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IN-SILICO STUDY OF BONE CANCER ACTIVITY OF PYRAZINE

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ABSTRACT

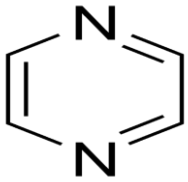
This study aims to describe the bone cancer activity of pyrazine, In this compound was predicted potential drug in medicinal field confirmed by swissADME software. Further, analaysed the bone cancer activity of puyazine by Autodocking study and find out the binding energy compound. in this study was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

KEYWORDS: Pyrazine, *bonecancer, Swiss ADME, Autodocking.*

INTRODUCTION

Pyrazine is an organic compound that belongs to the class of heterocyclic aromatic compounds. It consists of a six-membered ring containing four carbon atoms and two nitrogen atoms at alternate positions. Its molecular formula is $C_4H_4N_2$.

Structure Of Pyrazine



Pyrazine has a simple structure with a symmetrical arrangement of carbon and nitrogen atoms. The nitrogen atoms are positioned at opposite ends of the ring. Pyrazine is a colourless

to pale yellow liquid with a distinct, somewhat musty odour. It is highly soluble in water, alcohol, and ether. While pyrazine itself is not typically known for direct bone cancer activity, several pyrazine derivatives and compounds that contain a pyrazine ring have been studied for their biological activity, including bone cancer properties. The bone cancer potential of pyrazine derivatives may come from various mechanisms, including modulation of cell signaling pathways, induction of apoptosis, with cancer cell proliferation. Eman S. Tantawy *et al*[1] reported the synthesis of fused quinoxalines and pyrazines derivatives and due to the resultant pharmacological interest in compounds which belong to these heterocyclic derivatives.

Rakesh Sahu *et al*[2] explained the Pyrazine-based medications are a substantial contribution, as they are one of the most important pharmacophores found in heterocyclic compounds both synthetically and naturally. It's a six-membered aromatic heterocycle with two nitrogen atoms with a wide range of therapeutic applications in drug development and numerous prospects for future enhancement in anticancer drugs by targeting several critical receptors. A number of pyrazine compounds have been shown to inhibit enzymes, receptors, and a range of additional cancer-fighting targets.

Martin Dolezal & Jan Zitko[3] reported Pyrazine is a member of 1,4-diazines, which constitute an important class of heterocycles. Various pyrazine derivatives have been synthesized and successfully evaluated as agents with diverse pharmacological effects (including but not limited to antiproliferative, anti-infective, and effects on cardiovascular or nervous system) and some of them have become clinically used drugs worldwide.

EXPERIMENTAL METHODS

MATERIALS AND METHODS

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

Drug action and Bone cancer activity of pyrazine 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 pyrazine 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 pyrazine 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.**

RESULT AND DISCUSSSION

IN-SILICO DRUG ACTIVITY OF PYRAZINE BY SwissADME SOFTWARE

PHARMACOKINETICS PREDICTION OF PYRAZINE BY SwissADME SOFTWARE

First of all, Pyrazine 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.

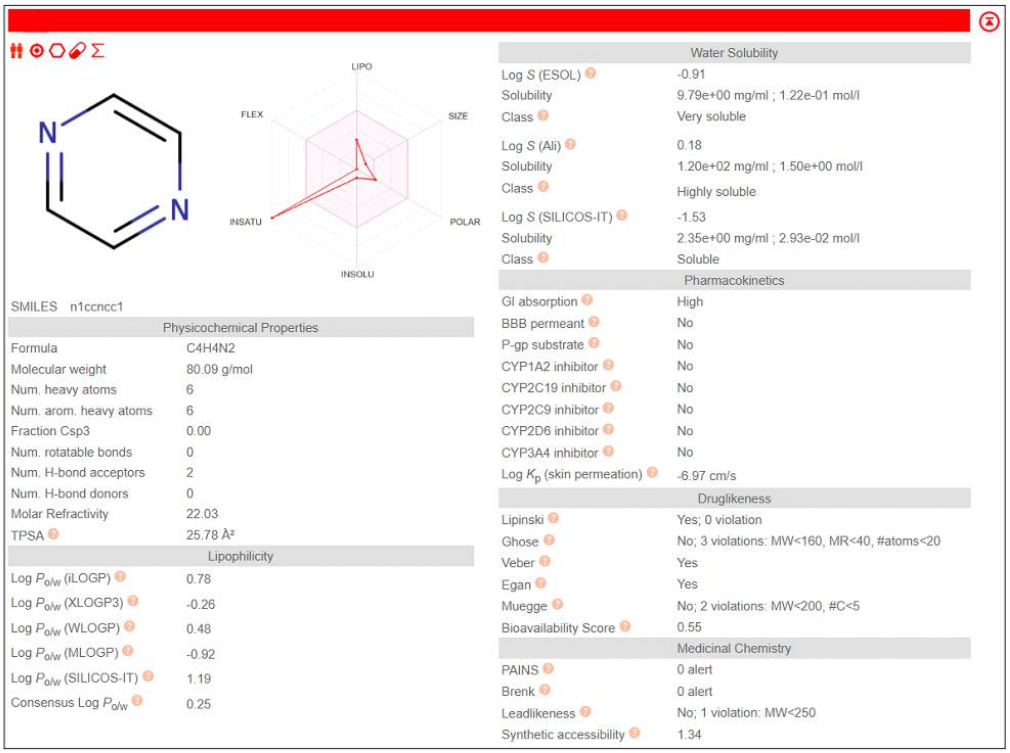


Figure 4: Pharmacokinetics Prediction diagram of pyrazine By Swiss ADME Software.

In figure 4, shows that data was confirmed by the pyrazine was used a potential drug molecule in Pharmacokinetics.

IN-SILICO BONE CANCER ACTIVITY OF PYRAZINE BY AUTO-DOCK SOFTWARE

Bone cancer activity of pyrazine 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 pyrazine was -3.63 calculated by auto -dock method.

Table 4: (a) Binding energy of pyrazine.

Clus-ter Rank	Lowest Binding Energy	Run	Mean Binding Energy	Num in Clus	Histogram 5 10 15 20 25 30 35
1	-3.63	10	-3.63	1	#
2	-3.62	3	-3.62	1	#
3	-3.62	6	-3.61	3	###
4	-3.60	8	-3.60	1	#
5	-3.57	4	-3.55	4	####

Number of multi-member conformational clusters found = 2, out of 10 runs.

Table 4(b) - Binding energy of pyrazine.

Rank	Sub-Rank	Run	Binding Energy	Cluster RMSD	Reference RMSD	Grep Pattern
1	1	10	-3.63	0.00	29.25	RANKING
2	1	3	-3.62	0.00	34.68	RANKING
3	1	6	-3.62	0.00	63.97	RANKING
3	2	2	-3.61	0.06	64.01	RANKING
3	3	5	-3.61	0.11	63.89	RANKING
4	1	8	-3.60	0.00	13.00	RANKING
5	1	4	-3.57	0.00	49.88	RANKING
5	2	1	-3.55	0.58	49.77	RANKING
5	3	7	-3.54	0.54	49.84	RANKING
5	4	9	-3.53	0.78	49.68	RANKING

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

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

CONCLUSION

In this study explained the study and calculation of bone cancer activity of pyrazine. The binding energy of pyrazine is -3.63. 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 pyrazine have the high binding energy value for bone cancer. In this work conclude that it is a best organic drug molecule.

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