# STN Express for the Macintosh, Version 3.12

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A survey of United Kingdom chemical searchers published in 1990 found that the preparation of a search strategy offline was considered to be particularly useful "...when a long complicated 'line' (which might be up to three lines), possibly containing several sets of parentheses, was involved."[1] STN Express is a front-end software package to assist with searching

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 QUERY NMR OR NQR OR N(W)M(W)R OR N(W)Q(W)R OR NOE OR N(W)O(W)E OR
OVERHAUSER  OR SPIN#(A)NUCLEAR OR (MAGNETIC OR  QUADR!POL?)(A)(RESONANCE#
OR RELAXATION#)

L1  QUE NMR OR NQR OR N(W)M(W)R OR N(W)Q(W)R OR NOE OR N(W)O(W)E OR OVER
        HAUSER OR SPIN#(A)NUCLEAR OR (MAGNETIC OR QUADR!POL?)(A)(RESONAN
        CE# OR RELAXATION#)
  .
   . [The portion of the search for publications of Malcolm H. Chisholm
     . which forms set L2 has been omitted from this example.]

=> s l1 and l2
        126174 NMR
          3695 NQR
        298159 N
         76055 M
         53417 R
          6608 N(W)M(W)R
        298159 N
          8598 Q
         53417 R
            27 N(W)Q(W)R
           723 NOE
        298159 N
        101401 O
         64993 E
             2 N(W)O(W)E
          3035 OVERHAUSER
        133769 SPIN#
        408084 NUCLEAR
         11034 SPIN#(A)NUCLEAR
        310272 MAGNETIC
         18575 QUADR!POL?
        214665 RESONANCE#
         63997 RELAXATION#
        119655 (MAGNETIC OR QUADR!POL?)(A)(RESONANCE# OR RELAXATION#)
L3          69 L1 AND L2

=> d bib ind

L3   ANSWER 1 OF 69  CA  COPYRIGHT 1994 ACS
AN   CA119(20):216227c  CA
TI   Mo4(H)3(O-Bu-tert)7(HNMe2): a novel hydrido cluster of molybdenum
AU   Chisholm, Malcolm H.; Huffman, John C.; Kramer, Keith S.; Streib,
     William E.
CS   Mol. Struct. Cent., Indiana Univ.
LO   Bloomington, IN 47405, USA
SO   J. Am. Chem. Soc., 115(21), 9866-7
SC   78-7 (Inorganic Chemicals and Reactions)
SX   75
DT   J
CO   JACSAT
IS   0002-7863
PY   1993
LA   Eng
OS   CJACS
KW   crystal structure molybdenum hydrido butoxo cluster; structure
     molybdenum amine hydrido butoxo cluster
IT   Crystal structure
     Molecular structure
     Nuclear  **magnetic**  **resonance**
        (of molybdenum amine hydrido butoxo cluster)
IT   Cluster compounds, coordinative
        (molybdenum, tetranuclear, hydrido diethylamine butoxo, prepn.
        and crystal structure of)
IT   150697-36-2P
        (prepn. and crystal structure of)
IT   150641-71-7P   150641-72-8P
        (prepn. of)
IT   84417-22-1
        (reaction of, with hydrogen and tert-butanol)
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**Figure 1.** Predefined search strategy in STN Express for a subject search on NMR in the CA File.

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L3   ANSWER 1 OF 50  COPYRIGHT 1994 ACS
RN   116049-04-8  LREGISTRY
CN   Carbamic acid,
[2-[1,3,3a,8,9,9a-hexahydro-3-hydroxy-5-methoxy-9a-

(phenylsulfonyl)phenanthro[4,5-bcd]furan-9b(2H)-yl]ethyl]methyl-,
     2-(trimethylsilyl)ethyl ester,
(3.alpha.,3a.beta.,9a.beta.,9b.beta.)-
     (.+-.)- (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Phenanthro[4,5-bcd]furan, carbamic acid deriv. (9CI)
FS   STEREOSEARCH
MF   C30 H41 N O7 S Si
SR   CA
LC   STN Files:   BEILSTEIN*, CA, CASREACT, CJACS
         (*File contains numerically searchable property data)
DES  *

Racemate.  One enantiomer shown.
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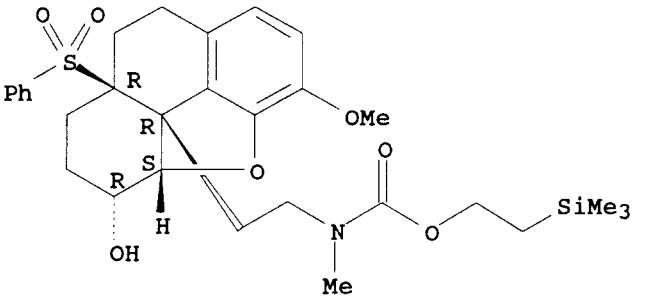


**Figure 2.** Example of search output downloaded from a structure search of the LRegistry File using STN Express.

bibliographic or chemical structure databases on the STN International and Questel systems. Since these are currently the only online systems that allow searching by chemical structure for all substances registered by Chemical Abstracts Service, the software should be very useful to chemists and chemical information specialists. The author of the 1990 paper found that even in 1987, end users in 33% of the 21 large companies surveyed were exploiting the ability of the software to create structures offline before going online to run a structure search.[2]

In version 3.12, we now have a much more mature version of the STN Express software than was available in 1987. (Version 3.2 of STN Express is due in early 1994.) Toward the end of 1993, the cost of the current version of STN Express was lowered from $460 to $199. (The 1991 price was $675.) The January 1994 issue of *STNews* carried the announcement that a range of pricing options would be available in 1994 for version 3.2 of the software. The new user will pay $248 for a single workstation application of STN Express. For $498, version 3.2 may be used simultaneously on a network by 1–5 users; for $996, up to 10 searchers may use the product on a server at the same time. It will also be possible to upgrade from the single-user license to the five-user option for $250, and two single-user licenses may be converted to a shared-use license for 1–5 concurrent users. Owners of single-user versions older than 3.2 will be required to pay the upgrade fee of $49 for each copy prior to selecting the last option. This more flexible pricing of STN Express is certainly welcome. However, the cost of the product is still considerably higher than the National Library of Medicine's Grateful Med front-end software, which currently sells for $29.95.

Setting up the software for modem use was relatively easy, but direct Internet connections required some assistance from network personnel, both at Indiana University and at STN. The vendor's login ID and password can be programmed into the software during the setup routine for automatic login, if desired.

Other STN Express features include guided search, chemical structure drawing, command files (scripts to run searches and to capture results to a file), and predefined search strategies. The main menu looks like the typical GUI menu for Windows or Macintosh applications. In addition to File and Edit choices, one finds Guided Search, Logon, Query, Results, Setup, and Help options.

"Guided Search" requires the choice of a broad subject category (physics, chemistry, energy, etc.), which is linked to a number of relevant databases. The user has the option of choosing the STN file as listed or choosing another file. There are over 50 predefined subject search strategies which can be used in a search session. These are undoubtedly more carefully constructed than strategies which novice or even many experienced searchers could construct. However, there is relatively little information on the predefined search strategies in either of the manuals, not even a full listing of the titles. This is a pity, because it is sometimes not easy to guess from the file names the subject of the strategy. Whereas one might figure in the IBM PC version that file CANMR.PSS is the strategy shown in Figure 1 for an NMR search on the CA File, I personally could not have deduced that CAALL.PSS is the strategy for "all analysis" documents in that database. The file naming conventions of the Macintosh solve that problem by calling the file "CA.all analysis".

The example illustrates how a predefined search strategy may be of use to a novice in retrieving articles that do not include in the indexing or title of the document the common acronym "NMR" yet are relevant for the search topic.

STN Express includes a superb structure-drawing component. The ability to prepare the structure query offline in STN Express obviates the need to learn the commands required on STN or Questel for constructing structures, but one must

still understand the types of searches that can be performed once connected to the systems. Chapter 6, "Structure Queries", in the *STN Expresss Action Guide* contains a concise description of the structure searching options on both systems. The structure drawing environment provides an opportunity to draw the molecule free hand or to utilize various predrawn structures and shortcut symbols. One can even import the structure from other graphics files, including ChemDraw and other popular chemical structure drawing programs. The "Draw" menu contains commands to choose bond value, atom and shortcut symbols, and system-defined or user-defined variables. Stereochemical bond depictions can be used but are treated as single bonds for searching in version 3.12. There is also a collection of predefined structures (templates), and more templates can be added by the user. Figure 2 shows a structure retrieved from a recent search of the LRegistry File using a predefined structure template as the search key. It is also possible to define reaction queries for uploading to STN reaction files. A query verification routine allows one to check structures for correctness and accuracy before saving them. Tautomeric systems are automatically translated into STN conventions.

STN Express is an excellent software package which is very highly recommended for both expert and novice searchers. The single greatest improvement this reviewer could hope for in the next revision is the inclusion of clearer instructions for Internet connections via STN Express.

## REFERENCES AND NOTES

(1) Smith, E. D. The Effects of New Technology on Information Work: Examples from Chemical Companies. *J. Librarianship* **1990**, *22* (3), 145–160; p 150.
(2) *Ibid.*, p 151.
(3) For a review of an earlier version of STN Express, see: Wolman, Y. STN Express (review). *J. Chem. Inf. Comput. Sci.* **1989**, *29*, 42–43.