

## **3D Structure Determinations and Cellular Mapping Using X-ray Absorption Spectroscopy**

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Three-dimensional structure determinations of complexes in any phase can be determined by the use of multiple-scattering analysis of XAFS (X-ray absorption fine structure) data. Apart from the advantage of being able to obtain structural information in any phase, there are several other advantages of XAFS over protein crystallography for structural studies with metalloproteins including: generally more precise and accurate bond lengths (and angles in some cases); and less photodamage-induced changes to bonding parameters at the active site during data collection. However, XAFS provides no information on the 3-D structure of the protein; hence, it is an important complementary technique to protein crystallography and, in most cases, it is preferable to combine the information from both techniques in order to obtain accurate structural information. The fact that X-ray absorption techniques can be used on any medium, also allows structural information to be obtained from species in organelles within cells using XANES (X-ray absorption near-edge structure) spectroscopy and XAFS for bulk cells and tissues. Microprobe X-ray fluorescence mapping also enables biodistribution studies on single cells down to the sub-organelle level. The applications of these techniques to various problems will be described, including: the biotransformations of drugs and carcinogens in cells and biological fluids; understanding the early stages of degenerative diseases at a cellular level; and solving important problems in heme biochemistry.