60 ANSWERS  REGISTRY  COPYRIGHT 2004 ACS on STN
IN 3-Pyridinecarbothioic acid, 6-(difluoromethyl)-4-
   (2-methylpropyl)-5-[[methylthio)methylene]amino]-
   2-(trifluoromethyl)-, S-methyl ester (9CI)
MF C15 H17 F5 N2 O S2

```



```

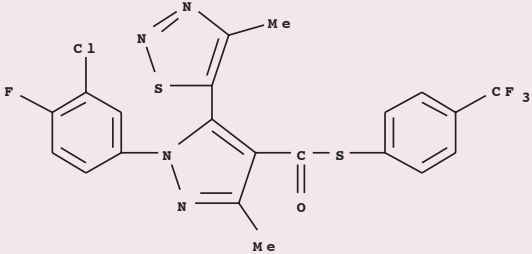
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

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

=> D L3 1-5

L3 ANSWER 1 OF 60  REGISTRY  COPYRIGHT 2004 ACS on STN
RN 264880-65-1  REGISTRY
CN 1H-Pyrazole-4-carbothioic acid, 1-(3-chloro-4-
   fluorophenyl)-3-methyl-5-(4-methyl-1,2,3-
   thiadiazol-5-yl)-, S-[4-(trifluoromethyl)phenyl]
   ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H13 Cl F4 N4 O S2
SR CAS Client Services

```



```

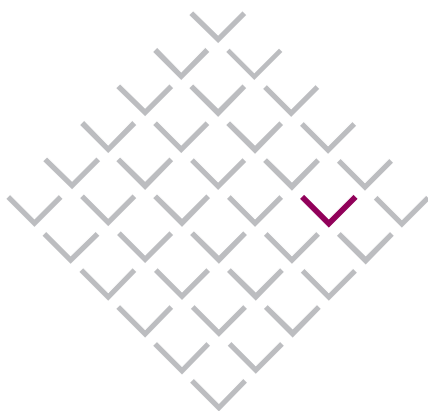
**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**
.
.
.

```

In D HIS, EXTEND is included with the L-number for the candidate search results.

You can SCAN the candidate structures from the screening part of the search.

You can view the CAS Registry Numbers for the candidate search results by using a display format, e.g., IDE, that includes the CAS Registry Number.



For more information

Enter HELP SET EXTEND at an arrow prompt for online information about the EXTEND option in structure searching.

For Web access to this STNote, visit:

www.cas.org/ONLINE/STN/STNOTES/stnotescover.html