# Studies of brine-oil interfaces based on molecular dynamics and sonification

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## Objectives

In order to develop a better enhanced oil recovery techniques, it is important to study the parameters that influence the oil / brine interfacial properties. Hydrogen bonds play a central role in these properties, and their network structure can form several geometric patterns known as oligomers. Given the capacity to differentiate sounds composed by varied frequencies and timbres, we aim to introduce in the context of the oil industry the sonification of statistical data on the formation of oligomers in the oil / brine interface. This technique aims to improve the simultaneous analysis of multiple data, in addition to disseminating knowledge in a creative way.

## Materials and Methods

We use molecular dynamics (MD) simulations using the LAAMPS code [2] to generate molecular paths of the oil / brine interface under normal conditions of temperature and pressure as described in reference [1]. With the help of ChemNetwork [3] it was possible to identify the types and quantities of oligomers based on geometric criteria applied to the network structure of hydrogen bonds. In addition, we have developed post-processing tools to extract static data on the formation of oligomers in the aqueous phase. These data were later converted into audible frequencies using sonication techniques in the SuperCollider program [4].

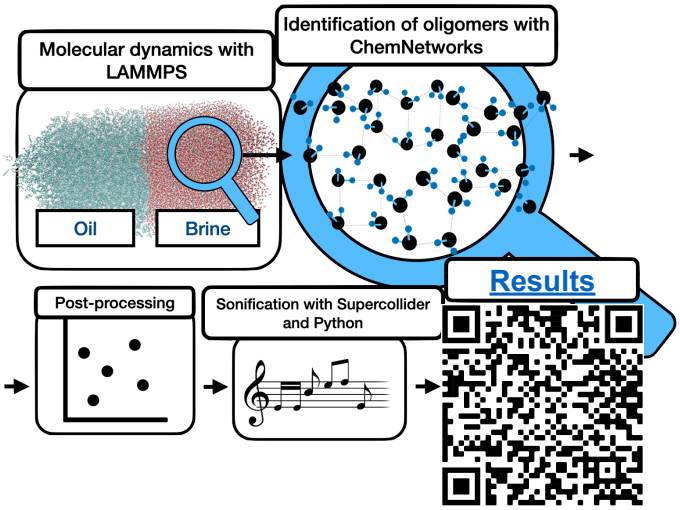


Figure 1. Computational protocol and QR code directing to the audio files generated by the sonification process.

## Results

The formation of oligomers is influenced by the interaction with the oil due to the break of hydrogen bonds in the water at the interface. In addition, the main oligomers formed were pentamers, boats, books, bags, tetramers and chairs. Finally, with sonification techniques, it was possible to have a more comprehensive perception of the effect of the interface on the formation of different oligomers in the aqueous phase.

## Conclusions

The combination of molecular dynamics and sonification allows the simultaneous analysis of the formation of several types of oligomers and the influence of the interface on these structures due to the great auditory ability to distinguish sounds composed of various frequencies and timbres. In addition, this technique contributes to the popularization of science by exploring senses beyond the visual.

## References

[1]Brine–Oil Interfacial Tension Modeling: Assessment of Machine Learning Techniques Combined with Molecular Dynamics,A.Kirch, YM.Celaschi, JM de Almeida, CR Miranda; ACS Applied Materials & Interfaces 12, 15837 (2020)
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