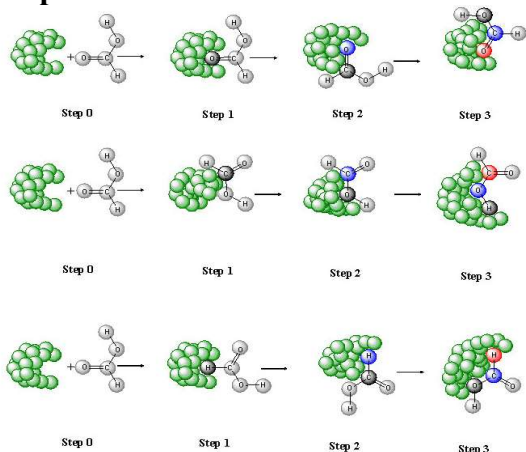


Leave-Species-Out Procedure in Multi-target QSAR models**Francisco J. Prado-Prado**

Biomedical Sciences Department, Health Sciences Division,

University of Quintana Roo, UQROO, 77039, Mexico.

Graphical Abstract**Abstract.**

In this paper we generalized QSAR models to predict the biological activity of antifungal drugs against 87 fungi species. The data was processed by Linear Discriminant Analysis (LDA) classifying drugs as active or non-active. The model correctly classifies 338 out of 368 active compounds (91.85%) and 89 out of 123 non-active compounds (72.36%). Overall training predictability was 86.97% (427 out of 491 compounds). Validation of the model was carried out by means of Leave-Species-Out (LSO) procedure. After elimination step-by-step of all drugs tested against one specific species we record the percentage of good classification of leave-out compounds (LSO-predictability). Ref: Bioorg Med Chem. 2006 Sep 1;14(17):5973-80.

Ref: Ref: Bioorg Med Chem. 2006 Sep 1;14(17):5973-80.<http://www.sciencedirect.com/science/article/pii/S096808960600383X?via%3Dihub>