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Phytochemical Screening and GC- MS analysis of *Aloe Barbadensis Miller* with *In Silico* Approach against Anticancer Activities

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Abstract—*The aim of the study was to investigate the phytochemical compounds, GC-MS analysis and anticancer (Small cell Lung Cancer) activity of different extracts of Aloe Barbadensis Miller (Aloe Vera). Plants have important source of medicine with qualities for thousands of years, mainly on traditional remedies such as herbs for their history plants have been used as popular folk medicine. Aloe Vera is one of the best examples of having medicinal values, and contains both medicine and cosmetic effects. The Screening of phytochemical (Qualitative) analysis of Aloe Vera shows that it contains almost all types of chemical constituents like; Tannin, Phlobatannins, Saponin, Flavonoids, Terpenoids, Cardiac glycosides, and Anthroquinones, which are used in medicinal purpose. Here, two different solvents such as Aqueous and Methanol were used to extract the bioactive compounds from the leaf and root of Aloe Vera. Qualitatively analyzed Alkaloid, Carbohydrates, Cardiac Glycosides, Saponin, Tannin, Phenol, Amino acids, Oxalate, Anthraquinones, Quinines and sterols gave positive results and Terpenoids, Flavonoids, Steroid and Phlabotannin gave negative results. In GC-MS analysis, 14 bioactive phytochemical compounds were identified in the Methanolic extract of Aloe Vera. This present investigation computationally predicted Guanine nucleotide binding protein subunit alpha-15, causes Small Cell Lung Cancer (SCLC) via a structure-based method. Because of the unknown nature of crystal structure of targeted protein, a robust three-dimensional homology model of Guanine nucleotide binding protein subunit alpha-15 (PDB ID: 4GNK) was constructed by comparative modelling in MODELLER (v 9.19). The best three dimensional structure of target protein was selected on the basis of lowest discrete optimized protein energy (DOPE) score. The target protein was successfully docked with 14 GC-MS compounds by AutoDock 1.5.6. Molecular docking study identified that the root compound 9, 12-Octadecanoic acid (z, z) possesses high binding affinity towards target protein and inhibit it. Propose of the new predicted structure is reliable for the structural insights and functional studies and the selected inhibitor might be more potent for Small Cell Lung Cancer. Overall, findings of this study may be helpful in designing the novel therapeutic targets to cure Small Cell Lung cancer.*

Keywords*: Aloe Vera, Phytochemical, GC-MS, Guanine nucleotide binding protein subunit alpha- 15, Small Cell Lung Cancer, Homology Modelling and Molecular Docking.*

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