





DataQ Intelligence (in Gründung) · Gebäude B9, Universitätsstraße 30 · 95447 Bayreuth · Germany

<u>To:</u> Daniel Chateigner, Xiaolong Chen, Marco Ciriotti, Robert T. Downs, Saulius Gražulis, Werner Kaminsky, Armel Le Bail, Luca Lutterotti, Yoshitaka Matsushita, Andrius Merkys, Peter Moeck, Peter Murray-Rust, Miguel Quirós Olozábal, Hareesh Rajan, Alexandre F.T. Yokochi

DataQ Intelligence

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Online Meeting

Dear members of the advisory board of COD,

your data base is about to reach half a million entries. Congratulations!

We are DataQ Intelligence, a startup from Bayreuth, Germany, (https://www.dataqintelligence.com/) supported by the European Union and the EXIST-Program.

Our topic is "systematic errors in diffraction data". We are looking for partners who are also concerned about data quality issues in crystallography. Our vision is that in 5-10 years each individual structure publication will include a small paragraph dedicated to the topic of systematic errors that addresses questions like:

- how much (to which degree) is the data set affected by systematic errors?
- how do systematic errors show up (characteristic appearance, descriptive side)?
- what are the likely consequences for model parameters and model parameter errors?
- what is a possible or likely source of this error?
- are there yet ways to remove this error known?

We think that this topic might be of interest to you as well and that we should talk to each other about this

if you feel so as well.

This is an informal request for an online meeting via Zoom or MS Teams for deepening this discussion. (We will send you the invitation mail after you confirmed).

We suggest to meet online on 13th of September at 9:00am.

Yours sincerely, Dr. rer. nat. habil. J. Henn



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