



Contribution ID: 6

Type: **Invited**

Exploring Ligand-Protein Interactions at Multiple Temperatures Using Macromolecular Crystallography

Thursday 5 June 2025 11:00 (30 minutes)

Cryogenic temperatures may introduce artefacts that limit the understanding of protein dynamics, crucial to their biological functions. To address this, we developed a room-temperature (RT) X-ray crystallographic method that captures movie-like structural snapshots triggered by temperature [1]. This method revealed binding-mode changes of TL00150, a 175.15 Da fragment in endothianensin. Building on this, we further developed Cryo2RT, a high-throughput RT de the cryo-crystallography workflow [2]. This fragments, thaumatin, and SARS-CoV-2 3CL_{pro} seen at cryogenic temperatures. To minimize a threshold considered safe for both cryo and slightly lower resolution and higher B-factor motion at RT. These findings provide insight potential for fragment-based screening and

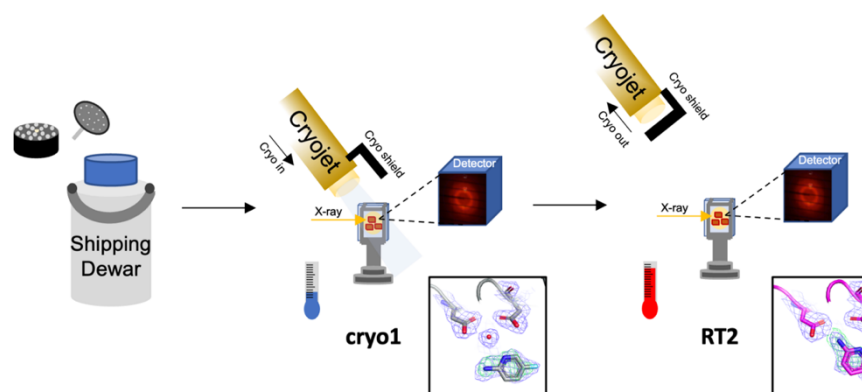


Figure 1: enter image description here

References

- [1] Huang, C.-Y., Aumonier, S., Engilberge, S., Eris, D., Smith, K. M. L., Leonarski, F., Wojdyla, J. A., Beale, J. H., Buntschu, D., Pauluhn, A., Sharpe, M. E., Metz, A., Olieric, V., and Wang, M. (2022) Acta Cryst. D78: 964-974. <https://doi.org/10.1107/S205979832200612X>
- [2]: Huang, C.-Y., Aumonier, S., Olieric, V., and Wang, M. (2024) Acta Cryst. D80: 620-628. <https://doi.org/10.1107/S2059798324006697>

Presenter: HUANG, Chia-Ying (PSI - Paul Scherrer Institut)**Session Classification:** Radiation Damage in Temperature Controlled Crystallography