ADBA
Computers and Electronics in Medicine
Cutting-Edge Scientific Solutions

e-ISSN: 3023-8609
RESEARCH ARTICLE
Vol.3 / No.1 / 2026 / pp.36-41
https://doi.org/10.69882/adba.cem.2026014

Exploring the Chemical Space of BACE-1 Inhibitors: Structure-Based Prediction with Deep Learning and Machine Learning

Duygu Selen Yılmazcan [*,1] **and Muhammed Ali Pala** [α,β,2]

*Department of Biomedical Engineering, Sakarya University of Applied Sciences, Sakarya 54050, Türkiye, αDepartment of Electrical and Electronics Engineering, Faculty of Technology, Sakarya University of Applied Sciences, Sakarya 54050, Türkiye, βBiomedical Technologies Application and Research Center (BIYOTAM), Sakarya University of Applied Sciences, Sakarya 54050, Türkiye.

ABSTRACT The identification of effective inhibitors targeting β-site amyloid precursor protein cleaving enzyme-1 (BACE-1) is crucial for developing therapeutic strategies for Alzheimer's disease. This study developed a structure-based computational framework for predicting BACE-1 inhibitory activity using both deep learning and conventional machine learning techniques. A publicly available BACE-1 dataset with chemical structures defined in SMILES (Simplified Molecular Input Line Entry System) format was subjected to feature extraction using the RDKit program. Global molecular characteristics and substructural information were captured using both molecular fingerprint representations and physicochemical descriptors. Circular (Morgan/ECFP4) fingerprints, RDKit fingerprints, and MACCS keys were used to encode molecular substructures into binary vectors. Subsequently, Support Vector Machines (SVM), k-Nearest Neighbors (kNN), deep neural networks (DNN), and enhanced deep neural networks were trained and validated using these features under the same experimental conditions. Confusion-matrix analysis and standard classification metrics (accuracy, precision, recall, and F1-score) were used to assess the model's performance. Deep learning models outperformed traditional machine learning techniques in capturing intricate nonlinear structure–activity correlations, according to comparison research. The proposed enhanced DNN demonstrated balanced precision and recall across both classes and achieved an accuracy of 0.99 on a test set of 303 molecules, including 138 active inhibitors and 165 inactive non-inhibitors. All things considered, these results imply that deep learning models, in conjunction with molecular fingerprints, offer a robust and reliable approach to BACE-1 inhibitor prediction and could accelerate early-stage virtual screening. All experiments were conducted using a fixed random seed and a held-out random split to ensure reproducibility.

KEYWORDS
BACE-1 inhibitors
Deep learning
Machine learning
Molecular fingerprints
Structure activity relationship

INTRODUCTION

The most common cause of dementia globally, Alzheimer's disease, is a progressive neurological condition that primarily affects older persons (Knopman et al. 2021). Memory and other cognitive abilities gradually deteriorate because of the illness, which eventually affects independence and day-to-day activities. Alzheimer's disease has a significant macroeconomic impact on healthcare systems in addition to its dramatic effects on patients and caregivers. The need for more potent disease-modifying therapies is highlighted by the fact that, despite symptomatic therapies, current therapeutic options remain limited in their ability to prevent or reverse disease progression.

The build-up of β-amyloid (β) peptides is one of the main pathogenic characteristics of Alzheimer's disease at the molecular level (Hampel et al. 2023). The amyloidogenic processing of the amyloid precursor protein, involving multiple cleavage events, results in the production of β (Hampel et al. 2023). The first cleavage step that commits amyloid precursor protein to β synthesis is catalysed by β-site amyloid precursor protein cleaving enzyme-1 (BACE-1, β-secretase). As a result, pharmacological inhibition of BACE-1 has been extensively studied as a tactic to lower β formation and impede downstream aggregation-related processes, making BACE-1 a significant therapeutic target and an ongoing focus of drug development research (Coimbra et al. 2024; Ghosh 2024).

Simultaneously, the availability of vast biochemical datasets and the expansion of computational resources have made machine learning, especially deep learning, increasingly crucial in early-stage drug discovery (Zhang and Saravanan 2024; Pala 2025a). By learning quantitative structure–activity relationships (QSAR) from molecular representations, machine-learning-based screening can save time and money compared to conventional trial-and-error methods (Pala 2025b). Previous studies have reported the effectiveness of deep neural network–based approaches for drug interaction and bioactivity-related prediction tasks (Pala 2025c). DNNs are particularly well-suited to capturing nonlinear patterns in chemical data (Pala 2025a; Qian et al. 2023). Deep learning-based

Manuscript received: 21 November 2025,
Revised: 18 January 2026,
Accepted: 21 January 2026.

[1]25500305002@subu.edu.tr (**Corresponding author**)
[2]pala@subu.edu.tr

methods have also been shown to outperform traditional machine learning baselines for BACE-1 inhibitor prediction.

Inspired by these advancements, this study proposes a structure-based computational framework that utilises molecular information derived from SMILES strings to classify BACE-1 inhibitors. We extract a feature set comprising physicochemical descriptors generated with RDKit tools and fingerprint-based representations that encode substructural patterns. To facilitate a fair and direct comparison, we integrate these molecular representations into both deep learning architectures and traditional machine learning models, such as SVM and KNN, within a single experimental setup. All models are trained and evaluated on the same dataset and shared feature space, providing a controlled, systematic comparison of DNN-based and traditional ML approaches for differentiating BACE-1 inhibitors from non-inhibitors, in contrast to prior studies that primarily focus on a single modelling paradigm.

MATERIALS AND METHODS

Dataset

The dataset used in this study was obtained from an open-access BACE-1 inhibitor classification dataset widely used in the literature and contains a total of 1513 compounds with experimentally reported BACE-1 inhibitory activity (Wu et al. 2018). Each compound is represented in SMILES format and annotated with binary class labels (active/inactive), framing the prediction task as a binary classification problem (Weininger 1988; Lenselink et al. 2017).

The raw data were preprocessed to remove any erroneous or illegible molecular structures. The RDKit chemical computing library was then used to calculate molecular descriptors that quantitatively represent the compounds' structural and physicochemical properties. The calculated descriptors include molecular weight (MolWt), octanol/water partition coefficient (LogP), numbers of hydrogen bond donors and acceptors (HBD, HBA), topological polar surface area (TPSA), numbers of rotatable bonds, rings, and heavy atoms, and the carbon sp^3 ratio (FractionCSP3) (Todeschini and Consonni 2009). These descriptors are widely used in structure–activity relationship (SAR) modelling and exhibit strong discriminatory power for predicting inhibitory activity.

In addition to global physicochemical descriptors, molecular structures were also encoded using fingerprint-based representations to capture local substructural information. Circular and key-based molecular fingerprints were generated for each compound using the RDKit library. Circular (Morgan/ECFP4) fingerprints, RDKit fingerprints, and MACCS keys were used to encode molecular substructures (Rogers and Hahn 2010; Durant et al. 2002; Yang et al. 2019). Fingerprints encode molecular substructure patterns as binary vectors, enabling machine learning and deep learning models to learn structural similarities and recurring motifs among compounds effectively. This representation facilitates the incorporation of local chemical features that are not fully captured by traditional descriptor-based approaches. After feature generation, the dataset was split into training and test sets using a stratified random split with an 80/20 ratio, ensuring that the class distributions of active and inactive compounds were preserved across both subsets.

Table 1 summarises the various fingerprint types, computational factors, and basic characteristics used in this study. In this study, predicting BACE-1 inhibitor activity is treated as a binary classification problem. Both standard machine learning techniques and deep learning models were trained on a high-dimensional feature space comprising chemical IDs and fingerprint images. All models attempt to distinguish between inhibitory and non-inhibitory substances.

Machine Learning Models

Support Vector Machine (SVM) Support vector machines are supervised learning algorithms that try to maximise class separation by defining an ideal decision boundary (Cortes and Vapnik 1995). They produce effective results, particularly on high-dimensional and nonlinear datasets. In this study, kernel functions were used to create the SVM model and capture intricate interactions between chemical characteristics. SVM's fundamental purpose is to identify a hyperplane that maximises the margin between classes. The optimisation problem presetnted in Equation 1./2. is solved by minimising a regularised loss function, where x_i represents the molecular feature vector, y_i the class label, w the weight vector, b the bias term, and ξ_i the slack variables. The regularisation parameter C controls the trade-off between maximising the margin and allowing classification errors.

$$\min_{w,b,\xi} \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{N}\xi_i \tag{1}$$

$$y_i(w \cdot x_i + b) \geq 1 - \xi_i \tag{2}$$

Equation 1./2. The Support Vector Machine (SVM) optimisation issue is formulated mathematically, with the goal of maximising the margin between classes while permitting controlled misclassification using slack variables and the regularisation parameter C.

k-Nearest Neighbors (kNN) The k-nearest neighbour (kNN) algorithm is a sample-based classification method that accounts for similarities among samples (Cover and Hart 1967). A test sample's class is determined by the class labels of its k nearest neighbours in the feature space. When predicting activity based on molecular similarities, the kNN algorithm produces intuitive and effective results.

Equation 3 illustrates the class prediction rule of the kNN classifier, where $N_k(x)$ represents the set of k nearest neighbours of the test sample x, and $I(\cdot)$ denotes the indicator function. Distance between samples is measured using the Euclidean distance.

$$\hat{y} = \arg\max_{c} \sum_{i \in N_k(x)} \mathbb{I}(y_i = c) \tag{3}$$

Equation 3 decision rule of the k-Nearest Neighbors (kNN) classifier, where the predicted class is determined by majority voting among the k nearest neighbors in the feature space.

Deep Learning Models

Deep Neural Network (DNN) For binary classification, a feed-forward deep neural network architecture was used. In addition to batch normalisation, dropout regularisation, and early stopping to enhance generalisation and avoid overfitting, the model was trained with class weighting to mitigate potential class imbalance. Based on validation performance, hyperparameters were selected empirically. Multilayer artificial neural networks have been successfully applied to model complex nonlinear structure–activity relationships in various molecular property and drug interaction prediction tasks (Pala 2025a,b). These networks provide a hierarchical learning process that begins at the input layer and propagates through one or more hidden layers to the output layer (LeCun et al. 2015).

The following equation defines the output of a neuron in a fully connected neural network layer:

Table 1 Summarises the descriptive features, parameter settings, vector types, and dimensionalities of the chemical fingerprint representations used in this investigation.

Fingerprint Type	Description	Parameters	Vector Type	Bit Length
Morgan (ECFP4)	Circular fingerprints encoding atomic neighbourhoods up to a radius of two bonds	Radius = 2	Binary	1024
RDKit Topological (RDKFingerprint)	Path-based fingerprint encoding linear atom paths and molecular bonding patterns	Default	Binary	2048
MACCS Keys	Predefined chemical substructure keys representing common chemical patterns	166 keys	Binary	166

$$\mathbf{h}^{(l)} = f\left(\mathbf{W}^{(l)}\mathbf{h}^{(l-1)} + \mathbf{b}^{(l)}\right) \tag{4}$$

Equation 4. Forward propagation in a fully connected layer, where $\mathbf{h}^{(l)}$ denotes the activation vector of layer l, $\mathbf{h}^{(l-1)}$ the activations from the previous layer, $\mathbf{W}^{(l)}$ the weight matrix, $\mathbf{b}^{(l)}$ the bias vector, and $f(\cdot)$ the activation function.

Here, $\mathbf{W}^{(l)}$ represents the weight matrix, $\mathbf{b}^{(l)}$ the bias vector, and $f(\cdot)$ the activation function. For the binary classification problem, the sigmoid activation function is used in the output layer:

$$\sigma(z) = \frac{1}{1+e^{-z}} \tag{5}$$

Equation 5. Sigmoid activation function for binary classification, where the function maps real-valued inputs to the interval $(0, 1)$.

A binary cross-entropy loss function was selected to reduce the discrepancy between the expected outputs and the actual class labels during model training:

$$\mathcal{L} = -\frac{1}{N}\sum_{i=1}^{N}[y_i \log(\hat{y}_i) + (1-y_i)\log(1-\hat{y}_i)] \tag{6}$$

Equation 6. Binary cross-entropy loss function used for training the deep neural network, where y_i denotes the true class label, $\hat{y}_i$ the predicted probability, and N the total number of samples.

Improved Deep Neural Network Architecture A binary cross-entropy loss function was selected to reduce the discrepancy between expected outputs and actual class labels during model training. Several regularisation strategies were incorporated into the baseline DNN architecture to improve model performance and prevent overfitting. During training, a proportion of the network's neurons was randomly deactivated using dropout layers, which helps reduce co-adaptation of neurons and enhances generalisation (Srivastava et al. 2014). To address potential class imbalance in the dataset, class weights were incorporated into the training process, following strategies adopted in previous deep learning studies (Pala 2025a). Furthermore, an early stopping mechanism was employed to monitor the model's validation loss and terminate training once performance ceased to improve, thereby preventing unnecessary overtraining (Prechelt 1998). The hyperparameter configuration of the improved DNN model is summarized in Table 2.

EXPERIMENTAL RESULTS

This section presents and analyses the experimental findings from using deep learning and classical machine learning models on the BACE-1 dataset. Standard classification metrics, including accuracy, precision, recall, F1-score, and confusion matrices, were used to assess the model's performance (Sokolova and Lapalme 2009). These criteria provide a thorough evaluation of each model's ability to differentiate between BACE-1 inhibitors and non-inhibitors accurately. To guarantee the validity and applicability of the presented findings, all experiment was carried out on a separate test set. The efficacy of the deep neural network model in capturing intricate nonlinear correlations between chemical fingerprints and BACE-1 inhibitory activity was evaluated.Table 3 summarises the classification performance of the DNN model on the test dataset.

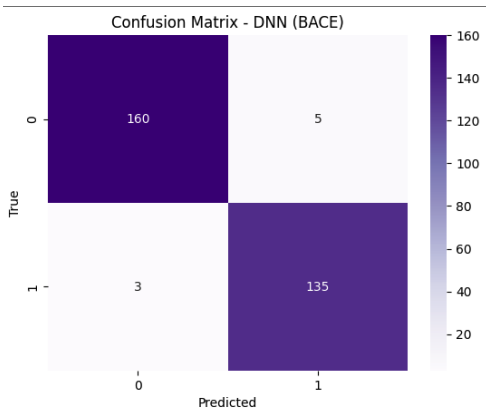

Figure 1 The confusion matrix of the DNN model illustrating its ability to correctly classify both inhibitory and non-inhibitory compounds, while revealing a limited number of misclassifications.

The performance of the proposed deep neural network (DNN) model was compared with that of traditional machine learning techniques, including Support Vector Machines (SVM) and k-Nearest Neighbours (kNN), to further evaluate the effectiveness of the proposed deep learning methodology. To ensure a fair and unbiased comparison, all models were trained and evaluated using identical molecular feature representations and the same held-out test dataset. Standard classification metrics were employed for the comparative analysis, enabling an objective assessment

Table 2 Hyperparameter configuration of the improved deep neural network (DNN) model used for BACE-1 inhibitor classification.

Hyperparameter	Value	Description
Neurons per layer	512–256–128	Decreasing layer sizes (funnel-shaped architecture)
Activation function	ReLU	Nonlinear activation for hidden layers
Output activation	Sigmoid	Binary classification output
Loss function	Binary cross-entropy	Optimization objective for binary labels
Optimizer	Adam	Adaptive gradient-based optimizer
Learning rate	0.001	Initial learning rate for Adam
Batch size	32	Number of samples per gradient update
Max epochs	100	Upper bound; training may stop earlier with early stopping
Dropout rate	0.30	Regularization to reduce overfitting
Validation split	0.20	Fraction of training data reserved for validation

Table 3 Classification performance on the BACE-1 inhibitor prediction problem.

Class	Precision	Recall	F1-Score	Support
0	0.98	0.97	0.98	165
1	0.96	0.98	0.97	138
Accuracy			**0.97**	303
Macro Avg	0.97	0.97	0.97	303
Weighted Avg	0.97	0.97	0.97	303

of each model's capability to distinguish BACE-1 inhibitors from non-inhibitors.

Table 4 Standard classification criteria used to compare the performance of deep neural network designs and classical machine learning models on the BACE-1 inhibitor prediction problem.

Model	Accuracy	Precision	Recall	F1-score
SVM	0.97	0.97	0.97	0.97
kNN	0.82	0.82	0.82	0.82
DNN	0.97	0.97	0.97	0.97
Improved DNN	**0.99**	**0.99**	**0.99**	**0.99**

As shown in Table 4, the improved DNN model achieved the highest overall performance across all evaluation metrics, outperforming both classical machine learning methods and the baseline DNN architecture. While the SVM and standard DNN models demonstrated strong and comparable predictive performance, with an accuracy of 0.97, the kNN model exhibited substantially lower performance, indicating a limited ability to capture complex structure–activity relationships. In contrast, the improved DNN architecture achieved an accuracy of 0.99, along with precision, recall, and F1-score values of 0.99, highlighting its superior capability to model nonlinear relationships between molecular fingerprints and BACE-1 inhibitory activity. These results demonstrate the effectiveness of deep learning–based approaches, particularly optimised DNN architectures, for reliable inhibitor classification.

In addition to threshold-dependent performance metrics, receiver operating characteristic (ROC) analysis was conducted to evaluate the models' discriminative capability across varying decision thresholds. Unlike accuracy-based measures, ROC curves provide a threshold-independent assessment of classification performance, making them particularly suitable for imbalanced datasets such as BACE-1. The area under the ROC curve (AUC) reflects the overall ability of the models to distinguish between inhibitors and non-inhibitors. ROC curves are reported for classical machine learning models (SVM and KNN) to highlight their threshold-independent discrimination. In contrast, deep learning models were primarily evaluated using confusion matrices and standard classification metrics.

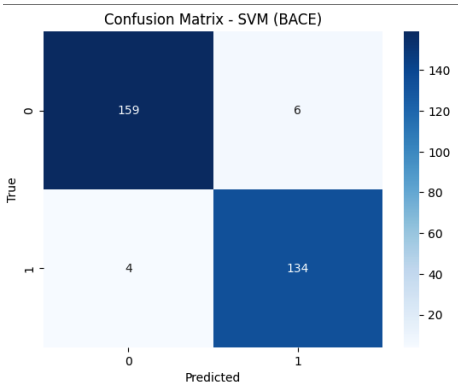

Figure 2 (a)

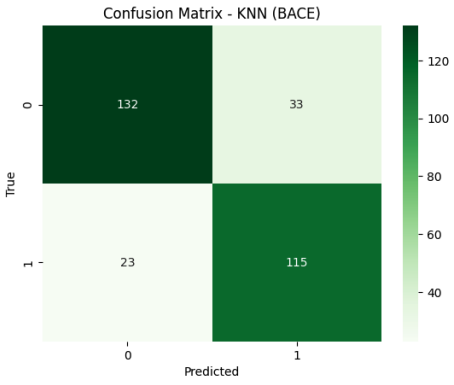

Figure 2 (b)

Figure 2 The confusion matrices of SVM and kNN highlight the differences in their classification behavior, with SVM exhibiting fewer misclassifications compared to kNN.

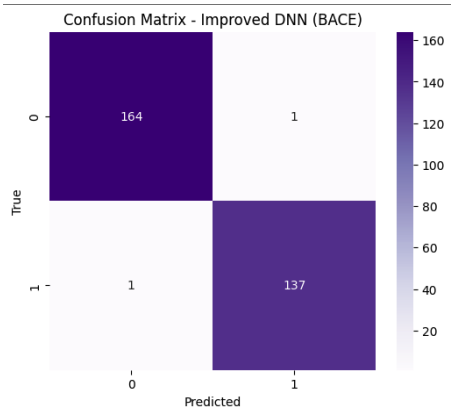

Figure 3 Compared to the baseline DNN, the improved DNN confusion matrix demonstrates a further reduction in classification errors, indicating enhanced generalisation capability.

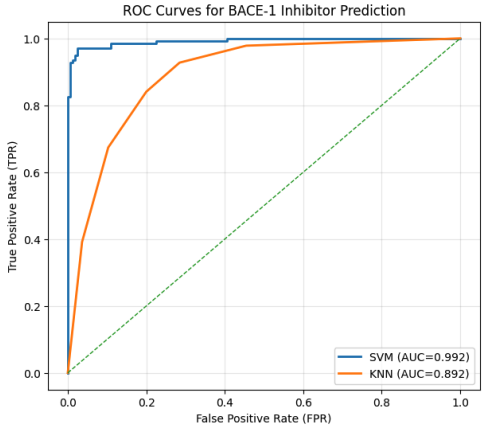

Figure 4 ROC curve analysis indicating that classical machine learning models, particularly SVM, exhibit strong discriminative capability for BACE-1 inhibitor prediction.

CONCLUSION

This study integrated chemical descriptors and fingerprint-based representations to develop a structure-based machine learning framework for predicting BACE-1 inhibitory activity. To assess how well deep learning techniques and classical machine learning models, such as Support Vector Machines and k-Nearest Neighbours, model the structure–activity relationships in the BACE-1 dataset. The experimental findings showed that deep neural network models outperform traditional techniques for extracting intricate nonlinear patterns from chemical fingerprint data. With an overall accuracy of 0.99, the enhanced DNN architecture outperformed SVM across prediction accuracy, precision, recall, and F1-score. These results show that for BACE-1 inhibitor classification tasks, deeper architectures in conjunction with optimised feature representations offer a substantial advantage. All things considered, the suggested method emphasises the promise of deep learning-based models as dependable and effective instruments for early-stage drug discovery, especially in the identification of prospective BACE-1 inhibitors. To improve predictive performance, future research might focus on extending this framework to regression-based activity prediction, external validation on separate datasets, and incorporating sophisticated representation learning methods, such as graph neural networks.

Ethical standard

The authors have no relevant financial or non-financial interests to disclose.

Availability of data and material

All datasets analysed in this manuscript are publicly available. The MoleculeNet datasets can be accessed at the following link: https://moleculenet.org/datasets-1.

Conflicts of interest

The authors declare that there is no conflict of interest regarding the publication of this paper.

LITERATURE CITED

Knopman, D.S., Amieva, H., Petersen, R.C. et al. Alzheimer disease. Nat Rev Dis Primers 7, 33 (2021). https://doi.org/10.1038/s41572-021-00269-y

Harald Hampel, Giuseppe Caruso, Robert Nisticò, Gaia Piccioni, Nicola B. Mercuri, Filippo Sean Giorgi, Fabio Ferrarelli, Pablo Lemercier, Filippo Caraci, Simone Lista, Andrea Vergallo, Neurodegeneration Precision Medicine Initiative (NPMI), Biological Mechanism-based Neurology and Psychiatry: A BACE1/2 andDownstream Pathway Model, Current Neuropharmacology; Volume 21, Issue 1, Year 2023, e011221198450. DOI: 10.2174/1570159X19666211201095701

Coimbra JRM, Resende R, Custódio JBA, Salvador JAR, Santos AE. BACE1 Inhibitors for Alzheimer's Disease: Current Challenges and Future Perspectives. Journal of Alzheimer's Disease. 2024;101(s1):S53-S78. doi:10.3233/JAD-240146

Arun K. Ghosh, BACE1 inhibitor drugs for the treatment of Alzheimer's disease: Lessons learned, challenges to overcome, and future prospects†, Global Health & Medicine, 2024, Volume 6, Issue 3, Pages 164-169, Released on J-STAGE July 02, 2024, Advance online publication June 06, 2024, Online ISSN 2434-9194, Print ISSN 2434-9186, https://doi.org/10.35772/ghm.2024.01033.

Haiping Zhang, Konda Mani Saravanan, Advances in Deep Learning Assisted Drug Discovery Methods: A Self-review, Current Bioinformatics; Volume 19, Issue 10, Year 2024, e290124226290. DOI: 10.2174/0115748936285690240101041704

Pala, M. A. (2025). XP-GCN: Extreme learning machines and parallel graph convolutional networks for high-throughput prediction of blood-brain barrier penetration based on feature fusion. Computational Biology and Chemistry, 120, 108755. https://doi.org/10.1016/j.compbiolchem.2025.108755

Pala, M. A. (2025). Graph-Aware AURALSTM: An attentive unified representation architecture with BiLSTM for enhanced molecular property prediction. Molecular Diversity. https://doi.org/10.1007/s11030-025-11197-4

Pala, M. A. (2025). DeepInsulin-Net: A deep learning model for identifying drug interactions leading to specific insulin-related adverse events. Sakarya University Journal of Computer and Information Sciences, 8(2), 245–259. https://doi.org/10.35377/saucis...1646658

Qian, C., Tang, H., Yang, Z., Liang, H., & Liu, Y. (2023). Can Large Language Models Empower Molecular Property Prediction? http://arxiv.org/abs/2307.07443

Wu, Z., Ramsundar, B., Feinberg, E. N., Gomes, J., Geniesse, C., Pappu, A. S., Leswing, K., & Pande, V. (2018). MoleculeNet: a benchmark for molecular machine learning. Chemical Science, 9(2), 513–530. https://doi.org/10.1039/C7SC02664A

Weininger, D. (1988). SMILES, a chemical language and information system. 1. Introduction to methodology and encoding rules. Journal of Chemical Information and Computer Sciences, 28(1), 31–36. https://doi.org/10.1021/ci00057a005

Lenselink, E. B., ten Dijke, N., Bongers, B., Papadatos, G., van Vlijmen, H. W. T., Kowalczyk, W., IJzerman, A. P., & van Westen, G. J. P. (2017). Beyond the hype: deep neural networks outperform established methods using a ChEMBL bioactivity benchmark set. Journal of Cheminformatics, 9(1), 45. https://doi.org/10.1186/s13321-017-0232-0

Todeschini, R., & Consonni, V. (2009). Molecular Descriptors for Chemoinformatics. Wiley. https://doi.org/10.1002/9783527628766

Rogers, D., & Hahn, M. (2010). Extended-Connectivity Fingerprints. Journal of Chemical Information and Modeling, 50(5), 742–754. https://doi.org/10.1021/ci100050t

Durant, J. L., Leland, B. A., Henry, D. R., & Nourse, J. G. (2002). Reoptimization of MDL Keys for Use in Drug Discovery. Journal of Chemical Information and Computer Sciences, 42(6), 1273–1280. https://doi.org/10.1021/ci010132r

Yang, K., Swanson, K., Jin, W., Coley, C., Eiden, P., Gao, H., Guzman-Perez, A., Hopper, T., Kelley, B., Mathea, M., Palmer, A., Settels, V., Jaakkola, T., Jensen, K., & Barzilay, R. (2019). Analyzing Learned Molecular Representations for Property Prediction. Journal of Chemical Information and Modeling, 59(8), 3370–3388. https://doi.org/10.1021/acs.jcim.9b00237

Cortes, C., & Vapnik, V. (1995). Support-vector networks. Machine Learning, 20(3), 273–297. https://doi.org/10.1007/BF00994018

Cover, T., & Hart, P. (1967). Nearest neighbor pattern classification. IEEE Transactions on Information Theory, 13(1), 21–27. https://doi.org/10.1109/TIT.1967.1053964

LeCun, Y., Bengio, Y., & Hinton, G. (2015). Deep learning. Nature, 521(7553), 436–444. https://doi.org/10.1038/nature14539

Srivastava, N., Hinton, G., Krizhevsky, A., Sutskever, I., & Salakhutdinov, R. (2014). Dropout: A simple way to prevent neural networks from overfitting. Journal of Machine Learning Research, 15(1), 1929–1958.

Prechelt, L. (1998). Early stopping—but when? In G. B. Orr & K.-R. Müller (Eds.), Neural networks: Tricks of the trade (pp. 55–69). Springer.

Sokolova, M., & Lapalme, G. (2009). A systematic analysis of performance measures for classification tasks. Information Processing & Management, 45(4), 427–437. https://doi.org/10.1016/j.ipm.2009.03.002

How to cite this article: Yılmazcan, D. S., and Pala, M. A. Exploring the Chemical Space of BACE-1 Inhibitors: Structure-Based Prediction with Deep Learning and Machine Learning. *Computers and Electronics in Medicine*, 3(1), 36-41, 2026.