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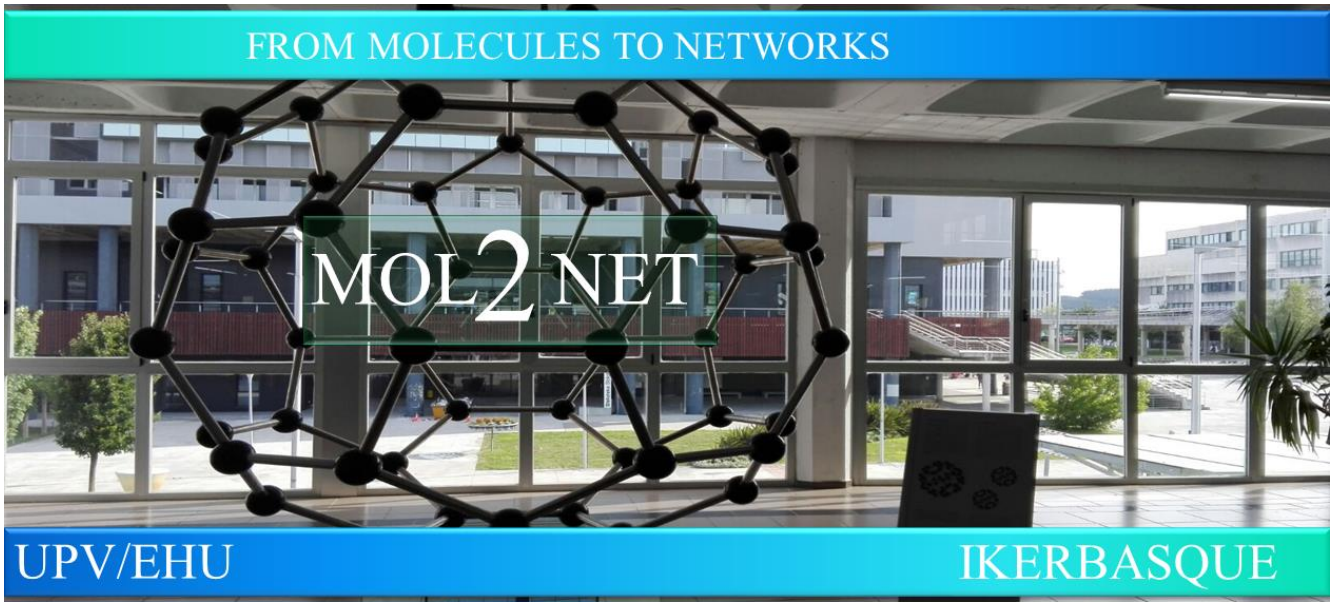
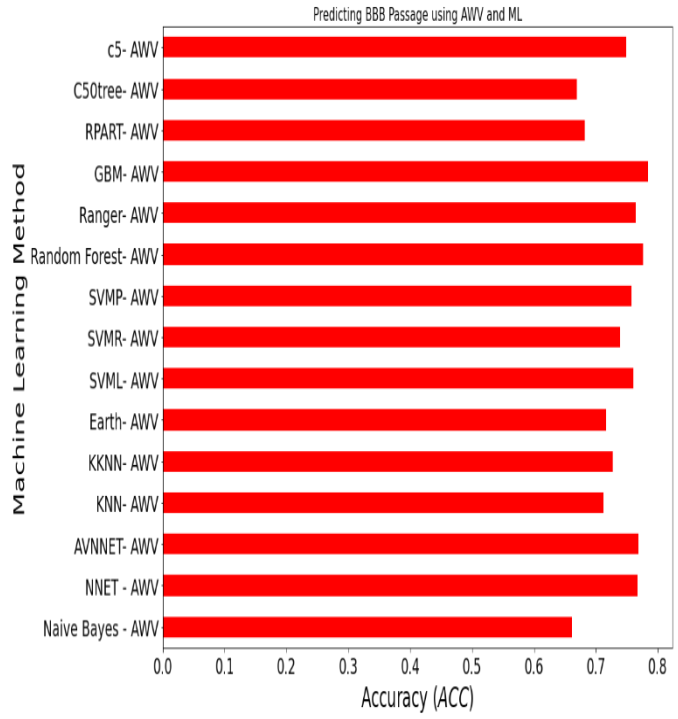


Predicting Blood-Brain Barrier Passage using Atomic Weighted Vector and Machine Learning

Yoan Martínez López[a], Yanaima Jauriga Ortiz[a], Ansel Rodríguez González[b], Juan A. Castillo Garit[c] , Gerardo M. Casanola-Martin[d] , Julio Madera Quintana[a]

[a] *Department of Computer Sciences, Faculty of Informatics, Camagüey University*
[b] *Unidad de Transferencia Tecnológica, Centro de Investigación Científica y de Educación Superior de Ensenada*
[c] *Unidad de Toxicología Experimental, Universidad de Ciencias Médicas de Villa Clara*
[d] *Department of Coatings and Polymeric Materials, North Dakota State University*

Graphical Abstract	**Abstract.**
	The blood-brain barrier (BBB) is a highly selective permeability barrier that separates circulating blood from brain extracellular fluid in the central nervous system (CNS). This barrier allows the passage of water, some gases, and lipid-soluble molecules by passive diffusion, as well as the selective transport of molecules such as glucose and amino acids that are crucial for neuronal function. In this research, we present an exploratory study, where several



machine learning techniques are applied to predict blood-brain barrier passage by applying molecular descriptors based on atomic vectors, obtained by MD-LOVIs software. Several techniques such as KNN-AWV(ACC= 0.712), AVNNET-AWV(ACC=0.768), Random Forest-AWV(ACC=0.776) and GBM-AWV(ACC=0.784) obtained good prediction performance. The results show that machine learning techniques are powerful tools for the prediction of this activity. The experiment file and dataset can be downloaded at: https://github.com/cybervalient/DeepMD_AWV/blob/main/BBB-AWV-ML.R and https://github.com/cybervalient/DeepMD_AWV/blob/main/BBB%20caret.rar

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