EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal: *https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do*

Deadlines for submission of Experimental Reports

Experimental reports must be submitted within the period of 3 months after the end of the experiment.

Experiment Report supporting a new proposal ("relevant report")

If you are submitting a proposal for a new project, or to continue a project for which you have previously been allocated beam time, you must submit a report on each of your previous measurement(s):

- even on those carried out close to the proposal submission deadline (it can be a *"preliminary report"),*
- even for experiments whose scientific area is different form the scientific area of the new proposal,
- carried out on CRG beamlines.

You must then register the report(s) as "relevant report(s)" in the new application form for beam time.

Deadlines for submitting a report supporting a new proposal

- 1st March Proposal Round - **5th March**
- 10th September Proposal Round - **13th September**

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report in English.
- include the experiment number to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** Assessing the structural, thermodynamical, and dynamical properties of crowded solutions of intrinsically disordered proteins	**Experiment number**: MX-2124
Beamline: BM29	**Date of experiment**: from: 31 Oct 2018 to: 01 Nov 2018	**Date of report**: 08 Jan 2020
Shifts: 3	**Local contact(s)**: Mark Tully	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

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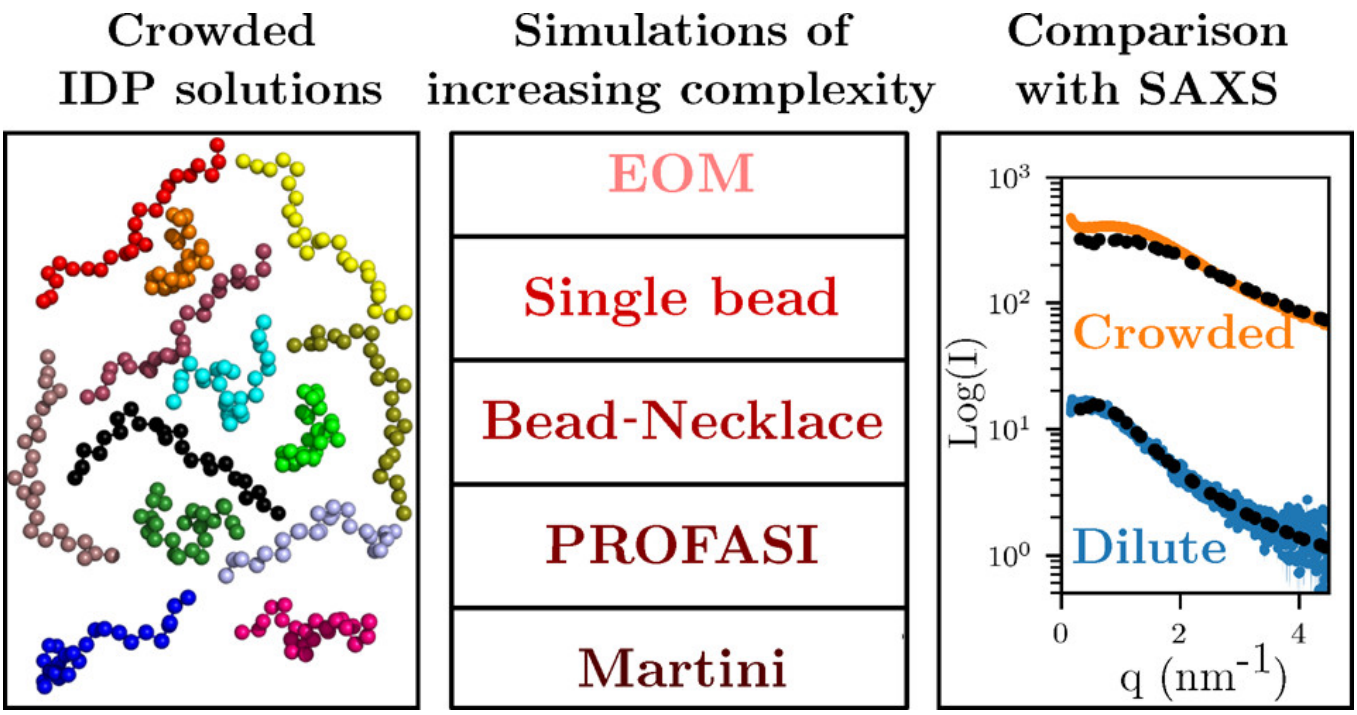
Report:

Published:

Eric Fagerberg, Samuel Lenton, and Marie Skepö
Journal of Chemical Theory and Computation **2019** *15* (12), 6968-6983
DOI: 10.1021/acs.jctc.9b00723

Intrinsically disordered proteins (IDPs) adopt heterogeneous conformational ensembles in solution. The properties of the conformational ensemble are dependent upon the solution conditions, including the presence of ions, temperature, and crowding, and often directly impact biological function. Many *in vitro* investigations focus on the properties of IDPs under dilute conditions, rather than the crowded environment found *in vivo*. Due to their heterogeneous nature, the study of IDPs under crowded conditions is challenging both experimentally and computationally. Despite this, such studies are worth pursuing due to the insight gained into biologically relevant phenomena. Here, we study the highly charged IDP Histatin 5 under self-crowded conditions in low and high salt conditions. A combination of small-angle X-ray scattering and different simulation models, spanning a range of computational complexity and detail, is used. Most models are found to have limited application when compared to results from experiments. The best performing model is the highly coarse-grained, bead-necklace model. This model shows that Histatin 5 has a conserved radius of gyration and a decreasing flexibility with increasing protein concentration. Due to its computational efficiency, we propose that it is a suitable model to study crowded IDP solutions, despite its simplicity.


Crowded
IDP solutions
Simulations of
increasing complexity
Comparison
with SAXS
EOM
Single bead
Bead-Necklace
PROFASI
Martini
Crowded
Dilute
Log(I)
q (nm-1)