

# Getting started with Simulis® Thermodynamics

## Use Case 10: Use of the Predictive Models Editor

Software & Services In Process Simulation

*We guide You to efficiency*



ProSim

# Introduction

This document presents the Predictive Models Editor that is used to configure predictive thermodynamic models based on group contributions.

- Editor presentation
- Use within Simulis Thermodynamics
- Installation of « private » matrices from the UNIFAC consortium

# Presentation: models

- Simulis Thermodynamics (ProSim's thermodynamic calculation server) includes several predictive models based on group contributions.
  - UNIFACs (Original, Dortmund, Larsen, PSRK, VTPR, NIST, ...)
  - PPR78
  - GC-PPC-SAFT
  - NRTL-PR
  - ...

# Presentation: groups and sub-groups

- A group can include several functional sub-groups
- Each sub-group has specific parameters that depend on the model
- Interaction coefficients between groups allow to describe the influence of the groups on each other
- In order for the model to work, it must be possible to do group assignment for each molecule

# Presentation: the software

- Accessible from the start menu in the ProSim directory, under the name: « predictive models editor »
- Open the files containing the groups and sub-groups information and their interaction parameters (.xud) located in the default directory:  
« C:\ProgramData\ProSim\StarDust\UNIFAC Models »

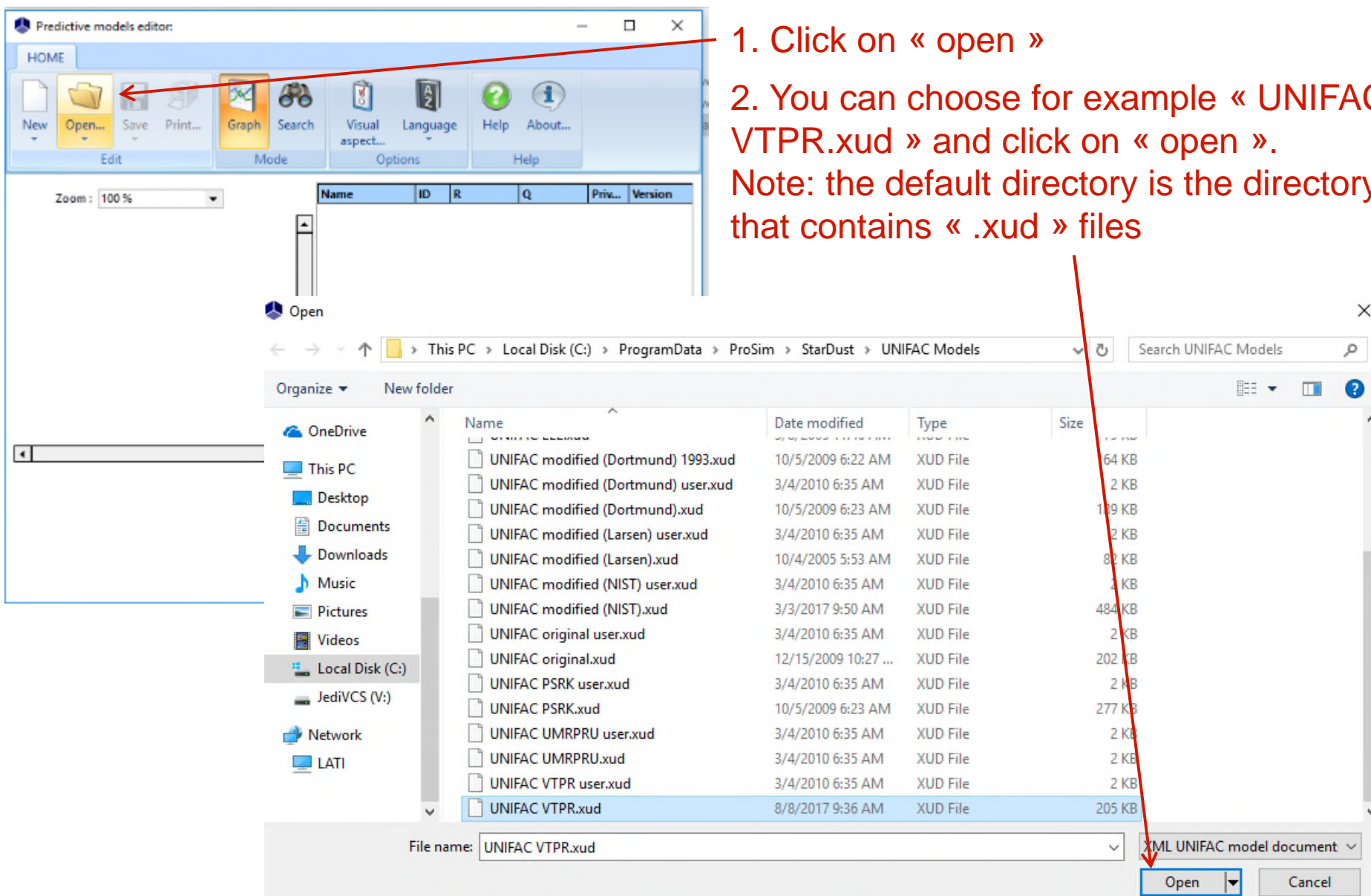


# Editor: open a « xud » file

1. Click on « open »

2. You can choose for example « UNIFAC VTPR.xud » and click on « open ».

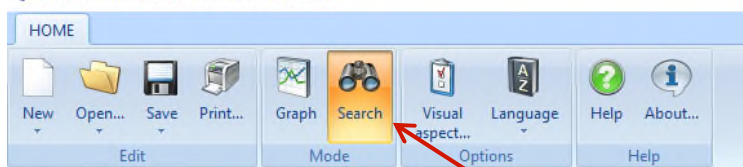
Note: the default directory is the directory that contains « .xud » files



# Editor: indication of use

Graph mode

Predictive models editor: UNIFAC VTPR.xud

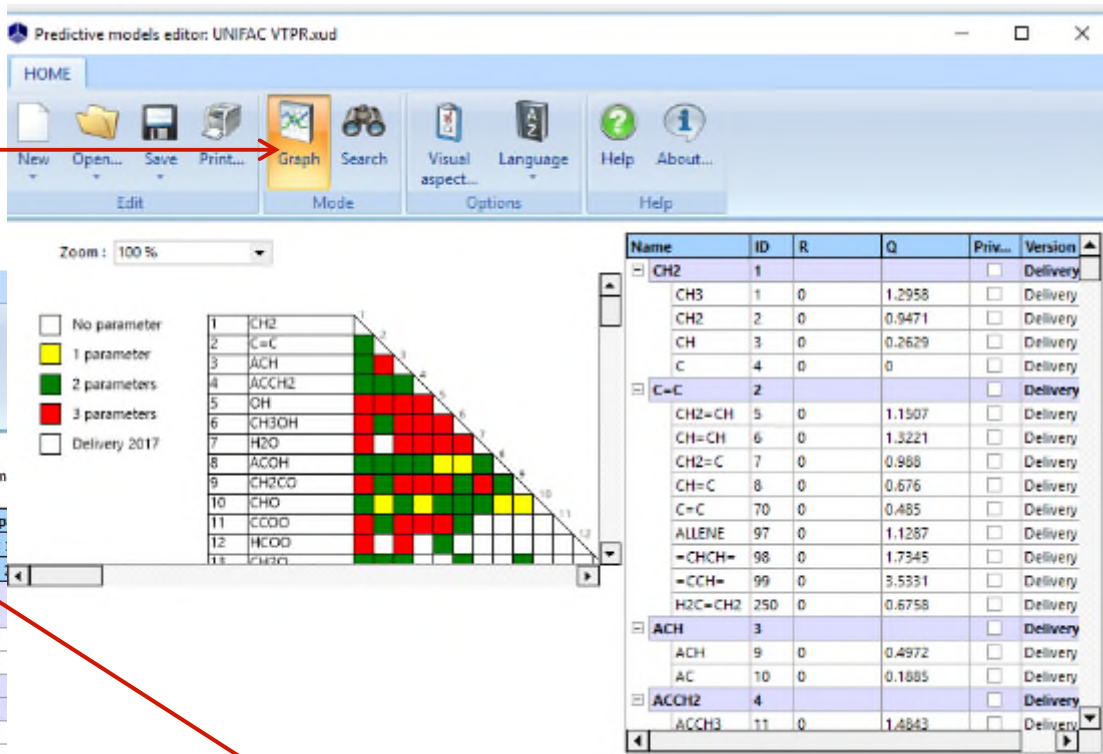


Search subgroups by ID or name:

Search now

☒ Show additional information

Sub-groups				Main groups				Binary interaction p			
Name 1	ID 1	Version 1	Pri...	Name 1	ID 1	Version 1	Pri...	A 1-2	B 1-2	C	
Name 2	ID 2	Version 2	Pri...	Name 2	ID 2	Version 2	Pri...	A 2-1	B 2-1	C	
CH3	1	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	Deliver
CH2=CH	5	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH3	1	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	
CH=CH	6	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH3	1	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	
CH2=C	7	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH3	1	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	
CH=C	8	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH3	1	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	
C=C	70	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH3	1	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	
ALLENE	97	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH3	1	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	
=CHCH=	98	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH3	1	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	
=CCH=	99	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH3	1	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	
H2C=CH2	250	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH2	2	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	
CH2=CH	5	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH2	2	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	
CH=CH	6	Delivery 20	<input type="checkbox"/>	C=C	2	Delivery 20	<input type="checkbox"/>	-87.61	-0.054411	0	
CH2	2	Delivery 20	<input type="checkbox"/>	CH2	1	Delivery 20	<input type="checkbox"/>	171.47	-0.043222	0	



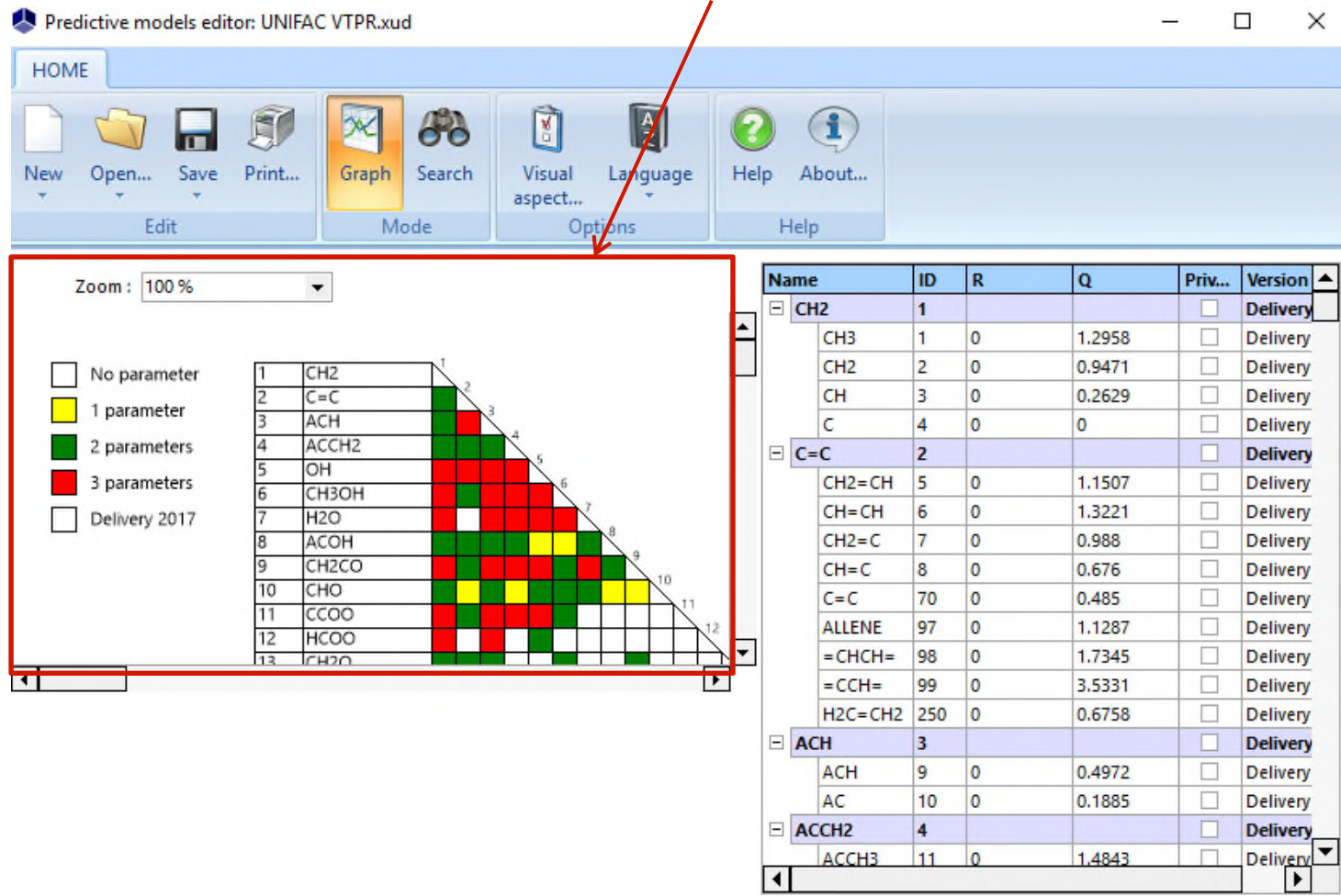
Search mode



# Editor: data visualization

## Group interactions matrix

- The color code indicates the number of parameters available for each interaction.
  - In the absence of parameters, the reliability of the predictive model is questionable.





# Editor: data visualization

By hovering the mouse on a colored box:

- Display the available parameters for the corresponding groups binary and therefore for associated sub-groups.

Predictive models editor: UNIFAC VTPR.xud

HOME

New Open... Save Print... Graph Search Visual aspect... Language Help About...

Edit Mode Options Help

Zoom : 100 %

☐ No parameter  
☐ 1 parameter  
☐ 2 parameters  
☐ 3 parameters  
☐ Delivery 2017

Main groups	Subgroups	Parameters
[6] CH3OH	[15] CH3OH	6→13 -35.988 -0.62428 0
[13] CH2O	[24] CH3O, [25] CH2O, [26] CHO	13→6 322.09 0.29426 0

Name	ID	R	Q	Priv...	Version
CH2	1				Delivery 2017
CH3	1	0	1.2958		Delivery 2017
CH2	2	0	0.9471		Delivery 2017
CH	3	0	0.2629		Delivery 2017
C	4	0	0		Delivery 2017
C=C	2				Delivery 2017
CH2=CH	5	0	1.1507		Delivery 2017
CH=CH	6	0	1.3221		Delivery 2017
CH2=C	7	0	0.988		Delivery 2017
CH=C	8	0	0.676		Delivery 2017
C=C	70	0	0.485		Delivery 2017
ALLENE	97	0	1.1287		Delivery 2017
=CHCH=	98	0	1.7345		Delivery 2017
=CCH=	99	0	3.5331		Delivery 2017
H2C=CH2	250	0	0.6758		Delivery 2017
ACH	3				Delivery 2017
ACH	9	0	0.4972		Delivery 2017
AC	10	0	0.1885		Delivery 2017
ACCH2	4				Delivery 2017
ACCH3	11	0	1.4843		Delivery 2017
ACCH2	12	0	1.1356		Delivery 2017
ACCH	13	0	0.4514		Delivery 2017
OH	5				Delivery 2017
OH (P)	14	0	1.0189		Delivery 2017
OH (S)	81	0	0.9326		Delivery 2017
OH (T)	82	0	0.8727		Delivery 2017
CH3OH	6				Delivery 2017
CH3OH	15	0	0.8779		Delivery 2017

# Editor: data visualization

## Groups and sub-groups description

- Groups and sub-groups number
- Sub-groups parameters

Predictive models editor: UNIFAC VTPR.xud

HOME

New Open... Save Print... Graph Search Visual aspect... Language Help About...

Edit Mode Options Help

Zoom : 100 %

☐ No parameter  
☐ 1 parameter  
☐ 2 parameters  
☐ 3 parameters  
☐ Delivery 2017

1 CH2  
 2 C=C  
 3 ACH  
 4 ACCH2  
 5 OH  
 6 CH3OH  
 7 H2O  
 8 ACOH  
 9 CH2CO  
 10 CHO  
 11 CCOO  
 12 HCOO  
 13 CH2O  
 14 CH2NH2  
 15 CH2NH  
 16 (C)3N  
 17 ACNH2  
 19 CH2CN  
 20 COOH  
 21 CCL  
 22 CCL2

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22

1 CH2  
 2 C=C  
 3 ACH  
 4 ACCH2  
 5 OH  
 6 CH3OH  
 7 H2O  
 8 ACOH  
 9 CH2CO  
 10 CHO  
 11 CCOO  
 12 HCOO  
 13 CH2O  
 14 CH2NH2  
 15 CH2NH  
 16 (C)3N  
 17 ACNH2  
 19 CH2CN  
 20 COOH  
 21 CCL  
 22 CCL2

Main groups Subgroups Parameters  
 [6] CH3OH [15] CH3OH 6→13 -35.988 -0.62428 0  
 [13] CH2O [24] CH3O, [25] CH2O, [26] CHO 13→6 322.09 0.29426 0

Name ID R Q Priv... Version  
 CH2 1 0 1.2958 Delivery 2017  
 CH3 1 0 0.9471 Delivery 2017  
 CH2 2 0 0.2629 Delivery 2017  
 CH 3 0 0 Delivery 2017  
 C 4 0 0 Delivery 2017  
 C=C 2 0 1.1507 Delivery 2017  
 CH2=CH 5 0 1.3221 Delivery 2017  
 CH=CH 6 0 0.988 Delivery 2017  
 CH2=C 7 0 0.676 Delivery 2017  
 CH=C 8 0 0.485 Delivery 2017  
 C=C 70 0 1.1287 Delivery 2017  
 ALLENE 97 0 1.7345 Delivery 2017  
 =CHCH= 98 0 3.5331 Delivery 2017  
 =CCH= 99 0 0.6758 Delivery 2017  
 H2C=CH2 250 0 0.6758 Delivery 2017  
 ACH 3 0 0.4972 Delivery 2017  
 ACH 9 0 0.1885 Delivery 2017  
 AC 10 0 0.4514 Delivery 2017  
 ACCH2 4 0 1.4843 Delivery 2017  
 ACCH3 11 0 1.1356 Delivery 2017  
 ACCH2 12 0 0.4514 Delivery 2017  
 ACCH 13 0 1.0189 Delivery 2017  
 OH 5 0 0.9326 Delivery 2017  
 OH (P) 14 0 0.8727 Delivery 2017  
 OH (S) 81 0 0.8727 Delivery 2017  
 OH (T) 82 0 0.8779 Delivery 2017  
 CH3OH 6 0 0.8779 Delivery 2017  
 CH3OH 15 0 0.8779 Delivery 2017

Group

SubGroup



# Editor: modifications

By clicking on a box, colored or not:

- Open a window for editing group interaction parameters
  - The parameters are not necessarily symmetrical

Predictive models editor: UNIFAC VTPR.xud

HOME

New Open... Save Print... Graph Search Visual aspect... Language Help About...

Edit Mode Options Help

Zoom: 100 %

Binary interaction parameters

Maingroup 1: [6] CH3OH

Maingroup 2: [13] CH2O

Version: Delivery 2017 ☐ Private

Parameters:

	A	B	C
6->13	-35.988	-0.62428	0
13->6	322.09	0.29426	0

Legend:

- ☐ No parameter
- ☒ 1 parameter
- ☒ 2 parameters
- ☒ 3 parameters
- ☒ Delivery 2017

Main groups	Subgroups	Parameters
[6] CH3OH	[15] CH3OH	6-13 -35.988 -0.62428 0
[13] CH2O	[24] CH3O, [25] CH2O, [26] CHO	13-6 322.09 0.29426 0

Name	ID	R	Q	Priv...	Version
CH2	1			<input type="checkbox"/>	Delivery 2017
			8	<input type="checkbox"/>	Delivery 2017
		1		<input type="checkbox"/>	Delivery 2017
		9		<input type="checkbox"/>	Delivery 2017
				<input type="checkbox"/>	Delivery 2017
				<input type="checkbox"/>	Delivery 2017
		7		<input type="checkbox"/>	Delivery 2017
		1		<input type="checkbox"/>	Delivery 2017
				<input type="checkbox"/>	Delivery 2017
				<input type="checkbox"/>	Delivery 2017
				<input type="checkbox"/>	Delivery 2017
		7		<input type="checkbox"/>	Delivery 2017
		5		<input type="checkbox"/>	Delivery 2017
		1		<input type="checkbox"/>	Delivery 2017
		8		<input type="checkbox"/>	Delivery 2017
				<input type="checkbox"/>	Delivery 2017
				<input type="checkbox"/>	Delivery 2017
		2		<input type="checkbox"/>	Delivery 2017
		5		<input type="checkbox"/>	Delivery 2017
				<input type="checkbox"/>	Delivery 2017
OH	5			<input type="checkbox"/>	Delivery 2017
OH (P)	14	0	1.0189	<input type="checkbox"/>	Delivery 2017
OH (S)	81	0	0.9326	<input type="checkbox"/>	Delivery 2017
OH (T)	82	0	0.8727	<input type="checkbox"/>	Delivery 2017
CH3OH	6			<input type="checkbox"/>	Delivery 2017
CH3OH	15	0	0.8779	<input type="checkbox"/>	Delivery 2017

Ok Cancel

# Editor: modifications

All fields are editable by following the procedure below:

- Select the field
  - In this example, the property R (Van der Waals volume) of CH3 sub-group is selected

Name	ID	R	Q	Priv...	Version
CH2	1			<input type="checkbox"/>	Delivery 2017
CH3	1	0	1.2958	<input checked="" type="checkbox"/>	Delivery 2017
CH2	2	0	0.9471	<input type="checkbox"/>	Delivery 2017
CH	3	0	0.2629	<input type="checkbox"/>	Delivery 2017
C	4	0	0	<input type="checkbox"/>	Delivery 2017

- Press « Enter » or « F2 » to activate the edit mode
  - The property R (Van der Waals volume) of CH3 sub-group is now editable

Name	ID	R	Q	Priv...	Version
CH2	1			<input type="checkbox"/>	Delivery 2017
CH3	1	0	1.2958	<input checked="" type="checkbox"/>	Delivery 2017
CH2	2	0	0.9471	<input type="checkbox"/>	Delivery 2017
CH	3	0	0.2629	<input type="checkbox"/>	Delivery 2017
C	4	0	0	<input type="checkbox"/>	Delivery 2017

- Validate the modification by pressing « Enter ». Since edit mode is active, the next cell becomes editable if necessary



# Editor: modifications

Adding a new main group:

- Right-click on any cell
- In the dropdown menu, choose « Add a main group »
  - The main group is automatically added at the end of the list

	C	4	0	0	<input type="checkbox"/>	Delivery 2017
[-]	C=C	2			<input type="checkbox"/>	Delivery 2017
	CH2=CH	5	0	1.1507	<input type="checkbox"/>	Delivery 2017
	CH=CH	6	0	1.2221	<input type="checkbox"/>	Delivery 2017
	CH2=C				<input type="checkbox"/>	Delivery 2017
	CH=C				<input type="checkbox"/>	Delivery 2017
	C=C				<input type="checkbox"/>	Delivery 2017
	ALLEN				<input type="checkbox"/>	Delivery 2017
	=CHC				<input type="checkbox"/>	Delivery 2017
	=CCH				<input type="checkbox"/>	Delivery 2017
	H2C=C				<input type="checkbox"/>	Delivery 2017
[-]	ACH				<input type="checkbox"/>	Delivery 2017
	ACH				<input type="checkbox"/>	Delivery 2017
	AC				<input type="checkbox"/>	Delivery 2017
[-]	ACCH2				<input type="checkbox"/>	Delivery 2017
	ACCH3				<input type="checkbox"/>	Delivery 2017
	ACCH2	12	0	1.1356	<input type="checkbox"/>	Delivery 2017
	ACCH	13	0	0.4514	<input type="checkbox"/>	Delivery 2017
[-]	OH	5			<input type="checkbox"/>	Delivery 2017

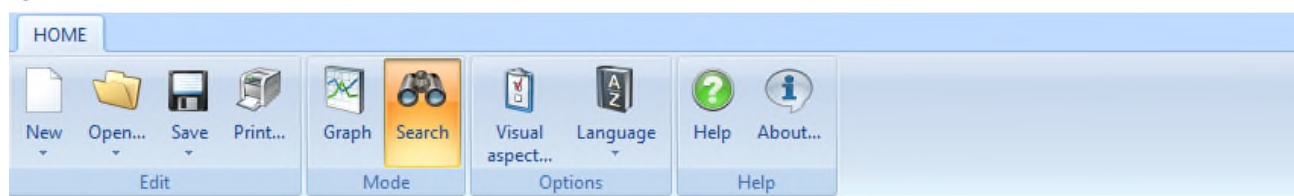
Adding a new sub-group:

- Right-click on the purple line of the desired main group
- In the drop down list, choose « Add a sub-group »

	C	4	0	0	<input type="checkbox"/>	Delivery 2017
[-]	C=C	2			<input type="checkbox"/>	Delivery 2017
	CH2=C				<input type="checkbox"/>	Delivery 2017
	CH=CH				<input type="checkbox"/>	Delivery 2017
	CH2=C				<input type="checkbox"/>	Delivery 2017
	CH=C				<input type="checkbox"/>	Delivery 2017
	C=C				<input type="checkbox"/>	Delivery 2017
	ALLEN				<input type="checkbox"/>	Delivery 2017
	=CHC				<input type="checkbox"/>	Delivery 2017
	=CCH				<input type="checkbox"/>	Delivery 2017
	H2C=C				<input type="checkbox"/>	Delivery 2017
[-]	ACH				<input type="checkbox"/>	Delivery 2017
	ACH				<input type="checkbox"/>	Delivery 2017
	AC				<input type="checkbox"/>	Delivery 2017
[-]	ACCH2	4			<input type="checkbox"/>	Delivery 2017
	ACCH3	11	0	1.4843	<input type="checkbox"/>	Delivery 2017
	ACCH2	12	0	1.1356	<input type="checkbox"/>	Delivery 2017
	ACCH	13	0	0.4514	<input type="checkbox"/>	Delivery 2017

# Editor: modifications

The « Search » mode allows to visualize the global set of parameters between a given group and the others, and easily edit them (rather than clicking on the corresponding cell of the triangular matrix presented previously).



Search subgroups by ID or name:

Search now

☐ Show additional information

Sub-groups		Main groups		Binary interaction parameters			Misc.
Name 1	ID 1	Name 1	ID 1	A 1-2	B 1-2	C 1-2	Notes
Name 2	ID 2	Name 2	ID 2	A 2-1	B 2-1	C 2-1	
CH3	1	CH2	1	171.47	-0.043222	0	
CH2=CH	5	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
CH=CH	6	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
CH2=C	7	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
CH=C	8	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
C=C	70	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
ALLENE	97	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
=CHCH=	98	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
=CCH=	99	C=C	2	-87.61	-0.054411	0	
CH3	1	CH2	1	171.47	-0.043222	0	
H2C=CH2	250	C=C	2	-87.61	-0.054411	0	
CH2	2	CH2	1	171.47	-0.043222	0	
CH2=CH	5	C=C	2	-87.61	-0.054411	0	

# Simulis Thermodynamics

For a group contribution model to work, the decomposition of the molecules must involve sub-groups that are available in that model (if the decomposition of the molecules involves a sub-group not recognized by the model, that predictive model cannot be used).

In Simulis Thermodynamics, the decomposition of a molecule must be specified in the « Compounds » tab of the calculator, using the « Standard » sub-folder of the « Group contribution model » folder in the compound editor.


The screenshot displays the 'Thermodynamic calculator editor' window. The 'COMPOUND' tab is selected, showing a list of compounds: ETHYLBENZENE and ETHANE. The 'COMPOUND' window is open, displaying the 'Properties' table for ETHYLBENZENE. The 'Group contribution model' folder is expanded, and the 'Standard' sub-folder is highlighted. The 'Properties' table lists various chemical structure models and their corresponding group contribution values.


Properties	Value
Identification	
Group contribution model	
Standard	
UNIFAC modified (Dortmund) 1993 chemical structure	[ACH] 5 [ACCH2] 1 [CH3] 1
UNIFAC original chemical structure	[ACH] 5 [ACCH2] 1 [CH3] 1
UNIFAC PSRE chemical structure	[ACH] 5 [ACCH2] 1 [CH3] 1
UNIFAC LLE chemical structure	[CH3] 1 [ACH] 5 [ACCH2] 1
UNIFAC modified (Dortmund) chemical structure	[ACH] 5 [ACCH2] 1 [CH3] 1
UNIFAC modified (Jensen) chemical structure	[CH3] 1 [CH2] 1 [ACH] 5 [AC] 1
PPR 78 chemical structure	[ACH] 5 [AC] 1 [CH2] 1 [CH3] 1
UNIFAC VPM chemical structure	[ACH] 5 [ACCH2] 1 [CH3] 1
UNIFAC UMRPRU chemical structure	<unknown>
NRTL PR chemical structure	[ACH] 5 [AC] 1 [CH2] 1 [CH3] 1
GC-PMC-SAF chemical structure	[EthylBz (GZ)(1, 0) 1 [CH3](1, ...
UNIFAC modified (NIST) chemical structure	[ACH] 5 [ACCH2] 1 [CH3] 1
User	
Atomic	
Phase change	
Combustion, security, toxicity	
Condensed phase	
Phase thermochemistry	
Interaction, gas phase reaction	
User properties	
PMC-SAF	
NRTL-SAC	



# Simulis Thermodynamics

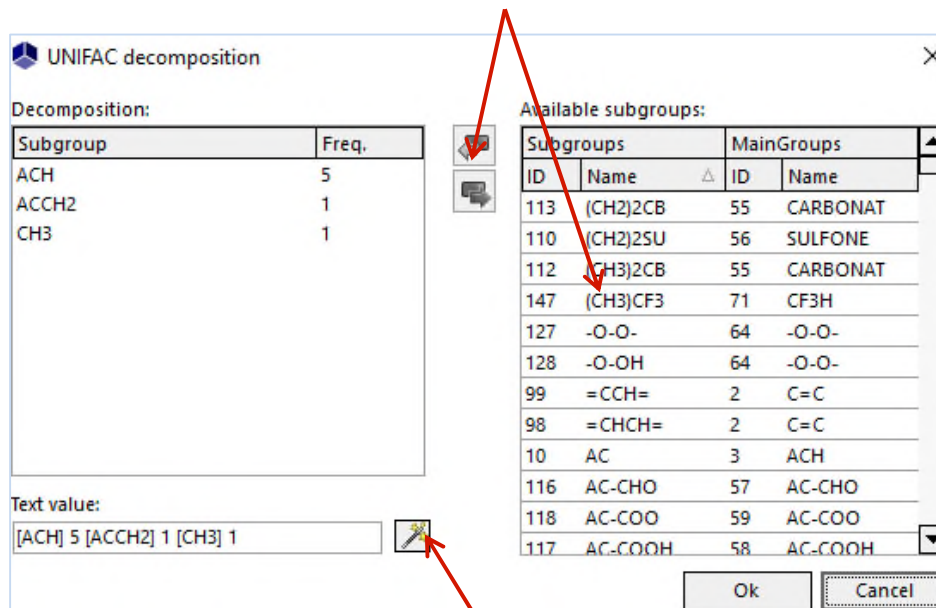
Create the decomposition specification by clicking on the « ... » button located at the end of the line for each decomposition

 UNIFAC VTPR chemical structure

[ACH] 5 [ACCH2] 1 [CH3] 1 

The editing window appears:

- Sub-groups are added by double clicking on the list located on the right or using the arrows located in the middle



- The magic wand allows an automatic prediction of the decomposition if it is possible and if the SMILES of the molecule has been provided (property available in the « identification » tab of the component).



# Simulis Thermodynamics

In a Simulis Thermodynamics « calculator », if a group contribution predictive model is selected (e.g. VTPR), click on “Predictive model parameters” to visualize the reduced matrix that only display the groups related to the components of the calculator.

**Thermodynamic calculator editor**

This window helps you to define the context of your thermodynamic calculator

**COMPOUNDS** **MODEL** **PARAMETERS**

**NAME** VTPR

**Category** All the profiles

**Profile** VTPR

**Approach type** Using Equation of state

**Equation of state** PR Generalized

**Alpha function** Twu

**Mixing rules** VTPR

**Activity coefficient model** UNIFAC VTPR

**Pure liquid fugacity standard state** Standard

**Liquid molar volume** Volume translation

**Transport properties** Ely-Hanley model (TRAPP method)

**Enthalpy calculation** H\*=0, ideal gas, 25°C, 1 atm

**User-defined thermodynamic model** None

**Model index** 1

**Comments :**

**THERMODYNAMIC MODEL**

**DOCUMENTATION**

- Thermodynamic assistant
- Thermodynamic help

**ADDITIONAL PARAMETERS**

**MODEL INFORMATION**

- Reactive model parameters...
- Predictive model parameters...**
- Polymers model parameters...

**WATER-HYDROCARBON**

**Predictive models editor:**

Zoom : 100 %

☐ No parameter

☒ 1 parameter

☒ 2 parameters

☒ 3 parameters


1	CH2	1			
3	ACH				
4	ACCH2				
5	OH				

Name	ID	R	Q	Priv...	Version
CH2	1			<input type="checkbox"/>	Delivery
CH3	1	0	1.2958	<input type="checkbox"/>	Delivery
CH2	2	0	0.9471	<input type="checkbox"/>	Delivery
ACH	3			<input type="checkbox"/>	Delivery
ACH	9	0	0.4972	<input type="checkbox"/>	Delivery
ACCH2	4			<input type="checkbox"/>	Delivery
ACCH2	12	0	1.1356	<input type="checkbox"/>	Delivery
OH	5			<input type="checkbox"/>	Delivery
OH (P)	14	0	1.0189	<input type="checkbox"/>	Delivery

# Simulis Thermodynamics

If the user wants to use a custom matrix it is possible to edit and import the « User » templates.

In the « C:\ProgramData\ProSim\StarDust\UNIFAC Models » folder, empty « .xud » files with the « User » indication are available for each model.

 UNIFAC VTPR user.xud	3/4/2010 6:35 AM	XUD File	2 KB
--	------------------	----------	------

These files need to be fully configured by the user. The thermodynamic model to choose is the one with the « (User) » extension.

Activity coefficient model

UNIFAC VTPR (User) ▼

The molecules decompositions need to be defined in the « User » sub-folder.  
**For these models, automatic decomposition may not be consistent since it is based on the groups involved in original models.**

Complete	
Properties	Value
<ul style="list-style-type: none"> <li>Identification</li> <li>Group contribution model           <ul style="list-style-type: none"> <li>Standard</li> <li>User</li> </ul> </li> </ul>	
<ul style="list-style-type: none"> <li>UNIFAC original user chemical structure</li> <li>UNIFAC PSRK user chemical structure</li> <li>UNIFAC LLE user chemical structure</li> <li>UNIFAC modified (Dortmund) user chemical structure</li> <li>UNIFAC modified (Larsen) user chemical structure</li> <li>PPR 78 user chemical structure</li> <li>UNIFAC VTPR user chemical structure</li> <li>UNIFAC IIMPRII user chemical structure</li> </ul>	<ul style="list-style-type: none"> <li>&lt;unknown&gt;</li> <li>&lt;unknown&gt;</li> <li>&lt;unknown&gt;</li> <li>&lt;unknown&gt;</li> <li>&lt;unknown&gt;</li> <li>&lt;unknown&gt;</li> <li>&lt;unknown&gt;</li> <li>&lt;unknown&gt;</li> </ul>

# Private matrices

If the user is member of the UNIFAC consortium, private « .xud » files are provided by the consortium to all members. An installation tool provided by ProSim, in addition to Simulis Thermodynamics, allows to upgrade the ProSim public databases with the UNIFAC member's private databases.

« UNIFAC Private [year] for Simulis Setup.exe »

In order to compare the results, the public databases are conserved in the « Public » folder within the directory containing the « .xud » files.

**WARNING:** The use of private databases implies new parameters, but especially new groups! The molecules decompositions must be updated to correspond with the private databases. The automatic decomposition tool takes into account the type of database (public/private) in order to provide a consistent decomposition.

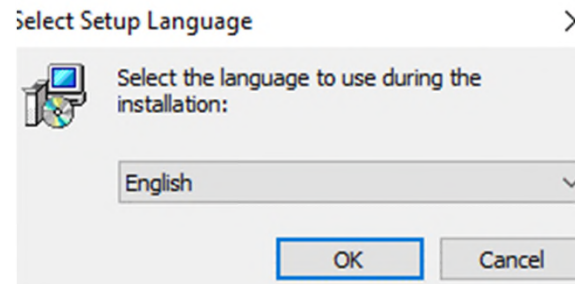
Text value:

[ACH] 5 [ACCH2] 1 [CH3] 1

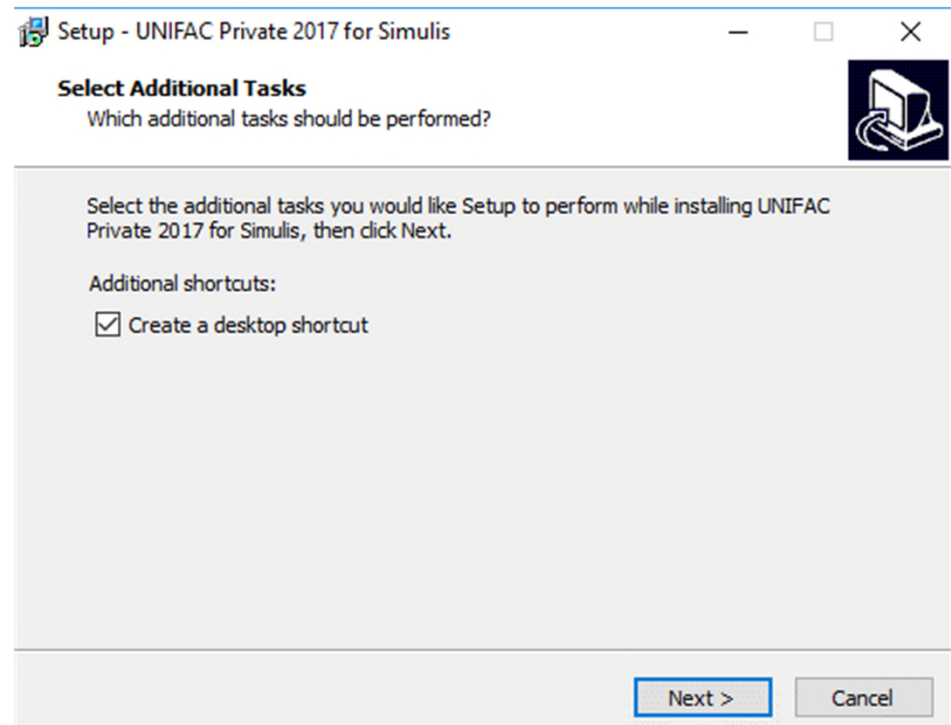


# Private matrices

- Select the installation language and press « OK »



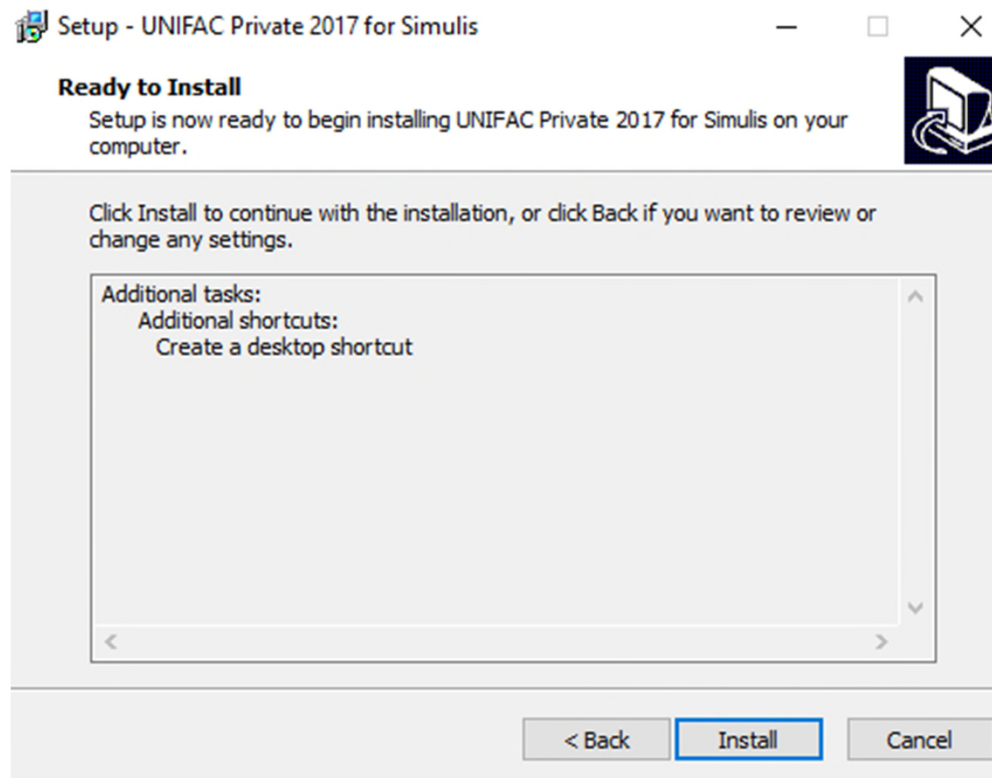
- Choose if a shortcut icon for the predictive model editor should be installed or not on the desktop and press « Next »





# Private matrices

- Click on « Install »



# Private matrices

- Note that in some cases, files are « read-only », therefore it is necessary to change the directory attribute « C:\ProgramData\ProSim »

Error



C:\ProgramData\ProSim\StarDust\UNIFAC Models\UNIFAC Modified (Dortmund).xud

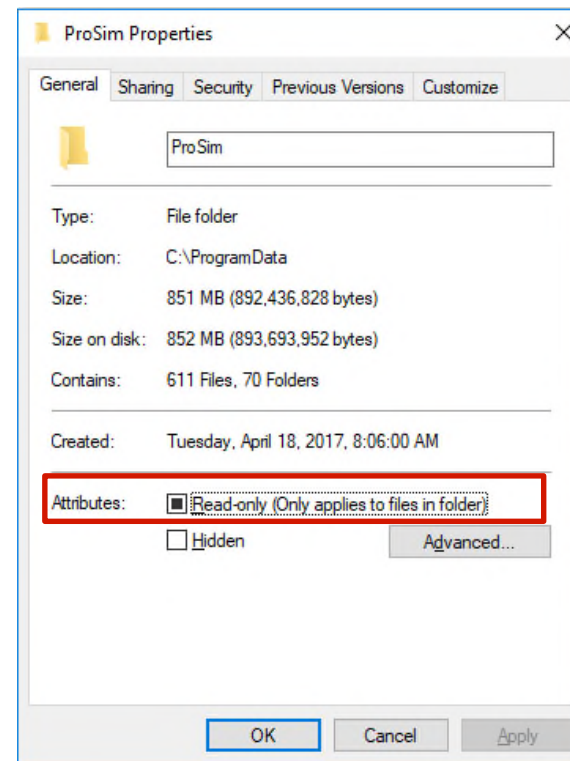
The existing file is marked as read-only.

Click Retry to remove the read-only attribute and try again, Ignore to skip this file, or Abort to cancel installation.

Abort

Retry

Ignore



# Private matrices

- Once the installation is complete, the installer offers to immediately run the predictive models editor.



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# ProSim

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