

University of Montana Small Molecule X-ray Diffraction Core Facility Co-Authorship Policy

The policy outlined are in accord with many crystallographic laboratories across the nation, with the American Crystallographic Association's [ethics policy](#), with the [ACS Ethical Authorship](#) tips (see number 2) and with the [ACS Ethical Guidelines to Publication of Chemical Research](#) (see section B number 11). Please note that the compliance by faculty and collaborators within these guidelines is voluntary, yet encouraged.

Authorship:

We ask for co-authorship if users of the facility ask us to contribute to the scientific interpretation of the data. We consider contribution to mean anything which goes beyond sending the user the completed CIF and report, be it detailed discussions, database searches or contributing figures, tables, or even paragraphs. Additionally we request that the PI (i.e. corresponding author) ask several questions: Is the structure a crucial part of the manuscript? Without it, would the other analytical data support the conclusions? If the structure is a critical component to the manuscript, co-authorship of the crystallographer is recommended. Most papers that have this component include parameters, diagrams, and structural discussions that fall within the expertise of the crystallographer. We encourage all collaborators to use the crystallographer's expertise in these discussions. As a co-author, the crystallographer is happy to assist in the preparation and revision of manuscripts.

Acknowledgement: If the data was used to confirm a structure that was well characterized by other methods (mass spectrometry, NMR, elemental analysis, etc.), and also lead to a routine structure (i.e. no disorder, small number of atoms in the asymmetric unit, not twinned, etc.) acknowledgement is sufficient.

From clients who just want the data and are happy to simply get a completed CIF and report back, we do not require co-authorship. An acknowledgement of the crystallographer here is also sufficient. Please note that without authorship the crystallographer reserves the right to not assist in response to any reviewer/editor concerns, or questions concerning the data at a future time. If these services are needed, they would then be available and billed accordingly for the crystallographer's time (i.e. dollars per hour charge).