

An *in silico* approach towards lung cancer with regard to chemokine receptors

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ABSTRACT

In our present study, it was identified that the chemokine receptors towards lung cancer has been synthesized with a multiple steps. *In vivo* methods can be used and it is a multi-step process which is used to identify biological molecules. Pharmacokinetic properties has been developed where the metabolism, production and pathogenicity was identified. The present study compares low binding lead compounds and their potential binding attraction leads to the identification of main pathogenic diseases such as lung cancer. It performs an experimental study to identify the similarities between normal lung cancer to contagious lung cancer. It has been proved by clinical studies to identify a difference between them and the inflammatory prostate cancer has been identified.

KEY WORDS: Enzymes, Inhibitors, Lung cancer, target drug.

1. INTRODUCTION

Cancer (medical term: malignant neoplasm) which is having undefined growth has been divided through normal metastatic method which can spread from normal cell to dead cells and protrude into it to destroy adjacent tissues and cells. In some cases, the contagious cells can spread to other parts of the body through blood ^[1]. The properties of malignant cancer can be varied from normal cells in many criteria but having slight variations with benign tumors.

Lung cancer: Lung cancer mainly affects lungs where the uncontrolled growth takes place in the lining of the lung. It grows by the mechanism of metastasis where it affects adjacent tissues of the lung and beyond it. Initially, the lung cancer can initiate in epithelial layer of cells and causes death in all ages of people annually from 2004. The most commonly occurring symptoms include weezing, cold, cough and loss of weight.

Types of lung cancer: Lung cancer can be treated by using radiotherapy and chemotherapeutic agents can be used. In terms of preliminary to contagious lung cancer radiation therapy can be used rather than chemotherapy. Larger airways usually refers to Oat cell carcinoma and the small cells leads to paraneoplastic syndrome association.

Treatment

Surgery: Surgery is limited based on non-small cell lung carcinoma limited to one lung, up to critical stage

Chemotherapy: Chemotherapy can be given to 5 or 10% and applied in most severe cases

Radiotherapy: Radiotherapy can be given instead of chemotherapy and in carcinoma cases.

2. MATERIALS AND METHODS

Pubmed:

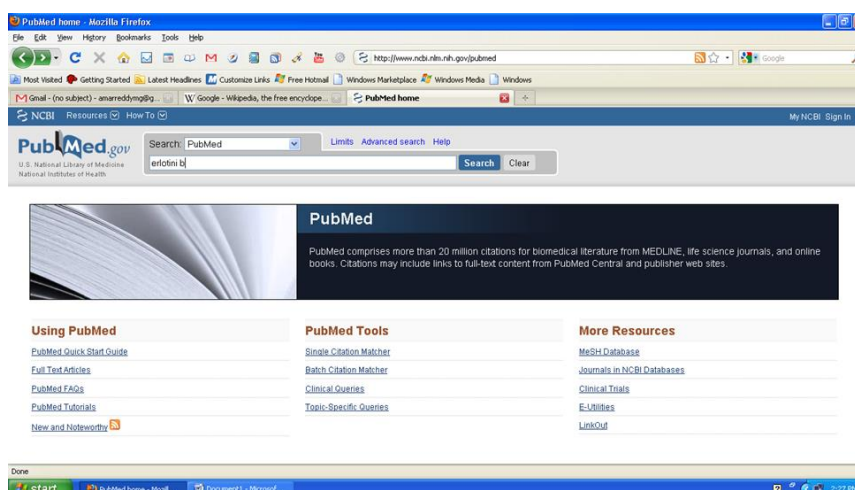


Figure.1. Pubmed snapshot



Figure.2.Pubchem snapshot

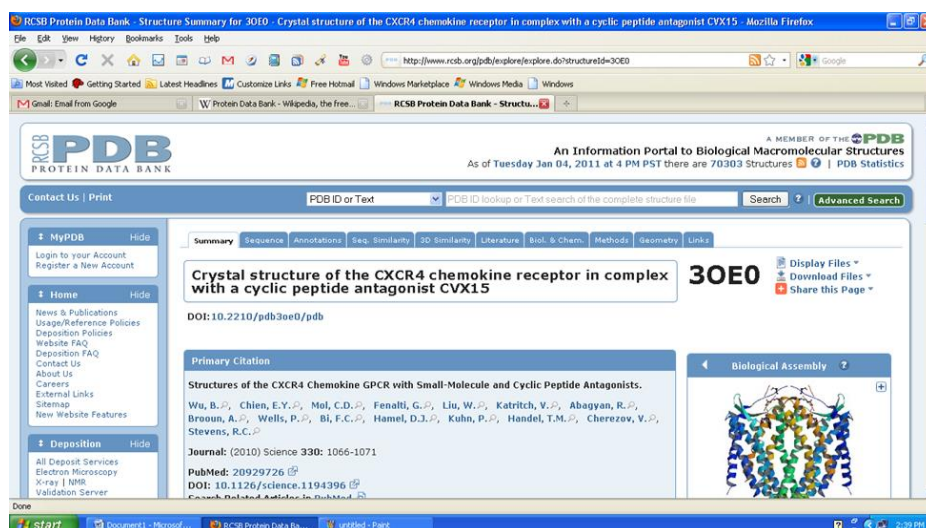


Figure.3.pdb page snapshot

3. RESULTS



Figure.4.TOPOTECAN structure retrieval from Pubchem

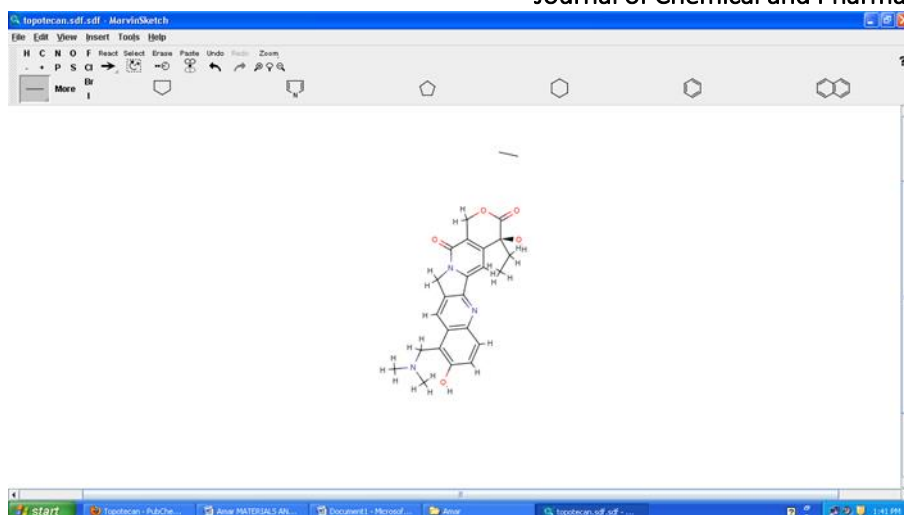
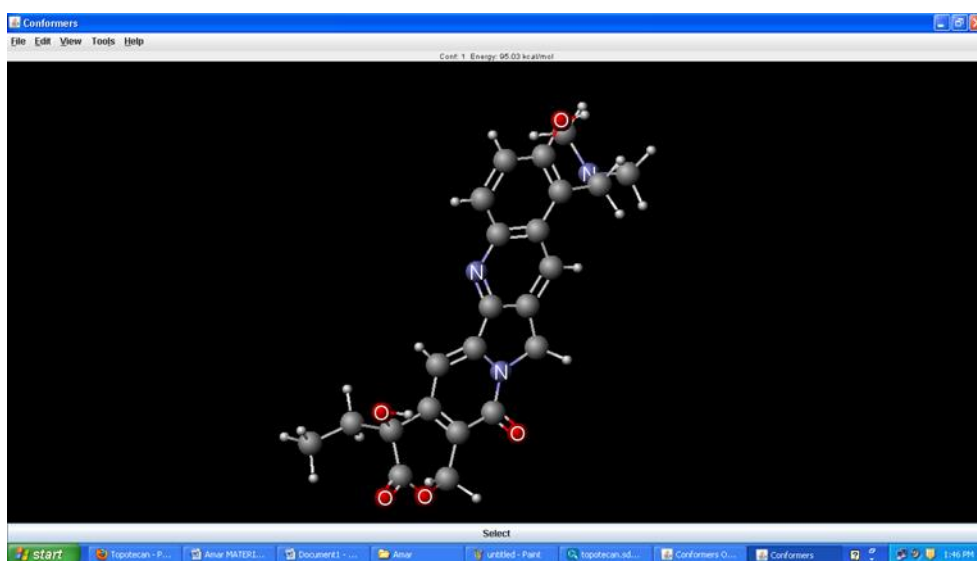


Figure.5. Structure of TOPOTECAN in PUBMED



**Figure.6. Shows 3d Structure with Energy Value
Table.1. Docking score value**

| Name of the molecule | G-value |
|----------------------|---------|
| acetogenins | -17.69 |
| Allicin | -14.17 |
| Allixin | -13.98 |
| allylsulphides | -10.68 |
| Apigenin | -19.62 |
| Artesunate | -21.57 |
| Betaglucan | -14.66 |
| Capsaicin | -19.75 |
| Catechin | -18.35 |
| Combretastatin A-4 | -20.23 |
| Diallyl disulfide | -12.60 |
| Ellagic acid | -17.54 |
| Ferulic acid | -17.83 |
| Glutathione | -12.78 |
| Hydroxytyrosol | -12.60 |

4. DISCUSSION AND SUMMARY

The molecules were allowed for receptor-ligand interaction by using docking tools. The score was identified and the molecules were showed by showing better interactions. It also finds the better score which results in receptor-ligand interaction by docking technique.

REFERENCES

- Arumugam S, Ramareddy S, Simulation comparison of class D/ Class E inverter fed induction heating", Journal of Electrical Engineering, 12 (2), 2012, 71-76.
- Camphausen KA How Cancer Arises, An explosion of research is uncovering the long-hidden molecular underpinnings of cancer—and suggesting new therapies, (PDF). Scientific American, 1996, 62–70.
- Clarke SJ, Clinical pharmacokinetics of docetaxel, Clin Pharmacokinet, 36 (2), 1999, 99-114.
- Fenton C, European Consensus Statement on Lung Cancer: risk factors and prevention. Lung Cancer Panel, CA Cancer J Clin (Smoking is the major risk factor, accounting for about 90% of lung cancer incidence) 48 (3), 1998, 167–176.
- Lydia Caroline M, Kandasamy A, Mohan R, Vasudevan S, Growth and characterization of dichlorobis l-proline Zn(II), A semiorganic nonlinear optical single crystal, Journal of Crystal Growth, 311(4), 2009, 1161-1165.
- Lyseng-Williamson KA, Docetaxel: a review of its use in metastatic breast cancer, Drugs, 65 (17), 2005, 2513-31.
- Pazdur R, Wagman LD, Hoskins WJ, Eds. Cancer Management: A Multidisciplinary Approach. 11th ed, 2009.
- Ramkumar Prabhu M, Reji V, Sivabalan A, Improved radiation and bandwidth of triangular and star patch antenna, Research Journal of Applied Sciences, Engineering and Technology, 4 (12), 2012, 1740-1748.
- Rivory LP, Improved survival in never-smokers vs current smokers with primary adenocarcinoma of the lung, Chest (American College of Chest Physicians), 126 (2), 2004, 347–351.
- Saravanan T, Srinivasan V, Udayakumar R, A approach for visualization of atherosclerosis in coronary artery, Middle - East Journal of Scientific Research, 18 (12), 2013, 1713-1717.
- Srinivasan V, Saravanan T, Reformation and market design of power sector, Middle - East Journal of Scientific Research, 16 (12), 2013, 1763-1767.
- Srivatsan P, Aravindha Babu N, Mesiodens with an unusual morphology and multiple impacted supernumerary teeth in a non-syndromic patient, Indian Journal of Dental Research, 18 (3), 2007, 138-140.
- Sundarraaj M, Study of compact ventilator, Middle - East Journal of Scientific Research, 16 (12), 2013, 1741-1743.
- Thooyamani KP, Khanaa V, Udayakumar R, An integrated agent system for e-mail coordination using jade, Indian Journal of Science and Technology, 6 (6), 2013, 4758-4761.
- Udayakumar R, Khanaa V, Kaliyamurthie KP, "Optical ring architecture performance evaluation using ordinary receiver", Indian Journal of Science and Technology, 6 (6), 2013, 4742-4747.
- Udayakumar R, Kumarave A, Rangarajan K, Introducing an efficient programming paradigm for object-oriented distributed systems, Indian Journal of Science and Technology, 6 (5), 2013, 4596-4603.
- Udayakumar R, Khanaa V, Kaliyamurthie K.P, Performance analysis of resilient fthh architecture with protection mechanism, Indian Journal of Science and Technology, 6 (6), 2013, 4737-4741.
- Uma Mageswaran S, Guna Sekhar N.O, Reactive power contribution of multiple STATCOM using particle swarm optimization", International Journal of Engineering and Technology, 5 (1), 2013, 122-126.
- Vidyalakshmi K, Kamalakannan, P, Viswanathan S, Ramaswamy S, Antinociceptive effect of certain dihydroxy flavones in mice, Pharmacology Biochemistry and Behavior, 96 (1), 2010, 1-6.
- Vijayaragavan SP, Karthik B, Kiran TVU, Sundar Raj M, Robotic surveillance for patient care in hospitals, Middle - East Journal of Scientific Research, 16 (12), 2013, 1820-1824.
- Vijayaragavan S.P, Karthik B, Kiran Kumar T.V.U, Sundar Raj M, Analysis of chaotic DC-DC converter using wavelet transform, Middle - East Journal of Scientific Research, 16 (12), 2013, 1813-1819.
- Vijayaragavan S.P, Karthik B, Kiran T.V.U, Sundar Raj M, Robotic surveillance for patient care in hospitals, Middle - East Journal of Scientific Research, 16 (12), 2013, 1820-1824.