LiqCryst 5.1

by

Volkmar Vill
in co-operation with Z. Galewski

User Manual

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The LiqCryst database series was created by Prof. Dr. Volkmar Vill.

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Introduction

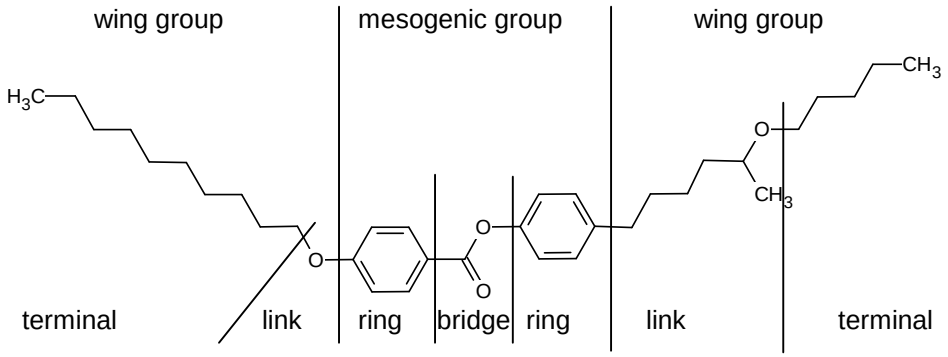
The term *liquid crystals* covers a wide area of systems. There are thousands of papers concerned with the chemical structures, physical properties and technical applications of liquid crystals. To give an easy access to this multitude of data, the literature has been screened and the database LiqCryst has been created.

LiqCryst contains the chemical structures and physical data of currently known thermotropic liquid crystals. Liquid crystals are found in numerous classes of substances, for example among biphenyls, soaps, cellulosics, elastomers, cholesterol esters, metallomesogens, combined polymers and lipids. For all these compounds (usually pure compounds, mixtures only in a few exceptional cases) the database documents all physical properties, that can be deduced from the chemical structure. These data include transition temperatures, enthalpies, elastic constants and other important physical properties.

Actually, the database contains entries for more than 92.000 compounds compiled from about 82.000 references including not only journals, books and monographs, but also patent literature, conference proceedings and Ph.D. theses. For every entry the consistency of the synthetic pathway, the structural formula, the name of the substances and the properties have been checked and evident typing errors have been corrected. Questionable data are pointed out by the **clearing parameter *un*** (for further explanation see Definitions, Parameters and Abbreviations) and additional texts. Obvious mistakes of authors have been corrected and marked with the **clearing parameter *chg***. In this case the original data can be found in the file for additional data. Outdated expressions have been replaced by modern terms, e.g. *Pocken-Phase* by **smectic phase**, smectic G and smectic H (*Gray-Nomenclature*) by smectic **H** and smectic **G** (*Demus-Nomenclature*). Part of the data have been published with Springer-Verlag in the Landolt-Börnstein series of Liquid Crystals.

Thus the database LiqCryst gives a complete documentation of information about currently known liquid crystals. The aim of LiqCryst is to use this knowledge to analyse and compare characteristics of liquid crystals. The conclusions drawn from this analysis give an insight into structure/property relationships and can be used to predict the physical properties of new compounds. Therefore LiqCryst is not only a topical work of reference, but an aid by which the user can, after careful evaluation of the stored data, methodically prepare new compounds that fit a given problem.

In principle all known chemical structures of liquid crystals can be represented by a simple model in which a compound is dissected into a few basic parts. In the case of a liquid crystal molecule this unit construction system (*LEGO*) results in a linear list of fragments. LiqCryst uses this principle to give the user an effective access to the information included in the database. Therefore each liquid crystalline compound can be put together from different fragments. An essential part is the main building block consisting of a **mesogenic group** and two **wing groups**. A **mesogenic group** consists of **rings** and **bridges**, whereas a **wing group** is composed of **links** and **terminal groups**. (For an explanation of specific expressions see Glossary).



The advantage of LiqCryst is that the search is possible not only by structures, but also by substructures defined by atoms and bonds and by substructures defined by a list of fragments (ring, bridge, link, terminal). Furthermore physical data such as transition temperatures, mesophases and transition ranges in their numerical values and chemical elements can be used as a search query. Even a search via trivial names, authors index and specific journals is possible.

Since physical properties and chemical structures are well defined by simple numbers, a statistical analysis of experimental data is possible. LiqCryst supplies a tool for the statistical analysis of the data using mean values and linear regression.

Multicomponent systems or lyotropic liquid crystals are not yet included in the database; nor are purely technical data, e.g. switching times. Future developments will enlarge the extent of the database, especially in the field of surfactants and non-linear optics.

This user manual has been written to be used alongside the liquid crystal database LiqCryst created by Volkmar Vill. The database aims to be an easily usable computerised system which enables the user to quickly and easily find further information on specific liquid crystals or liquid crystal types. The database is also designed to be not only a reference but to act as a tool for the user to prepare new compounds to fit a given problem. This is done by carrying out quick and simple searches through the copious data stored in the system. The data can be searched by using numerous different types of searches, which are specifically designed with reference to the types of data that may be available to the user.

This guide has been created to make it much easier for the first-time user to become acquainted with the database and make fast and easy use of this very powerful and potentially time saving tool.

A certain degree of knowledge on general computer use and liquid crystal science has been assumed in the writing of this manual. It is assumed that the user is fairly computer literate and has already experienced menu-based Windows packages such as Microsoft's 'Word' and 'Excel'. It is expected that the user can follow instructions, such as 'Click on...' and 'select...' during explanations of how the database is used. It is also expected that the user has a basic comprehension of the general behaviour of liquid crystals and the terminology used in liquid crystal research as these are not explained in these pages.

Advisory Board on Liquid Crystals

The advisory board of LiqCryst is a platform for the future development of LiqCryst. The board takes a constructively critical view of the database and makes suggestions for ways in which the database might be expanded and enhanced. Furthermore, the board members should be aware that the database itself has possibilities beyond its application in liquid crystals, and therefore be alive to possibilities for its expansion into other disciplines.

Member	**Function, Research Area**
Prof. Duncan Bruce, University of Exeter, UK	Head, Inorganic Chemistry
Prof. George Gray, Merck Ltd, UK	Organic Chemistry, Industry
Prof. Takashi Kato, University of Tokyo, Japan	Organic Chemistry, Polymers
Dr. Joseph Maclennan, University of Colorado, USA	Physics

File Storage

The data obtained from LiqCryst can be stored in a number of different file types depending on what kind of data has to be stored. The different file types are :

1) '.mol' files : Molecular drawings of liquid crystals.
2) '.sxc' files : Lists of liquid crystal compounds.
3) '.sxr' files : Lists of liquid crystal references.
4) '.sx2' files : Pairs of liquid crystal compounds obtained from a comparison.
5) '.sxp' files : Lists of selected properties of liquid crystal compounds.
6) '.lxl' files : List files

Content of the Database

The following lists sum up the scope of the information available through LiqCryst.

Data can be found on:

- thermotropic liquid crystals
  (e.g. calamitic, discotic, polymeric, amphiphilic liquid crystals)
- basic structural units for liquid crystalline compounds (e.g. biphenyl)
- compounds with mesogenic structures, which have not been studied as liquid crystals
- compounds with mesogenic structures, which do not show liquid-crystalline behaviour (dopants).

For all these compounds the following data have been collected:

- phase schemes
- structure-related measured data
  (e.g. dielectric constant, enthalpy, refraction index, density, spontaneous polarization)
- references to spectroscopy and X-ray studies
- others

The following search options are available:

- chemical substructures defined by their connectivity (atoms and bonds)
- chemical substructures defined as linear lists of fragments
- chemical substructures defined as text strings
- structural fragments (such as rings, bridges)
- ring types by specifying allowed sizes, elements present or absent, etc.
- phase sequences
- transition temperatures
- similarity (see Compare Menu)
- chemical elements / molecular formula
- physical data, searchable by numerical value, including ranges
- trivial names / IUPAC names
- specific characteristics (e.g. chiral, forked, acids)
- references in the form of authors, titles, form and year of the publication, ...

The following information is searchable by numerical values and usable for a statistical analysis:

- chemical structures as a sequence of structural fragments
- up to seven liquid crystalline phases
- melting points or glass temperatures, solid-solid transitions, recrystallisation temperatures
- literature references
- chemical elements, classifications according to chemical and physical properties

Information for bibliographical use:

- additional information on phase schemes
- alternative phase schemes
- pressure-dependent phase schemes
- transition enthalpies, heat capacities
- viscosities, elastic constants
- dielectricity constants, susceptibilities, dipol moments
- densities
- twisting powers, selective reflexions
- activation energies
- refraction indices
- pitches
- order parameters
- spontaneous polarizations, tilt angles
- layer sizes
- references to X-ray structures and crystal data, X-ray scattering
- neutron scattering
- spectroscopy (NMR, UV, IR and others)
- ultrasonic properties
- force field microscopy (AFM, STM)
- non-linear optics (SHG)
- stationary phases for gas chromatography
- LB films, FSLC films
- text indications

Many entries are hyperlinked to online-sources, so that it is easy to research in deeper details where the LiqCryst database itself can only offer a short extract. URLs to full papers are often listed for patents, and important journals.

Shortcut Buttons

A selection of shortcut buttons are available in the toolbar to help you use LiqCryst as quickly and efficiently as possible. These are :


Open a file


Save


Print


Copy text to clipboard


Copy picture to clipboard


Help


Extract the selected entries to a new window


Extract compounds


Extract properties


Extract references


Graphical display of data (homologous series / statistical analysis).

Execute an external hyperlink

These buttons are only active when the appropriate function can be undertaken.

Assignment of Keys and Mouse

F1	Help Key
F2	Edit Current Record (Advanced only)
F3	New Property (Advanced only)
Ctrl + F2	Edit current structure
Ctrl + T	Copy Text from active window
Ctrl + I	Copy Image / Structure from active window
Ctrl + V	Copy Text into active textbox
Ctrl + W	Copy Image / Structure into active window
Left mouse button	select an item or execute a (blue underlined) external hyperlink
Right mouse button	enlarge a screen display or show additional information (keep the button pressed)
Double click	open the clicked thingy in a new window
Left mouse button + ALT-key	drag and drop
Left mouse button + SHIFT-key	execute an external hyperlink
Right mouse button + CTRL-key	copy item to the clipboard

Use drag and drop to fill fragment pictures.

Information on Searching

Before commencing a search in LiqCryst it is important that you decide how precise you require the results to be, that is, whether you require information on just one molecule or all molecules sharing certain characteristics. These choices will also depend on the type of information that is available for the search to be based on. This will enable you to use the search that is most suited to your needs.

The types of searches can be split into three groups :

1) Searches for liquid crystals that are similar/identical in molecular structure.

2) Searches for liquid crystals that are similar/identical in properties.

3) Searches for bibliographical information (details of who wrote about a specific molecule first, in what publication and when).

1) Liquid Crystals that are Similar/Identical in Molecular Structure

It is possible to search for molecular structures of liquid crystals in a variety of ways depending on the preciseness of the search and the information available.

i) **By Fragments** :- This search allows you to build up a liquid crystal structure in the form of specific segments of the molecule as precisely as required. A display of all molecules that fit the criteria will be produced.

ii) **By Identifier** :- This is a fairly precise search that involves the input of specific liquid crystal data. These include trivial name, various registration numbers and molecular mass.

iii) **By Line Notation** :- This search involves entering an abbreviated molecular formula and is best used for simpler liquid crystal structures.

iv) **By Drawing** :- This search can be as precise or as indistinct as you require. It is based around the drawing of a liquid crystal molecule which can either be loaded from a '.Mol' file (that is a file produced from a compatible molecular drawing package with the suffix '.Mol') and adapted if required or can be drawn directly.

v) **By Classifications** :- A very general search in which groups of liquid crystals are searched for which obey certain pre-selected molecular classifications.

2) Liquid Crystals that are Similar/Identical in Properties

There are two main ways to search by properties and the chosen option would depend on the type of data that is to be search with.

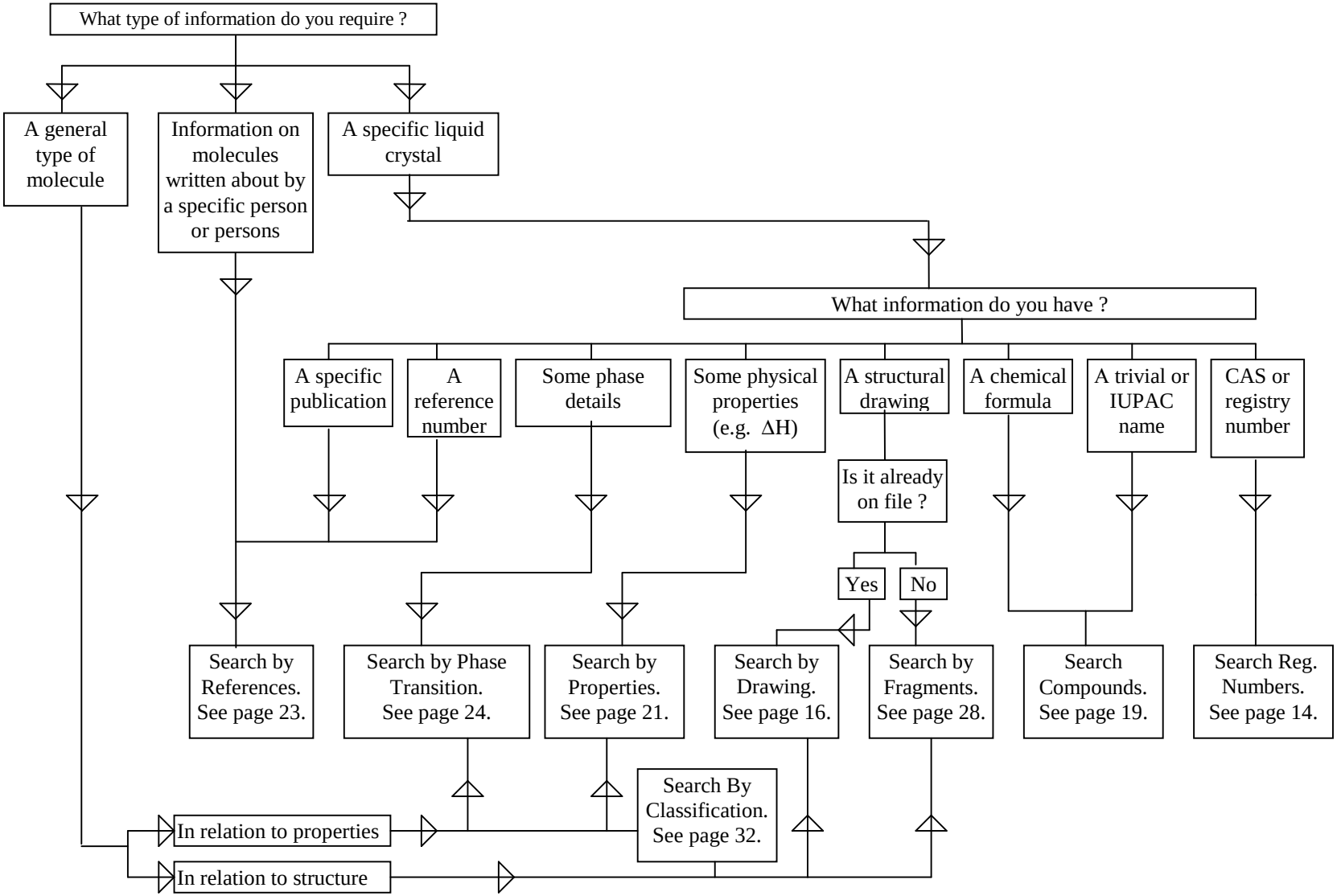
i) **By Mesophase** :- A search which can be carried out to produce liquid crystals with similar/identical phase behaviour.

ii) **By Generic Properties** :- This search will produce tables of molecules with similar physical properties (e.g. energy values ΔH or dielectrics ε etc.).

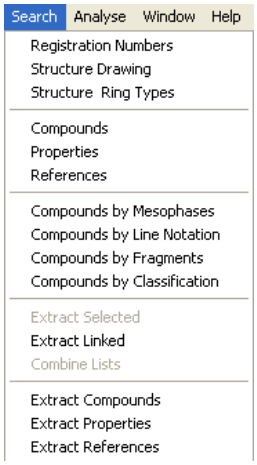
3) Bibliographic Information

All the liquid crystal molecules in the database have been referenced to all the publications they have appeared in. When carrying out any of the above searches, individual liquid crystals displayed will also have a reference number from which the bibliographic information is available.

i) **By Reference** :- with this search bibliographic information can be produced referring either to a specific reference number, a specific person or persons, a specific journal, title of publication, volume number, page and year of publication. It is also possible to limit the sources of data to specific types of publications.


What type of information do you require ?
A general type of molecule
Information on molecules written about by a specific person or persons
A specific liquid crystal
What information do you have ?
A specific publication
A reference number
Some phase details
Some physical properties (e.g. ΔH)
A structural drawing
A chemical formula
A trivial or IUPAC name
CAS or registry number
Is it already on file ?
Yes
No
Search by References. See page 23.
Search by Phase Transition. See page 24.
Search by Properties. See page 21.
Search by Drawing. See page 16.
Search by Fragments. See page 28.
Search Compounds. See page 19.
Search Reg. Numbers. See page 14.
Search By Classification. See page 32.
In relation to properties
In relation to structure

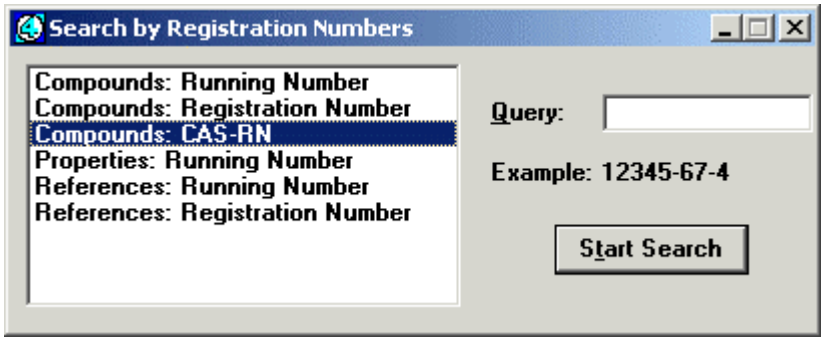
Using the Searches



Various search options are available from the LiqCryst Search - menu as shown on the graphics at the right.

Search Registration Numbers

This very simple search allows to look directly for registration numbers, or also running numbers of compounds, properties and references. It is also possible to specify *ranges* of numbers, e.g. to find all CAS-RN within a specific range.



It is possible to search by :

i) **Compound Running Number**: The sequential number of the molecule with respect to its position in the file. It is also possible to specifiy a range: e.g. 100-200.

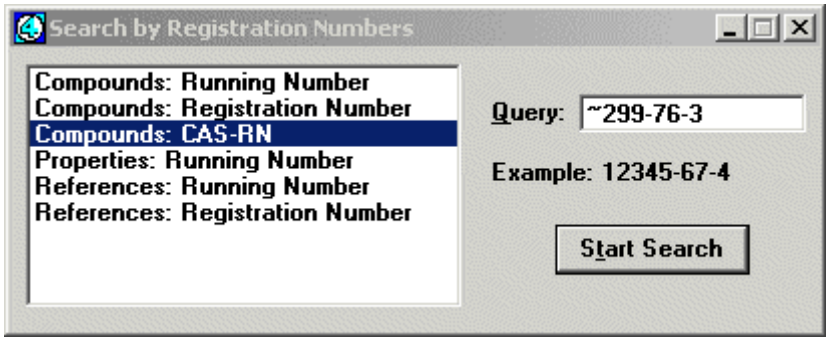
ii) **Compound Registration Number**: Each compound entered in the LiqCryst is assigned a permanent registration number that can be used for searching purposes as an identifier. Entering a known registration number leads directly to a display of that compound.

iii) **Compound CAS-RN**: The Chemical Abstracts Registration Number can be used to search for a limited number of compounds in LiqCryst. Entering "*" in the box provided will produce a list of all compounds with a known CAS-RN that are present in the database. An internal list of "deleted registry numbers" will translate older numbers to current one, so the search for the number 26227-73-6 will yield MBBA, although the CAS-RN of that ist now 97402-82-9.

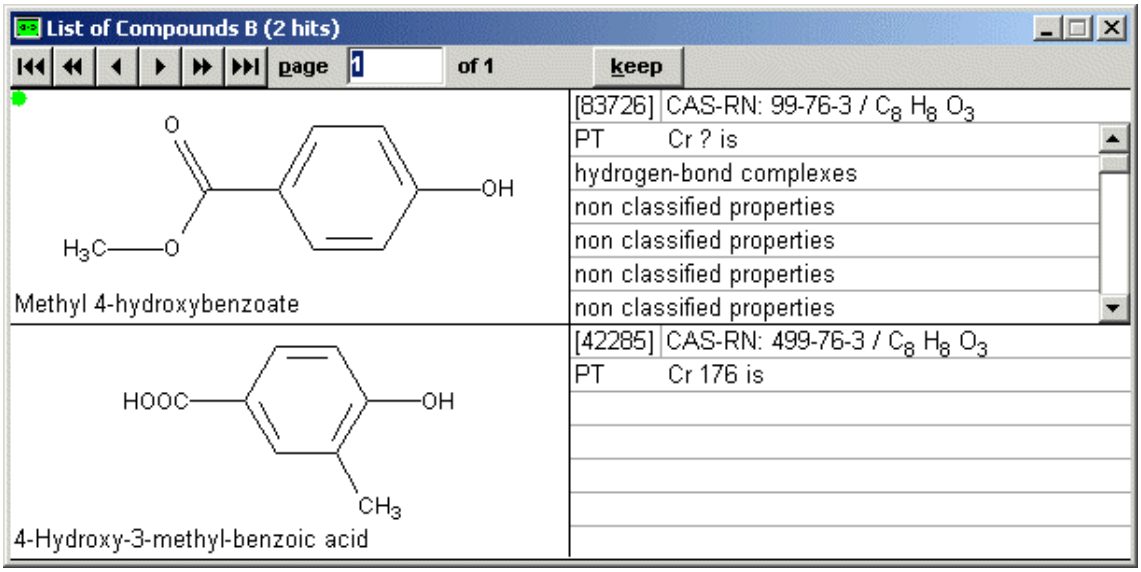
iv) **Reference Running Number**: The sequential number of the reference with respect to its position in the file. It is also possible to specifiy a range: e.g. 100-200.

v) **Reference Registration Number**: Each reference entered in the LiqCryst is assigned a permanent registration number that can be used for searching purposes as an identifier. Entering a known registration number leads directly to a display of that reference.

Example 1 Search CAS-RN as "fuzzy" search.



299-76-3 is an invalid CAS-RN (the checksum is not correct), however when the search is entered with the preceding tilde, then a fuzzy search will be done which allows up to one mistake in the number. The result of this search is shown below:



Found were the CAS-RN 99-76-3 (which has one digit less than the searched RN), and 499-76-3 (which has the first digit changed in comparison to the searched-for number). In many cases this allows the finding of a compound even if there are typographic errors.

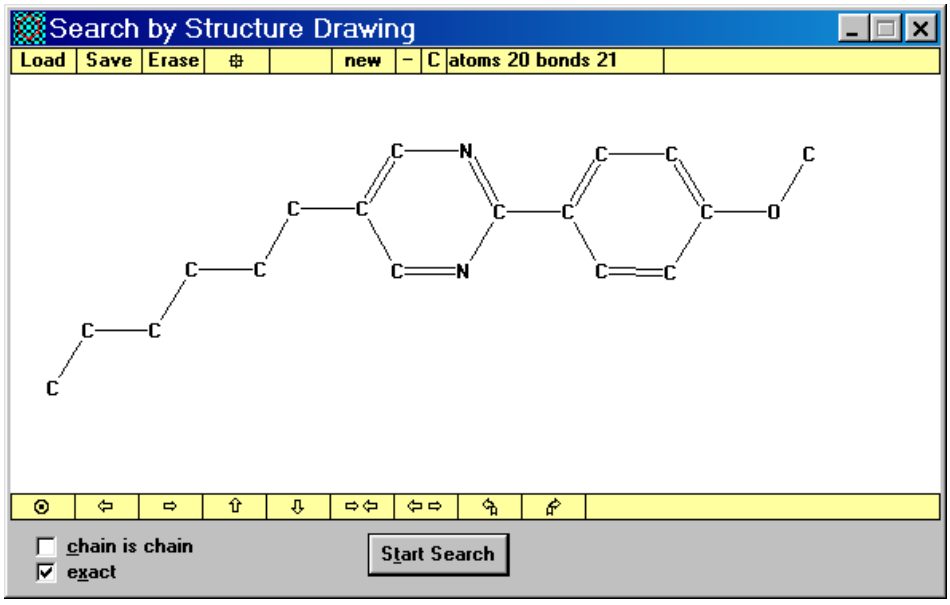
Search by Structure Drawing

This search is based around the drawing of a liquid crystal molecule. The search allows you to either edit a previously saved molecule or create a new one.

If you already have a drawing of the molecule you wish to search saved in an appropriate format (a .Mol file) then click on the <**Load**> button and select the correct drive and pathway and open your file in the normal way. Alternatively, paste a structure drawing to this window which has been copied from somewhere else (using the menu Edit → Paste Image, or the key-combination Shift + Ins).

A picture of your molecule should now have appeared in the window. A search can now be carried out on this molecule. If the molecule is incomplete and needs editing or you do not have a pre-drawn molecule then you can draw a structure.

Example 2 Search By Drawing



Editing the structure may be necessary if, for example, there is an unrecognised atom present in your molecule, as this will have to be replaced. The drawing options enables you to :

i) **Load a New Molecule:** This can be achieved by simply clicking on the **<Load>** button in the top left hand corner. This will however remove any drawing without saving.

ii) **Create Atoms and Bonds:** To create an atom the mouse is placed in the required area and the left mouse button is pressed. This will produce an atom which has been previously nominated (or otherwise a Carbon atom will be produced). A line will now be present which is attached to the newly positioned atom and the mouse pointer, this represents the bond from that atom. The line can either be attached to an existing atom (by clicking on the atom to be attached to), can be attached to a new atom (done simply by clicking the left mouse button at point at which you require the new atom) or alternatively if no bond is required the right mouse button is pressed and the line will removed.

iii) **Alter the Type of Atom or Bond:** To alter the type of atom before it is created there are a number of keyboard functions that can be used to change the nature of the next atom drawn. These are :

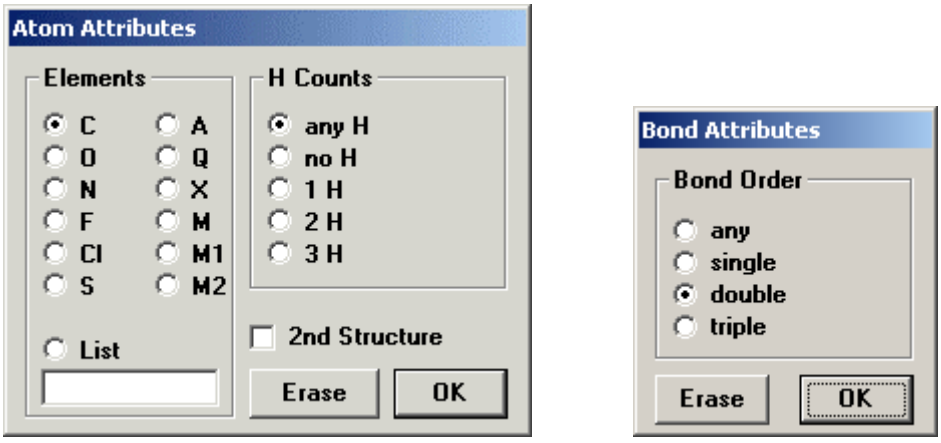
C, O, N, F, S, P, B, A, Q, X, M

By pressing one of these keys the next atom that is drawn will correspond to it (with A being any element except hydrogen, Q being any element except hydrogen and carbon, X being a Halogen, M being any metal). To alter the type of bond before it is drawn the following keyboard functions are available:

0, 1, 2, 3

This will alter the bond type to any bond, a single bond, a double bond or a triple bond respectively.

To alter an atom or bond that has already been drawn, place the mouse pointer over the item to be changed and click the right mouse button. You will now be able to choose the atom or bond you wish to change it to from the attributes windows :



The ‘atom attributes’ box allows you to either change the selected atom to a specific element or a list of elements. These lists are :

2nd Structure: Used for comparing compounds based on two substructures. See Compare by Drawing for more information

A : Any element other than H

Q : Any element other than H and C

X : Any halogen

M : Any metal

M1 : Any ionic metal (Li, Na, K, Rb, Cs, Mg, Ca, Sr, Ba)

M2 : Any metal except Li, Na, K, Rb, Cs, Mg, Ca, Sr, Ba

List : A list of elements, such as N, O and S are available

H Counts : Exact number of hydrogens. Should only be used for C, N and O. Use this option to avoid further substitution of the substructure at a specific position.

These letters are there so that searches can be carried out with groups of atoms, such as halogens, all being included rather than having to carry out different searches for each separate halogen.

Cycling through the type of bonds is possible by clicking the left mouse button on an existing bond and repeat that until the desired bond is found.

iv) **Erasing** : The **<Erase>** button in the top left hand corner of the drawing window can only be used to erase the entire molecule. To erase any particular atom or bond you must first activate the eraser by clicking on the symbol to the right of the Erase - button. This will turn black once activated and the mouse pointer will delete any atom or bond that is selected. To deactivate the eraser function simply click on the eraser box, which should return to its normal colour.

Eraser inactive:  Eraser active: 

v) **Moving the molecule** : The symbols on the bottom row will shift the molecule. The molecule can be move left, right, up and down, it can be rotated clockwise and anticlockwise around the centre of the editor window. It can be enlarged or decreased in size and it can be centered on the screen to give the best fit. All these can be accomplished by simply clicking on the symbol that corresponds to the appropriate motion.

vi) **Save the Drawing** : Choosing the save function saves the structure to file.

vii) **Templates :** All drawings of the program can be used as template for the editor, e.g. the drawing in the windows of single compounds, list of compounds, pairs of compounds, list of fragments. Move the mouse to the structures, which you want to use. Push the ALT-key and then the left mouse key. Keep the mouse key pressed and move the mouse pointer to the drawing area of the editor. Now release the mouse key. The selected structure will be drawn in the editor.

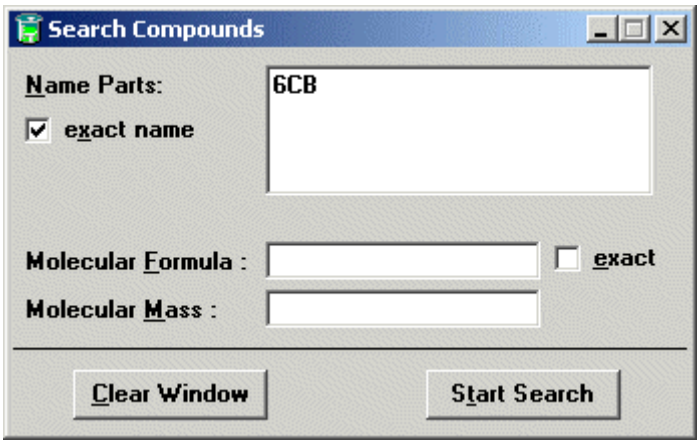
Rules for the **MOL files**:

- Please use only the following types of bonds: single, double, triple or unspecified and not complex wild cards, e.g. single or double bonds and single or aromatic bonds
- include all necessary hydrogens to prevent substitution by other groups

Options include "exact": search for an exact structure, i.e. further substitution of the molecule is not allowed; and "chain is chain": open alkyl-chains in the drawing can not be part of ring systems.

Search Compounds

This is the most general search for compounds, using names, molecular formula or mass as search parameters.



i) **Name Parts**: For this search you can query for (parts of) IUPAC-names of most of the compounds or also for exact trivial names (usually an abbreviation of a systematic name, e.g. MBBA, 6CB). To carry out the search simply enter the name in the box provided. The ‘exact name’ checkbox switches from searching of name-parts to searching of exact names. Name parts should be entered one per line. *The molecule name can be entered regardless of case.*

ii) **Molecular Formula**: This option allows you to choose the number of different types of atoms that are in the molecule that you are searching for. When the exact button is activated the resultant compound will only possess the atoms requested and in the ratio stated.

iii) **Molecular Mass** : This search can be used to provide a list of compounds either :

a) With the same molecular mass, e.g. 230
b) With a molecular mass within a specified range, e.g. 220-240
c) With a molecular mass above a specified weight, e.g. >220
d) With a molecular mass below a specified weight., e.g. <240

Example 3.1 Name Parts.

Search for all compounds which contain all the parts as “benzene”, as well as “chloro” AND “methyl” anywhere in any name, the order of appearance is irrelevant, hence one of the possible results is 1-(4-**Chloro**methyl-cyclohexyl)-4-fluoro-**benzene**

Example 3.2 Molecular Formula.

Search for all compounds which have exactly 20 carbon-atoms, 2 to 4 fluorine atoms and any number of hydrogens. The checkbox “exact” implies that no other elements may be present. So the molecular formula C_{20} H_{20} F_2 O_4 would *not* be present in the results, but it *would* be included if the checkbox “exact“ were unchecked

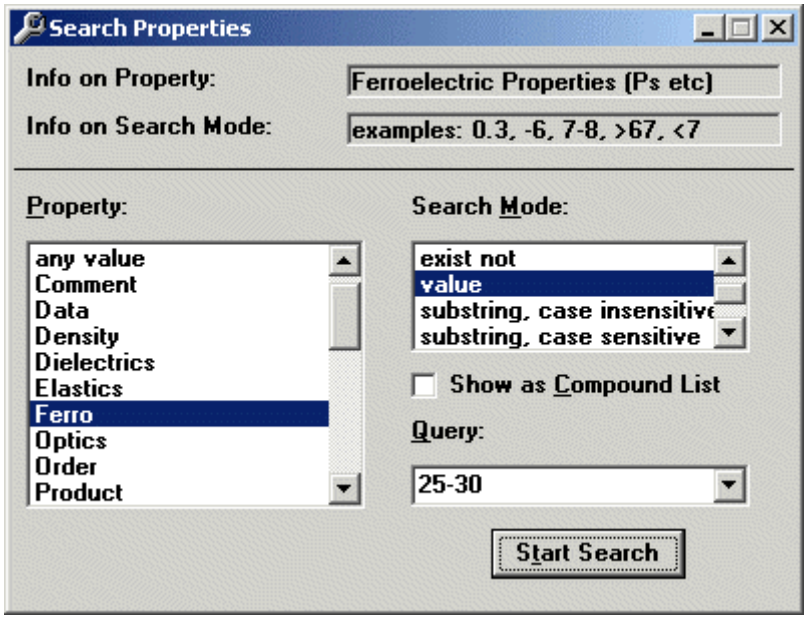
Example 3.3 Exact Mass.

Search for all compounds with a molecular mass of 263. This includes molecules with a mass of between 262.5 and 263.5

Please Note: When searching by molecular mass, there is always a variance of +/- 0.5 in the last digit allowed. 263 will be expanded to ”262.5 - 263.5” *and 262.2 will be expanded to* “262.15 - 262.25”

Search Properties

The property search allows you to enter physical information and receive data on liquid crystals which have physical properties corresponding to those entered. It is possible to search for numerical values, including ranges, as well as for substrings of properties.



This "Property" list window shows all property types which are present in the database. Now LiqCryst includes some physical properties as table too. These tables could be searched directly into the "Property" list window by the new fields "Table", "Table.Title" and "Table.Table". Additionally the fields "any text" and "any value" are present, which allow for searching across all different property types. Information on the selected property as well as examples how to formulate a query will always be given in the two lines on the top.

"any value" will search all properties which are of the type "Value" or "Text/Value". Currently all properties of LiqCryst are of the type Text/Value, i.e. the text shown is internally additionally interpreted as a numerical value, using the first number found in the textstring.

"any text" will search all properties which are of the type "Text" or "Text/Value".

The available Search Modes are:

"exist"
"exist multiple" (useful mainly when “Show as Compound List” is enabled)
"exist not"
: always available when a "regular" property is selected in the Property list (i.e. not for "any text" and "any value")

"value"
: available for properties which are of the type "value" or "text/value", currently all properties in LiqCryst are searchable as value.

"substring, case insensitive"
"substring, case sensitive"
"exact string case insensitive"
"exact string, case sensitive"
: Various methods to search for text-contents in a property. Always available, when the property is of the type "text" or "text/value", currently all properties in LiqCryst are searchable as text.

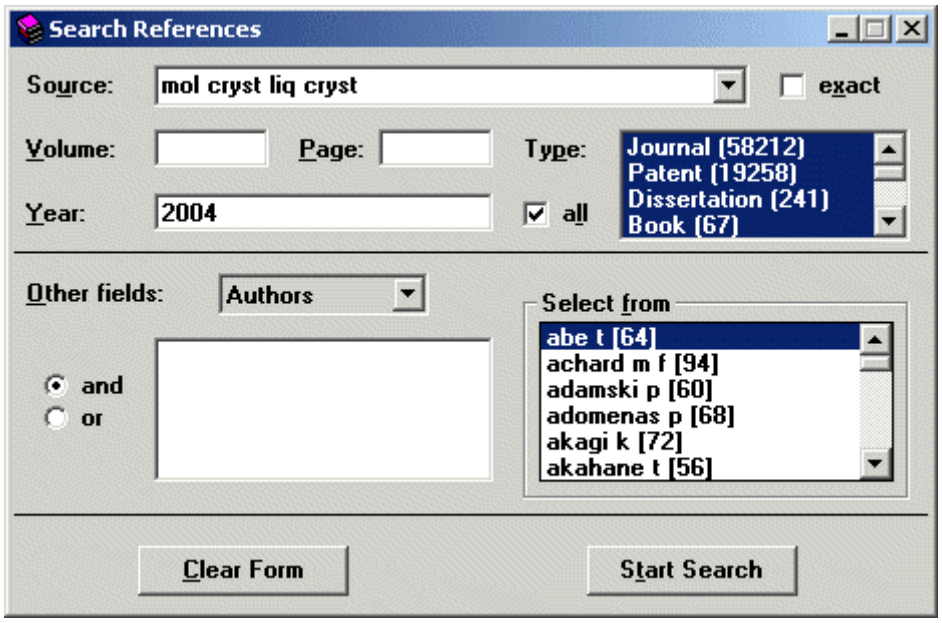
Greek letters in property texts have to be represented by their Latin equivalents, see appendix D.

Checkbox “Show as Compound List”:

When selected, the resulting display will not be as usual a list of properties, but instead all compounds which contain at least one of the found properties will be shown in a compound-list. The effect is the same as doing a normal property search followed by the function “Search → Extract Compounds”.

Search References

Once the reference search window has been selected then the data to be searched can be entered into the relevant box on the screen.



Elements of the Window:

i) **Source:** The combo box contains a list of all sources contained in the database, or when a maximum number of sources is exceeded, all the most frequent sources. Either choose one of the sources from the drop-down box, or type the full or partial title into the textbox directly. The text will be normalised, so that capitalisation and punctuation is ignored.

For example searching for the British Patent GB 1.603.075: The Country of the patent will be listed under "Source: brit uk patent", the Patent number has to be specified using "Other fields: [Search Terms]: PI 1.603.075"

ii) **Volume:** Give the volume number of the reference. Depending on the source this can be a purely numerical value, or something like "87A", e.g. for conference proceedings.

iii) **Page:** Give the starting page of the reference, or when known the range of pages of the reference. This is not a numerical search, but compares the given string with the "page" string of the stored references.

For example for the reference "Science 172, 1044-1046 (1971)" one can specify in the page field either "1044" or "1044-1046" but not "1040-1050", which would include the range of the searched-for reference as well.

A string search is used instead of a numerical search because some journals are using combinations of letters, arabic number and roman numbers to count pages.

iv) **Year:** Give the publication year of the reference, or a range of years.

For example for the reference "Science 172, 1044-1046 (1971)" one can specify in the year field "1971" or also "1970-1980". For looking from the year 1970 onward the search string must be "1970-" or vice versa from the year 1970 backwards "-1970" can be entered.

v) **Type**: Select in this listbox, which document types to allow for a search. In brackets is given the number of occurrences for each document type. Check the box "all", to allow all types of documents at once, this is the default.

vi) **Other fields:** All other reference fields can be searched singly or in combination via the textbox in the lower part. Each entry has to be specified as <Search Field> <Space> <Query> The "Search Field" can be "AU", "ED" and "KW" for Authors, Editors and Keywords, respectively. For these three, an index is generated, which allows to select entries from the listbox on the right, and to see the counter how often they are referenced. This box only will list the 100 auhtors with the highest amount of papers. Selecting an entry will copy it to the textbox on the left, but one can also type in search strings manually.

Other Search Fields that are available for searching include "PI" for Patent Information: "AI", Patent Application Number; "PRAI", Previous Application Number; "TI", title of publication.; “URL” for external hyperlinks

vii) "**And/Or**": Choose whether the entries made in the textbox "Other Fields" in the lower part have to be matched all in one source ("and") or if only any one of the given entries needs to occur in the reference found ("or"). Even if "or" is specified, all entries made in the upper part of the window have to be matched.

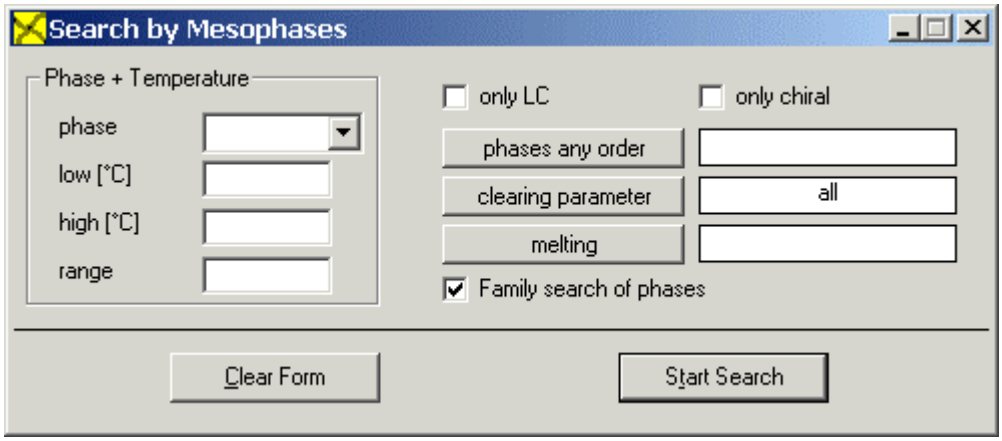
The compounds can then be found using the extract function from the edit menu.

Search Compounds by Mesophase

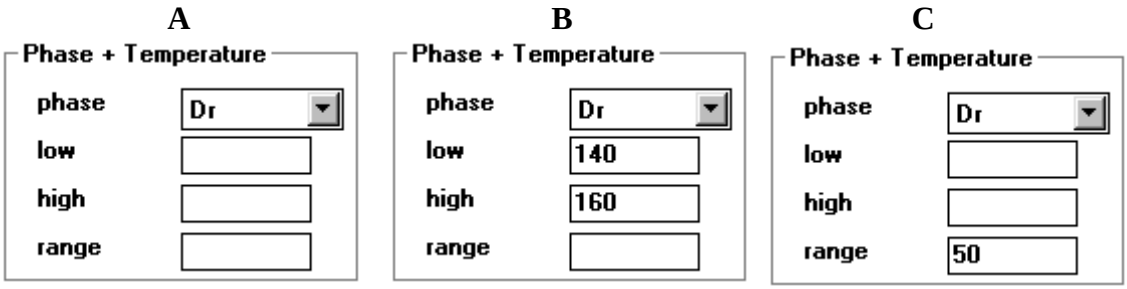
A ‘**Search by Mesophase**’ is usually based around specific phase behaviour with the result being a list of compounds which all have similar phase transitions. The search can be based around a specific phase with or without temperature boundaries applied (these can be in the form of a temperature range and/or high and low temperature values). A search can also be done on the phase sequence, clearing parameter, and melting or glass point or reference. These options can all be used individually to search

with, or in any combination to narrow the search. To make the search more specific there are also checkboxes available to further specify the search by making all molecules found real liquid crystals and/or chiral if requested. A melting point can also be included in the search.

There is also an option to include a family search of phases. This means that if, for example you wish to examine the smectic phase then ticking the family search box will include all types of smectic phases.



Example 4.1 Searching by Phase Transitions



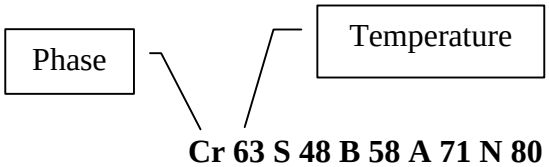
A : Search for all compounds which exhibit the Dr phase

B : Search for all compounds which exhibit the Dr phase at temperatures of at least 140°C and 160°C

C : Search for all compounds which exhibit a Dr phase with a temperature range greater than 50°C

Example 4.2 Searching by exact Phase Sequence

For the following phase sequence :



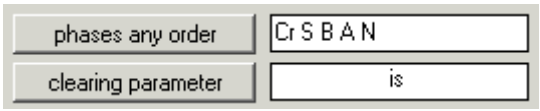
Cr 63 S 48 B 58 A 71 N 80 is

The phases are entered in temperature order with a space between each phase identifier:

The search done in this way will lead to 19 compounds, which have this exact appaearence of phases. (Family search deactivated)

Example 4.3 Searching by Phases in any Order

A slightly more fuzzy search allows finding of phases where the order is not exactly known.



This variant of the search will lead to 36 hits, where the phases do not follow directly each other or are in a different order, so for example the following phase scheme will be also among the results.

Cr 56 S 26 B 34.9 C 63.8 A 74.1 N 85.1 is

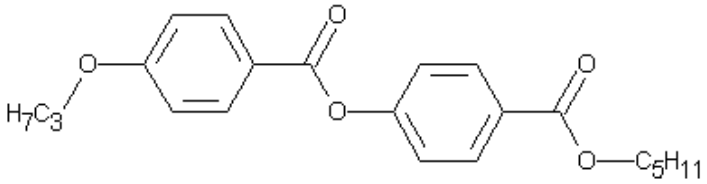
The search can be made even more fuzzy, when the checkbox “family search of phases” is checked, leading to 39 and 158 hits, respectively.

Search by Line Notation

To search by line notation you must have the molecule you wish to search for available in the form of an empirical formula. This can be done by selecting the ‘**Search String**’ box. You should now see the cursor flashing and you can begin to enter the formula. When entering a string you should group together the carbon chains and separate all links, chains and bridges with the relevant bond. There is also a checkbox present in the window marked ‘**compare with**’. This function is for use when comparing structurally similar molecules and so can be ignored for the moment (see later). Once the string has been entered you can now press the **<Start search>** button. You must take care when entering strings for this search as it can be very easy to enter substituents incorrectly and thereby produce a negative result. It is for this reason that a number of abbreviations for more complex substructures are available for use, and these are listed in Appendix G.

Example 5 Search By Line Notation

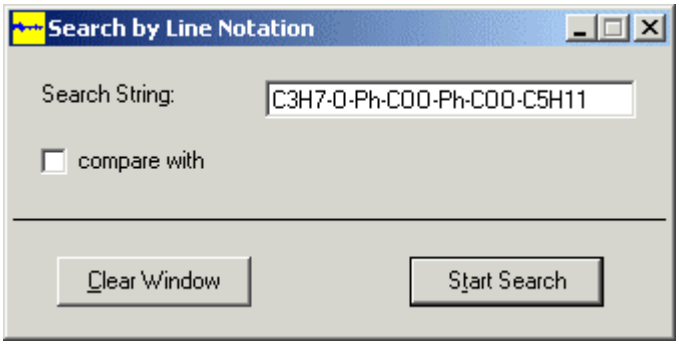
To search for the molecule :



It must first be converted to the form of line notation :

C_3H_7-O-Ph-COO-Ph-COO-C_5H_{11}

This can now be entered as the search string.



The symbols '|' and '**?**' can also be used in searches. These are very useful in either increasing or decreasing the preciseness of the search. By entering '|' on a search string the end of the string is defined, meaning that no further substituents will be added to that end of the string. By using '**?**' in the string, this means that any or no group can appear in the position it is entered in the formula. For example, entering the string :

C_3H_7-O-Ph-?-Ph-COO-C_5H_{11}

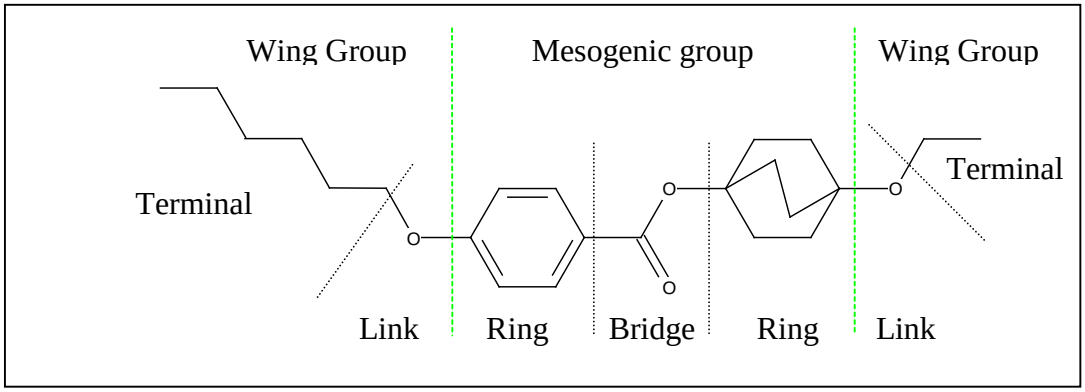
will display all molecules which fit the formula but have any or no bridging group between the two phenyl groups.

Further examples of the use of these symbols are given in Appendix G.

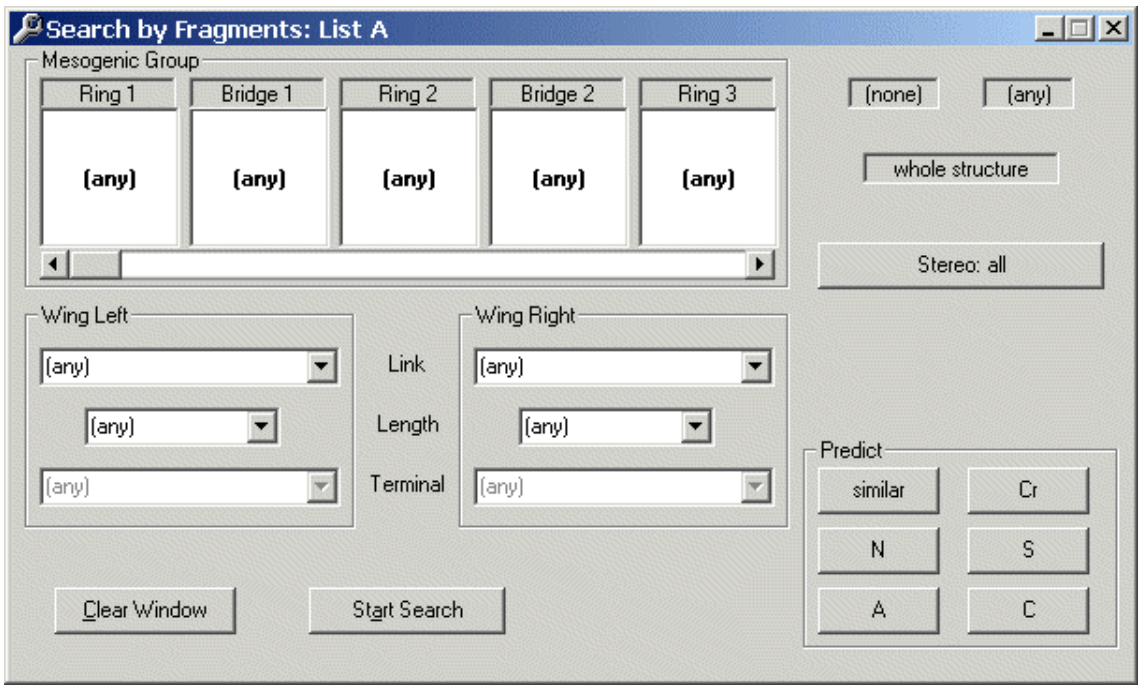
Search by Fragments

This involves the creation of a chemical substructure by choosing a structure for the various sections of the molecule. The 2-D structural formula that is created is split into a mesogenic group consisting of the main ring system and the bridges that are used between the rings if more than one ring group is present, and two wing groups which are at either side of the mesogenic group and consist of a terminal (often an alkyl chain) and a link which joins the terminal group to the mesogenic group.

Example 6 Mesogenic and wing groups



To create a substructure such as the one shown above, choose the '**Compounds by Fragments**' option from the '**search**' menu. You should then be faced with a display as shown below.



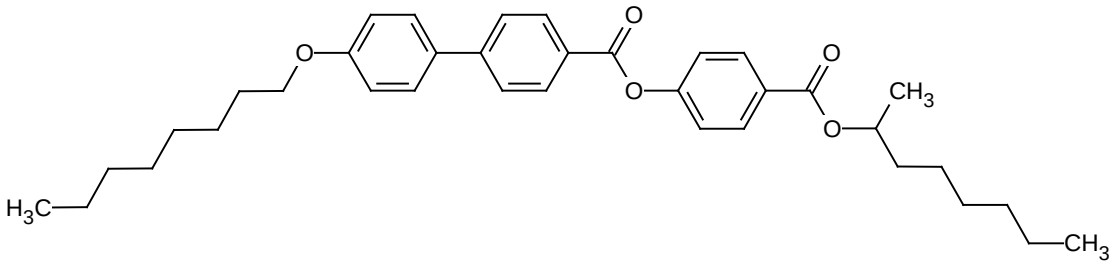
You should now enter in the spaces provided the types of groups that are present in the liquid crystal that you are searching for. For the mesogenic group this can be achieved most easily by double clicking on the box that corresponds to the position that the group is to be placed in. This will result in the appearance of a pop-up window that

contains a pictorial display of the rings or bridges that can be used. To choose a ring, simply position the mouse pointer over the ring, hold down the left mouse button and move the pointer over the corresponding ring box. Release the mouse button to 'drop' the ring in the box. It is also possible to enter a short description of the desired ring or bridge rather than the molecular structure by clicking on the box title and entering the name. If no ring or bridge is required then insert '**none**' into the box. To choose the appropriate wing groups the drop down menus can be used by clicking on the down arrow to show the available groups. The search can also be made less specific by choosing 'any' for one or more of the sections.

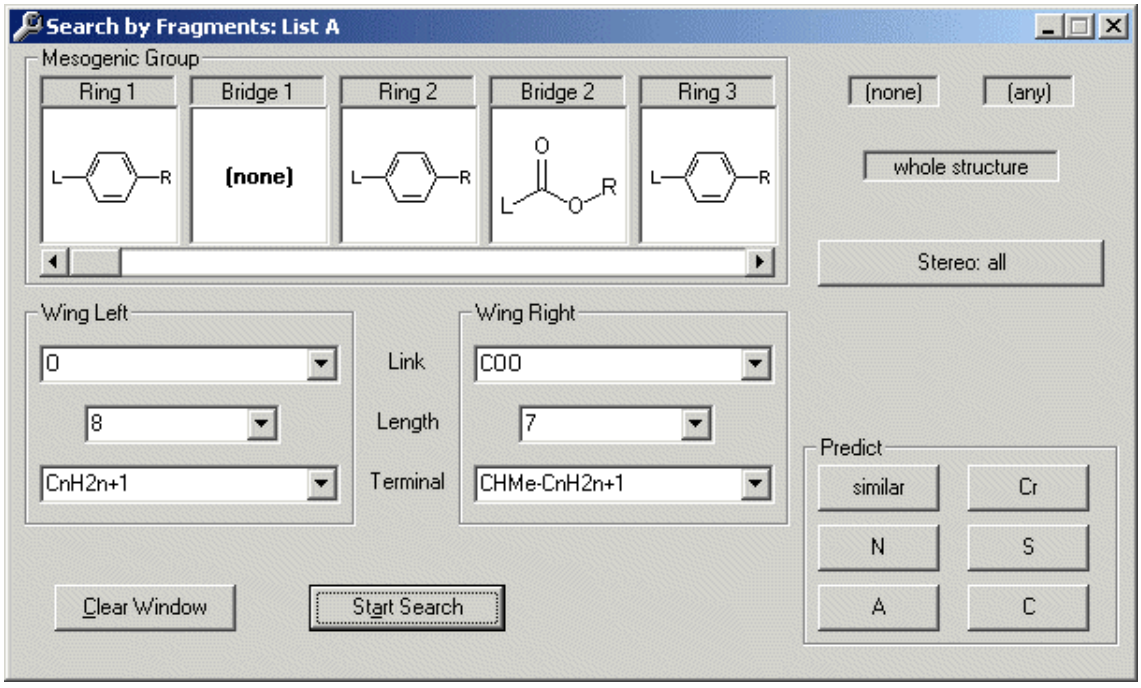
To limit the number of rings that appear in the structure place '**none**' in the adjacent box. For instance, if you require molecules with no more than 3 rings place '**none**' in ring 4. This is down by holding down the left mouse - button over the box "none" at the right of the search window and then dragging and dropping the "none" into the desired fragment - box. (e.g. ring or bridge)

Example 7.1 Search by Fragments

To search for the structure :



The following details should be entered :

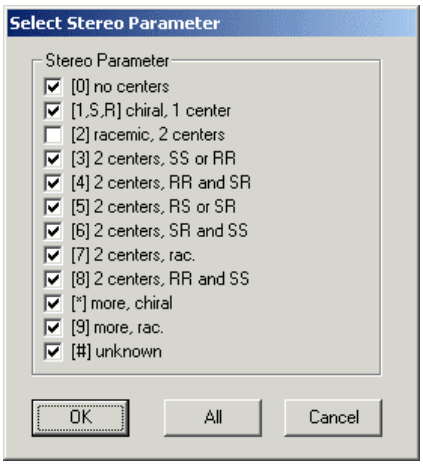


Once the <**Start Search**> button has been pressed a successful search should lead you to a table of compounds which fit the criteria of the search. In this case there are two molecules which are produced. This is simply because the molecule has been entered twice due to different stereochemistry and data.

The scope of the search can be widened by changing any of the data entered to ‘any’ and thereby producing a range of similar molecules.

The box marked ‘stereo : …’ is made available to narrow down the search by specifying the type of stereochemistry that is required in the target molecule.

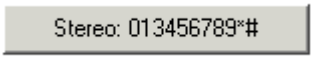
Example 7.2 Stereo Parameters in Fragment Searching



The selction button shows the currently selected parameters which will be included in the search.

All Parameters selected

Parameters selected in this example



In the previous example 2 molecules were found due to their different stereochemistry. By using the ‘stereo’ option the search can be used to produce only the chiral (R or S) enantiomer rather than the racemate.

In this example the option to show all chiral molecules with two centres is the only one not selected, which results in only one of the two molecules produced in the previous example being displayed.

There is also a ‘whole structure’ box available in this window. This box accepts full structures of molecules that have been produced as part of a search. This is done by clicking on the display of the molecule required and ‘dropping’ it in the ‘whole structure’ box. The structure can now be used as a base to search for structurally similar compounds.

Examples of more complex liquid crystal structures and how to search for them can be found in Appendix A and a list of abbreviations for stereochemistry can be found in Appendix E .

Example 7.3 Fragmentation of Wing Groups into Links and Terminal Groups

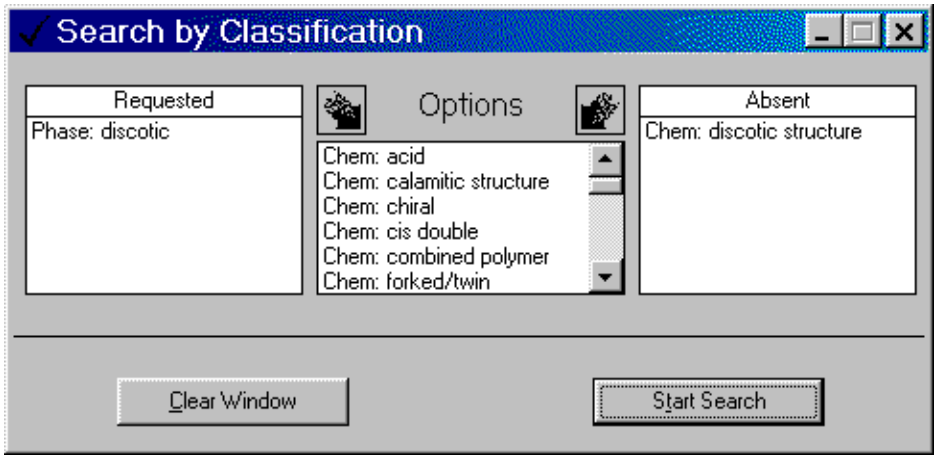
wing group	**link**	**terminal group**
-CN	**-**	-CN
-OCN	**-O-**	-CN
-NCS	**-**	-NCS
		e.g. only single bonded hetero atoms act as links
$-CH_3$	**-**	$-CH_3$
$-O-CH_2-CH=CH_2$	**-O-**	$-CH_2-CH=CH_2$
$-OOC-CH_3$	**-OOC-**	$-CH_3$
$-O-CHMe-C_6H_{13}$	**-O-**	$-CHMe-C_6H_{13}$
$-CHF-C_3H_7$	**-**	$-CHF-C_3H_7$
		mono subst. chains have their own type of terminal
$-CF_2-C_3H_7$	**-CF_2-**	$-C_3H_7$
		di subst. chains do not have their own type of terminal
$-OOC-CHF-CHMe-C_2H_5$	**-OOC-CHF-**	$-CHMe-C_2H_5$
		longest possible terminal group
$-OOC-CH=CH_2$	**-OOC-**	$-CH=CH_2$
		part of the $CH=CH-C_n$ homologous series
$-OOC-CMe=CH_2$	**-OOC-CMe=CH-**	-H

Search Compounds by Classification

A '**Search by Classification**' involves the selection of key features of liquid crystal molecules. These features can be requested or rejected to ensure that either all (if requested) or none (if rejected) of the molecules found in the search have the selected characteristic.

Example 8 Search By Classification

To search for liquid crystals that undergo a discotic phase but do not have discotic structure :



To narrow down the range of the search it is suggested that one or more items are rejected for each search that is attempted.
A list of explanations of the classifications can be found in Appendix B.

Combine Lists

The combine lists search, including lists of pairs, allows you to manipulate previously saved searches. This can be done in three ways :

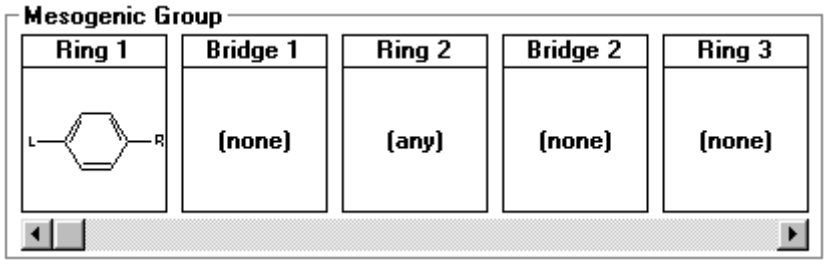
1) add all: Creates a list that contains the sum of all the selected lists.
2) intersection: Creates a list of common entries in all the selected lists.
3) substract: Creates a list of compounds that are present in the first selected file but are not in any of the other files.
4) invert list: Shows all entries in the database other than those in the selected file.

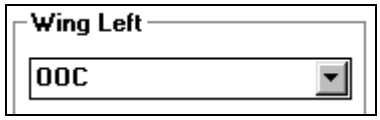
For all options other than 'invert list' it is necessary that more than one list is opened at the same time.

Example 9 Combine Lists

For the following examples consider 3 searches that have been completed and saved.

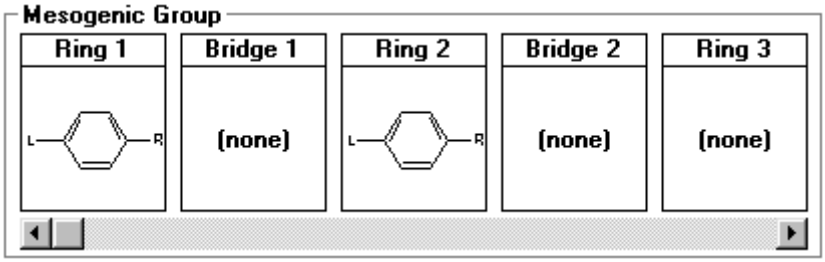
The first searched for all liquid crystals with consisting of an unbridged, two ring system with one of the rings being benzene and the other unspecified. The link to the left side was also specified as a carboxy group.





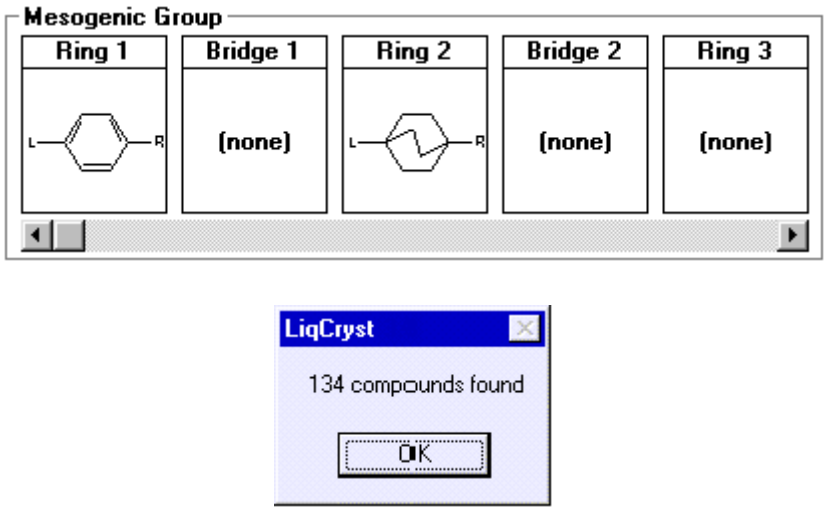
All other areas unspecified

The second searched for compounds containing a biphenyl group :



All other areas unspecified

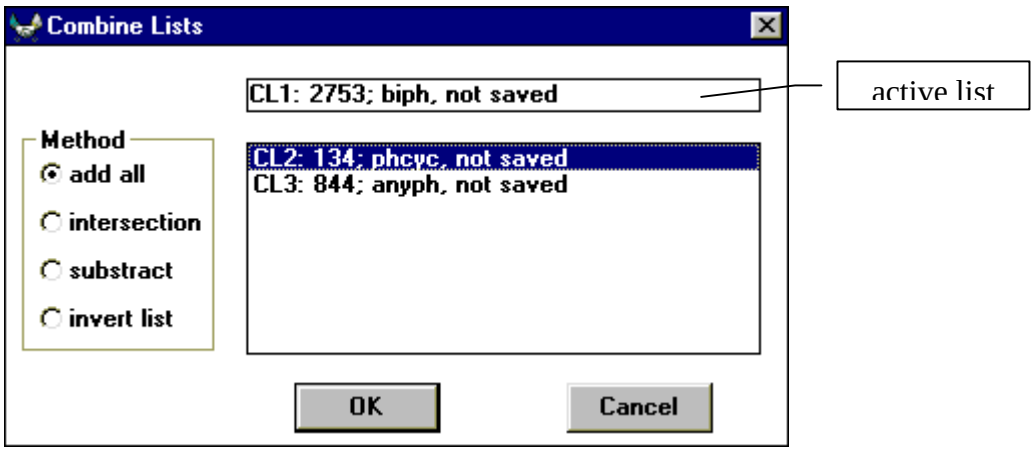
and the third searched for all compounds with the phenyl-bicyclooctane ring system.



The three searches were saved as ‘anyph’, ‘biph’ and ‘phcyc’ respectively. After each search is completed click on the ‘**keep**’ box to keep the molecular lists active.

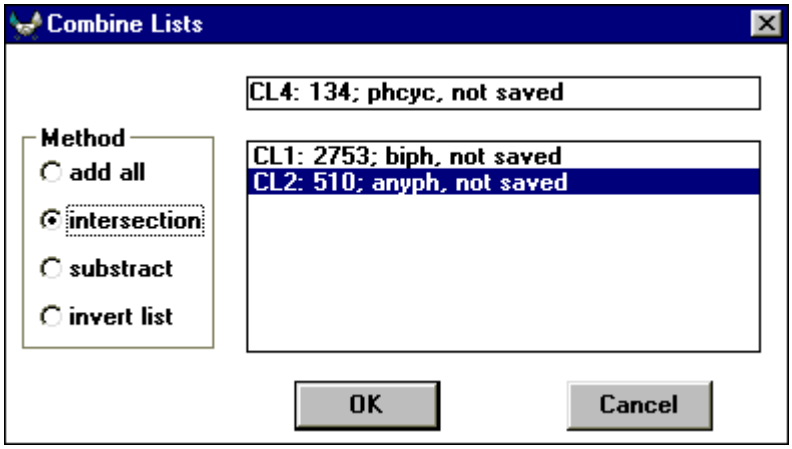
Example 9.1 Add All

This will produce tables of the contents of all selected files. So, to produce all molecules with the biphenyl and phenyl-bicyclooctane ring systems described above, choose ‘**add all**’ from the ‘**Method**’ section and click on the files to select them. The last active window becomes the main list and is separated at the top of the window lists (this is done by clicking on the list - window you wish to appear first in the "combine list" - window). To select more than one window hold down the shift key.



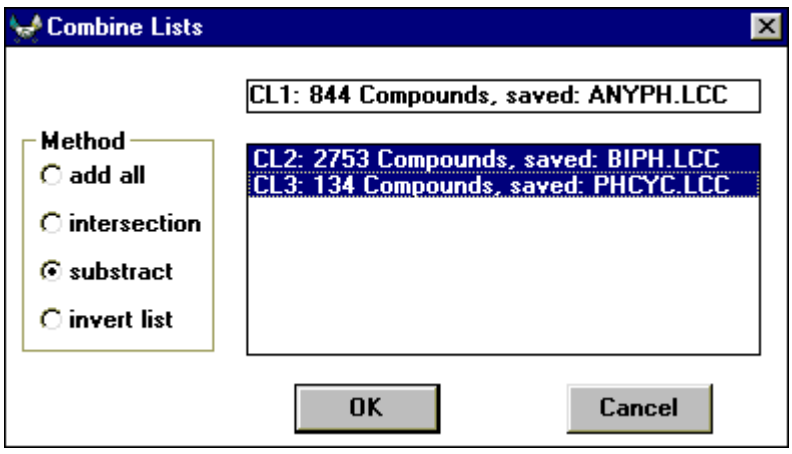
Example 9.2 Intersection

This will produce common molecules in the selected files, so the result should be tables of molecules with the phenyl-bicyclooctane ring system with a carboxy link.



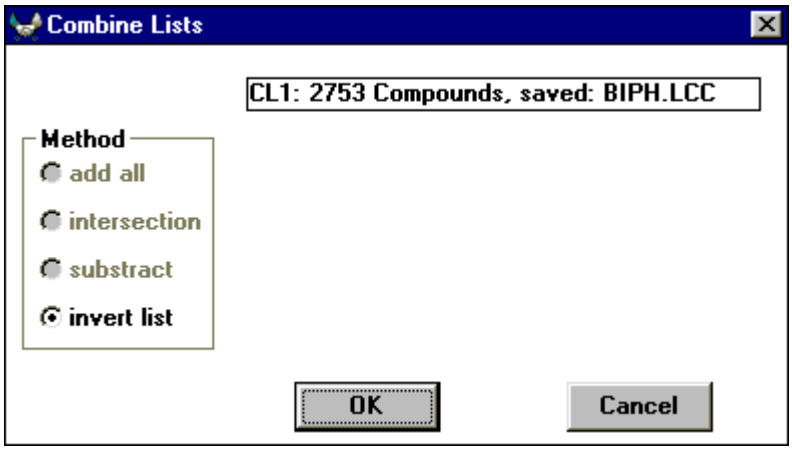
Example 9.3 Substract

To produce molecules with two rings and a -COO link, but not biphenyl or phenyl-cyclooctane, the active file is selected as ‘anyph’ but it can be any. The other files created are then highlighted and the <**OK**> button pressed. This will produce tables of molecules which are present in the ‘anyph’ file but not in either the ‘biph’ or ‘phcyc’ files.



Example 9.4 Invert list

Choosing the list of compounds that contain the biphenyl group and inverting will provide a list of all the liquid crystal compounds that do not have the biphenyl group.

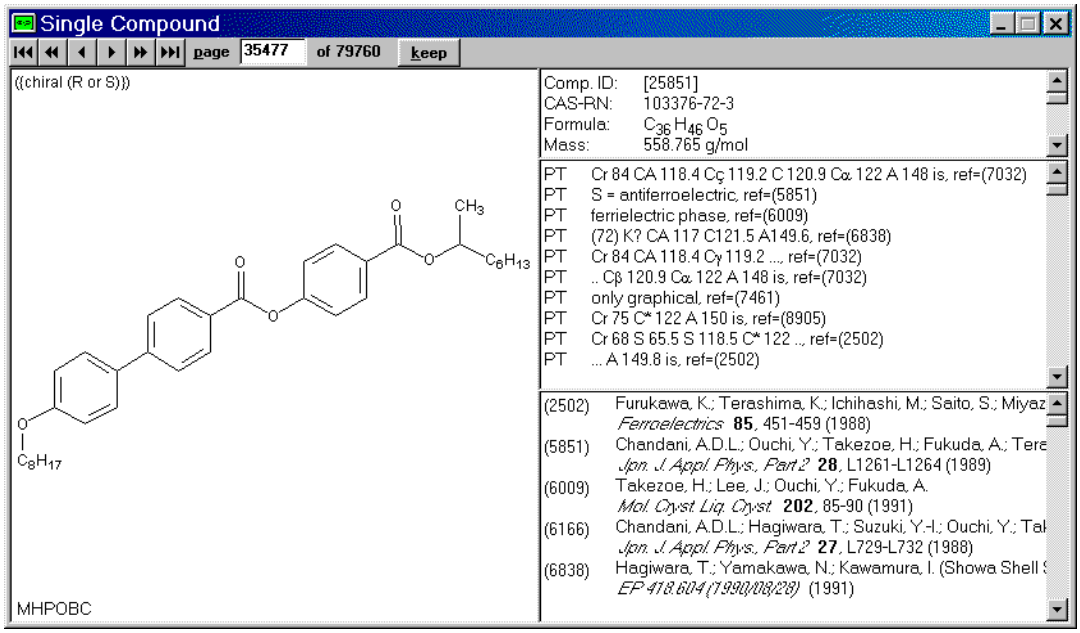


Results of the Searches

The results of the main searches can either be one specific liquid crystal molecule, a group of similar molecules in tabulated form or a list of references.

1) A Specific Liquid Crystal

If your search has resulted in only one liquid crystal being found which fits the criteria of the search then you should see a screen display similar to the one below (obtained from an exact name search for 'MHPOBC') :

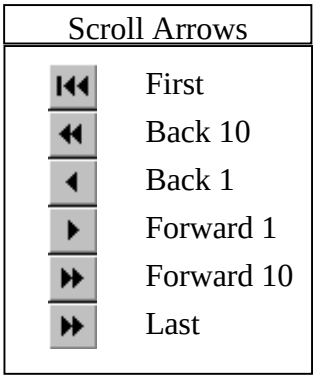


As you can see the display is split into five distinct areas.

The first row is the function bar. It displays the running number of the current molecule, the scroll arrows which are used to control the file number by moving backwards or forwards within the file sequence and a button marked <**keep**>. In normal operation the LiqCryst program will remove any windows of a previous search, once a

new search has been completed. If the **<keep>** button is pressed you will see that it changes to 'kept' and the current window will be kept active until closed manually

.



The left side of the window shows a pictorial representation of the molecular structure along with the name of the molecule which can be enlarged by holding down the right mouse button over the drawing or over the required data.

The right side of the window, row 1, shows molecules identifiers (LC Reg number, CAS-RN, Molecular formula, MW (molecular mass) etc.).

The right side of the window, row 2, shows phase information on the liquid crystal and the main reference for the molecule as well as the physical data and the reference from which it was taken. A list of abbreviations that are used when assigning physical data are shown in Appendix D. this reference can be displayed in full by double-clicking the left mouse button in this area. The phase information for this molecule is as follows :

Cr 84 CA* 118.4 Cγ* 119.2 C* 120.9 Cα* 122 A 148 is

The letters are abbreviations for the specific phases that the liquid crystal undergoes and the numbers represent the temperatures of the phase boundary. So in the above example 'Cr' represents crystal and it is before the number 84, this means that this liquid crystal is crystalline below 84^{o}C. Above this temperature it is chiral antiferroelectric 'S_{CA}' (abbreviated to 'CA*') until it reaches 118.4^{o}C where it becomes chiral ferrielectric 'Scγ' (abbreviated to 'Cγ*') and so on until it reaches 148^{o}C above which it is isotropic (abbreviated to 'is'). For a full list of phase abbreviations used see Appendix C.

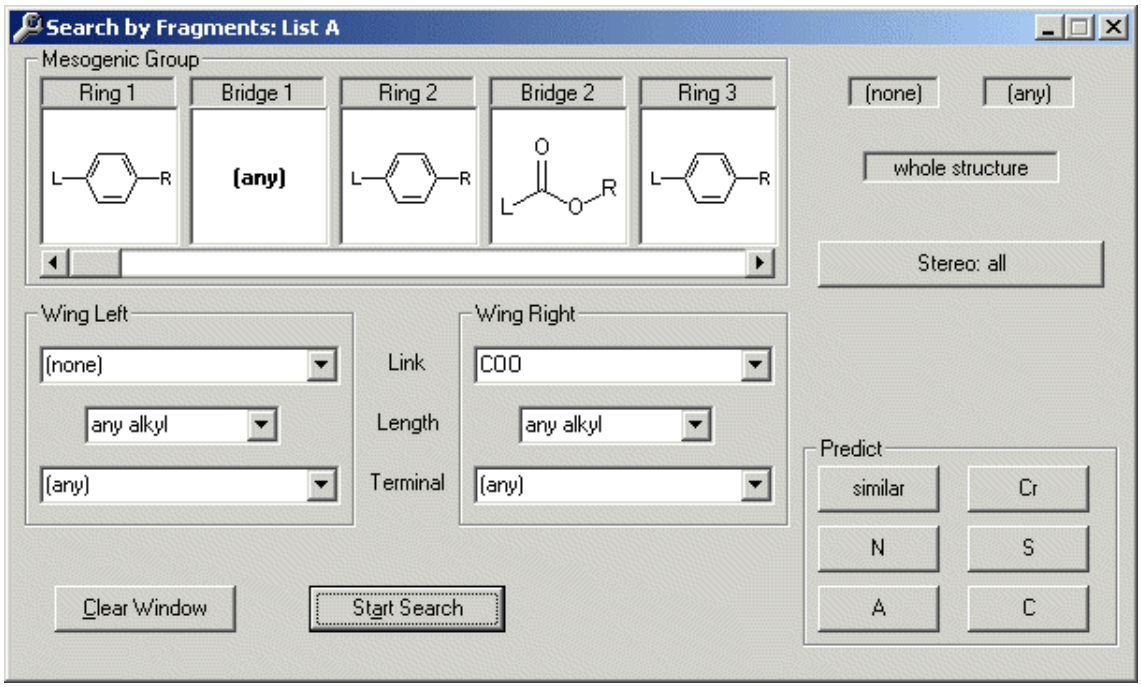
The right side of the window, row 3, is a full numerically ordered display of all the references shown in row three and four.

2) A Group of Similar Molecules

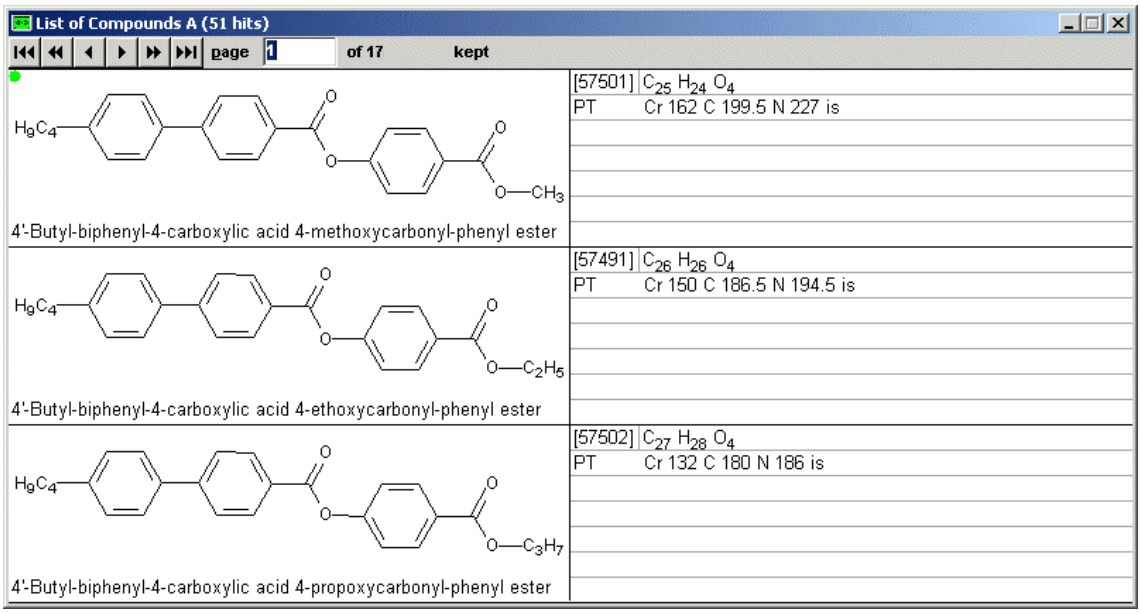
If your search has resulted in more than one liquid crystal fitting the criteria described in the search the results will be presented in a tabulated form.

Example 10 Display of a tabular Compound List

The following search was used to obtain the data for the compound table:



The list of fragments (-ph-?-ph-coo-ph-coo-) gives the following hit-list:



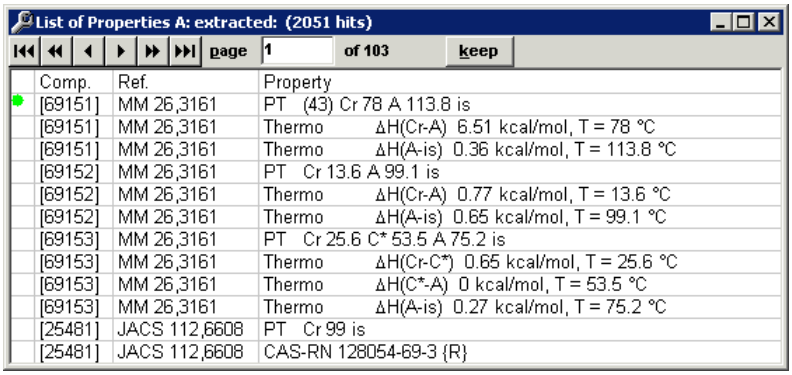
The table lists the full structures and associated data. The left hand column of the window shows the full molecular structure of the liquid crystal and the right hand column carries the data, with the first line showing the liquid crystal registration number and further lines giving phase information and physical data along with the relevant reference numbers. The right mouse button can be used to enlarge the structure and phase information.

Example 11 Extracting Properties or References

When a list of molecules has been produced after a successful search, such as in the example above, then the extraction features (available from the file menu or via the shortcut buttons) becomes active.

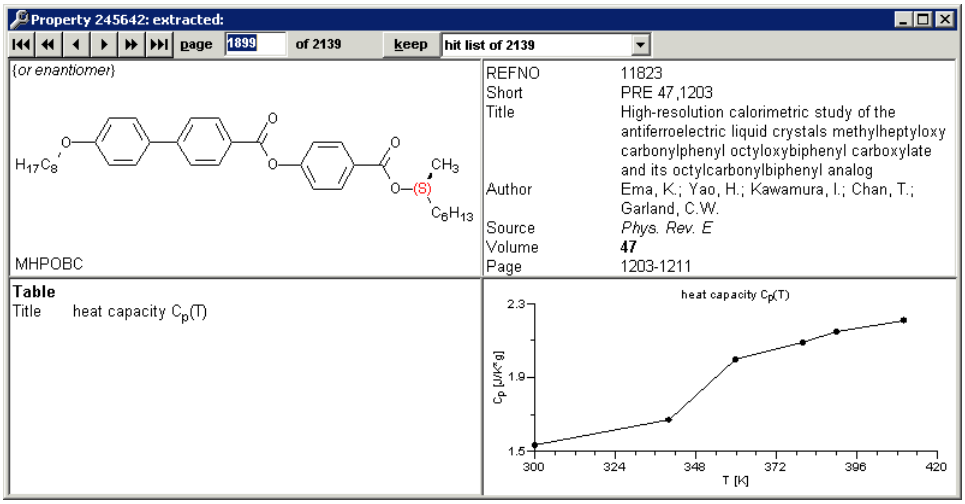
Using the search-result from above go to the Search Menu,

Choosing the option ‘extract properties’ from a compound or reference list will produce a list of all the different properties that were present in the original list along with the molecule from which they originated, and the reference (similarly ‘Extract references’ will show all the different references that are present in the original list). To obtain a list of certain compounds, highlight the relevant LC registration number by clicking on the appropriate number, and choose "Extract selected" from the "Search" -menu.



Comp.	Ref.	Property
[69151]	MM 26,3161	PT (43) Cr 78 A 113.8 is
[69151]	MM 26,3161	Thermo ΔH(Cr-A) 6.51 kcal/mol, T = 78 °C
[69151]	MM 26,3161	Thermo ΔH(A-is) 0.36 kcal/mol, T = 113.8 °C
[69152]	MM 26,3161	PT Cr 13.6 A 99.1 is
[69152]	MM 26,3161	Thermo ΔH(Cr-A) 0.77 kcal/mol, T = 13.6 °C
[69152]	MM 26,3161	Thermo ΔH(A-is) 0.65 kcal/mol, T = 99.1 °C
[69153]	MM 26,3161	PT Cr 25.6 C* 53.5 A 75.2 is
[69153]	MM 26,3161	Thermo ΔH(Cr-C*) 0.65 kcal/mol, T = 25.6 °C
[69153]	MM 26,3161	Thermo ΔH(C*-A) 0 kcal/mol, T = 53.5 °C
[69153]	MM 26,3161	Thermo ΔH(A-is) 0.27 kcal/mol, T = 75.2 °C
[25481]	JACS 112,6608	PT Cr 99 is
[25481]	JACS 112,6608	CAS-RN 128054-69-3 {R}

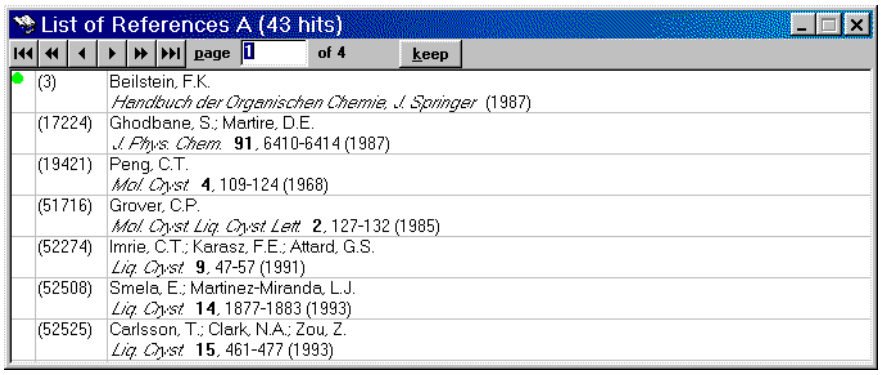
The ‘Extract compounds’ option should now be active. This will produce again a list of all the compounds from which the properties were extracted. To see more details of the properties, double-click one of them, and the current property-list will be “captured” in a single-property display, to get easy access to the full property and reference details complete with the corresponding chemical structure.



3) A List of References

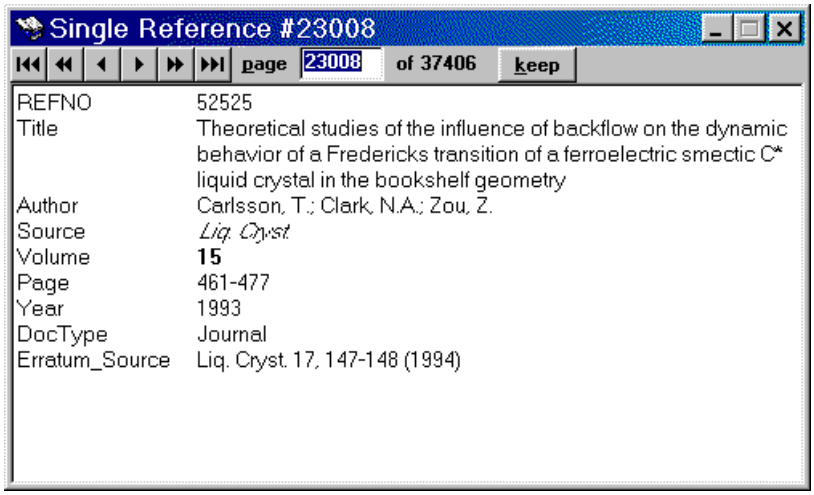
By choosing the "Extract References" from the "Search" -menu, a list of references from all properties in a compound- or reference - list can be obtained.

References are generally produced as a list :



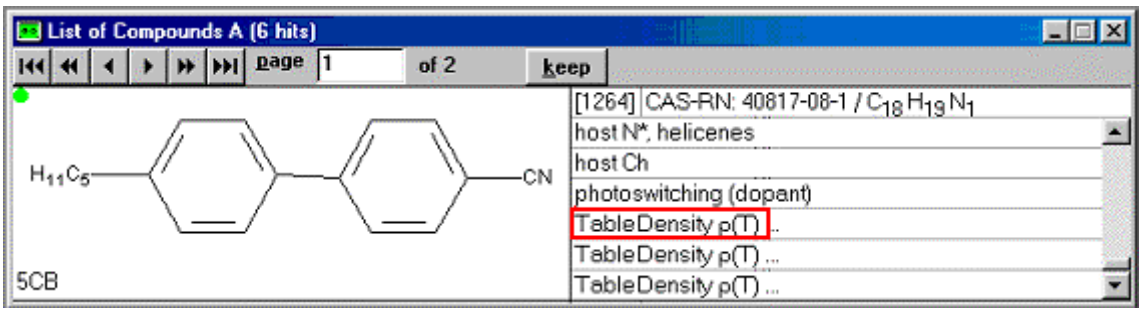
This shows the reference number, the author(s), the journal it appeared in (along with volume and page number if available) and the year of publication.

Double click will open a single reference window including title.

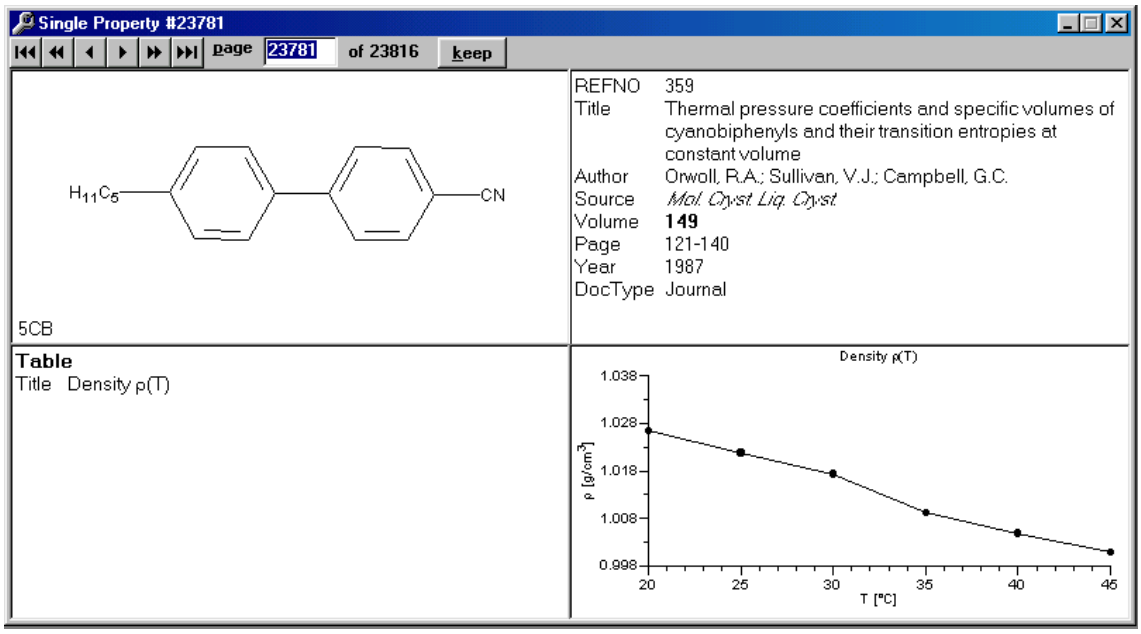


4) A Table and Diagram Representation

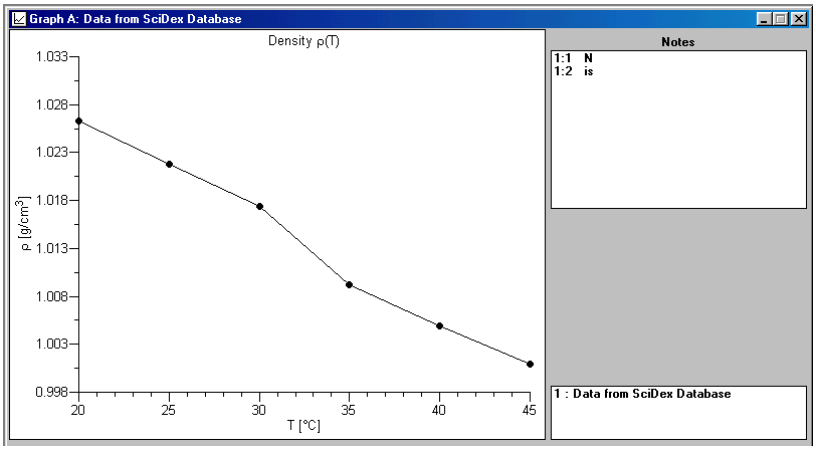
LiqCryst includes now temperature dependent properties, that are displayed as tables and diagrams.

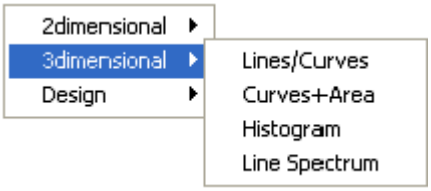


This window shows the temperature dependent properties like density versus temperature, "Table Density ρ(T)". Double click on the property will open a single property window including a diagram.



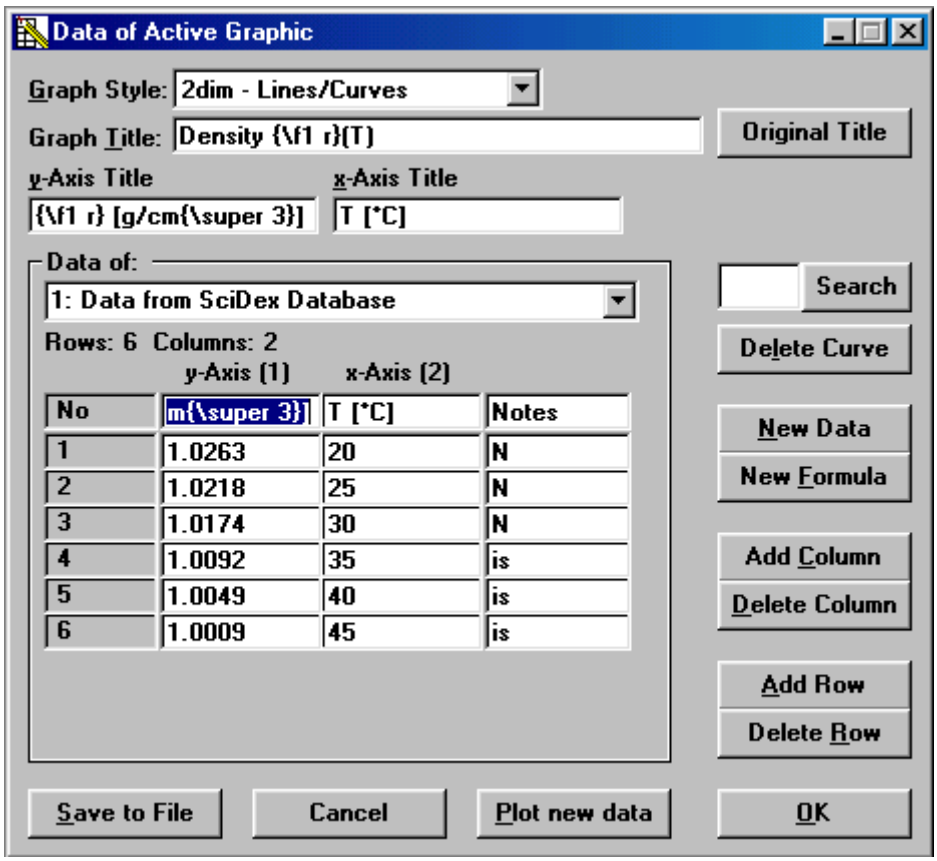
Double click on the diagram will open a single diagram window as well as a table tool window. Mouse down on a diagram point allows to view the x,y values.





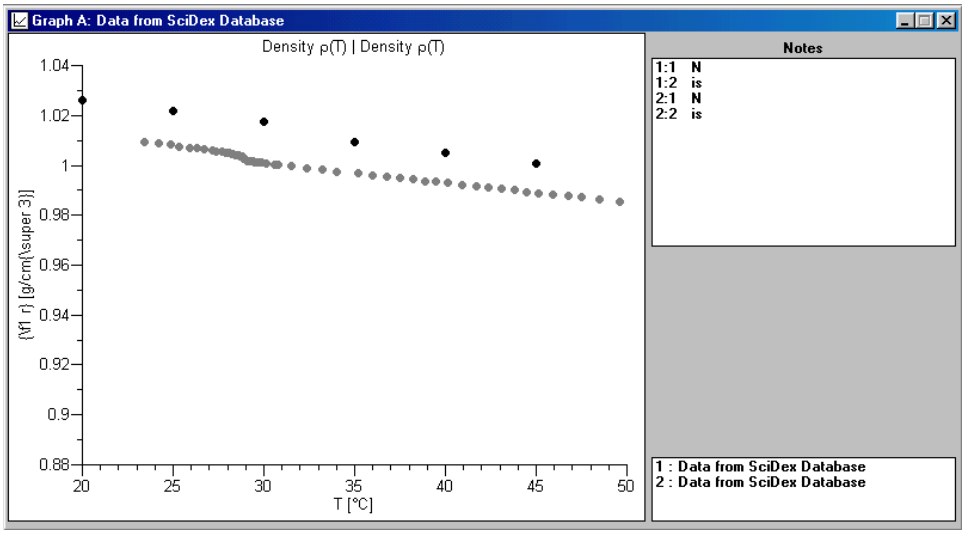
Click on the right mouse button to change the design of the current graph (diagram) to e.g. 3dimensional.

Each time a single diagram window is opened another window called "Data of Active Graphic" will be opened in the bottom left corner. By double clicking at the title bar of this window it will be enlarged and presented as follows.



This window will allow you to add new values to the current diagram and to work temporary with it. Please take care that new added values will not be saved into the current LiqCryst database. The "Save to File" button will only save your changes as .SDG files. Such files could not be opened with LiqCryst itself, but only with SciDex, the Scientific Data Explorer by LCI.

If you wish to compare some different opened diagrams, just press Alt and the left mouse button to drag a diagram into the other one.



Saving and Editing

When a search has been completed various options should become available from the '**File'** and '**Edit**' menus.

1) From The File Menu

Print data : when viewing a single molecule the '**Print**' option from the file menu will produce a full printout of all the data in the active window. When viewing a table of similar molecules the '**Print**' option will produce a printout of the molecular display and the table shown.

Save : After a successful search choosing the '**Save**' option will save the search data that has just been compiled. (in *.sxc files)

Export List file : Export a list file.

Export Mol file : Saves the selected molecule as a .Mol file for use in other packages.

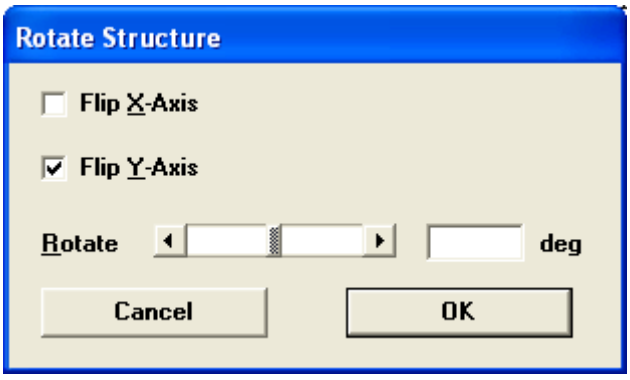
2) From The Edit Menu

Copy Image : Copies the molecular display in the main window to the clipboard.

Copy Text : Copies the data and the reference list to the clipboard.

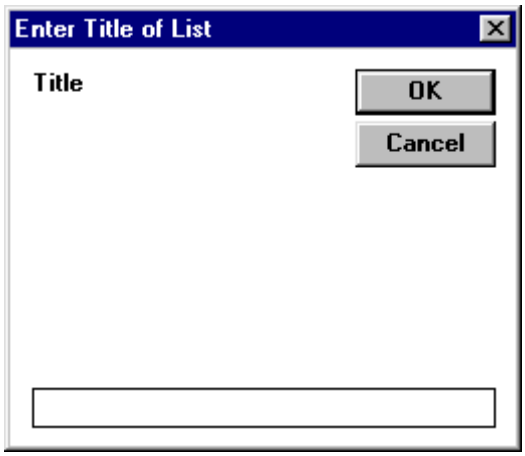
Rotating the Molecule

If this option is available from the main menu bar ("Edit" - menu → "Rotate Structure") then it is possible to rotate the 2-D molecular drawing. The molecule can be rotated clockwise by entering negative angles and counterclockwise by entering positive angles, or using the scroll bar. Or it can be flipped about the X or Y axis. If both a rotation angle and an axis-flip is selected, the rotation will be performed first, then the flip(s).



Naming the Window

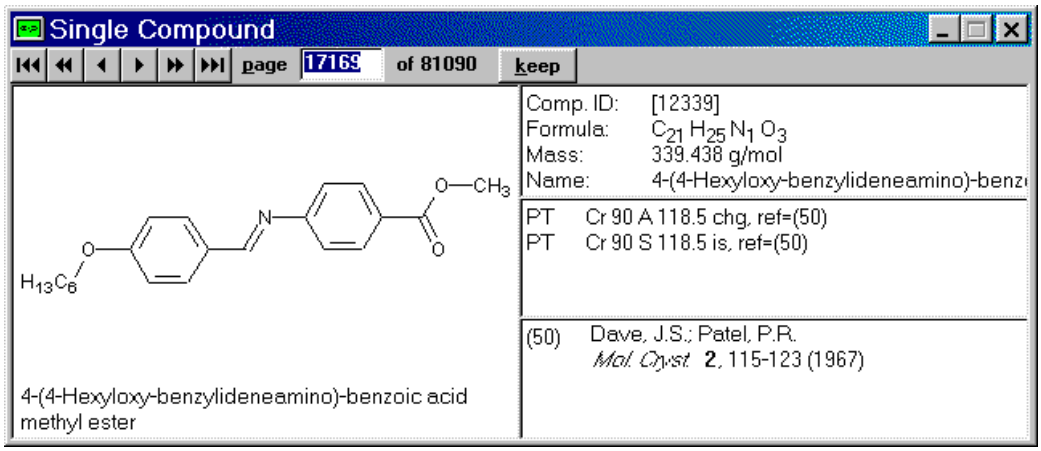
Available from the edit menu, this option allows you to change the name of the active window.

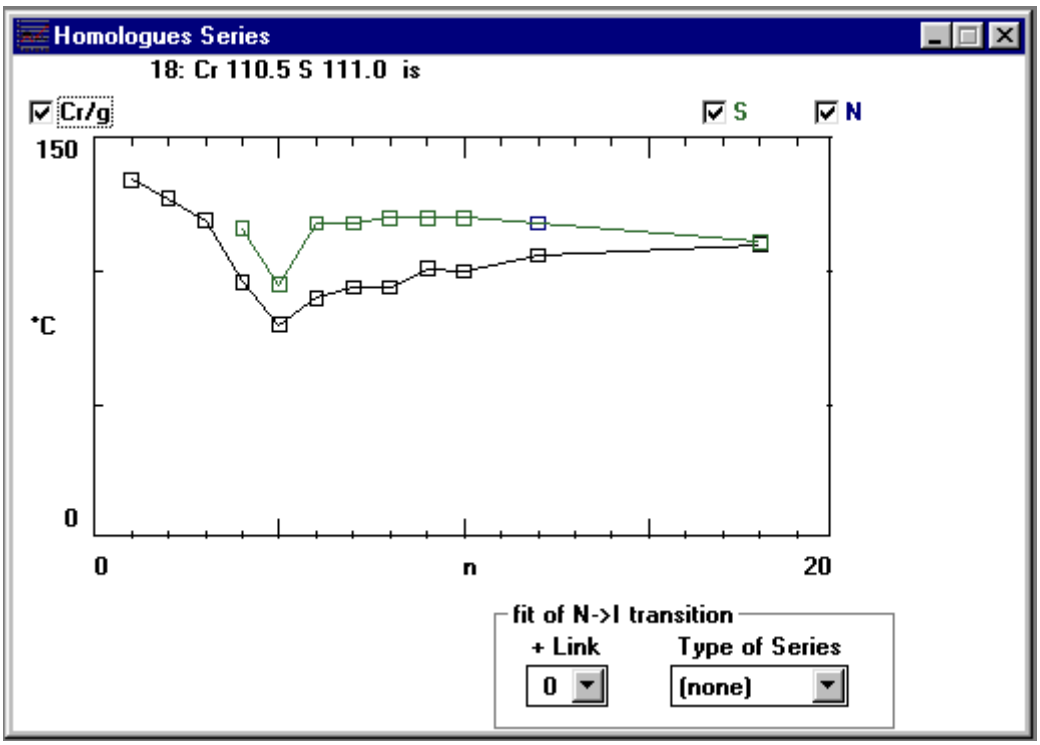


Homologous Series

The homologous series option should become available after a successful search has been carried out. It is primarily used to compare phase transitions of homologous molecules to the liquid crystal that is currently being displayed. When the '**homologues**' menu is active in the analyse menu, clicking on the option will provide a graph of phase transitions exhibited by the liquid crystal series from which comparisons can be drawn. An example is shown below :

The function "Show Homologues Series" can only be successfully executed when a compound is active which as an alkyl-chain at either left or right or both ends of the molecule.





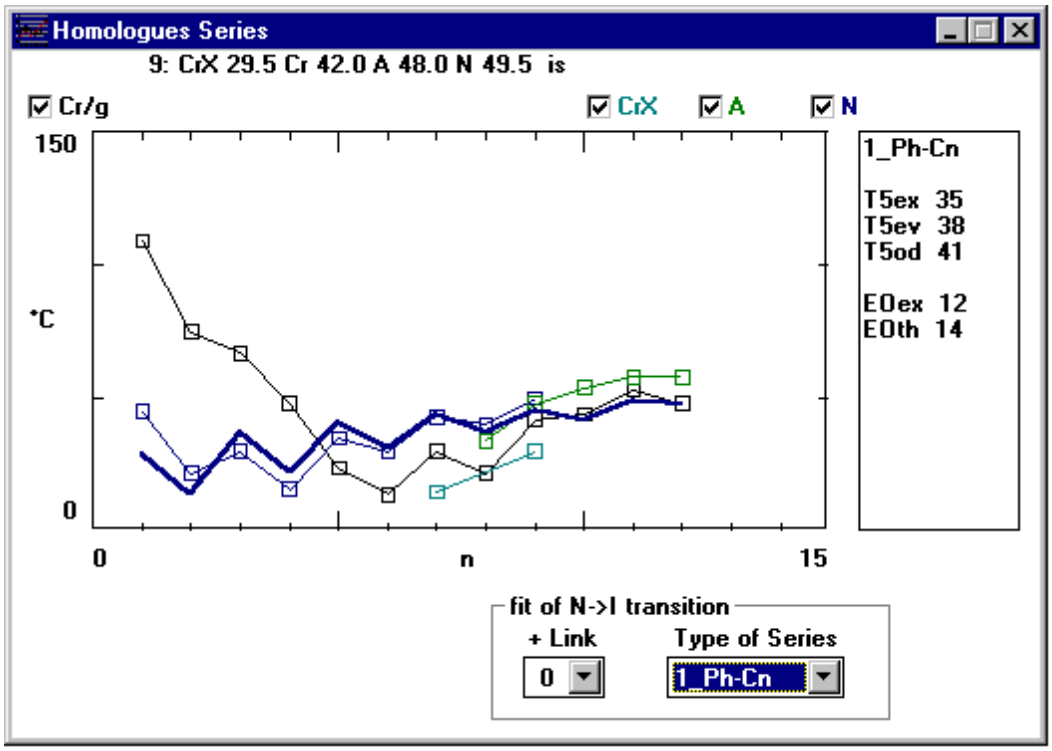
By moving the mouse pointer over the graph, phase data is displayed at the top of the window for the particular homologue.

The check boxes show the types of phases exhibited by the homologues. The colour of the check box corresponds to the line of the same colour on the graph that represents an individual phase. By clicking on one of the check boxes the tick can be removed, this removes the line to which that checkbox corresponds on the graph, and therefore the behaviour of that phase is not shown. By clicking on an empty box the tick is replaced and the line is again drawn.

To export data use '**Copy text**' and '**copy image**' from the '**edit**' menu.

If the homologous series produced shows the nematic phase then it may be possible to use a new **tool for nematic phase fitting**. The fitting is used to determine the odd/even effect of the number of atoms in the wing group and plot a theoretical curve of the combination.

Tool for the Fit of the Nematic Transition Temperatures



For the fit two curves are compiled by the program (These curves are not displayed): one curve connects the transition temperatures for all members of a homologous series with an even number of atoms in the wing group (T2, T4, T6, ...), while the other connects all transition temperatures of the members of a homologous series with uneven numbers of atoms in the wing group (T1, T3, T5, T7, ...). These curves are used to determine the even/odd effect. The final curve represents a combination of theoretical curves (curve in bold type in the above display).

Then the experimental data can be compared with the statistical data.
The diagram of the nematic phase will be characterized by:

T_n Temperature for wing length n. In this case n is the number of atoms including links. $T_n = m_n \bullet T5 + b_n$
m_n and b_n are statistical data
m,b are parameters of the linear regression function (y = m*x + b).

T5 The transition temperature for n = 5. In this case n is the number of atoms in a wing group including links, e.g. C5H11, O-C4H9 or OOC-C3H7.

EO The value of the even/odd effect: EO = T5 - (T4 + T6) / 2

Two parameters are needed:

- The additional length of the linking group
- The type of the homologous series.

Please use these values for the additional length of the linking group:

0	for alkyl (CnH2n+1)
1	for alkoxy etc.(e.g. O-CnH2n+1, CO-CnH2n+1)
2	OOC-CnH2n+1, COO-CnH2n+1, etc
3	OCOO-CnH2n+1, etc.

Possible types of homologous series are (Use the mouse to select a type):

1_Cy-Cn	one alkyl chain on a cyclohexane ring
1_Ph-Cn	one alkyl chain on a phenyl ring
1_Ph-OCn	one alkoxy chain on a phenyl ring
1_BCO-Cn	one alkyl ring on a bicyclooctane ring
2_Ph-Cn	two alkyl groups on a phenyl ring
2_Ph-OCn	two alkoxy groups on a phenyl ring

The data box on the right hand side of the screen display contains information about the fit:

T5ex	experimental data for n = 5
T5ev	theoretical value for n = 5, calculated from even members of the homologous series
T5od	theoretical value for n = 5, calculated from odd members of the homologous series
EOex	experimental value for the even/odd effect
EOth	theoretical value for the even/odd effect

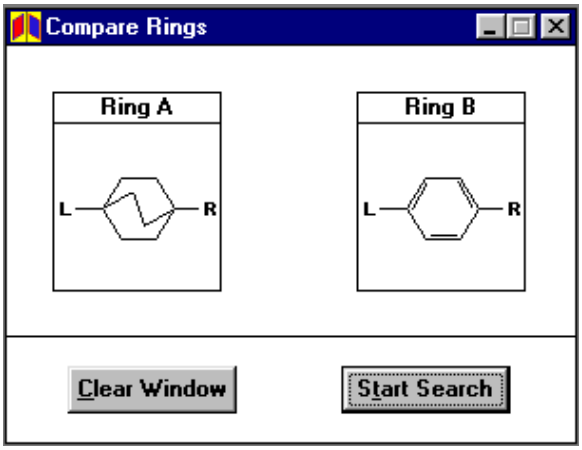
Comparing Liquid Crystals

The compare function in LiqCryst allows comparisons to be made between specific molecules or molecular groups found in liquid crystals (bridges and rings). To compare molecules or groups choose one of the following options from the '**Analyse**' menu :

Compare Rings

The two rings are chosen in the same way as in the '**Search by Fragment**' window. A search is then carried out through the nominated file with the result being pairs of compounds that are identical except for one of the rings.

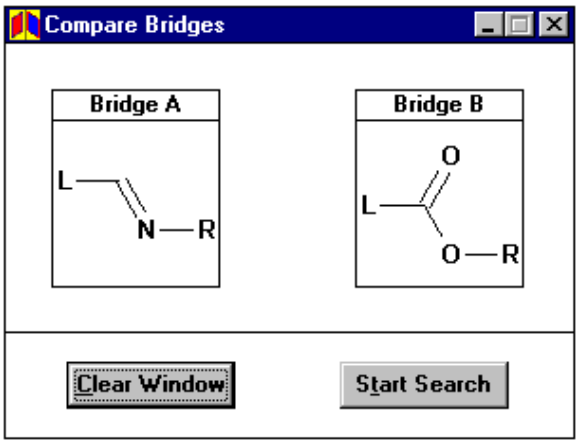
Example 12 Compare Rings



Compare Bridges

This comparison search works on the same principle as the '**Compare Rings**' function.

Example 13 Compare Bridges



The program compares the bridge CH=N with the COO fragment under the aspect of the transition temperatures for the nematic phase. LiqCryst creates the following table:

structure 1	structure 2	y (temp. of 1)	x (temp. of 2)
EtO-Ph-CH=N-Ph-CN	EtO-Ph-COO-Ph-CN	129	105
MeO-Ph-CH=N-Ph-Bu	MeO-Ph-COO-Ph-Bu	48	25
EtO-Ph-CH=N-Ph-OEt	EtO-Ph-COO-Ph-OEt	143	117

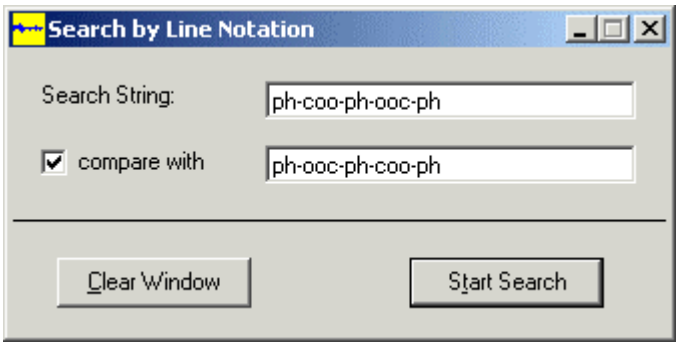
The pair of data x,y can be used for statistical analysis by LiqCryst itself or by Excel or other programs.

Compare Line Notation

This search also works on a similar principle but involves the entry of one exact line notation which can then be entered again with a slight alteration so that a comparison can be made between the two.

Example 14 Compare Line Notation

Entering the following will compare similar compounds that differ in the bridges between phenyl groups:



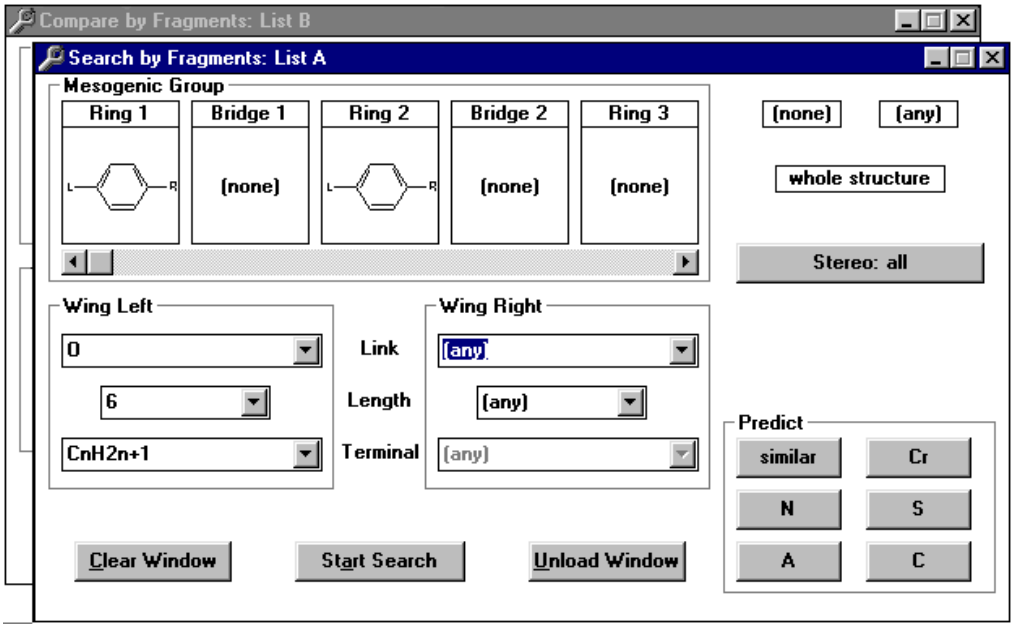
The results will be displayed in a "List of Pairs"

Compare Fragments

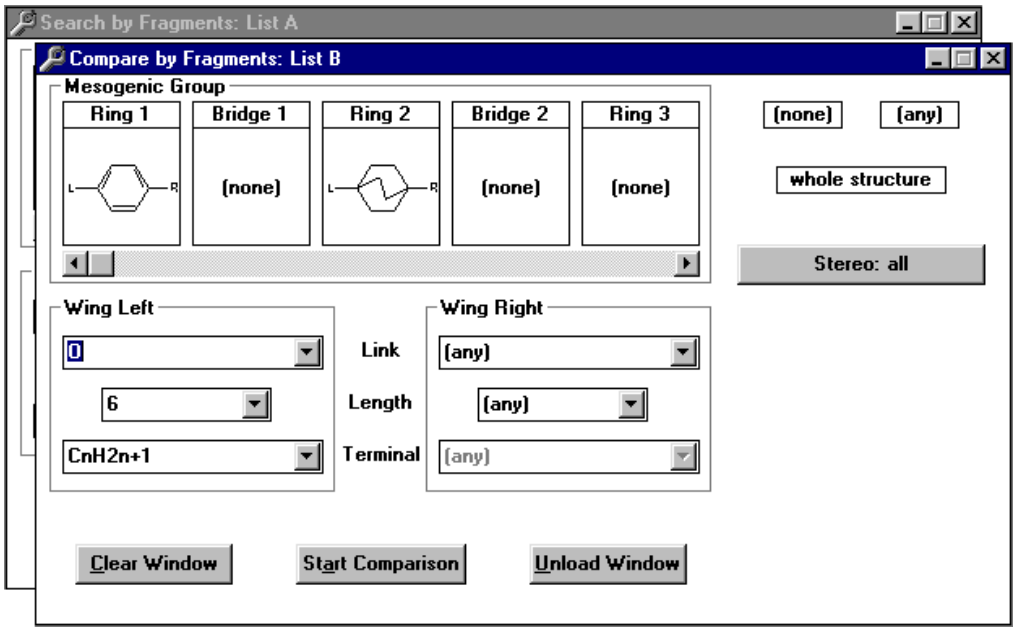
Comparing by substructure involves the entry of two full substructures in the windows provided. These are then used as a reference for pairs of similar compounds. For more information on entering substructures see '**Search by Fragments**'.

Example 15 Compare by Fragment

To compare the effect of replacing a bicyclooctane ring with a benzene ring you must firstly enter the two substructures to be compared :



To save time entering the structure again, hold down the left mouse button over the whole structure box in list A and drag the structure to the whole structure box in list B. Now simply change the factor that is to be compared.



The <**Start Search**> button can now be pressed and a display of how many pairs fit the criteria will be shown.

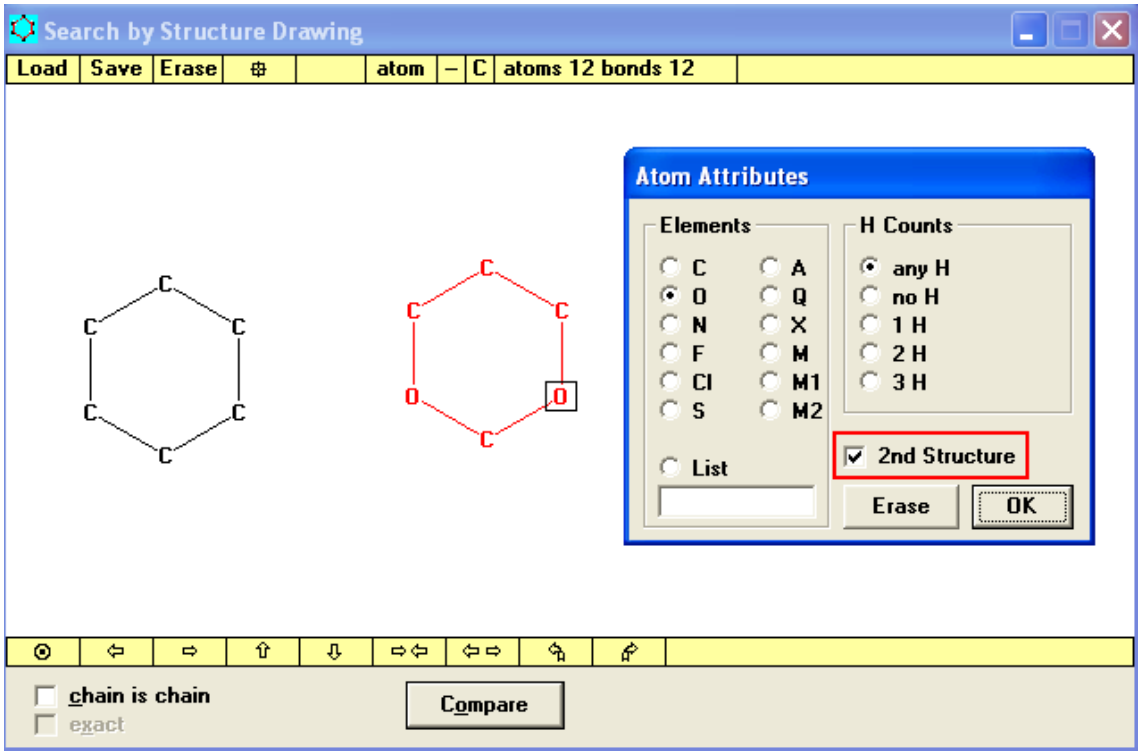
Similarity

The Similarity option is based around the '**Search by Fragment**' window. A substructure must first be entered up to ring 3 before a search can be carried out that will produce a range of similar molecules. Its use is described in the '**predict**' section.

Compare Compounds by Drawing

This function allows a comparison of structures based on a classical substructure search as used by other chemical databases. For Compare by Drawing, two substructures have to be defined. One of these gets the option "second structure" by right-clicking on any atom of the substructure and selecting the checkbox "2nd Structure" in the Atom Attributes window. The second structure will be shown in red.

Structures can either drawn directly in the window or can be inserted into the window by drag and drop or can be imported as a MOL file



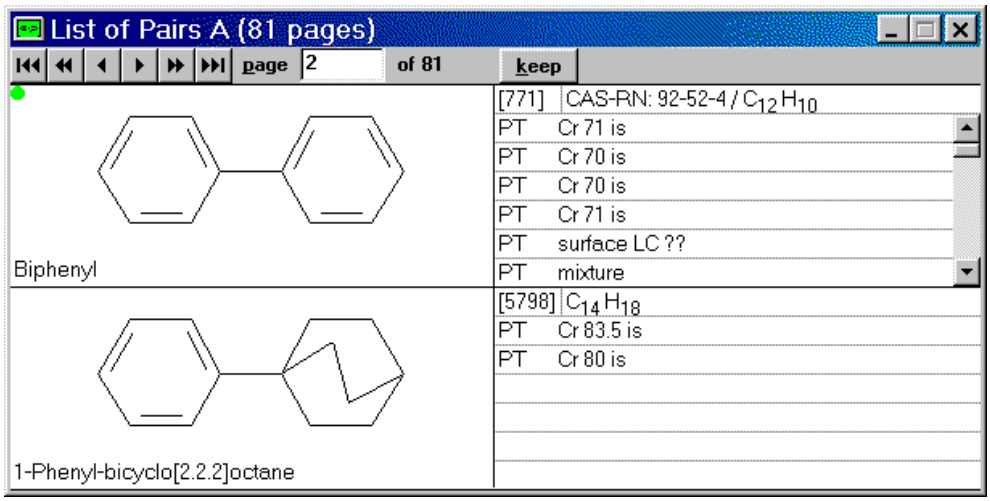
The above example would compare Cyclohexane with 1,3-Dioxane based on a substructure. This search will give more hits than the similar but not identical search, in which Cyclohexane and 1,3-Dioxane are compared as Fragments, since a substructure search allows flexible substitution on the rings, while the fragment search defines the rings unsubstituted except for the direct connections to the rest of the structures on the left and the right side.

See Search by Drawing for details on how to draw a structure.

The result of the comparison is a list of pairs.

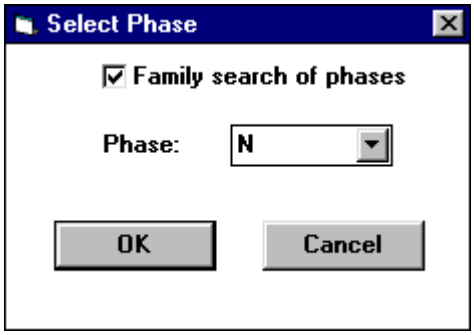
Results of Comparing Molecules

On completion of a successful comparison a display of the pairs of similar molecules should be produced.



On the display above the active molecule (the molecule that will be copied, exported or rotated should it be requested from the edit or file menu) is shown by the green dot in the top right hand corner of the molecule display window. The phase behaviour is shown in the middle columns.

The pairs of molecules can be further analysed by choosing the '**Analyse Comparison**' option from the analyse menu. This option allows the investigation of the pairs with regards to phase behaviour. If you choose to analyse your data you will then be asked to enter the phase that you wish to investigate.

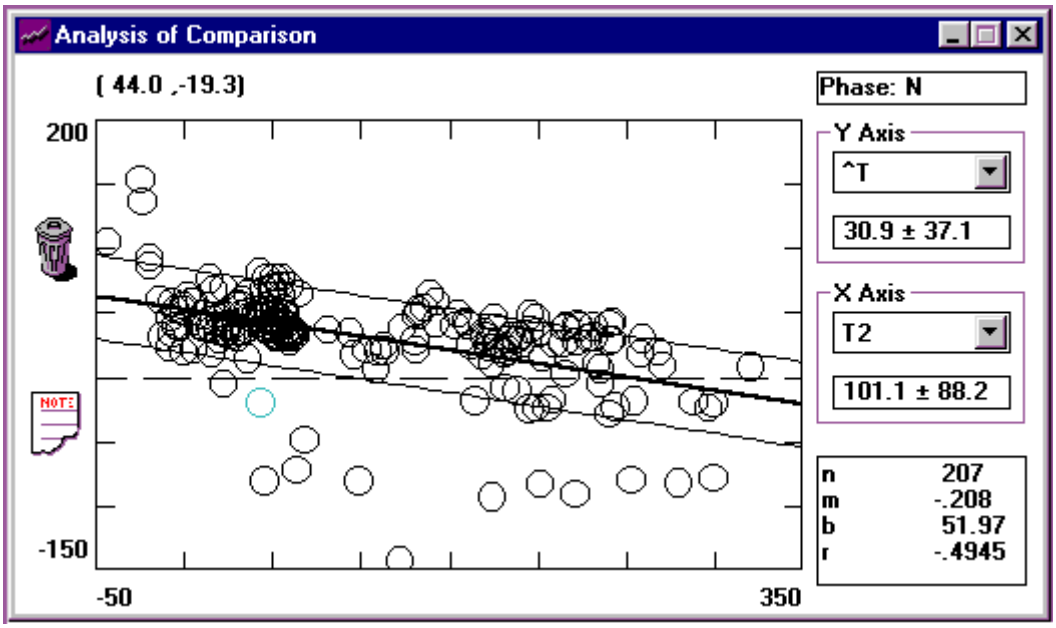


There is also an option to include a family search of phases. This means that if, for example, you wish to examine the smectic phase then ticking the family search box will include all types of smectic phases.

Once the required phase has been entered, if enough pairs exhibit the requested phase, then you will be presented with a graph showing the pairs.

Each circle on the next graph represents a pair of molecules, clicking on any of the circles will show the pair in question in the active list window. The circle corresponding

to the pairs you have just viewed should be highlighted. A 'Trashcan' is also now available on the left of the analyse window, this can be used to dispose of the pair of compounds just viewed (clicking on the 'Trashcan' will remove the highlighted pair).

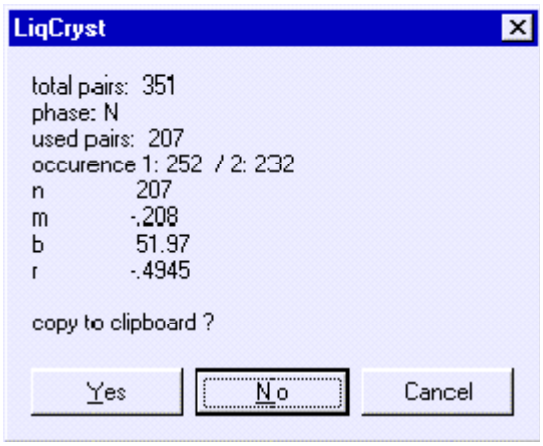


Linear regression : Y = mX + b

The axis of the graph can be changed from the drop down menus available (the down arrow on the right of the box). On first view of the graph X will always be shown as **T2** and the Y axis as **^T**, but can be replaced by **T1**, **(T1+T2)/2** or **Chain Length**

T1	Transition temperatures of structures with search pattern 1
T2	Transition temperatures of structures with search pattern 2
^T	=T1-T2; difference of temperatures
(T1+T2)/2	Average temperature calculated from both compounds
Chain Length	Sum of both wing groups, including links and terminal groups

Clicking on the note icon will give the complete statistical information and the option to copy it to the clipboard :



This shows that in total the comparison contains 351 compounds, but not all of the molecules had a nematic phase. If one of the molecules in a pair does not have a nematic phase then this negates the pair of similar molecules from the comparison. This accounts for the difference in the number of pairs used and the total number of pairs. the data also reveals that 252 molecules with pattern 1 and 232 molecules with pattern 2 have the required nematic phase. Therefore 207 molecules have been used for the statistical analysis.

The letters ‘n’, ‘m’, ‘b’ and ‘r’ are parameters for the linear regression.

A list of abbreviations and formulas used in the ‘**Analyse Comparison**’ function are shown in Appendix F.

Predicting Phase Behaviour and Similarity

The ‘**Predict by Similarity**’ function is available from the ‘**Analyse**’ menu and can be used to show similarity between molecules or to predict values for the phase transitions :

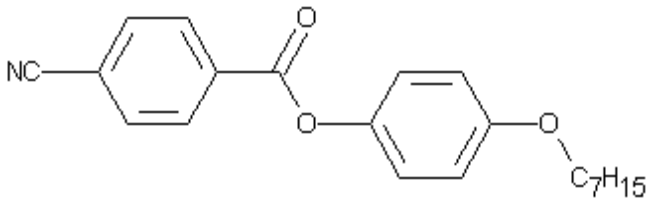
Cr : The melting point
N : Nematic phase transition temperature
S : Smectic phase transition temperature
A : Smectic A phase transition temperature
C : Smectic C phase transition temperature

It involves the entry of a complete chemical structure which can then be used as a reference for a search for all similar molecules via the search by fragment window.

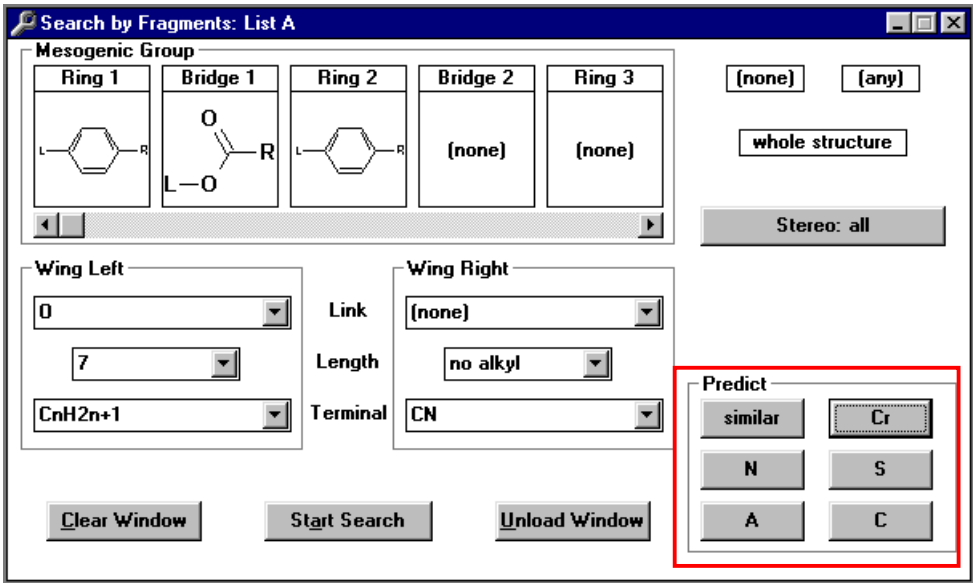
The search allows you to either simply search for the similar molecules and view them by clicking on the <**similar**> button or to search for similar molecules and then extrapolate the data obtained to predict phase temperatures for the molecule entered. To estimate the phase data click on the phase that you wish to extrapolate.

Example 16 Predicting Phase Behaviour

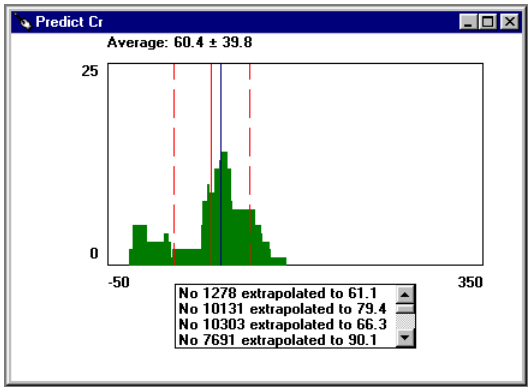
To predict the melting point of the molecule :



The following should be entered in the predict window :



When the search has been completed after pressing any of the “Predict” buttons for melting-point, or the phase transitions for N, S, A or C-phase, a graphical representation of the prediction will be produced along with the tables of compounds used to make the prediction.

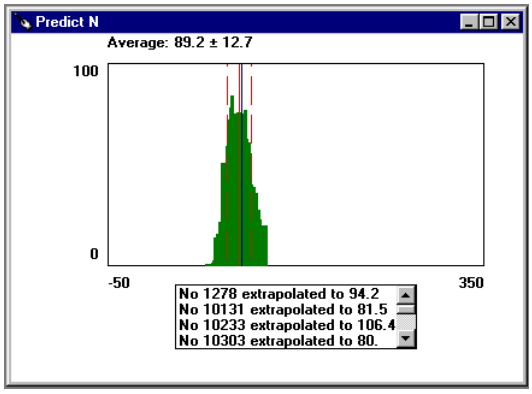


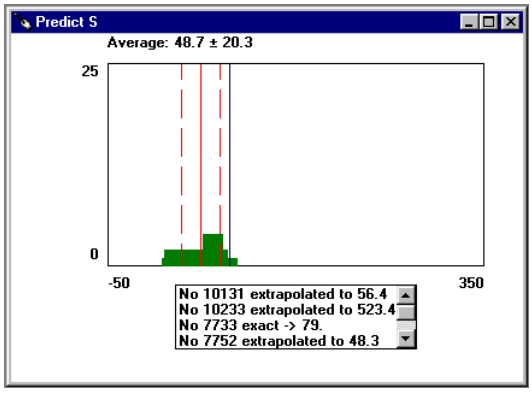
The prediction is based around the average value which is calculated along with the estimated uncertainty in the value.

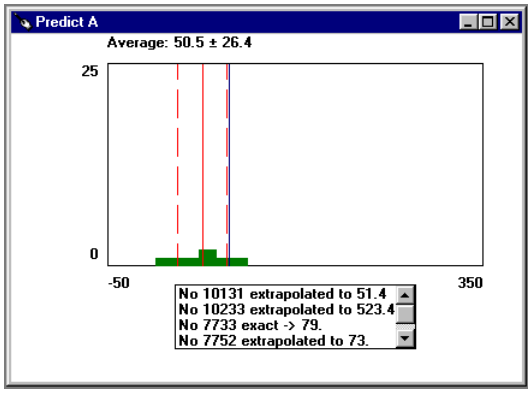
The **X-axis** on the graph represents the temperature and the **Y-axis** shows the statistical distribution.

The **green area** represents the sum of the predictions derived from the different molecules.

The **solid red line** gives the average prediction with the **dashed red lines** showing the deviation.
If a **blue line** is present it means the prediction has been made on a known compound which is in the database and its position represents the value of the relevant phase data.
In the box below the graph the molecules that were used to make the prediction are listed along with the data used. The same search structure can then be used to make predictions for the other phases if required.

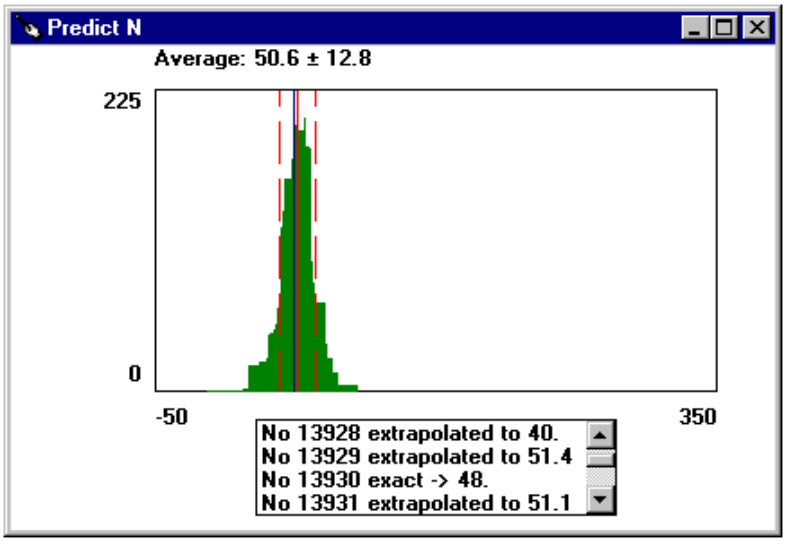






No data produced for the smectic C phase.

Example 17 Prediction for a Nematic Phase



The list box: No 13928 and No 13929 are similar to the compound for which the prediction of the transition temperature was requested. The extrapolation of the transition temperatures for these compounds give the values 40 and 51.4. No 13930 has exactly the structure of the investigated compound with a measured value of 48°C for the transition temperature.
The user enters a complete description of the chemical structure, e.g. MeO-Ph-CH=N-Ph-Bu, and defines the requested property, e.g. transition from nematic to isotropic. The program looks for all similar compounds, which already have this property, e.g.:

similar compound	measured value	extrapolation
MeO-Ph-COO-Ph-Bu	25	50 (by COO/CH=N statistics)
EtO-Ph-CH=N-Ph-Bu	80	58 (by EtO/MeO statistics)
.. further molecules ..		

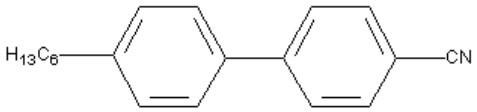
All these single extrapolations are summarized and evaluated according to the standard deviation of the single statistic to give the final prediction, e.g. 50.6 ± 12.8 °C .

Predicting N by Increments

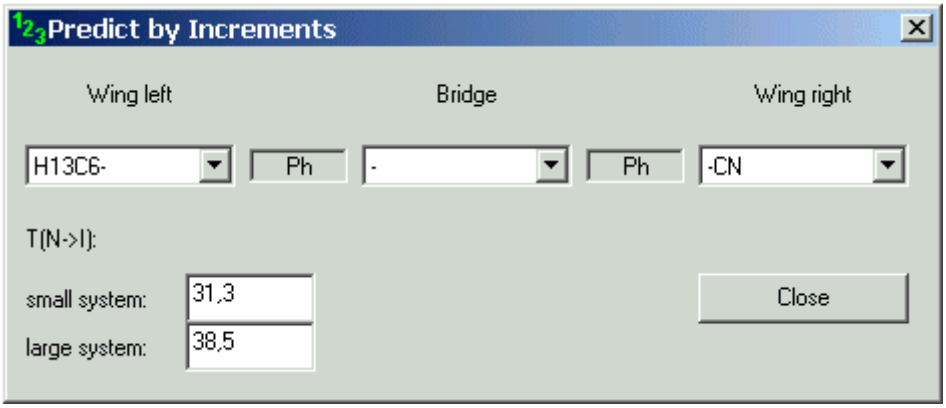
A simple increment system is now included in LiqCryst to predict the Nematic-Isotropic transition temperature of a limited number of molecules. The Nematic-Isotropic transition temperature can be predicted for a limited number of liquid crystals which follow the general scheme “Wing1-Phenyl-Bridge-Phenyl-Wing2”.

Example 18 Prediction for a Nematic-Isotropic transition temperature

To predict the Nematic-Isotropic transition temperature of the molecule:



The following should be entered in the predict window:



(correct transition temperature: 30.1 °C)

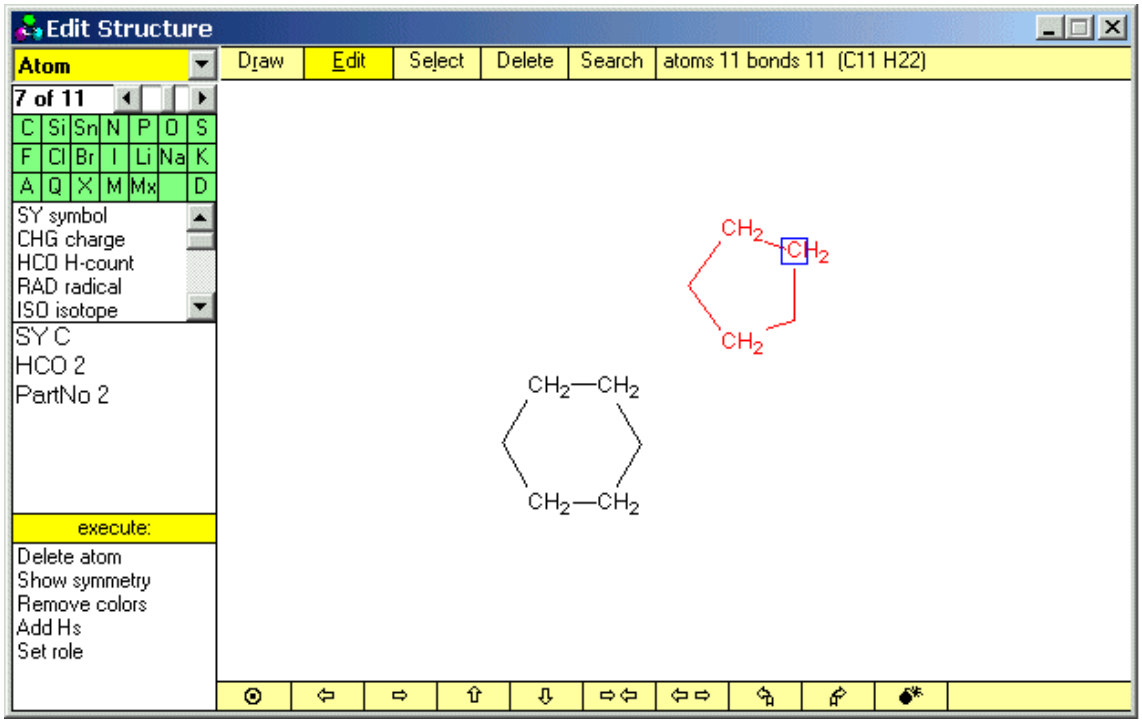
The “small system” has less fragments defined and gives more exact results, if it gives a result at all. The small system is derived from data from about 2000 compunds. The larger system contains a broader variation and allows prediction of the N->is temperature for about 20000 compounds. (56 wing-groups on each side, and 9 different types of bridges between the phenyl-rings)

The small system has been published in Liq.Cryst. 22, 519-523 (1997)
The large system is as of yet unpublished.

Edit Structure

The window Edit Structure is the general structure editor of the SciDex database system. Many of the available options are not important for LiqCryst, since the database is not editable. The main interest of this window is the possibility to search or compare substructures with specific stereochemistry.

Additionally this window allows an advanced search for homologous series which can find homologous also in middle of the molecule, e.g. within the mesogenic groups or varying lengths of spacers. This search will only create a list of compounds, no graphical analysis of the mesogenic properties.



Elements of the top line

Five different modi exist, which can be chosen from the top line:

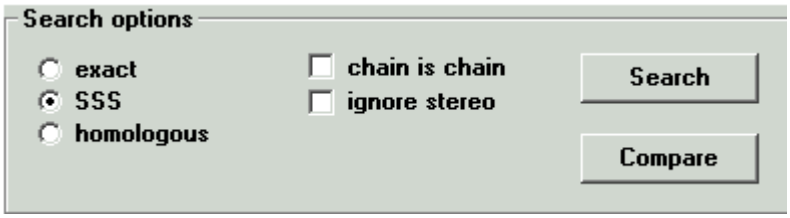
Draw To draw a structure, use the left mouse button to click at the positions where you want to place atoms. The default atom-type is Carbon, and the default bond-order is Single. To stop drawing, click the right mouse-button once. To enter the Edit Mode, right-click a second time.

Edit To modify an atom or a bond, left click on that atom/bond once, and choose an option from the list on the upper left of the window or type the changed value into the edit box below. Atoms or bonds can be moved by using the right mouse button. For bonds it is possible to cycle through the bond-orders (single, double, triple, unspecified, single, ...) by using the left mouse button to click on the bond multiple times. Holding the Control button during clicking on a single bond will switch between stereo-bond and normal bond. To go from the Edit Mode back to Drawing Mode, click twice with the left mouse-button (two single clicks, not a double click) on the atom you wish to alter.

Select Atoms can be selected by clicking on the atoms one by one or, alternatively, by drawing a rectangle around the atoms to be selected. The parts of the molecule inside of the selection will be marked blue. All structure modification commands on the bottom of the screen will then only apply to the selected atoms.

Delete In Delete Mode, the mouse cursor will change to an eraser and can be used to delete atoms and/or bonds. In order to go back to Edit Mode, click the right mouse-button once.

Search



Three different types of search exist:

- exact match
- substructure search
- search homologous series

Additional options are:

“chain is chain” -> chain atoms of the substructure will also be chain atoms in the complete structure; in other words, bonds that are no part of a ring in the substructure may not be part of a ring in the complete structure;

“ignore stereo” -> Stereo-attributes of atoms/single bonds (R/S) or double bonds (E/Z) will be ignored in the search

The “Compare” command from the "Search"-menu in the Editor-window is only available, if two separate structures are defined. This can be done via the command “set role” (from the Edit Structure-window), which is available when any atom is selected in the Edit mode (first left click on the atom then right click on the same atom to activate the Edit mode) .

The rightmost part is only for informative purposes and lists the current number of atoms and bonds as well as the calculated Molecular Formula (including implicit hydrogen atoms).

Elements of the bottom line

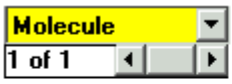
The symbols of the bottom line can be used to resize or move the structure within the drawing canvas

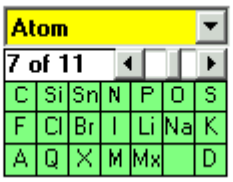
⊙	Centers the drawing, best fit to the screen
⇦ ⇨ ⇧ ⇩	Moves the drawing left, right, up or down
⇨⇦ ⇦⇨	Decreases or increases the size of thew drawing
↺ ↻	Rotates the drawing anti clockwise. or clockwise
💣	Erases the structure or selected atoms (in select mode)

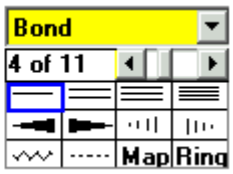
Elements on the left side of the window

The left hand side shows the settable options for molecules, the bond editor or the atom table. The contents will change, depending on the selection in the drawing canvas to the right. If no part of the molecule is active, this list shows the options for the whole molecule. In the above drawing an atom is active (blue box, see above). To view the bond options place the mouse-pointer over the middle of a bond in the drawing, to view the atom options place the mouse-pointer over any atom.

Area







Settable Options

ST	Stereo (chir,rac)	SY	symbol	BO	bond order
INFO	info text	CHG	charge	CL	color
CL	color	RAD	radical	CO	comment
CO	comment	ISO	isotope	J	NMR coupling
UQ	unique ID	LB	label	ST	E/Z Stereo (yes,no)
V1	value No 1	CL	color	V1	value No 1
V2	value No 2	CO	comment	V2	value No 2
V3	value No 3	UQ	unique ID	V3	value No 3
V4	value No 4	d	NMR shift	V4	value No 4
		ST R/S	Stereo (yes,no)		
		POS	position nmber		
		partChg	partial Charge		
		V1	value No 1		
		V2	value No 2		
		V3	value No 3		
		V4	value No 4		

Functions to Execute	Check Drawing	Delete atom	Delete bond
	Delete all	Show symmetry(color)	Align horizontal
	Undo/Redo	Show symmetry(pos.label)	Align vertical
	Remove colors	Remove colors	Flip Side A
	CH_Analysis	Add Hs	Flip Side B
	MS_Molpeak	Remove Hs	
	Rotate/Enantiomer	Set role	
	Add Hs		
	Remove Hs		
	Get SMILES string		
	Get ROSDAL string		

Comments on the "Functions to execute"

"Show symmetry" will analyse the symmetry of the atoms which have the same type as the selected atom. This can be used e.g. for NMR-data which are the same for symmetric atoms. Atoms which are chemically identical will be displayed in the same color.

"Remove colors" exist in both "Molecule" and "Atom"-mode. If this function is chosen when an atom is active, only the colors of the selected atom-type will be removed. This is meant to remove the symmetry-information for the atom-type (e.g. C; Si). In "Molecule-mode", all colours of all atoms and all bonds will be reset.

"Add Hs" also exists in both Atom and Molecule-mode. In the former case it will add hydrogens only to the selected atom, in the latter it will add hydrogens to all atoms of type C, N, O, S.

"MS_Molpeak" will generate a graphical display of the "M+" peak of a mass spectrum, taking into account the natural frequency of occurrence of the isotopes. The resolution can be specified to varying degrees of exactness.

"Set role" can be used to assign a role (2^{nd} structure or no role) to a drawn fragment. Currently this is only used for comparison of molecules by substructure.

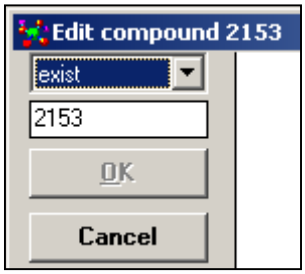
Functions of LiqCryst Advanced

The "advanced" version of LiqCryst allows now to add your own (private) data into the database. The stock-data cannot be modified, but you can add new properties to all compounds, and you can also add new compounds into the database which are not yet registered by LCI Publisher.

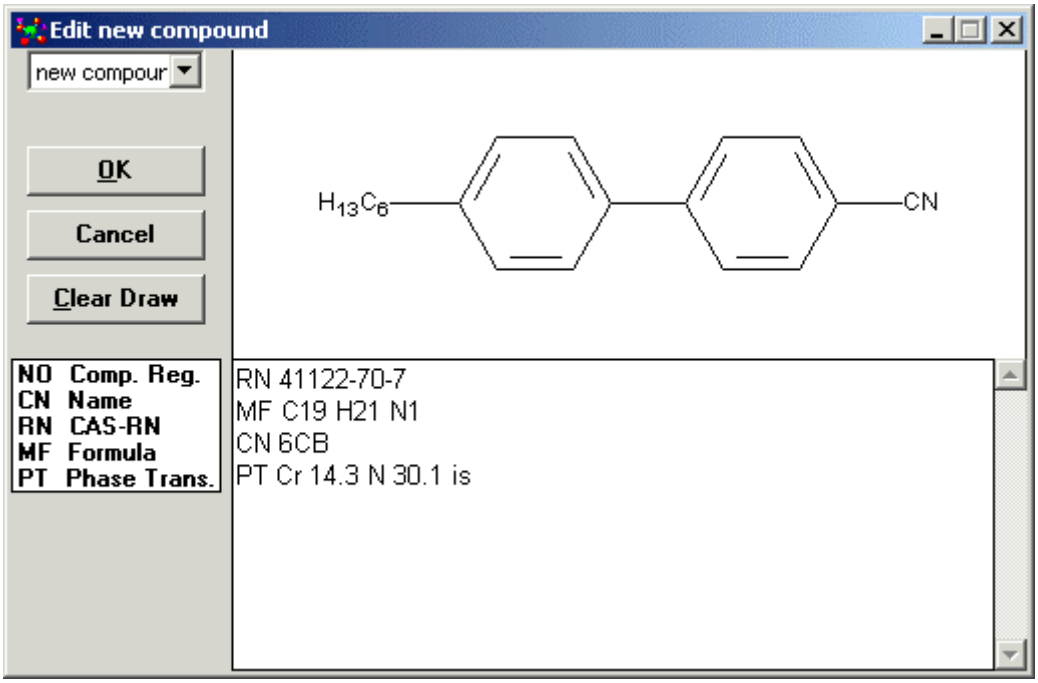
You are free to share your custom data with us, to be included into the next update of LiqCryst (publishing within this database), or keep the private data for yourself. Any new version of LiqCryst will have the option to transport your private data to the newer versions. You only will have to export all your data into an SDF-file, and re-import this SDF-file into the new version of LiqCryst. Since the association of new properties to existing compounds is done via the unique LiqCryst registry number, it is assured that the data will be assigned properly to the new databse.

1) Add New Compounds / Edit Existing Compound

The window for editing an existing compound and adding a new compound is identical, with the exception that for editing an existing compound the running number of the compound will be displayed on the left.To obtain the window for editing a new compound go to the "New Compound" point in the "Edit"-menu. LiqCryst stock-data cannot be edited, so that OK-button is disabled, when such a compound is displayed.



The small field shown above which shows the “2153” can be used to enter a compound identification which can then be loaded into the edit window.



The compound fields are displayed in the list-box on the left side, the meaning is as follows:

NO Compound registry number – it's recommended not to use registry numbers for your own compounds within LiqCryst, because of the possibility of clashing with future officially registered LiqCryst compounds.

CN Compound names, one per line. There can be an arbitrary amount of compound names (IUPAC-names, or trivial names), the limit is about 32 kbyte of data for one compound.

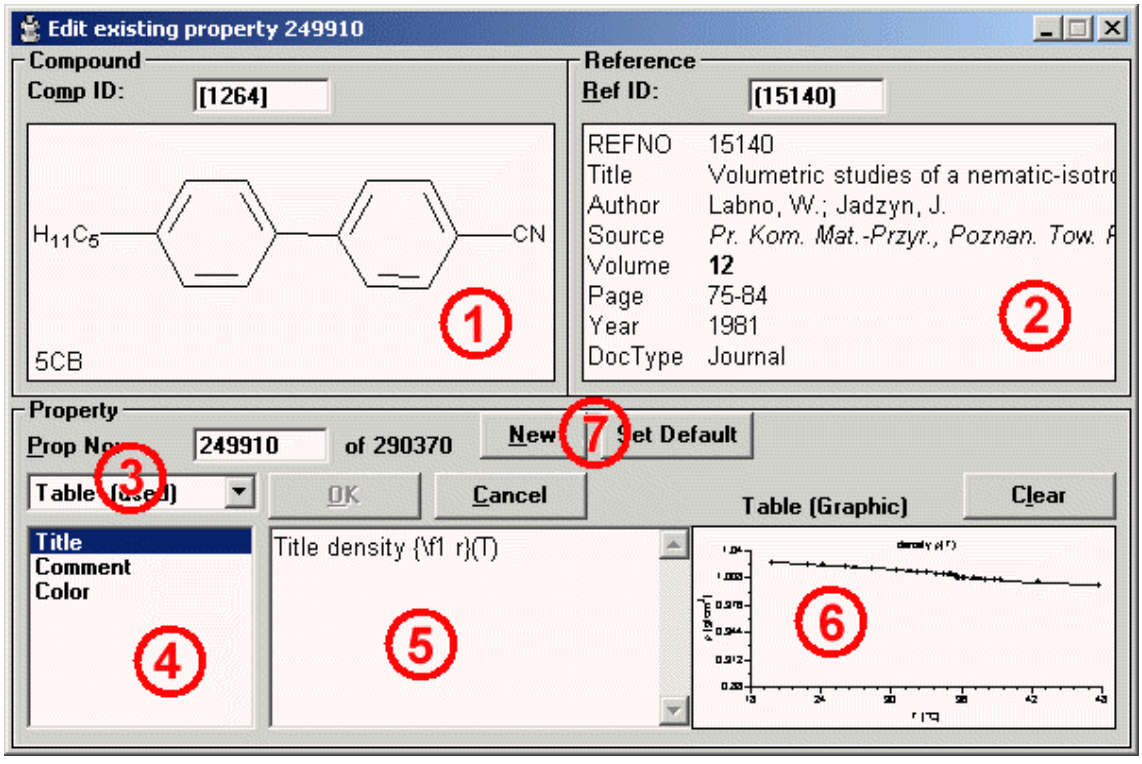
RN CAS-Registry number. Only one registry number can be assigned to a compound in this way, in case you need multiple CAS-RN, you need to register the others as properties (see below)

MF Molecular Formula

PT Liquid Crystal Phase Transition. This is the phase sequence which is used for searches with the "Search by Mesophase" function. Note that this entry will not be shown within the normal property list of the single compound display, so you might want to register the same phase transtions as a new property additionally

2) Add New Properties / Edit Existing Property

The window for editing an existing property and adding a new property is identical. LiqCryst stock-data cannot be edited, so that the OK-button is disabled, when such a property is displayed like in the example below. Description of the coloured circled numbers follows on the next page

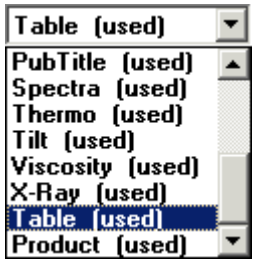


Description of the areas of the Edit Property Window

1 The Compound currently associated with the property is shown in this area. To add a different compound, either enter the number of the compound (running-number, registry number in square braces or a CAS-RN) in the textbox above and press return, or use the “drag and drop” feature by clicking on a compound in any other window (hold the mouse-button down) and drag it over the compound area in the Edit Property Window and release the mouse button.

2 The Reference currently associated with the property is shown in this area. To add a different reference, either enter the number of the reference (running-number or registry number in brackets) in the textbox above and press return, or use the “drag and drop” feature by clicking on a reference in any other window (hold the mouse-button down) and drag it over the reference area in the Edit Property Window and release the mouse button.

3 This drop-down list contains all the defined property types, a selection is shown on the right. To define new property types of your own, choose from the Edit Menu “Edit Property Definitions”. Upon selecting one of these types, its subfields will be copied into the area below (marked (4)). Used Properties will always be listed first, followed by Property-Types for which there is not yet anything registered.



4 This list shows all the available sub-fields of the property-type selected from the box above. The subfields “comment” and “color” are always present, the rest depends on the specific property-type chosen. In the shown example, the property-type “Table” has as a subfield “Title”.

5 The actual text of the property. The format of this is the subfield followed by a blank and the content of the field. Different subfields go on different lines. Text-formatting can be done with a subset of RTF (RichText) definitions, see the list below.

6 For properties that also have a binary sub-type (like “Table” does), a representation of the binary data will be displayed in this part of the window. Double-clicking on this sub-window will allow you to edit the table itself.

7 The buttons “New” and “Set Default”.

“New” allows to create a copy of an existing property, which you want to associate to a different compound for example, or which you want to modify slightly. All it does is remove the current property-number, and act the same as if you had chosen “New Property” from the Edit-Menu, instead of going to “Edit Current Record”.

“Set Default” allows to set the current content of the box marked as (5) as a default text for any new property, thereby saving a lot of typing if you need to register many very similar properties.

Using formatted Fonts in the Edit Property Window

It is possible to use formatted fonts in Properties and in Compound names, by using a subset of the RTF ("Rich Text Format") specification. To use one of these special character types, include the formatted text in curly braces, and precede the text in the braces with a backslash and the formatation symbol.

The available formatations include:

H{\sub 2}O{\sub 2}	H_2O_2 (subscript)
{\super 13}C	^{13}C (superscript)
{\b Bold}	**Bold**
{\i Italic}	*Italic*
{\ul Underline}	Underline
{\f1 abgd}	αβγδ (Greek letters)
{\gr abgd}	Same as "\f1", but not a standard RTF-tag.

For greek letters, both "\f1" and "\gr" are valid for input of data, but SciDex itself will always use "\f1" for display. Tags can be combined in any which way (with the obvious exception of "\sub" and "\super"), and the curly braces can be stacked and nested at will.

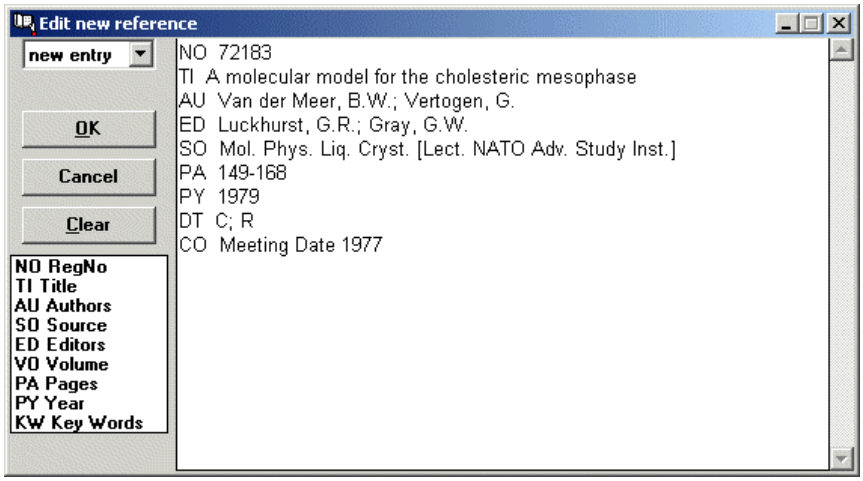
Example for combination:

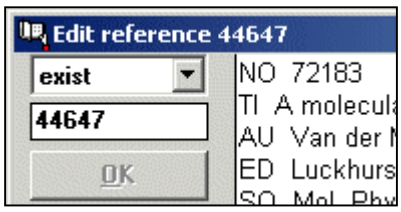
{\b\i Bold & Italic {\ul and underlined}, not underlined {\gr with greek}}

Bold & Italic and underlined, not underlined ωιτη γρεεκ

3) Add New References / Edit Existing Reference

The window for editing an existing reference and adding a new reference is identical, with the exception that for editing an existing reference the running number of the reference will be displayed on the left. LiqCryst stock-data cannot be edited, so that OK-button is disabled, when such a reference is displayed.





The textbox with the number can be used to jump to a particular reference number (to enter a registration number, put the number in brackets)

List of Reference Fields

NO Reference registry number – it's recommended not to use registry numbers for your own references within LiqCryst, because of the possibility of clashing with future officially registered LiqCryst references.

TI The title of the publication

AU Authors – the format should be "<Surname>, <Initial>." separate multiple authors by a semicolon, as shown in the example above, or put them one per line, each line starting with AU, a blank, and then the name.
As an additional help for entering names, a listbox with the more frequent author names will pop up to select from, if you click on the AU-field in the select-box on the left.

SO The Source (e.g. Journal) of the publication, as with the authors, a list of the often-used sources will pop up when you click on that entry.

ED Editors of the Article, formatting of the names should be done identical as with the authors: "<Surname>, <Initial>." Separate multiple editors by semicolon, or put them one per line, starting each line with ED and a blank, followed by the name.

VO Volume number, this is internally a text-field, so both numerical and textual data are possible, and searching for this field is based on a text-search, not on a number-search.

PA Pages of the article in the format <start-page>-<endpage>, if only the startpage is known, simply omit the dash and the endpage. Please keep in mind that currently only the start-page is searchable, though this might be extended in the future.

PY Publication Year

KW Keywords associated to the article, separate multiple keywords by semicolon, or put them one per line, starting each line with KW and a blank, followed by the keyword.

There are a few additional reference fields which can't be chosen directly from the list on the left, but can still be entered manually in the textbox on the right, these are:

CO Reference Comment – any additional information that you deem useful

AN CAS-AN number (CAS referecne registry number)

SH Short label for this reference, if given, this will be used instead of the reference registration number when referring to a reference in a property list

DT Document type, for possible values look at the table below

ISBN ISBN-Number of the book this article appeared in

URL An internet-ressource (http:// or doi://) these are currently not yet hotlinked, but will be in a future version to allow double-click on a reference to reach the full-text online provided you are allowed to access said full-text.

LA Language

PI Patent Number

AI Patent Application Number

List of possible Document Types

J	Journal
P	Patent
D	Dissertation
B	Book
C	Conference
2	2nd Source
I	Information Sheet
U	Unpublished
W	WWW Source
A	Annals or Laboratory Journals
M	Master Thesis
L	Legal Document
R	Review
O	Other Source
T	Translated Source

Every Reference may have multiple document-types, if there's more than one, separate the entries by a semicolon.

4) Data Import and Export of LiqCryst Advanced

To integrate your own private data into LiqCryst, it is possible to go record by record, using the methods described above for input. However, if you already have another database system which is capable of exporting its data to an MDL SDF-file, then this SDF-file can easily be integrated into LiqCryst.

The relevant Compound-definition fields are mentioned above under "Add New Compounds", the main ones being CN → compound name; MF → Molecular Formula and RN → CAS-Number, etc.

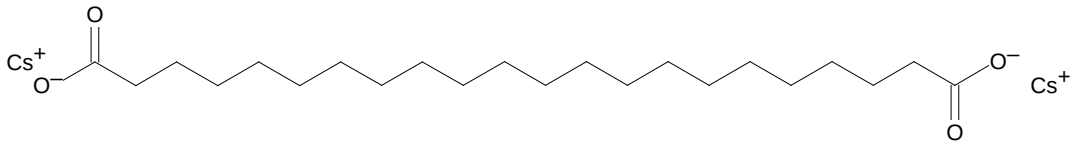
When exporting data out of LiqCryst, only your **own** data will be exported, LiqCryst stock-data will not be contained in the exported SDF-file. As a result, if you import an SDF-file, and later on choose "export all data", the resulting SDF-file might contain *less* information than the original one, because of properties which have been added to LiqCryst stock-compounds. These properties will be exported as well, but instead of the entire compound identification only the LiqCryst registry number will be used to refer to the compound. Nonetheless the exported data are in any case sufficiently defined to be importable intop any future version of LiqCryst without loss of data or precision.

Appendix

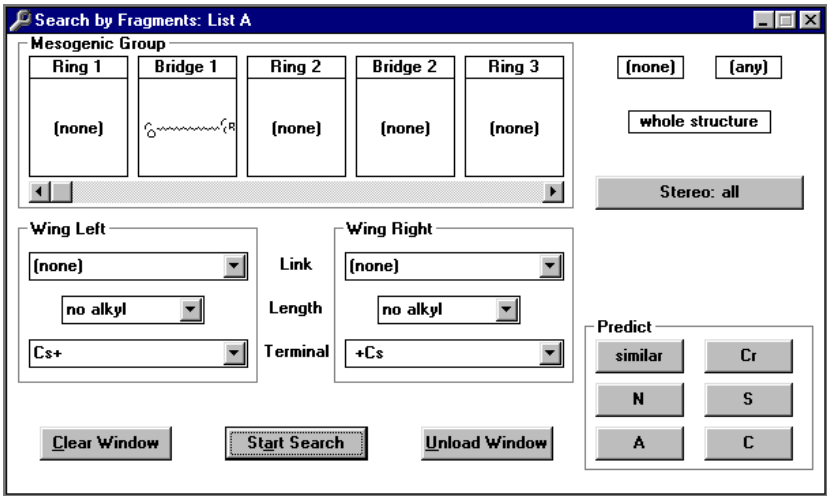
Appendix A: Examples of Searching For Complex Molecular Structures

Salts :

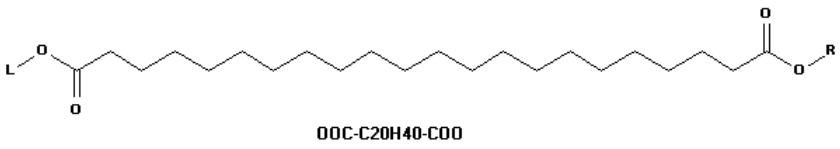
To search for the compound :



Enter in the fragment box :



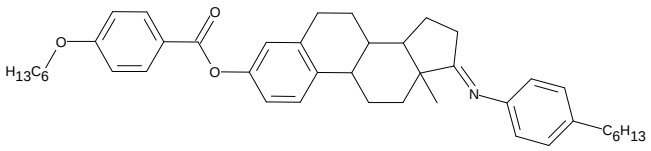
where bridge 1 is :



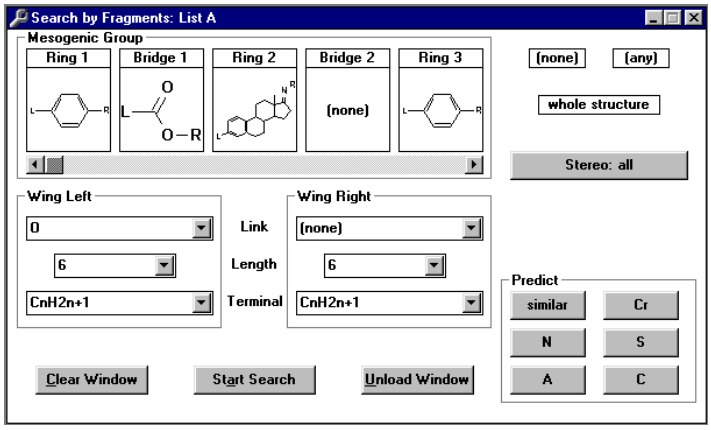
OOC-C20H40-COO

Steroids :

To search for the structure:

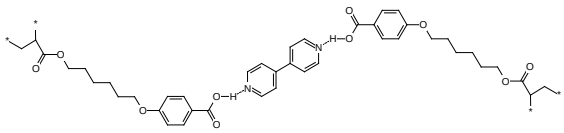


Enter :

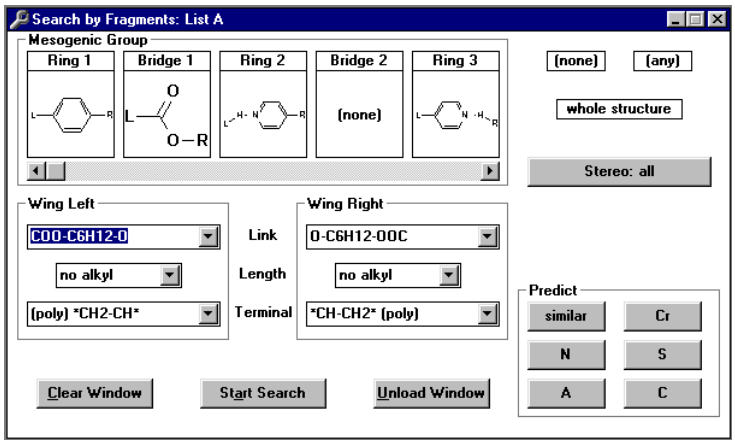


Polymers :

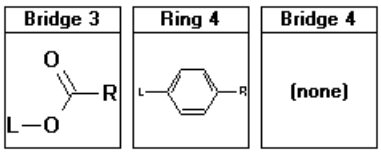
To search for the compound :



Enter in the fragment box :

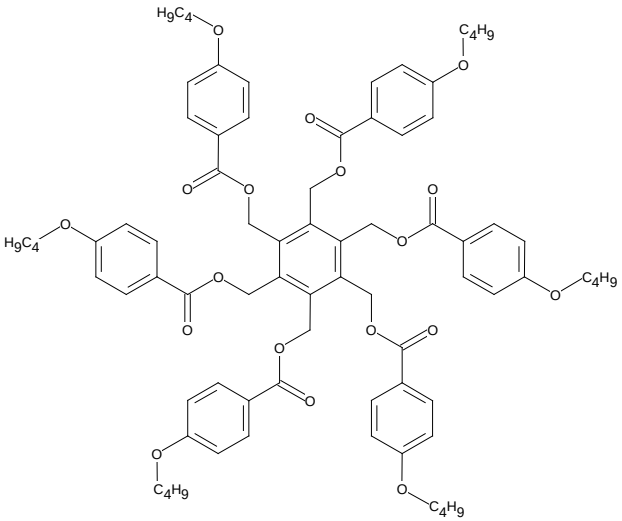


The remainder of the mesogenic group is :

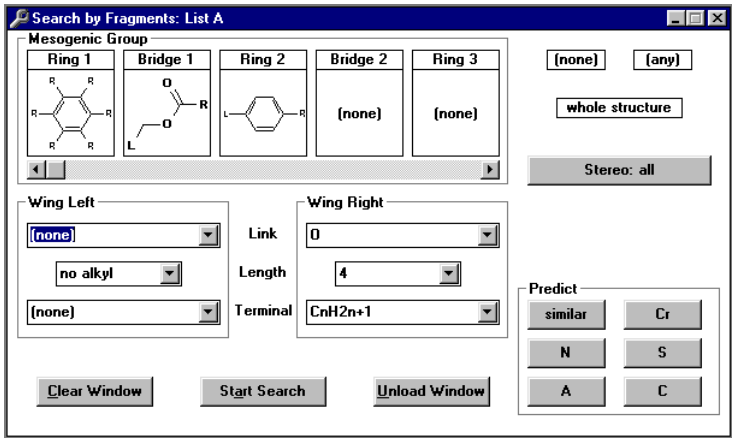


Discotics :

To search for the structure :



Enter :



Appendix B: Explanation of Classifications

Classification	Meaning
Chem : acid	Compound contains free acid group (-COOH, -SO_3H...).
Chem : calamatic structure	Compound without disc-like structure.
Chem : chiral	Chiral compound.
Chem : cis double	A *cis* double bond in a chain fragment.
Chem : combined polymer	Polymer, containing mesogenic groups in the main chain and in the side chain.
Chem : discotic structure	Compounds with a disc-like fragment or a disubstituted, polar head group.
Chem : forked/twin	Unusual chemical structures, such as T-shaped molecules, twin-structures, polycatenars etc.
Chem : H-bonded	Compound with an intramolecular H-bond.
Chem : ionic	Compound with an ionic structure.
Chem : M-C bond	Compound has a carbon-metal-bond.
Chem : mixture	Compound is a mixture of isomers; regioisomers or stereoisomers.

Chem : poly network	Crosslinked polymer, more than two repeating positions of the polymer backbone.
Chem : polymer	All kinds of polymers.
Chem : radical	Compound has a free radical, for example a nitroxide structure.
Chem : side chain poly	Side chain polymer.
Chem : standard structure	Simple calamitic structure, e.g. a compound with one, two or three rings without disc-like or polymer structures; no acids, ions or steroids.
Chem : steroid	Steroid structure.
Chem : sugar/polyol	Compound has an amphiphilic polyol structure, most probably a sugar backbone.
Chem : symmetrical structure	Inversion of the list of fragments will give the same compounds, e.g. wing group left is the same as wing group right, the left ring is the same as the right wing, etc.
Chem : trans double	A trans double bond in a chain fragment.
Ele : F	Compound has at least one fluorine atom.
Ele : Halogen	Compound has at least one halogen atom (F, Cl, Br, I).
Ele: metal	Compound has at least one metal atom.
Ele : N	Compound has at least one nitrogen atom.
Ele : O	Compound has at least one oxygen atom.
Ele : S	Compound has at least one sulfur atom.
Ele : Si	Compound has at least one silicon atom.
Group : cyano	Compound has a cyano group.
Group : nitro	Compound has a nitro group.
Phase : antiferroelectric	Compound has a antiferroelectric phase, e.g. CA, IA.
Phase : calamatic	Compound has a lamellar phase.
Phase : chirality required	Compound has a phase which requires chirality for its existence (TGBA, BP).
Phase : discotic	Compound has a columnar phase.
Phase : ferroelectric	Compound has a chiral, tilted smectic phase, e.g. C, I, F.
Phase : helical, if chiral	Compound has phase, which has a helical structure for chiral compounds, e.g. N, C
Phase : liquid crystalline	Compound has at least one mesophase.
Phase : nematic	Compound has a phase from the family of nematic phases (N, Nd, BP).
Phase : ordered phase	Compound has an ordered smectic phase (B, I, F, G, H, etc.) or an ordered columnar phase (Dho, etc.).
Phase : re-entrant phase	Compound has a re-entrant phase, e.g. Nre, Are, re-entrant isotropic phase.
Phase : solid phase	Melting point or crystal/crystal transitions are given.
Phase : TGB phase	Compound has TGB phase, e.g. TGBA or TGBC.

Phase : tilted phase	Compound has a tilted lamellar or columnar phase (C, I, F).
Ring : aliphatic	Compound contains aliphatic rings (cyclohexane, dioxane, bicyclohexane, etc.)
Ring : aromatic	Compound contains aromatic rings (phenyl, pyrimidine, naphthalene, etc.).
Ring : carbocycles	Compound contains carbocyclic rings (phenyl, cyclohexane, etc.).
Ring : crown ethers	Compound contains crown ethers.
Ring : fused	Compound contains fused rings (naphthalene, cholesterol, etc.)
Ring : large	Compound contains rings with more than 6 members (cyclooctane, etc.).
Ring : N-heteros	Compound contains nitrogen heterocycles (pyrimidine, phorphyrin, etc.)
Ring : O-heteros	Compound contains oxygen heterocycles (furan, dioxane, etc.)
Ring : only 6-membered	Compound contains only six membered rings (phenyl, cyclohexane, pyrimidine) and no rings as naphthalene, thiophene etc.
Ring : other heteros	Compound contains heterocycles containing metals or B, P, etc.
Ring : S-heteros	Compound contains sulfur heterocycles (thiophene, etc.)
Ring : small	Compound contains small rings (cyclopropane, epoxids)

Appendix C: Phase Abbreviations

A	smectic A or neat or Lα	**G**	smectic G
A#	TGB_A, smectic A*	**I**	smectic I
A-M	smectic phases : S_A - S_M	**IA**	antiferroelectric S_{IA}
B	smectic B (smectic B_{hex})	**J**	smectic G', smectic J
BP	blue phase	**K**	smectic K
C	smectic C	**L**	smectic B_{cryst}
C#	TGB_C	**N**	nematic or cholesteric
CA	antiferroelectric S_{CA}	**N***	cholesteric
Cα	$S_{c\alpha}$ (use C~a for input)	**Nd**	discoid-nematic
Cγ	ferrielectric $S_{c\gamma}$ (use C~g for input)	**P**	plastic crystalline, α-phase of lipids
Cr	used as general description for crystalline state in table display (as K)	**Q**	cubic phase
C*	ferroelectric C, chiral C	**R**	re-entrant nematic
CrX	crystal/crystal transition	**S**	smectic
D	discotic	**Are**	re-entrant S_A, or low temperature

			S_A
Dh	hexagonal columnar discotic	**Tg**	glass transition
Dhd	disordered hexagonal columnar discotic	**tr**	unknown transition
Dho	ordered hexagonal columnar discotic	**X**	unknown liquid crystalline phase
Dr	rectangular columnar discotic	**Y**	re-entrant isotropic phase
Dt	tilted columnar discotic	**( )**	consolidation temperature

Clearing Parameters

is	isotropic, nothing unusual
ch	data that have been corrected and assessed
ex	extrapolated temperatures
dec	decomposition at clearing temperature
un	unclear, uncertain data
no	no hints given as to liquid crystalline behaviour, not tested

Appendix D: Abbreviations For Physical Data

α	polarisability (a for input)	**S**	order parameter
α1 – α 6	Viscosity	**ΔS**	entropy (only if enthalpy is not given) (DS for input)
β	helical twisting power (HTP) (b for input)	**Tilt**	tilt angle (SC)
γ1	rotational viscosity (g for input)	**ΔV**	change in volume (only in special cases, see r) (DV for input)
ε	dielectric constant (e for input)	**X-ray structure**	X-ray analysis (exact data on x,y,z for all atoms)
κ	k11+(k33-k22)/4 (k for input)	**X-ray diff**	X-ray diffraction
λ	wave length of selective reflection (l for input)	**neutron diff**	neutron diffraction, neutron scattering
μ	electric dipole moment (m for input)	**PT :**	alternative phase scheme
ρ	density (r for input)	**PT : Tg**	glass temperature
σ	electric conductivity (s for input)	**PT : Tm2**	melting point of a metastable modification
χ	magnetic susceptibility (c for input)	**PT : no LC**	substance is not liquid crystalline

η	viscosity (h for input)	**PT : ^LC**	broadness of liquid crystalline phase(s)
ν	dynamic viscosity (n for input)	**PT : pressure dep.**	temperature / pressure / phase diagram
Cp	heat capacity	**ESR**	electron spin resonance
D	diffusion coefficient	**1H-NMR**	magnetic resonance: proton
d	layer thickness	**2H-NMR**	magnetic resonance: deuterium
E	Exponent	**IR**	infrared spectroscopy
Ea	activation energy	**RAMAN**	raman spectroscopy
ΔH	enthalpy (use DH for input)	**UV**	ultraviolet spectroscopy
k11	elastic constants (k11, k22, k33)	**GC**	liquid crystal used as stationary phase
Mn	average molar mass	**LB film**	Langmuir-Blodgett film
n	refraction index	**FSLC film**	free-standing film
p	pitch (cholesteric phase, SC*)	**film pressure**	surface pressure, p-A isotherm
Ps	spontaneous polarisation	**STM**	scanning tunnel microscopy
PT	alternative phase scheme	**SHG**	second harmonic generation
<P2>	order parameter	**THG**	third harmonic generation
<P4>	order parameter	**r**	intercolumnar distance

Data may also be given on :

Rayleigh scattering
light scattering
ultrasonic velocity
conformation
.....

Additional symbols

Δ	generally used for differences (use D for input) e.g. Δe anisotropy of dielectric constant
⊥	perpendicular e.g. ε ⊥ perpendicular dielectric constant
|	parallel e.g. ε | parallel dielectric constant
“	imaginary part e.g. ε " imaginary part of the dielectric constant
is	isotropic e.g. εis dielectric constant in the isotropic phase
(T)	temperature dependent e.g. ε(T) reference to a diagram : dielectric constant versus temperature

(f)	frequency dependent
(p)	pressure dependent
(λ)	wavelength dependent
(E)	variation of the electric field
(B)	variation of the magnetic field

Frequently used text tags

calculation	computer-based calculations of the conformation
(extra)	extrapolated values
(Dioxane)	solvent
(N)	phase
(589nm)	wavelength
(1 kHz)	measured frequency
(0.98Tc)	relative temperature
(Tc-3)	relative temperature

Units

ΔH	kJ/mol , kcal/mol , cal/g
η	CP
ν	mm^2/s
p	μm
Ps	nC/cm^2
μ	D, Cm

Appendix E: Abbreviations For Stereochemistry

	no chiral fragment (achiral) or static chiral
1	chiral (R or S)
R	chiral (R)
S	chiral (S)
2	racemate, i.e. a mixture of both enantiomers
3	chiral (SS or RR)
4	chiral racemate (RR + RS), i.e. a mixture of two diastereomers
5	chiral (SR or RS)
6	chiral racemate (SS + SR), i.e. a mixture of two diastereomers

7	racemate RR + RS + SS + SR
8	racemate RR + SS
*****	Chiral
9	Racemate
#	unknown chirality

Appendix F: Abbreviations and Formulas for Analyse Comparison

LiqCryst uses the classical formulas for mean value statistics and linear regression as described in all statistic books.

Abbreviations used:

x, y	pair of data (e.g. transition temperature of compound 1 and 2)
n	number of pairs
X	mean value of x
Y	mean value of y
sx	standard deviation of the x data (scattering of the x values)
sX	standard deviation of the X mean value (error of X)
r	correlation coefficient for the linear regression function between y and x
m,b	parameters of the linear regression function (y = m*x + b)
S	symbol for the sum of all data sets
sqr	square root

Formulae used:

X =	S x / n
sx =	sqr ((S (x · x) - S x · S x) / n · (n-1))
sy =	sqr ((S (y · y) - S y · S y) / n · (n-1))
sX =	sx / sqr (n-1) (sX is not used yet in the display)
m =	(S x · y - S x · S y / n) / (S (x · x) - S x· S x / n)
b =	(S y - m · S x) / n
r =	m · sx / sy

Appendix G: Abbreviations Used For Line Notation

NO2	Nitro group on the right hand side of a molecule.
O2N	Nitro group on the left hand side.
-CH2-	Normal methylene group
H2C-	Terminal methylene group on the left hand side of a molecule, e.g. H_2C=CMe-COO ...
|	Marks the beginning or the end of a Search String. This symbol is needed when an exact definition of a Search String is wanted (no similar compounds will be searched for)
Cl	Chlorine in an unspecified position.
|Cl	Chlorine as a terminal group on the left hand side of a molecule.
OOC-?-COO	One '?' symbol can be used in a query. This symbol can be used to define parts of a bridge, whereas in a Search by Similarity only complete bridges can be defined and searched for.
Ph-?COO-Ph	Will find Ph-COO-Ph and Ph-CH=CH-COO-Ph.
C5H11-Ph-Ph-CN	Will search for a compound that includes 5CB (see table of trivial names) as a substructure.
|C5H11-Ph-Ph-CN|	Will search for 5CB as a complete structure..
HPC	Abbreviation for hydroxypropyl cellulose (as a fragment)
HPC-OH	Hydroxypropyl cellulose (unmodified)
PA	Abbreviation for poly acrylates
PA-Ph-Ph-CN	*CH-CH*-COO-Ph-PH-CN The symbol * is used to mark the connection of a polymer with its backbone.
PMA	Abbreviation for poly methacrylates
PMA-Ph-Ph-CN	*CH-CMe*-COO-Ph-PH-CN The symbol * is used to mark the connection of a polymer with its backbone.
2pyr5	Pyrimidine has a substituent on the left hand side in 2-position and a substituent on the right hand side in 5-position.
2py5	Pyridine has a substituent on the left hand side in 2-position and a substituent on the right hand side in 5-position.
BCO	Bicyclooctane
Thiophene	Thiophene has a substituent on the left hand side in 2-position and a substituent on the right hand side in 5-position.
PhMe	3-methyl-phenyl has a substituent on the left hand side in 1-position and a substituent on the right hand side in 4-position. Examples substitutions Cy-COO-Ph-Me 1-(Cy-COO) 4-methyl Cy-COO-PhMe 1-(Cy-COO) 3-methyl Cy-COO-PhMe-Me 1-(Cy-COO) 3-methyl and 4-methyl
MePh	2-methyl-phenyl has a substituent on the left hand side in 1-position and a substituent on the right hand side in 4-position.
Naph	2,6-disubstituted naphthalene
2Dio5	1,3-dioxane has a substituent on the left hand side in 2-position and a substituent on the right hand side in 5-position.
Ph-COO-Ph|	no further substitution on the right hand side, i.e. a hydrogen.

Glossary

Term	Definition
bridge	A fragment: a chain between two rings.
calamatic LC	Liquid crystal without a disc-like fragment.
clearing parameter	A letter or symbol used to complete and evaluate the phase scheme.
combined polymer	Elastomers, polymers with mesogenic groups in the main chain and in the side chain.
discotic LC	Liquid crystal with a disc shaped fragment or columnar phase.
forked	Special ring, bridge and link fragments allow the composition of forked molecular structures. These fragments have more than one connectivity on one side, e.g. linking group N(is used for wing groups as $N(C_2H_5)_2$ (input: link right side N, length 2, type CnH2n+1).
fragment	Part of a molecule. Fragments are connected with single bonds. A fragment can be a ring, a bridge, a link or a terminal group.
isotropic	The normal liquid phase, isotropic liquid phase.
link	A fragment: a chain between a ring and a terminal group.
lyotropic	Liquid crystalline behaviour is induced by a solvent (These compounds are not registered in LiqCryst).
main chain polymer	Polymers with a mesogenic group in the backbone.
mesogenic group	The main body of the liquid crystal structure, containing the rings and bridges.
monotropic	The clearing temperature is lower than the melting temperature. The mesophase of these compounds can only be observed in the supercooled melt.

.Mol File	The type of file as defined by MDL Corp. .Mol Files can be imported from and exported to most of the commonly used chemistry programs.
polymeric LC	Liquid crystal that is part of a polymer
ring	A fragment: this can be a single ring or a fused ring system.
real LC	Compounds with a mesophase.
side chain polymer	Comb-like polymer, a polymer with the mesogenic group in the side chains and not in the main chain (backbone).
similarity	Two compounds are similar, if they differ only in one fragment (see Compare Menu).
static chiral	Compounds where only one enantiomer is predominantly available, e.g. steroids or sugars.
thermotropic	Liquid crystalline behaviour as a result of pure compounds, opposite to lyotropic.
wing group	the side groups of the liquid crystal, comprising of the links and terminal groups.