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SAMET: A machine- learning web based platform for management, interpretation and analysis of IR spectral data

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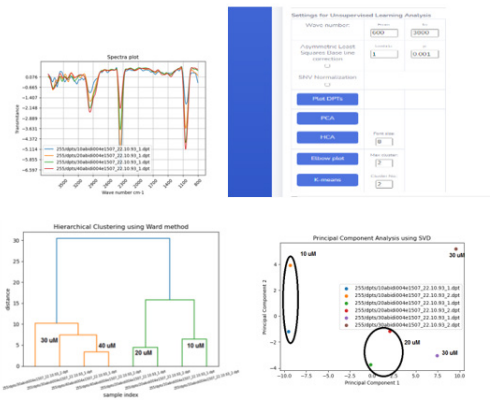
Versatile supervised and unsupervised machine learning techniques are widely used in different branches of pharmaceutical sciences. Application of supervised techniques including hierarchical cluster analysis (HCA), k-means and kohonen neural network in clustering of different spectral data such as infra-red (IR) spectroscopy can lead to better interpretation as well as investigation of batch to batch variations in chemicals (1). To integrate different unsupervised learning methods as well as providing a suitable management platform in an easy to use interface, we designed and developed a web based software in django frame work by means of python and JS programming (2). SAMET (Spectral Analysis via Machine Learning Estimation of Trained models) can be hosted in both windows and linux operating systems for management and analysis of IR spectral data. This software can visualize, present descriptive interpretation for IR spectroscopy and perform unsupervised learning methods on dpt files resulting from IR spectroscopy. This platform can be utilized in different branches of pharmaceutical industry such as quality control labs.



Biography

Dr. Maryam Kabiri is a PharmD,MPH student with experience in molecular modeling,computational drug discovery, toxicological screening of synthetic and natural products and bioinformatics.The most prominent goal of her research is to find out novel in silico pipelines in drug design and discovery,molecular dynamics simulation of membrane proteins and drug delivery

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