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Comparative in silico and in vitro Study of N-(1-Methyl-2-Oxo-2-N-Methyl Anilino-Ethyl) Benzene Sulfonamide and Its Analogues as an Anticancer Agent

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Abstract : Doxorubicin, also known as adriamycin, is an anthracycline class of drug used in cancer chemotherapy. It is used in the treatment of non-Hodgkin's lymphoma, multiple myeloma, acute leukemias, breast cancer, lung cancer, endometrium cancer and ovary cancers. It functions via intercalating DNA and ultimately killing cancer cells. The major side effects of doxorubicin are hair loss, myelosuppression, nausea & vomiting, oesophagitis, diarrhoea, heart damage and liver dysfunction. The minor modifications in the structure of compound exhibit large variation in the biological activity, has prompted us to carry out the synthesis of sulfonamide derivatives. Sulfonamide is an important feature with broad spectrum of biological activity such as antiviral, antifungal, diuretics, anti-inflammatory, antibacterial and anticancer activities. Structure of the synthesized compound N-(1-methyl-2-oxo-2-N-methyl anilino-ethyl)benzene sulfonamide confirmed by proton nuclear magnetic resonance (1H NMR),13C NMR, Mass and FTIR spectroscopic tools to assure the position of all protons and hence stereochemistry of the molecule. Further we have reported the binding potential of synthesized sulfonamide analogues in comparison to doxorubicin drug using Auto Dock 4.2 software. Computational binding energy (B.E.) and inhibitory constant (Ki) has been evaluated for the synthesized compound in comparison of doxorubicin against Poly (dA-dT).Poly (dA-dT) and Poly (dG-dC).Poly (dG-dC) sequences. The in vitro cytotoxic study against human breast cancer cell lines confirms the better anticancer activity of the synthesized compound over currently in use anticancer drug doxorubicin. The IC50 value of the synthesized compound is 7.12 µM where as for doxorubicin is 7.2 µ.

Keywords : Doxorubicin, auto dock, in silco, in vitro
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