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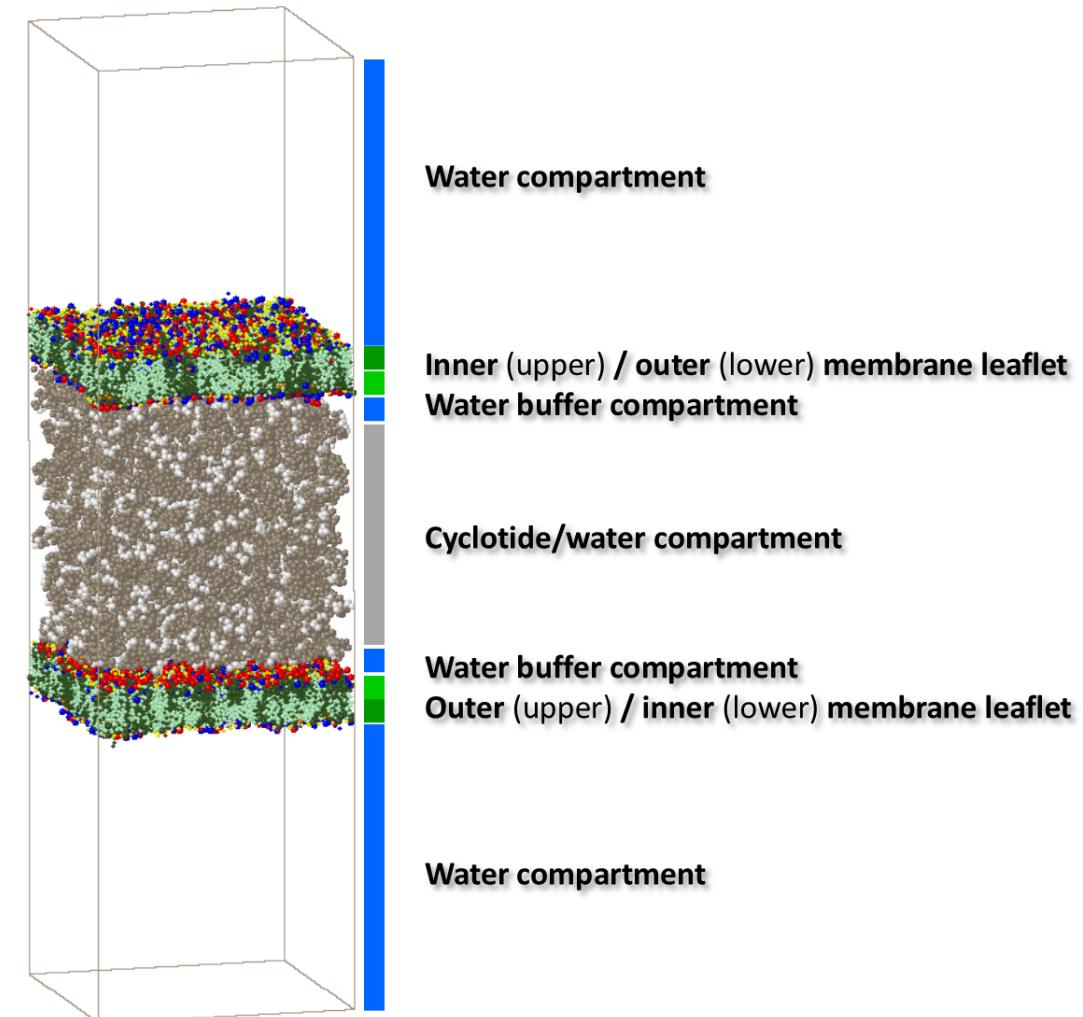
www.molecular-dynamics.de



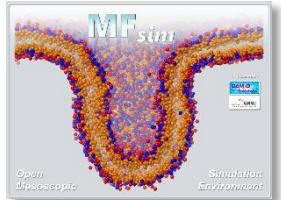
www.gnwi.de

Introduction

This tutorial demonstrates details of the preparation-simulation-evaluation triad of a cyclotide/membrane sandwich interaction model. It consists of two plasma bilayer membranes enclosing a cyclotide/water compartment with the cyclotide Kalata B1 (kB1) single-spot mutant kB1-W19Y. This mutant exhibits a replacement of amino acid tryptophan (W) at position 19 by amino acid tyrosine (Y).



MF_{sim}
2.3.0.0



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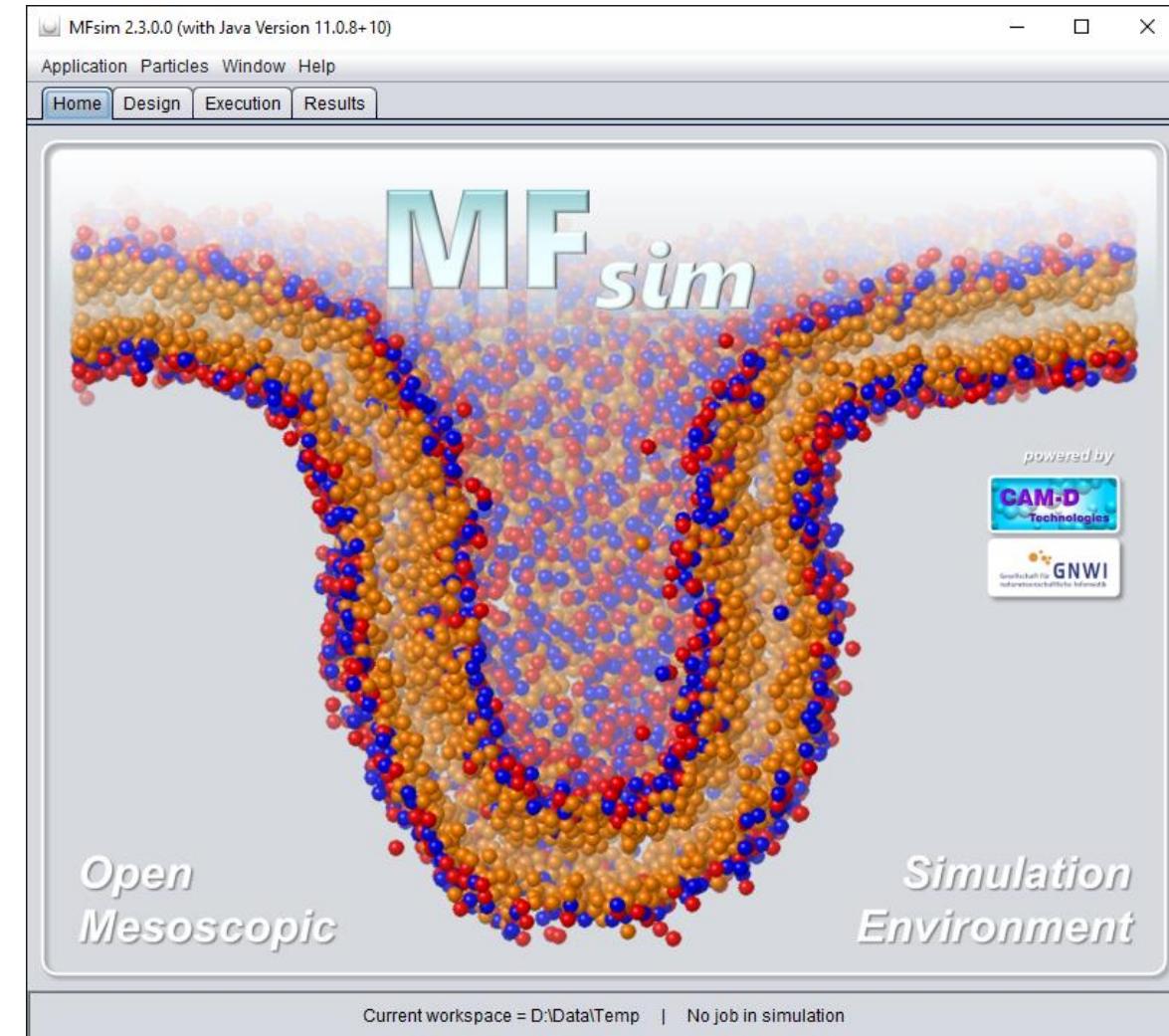


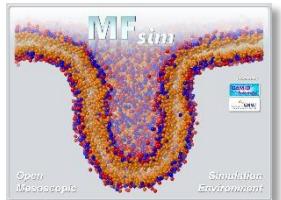
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GitHub repository:
<https://github.com/ziesensy/MFsim>

Application Start

Start MFsim ...





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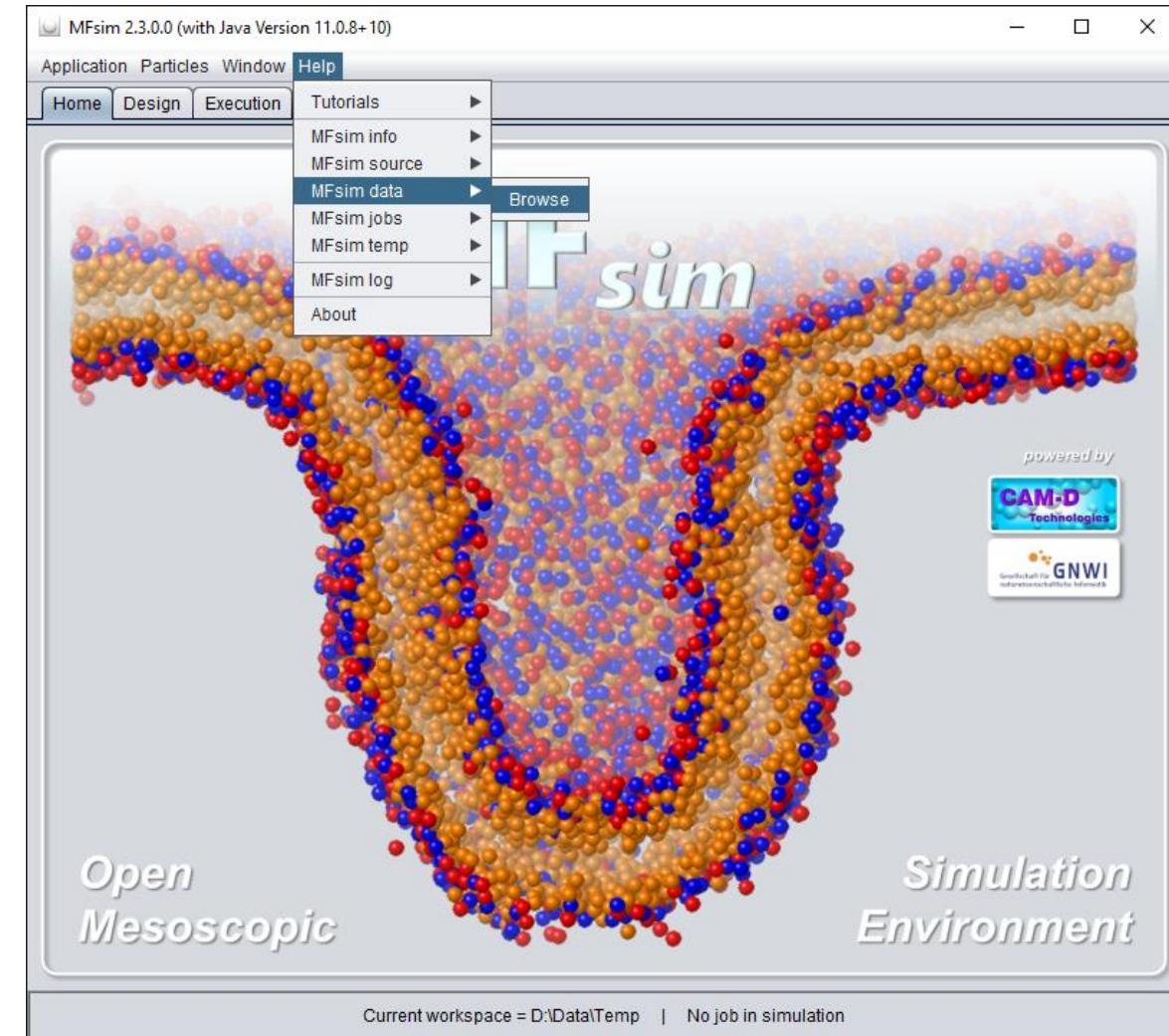


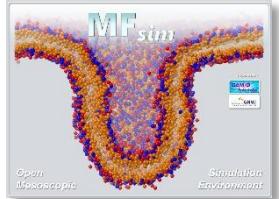
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Particle Set Download

... select menu item **Help / MFsim data / Browse** to browse the MFsim data directory

...





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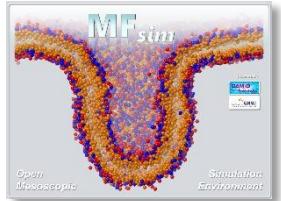


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Particle Set Download

... and download particle set text file *ParticleSet_AA_V03_pm.txt* from the MFsim GitHub repository (located in subfolder *tutorials/Supplement*) into the *CustomParticles* subfolder.

Name	Date modified	Type	Size
CustomParticles	20/02/2020 18:29	File folder	
JobInputs	13/02/2020 10:43	File folder	
JobResults	13/02/2020 10:40	File folder	
Temp	04/02/2020 12:16	File folder	
BasicPreferences.xml	20/02/2020 19:08	XML File	9 KB
MFsim_Logfile.txt	21/02/2020 10:04	Text Document	2 KB
MFsim_SingleInstance.txt	21/02/2020 10:04	Text Document	0 KB



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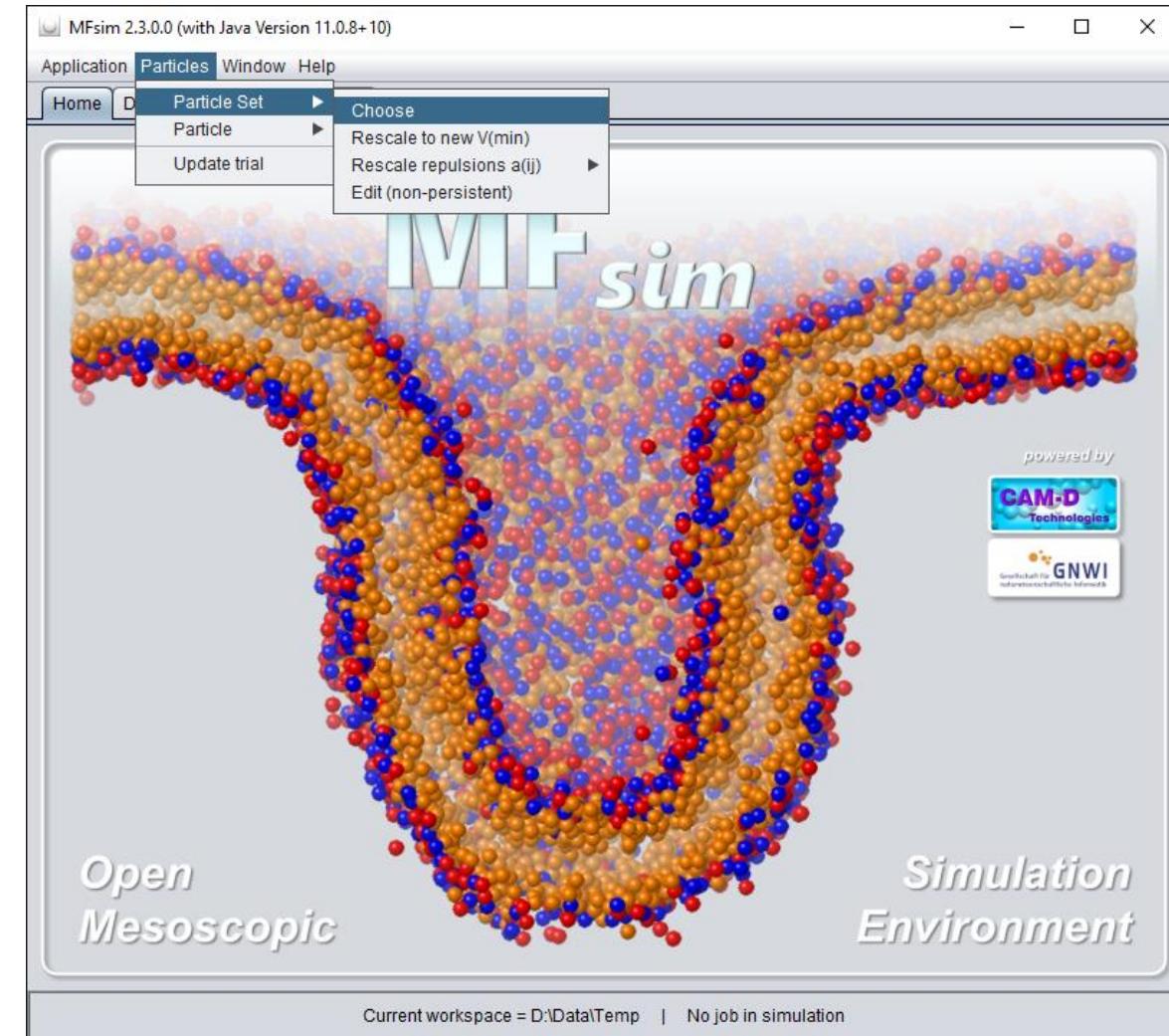
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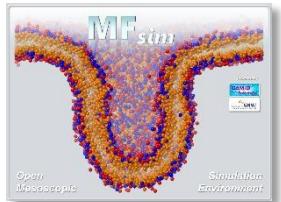


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Particle Set Choice

Select menu item **Particles / Particle set / Choose**





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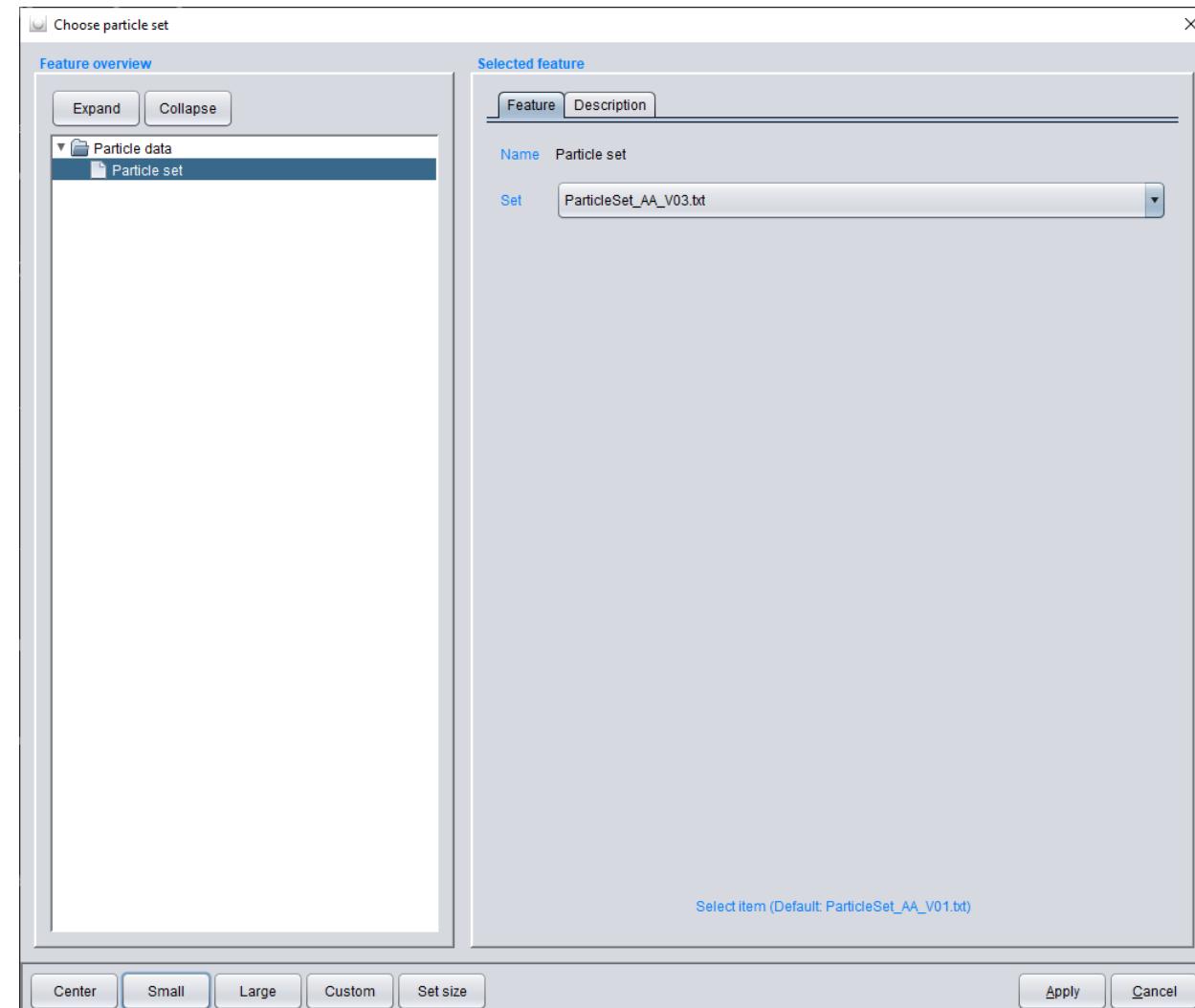
www.molecular-dynamics.de

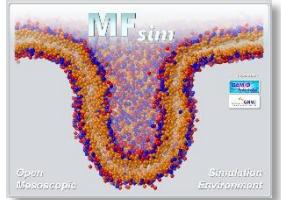


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Particle Set Choice

... choose *ParticleSet_AA_V03_pm.txt* and confirm with **Apply**.





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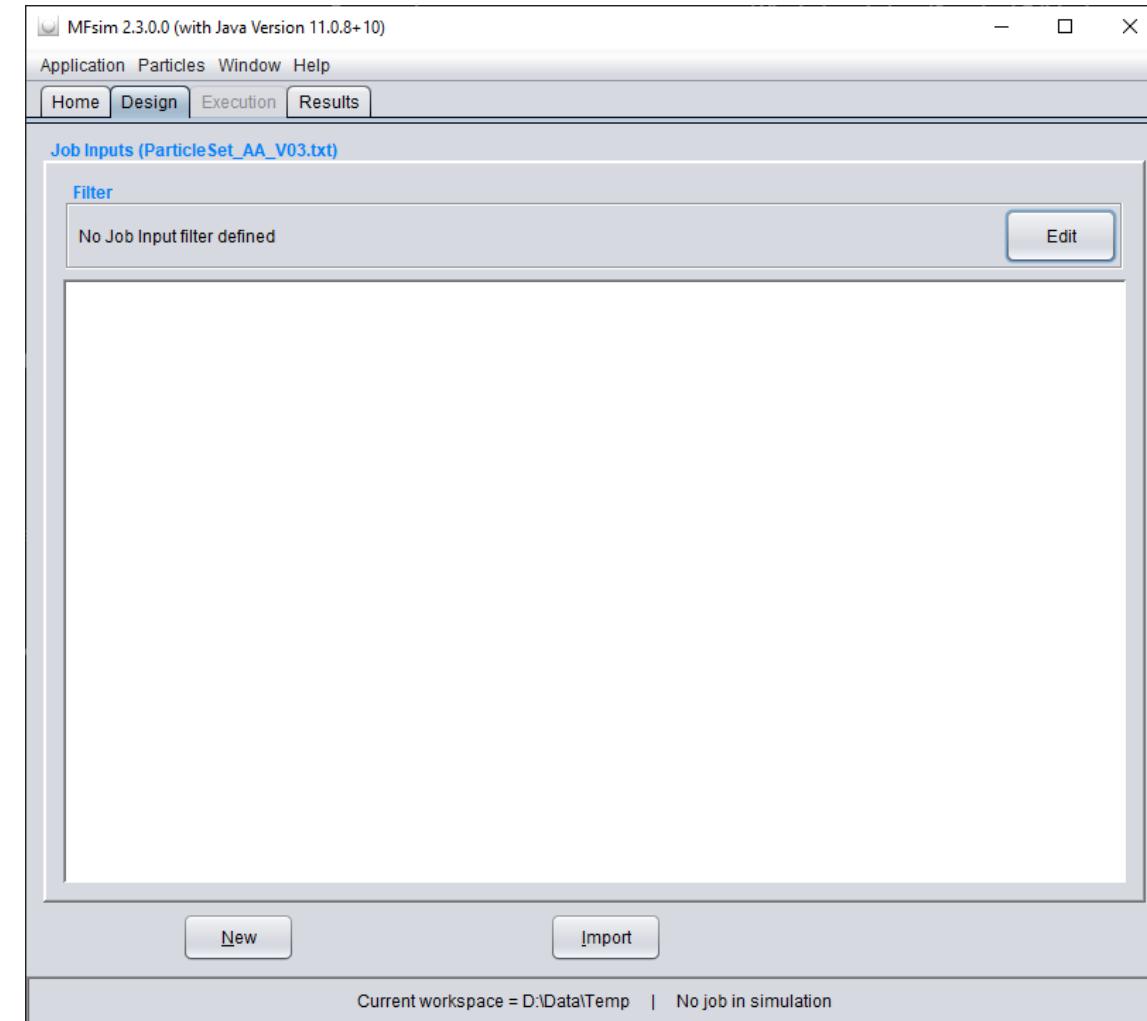
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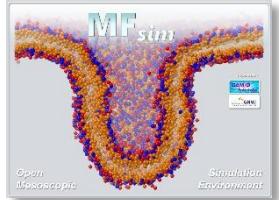


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New Job Input

Activate the **Design** tab and create a new job input with button **New**.





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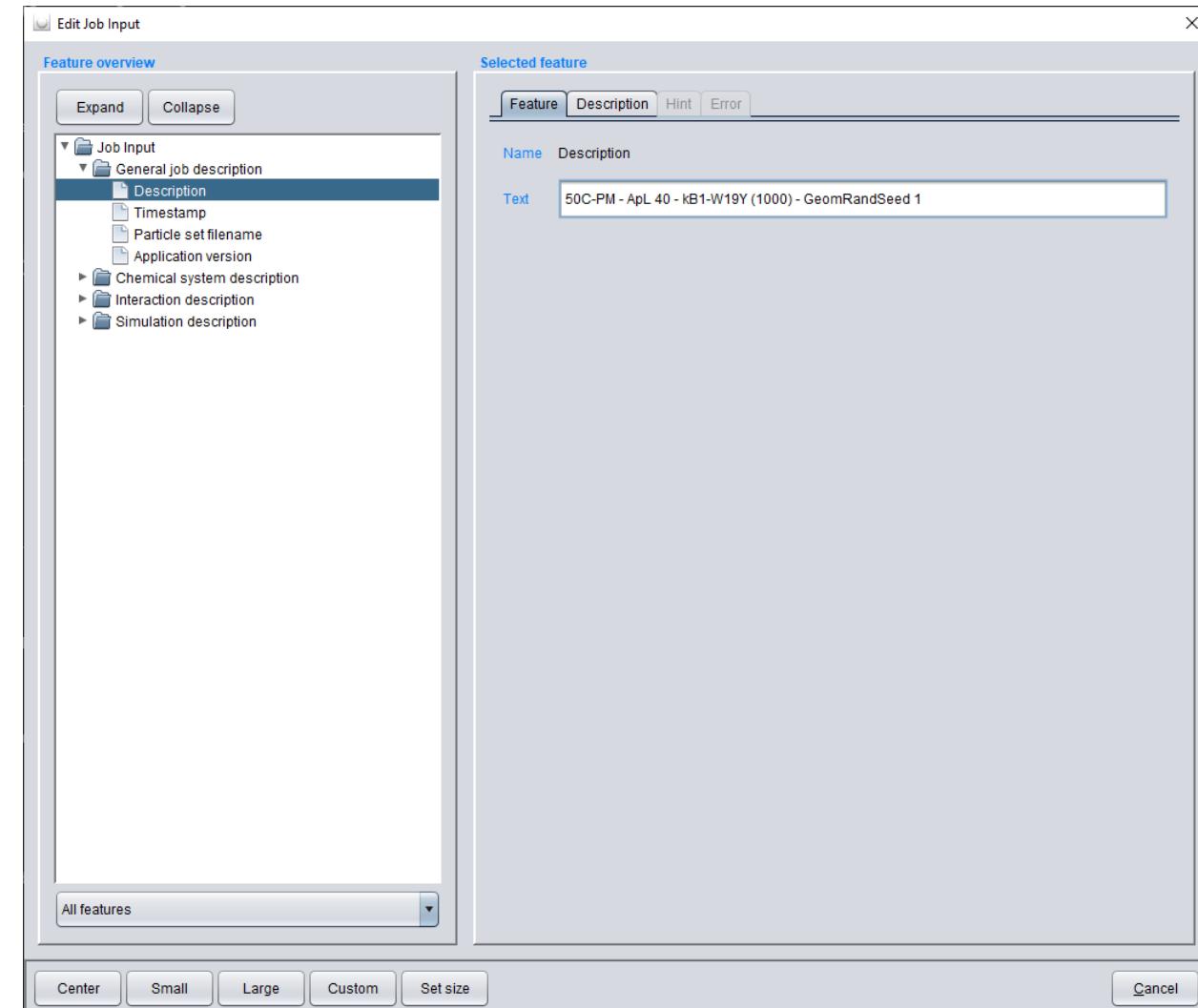
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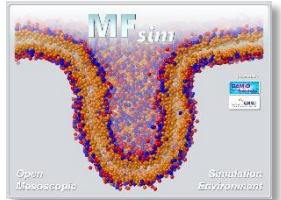


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General Job Description

Select **Job Input / General job description / Description** and change the description to **50C-PM - ApL 40 - kB1-W19Y (1000) - GeomRandSeed 1.**





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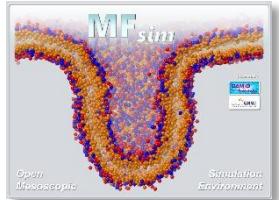
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Molecule Definition

Select **Job Input / Chemical system description / Molecule definition ...**

The screenshot shows the 'Edit Job Input' dialog box. On the left, under 'Feature overview', the 'Molecule definition' item is selected and highlighted in blue. On the right, the 'Selected feature' panel displays a table for 'Molecule definition' with one row for 'Water'. The table has columns for 'Molecule name' (Water), 'Molecular structure' (H₂O), and 'Graphics color' (CYAN). The 'CYAN' cell is highlighted with a cyan background.

Name	Molecule definition
Molecule name	Water
Molecular structure	H ₂ O
Graphics color	CYAN



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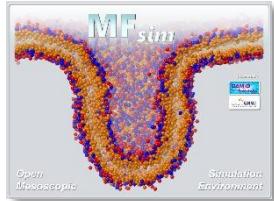


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Molecule Definition

... and rename the default water molecule to **WaterIn1** (the water molecules for the upper “inside” water compartment, see introduction).

Name	Molecular structure	Graphics color
WaterIn1	H2O	CYAN



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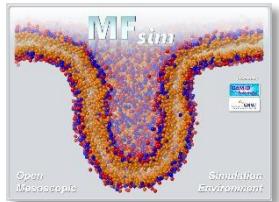
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GitHub repository:
<https://github.com/zieseny/MFsim>

Molecule Definition

Insert a new row and rename to *WaterOut* (the water molecules for the enclosed “outside” cyclotide/water compartment, see introduction). **Insert** a second new row and rename to *WaterIn2* (the water molecules for the lower “inside” water compartment, see introduction).

Name	Molecular structure	Graphics color
WaterIn1	H2O	CYAN
WaterOut	H2O	CYAN
WaterIn2	H2O	CYAN

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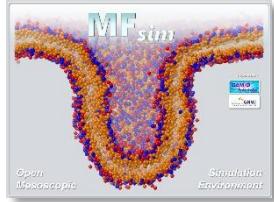
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Molecule Definition

Insert a new row and rename to *CHOLin* (the cholesterol molecules of the inner membrane leaflets). Change the **Graphics color** to **OLIVE**. Open the molecular structure editor dialog by double-click on the **Molecular structure** column entry.

Name	Molecular structure	Graphics color
WaterIn1	H2O	CYAN
WaterOut	H2O	CYAN
WaterIn2	H2O	CYAN
CHOLin	H2O	OLIVE

Double-click the **Molecular structure** column entry to open the molecular structure editor dialog (or press function key F2 if column entry has focus)

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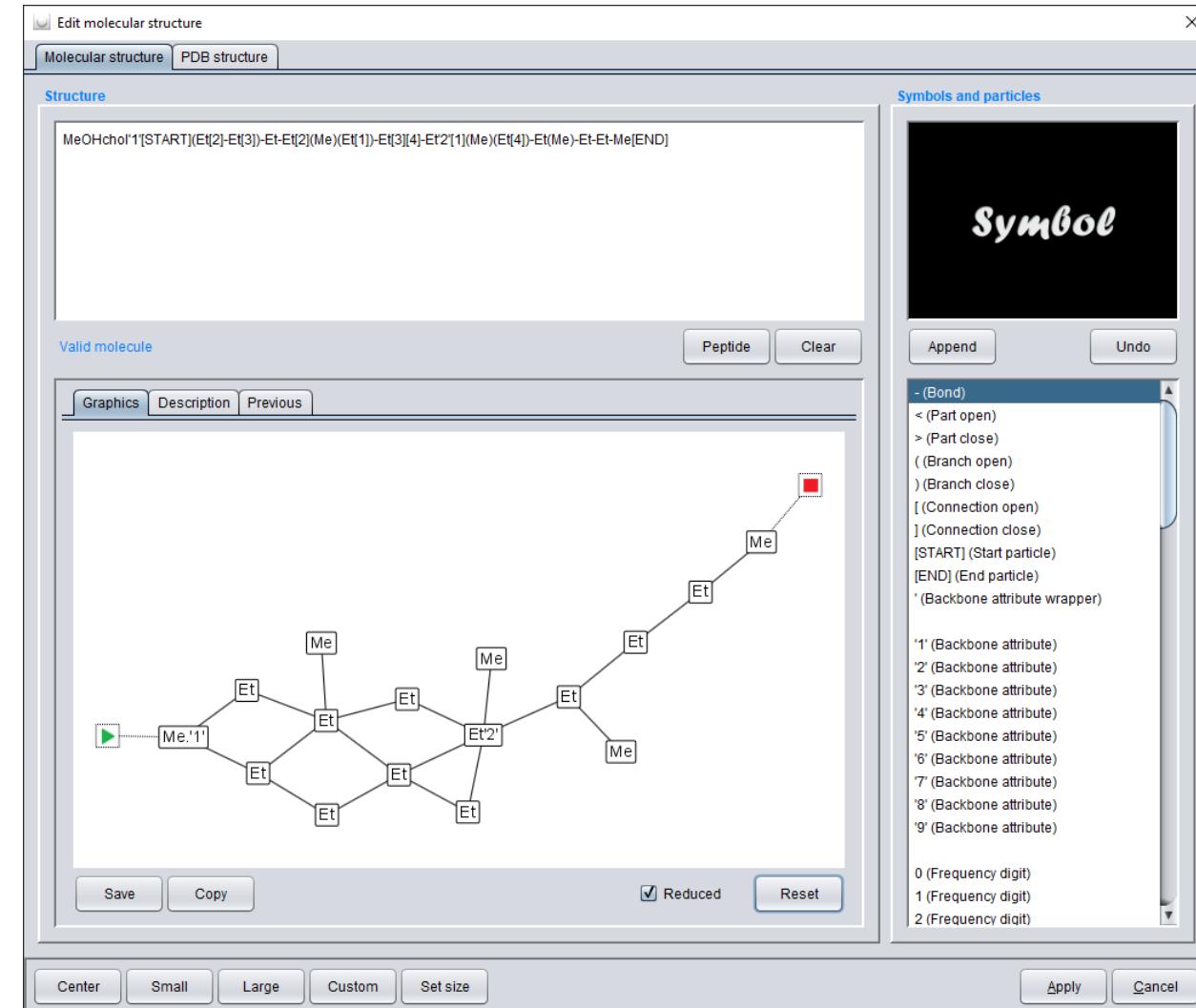
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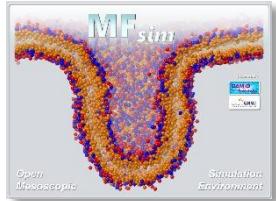
Molecular Structure Editor

Insert the SPICES string

MeOHchol'1'[START](Et[2]-Et[3])-Et-Et[2](Me)(Et[1])-Et[3][4]-Et'2'[1](Me)(Et[4])-Et(Me)-Et-Et-Me[END]

for cholesterol in the **Structure** box. A topological graph display of the **Valid molecule** definition is directly created below in the **Graphics** panel. The [START]/[END] tags allow for later orientation of the cholesterol molecules in the simulation box. The backbone tags '1' and '2' support the definition of molecular backbone forces (harmonic springs) between the tagged particles to control molecular stiffness. Particle *MeOHchol* is a duplicated physical MeOH particle to be exclusively used in the cholesterol molecule (e.g. for later specific display or analysis purposes). Hit **Apply** to confirm the entry.





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Molecule Definition

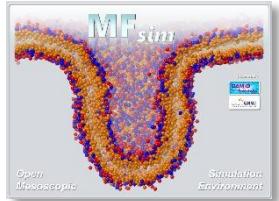
The SPICES definition is shown in the **Molecule structure** field. Define the following molecules in the same manner ...

- Cholesterol of the outer membrane leaflets:
 - **Molecule name:** CHOLout
 - SPICES **Molecular structure:**
MeOHchol'1'[START](Et[2]-Et[3])-Et-Et[2](Me)(Et[1])-Et[3][4]-Et'2'[1](Me)(Et[4])-Et(Me)-Et-Et-Me[END]
 - **Graphics color:** OLIVE

The screenshot shows the 'Edit Job Input' dialog box with the 'Feature overview' tree expanded to show the 'Molecule definition' node under 'Chemical system description'. The 'Selected feature' panel shows a table for defining molecules:

Name	Molecule definition	Graphics color
WaterIn1	H2O	CYAN
WaterOut	H2O	CYAN
WaterIn2	H2O	CYAN
CHOLin	MeOHchol'1'[START](Et[2]-Et[3])-Et-Et[2](Me)(Et[1])-Et[3][4]-Et'2'[1](Me)(Et[4])-Et(Me)-Et-Et-Me[END]	OLIVE

Buttons at the bottom include 'Set', 'Click cell to edit', 'Remove', 'Insert', 'Copy', 'New', 'Center', 'Small', 'Large', 'Custom', 'Set size', 'Apply', and 'Cancel'.



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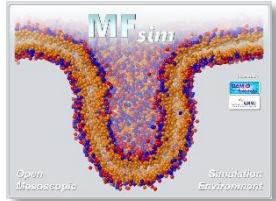


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Molecule Definition

- DMPC of the inner membrane leaflets:
 - **Molecule name:** *DMPCin*
 - **SPICES Molecular structure:** *TriMeNPpI[START]-DMPN(MeAc-6Et[END])(MeAc-6Et)*
 - **Graphics color:** GREEN
- DMPC of the outer membrane leaflets:
 - **Molecule name:** *DMPCout*
 - **SPICES Molecular structure:** *TriMeNPpI[START]-DMPN(MeAc-6Et[END])(MeAc-6Et)*
 - **Graphics color:** GREEN

Molecule name	Molecular structure	Graphics color
WaterIn1	H2O	CYAN
WaterOut	H2O	CYAN
WaterIn2	H2O	CYAN
CHOLin	MeOHchol1[...	OLIVE
CHOLout	MeOHchol1[...	OLIVE
DMPCin	TriMeNPpI[ST...	GREEN
DMPCout	TriMeNPpI[ST...	GREEN
DOPEin	MeNH2PpI[STA...	PLUM
DOPEout	MeNH2PpI[STA...	PLUM
PIP2in	DMPN[1](MeAc...	ORANGE
PIP2out	DMPN[1](MeAc...	ORANGE
PSin	HAcNpI[START...	MAGENTA
SMin	TriMeNPpI[ST...	MINT
SMout	TriMeNPpI[ST...	MINT



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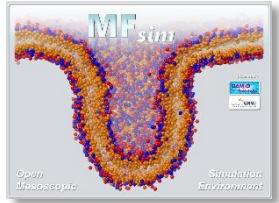
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Molecule Definition

- DOPE of the inner membrane leaflets:
 - Molecule name:** DOPEin
 - SPICES Molecular structure:** MeNH2Ppl[START]-DMPN(MeAc-8Et)(MeAc-8Et[END])
 - Graphics color:** PLUM
- DOPE of the outer membrane leaflets:
 - Molecule name:** DOPEout
 - SPICES Molecular structure:** MeNH2Ppl[START]-DMPN(MeAc-8Et)(MeAc-8Et[END])
 - Graphics color:** PLUM

The screenshot shows the 'Edit Job Input' dialog with the 'Feature overview' tree expanded. The 'Molecule definition' node under 'Chemical system description' is selected. To the right, a table lists various molecules with their names, SPICES structures, and graphics colors.

Name	Molecule definition	
WaterIn1	H2O	CYAN
WaterOut	H2O	CYAN
WaterIn2	H2O	CYAN
CHOLin	MeOHchol[1]...	OLIVE
CHOLout	MeOHchol[1]...	OLIVE
DMPCin	TriMeNPpl[ST...	GREEN
DMPCout	TriMeNPpl[ST...	GREEN
DOPEin	MeNH2Ppl[STA...	PLUM
DOPEout	MeNH2Ppl[STA...	PLUM
PIP2in	DMPN[1](MeAc...	ORANGE
PIP2out	DMPN[1](MeAc...	ORANGE
PSin	HAcNpl[START...	MAGENTA
SMin	TriMeNPpl[ST...	MINT
SMout	TriMeNPpl[ST...	MINT



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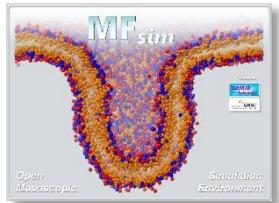
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Molecule Definition

- PIP2 of the inner membrane leaflets:
 - **Molecule name:** *PIP2in*
 - **SPICES Molecular structure:**
 $DMPN[1](MeAc-8Et)(MeAc-9Et[END])-MeOH-DMPNpl-DMPNpl[START]-MeOH-MeOH[1]$
 - **Graphics color:** ORANGE

- PIP2 of the outer membrane leaflets:
 - **Molecule name:** *PIP2out*
 - **SPICES Molecular structure:**
 $DMPN[1](MeAc-8Et)(MeAc-9Et[END])-MeOH-DMPNpl-DMPNpl[START]-MeOH-MeOH[1]$
 - **Graphics color:** ORANGE

Name	Molecule definition	
WaterIn1	H2O	CYAN
WaterOut	H2O	CYAN
WaterIn2	H2O	CYAN
CHOLin	MeOHchol'1[...	OLIVE
CHOLout	MeOHchol'1[...	OLIVE
DMPCin	TriMeNPpl[ST ...	GREEN
DMPCout	TriMeNPpl[ST ...	GREEN
DOPEin	MeNH2Ppl[STA ...	PLUM
DOPEout	MeNH2Ppl[STA ...	PLUM
PIP2in	DMPN[1](MeAc ...	ORANGE
PIP2out	DMPN[1](MeAc ...	ORANGE
PSin	HAcNpl[START ...	MAGENTA
SMin	TriMeNPpl[ST ...	MINT
SMout	TriMeNPpl[ST ...	MINT



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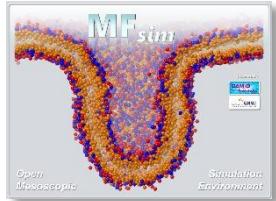


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Molecule Definition

- PS of the inner membrane leaflets:
 - **Molecule name:** PSin
 - **SPICES Molecular structure:**
 $HAcNpI[START]-$
 $DMPN(MeNH2PpI)(MeAc-8Et)(MeAc-$
 $8Et[END])$
 - **Graphics color:** MAGENTA

Name	Molecule definition	
WaterIn1	H2O	CYAN
WaterOut	H2O	CYAN
WaterIn2	H2O	CYAN
CHOLin	MeOHchol ¹ [...	OLIVE
CHOLout	MeOHchol ¹ [...	OLIVE
DMPCin	TriMeNPpI[ST ...	GREEN
DMPCout	TriMeNPpI[ST ...	GREEN
DOPEin	MeNH2PpI[STA ...	PLUM
DOPEout	MeNH2PpI[STA ...	PLUM
PIP2in	DMPN[1](MeAc ...	ORANGE
PIP2out	DMPN[1](MeAc ...	ORANGE
PSin	HAcNpI[START ...	MAGENTA
SMin	TriMeNPpI[ST ...	MINT
SMout	TriMeNPpI[ST ...	MINT



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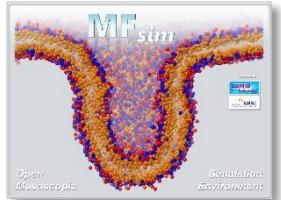
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Molecule Definition

- SM of the inner membrane leaflets:
 - Molecule name:** SMin
 - SPICES Molecular structure:** TriMeNPpI[START]-DMPN(MeAcNH-7Et)(MeOH-7Et-Me[END])
 - Graphics color:** MINT
- SM of the outer membrane leaflets:
 - Molecule name:** SMout
 - SPICES Molecular structure:** TriMeNPpI[START]-DMPN(MeAcNH-7Et)(MeOH-7Et-Me[END])
 - Graphics color:** MINT

The screenshot shows the 'Edit Job Input' dialog with the 'Feature overview' tree expanded. The 'Molecule definition' node under 'Chemical system description' is selected. To the right, a table lists molecules with their names, SPICES structures, and graphics colors.

Molecule name	Molecular structure	Graphics color
WaterIn1	H2O	CYAN
WaterOut	H2O	CYAN
WaterIn2	H2O	CYAN
CHOLin	MeOHchol1[...	OLIVE
CHOLout	MeOHchol1[...	OLIVE
DMPCin	TriMeNPpI[ST...	GREEN
DMPCout	TriMeNPpI[ST...	GREEN
DOPEin	MeNH2PpI[STA...	PLUM
DOPEout	MeNH2PpI[STA...	PLUM
PIP2in	DMPN[1](MeAc...	ORANGE
PIP2out	DMPN[1](MeAc...	ORANGE
PSin	HAcNpI[START...	MAGENTA
SMin	TriMeNPpI[ST...	MINT
SMout	TriMeNPpI[ST...	MINT



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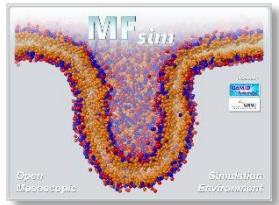
GitHub repository:
<https://github.com/zieseny/MFsim>

Molecule Definition

... for a complete membrane compound description.

The screenshot shows the 'Edit Job Input' dialog box. On the left, a tree view under 'Job Input' shows 'General job description', 'Chemical system description' (with 'Monomer definition (Off)' and 'Molecule definition' expanded), and 'Simulation box', 'Property calculation', 'Interaction description', and 'Simulation description'. On the right, a table lists molecules with their names, molecular structures (represented by small icons), and graphics colors. Buttons at the bottom include 'Set', 'Select item (Default: CYAN)', 'Remove', 'Insert', 'Copy', 'New', 'Center', 'Small', 'Large', 'Custom', 'Set size', 'Apply', and 'Cancel'.

Name	Molecule definition	
WaterIn1	H ₂ O	CYAN
WaterOut	H ₂ O	CYAN
WaterIn2	H ₂ O	CYAN
CHOLin	MeOHchol[1]...	OLIVE
CHOLout	MeOHchol[1]...	OLIVE
DMPCin	TriMeNPp[IST ...	GREEN
DMPCut	TriMeNPp[IST ...	GREEN
DOPEin	MeNH2Pp[STA ...	PLUM
DOPEout	MeNH2Pp[STA ...	PLUM
PIP2in	DMPN[1](MeAc ...	ORANGE
PIP2out	DMPN[1](MeAc ...	ORANGE
PSin	HAcNp[START ...	MAGENTA
SMin	TriMeNPp[IST ...	MINT
SMout	TriMeNPp[IST ...	MINT



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<https://github.com/zieseny/MFsim>

Molecule Definition

For the cyclotide definition **Insert** a new row, rename to *KB1Y19* and choose *WHITE* as **Graphics color**. Click the **Molecular structure** field ...

MFsim

2.3.0.0

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Gesellschaft für naturwissenschaftliche Informatik GNWI

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GitHub repository: https://github.com/zieseny/MFsim

Edit Job Input

Feature overview

Selected feature

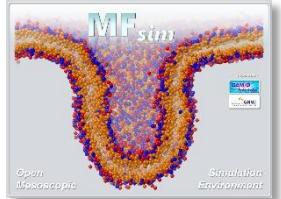
Name	Molecule name	Molecular structure	Graphics color
Water	H2O		CYAN
WaterOut	H2O		CYAN
WaterIn2	H2O		CYAN
CHOLin	MeOHchol[1][...]		OLIVE
CHOLOut	MeOHchol[1][...]		OLIVE
DMPClin	TriMeNPpl[ST...]		GREEN
DMPCout	TriMeNPpl[ST...]		GREEN
DOPEin	MeNH2Ppl[STA...]		PLUM
Water2	MeNH2Ppl[STA...]		PLUM
PIP2in	DMPN[1](MeAc...)		ORANGE
PIP2out	DMPN[1](MeAc...)		ORANGE
PSin	HAcNpl[START...]		MAGENTA
SMin	TriMeNPpl[ST...]		MINT
SMout	TriMeNPpl[ST...]		MINT
KB1Y19	H2O		WHITE

All features Hint

Set Click on table cell to edit Remove Insert Copy

New Table-data schema

Center Small Large Custom Set size Apply Cancel



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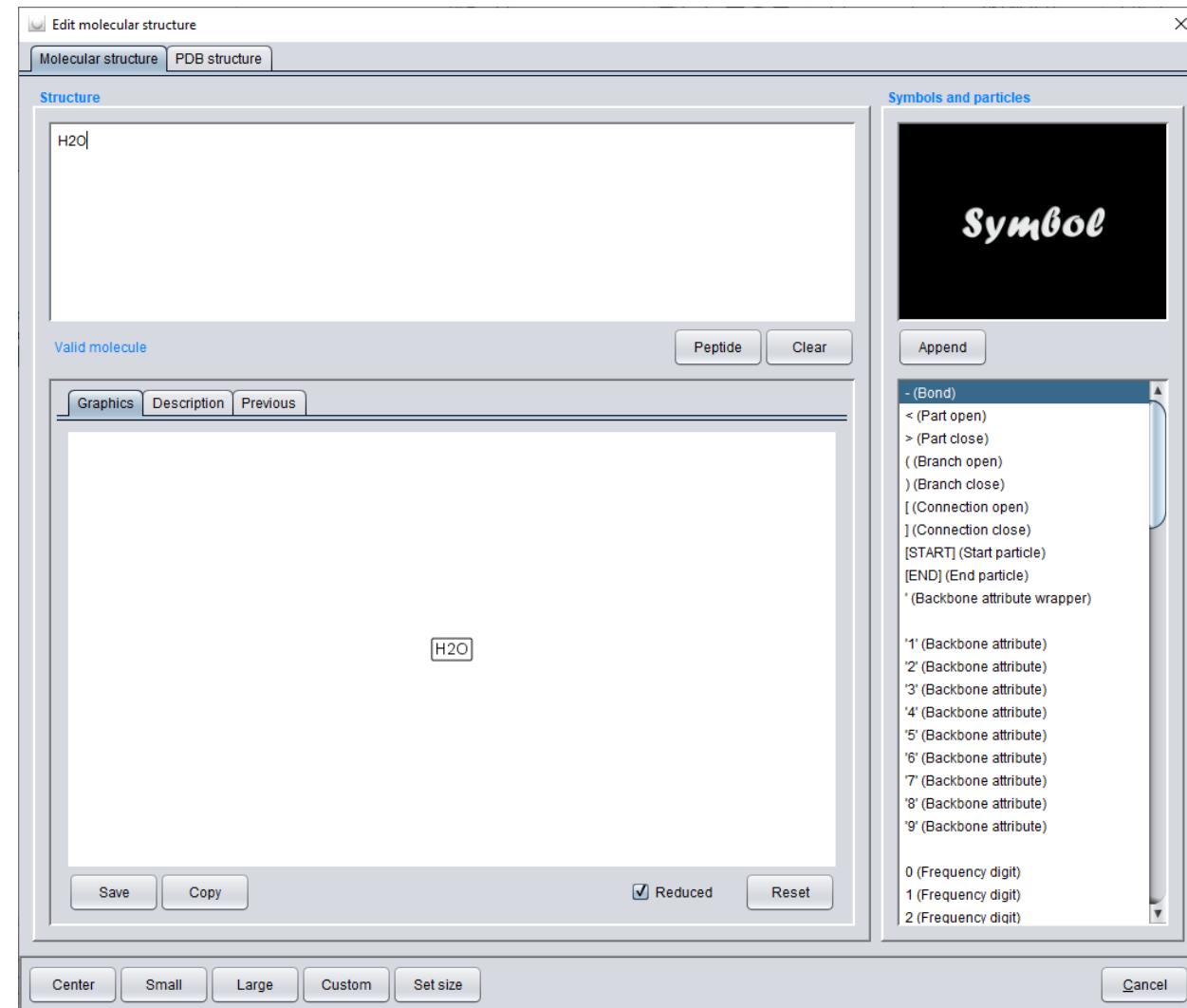


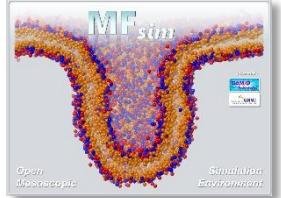
www.gnwi.de

GitHub repository:
<https://github.com/zieseny/MFsim>

Molecular Structure Editor

... and select the **PDB structure** tab ...





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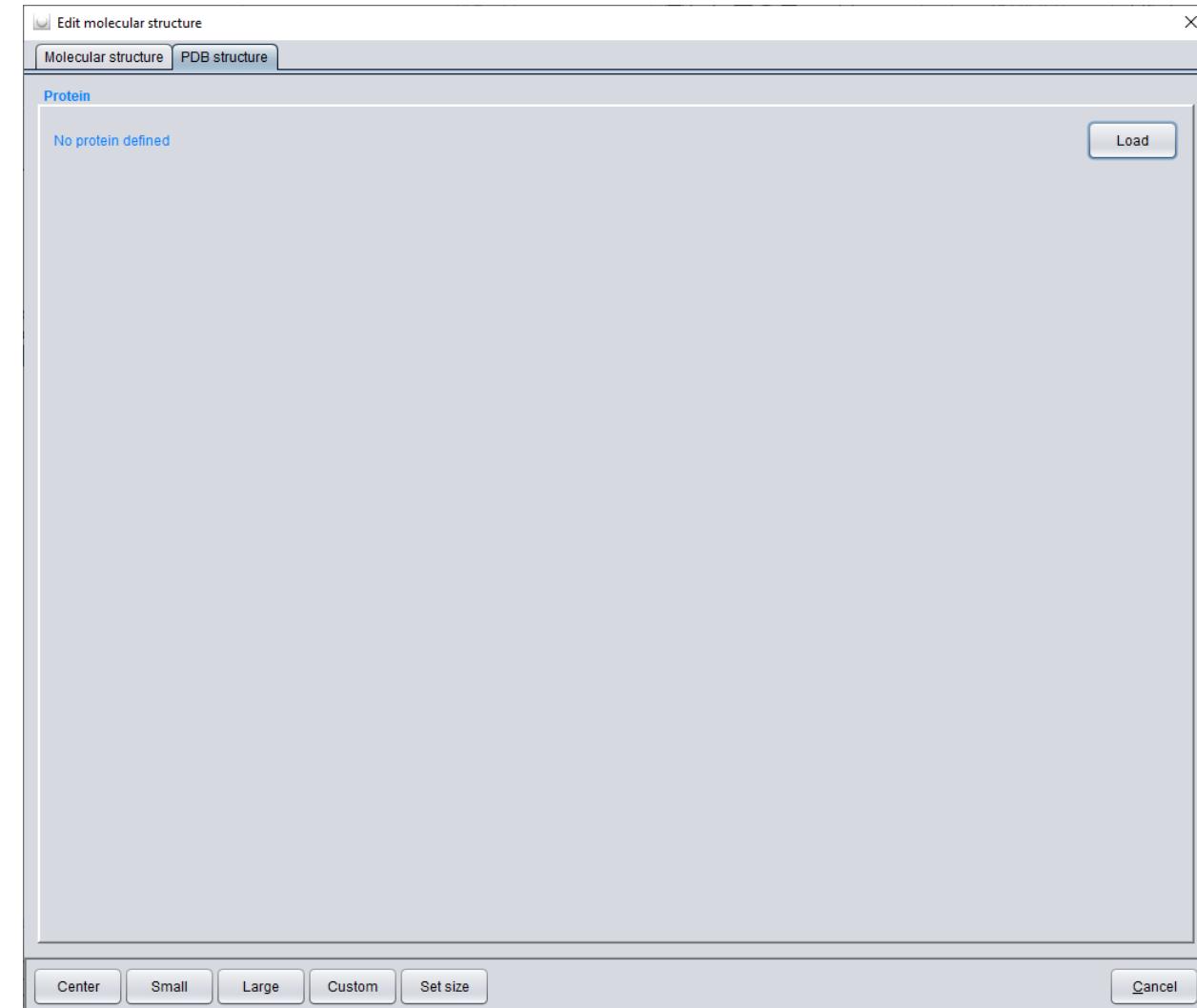
www.molecular-dynamics.de

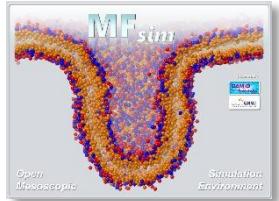


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Molecular Structure Editor

... to import the 3D structure of Kalata B1 from its PDB file. Hit the **Load** button ...





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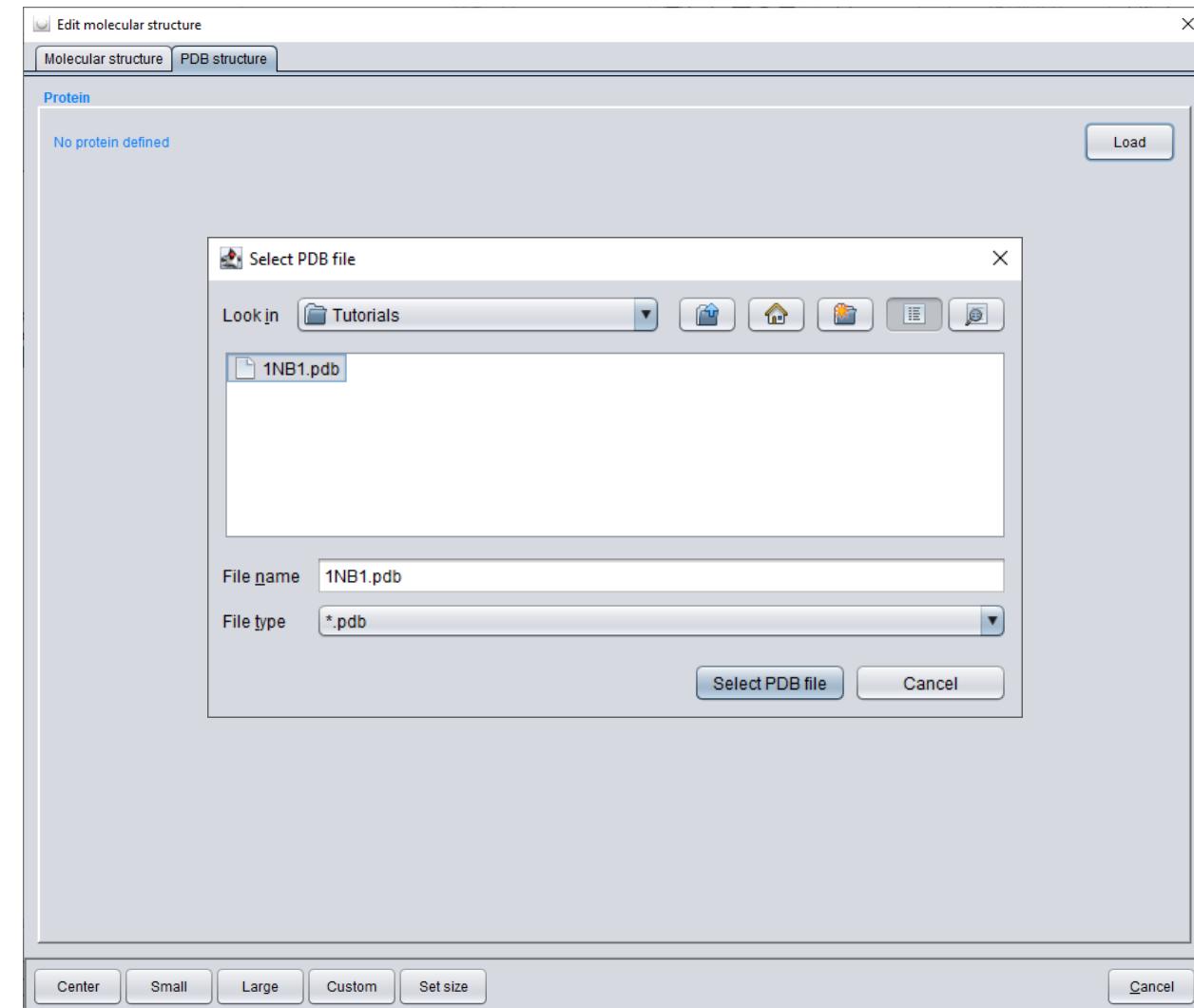


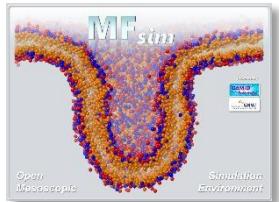
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Molecular Structure Editor

... and **Select PDB file 1NB1.pdb** for cyclotide Kalata B1 ...

Note: PDB file 1NB1.pdb can be downloaded from <https://www.rcsb.org/structure/1NB1> or from the *tutorials/Supplement* subfolder of the MFsim GitHub repository.





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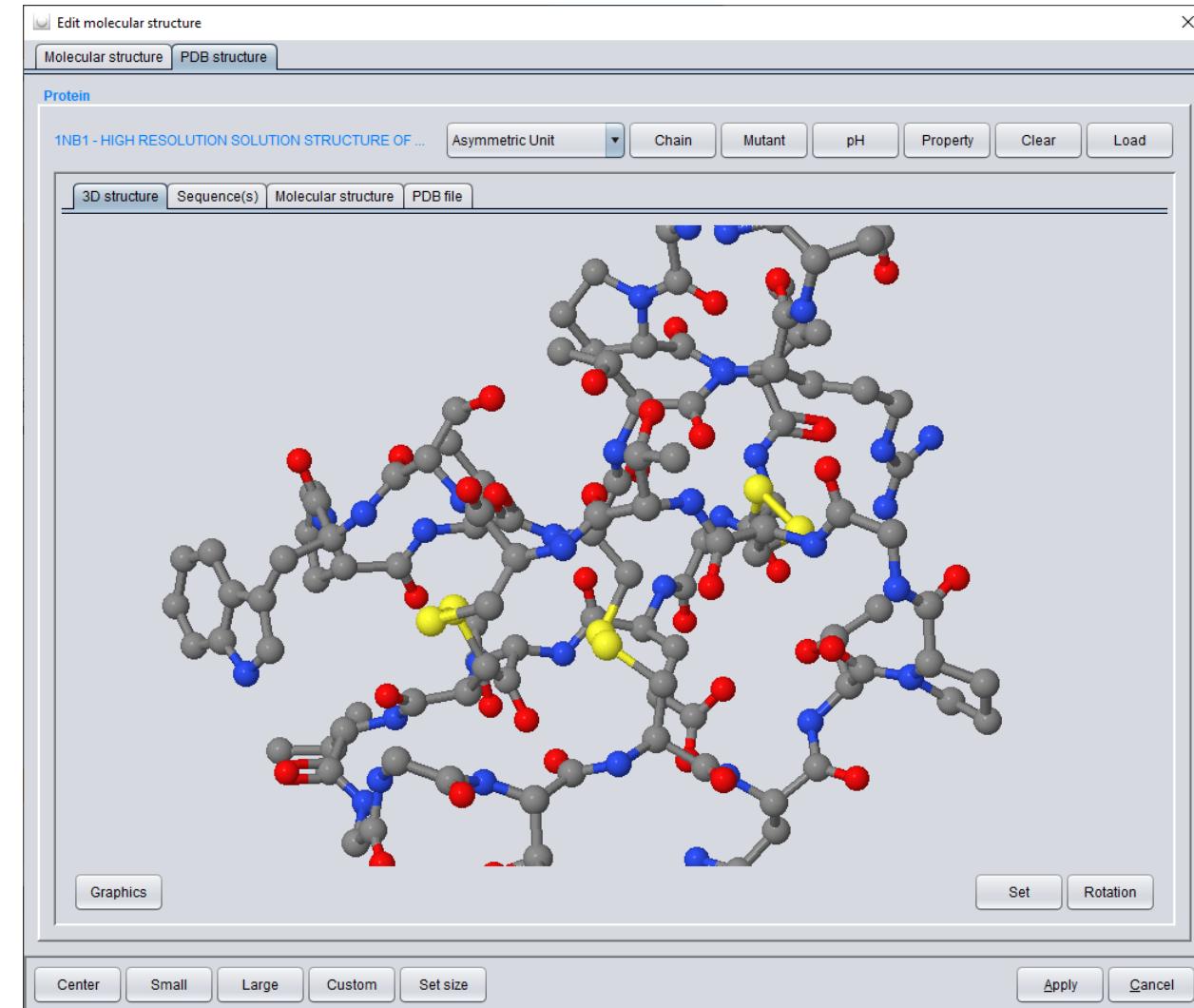
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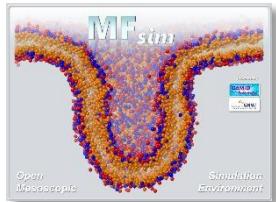


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Molecular Structure Editor

... to import and display cyclotide related PDB information. Hit the ***Mutant*** button ...





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Molecular Structure Editor

... to replace an amino acid via the **Replacement** column:
Choose **Amino acid Tryptophan** with **Index in chain 19** ...

Define mutated protein

Feature overview

Selected feature

Feature	Description		
Name	Amino acid replacement		
Chain	Index in chain	Amino acid	Replacement

KALATA B1 14 Glycine Glycine

KALATA B1 15 Cysteine Cysteine

KALATA B1 16 Threonine Threonine

KALATA B1 17 Cysteine Cysteine

KALATA B1 18 Serine Serine

KALATA B1 19 Tryptophan Tryptophan

KALATA B1 20 Proline Proline

KALATA B1 21 Valine Valine

KALATA B1 22 Cysteine Cysteine

KALATA B1 23 Threonine Threonine

KALATA B1 24 Arginine Arginine

KALATA B1 25 Asparagine Asparagine

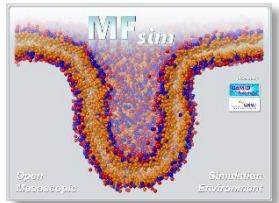
KALATA B1 26 Glycine Glycine

KALATA B1 27 Leucine Leucine

KALATA B1 28 Proline Proline

KALATA B1 29 Valine Valine

- Tryptophan
- Methionine
- Phenylalanine
- Proline
- Serine
- Threonine
- Tryptophan**
- Tyrosine
- Valine



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Molecular Structure Editor

... and replace by *Tyrosine*.
Confirm the replacement with
Apply.

Define mutated protein

Feature overview

Expand Collapse

Mutant

Amino acid replacement

Feature	Description		
Name	Amino acid replacement		
Chain	Index in chain	Amino acid	Replacement

KALATA B1 14 Glycine Glycine

KALATA B1 15 Cysteine Cysteine

KALATA B1 16 Threonine Threonine

KALATA B1 17 Cysteine Cysteine

KALATA B1 18 Serine Serine

KALATA B1 19 Tryptophan Tryptophan Tyrosine

KALATA B1 20 Proline Proline

KALATA B1 21 Valine Valine

KALATA B1 22 Cysteine Cysteine

KALATA B1 23 Threonine Threonine

KALATA B1 24 Arginine Arginine

KALATA B1 25 Asparagine Asparagine

KALATA B1 26 Glycine Glycine

KALATA B1 27 Leucine Leucine

KALATA B1 28 Proline Proline

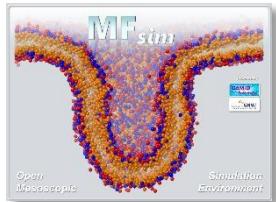
KALATA B1 29 Valine Valine

Set Select item (Default: Tryptophan)

Table-data schema

New

Center Small Large Custom Set size Apply Cancel



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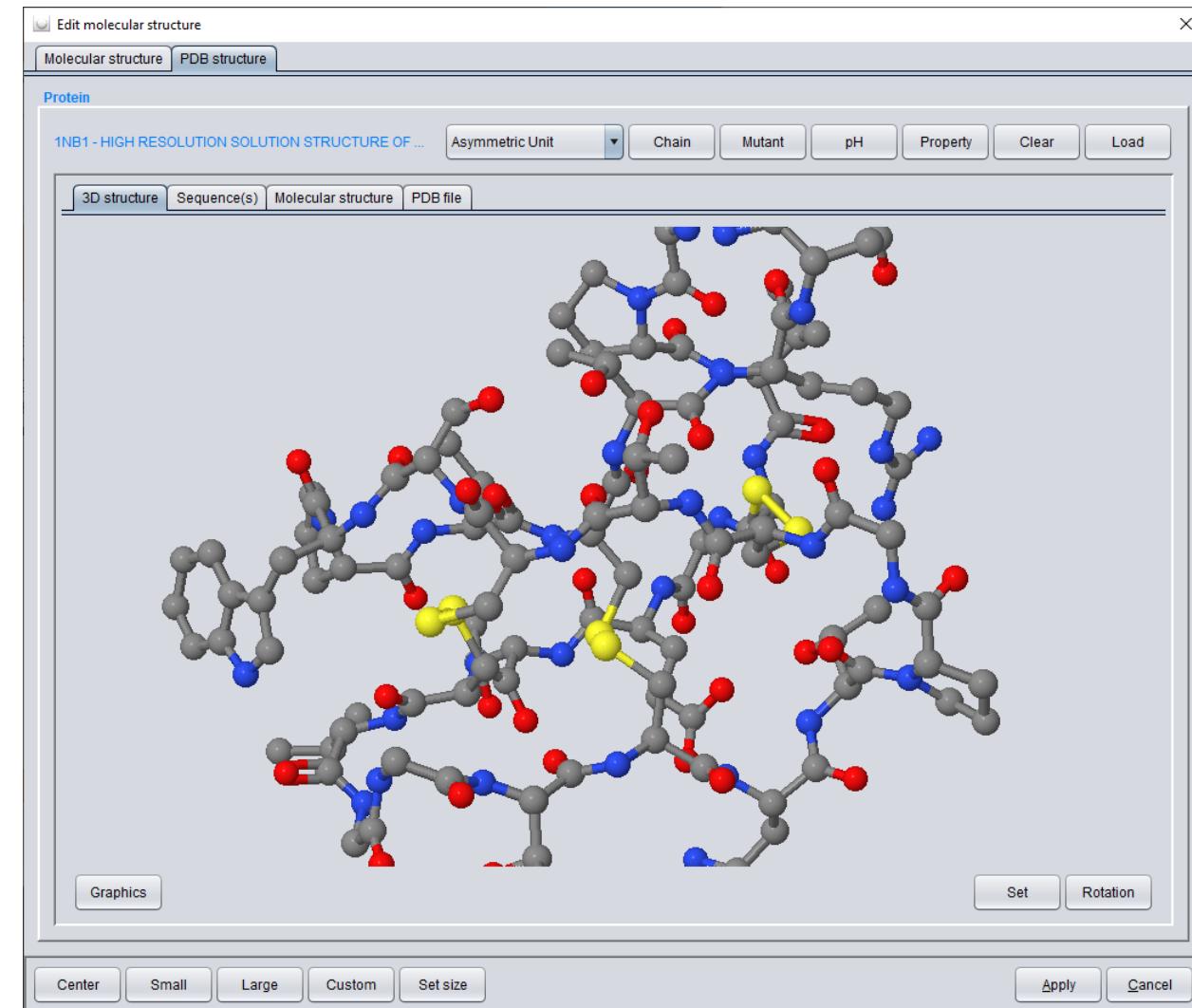


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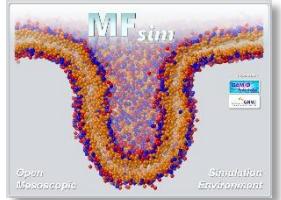
GitHub repository:
<https://github.com/zieseny/MFsim>

Molecular Structure Editor

Hit the **pH** button ...



Cyclotide-membrane sandwich interaction model (Lisa Sophie Kersten)



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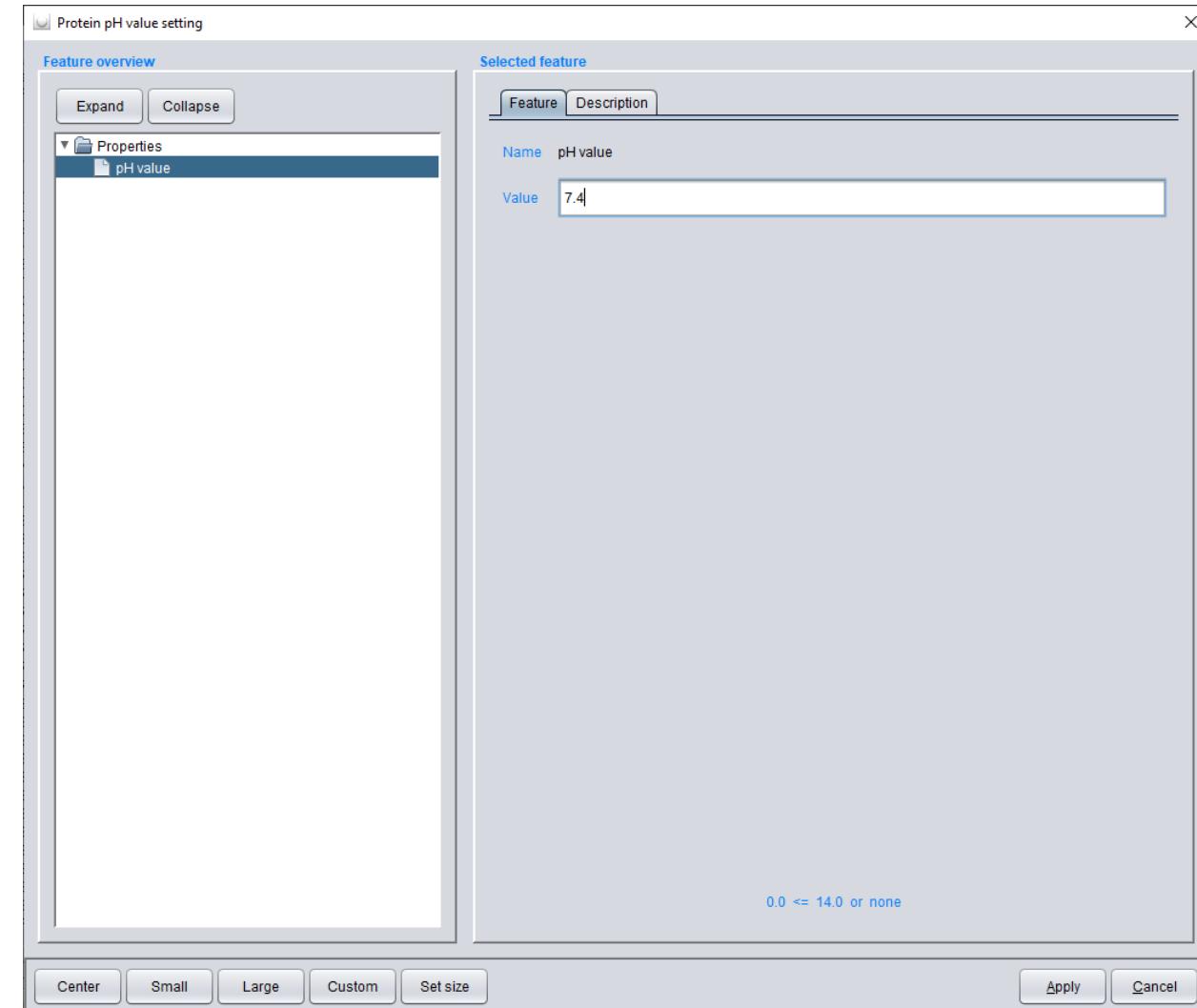
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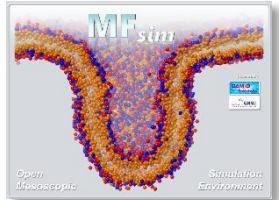


www.gnwi.de

Molecular Structure Editor

... to set the **pH value** to (its physiological value of) 7.4. Confirm with **Apply**.





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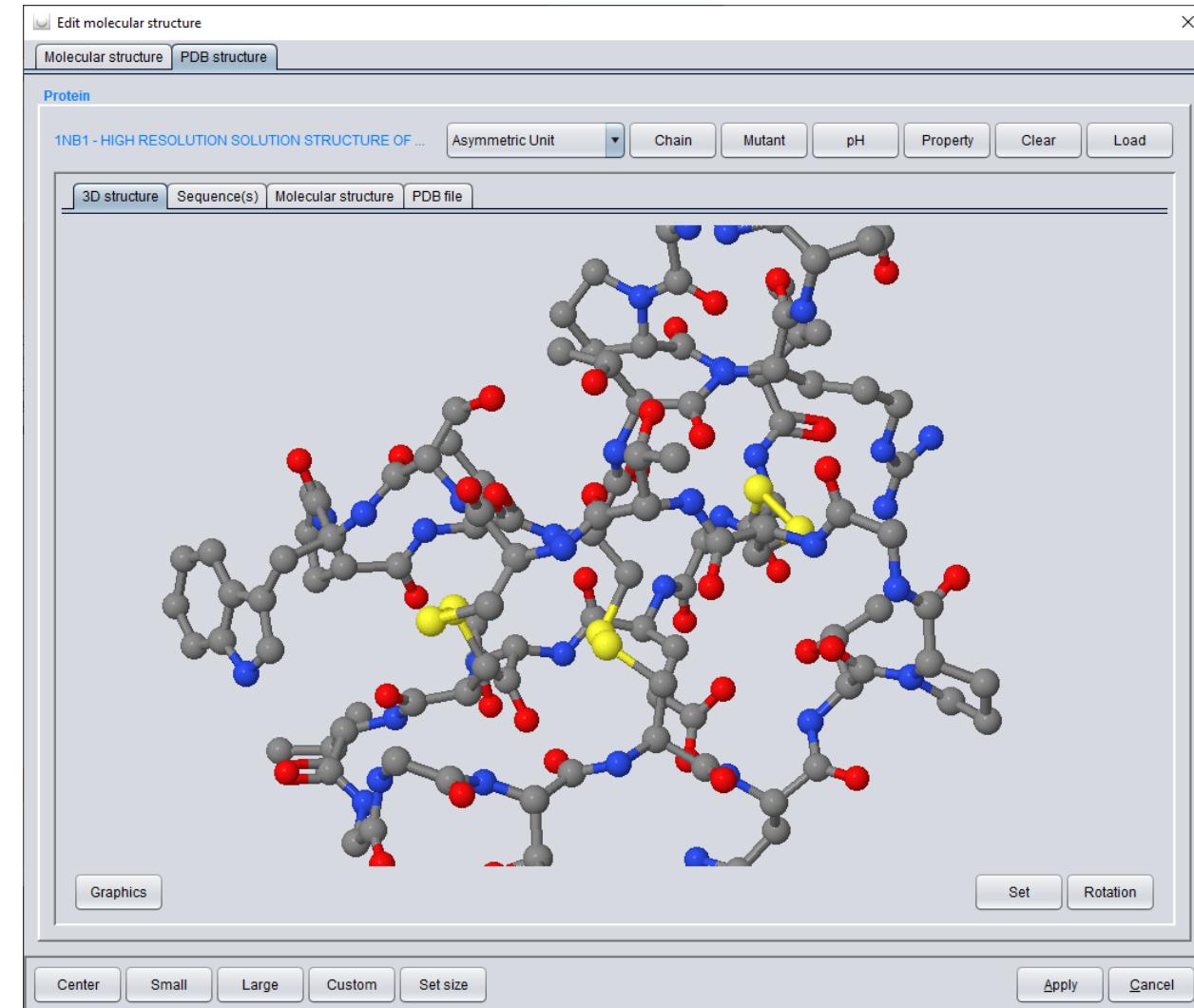
www.molecular-dynamics.de

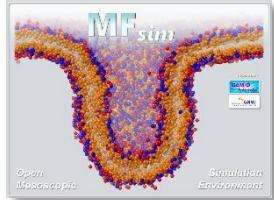


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Molecular Structure Editor

Hit the **Property** button ...



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GitHub repository:
<https://github.com/zieseny/MFsim>

Molecular Structure Editor

... and select **Properties / Backbone probes** to replace protein backbone particles by probe particles which allow for later specific display in the simulation box (without any change of “the physics”).

Protein property settings

Feature overview

Selected feature

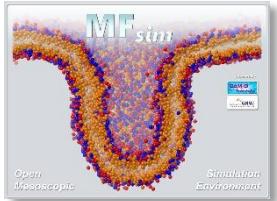
Index	Amino acid	Backbone particle	Probe particle
1	Cysteine	[CYS]1:A.CA #2	None
2	Glycine	[GLY]2:A.CA #12	None
3	Glutamic Acid	[GLU]3:A.CA #19	None
4	Threonine	[THR]4:A.CA #34	None
5	Cysteine	[CYS]5:A.CA #48	None
6	Valine	[VAL]6:A.CA #58	None
7	Glycine	[GLY]7:A.CA #74	None
8	Glycine	[GLY]8:A.CA #81	None
9	Threonine	[THR]9:A.CA #88	None
10	Cysteine	[CYS]10:A.CA #102	None
11	Asparagine	[ASN]11:A.CA #112	None
12	Threonine	[THR]12:A.CA #126	None
13	Proline	[PRO]13:A.CA #140	None
14	Glycine	[GLY]14:A.CA #154	None
15	Cysteine	[CYS]15:A.CA #161	None
16	Threonine	[THR]16:A.CA #171	None

Set Click on table cell to edit

Table-data schema

New

Center Small Large Custom Set size Cancel



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Molecular Structure Editor

Replace **Backbone particles** of **Amino acids** with **Index** 3, 19, 20, 21, 24, 27, 28 and 29 by the following **Probe particles**

- index 3 to probe particle MeAcNHPD2
- ...

Protein property settings

Feature overview

Selected feature

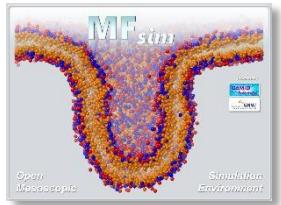
Feature		Description		
Name	Backbone probes	Amino acid	Backbone particle	Probe particle
1	Cysteine	[CYS]1:A.CA #2	None	None
2	Glycine	[GLY]2:A.CA #12	None	None
3	Glutamic Acid	[GLU]3:A.CA #19	MeAcNHPD2	MeAcNHPD2
4	Threonine	[THR]4:A.CA #34	None	None
5	Cysteine	[CYS]5:A.CA #48	MeAcNHPD3	MeAcNHPD3
6	Valine	[VAL]6:A.CA #58	MeAcNHPD4	MeAcNHPD4
7	Glycine	[GLY]7:A.CA #74	MeAcNHPD5	MeAcNHPD5
8	Glycine	[GLY]8:A.CA #81	MeAcNHPD6	MeAcNHPD6
9	Threonine	[THR]9:A.CA #88	MeAcNHPD7	MeAcNHPD7
10	Cysteine	[CYS]10:A.CA #102	None	None
11	Asparagine	[ASN]11:A.CA #112	None	None
12	Threonine	[THR]12:A.CA #126	None	None
13	Proline	[PRO]13:A.CA #140	None	None
14	Glycine	[GLY]14:A.CA #154	None	None
15	Cysteine	[CYS]15:A.CA #161	None	None
16	Threonine	[THR]16:A.CA #171	None	None

Set Select item (Default: None)

Table-data schema

New

Center Small Large Custom Set size Cancel

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Molecular Structure Editor

...

- index 19 to probe particle *MeAcNHPD4*
- index 20 to probe particle *AzolidPD1*
- index 21 to probe particle *MeAcNHPD1*
- index 24 to probe particle *MeAcNHPD3*
- index 27 to probe particle *MeAcNHPD1*
- index 28 to probe particle *AzolidPD1*
- index 29 to probe particle *MeAcNHPD1*

Protein property settings

Feature overview

Selected feature

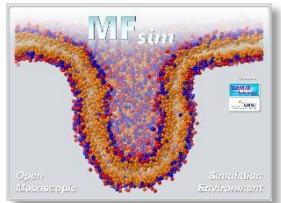
Feature		Description	
Name	Backbone probes	Backbone particle	Probe particle
Index	Amino acid	Backbone particle	Probe particle
14	Glycine	[GLY]14:A.CA #154	None
15	Cysteine	[CYS]15:A.CA #161	None
16	Threonine	[THR]16:A.CA #171	None
17	Cysteine	[CYS]17:A.CA #185	None
18	Serine	[SER]18:A.CA #195	None
19	Tyrosine	[TRP]19:A.CA #206	MeAcNHPD4
20	Proline	[PRO]20:A.CA #230	AzolidPD1
21	Valine	[VAL]21:A.CA #244	MeAcNHPD1
22	Cysteine	[CYS]22:A.CA #260	None
23	Threonine	[THR]23:A.CA #270	None
24	Arginine	[ARG]24:A.CA #284	MeAcNHPD3
25	Asparagine	[ASN]25:A.CA #308	None
26	Glycine	[GLY]26:A.CA #322	None
27	Leucine	[LEU]27:A.CA #329	MeAcNHPD1
28	Proline	[PRO]28:A.CA #348	AzolidPD1
29	Valine	[VAL]29:A.CA #362	MeAcNHPD1

Set Select item (Default: None)

Table-data schema

New

Center Small Large Custom Set size Apply Cancel



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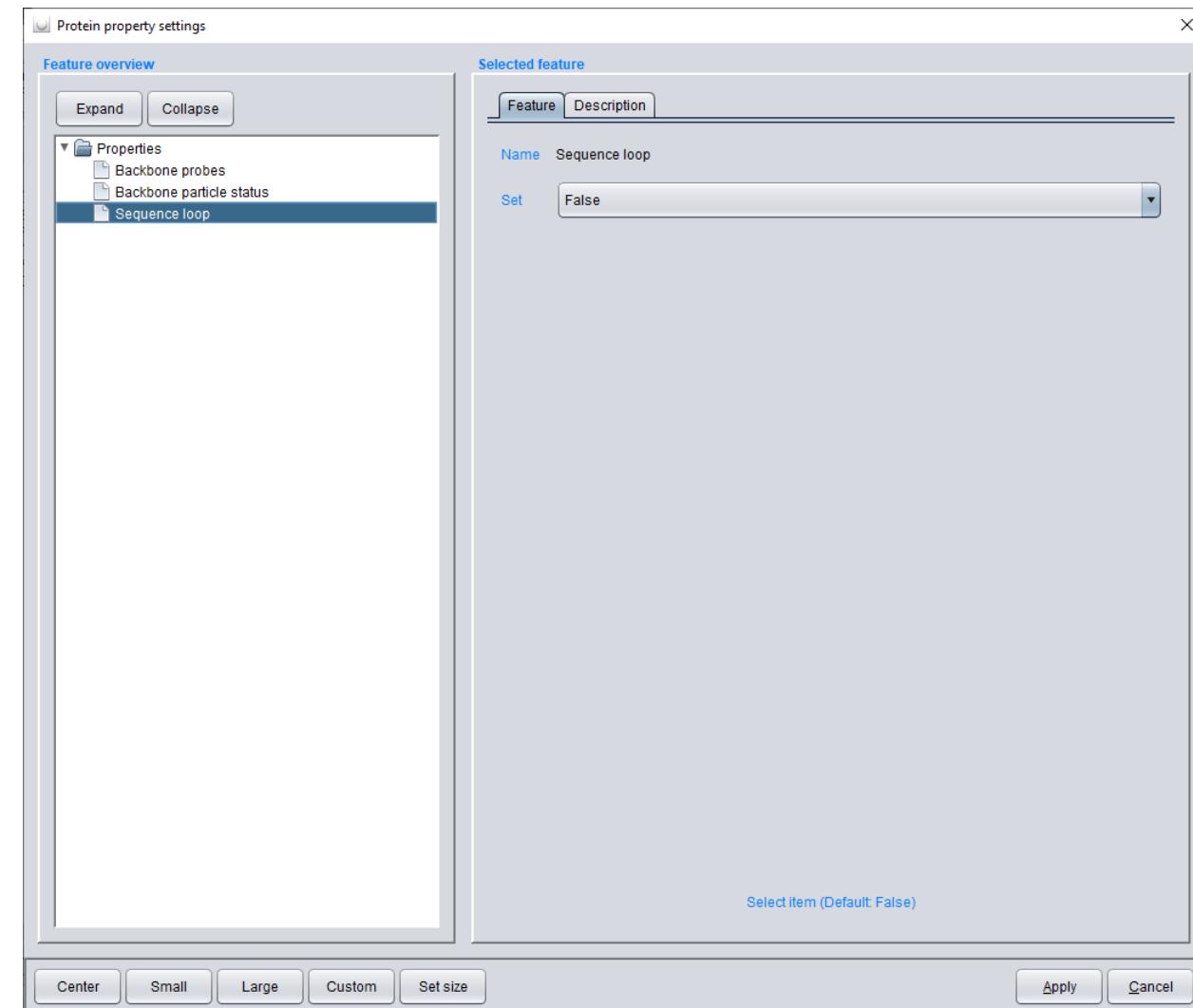
www.molecular-dynamics.de

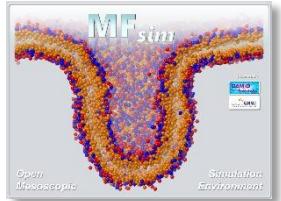


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Molecular Structure Editor

Select **Properties / Sequence loop ...**





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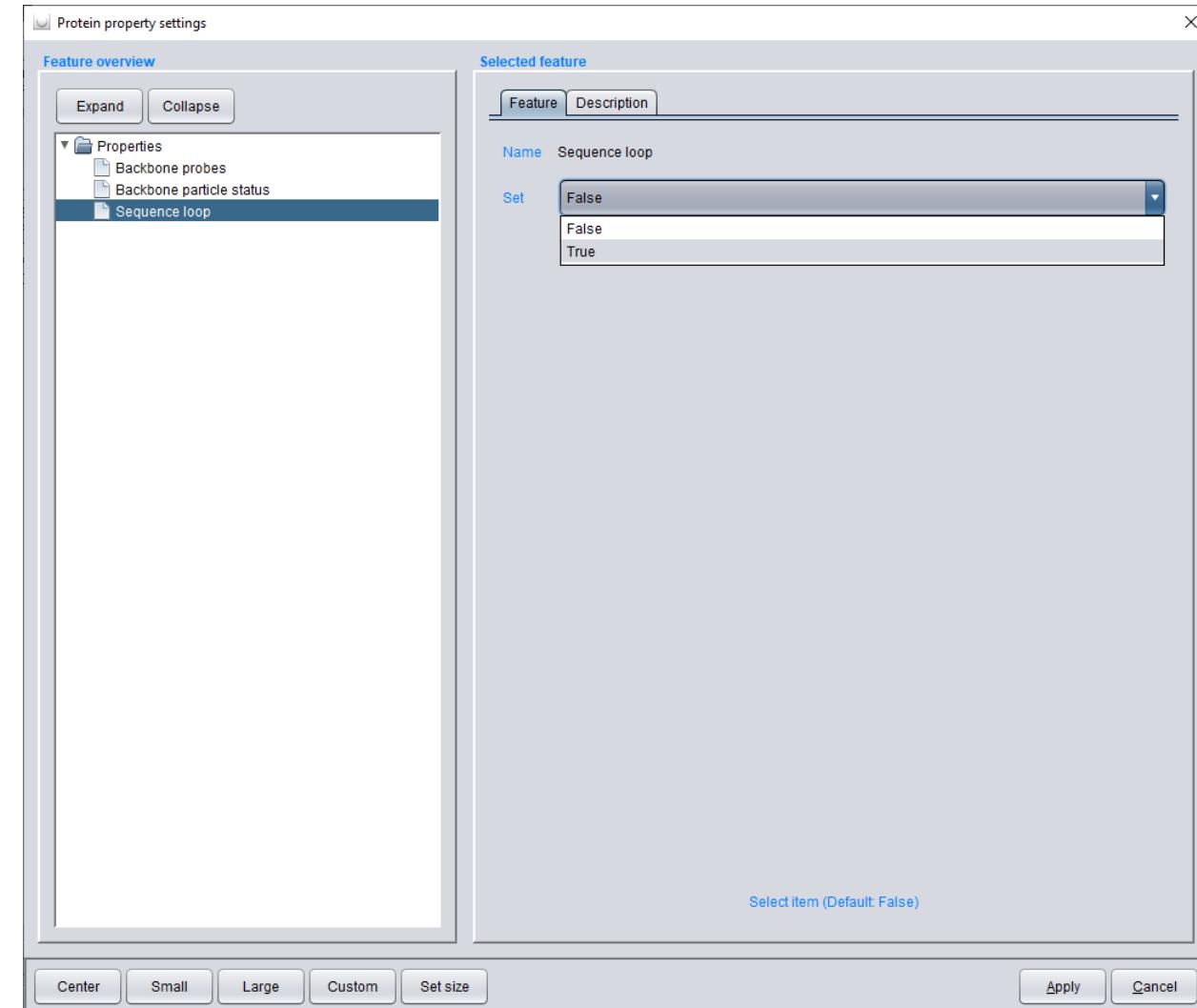
www.molecular-dynamics.de

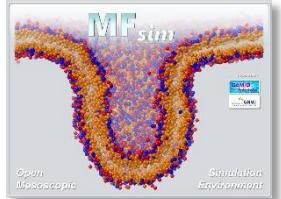


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Molecular Structure Editor

... and select *True* (since KalataB1 is a cyclic peptide). Confirm with **Apply**.





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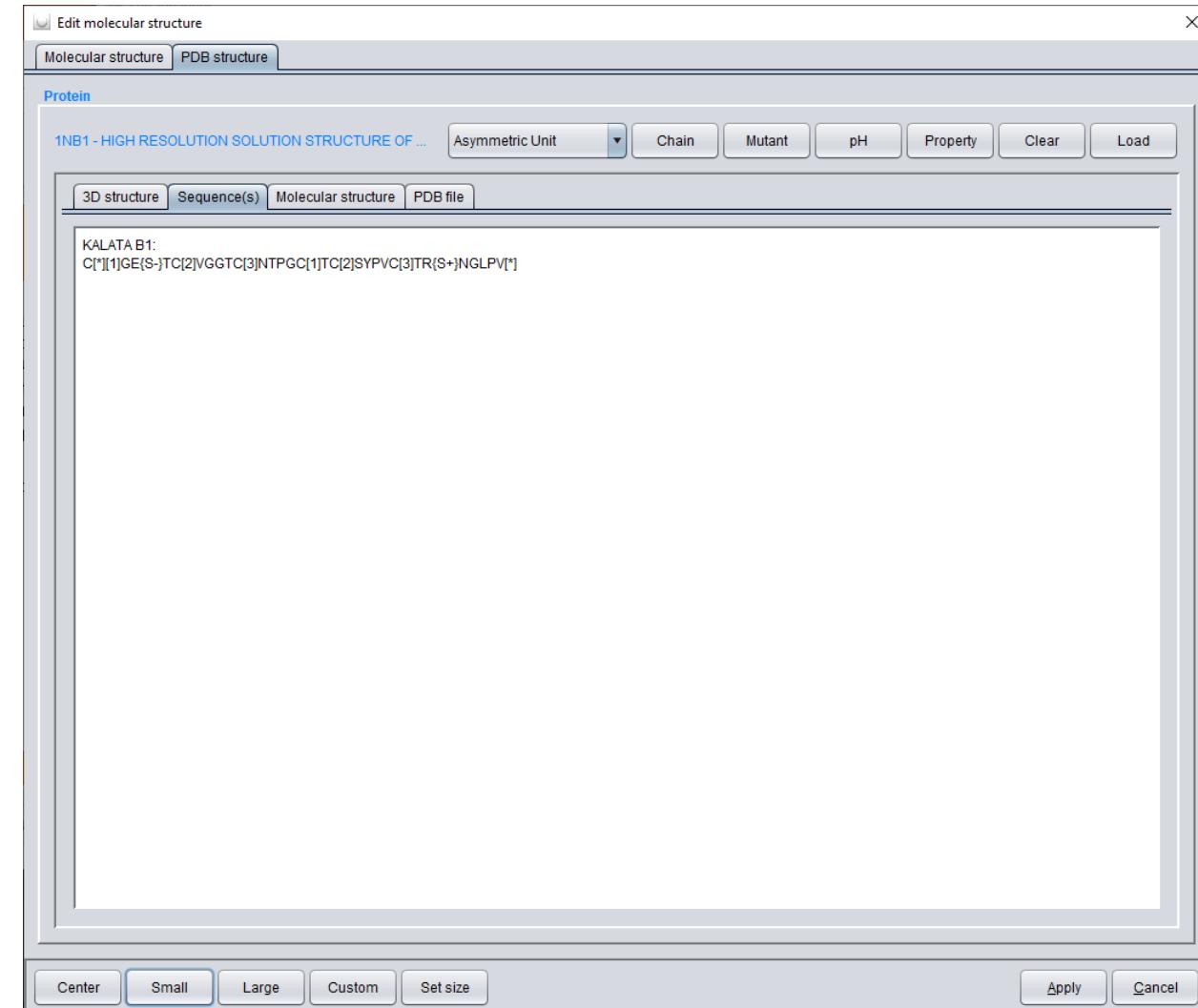
www.molecular-dynamics.de

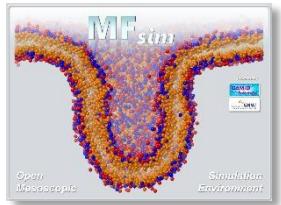


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Molecular Structure Editor

The applied settings can be viewed with the
Sequence(s) tab ...





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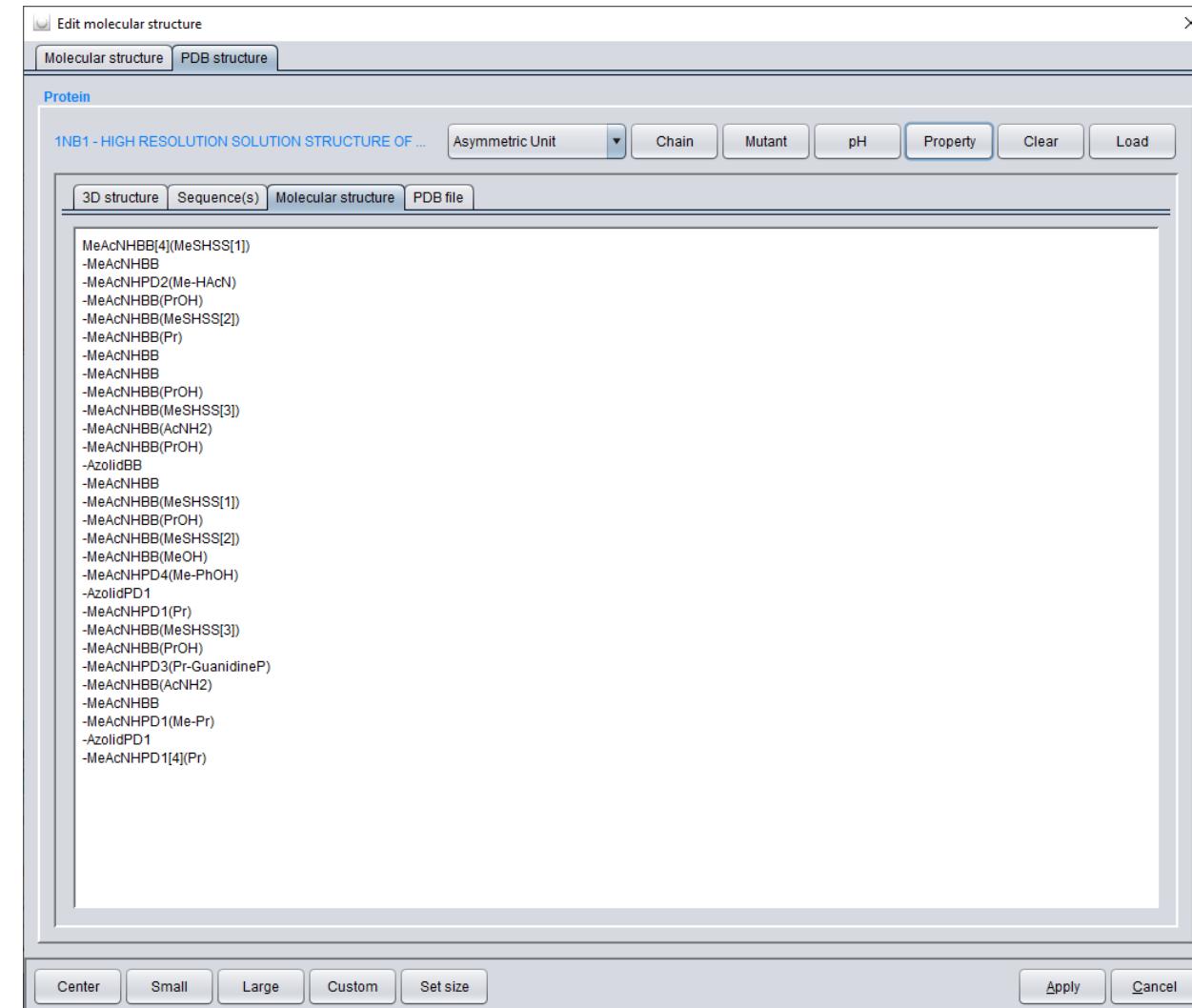
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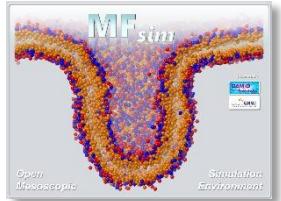


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Molecular Structure Editor

... and the **Molecular structure** tab (where each line of the SPICES string corresponds to a single amino acid representation). Confirm the entries with **Apply** ...





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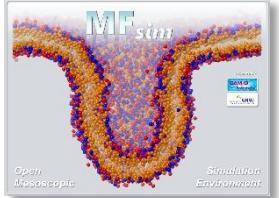
GitHub repository:
<https://github.com/zieseny/MFsim>

Molecule Definition

... to view the completed **Molecule definition**.

The screenshot shows the 'Edit Job Input' dialog with the 'Feature overview' tree expanded. The 'Molecule definition' node under 'Chemical system description' is selected. To the right, the 'Selected feature' panel displays a table of molecules with their names, structures, and graphics colors.

Molecule name	Molecular structure	Graphics color
WaterIn1	H ₂ O	CYAN
WaterOut	H ₂ O	CYAN
WaterIn2	H ₂ O	CYAN
CHOLin	MeOHchol[1][...	OLIVE
CHOLout	MeOHchol[1][...	OLIVE
DMPCin	TriMeNPp[IST ...	GREEN
DMPCut	TriMeNPp[IST ...	GREEN
DOPEin	MeNH2Pp[STA ...	PLUM
DOPEout	MeNH2Pp[STA ...	PLUM
PIP2in	DMPN[1](MeAc ...	ORANGE
PIP2out	DMPN[1](MeAc ...	ORANGE
PSin	HAcNp[START ...	MAGENTA
SMin	TriMeNPp[ST ...	MINT
SMout	TriMeNPp[ST ...	MINT
KB1Y19	MeAcNHBB[4](...	WHITE

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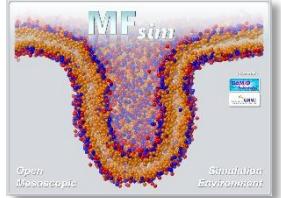
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Quantity Definition

Select **Job Input / Chemical system description / Simulation box / Composition / Quantity ...**

The screenshot shows the 'Edit Job Input' dialog box. On the left, the 'Feature overview' tree view is expanded to show 'Job Input' > 'Chemical system description' > 'Simulation box' > 'Composition' > 'Quantity'. The 'Quantity' node is selected, highlighted with a blue selection bar. On the right, the 'Selected feature' panel displays a table titled 'Name Quantity' with 16 rows. Each row contains a molecule name and its value, all set to 24000. The table includes columns for 'Name', 'Quantity', 'Molecule name', and 'Value'. Buttons for 'Set' and 'Apply' are at the bottom.

Name	Quantity
Molecule name	Value
WaterIn1	24000
WaterOut	24000
WaterIn2	24000
CHOLin	24000
CHOLout	24000
DMPCin	24000
DMPCout	24000
DOPEin	24000
DOPEout	24000
PIP2in	24000
PIP2out	24000
PSin	24000
SMin	24000
SMout	24000
KB1Y19	24000



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GitHub repository:
<https://github.com/zieslesny/MFsim>

Quantity Definition

... and define the individual molecule quantities in the **Value** column of every **Molecule name** row as shown in the screenshot.

Screenshot of the 'Edit Job Input' dialog showing the 'Quantity' feature definition and a table for defining molecule quantities.

Feature overview:

- Job Input
 - General job description
 - Chemical system description
 - Monomer definition (Off)
 - Molecule definition
 - Simulation box
 - Composition
 - DPD density
 - Concentration (Off)
 - Quantity
 - Box size
 - Colors
 - Particles and molecules display
 - Geometry random seed
 - Compartments and box view
 - Movement
 - Property calculation
 - Interaction description
 - Simulation description

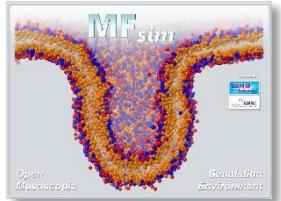
Selected feature: Quantity

Name	Quantity
WaterIn1	200000
WaterOut	146000
WaterIn2	200000
CHOLin	890
CHOLout	710
DMPCin	154
DMPCout	486
DOPEin	248
DOPEout	72
PIP2in	60
PIP2out	20
PSin	160
SMin	88
SMout	312
KB1Y19	1000

Table-data schema:

- New

Buttons at the bottom: All features, Hint, Center, Small, Large, Custom, Set size, Apply, Cancel.



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Box Size Definition

Choose **Job Input / Chemical system description / Simulation box / Composition / Box size ...**

The screenshot shows the 'Edit Job Input' dialog with the 'Feature overview' tree on the left and the 'Selected feature' table on the right.

Feature overview:

- Job Input
 - General job description
 - Chemical system description
 - Monomer definition (Off)
 - Molecule definition
 - Simulation box
 - Composition
 - DPD density
 - Concentration (Off)
 - Quantity
 - Box size** (selected)
 - Colors
 - Particles and molecules display
 - Geometry random seed
 - Compartments and box view
 - Movement
 - Property calculation
 - Interaction description
 - Simulation description

Selected feature:

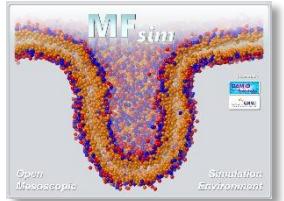
Feature	Description	Hint	Error														
Name	Box size																
x [DPD]	60.221405	y [DPD]	60.221405	z [DPD]	60.221405	State x	flexible	x [Å]	285.75568	State y	flexible	y [Å]	285.75568	State z	flexible	z [Å]	285.75568

Click on table cell to edit

Table-data schema:

New

Buttons at the bottom: Center, Small, Large, Custom, Set size, Apply, Cancel.



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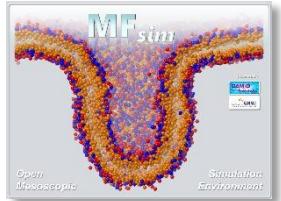
GitHub repository:
<https://github.com/zieslesny/MFsim>

Box Size Definition

... select *fixed* for **State X** ...

The screenshot shows the 'Edit Job Input' dialog with the 'Feature overview' tree expanded to show the 'Box size' node under 'Job Input / Chemical system description / Simulation box / Composition'. In the 'Selected feature' table, the 'Box size' row is selected. The 'State x' column dropdown menu is open, showing 'flexible' and 'fixed' options. A tooltip 'Select item (Default: flexible)' is visible near the dropdown. The table has columns for Name (Box size), x [DPD], y [DPD], z [DPD], State x, x [Å], State y, y [Å], State z, and z [Å]. The 'x [Å]' column contains values 285.75568, 285.75568, and 285.75568 respectively for the three rows.

Name	x [DPD]	y [DPD]	z [DPD]	State x	x [Å]	State y	y [Å]	State z	z [Å]
Box size	60.221405	60.221405	60.221405	flexible	285.75568	flexible	285.75568	flexible	285.75568
Box size	60.221405	60.221405	60.221405	fixed	285.75568	fixed	285.75568	fixed	285.75568
Box size	60.221405	60.221405	60.221405	fixed	285.75568	fixed	285.75568	fixed	285.75568



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Box Size Definition

... and change the fixed simulation box length $x [A]$ to 185.1 Angstrom.

The screenshot shows the 'Edit Job Input' dialog box with the 'Feature overview' tree on the left and the 'Selected feature' panel on the right.

Feature overview:

- Job Input
 - General job description
 - Chemical system description
 - Monomer definition (Off)
 - Molecule definition
 - Simulation box
 - Composition
 - DPD density
 - Concentration (Off)
 - Quantity
 - Box size (selected)
 - Colors
 - Particles and molecules display
 - Geometry random seed
 - Compartments and box view
 - Movement
 - Property calculation
 - Interaction description
 - Simulation description

Selected feature:

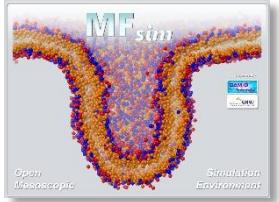
Feature	Description	Hint	Error														
Name	Box size																
x [DPD]	60.221405	y [DPD]	60.221405	z [DPD]	60.221405	State x	fixed	x [A]	185.1	State y	flexible	y [A]	285.755678	State z	flexible	z [A]	285.755678

Below the table, a note says: $0.100000 \leq 89.628095$ (default) $\leq \infty$.

Table-data schema:

- New

At the bottom, there are buttons: Center, Small, Large, Custom, Set size, Apply, and Cancel.

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Box Size Definition

Repeat these operations for a fixed simulation box y length of 185.1 Angstrom. The value of the *flexible* z length is automatically adjusted accordingly (depending on the number and volume of the particles in the box and the DPD density).

The screenshot shows the 'Edit Job Input' dialog with the 'Feature overview' tree on the left and the 'Selected feature' panel on the right.

Feature overview:

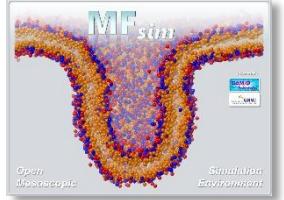
- Job Input
 - General job description
 - Chemical system description
 - Monomer definition (Off)
 - Molecule definition
 - Simulation box
 - Composition
 - DPD density
 - Concentration (Off)
 - Quantity
 - Box size** (selected)
 - Colors
 - Particles and molecules display
 - Geometry random seed
 - Compartments and box view
 - Movement
 - Property calculation
 - Interaction description
 - Simulation description

Selected feature:

Feature	Description	Hint	Error														
Name	Box size																
x [DPD]	60.221405	y [DPD]	60.221405	z [DPD]	60.221405	State x	fixed	x [Å]	285.75568	State y	fixed	y [Å]	185.1	State z	flexible	z [Å]	285.755678

Table-data schema:

Buttons at the bottom: Center, Small, Large, Custom, Set size, Apply, Cancel.



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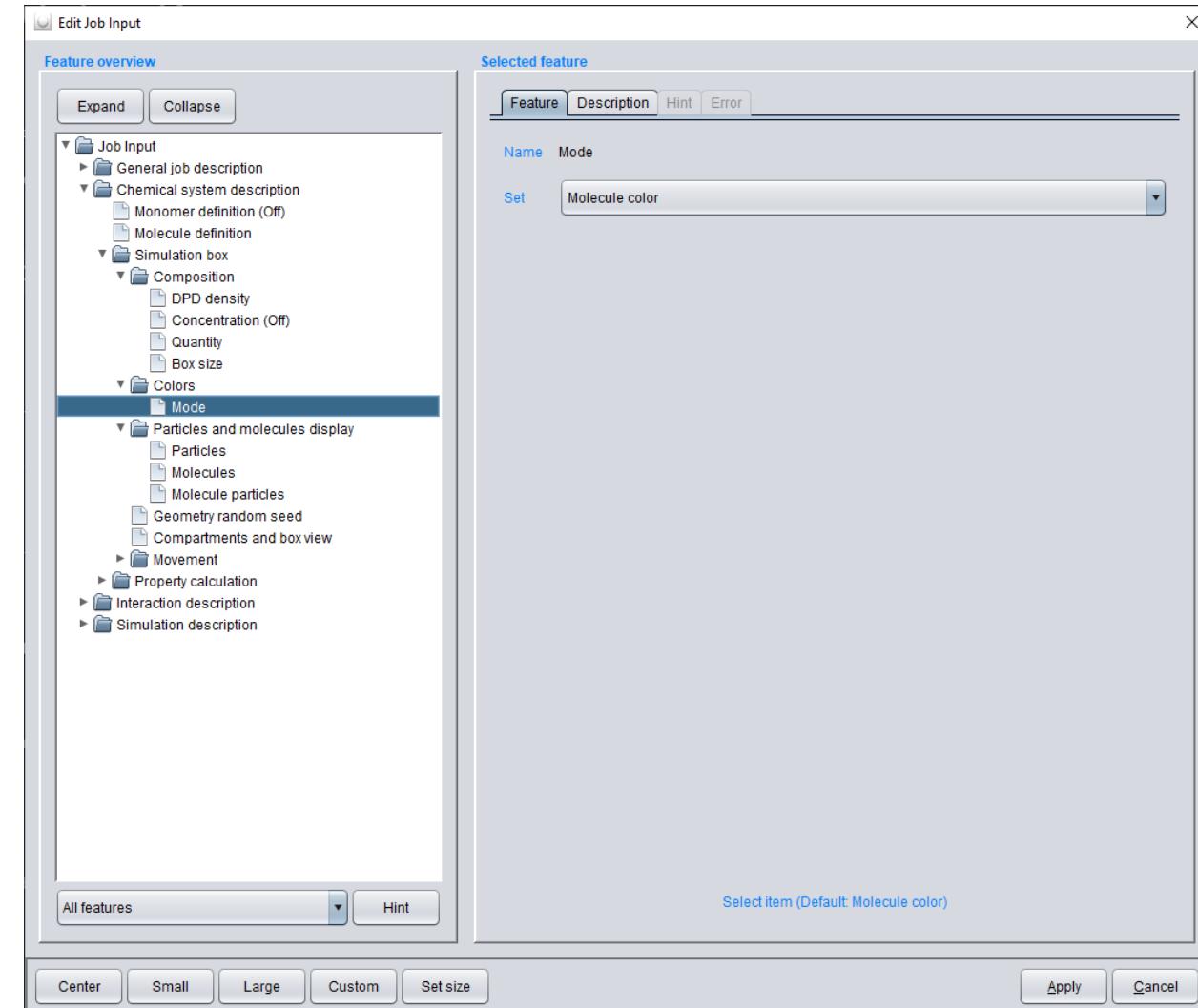


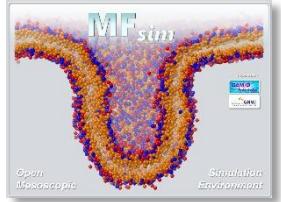
www.gnwi.de

GitHub repository:
<https://github.com/zieseny/MFsim>

Particle Display

Select **Job Input / Chemical system description / Simulation box / Colors / Mode ...**





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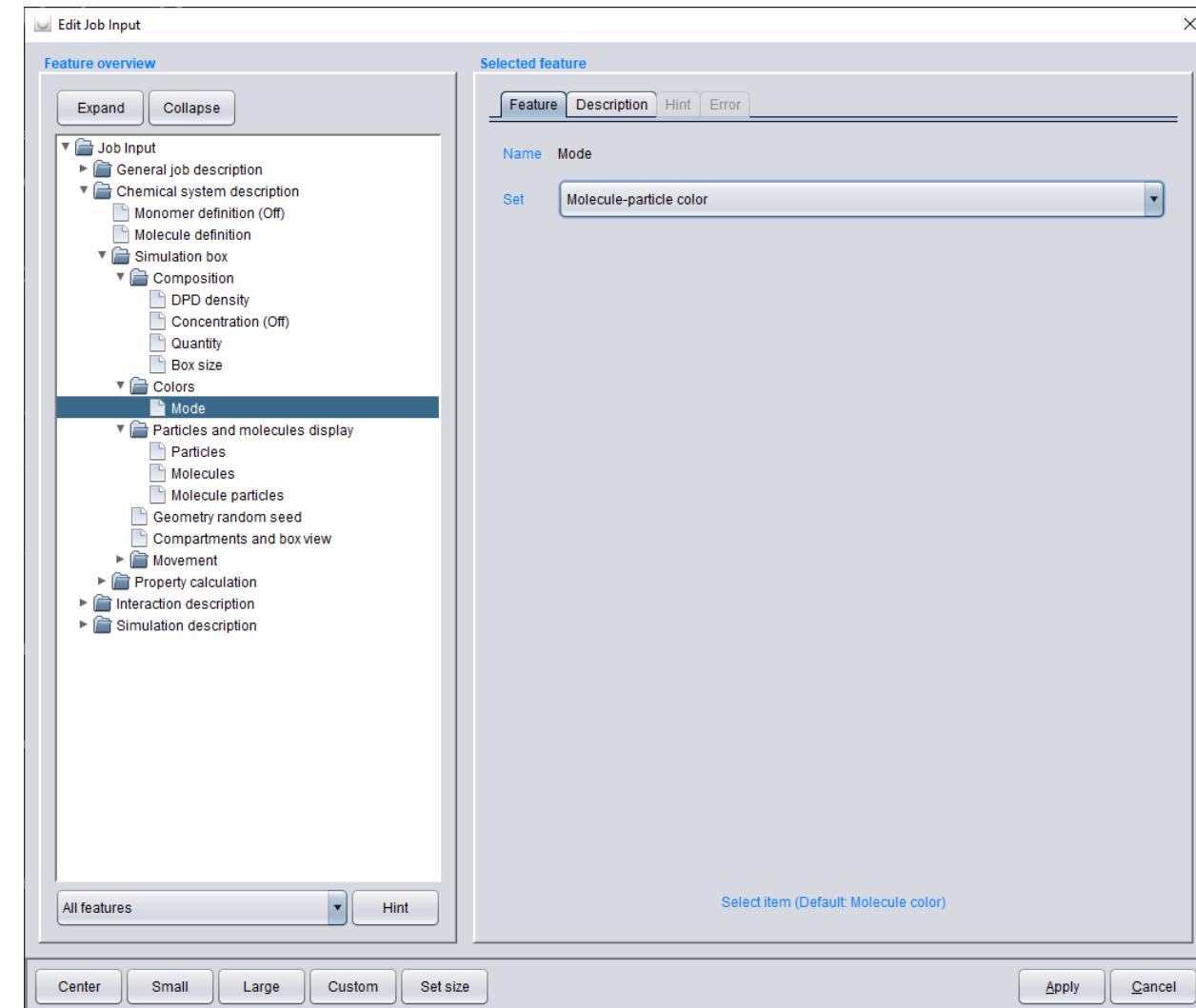


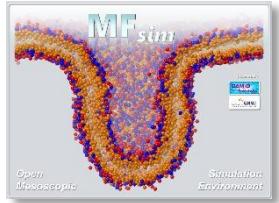
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GitHub repository:
<https://github.com/zieseny/MFsim>

Particle Display

... and choose *Molecule-particle color*.





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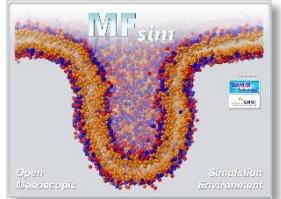
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Particle Display

Select **Job Input / Chemical system description / Simulation box / Particles and molecules display / Molecule particles** to define **Display** and **Graphics color** of all particles within their related molecules. To turn off the display of all H₂O particles hit the **Set** button for (filtered) bulk settings ...

The screenshot shows the 'Edit Job Input' dialog with the 'Selected feature' tab selected. The tree view on the left shows the 'Molecule particles' node under 'Particles and molecules display'. The table on the right lists molecule names, particle types, particle names, display status, graphics color, radius scale, and transparency for each entry.

Molecule name	Particle	Particle name	Display	Graphics color	Radius scale	Transparency
CHOLin	Et	Ethane	On	OLIVE	100	0
CHOLin	Me	Methane	On	OLIVE	100	0
CHOLin	MeOHchol	Methanol	On	OLIVE	100	0
CHOLout	Et	Ethane	On	OLIVE	100	0
CHOLout	Me	Methane	On	OLIVE	100	0
CHOLout	MeOHchol	Methanol	On	OLIVE	100	0
DMPClin	DMPN	Dimethylphosphate	On	GREEN	100	0
DMPClin	Et	Ethane	On	GREEN	100	0
DMPClin	MeAc	MethylAcetate	On	GREEN	100	0
DMPClin	TriMeNPpl	TriMethylamine	On	GREEN	100	0
DMPCout	DMPN	Dimethylphosphate	On	GREEN	100	0
DMPCout	Et	Ethane	On	GREEN	100	0
DMPCout	MeAc	MethylAcetate	On	GREEN	100	0
DMPCout	TriMeNPpl	TriMethylamine	On	GREEN	100	0
DOPEin	DMPN	Dimethylphosphate	On	PLUM	100	0
DOPEin	Et	Ethane	On	PLUM	100	0



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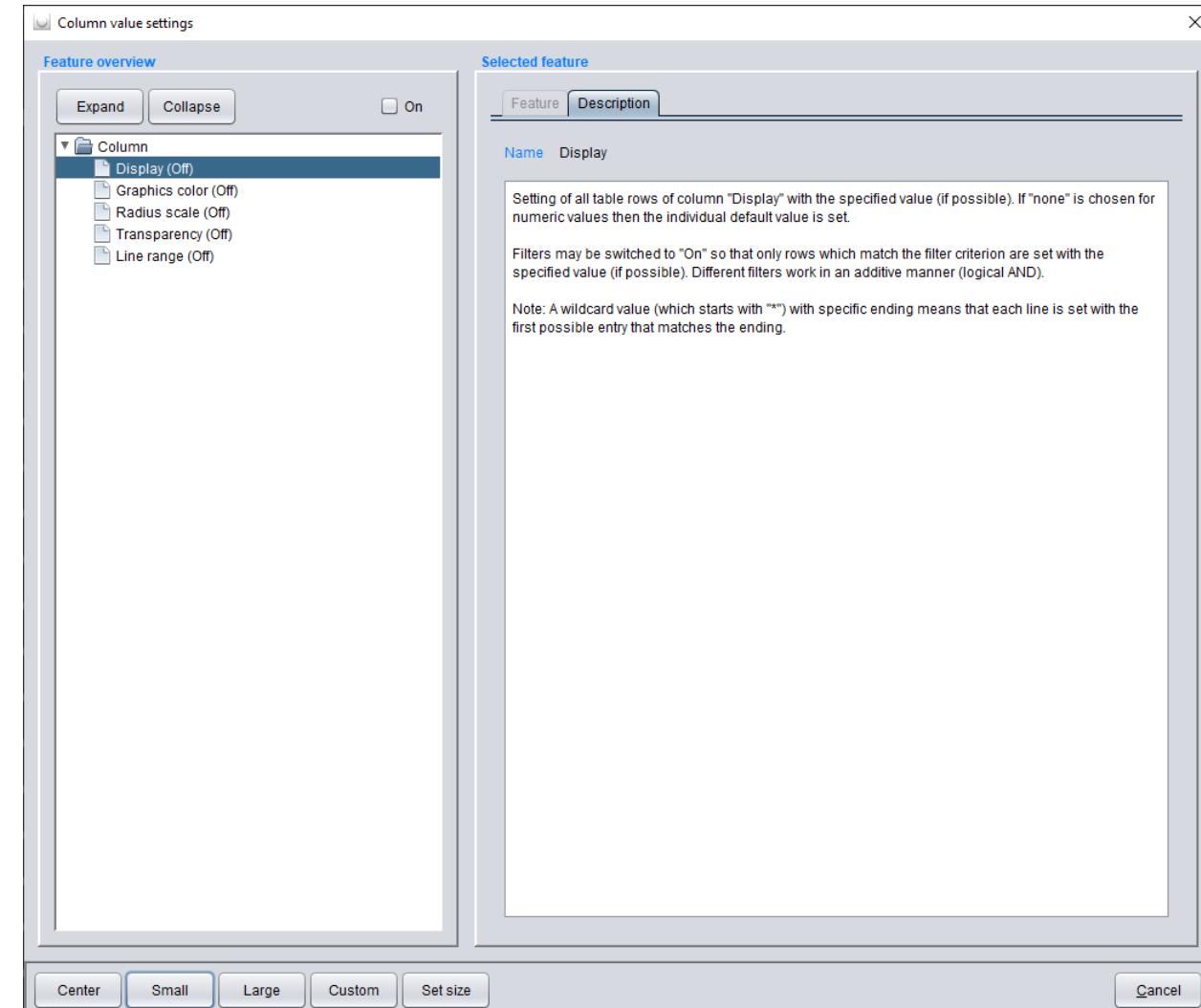
www.molecular-dynamics.de

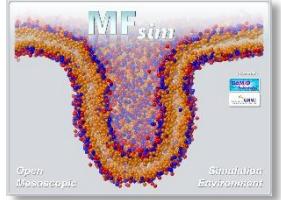


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Particle Display

... select the (by default disabled) **Display** setting ...



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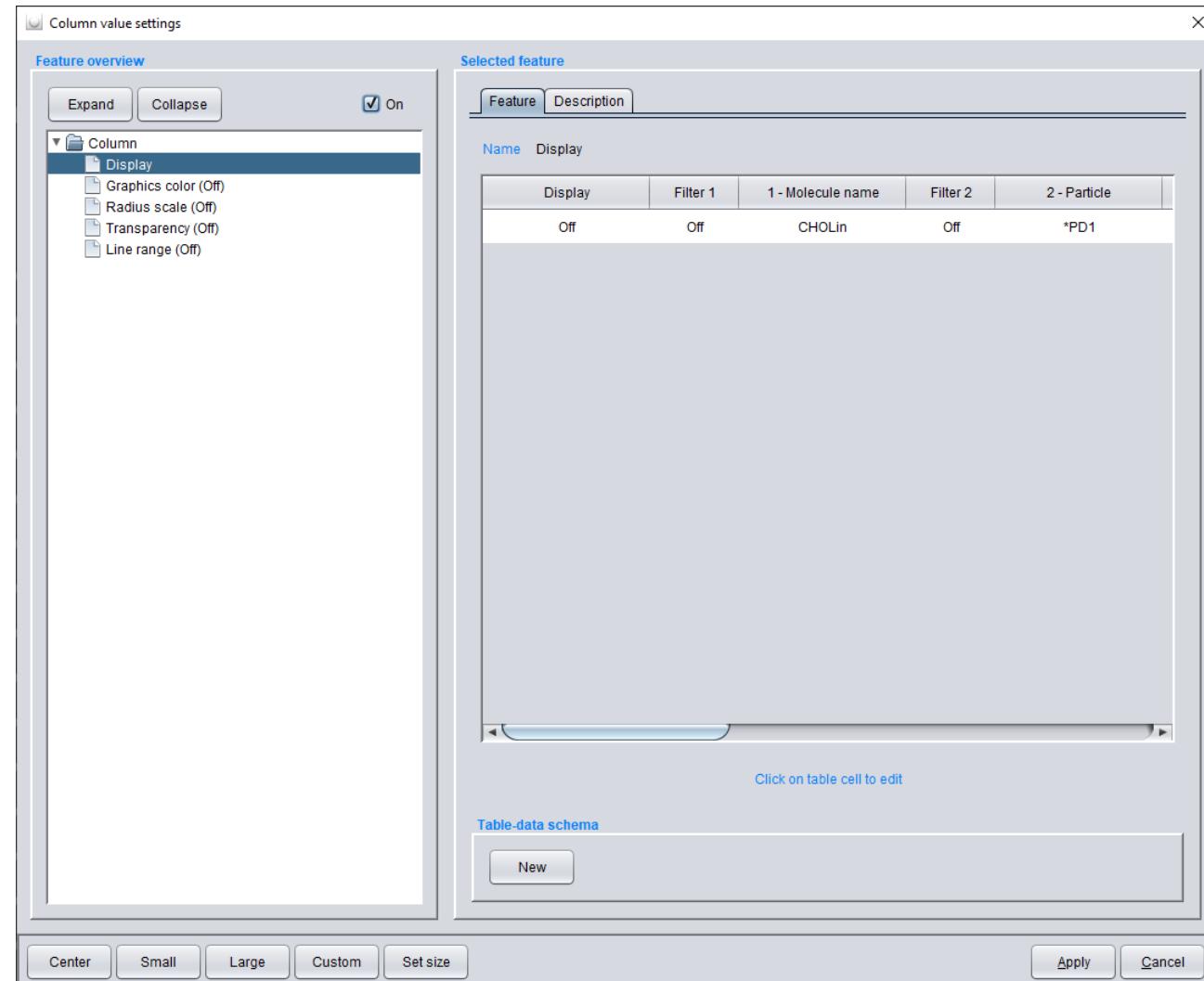
www.molecular-dynamics.de

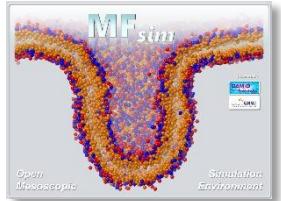


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Particle Display

... and enable this setting by ticking the **On** checkbox. The bulk setting for **Display** is set to *Off* (i.e. no display) by default. Change particle **Filter 2** ...



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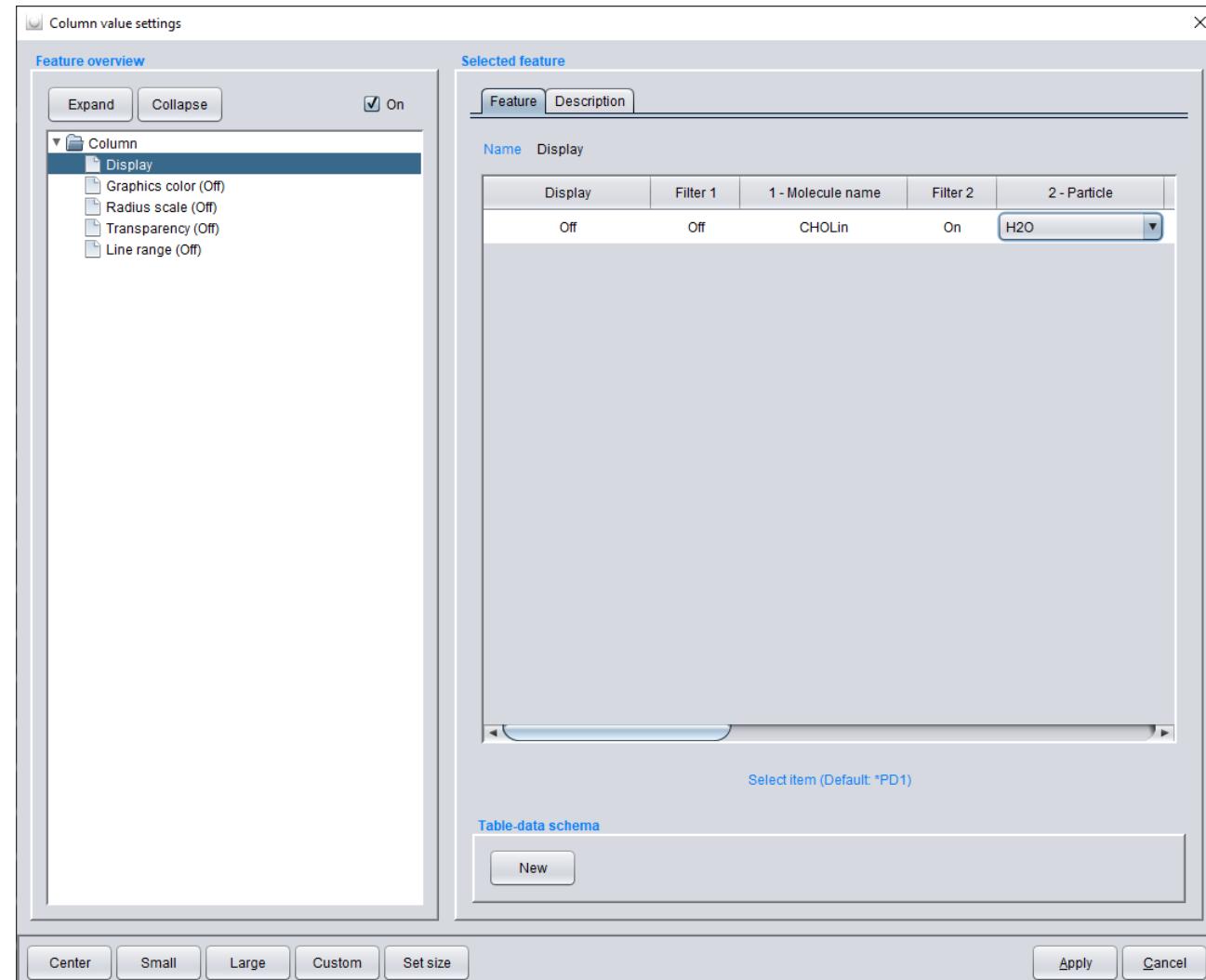
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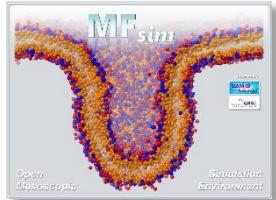


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Particle Display

... to **On** and select the target *H₂O* particle (to which the bulk setting will be applied exclusively) under **2 - Particle**. Confirm the entries with **Apply**.





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Particle Display

The **Display** of all H₂O particles in the simulation box is turned *Off*.

Define all other entries by individual or filtered bulk settings ...

MFsim Edit Job Input

Feature overview

Selected feature

Name Molecule particles

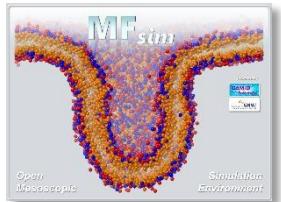
Molecule name	Particle	Particle name	Display	Graphics color	Radius scale	Transparency
PSin	MeNH2Ppl	Methylamine	On	MAGENTA	100	0
SMin	DMPN	Dimethylphosphate	On	MINT	100	0
SMin	Et	Ethane	On	MINT	100	0
SMin	Me	Methane	On	MINT	100	0
SMin	MeAcNH	MethylAcetamide	On	MINT	100	0
SMin	MeOH	Methanol	On	MINT	100	0
SMin	TriMeNPpl	TriMethylamine	On	MINT	100	0
SMout	DMPN	Dimethylphosphate	On	MINT	100	0
SMout	Et	Ethane	On	MINT	100	0
SMout	Me	Methane	On	MINT	100	0
SMout	MeAcNH	MethylAcetamide	On	MINT	100	0
SMout	MeOH	Methanol	On	MINT	100	0
SMout	TriMeNPpl	TriMethylamine	On	MINT	100	0
WaterIn1	H2O	Water	Off	CYAN	100	0
WaterIn2	H2O	Water	Off	CYAN	100	0
WaterOut	H2O	Water	Off	CYAN	100	0

Table-data schema

New Schema 1 Show Apply Remove

Center Small Large Custom Set size

Click on table cell to edit



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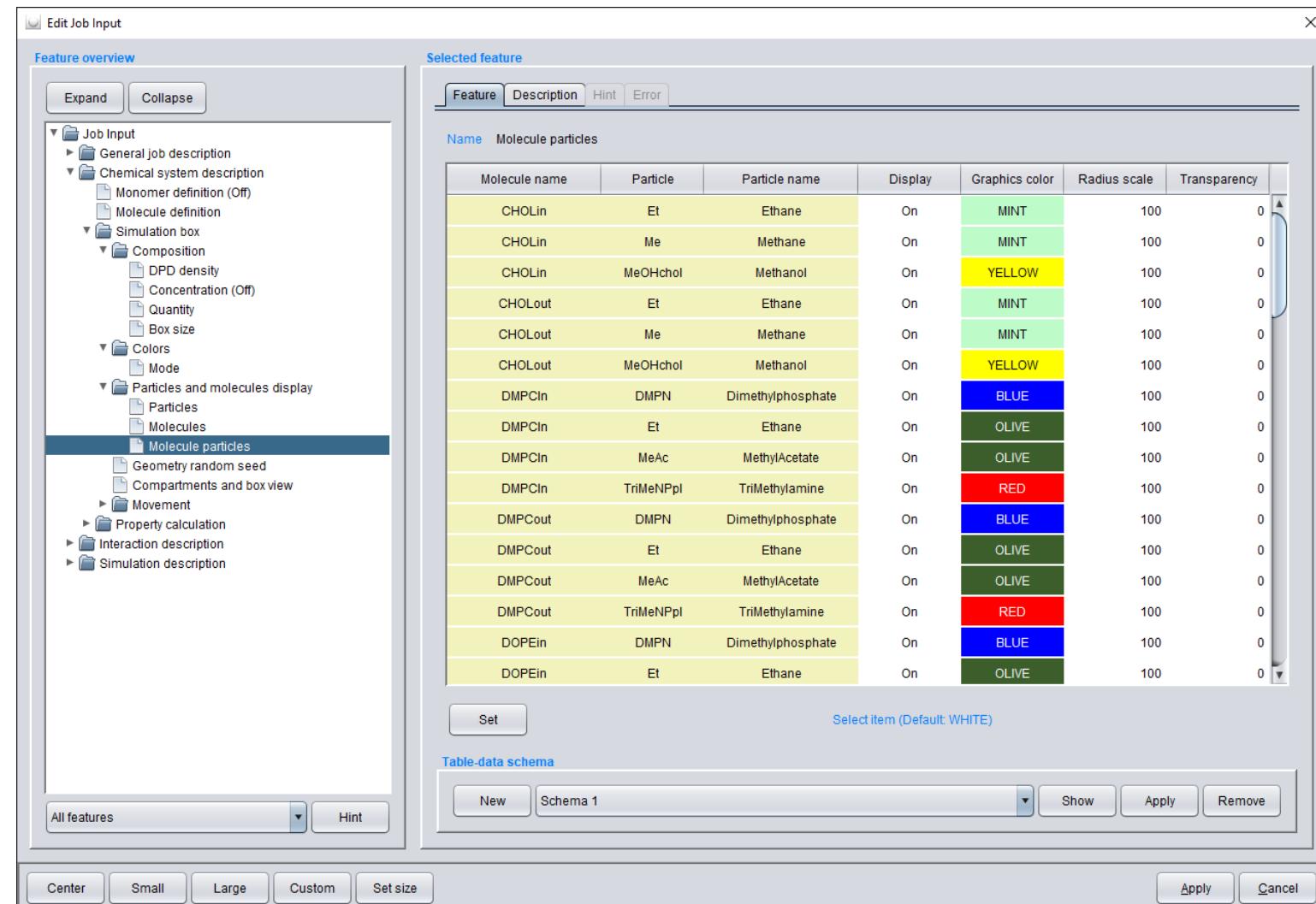


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Particle Display

... 

The dialog box displays the 'Feature overview' tree on the left and the 'Selected feature' table on the right.

Feature overview:

- Job input
 - General job description
 - Chemical system description
 - Monomer definition (Off)
 - Molecule definition
 - Simulation box
 - Composition
 - DPD density
 - Concentration (Off)
 - Quantity
 - Box size
 - Colors
 - Mode
 - Particles and molecules display
 - Particles
 - Molecules
 - Molecule particles
 - Movement
 - Property calculation
 - Interaction description
 - Simulation description

Selected feature:

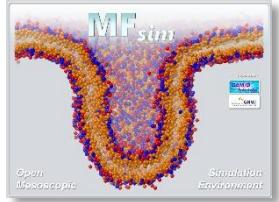
Name	Molecule particles					
CHOLin	Et	Ethane	On	MINT	100	0
CHOLin	Me	Methane	On	MINT	100	0
CHOLin	MeOHchol	Methanol	On	YELLOW	100	0
CHOOut	Et	Ethane	On	MINT	100	0
CHOOut	Me	Methane	On	MINT	100	0
CHOOut	MeOHchol	Methanol	On	YELLOW	100	0
DMPClin	DMPN	Dimethylphosphate	On	BLUE	100	0
DMPClin	Et	Ethane	On	OLIVE	100	0
DMPClin	MeAc	MethylAcetate	On	OLIVE	100	0
DMPClin	TriMeNPpl	TriMethylamine	On	RED	100	0
DMPCout	DMPN	Dimethylphosphate	On	BLUE	100	0
DMPCout	Et	Ethane	On	OLIVE	100	0
DMPCout	MeAc	MethylAcetate	On	OLIVE	100	0
DMPCout	TriMeNPpl	TriMethylamine	On	RED	100	0
DOPEin	DMPN	Dimethylphosphate	On	BLUE	100	0
DOPEin	Et	Ethane	On	OLIVE	100	0

Table-data schema:

New	Schema 1	Show	Apply	Remove
-----	----------	------	-------	--------

Buttons at the bottom:

- Center
- Small
- Large
- Custom
- Set size
- Apply
- Cancel



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Particle Display

... where only backbone particles of KB1Y19 are to be displayed, i.e. *AzolidBB*, *AzolidPD1*, *MeAcNHBB*, *MeAcNHPD1*, *MeAcNHPD2*,

...

MFsim Edit Job Input

Feature overview

Selected feature

Molecule name	Particle	Particle name	Display	Graphics color	Radius scale	Transparency
DOPEin	Et	Ethane	On	OLIVE	100	0
DOPEin	MeAc	MethylAcetate	On	OLIVE	100	0
DOPEin	MeNH2Ppl	Methylamine	On	RED	100	0
DOPEout	DMPN	Dimethylphosphate	On	BLUE	100	0
DOPEout	Et	Ethane	On	OLIVE	100	0
DOPEout	MeAc	MethylAcetate	On	OLIVE	100	0
DOPEout	MeNH2Ppl	Methylamine	On	RED	100	0
KB1Y19	AcNH2	Acetamide	Off	WHITE	100	0
KB1Y19	AzolidBB	Azolidine	On	BEIGE	100	0
KB1Y19	AzolidPD1	Azolidine	On	WHITE	100	0
KB1Y19	GuanidineP	Guanidine	Off	WHITE	100	0
KB1Y19	HAcN	AceticAcid	Off	WHITE	100	0
KB1Y19	Me	Methane	Off	WHITE	100	0
KB1Y19	MeAcNHBB	MethylAcetamide	On	BEIGE	100	0
KB1Y19	MeAcNHPD1	MethylAcetamide	On	WHITE	100	0
KB1Y19	MeAcNHPD2	MethylAcetamide	On	BEIGE	100	0

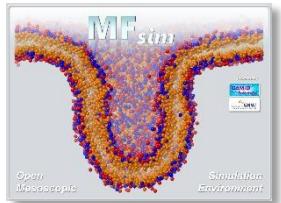
Set Select item (Default: WHITE)

Table-data schema

New Schema 1 Show Apply Remove

Center Small Large Custom Set size

Apply Cancel



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Particle Display

... MeAcNHPD3 and
MeAcNHPD4, ...

MFsim Simulation Environment

Edit Job Input

Feature overview

Selected feature

Name Molecule particles

Molecule name	Particle	Particle name	Display	Graphics color	Radius scale	Transparency
KB1Y19	MeAcNHPD2	MethylAcetamide	On	BEIGE	100	0
KB1Y19	MeAcNHPD3	MethylAcetamide	On	BEIGE	100	0
KB1Y19	MeAcNHPD4	MethylAcetamide	On	PLUM	100	0
KB1Y19	MeOH	Methanol	Off	WHITE	100	0
KB1Y19	MeSHSS	Methanethiol	Off	WHITE	100	0
KB1Y19	PhOH	Phenol	Off	WHITE	100	0
KB1Y19	Pr	Propane	Off	WHITE	100	0
KB1Y19	PrOH	Propanol	Off	WHITE	100	0
PIP2in	DMPN	Dimethylphosphate	On	BLUE	100	0
PIP2in	DMPNpl	Dimethylphosphate	On	BLUE	100	0
PIP2in	Et	Ethane	On	OLIVE	100	0
PIP2in	MeAc	MethylAcetate	On	OLIVE	100	0
PIP2in	MeOH	Methanol	On	ORANGE	100	0
PIP2out	DMPN	Dimethylphosphate	On	BLUE	100	0
PIP2out	DMPNpl	Dimethylphosphate	On	BLUE	100	0
PIP2out	Et	Ethane	On	OLIVE	100	0

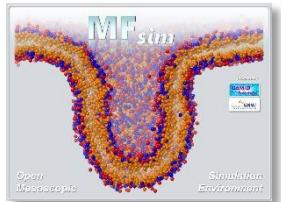
All features Hint

Center Small Large Custom Set size

Table-data schema

New Schema 1 Show Apply Remove

Apply Cancel



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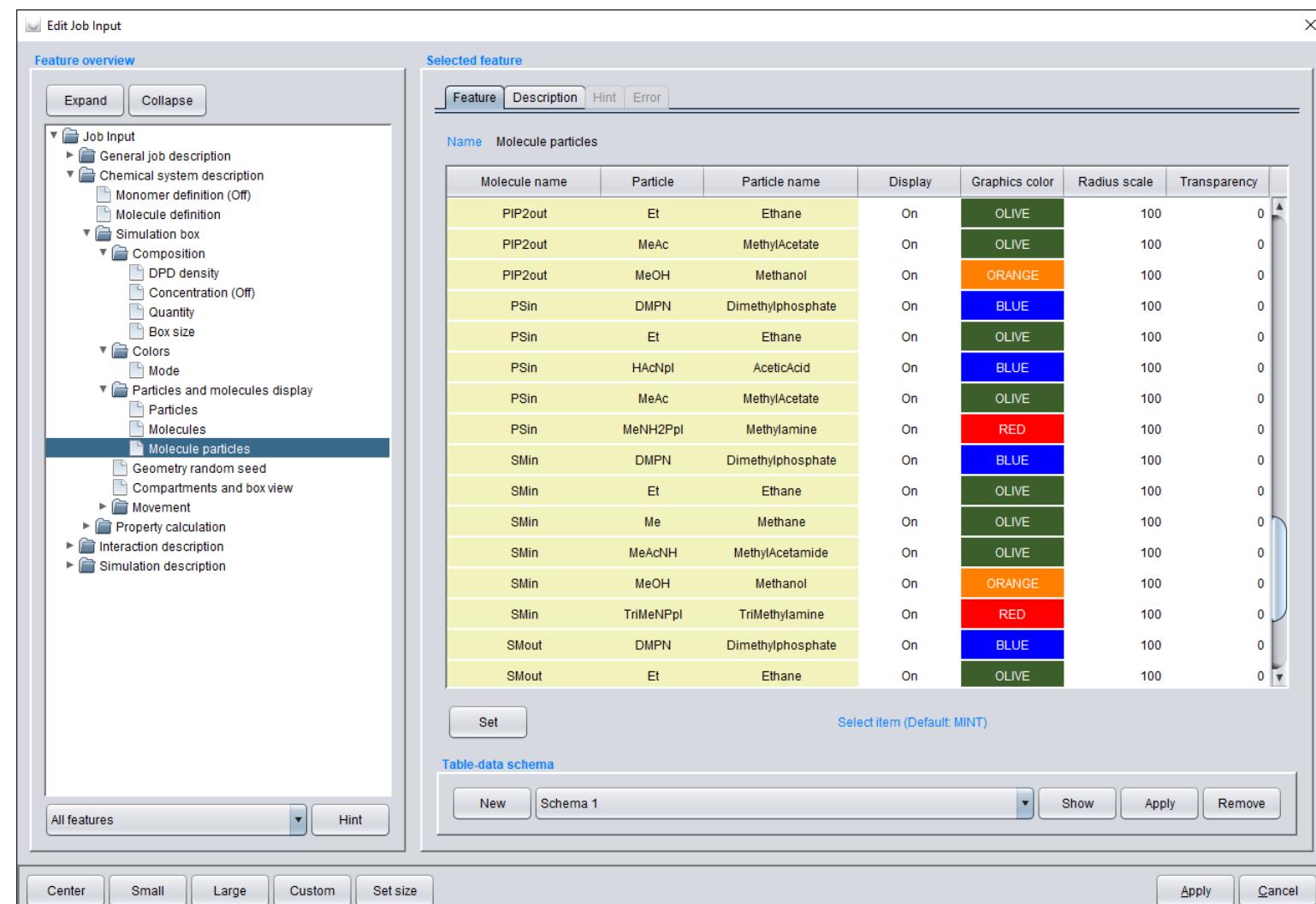
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GitHub repository:
<https://github.com/zieseny/MFsim>

Particle Display

... 

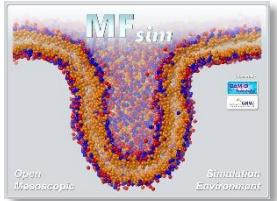
The dialog box displays the 'Edit Job Input' interface. The 'Feature overview' tree view shows the following structure:

- Job input
 - General job description
 - Chemical system description
 - Monomer definition (Off)
 - Molecule definition
 - Simulation box
 - Composition
 - DPD density
 - Concentration (Off)
 - Quantity
 - Box size
 - Colors
 - Mode
 - Particles and molecules display
 - Particles
 - Molecules
 - Molecule particles
 - Movement
 - Property calculation
 - Interaction description
 - Simulation description

The 'Selected feature' tab is active, showing a table titled 'Name Molecule particles' with the following data:

Molecule name	Particle	Particle name	Display	Graphics color	Radius scale	Transparency
PIP2out	Et	Ethane	On	OLIVE	100	0
PIP2out	MeAc	MethylAcetate	On	OLIVE	100	0
PIP2out	MeOH	Methanol	On	ORANGE	100	0
PSin	DMPN	Dimethylphosphate	On	BLUE	100	0
PSin	Et	Ethane	On	OLIVE	100	0
PSin	HAcNpl	AceticAcid	On	BLUE	100	0
PSin	MeAc	MethylAcetate	On	OLIVE	100	0
PSin	MeNH2Ppl	Methylamine	On	RED	100	0
SMin	DMPN	Dimethylphosphate	On	BLUE	100	0
SMin	Et	Ethane	On	OLIVE	100	0
SMin	Me	Methane	On	OLIVE	100	0
SMin	MeAcNH	MethylAcetamide	On	OLIVE	100	0
SMin	MeOH	Methanol	On	ORANGE	100	0
SMin	TriMeNPpl	TriMethylamine	On	RED	100	0
SMout	DMPN	Dimethylphosphate	On	BLUE	100	0
SMout	Et	Ethane	On	OLIVE	100	0

Buttons at the bottom include 'Set', 'Select item (Default: MINT)', 'Table-data schema' (with 'New' and 'Schema 1' buttons), and 'Apply' and 'Cancel' buttons.



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Particle Display

... to complete the particle display definitions which can be saved to a **Table-data schema** by hitting the **New** button for comfortable re-use (not covered by this tutorial).

The screenshot shows the 'Edit Job Input' dialog with the 'Feature overview' tree on the left and a table-based configuration area on the right.

Feature overview:

- Job input
 - General job description
 - Chemical system description
 - Monomer definition (Off)
 - Molecule definition
 - Simulation box
 - Composition
 - DPD density
 - Concentration (Off)
 - Quantity
 - Box size
 - Colors
 - Mode
 - Particles and molecules display
 - Particles
 - Molecules
 - Molecule particles
 - Geometry random seed
 - Compartments and box view
 - Movement
 - Property calculation
 - Interaction description
 - Simulation description

Selected feature:

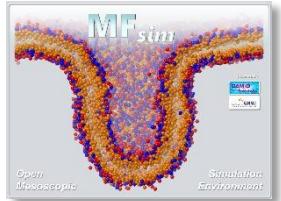
Feature	Description	Hint	Error
Name Molecule particles			
Molecule name	Particle	Particle name	Display
PSin	MeNH2Ppl	Methylamine	On
SMin	DMPN	Dimethylphosphate	On
SMin	Et	Ethane	On
SMin	Me	Methane	On
SMin	MeAcNH	MethylAcetamide	On
SMin	MeOH	Methanol	On
SMin	TriMeNPpl	TriMethylamine	On
SMout	DMPN	Dimethylphosphate	On
SMout	Et	Ethane	On
SMout	Me	Methane	On
SMout	MeAcNH	MethylAcetamide	On
SMout	MeOH	Methanol	On
SMout	TriMeNPpl	TriMethylamine	On
WaterIn1	H2O	Water	Off
WaterIn2	H2O	Water	Off
WaterOut	H2O	Water	Off

Table-data schema:

- New
- Schema 1
- Show
- Apply
- Remove

Buttons at the bottom:

- Center
- Small
- Large
- Custom
- Set size
- Apply
- Cancel



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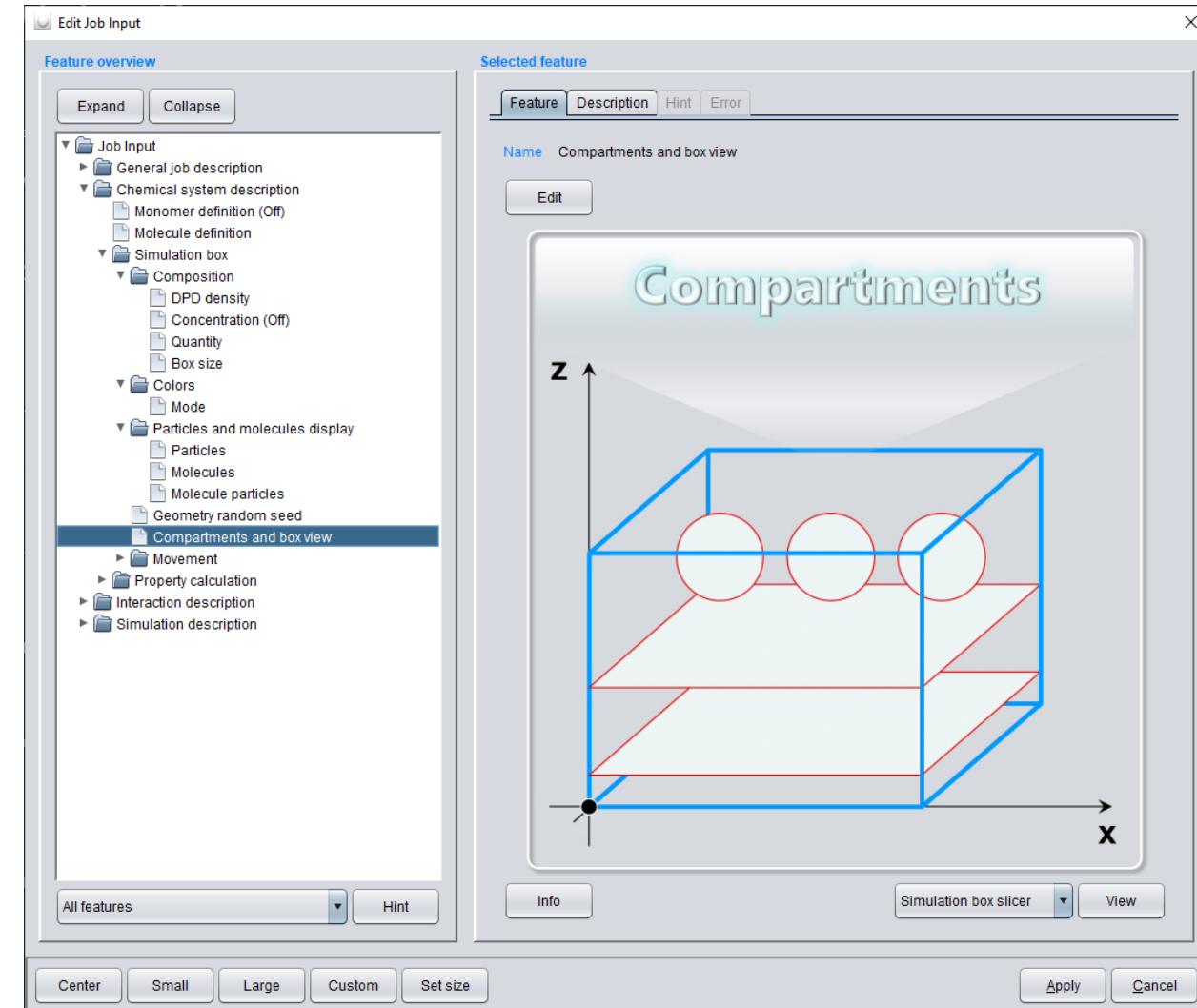
www.molecular-dynamics.de

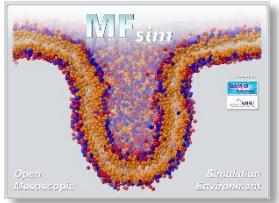


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Compartment Definition

Select **Job Input / Chemical system description / Simulation box / Compartments and box view ...**





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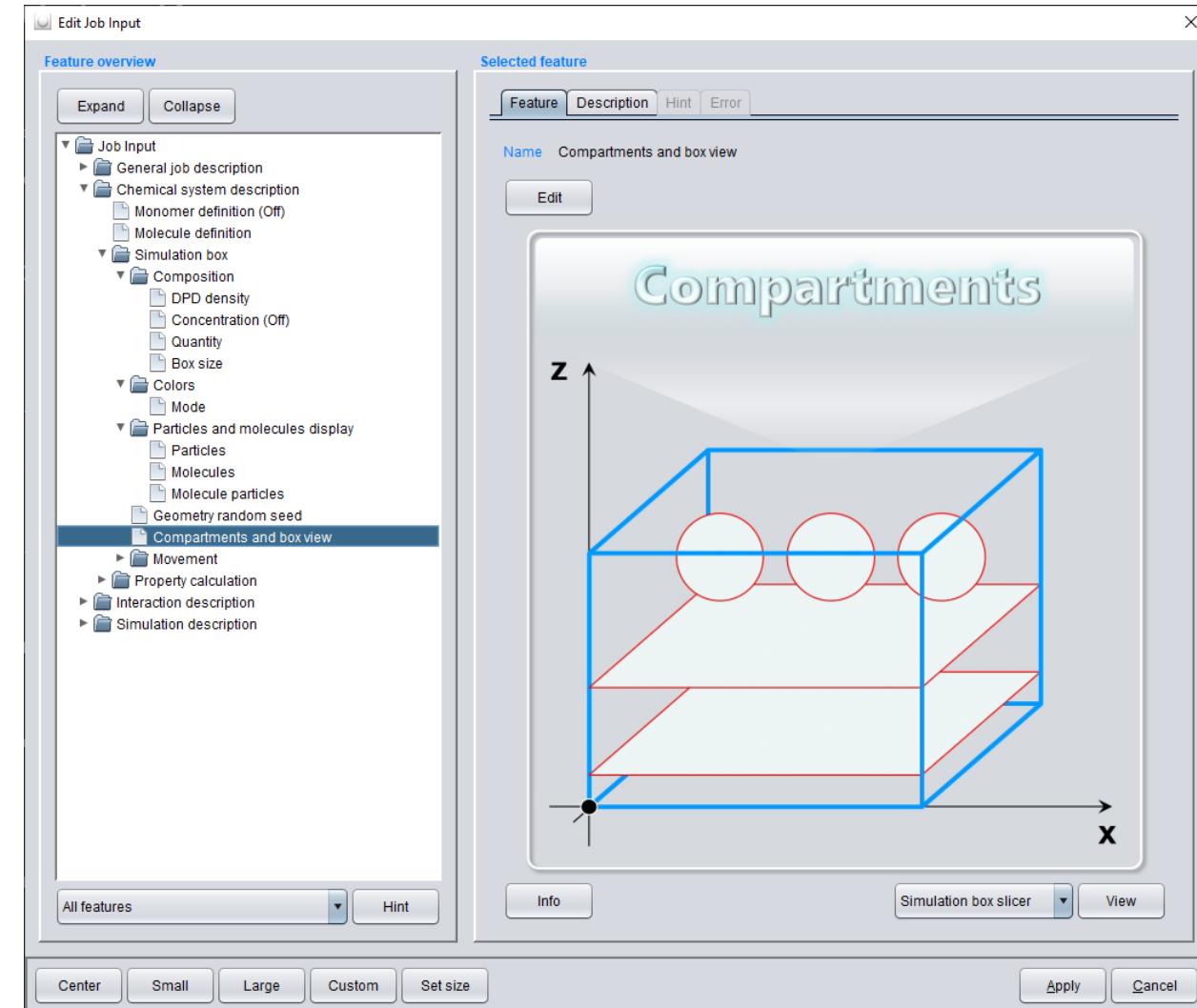
www.molecular-dynamics.de

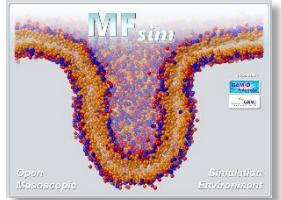


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Compartment Definition

... and hit the **Edit** compartments button ...



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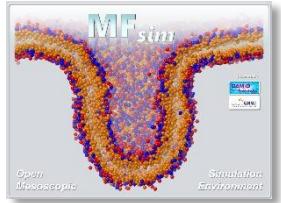


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Compartment Definition

... to open the **Edit compartments of simulation box** dialog with all molecules being initially located in the simulation box **Bulk** volume. Hit the **Name** button ...

Name	Chemical composition	Molecule name	Molecular structure	%	Quantity	Orientation
WaterIn1	H ₂ O	100	200000	Random		
WaterOut	H ₂ O	100	146000	Random		
WaterIn2	H ₂ O	100	200000	Random		
CHOLin	MeOHchol[1]...	100	890	Random		
CHOLout	MeOHchol[1]...	100	710	Random		
DMPCin	TriMeNPpl ST ...	100	154	Random		
DMPCout	TriMeNPpl ST ...	100	486	Random		
DOPEin	MeNH2Ppl STA ...	100	248	Random		
DOPEout	MeNH2Ppl STA ...	100	72	Random		
PIP2in	DMPN[1](MeAc ...	100	60	Random		
PIP2out	DMPN[1](MeAc ...	100	20	Random		
PSin	HAcNpl START ...	100	160	Random		
SMin	TriMeNPpl ST ...	100	88	Random		
SMout	TriMeNPpl ST ...	100	312	Random		
KB1Y19	MeAcNHBB[4](...	100	1000	3D random		



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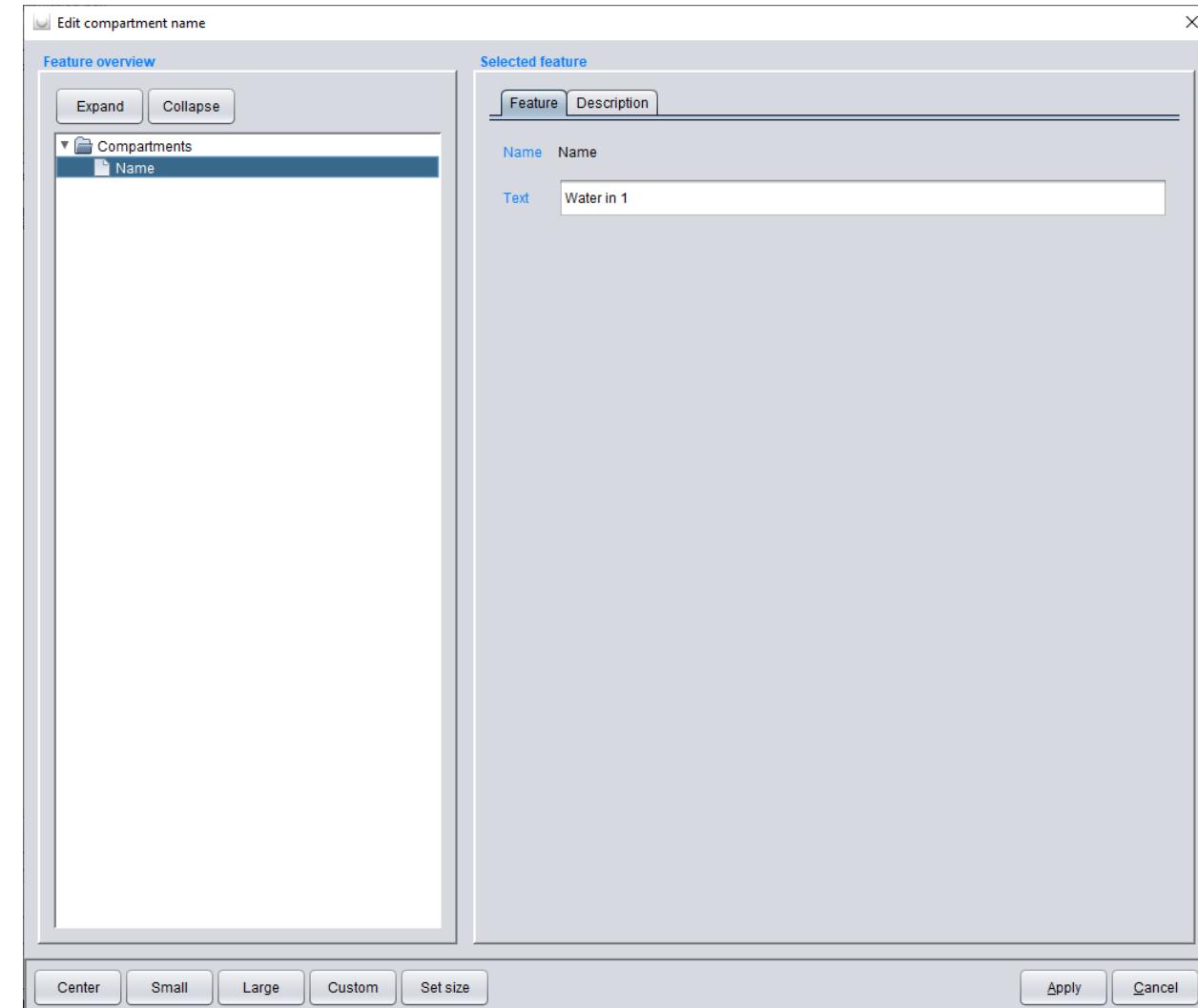
www.molecular-dynamics.de

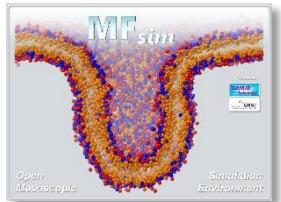


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Compartment Definition

... input *Water in 1* and hit **Apply**.





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Compartment Definition

Hit button **Add xy-layer: Water in 1 ...**

Edit compartments of simulation box

Compartments Geometry

Feature overview

Expand Collapse

Selected feature

Feature	Description	Hint	Error	
Name	Chemical composition			
Molecule name	Molecular structure	%	Quantity	Orientation

Chemical composition

Molecule name	Molecular structure	%	Quantity	Orientation
WaterIn1	H ₂ O	100	200000	Random
WaterOut	H ₂ O	100	146000	Random
WaterIn2	H ₂ O	100	200000	Random
CHOLin	MeOHchol[1]...	100	890	Random
CHOLout	MeOHchol[1]...	100	710	Random
DMPCin	TriMeNPpl ST ...	100	154	Random
DMPCout	TriMeNPpl ST ...	100	486	Random
DOPEin	MeNH2Ppl STA ...	100	248	Random
DOPEout	MeNH2Ppl STA ...	100	72	Random
PIP2in	DMPN[1](MeAc ...	100	60	Random
PIP2out	DMPN[1](MeAc ...	100	20	Random
PSin	HAcNp START ...	100	160	Random
SMin	TriMeNPpl ST ...	100	88	Random
SMout	TriMeNPpl ST ...	100	312	Random
KB1Y19	MeAcNHBB[4](...	100	1000	3D random

Set Click on table cell to edit

Table-data schema

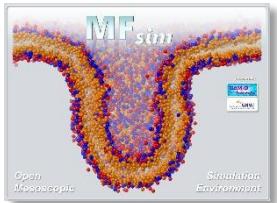
New

All features

Name Add sphere: Water in 1 Add xy-layer: Water in 1

Center Small Large Custom Set size

Cancel

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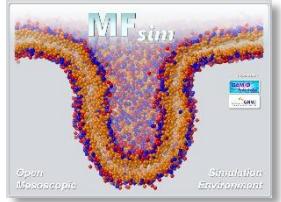


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Compartment Definition

... to create the *Water in 1* layer for the water molecules at the top of the simulation box. Specify 100 % of WaterIn1 to be located within this compartment. Select the **Geometry** tab ...

Molecule name	Molecular structure	%	Quantity	% Surface	Quantity in volume	Quantity on surface	Orientation
WaterIn1	H ₂ O	100	0	0	0	0	None
WaterOut	H ₂ O	0	0	0	0	0	None
WaterIn2	H ₂ O	0	0	0	0	0	None
CHOLin	MeOHcho[1]...	0	0	0	0	0	None
CHOLout	MeOHcho[1]...	0	0	0	0	0	None
DMPCin	TriMeNPp[IST ...	0	0	0	0	0	None
DMPCout	TriMeNPp[IST ...	0	0	0	0	0	None
DOPEin	MeNH2Pp[STA ...	0	0	0	0	0	None
DOPEout	MeNH2Pp[STA ...	0	0	0	0	0	None
PIP2in	DMPN[1](MeAc ...	0	0	0	0	0	None
PIP2out	DMPN[1](MeAc ...	0	0	0	0	0	None
PSin	HAcNp[START ...	0	0	0	0	0	None
SMin	TriMeNPp[ST ...	0	0	0	0	0	None
SMout	TriMeNPp[ST ...	0	0	0	0	0	None
KB1Y19	MeAcNHBB[4) ...	0	0	0	0	0	None



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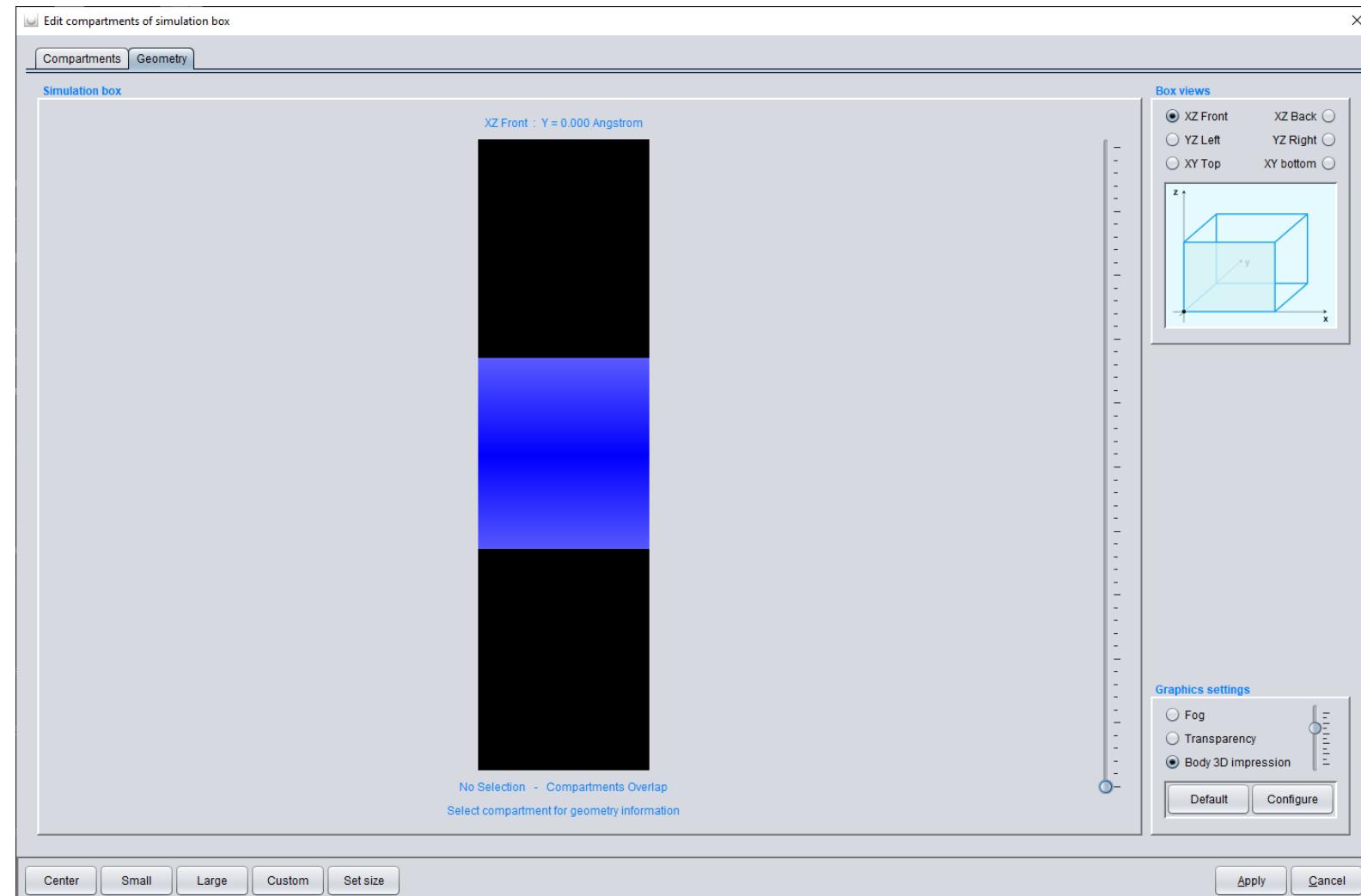
www.molecular-dynamics.de

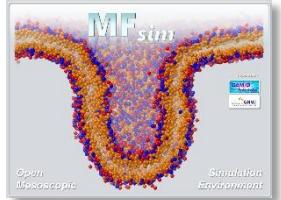


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Compartment Definition

... where the new layer compartment is placed in the middle of the simulation box by default. Click (the compartment color is changed to white) & drag the Water in 1 layer ...





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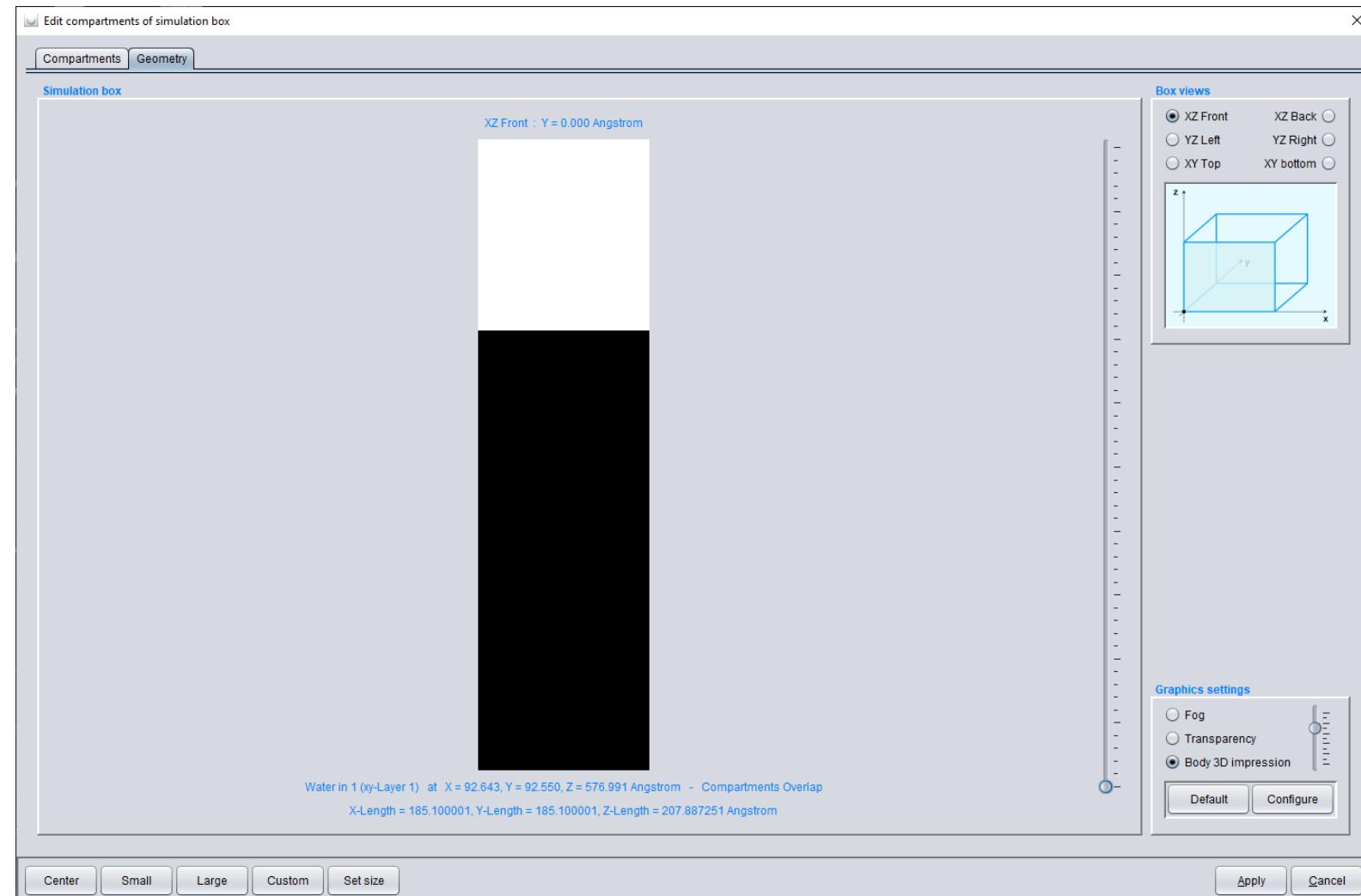
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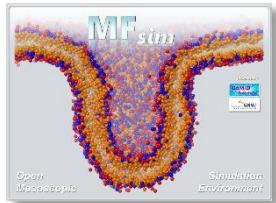


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Compartment Definition

... to the top of the simulation box. Switch back to the **Compartments** tab.





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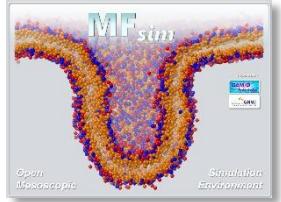


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Compartment Definition

Create a new *M1* in layer for the inner leaflet of the upper plasma bilayer membrane. 50 % of the inner membrane molecules are to be located here with 100 % at the **Surface** with a **Random xy top Orientation** so that the particles labeled with a [START] tag are positioned at the top of this compartment. Select the **Geometry** tab ...

Name	Molecular structure	%	Quantity	% Surface	Quantity in volume	Quantity on surface	Orientation
Waterin1	H2O	0	0	0	0	0	None
WaterOut	H2O	0	0	0	0	0	None
Waterin2	H2O	0	0	0	0	0	None
CHOLin	MeOHchol'1[...	50	445	100	0	445	Random xy top
CHOOut	MeOHchol'1[...	0	0	0	0	0	None
DMPCin	TriMeNPpl(ST ...	50	77	100	0	77	Random xy top
DMPCout	TriMeNPpl(ST ...	0	0	0	0	0	None
DOPEin	MeNH2Ppl(STA ...	50	124	100	0	124	Random xy top
DOPEout	MeNH2Ppl(STA ...	0	0	0	0	0	None
PIP2in	DMPN[1](MeAc ...	50	30	100	0	30	Random xy top
PIP2out	DMPN[1](MeAc ...	0	0	0	0	0	None
PSin	HAcNpl[START ...	50	80	100	0	80	Random xy top
SMin	TriMeNPpl(ST ...	50	44	100	0	44	Random xy top
SMout	TriMeNPpl(ST ...	0	0	0	0	0	None
KB1Y19	MeAcNHBB[4](...	0	0	0	0	0	None



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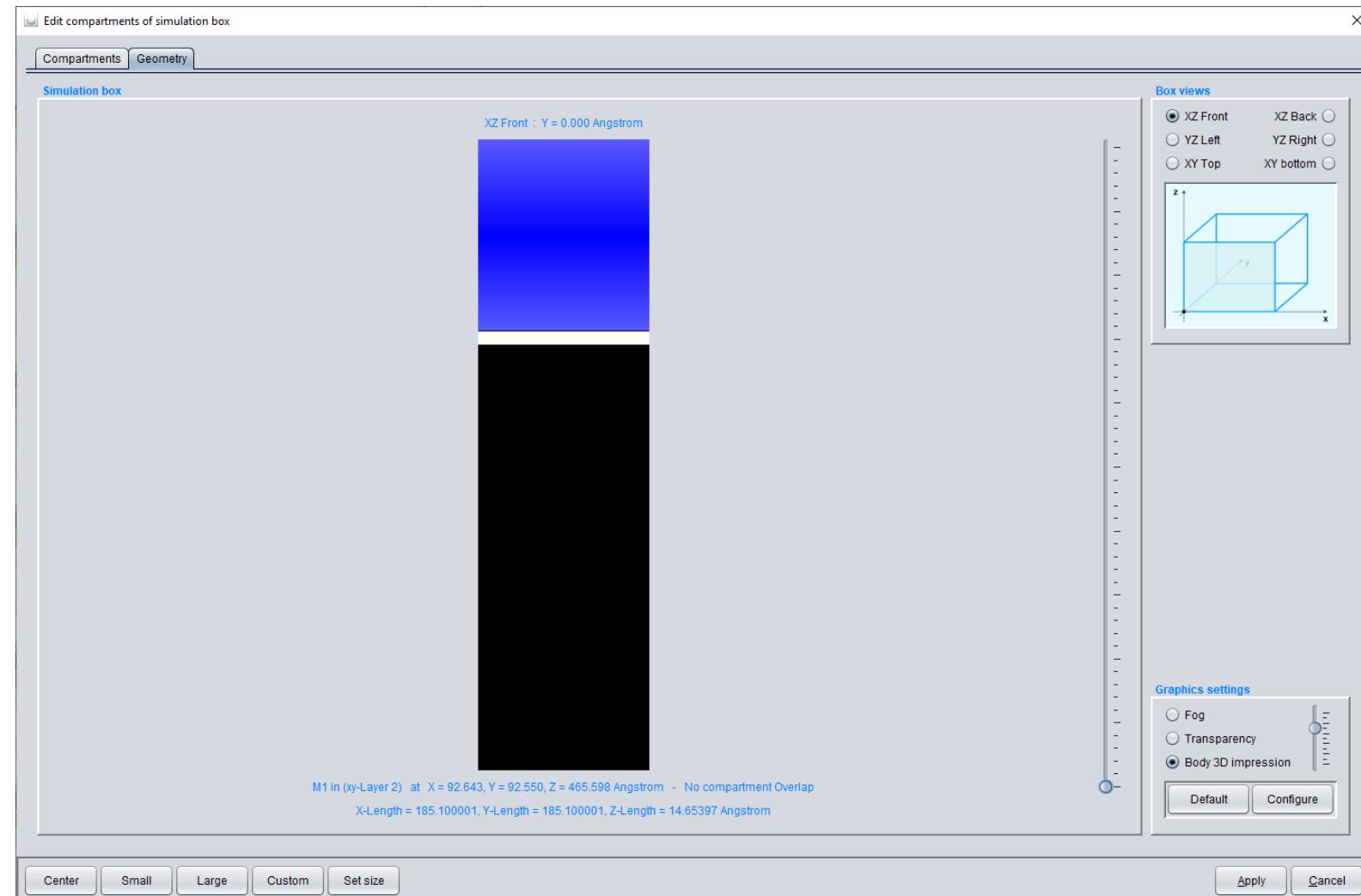


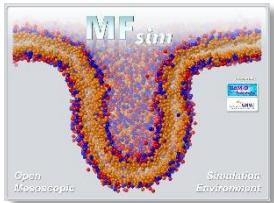
www.gnwi.de

GitHub repository:
<https://github.com/zieseny/MFsim>

Compartment Definition

... and click & drag the *M1* in layer directly below the *Water in 1* layer. Switch back to the **Compartments** tab.





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GitHub repository:
<https://github.com/zieseny/MFsim>

Compartment Definition

Create a new **M1 out** layer for the outer leaflet of the upper plasma bilayer membrane. 50 % of the outer membrane molecules are to be located here with 100 % at the **Surface** with a *Random xy bottom Orientation* so that the particles labeled with a [START] tag are positioned at the bottom of this compartment. Select the **Geometry** tab ...

MFsim
Edit compartments of simulation box

Compartments Geometry

Feature overview

Expand Collapse

- Simulation box
 - Bulk
 - xy-Layer compartments
 - Water in 1 (xy-Layer 1)
 - M1 in (xy-Layer 2)
 - M1 out (xy-Layer 3)
 - Chemical composition
 - Geometry

Selected feature

Feature Description Hint Error

Name Chemical composition

Molecule name	Molecular structure	%	Quantity	% Surface	Quantity in volume	Quantity on surface	Orientation
WaterIn1	H ₂ O	0	0	0	0	0	None
WaterOut	H ₂ O	0	0	0	0	0	None
WaterIn2	H ₂ O	0	0	0	0	0	None
CHOLin	MeOHcho[1]...	0	0	0	0	0	None
CHOOut	MeOHcho[1]...	50	355	100	0	355	Random xy bottom
DMPCin	TriMeNpp[IST ...	0	0	0	0	0	None
DMPCout	TriMeNpp[IST ...	50	243	100	0	243	Random xy bottom
DOPEin	MeNH2Ppl[STA ...	0	0	0	0	0	None
DOPEout	MeNH2Ppl[STA ...	50	36	100	0	36	Random xy bottom
PIP2in	DMPN[1](MeAc ...	0	0	0	0	0	None
PIP2out	DMPN[1](MeAc ...	50	10	100	0	10	Random xy bottom
PSin	HAcNpl[START ...	0	0	0	0	0	None
SMin	TriMeNpp[ST ...	0	0	0	0	0	None
SMout	TriMeNpp[ST ...	50	156	100	0	156	Random xy bottom
KB1Y19	MeAcNHBB[4]...	0	0	0	0	0	None

Set Click on table cell to edit

Table-data schema

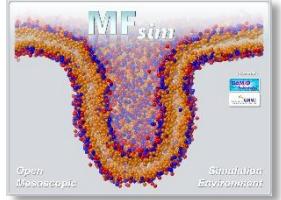
New

Remove

Add sphere Add xy-layer

Center Small Large Custom Set size

Apply Cancel



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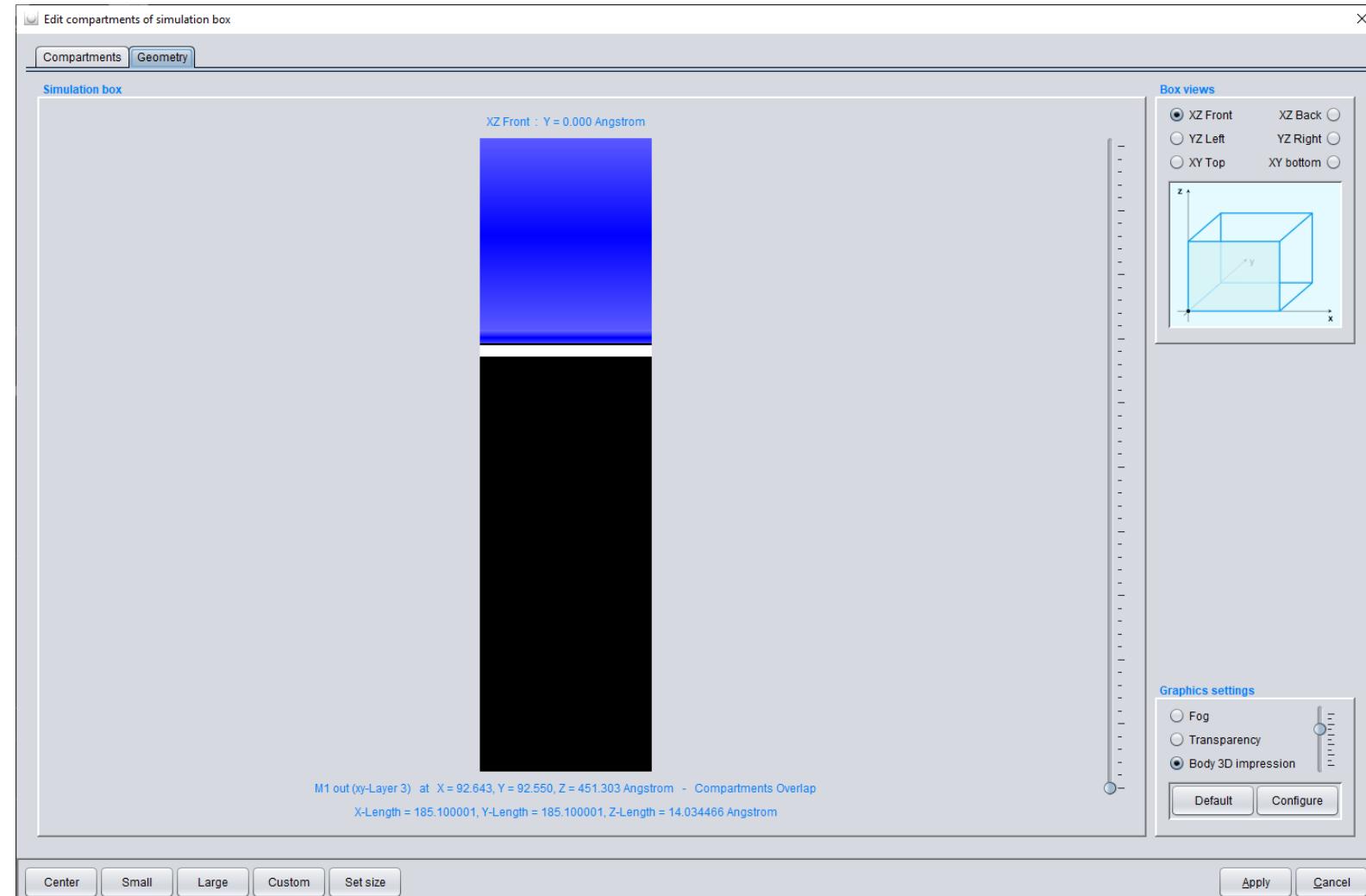


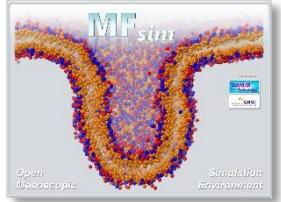
www.gnwi.de

GitHub repository:
<https://github.com/ziesnsy/MFsim>

Compartment Definition

... and click & drag the *M1 out* layer directly below the *M1 in* layer. Switch back to the **Compartments** tab.



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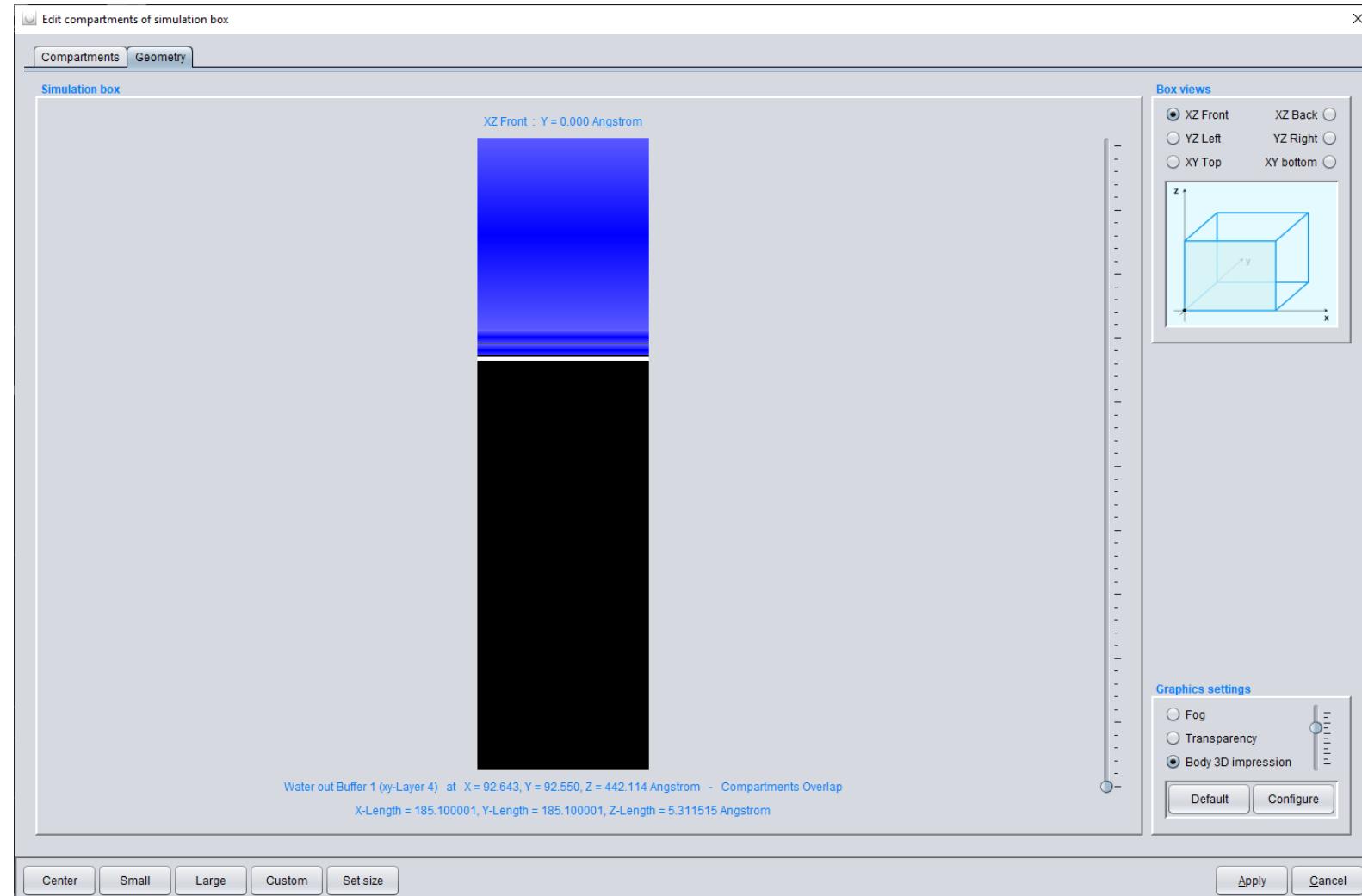
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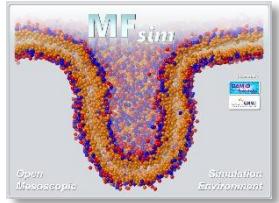


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Compartment Definition

Create a new *Water out Buffer 1* layer for the upper water buffer with 3.5 % of *WaterOut* molecules. Select the **Geometry** tab and click & drag this layer directly below the *M1 out* layer. Switch back to the **Compartments** tab.





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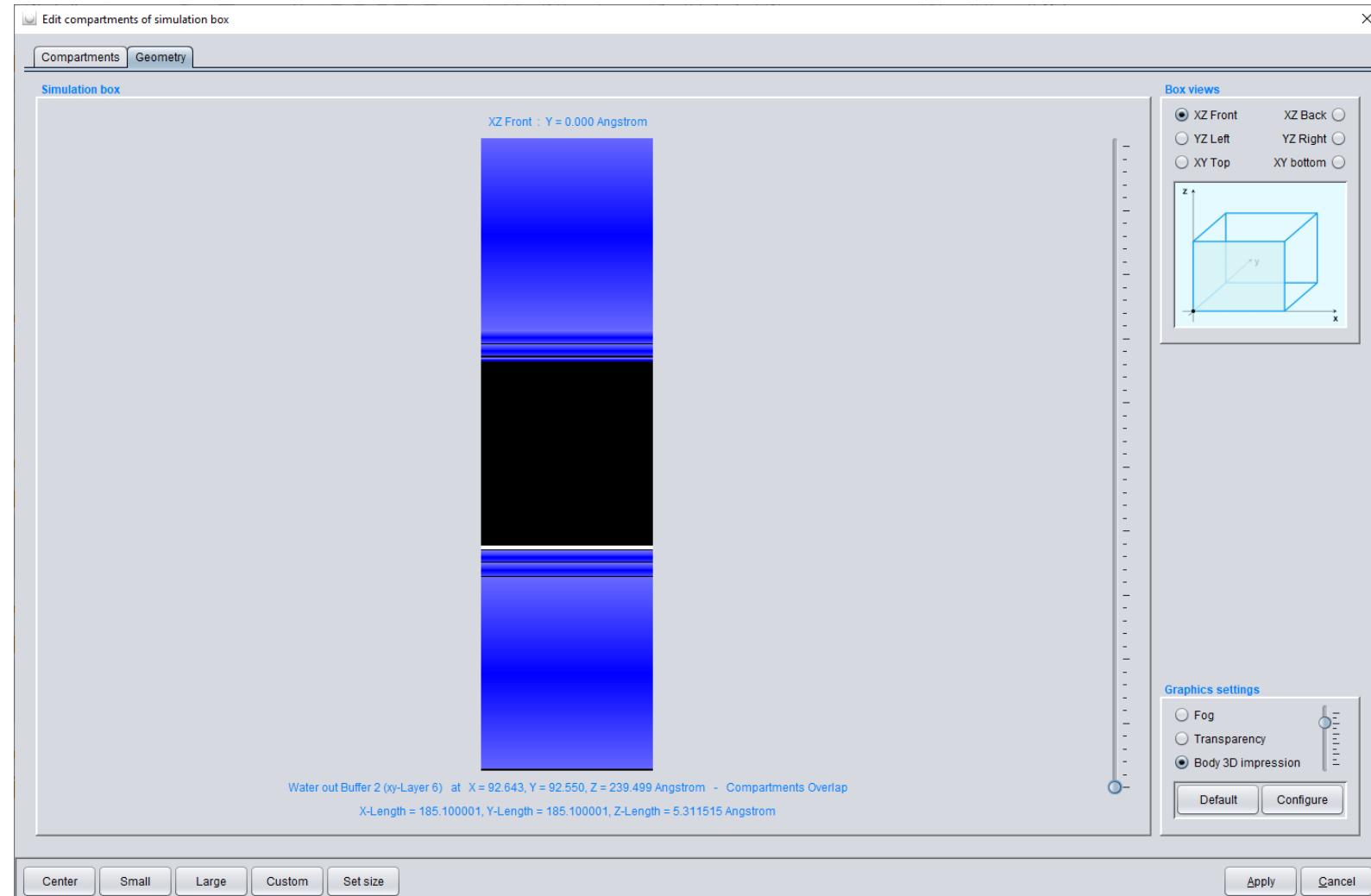


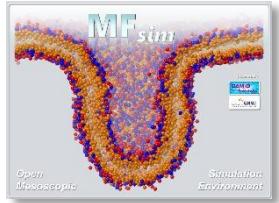
www.gnwi.de

GitHub repository:
<https://github.com/ziesny/MFsim>

Compartment Definition

Create and position a new *Water in* 2 layer at the bottom of the simulation box, a new *M2 in* layer (above), a new *M2 out* layer (above) and a new *Water out Buffer 2* layer (above) accordingly.





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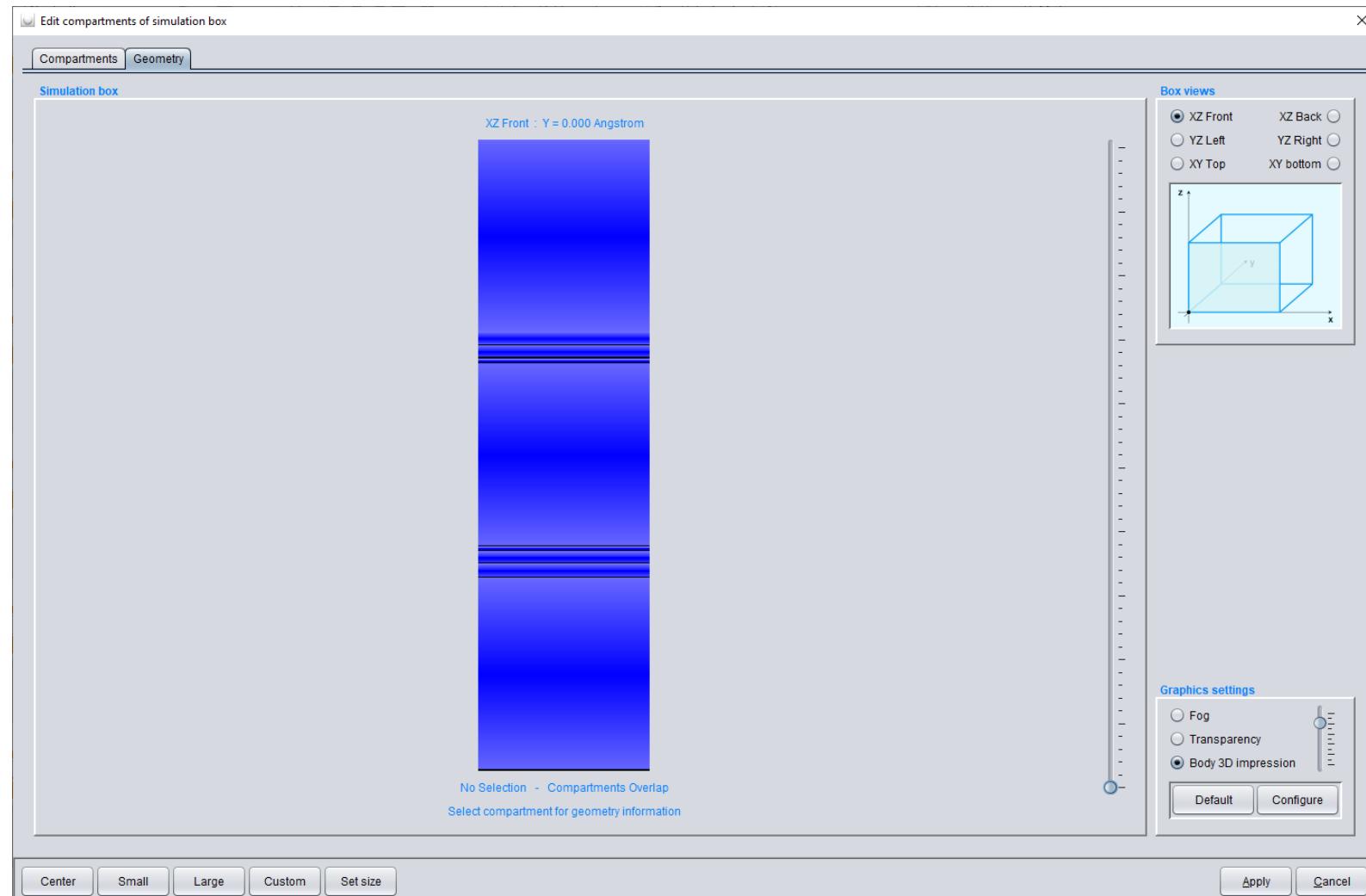


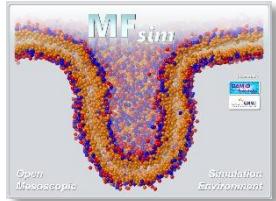
www.gnwi.de

GitHub repository:
<https://github.com/ziesny/MFsim>

Compartment Definition

Finally create a new *Water out + Cyclotides* layer with 93 % of *WaterOut* molecules and 100 % of KB1Y19 cyclotides which are positioned *3D random* by default, i.e. the cyclotides are located randomly rotated at random positions within the layer without overlap. Select the **Geometry** tab to view the new layer in the (default and intended) middle of the simulation box. Switch back to the **Compartments** tab ...





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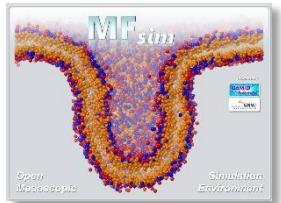


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Compartment Definition

... to control that all molecules have been assigned to compartments so that the **Bulk** volume is empty. **Apply** the compartment settings ...

Molecule name	Molecular structure	%	Quantity	Orientation
WaterIn1	H2O	0	0	Random
WaterOut	H2O	0	0	Random
WaterIn2	H2O	0	0	Random
CHOLin	MeOHcho[1]...	0	0	Random
CHOLout	MeOHcho[1]...	0	0	Random
DMPCin	TriMeNpp[IST ...	0	0	Random
DMPCout	TriMeNpp[IST ...	0	0	Random
DOPEin	MeNH2Ppl[STA ...	0	0	Random
DOPEout	MeNH2Ppl[STA ...	0	0	Random
PIP2in	DMPN[1](MeAc ...	0	0	Random
PIP2out	DMPN[1](MeAc ...	0	0	Random
PSin	HAcNpl[START ...	0	0	Random
SMin	TriMeNpp[ST ...	0	0	Random
SMout	TriMeNpp[ST ...	0	0	Random
KB1Y19	MeAcNHBB[4]...	0	0	3D random



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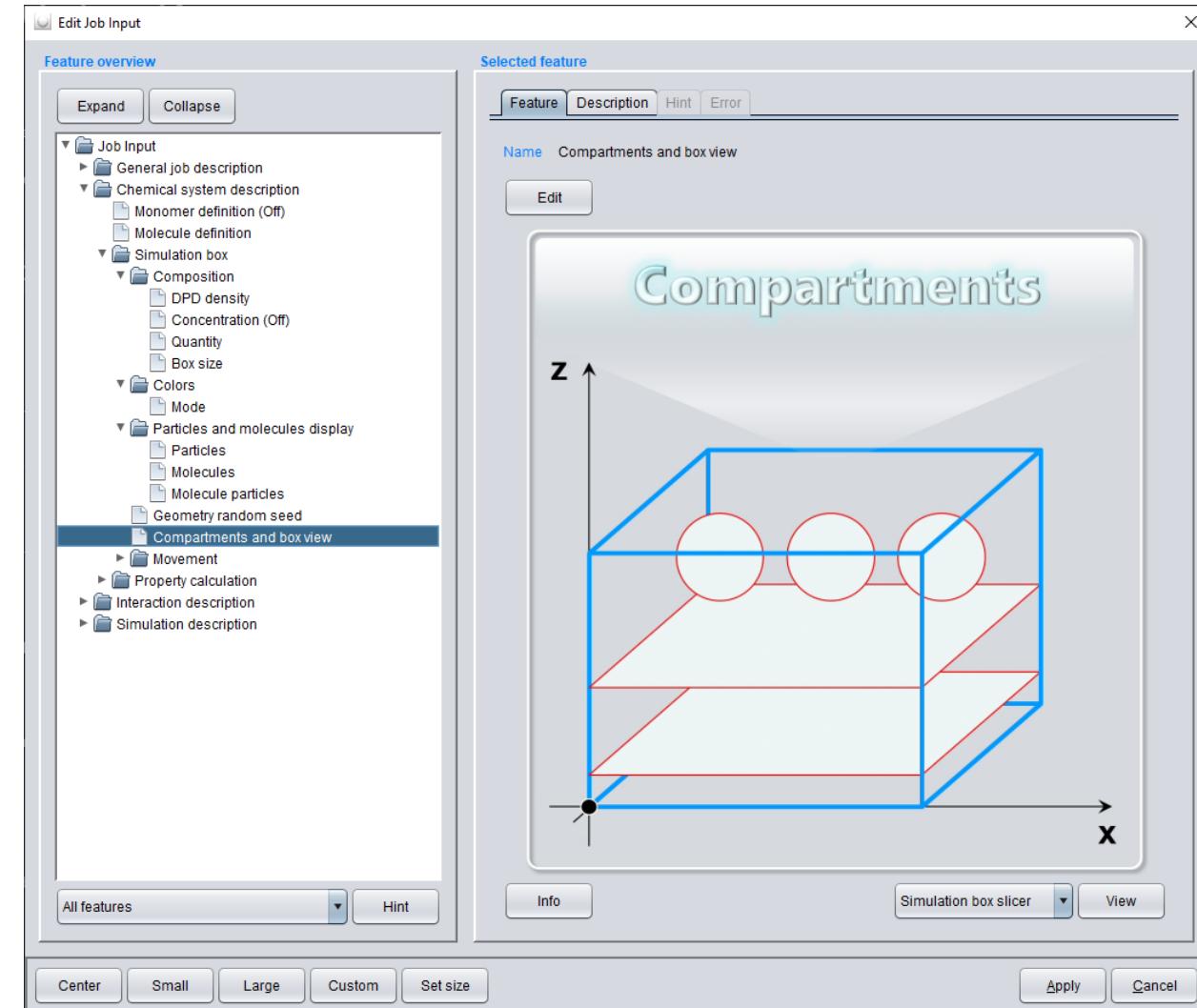
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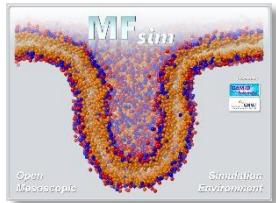


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Compartment Definition

... and press **View** ...



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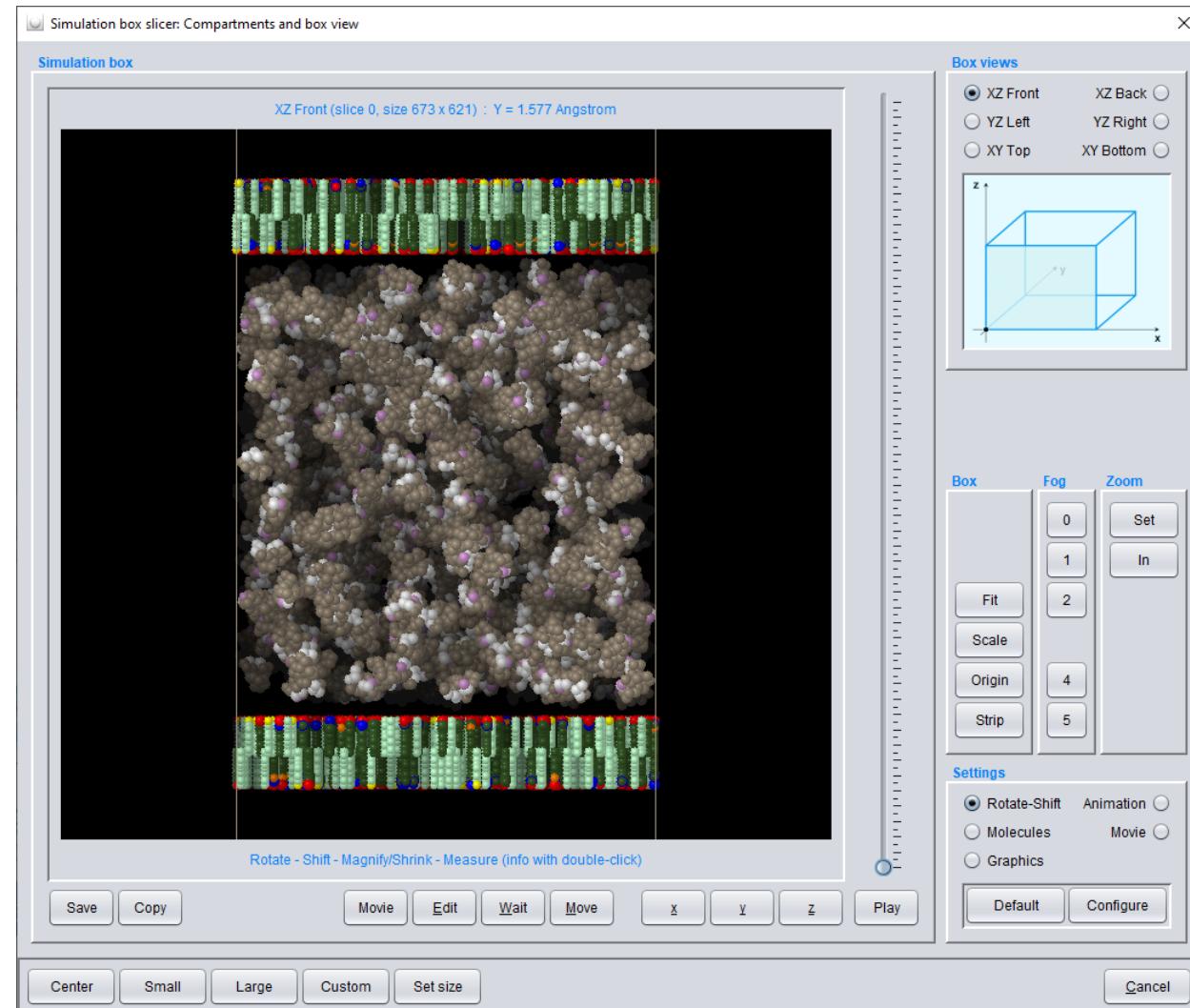
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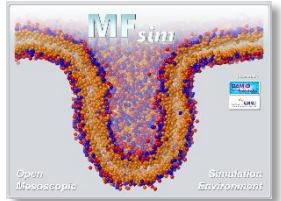


www.gnwi.de

Simulation box view

... to open the simulation box view dialog which allows for an inspection of the (correct) compartment assignment (note, that all water molecules and side chain particles of the cyclotides are excluded from display due to their particle display setting – the mutated amino acid of the cyclotide is shown in *PLUM*, the other “hydrophobic patch” amino acids in *WHITE*). **Cancel** the dialog.



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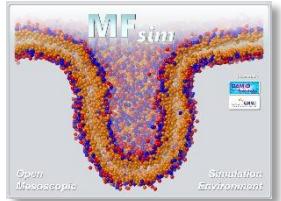
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Molecule Backbone Forces

Select **Job Input / Interaction Description** / **Molecules backbone forces** to define backbone forces (harmonic springs) between particles with corresponding backbone tags in the SPICES string for the stiffness of a molecule's backbone.

The screenshot shows the 'Edit Job Input' dialog box. On the left, the 'Feature overview' tree view is expanded, showing 'Job Input' and 'Interaction description'. Under 'Interaction description', 'Molecule backbone forces' is selected and highlighted in blue. On the right, the 'Selected feature' panel displays the configuration for 'Molecule backbone forces'. The table has columns: Name, Attribute 1, Attribute 2, Distance [Å], Distance [DPD], k(BB), and Behaviour. A single row is present for 'CHOLin' with values: Attribute 1=1, Attribute 2=2, Distance [Å]=0, Distance [DPD]=0, k(BB)=0, and Behaviour=DEFAULT. Below the table are buttons for Set, Insert, Copy, and Apply/Cancel.

Feature	Description	Hint	Error			
Name Molecule backbone forces						
CHOLin	1	2	0	0	0	DEFAULT

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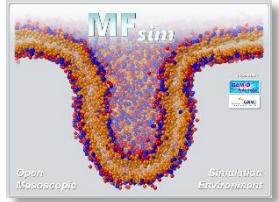
Molecule Backbone Forces

For the default *CHOLin* molecule change the **Distance [A]** to 8.73 Angstrom and force constant **k(BB)** to 4. Hit **Insert** to add a new line and change the **Molecule name** to *CHOLout*. Again change the **Distance [A]** to 8.73 Angstrom and force constant **k(BB)** to 4.

The screenshot shows the 'Edit Job Input' dialog box with the 'Selected feature' tab selected. The 'Name' field is set to 'Molecule backbone forces'. The table below lists two entries:

Molecule name	Attribute 1	Attribute 2	Distance [A]	Distance [DPD]	k(BB)	Behaviour
CHOLin	1	2	8.73	1.839798	4	DEFAULT
CHOLout	1	2	8.73	1.839798	4	DEFAULT

Buttons at the bottom include 'Set', 'Remove', 'Insert', 'Copy', 'Table-data schema' (with 'New' button), and 'Apply'/'Cancel'.

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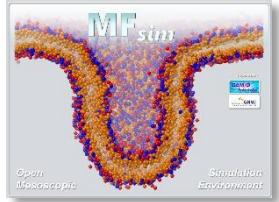


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Protein Distance Forces

Select **Job Input / Interaction Description / Protein distance forces** to set the backbone distance force constants $k(\text{BB})$ for all possible harmonic backbone springs to control the stiffness of the protein backbone. Hit the **Set** button for bulk settings ...

Distances 1-i, i = ...	KB1Y19 - k(BB)
2	0
3	0
4	0
5	0
6	0
7	0
8	0
9	0
10	0
11	0
12	0
13	0
14	0
15	0
16	0
17	0



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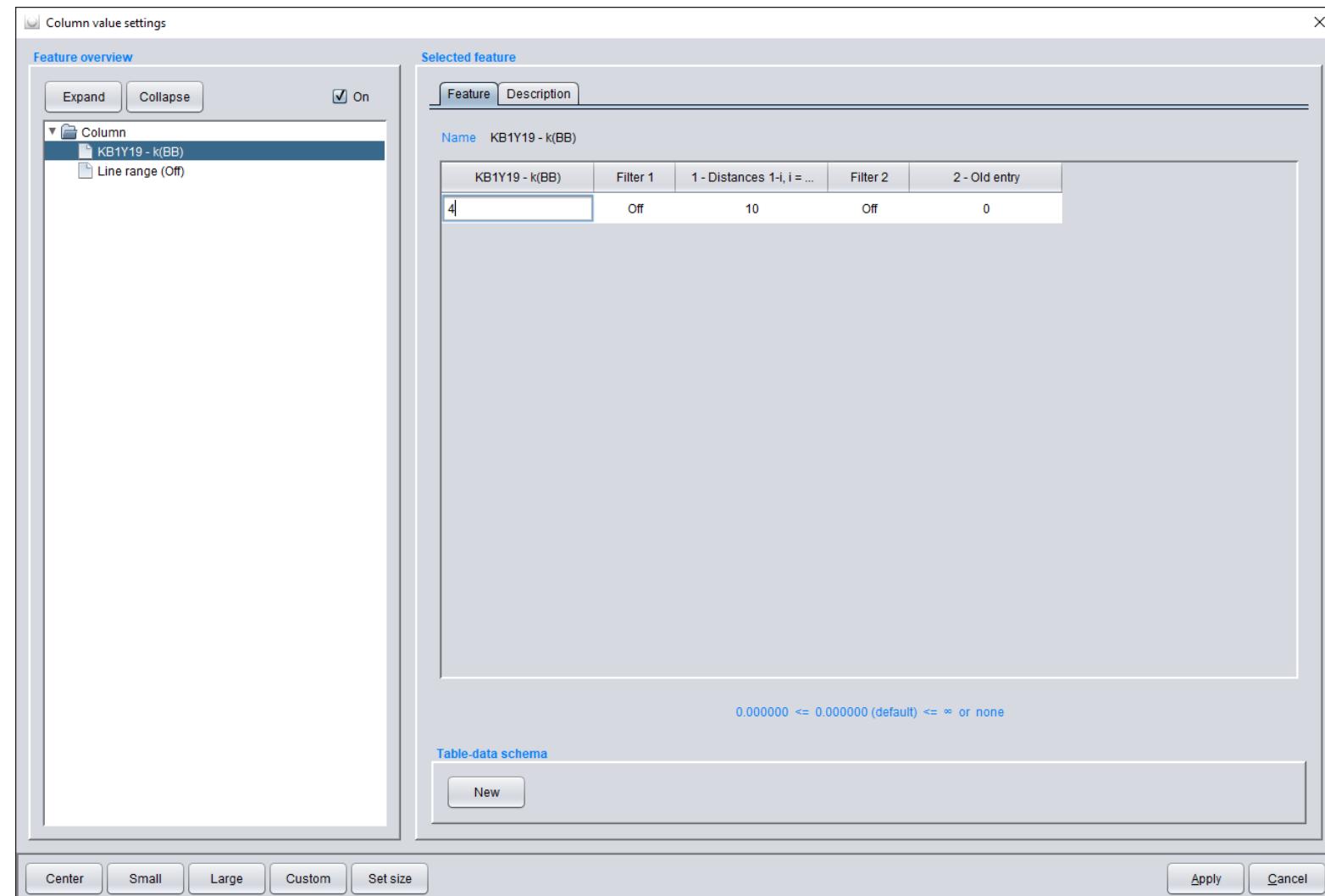
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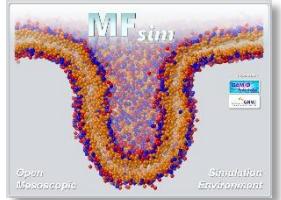


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Protein Distance Forces

... select the (by default disabled) **KB1Y19 – k(BB)** setting and enable this setting by ticking the On checkbox. Change the **KB1Y19 – k(BB)** value to 4. Confirm the entry with **Apply** ...





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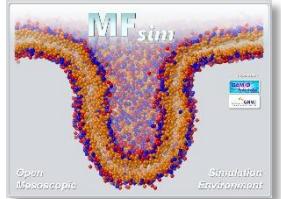
www.gnwi.de

GitHub repository:
<https://github.com/zieseny/MFsim>

Protein Distance Forces

... to set all $KB1Y19 - k(BB)$ values to 4.

Distances 1-i, i = ...	KB1Y19 - k(BB)
2	4
3	4
4	4
5	4
6	4
7	4
8	4
9	4
10	4
11	4
12	4
13	4
14	4
15	4
16	4
17	4



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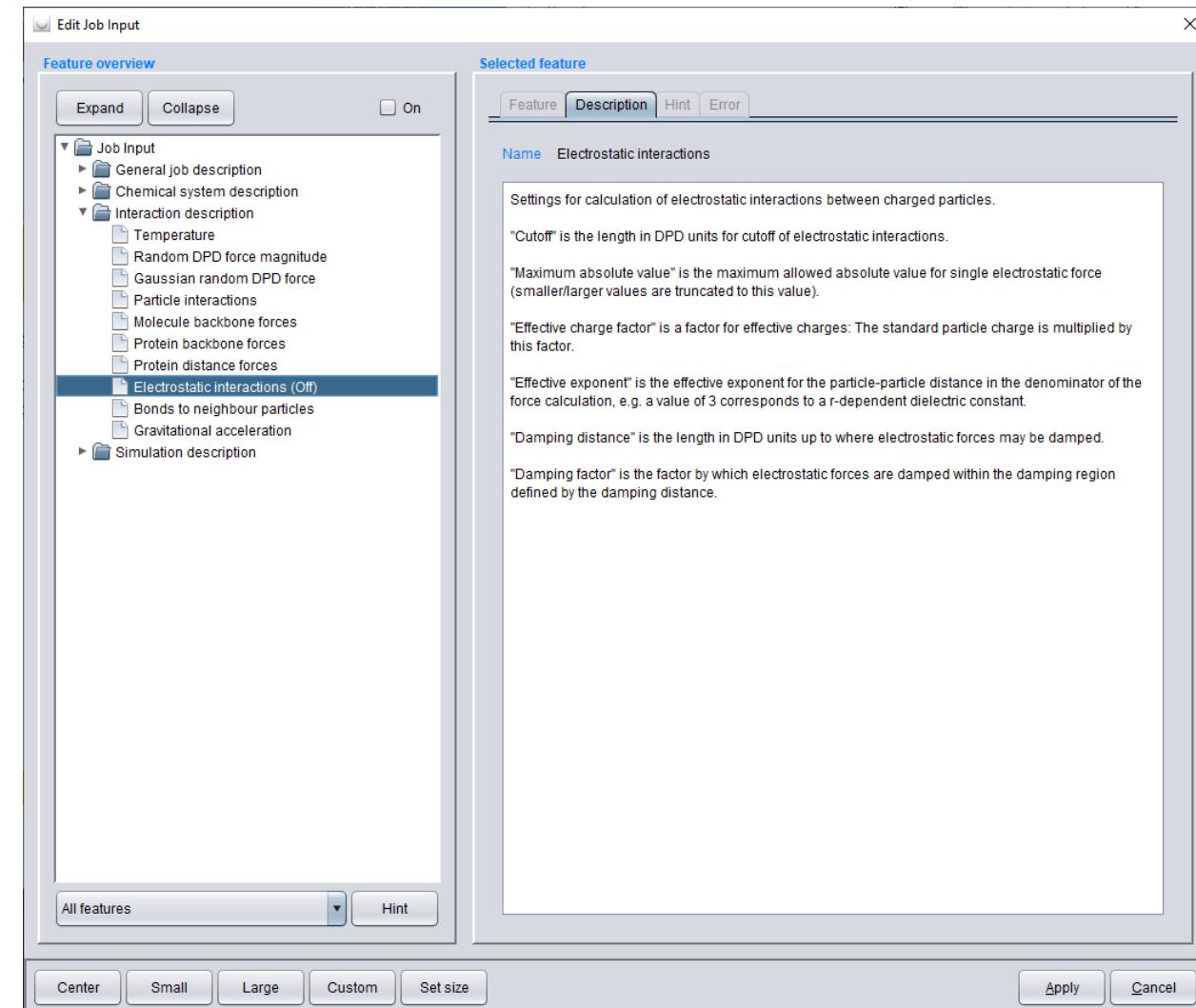
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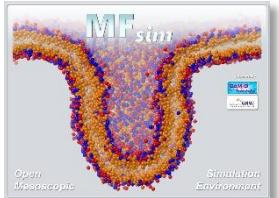
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Electrostatic Interactions

Select disabled **Job Input / Interaction Description / Electrostatic interactions ...**



Electrostatic Interactions



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... and enable by ticking the On checkbox. Do not change the default settings.

Name	Electrostatic interactions
Cutoff	5
Maximum absolute value	25
Effective charge factor	1
Effective exponent	

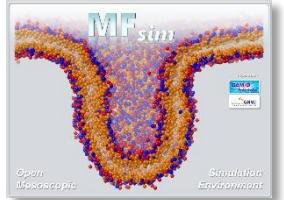
Click on table cell to edit

Table-data schema

New

All features Hint

Center Small Large Custom Set size Apply Cancel



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Simulation Steps

Select **Job Input / Simulation description / Simulation steps ...**

Edit Job Input

Feature overview

Expand Collapse

Job Input

- General job description
- Chemical system description
- Interaction description
- Simulation description

Selected feature

Feature Description Hint Error

Name Simulation steps

Number of steps	Single step [ns]	Full simulation [ns]
1000	0.049	48.753

All features

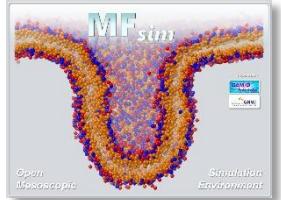
Center Small Large Custom Set size

Click on table cell to edit

Table-data schema

New

Apply Cancel



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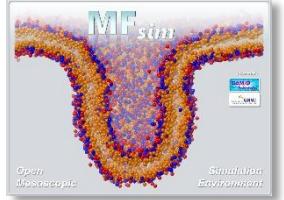
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Simulation Steps

... and change the **Number of steps** to 125000.

The screenshot shows the 'Edit Job Input' dialog box. On the left, the 'Feature overview' tree is expanded, showing 'Job Input' with 'General job description', 'Chemical system description', 'Interaction description', and 'Simulation description'. 'Simulation description' is further expanded to show 'Simulation steps' and other parameters like 'Time step length', 'Output frequency', etc. A blue bar highlights 'Simulation steps'. On the right, the 'Selected feature' panel shows a table for 'Simulation steps'. The table has three columns: 'Number of steps', 'Single step [ns]', and 'Full simulation [ns]'. The values are 125000, 0.049, and 6094.115 respectively. Below the table, a note says 'Click on table cell to edit'. At the bottom of the dialog are buttons for 'All features', 'Center', 'Small', 'Large', 'Custom', 'Set size', 'Apply', and 'Cancel'.

Name	Simulation steps
Number of steps	125000
Single step [ns]	0.049
Full simulation [ns]	6094.115



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Integration Type

Select **Job Input / Simulation description / Integration type ...**

MFsim 2.3.0.0

Open Mesoscopic Simulation Environment

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GitHub repository:
<https://github.com/ziesensy/MFsim>

Integration Type

Selected feature

Name: Integration type

Type	Parameter 1	Parameter 2
GWMVV	0.65	none

All features

Center Small Large Custom Set size Cancel

Click on table cell to edit

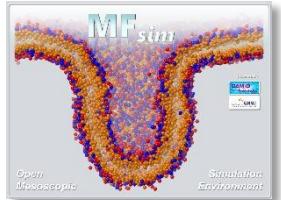
Table-data schema

New

Integration Type

Job Input

- General job description
- Chemical system description
- Interaction description
- Simulation description
 - Simulation steps
 - Time step length
 - Output frequency
 - Integration type
 - Initial minimization steps
 - Minimization step output
 - Periodic boundaries
 - DPD unit mass
 - Initial velocity scaling steps
 - Random number generator



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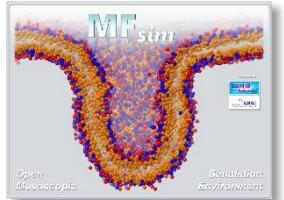


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Integration Type

... and change **Type** to **S1MVV** (with **Parameter 1** being *true*).

Feature	Description	Hint	Error
Name	Integration type		
Type	S1MVV	true	none



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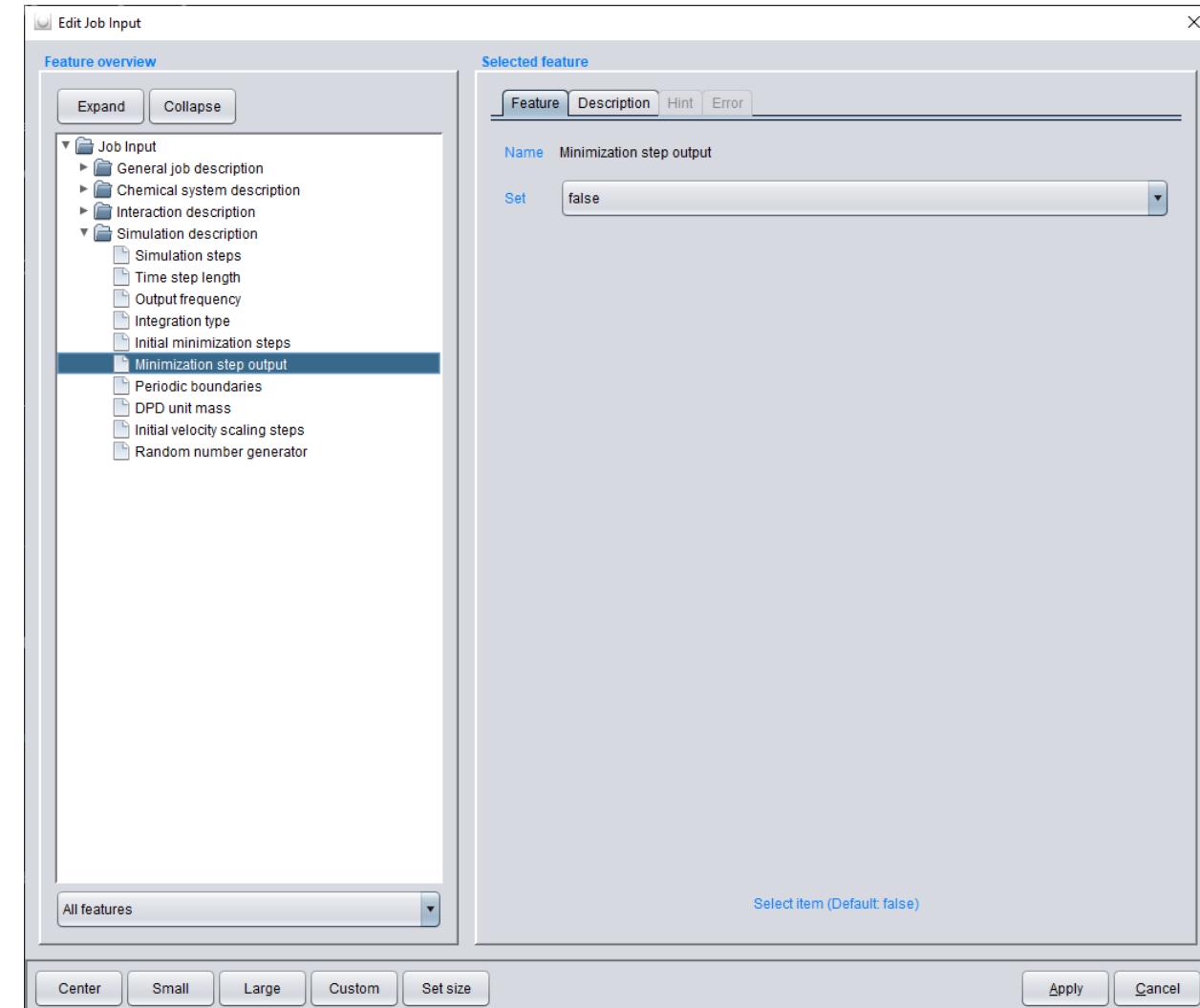
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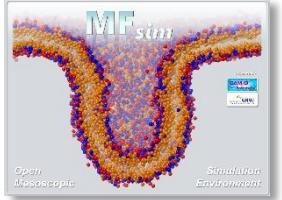


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Minimization Step Output

Select **Job Input / Simulation description / Minimization step output ...**





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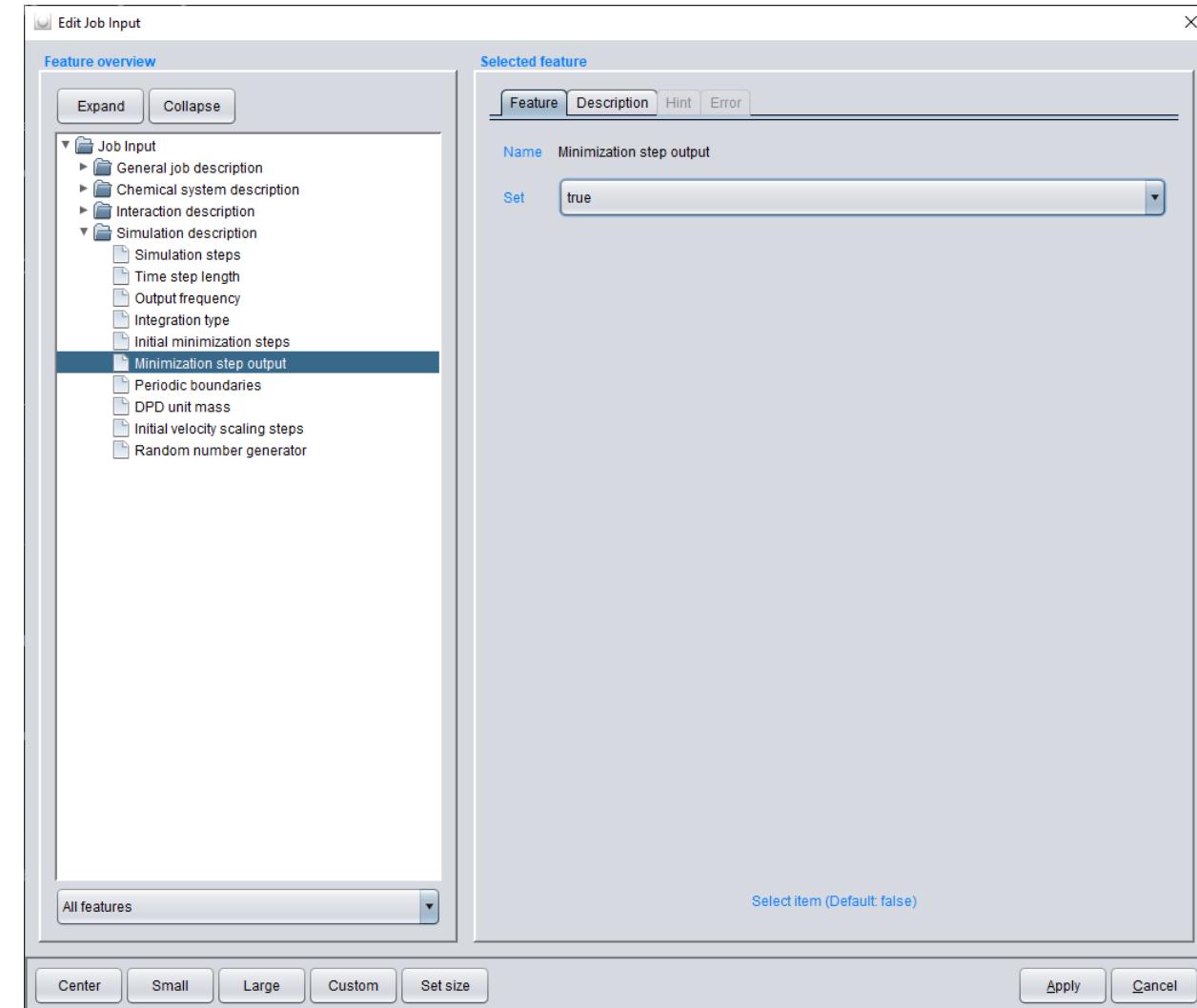
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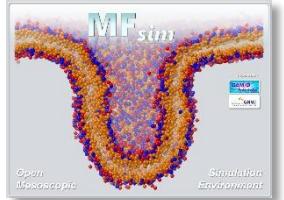


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Minimization Step Output

... and change to *true*.





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Periodic Boundaries

Select **Job Input / Simulation description / Periodic boundaries ...**

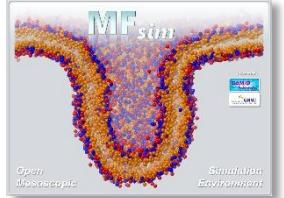
The screenshot shows the 'Edit Job Input' dialog box. On the left, the 'Feature overview' tree is expanded to show 'Job Input', 'Chemical system description', 'Interaction description', and 'Simulation description'. Under 'Simulation description', 'Periodic boundaries' is selected and highlighted in blue. On the right, the 'Selected feature' panel shows a table for 'Periodic boundaries' with columns for 'Name', 'x', 'y', and 'z'. The table contains the values 'true', 'true', and 'true' respectively. Below the table, there is a note: 'Click on table cell to edit'. At the bottom of the dialog, there are buttons for 'All features', 'Center', 'Small', 'Large', 'Custom', 'Set size', 'Apply', and 'Cancel'.

Name	x	y	z
Periodic boundaries	true	true	true

Click on table cell to edit

All features

Center Small Large Custom Set size Apply Cancel



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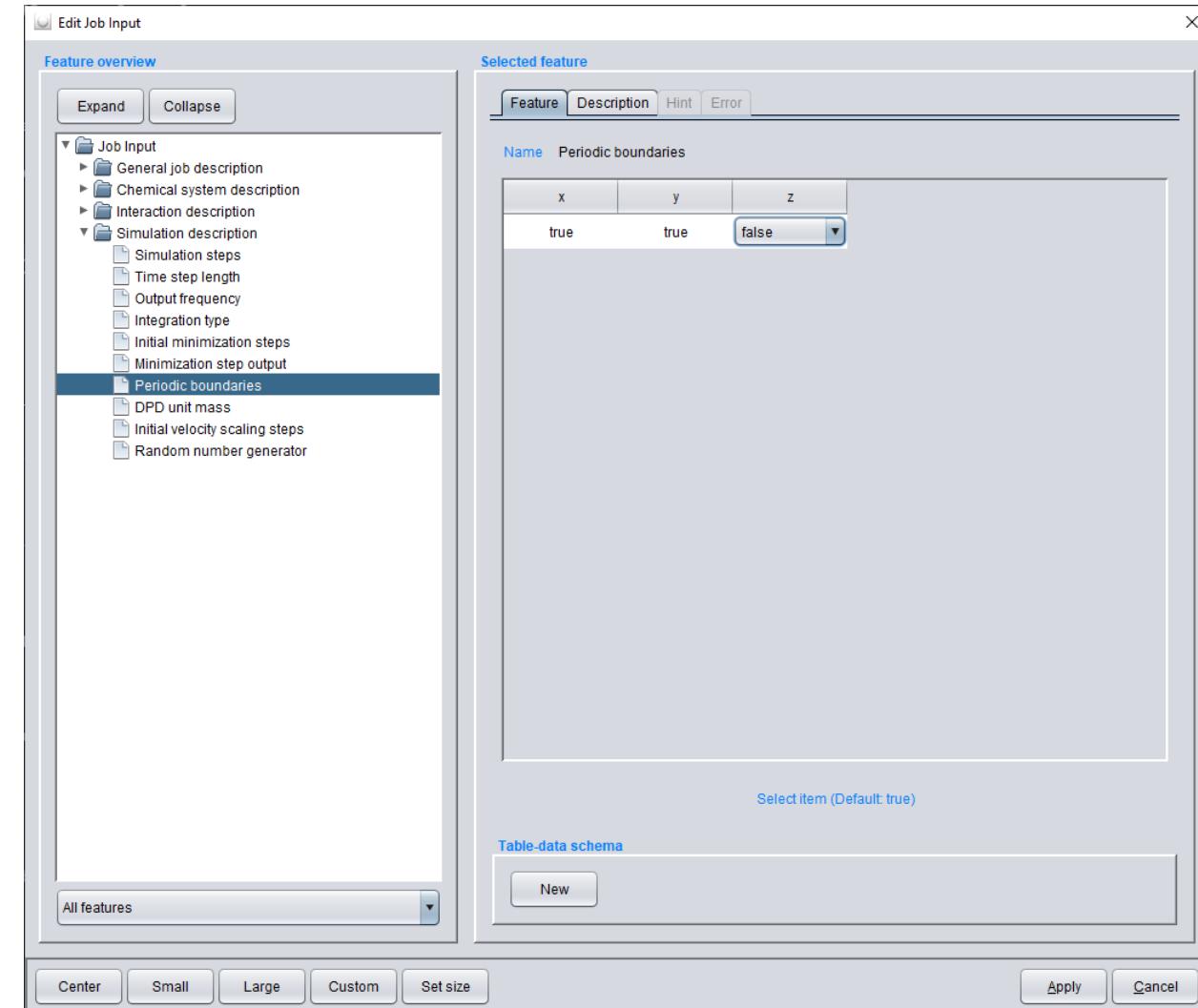
www.molecular-dynamics.de

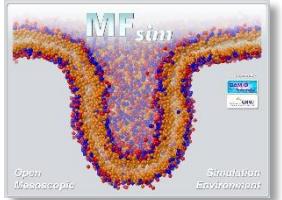


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Periodic Boundaries

... and change **Periodic boundaries** for the z axis to *false*.





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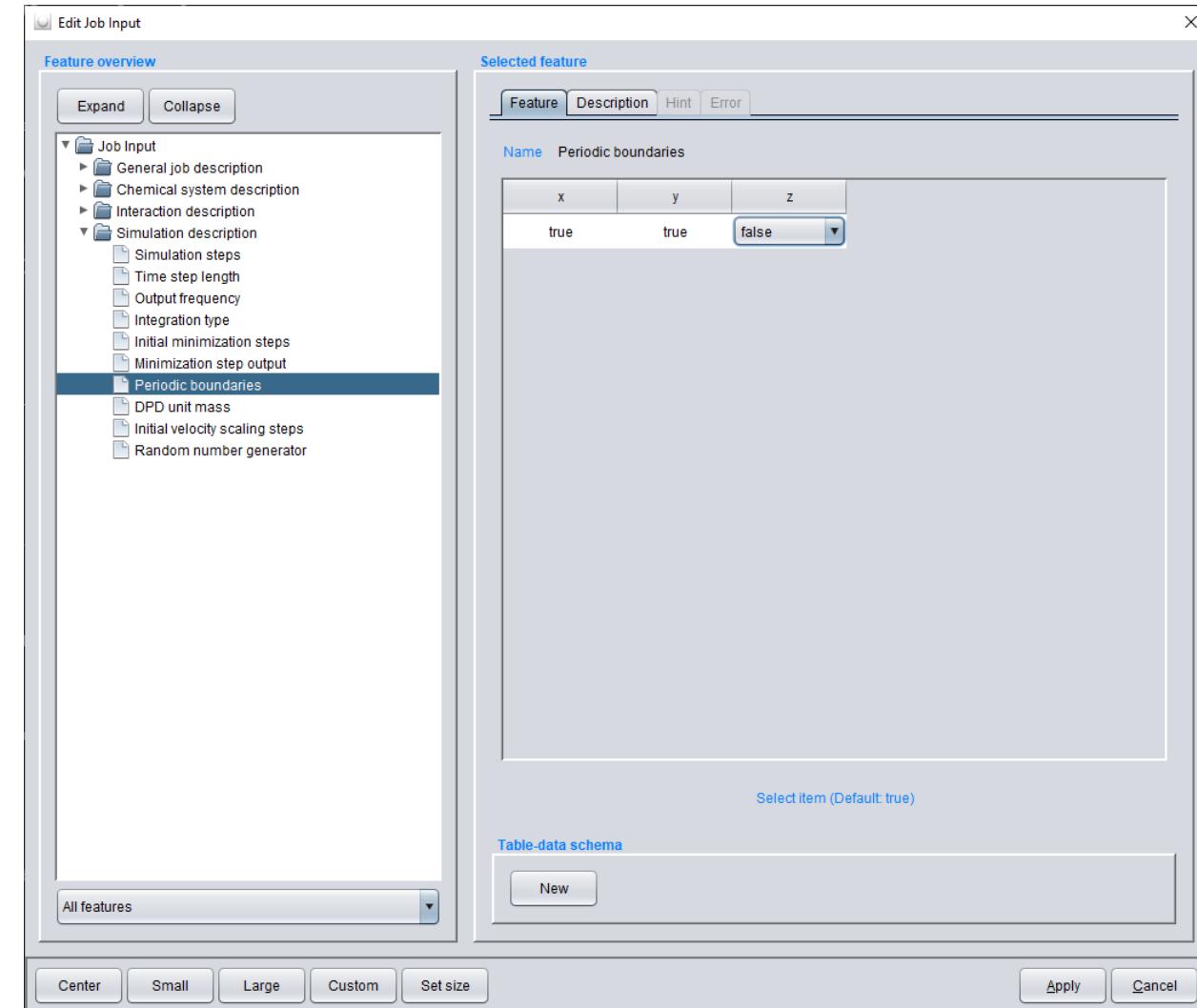


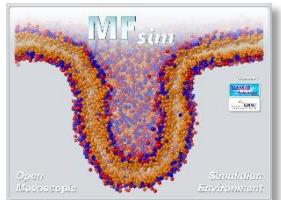
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New Job Input

Finally confirm all job input settings with **Apply**

...





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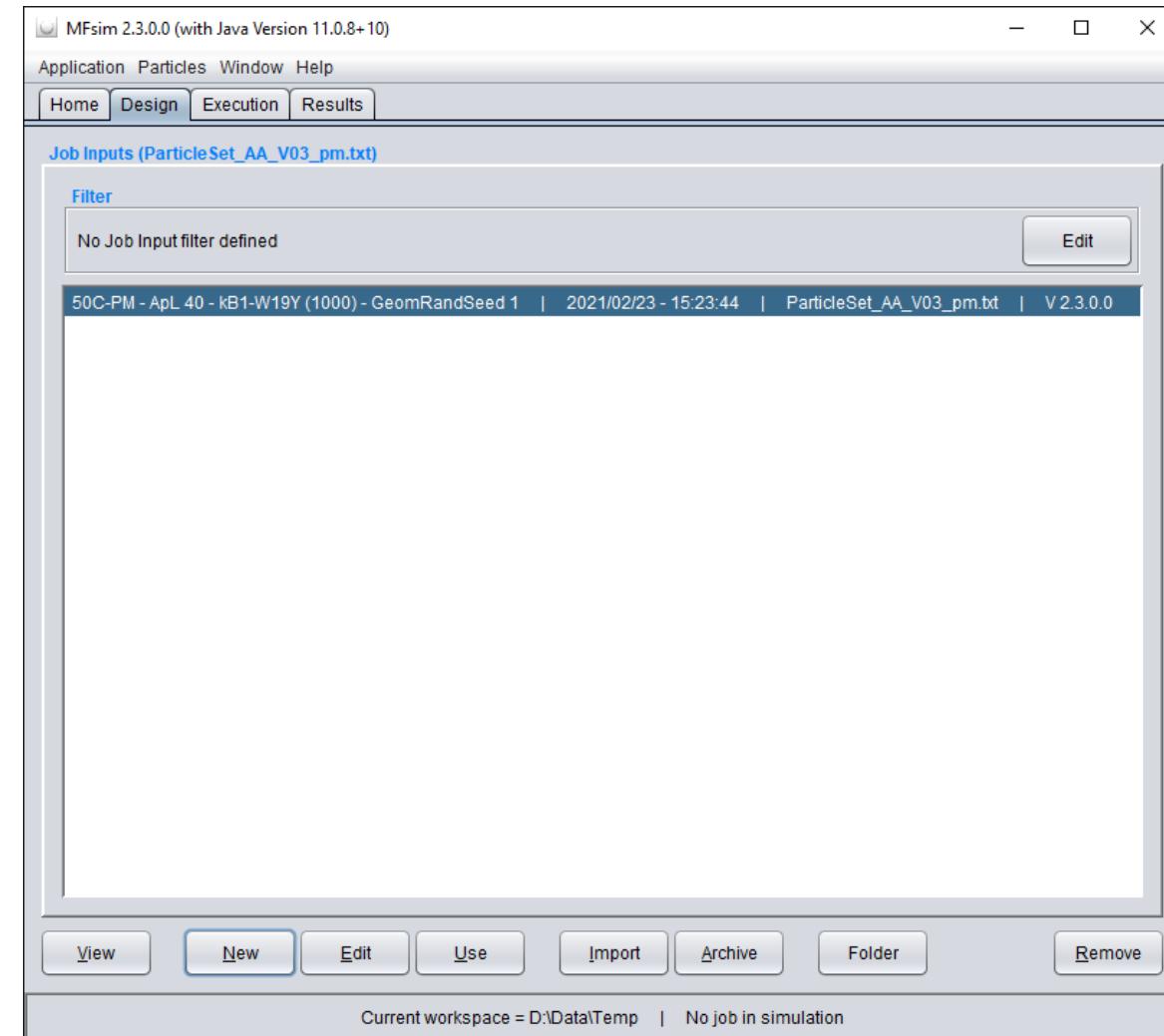
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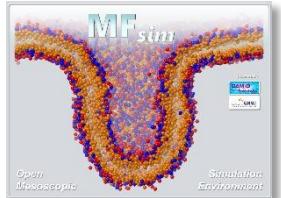


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New Job Input

... so that the new Job Input appears in the **Job Inputs** list.





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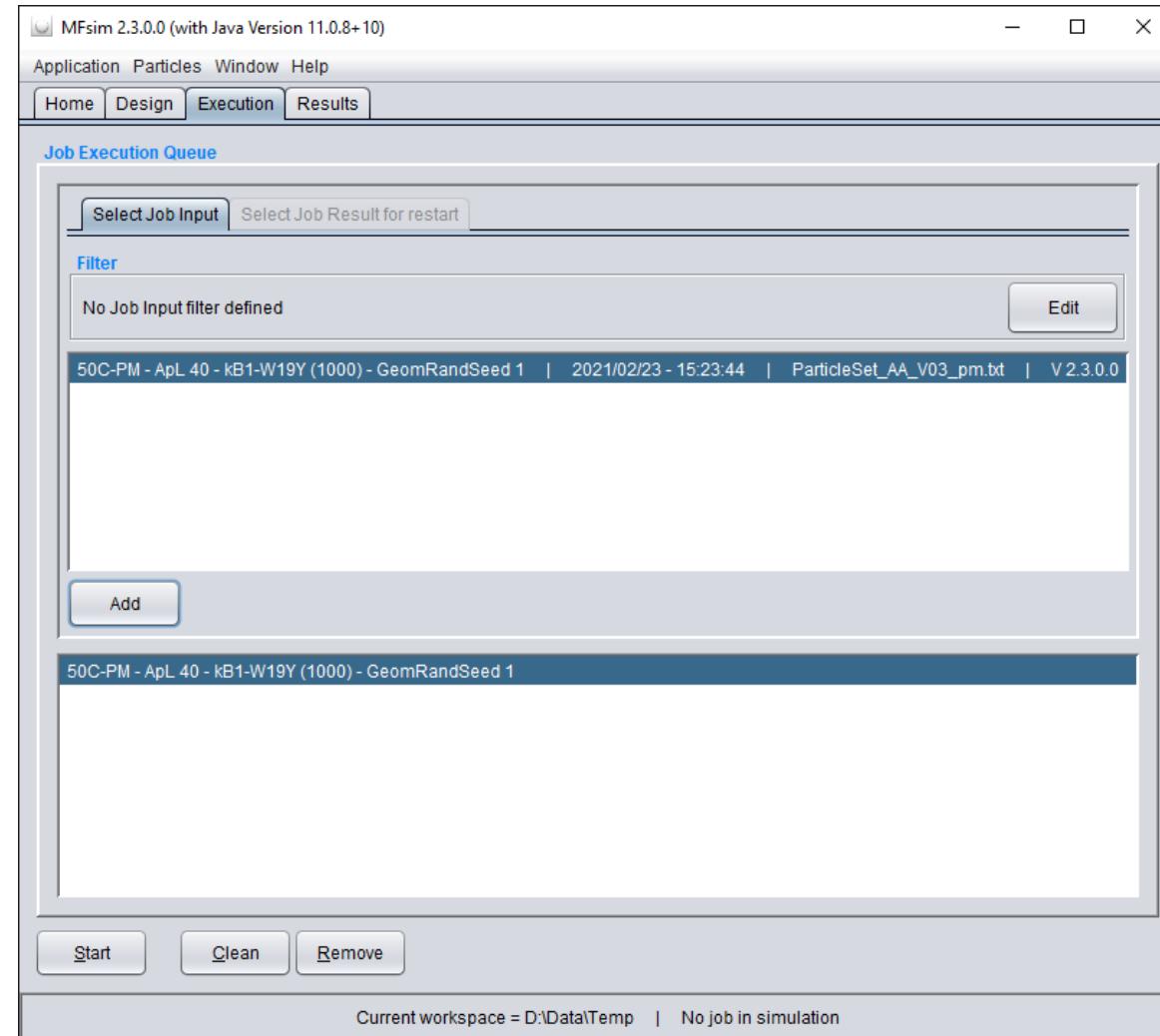
www.molecular-dynamics.de

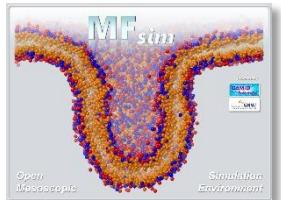


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Job Execution

Execute the new job (details are not covered by this tutorial).





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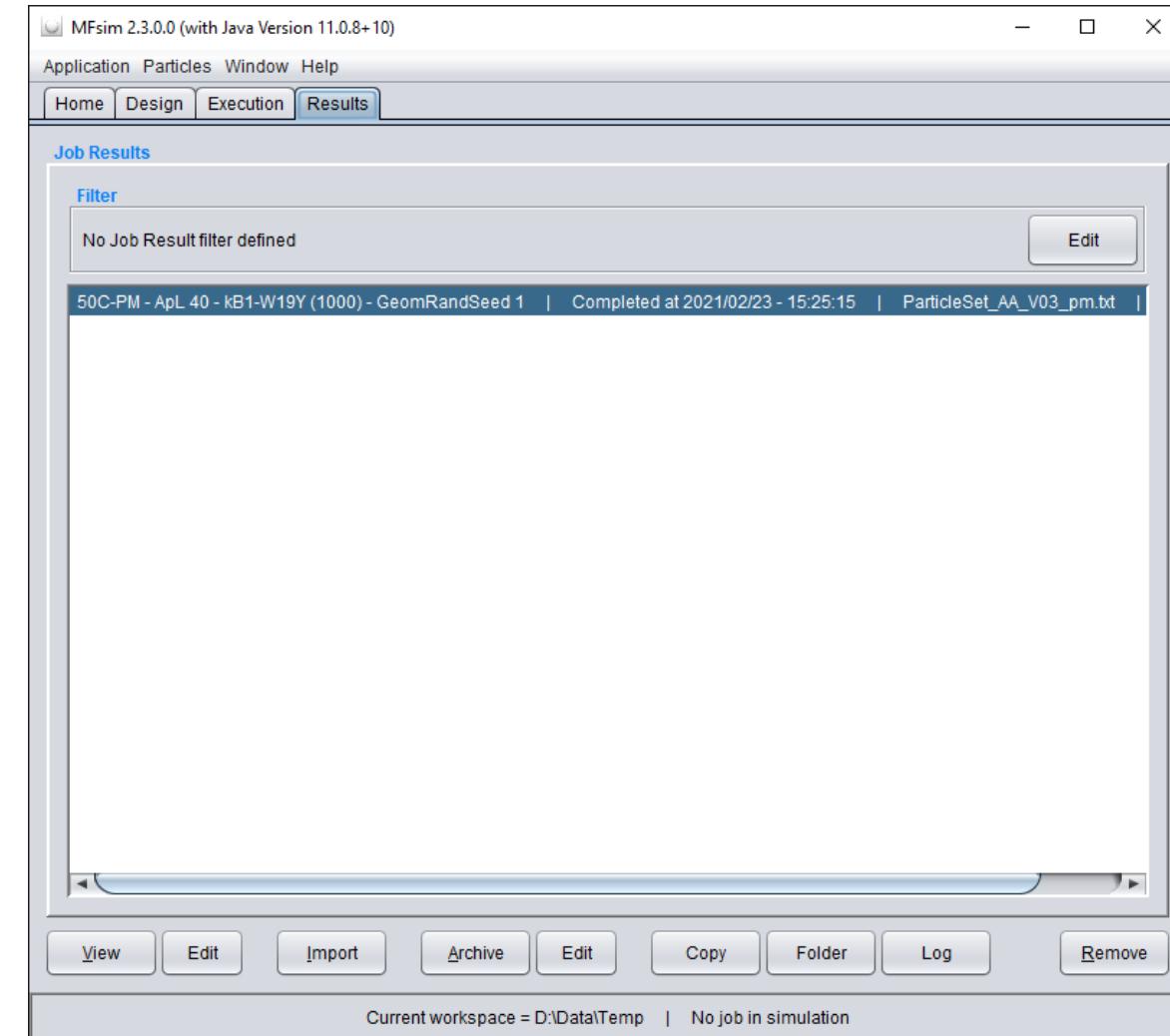


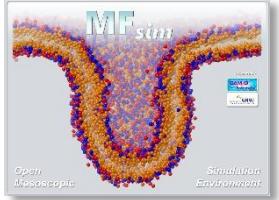
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Job Result Evaluation

The successfully executed job generates a job result on the **Results** tab. Hit the **View** button

...





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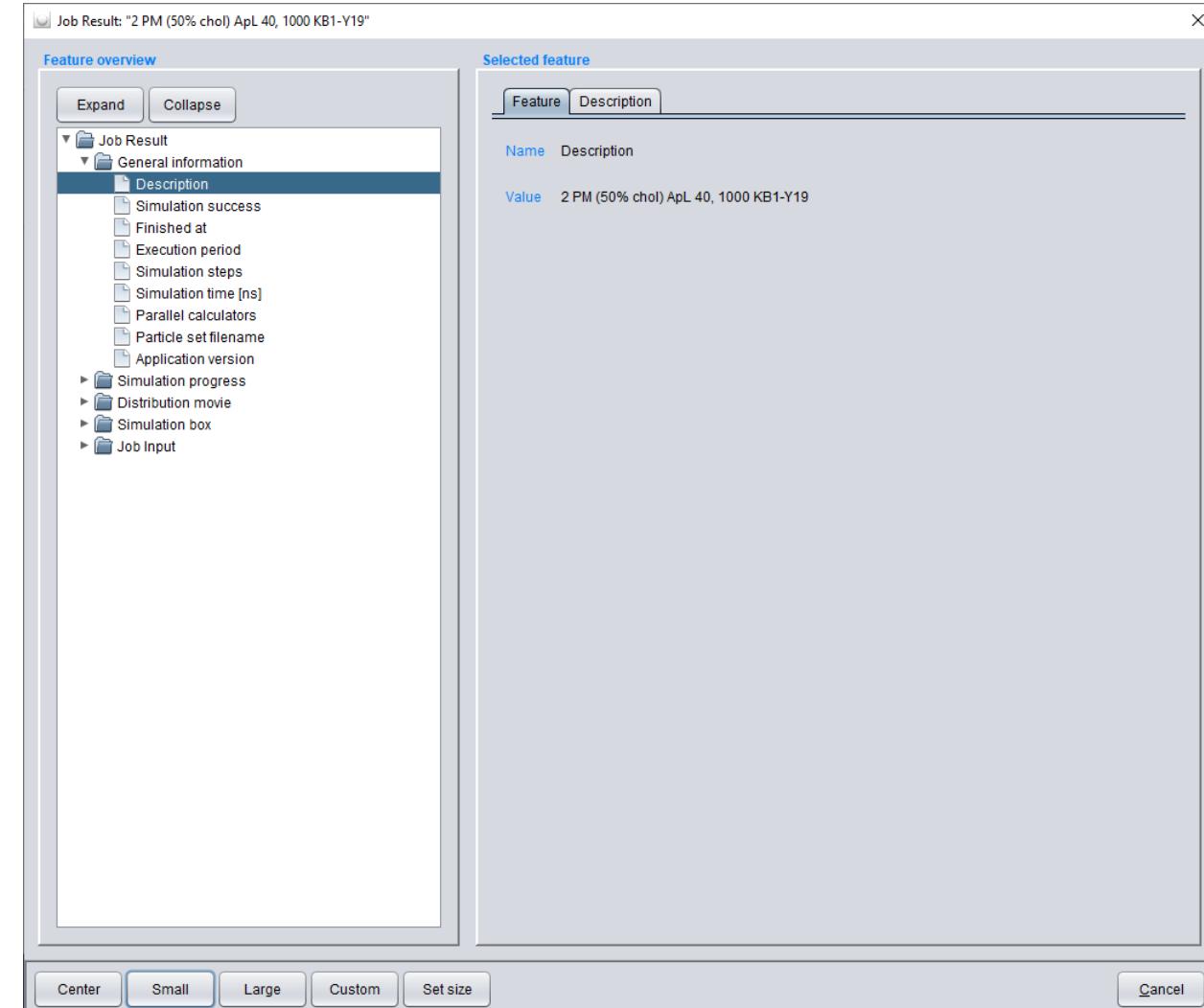
www.molecular-dynamics.de

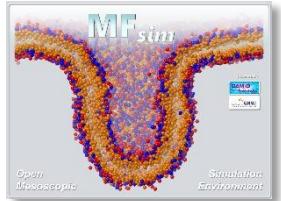


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Job Result Evaluation

... to inspect the simulation results.





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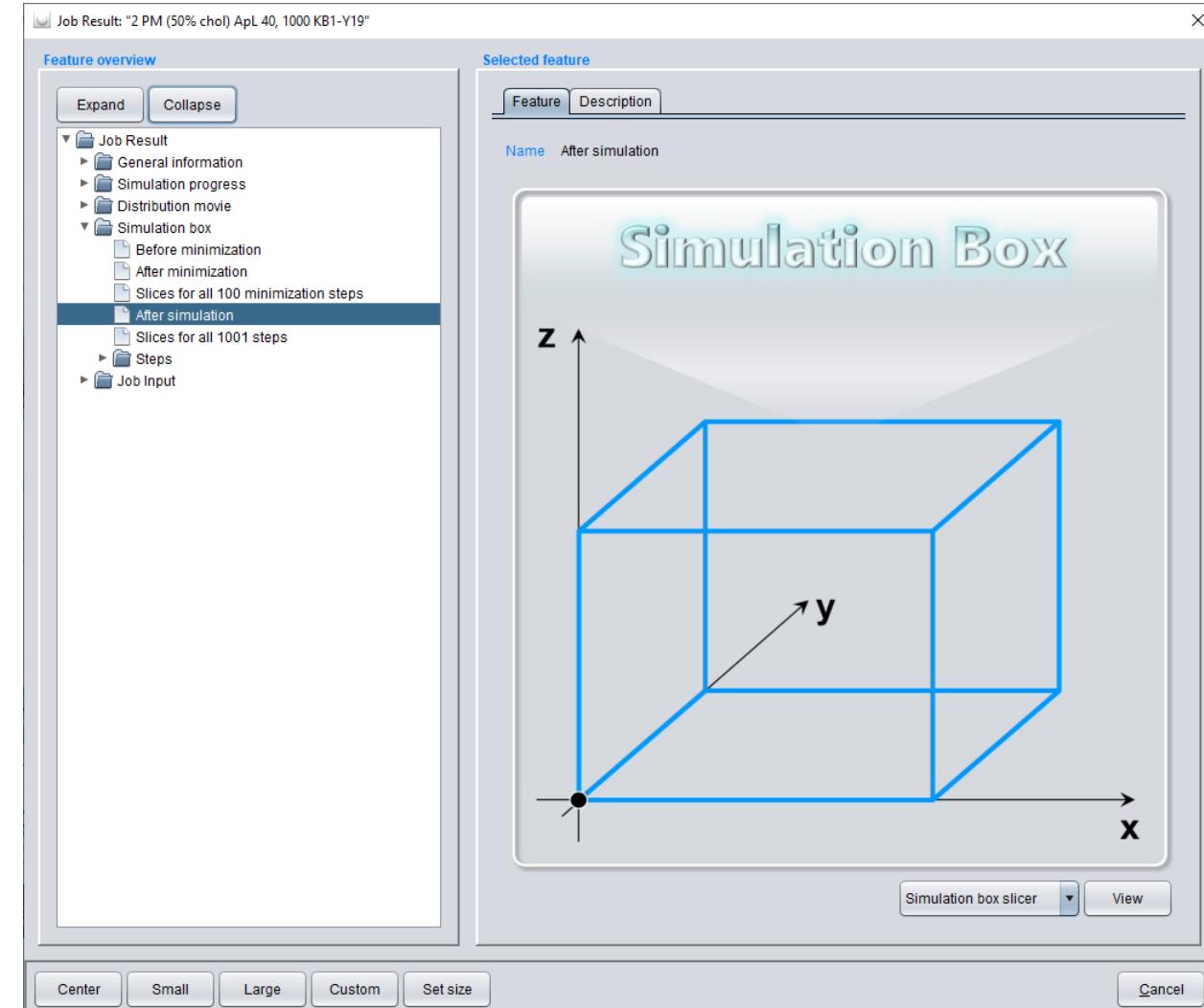
www.molecular-dynamics.de

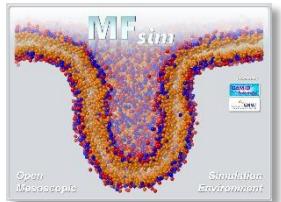


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Job Result Evaluation

Select **Job Result / Simulation box / After simulation** and hit the **View** button ...





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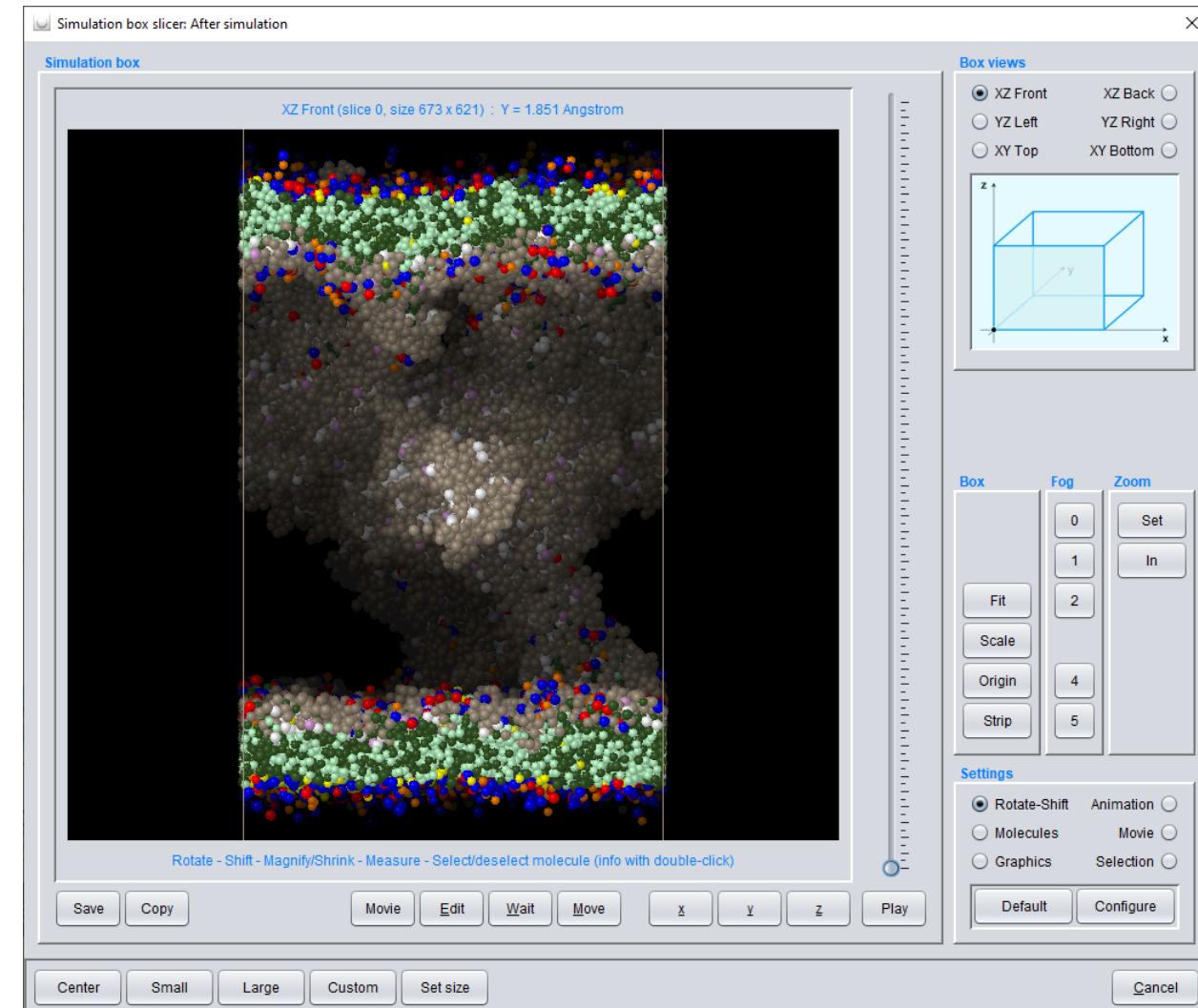
www.molecular-dynamics.de

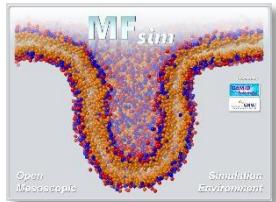


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Job Result Evaluation

... to open the simulation box view dialog for the last simulation step. Hit the **Set** button of the **Zoom** quick settings panel ...





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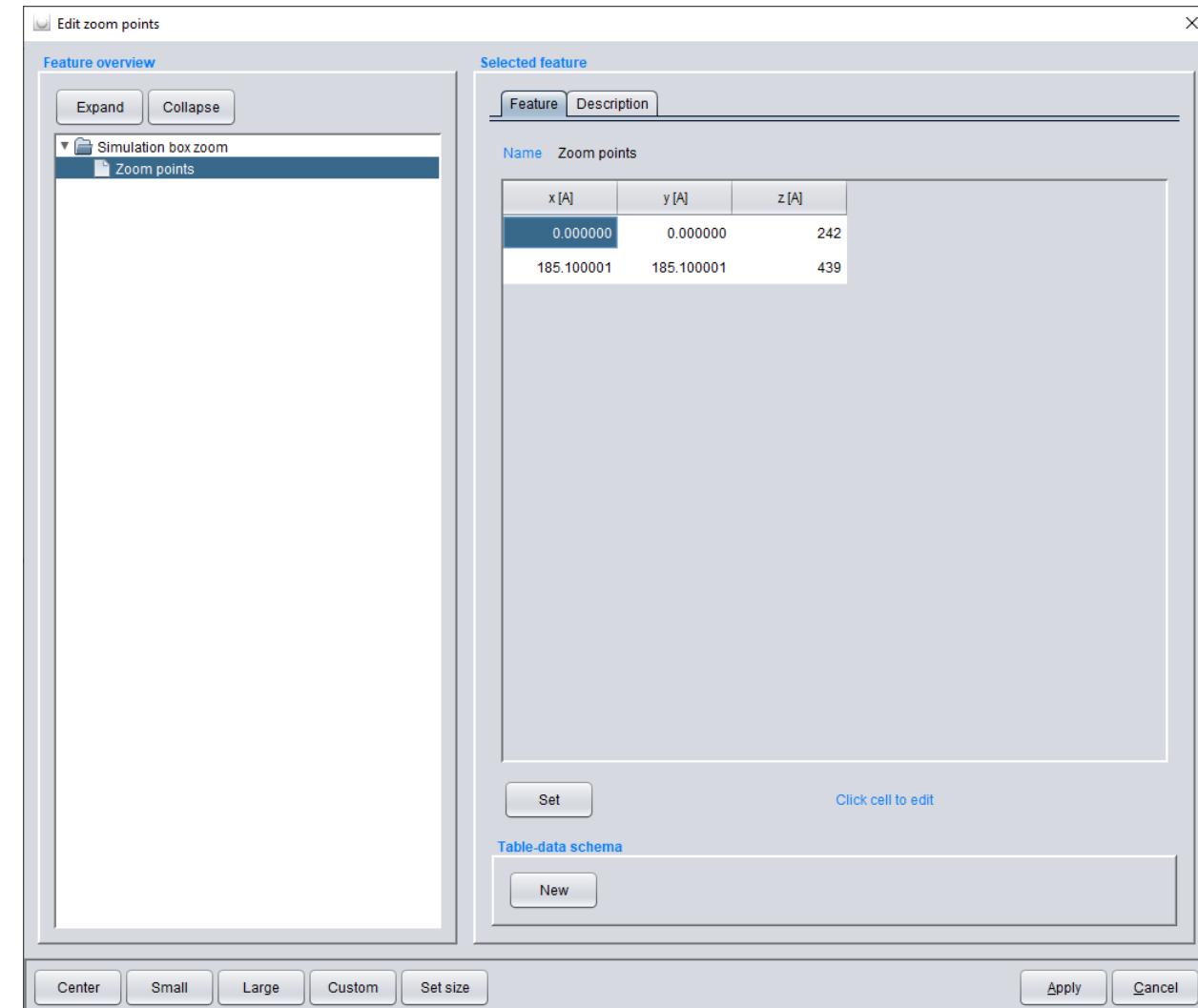
www.molecular-dynamics.de

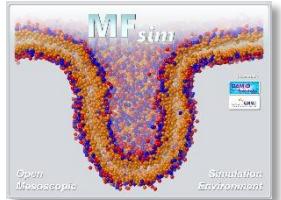


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Job Result Evaluation

... to zoom into the cyclotide/water compartment by changing **z [Å]** from 242 to 439 Angstrom (these boundaries are to be derived from the corresponding compartment settings). Confirm with **Apply**.





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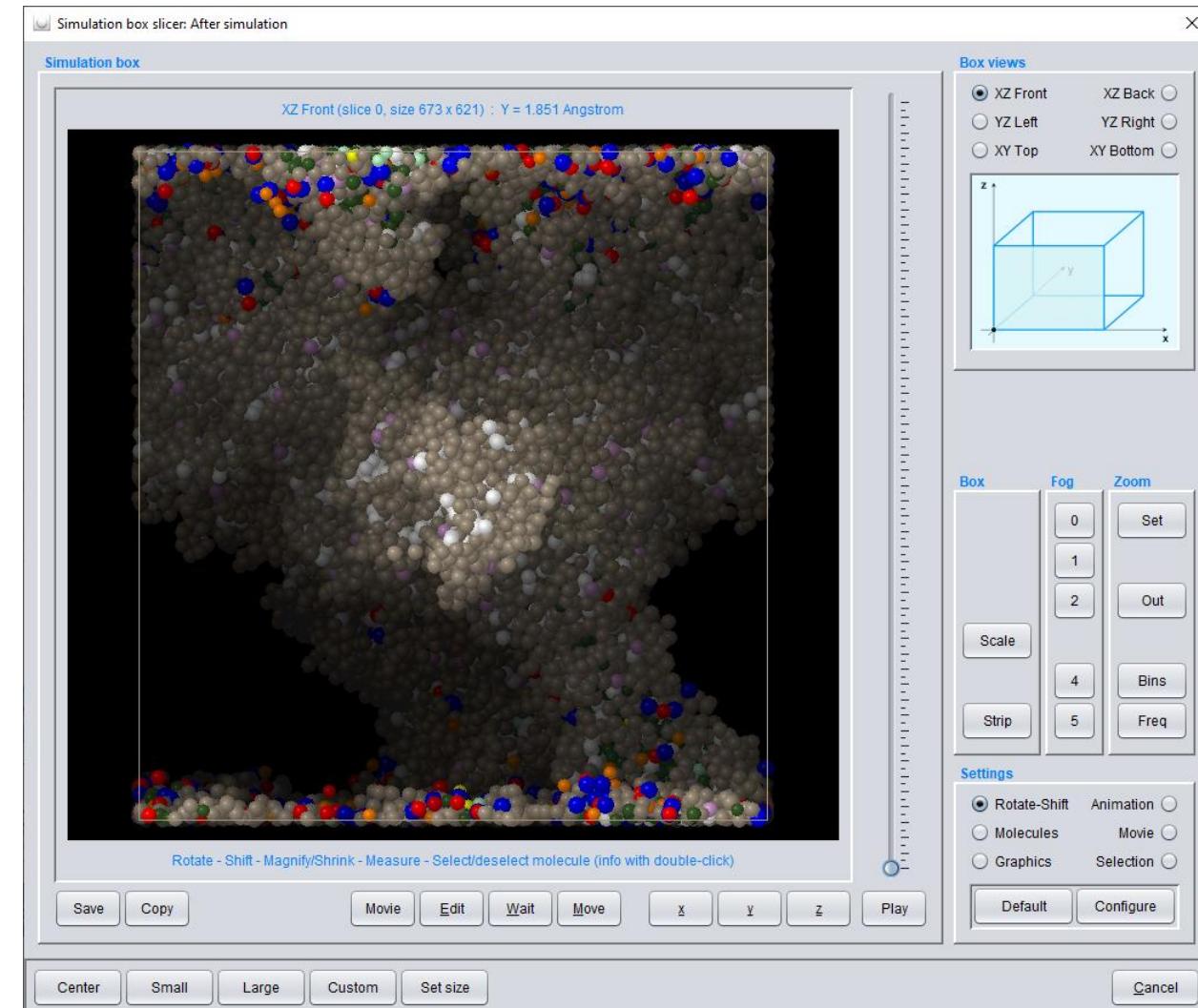
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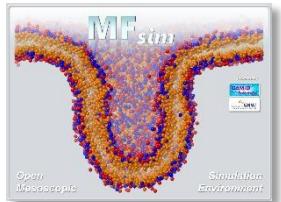


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Job Result Evaluation

Hit the **Bins** button of the **Zoom** quick settings panel ...





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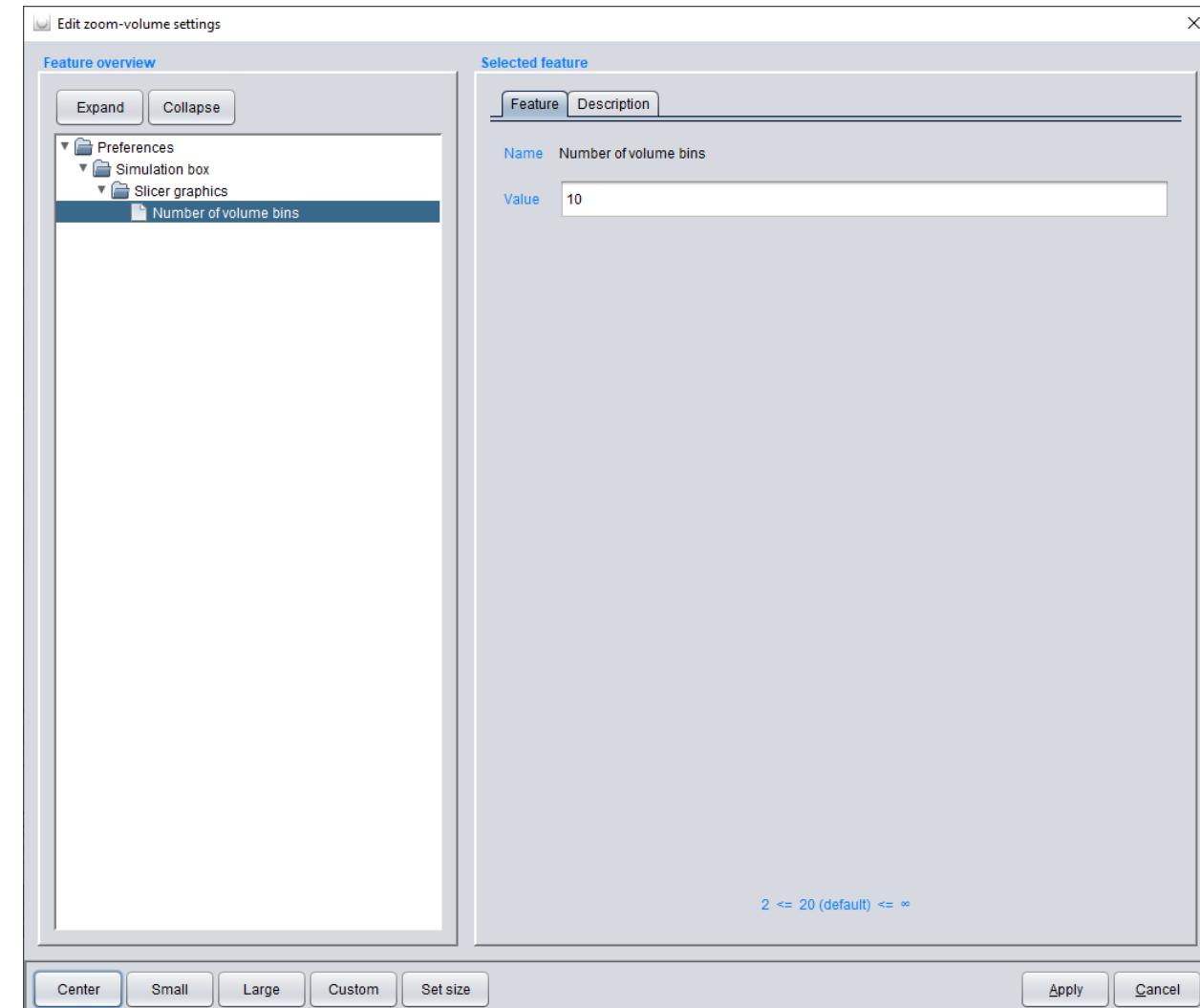
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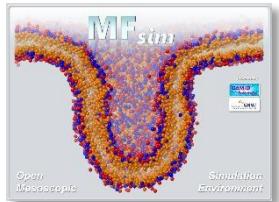


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Job Result Evaluation

... and change the **Number of volume bins** to 10. Confirm with **Apply**.





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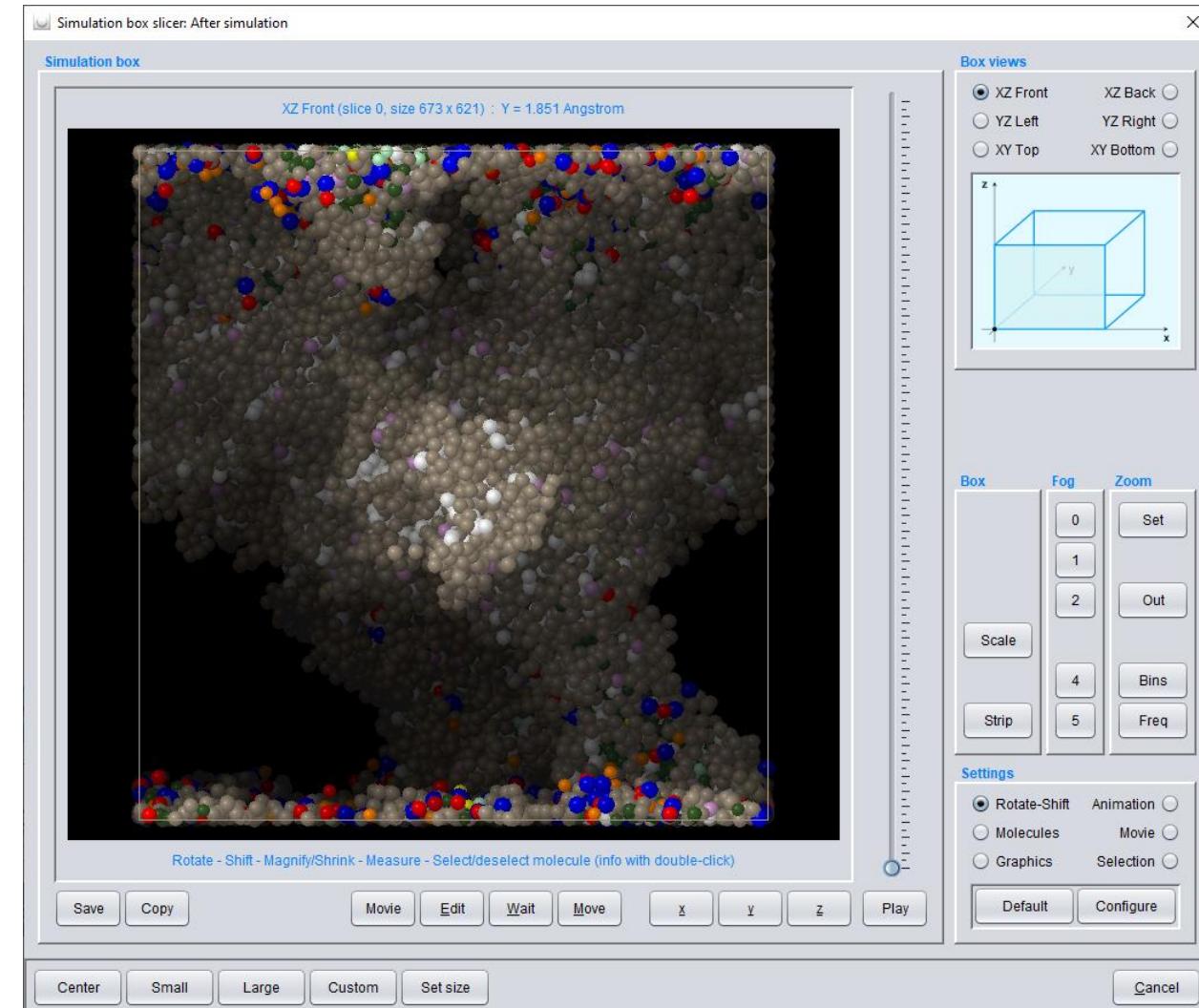
www.molecular-dynamics.de

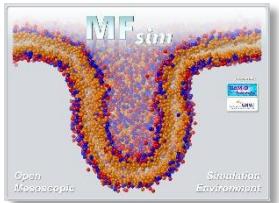


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Job Result Evaluation

Hit the **Freq** button of the **Zoom** quick settings panel ...





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Job Result Evaluation

... to open the **Zoom-volume information** dialog.

Zoom-volume information

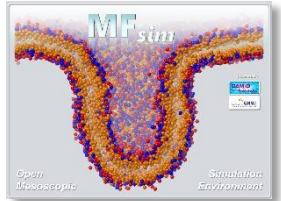
Feature overview

		Expand	Collapse
Zoom-volume frequency distributions			
Molecule particles			
Along x direction			
Along y direction			
Along z direction			

Selected feature

Feature		Description	
Name Molecule particles			
Molecule name	Particle	Particle name	Particle count
CHOLin	Et	Ethane	420
CHOLin	Me	Methane	148
CHOLin	MeOHchol	Methanol	55
CHOOut	Et	Ethane	292
CHOOut	Me	Methane	92
CHOOut	MeOHchol	Methanol	30
DMPCin	DMPN	Dimethylphosphate	1
DMPCin	Et	Ethane	13
DMPCin	MeAc	MethylAcetate	2
DMPCin	TriMeNPpl	TriMethylamine	1
DMPCout	DMPN	Dimethylphosphate	217
DMPCout	Et	Ethane	1455
DMPCout	MeAc	MethylAcetate	296
DMPCout	TriMeNPpl	TriMethylamine	250
DOPEin	Et	Ethane	14
DOPEout	DMPN	Dimethylphosphate	34
DOPEout	Et	Ethane	251
DOPEout	MeAc	MethylAcetate	39
DOPEout	MeNH2Ppl	Methylamine	40
KB1Y19	AzolidBB	Azolidine	878

Center Small Large Custom Set size Cancel

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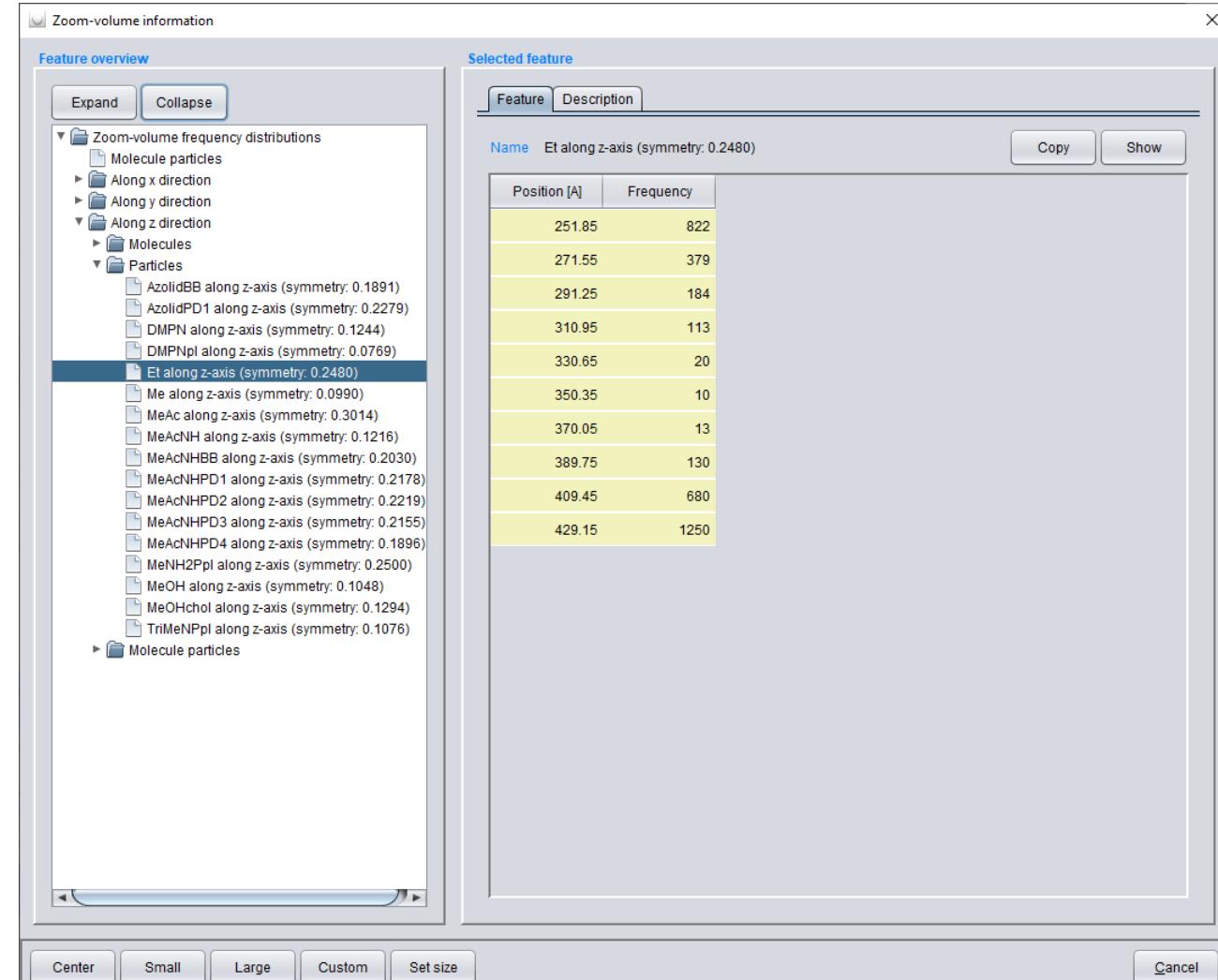
www.molecular-dynamics.de

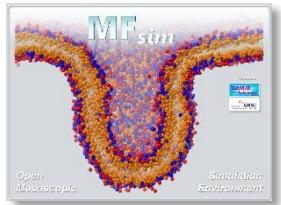


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Job Result Evaluation

Select **Zoom-volume frequency distributions / Along z direction / Particles / Et along z-axis ...** to view the Et particle distribution (partitioned into 10 bins) along the z-axis in the compartment. Hit the **Show** button ...





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Job Result Evaluation

... for a diagram chart of the Et distribution.
Particle distributions may be used for further evaluation operations concerning the cyclotide/membrane interaction.

