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PTML in optimizing preclinical plasmodium assays

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Abstract:

The use of algorithms to predict optimal results in preclinical malaria assays from a data set that includes the experimental conditions of preclinical assays and characteristics of proteins, genes and chromosomes is a breakthrough in research. The process from data collection to data processing takes 70 percent of the time to develop. The process from the creation of preliminary models to the production of the model takes 30 percent of the total research time. There are several databases such as ChEMBL, Uniprot and NCBI-GDV that allow the collection of information on both preclinical assays and characteristics of any species, in this case study is *plasmodium falciparum*. This species is a major public health problem in tropical and subtropical countries. *P. falciparum* usually causes high fever, diarrhea, chills and in a few hours, it can evolve to a severe case causing death. The use of different algorithms such as: Linear Discriminant Analysis (LDA), Classification Tree with Univariate Splits (CTUS), Classification Tree with Linear Combinations (CTLC), and so on. The use of these algorithms and the perturbation theory allows pharmaceutical industries to optimize preclinical testing processes obtaining the most optimal models with a high percentage of specificity and sensitivity.

References:

1. DiMasi, J. A.; Grabowski, H. G.; Hansen, R. W., Innovation in the pharmaceutical industry: New estimates of R&D costs. *J Health Econ* 2016, 47, 20-33.
2. Gaillard, T.; Boxberger, M.; Madamet, M.; Pradines, B., Has doxycycline, in combination with anti-malarial drugs, a role to play in intermittent preventive treatment of Plasmodium falciparum malaria infection in pregnant women in Africa? *Malar J* 2018, 17, 469.
3. Gaulton, A.; Hersey, A.; Nowotka, M.; Bento, A. P.; Chambers, J.; Mendez, D.; Mutowo, P.; Atkinson, F.; Bellis, L. J.; Cibrian-Uhalte, E.; Davies, M.; Dedman, N.; Karlsson, A.; Magarinos, M. P.; Overington, J. P.; Papadatos, G.; Smit, I.; Leach, A. R., The ChEMBL database in 2017. *Nucleic Acids Res* 2017, 45, D945-D954.
4. Gaulton, A.; Bellis, L. J.; Bento, A. P.; Chambers, J.; Davies, M.; Hersey, A.; Light, Y.; McGlinchey, S.; Michalovich, D.; Al-Lazikani, B.; Overington, J. P., ChEMBL: a large-scale bioactivity database for drug discovery. *Nucleic Acids Res* 2012, 40, D1100-7.
5. Gonzalez-Diaz, H.; Arrasate, S.; Gomez-SanJuan, A.; Sotomayor, N.; Lete, E.; Besada-Porto, L.; Russo, J. M., General Theory for Multiple Input-Output Perturbations in Complex Molecular Systems. 1. Linear QSPR Electronegativity Models in Physical, Organic, and Medicinal Chemistry. *Current Topics in Medicinal Chemistry* 2013, 13, 1713-1741.
6. Kalanon, M.; McFadden, G. I., Malaria, Plasmodium falciparum and its apicoplast. *Biochem Soc Trans* 2010, 38, 775-82.
7. Martinez, S. G.; Tenorio-Borroto, E.; Barbabosa Pliego, A.; Diaz-Albiter, H.; Vazquez-Chagoyan, J. C.; Gonzalez-Diaz, H., PTML Model for Proteome Mining of B-cell Epitopes and Theoretic-Experimental Study of Bm86 Protein Sequences from Colima Mexico. *J Proteome Res* 2017.
8. Quevedo-Tumailli, V. F.; Ortega-Tenezaca, B.; Gonzalez-Diaz, H., Chromosome Gene Orientation Inversion Networks (GOINs) of Plasmodium Proteome. *J Proteome Res* 2018, 17, 1258-1268.
9. Wolfsberg, T. G., Using the NCBI Map Viewer to browse genomic sequence data. *Curr Protoc Hum Genet* 2011, Chapter 18, Unit18 5.
10. UniProt Consortium, T., UniProt: the universal protein knowledgebase. *Nucleic Acids Res* 2018, 46, 2699.