WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
Coden USA: WJPRAP Impact Factor 8.63
Volume 15, Issue 6, 946-958. Research Article ISSN 2277–7105

COMPUTATIONAL EVALUATION OF 1H-3-INDAZOLE DERIVATIVES AGAINST CANCER PROTEIN TARGETS

Murugan R.[1]*, Senthil Kumar S.K.[2], Muthuram M.[3], Nadhiya R.[3], Nagaraj R.[3], Naveen Kumar M.[3], Naveena Priya S.[3]

[1]Associate Professor, Department of Pharmaceutical Chemistry, Arunai College of Pharmacy, Tiruvannamalai.

[2]Principal Cum Professor, Department of Pharmaceutics, Arunai College of Pharmacy, Tiruvannamalai.

[3]B. Pharm Final Year Students, Arunai College of Pharmacy, Tiruvannamalai, Tamil Nadu, India.

Article Received on 15 Feb. 2026,
Article Revised on 05 March 2026,
Article Published on 16 March 2026,

https://doi.org/10.5281/zenodo.19046192

***Corresponding Author**

Murugan R.

Associate Professor, Department of Pharmaceutical Chemistry, Arunai College of Pharmacy, Tiruvannamalai.
akshithakuncha16@gmail.com

How to cite this Article: Murugan R.1*, Senthil Kumar S.K.2, Muthuram M.3, Nadhiya R.3, Nagaraj R.3, Naveen Kumar M.3, Naveena Priya S.3. (2026). Computational Evaluation of 1h-3-Indazole Derivatives Against Cancer Protein Targets. World Journal of Pharmaceutical Research, 15(6), 946–958.
This work is licensed under Creative Commons Attribution 4.0 International license.

ABSTRACT

Cancer remains a major global health burden requiring the development of novel therapeutic scaffolds with improved efficacy and reduced toxicity. Indazole-based heterocycles have emerged as promising pharmacophores due to their kinase inhibitory and multi-target anticancer potential. The present study evaluates four 1H-3-indazole derivatives using structure-based computational approaches. Molecular docking was performed against twelve cancer-associated protein targets. Drug-likeness and ADME properties were predicted using SwissADME, and toxicity assessment was conducted using Pro tox-III. All compounds satisfied Lipinski's Rule of Five and Veber's criteria. Docking scores ranged from −7.4 to−13.0 kcal/mol, with Ligand-3 exhibiting consistent strong binding across multiple targets. Toxicity prediction classified the compounds under Class IV with acceptable safety margins. These findings suggest that 1H-3-indazole derivatives, particularly Ligand-3, may serve as promising multi-target anticancer lead candidates requiring further experimental validation.

KEYWORDS: 1H-Indazole, Molecular docking, Anticancer agents, ADME prediction, Drug design, In silico toxicity.

INTRODUCTION

Cancer

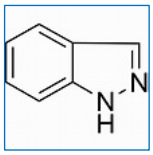
Cancer is "a group of diseases characterized by uncontrollable growth and spread of abnormal cells, which can then invade adjoining parts of the body and spread to other organs". Globally, after cardiovascular diseases, cancer is the second leading cause of death.

Mechanism Action of cancer

1. Inhibition of DNA synthesis – Prevents cancer cell replication
2. DNA damage – Causes breaks or cross-linking in DNA leading to cell death
3. Inhibition of cell division (mitosis) – Stops cancer cells from dividing
4. Induction of apoptosis – Triggers programmed cell death
5. Hormonal action – Blocks hormones required for cancer growth
6. Targeted action – Inhibits specific receptors or enzymes in cancer cells
7. Immune system activation – Helps the immune system destroy cancer cells.

Indazole

- Synonym: Benzopyrazole, 2-Azaindole, 1,2-Diazaindene
- IUPAC: Indazole
- Structure:



- Mol. Formula: $C_7H_6N_2$
- Therapeutic: Anticancer, NSAID, Spermatogenetic etc.
- Basic character:

Indazole is a fused heterocyclic compound consisting of a benzene ring fused with a pyrazole ring, bicyclic systems of benzo–azole are weaker base than the corresponding monocyclic heterocycles azole compounds but indazole is a slightly weaker acid than pyrazole. The heterocyclic aromatic organic chemical indazole, also known as benzopyrazole, is a rare heterocyclic aromatic organic compound discovered in nature.

INTRODUCTION TO MOLECULAR DOCKING

Molecular docking is a computational technique used to predict the preferred orientation of one molecule (typically a small ligand) when bound to a target macromolecule (usually a protein). This approach plays a pivotal role in drug discovery and design by helping researchers understand how potential drug candidates interact with biological targets at the molecular level. Molecular docking relies on various algorithms and scoring functions to evaluate the binding modes and affinities, making it an essential tool in pharmacology, biochemistry, and structural biology. The primary goal of molecular docking is to model the interaction between the ligand and the target protein, providing insights into binding affinities and the structural features that influence these interactions. By simulating these docking scenarios, scientists can identify promising compounds, optimize lead candidates, and streamline the drug development process. For example, protein-ligand docking. More recently, docking is also applied to predict the binding mode between two macromolecules, for instance protein-protein docking.

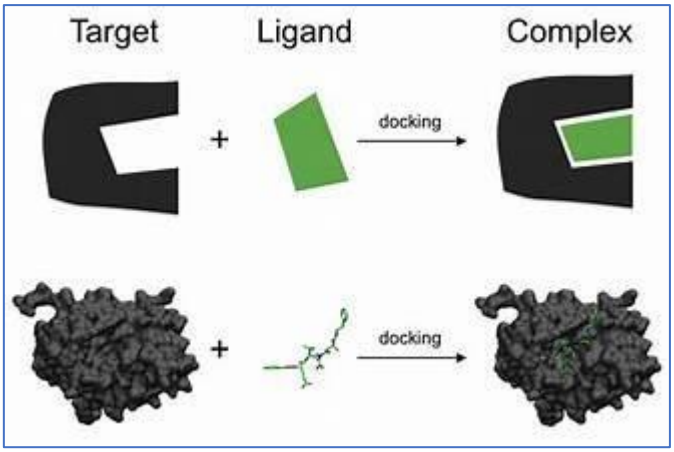


Fig no. 1: Molecular Docking.

MAJOR STEPS INVOLVED IN MECHANICS OF MOLECULAR DOCKING

Molecular Docking is the process in which the intermolecular interaction between 2 molecules was studied in In-silico. In this process, the Macromolecule is the protein receptor. The micro molecule is the Ligand molecule which can be acted as an inhibitor.

Docking process involves the following steps

Step-1: Preparation of Protein: Retrieving the 3D structure of the protein from a Protein Data Bank (PDB) and preprocessing it by removing water molecules, stabilizing charges, and addressing missing residues or side chains.

Step-2: Active site prediction: Identifying the specific active site on the protein receptor that is relevant for docking, often involving the removal of water molecules and heteroatoms.

Step-3: Preparation of ligand: Obtaining from databases or sketching them and applying Lipinski's Rule of 5 to select suitable drug like candidates.

According to Lipinski's Rule of 5, for the choice of ligand, the following criteria should be met:

- Less than five hydrogen bond donors
- Less than 10 hydrogen bond acceptors
- Molecular mass less than 500 Da
- High Lipophilicity (expressed as Log P not over 5)
- Molar refractivity should be between 40-130.

Step-4: Docking: Docking the prepared ligand against the protein and analyzing the interaction to identify the best docked ligand complex based on scoring.

MATERIALS AND METHODS

Selection of Ligands: Four 1H-indazole derivatives were selected based on reported anticancer activity.

Chemical structures were optimized prior to docking.

Protein Preparation: 12 cancer-related protein structures were retrieved from the Protein Data Bank (PDB IDs: 1HCK, 1T46, 3ERT, 3EYG, 3VHE, 4XHK, 5EW8, 6FEW, 6GR8, 6JOL, 7A2A, 7PCD). Water molecules and heteroatoms were removed. Hydrogen atoms were added and the structures were energy minimized before grid generation.

Molecular Docking: Docking simulations were performed using Auto Dock.

- Protein: Treated as rigid
- Ligands: Flexible
- Grid box: Centered on active site
- Output: Binding energy (kcal/mol)
- Lower docking scores indicate stronger binding affinity.

ADME and Drug-Likeness Prediction: Swiss ADME was used to evaluate:

- Molecular weight
- Log P

- H-bond donors and acceptors
- GI absorption
- BBB permeability
- TPSA
- Rotatable bonds
- Lipinski's Rule of Five and Veber's Rules were applied.
- Toxicity Prediction:
- In silico toxicity prediction was performed using Pro Tox-III to determine:
- LD_{50}
- Toxicity class
- Hepatotoxicity
- Mutagenicity
- Carcinogenicity

METHODOLOGY

- Open Browser and search and open the website www.rcsb.org and Download Random Cancer Proteins as PDB File Format.
- Then search and open the website www.molinpiration.com and draw the structure as indazole Derivatives and copy the SMILES of drawn structure.
- Then search and open the website www.biotech.fyicenter.com and paste the
- Smiles of drawn structure and convert into SDF File to download. Then search and open www.software.informer.com and download the Molegro Molecular software and install it.
- Open the software and select 'open' and select protein and import it. Then select only protein and save as PDB file. Then select the ligand and save as PDB file.
- Search and open the www.ccsb.scripps.edu and download the mgl tools and download and install the software version 1.5.7
- Open Autodock software, select the preference, select setup directory and paste the designated directory and set.

- **Preparation of Targeted Protein**

Open File →Read molecules →select the protein edit→ Hydrogen →add polar only → Click ok edit → Hydrogen → Merge Non-polar

Edit→ Compute Gasteiger charges

File → write pdb → click sort nodes →click ok

❖ **Preparation of Ligand**

Open Ligand → input → open → select pdb → select ligand → click ok Edit → Add Kollman Charges

Open Ligand → select Output → save as pdbqt file.

❖ **Preparation of Grid Parameter File**

Open Grid → Click Macromolecules → choose protein → ok → save as pdbqt file Grid → set map types → choose ligand → select ligand

Grid → Grid box → click close saving current

(*We have used X, Y, Z dimensions as 60x60x60. Further X,Y,Zcenter (Center Grid Box) can be changed according to the requirements but we are taking them as Default)

Grid → click output → save as GRID.gpf.

❖ **Preparation of Docking Parameter File**

Open Docking → click Macromolecules → set rigid filenames → select protein → open Docking → Click Ligand → Choose →select Ligand → Accept it

Docking → Click Search parameter → Click Genetic Algorithm →Accept it Docking → Output → click Lamarckian GA→ save as DOCK.dpf.

❖ Go to the selected directory and then command prompt and type as same as below in the selected directory to make the docking process.

autogrid4.exe -p grid.gpf -l grid.glg

autodock4.exe -p dock.dpf -l dock.dlg

❖ After docking process, In autodock tool

Open Analyze → select dockings → select dpf file → open

Analyze → select macromolecules → choose → select protein

Analyze → select conformations → click Play, ranked by energy → select play options → select Build H-Bonds → show info →note Binding energy → select Build Current → select write complex → save as pdbqt.

❖ By using this saved file, we can see the Binding interactions within the protein and ligand.

RESULTS AND DISCUSSION

Symptoms can vary greatly among individuals affected by cancer. Common symptoms of

cancer include persistent or burning abdominal pain, often worsening at night, nausea and vomiting, bloating and discomfort, loss of appetite, heartburn-like sensations, unexplained weight loss, fatigue, and the presence of blood in the stool, depending on the type and stage of the disease. Although various treatment strategies for cancer are available worldwide, it remains a serious and life-threatening condition, highlighting the severity of the disease.

Considering the seriousness of cancer, the present study focuses on enhancing drug-likeness properties to act against cancer by evaluating the anticancer activity of various compounds. The compounds investigated in this study were Indazole.

Indazole Against Anti-Cancer Activity

In this study, we have collected 4 selected compounds of 1H-3-indazole Derivative. They were examined to recognize the prospects of various compounds that can act as a drug against cancer causing agent. The protein structure was downloaded from the protein data bank and then structure was MOLINSPIRATION software. The observed compound, and their structure.

Table no. 1: Core Structure of 1H-3-Indazole Derivative.

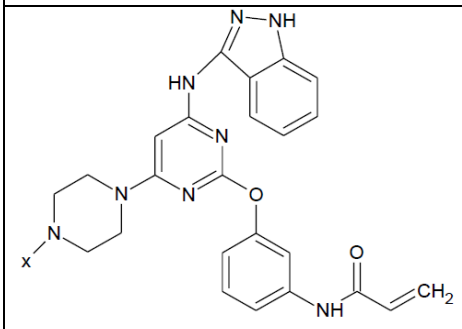
CORE STRUCTURE	SUBSTITUTION
	Where x=, • Ligand 1 – CH2=CH2 • Ligand 2 – CH2-CH3 • Ligand 3 – Cl • Ligand 4 – F

Table no. 2: IUPAC Names of 1H-3-Indazole Derivatives.

S.no	IUPAC NAMES
1	N-(3-((5-((1H-indazol-3-yl)amino)-2-(4-vinylpiperazin-1-yl)pyrimidin-4-yl)oxy)phenyl) acrylamide
2	N-(3-((5-((1H-indazol-3-yl)amino)-2-(4-ethylpiperazin-1-yl)pyrimidin-4-yl)oxy)phenyl) acrylamide
3	N-(3-((5-((1H-indazol-3-yl)amino)-2-(4-chloropiperazin-1-yl)pyrimidin-4-yl)oxy)phenyl) acrylamide
4	N-(3-((5-((1H-indazol-3-yl)amino)-2-(4-fluoropiperazin-1-yl)pyrimidin-4-yl)oxy)phenyl) acrylamide

THE ADME STUDY REPORT OF THE COMPOUNDS OF INDAZOLE DERIVATIVE ARE

The captured various compounds were then subjected to ADME testing using SWISSADME software. The forecasted ADME property of various compound based on their structure, functional groups and molecular properties such as Mol/ M.W (molecular weight), BBB permeant (Blood-Brain Barrier parameter of compounds), GI (Gastrointestinal absorption), H-bond acceptors, H-bond donors, Violation and mLogP (Moriguchi octanol-water partition coefficient). Few compounds transgressed drug-likeness tests were removed as those compounds have poor ability to cross the biological membrane. The ADME report are mentioned under the following table.

Table no. 3: The ADME Study Report or Lipinski's Rule of Selected Indazole Derivatives.

PROPERTIES	LIGAND 1	LIGAND 2	LIGAND 3	LIGAND 4	RECOMMEND VALUE
MOLECULAR WEIGHT {g/mol}	490.94	474.49	484.55	482.54	< 500
BLOOD BRAIN BARRIER	NO	NO	NO	NO	NO
GI ABSORPTION	HIGH	HIGH	HIGH	HIGH	HIGH
H-BOND ACCEPTOR	6	7	6	5	< 10
H-BOND DONOR	3	3	3	3	< 5
VIOLATION	0	0	0	0	0
mLOG P	2.23	2.13	2.44	2.37	< 4.15

Table no. 4: Veber's Rule.

LIGAND	ROTATABLE BONDS	POLAR SURFACE AREA Å^2
1	9	111.30
2	9	111.30
3	8	111.30
4	8	111.30
RECOMMEND VALUE	≤ 10	≤140 Å^2

THE RESULT OF MOLECULAR DOCKING SCORE OF INDAZOLE DERIVATIVE:

The docking studies of the ligands to protein active sites were done by the modern molecular docking program AutoDock version to determine compounds binding affinity. In silico approach between selected ligands and Protein Data Bank ID of the Cancer disease. The good drug-likeness properties containing the ligand's docking score, yield [%].

Table no. 5: In Silico Toxicity Prediction of Anticancer Compounds Using Protox-III.

Toxicity Profile	LIGAND 1	LIGAND 2	LIGAND 3	LIGAND 4
LD_{50} (mg/kg)	700	700	700	700
Toxicity Class	Class IV	Class IV	Class IV	Class IV
Hepatotoxicity	NO	NO	NO	NO
Carcinogenicity	YES	YES	NO	NO
Mutagenicity	NO	NO	NO	NO
Immunotoxicity	NO	NO	NO	NO
Cytotoxicity	NO	NO	NO	NO

MOLECULAR DOCKING RESULT OF INDAZOLE

- Docking simulations were performed for Four Indazole derivatives against twelve cancer-related proteins. The Binding affinities (kcal/mol) for each ligand-protein complex are shown in Table.
- The molecular docking study was carried out for four indazole derivatives (Compounds 1–4) against multiple cancer-related protein targets using Auto Dock
- Docking scores were expressed in kcal/mol, where more negative values indicate stronger binding affinity between ligand and protein.
- All Four Compounds showed good binding interactions with the selected proteins, suggesting their Potential Anticancer Activity.

Table no. 6: Docking Score of Ligands with Proteins.

S.NO	PROTEIN	LIGAND 1	LIGAND 2	LIGAND 3	LIGAND 4
1	1HCK	-11.09	-10.5	-11.37	-9.74
2	1T46	-9.90	-11.49	-10.62	-11.81
3	3ERT	-10.76	-10.97	-10.76	-9.67
4	3EYG	-9.89	-10.66	-12.44	-10.14
5	3VHE	-11.08	-10.56	-11.49	-10.09
6	4XHK	-11.06	-9.29	-9.87	-9.34
7	5EW8	-8.46	-8.70	-10.82	-11.12
8	6FEW	-13.01	-10.84	-11.25	-10.64
9	6GR8	-11.19	-10.49	-10.39	-9.06
10	6JOL	-12.54	-10.71	-9.89	-12.55
11	7A2A	-10.91	-11.08	-10.66	-7.45
12	7PCD	-7.55	-10.49	-9.30	-10.00

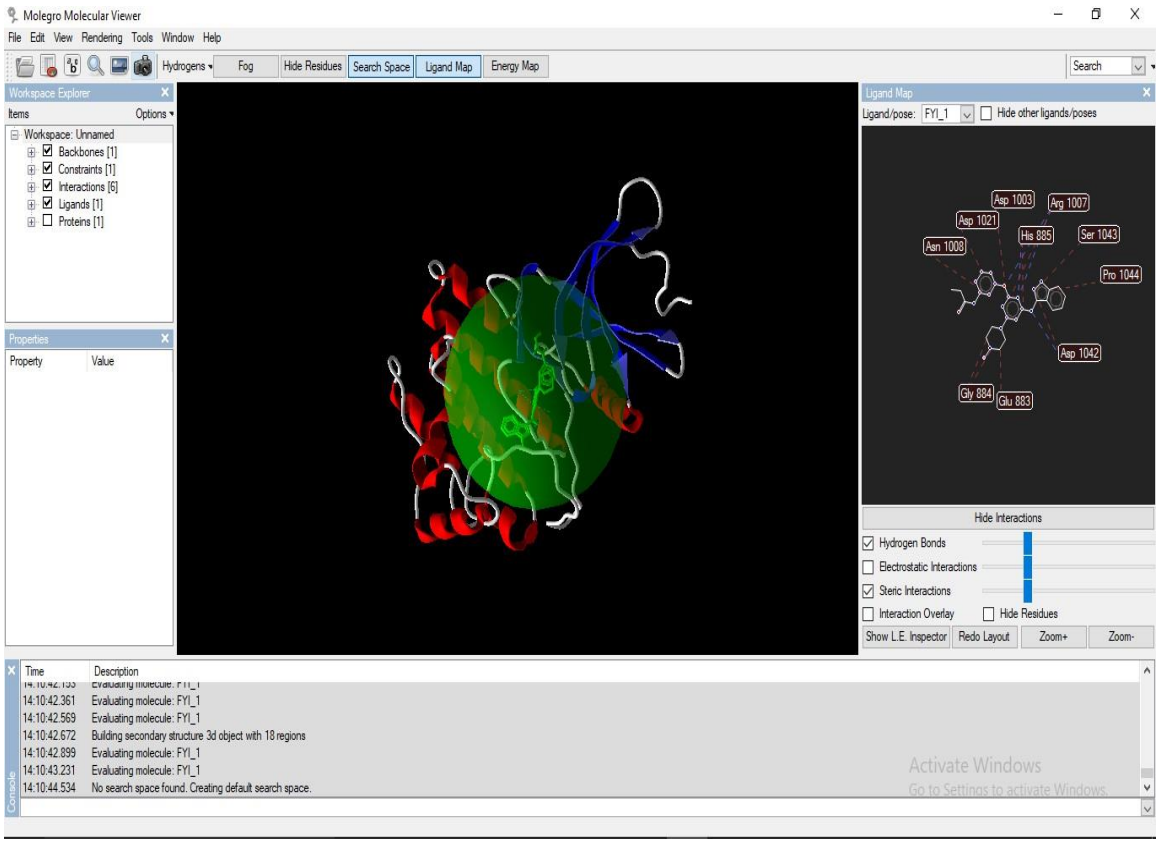


Fig. no. 2: Docking Interaction of Ligand 4 With Protein 3eyg.

CONCLUSION

The present study investigated the molecular docking interactions of four indazole derivatives against twelve different cancer-related receptor proteins using Auto Dock. According to the docking data, the ligand-receptor interactions were favorable, with binding energies ranging from around -7.4 to -13.0 kcal/mol.

Among the compounds that were examined, Ligand 3 showed a strong and consistent binding affinity across a variety of receptor targets. It showed notable interaction with proteins including 3EYG (-12.44 kcal/mol), 3VHE (-11.49 kcal/mol), 1HCK (-11.37 kcal/mol), and 6FEW (-11.25 kcal/mol). In the active binding sites, several docking scores < -10 kcal/mol indicate persistent complex formation and efficient interaction.

The structural characteristics that improve hydrophobic interactions, van der Waals forces, and potential hydrogen bonding within the receptor binding pockets—such as halogen substitution and improved molecule orientation—may be responsible for the reported binding affinity.

Overall, the results indicate that Ligand 3 possesses promising multi-target anticancer potential. However, as molecular docking provides only computational prediction of binding affinity, further in vitro and in vivo experimental studies are necessary to validate its biological activity and therapeutic applicability.

REFERENCES

1. Wermuth CG, Ganellin CR, Lindberg P, Mitscher LA. Glossary of terms used in medicinal chemistry. IUPAC Recommendations 1997, Part I. In: Adam J, editor. Annual reports in medicinal chemistry. San Diego, CA: Academic Press; 1998. p.385 95. For Part II, http://www.iupac.org/home/publications/provisional-recommendations/published/published- container/glossary-of-terms-usedin- medicinal-chemistry-part-ii.html.
2. http://en.wikipedia.org/wiki/medicinal_chemistry
3. National Cancer Institute. What Is Cancer? Available online: https://training.seer.cancer.gov/disease/cancer/review.html (accessed on 26 Mar 2021).
4. PKM2 inhibition decreases glycolysis and cancer cell proliferation, Youyou Zhou., et., al, International Journal of Cancer, 2020.
5. Tomlinson, D.R. 'Aldose reductase inhibitors and diabetic complications', Diabetes Research and Clinical Practice, 1992; 17(2): 77–83.
6. Robbins and Cotran Pathologic Basis of Disease, Vinay Kumar, Abul K. Abbas, Jon C. AsterElsevier, 2020; Chapter 6: Neoplasia 261–272.
7. Harrison's Principles of Internal Medicine,J. Larry Jameson et al., McGraw-Hill, Part 8 – Oncology, 2022; 667–675, 676–680.
8. Chen, W.Q. Cancer statistics: Updated cancer burden in China Preface. Chin. J. Cancer Res., 2015; 27: 1.
9. Joule and mills, Heterocyclic chemistry, 4th edition, [449].
10. Kerru, N.; Singh, P.; Koorbanally, N.; Raj, R.; Kumar, V. Recent advances (2015–2016) in anticancer hybrids. Eur. J. Med. Chem., 2017; 142: 179–212. [CrossRef] [PubMed]
11. Doing J, Zhang Q, Wang Z, Huang G, Li S. Recent Advances in the Development of indazole - based Anticancer Agents. Chem Chem., 2018; 13: 1-19. doi: 10.1002/cmdc.201800253.
12. Shrivastava A, Chakraborty AK, Upmanyu N, et al. Recent progress in chemistry and biology of indazole and its derivatives: A brief review. Austin J Anal Pharm Chem., 2016;

3(4): 1076.

13. Tanitame A, Oyamada Y, Ofuji K, Kyoya Y, Suzuki K, Ito H, Kawasaki M, Nagai K, Wachi M, Yamagishi J. Design, synthesis and structure–activity relationship studies of novel indazole analogues as DNA gyrase inhibitors with Gram-positive antibacterial activity. Bioorg Med Chem Lett., Jun. 7, 2004; 14(11): 2857-62. doi: 10.1016/j.bmcl.2004.03.044, PMID 15125947.
14. Minu M, Thangadurai A, Wakode SR, Agrawal SS, Narasimhan B. Synthesis, antimicrobial activity and QSAR studies of new 2, 3-disubstituted-3, 3a, 4, 5, 6, 47 7-hexahydro- 2Hindazoles. Bioorg Med Chem Lett., 2009; 19(11): 2960-4. doi: 10.1016/j.bmcl.2009.04.052, PMID 19410452.
15. López-Vallejo F, Castillo R, Yépez-Mulia L, et al, Medina-Franco JL. Benzotriazoles and indazoles are scaffolds with biological activity against Entamoeba histolytica. J. Biomol. Screening, 2011; 16(8): 862-8. doi: 10.1177/1087057111414902, PMID 21821786.
16. Pérez-Villanueva J, Hernández-Campos A, Yépez-Mulia L, Méndez-Cuesta C, Méndez-Lucio O, Hernández-Luis F, Castillo R. Synthesis and antiprotozoal activity of novel 2-{[2-(1H-imidazol- 1-yl) ethyl]sulfanyl}-1H-benzimidazole derivatives. Bioorg Med Chem Lett., 2013; 23(14): 4221-4. doi: 10.1016/j.bmcl.2013.05.012, PMID 23731944.
17. Cedillo-Rivera R, Chávez B, González-Robles A, Tapia A, YépezMulia L. In vitro effect of nitazoxanide against Entamoeba histolytica, Giardia intestinalis and Trichomonas vaginalis trophozoites. J Eukaryot Microbiol, 2002; 49(3): 201-8. doi: 10.1111/j.1550-7408. 2002.tb00523.x, PMID 12120985.
18. Orlando BJ, Malkowski MG. Crystal structure of rofecoxib bound to human cyclooxygenase-2. Acta Crystallogr F Struct Biol Commun, 2016; 72(10): 772-6. doi: 10.1107/S2053230X16014230, PMID 27710942.
19. Cheekavolu C, Muniappan M. In vivo and in vitro anti-inflammatory activity of indazole and its derivatives. J. Clin Diagn Res., 2016; 10(9): FF01–FF06. doi: 10.7860/JCDR/2016/19338.8465, PMID 27790461.
20. Woods KW, Fischer JP, Claiborne A, Li T, Thomas SA, Zhu GD, Diebold RB, Liu X, Shi Y, Klinghofer V, Han EK, Guan R, Magnone SR, Johnson EF, Bouska JJ, Olson AM, de Jong R, Oltersdorf T, Luo Y, Rosenberg SH, Giranda VL, Li Q. Synthesis and SAR of indazolepyridine based protein kinase B/Akt inhibitors. Bioorg Med Chem., 2006; 14(20): 6832-46. doi: 10.1016/j.bmc.2006.06.047, PMID 16843670.
21. Patel M, Rodgers JD, McHugh RJ, Johnson BL, Cordova BC, Klabe RM, Bacheler LT, Erickson- Viitanen S, Ko SS. Unsymmetrical cyclic ureas as HIV-1 protease

inhibitors: novel biarylindazoles as P2/P2’ substituents. Bioorg Med Chem Lett., 1999; 9(22): 3217-20. doi: 10.1016/s0960-894x(99)00564-8, PMID 10576691. 48

22. Moore PK, Babbedge RC, Wallace PZ, Gaffen ZA, Hart SL. 7 -nitro indazole, an inhibitor of nitric oxide synthase, exhibits antinociceptive activity in the mouse without increasing blood pressure. Br J Pharmacol, 1993; 108(2): 296-7. doi: 10.1111/j.1476-5381. 1993. tb12798.x, PMID 7680591.
23. Tzvetkov NT, Hinz S, Küppers P, Gastreich M, Müller CE. Indazole-and indole5-carboxamides: selective and reversible monoamine oxidase B inhibitors with subnanomolar potency. J Med Chem., 2014; 57(15): 6679-703. doi: 10.1021/jm500729a, PMID 24955776.
24. N. A. Ali, B. A. Dar, V. Pradhan, M. Farooqui, Mini Rev. Med. Chem., 2013; 13: 1792 – 1800.
25. P. S. Kuhn, G. E. Buchel, K. K. Jovanovic, L. Filipovic, S. Radulovic, P. Rapta, V. B. Arion, Inorg. Chem., 2014; 53: 11130 –11139.
26. Ferreira, L.G., Dos Santos, R.N., Oliva, G. and Andricopulo, A.D., Molecular docking and structure-based drug design strategies. Molecules, 2015; 20(7): 13384-13421.
27. Azad, I., 2023. Molecular docking in the study of ligand-protein recognition: an overview. Molecular Docking-Recent Advances.
28. Patil, V.S. and Patil, P.A., Molecular Docking: A useful approach of Drug Discovery on the Basis of their Structure. Asian Journal of Pharmaceutical Research, 2023; 13(3): 191-195.
29. Raval, K.Y, et.al., Basics, types and applications of molecular docking: A review. IP International Journal of Comprehensive and Advanced Pharmacology, 2022; 7(1): 12–16.