Chapter 8
References

8 References

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Appendices

Tables

Table-S1 Number of features calculated and used for model building

S.No.	Name of features	No. of features calculated	No. of features used for building model
1	Modred	1613	22
2	MACCS	166	151
3	PUBCHEM	881	610
4	KRFP	4861	1753

Table-S2 List of MACCS, PUBCHEM and KRFP fingerprints used in building models

Fingerprints	Bits
MACCS	MACCSFP8, MACCSFP11, MACCSFP13, MACCSFP14, MACCSFP16, MACCSFP17, MACCSFP18, MACCSFP19, MACCSFP20, MACCSFP21, MACCSFP22, MACCSFP23, MACCSFP24, MACCSFP25, MACCSFP26, MACCSFP27, MACCSFP28, MACCSFP29, MACCSFP30, MACCSFP32, MACCSFP33, MACCSFP34, MACCSFP36, MACCSFP37, MACCSFP38, MACCSFP39, MACCSFP40, MACCSFP41, MACCSFP42, MACCSFP43, MACCSFP45, MACCSFP46, MACCSFP47, MACCSFP48, MACCSFP49, MACCSFP50, MACCSFP51, MACCSFP52, MACCSFP53, MACCSFP54, MACCSFP55, MACCSFP56, MACCSFP57, MACCSFP58, MACCSFP59, MACCSFP60, MACCSFP61, MACCSFP62, MACCSFP63, MACCSFP64, MACCSFP65, MACCSFP66, MACCSFP67, MACCSFP68, MACCSFP69, MACCSFP70, MACCSFP71, MACCSFP72, MACCSFP73, MACCSFP74, MACCSFP75, MACCSFP76, MACCSFP77, MACCSFP78, MACCSFP79, MACCSFP80, MACCSFP81, MACCSFP82, MACCSFP83, MACCSFP84, MACCSFP85, MACCSFP86, MACCSFP87, MACCSFP88, MACCSFP89, MACCSFP90, MACCSFP91, MACCSFP92, MACCSFP93, MACCSFP94, MACCSFP95, MACCSFP96, MACCSFP97, MACCSFP98, MACCSFP99, MACCSFP100, MACCSFP101, MACCSFP102, MACCSFP103, MACCSFP104, MACCSFP105, MACCSFP106, MACCSFP107, MACCSFP108, MACCSFP109, MACCSFP110, MACCSFP111, MACCSFP112, MACCSFP113, MACCSFP114, MACCSFP115, MACCSFP116, MACCSFP117, MACCSFP118, MACCSFP119, MACCSFP120, MACCSFP121, MACCSFP122, MACCSFP123, MACCSFP124, MACCSFP125, MACCSFP126, MACCSFP127, MACCSFP128, MACCSFP129, MACCSFP130, MACCSFP131,

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Table S3- AUC of ROC plot of models built on 3D descriptors

Model No.	Parameters	AUC of ROC score
NB-5	Type- Gaussian Var smoothing- 10^{-9}	0.80
KNN-5	N neighbours -7	0.90
SVM-5	C=0.01 Gamma=0.1 Kernel=Rbf	0.88
RF-5	N estimator=500 Max depth=15 Min samples split= 4	0.93
GB-5	N estimator=500 Max depth=4 Min samples split= 7	0.92

Table S4- Summary of parameters for Random Forest classifier

Descriptors	**Parameters**
MACCS	max_depth=20, min_samples_leaf=5, n_estimators=200, n_jobs=-1,
ECFP-4	max_depth=0, min_samples_leaf=5, n_estimators=50, n_jobs=-1,

ECFP-6	max_depth=5, min_samples_leaf=5, n_estimators=10, n_jobs=-1,
PubChem	max_depth=20, min_samples_leaf=5, n_estimators=50, n_jobs=-1,
Estate	max_depth=5, min_samples_leaf=5, n_estimators=300, n_jobs=-1,

Table S5- Summary of parameters for XGBoost classifier

Descriptors	**Parameters**
MACCS	colsample_bytree: 0.5, gamma: 0, learning_rate: 0.1, max_depth: 11, reg_lambda: 1, scale_pos_weight: 5, subsample: 0.8, tree_method: 'gpu_hist'
ECFP-4	colsample_bytree: 0.5, gamma: 0, learning_rate: 0.05, max_depth: 7, reg_lambda: 10, scale_pos_weight: 1, subsample: 0.8, tree_method: 'gpu_hist'
ECFP-6	colsample_bytree: 0.5, gamma: 0, learning_rate: 0.1, max_depth: 11, reg_lambda: 3, scale_pos_weight: 3, subsample: 0.8, tree_method: 'gpu_hist'
PubChem	colsample_bytree: 0.5, gamma: 0, learning_rate: 0.1, max_depth: 9, reg_lambda: 0, scale_pos_weight: 9,

	subsample: 0.8, tree_method: 'gpu_hist'
Estate	colsample_bytree: 0.5, gamma: 0, learning_rate: 0.1, max_depth: 7, reg_lambda: 0, scale_pos_weight: 5, subsample: 0.8, tree_method: 'gpu_hist'

Table S6- Summary of parameters for LightGBM classifier

Descriptors	**Parameters**
MACCS	num_leaves=15, reg_alpha=0.1, min_data_in_leaf=50, learning_rate=0.01, lambda_l1=0, lambda_l2=1
ECFP-4	num_leaves=30, reg_alpha=0.1, min_data_in_leaf=30, learning_rate=0.5, lambda_l1=1, lambda_l2=0
ECFP-6	num_leaves=20, reg_alpha=0.1, min_data_in_leaf=30, learning_rate=0.5, lambda_l1=1, lambda_l2=0
PubChem	num_leaves=10, reg_alpha=0.1, min_data_in_leaf=50, learning_rate=0.7, lambda_l1=1, lambda_l2=1
Estate	num_leaves=20, reg_alpha=0.1, min_data_in_leaf=30, learning_rate=0.3, lambda_l1=0, lambda_l2=1

Table S7. List of all the unique features extracted from the training dataset:

Features	['','[UNK]','C','=C','Branch1','Ring1', 'O','=Branch1', 'N','=O', 'Ring2', 'C@H1', 'C@@H1', 'Branch2', '#Branch1', 'S', '=N', '=Branch2', '#Branch2', 'F', 'Cl', 'C@@', '#C', 'C@', 'P', '/C', 'NH1', '=Ring1', 'N+1', '\\C', 'O-1', '/N', 'Br', '#N', 'I', '=S', '=N+1', '/O', '=Ring2', '\\O', 'S+1', '/C@@H1', '/C@H1', '\\C@H1', '\\N', '\\C@@H1', '=P', '=N-1', '/S', '/N+1', 'S@@+1', 'N@+1', 'N.N', 'N-1', 'C+1', '/Cl', '\\S', 'N@@+1', '/F', '-\\Ring2', 'S@+1', 'O.C', 'NH0', 'B', '=O+1', '#N+1', '\\F', '\\Cl', 'Xe', 'SiH3', 'SH0', 'S@@', 'Ring1.N', 'P+1', 'O+1', 'Ne', 'NH1-1', 'Li', 'Kr', 'CH1', 'C.N', 'C.C', 'C-1', 'Branch2.C', 'Ar', '=SH1','=P@@','/I','-/Ring2','#S@','#C-1']

Figures:

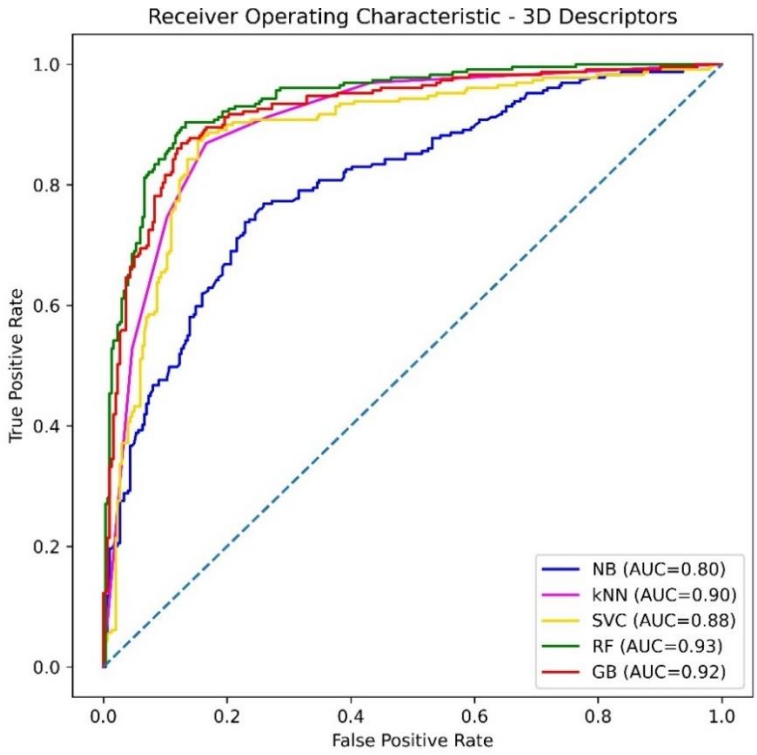


Figure S1- Receiver operating characteristics (ROC) curves of models build on 3D descriptors.

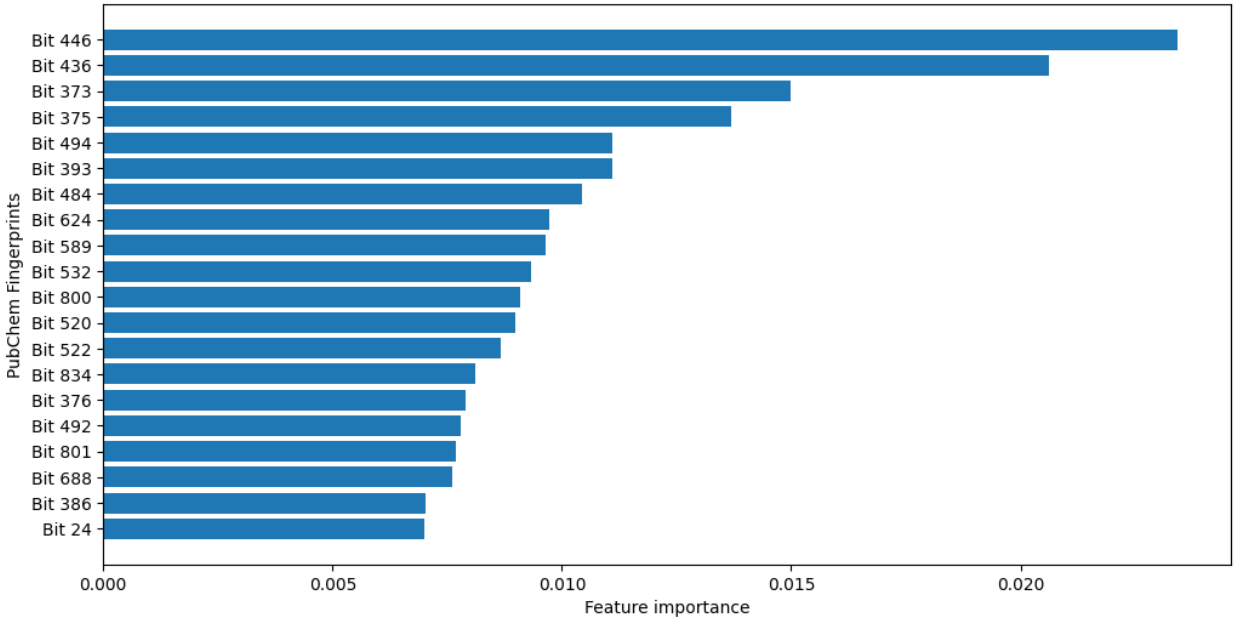


Figure S2- Feature importance of top 20 PubChem fingerprints obtained from the XGBoost model

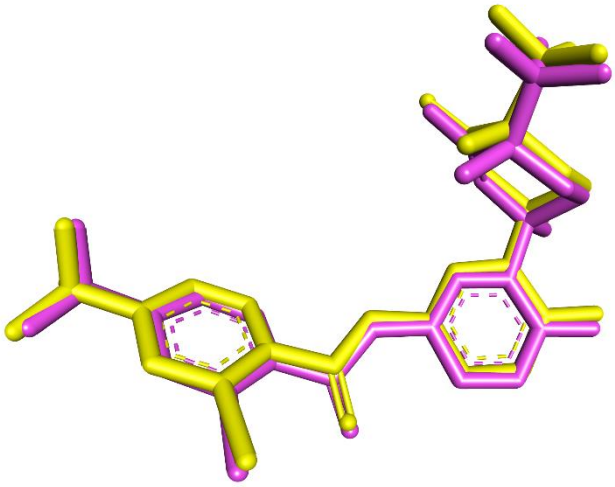


Figure S3- Superimposed structure of co-crystallized ligand (Yellow) and docked pose (Pink).

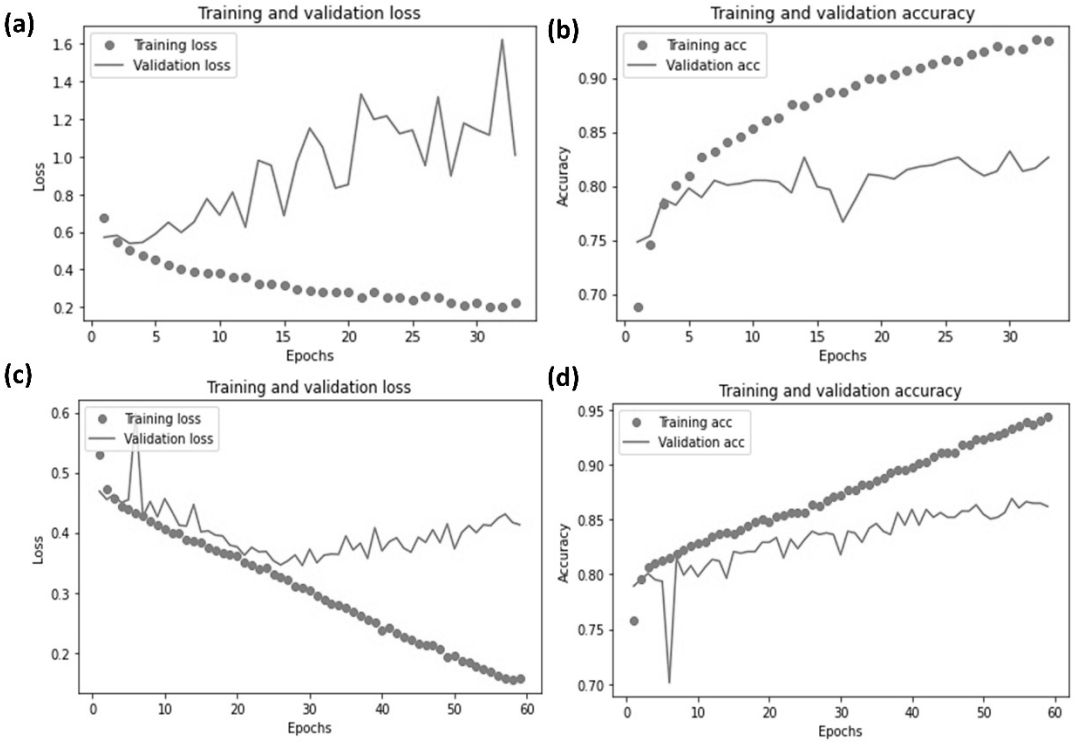


Figure S4- Performance of Model while training: (a) Training loss and validation loss for ANN-1 Model (b) Training and Validation accuracy for ANN-1 model (c) Training loss and validation loss for LSTM-1 Model (d) Training and Validation accuracy for LSTM-1 model

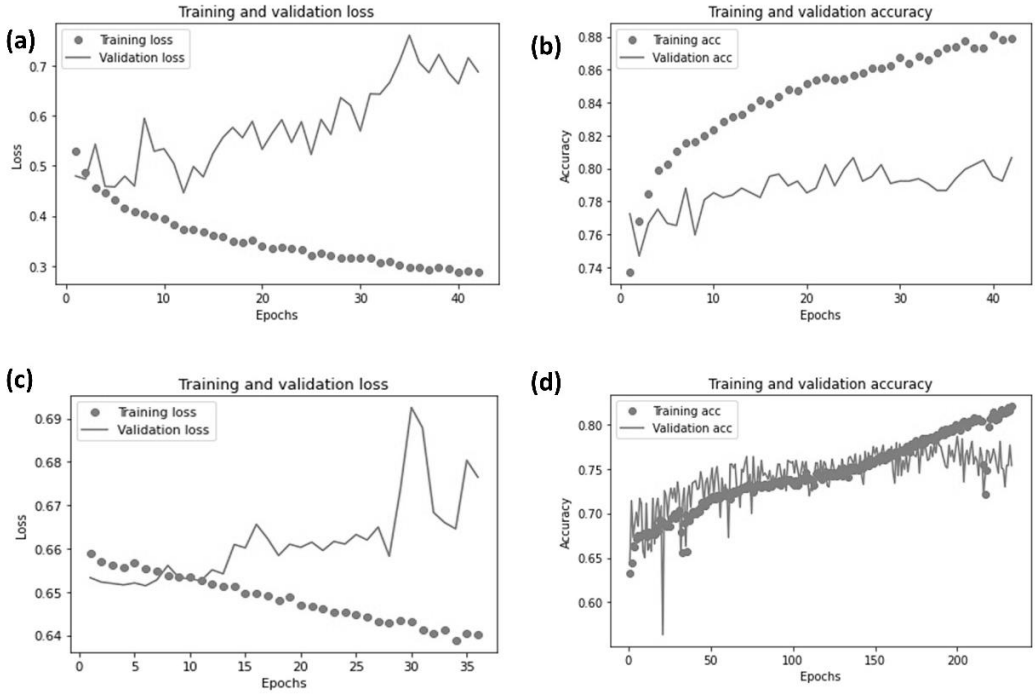


Figure S5- Performance of Model while training: (a) Training loss and validation loss for ANN-2 Model (b) Training and Validation accuracy for ANN-2 model (c) Training loss and validation loss for LSTM-2 Model (d) Training and Validation accuracy for LSTM-2 model

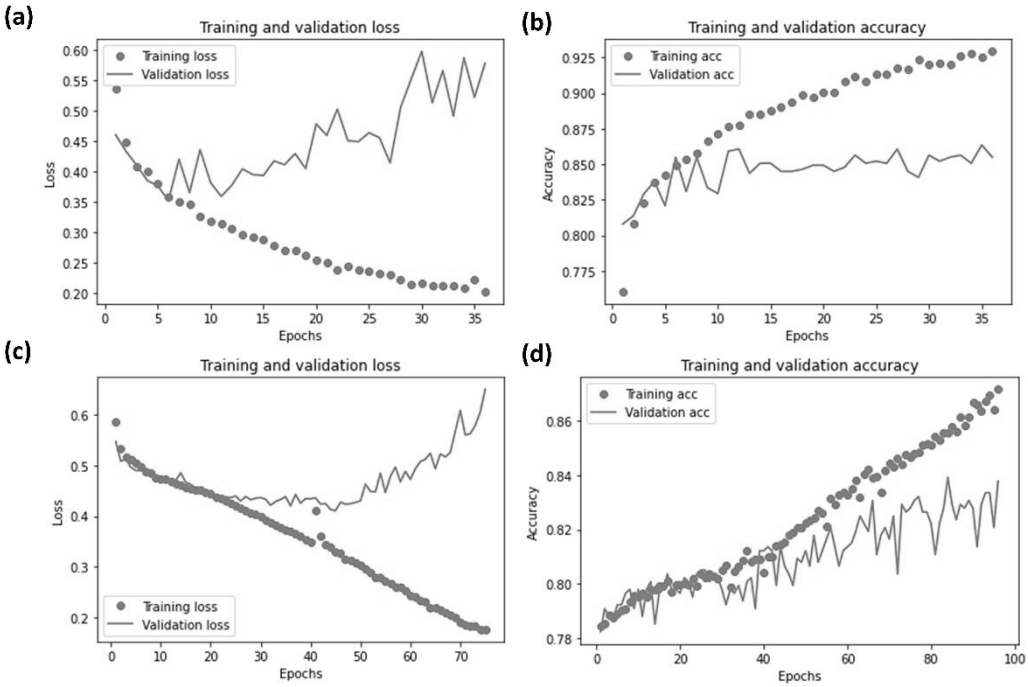


Figure S6- Performance of Model while training: (a) Training loss and validation loss for ANN-3 Model (b) Training and Validation accuracy for ANN-3 model (c) Training loss and validation loss for LSTM-3 Model (d) Training and Validation accuracy for LSTM-3 model

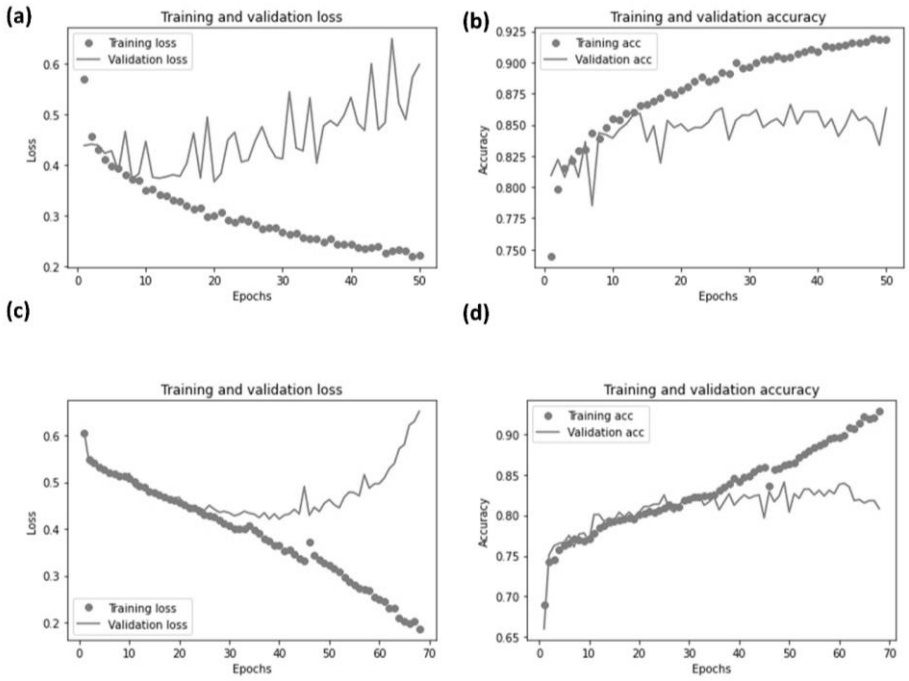


Figure S7- Performance of Model while training: (a) Training loss and validation loss for ANN-4 Model (b) Training and Validation accuracy for ANN-4 model (c) Training loss and validation loss for LSTM-4 Model (d) Training and Validation accuracy for LSTM-4 model

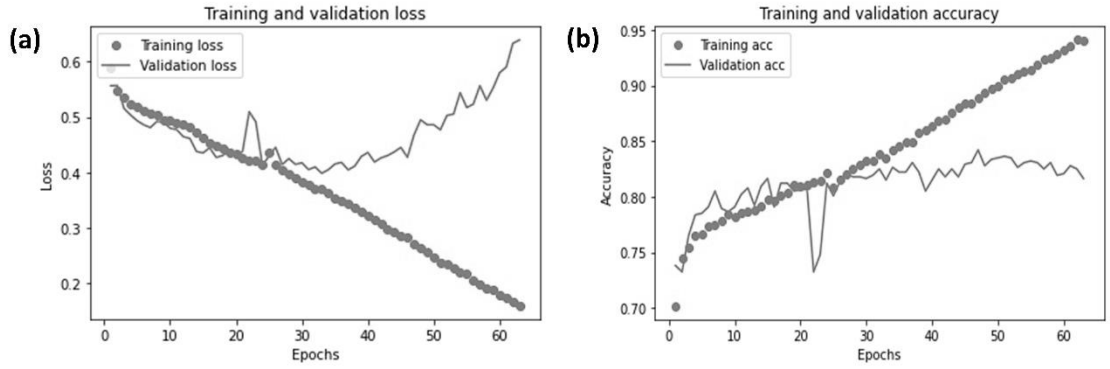


Figure S8- Performance of Model while training: (a) Training loss and validation loss for LSTM-5 Model (b) Training and Validation accuracy for LSTM-5 model

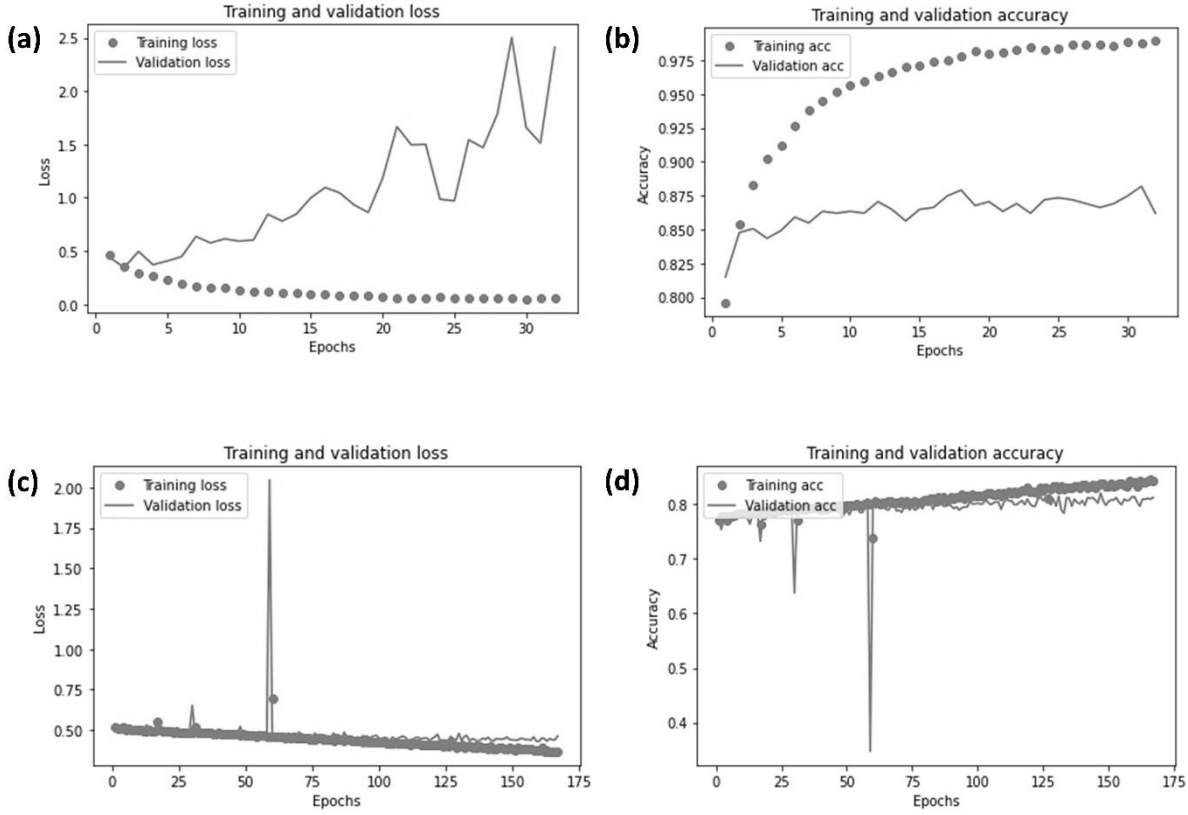


Figure S9- Performance of Model while training: (a) Training loss and validation loss for ANN-6 Model (b) Training and Validation accuracy for ANN-6 model (c) Training loss and validation loss for LSTM-6 Model (d) Training and Validation accuracy for LSTM-6 model

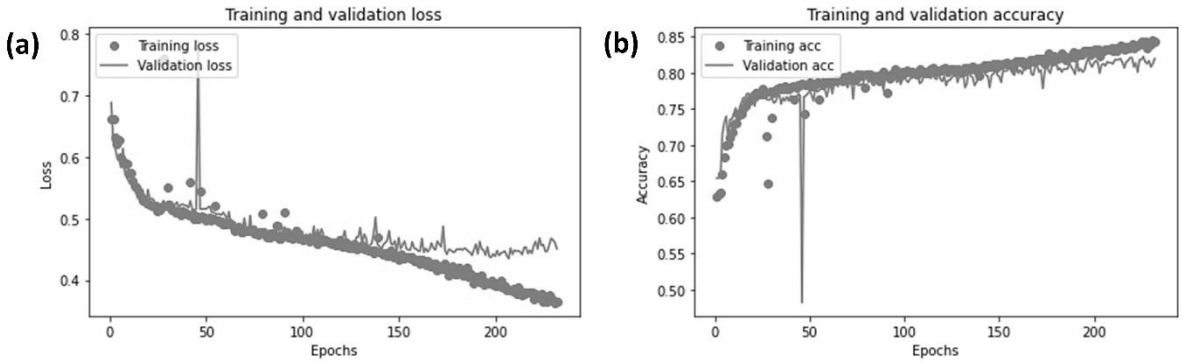


Figure S10- Performance of Model while training: (a) Training loss and validation loss for LSTM-7 Model (b) Training and Validation accuracy for LSTM-7 model

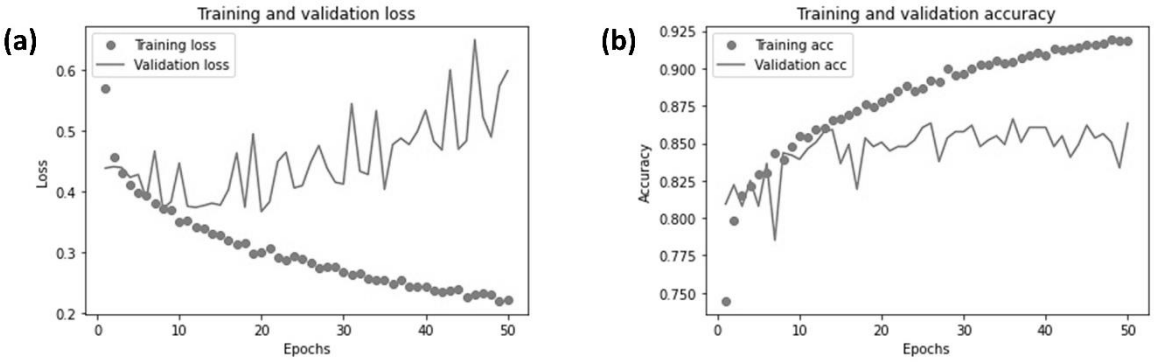


Figure S11- Performance of Model while training: (a) Training loss and validation loss for ANN-8 Model (b) Training and Validation accuracy for ANN-8 model

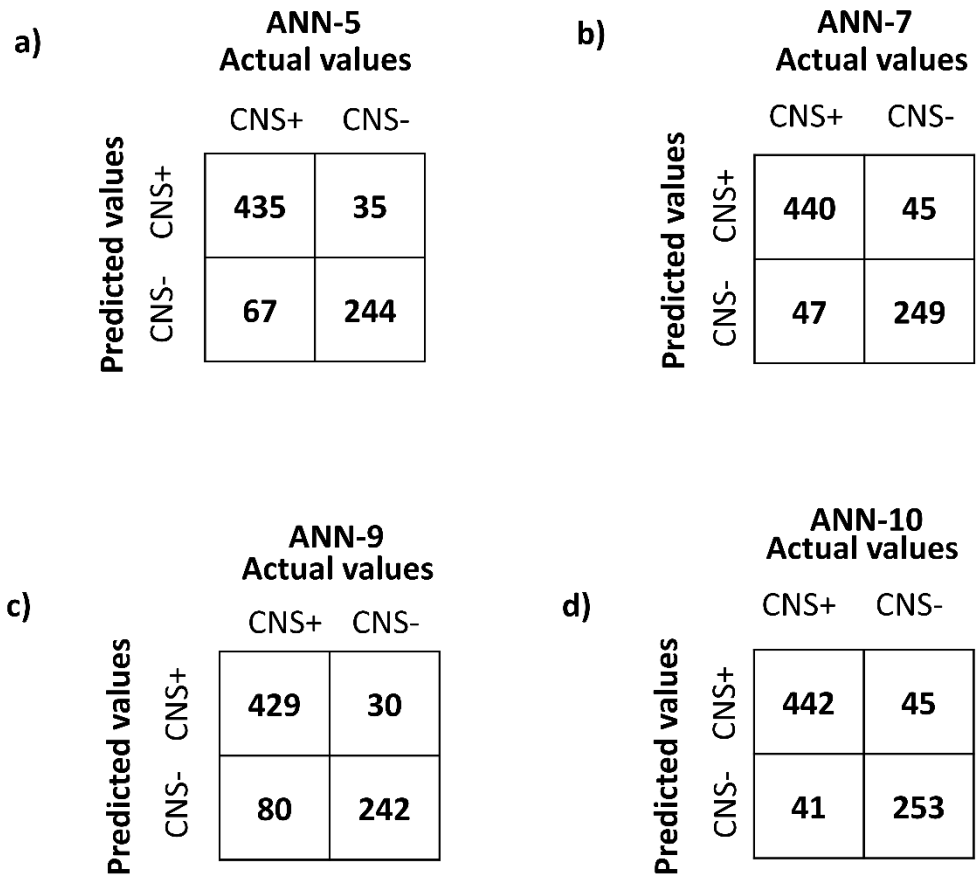
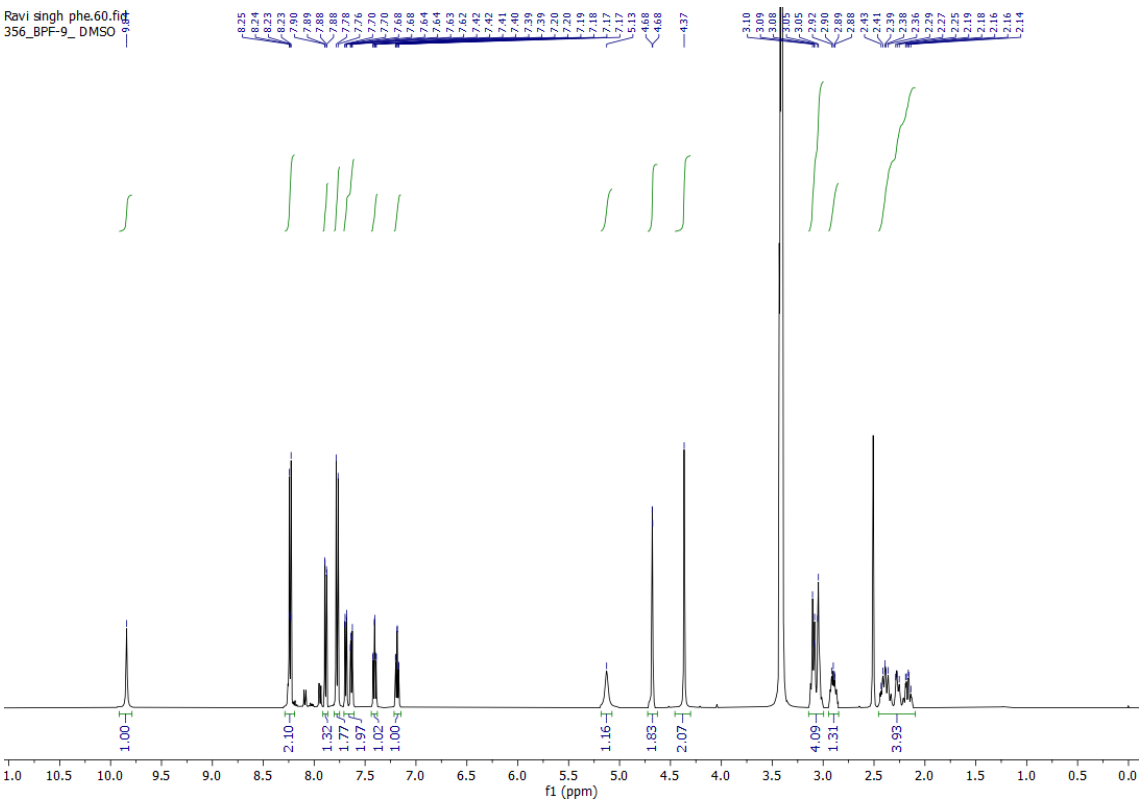


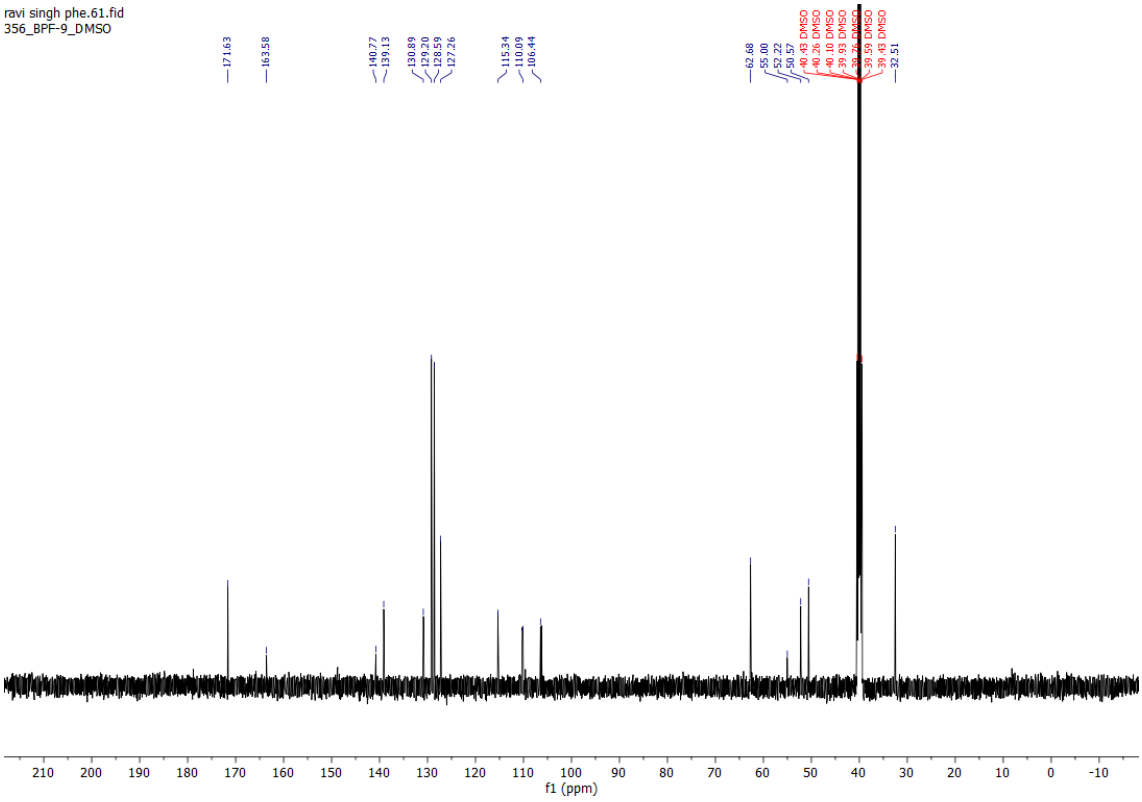
Figure S12- Confusion matrix of models on Test set: (a) ANN-5 model (b) ANN-7 (c) ANN-9 (d) ANN-10

Spectral data:

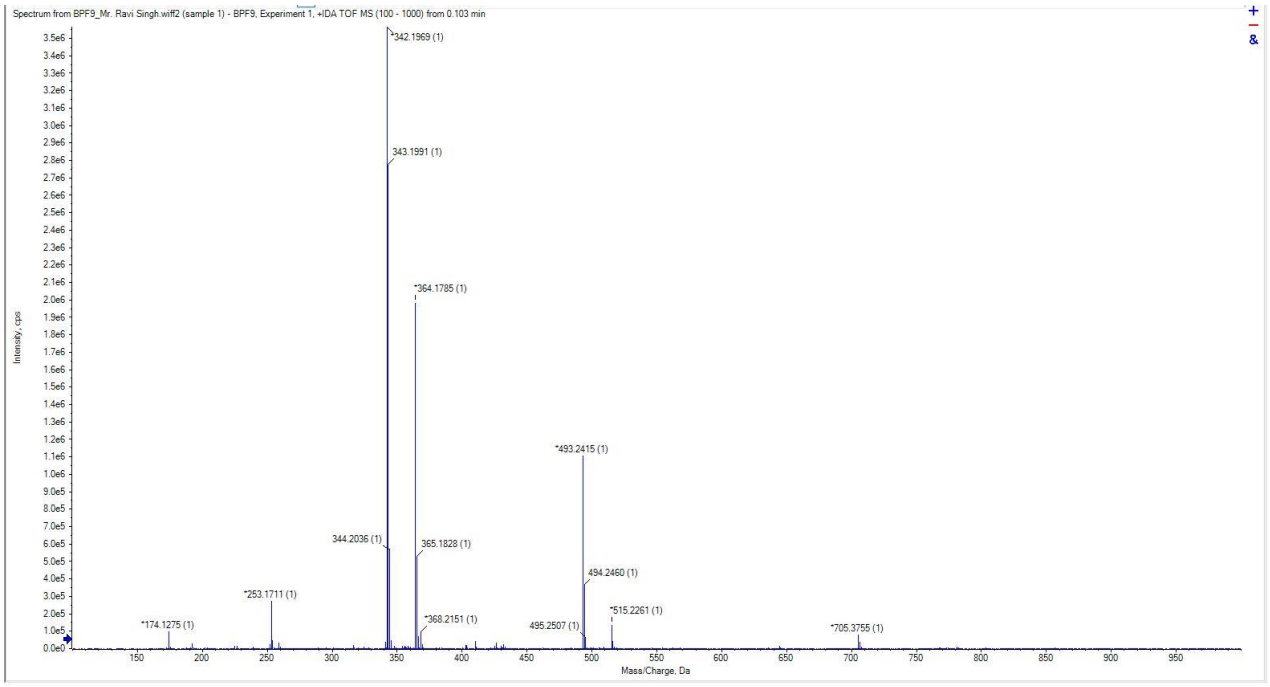
2-((1-benzylpiperidin-4-yl)amino)-N-(2-fluorophenyl)acetamide



Spectra 1. ^{1}H-NMR spectra of compound 66



Spectra 2. ^{13}C-NMR spectra of compound 66



Spectra 3. HRMS of compound 66

List of Publications

1. **Singh R**, Ganeshpurkar A, Ghosh P, Pokle AV, Kumar D, Singh Rb, Singh SK, Kumar A. 2021. Classification of beta-site amyloid precursor protein cleaving enzyme 1 inhibitors by using machine learning methods. *Chemical Biology & Drug Design*. 98(6):1079-1097.
2. **Singh R**, Anand A, Ganeshpurkar A, Ghosh P, Chaurasia T, Singh RB, Kumar D, Singh SK, Kumar A. 2023. Machine learning-based screening of in-house database to identify BACE-1 inhibitors. *Chemical Papers*. 77(11):6849-6858.
3. **Singh R**, Ghosh P, Ganeshpurkar A, Anand A, Swetha R, Singh RB, Kumar D, Singh SK, Kumar A. 2023. Natural-Language Processing (NLP) based feature extraction technique in Deep-Learning model to predict the Blood-Brain-Barrier permeability of molecules. *Molecular Informatics*. 42(10):2200271.
4. **Singh R**, Ganeshpurkar A, Singh SK, Kumar A, Design, synthesis and biological evaluation of N-benzylpiperidines as multi-target directed ligands for the treatment of Alzheimer's disease *(Manuscript under review*)