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Original Article

Development Of Novel Benzimidazole Derivative: Synthesis Structural And Anti-Microbial Activity

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ABSTRACT

Benzimidazole plays an important role in the medicinal chemistry and drug discoverx with many pharmacological activities which have made an indispensable anchor for discovery of novel therapeutic agents. Substitution of benzimidazole nucleus is an important synthetic strategy in the drug discovery process. Therapeutic properties of the benzimidazole related drugs have encouraged the medicinal chemists to synthesize novel therapeutic agents Therefore, it is required to couple the latest information with the earliest information to understand the status of benzimidazole nucleus in drug discovery. In the present review, benzimidazole derivatives with different pharmacological activities are described on the basis of substitution pattern around the nucleus with an aim to help medicinal chemists for the development of SAR on benzimidazoles for each activity. This article aims to review the work reported, chemistry and pharmacological activities of benzimidazole derivatives during past years.

Keywords: Benzimidazole derivatives, Molecular docking, ADMET, Drug-likeness, Lipinski rule, Pharmacokinetics, Toxicity profiling, 2VH1 protein, Albendazole, Drug design, antimicrobial activity, antifungal activity.

INTRODUCTION

Benzimidazole is an important heterocyclic compound widely recognized for its diverse pharmacological activities, including antimicrobial, antifungal, antiviral, and antiparasitic properties. Due to its structural similarity with naturally occurring nucleotides, benzimidazole derivatives have gained significant attention in medicinal chemistry for the development of novel therapeutic agents. In recent years, computational approaches such as molecular docking and ADMET prediction have become essential tools in drug discovery, allowing rapid screening of compounds and reducing experimental costs. These techniques help in understanding the binding interactions between ligands and target proteins, as well as predicting pharmacokinetic and toxicity profiles. In this study, a series of benzimidazole derivatives (CB-1 to CB-8) were synthesized using different substituted aldehydes. The compounds were evaluated for their binding affinity against the target protein (PDB ID: 2VH1) through molecular docking studies. Furthermore, drug-likeness, pharmacokinetics, and toxicity assessments were performed to determine their suitability as potential drug candidates. The objective of this work is to identify promising benzimidazole-based compounds with enhanced biological activity and favorable safety profiles, which may serve as lead molecules for future pharmaceutical development.

LITERATURE REVIEW

Patel et al. (2018): - reported benzimidazole derivatives with significant antibacterial activity against S. aureus and E. coli, enhanced by halogen substitution.

Khan et al. (2019): - demonstrated antifungal potential of nitro-substituted benzimidazoles, showing comparable activity to fluconazole.

Singh et al. (2020): - highlighted that benzimidazole analogs inhibit DNA-binding enzymes and microbial topoisomerases.

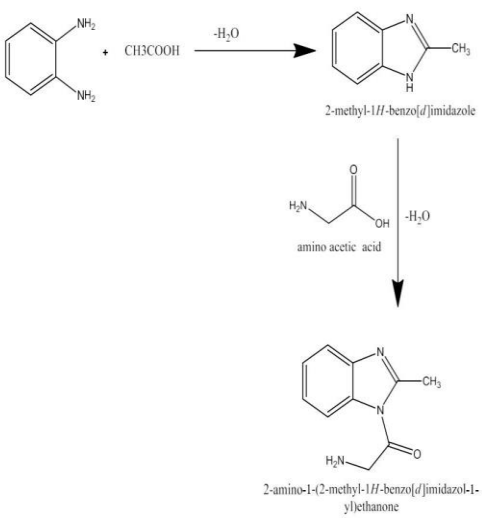
De Clercq (2021): - suggested benzimidazole derivatives as promising scaffolds for designing broad-spectrum antimicrobial agents.

These studies highlight that substitutions at C-2 and N-1 positions of benzimidazole strongly influence antimicrobial activity.

Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

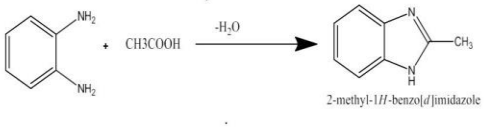
SCHEME OF DESIGN

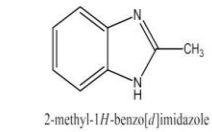
- **Synthesis CB-B**

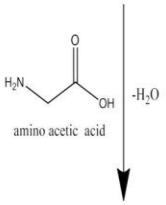


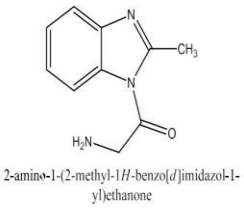
Experimental procedure

- **Synthesis CB-A-**

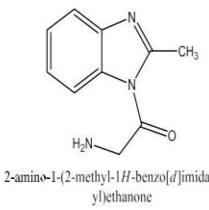








- **Synthesis CB-derivatives (aldehyde)**



METHOD AND MATERIAL:

Procedure for Synthesis of Benzimidazole:

1. Dissolve 27g of o-phenylenediamine in a 250mL round-bottom flask.

2. Add 17.5g of formic acid to the solution.

3.Heat the mixture at 100°C for 2 hours using a water bath.

4. Allow the mixture to cool, then slowly add a 10% sodium hydroxide solution while constantly rotating the flask, until the mixture reaches a slightly alkaline ph.

5. Filter the resulting crude benzimidazole using a vacuum pump and wash it with ice-cold water.

6. Repeat the washing step with an additional 25mL of cold water to ensure complete purification

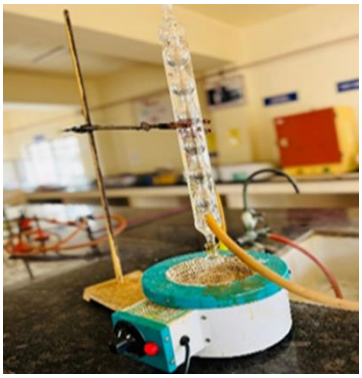


Fig1. Boiling Method

RECRYSTALLIZATION

1. To purify the synthesized product, dissolve it in 400 mL of boiling water.

2. Add 2 g of activated carbon to remove impurities and heat the mixture for 15 minutes.

3. Filter the solution rapidly through a preheated Buchner funnel under vacuum.

4. Allow the filtrate to cool to approximately 10°C, then collect the crystallized benzimidazole by filtration. 5. Wash the product with 25 mL of cold water and dry it at 100°C. This recrystallization process yields 25 g of pure benzimidazole, characterized by a melting point of 171-172°C.

Fig.2 Heating Phenylenediamine

Fig.3 After Heating

Fig.4 Final Product

PROCEDURE OF TLC(THIN LAYER CHROMATOGRAPHY

1) PREPARATION OF MOBILE PHASE :

Prepare the mobile phase by mixing Chloroform and Methanol in a suitable ratio.

Commonly used ratios:

9:1 (Chloroform: Methanol) – for non-polar to moderately polar compounds

8:2 or 7:3 – for more polar compounds

Mix well and pour into the TLC chamber to a depth of about 0.5–1 cm.

Close the chamber and allow it to saturate for 10–15 minutes.

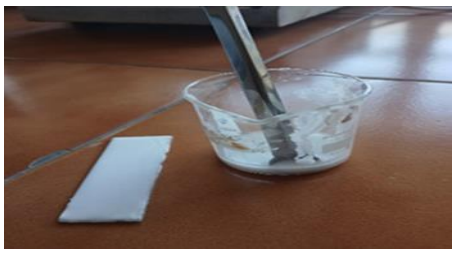


Fig.5 Mobile Phase

2) PREPARATION OF SAMPLE :

1). Dissolve a small quantity of the sample in a suitable solvent (often methanol or chloroform).

2). The solution should be clear and dilute.

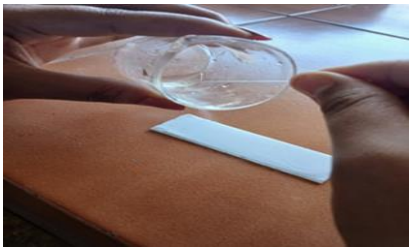


Fig.6 Spotting of sample

3) PROCEDURE OF SPOTTING SAMPLE :

1.Take a TLC plate.

2.Draw a pencil line about 1–1.5 cm from the bottom (baseline).

3.Using a capillary tube, apply a small spot of the sample on the baseline.

4. Allow the spot to dry completely (do not blow).

5. Development of TLC Plate

6. Carefully place the TLC plate vertically in the developing

4) DRYING THE PLATE :

1.Remove the plate and immediately mark the solvent front with a pencil.

2. Allow the plate to dry at room temperature.

5) DETECTION OF SPOTS:

1. Observe the plate under: UV light (254 nm or 366 nm)

OR

2. Spray with suitable reagent (iodine vapour, anisaldehyde, ninhydrin, Dragendorff's reagent etc.)

3. Mark the visible spots.

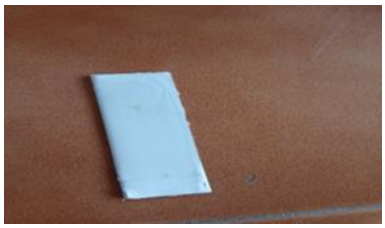


Fig.7 Detection of spot

6) CALCULATION OF *RF* VALUE

$$Rf = \frac{\text{Distance travelled by solute}}{\text{Distance travelled by solvent front}}$$

1). Distance From Baseline to Spot Centre = 4.5cm

2). Distance from Baseline to Solvent Front = 6.2cm

$$\mathbf{R}f = \frac{4.5}{6.5} = 0.72$$

COMPOUND SYNTHESIZED:

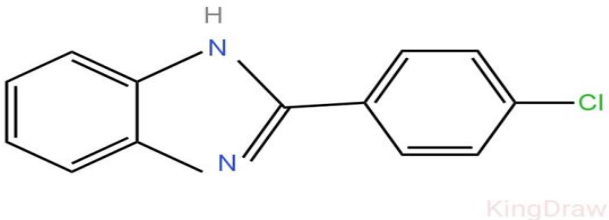
1) Compound: -

IUPAC Name-: 2-(4-chlorophenyl)-1H-benzimidazole

Molecular Formula- C13H9CIN2

Molecular weight-228.68g/mol

Structure:



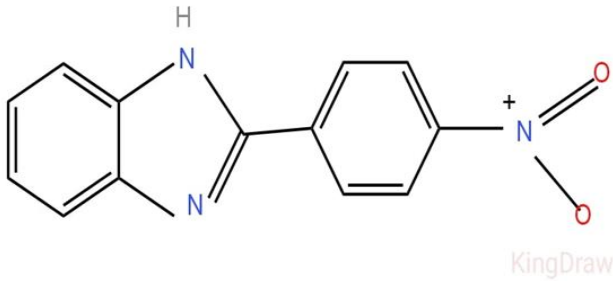
2) Compound: -

IUPAC Name-: 2-(4-nitrophenyl)-1H-benzimidazole

Molecular Formula-C13H9N302

Molecular weight-239.23g/mol

Structure-



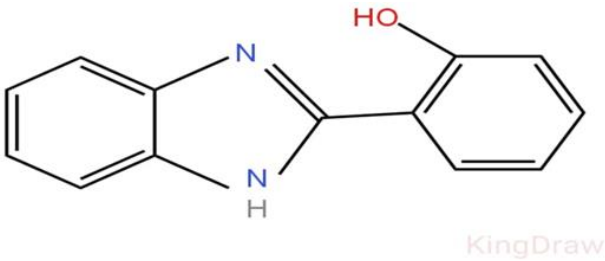
3) Compound-

IUPAC Name-: 2-(2-hydroxyphenyl)-1H-benzimidazole

Molecular Formula – C13H10N2O

Molecular weight- 210.23g/mol

Structure-



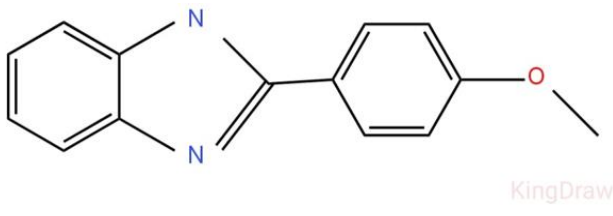
4) Compound-

IUPAC Name-: 2-(4-methoxyphenyl)-1H-benzimidazole

Molecular Formula-C14H12N2O

Molecular weight- 224.26g/mol

Structure-



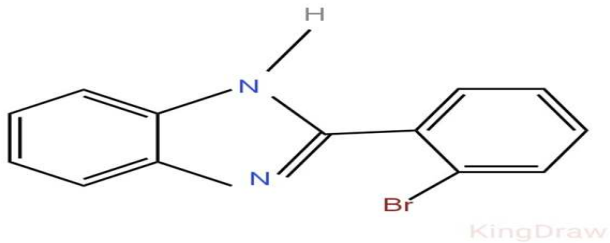
5) Compound-

IUPAC Name-: 2-(2-bromophenyl)-1H-benzimidazole

Molecular Formula- C13H9BrN2

Molecular weight- 273.13g/mol

Structure-



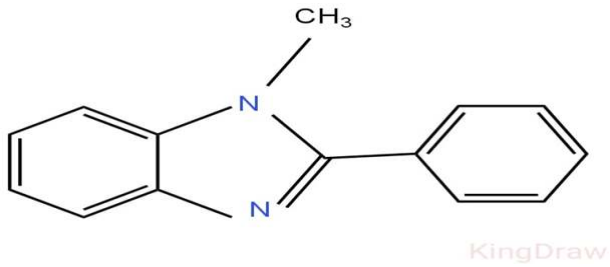
6) Compound-

IUPAC Name-:1-methyl-2-phenylbenzimidazole

Molecular Formula-C14H12N2

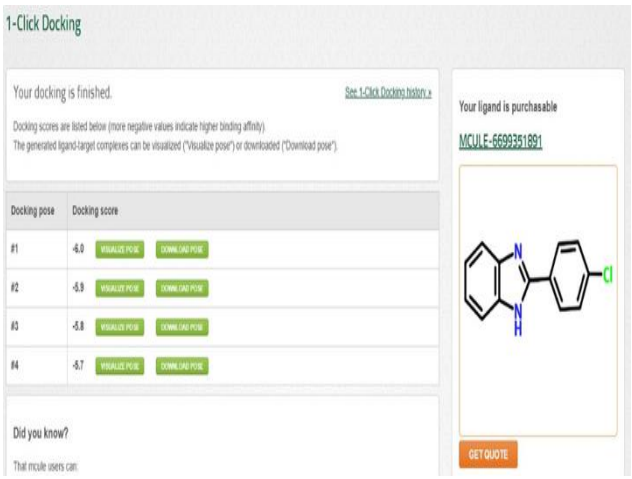
Molecular weight-208.26g/mol

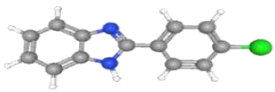
Structure-



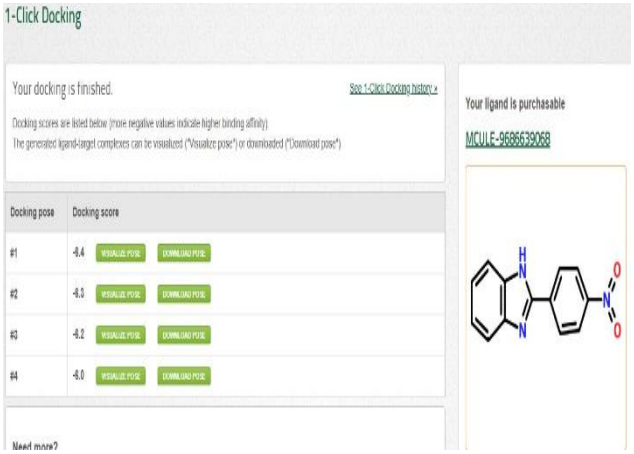
ONE CLICK DOCKING ;-

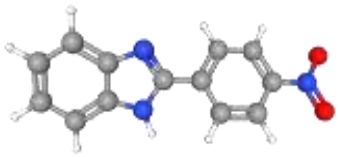
1) Compound: - IUPAC Name-: 2-(4-chlorophenyl)-1H-benzimidazole



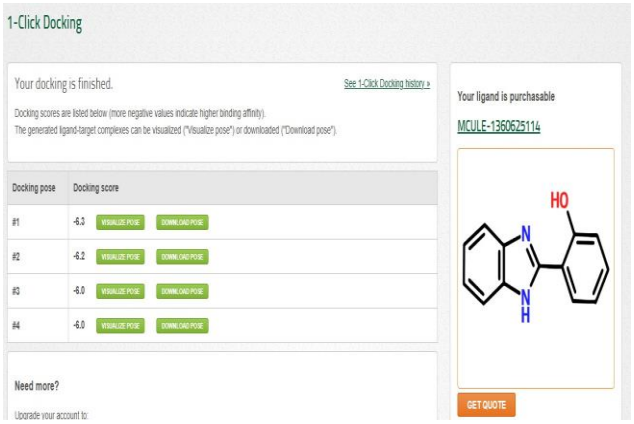


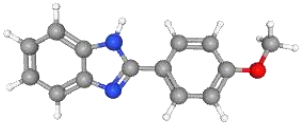
2) Compound: - IUPAC Name-: 2-(4-nitrophenyl)-1H-benzimidazole



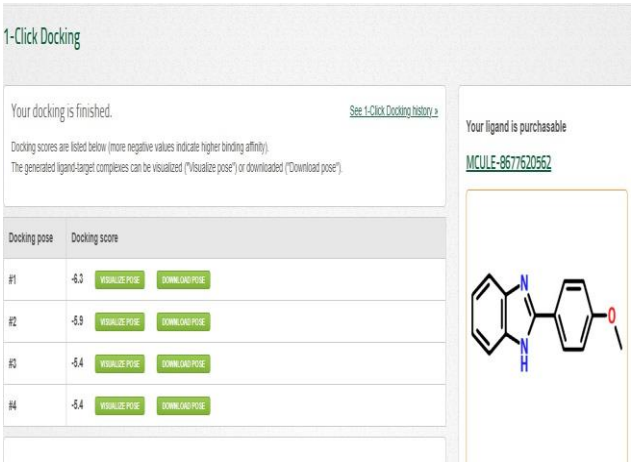


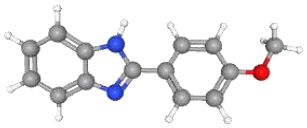
3) Compound- IUPAC Name-: 2-(2-hydroxyphenyl)-1H-benzimidazole



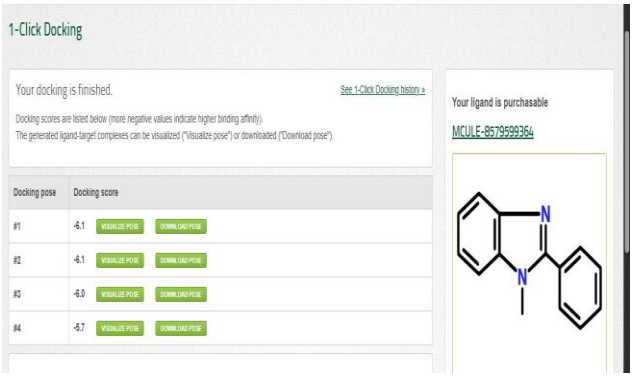


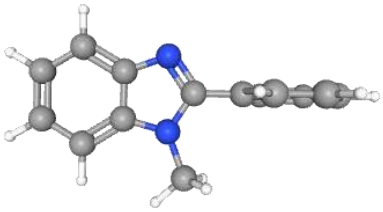
4) Compound- IUPAC Name-: 2-(4-methoxyphenyl)-1H-benzimidazole



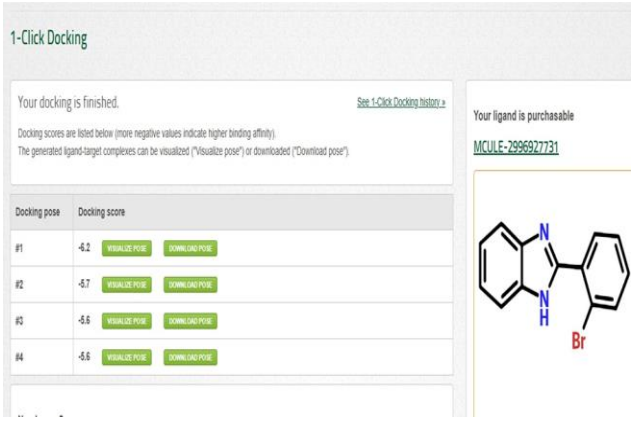


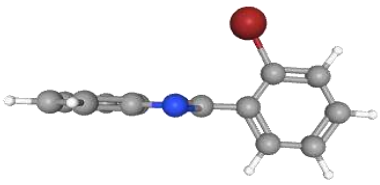
6) Compound- IUPAC Name-:1-methyl-2-phenylbenzimidazole



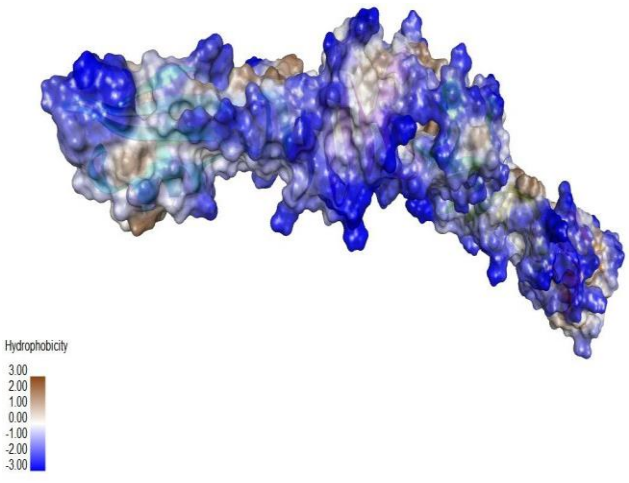


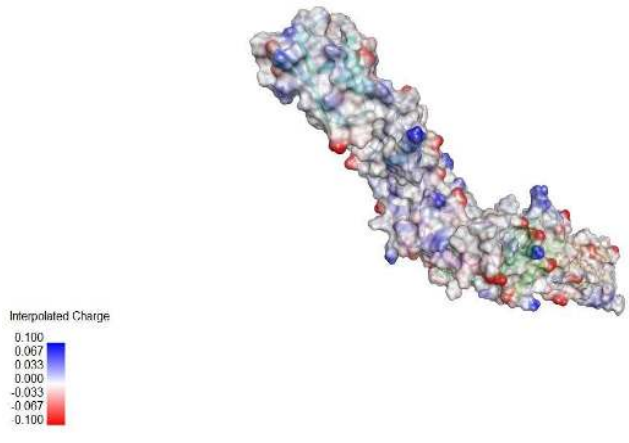
5) Compound- IUPAC Name-: 2-(2-bromophenyl)-1H-benzimidazole



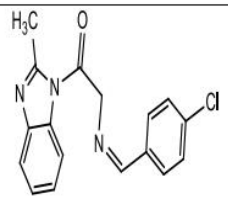
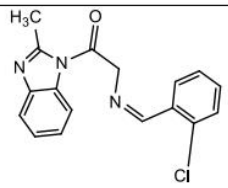
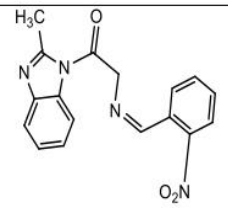
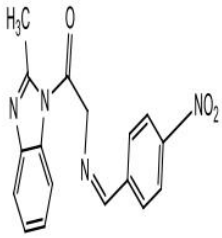
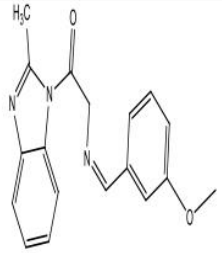


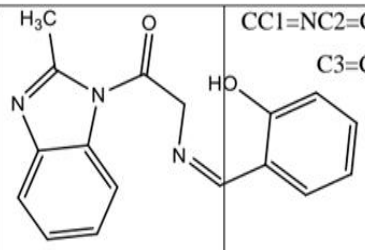
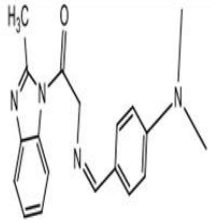
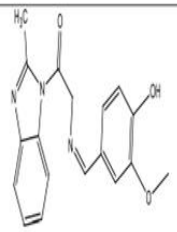
Protein (PDB:2VH1)





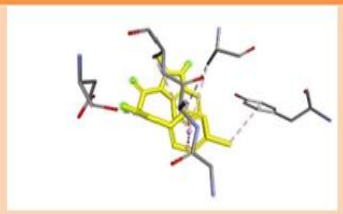
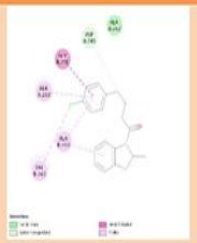
STUCTRAL DATA OF Benzimidazole

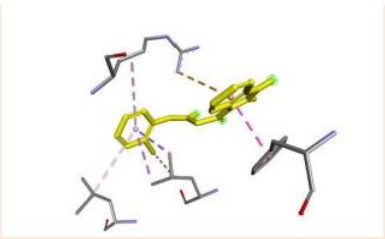
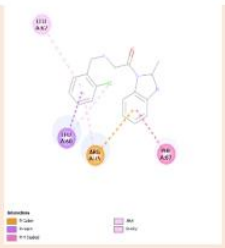
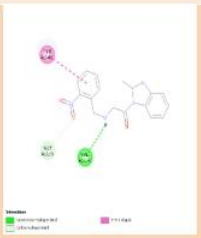
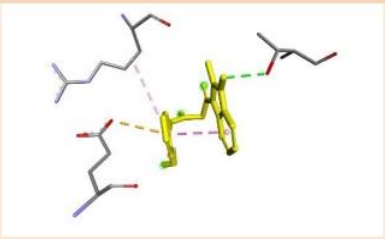
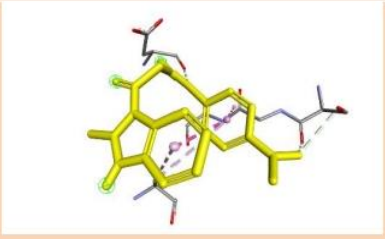
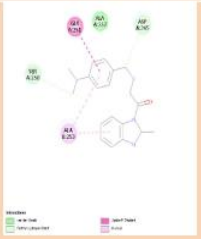
Comp. Code	Structure	SMILES	IUPAC	MW (g/mol)	DER
CB-1		CC1=NC2=CC=CC=C2N1C(C/N=C\C3=CC=C(Cl)C=C3)=O	(Z)-2-((4-chlorobenzylidene)cbino)-1-(2-methyl-1H-benzo[d]imidazol-1-yl)ethanone	311.77	4-chlorobenzaldehyde
CB-2		CC1=NC2=CC=CC=C2N1C(C/N=C\C3=C(Cl)C=CC=C3)=O	(Z)-2-((2-chlorobenzylidene)cbino)-1-(2-methyl-1H-benzo[d]imidazol-1-yl)ethanone	311.77	2-chlorobenzaldehyde
CB-3		CC1=NC2=CC=CC=C2N1C(C/N=C\C3=C([N+]([O-])=O)C=CC=C3)=O	(Z)-1-(2-methyl-1H-benzo[d]imidazol-1-yl)-2-((2-nitrobenzylidene)cbino)ethanone	322.32	2-NITROBENZALDEHYDE
CB-4		CC1=NC2=CC=CC=C2N1C(C/N=C\C3=CC=C([N+]([O-])=O)C=C3)=O	(Z)-1-(2-methyl-1H-benzo[d]imidazol-1-yl)-2-((4-nitrobenzylidene)cbino)ethanone	322.32	4-NITROBENZALDEHYDE
CB-5		CC1=NC2=CC=CC=C2N1C(C/N=C\C3=CC(OC)=CC=C3)=O	(Z)-2-((3-methoxybenzylidene)cbino)-1-(2-methyl-1H-benzo[d]imidazol-1-yl)ethanone	307.13	ANISALDEHYDE

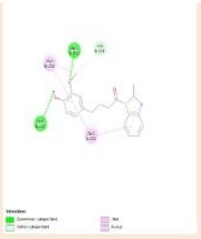
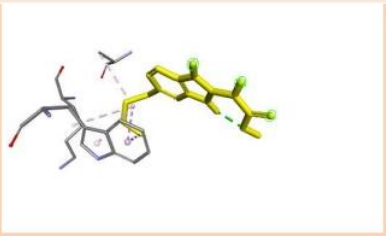
CB -6		CC1=NC2=CC=CC=C2N1C(C/N=C\C3=CC=CC=C3O)=O	(Z)-2-((2-hydroxybenzylidene)cbino)-1-(2-methyl-1H-benzo[d]imidazol-1-yl)ethanone	293.12	SALICYLALDEHYE
CB -7		CC1=NC2=CC=CC=C2N1C(C/N=C\C3=CC=C(N(C)C)C=C3)=O	(Z)-2-((4-(dimethylcbino)benzylidene)cbino)-1-(2-methyl-1H-benzo[d]imidazol-1-yl)ethanone	320.16	P-dimethyl benzaldehyde
CB -8		CC1=NC2=CC=CC=C2N1C(C/N=C\C3=CC(OC)=C(O)C=C3)=O	(Z)-2-((4-hydroxy-3-methoxybenzylidene)cbino)-1-(2-methyl-1H-benzo[d]imidazol-1-yl)ethanone	323.25	VANILINE

DOCKING STUDY DATA

My protein (PDB:2VH1)

SR.NO	DER	3D	2D	DOCK SCORE
CB-1	4-chlorobenzaldehyde			-6.4

CB-2	2-chlorobenzaldehyde			-7.2
CB-3	2-NITROBENZALDEHYDE			-5.6
CB-4	4-NITROBENZALDEHYDE			-6.6
CB-5	ANISALDEHYDE			-7.0
CB-6	SALICYLALDEHYE			-5.4
CB-7	P-dimethyl benzaldehyde			-6.4

CB-8	VANILINE			-7.1
Std	Albendazole			-5.9

AMINO ACID DATA

SR.NO	NAME	DISTANCE	CATEGORY	FROM CHEMISTRY	TO CHEMISTRY
CB-1	2vh1_pdb_clea_fragment_uff_e=407.99_0: C16 - A:ASP245:O 2vh1_pdb_clea_fragment_uff_e=407.99_0 - 2vh1_pdb_clea_fragment_uff_e=407.99_0 A:GLY251:C,O;ALA252:N - 2vh1_pdb_clea_fragment_uff_e=407.99_0 B:TYR243 - 2vh1_pdb_clea_fragment_uff_e=407.99_0: Cl23 2vh1_pdb_clea_fragment_uff_e=407.99_0 - B:ALA253 2vh1_pdb_clea_fragment_uff_e=407.99_0 - A:ALA253 2vh1_pdb_clea_fragment_uff_e=407.99_0 - B:ALA253	3.78322 4.02384 4.0727 4.89196 4.58002 5.46541 4.82942	Hydrogen Bond Pi-Orbitals Amide Hydrophobic Pi-Orbitals Alkyl Hydrophobic Pi-Orbitals Alkyl Hydrophobic Pi-Orbitals Alkyl	H-Donor Pi-Orbitals Pi-Orbitals Pi-Orbitals Pi-Orbitals Pi-Orbitals Pi-Orbitals	H-Acceptor Pi-Orbitals Pi-Orbitals Alkyl Alkyl Alkyl Alkyl
CB-2	A:ARG75:NH2 - 2vh1_pdb_clea_fragment_uff_e=422.83_0 A:LEU60:CD1 - 2vh1_pdb_clea_fragment_uff_e=422.83_0 A:LEU60:CD2 -	4.73243 3.624 3.99187 3.89531 4.42238	Electrostatic Hydrophobic Hydrophobic	Positive C-H C-H Pi-Orbitals Alkyl	Pi-Orbitals Pi-Orbitals Pi-Orbitals Pi-Orbitals Alkyl

	2vh1_pdb_clea_fragment_uff_e=422.83_0 A:PHE87 - 2vh1_pdb_clea_fragment_uff_e=422.83_0 2vh1_pdb_clea_fragment_uff_e=422.83_0: Cl21 - A:LEU60 2vh1_pdb_clea_fragment_uff_e=422.83_0 - A:LEU62 2vh1_pdb_clea_fragment_uff_e=422.83_0 - A:ARG75	5.37049 5.34153	Hydrophobic Hydrophobic Hydrophobic Hydrophobic	Pi-Orbitals Pi-Orbitals	Alkyl Alkyl
CB-3	2vh1_pdb_clea_fragment_uff_e=579.68_0: H17 - A:VAL254:O A:GLY255:CA - 2vh1_pdb_clea_fragment_uff_e=579.68_0: O25 2vh1_pdb_clea_fragment_uff_e=579.68_0 - 2vh1_pdb_clea_fragment_uff_e=579.68_0 A:TYR243 - 2vh1_pdb_clea_fragment_uff_e=579.68_0	2.44535 3.2309 3.84909 4.81792	Hydrogen Bond Hydrogen Bond Hydrophobic Hydrophobic	H-Donor H-Donor Pi-Orbitals Pi-Orbitals	H-Acceptor H-Acceptor Pi-Orbitals Pi-Orbitals
CB-4	B:GLY255:CA - 2vh1_pdb_clea_fragment_uff_e=436.25_0: O26 2vh1_pdb_clea_fragment_uff_e=436.25_0: C16 - A:ASP245:O 2vh1_pdb_clea_fragment_uff_e=436.25_0 - 2vh1_pdb_clea_fragment_uff_e=436.25_0 A:GLY251:C,O;ALA252:N - 2vh1_pdb_clea_fragment_uff_e=436.25_0 2vh1_pdb_clea_fragment_uff_e=436.25_0 - B:ALA253 2vh1_pdb_clea_fragment_uff_e=436.25_0 - B:ALA253	3.5415 3.75552 4.20215 4.05515 4.43237 4.99615	Hydrogen Bond Hydrogen Bond Hydrophobic Hydrophobic Hydrophobic Hydrophobic	H-Donor H-Donor Pi-Orbitals Amide Pi-Orbitals	H-Acceptor H-Acceptor Pi-Orbitals Pi-Orbitals Alkyl Alkyl
CB-5	B:ALA252:N - 2vh1_pdb_clea_fragment_uff_e=426.94_0: O24 2vh1_pdb_clea_fragment_uff_e=426.94_0: C25 - A:VAL254:O	3.20027 3.67208 3.84759 5.33795 3.60145	Hydrogen Bond Hydrogen Bond Hydrophobi	H-Donor H-Donor C-H Pi-Orbitals Alkyl	H-Acceptor H-Acceptor Pi-Orbitals Pi-Orbitals Alkyl

	B:ALA253:CB - 2vh1_pdb_clea_fragment_uff_e=426.94_0 B:TYR248 - 2vh1_pdb_clea_fragment_uff_e=426.94_0 A:ALA253 - 2vh1_pdb_clea_fragment_uff_e=426.94_0: C25 2vh1_pdb_clea_fragment_uff_e=426.94_0 - B:ALA253 2vh1_pdb_clea_fragment_uff_e=426.94_0 - A:ALA253	5.21425 4.81366	c Hydrophobic Hydrophobic Hydrophobic Hydrophobic	Pi-Orbitals Pi-Orbitals	Alkyl Alkyl
CB-6	2vh1_pdb_clea_fragment_uff_e=516.55_0: H8 - A:THR216:OG1 A:GLU169:OE1 - 2vh1_pdb_clea_fragment_uff_e=516.55_0 2vh1_pdb_clea_fragment_uff_e=516.55_0 - 2vh1_pdb_clea_fragment_uff_e=516.55_0 2vh1_pdb_clea_fragment_uff_e=516.55_0 - A:ARG197	2.73256 3.72949 3.73433 5.4007	Hydrogen Bond Electrostatic Hydrophobic Hydrophobic	H-Donor Negative Pi-Orbitals Pi-Orbitals	H-Acceptor Pi-Orbitals Pi-Orbitals Alkyl
CB-7	2vh1_pdb_clea_fragment_uff_e=453.28_0: C16 - A:ASP245:O 2vh1_pdb_clea_fragment_uff_e=453.28_0: C25 - A:SER250:O 2vh1_pdb_clea_fragment_uff_e=453.28_0: C25 - A:SER250:OG 2vh1_pdb_clea_fragment_uff_e=453.28_0 - 2vh1_pdb_clea_fragment_uff_e=453.28_0 A:GLY251:C,O;ALA252:N - 2vh1_pdb_clea_fragment_uff_e=453.28_0 2vh1_pdb_clea_fragment_uff_e=453.28_0 - B:ALA253 2vh1_pdb_clea_fragment_uff_e=453.28_0 - B:ALA253	3.78352 3.32613 3.48712 4.10874 4.14456 4.81834 5.04147	Hydrogen Bond Hydrogen Bond Hydrogen Bond Hydrophobic Hydrophobic Hydrophobic Hydrophobic	H-Donor H-Donor H-Donor Pi-Orbitals Amide Pi-Orbitals Pi-Orbitals	H-Acceptor H-Acceptor H-Acceptor Pi-Orbitals Pi-Orbitals Alkyl Alkyl
CB-8	A:ALA252:N - 2vh1_pdb_clea_fragment_uff_e=443.99_0: O24	3.3262 2.44267 3.06589	Hydrogen Bond Hydrogen	H-Donor H-Donor H-Donor	H-Acceptor H-Acceptor H-Acceptor

	2vh1_pdb_clea_fragment_uff_e=443.99_0: H27 - A:ASP245:O 2vh1_pdb_clea_fragment_uff_e=443.99_0: C25 - B:VAL254:O B:ALA253 - 2vh1_pdb_clea_fragment_uff_e=443.99_0: C25 2vh1_pdb_clea_fragment_uff_e=443.99_0 - A:ALA253 2vh1_pdb_clea_fragment_uff_e=443.99_0 - A:ALA253 2vh1_pdb_clea_fragment_uff_e=443.99_0 - B:ALA253	3.77382 4.10036 4.29147 5.38383	Bond Hydrogen Bond Hydrophobic Hydrophobic Hydrophobic Hydrophobic	Alkyl Pi-Orbitals Pi-Orbitals Pi-Orbitals	Alkyl Alkyl Alkyl Alkyl

Drug-Likeness and Physicochemical Properties

Compound Codes	Lipinski rule of five					Veber's rule	
	M Log P	Mol. Wt. (g/mol)	HBA	HBD	Violations	TPSA (Å²)	No. Of rotatable bonds
CB-1	2.58	311.77	3	0	(yes) 0	47.25 Å²	4
CB-2	2.58	311.77	3	0	(yes) 0	47.25 Å²	4
CB-3	1.80	322.32	4	0	(yes) 0	93.07 Å²	5
CB-4	2.00	322.32	4	0	(yes) 0	93.07 Å²	5
CB-5	2.22	307.35	4	0	(yes) 0	67.48 Å²	5
CB-6	1.95	293.32	4	4	(yes) 0	68.48 Å²	4
CB-7	2.86	320.39	3	0	(yes) 0	50.49 Å²	5
CB-8	2.69	323.35	5	1	(yes) 0	76.71 Å²	5
Std (Albendazole)	1.62	265.33	2	3	(yes) 0	92.31 Å²	6

Pharmacokinetics &Lipophilicity

Compound codes	Log S	GI absorption	BBB permeant	P-gp substrate	Log-kp	CYP3A4 inhibitor
CB-1	-4.42	High	Yes	No	-5.49	No

CB-2	-4.42	High	Yes	No	-5.49	No
CB-3	-3.87	High	No	No	-6.12	No
CB-4	-3.87	High	No	No	-6.12	No
CB-5	--3.89	High	No	No	-5.93	No
CB-6	-3.68	High	No	No	-6.08	No
CB-7	-4.04	High	No	No	-5.90	No
CB-8	-3.75	High	No	No	-6.28	No
Std (Albendazole)	-3.23	High	No	No	-5.92	No

ADMET and Toxicity Profiling

Compound codes	**Parameters**									
	LD_{50} (mg/kg)	**Toxicity class**	**Prediction accuracy (%)**	**Hepatotoxicity**	**Nephrotoxicity**	**Carcinogenicity**	**Immunotoxicity**	**Mutagenicity**	**Cytotoxicity**	**Clinical toxicity**
				(Probability)						
CB-1	4000	5	53.51	I-0.79	I-0.77	I-0.70	I-0.76	I-0.69	I-0.68	I-0.55
CB-2	4000	5	52.41	I-0.79	I-0.77	I-0.70	I-0.76	I-0.67	I-0.68	I-0.55
CB-3	200	3	45.01	I-0.61	I-0.65	I-0.76	A-0.85	A-0.86	I-0.64	I-0.54
CB-4	2200	5	46.91	I-0.61	I-0.65	I-0.76	A-0.85	A-0.87	I-0.60	I-0.54
CB-5	4000	5	50.99	I-0.67	I-0.69	I-0.76	I-0.76	A-0.87	I-0.60	I-0.54
CB-6	4000	5	50.05	I-0.77	I-0.69	I-0.76	I-0.86	A-0.87	I-0.60	I-0.54
CB-7	4000	5	49.12	I- 0.80	I- 0.81	I- 0.56	I- 0.61	I- 0.56	I- 0.65	I- 0.58
CB-8	4000	5	50.04	I-0.74	I-0.58	I-0.60	A-0.96	I-0.53	I-0.50	I-0.57
Std (Albendazole)	970	4	50.00	A- 0.78	I- 0.54	I- 0.50	I- 0.83	I- 0.71	I- 0.75	I- 0.52

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