Journal of Neonatal Surgery
ISSN(Online): 2226-0439
Vol. 14,issue.32s (2025)
https://www.jneonatalsurg.com

OPEN ACCESS

In-Silico Study Of Bone Cancer Activity Of Indole 3-Carbinol

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Cite this paper as Dr. S.K.Periyasamy, Dr. C. Karikal Chozhan, R. Rajeshkannan, K. Muralidharan (2025) In-Silico Study Of Bone Cancer Activity Of Indole 3-Carbinol.Journal of Neonatal Surgery, 14, (32s), 9818-9822

ABSTRACT

This study aims to describe the bone cancer activity of Indole-3- carbinol. This compound is predicted as a potential drug in medicinal field confirmed by Swiss ADME software. Further, the bone cancer activity of Indole-3-carbinol was analyzed by Auto docking study and found out the binding energy of compound which confirms that this can be a potential bone cancer drug. Hence, Indole – 3 carbinol is expected to be an effective bone cancer drug in medicinal field as well as in the society.

Keywords: *Indole -3-carbinol, bone cancer, Swiss ADME, Auto docking.*

1. INTRODUCTION

Indole-3-carbinol (I3C) is an organic compound with significant biological relevance, particularly in the context of cancer research and health aspects. It is a natural product found in cruciferous vegetables like Broccoli, Brussels sprouts, Cabbage, and Kale. Below is a detailed description of Indole-3-carbinol, including its chemical structure, properties, biological activities and applications. Jing-Ru Wen et al1 investigated during the course of on cogenesis and tumor progression, cancer cells constitutively up regulate signaling pathways relevant to cell proliferation and survival as a strategy to overcome genomic instability and acquire resistance phenotype to chemotherapeutic agents. This broad spectrum of anti- tumor activities in conjunction with low toxicity underscores the translational value of Indole-3-carbinol and its metabolites in cancer therapy. Bharat B. Aggarwal & Haruyo Ichikawa2 explained that Indole-3- carbinol is produced by members of the family Cruciferae, and particularly members of the Genus Brassica (e.g., cabbage, radishes, cauliflower, broccoli, brussels sprouts, and daikon). Under acidic conditions, 13C is converted to a series of oligomeric products (among which 3,3'-diindolylmethane is a major component) thought to be responsible for its biological effects in vivo. In vitro, 13C has been shown to suppress the proliferation of various tumor cells including breast cancer, prostate cancer, endometrial cancer, colon cancer, and leukemic cells; induce G1/S arrest of the cell cycle, and induce apoptosis.

Karimabad, Mojgan N. *et al*[3] stated that the Indole-3-carbinol (I3C) displays anti- cancer/proliferative activities against human cancer cells.

Yichao Wan *et al*[4] reported heterocyclic compounds are a significant source of pharmacologically active compounds. Among them, the Indole scaffold widely distributes in natural products and bioactive molecules including anti-cancer agents.

Sarkar Fazlul H & Li Yiwei[5] informed that Epidemiological and dietary studies have revealed an association between high dietary intake of cruciferous vegetables and decreased prostate cancer risk. Our studies have shown that Indole-3-carbinol (I3C), a common phytochemical in cruciferous vegetables, and its in vivo dimeric product 3,3′-diindolylmethane (DIM) upregulate the expression of phase I and phase II enzymes, suggesting increased capacity for detoxification and inhibition of carcinogens. Studies from our laboratory and others have found that I3C can induce G1 cell-cycle arrest and apoptosis in prostate cancer cells. Young S. Kim & J.A. Milner[6] explained that mounting preclinical and clinical evidence indicates that Indole-3-carbinol (I3C), a key bioactive food component in cruciferous vegetables, has multiple anti-carcinogenic and anti-tumorigenic properties.

Indole-3-carbinol has been studied extensively for its potential anti-cancer properties. Research has shown that it may help in the prevention of hormone-related cancers, such as breast cancer, prostate cancer, and endometrial cancer. I3C may influence estrogens metabolism, leading to the production of more favourable estrogens metabolites that are less likely to promote cancerous growth. It has been shown to regulate the expression of certain genes involved in detoxification (e.g., phase I and phase II enzymes) and apoptosis (programmed cell death) in cancer cells. Indole-3-carbinol exhibits potential anti-inflammatory properties. It has been shown to inhibit the expression of inflammatory mediators such as cyclooxygenase-2 (COX-2), an enzyme involved in the inflammatory process. This makes it possible of interest in inflammatory conditions like arthritis.

2. EXPERIMENTAL METHODS

Materials and Methods:

All the study was carried out by the in-*silico* methods.

Drug action and Bone cancer activity of Indole -3 –Carbinol was followed by two methods of *in - silico* studies.

I Method: *In silico* drug-likeness evaluation on Swiss ADME Method:

In order to predict the potential of Indole-3-carbinol compound to become a medicine, we driven an in silico evaluation of physicochemical properties, pharmacokinetics, drug- likeness and medicinal chemistry friendliness tests on *Swiss ADME*, a free-on-line platform that gives free access to a pool of

predictive models.

Operation of Swiss ADME

Go to Swiss ADME.

Input the chemical structure using:

SMILES notation (e.g., CC(=O)OC1=CC=CC=C1C(=O)O for Aspirin)

Molecular name or **draw the structure** using the provided tool.

Click "**Run**" to generate ADME properties. Analyze the predicted data, particularly drug- likeness and pharmacokinetics

II Method: *In silico* Bone cancer activity on Autodocking Method:

In this method Indole-3-carbinol compound was done by bone cancer activity. Bone cancer activity investigated by the Auto-dock 4.0 free soft ware.

Steps for AutoDock-Based Docking Studies in Bone Cancer

Preparation of Target Protein (Receptor)

Select a **bone cancer-related protein** from the **Protein Data Bank (PDB)** (e.g., osteosarcoma- related targets like MMPs, VEGFR, or ALK).

Remove water molecules, heteroatoms, and non-essential ligands using **AutoDockTools (ADT)**

or PyMOL.

Add **polar hydrogens** and calculate **Gasteiger charges**.

Convert to **PDBQT format** (required by AutoDock).

Preparation of Organic Compounds (Ligands)

Obtain or **draw the structure** using ChemDraw, Avogadro, or similar software.

Convert the structure into **PDB** format (use Open Babel if needed).

Optimize geometry and **add hydrogen atoms**.

Convert to **PDBQT format** using AutoDockTools.

Grid Box and Docking Parameter Setup

Define a **grid box** around the active site of the target protein.

Choose an **appropriate docking algorithm** (Genetic Algorithm in AutoDock4 or AutoDock Vina).

Set the **number of docking runs** (higher runs provide better accuracy).

Running the Docking Simulation.

Run **AutoDock Vina** or **AutoDock4** to perform docking.

Analyze the **binding affinity (kcal/mol)** and interaction type (H-bonds, hydrophobic, electrostatic).

Post-Docking Analysis

Use **PyMOL, Discovery Studio, or LigPlot+** to visualize interactions.

Rank compounds based on **binding energy** (lower energy = stronger binding).

Identify key interactions with **cancer-related residues**

3. RESULT AND DISCUSSSION:

IN-SILICO DRUG ACTIVITY OF INDOLE 3-CARBINOL BY Swiss ADME SOFTWARE:

PHARMACOKINETICS PREDICTION OF INDOLE 3-Carbinol BY SwissADME SOFTWARE:

First of all, INDOLE 3-Carbinol drug action confirmed by the *in-silico* evaluation of physicochemical properties, pharmacokinetics, drug-likeness and medicinal chemistry friendliness tests on *Swiss ADME*, a free-on- line platform that gave a free access to a pool of predictive models

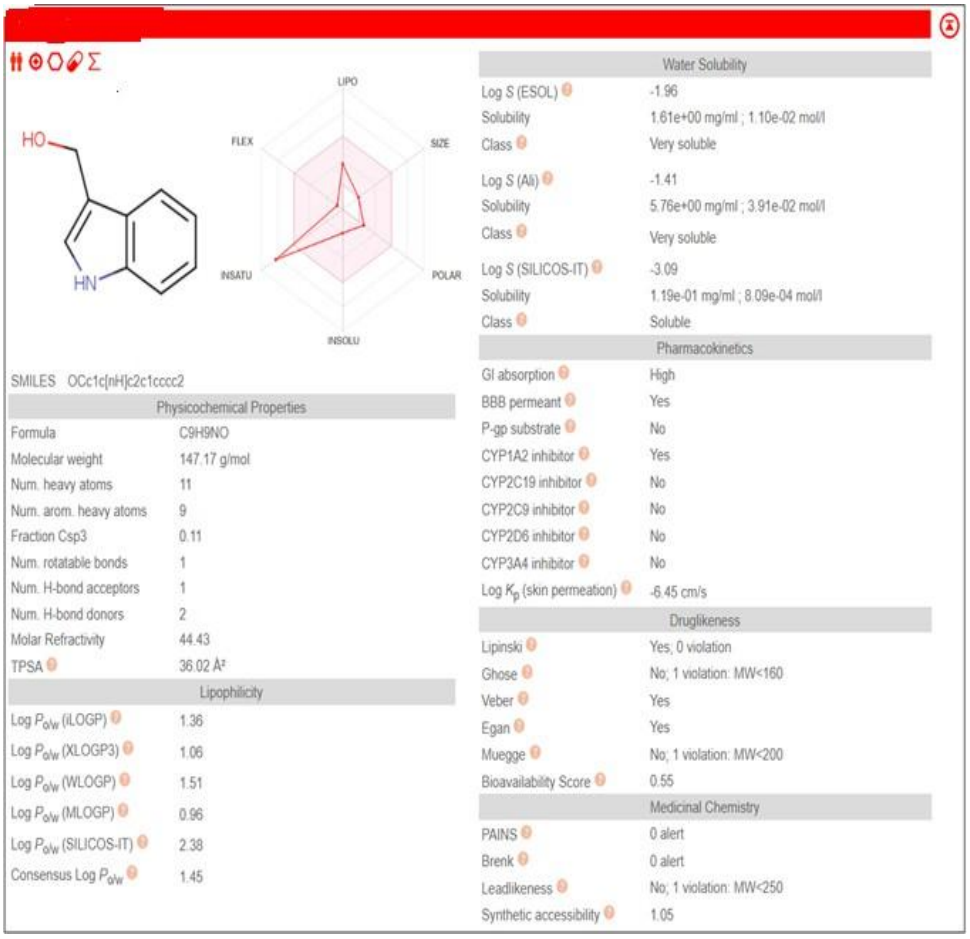

Figure:2 Pharmacokinetics Prediction diagram of Indole 3-Carbinol By Swiss ADME Software

In Figure 2, shows that data was confirmed by the Indole-3-Carbinol was used a potential drug molecule in Pharmacokinetics.

IN-SILICO BONE CANCER ACTIVITY OF INDOLE 3 CARBINOL BY AUTO-DOCK SOFTWARE:

Bone cancer activity of Indole-3-carbinol was carried out by auto docking study of *in-silico* method. In this method binding energy of protein was calculated. The binding energy score of Indole - 3 carbinol is -1.72 calculated by auto-dock method

Table 2(a) Binding energy of Indole-3-carbinol

Cluster Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-1.72	9	-1.69	2	##
2	-1.63	7	-1.63	2	##
3	-1.42	1	-1.42	1	#
4	-1.11	3	-1.11	2	##
5	-1.07	6	-1.07	1	#
6	-1.06	10	-1.06	1	#
7	-1.05	8	-1.05	1	#

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	9	-1.72	0.00	28.00	RANKING
1	2	4	-1.66	0.28	28.05	RANKING
2	1	7	-1.63	0.00	28.28	RANKING
2	2	2	-1.63	0.03	28.27	RANKING
3	1	1	-1.42	0.00	21.69	RANKING
4	1	3	-1.11	0.00	50.68	RANKING
4	2	5	-1.11	0.13	50.75	RANKING
5	1	6	-1.07	0.00	41.88	RANKING
6	1	10	-1.06	0.00	16.46	RANKING
7	1	8	-1.05	0.00	40.04	RANKING

Table 2(b) Binding energy of Indole-3-carbinol.

This is our docking results for the Indole-3-carbinol compound. We get peak value ranging of **-1.72**. On docking of Cancer Protein and Indole-3-carbinol drug.

From this data, we confirmed that Indole-3-carbinol is a good drug molecule used in pharmaceuticals and other medicinal fields.

4. CONCLUSION:

In this report, we explained the study and calculation of bone cancer activity of Indole -3 - carbinol. The binding energy of Indole -3 - carbinol is -1.72. Molecular docking is an important tool in computational chemistry and computer-aided drug design. The goal of ligand-protein docking is to identify favoured binding modes of a ligand with a protein of known three-dimensional structure. This study is focused on describing several approaches and algorithms used to find the optimal conformation of resulting ligand protein complex. It also aims to provide overview and assessment of several commonly used docking software. We tested the programs on a set of matrix

metalloproteinase to evaluate their accuracy and treatment of metal atoms. The initial protein and ligand structures have been optimized, docked with each software and the results have been compared with experimental data. While the software was often able to find correct ligand conformations, the results revealed significant problems of tested docking software in prediction of binding energy. From *in-silico* study of compound Indole -3 - carbinol have the high binding energy value for bone cancer. In this work conclude that it is a best organic drug molecule.

Acknowledgement

The authors thank the Management and Principal Jamal Mohamed College (Autonomous), Tiruchirappalli, Tamil Nadu, India for providing necessary facilities and encouragement

REFERENCES

[1] Jing-Ru Weng a b, Chen-Hsun Tsai c, Samuel K. Kulp c, Ching-Shih Chen , Indole-3-carbinol as a chemopreventive and anti-cancer agent,Cancer Letters,262, 2, 153-163(2008), https://doi.org/10.1016/j.canlet.2008.01.033

[2] Bharat B. Aggarwal & Haruyo Ichikawa , Molecular Targets and Anticancer Potential of Indole-3-Carbinol and Its Derivatives, Cell Cycle,4, 9:

[3] (2005),https://doi.org/10.4161/cc.4.9.1993

[4] Karimabad, Mojgan N.; Mahmoodi, Mehdi; Jafarzadeh, Abdolah; Darekordi, Ali; Hajizadeh, Mohamad Reza; Hassanshahi, Gholamhossein, Molecular Targets, Anti-cancer Properties and Potency of Synthetic Indole-3-carbinol Derivatives, Mini-Reviews in Medicinal Chemistry,19, 7, 540 – 554, (2019), https://doi.org/10.2174/1389557518666181116120145

[5] Yichao Wan, Yuanhua Li , Chunxing Yan , Mi Yan , Zilong Tang, Indole: A privileged scaffold for the design of anti-cancer agents, European Journal of Medicinal Chemistry

[6] 183 (2019),https://doi.org/10.1016/j.ejmech.2019.111691

[7] Sarkar Fazlul H. &, Li Yiwei,Indole-3-Carbinol and Prostate Cancer, The Journal of Nutrition, 134, 12, 3493S-3498S(2004), https://doi.org/10.1093/jn/134.12.3493S

[8] Young S. Kim & J.A. Milner,Targets for indole-3-carbinol in cancer prevention

[9] The Journal of Nutritional Biochemistry,16, 2, 65-73(2005), https://doi.org/10.1016/j.jnutbio.2004.10.007..

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