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Dose calculations for microcrystallography, XFELs, and electron microscopy: extensions to RADDOSE-3D

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Radiation damage remains a fundamental limitation to the success of X-ray macromolecular crystallography (MX) experiments. The program RADDOSE-3D [1,2] estimates the dose absorbed by samples during data collection at synchrotron sources, allowing direct comparison of radiation damage between experiments carried out with different samples and beam parameters. Here, I present a number of extensions to RADDOSE-3D, which perform Monte Carlo simulations to improve the accuracy and applicability of RADDOSE-3D. The first of these extensions provides more accurate dose estimates for synchrotron data collection on microbeams or microcrystals by taking into account the redistribution of photoelectrons produced both in the crystal and the surrounding. These emphasise the importance of beam energy [3,4,5], surrounding material, and crystal orientation on radiation damage to microcrystals. The second extension, RADDOSE-XFEL, calculates the time-resolved dose during XFEL data collection. The final extension, RADDOSE-EM, calculates the dose absorbed during single particle electron cryomicroscopy and micro-electron diffraction (MicroED) data collection. It is hoped that these extensions can be used to facilitate the study of radiation damage in new experiments and be used to maximise data collection efficiency.

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