Contribution ID: **121** Type: **Oral presentations**

Phasing your XALOC data with ARCIMBOLDO

Thursday, 18 June 2015 10:20 (20 minutes)

Phasing your XALOC data with ARCIMBOLDO

Macromolecular Ab Initio phasing, from the native intensities alone with no experimental phase information or previous particular structural knowledge has been the object of a long quest, limited by two main barriers: structure size and data resolution. Beyond the first atomic resolution successes, current approaches have been developed, exploiting alternative constraints to atomicity, through use of the Patterson function, density modification and data extrapolation [1].
Our own approach relies on the combination of locating model fragments with the program PHASER [2] and density modification with the program SHELXE [3]. Appropriate search models are polyalanine alpha-helices[4], small polypeptide folds[5], DNA-binding motifs[6] or fragments from distant homologs[7]. Given the difficulties in discriminating correctly positioned fragments, many putative hypotheses have to be tested in parallel, thus calculations are performed on a grid or supercomputer. The method has been called after the Italian painter Arcimboldo, who used to compose portraits out of fruits and vegetables. In the case of our program, most collections of fragments remain a "still-life", but some are correct enough for density modification to reveal the protein's true portrait (http://chango.ibmb.csic.es/ARCIMBOLDO). Using these methods, a number of unknown macromolecules with a few thousand atoms and resolutions around 2 Å have been solved.
Performance of the single-workstation implementation ARCIMBOLDO_LITE available at XALOC will be presented.

References

[1] Sheldrick, G.M., Gilmore, C., Hauptman, H.A., Weeks, C.M., Miller, R. and Usón, I. International Tables for Crystallography (2012). Vol. F, ch. 16.1, pp. 413-432; Burla, M.C., Carrozzini, B., Cascarano, G.L., Giacovazzo, C., Polidori,M. J. Appl. Cryst. 45, 1287-1294 (2011).
[2] McCoy, A.J. Grosse-Kunstleve RW, Adams PD, Winn MD, Storoni LC, Read RJ.. J. Appl. Crystallogr. 40, 658–674 (2007).
[3] A. Thorn and G.M. Sheldrick. Acta Crystallogr. D69, 2251-2256 (2013).
[4] Rodríguez D.D., Grosse, C., Himmel, S., González, C., de Ilarduya, I. M., Becker, S., Sheldrick, G. M. and Usón, I. Nature Methods 6: 651-653 (2009).
[5] Sammito, M., Millán, C., Rodríguez, D.D., de Ilarduya, I.M., Meindl, K., De Marino, I., Petrillo, G., Buey, R.M., de Pereda, J.M., Zeth, K, Sheldrick, G. M. and Usón, I. Nature Methods 10: 1099-1101 (2013).
[6] Pröpper, K., Meindl, K., Sammito, M., Dittrich, B., Sheldrick, G.M., Pohl, E. and Usón, I. Acta Cryst. D70, 1743-1757 (2014).
[7] Sammito, M., Meindl, K., de Ilarduya, I.M., Millán, C., Artola-Recolons, C., Hermoso, J.A. and Usón, I. FEBS Journal 281: 4029–4045 (2014)

Primary author: Prof. USÓN, Isabel (ICREA at IBMB-CSIC)

Co-authors: MILLÁN, Claudia (IBMB-CSIC); Dr JUANHUIX, Jordi (Experiments); SAMMITO, Massimo (IBMB_CSIC); BORGES, Rafael Junqueira (IBMB-CSIC, UNESP)

Presenter: BORGES, Rafael Junqueira (IBMB-CSIC, UNESP)

Session Classification: Session 6 - II ALBA User's Meeting 2015

Track Classification: II ALBA User's Meeting