

Preface

This first issue of Section D contains a set of papers directed at the timely topic of direct methods of phasing in macromolecular crystallography. These papers resulted from a conference of that title which was held at Panama City Beach, Florida, USA, 24–27 April 1992. A total of 96 delegates and speakers attended this conference, including representation from the USA, Canada, Western Europe and Russia. The conference was organized to cover the latest developments in phasing techniques applied to crystal structures of large biological macromolecules, especially proteins, in the molecular weight range 5000–100 000. Within this framework, speakers were invited to cover several themes, including *ab initio* phasing from native amplitudes; phase extension; phase improvement starting with approximate phases from SIR, MIR, molecular replacement or MAD techniques; improved refinement of macromolecular structures; and location and refinement of sites for heavy atoms and anomalous scatterers. The papers presented at this meeting were then submitted for review through regular refereeing mechanisms before being accepted for publication in this special issue of *Acta Crystallographica* Section D.

Throughout the discussions at this conference, the participants reminisced about the slow evolution of direct methods that occurred in the small-molecule field between the original theoretical developments in the late 1940's and early 1950's, and the time that direct methods were actually widely accepted and used beginning in the mid- to late 1960's. It was the hope of many participants that we might move more rapidly to assimilate new developments in the macromolecular field, and that the papers presented at this

meeting might lay the groundwork for accelerating future applications of direct methods in the phasing of macromolecular diffraction data. At the conclusion of the conference, there was general excitement about the progress that had been reported. Considering the primary importance of phasing methods in macromolecular crystallography, it is appropriate that this first issue of Section D, 'Biological Crystallography,' includes the forefront papers that were presented and discussed at this conference.

Although each of these individual papers stands on its own merit, the Panama City Beach conference provided an excellent opportunity to bring these latest developments together, and to exchange ideas, experiences, and strategies for the future efforts to apply direct methods to macromolecular phasing. We are indebted to Penny Mann from the University of Alabama at Birmingham for her many contributions toward the organization of this conference, and for the generous financial support provided by the International Union of Crystallography, the National Aeronautics and Space Administration, the Center for Macromolecular Crystallography at the University of Alabama at Birmingham, the Schering Corporation, SmithKline Beecham Pharmaceuticals, Sterling Winthrop, Inc., The Du Pont Merck Pharmaceutical Company and The Upjohn Company.

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