



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://www.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 from 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.



Experiment title: Study of the incorporation of metabolic molecules into calcite for the improvement of metabolic magnetic resonance imaging of tumors.	Experiment number: CH-6555	
Beamline: ID22	Date of experiment: from: 20.06.23 to: 25.06.23	Date of report: 01.09.2023
Shifts: 12	Local contact(s): Ola Gjonnes Grendal	<i>Received at ESRF:</i>

Names and affiliations of applicants (* indicates experimentalists):

Boaz Pokroy* – Department of Materials Science and Engineering, Technion – Israel Institute of Technology.

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Elena Prudnikov* – Department of Materials Science and Engineering, Technion – Israel Institute of Technology. Lotan Portal* – Department of Materials Science and Engineering, Technion – Israel Institute of Technology.

Report:

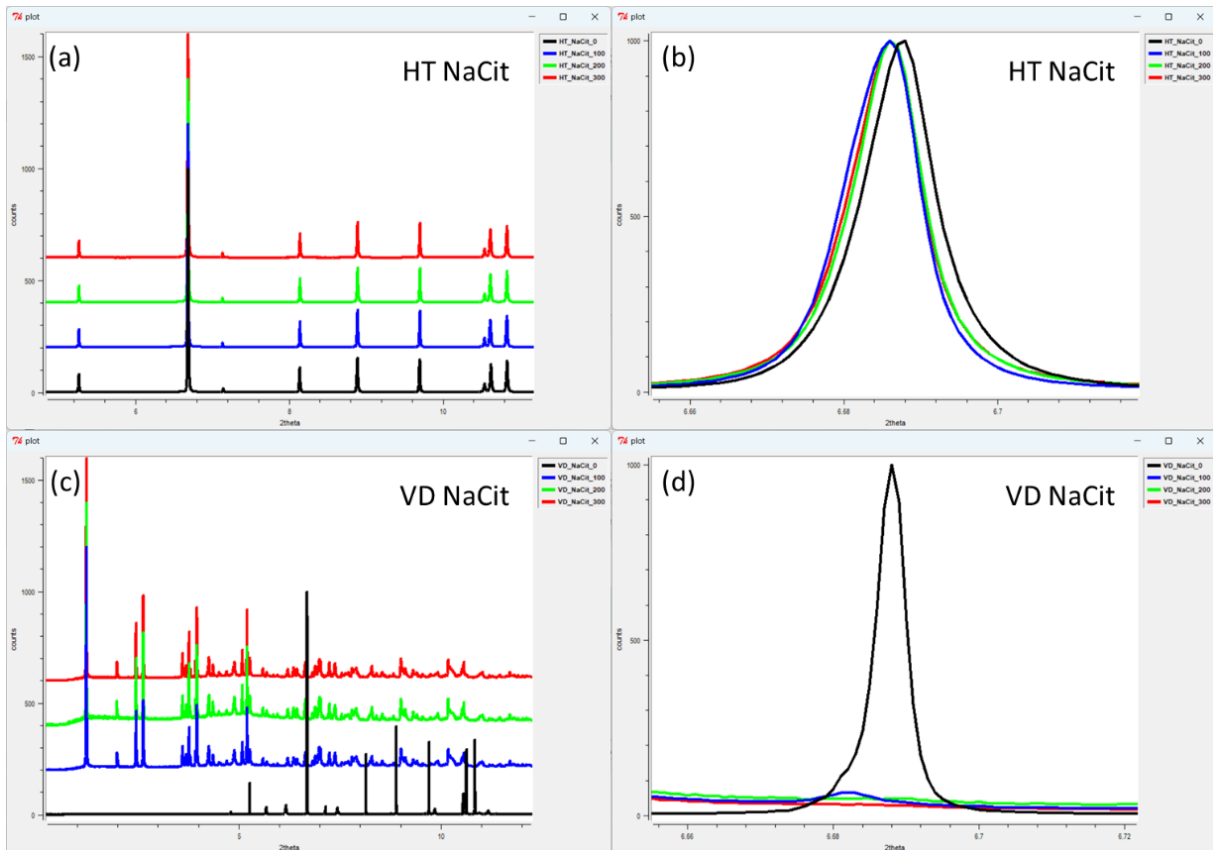


Figure 1. (a+c) HR-PXRD patterns of CaCO_3 , and (b+d) zoom-in on calcite (104) reflection, grown in the presence of (a+b) sodium citrate using a hydrothermal route, and (c+d) citric acid using the vapor diffusion method.

Figure 1 presents the HR-PXRD results of CaCO_3 grown in the presence of one metabolite – citrate, using two different routes – hydrothermal (HT) and vapour diffusion (VD). When grown using the HT route, the metabolite is added to the carbonate solution, hence, we used its alkaline form, namely sodium citrate (NaCit). In this case, the formation of CaCO_3 is fast, and the resulting phase is pure calcite (Figure 1a). when taking a closer look at the most intense calcite reflection (104), a slight shift is observed when NaCit is added. This may be an indication of lattice expansion as a result of citrate incorporation. On the other hand, when grown using the VD route, the metabolite is added to the calcium solution. When adding NaCit, the solution becomes opaque after a few seconds, due to the formation of insoluble calcium citrate (CaCit). Hence, in this case, we used citric acid (HCit), which inhibits the formation of CaCit. However, due to the slow pH increase of the solution (ammonia diffusion), CaCit still forms (Figure 1c), and completely eliminates the formation of CaCO_3 (Figure 1d).

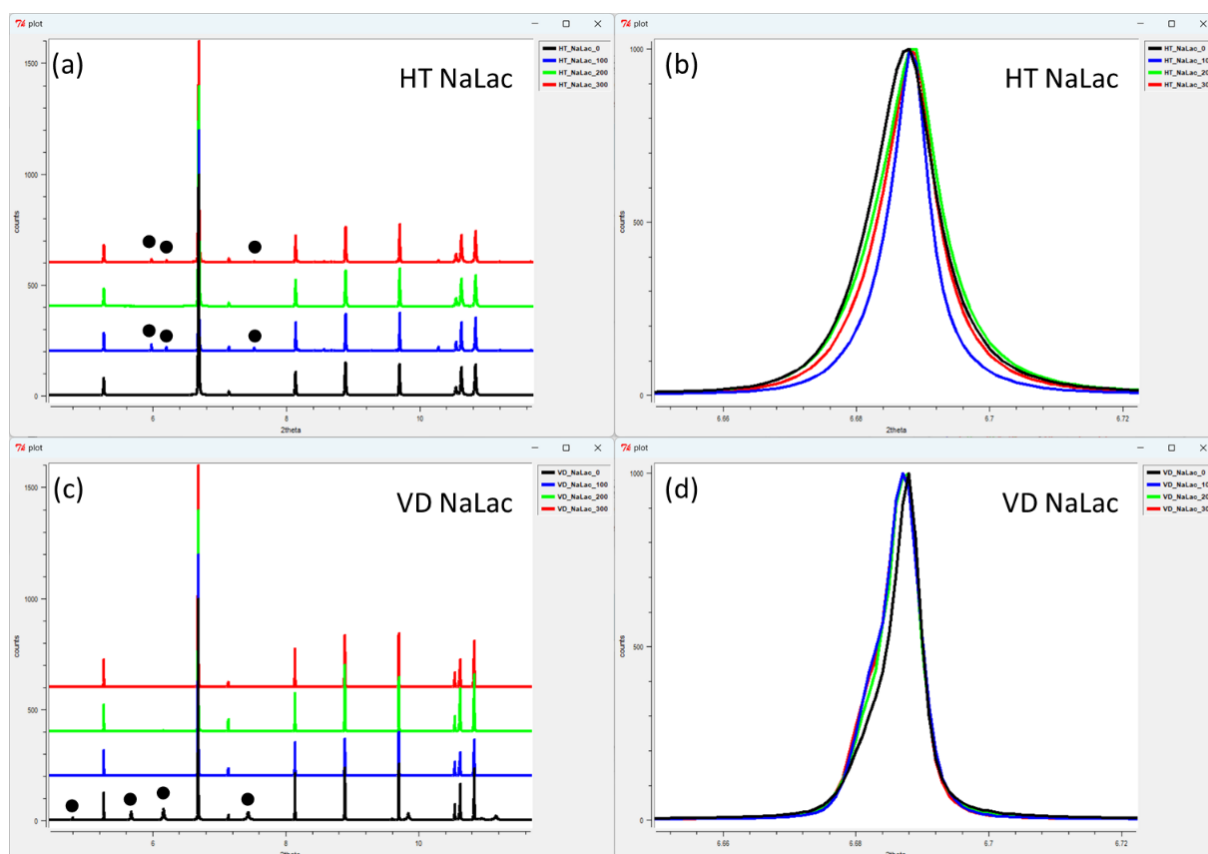


Figure 2. (a+c) HR-PXRD patterns of CaCO_3 , and (b+d) zoom-in on calcite (104) reflection, grown in the presence of sodium lactate using (a+b) a hydrothermal route, and (c+d) the vapor diffusion method.

Figure 2 presents the HR-PXRD results of CaCO_3 grown in the presence of another metabolite – lactate. In this case, calcium lactate does not precipitate, so we could use the alkaline form (sodium lactate, NaLac) in both synthetic routes. In all of the samples the dominant CaCO_3 polymorph is calcite, with small amounts of aragonite or vaterite impurities in some of the cases (labelled with dots in Figure 2a,c). However, zooming in on the (104) reflection does not indicate any significant incorporation (Figure 2b,d).

Future work

1. Analysing all the data and understanding which metabolite can be incorporated into the calcitic structure.
2. Performing analytical metabolites detection on the relevant sample, to correlate between the concentration of metabolite in each sample and the lattice distortion it induces.
3. Trying to understand the incorporation mechanism of the metabolites into calcite.