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LTP III: Detection of ice-crystal artifacts in macromolecular diffraction data through machine learning

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Contamination with diffraction from ice crystals can negatively affect, or even impede, macromolecular structure determination and therefore detecting the resulting artefacts in diffraction data is crucial. However, once the data have been processed it can be very difficult to automatically recognize this problem. To address this, a set of convolutional neural networks named Helcaraxe has been developed which can detect ice-diffraction artefacts in processed diffraction data from macromolecular crystals.
Our work shows that the multi-dimensional pattern-recognition abilities of convolutional neural networks are a valuable addition to the toolbox of diffraction data analysis. Helcaraxe is currently already in use in the Coronavirus Structural Task Force pipeline and has been integrated into the newest version of AUSPEX.

Primary author: NOLTE, Kristopher (Institut für Nanostruktur und Festkörperphysik, Universität Hamburg, Germany)

Co-authors: GAO, Yunyun (University Hamburg); STÄB, Sabrina (Institut für Nanostruktur und Festkörperphysik, Universität Hamburg, Germany); KOLLMANSBERGER, Philip (CCTB, Julius-Maximilians-Universität Würzburg, Germany); THORN, Andrea (Universität Hamburg)

Presenter: NOLTE, Kristopher (Institut für Nanostruktur und Festkörperphysik, Universität Hamburg, Germany)

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