I'm not a robot

Dr. John C. Lindon is a professor and senior research investigator in the Division of Computational and Systems Medicine, part of the Department of Surgery and Cancer, Imperial College London. He is also a founder, director of, and a consultant to Metabometrix Ltd, a company spun out of Imperial College to exploit the commercial possibilities of metabolic phenotyping. He is editor in chief of the Encyclopedia of Spectroscopy and Spectrometry and is on the editorial board of several journals. His major research interest is the use of NMR and other analytic methods coupled with multivariate statistics to study biofluids and tissues, a field now termed metabolic phenotyping. George E. Tranter PhD MA BSc FRSC CChem CSci, has held senior R&D positions in both industry and academia (including at London University, Oxford University, the Wellcome Foundation and GlaxoWellcome). Until 2006 he led the Biospectroscopy Centre of Imperial College London and subsequently was Senior Research Fellow of the Department of Chemistry, University of Oxford. He is a recognized international authority in the field of molecular chirality and the spectroscopic/physicochemical features of drugs and biopharmaceuticals. He is named as inventor on drug patents, has published widely in the scientific literature, co-edited The Encyclopedia of Spectroscopy & Spectrometry (Academic Press), editor of the Separations and Analysis volume of Comprehensive Chirality (Elsevier), has been a member of scientific journal editorial boards (inc. CHIRALITY) and appeared on radio and television programmes in the UK and abroad. He is also a member of various scientific advisory panels and is a key partner in collaborations that bring together the biopharmaceutical industry, academia, and governmental institutions to investigate and validate biopharmaceutical structure and function. His particular interests are in the rational discovery of new therapeutics, with a passion for the role chirality plays in nature, from the molecular level through to macroscopic structures (e.g., helical shells) and beyond.istics of marine creatures. David W. Koppenaal is Chief Technology Officer at the Enviromental Molecular Sciences Center (EMSL) at Pacific Northwest National Laboratory in Richland, WA. Dr. Koppenaal’s research interests include the development of new instrumental and spectroscopic techniques for metallomics applications and the metallomic study of cyanobacterial systems. Dr. Koppenaal was an early proponent of metallomics as a new science discipline, serving as an advocate and speaker on this topic since 2000, organizing the first symposia focused on this topic in the US, and serving as co-chair of the 2nd International Metallomics Symposium (2009). Dr. Koppenaal is well-known for his fundamental science investigations and innovations in atomic mass spectrometry, including the initial development and demonstration of effective reaction cell technology and associated ion molecule reaction approaches for interference reduction in ICPMS. More recently he has developed and applied ultra-high resolution orbital trapping MS techniques to metallomics applications. Dr. Koppenaal has also served as Editorial Board member of JAAS, and as Chair of the Analytical Division of the American Chemical Society. He is a Fellow of the Royal Society of Chemistry, the American Association for the Advancement of Science, and the American Chemical Society. Ask the publishers to restore access to 500,000+ books. This paper discusses the methodologies and considerations involved in small-molecule crystallography, particularly focusing on the refinement of crystal structures through various software such as SHELX and CRYSTALS. It outlines the general workflow of crystallographic structure determination, emphasizing the importance of model fitting and the statistical considerations related to the precision and accuracy of measurements. Key challenges including systematic errors and the correlation of uncertainties are also highlighted. 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