Simulation Foundry: scalable and FAIR molecular modelling

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Thursday 7\textsuperscript{th} November, 2019
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1 Quality Control

This report was generated using the workflow developed by G. Gygli in 2018-2019. It allows you to easily get an overview of your data, or estimate the quality of your simulations.

Here follows a list of things to check manually - if the list is empty, it is still recommended to check things yourself!

missing simulations:
This is a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 20 ° celsius.

Figure 1: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 20 ° celsius.
Figure 1: ... continued
3 energy

This is a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 20 ° celsius.

Figure 2: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 20 ° celsius.
Figure 2: ... continued
This is a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 20 ° celsius.

Figure 3: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 20 ° celsius.
Figure 3: ... continued
5 energy

This is a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 20 ° celsius.

Figure 4: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 20 ° celsius.
Figure 4: ... continued
This is a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 20 ° celsius.

Figure 5: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 20 ° celsius.
Figure 5: ... continued

(e) Density

(f) Enthalpy

(g) Volume
7 energy

This is a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 20 ° celsius.

Figure 6: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 20 ° celsius.
Figure 6: ... continued
8 energy

This is a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 20 ° celsius.

Figure 7: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 20 ° celsius.
Figure 7: ... continued
9 energy

This is a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 20 ° celsius.

Figure 8: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 20 ° celsius.
Figure 8: ... continued
10 energy

This is a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 20 ° celsius.

Figure 9: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 20 ° celsius.
Figure 9: ... continued
11 energy

This is a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 20 ° celsius.

Figure 10: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 20 ° celsius.
Figure 10: ... continued
12 energy

This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 20 ° celsius.

![Graphs showing potential, total-energy, temperature, and pressure over time for a mixture of H2O and MEOH.](image)

Figure 11: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 20 ° celsius.
Figure 11: ... continued
This is a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 30 ° celsius.

Figure 12: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 30 ° celsius.
Figure 12: ... continued
14 energy

This is a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 30 ° celsius.

Figure 13: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 30 ° celsius.
Figure 13: ... continued
This is a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 30 ° celsius.

Figure 14: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 30 ° celsius.
Figure 14: ... continued
This is a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 30 ° celsius.

Figure 15: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 30 ° celsius.
Figure 15: ... continued
This is a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 30 ° celsius.

Figure 16: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 30 ° celsius.
Figure 16: ... continued
This is a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 30 ° celsius.

Figure 17: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 30 ° celsius.
Figure 17: ... continued
This is a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 30 ° celsius.

Figure 18: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 30 ° celsius.
Figure 18: ... continued
This is a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 30 ° celsius.

Figure 19: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 30 ° celsius.
Figure 19: ... continued
21 energy

This is a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 30 ° celsius.

Figure 20: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 30 ° celsius.
Figure 20: ... continued
This is a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 30 ° celsius.

Figure 21: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 30 ° celsius.
Figure 21: ... continued
energy

This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 30 ° celsius.

Figure 22: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 30 ° celsius.
Figure 22: ... continued
This is a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 40 ° celsius.

Figure 23: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 40 ° celsius.
Figure 23: ... continued
This is a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 40 ° celsius.

Figure 24: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 40 ° celsius.
Figure 24: ... continued
This is a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 40 ° celsius.

Figure 25: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 40 ° celsius.
Figure 25: ... continued
This is a mixture of H₂O and MEOH, with 30 w/w % H₂O and 70 w/w % MEOH at 40 ° celsius.

Figure 26: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H₂O and MEOH, with 30 w/w % H₂O and 70 w/w % MEOH at 40 ° celsius.
Figure 26: ... continued
This is a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 40 ° celsius.

Figure 27: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 40 ° celsius.
Figure 27: ... continued
This is a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 40 ° celsius.

Figure 28: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 40 ° celsius.
Figure 28: ... continued
This is a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 40 ° celsius.

Figure 29: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 40 ° celsius.
Figure 29: ... continued
This is a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 40 ° celsius.

Figure 30: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 40 ° celsius.
Figure 30: ... continued
This is a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 40 ° celsius.

Figure 31: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 40 ° celsius.
Figure 31: ... continued
This is a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 40 ° celsius.

Figure 32: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 40 ° celsius.
Figure 32: ... continued
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 40 ° celsius.

Figure 33: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 40 ° celsius.
Figure 33: ... continued
This is a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 50 ° celsius.

Figure 34: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 50 ° celsius.
Figure 34: ... continued
This is a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 50 ° celsius.

Figure 35: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 50 ° celsius.
Figure 35: ... continued
This is a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 50 ° celsius.

Figure 36: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 50 ° celsius.
Figure 36: ... continued
This is a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 50 ° celsius.

Figure 37: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 50 ° celsius.
Figure 37: ... continued
This is a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 50 ° celsius.

Figure 38: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 50 ° celsius.
Figure 38: ... continued
This is a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 50 ° celsius.

Figure 39: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 50 ° celsius.
Figure 39: ... continued
This is a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 50 ° celsius.

Figure 40: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 50 ° celsius.
Figure 40: ... continued
This is a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 50 ° celsius.

Figure 41: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 50 ° celsius.
Figure 41: ... continued
This is a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 50 ° celsius.

Figure 42: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 50 ° celsius.
Figure 42: ... continued
This is a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 50 ° celsius.

Figure 43: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 50 ° celsius.
Figure 43: ... continued
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 50 ° celsius.

Figure 44: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 50 ° celsius.
Figure 44: ... continued
This is a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 60 ° celsius.

Figure 45: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 60 ° celsius.
Figure 45: ... continued
This is a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 60 ° celsius.

Figure 46: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 60 ° celsius.
Figure 46: ... continued
This is a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 60 ° celsius.

Figure 47: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 60 ° celsius.
Figure 47: ... continued
This is a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 60 ° celsius.

Figure 48: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 60 ° celsius.
Figure 48: ... continued
50 energy

This is a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 60 ° celsius.

Figure 49: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 60 ° celsius.
Figure 49: ... continued
51 energy

This is a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 60 ° celsius.

Figure 50: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 60 ° celsius.
Figure 50: ... continued
This is a mixture of H₂O and MEOH, with 60 w/w % H₂O and 40 w/w % MEOH at 60 ° celsius.

Figure 51: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H₂O and MEOH, with 60 w/w % H₂O and 40 w/w % MEOH at 60 ° celsius.
Figure 51: … continued
This is a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 60 ° celsius.

Figure 52: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 60 ° celsius.
Figure 52: ... continued
54 energy

This is a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 60 ° celsius.

Figure 53: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 60 ° celsius.
Figure 53: ... continued
This is a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 60 ° celsius.

Figure 54: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 60 ° celsius.
Figure 54: ... continued
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 60 ° celsius.

Figure 55: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 60 ° celsius.
Figure 55: ... continued
This is a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 70 ° celsius.

Figure 56: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 70 ° celsius.
Figure 56: ... continued
This is a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 70 ° celsius.

Figure 57: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 70 ° celsius.
Figure 57: ... continued
This is a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 70 ° celsius.

Figure 58: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 70 ° celsius.
Figure 58: ... continued
This is a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 70 ° celsius.

Figure 59: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 70 ° celsius.
Figure 59: ... continued
This is a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 70 ° celsius.

Figure 60: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 70 ° celsius.
Figure 60: ... continued
This is a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 70 ° celsius.

Figure 61: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 70 ° celsius.
Figure 61: ... continued
This is a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 70 ° celsius.

Figure 62: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 70 ° celsius.
Figure 62: ... continued
This is a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 70 ° celsius.

Figure 63: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 70 ° celsius.
Figure 63: ... continued
This is a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 70 ° celsius.

Figure 64: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 70 ° celsius.
Figure 64: ... continued
This is a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 70 ° celsius.

Figure 65: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 70 ° celsius.
Figure 65: ... continued
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 70 ° celsius.

Figure 66: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 70 ° celsius.
Figure 66: ... continued
This is a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 80 ° celsius.

Figure 67: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 80 ° celsius.
Figure 67: ... continued
This is a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 80 ° celsius.

Figure 68: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 80 ° celsius.
Figure 68: ... continued
This is a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 80 ° celsius.

Figure 69: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 80 ° celsius.
Figure 69: ... continued
This is a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 80 ° celsius.

Figure 70: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 80 ° celsius.
Figure 70: ... continued
This is a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 80 ° celsius.

Figure 71: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 80 ° celsius.
Figure 71: ... continued
This is a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 80 ° celsius.

Figure 72: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 80 ° celsius.
Figure 72: ... continued
This is a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 80 ° celsius.

Figure 73: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 80 ° celsius.
Figure 73: ... continued
This is a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 80 ° celsius.

Figure 74: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 80 ° celsius.
(e) Density

(f) Enthalpy

(g) Volume

Figure 74: ... continued
This is a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 80 ° celsius.

Figure 75: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 80 ° celsius.
(e) Density

(f) Enthalpy

(g) Volume

Figure 75: ... continued
This is a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 80 ° celsius.

Figure 76: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 80 ° celsius.
Figure 76: ... continued
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 80 ° celsius.

Figure 77: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 80 ° celsius.
Figure 77: ... continued
This is a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 90 ° celsius.

Figure 78: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and 100 w/w % MEOH at 90 ° celsius.
Figure 78: ... continued
This is a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 90 ° celsius.

Figure 79: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and 90 w/w % MEOH at 90 ° celsius.
Figure 79: ... continued
energy

This is a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 90 ° celsius.

Figure 80: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and 80 w/w % MEOH at 90 ° celsius.
Figure 80: ... continued
This is a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 90 ° celsius.

Figure 81: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and 70 w/w % MEOH at 90 ° celsius.
Figure 81: ... continued
This is a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 90 ° celsius.

Figure 82: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and 60 w/w % MEOH at 90 ° celsius.
Figure 82: ... continued
This is a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 90 ° celsius.

Figure 83: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and 50 w/w % MEOH at 90 ° celsius.
Figure 83: ... continued
This is a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 90 ° celsius.

Figure 84: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and 40 w/w % MEOH at 90 ° celsius.
(e) Density

(f) Enthalpy

(g) Volume

Figure 84: ... continued
energy

This is a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 90 ° celsius.

Figure 85: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and 30 w/w % MEOH at 90 ° celsius.
Figure 85: ... continued
This is a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 90 ° celsius.

Figure 86: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and 20 w/w % MEOH at 90 ° celsius.
Figure 86: ... continued
This is a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 90 ° celsius.

Figure 87: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and 10 w/w % MEOH at 90 ° celsius.
Figure 87: ... continued
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 90 ° celsius.

Figure 88: Overview of properties (Potential Total-Energy Temperature Pressure Density Enthalpy Volume) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 90 ° celsius.
Figure 88: ... continued
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 20 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 89: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 20 ° celsius.
Figure 90: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 20 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 20 ° celsius.

Figure 91: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 20 ° celsius.
Figure 92: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 20 ° celsius.
92 msd

This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 20 ° celsius.

Figure 93: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 20 ° celsius.
Figure 94: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 20 ° celsius.

Figure 95: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 20 ° celsius.
Figure 96: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 20 ° celsius.

Figure 97: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 20 ° celsius.
Figure 98: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 20 ° celsius.

Figure 99: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 20 ° celsius.
Figure 100: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 20 ° celsius.

Figure 101: Overview of MSD for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 20 ° celsius.
Figure 102: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 20 ° celsius.

Figure 103: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 20 ° celsius.
Figure 104: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 20 ° celsius.

Figure 105: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 20 ° celsius.
Figure 106: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 20 ° celsius.

Figure 107: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 20 ° celsius.
Figure 108: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 20 ° celsius.

Figure 109: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 20 ° celsius.
Figure 110: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 20 ° celsius.
msd

This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 30 ° celsius.

Figure 111: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 30 ° celsius.
Figure 112: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 30 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.
msd

This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 30 ° celsius.

Figure 113: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 30 ° celsius.
Figure 114: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 30 ° celsius.

Figure 115: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 30 ° celsius.
Figure 116: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 30 ° celsius.
This is a mixture of H₂O and MEOH, with 30 w/w % H₂O and -70 w/w % MEOH at 30 ° celsius.

Figure 117: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H₂O and MEOH, with 30 w/w % H₂O and -70 w/w % MEOH at 30 ° celsius.
Figure 118: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 30 ° celsius.

Figure 119: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 30 ° celsius.
Figure 120: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 30 ° celsius.

Figure 121: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 30 ° celsius.
Figure 122: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 30 ° celsius.

Figure 123: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 30 ° celsius.
Figure 124: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 30 ° celsius.

Figure 125: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 30 ° celsius.
Figure 126: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 30 ° celsius.

Figure 127: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 30 ° celsius.
Figure 128: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 30 ° celsius.

Figure 129: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 30 ° celsius.
Figure 130: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 30 ° celsius.
111 msd

This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 30 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 131: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 30 ° celsius.
Figure 132: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 40 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 133: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 40 ° celsius.
Figure 134: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 40 ° celsius.

Figure 135: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 40 ° celsius.
Figure 136: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 40 ° celsius.
This is a mixture of H₂O and MEOH, with 20 w/w % H₂O and -80 w/w % MEOH at 40 ° celsius.

Figure 137: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H₂O and MEOH, with 20 w/w % H₂O and -80 w/w % MEOH at 40 ° celsius.
Figure 138: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 40 ° celsius.

Figure 139: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 40 ° celsius.
Figure 140: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 40 ° celsius.

Figure 141: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 40 ° celsius.
Figure 142: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 40 ° celsius.
msd

This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 40 ° celsius.

Figure 143: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 40 ° celsius.
Figure 144: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 40 ° celsius.

Figure 145: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 40 ° celsius.
Figure 146: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 40 ° celsius.

Figure 147: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 40 ° celsius.
Figure 148: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 40 ° celsius.

Figure 149: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 40 ° celsius.
Figure 150: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 40 ° celsius.

Figure 151: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 40 ° celsius.
Figure 152: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 40 ° celsius.

Figure 153: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 40 ° celsius.
Figure 154: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 50 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 155: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 50 ° celsius.
Figure 156: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 50 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 50 ° celsius.

Figure 157: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 50 ° celsius.
Figure 158: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 50 ° celsius.

Figure 159: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 50 ° celsius.
Figure 160: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 50 ° celsius.

Figure 161: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 50 ° celsius.
Figure 162: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 50 ° celsius.

Figure 163: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 50 ° celsius.
Figure 164: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 50 ° celsius.

Figure 165: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 50 ° celsius.
Figure 166: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 50 ° celsius.

Figure 167: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 50 ° celsius.
Figure 168: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 50 ° celsius.

Figure 169: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 50 ° celsius.
Figure 170: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 50 ° celsius.

Figure 171: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 50 ° celsius.
Figure 172: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 50 ° celsius.

Figure 173: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 50 ° celsius.
Figure 174: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 50 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 175: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 50 ° celsius.
The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 176: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 60 ° celsius.

Figure 177: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 60 ° celsius.
Figure 178: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 60 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 60 ° celsius.

Figure 179: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 60 ° celsius.
Figure 180: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 60 ° celsius.

Figure 181: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 60 ° celsius.
Figure 182: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 60 ° celsius.

Figure 183: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 60 ° celsius.
Figure 184: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 60 ° celsius.

Figure 185: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 60 ° celsius.
Figure 186: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 60 ° celsius.

Figure 187: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 60 ° celsius.
Figure 188: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 60 ° celsius.
This is a mixture of H₂O and MEOH, with 60 w/w % H₂O and -40 w/w % MEOH at 60 ° celsius.

Figure 189: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H₂O and MEOH, with 60 w/w % H₂O and -40 w/w % MEOH at 60 ° celsius.
Figure 190: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 60 ° celsius.

Figure 191: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 60 ° celsius.
Figure 192: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 60 ° celsius.

Figure 193: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 60 ° celsius.
Figure 194: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 60 ° celsius.

![Graphs](image)

(a) MEOH  
(b) Water  
(c) System

Figure 195: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 60 ° celsius.
Figure 196: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 60 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 197: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 60 ° celsius.
Figure 198: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 70 ° celsius.

Figure 199: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 70 ° celsius.

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You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.
The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 200: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 70 ° celsius.

Figure 201: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 70 ° celsius.
Figure 202: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 70 ° celsius.

Figure 203: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 70 ° celsius.
Figure 204: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 70 ° celsius.

Figure 205: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 70 ° celsius.
Figure 206: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 70 ° celsius.
msd

This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 70 ° celsius.

Figure 207: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 70 ° celsius.
Figure 208: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 70 ° celsius.

Figure 209: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 70 ° celsius.
Figure 210: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 70 \degree celsius.

Figure 211: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 70 \degree celsius.
Figure 212: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 70 ° celsius.

Figure 213: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 70 ° celsius.
Figure 214: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 70 ° celsius.

Figure 215: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 70 ° celsius.
Figure 216: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 70 ° celsius.

Figure 217: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 70 ° celsius.
Figure 218: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 70 ° celsius.

Figure 219: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 70 ° celsius.
Figure 220: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 80 ° celsius.

Figure 221: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 80 ° celsius.

The png you were looking for does NOT exist. You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.
Figure 222: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 80 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 80 ° celsius.

Figure 223: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 80 ° celsius.
Figure 224: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 80 ° celsius.

Figure 225: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 80 ° celsius.
Figure 226: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 80 ° celsius.

Figure 227: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 80 ° celsius.
Figure 228: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 80 ° celsius.

Figure 229: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 80 ° celsius.
Figure 230: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 80 ° celsius.

Figure 231: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 80 ° celsius.
Figure 232: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 80 ° celsius.

(a) MEOH

(b) Water

(c) System

Figure 233: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 80 ° celsius.
Figure 234: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 80 ° celsius.

Figure 235: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 80 ° celsius.
Figure 236: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 80 ° celsius.

Figure 237: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 80 ° celsius.
Figure 238: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 80 ° celsius.

Figure 239: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 80 ° celsius.
Figure 240: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 80 ° celsius.

Figure 241: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 80 ° celsius.
The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

(a) MEOH

(b) Water

(c) System

Figure 242: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 90 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 243: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 90 ° celsius.
The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 244: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 90 ° celsius.

Figure 245: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 90 ° celsius.
Figure 246: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 90 ° celsius.

Figure 247: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 90 ° celsius.
Figure 248: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 90 ° celsius.

Figure 249: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 90 ° celsius.
Figure 250: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 90 ° celsius.
msd

This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 90 ° celsius.

Figure 251: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 90 ° celsius.
Figure 252: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 90 ° celsius.

Figure 253: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 90 ° celsius.
Figure 254: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 90 ° celsius.

Figure 255: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 90 ° celsius.
Figure 256: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 90 ° celsius.

Figure 257: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 90 ° celsius.
Figure 258: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 90 ° celsius.

Figure 259: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 90 ° celsius.
Figure 260: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 90 ° celsius.

Figure 261: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 90 ° celsius.
Figure 262: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 90 ° celsius.

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You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 263: Overview of msd for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 90 ° celsius.
Figure 264: Overview of regression quality used to determine diffusion coefficients for selected groups (MEOH Water System) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 20 ° celsius.

Figure 265: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 20 ° celsius.

Figure 266: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 20 ° celsius.

Figure 267: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 20 ° celsius.
This is a mixture of H$_2$O and MEOH, with 30 w/w % H$_2$O and -70 w/w % MEOH at 20 ° celsius.

Figure 268: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H$_2$O and MEOH, with 30 w/w % H$_2$O and -70 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 20 ° celsius.

Figure 269: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 20 ° celsius.
183 hbonds

This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 20 ° celsius.

Figure 270: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 20 ° celsius.

Figure 271: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 20 ° celsius.

(a) MEOH with Water

(b) MEOH with MEOH

(c) Water with Water

Figure 272: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 20 ° celsius.

Figure 273: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 20 ° celsius.

- **(a) MEOH with Water**
- **(b) MEOH with MEOH**
- **(c) Water with Water**

Figure 274: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 20 ° celsius.

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(a) MEOH with Water  (b) MEOH with MEOH  (c) Water with Water

Figure 275: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 20 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 30 ° celsius.

Figure 276: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 30 ° celsius.

Figure 277: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 30 ° celsius.

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<th>(c) Water with Water</th>
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Figure 278: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 30 ° celsius.

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<th>(c) Water with Water</th>
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Figure 279: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 30 ° celsius.

Figure 280: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 30 ° celsius.

Figure 281: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 30 ° celsius.
195  hbonds

This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 30 ° celsius.

Figure 282: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 30 ° celsius.

Figure 283: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 30 ° celsius.

Figure 284: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 30 ° celsius.

Figure 285: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 30 ° celsius.

(a) MEOH with Water
(b) MEOH with MEOH
(c) Water with Water

Figure 286: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 30 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 40 ° celsius.

Figure 287: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 40 ° celsius.
201  hbonds

This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 40 ° celsius.

Figure 288: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 40 ° celsius.

(a) MEOH with Water
(b) MEOH with MEOH
(c) Water with Water

Figure 289: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 40 ° celsius.

Figure 290: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 40 ° celsius.
This is a mixture of H₂O and MEOH, with 40 w/w % H₂O and -60 w/w % MEOH at 40 ° celsius.

Figure 291: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H₂O and MEOH, with 40 w/w % H₂O and -60 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 40 ° celsius.

Figure 292: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 40 ° celsius.

Figure 293: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 40 ° celsius.
207 hbonds

This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 40 ° celsius.

(a) MEOH with Water

(b) MEOH with MEOH

(c) Water with Water

Figure 294: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 40 ° celsius.

Figure 295: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 40 ° celsius.
This is a mixture of H$_2$O and MEOH, with 90 w/w % H$_2$O and -10 w/w % MEOH at 40 ° celsius.

Figure 296: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H$_2$O and MEOH, with 90 w/w % H$_2$O and -10 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 40 ° celsius.

Figure 297: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 40 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 50 ° celsius.

Figure 298: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 50 ° celsius.

Figure 299: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 50 ° celsius.
213  hbonds

This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 50 ° celsius.

Figure 300: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 50 ° celsius.

Figure 301: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 50 ° celsius.

Figure 302: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 50 ° celsius.

Figure 303: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 50 ° celsius.

Figure 304: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 50 ° celsius.

Figure 305: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 50 ° celsius.
hbonds

This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 50 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

(a) MEOH with Water

(b) MEOH with MEOH

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You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

(c) Water with Water

Figure 306: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 50 ° celsius.

| (a) MEOH with Water | (b) MEOH with MEOH
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Figure 307: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 50 ° celsius.

Figure 308: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 50 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 60 ° celsius.

(a) MEOH with Water

(b) MEOH with MEOH

(c) Water with Water

Figure 309: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 60 ° celsius.

Figure 310: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 60 ° celsius.

(a) MEOH with Water

(b) MEOH with MEOH

(c) Water with Water

Figure 311: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 60 ° celsius.

Figure 312: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 60 ° celsius.

(a) MEOH with Water

(b) MEOH with MEOH

(c) Water with Water

Figure 313: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 60 ° celsius.

Figure 314: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 60 ° celsius.

Figure 315: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 60 ° celsius.

Figure 316: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 60 ° celsius.

(a) MEOH with Water

(b) MEOH with MEOH

(c) Water with Water

Figure 317: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 60 ° celsius.

Figure 318: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 60 ° celsius.

Figure 319: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 60 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 70 ° celsius.

Figure 320: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 70 ° celsius.
234  hbonds

This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 70 ° celsius.

(a) MEOH with Water

(b) MEOH with MEOH

(c) Water with Water

Figure 321: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 70 ° celsius.
This is a mixture of H$_2$O and MEOH, with 20 w/w % H$_2$O and -80 w/w % MEOH at 70 ° celsius.

Figure 322: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H$_2$O and MEOH, with 20 w/w % H$_2$O and -80 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 70 ° celsius.

Figure 323: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 70 ° celsius.

Figure 324: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 70 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

(a) MEOH with Water
(b) MEOH with MEOH
(c) Water with Water

Figure 325: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 70 ° celsius.
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This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 70 ° celsius.

(a) MEOH with Water

(b) MEOH with MEOH

(c) Water with Water

Figure 326: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 70 ° celsius.

Figure 327: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 70 ° celsius.

Figure 328: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 70 ° celsius.

Figure 329: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 70 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

(a) MEOH with Water  
(b) MEOH with MEOH

(c) Water with Water

Figure 330: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 70 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 80 ° celsius.

(a) MEOH with Water
(b) MEOH with MEOH
(c) Water with Water

Figure 331: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 80 ° celsius.

Figure 332: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 80 ° celsius.

Figure 333: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 80 ° celsius.

Figure 334: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 80 ° celsius.

Figure 335: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 80 ° celsius.

Figure 336: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 80 ° celsius.

Figure 337: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 80 ° celsius.

Figure 338: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 80 ° celsius.

Figure 339: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 80 ° celsius.

Figure 340: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 80 ° celsius.

The png you were looking for does NOT exist.
You may want to check in the workflow if something went wrong or if the mixture you are working with does not have the components you wanted to analyse, e.g. no Water in 100% Methanol.

Figure 341: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 80 ° celsius.
This is a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 90 ° celsius.

Figure 342: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 0 w/w % H2O and -100 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 90 ° celsius.

Figure 343: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 10 w/w % H2O and -90 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 90 ° celsius.

Figure 344: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 20 w/w % H2O and -80 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 90 ° celsius.

Figure 345: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 30 w/w % H2O and -70 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 90 ° celsius.

Figure 346: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 40 w/w % H2O and -60 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 90 ° celsius.

Figure 347: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 50 w/w % H2O and -50 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 90 ° celsius.

Figure 348: Overview of hydrogen bonds of molecules in the system (MEOH-Water, MEOH-MEOH, Water-Water) of all replicates of a mixture of H2O and MEOH, with 60 w/w % H2O and -40 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 90 ° celsius.

Figure 349: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 70 w/w % H2O and -30 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 90 ° celsius.

(a) MEOH with Water

(b) MEOH with MEOH

(c) Water with Water

Figure 350: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 80 w/w % H2O and -20 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 90 ° celsius.

Figure 351: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 90 w/w % H2O and -10 w/w % MEOH at 90 ° celsius.
This is a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 90 ° celsius.

Figure 352: Overview of hydrogen bonds of molecules in the system (MEOH-Water MEOH-MEOH Water-Water) of all replicates of a mixture of H2O and MEOH, with 100 w/w % H2O and 0 w/w % MEOH at 90 ° celsius.
265.1 Methods

Molecular dynamics simulations were performed with the GROningen MAChine for Chemical Simulation (GROMACS) package (GROMACS 5.1.4-gnu-4.9/2016.5, GROMACS1, GROMACS2, GROMACS3, GROMACS4, GROMACS5, GROMACS6, GROMACS7), on the high performance infrastructure of the homer. A bash (version 4.4.19) script was used to simultaneously launch replicates of each of 1 solvent mixtures of molecules at different temperatures (20, degrees celsius), thus 33 simulations were performed in total. The oplsaa and spce water model were used (oplsaa, spce). Non-standard molecules were parametrized using the LigParGen webserver with the 1.14*CM1A charge model (LigParGen1, LigParGen2, LigParGen3).

A Simulation Foundry (DOI of our PUBLICATION) was used to automatically perform the ensemble of simulations (simulation foundry). The simulation box was 8 by 8 by 8 nm large, and was neutral due to the partial charges of the molecules in the system being zero, by adding 0 None ions.

Minimisation was performed for 50000 steps using steep (a steepest descent algorithm implemented in GROMACS). Equilibration was performed for 10 ns using the md integrator (a leap-frog algorithm implemented in GROMACS), the V-rescale thermostat (V-rescale) with isotropic coupling (tauT=0.1) and the barostat (), and electrostatic interactions were calculated with the particel-mesh Ewald summation (PME1, PME2). While equilibration was performed under NPT conditions, production was performed under NPT conditions by adding a Berendsen pressure coupling (Berendsen, tauP=0.6) for 100 ns. Check the mdp files of the Simulation Foundry for more parameters.