

# Artist Property Estimation

Structure Editor

Structure Data Base

Automatic Group Assignment

and

Property Estimation from Structure

**DDBSP** - Dortmund Data Bank Software Package



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## Introduction

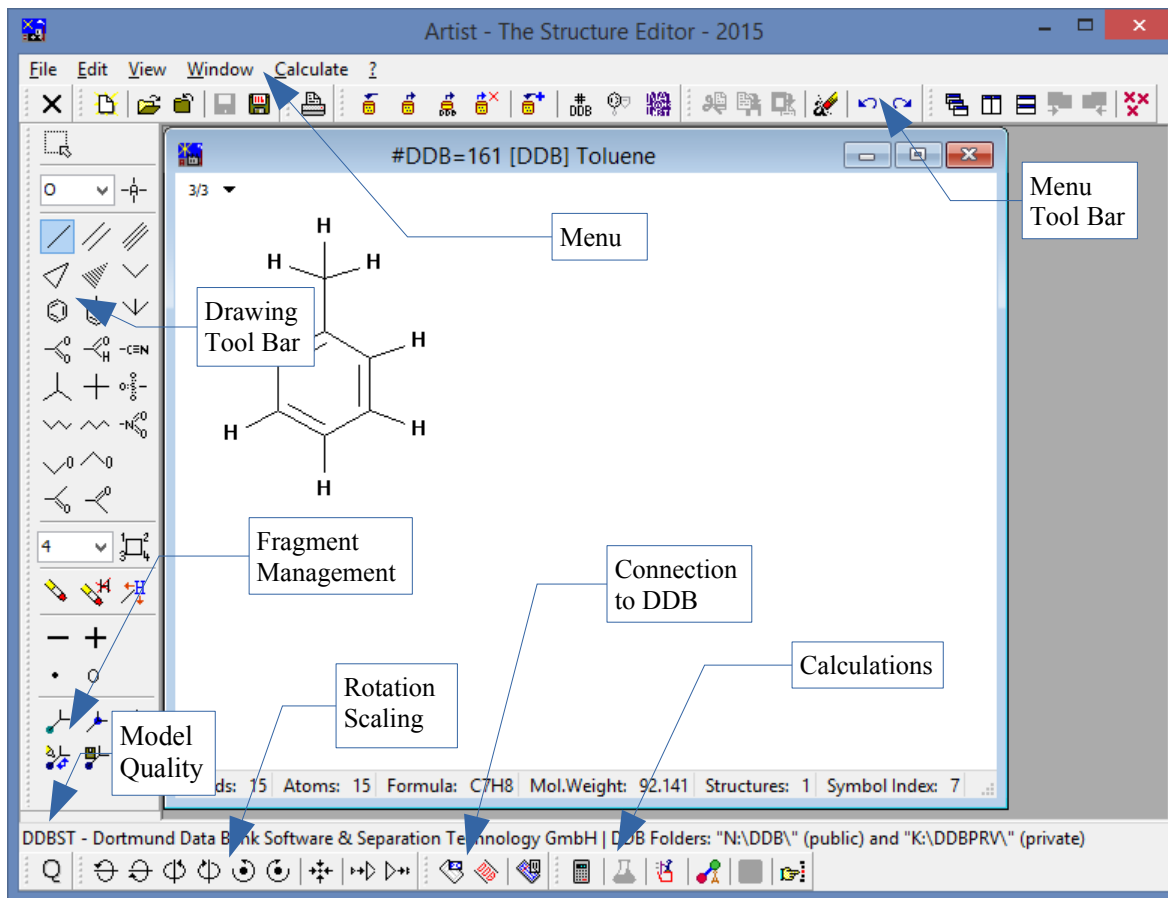
Artist is a tool for editing molecular structures and estimating thermophysical and transport properties from molecular structure directly. Artist contains a structure data bank (ChemDB) with structures for over 31000 components.

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

Artist 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. Artist adds the ability to determine the DDB number from the drawn structure.

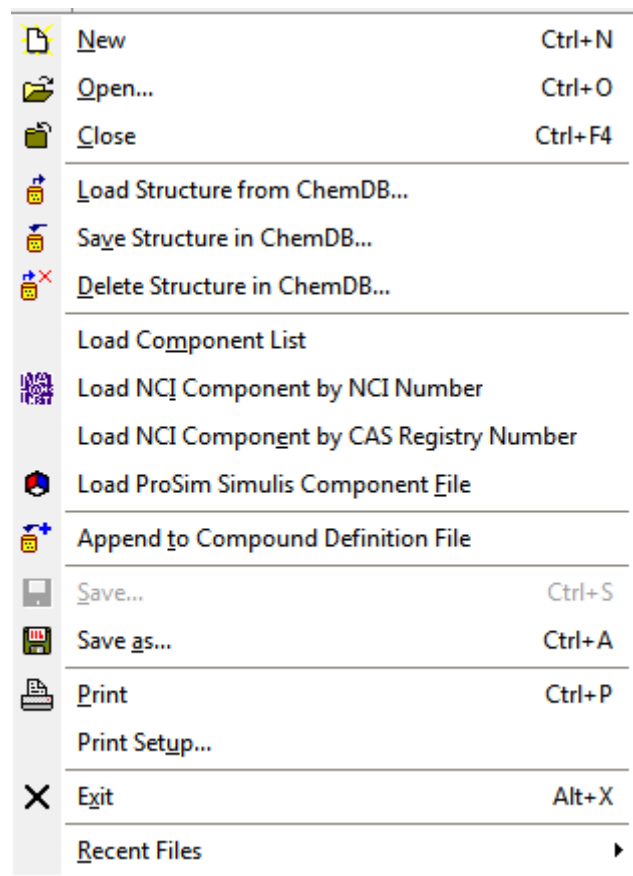
## The Main User Interface



Artist 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.

## The Menus

### 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 in ChemDB:** Save a molecular structure in the structure data bank. If the data bank already contains a structure, a dialog will be displayed for either replacing a structure or adding the new structure.

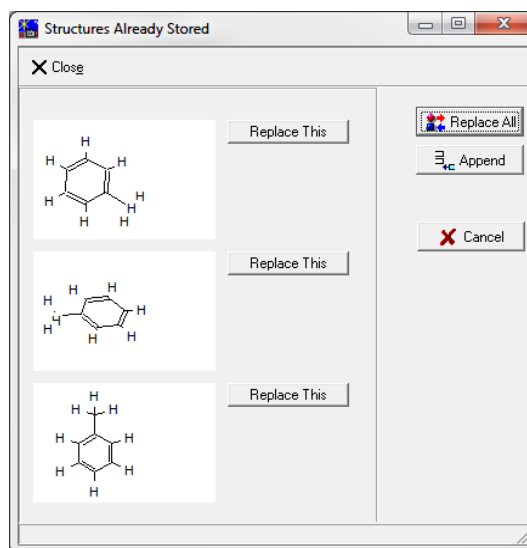


Figure 1: Saving Structures in ChemDB

**Delete Structure in ChemDB:** Removes a structure from the data bank. Artist displays a dialog from which the structure to be deleted can be selected.

*Common note for ChemDB access functions:* Artist opens the standard DDB component selection dialog for obtaining the component's DDB number because the structures are indexed (main index) by this component number.

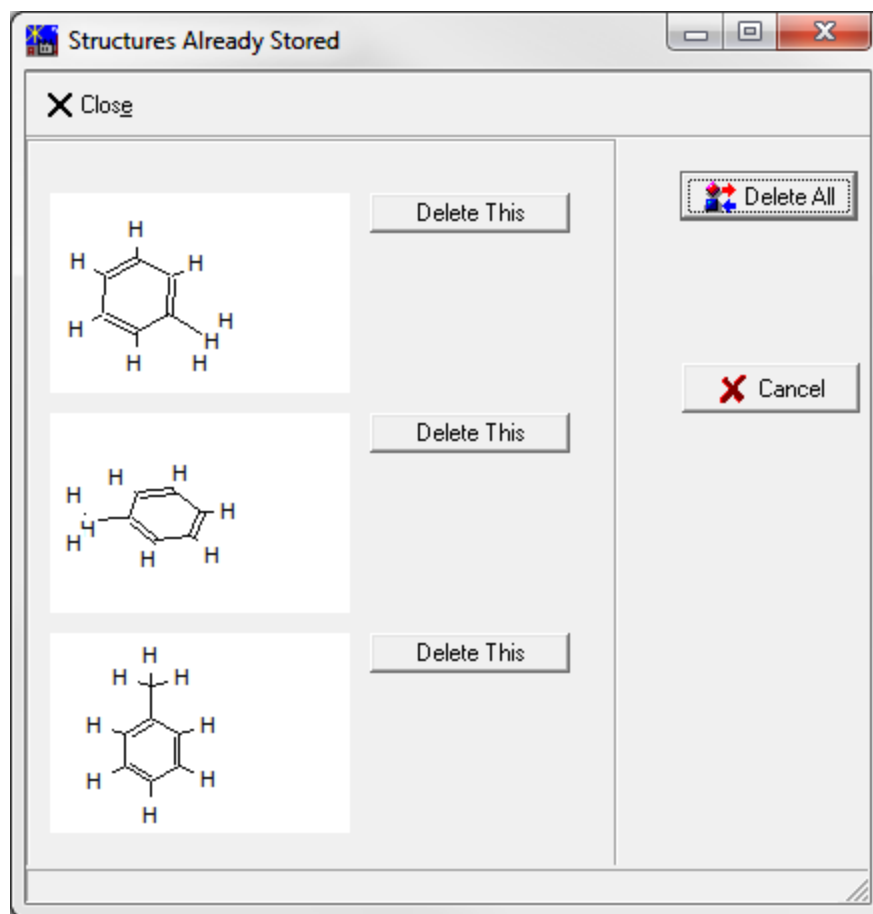


Figure 2: Deleting Structures From ChemDB

**Load Component List:** Component lists are containing DDB code numbers. Files with component lists have the extension “.stl”. If a line is selected the molecular structure of the component will be loaded and displayed in a new drawing window.

#### Load NCI Component by NCI

**Number:** Artist 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 to load a NCI component by its NCI number.

#### Load NCI Component by CAS Registry

**Number:** This menu entry allows to load a NCI component by its CAS registry number.

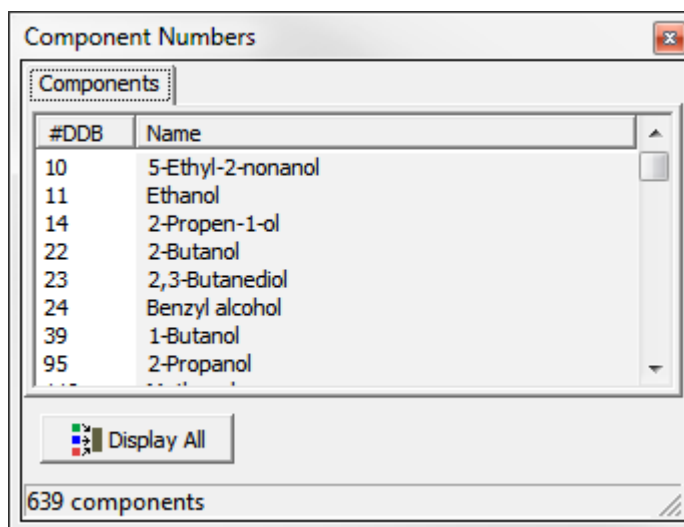


Figure 3: Component List

**Load ProSim Compound Definition File:** Artist can load and update compound definition files used and created by the ProSim<sup>1</sup> Simulis process simulation software. See chapter “ProSim Simulis Component File Update” on page 42 and following for more information.

**Append to Compound Definition File:** For adding new components Artist provides a dialog which allows to enter name, formula, CAS registry number and molecular weight.

The screenshot shows the 'New Component' dialog box. It has a title bar with the text 'New Component' and a close button. The dialog is divided into two main sections. The top section, 'Current Component Count', contains three input fields: 'Private Component List' with the value '23', 'Public Component List' with the value '45867', and 'Other Component List' with the value 'n.a.'. To the right of these fields are three buttons: 'Append to Private List', 'Append to Public List', and 'Append to Other List', each with a list icon. A 'Cancel' button is also present. The bottom section, 'New Component', contains several input fields and checkboxes. The 'English Name' field contains 'New Name'. The 'Alternative Name (German Name?)' field contains 'Neuer Name'. The 'CAS Registry Code' field is empty, with a note 'Maximum 127 characters per name' to its right. The 'Molecular Weight [g/mol]' field contains '92.141' and has a calculator icon. The 'Formula' field contains 'C7H8' and has a note 'Max. 31 characters' to its right. There are six checkboxes: 'Is Ionic Liquid', 'Is Carbohydrate', 'Is Polymer', 'Is Pharmaceutical', 'Biodiesel', and 'Oil & Gas', all of which are currently unchecked.

Figure 4: Adding a New Component

Artist can provide the molecular weight and the formula. After entering the necessary values (two names) the component can be appended either to the private (customer) or to the public (DDBST) data bank. Artist automatically updates the necessary files including the component basic file and the structure data bank. Other component lists are not supported in Artist.

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

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

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

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

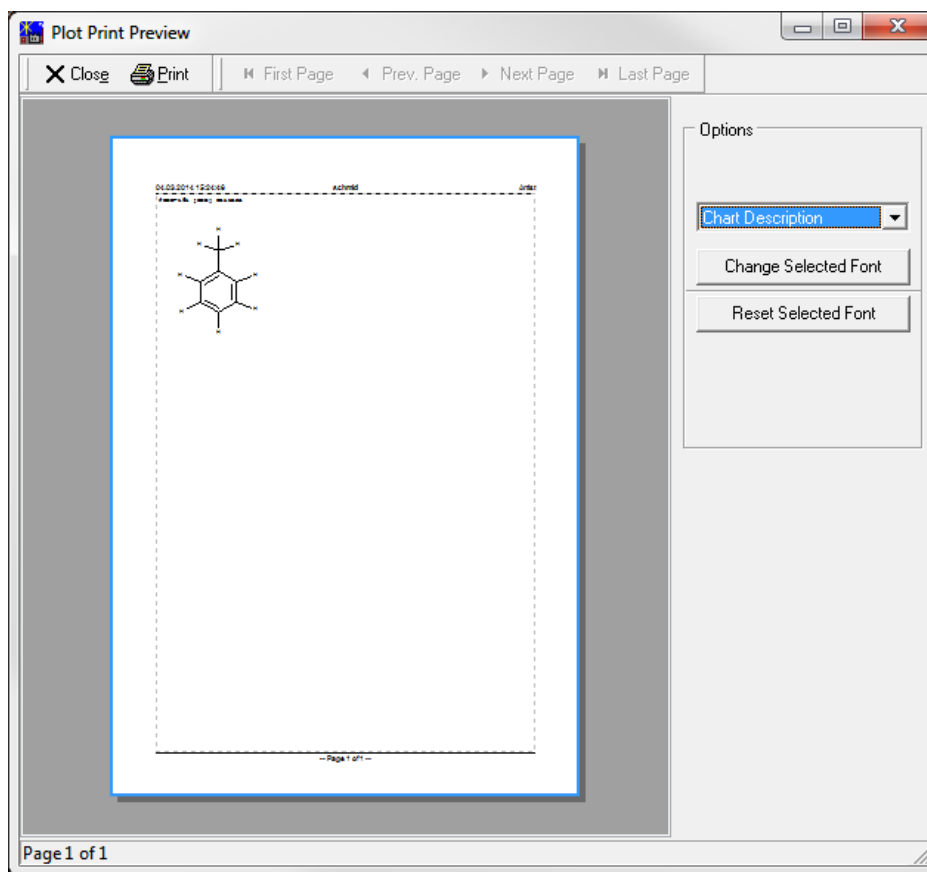
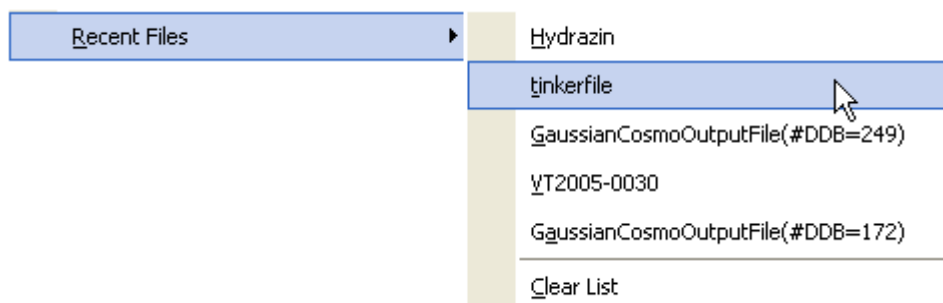


Figure 5: Print Preview Dialog

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

**Exit:** Closes Artist.

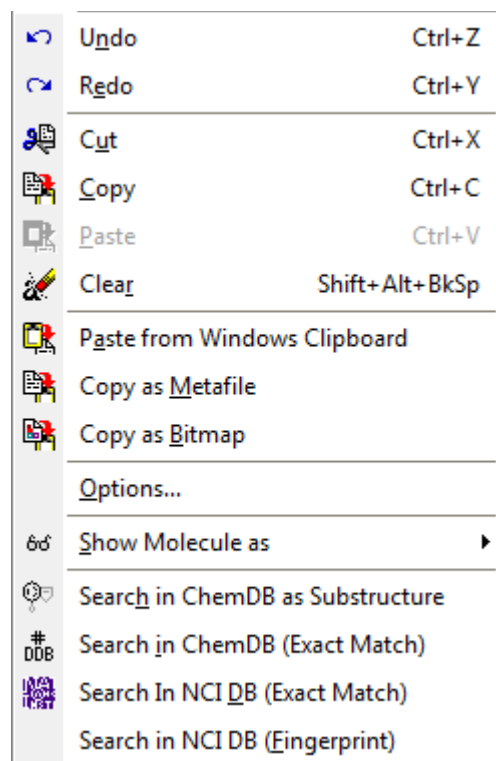
**Recent Files:** The sub menu is only visible if at least a single file has been loaded and contains the list of the recently load files.



“Clear List” removes all entries from this sub menu.



## The Edit Menu



**Undo:** Undoes the latest action

**Redo:** Redoes the latest undone action

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

**Copy:** Copies a marked area in the Artist internal buffer

**Paste:** Paste a marked area from the Artist internal buffer

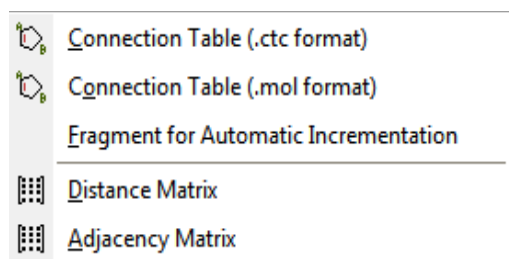
**Clear:** Removes the current drawing

**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 Incrementation:** 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)

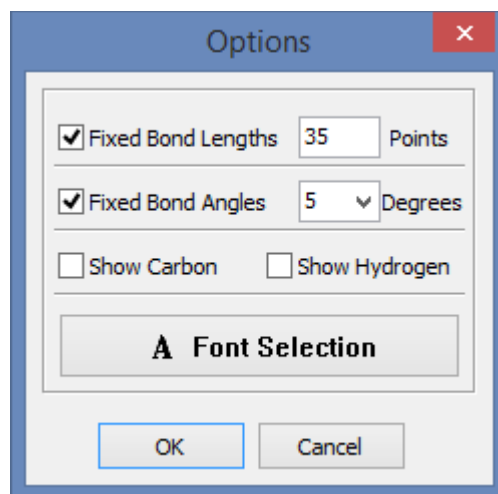


Figure 6: Options

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

The dialog displays the found component as a checkable list and 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

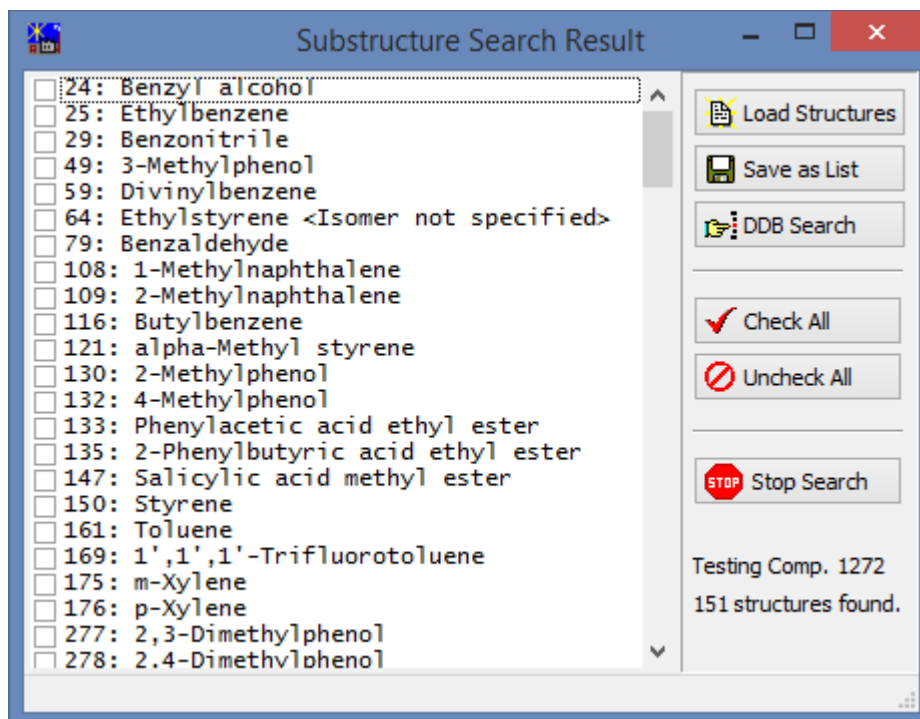


Figure 7: ChemDB Substructure Search

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

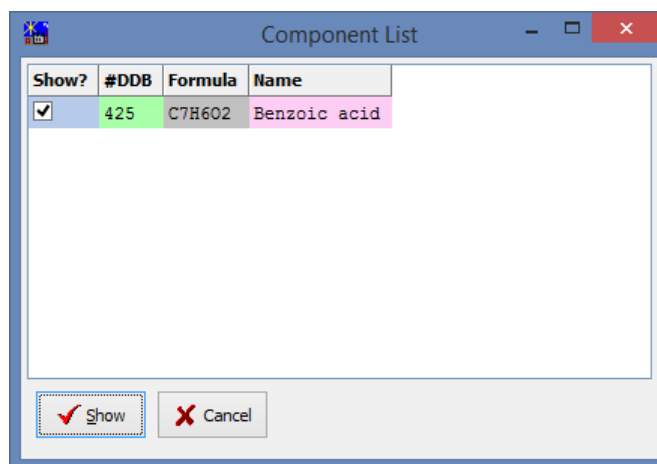


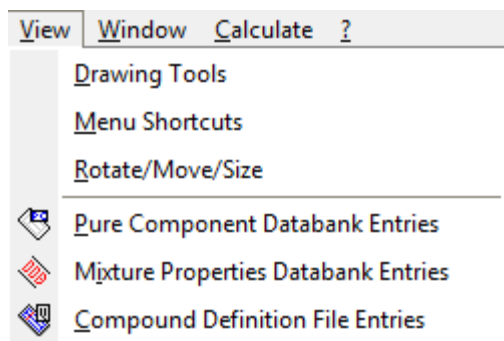
Figure 8: Search for Exact Match - Result

This allows to identify 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.

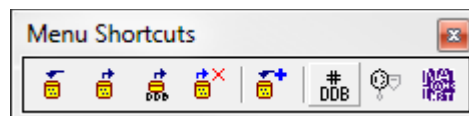
**Search in NCI DB (Exact Match):** This function searches the NCI data bank for matching structures.

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

## The View Menu



The first three entries (“Drawing Tools”, “Menu Shortcuts”, “Rotate/Move/Size”) allow to make tool bars visible if they have been teared off and closed.



The three other functions allow to start other programs in the DDB Software Package by OLE access. These function are only available if the DDB number of the component is available (see page 10 for “Search in ChemDB – Exact Match”)

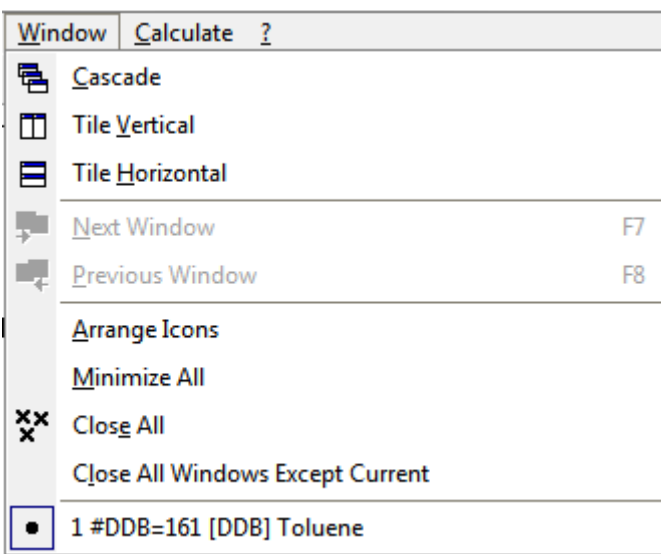
**Pure Component Properties:** Calling the Dortmund Data Bank main retrieval program and start a search for pure component properties of the current molecule.

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

**Compound Definition File Entries:** Calls the Component Editor and displays the component basic file

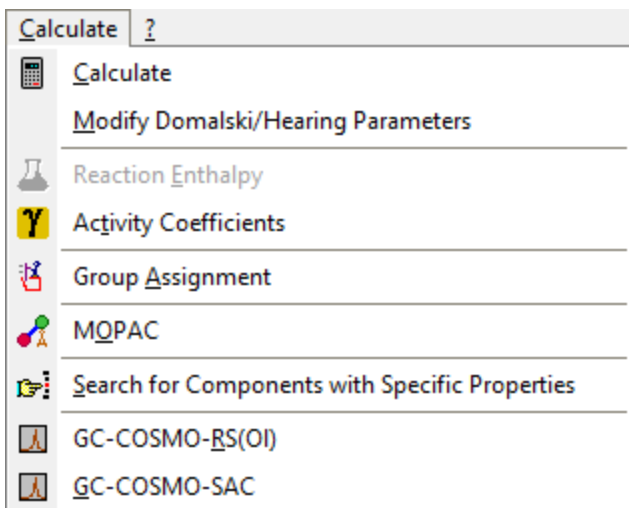
entries (like names, formula, CAS registry number)

### 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.

### The Calculate Menu



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

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

Group	Description	hf_gas	cp0_gas	s0_gas	hf_li
1	C-(H)3(C)	-42.26	25.73	127.32	-47
2	C-(H)2(C)2 ; chain	-20.63	22.89	39.16	-25
3	C-(H)(C)3 ; chain	-1.17	20.08	-53.6	-4
4	-CH3 corr (tertiary)	-2.26	0	0	-2

Figure 9: Editor for Domalski/Hearing Parameters

**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.

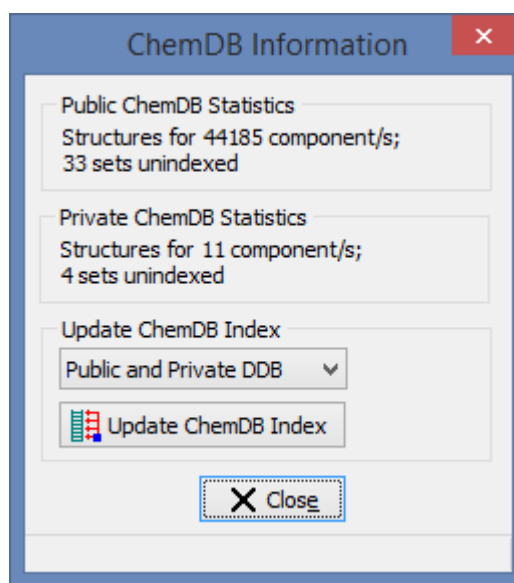
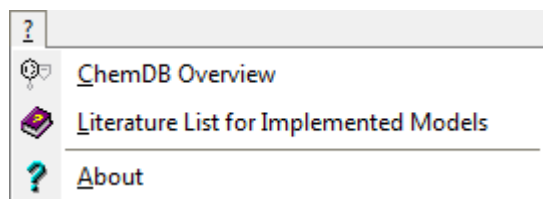
**MOPAC:** Display the dialog for calling MOPAC, Tinker, and RasMol. See chapter *MOPAC, Tinker, RasMol* for details.

**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(OI):** Opens a dialog with the results of the GC-COSMO-RS(OI) method. This method allows the estimation  $\sigma$ -profiles for the COSMO-RS(OI) 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  $\sigma$ -profiles for the COSMO-SAC model by a group contributions method.

### The Help Menu



1. “ChemDB Overview” shows the content of the structure data base ChemDB. It also allows

update the index of the data bank to accelerate the access.

2. “**Literature List for Implemented Models**” shows all references of the model and methods implemented in Artist.

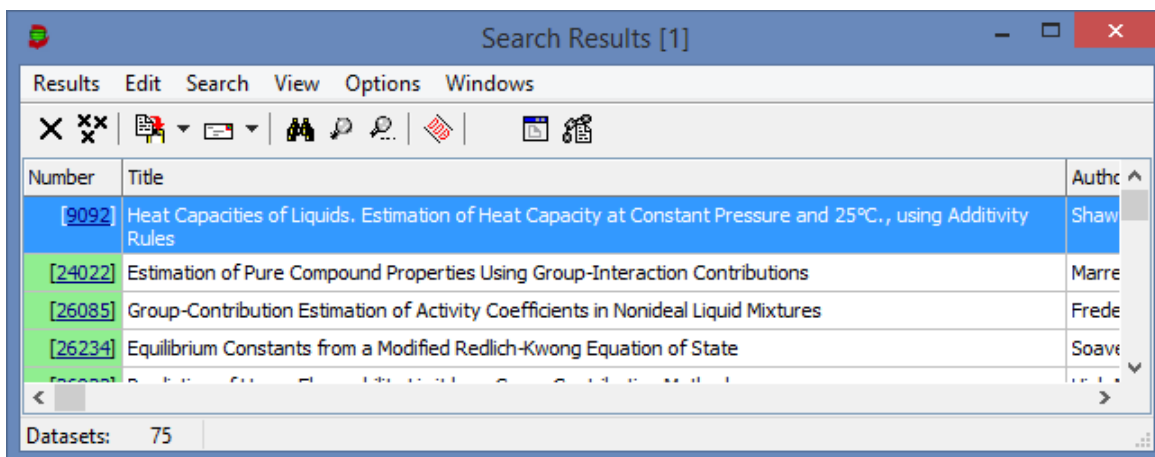


Figure 10: Literature List of Implemented Models

3. “**About**” shows Artist program details

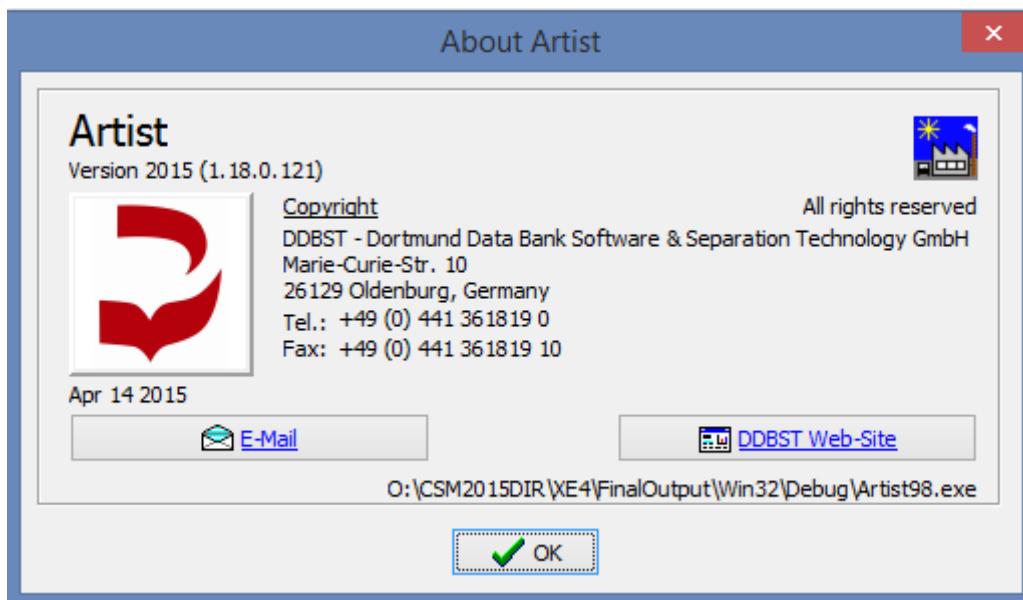
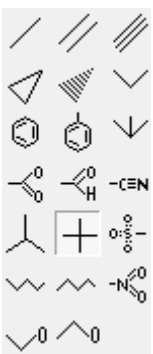


Figure 11: About

## Drawing Structures



Selection of 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)



Rings



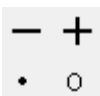
Delete bonds and atoms



Delete all hydrogens

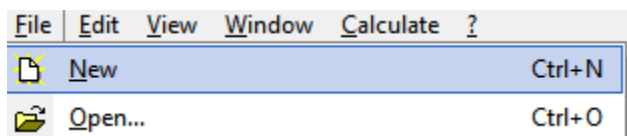



Add hydrogens including a simple coordinates generation



Charges (minus, plus, radical, none)

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



The drawing tools allow to select some predefined fragments. The most simple 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.



Artist 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 Artist 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.

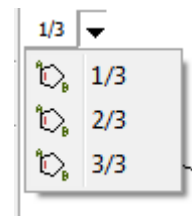
## Multiple Structures for a Single Component

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.

1/3 ▼



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



Artist selects the flattest structure to be shown first.

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



## Fragment Management

Artist allows to use drawn structures as fragments.



The single icons have the following functions.



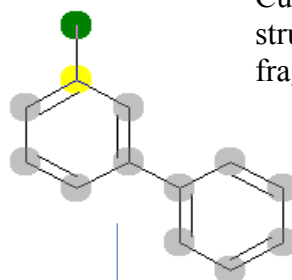
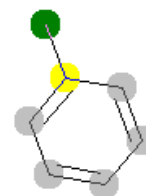
Define fragment anchor atom. This atom of a fragment is set with the mouse.  
The green circle defines the fragment center.



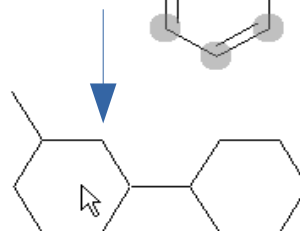
Define an atom connected to the anchor atom which will follow the mouse movement.  
This is the yellow circle in the figure above.



Directly use the current structure as fragment



Current  
structure as  
fragment



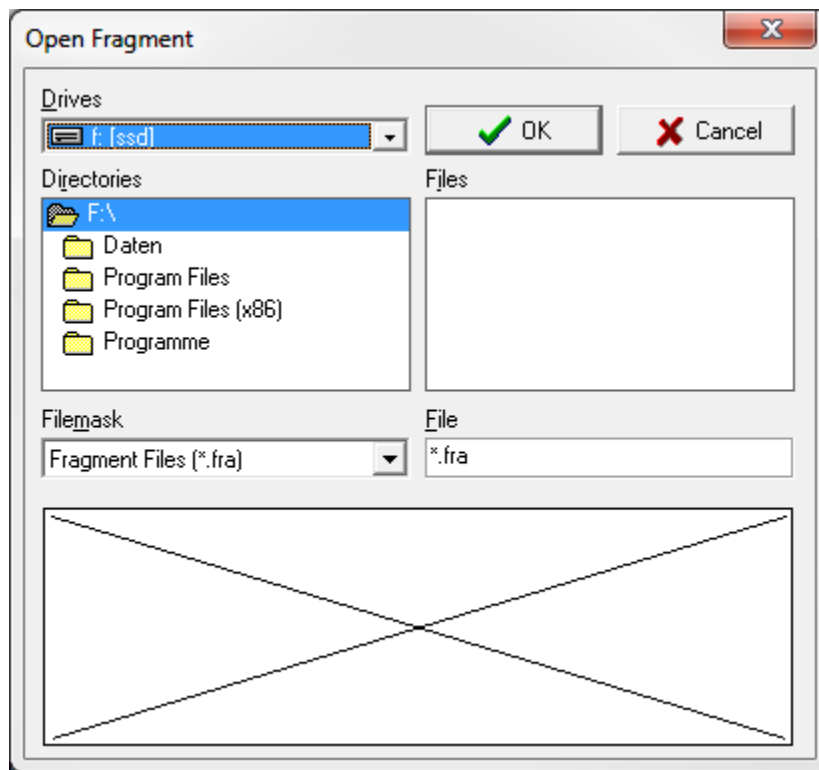
Drawing a  
new structure  
using the  
fragment



Save fragment to disk (".FRA" file)



Load fragment



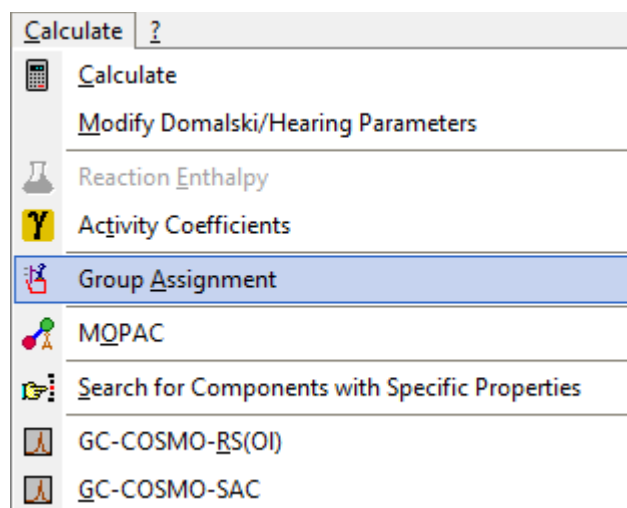
*Figure 12: Open Dialog for Fragments*

## Automatic Group Assignment

The core technology of Artist is the automatic fragmentation algorithm which allows to break 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 Artist provides a bulk of group assignment schemes separately for each model.

The automatic group assignment can be called from the Calculation menu or by the icon from the tool bar.



The dialog list all files with group assignments (".INK" files). Many of these "files" are integrated in the Artist programs.

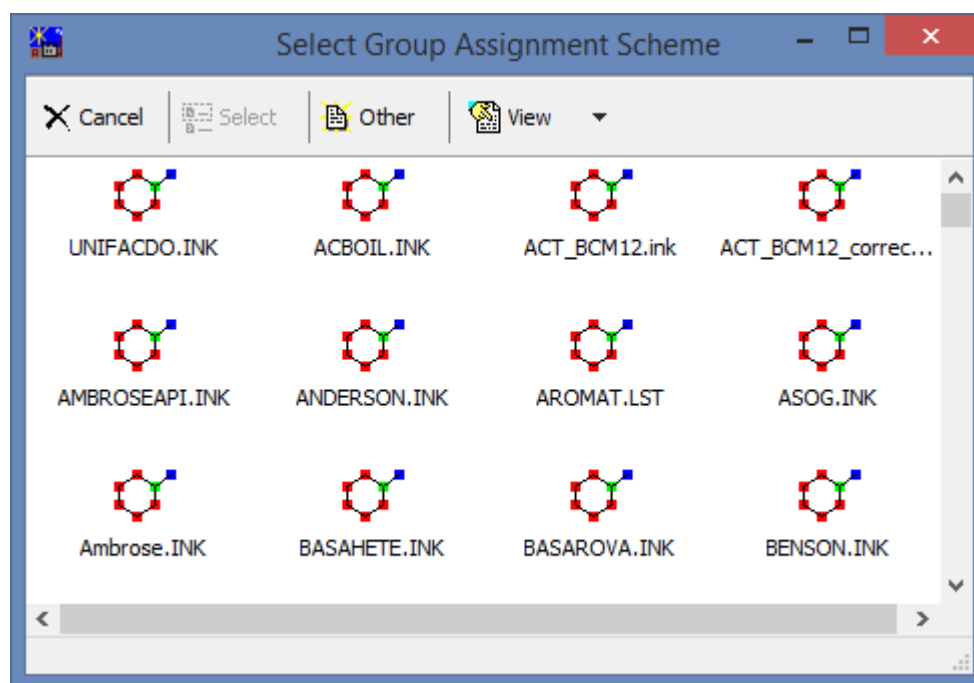
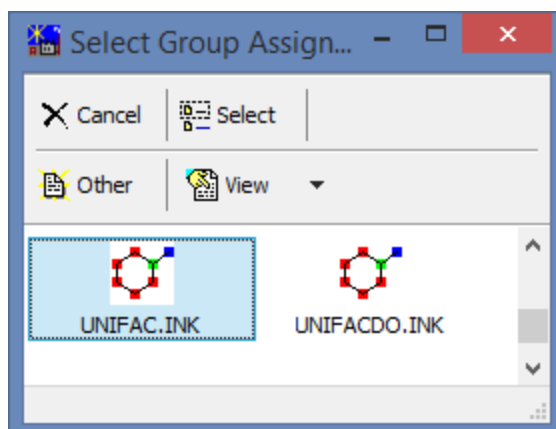


Figure 13: List of Group Assignment Schemes

The latest group assignment file used will be put on top of the list (here "UNIFACDO.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

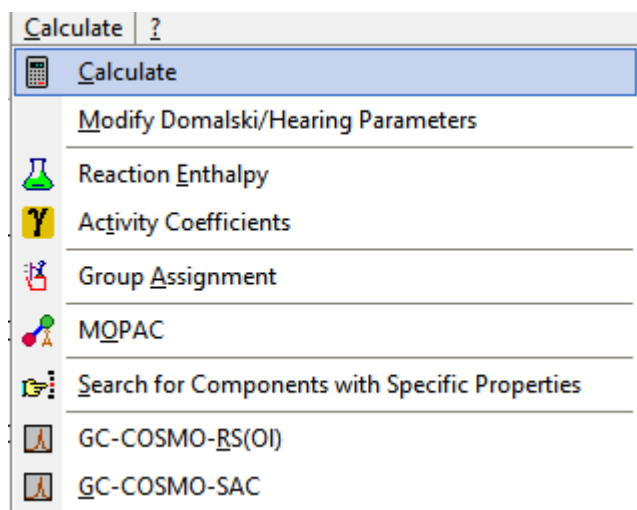
The group assignment found the UNIFAC subgroups 64 (Bromine), 10 (aromatic carbon with three bonds), and 9 (aromatic carbon with two bonds).

The DDB encoded groups ("3 1064 1010 5009") can be used in the component editor. The "3" determines the number of different groups, "1064" means 1 time the group number 64 [BR], "5009" means that group 9 [ACH] has been found five times.

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..

## Estimation of Properties

### Overview



Artist was originally designed for the estimation of pure component properties using group contribution methods, Artist 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 menu 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. Artist 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.

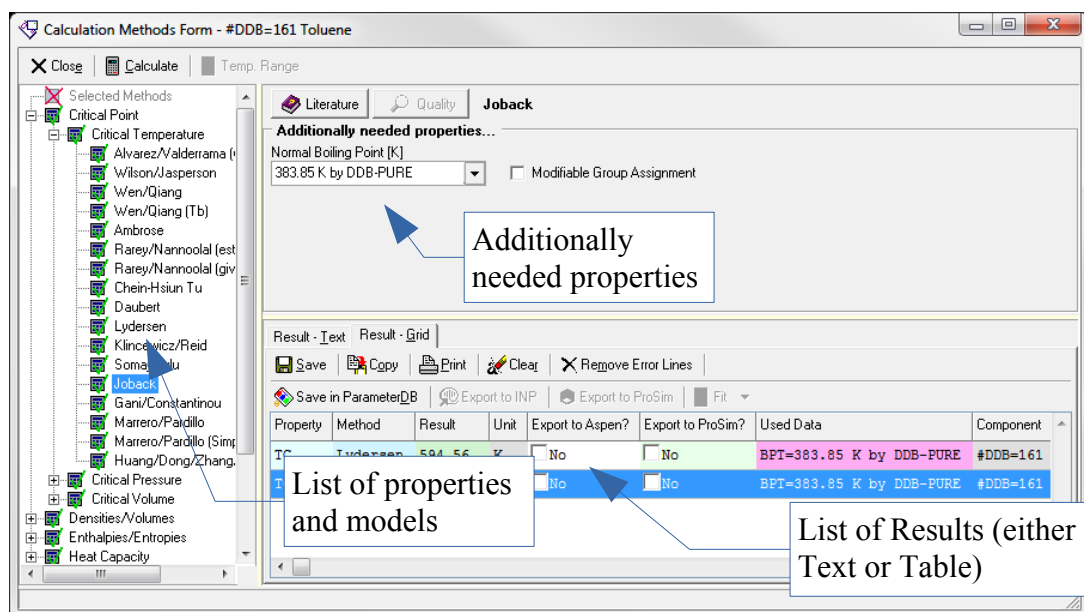
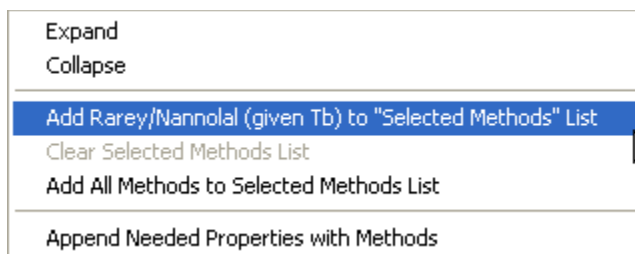


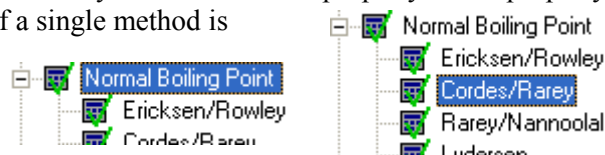
Figure 14: Property Estimation

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



Artist allows 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.



Artist 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).

## Prediction Output

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

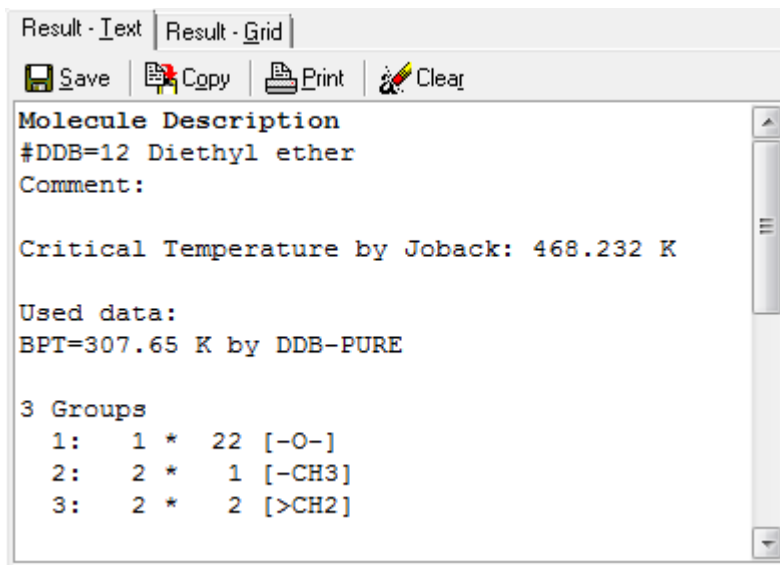


Figure 15: Property Estimation - Text Result

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

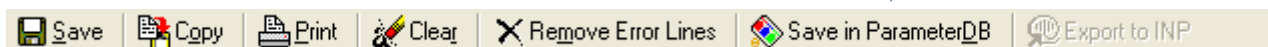
The table output

Property	Method	Result	Unit	Export to Aspen?	Export to ProSim?	Used Data
TC	Wen/Qiang (Tb)	591.437	K	<input type="checkbox"/> No	<input type="checkbox"/> No	BPT=383.85 K by DDB-PURE
BPT	Lydersen	382.004	K	<input type="checkbox"/> No	<input type="checkbox"/> No	TC=591.70 K by DDB-PURE
BPT	Gani/Constantinou	392.074	K	<input type="checkbox"/> No	<input type="checkbox"/> No	

Figure 16: Property Estimation - Table Output

is more concise and allows to copy the result to a spreadsheet program. Results can also be stored in the DDB parameter data bank (ParameterDB) or as Aspen INP file (selected properties only).

## Storing Results in the ParameterDB



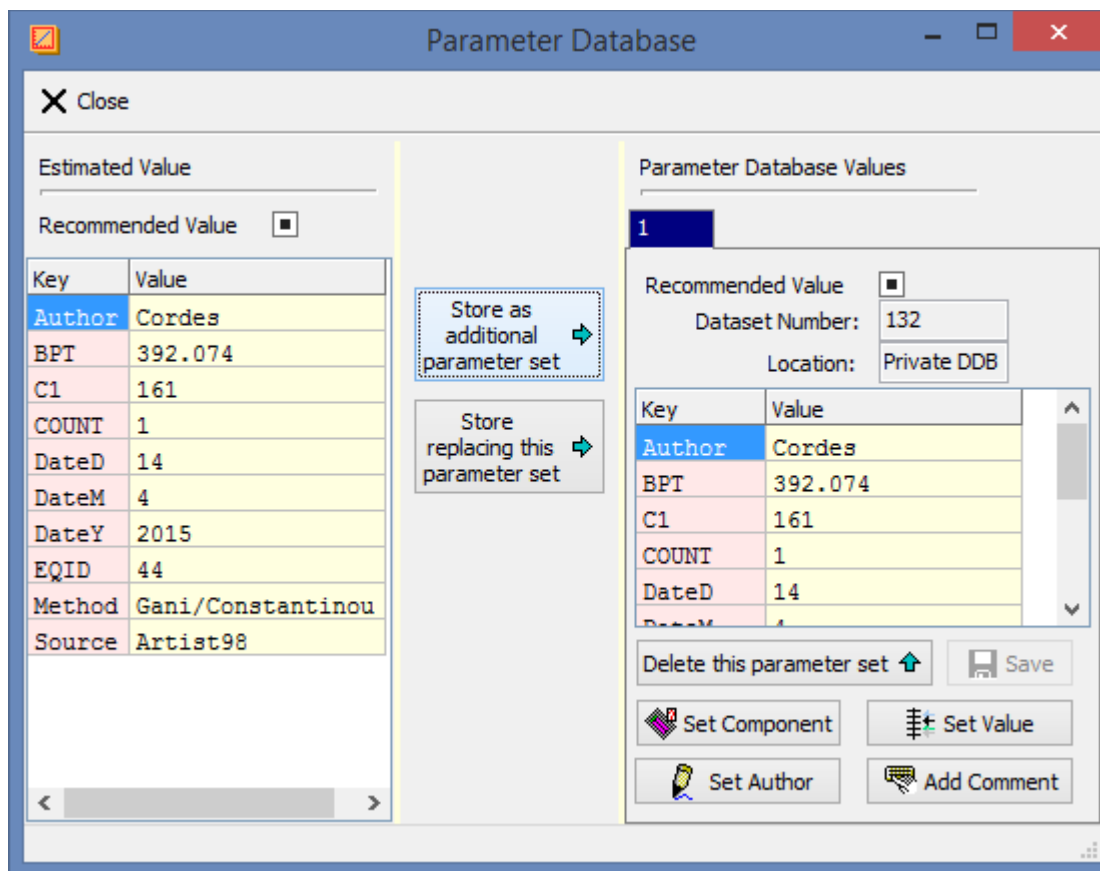


Figure 17: Property Estimation - Storing Results in Parameter Data Bank

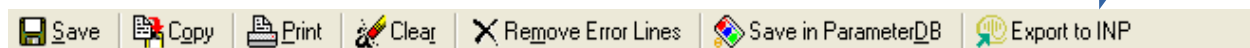
The dialog allows to replace or delete already stored sets and to add the current result as a new data set. It also allows to alter some of the data set entries (Component, Author, Value, Comment).

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

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

670.00 K by DDB-PURE  
659.017 - by Artist98/ParameterDB/325

## Storing Results as Aspen INP File



Artist can store

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





- Acentric Factor
- UNIQUAC r and q


Artist allows 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.


Result - Text


Result - Grid


 Save


 Copy

 Print



 Clear

 Remove Error Lines

 Save in ParameterDB

 Export to INP

Property	Method	Result	Unit	Export to Aspen?	Used Data	Comp
TC	Wen/Qiang (Tb)	669.695	K	<input checked="" type="checkbox"/> Yes	BPT=429.25 K by DDB-PURE	#DDB=
BPT	Lydersen	426.94	K	<input type="checkbox"/> No	TC=670.00 K by DDB-PURE	#DDB=
BPT	Gani/Constantinou	435.93	K	<input checked="" type="checkbox"/> Yes		#DDB=
BPT	Ericksen/Rowley	440.15	K	<input type="checkbox"/> No	UNIQUAC_R=4.02000 - by DDB-PURE	#DDB=




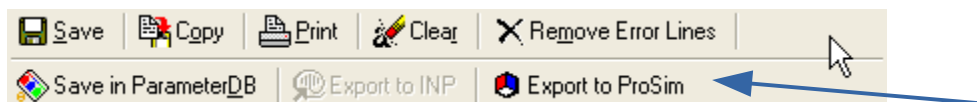


Figure 18: Aspen INP File Export

## Storing Results for ProSim Software



Artist allows storing the properties

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

Artist allows 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.

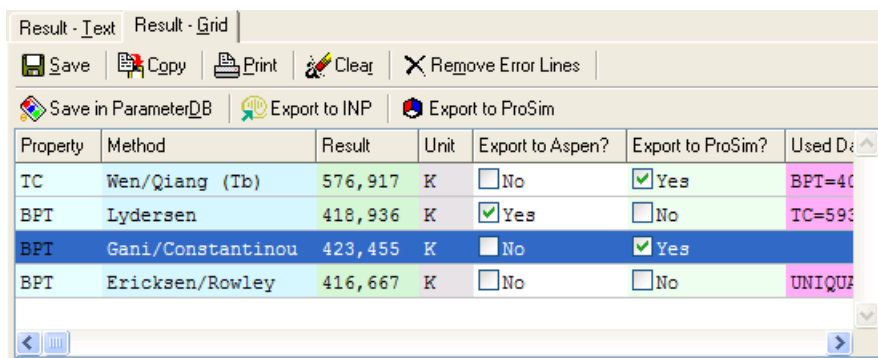


Figure 19: ProSim Component File Export

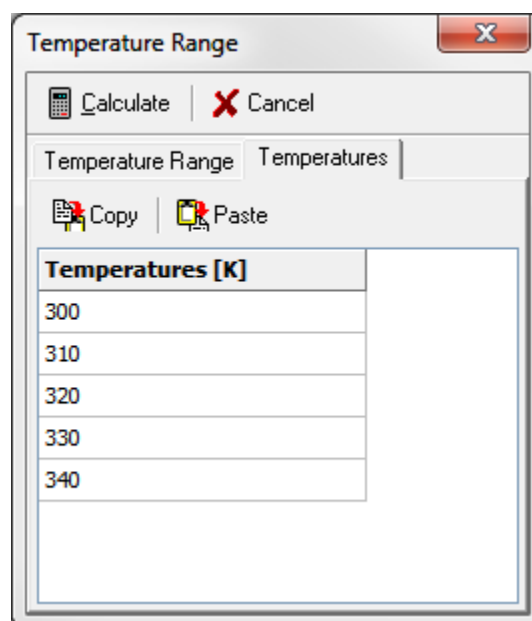
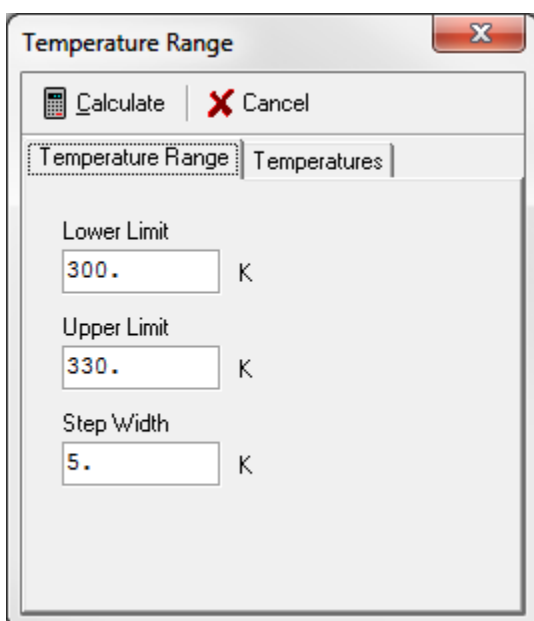
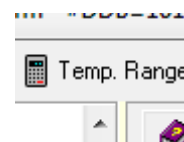
See also chapter “ProSim Simulis Component File Update” on page 42 and following for updating existing ProSim component files.

## 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 select. 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.



Result - Text

Result - Grid

Save

Copy

Print

Clear

Remove Error Lines

Save in ParameterDB

Export to INP

Property	Method	Result	Unit	Export to Aspen?	Used Data	Component	Used T	Un
LIQDEN	GCVOL	886.437	kg/m3	No	T=260.00 K by User	#DDB=25 Ethylbenzene	260.00 K	
LIQDEN	GCVOL	877.365	kg/m3	No	T=270.00 K by User	#DDB=25 Ethylbenzene	270.00 K	
LIQDEN	GCVOL	868.477	kg/m3	No	T=280.00 K by User	#DDB=25 Ethylbenzene	280.00 K	
LIQDEN	GCVOL	859.767	kg/m3	No	T=290.00 K by User	#DDB=25 Ethylbenzene	290.00 K	
LIQDEN	GCVOL	851.23	kg/m3	No	T=300.00 K by User	#DDB=25 Ethylbenzene	300.00 K	
LIQDEN	GCVOL	842.861	kg/m3	No	T=310.00 K by User	#DDB=25 Ethylbenzene	310.00 K	
LIQDEN	GCVOL	834.655	kg/m3	No	T=320.00 K by User	#DDB=25 Ethylbenzene	320.00 K	

Figure 20: Result of a Temperature Range Prediction

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

Antoine Fit			
Close			
Table Diagram			
Copy			
T [K]	P [kPa]	P calc. [kPa] AB	P calc. [kPa] ABC
300.0	4.03079	4.04417	4.03079
305.0	5.18214	5.18108	5.18214
310.0	6.59878	6.58476	6.59878
315.0	8.32699	8.30529	8.32698
320.0	10.4183	10.3996	10.4183
325.0	12.9299	12.9324	12.9299
330.0	15.9245	15.976	15.9245
<div> <div>A=8.04496 B=1968.909 C=273.15</div> <div>A=7.08956 B=1413.576 C=225.17</div> <div>P [mm Hg] T [°C]</div> </div> <div> <div>Copy Private ParameterDDB</div> <div>Copy Private ParameterDDB</div> <div>Export T/P to Aspen INP File</div> <div>Write Antoine-ABC</div> </div>			

Figure 21: Fitted Antoine Parameters

bank.

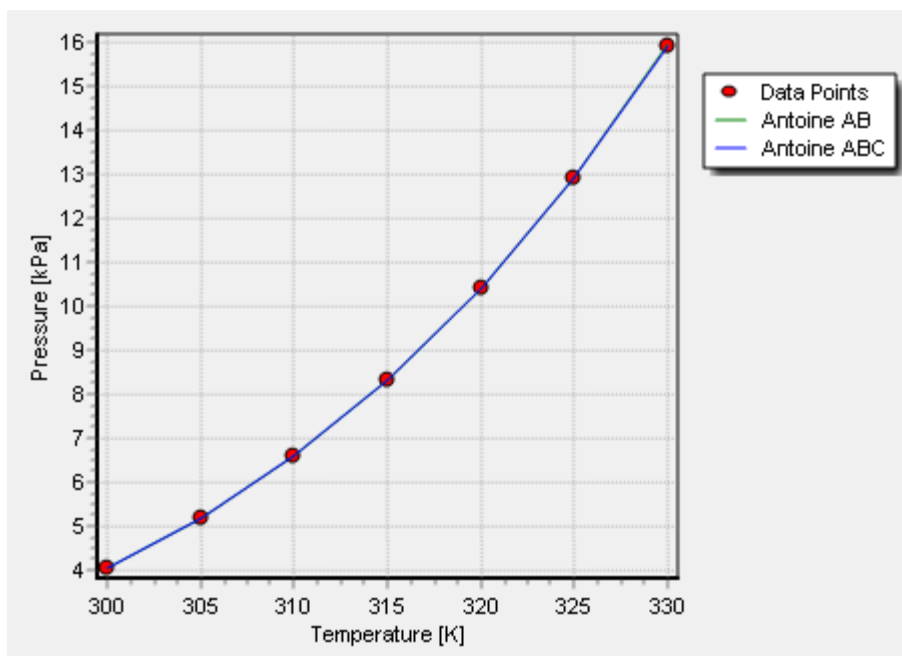


Figure 22: Graphical Result

The diagram shows the fitted blue line together with the estimated red circles.

### Fit Prediction Results with Other Equations

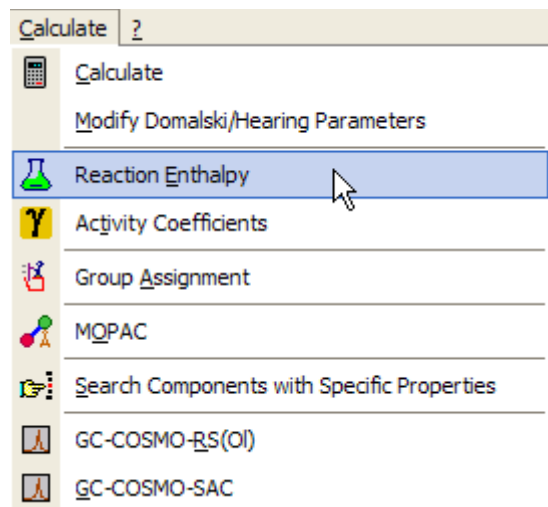
Result - Text			
Result - Grid			
<div> <div>Save</div> <div>Copy</div> <div>Print</div> <div>Clear</div> <div>Remove Error Lines</div> </div> <div> <div>Save in ParameterDB</div> <div>Export to INP</div> <div>Export to ProSim</div> <div>Fit</div> </div>			
Property	Method	Result	Unit
H_VAP	Rarey/Nannoolal	36.7558	kJ/mol

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.

Equation
Ideal Gas Heat Capacity
Heat of Vaporization
DIPPR 106 Equation
Extended Watson
PPDS 12 Equation
Liquid Saturated Density
Liquid Density

Figure 23: PCP Equation Fit

## Reaction Enthalpy



Artist allows 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 or more structures have been drawn or loaded.

Number	Description	Comm	Formula	Mol.Weight	Heat of Formation	State	Moles
1	#DDB=11 [DDB] Ethanol		C2H6O	46.069	-234.49 kJ/mol	Gas	1
2	#DDB=84 [DDB] Acetic acid		C2H4O2	60.053	-436.06 kJ/mol	Gas	1
3	#DDB=174 [DDB] Water		H2O	18.015	0 kJ/mol	Gas	1
4	#DDB=21 [DDB] Ethyl acetate		C4H8O2	88.106	-445.79 kJ/mol	Gas	1

Educts			Products		
Number	Description	Mol Count	Number	Description	Mol Count

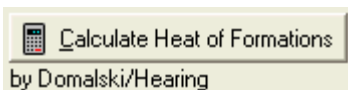
  

Heat of Form. (Educts)	Heat of Form. (Products)	Reaction Enthalpy

Figure 24: Reaction Enthalpy Calculation

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 Domalski/Hearing method, typed, or search in the Dortmund Data Bank.



2. The state of the component – liquid, gas, solid. This determines the result of the Domalski/Hearing method.
3. The number of moles for all components.

The next step is the assignment of molecules as educts 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.

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

The button Search Heat of Formations in DDB Database starts a search in the pure component properties

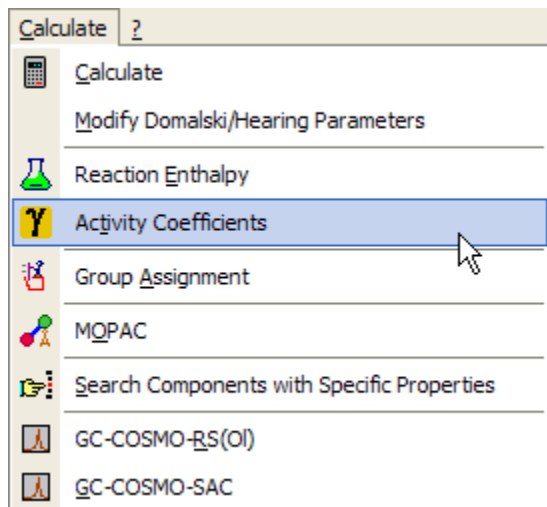
(PCP) branch of the Dortmund Data Bank for heats of formation of the components in the reaction enthalpy dialog.

Only a single heat of formation can be selected for a specific component. The links “[230]” etc. display the reference of the heat of formation.

Component	Heat of Formation [J/mol]	State	T [K]	Literature
<b>11 Ethanol</b>				
<input type="checkbox"/>	-276981.0	2 Liquid	298.00	[6343]
<input type="checkbox"/>	-236919.0	3 Vapor	298.00	[6834]
<input type="checkbox"/>	-236940.0	3 Vapor	298.00	[13191]
<input type="checkbox"/>	-235099.0	3 Vapor	298.00	[31282]
<input type="checkbox"/>	-277692.1	2 Liquid	298.00	[31282]
<b>84 Acetic acid</b>				
<input type="checkbox"/>	-484507.0	2 Liquid	298.00	[230]
<input type="checkbox"/>	-484089.0	2 Liquid	298.00	[6698]
<input type="checkbox"/>	-437353.5	48 Ideal Gas	298.16	[9100]
<input type="checkbox"/>	-437437.2	48 Ideal Gas	300.00	[9100]
<input type="checkbox"/>	-441119.1	48 Ideal Gas	400.00	[9100]
<input type="checkbox"/>	-445763.3	48 Ideal Gas	600.00	[9100]
<input type="checkbox"/>	-448775.8	48 Ideal Gas	800.00	[9100]
<input type="checkbox"/>	-450240.2	48 Ideal Gas	1000.00	[9100]
<input type="checkbox"/>	-450700.5	48 Ideal Gas	1200.00	[9100]
<input type="checkbox"/>	-450198.4	48 Ideal Gas	1500.00	[9100]

Figure 25: Search Heats of Formation in Dortmund Data Bank

## Activity Coefficients



Artist allows to calculate activity coefficients of binary and higher mixtures with the activity coefficient models

- original UNIFAC
- modified UNIFAC (Dortmund)
- modified UNIFAC (Lyngby)
- ASOG

**Calculation of Activity Coefficients**

Close

Number	Remove?	Description	Comment	Formula	Mol.Weight	Groups
1	<input type="button" value="Remove"/>	#DDB=11 [DDB] Ethanol		C2H6O	46.069	1014 1002 1001
2	<input type="button" value="Remove"/>	#DDB=84 [DDB] Acetic acid		C2H4O2	60.053	1042 1001
3	<input type="button" value="Remove"/>	#DDB=174 [DDB] Water		H2O	18.015	1016
4	<input type="button" value="Remove"/>	#DDB=21 [DDB] Ethyl acetate		C4H8O2	88.106	1021 1002 1001

Group Contribution Method  
mod. UNIFAC (Dortmund)

Constant Temperature  
  
0 Points  
Temperature [K]  
298

Constant Composition  

x1	x2	x3	x4
0.2	0.3	0.1	0.4000

☒ Mole Fractions  
☐ Weight Fractions

Temperature Range  

Start	End	Stepwidth
298	323	5

	x1	x2	x3	x4	T [K]	Gamma1	Gamma2	Gamma3	Gamma4
1	0.2000	0.3000	0.1000	0.4000	298	1.4084	1.0044	3.6629	1.32
2	0.2000	0.3000	0.1000	0.4000	303	1.3947	1.0066	3.6359	1.31
3	0.2000	0.3000	0.1000	0.4000	308	1.3798	1.0082	3.6058	1.30
4	0.2000	0.3000	0.1000	0.4000	313	1.3640	1.0092	3.5729	1.30
5	0.2000	0.3000	0.1000	0.4000	318	1.3475	1.0099	3.5372	1.29
6	0.2000	0.3000	0.1000	0.4000	323	1.3303	1.0101	3.4989	1.28

Figure 26: Activity Coefficient Calculation

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  button opens a dialog where the composition can be specified.

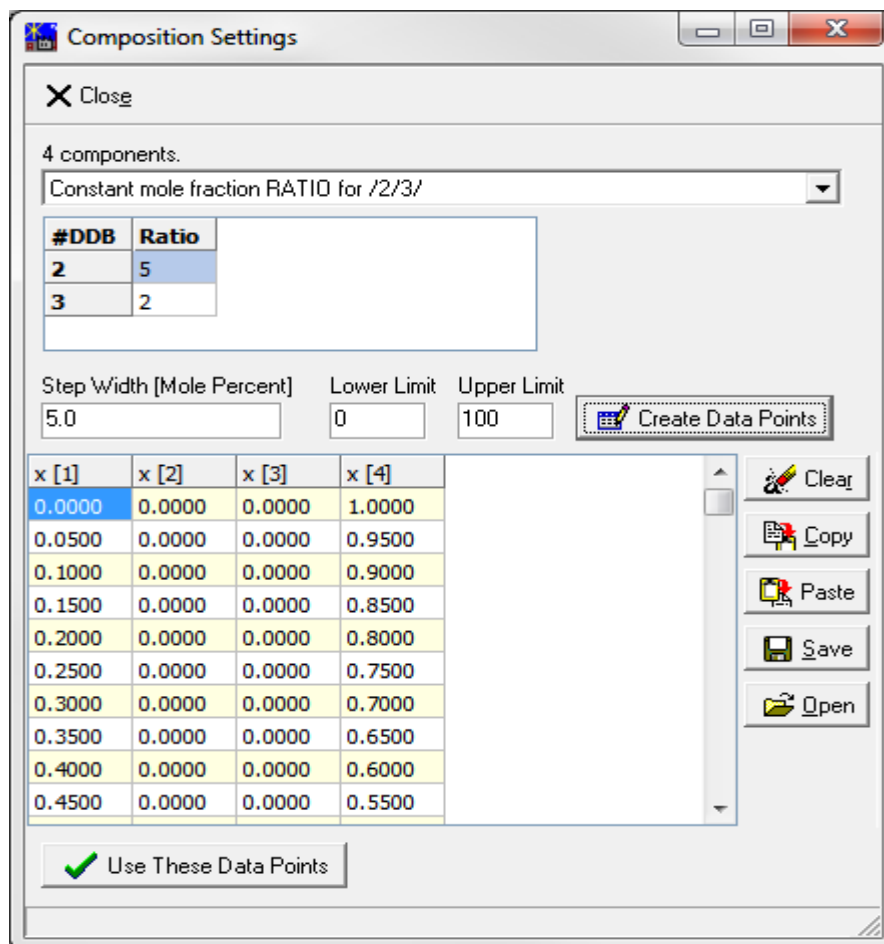


Figure 27: Composition Settings

This dialog allows 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.

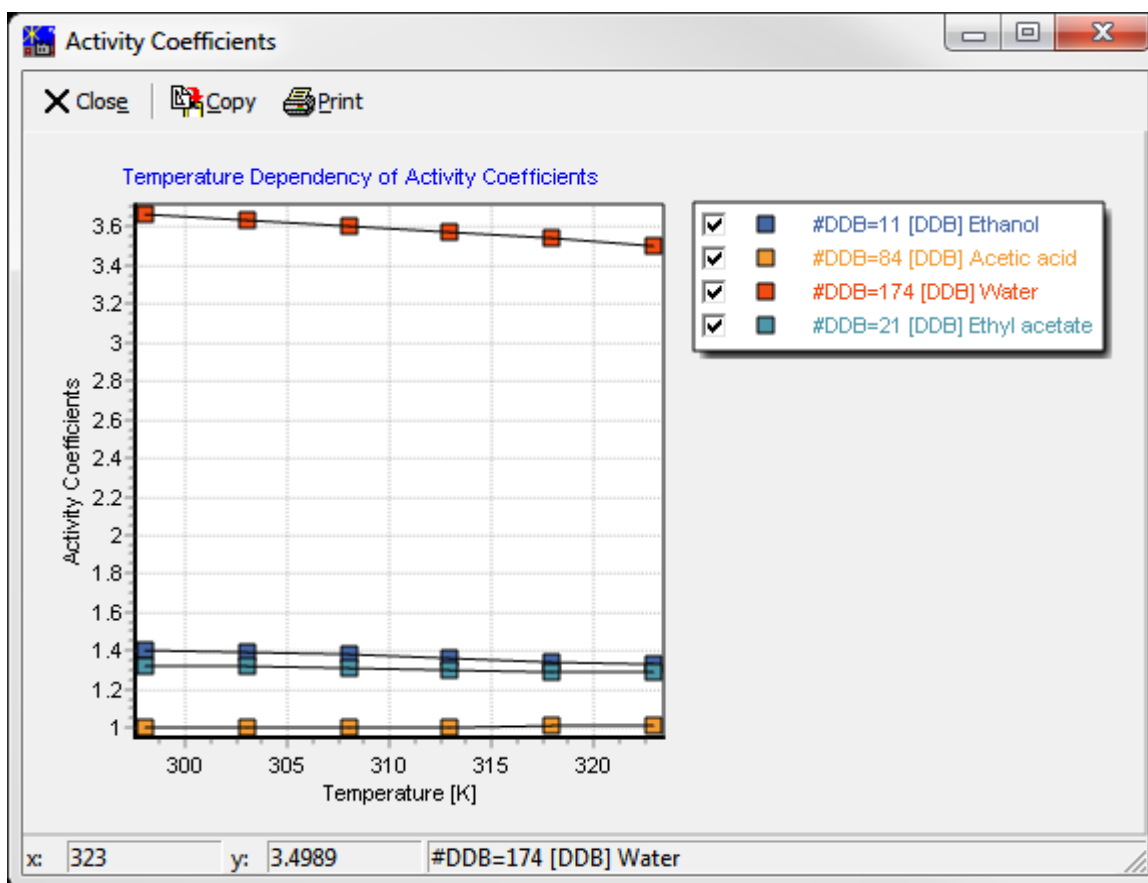


Figure 28: Temperature-Dependent Activity Coefficients

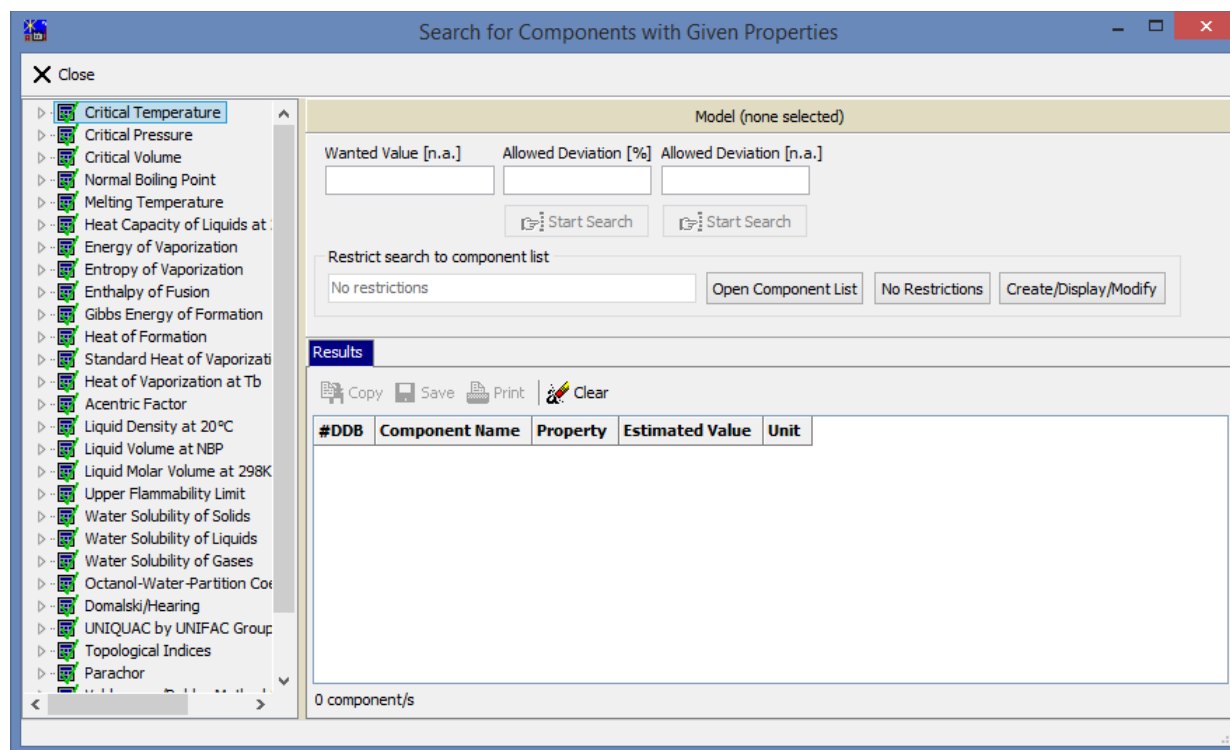
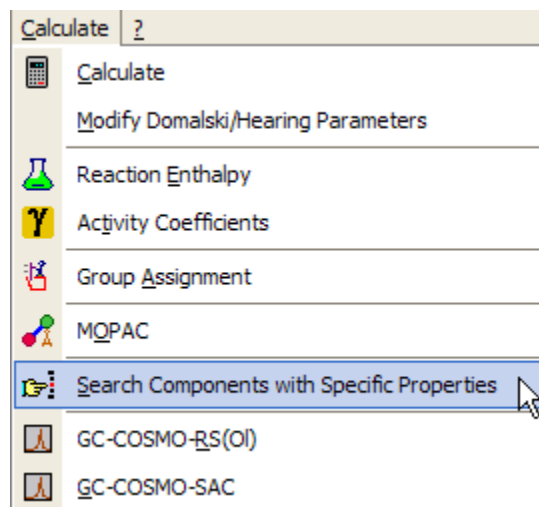
## Search for Components with Specified Properties

Artist 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 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) in percents.



The search can be restricted to a component list which can be created in the other DDB software (Component Selection program).

The software works through the entire component list and tries to estimate a value for all components stored in the chemical structure data base (more than 35000 structures).

A typical result looks like

Results				
Copy            Save            Print            Clear				
#DDB	Component Name	Property	Estimated Value	Unit
60	Decane	BPT	446.944	K
81	Acetic acid cyclohexyl ester	BPT	448.071	K
138	Phenol	BPT	440.863	K
158	Tetrahydrofurfuryl alcohol	BPT	446.78	K
236	4-Hydroxy-2-butanone	BPT	446.567	K
341	2-Methylcyclohexanol	BPT	441.228	K
354	1-Decene	BPT	446.736	K
8 component/s				

A normal boiling point of 444 K has been search and the lowed deviation was 1%. The model was

Search for Components with Given Properties

Close

☒ Critical Temperature  
☒ Critical Pressure  
☒ Critical Volume  
☒ Normal Boiling Point  
☐ Cordes/Rarey  
☐ Rarey/Nannoolal  
☐ Stein/Brown  
☐ Devotta/Rao  
☐ Joback  
☐ GVS  
☐ Gani/Constantinou  
☐ Marrero/Pardillo  
☐ Marrero/Pardillo (Simple C  
☐ Marrero/Pardillo (Simple C  
☐ Palatinus et al.  
☐ Huang/Dong/Zhang/Li/Zh  
☒ Melting Temperature  
☒ Heat Capacity of Liquids at 2  
☒ Energy of Vaporization  
☒ Entropy of Vaporization  
☒ Enthalpy of Fusion  
☒ Gibbs Energy of Formation  
☒ Heat of Formation

Cordes/Rarey

Wanted Value [K] 444    Allowed Deviation [%] 1    Allowed Deviation [K]

Restrict search to component list

Copy
 Save
 Print
 Clear

#DDB	Component Name	Property	Estimated
60	Decane	BPT	446.944
81	Cyclohexyl acetate	BPT	448.071
138	Phenol	BPT	440.863
158	Tetrahydrofurfuryl alcohol	BPT	446.78
236	4-Hydroxy-2-butanone	BPT	446.567

152 component/s

Working on component 6962 of 40779

“Cordes/Rarey”.

## MOPAC, Tinker, RasMol

We can distribute neither MOPAC nor Tinker and RasMol. The user has to download the programs from the Internet. All these programs are freely available (MOPAC at least up to version 7).

### MOPAC

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

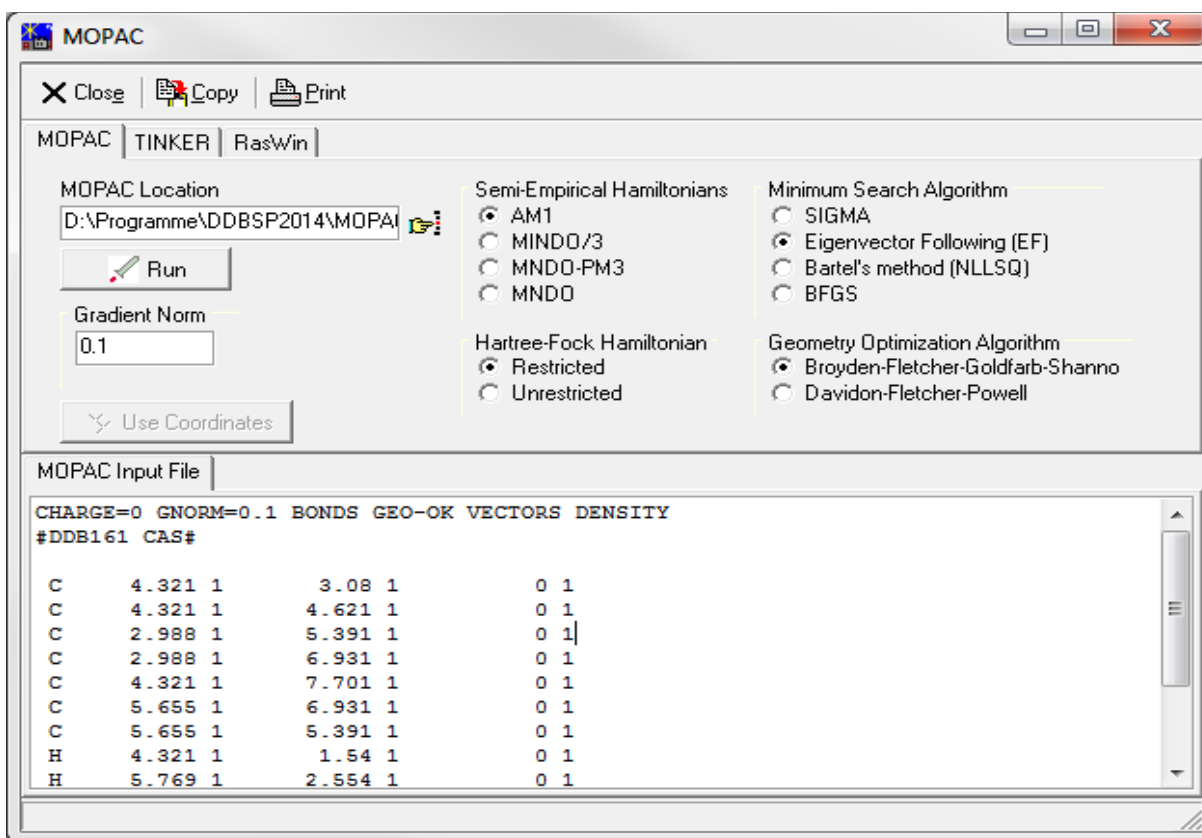
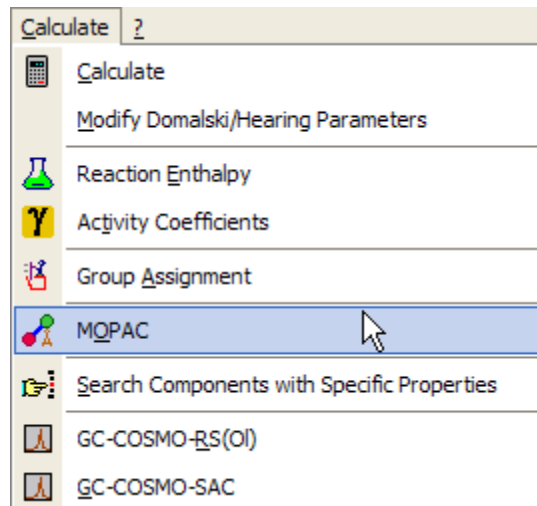
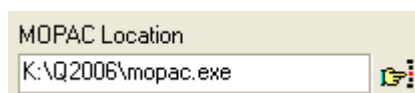



Figure 29: MOPAC Interface Dialog

Since MOPAC is a standalone program, the first step for using the program is defining its location in Artist.

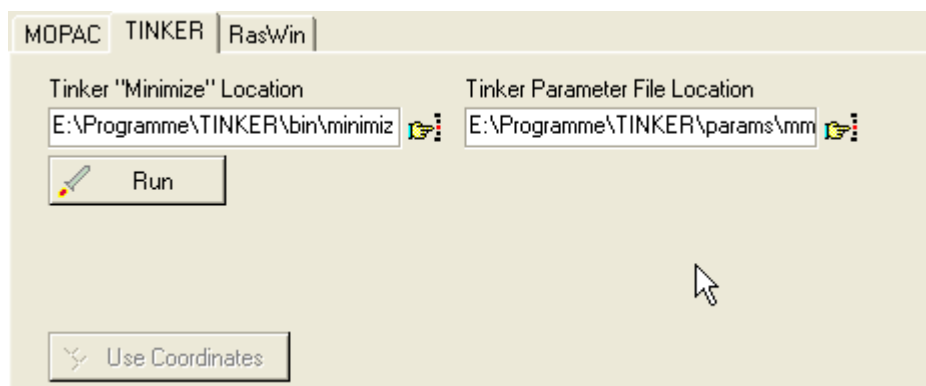


Artist does not much more than writing a MOPAC compatible molecular structure file (shown in the dialog), calling MOPAC


by command line and presenting the results. For a description of the different options please use the MOPAC manuals.

The button  Use Coordinates allows to load the coordinates generated by MOPAC.

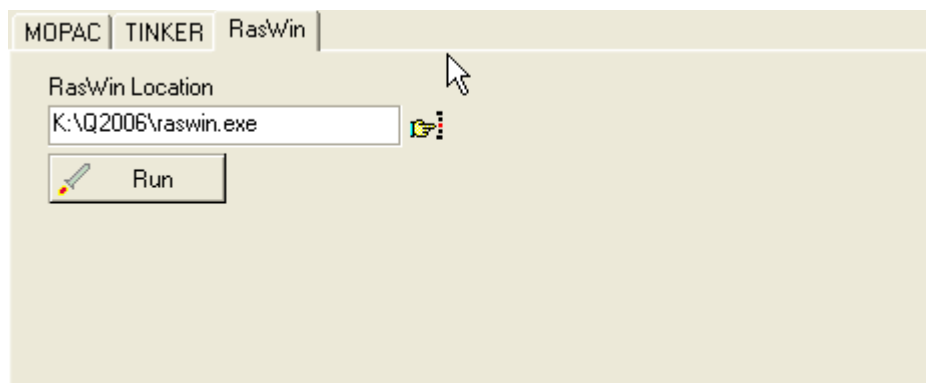
## Tinker



Tinker is a molecular mechanics programs used in Artist 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  Use Coordinates can be used to read the coordinates generated by Tinker.

## RasMol




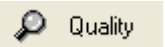
RasMol is a rather simple, but free, display program for chemical structures. Before first use the location of the program has to be specified.

## Model Quality

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

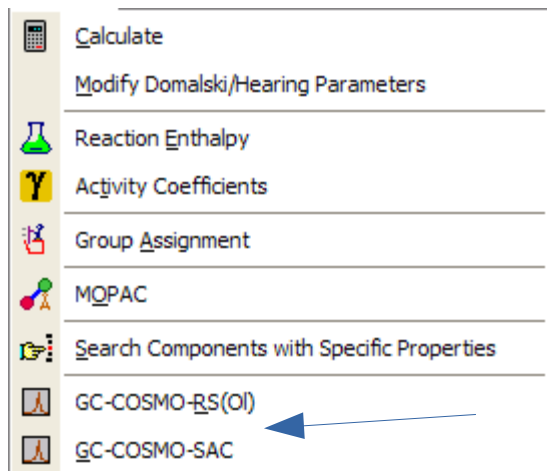
Component	Toluene		
DDB Number	161		
<b>Hydrocarbons (annotated HC) [1]</b>			
All components that belong to a Hydrocarbon Filter			
	AAD	Component Count	Quality
Ambrose	3.06 K	134	Excellent
Rarey/Nanolal	3.5 K	141	Excellent
Somayajulu	4.86 K	141	Good
Wen/Qiang(Tb)	4.99 K	124	Good
Joback	5.68 K	141	Good
Lydersen	6.36 K	141	Good
Marrero/Pardillo	7.06 K	123	Good
Klincewicz/Reid	7.42 K	141	Good
Gani/Constantinou	10.25 K	142	Unreliable
Chein-Hsiun_Tu	13.55 K	143	Unreliable
Daubert	14.29 K	140	Unreliable
Wen/Qiang	14.55 K	126	Unreliable
<b>Aromatic HC [6]</b>			
All components that belong to a Aromatic Hydrocarbon Filter			
	AAD	Component Count	Quality
Ambrose	3.83 K	31	Excellent
Rarey/Nanolal	4.07 K	37	Good
Somayajulu	4.69 K	37	Good
Lydersen	6.46 K	37	Good
Joback	6.89 K	37	Good

Figure 30: Quality Data Bank

The quality dialogs can be called either by the  button from the main dialog or by the  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.



## COSMO-RS $\sigma$ -Profiles



In a new publication<sup>2</sup> a group contribution method for creating COSMO-RS  $\sigma$ -profiles ("Surface Charge Density Profiles) and cavity volumes for COSMO-RS(OI) has been developed.

Additionally to the published method for COSMO-RS(OI) a second method for COSMO-SAC is already available but not yet published.

Artist allows the creation of  $\sigma$ -profiles by these two new methods.

The result dialog display three different output pages.

1. The  $\sigma$ -profile diagram. For COSMO-RS(OI) 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.

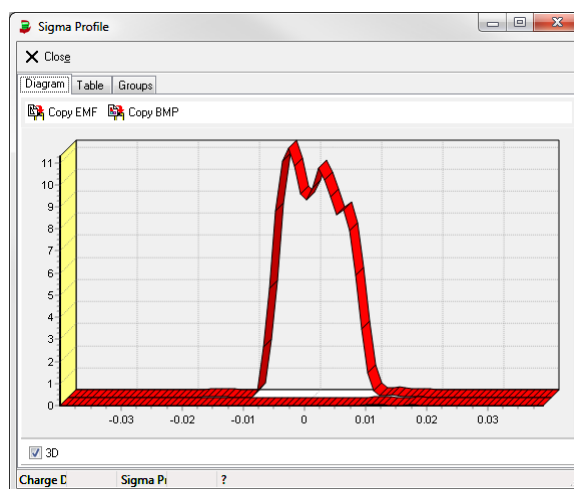
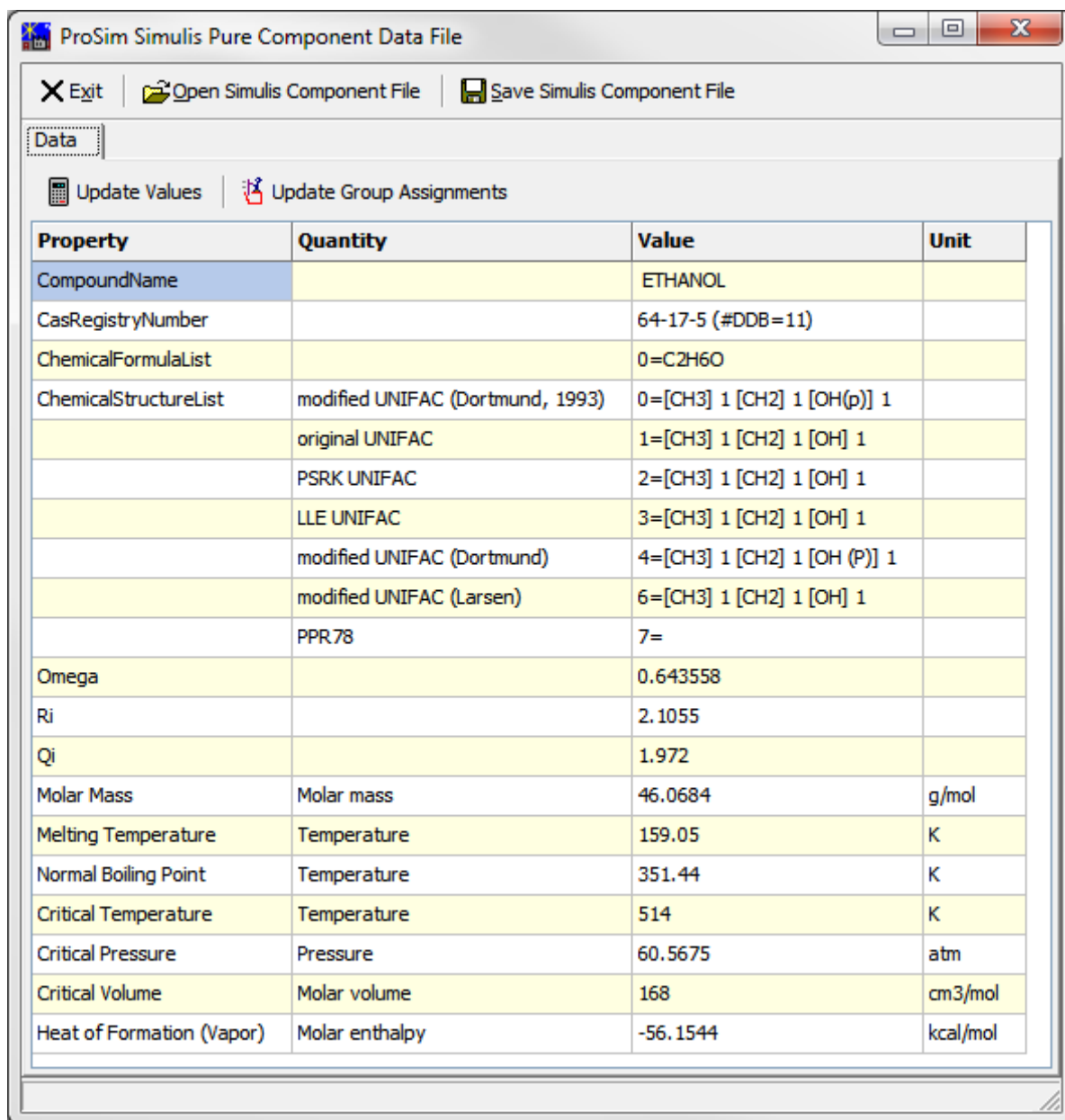


Figure 31:  $\sigma$ -Profile

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

## ProSim Simulis Component File Update

Artist can load and update compound definition files used and created by the ProSim<sup>3</sup> Simulis process



Property	Quantity	Value	Unit
CompoundName		ETHANOL	
CasRegistryNumber		64-17-5 (#DDB=11)	
ChemicalFormulaList		0=C2H6O	
ChemicalStructureList	modified UNIFAC (Dortmund, 1993)	0=[CH3] 1 [CH2] 1 [OH(p)] 1	
	original UNIFAC	1=[CH3] 1 [CH2] 1 [OH] 1	
	PSRK UNIFAC	2=[CH3] 1 [CH2] 1 [OH] 1	
	LLE UNIFAC	3=[CH3] 1 [CH2] 1 [OH] 1	
	modified UNIFAC (Dortmund)	4=[CH3] 1 [CH2] 1 [OH (P)] 1	
	modified UNIFAC (Larsen)	6=[CH3] 1 [CH2] 1 [OH] 1	
	PPR.78	7=	
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	Molar volume	168	cm3/mol
Heat of Formation (Vapor)	Molar enthalpy	-56.1544	kcal/mol

Figure 32: ProSim Simulis Component File Update

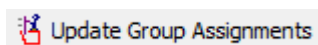
simulation software. The component identification relies on the CAS registry number. If a CAS-RN is not specified in the ProSim component file the assignment will fail.

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

A ProSim component file contains some basic properties that Artist can add or modify. The list of properties are

1. Groups assignments for
  1. original UNIFAC
  2. modified UNIFAC (Dortmund)
  3. PSRK
2. Acentric factor (Omega,  $\omega$ )
3. Volume and Surface for UNIQUAC
4. Molar mass
5. Melting temperature
6. Critical temperature, pressure, volume
7. Heat of formation of gases

## Updating Group Assignments



After selecting one of the three supported models

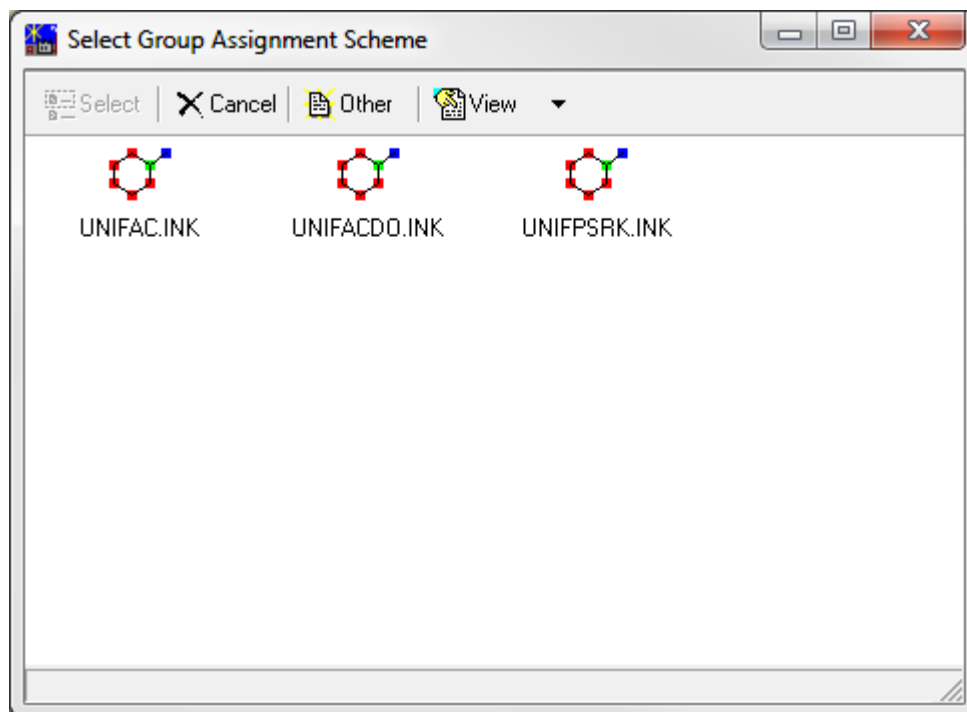


Figure 33: Group Assignment Scheme Selection for ProSim Component File Update

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

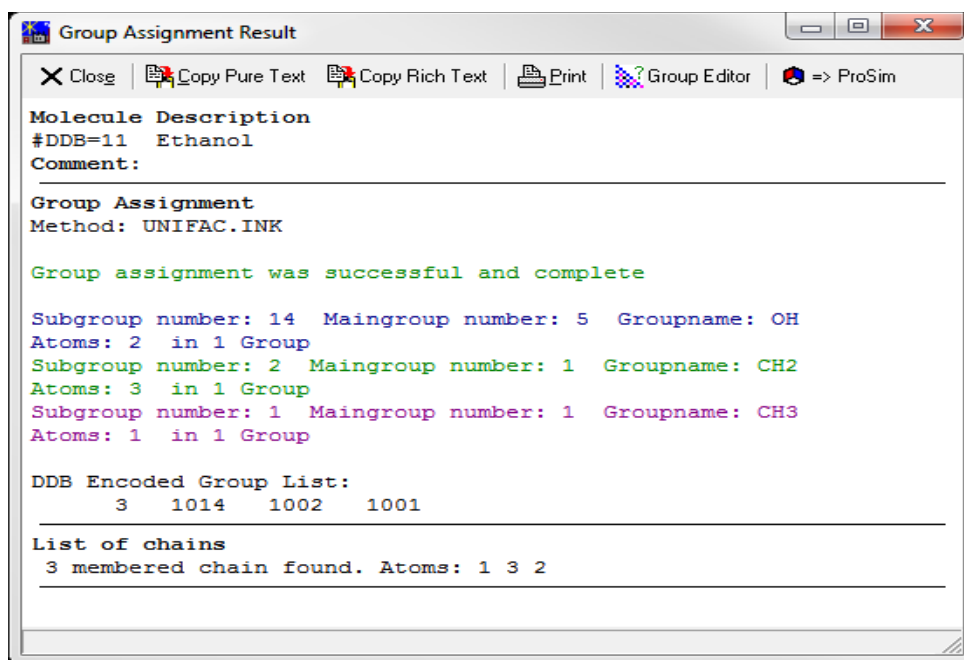

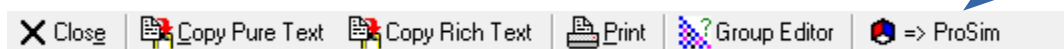


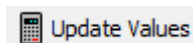
Figure 34: Group Assignment Result for ProSim Component File Update

The button “ => ProSim” in the toolbar



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

## Update Values




This function opens the standard Artist calculation dialog (see chapter “Estimation of Properties” on page 21 and following).

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

Result - Text		Result - Grid					
Save		Copy		Print		Clear	
				Remove Error Lines		Save in ParameterDB	
						Export to INP	
						Export to ProSim	
Property	Method	Result	Unit	Export to Aspen?	Export to ProSim?	Used Data	
TC	Alvarez/Valderrama (w/o isomer corr.)	521.429	K	<input type="checkbox"/> No	<input type="checkbox"/> No	BPT=351.45 K	
TC	Wilson/Jasperson	522.691	K	<input type="checkbox"/> No	<input type="checkbox"/> No	BPT=351.45 K	
TC	Wen/Qiang	514.629	K	<input type="checkbox"/> No	<input type="checkbox"/> No		
TC	Wen/Qiang (Tb)	528.409	K	<input type="checkbox"/> No	<input type="checkbox"/> No	BPT=351.45 K	
TC	Ambrose	512.592	K	<input type="checkbox"/> No	<input checked="" type="checkbox"/> Yes	BPT=351.45 K	
TC	Rarey/Nannolal (est.Tb)	495.984	K	<input type="checkbox"/> No	<input type="checkbox"/> No		
TC	Rarey/Nannolal (given Tb)	523.34	K	<input type="checkbox"/> No	<input type="checkbox"/> No	BPT=351.45 K	
TC	Chein-Hsiun Tu	490.2	K	<input type="checkbox"/> No	<input type="checkbox"/> No		
TC	Daubert	508.182	K	<input type="checkbox"/> No	<input type="checkbox"/> No	BPT=351.45 K	
TC	Lydersen	521.349	K	<input type="checkbox"/> No	<input type="checkbox"/> No	BPT=351.45 K	


Figure 35: Property Estimation for ProSim Component File Update

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.

## Store Component File

The ProSim component saving routine

 Save Simulis Component File

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

## Appendix

### File Formats

Artist allows to store four and read four 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

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.

The format of the MOL format can be obtained from MDL ([http://www.mdli.com/solutions/white\\_papers/ctfile\\_formats.jsp](http://www.mdli.com/solutions/white_papers/ctfile_formats.jsp)).

### The CTC File Format

The CTC format is specially designed to match the requirements of the program Artist 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:

<b>Tag</b>	<b>Description</b>
#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
#PROGRAM	program the file was created with
#COMMENT	comment

<i>Tag</i>	<i>Description</i>
#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 NO<sub>2</sub> 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 ( German “**Kette**” 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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