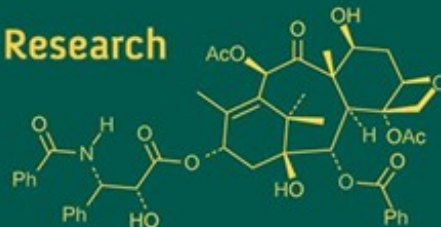
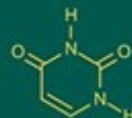


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Next-generation sequencing and computer-aided drug design for identification of novel therapeutic targets and drug candidates in glioblastoma

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ABSTRACT

Glioblastoma (GBM) is an aggressive primary brain tumour characterised by rapid proliferation, infiltrative growth, and resistance to conventional therapies. Mutations in isocitrate dehydrogenase 1 (IDH1), particularly at codon R132, are associated with glioma development and altered cellular metabolism. This study investigated the structural and functional characteristics of human IDH1 and identified potential drug candidates using an integrative computational biology and computer-aided drug design (CADD) approach. We retrieved the three-dimensional crystal structure of IDH1 (PDB ID: 8T7O) from the Protein Data Bank. We assessed sequence similarity, phylogenetic relationships, structural quality, conserved domains, and protein flexibility using BLASTP, BLAST Distance Tree Viewer, SAVES, ERRAT, PROCHECK, PyMOL, Jalview, InterProScan, and GeneWise. Molecular docking was performed with CB-Dock and AutoDock Vina to evaluate five candidate compounds: doxycycline calcium, minocycline hydrochloride, azithromycin, tigecycline, and dalfopristin. Structural validation yielded an ERRAT quality factor of 98.054%, with 91.7% of residues in the most favoured Ramachandran regions and no residues in disallowed regions. Sequence analysis revealed high conservation, while structural alignment produced RMSD values of 1.028 Å and 1.661 Å against PDB structures 8T7N and 3MAP, respectively. Docking analysis identified doxycycline calcium as the highest-scoring candidate, with a binding energy of -9.0 kcal/mol, followed by dalfopristin (-8.6 kcal/mol), minocycline hydrochloride (-8.5 kcal/mol), tigecycline (-8.0 kcal/mol), and azithromycin (-7.4 kcal/mol). These findings provide a computational foundation for further investigation of IDH1-associated glioblastoma therapeutics. Experimental validation and additional analyses are required to establish biological activity and therapeutic relevance.

Keywords: Glioblastoma, IDH, Next-generation sequencing, Bioinformatics, Computer-aided drug design, Molecular docking, Structural bioinformatic, Drug discovery

1. Introduction

Glioblastoma (GBM) is the most common and aggressive primary brain cancer, characterised by rapid proliferation, a highly infiltrative nature and intrinsic resistance to therapy [1-3]. These are intrinsic brain tumours thought to be of neuroglial progenitor cells origin [3]. Some subtypes of glioblastoma can be treated using surgery, and most of them are even resistant to surgery, radiotherapy and systemic chemotherapy [2, 3]. Recently, researchers found that somatic mutations in the gene encoding IDH1 cause 70% of secondary GBM and about 5% of primary GBM [4]. Most IDH1 mutations involve a single amino acid substitution at Arg132 (R132), and tumours show no loss of heterozygosity (LOH), leading to oncogenic activation of the enzyme [4, 5]. Isocitrate dehydrogenases (IDHs) catalyse the conversion of isocitrate to α -ketoglutarate. First, isocitrate is oxidised to oxalosuccinate, reducing NADP⁺ to NADPH. Then, in the second step, oxalosuccinate is converted to α -ketoglutarate by decarboxylation [6]. As an important enzyme in cellular metabolism, mutations can cause different types of cancer, including glioblastoma, acute myeloid leukaemia (AML), and chondrosarcoma [7].

Traditional drug discovery processes and clinical trials require time and are very costly. To address this, we use Modern bioinformatics tools. One of these is next-generation sequencing (NGS), which is a cost-effective tool and a revolution in the molecular biology field [8, 9]. Computational tools can be used for genomic-level detection and to understand their effect on the resulting protein. Next, at the sequence level, structural databases of IDH1 can be accessed from Protein Data Banks [10, 11].

Furthermore, Structure-based and ligand-based investigation of potential therapeutics related to mutant IDH1 can be done using computer-aided drug design (CADD) [12]. By using Molecular docking, interactions between the mutant IDH1 and the candidate compounds can be evaluated [12, 13]. This research inte

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grated next-generation sequencing tools and computer-aided drug design to identify novel therapeutic targets and drug candidates in glioblastoma.

2. Materials and methods

This study followed an integrative computational workflow in which we retrieved and validated protein structures. After validation, we performed sequence similarity, structural alignment, phylogenetic analysis, and structure-based molecular docking. A summary of these is discussed in the following subsection:

1. IDH1 Protein Structure and Sequence Retrieval:

The three-dimensional crystal structure of human IDH1 was retrieved from the Protein Data Bank (PDB ID: 8T7O) and downloaded in .pdb format [14, 15]. Along with the structure, the corresponding amino acid sequence was obtained in FASTA format from the NCBI Molecular Modelling Database (MMDB). This creates a connecting network among structural, sequence, and conserved-domain annotations to each PDB entry [15, 16].

2.2 Sequence Similarity and Phylogenetic Analysis

The retrieved FASTA sequence was submitted as a query to BLASTP (Basic Local Alignment Search Tool for Proteins) against the PDB protein database using default parameters [17-19]. Maximum score, query coverage, *E*-value, and percentage identity were used to evaluate homologous sequences [18, 19]. Phylogenetic relationships among the homologues were visualised using BLAST Distance Tree Viewer [20].

2.1 Protein structure validation

SAVES v6.0 server was used to assess the structure quality of the protein [21]. Overall model quality was evaluated using ERRAT on the basis of non-bonded atomic interaction statistics [22]. The structures are qualified as excellent ($\geq 95\%$), acceptable (80-90%) or requiring refinement ($< 80\%$) [22, 23]. Stereochemical quality was analysed using a Ramachandran plot, which shows the distribution of backbone dihedral (ϕ/ψ) angles across the most favoured, additionally allowed, generously allowed, and disallowed regions, generated through PROCHECK [24, 25].

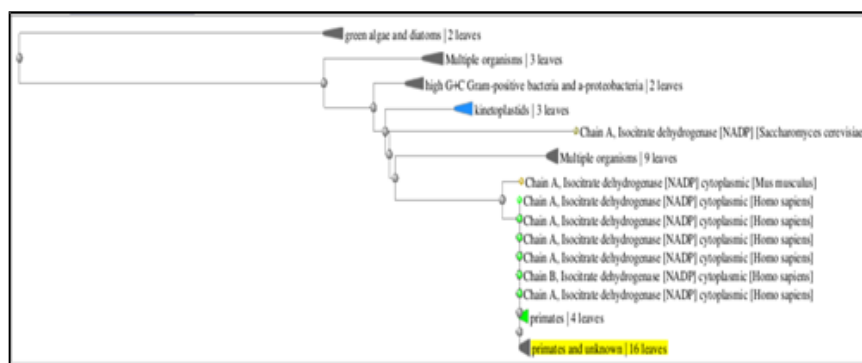


Figure 2. Phylogenetic tree generated with the Fast Minimum Evolution algorithm, showing evolutionary relationships among IDH1 homologues retrieved from the Protein Data Bank.

Structure visualisation, ligand contacts, and B-factor analysis

The validated IDH1 structure was visualized in PyMOL (Version 3.0, Schrödinger, LLC) [26]. The protein was visualised in cartoon (ribbon) representation with a white background, and water molecules were removed. The co-crystallised ligand was highlighted, and its binding pocket was visualised as a molecular surface, with contact residues labelled using PyMOL's annotation tools. PyMOL'S built-in distance tools were used to measure Hydrogen bonds and interatomic distances. To distinguish flexible, solvent-exposed regions from the

Multiple sequence alignments and Sequence conservation analysis
Jalview Desktop a cross-platform program was used for multiple sequence alignment editing, analysis and sequence conservation analysis of the protein [32]. 3D molecular structures of the protein (PDB ID: 8T7O) were uploaded in PDB format, and Jalview interpreted the structure in three ways: temperature factor, AlphaFold reliability, and Model quality. The alignment conservation is measured by the Conservation score or conservation factor [33, 34].

3. Results

3.1 Retrieval and Overview of IDH1

The crystal structure of human IDH1 (PDB ID: 8T7O) was successfully retrieved from the Protein Data Bank. It contains two chains: Chain A, the target protein, and Chain B, its binding partner. IDH1 catalyses the conversion of isocitrate into α -ketoglutarate. [4, 6]

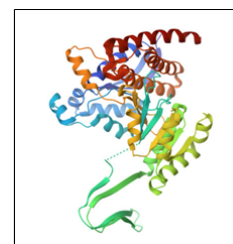


Figure 1. Crystal structure of the human IDH1 (PDB ID: 8T7O) retrieved from the Protein Data Bank.

3.2 Sequence Similarity Analysis and Phylogenetic Analysis

BLAST analysis demonstrates that the query protein exhibits 100% query coverage, 99–100% sequence identity, and an *E*-value of 0.0 with multiple experimentally resolved human Isocitrate Dehydrogenase 1 (IDH1) structures in the Protein Data Bank. These findings confirm that the query sequence is highly conserved and corresponds to human cytoplasmic NADP-dependent IDH1. The availability of several high-quality PDB structures makes this protein a reliable candidate for structural bioinformatics studies, molecular docking, mutation analysis, and structure-based drug discovery [35, 36].

stable protein core, pre-residue B-factors were extracted and mapped onto the structure [25, 26].

Molecular docking

Molecular docking was performed using the Cavity-detection guided blind docking tool server which automatically detects candidate binding cavities on the protein surface [27]. This all is done using its CurPocket algorithm and docks ligands into each predicted cavity with AutoDock Vina (version 1.1.2), without the need of predefined grid box [27-29]. The validated receptor (PDB ID: 8T7O) was uploaded in PDB format. Structure data files (SDF) for five candidate

ligands, Doxycycline calcium (PubChem CID 73415789), Minocycline hydrochloride (54685925), Azithromycin (447043), Tigecycline (54686904), Dalfopristin (6323289) were retrieved from PubChem and docked individually [30]. Predicted cavities were ranked by AutoDock Vina Score (kcal/mol) for each ligand. A more negative score indicated more favourable predicted binding. Alongside cavity volume ($\text{\AA}^3$) and docking-box dimensions [31].

Structural Quality Validation

ERRAT analysis of the IDH1 structure yielded an overall quality factor of 98.054%. PROCHECK requires a modelled protein file as input and generates a Ramachandran plot showing that, for the given pro-

tein, 91.7% (645), 7.7% (54), 0.6% (4), and 0% (0.0) of residues belong to the most favored, additionally allowed, generously allowed, and disallowed regions, respectively. The PROCHECK Ramachandran plot analysis showed that most amino acid residues occupy the most favored region, while the remaining residues further indicate that the experimental protein structure has good backbone stereochemical quality and is suitable for structural analyses, including docking and protein–ligand interaction studies. [37, 38]

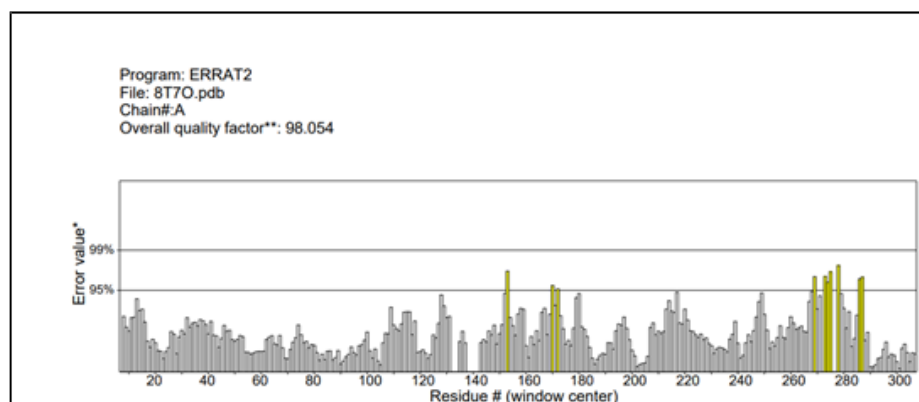


Figure 3. ERRAT validation plots of human IDH1 (PDB ID: 8T7O), showing an overall quality factor of 98.054%, indicative of excellent structural quality

Ramachandran plot for all residue types

PROCHECK Ramachandran plot for all residue types shows residue-specific Ramachandran plots, including Ala, Arg, Asn, Asp, Cys, Gln, Glu, Gly, His and other amino acids. Most residues are concentrated in the favourable regions around alpha- and beta-helix conformations; glycine shows a broader distribution, and proline shows a more restricted distribution. Overall, the protein structure appears to have a generally acceptable backbone conformation. [39, 40]

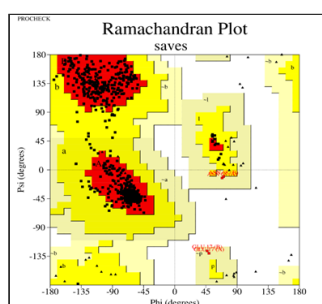


Figure 4. Ramachandran plot of human IDH1 (PDB ID: 8T7O) generated by PROCHECK, showing 91.7% of residues in the most favoured region and no residues in disallowed regions.

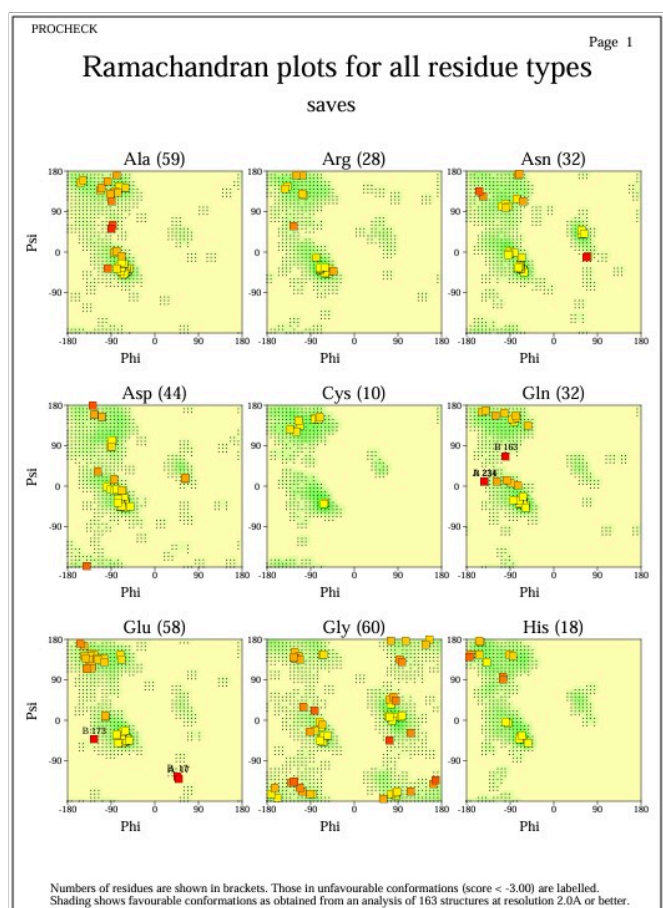


Figure 5. ProCheck Ramachandran plot for all residue types

3.6 Jalview analysis

The Secondary structure annotation shows alternating α -helices (red) and β -strands (green), demonstrating that both chains possess the same secondary structural architecture.

The sequence alignment indicates that chains A and B of PDB ID 8T70 are highly conserved, with nearly identical amino acid se-

quences across the aligned regions (residues 3–416 and 3–413). The Conservation track is predominantly high (yellow), showing that most amino acid positions are conserved between the chains and suggesting strong structural and functional similarity. The Quality score remains high for most residues, indicating a reliable alignment with only a few variable positions near the C-terminal region. The Temperature factor

(B-factor) profile is relatively stable, with minor fluctuations, suggesting that most of the protein is structurally ordered, while a few terminal or loop regions are more flexible. The Consensus sequence confirms that the aligned residues are largely identical, supporting a high degree of sequence identity and conservation. [41, 42]

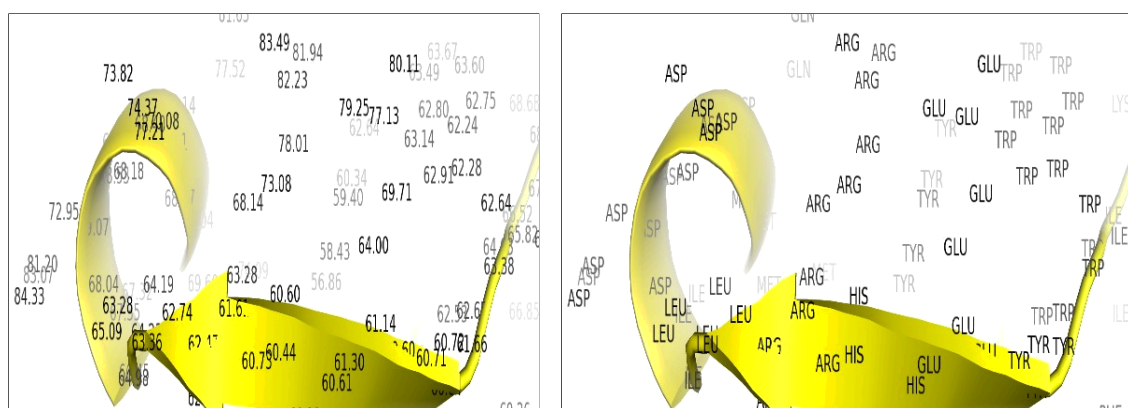


Figure 6. B-factor Analysis in PyMOL visualisation of a protein in cartoon (ribbon) representation with amino acid residues

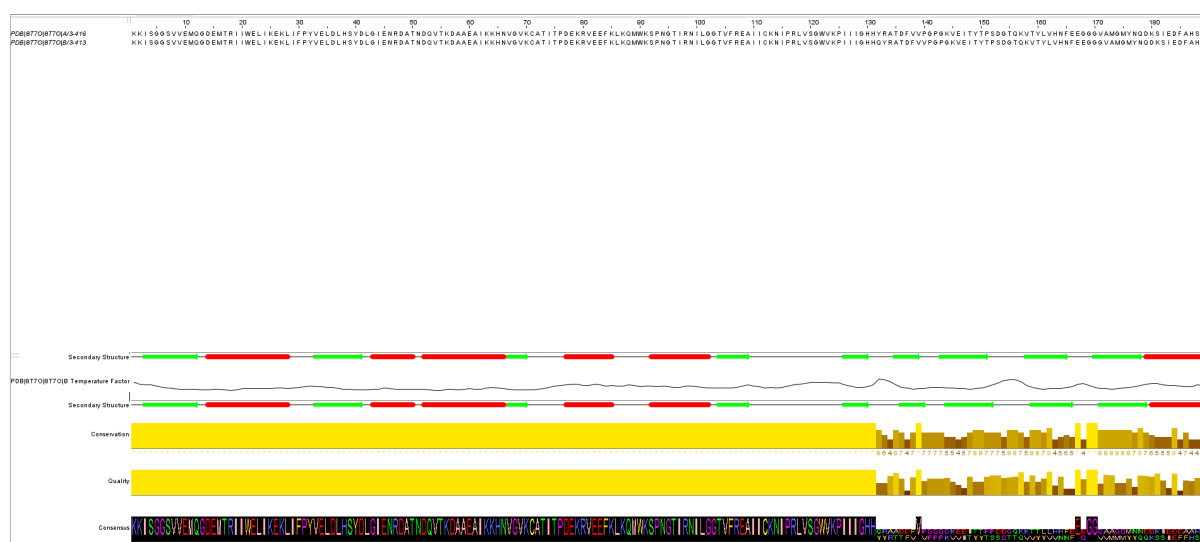


Figure 7. Jalview multiple sequence alignment of 8T70 analysis

RMSD Calculation:

Figure A shows excellent alignment, as typically observed for highly similar or identical structures, such as different models derived from the same crystallographic data or high-quality homologs. The large number of aligned atoms confirms that the overall protein architecture is nearly identical in the two structures. The alignment of PDB 8T70 and 8T7N demonstrates strong structural conservation, supported by an RMSD of 1.028 Å across 5,528 aligned atoms. This high-quality alignment provides a reliable basis for comparative analyses, including molecular docking, binding-site characterisation, mutational studies, and molecular dynamics simulations. [43, 44]

InterProScan

The following results were obtained from InterProScan after uploading protein sequences in FASTA format: Family: NADP-specific isocitrate dehydrogenase, Integrated: IPR004790, Model: PTHR11822:SF28 (3–410)

Domain: CATH-Gene3D; G3DSA:3.40.718.10; isopropylmalate dehydrogenase; Model: 5yzhB00 (1–414); Conserved site: detected around the middle region

PROSITE pattern: PS00470; isocitrate and isopropylmalate dehydrogenases signature; Integrated: IPR019818 (271–290), supporting en-

zyme activity

Conserved residue: PIRSR-PIRSR000108-1, residues 9–362 (functionally important amino acids); FunFam: (Functional family) FUNFAM G3DSA:3.40.718.10: FF: 000002, Isocitrate dehydrogenase [NADP], Model: 3.40.718.10-FF-000002 (2 – 413) [45, 46]

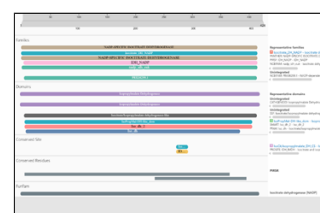


Figure 10. Protein Functional annotation/domain analysis of the protein sequence of 424 amino acids

GENEWISE Analysis

GENEWISE analysis generated an overall alignment score of 1003.21, indicating a strong protein-to-nucleotide alignment between

PDB ID 8T7O chain A and the IDH1 nucleotide sequence under the selected scoring and gene prediction parameters.

```

GENEWISE (Rfam: v1.2.1) (unreleased release)
This program is freely distributed under a GPL. See source directory
Copyright (c) 1998, Institute of the code and from separate copyright

Query protein:      pdh187701A
Comp Matrix:       BL05P02.his
Gap open:          12
Gap extension:     2
Start/End:         1-101
Target sequence:   101
Start/End:         101
Gene Parameter File: gow-1st
Updote site model: 07/00 only
07/00 site penalty: -9.96
Codon Table:       1a-06
Index score:       1a-06
Null model:       1a-06
Algorithm:         623

GENEWISE output
Score 1000.21 bits over entire alignment
Scores on bits over a synchronous coding model
Warning: The bits scores is not probabilistically correct for single steps
See 1000 help for more info

```

Figure 11. GENEWISE Alignment Analysis using query protein and target nucleotide sequence (IDH1 gene)

3.10 Molecular docking:

Five candidate ligands, Doxycycline calcium (PubChem CID 73415789), Minocycline hydrochloride (54685925), Azithromycin (447043), Tigecycline (54686904), and Dalfofpristin (6323289), were docked against the validated DYRK1A kinase domain using CB-Dock. For each ligand, CB-Dock evaluated five candidate cavities detected by its CurPocket algorithm, and we identified the top-ranked cavity for each ligand by its most negative AutoDock Vina score, as summarised in Table 1.

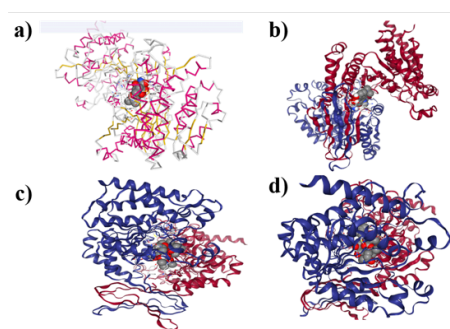
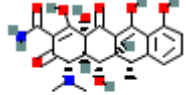
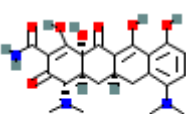


Figure 12. a) 3D molecular docking interaction of Doxycycline calcium within the binding region of the protein structure 8T7O (C1, most favourable docking cavity); b) 3D molecular docking interaction Minocycline hydrochloride with C1 as the most favourable docking cavity. c) 3D molecular docking interaction of Azithromycin with C4 as the most favourable docking cavity; d) 3D molecular docking interaction of Dalfofpristin with C1 as the most favourable docking cavity.

PubChem ID	Drug	Cur Pocket Id	Vina score(kcal/mol)	Cavity volume (Å ³)	Center (x,y,z)	Remarks
73415789		C1	-9.0	11423	32,-9,3	Best Docking affinity among the tested compounds
Doxycycline calcium						
54685925		C1	-8.5	11423	32,-9,3	Strong predicted binding affinity
Minocycline hydrochloride						

(continued on next page)



Table 1. Comparative molecular docking analysis of five candidate ligands against the IDH1 (PDB ID: 8T7O)

Figure 8. RMSD analysis of two proteomic sample with structural alignment (8T7O display green, 8T7N in yellow)

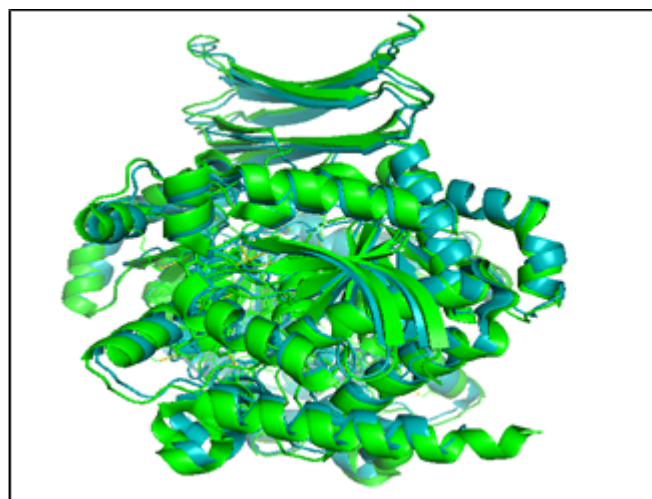
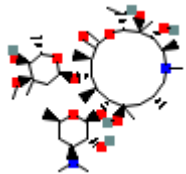
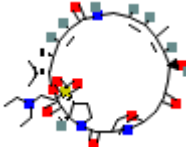


Figure 9. RMSD analysis of two proteomic samples with structural alignment (8T7O in green, 3MAP in teal)

447043		C4	-7.4	959	32,-5,17	Moderate Binding Affinity
Azithromycin						
54686904		C1	-8.0	11423	32,-9,3	Good binding affinity
Tigecycline						
6323289		C1	-8.6	11423	32,-9,3	Very Strong Binding affinity (second ranked among tested compound)
Dalfoprstin						

4.

Conclusion:

BLAST analysis: These analyses confirm the correct identification of the query protein and support the use of the protein, as well as the human and primate IDH1 Structure, for Comparative Structural analysis, Functional Studies, and Computer-aided drug design.

Jalview analysis of PDB ID 8T70 demonstrates very high sequence conservation and nearly identical secondary structural organisation between chains A and B. The consistently high conservation and quality scores indicate that these chains are structurally and functionally equivalent. Minor variations are limited to a few residues, mainly near the terminal region, and are unlikely to affect the overall protein fold or biological function significantly. [47, 48, 49, 50] Overall, the alignment supports the structural stability, evolutionary conservation, and functional reliability of the 8T70 protein, making it a suitable candidate for downstream structural analyses such as molecular docking, molecular dynamics simulation, and structure-based drug design. InterProScan annotation strongly indicates that the 424-amino-acid protein is an NADP-dependent isocitrate dehydrogenase (IDH). [51] Agreement among multiple protein-family and domain databases, along with conserved functional sites and residues, strongly supports that the protein contains the characteristic isocitrate dehydrogenase catalytic domain and likely catalyses NADP-dependent oxidative decarboxylation of isocitrate, producing α -ketoglutarate, CO_2 , and NADPH

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