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In-Silico Study of Bone Cancer Activity of N-Benzylideneaniline

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ABSTRACT

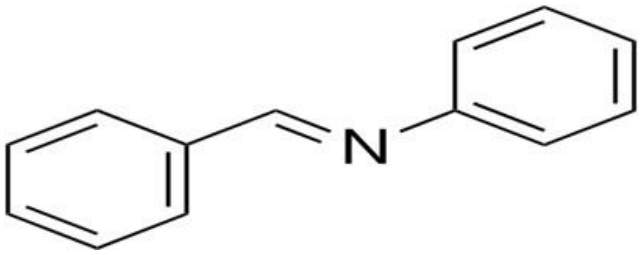
This study aims to describe the bone cancer activity of N-Benzylideneaniline , In this compound was predicted potential drug in medicinal field confirmed by swiss ADME software. Further, analaysed the bone cancer activity of N-Benzylideneaniline by Autodocking study and find out the binding energy compound. in this study was confirmed is very potential bone cancer drug. So, In future, N-Benzylideneaniline may be very effective bone cancer drug in the soceity and medicinal field.

Keywords: *N-Benzylideneaniline, bonecancer, Swiss ADME , Autodocking*

1. INTRODUCTION

N-Benzylideneaniline, also known as benzeneamine, N-benzylidene or benzylideneaniline, is an organic compound that belongs to the class of Schiff bases. It is synthesized by the condensation reaction of aniline and benzaldehyde, resulting in the formation of a double bond between the nitrogen atom of aniline and the carbon of the benzylidene group.

STRUCTURE OF N-BENZYLIDENEANILINE:



N-Benzylideneaniline is used in organic synthesis as an intermediate for preparing other chemicals, including ligands for coordination chemistry.It has applications in the production of dyes due to the unique reactivity of the Schiff base.It can be used in some analytical methods to detect certain metals or ions.N-Benzylideneaniline, as a Schiff base, exhibits various biological activities due to its chemical structure and ability to interact with biological systems. Here are some key biological activities associated with N-benzylideneaniline.Several studies have reported that N-benzylideneaniline and its derivatives exhibit anticancer activity. These compounds can interfere with cell proliferation and induce apoptosis (programmed cell death) in certain cancer cell lines. The Schiff base may disrupt critical pathways in cancer cell survival, such as the inhibition of specific enzymes or receptor-mediated pathways. N-Benzylideneaniline has shown anti-inflammatory effects in various models, suggesting it can reduce inflammation and associated pain. This could make it a potential candidate for the treatment of inflammatory diseases such as arthritis or colitis. It might modulate inflammation through the inhibition of pro-

inflammatory cytokines or enzymes like COX-2 (cyclooxygenase-2).Some derivatives of N-benzylideneaniline have been studied for their antidiabetic effects. These compounds may help in regulating blood sugar levels by influencing insulin secretion or enhancing the insulin sensitivity of target tissue

Shaoyi Cai *et al*[1], reported the Toll-like receptor 2 (TLR2) can recognize pathogen-associated molecular patterns to defense against invading organisms and has been represents an attractive therapeutic target. Until today, none TLR2 small molecule antagonist have been developed in clinical trial. Herein, we designed and synthesized 50 *N*-benzylideneaniline compounds with the help of CADD. And subsequent *in vitro* studies leading to the optimized compound SMU-A0B13 with most potent inhibitory activity to TLR2 (IC_{50}=18.21 ± 0.87 μM). Preliminary mechanism studies indicated that this TLR2 inhibitor can work through the NF-κB signaling pathway with high specificity and low toxicity, and can also efficiently downregulate inflammatory cytokines, such as SEAP, TNF-α and NO in HEK-Blue hTLR2, human PBMC and Raw 264.7 cell lines. Additionally, the docking situation also indicate SMU-A0B13 can well bind to the TLR2-TIR (PDB: 1FYW) active domain, which probably explains the bioactivity.

Yusuf Özkay *et al*[2] explained, A series of Schiff bases including N-benzylideneaniline (NBA) nuclei were prepared. The chemical products obtained were characterized by mass spectrometry (APCI), ^{1}H NMR, and IR spectroscopy in order to seek their cytotoxic and proliferation effects on human small lung (A549) and cervical (HeLa) cancer cell lines with biochemical assays. All of the synthesized compounds showed antiproliferative effects to different extents

2. EXPERIMENTAL METHODS

Materials and Methods:

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

Drug action and Bone cancer activity of N-Benzylideneaniline 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 N-Benzylideneaniline compound to become a medicine, we driven an in silico evaluation of physicochemical properties, pharmacokinetics, drug- likeness and medicinal chemistry friendliness tests on *SwissADME*, a free-on-line platform that gives free access to a pool of predictive models.

Operation of SwissADME

1. Go to SwissADME.
2. 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.
3. 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 N-Benzylideneaniline 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

A. 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).

B. 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.

C. 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).

D. 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).

E. 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

Docking Result:

***In-Silico* Drug Activity Of N-Benzylideneaniline By Swissadme Software:**

Pharmacokinetics Prediction Of N-Benzylideneaniline By Swissadme Software:

First of all, N-Benzylideneaniline drug action confirmed by the *In-silico* evaluation of physicochemical properties, pharmacokinetics, drug-likeness and medicinal chemistry friendliness tests on *SwissADME*, a free-on-line platform that gave a free access to a pool of predictive models.

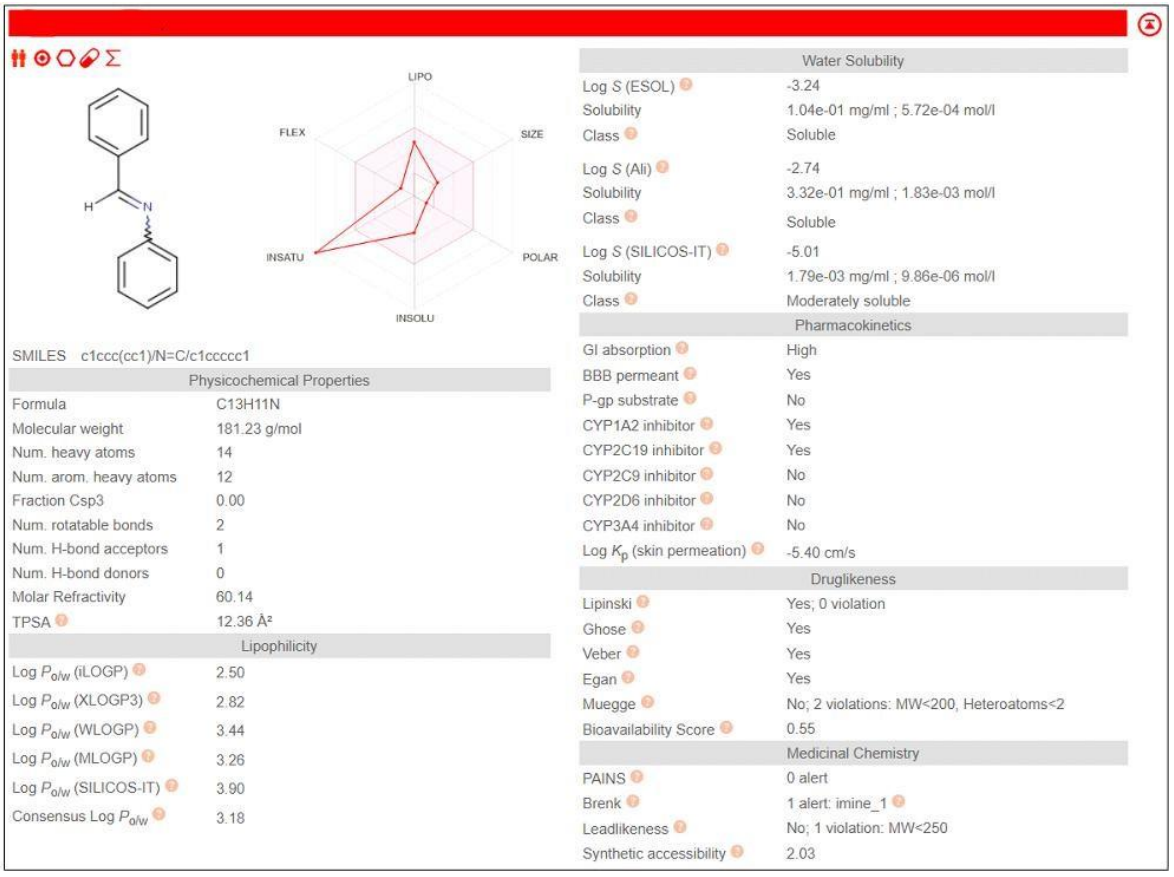


Figure:3 Pharmacokinetics Prediction diagram of N-Benzylidene aniline By Swiss ADME Software

In figure 3, shows that data was confirmed by the N-Benzylideneaniline was used a potential drug molecule in Pharmacokinetics

***IN-SILICO* BONE CANCER ACTIVITY OF N-BENZYLIDENEANILINE BY AUTO-DOCK SOFTWARE:**

Bone cancer activity of N-Benzylideneaniline 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 N-Benzylideneaniline is -4.63 calculated by auto-dock method.

Table 3 (a) Binding energy of N-Benzylideneaniline.

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-4.63	10	-4.63	1	#
2	-4.62	3	-4.62	1	#
3	-4.62	6	-4.61	3	###
4	-4.60	8	-4.60	1	#
5	-4.57	4	-4.55	4	####

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	10	-4.63	0.00	29.25	RANKING
2	1	3	-4.62	0.00	34.68	RANKING
3	1	6	-4.62	0.00	63.97	RANKING
3	2	2	-4.61	0.06	64.01	RANKING
3	3	5	-4.61	0.11	63.89	RANKING
4	1	8	-4.60	0.00	13.00	RANKING
5	1	4	-4.57	0.00	49.88	RANKING
5	2	1	-4.55	0.58	49.77	RANKING
5	3	7	-4.54	0.54	49.84	RANKING
5	4	9	-4.53	0.78	49.68	RANKING

Table 3 (b) Binding energy of N-Benzylideneaniline.

This is our docking results for the N-Benzylideneaniline compound. We get peak value ranging of -4.63. On docking of Cancer Protein and N-Benzylideneaniline drug.

From this data we confirmed that N-Benylideneaniline is a good drug molecule used in pharmaceuticals and other medicinal fields.

4. CONCLUSION

In this study explained the study and calculation of bone cancer activity of N-Benzylideneaniline l. The binding energy of N-Benzylideneaniline is -4.63. 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 were often able to find correct ligand conformations, the results revealed significant problems of tested docking software in prediction of binding energy. From the *in-silico* study of compound N-Benzylideneaniline have the high binding energy value for bone cancer. In this work conclude that it is a best organic drug molecule.

5. ACKNOWLEDGEMENT

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