IOSR Journal of Biotechnology and Biochemistry (IOSR-JBB)
ISSN: 2455-264X, Volume 11, Issue 6 Series 1 (Nov. – Dec. 2025), PP 01-10
www.iosrjournals.org

Integrative Workflow Of Biopython And Molecuar Docking To Explore Novel Therapeutics Targeting PARK7-DJ1

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Abstract
Parkinson's disease (PD) is a neurodegenerative affecting around 1 % population above the age of 50. Symptoms of PD usually show up post 50 years of age, however, young are not entirely exempted. Deregulation of cellular process associated with highly sensitivity of dopaminergic neurons and aging are one of the prime factors linked with PD. This study involves computational workflow combination of molecular docking and Biopython for the identification of prospective therapeutics that can potentially target the alpha-synuclein protein structure (PDB ID: 7C62). We used Biopython to retrieve and analyze the protein structure from the Protein Data Bank (PDB) and carried out both structural and sequence analyses to identify potential binding sites. A cavity detection–guided docking tool, B-dock, was applied to screen a library of natural and synthetic compounds for their binding affinity to the target protein. Docking results were further validated using AutoDock Vina. Protein–ligand interactions were examined using bioinformatics pipeline, while PDBsum was employed to generate interaction maps and confirm binding site predictions. This workflow identified several compounds with strong binding affinities that may inhibit α-synuclein aggregation, providing promising leads for Parkinson's disease therapeutics. The combination of bioinformatics, molecular docking, and structure-based drug discovery approaches enables efficient identification of potential candidates in the early stages of neurodegenerative disease research. Using in silico screening methods also reduces the need for extensive preliminary wet-lab work, minimizing resource use and supporting a more sustainable approach to drug discovery.

Keyword: *Parkinson's disease, Biopython, molecular docking, CB-DOCK, AutoDock Vina, Structure Analysis, PDBsum, drug discovery, Homology Modeling*

Date of Submission: 01-11-2025 Date of Acceptance: 10-11-2025

I. Introduction

Neurodegenerative diseases involve gradual degeneration and death of specific, vulnerable groups of neurons. (Ghosh, 2020). Some classic example of neurodegenerative diseases include: Parkinson's disease (PD), Huntington disease (HD), Amyotrophic lateral sclerosis (ALS), Alzheimer's disease (AD) Neurodegenerative diseases involve gradual deposition of proteins within specific brain areas (Logroscino *et al.*, 2022) Age is known to be the most significant risk factor contributing to the development of all neurodegenerative diseases, some studies suggest that the environmental factors and an individual's genetic makeup can equally be responsible for an increased risk of developing neurodegenerative diseases (Lamptey *et al.*, 2022). Neurons are not immortal however; the progressive loss of their function and/or structure is instrumental in the development of various brain related disorders.

As the brain has a control over many aspects of the bodily functions, neurodegenerative diseases can affect several facets of an individual's functioning and restrains the ability to perform complicated and basic tasks. Majority of the neurodegenerative disorders progress with remission whereas in certain cases, treatments can potentially show improvement in symptoms, pain relief if any characterized by restoration of mobility. (Lamptey *et al.*, 2022).

Parkinson's is a neurodegenerative disease that is age-dependent and progressive affecting around 1% of population over the age of 50. Its clinical manifestations include bradykinesia, tremor, postural instability, and cogwheel rigidity. (Krokidikis, 2019). Movement disorders such as tremor, elements of bradykinesia, rigidity, akinesia and hypokinesia along with postural abnormalities highly dominate the clinical syndrome called Parkinson's. Clinical syndrome of parkinsonism is linked with a distinct pathology that includes degeneration of pigmented brain stem nuclei consisting the dopaminergic substantia nigra pars compacta, with the appearance of Lewy bodies in remaining nerve cells. Some of the earliest recorded pathological modifications in PD have been

noted in olfactory bulb, pontine tegmentum/medulla oblongata. In early stages 1 and 2 patients often are pre-symptomatic. With the advancement in stages, 3 and 4 the basal forebrain, midbrain areas and substantia nigra begin getting involved. (Davie, 2008) Increasing number of single gene mutations have been detected even though PD is a sporadic disease. To date, the LLRK 2 gene or PARK 8 is the most prevalent cause of genetic or the 'sporadic' PD. KRRK2 mutations are detected in approximately 5-7% of patients with a family history of PD. Numerous single gene mutations such as DJ-1 and parkin having autosomal recessive pattern of inheritance may present with an early onset and relatively benign progression. (Davie, 2008)

Some common therapies administered for the management of PD include functional stereotaxic neurosurgery, pharmacotherapy, and supportive therapies including speech therapy, dietary measures, and physiotherapy. All therapies are for symptomatic management and as of now there is no therapy available that can prevent, stop, or slow down the manifestation of PD. (Oertel & Schulz, 2016) The risk of PD amyotrophic lateral sclerosis, and late-onset multiple sclerosis has significantly increased particularly in high income countries. Over the past few decades changing trends associated with neurological disorders have been reported. (Rocca, 2018)

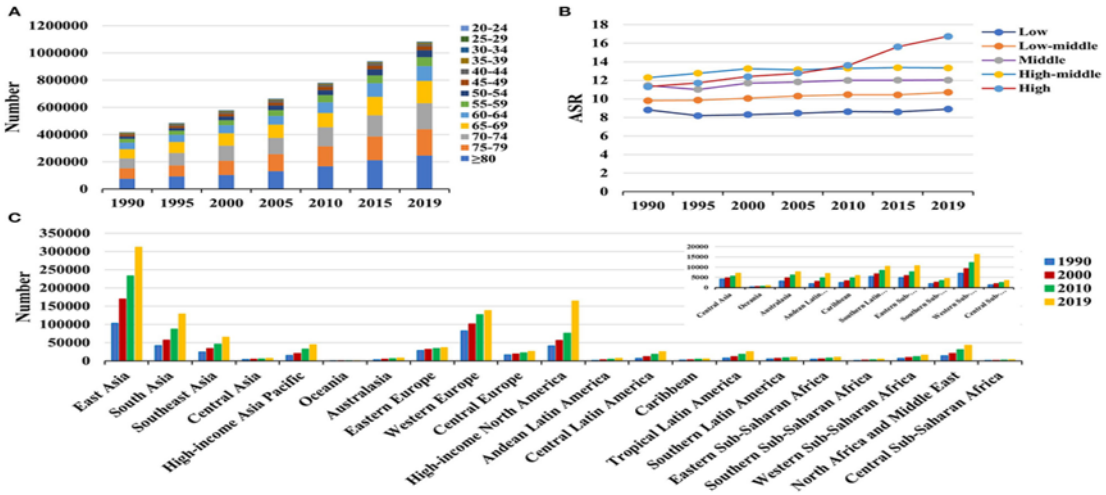


Figure 1: Incidence of Parkinson's disease from 1990 to 2019 is shown by age groups (A), age-standardized incidence rates in sociodemographic index areas (B), and case numbers by geographic regions (C). (Ou *et al.*, 2021)

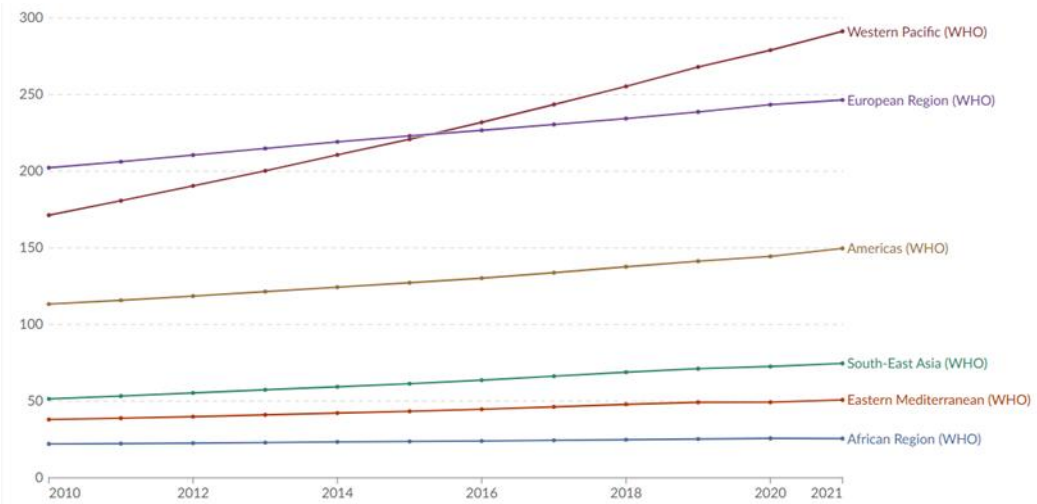


Figure 2: Parkinson's disease prevalence 2010 -2021 (Our World in Data. (2024)) Institute for Health Metrics and Evaluation (IHME) Global Burden of Disease Study 2021 (GBD 2021).

Computational methodologies, including molecular docking and bioinformatics, have arisen as potent instruments for discovering novel drug candidates by accurately predicting ligand-protein interactions (Meng et al., 2011). Molecular docking facilitates the prediction of binding affinities and orientations of small molecules within a protein's active site, hence optimizing drug discovery (Morris & Lim-Wilby, 2008). Tools such as CB-DOCK employ cavity-detection algorithms to enhance docking precision by identifying potential binding sites

(Liu et al., 2020). Molecular docking methods provide an efficient alternative to high-throughput random screening by enabling rapid virtual screening of ligand databases to identify potential leads (Gschwend et al., 1996). Visualization software such as PyMOL and RasMol allows detailed examination of ligand–protein interactions, while PDBsum generates comprehensive interaction maps to validate docking results (Laskowski et al., 2018). Protein structures from the Protein Data Bank (PDB) can be easily retrieved, analyzed, and modified using the open-source bioinformatics library Biopython (Cock et al., 2009). The protein DJ-1 (PARK7) plays a crucial role in Parkinson's disease (PD), influencing cellular defense against oxidative stress, mitochondrial function, and antioxidant activity. Mutations in the PARK7 gene, which encodes DJ-1, are linked to autosomal recessive juvenile Parkinsonism (ARJP), an early-onset form of PD. This study outlines a computational workflow integrating Biopython, molecular docking tools such as AutoDock Vina, and visualization platforms to identify potential therapeutic compounds targeting α-synuclein in PD. The workflow combines sequence analysis, structural modelling, and docking simulations to screen molecules with strong binding affinity. Since α-synuclein aggregation is central to PD pathology, compounds predicted to disrupt this process may serve as promising therapeutic leads. Furthermore, the framework is adaptable and reproducible, allowing its application to other protein targets implicated in neurodegenerative diseases

II. Materials And Methods

Molecular Visualization and Structural Analysis Using RasMol

The PARK7-DJ1 protein structure was examined using RasMol, a lightweight and easily accessible visualization tool widely used for molecular graphics. Its minimal processing requirements and open-source availability made it appropriate for a research workflow emphasizing energy efficiency and sustainability, avoiding the heavy computational load of larger visualization platforms. Protein structure files in PDB format were obtained from the Protein Data Bank (PDB). Before visualization, each file was checked for completeness and accuracy, and necessary corrections were made to address missing residues or atoms. Appropriate chain selection and symmetry operations ensured a biologically relevant representation of the protein complex. The use of RasMol's command-line features allowed visualization to be automated across multiple datasets, maintaining consistent orientations and display settings while saving time and computational effort. Different molecular representations were selected according to the focus of analysis. Colour coding was used to distinguish protein chains, secondary structures, and flexible regions, improving clarity without the need for additional software. RasMol also enabled direct measurements of angles, distances, and geometric relationships important for understanding active site configuration and molecular interactions. Comparative analyses were carried out by aligning similar protein structures to highlight conserved features and structural variations. For documentation, molecular images were exported using optimized settings that provided clear, publication-quality graphics without further rendering steps. This workflow supported a responsible, resource-conscious approach to structural bioinformatics, integrating scientific rigor with sustainable research practices.

Structural Validation Using the SAVE Server: A Sustainable Approach to Structural Integrity

To ensure structural reliability and maintain a sustainability-oriented workflow, all protein models used in this study were carefully validated through the SAVE (Structural Analysis and Verification Server) (Laskowski *et al.*, 1993; Pontius *et al.*, 1996). This integrated platform combines several trusted programs—PROCHECK, WHAT_CHECK, ERRAT, and VERIFY_3D—providing a comprehensive framework for assessing geometric and stereochemical integrity. Such validation minimized the risk of structural inaccuracies and prevented unnecessary computational effort associated with low-quality data.

Protein structures, submitted in PDB format, underwent detailed quality evaluation before inclusion in molecular docking or functional analyses. PROCHECK was used to examine both backbone and side-chain geometries, emphasizing Ramachandran plot distributions to identify residues in disallowed regions that might affect predictive accuracy. Chi-1/Chi-2 conformational checks verified side-chain orientations, while backbone parameters were compared against reference databases of high-resolution crystal structures. This early-stage scrutiny allowed potentially flawed models to be corrected or replaced, conserving time and computational energy in later stages. Additional assessment of atomic interaction patterns produced model quality scores that were benchmarked against experimentally validated structures. These comparisons helped filter out unreliable candidates before performing intensive docking simulations. VERIFY_3D further evaluated the sequence-to-structure compatibility of each model, analyzing residue environments against statistically derived profiles. This step was particularly valuable for detecting uncertain regions in homology-based or low-resolution structures, ensuring that computational resources were allocated efficiently. In keeping with principles of scientific transparency and resource-conscious research, models not meeting the established quality standards were either excluded from further analyses or clearly marked for conditional interpretation. When possible, alternative high-quality structures were substituted, reinforcing both reproducibility and robustness in the molecular docking studies of PARK7/DJ-1 (Protein Deglycase).

Eco-Efficient Structural Summary and Analysis with PDBsum in Drug Discovery

PDBsum serves as a critical resource in the structural analysis of protein structures, enabling detailed insights into protein architecture and function (Laskowski, 2001; Laskowski et al., 2018). This comprehensive database offers a range of tools to assess key structural features such as secondary structure, domain organization, ligand interactions, and structural integrity. By providing accurate structural summaries, Protein database sum helps establish a sustainable framework for understanding protein structure-function relationships, which is essential for advancing drug discovery while minimizing resource use and maximizing scientific impact. Protein database sum was utilized to systematically analyze all Protein Data Bank (PDB) entries associated with our research on the PARK7-DJ1 protein (a protein deglycase). Key aspects of the analysis, including secondary structure content, domain organization, and the identification of ligands or cofactors, were examined to ensure that structural interpretations align with the most reliable and sustainable scientific methods. The unification of PROMOTIF analysis in the scope of PDB sum was proven to be highly insightful due to its streamlining role in the pinpointing the structural motifs and super secondary elements, broadening our understanding for studying evolutionary linkages and potential treatment targets avoiding the need of excessive experimental efforts.

To ensure high-quality structural assessments, Ramachandran plot summaries were utilized to evaluate protein conformations, identifying any regions of concern to avoid errors in subsequent computational analyses. The contact analysis further provided valuable data on intramolecular interactions, offering insights into protein stability and minimizing the need for time-consuming manual exploration. Importantly, ligand interaction analyses allowed for an in-depth understanding of enzyme active sites, which is crucial for designing sustainable therapeutic interventions aimed at modulating PARK7-DJ1 activity, potentially with minimal environmental and material costs in future drug development. The CATH domain classification system was employed to explore protein fold families, thereby revealing evolutionary connections and identifying potential targets for therapeutic intervention. Structural alignment summaries provided quantitative data on protein similarities, further aiding the sustainable identification of novel druggable sites across related proteins. This streamlined process significantly reduces the time and resources typically required for structural exploration, promoting a more eco-efficient approach to drug discovery. The assembly of functional annotations into PDBsum enabled us to link structural characteristics with established functional properties of PARK7-DJ1, bolstering structure-based functional forecasting and the understanding of evolutionary influences. Moreover, quality assessment summaries, including validation metrics and geometric statistics, were scrutinized to confirm that the structural analyses were conducted with dependable and sustainable practices. By leveraging PDBsum's advanced capabilities, practices but also upholds the principles of sustainability in computational biology and drug discovery.

CLEFT: Sustainable Approaches in Ligand Binding Site Prediction and Drug Design

CLEFT (Computational Ligand Efficiency and Flexibility Tool) is a computational approach that aids in the identification and analysis of potential ligand-binding sites within protein structures, crucial for the rational design of therapeutics. By emphasizing the geometry and flexibility of protein binding sites, CLEFT provides valuable insights that support sustainable drug discovery processes, minimizing resource usage while maximizing scientific output. The tool plays a pivotal role in understanding the conformational flexibility of proteins, an essential factor in recognizing how proteins can interact with ligands in both static and dynamic forms. These insights are crucial in drug design, where reducing material waste, experimental efforts, and unnecessary synthesis steps aligns with the principles of sustainable science. By computationally mapping clefts, pockets, and cavities on the protein surface, CLEFT not only identifies potential binding sites but also evaluates their sustainability in the context of drug development. This includes an emphasis on designing molecules that can be synthesized with fewer resources, leading to more environmentally friendly processes.

Key features of CLEFT include:

1. **Binding Site Prediction and Sustainability**: The tool identifies and evaluates potential ligand-binding sites, emphasizing the discovery of sites that can be targeted using minimal experimental resources. By reducing the need for trial-and-error experiments, CLEFT streamlines the process, contributing to more resource-efficient drug discovery.
2. **Ligand-Protein Interaction Analysis**: CLEFT aids in understanding the interactions between ligands and protein targets, facilitating the development of drugs that are both effective and sustainable. This computational approach enables the identification of critical residues involved in ligand binding, allowing for the design of compounds with higher specificity, reducing the likelihood of off-target effects.
3. **Ligand Efficiency and Eco-friendly Drug Design**: By assessing ligand efficiency, CLEFT helps prioritize compounds that exhibit strong binding affinities with minimal structural modification, promoting the use of fewer chemical resources and optimizing lead compounds for sustainability in drug development. This efficiency also translates to lower environmental impacts during synthetic processes.

The integration of CLEFT into computational drug design not only accelerates the process of identifying promising therapeutic candidates but also contributes to reducing the environmental footprint of drug development, focusing on high-efficiency ligand-protein interactions, researchers can design more targeted and effective drugs, minimizing material usage and reducing the waste associated with traditional experimental drug screening methods.

Sustainable drug discovery depends primarily on computational tools like CLEFT that accelerate the design process and limit the use of unnecessary resources. through precise identification and evaluation of ligand-binding sites, CLEFT allows researchers to design therapeutics that are not only innovative but also eco-conscious. (Huggins et al., 2018; Ghosh et al., 2020).

Web server Docking: A Key Tool for Sustainable Docking Studies in Drug Discovery

In this study, **CB-Dock**, a computational docking platform, was incorporated to enhance the process of identifying potential therapeutic targets within the **PARK7-DJ1 protein**, an important molecule associated with **neurodegenerative disorders**. The use of CB-Dock streamlined protein–ligand docking simulations, improving both scientific efficiency and environmental sustainability (Uma Kumari, Karren *et al.*, 2025). As an open-access docking framework, CB-Dock accurately predicts ligand-binding pockets and optimizes docking conformations, enabling efficient exploration of protein–ligand interactions without extensive laboratory experimentation. This computational approach reduced the environmental and financial costs typically involved in early-stage drug discovery, aligning with the principles of sustainable biomedical research.

Key Contributions of CB-Dock to the Research Workflow

Efficient Protein–Ligand Docking: CB-Dock employs a refined docking algorithm capable of rapidly modelling the interaction between small molecules and target proteins. This allowed us to perform **virtual screening** of a large chemical library against PARK7-DJ1, leading to the identification of promising inhibitor candidates with minimal resource utilization. The reduced reliance on laboratory assays significantly decreased the carbon footprint of the initial screening process.

Accurate Binding Site Prediction: CB-Dock effectively identified potential ligand-binding regions within the PARK7-DJ1 structure. The high accuracy of this prediction minimized the need for experimental approaches such as **X-ray crystallography** or **NMR spectroscopy**, which are costly, time-consuming, and resource-intensive. This predictive strength is particularly beneficial given the structural complexity of PARK7-DJ1 and its functional significance in neuronal protection.

Sustainability in Drug Design: Automating the docking workflow through CB-Dock reduced the requirement for chemical reagents and biological samples commonly used in conventional drug discovery. Consequently, this contributed to an **eco-conscious drug design** model, lowering energy and material consumption while maintaining research precision and reproducibility.

High-Throughput Virtual Screening: Using CB-Dock's server-based environment, a high-throughput virtual screening was conducted to evaluate diverse chemical scaffolds as potential PARK7-DJ1 inhibitors. This entirely computational step enabled the prioritization of viable candidates for later experimental validation, minimizing unnecessary wet-lab efforts.

Open-Source Accessibility: The open-access nature of CB-Dock promotes collaboration and equitable access to computational resources. By eliminating licensing costs and enabling data sharing, it supports sustainable and inclusive research practices. Incorporating CB-Dock into our workflow not only improved the predictive accuracy of docking simulations but also advanced the goal of environmentally responsible drug discovery.

Biopython: Enabling Sustainable Bioinformatics in Drug Design

Biopython is a comprehensive, open-source bioinformatics library that simplifies the analysis of biological data, including protein sequences, structural information, and molecular simulations. In this study, Biopython was integrated into the computational framework to process and analyze PARK7-DJ1 (Protein Deglycase) efficiently. Its broad functionality supported sustainable research by automating data handling and reducing time, computational cost, and material use.

The automation of protein structure analysis through Biopython's parsing modules enabled rapid extraction and interpretation of PARK7-DJ1 features, such as secondary structures and binding motifs. This computational approach replaced several manual steps, minimizing experimental resource consumption. Additionally, sequence alignment tools in Biopython facilitated comparison with homologous proteins, revealing conserved motifs that could indicate potential binding sites — improving the precision of subsequent docking analysis.

Another major benefit of Biopython was its data visualization capability. By employing its graphical components, protein structures and docking outcomes were efficiently visualized without the need for additional

commercial software. This not only streamlined result interpretation but also optimized computational resource usage. The seamless integration between Biopython and CB-Dock ensured an automated and coherent workflow from structural analysis to docking simulation, maintaining both scientific rigor and sustainability. From an environmental standpoint, Biopython contributed significantly by minimizing dependency on physical reagents, biological samples, and energy-demanding experimental assays. Its open-source nature and automated pipelines enhanced both the efficiency and eco-friendliness of the research process. The adoption of Biopython in this study underscores how **open-source computational tools** can drive sustainable innovation in drug discovery — promoting high-quality, reproducible, and environmentally responsible scientific exploration.

III. Results

Structure Validation Prediction

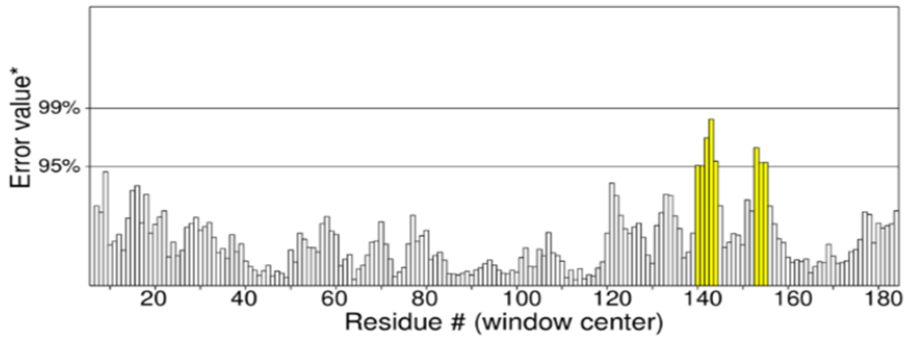


Figure 3: Structure validation graph shows per-residue error value mapped along a protein sequence (residue 1-180)

(Highlighted region (Yellow – residue (135-155) short segment show significant error)

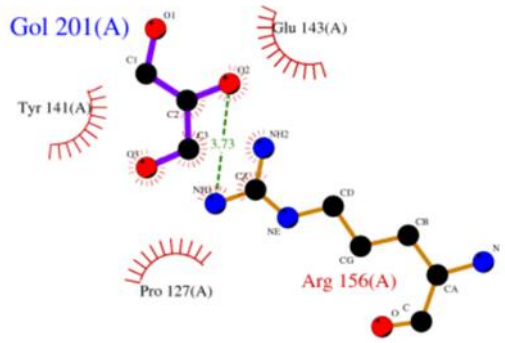


Figure 4: LIGPLOT analysis (ligand protein interactions) diagram highlight key residues involved in binding

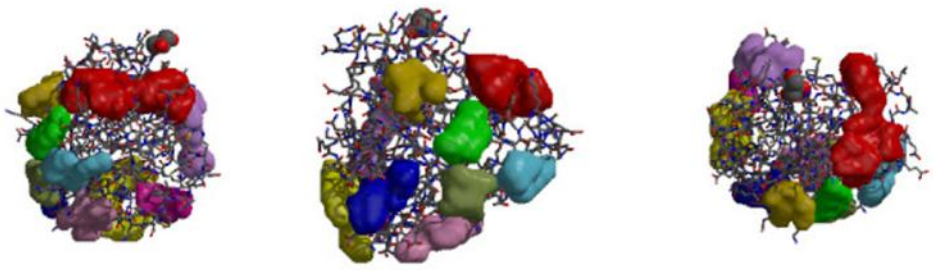
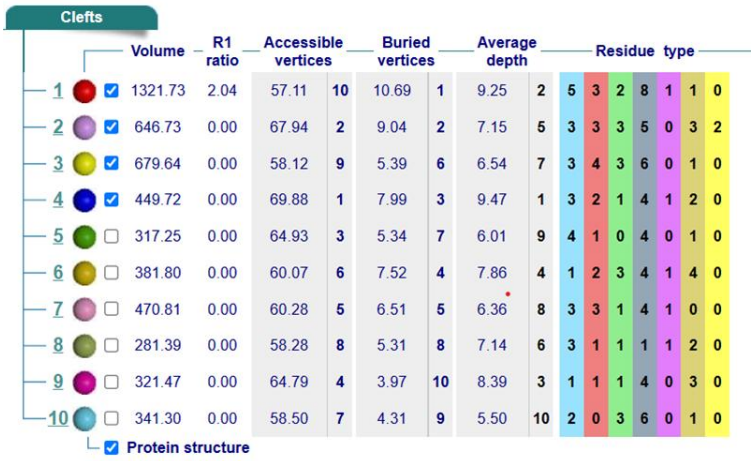


Figure 5: cleft analysis marked red area (pocket region) in protein structure

Analysis protein sample – 7c62 –

In PDBSUM, refers to the identification of cavities or pocket on the surface of protein structure. Structural biology tools (pdbsum) and computational drug discovery tools providing crucial in to protein function.



Clefts	Volume	R1 ratio	Accessible vertices		Buried vertices		Average depth		Residue type						
1	1321.73	2.04	57.11	10	10.69	1	9.25	2	5	3	2	8	1	1	0
2	646.73	0.00	67.94	2	9.04	2	7.15	5	3	3	3	5	0	3	2
3	679.64	0.00	58.12	9	5.39	6	6.54	7	3	4	3	6	0	1	0
4	449.72	0.00	69.88	1	7.99	3	9.47	1	3	2	1	4	1	2	0
5	317.25	0.00	64.93	3	5.34	7	6.01	9	4	1	0	4	0	1	0
6	381.80	0.00	60.07	6	7.52	4	7.86	4	1	2	3	4	1	4	0
7	470.81	0.00	60.28	5	6.51	5	6.36	8	3	3	1	4	1	0	0
8	281.39	0.00	58.28	8	5.31	8	7.14	6	3	1	1	1	1	2	0
9	321.47	0.00	64.79	4	3.97	10	8.39	3	1	1	1	4	0	3	0
10	341.30	0.00	58.50	7	4.31	9	5.50	10	2	0	3	6	0	1	0

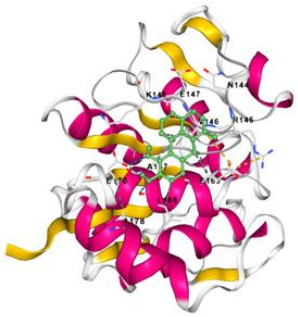
Protein structure

Figure 6: CLEFT analysis color chart used to represent various properties of CLEFT (binding pocket) on the protein surface.

(Each colour represents a specific type of residue on the basis of physiochemical properties around CLEFT)

Molecular Docking Analysis

1. APOMORPHINE

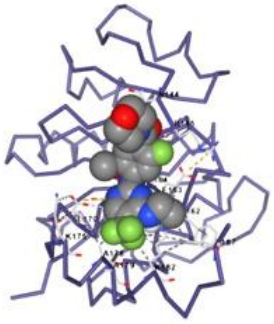


CurPocket ID	Vina score	Cavity volume (Å^3)	Center (x, y, z)	Docking size (x, y, z)
C5	-6.9	77	-16, 26, 8	19, 19, 19
C4	-6.5	84	-22, 42, 7	19, 19, 19
C3	-5.7	129	-36, 42, 9	19, 19, 19
C2	-5.6	207	-33, 38, -10	19, 19, 19
C1	-5.1	873	-34, 29, 9	19, 19, 19

Figure 7:(a) Protein -Ligand Interaction (b) Molecular docking Table with apomorphine

In this analysis this protein structure relevance to Parkinson disease where find Pocket Id C5 showing best binding site for ligand (Highlight by top vina score),vina score -6.9 indicate strong binding affinity, with cavity volume 77 Angstrom ,centre -16.28,8 (grid centre in molecular Docking, Docking Size 19,19,19 (grid box dimension).Protein structure ribbon form ,Ligand (green) docked in the active site pocket C5,interacting residue Chain A: MET17 ILE21 ASN144 ARG145 VAL146 GLU147 LYS148 PRO158 GLY159 THR160 SER161 PHE162 GLU163 LEU166 ALA167 GLU170 ALA178 LYS182 LEU185 VAL186 LEU187 LYS188 forming the interaction with ligand. Pocket C5 is the best site for docking inhibitor based on highest binding affinity (-6.9 Kcal/mol). The ligand fit in binding pocket with multiple interaction involving key active site residue this potential inhibition that help preserve dopamine level in Parkinson disease.

2.Gne-7915



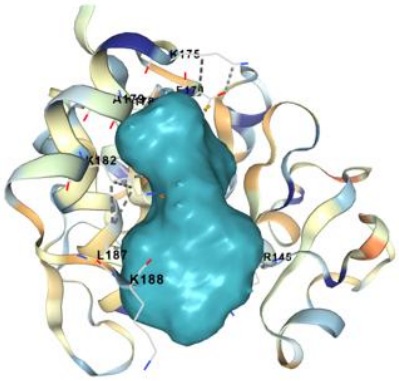
CurPocket ID	Vina score	Cavity volume (Å^3)	Center (x, y, z)	Docking size (x, y, z)
C5	-7.3	77	-16, 26, 8	25, 25, 25
C1	-6.2	873	-34, 29, 9	25, 25, 25
C2	-6.1	207	-33, 38, -10	25, 25, 25
C3	-6.0	129	-36, 42, 9	25, 25, 25
C4	-6.0	84	-22, 42, 7	25, 25, 25

Figure 8: (a) Protein – Ligand (Gne-7915) interaction (b) Molecular Docking table (7C62)

Crystal structure of the LRRK2 kinase domain analysis with vina score (C5) -7.3 Kcal/Mol (Strong binding affinity), cavity volume 77A, centre -16, 26, 8 and docking size (25*25*25). C5 pocket is the best binding site for GNE- 7915 based on negative vina score, despite its smaller cavity, it fits GNE- 7915 well, indicating specific binding site rather than random surface binding.

Gne-7915 binds effectively to the kinase domain LKKR2 (PDB: 7C62) with strong docking score suggesting it is high affinity inhibitor.

3.Opicapone



CurPocket ID	Vina score	Cavity volume (Å^3)	Center (x, y, z)	Docking size (x, y, z)
C5	-7.0	77	-16, 26, 8	23, 23, 23
C1	-6.6	873	-34, 29, 9	23, 23, 23
C2	-6.3	207	-33, 38, -10	23, 23, 23
C3	-6.3	129	-36, 42, 9	23, 23, 23
C4	-6.0	84	-22, 42, 7	23, 23, 23

Figure 9: (a) Protein – Ligand (Opicapone) interactions (b) Molecular docking Table with score (-7.0) Kcal/mol Opicapone and 7C62 show a strong binding affinity as there docking score results the value -7.0 Kcal/mol. The score -7.0 Kcal/mol is a favorable score in the docking studies as it is known to represent the compounds inhibitory action towards the protein. The docking score for Opicapone values -7.0 kcal/mol with COMT enzyme (PDB ID: 7C62) which indicates a strong, favorable binding affinity, supporting its role as a potent COMT inhibitor. The docking outcome reinforces its therapeutic potential and molecular efficacy.

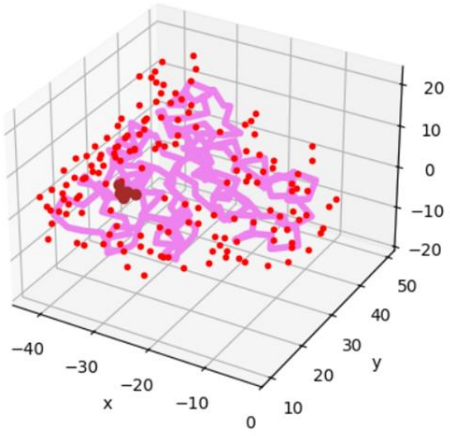


Figure 10: image of 3D Visualization of a protein structure in Biopython (Colab with Biopython and Matplotlib) (mpl_toolkits)

Above image showing backbone of the protein is represented by the purple ribbon or cartoon which trace the path of the main chain of the amino acid and the red dots scattered around the structure represent water molecules, dark brown cluster highlight specific ligand or active site component.

IV. Discussion

In this study we developed a computational workflow that integrated molecular docking tools such as AutoDock Vina, visualization tools including PyMol, RasMol for the identification of potential inhibitors against PD. This combination of workflow that incorporates structural modelling, sequence analysis and docking simulations has successfully resulted in recognition of compounds with high binding affinities. The result outcomes signal that these computational pipelines are significantly important for accelerating the research for potential candidate therapeutics against Parkinsons disease. Several such attempts have been made with studies focusing on Parkinson's and other disorders however; this approach integrates BioPython for pre-processing and its combination with other tools ensures a reproducible and streamlined computational pipeline. Another key

advantage of this strategy lies in its contribution to medical sustainability. Traditional drug discovery requires advanced laboratory setups, multiple experimental screenings, and considerable financial and material resources. In contrast, computational approaches can reduce dependence on such extensive wet-lab procedures during the initial stages of research, thereby saving time, minimizing waste, and lowering overall costs. This ensures that only the most promising drug candidates proceed to experimental validation. Such resource-conscious methodologies are especially valuable in neurodegenerative disease research, where complex disease mechanisms often make laboratory investigations both costly and labor-intensive.

V. Conclusion:

The workflow Combining with biopython for sequence/structure analysis with molecular docking using bioinformatics tools and software were precise identification of high -affinity ligands targeting the PARK7/DJ-1 protein, a key regulator in neurodegenerative disorders. The computational approach minimizes experimental waste, reduce the hazardous wet-lab screening and accelerates the discovery of potential therapeutic candidates. But using Insilco pipeline, research laboratory can lower their environmental footprints, promote safer occupational practices by limiting exposure of toxic chemicals

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