# Predict Pure

Structure Editor

Structure Data Base

Automatic Group Assignment

and

Property Estimation from Structure


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## Contents

# 1 Introduction

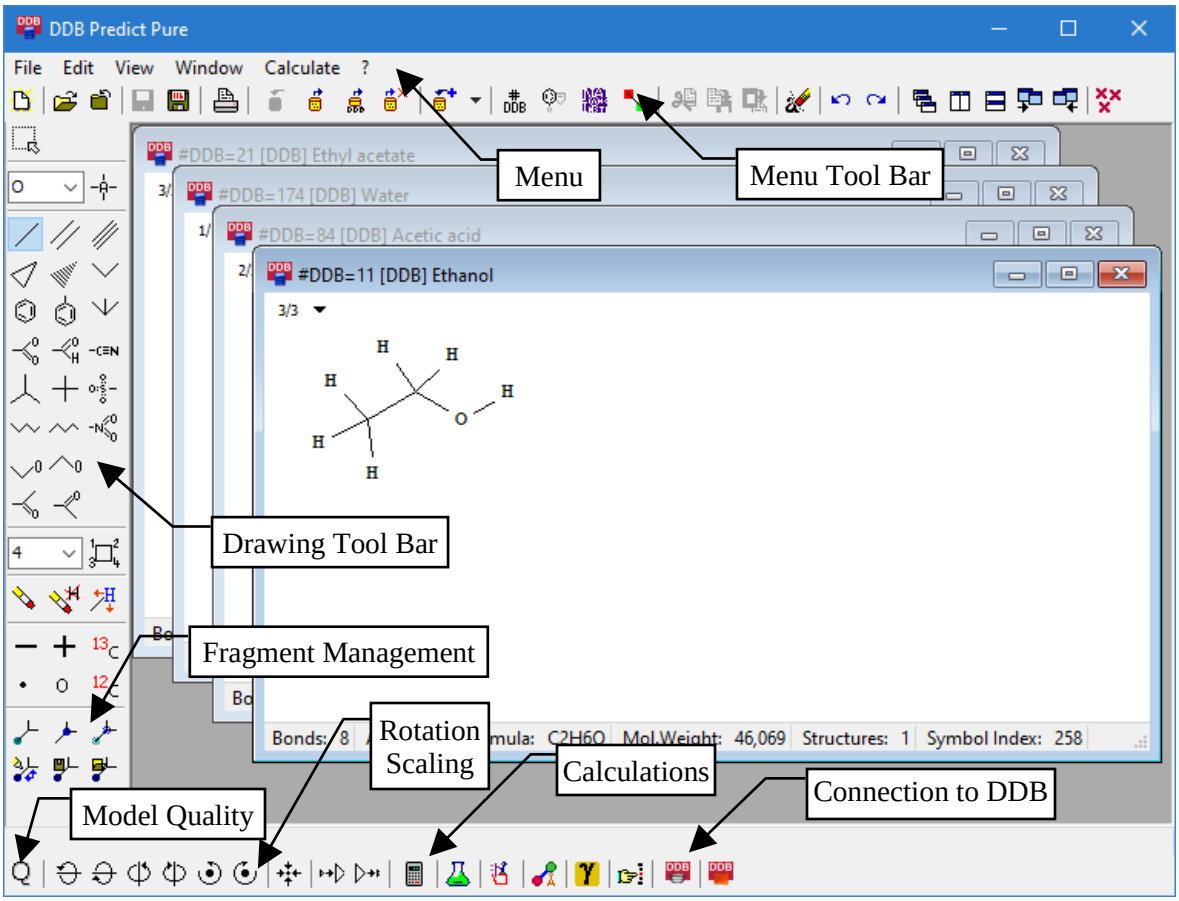
Predict Pure is a tool for editing molecular structures and estimating thermophysical and transport properties from molecular structure directly. Predict Pure contains a structure data bank (ChemDB) with structures of the DDB.

The core algorithm of Predict Pure is an automatic fragmentation which allows to implement a wide range of group contribution methods in a quick and reliable manner. A list of the properties and methods is appended to this document.

The list of methods comprises mainly group contribution methods – because of the underlying fragmentation algorithm – but also some corresponding states methods (equation of states etc.).

Predict Pure can additionally be used as retrieval program for components. The Dortmund Data Bank uses a component number index and this number has to be found either by name, formula, CAS registry number and several other techniques. Predict Pure adds the ability to determine the DDB number from the drawn structure.

# 2 The Main User Interface




Predict Pure is a typical example for a multi-document program contain multiple drawings in a parent window. All functions either in the menus, in the tool bars, or in the context menus are operating on the drawing in the topmost window.

## 2.1 The Menus

### 2.1.1 The File Menu

**New:** Open a new and empty drawing window.

**Open**: Opens a molecular structures file. The list of supported file formats is shown in the appendix.

**Close**: Close current drawing window. If the structure has been modified the program asks if the drawing should be saved.

**Load Structure from ChemDB**: Read a molecular structure from the structure data bank.

**Save structure to database**: Save a (modified) molecular structure in the structure data bank. The structure(s) will be shown in the data sheet of the *DDB Components* application. There the *Save* button can be used make all modifications permanent.

**Add structure to existing component**: If at least one structure has been loaded from the database, then this function can be used to quickly add a new structure to the existing component. The sub-menu lists only component numbers with matching formulas. The structure will be added without confirmation.

**Delete Structure in ChemDB**: Removes a structure from the data bank. If multiple structures exist for the component, then Predict Pure displays a dialog from which the structure to be deleted can be selected.

**Load Component List:** Component lists are containing DDB code numbers. Files with component lists have the extension ".stl", ".stx", or ".txt". The component list is displayed within the *DDB Components* application.

**Load NCI Component by NCI Number**: Predict Pure comes with the NCI (National Cancer Institute, U.S.A.) structure data bank which contains approx. a quarter of a million structures mainly for pharmaceutical components. This menu entry allows loading an NCI component by its NCI number.

**Load NCI Component by CAS Registry Number:** This menu entry allows loading an NCI component by its CAS registry number.

**Load ProSim Compound Definition File:** Predict Pure can load and update compound definition files used and created by the ProSim[1] Simulis process simulation software. See chapter "ProSim Simulis Component File Update" on page 34 and following for more information.

**Add private component**: For adding new components to the data bank Predict Pure opens the program *DDB Components*, which allows to enter name, formula, CAS registry number and molecular weight. The molecular weight and the formula are provided. After entering the necessary values, the component can be appended.

**Save**: Stores the current structure in the file it has been loaded from.

**Save as**: Stores the current drawing in a new file.

[1] ProSim Web Site (http://www.prosim.net)

**Print**: Prints the current drawing. This function always shows a print preview first.

**Print Setup**: Allows the user to select the printer and its properties.

**Exit**: Closes Predict Pure.

**Recent Files**: The sub menu is only visible if at least a single file has been loaded and contains the list of the recently load files.

### 2.1.2 The Edit Menu

**Undo:** Undoes the latest action.

**Redo**: Redoes the latest undone action.

**Cut**: Copies a marked area in the Predict Pure internal buffer and deletes the source.

**Copy**: Copies a marked area in the Predict Pure internal buffer.

**Paste**: Paste a marked area from the Predict Pure internal buffer.

**Clear**: Removes the current drawing.

**Paste from Windows Clipboard:** Pastes a MOL or CTC file from the Windows clipboard.

**Copy as Metafile**: Copies the current drawing as Windows meta file to the Windows clipboard.

**Copy as Bitmap:** Copies the current drawing as Windows bitmap to the Windows clipboard.

**Options**: Displays an option dialog.

**Show Molecule as**

- **Connection Table**: Displays the current structure in CTC format (see description in appendix) or in the MOL format.
- **Fragment for Automatic Group Assignment**: Displays the current structure in a format usable for the automatic fragmentation algorithm.
- **Distance Matrix**: Displays the distance matrix of the molecule (number of bonds between atoms, used mainly for topological indexes).
- **Adjacency Matrix**: Displays the adjacency matrix of the molecule (1 if a bond exists, 0 if not, used mainly for topological indexes).

**Search in ChemDB as Substructure**: This function allows searching the molecular structure data bank for components containing the current structure as substructure.

The dialog displays the found components in a list where the components can be selected. It allows

- loading and displaying the checked components,
- saving the list as a DDB component list (“stl” file) which then can be used in other DDB programs,
- moving the components to the main DDB retrieval program and searching experimental data.

**Search in ChemDB (Exact Match)**: This function searches the structure database for exactly matching structures.

This allows identifying the DDB component number for a molecule which is the main index number in the Dortmund Data Bank. This list can contain multiple structures if conformers are available.

**Search in NCI DB (Exact Match)**: This function searches the NCI data bank for matching structures.

**Search in NCI DB (Fingerprint)**: This allows searching the NCI data bank for components with same (or at least similar) formula.

### 2.1.3 The View Menu

The first three functions call other DDB software applications. These functions are only available if the DDB number of the component is available.

**Pure Component Databank Entries**: Calling the Dortmund Data Bank main retrieval program and start a search for pure component properties of the current molecule.

**Mixture Properties Databank Entries**: Calls the Dortmund Data Bank program and retrieves all data from mixture properties data banks.

**Compound Definition File Entries:** Calls the program *DDB Components* and displays the component file entries (like names, formula, CAS registry number).

**List of Structures from Component List with Group Assignments:** Opens a list of components and shows the group assignments based on a chosen method.

### 2.1.4 The Window Menu

The Window menu contains the standard Windows functions for windows like arrangement, switching to the previous and next window, closing all or some windows, and a list of all windows.

### 2.1.5 The Calculate Menu

**Calculate**: Display the calculation dialog – see details in the "Estimation of Properties" chapter.

**Modify Domalski/Hearing Parameters**: Displays a dialog where group contribution parameters for the Domalski/Hearing models can be modified.

**Reaction Enthalpy**: Display the dialog for estimating the reaction enthalpy – see chapter *Reaction Enthalpy* for details.

**Activity Coefficients**: Displays the dialog for estimating activity coefficients – see chapter *Activity Coefficients* for details.

**Group Assignment**: Display the dialog for the automatic group assignment – see chapter *Automatic Group Assignment* for details.

**MOPAC**: Display the dialog for calling MOPAC, Tinker, and RasMol. See chapter *MOPAC, Tinker, RasWin* for details.

**Search Components with Specific Properties**: Display the dialog for searching components with wanted properties – see chapter *Search for Components with Specified Properties* for details.

**GC-COSMO-RS(Ol):** Opens a dialog with the results of the GC-COSMO-RS(Ol) method. This method allows the estimation σ-profiles for the COSMO-RS(Ol) model by a group contributions method.

**GC-COSMO-SAC**: Opens a dialog with the results of the GC-COSMO-SAC method. This method allows the estimation σ-profiles for the COSMO-SAC model by a group contributions method.

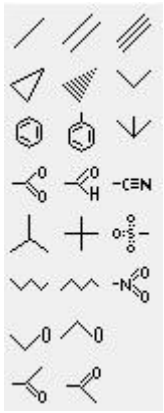
### 2.1.6 The Help Menu

1. **"Manual"** opens the manual.

2. **"ChemDB Overview**" shows the content of the structure data base ChemDB. It also allows updating the index of the data bank to accelerate the access.
3. "**Literature List for Implemented Models**" shows all references of the model and methods implemented in Predict Pure. This function requires the *DDB Access Package*.
4. "**About**" shows Predict Pure program details (like the version number).

# 3 Drawing Structures

Selection of an atomic symbol



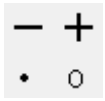
Drawing tools (single bond, double bond, triple bond, wedges, dimethyl group, benzene, methyl benzene, trimethyl group, carboxylic acids, aldehydes, nitriles, isopropyl, tert-butyl, sulfonate, alkyl chains, nitro, glycol chains, ketones)

Rings

Delete bonds and atoms

Delete all hydrogens

Add hydrogens including a simple generation of coordinates.



Charges (minus, plus, radical, none)

Specifying isotope information. The specific mass has to entered in a dialog.

The button  removes all isotope information.

After creating a new drawing window (by File-New or  ) an empty sheet is displayed.

The drawing tools allow the selection of some predefined fragments. The simplest fragment is the single bond 

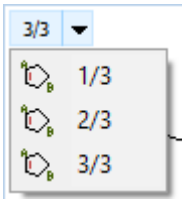
The drawing mode is 'click and drag'. After selecting the position of the start atom of the bond with pressing the left mouse key the structure can be drawn by moving the mouse while keeping the mouse pressed down.

Predict Pure displays a small green box when the left mouse key is pressed down. This box is the area where drawing of the bond can be canceled. The mouse cursor has to be moved inside this box before the mouse key is released.

The bond itself follows the movement of the mouse while the left mouse key is kept down. When releasing the mouse key while the mouse pointer is outside the initial green box Predict Pure fixes the bond. The green box is also shown when the mouse cursor floats above already drawn atoms and bonds. If a new bond is started on an existing atom the bond is fixed to this atom.

If a fragment has more than a single bond and two atoms there's always one atom dedicated as anchor (center) atom which is set with the initial mouse click and an atom connected to the anchor which follows the mouse movement. The other fragment parts are defined by the position of this atom pair and their bond.

## 3.1 Multiple Structures for a Single Component




The structure data base ChemDB can contain several structures for a single component. These are normally a flat 2D and a 3D structure or structures with or without hydrogens.


If multiple structures are loaded from the ChemDB all these structures are added to a single drawing window and drop down menu in the top left corner indicates how many structures are available and allows switching between them.

Predict Pure selects the flattest structure to be shown first.

The structure shown in the drawing windows is used for calculations and group assignment.

## 3.2 The Context Menu

The drawing window has a context menu with several functions. Some are replicating functions from the main menu (“Search” and “Copy” functions) and one is a short-cut for a function from the drawing tools panel (“Add Hydrogens”).

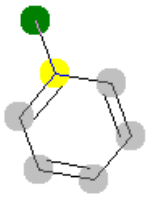
The other functions are only available through this context menu:

- “New Window from Structure” creates a new window with the chosen structure.
- “Add Empty Structure” adds an additional multiple structure to the given window.
- “Make Bond Vertical” and “Make Bond Horizontal”: This allows to change the orientation of the drawn molecule by making the selected bond either vertical or horizontal.
- “Flip Horizontal” and “Flip Vertical”: These functions allow to mirror the drawn molecule.
- “Check Consistency of Multiple Structures”: If two or more structures are available for the current molecules (see also previous chapter “Multiple Structures for a Single Component”) this function allows the user to check if the drawn or loaded structures are identical.

- “Create 2D Structure with OpenBabel” and “Create 3D Structure with OpenBabel”: If OpenBabel is installed it is possible to use it to create 2D or 3D structures with OpenBabel. OpenBabel is invoked by command line and the program “obabel.exe” must be in the Windows search path.
- “Search for Similar Components”. This function is described in chapter 10, “Search for Similar Components”.

# 4 Fragment Management

Predict Pure allows the user to use drawn structures as fragments.



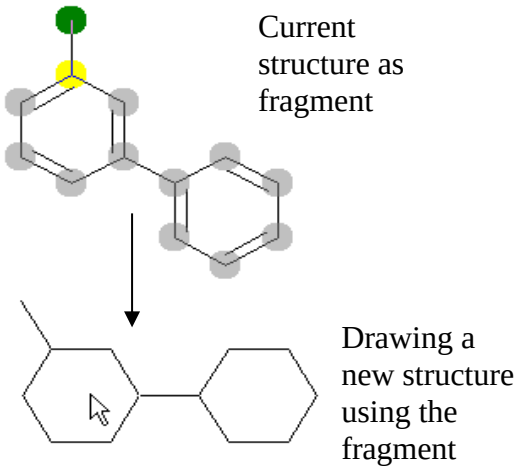
The single icons have the following functions.

Define fragment anchor atom. This atom of a fragment is set with the mouse.

The green circle defines the fragment center.

Define an atom connected to the anchor atom which will follow the mouse movement.

This is the yellow circle in the picture above.




Directly use the current structure as fragment

Save fragment to disk (“.FRA” file)

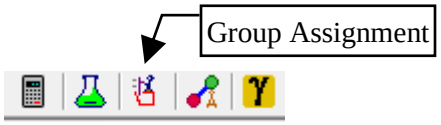
Load fragment

# 5 Automatic Group Assignment

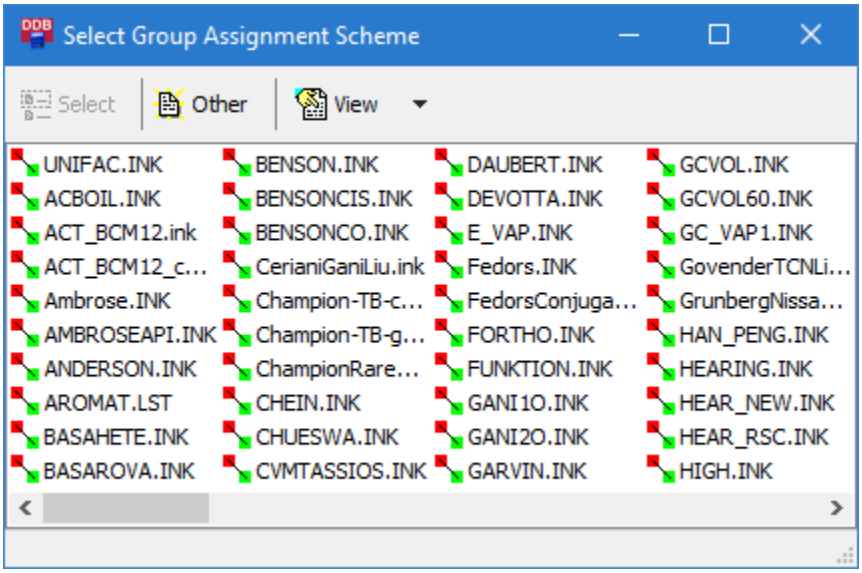
The core technology of Predict Pure is the automatic fragmentation algorithm which breaks a molecule into groups. The groups are the basis for the implementation of group contribution methods.

Since almost every method has its own specific list of groups, Predict Pure provides a bulk of group assignment schemes separately for each model.

The automatic group assignment can be called from the “Calculate” menu by the “Group Assignment” option or by the icon from the tool bar.




The dialog list all files with group assignments (“.INK” files). Most of these “files” are integrated in the Predict Pure program.




The latest group assignment file used will be put on top of the list (here “UNIFAC.INK”). A typical result for the fragmentation of bromo benzene by the UNIFAC model is shown here:

```
Molecule Description
#DDB=26  Bromobenzene
Comment:


Group Assignment
Method: UNIFAC.INK

Group assignment was successful and complete

Subgroup number: 64  Maingroup number: 33  Groupname: Br
Atoms: 1  in 1 Group
Subgroup number: 10  Maingroup number: 3  Groupname: AC
Atoms: 2  in 1 Group
Subgroup number: 9  Maingroup number: 3  Groupname: ACH
Atoms: 3 4 5 6 7  in 5 Groups

DDB Encoded Group List:
      3   1064   1010   5009


List of rings
 6 membered aromatic ring found. Atoms: 2 3 4 5 6 7
```

The group assignment found the UNIFAC subgroups 64 (Bromine), 10 (aromatic carbon with three bonds), and 9 (aromatic carbon with two bonds).

The group assignment can deliver also a list of ortho/meta/para pairs, a list of rings, a list of chains, and the graphical representation of the assignment. The list of rings, chains, and o-, m-, p-pairs are suppressed if no such structural part are present.

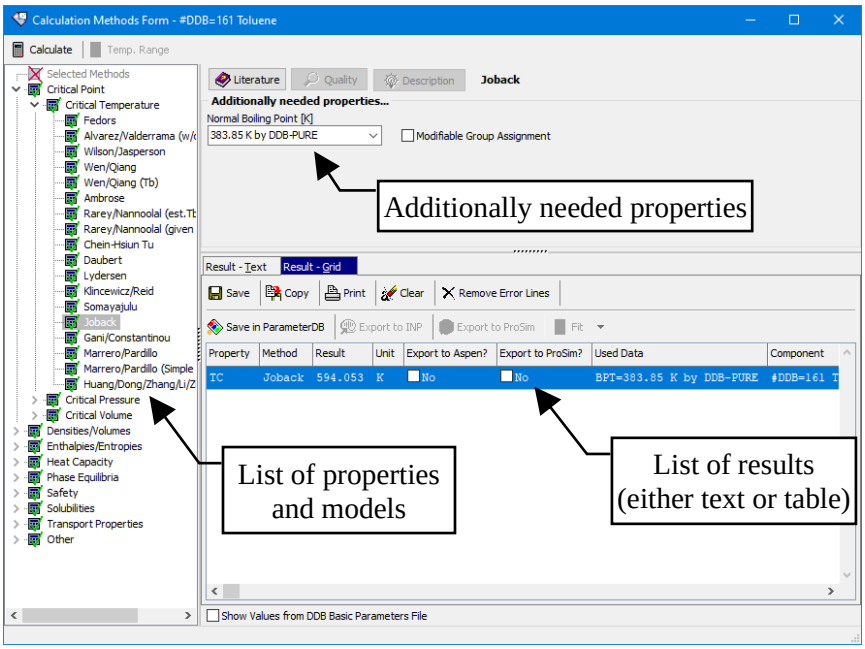
# 6 Estimation of Properties

## 6.1 Overview

Predict Pure was originally designed for the estimation of pure component properties using group contribution methods. Predict Pure now contains several dozens of different estimation methods. A list of models together with the references can be found in the appendix. The calculation dialog can be called either from the menu (Calculate-Calculate) or from an  icon in the tool bar.

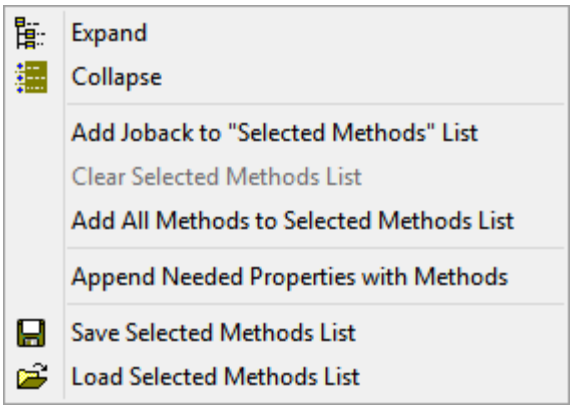
The calculation dialog contains three major parts:

1. The list of properties in a tree view with the different models grouped below the properties.
2. A dialog part where additionally needed properties (besides the model specific group contributions) can be entered. Predict Pure collects result from previous calculations (a "history" of results) and allows to use these results as input for other models.

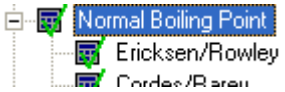



3. The list of results either in a table format or as – in some cases more detailed – text output.

The branch "Selected Methods" can be used to collect methods from different properties branches. This allows the user to make a "selected methods list" for an even quicker access. The different methods can be added by the tree view's context menu entries.




Predict Pure allows the user to calculate properties by single methods and by all methods for a property. If the property line is selected all methods are calculated in a row. If a single method is selected only this single method is used.





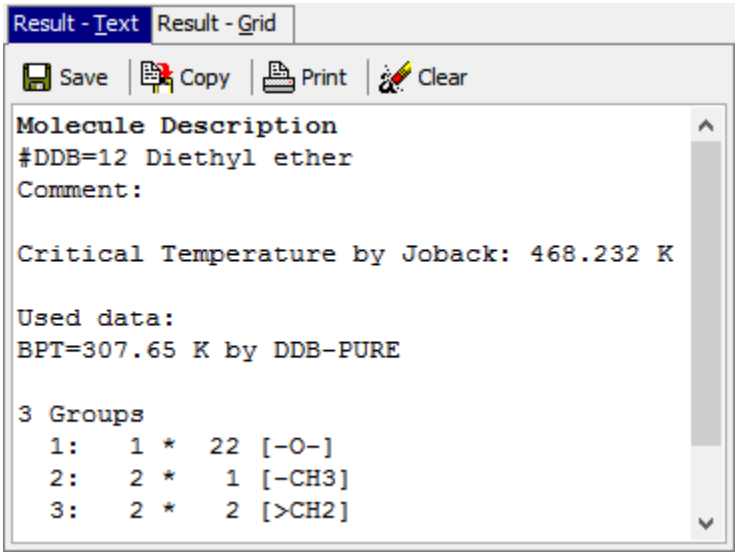
Some methods need additional input besides the structural information. The list of additionally needed properties is displayed in the dialog and the user has to fill the missing information. If data are missing and a complete property calculation is started the methods with missing values will fail.

Predict Pure provides a history of all results calculated or entered before and from the pure component basic file (which are e. g. critical data, see component editor for more details).

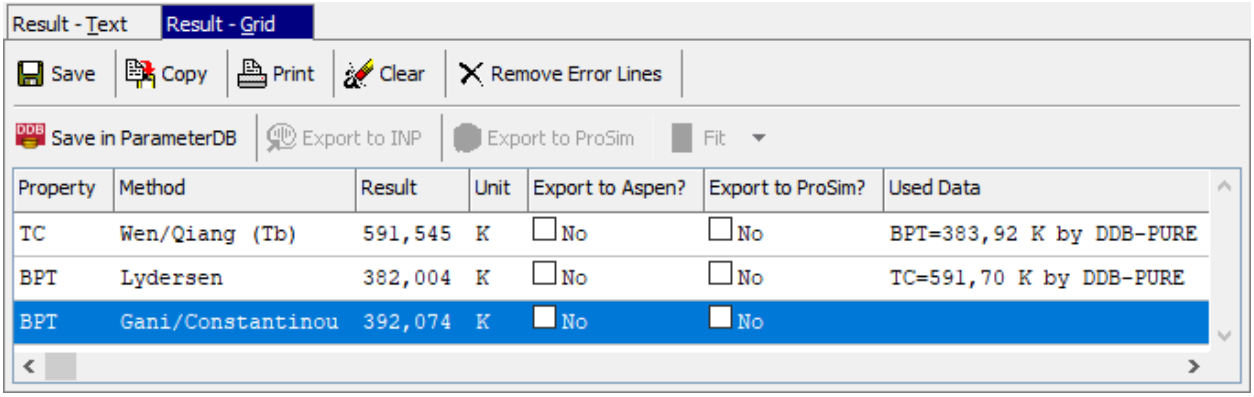
## 6.2 Prediction Output

Predict Pure presents the estimation results in two different modes – a table and a text output.

The text output contains additional information – especially the list of groups from the automatic fragmentation.




The table outputs are more concise and allows copying the result to a spread sheet program. Results can also be stored in the DDB parameter data bank (ParameterDDB), as Aspen INP file (selected properties only), or as ProSim compatible XML file.



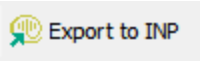
## 6.3 Storing Results in the ParameterDDB


The dialog allows the user to replace or delete already stored sets and to add the current result as a new data set. It also allows the user to alter some of the data set entries (Component, Author, Value, Comment).

This dialog only allows the user to store values in a private (customer) data base. The public data sets (delivered from DDBST GmbH) cannot be modified or removed here.

The values stored in the ParameterDDB will be available for further calculations.

## 6.4 Storing Results as Aspen INP File

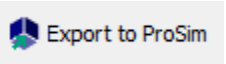



Predict Pure can store

- Critical temperature, pressure, volume
- Normal boiling point
- Melting temperature
- Heat of formation
- Acentric Factor
- UNIQUAC r and q

Predict Pure allows the user to export only single values of each property for a component. The result grid contains check boxes which allow the user to select the values intended for export.

## 6.5 Storing Results for ProSim Software



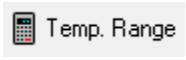

Predict Pure allows storing the properties

- Critical data (temperature, pressure, volume)
- Normal boiling point
- Melting temperature
- Heat of formation

Predict Pure allows the user to export only single values of each property for a component. The result grid contains check boxes which allow to select the values intended for export.

See also chapter “ProSim Simulis Component File Update” on page 34 and following for updating existing ProSim component files.

## 6.6 Temperature-Dependent Properties




For temperature-dependent properties like viscosities, densities, heat capacities and others the input of a temperature range is possible if a single method has been selected. This function does not work for multiple models.

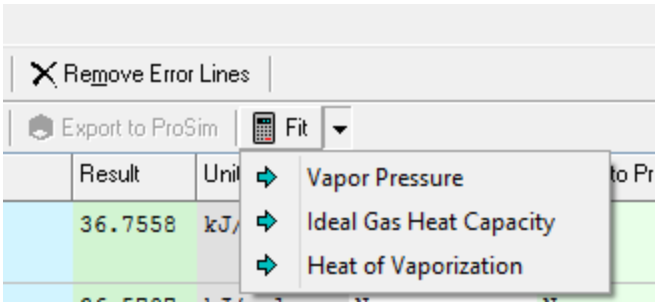
The dialog allows entering a start, an end temperature and a step width or, alternatively, a list of temperatures which can also be copied and pasted.

The results of the prediction are all listed in the normal result grid.

For predicted vapor pressure data an additional dialog is shown with automatically fitted Antoine parameters which then could be copied to the Windows clipboard or saved to the DDB parameter data bank.

The Diagram shows the fitted blue line together with the estimated red circles

### 6.6.1 Fit Prediction Results with Other Equations




Predicted temperature-dependent data like vapor pressures, heats of vaporization, heat capacities, etc. can be transferred to the program “PCPEquationFit” (see separate documentation). This program allows fitting of parameters to a variety of different equations.

# 7 Reaction Enthalpy

Predict Pure allows the user to calculate the reaction enthalpy from estimated and known heats of formation. The calculation dialog is called from the 'Calculate' menu – 'Reaction Enthalpy' or by the  icon in the tool bar. The menu entry is only activated if three of more structures have been drawn or loaded.

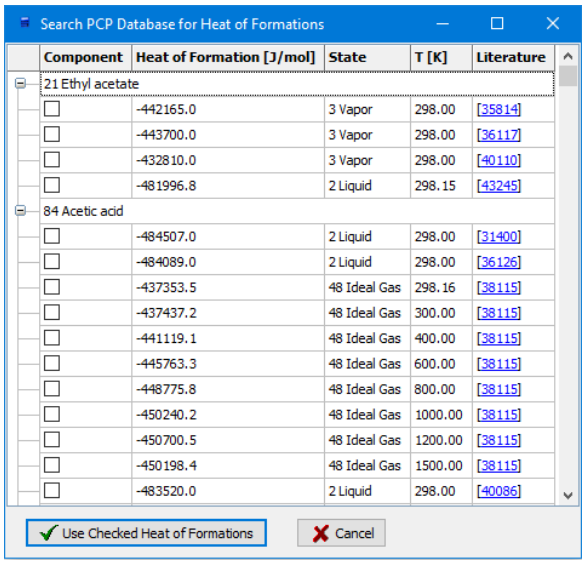
All components are listed initially in the “Available Components” grid. Three types of data have to be provided.

1. The heat of formation of the components – which can be estimated by the methods Domalski/Hearing, Benson, Joback and Gani/Constantinou, typed in, or searched in the Dortmund Data Bank.
2. The state of the component – liquid, gas, solid. This determines the result of the selected method.
3. The number of moles for all components.

The next step is the assignment of molecules as educts (reactants) and products. This can be done by selecting the component in the main grid and using the green and red triangle to add and remove them from the sub grids or by drag and drop. If all data are available the button starts the calculation and displays the result.

## *7.1 Search of Heats of Formation in the Dortmund Data Bank*

The button *Search Heat of Formations in the DDB Database* starts a search in the pure component properties (PCP) branch of the Dortmund Data Bank for heats of formation of the components in the reaction enthalpy dialog.




Only a single heat of formation can be selected for a specific component. The links in the *Literature* column display the reference of the heat of formation.

# 8 Activity Coefficients

Predict Pure allows the user to calculate activity coefficients of binary and higher mixtures with the activity coefficient models

- original UNIFAC
- modified UNIFAC (Dortmund)
- modified UNIFAC (Lyngby)
- NIST mod. UNIFAC

The calculation dialog is called from the 'Calculate' menu by the 'Activity Coefficients' option or by the  icon in the tool bar.

The activity coefficient dialog automatically uses all components currently displayed and performs an automatic fragmentation for the chosen model. The groups are shown encoded – e. g. “4002” means 4 times sub group no. 2.

Two calculation modes are available.

1. Calculate activity coefficients for a list of compositions for a constant temperature
2. Calculate activity coefficients for a list of temperatures for a constant composition

The results of the calculation can be saved as an Excel file or copied to the Windows clipboard.

The *Details* Button opens a dialog with detailed information about the group assignment and the available or missing parameters.

The *Set Compositions* button opens a dialog where the composition can be specified. This dialog allows the user to keep some compositions constant or to set some composition in a specified ratio. The other compositions are calculated as equally distributed points.

If the activity coefficients have been calculated at a constant composition a diagram with the temperature-dependent activity coefficients is displayed.

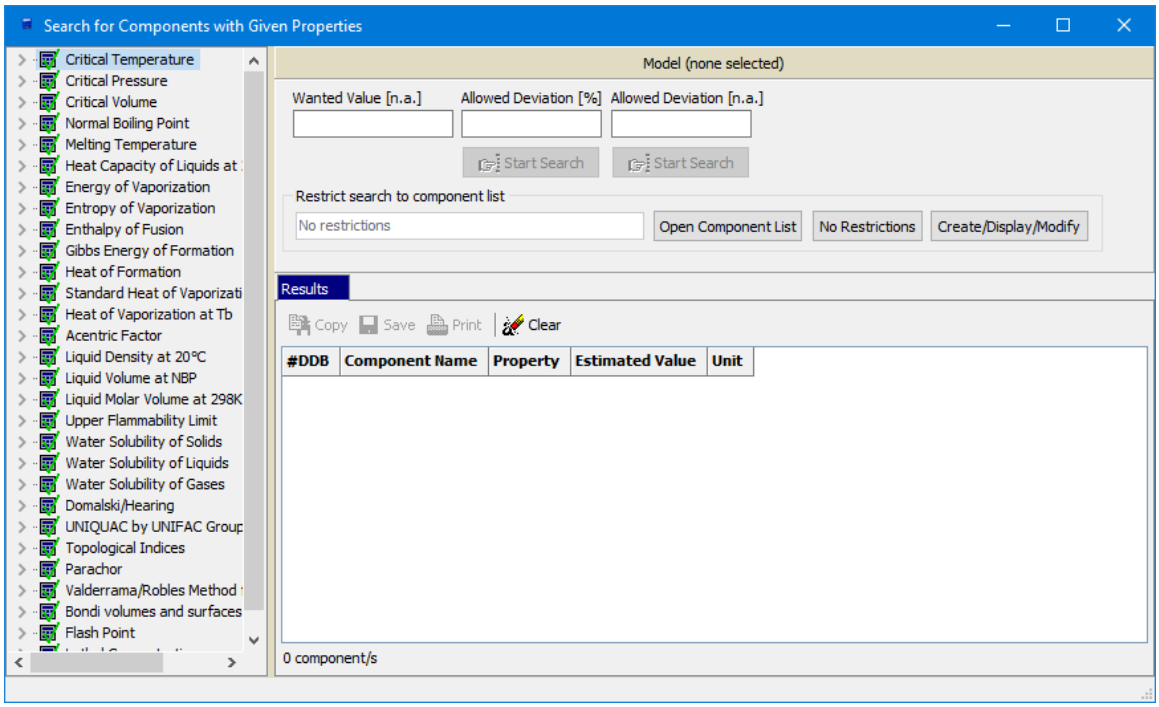
# 9 Search for Components with Specified Properties

Predict Pure can use the built-in models to search for components with specified properties.

The current version is limited to models estimating non-temperature-dependent single values like the critical temperature or the normal boiling point.

The dialog can be opened in the *Calculate* menu by the *Search for components with Specific Properties* menu item or by the icon in the tool bar. It is very similar to the normal calculation dialog. The left pane contains a tree with properties at the top and the models list in the second level.

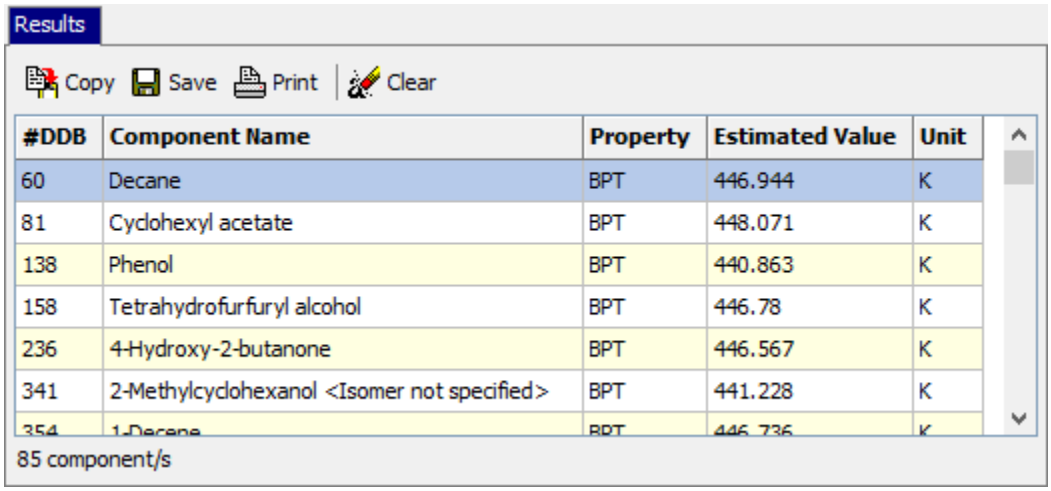
A search is only possible for a single model at a time and it needs the specification of a wanted value and a deviation either in absolute values (e. g. Kelvin for normal boiling points) or in percent.



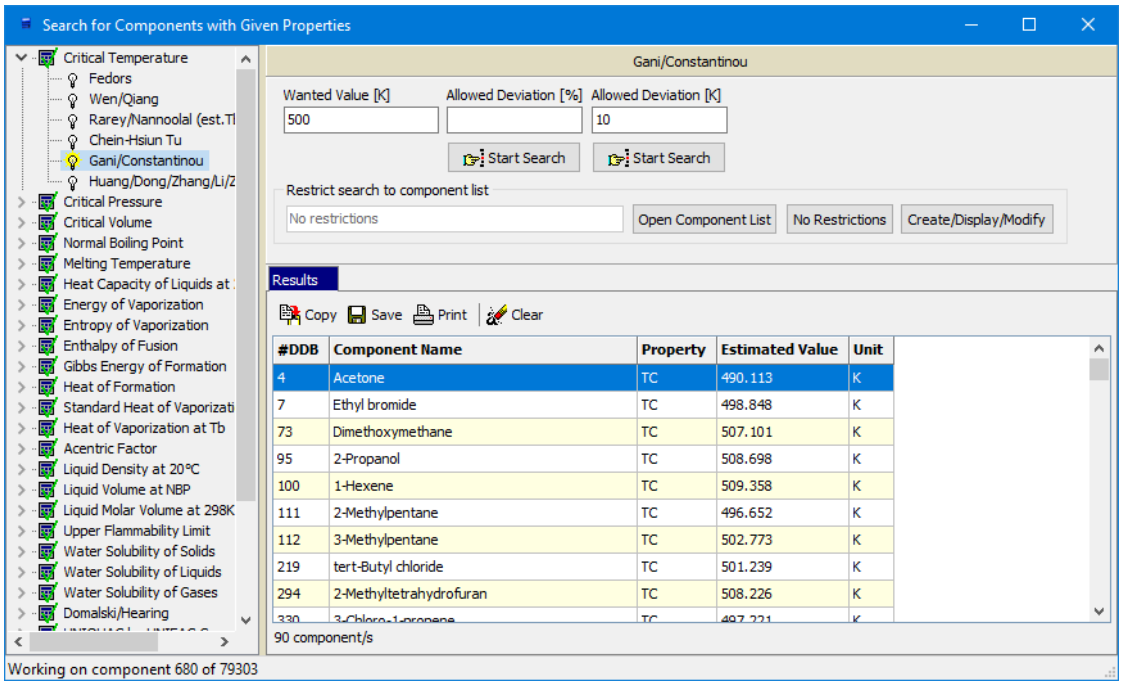

The search can be restricted to a component list which can be created in the other DDB software DDB Components).

The software works through the entire component list and tries to estimate a value for all components stored in the chemical structure data base.

Typical results look like this:




A normal boiling point of 444 K has been searched and the lowed deviation was 1%. The model was "Cordes/Rarey".

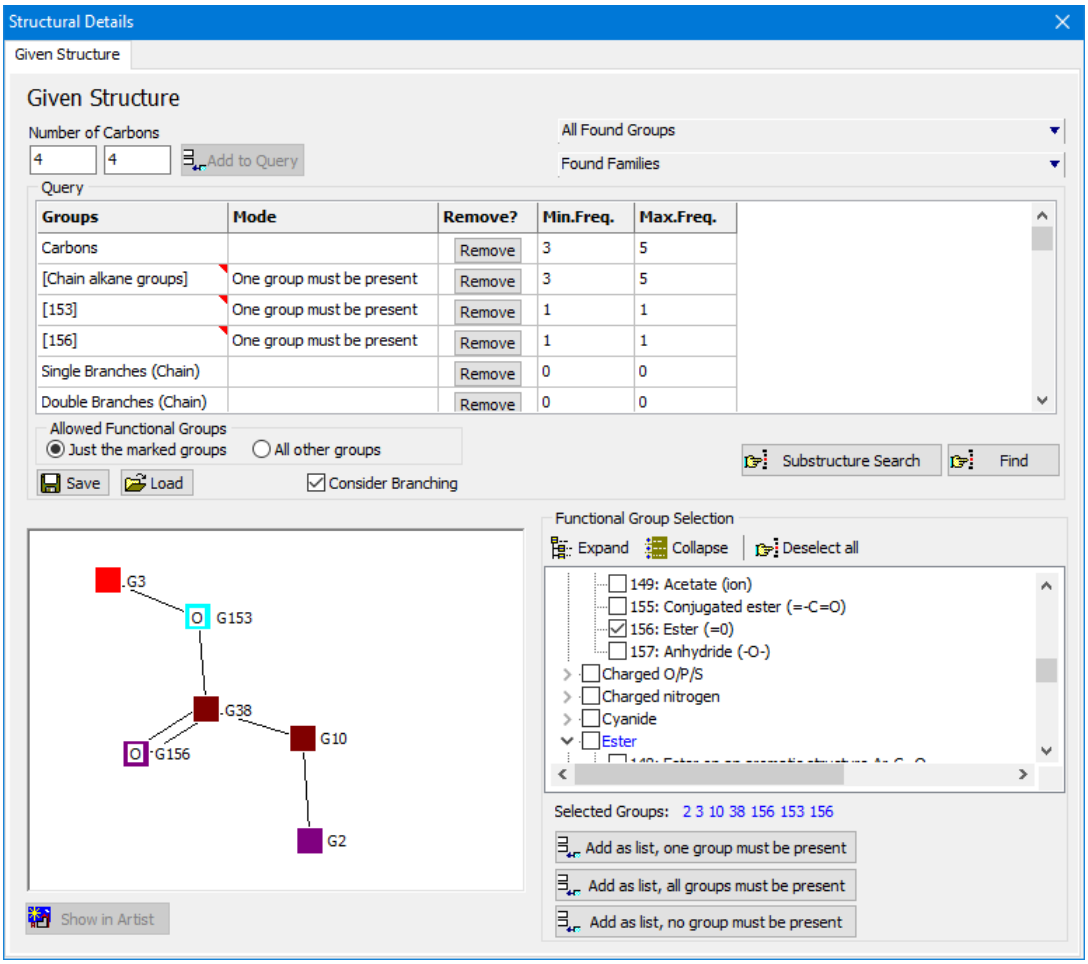



Here a critical temperature of 500 K ± 10 K has been searched with the model of Gani and Constantinou.

# 10 Search for Similar Components

## *10.1 Component Similarity search*

The first way to use the similarity search is to find a list of related components for a given component. This list allows, for example, a broader search for comparable experimental data. When the "Similarity Search" dialog opens, it will automatically create search criteria on basis of the starting component to find comparable components. These criteria can be found in the query window.



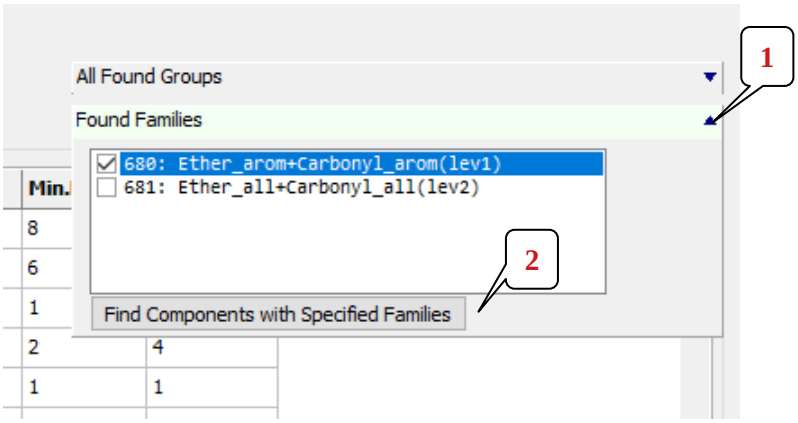

The user can now modify this criteria list for his specific needs if this is necessary

1. **"Carbons"**
   This criterion specifies the limits for the frequency of C-Atoms which are allowed in the wanted related components.
2. **"Aromatic groups"**
   This criterion specifies the limits for the frequency of aromatic carbon groups which are allowed in the related components (e. g. CH group in a benzene).

3. **“Chain alkane groups”**
   This criterion specifies the limits for the frequency of chain-alkane carbon groups which are allowed in the related components (e. g. CH3 or CH2 groups in n-Hexane).
4. **“Cyclo alkane groups”**
   This criterion specifies the limits for the frequency of cyclo-alkane carbon groups which are allowed in the related components (e. g. CH2 group in Cyclohexane).
5. **“Allowed Functional Groups”**
   This criterion specifies the limits of the frequency of the functional groups which are allowed (e. g. OH group in Alcohols). These functional groups are all groups which do not belong to the structure groups named above.
   a) **“Just the marked groups”**
      Only the given functional groups in the query are allowed in the related components.
   b) **“All other groups”**
      The given functional groups have to be in the wanted components, but all other functional groups are allowed.
6. **“Consider Branching”**
   When this option is marked, branching criteria are created on basis of the analysis of the chosen molecule. Only components with a similar branching will be in the list of related components (e. g. n-Pentane and n-Heptane for a given n-Hexane).
7. **“Find”**
   This button will start the search for similar components. After the search a component list is opened.
8. “**Substructure Search**”
   This will also conduct a search but will use the component list to start a substructure for just the found components.

## *10.2 Family Search*

It is also possible to start the similarity search with already predefined component families which contain the given component. For this option the “Found Families” drop down control (1) has to be opened and the wanted family has to be marked.



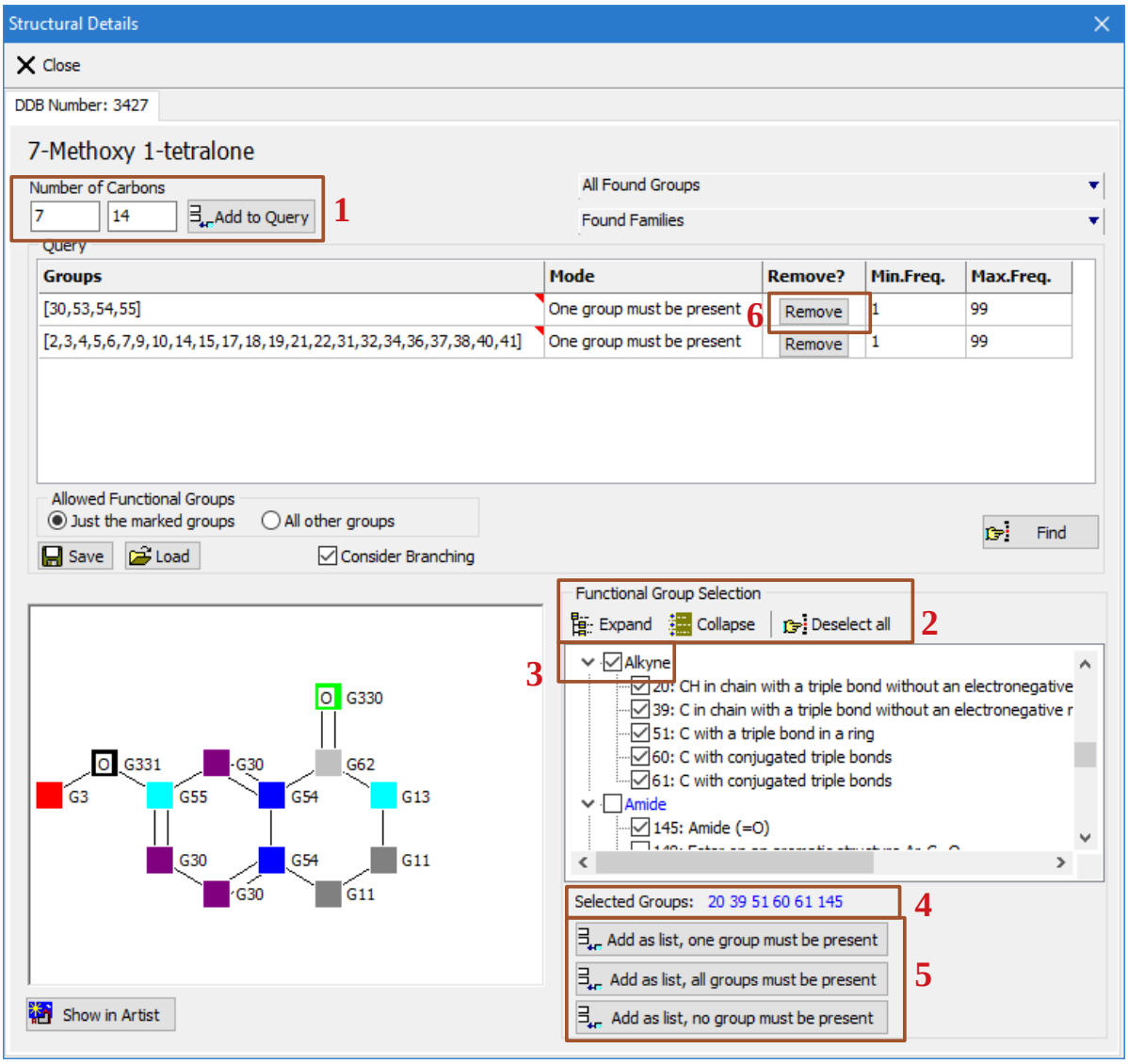
The button “Find Components with Specified Families” (2) will start the search. At the end a list of components with all family members will be shown.

## *10.3 Custom Search*

Another way to use the similarity search is to create own search criteria. Open the “Similarity Search” with a random component. After all unneeded criteria have been deleted by the “Remove” button (6) in the query, new criteria can be defined by the “Functional Group Selection” entries. Specific groups can be marked. If a main group like “Alcohol” is chosen, every sub group is marked. Main groups can be expanded or collapsed by the arrow at the main group (3). It is also possible to expand or collapse all main groups with the “Expand” and “Collapse” buttons at the top (2). The “Deselect all” button removes all marks (2). The selected groups (4) can be added as criterion to the query by the following three buttons (5):

- **“Add as list, one group must be present”**
  Components which fulfill this criterion consist at least of one of the defined groups.
- **“Add as list, all groups must be present”**
  Components which fulfill this criterion consist of all defined groups.
- **“Add as list, no group must be present”**
  Components which fulfill this criterion consist of none of the defined groups.

The frequency of C atoms can be defined by the “Number of Carbons” dialog (1) at the top of the menu (the “Add to query” button will add this criterion). The “Allow functional groups” function can be used in the same way described in chapter A. At the end the list of components which fulfill all criteria can be created by the “Find” button.


Structural Details
Close
DDB Number: 3427
7-Methoxy 1-tetralone
Number of Carbons
7
14
Add to Query
1
All Found Groups
Found Families
Query
Groups
Mode
Remove?
Min.Freq.
Max.Freq.
[30,53,54,55]
One group must be present
Remove
6
1
99
[2,3,4,5,6,7,9,10,14,15,17,18,19,21,22,31,32,34,36,37,38,40,41]
One group must be present
Remove
1
99
Allowed Functional Groups
Just the marked groups
All other groups
Find
Save
Load
Consider Branching
Functional Group Selection
Expand
Collapse
Deselect all
2
3
Alkyne
39: C in chain with a triple bond without an electronegative r
51: C with a triple bond in a ring
60: C with conjugated triple bonds
61: C with conjugated triple bonds
Amide
145: Amide (=O)
G330
G331
G30
G62
G3
G55
G54
G13
G30
G54
G11
G30
G11
Selected Groups: 20 39 51 60 61 145
4
Add as list, one group must be present
Add as list, all groups must be present
Add as list, no group must be present
5
Show in Artist

# 11 MOPAC, Tinker, RasWin

We can distribute neither MOPAC nor Tinker nor RasWin. The user has to download the programs from the Internet. All these programs are freely available (MOPAC at least up to version 7). The calculation dialog can be opened by the *MOPAC* menu item in the *Calculate* menu or by the icon in the tool bar.

## *11.1 MOPAC*

Predict Pure can use MOPAC for some calculations and for structure optimization. Predict Pure has been tested to work with MOPAC version 7, the last freely available version.

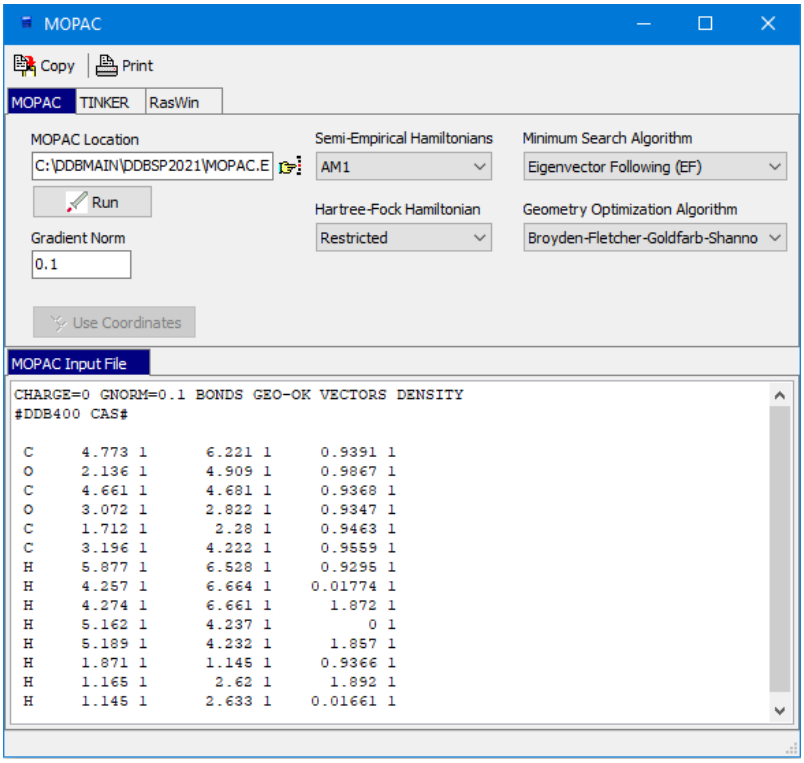
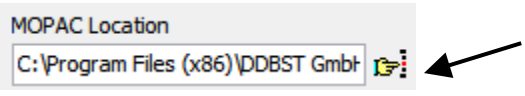



*Figure 1: MOPAC Interface Dialog*

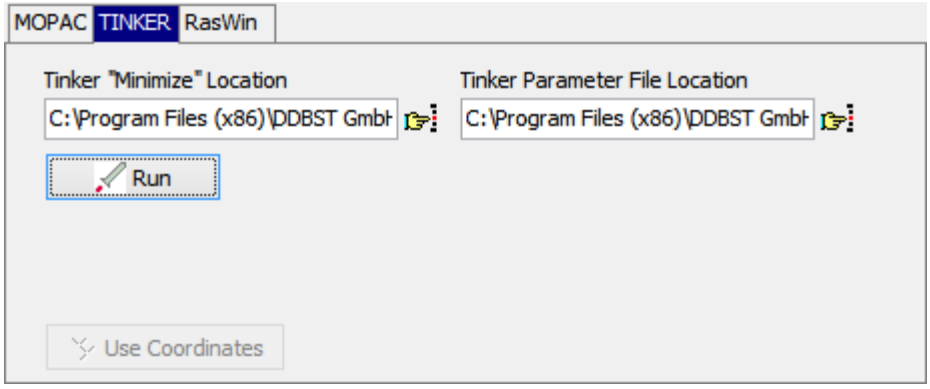
Since MOPAC is a standalone program, the first step for using the program is defining its location in Predict Pure. Predict Pure does not much more than writing a MOPAC compatible molecular structure file (shown in the dialog), calling MOPAC by command line and presenting the results. For a description of the different options please use the MOPAC manuals.




The button 

allows the user to load the coordinates generated by MOPAC.

## 11.2 Tinker

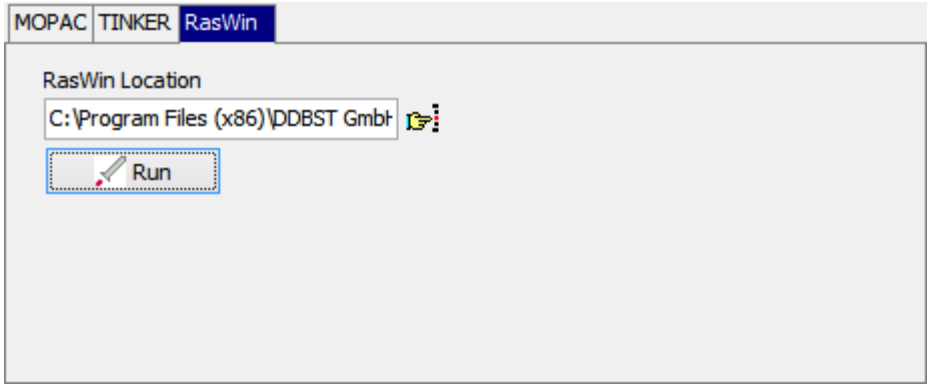



Tinker is a molecular mechanics programs used in Predict Pure for generating 3D structures. The location of the "minimize.exe" program and the location of the "mm3.prm" have to be specified before Tinker can be used.

The button  can be used to read the coordinates generated by Tinker.



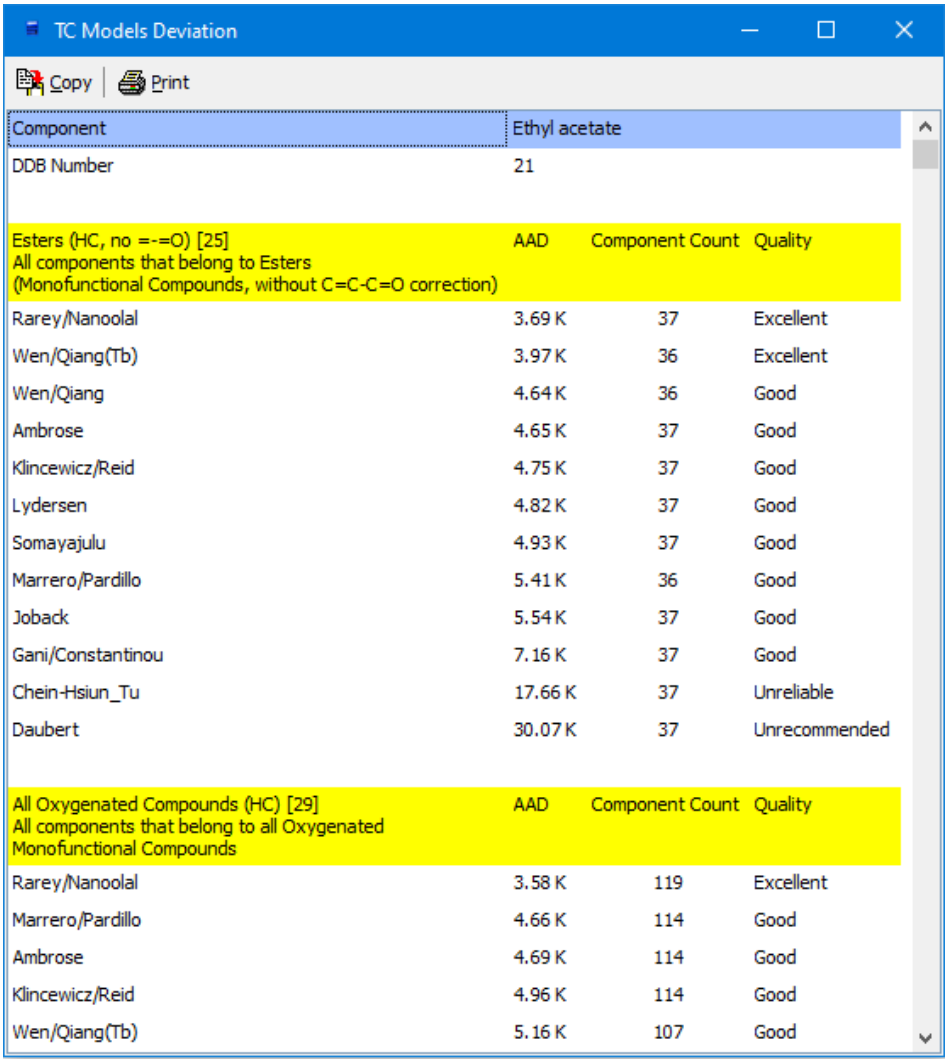
## 11.3 RasWin




RasWin is a rather simple, but free display program for chemical structures. Before first use the location of the program has to be specified.

# 12 Model Quality

Predict Pure contains information on mean deviation for different models estimating normal boiling points, critical temperature, critical pressure, and critical volume.




| Component | Ethyl acetate | | |
|---|---|---|---|
| DDB Number | 21 | | |
| | | | |
| Esters (HC, no =-=O) [25]<br>All components that belong to Esters<br>(Monofunctional Compounds, without C=C-C=O correction) | AAD | Component Count | Quality |
| Rarey/Nanoolal | 3.69 K | 37 | Excellent |
| Wen/Qiang(Tb) | 3.97 K | 36 | Excellent |
| Wen/Qiang | 4.64 K | 36 | Good |
| Ambrose | 4.65 K | 37 | Good |
| Klincewicz/Reid | 4.75 K | 37 | Good |
| Lydersen | 4.82 K | 37 | Good |
| Somayajulu | 4.93 K | 37 | Good |
| Marrero/Pardillo | 5.41 K | 36 | Good |
| Joback | 5.54 K | 37 | Good |
| Gani/Constantinou | 7.16 K | 37 | Good |
| Chein-Hsiun_Tu | 17.66 K | 37 | Unreliable |
| Daubert | 30.07 K | 37 | Unrecommended |
| | | | |
| All Oxygenated Compounds (HC) [29]<br>All components that belong to all Oxygenated<br>Monofunctional Compounds | AAD | Component Count | Quality |
| Rarey/Nanoolal | 3.58 K | 119 | Excellent |
| Marrero/Pardillo | 4.66 K | 114 | Good |
| Ambrose | 4.69 K | 114 | Good |
| Klincewicz/Reid | 4.96 K | 114 | Good |
| Wen/Qiang(Tb) | 5.16 K | 107 | Good |

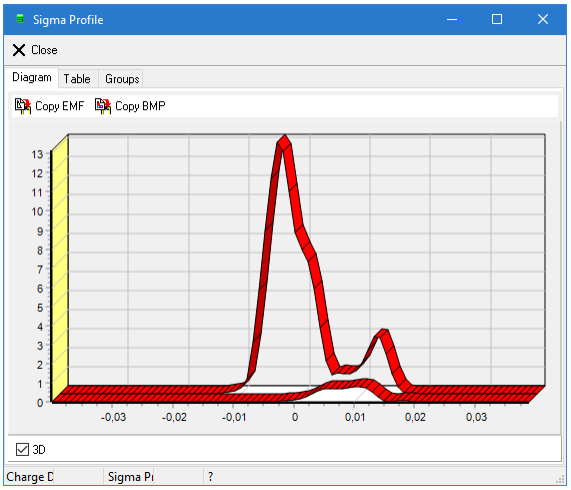
The quality dialogs can be called either by the Q button from the main dialog or by the Quality button from the calculation dialog. The data bank contains quality information for component classes. The current atom is assigned to these classes and the stored information for the appropriate component classes. The component classes are organized hierarchical. There are comprehensive classes like “Hydrocarbons” and more detailed classes like “Aromatic Hydrocarbons”. The AAD (average absolute deviation) is given in Kelvin, the “Component Count” column displays the number of tested components and the “Quality” column gives a (quite arbitrary) comment on the quality.

# 13 COSMO-RS σ-Profiles

In a 2007 publication[2] a group contribution method for creating COSMO-RS σ-profiles ("Surface Charge Density Profiles) and cavity volumes for COSMO-RS(Ol) has been developed.

In 2009 a second method for COSMO-SAC has been published[3].

Predict Pure allows the creation of σ-profiles by these two new methods in the 'Calculate' menu by using the 'GC-COSMO-RS(Ol)' or the 'GC-COSMO-SAC' option.




The result dialog display three different output pages.

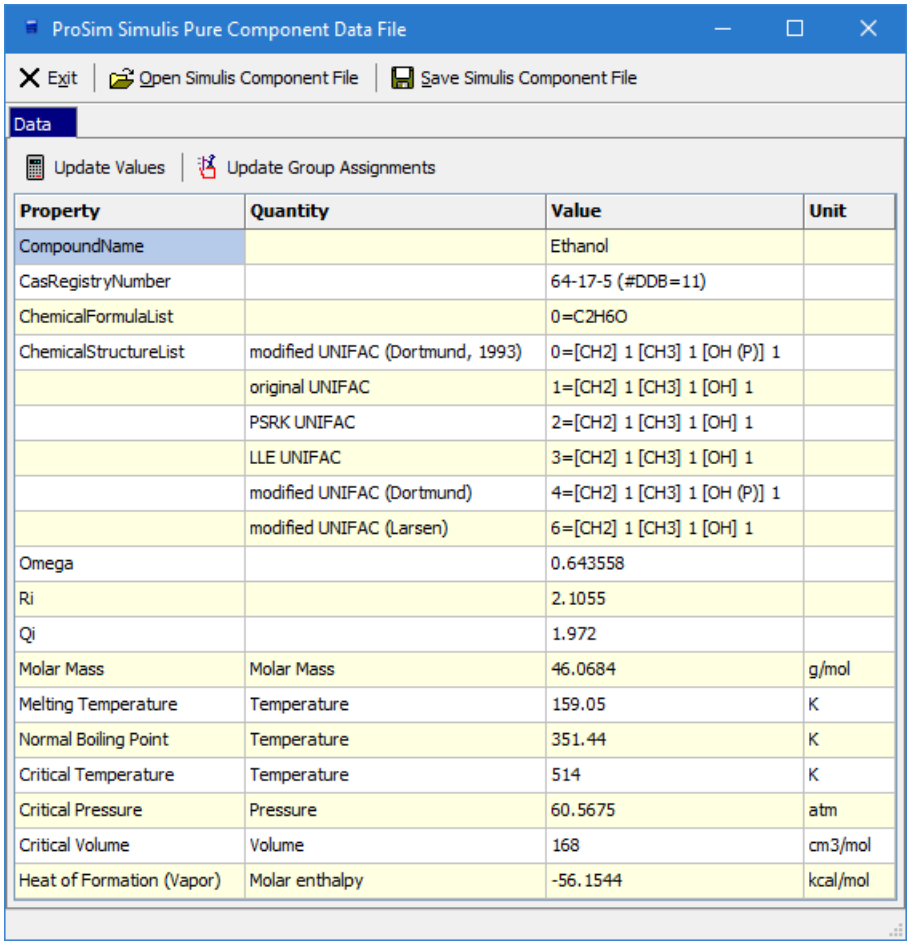
1. The σ-profile diagram. For COSMO-RS(Ol) two lines with 80 intervals are shown. The additional line contains charge densities covering hydrogen-bonding. COSMO-SAC only uses 50 intervals and no separate hydrogen-bonding profile.
2. The second page contains the table with the actual data. This table can be saved to a file in a format usable by DDB software.
3. The third page shows the groups found in the current molecular structure.

[2] Mu T., Rarey J., Gmehling J., "Group Contribution Prediction of Surface Charge Density Profiles for COSMO-RS(Ol)", AIChE J., 53(12), 3231-3240, 2007

[3] Mu T., Rarey J., Gmehling J., "Group Contribution Prediction of Surface Charge Density Distribution of Molecules for COSMO-SAC", AIChE J., 55(12), 3298-3300, 2009

# 14 ProSim Simulis Component File Update

Predict Pure can load and update compound definition files used and created by the ProSim[4] Simulis process simulation software. The component identification relies on the CAS registry number. If a CAS-RN is not specified in the ProSim component file the assignment will fail.




| Property | Quantity | Value | Unit |
|---|---|---|---|
| CompoundName | | Ethanol | |
| CasRegistryNumber | | 64-17-5 (#DDB=11) | |
| ChemicalFormulaList | | 0=C2H6O | |
| ChemicalStructureList | modified UNIFAC (Dortmund, 1993) | 0=[CH2] 1 [CH3] 1 [OH (P)] 1 | |
| | original UNIFAC | 1=[CH2] 1 [CH3] 1 [OH] 1 | |
| | PSRK UNIFAC | 2=[CH2] 1 [CH3] 1 [OH] 1 | |
| | LLE UNIFAC | 3=[CH2] 1 [CH3] 1 [OH] 1 | |
| | modified UNIFAC (Dortmund) | 4=[CH2] 1 [CH3] 1 [OH (P)] 1 | |
| | modified UNIFAC (Larsen) | 6=[CH2] 1 [CH3] 1 [OH] 1 | |
| Omega | | 0.643558 | |
| Ri | | 2.1055 | |
| Qi | | 1.972 | |
| Molar Mass | Molar Mass | 46.0684 | g/mol |
| Melting Temperature | Temperature | 159.05 | K |
| Normal Boiling Point | Temperature | 351.44 | K |
| Critical Temperature | Temperature | 514 | K |
| Critical Pressure | Pressure | 60.5675 | atm |
| Critical Volume | Volume | 168 | cm3/mol |
| Heat of Formation (Vapor) | Molar enthalpy | -56.1544 | kcal/mol |

A ProSim component file contains some basic properties that Predict Pure can add or modify. The list of properties is

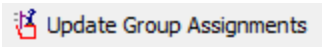
1. Groups assignments for
   a) original UNIFAC
   b) modified UNIFAC (Dortmund)

[4] ProSim Web Site (http://www.prosim.net)

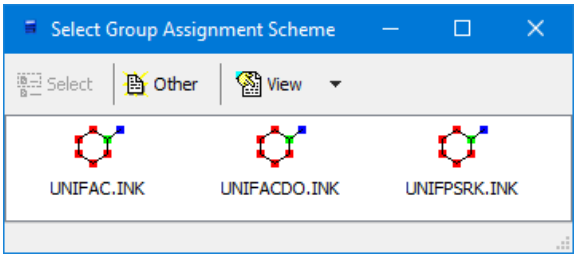
c) PSRK

2. Acentric factor (Omega, ω)
3. Volume and Surface for UNIQUAC
4. Molar mass
5. Melting temperature
6. Critical temperature, pressure, volume
7. Heat of formation of gases

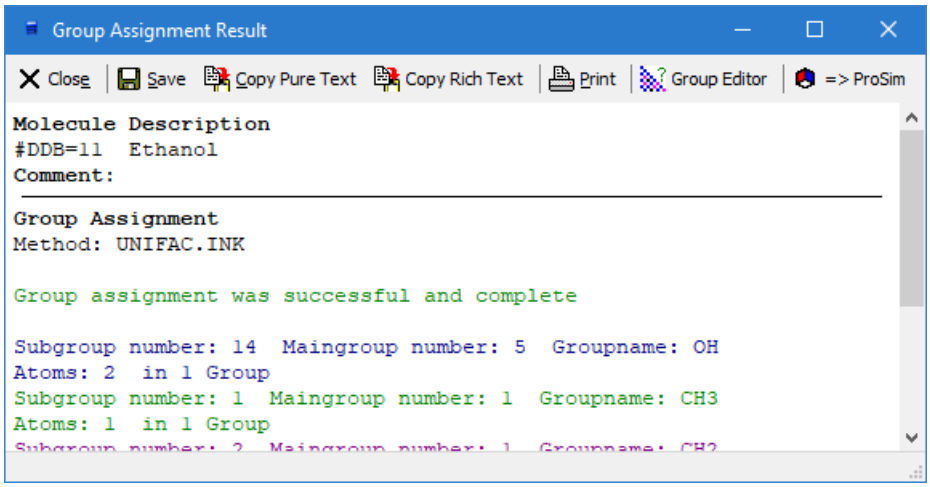
## 14.1 Updating Group Assignments




After selecting one of the three supported models




Predict Pure shows a dialog with the groups assigned to the component's molecule.



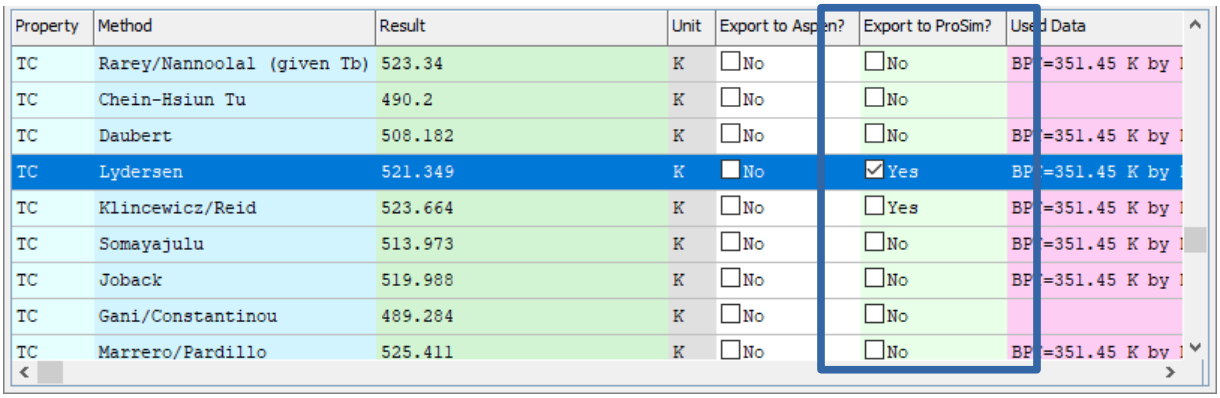

The button 

in the toolbar


will close the group assignment result dialog and enter the obtained groups in the component dialog.

## 14.2 Update Values


This function opens the standard Predict Pure calculation dialog (see chapter “Estimation of Properties” on page 17 and following).



| Property | Method | Result | Unit | Export to Aspen? | Export to ProSim? | Used Data |
|---|---|---|---|---|---|---|
| TC | Rarey/Nannoolal (given Tb) | 523.34 | K | No | No | BP=351.45 K by |
| TC | Chein-Hsiun Tu | 490.2 | K | No | No | |
| TC | Daubert | 508.182 | K | No | No | BP=351.45 K by |
| TC | Lydersen | 521.349 | K | No | Yes | BP=351.45 K by |
| TC | Klincewicz/Reid | 523.664 | K | No | Yes | BP=351.45 K by |
| TC | Somayajulu | 513.973 | K | No | No | BP=351.45 K by |
| TC | Joback | 519.988 | K | No | No | BP=351.45 K by |
| TC | Gani/Constantinou | 489.284 | K | No | No | |
| TC | Marrero/Pardillo | 525.411 | K | No | No | BP=351.45 K by |

The result grid contains an additional column “Export to ProSim?”

where a single line for every property can be selected. Only supported properties can be selected.

The button *Export to ProSim* will enter the selected value in the ProSim component dialog.

## 14.3 Store Component File


The ProSim component saving routine always asks for a file name. The previously loaded file is preselected and can be used to overwrite the old file.

# 15 Appendix

## 15.1 File Formats

Predict Pure supports several file formats. Readable formats are

1. The proprietary DDBST format with the extension ".CTC".
2. The MOL format ".MOL" defined by MDL Information Systems (http://www.mdli.com/).
3. The Tinker ".XYZ" format.
4. The COSMO formats from Gaussian and Turbomole
5. The SDF format; a file containing single or multiple MOL files
6. The SMILES format (file extension *.smi), if OpenBabel is installed

Writable formats are

1. The proprietary DDBST format with the extension ".CTC".
2. The MOL format ".MOL" defined by MDL Information Systems (http://www.mdli.com/).
3. The MOPAC-Z format
4. The Gaussian ".gjf" format.

A description of the MOL format can be found the English Wikipedia:
https://en.wikipedia.org/wiki/Chemical_table_file

### 15.1.1 The CTC File Format

The CTC format is specially designed to match the requirements of the program Predict Pure with respect to storing molecular structures. It is a simple tagged format in pure ASCII. It can be viewed and edited by simple text editors.

The program uses the following tags:

| *Tag* | *Description* |
|---|---|
| #ATOMS | list and description of atoms in the molecule |
| #BONDS | list and description of bonds between the atoms |
| #CAS | CAS registry number of the component |
| #FORMULA | empirical formula of the component |
| #ENAME | English name of the component |
| #TIME | file creation time |

| Tag | Description |
|---|---|
| #PROGRAM | program the file was created with |
| #COMMENT | comment |
| #FILE | original filename |

These tags start blocks within the file. Blocks are ended by another tag or the end of file. There is no special order in which the blocks must appear.

#### #ATOMS

This block contains a list and description of the atoms in the molecule. Hydrogen atoms can be included or may be omitted. The first line must contain the number of atoms in the molecule. The following lines, one for each atom, contain the following entries separated by at least one blank character:

- x-, y- and z-coordinate (Cartesian).
- Atomic symbol. Only symbols from the standard periodic system of elements (PSE) are allowed. Functional groups like COOH or NO2 are not legal entries.
- Charge or radical. The following predefined numbers are used to encode the different types of charges or radicals:
  - **0** → no charge, no radical
  - **1** → charge +3
  - **2** → charge +2
  - **3** → charge +1
  - **4** → radical
  - **5** → charge -1
  - **6** → charge -2
  - **7** → charge -3

The same way of encoding is used in mol files by MDL (Molecular Design). Additional number are

  - **13** → charge +4
  - **12** → charge +5
  - **11** → charge +6
  - **15** → charge -4
  - **16** → charge -5
  - **17** → charge -6
- mass differences to the most common isotope to specify different isotopes.
- chemical environment. The following environment are defined:

- **K** → aliphatic chain ("K" for German "**K**ette" means chain)
- **R** → aliphatic ring
- **A** → aromatic system
- **N** → non-aromatic neighborhood
- **C** → aromatic or ring (cyclic neighborhood)
- ***** → not specified

- molecule number (a ctc structure can contain multiple structures)

#### #BONDS

This block contains a list and description of the bonds between the atoms. The first line must contain the number of different bonds, double and triple bonds are counted as one bond. The following lines, one for each bond, contain the following entries separated by at least one blank character:

- atom counter of the first atom.
- atom counter of the second atom.
- bond multiplicity (1 – single bond, 2 – double bond, 3 – triple bond)
- bond orientation allows simple coding of stereo chemistry.
  - **0** → not specified
  - **1** → in plane
  - **5** → in front of plane
  - **6** → behind plane
- chemical environment in format %c. The following environment are used:
  - **K** → aliphatic chain
  - **R** → aliphatic ring
  - **A** → aromatic system
  - **N** → non-aromatic neighborhood
  - **C** → aromatic or ring (cyclic neighborhood)
  - ***** → not specified

#### #CAS

This block contains the CAS registry number of the component.

#### #FORMULA

This block contains the empirical formula of the component.

#### #ENAME

This block contains the English name of the component.

#### #DATE

This block contains the file creation date. The format is (day. Month. year).

#### #TIME

This block contains the file creation time as the only entry. The format is (hour: minute: second).

#### #PROGRAM

This block contains the name of the program the file was created with as the only entry.

#### #COMMENT

This block contains comments in free format (single line).

#### #FILE

This block contains the original filename.

#### *Examples:*

The following examples illustrate the use of the ctc format.

Ethanol (hydrogen atoms omitted)

```
#DDB
11
#DATE
20.6.2000
#TIME
19:50:59
#ATOMS
3
    87.97         35          0  C  0  0 *  1
       35     42.93     14.03  O  0  0 *  1
    65.88     48.36     23.63  C  0  0 *  1
#BONDS
2
 1  3  1  1 *
 2  3  1  1 *
```

Ethyl benzene (hydrogen atoms included)

```
#DDB
25
#DATE
20.6.2000
#TIME
19:53:30
#ATOMS
18
    149.4      59.29      41.23  C  0  0 *  1
    68.11      116.3      31.62  H  0  0 *  1
    171.1      113.6      93.87  C  0  0 *  1
    224.4      82.79      44.89  C  0  0 *  1
    238.7      131.1      93.24  H  0  0 *  1
       35      126.7      77.62  H  0  0 *  1
    92.86      98.73      125.6  H  0  0 *  1
    68.21      124.8      65.88  C  0  0 *  1
    200.3         35          0  H  0  0 *  1
    257.4      80.93      33.24  H  0  0 *  1
    192.2      56.86      26.11  C  0  0 *  1
      163      135.4        120  H  0  0 *  1
    124.6      39.28      26.76  H  0  0 *  1
       77      58.97      87.07  H  0  0 *  1
    138.9      87.63       75.1  C  0  0 *  1
    213.9      111.1      78.76  C  0  0 *  1
    84.01        156       70.2  H  0  0 *  1
     92.8      90.24      91.39  C  0  0 *  1
#BONDS
18
 4 10  1  1 *
 1 13  1  1 *
11  9  1  1 *
 3 12  1  1 *
 4 11  1  1 *
 8 17  1  1 *
 8  2  1  1 *
 8  6  1  1 *
 4 16  2  1 *
 1 15  1  1 *
16  5  1  1 *
11  1  2  1 *
 3 15  2  1 *
 8 18  1  1 *
15 18  1  1 *
16  3  1  1 *
18  7  1  1 *
18 14  1  1 *
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