

# Assessing the Value of Small Molecule Service Crystallography in the Face of Advancing Technology

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For many universities with X-ray diffraction equipment, the safest and most cost-effective way to allow access to this equipment has been to house it in user facilities run by staff scientists. However, recent developments in low power X-ray sources and detectors allow a diffractometer to be housed in nearly any laboratory. Furthermore, structural methods such as solid state NMR and electron diffraction are increasingly used to get structures from materials that are inaccessible to single crystal X-ray diffraction. Powerful computer fitting programs have increased the accessibility of structure interpretations from scattering on non-crystalline materials. Finally, improvements in synchrotron sources have led to crystal structure determination pipelines with such high throughput that they are being applied towards routine small molecule crystallography. These developments have drastically rewritten the role of the university service crystallographer in a fairly short time. This talk will explore the costs in running a user facility at a mid-sized R1 research university in the United States and compare it to other models for user access such as single investigator-led labs or larger instrument centers. Fundraising opportunities at many universities are limited for staff scientists, so sources of value given to the institution must be identified. As the accessibility of structural science increases for everybody, it can be seen that the value of a staff scientist-led user facility shifts away from research productivity and towards the university's educational mission.