

## Neutron research, Contr. talk 2 - Sucrose versus trehalose as possible preservatives for proteins

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Sucrose and trehalose are well-known industrial preservatives for various purposes: they are widely used in cosmetics, food conservation and pharmaceutical industry [1,2]. For instance, sucrose is a stabilizing compound of covid-19 vaccine produced by Pfizer [3]. In this work with the help of atomistic molecular dynamics simulations sucrose and trehalose were considered as agents for preservation of two model-proteins (myoglobin and A $\beta$ (1-42) peptide) at three different water contents. Results of calculations of self-intermediate scattering functions demonstrated that systems containing sugars with the smaller amount of water needed more than 100 ns, while similar systems without sugars could be relaxed in at around 60-80 ns. Trehalose was the best stabilizing agent in all studied cases which could be a consequence of a slower dynamics of this sugar.

[1] Olsson, Christoffer, Samuel Genheden, Victoria García Sakai, and Jan Swenson. "Mechanism of trehalose-induced protein stabilization from neutron scattering and modeling." *The Journal of Physical Chemistry B* 123, no. 17 (2019): 3679-3687.

[2] Starciuc, Tatiana, Benjamin Malfait, Florence Danede, Laurent Paccou, Yannick Guinet, Natalia T. Correia, and Alain Hedoux. "Trehalose or Sucrose: Which of the Two Should be Used for Stabilizing Proteins in the Solid State? A Dilemma Investigated by In Situ Micro-Raman and Dielectric Relaxation Spectroscopies During and After Freeze-Drying." *Journal of pharmaceutical sciences* 109, no. 1 (2020): 496-504.

[3] Vogel, Annette B., Isis Kanevsky, Ye Che, Kena A. Swanson, Alexander Muik, Mathias Vormehr, Lena M. Kranz et al. "BNT162b vaccines protect rhesus macaques from SARS-CoV-2." *Nature* (2021): 1-7.

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**Session Classification** : Contributed talks