s8b.m2.p3 **On the significance of an accurate vector-set selection in molecular replacement: a practical example.** C. Alvarez-Rúa, J. Borge, S. García-Granda. *Departamento de Química Física y Analítica. Facultad de Química. Universidad de Oviedo. C/ Julián Clavería, 8. 33006 Oviedo. SPAIN.*
Keywords: vector-search, rotation function, molecular replacement.

Vector-search rotation functions try to locate a vector-set from the search model in the Patterson map of the unknown crystal structure. Therefore, the performance of this sort of functions is greatly influenced by an accurate selection of this vector-set [1].

Many vector selection procedures have been proposed and successfully implemented for small molecules. Most of them are based on the fact that atoms are clearly distinguishable in the crystal and interatomic vectors can be geometrically derived from the atomic positions. However, these procedures are no longer valid when working with macromolecular data and the vector-set has to be directly obtained from the Patterson map of the search model. This is not a simple task because of the great number of atoms in the unit cell and the lack of high resolution data, which make the Patterson peaks be not well-resolved.

A number of vector-set selection procedures in macromolecular crystallography have been tested and their influence on the performance of a new vector-search rotation function has been studied. Practical examples will be presented that illustrate the significance of the vector-selection step in the rotation search process.

[1] Borge, J., Alvarez-Rúa, C. & García-Granda, S. (2000). *Acta Cryst.* D**56** (in press).

s8b.m2.p4 **Vector-search methods revisited in macromolecular crystallography: a new rotation function in Patterson space.** J. Borge, C. Alvarez-Rúa, S. García-Granda. *Departamento de Química Física y Analítica. Facultad de Química. Universidad de Oviedo. C/ Julián Clavería, 8. 33006 Oviedo. SPAIN.*
Keywords: vector-search, rotation function, molecular replacement.

Rotation functions can be mathematically implemented in two different forms: reciprocal space and vector (or Patterson) space algorithms. The latter are usually called vector-search methods. Functions belonging to the first class dominate the present software. However, vector-search rotation functions can be as quick and successful as reciprocal space algorithms provided that the input data to the rotation function are appropriately prepared.

Image Seeking Functions (ISFs) can be regarded as a criterion of fit between an observed Patterson map and a vector-set from a search model. This particularity makes them appear as potentially useful Patterson space rotation functions.

The application of ISFs in the molecular replacement method will be presented [1]. Attention will be focused on the effect of the magnitude of some statistical parameters relating both crystal and model Patterson maps on the performance of the ISFs [2]. It will be shown that the success of the whole proposed procedure heavily depends on the vector-set selection step. Results of the application of the method will be discussed.

[1] Borge, J., Alvarez-Rúa, C. & García-Granda, S. (2000). *Acta Cryst.* D**56** (in press).
[2] García-Granda, S., Borge, J. & Gutiérrez-Rodríguez, A. (1996). *Anales de Química*, Int. Ed. **92**, 294-298.