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| S.No | Algorithm | Purpose | Optimized Hyper-Parameters |
| 1 | t-Distributed Stochastic Neighbor Embedding | Feature Selection | perplexity 18, learning rate 185, and 500 iterations |
| 2 | Deep Neural Network | Model Training | Optimizer: Adam, Activation Function: ‘ReLu’, Drop out layer = 0.05, Loss Function: MSE (Mean Square Error), Epochs = 150, Batch size of 64, Learning Rate = 0.001, Early Stopping with Patience of 10, Validation Split: 0.25, verbose = 1, Restore best weights = True, Input layer with 500 nodes, four hidden layers with 3000, 6000, 3000, 2000 nodes and single output node with ‘Linear’ Activation function. |
| 3 | Standard Autoencoders | Dimensionality reduction | Optimizer: RMS prop, Activation Function: ‘ReLu’, Gaussian Noise with Standard deviation of 0.01, Loss Function: MSE (Mean Square Error), Epochs = 100, Batch size of 25, Learning Rate = 0.01, Early Stopping with Patience of 10, Validation Split: 0.3, Bottle Neck layer: 500 features, Input layers varied based on the dataset. |

Table 1: Optimized Hyperparameters Employed for MM-DNN Model Development. This table presents the hyperparameters optimized using Hyperopt for the development of the MM-DNN (Multi-Modal Deep Neural Network) model. t-SNE was employed for feature selection based on drug molecular descriptors, while autoencoder reduced dimensionality and facilitated data concatenation for model training, thereby simplifying data complexity. Deep neural network architecture was utilized for training the model on preprocessed datasets.