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Elemental analysis, phytochemical screening and evaluation of antioxidant, antibacterial and anticancer activity of *Pleurotus ostreatus* through *in-vitro* and *in-silico* approaches

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Pleurotus ostreatus (Oyster mushroom) is second to only Agaricus bisporus in their consumption pattern and cultivation across the world. The mushroom is reservoir of important bioactive compounds e.g., β- glucans, lentinan, lipopolysaccharides, resveratrol, Cibacron blue affinity purified protein, concanavalin, rutin, p-coumaric acid, ascorbic acid etc. These compounds impart on these natural herbs various healing effects e.g., hypocholesterolemia, free radical scavenging, antioxidant, antiatherogenic, antitumor, immunomodulatory and anti-bacterial properties. Thus, in this study we examined Oyster mushroom sample for presence of biologically essential elements using direct current arc optical emission spectroscopy. We also screened presence of volatile bioactive compounds by GC-MS in ethanolic extract of *Pleurotus Astreatus*. Additionally, in-vitro antioxidant, antibacterial and anticancer activities of ethanolic extract was studied. Molecular docking was performed between ligands as obtained from GC-MS data and proteins which are overexpressed in breast cancer e.g., EGFR, PR and NF-kB. The result of direct current arc optical emission spectroscopy revealed the presence of Fe, K, Na, Ca, Mg, Cr and Sr in the mushroom sample. Moreover GC-MS analysis showed that ethanolic extract of oyster mushroom possessed 32 biologically active compounds with a concentration maxima of linoleic

acid ethyl ester. The extract displayed remarkable free radical scavenging activity against DPPH. Additionally, the mushroom showed significant antibacterial activity against both gram positive (S. aureus) and gram-negative bacterial strains (Pseudomonas aeruginosa, Proteus vulgaris, Proteus mirabilis). In-vitro studies confirmed the anti-cancer activity of extract. It inhibited growth and proliferation of MCF-7 cells and simultaneously induced apoptosis. The result of molecular docking study unfolded the probable mechanism of action behind in-vitro effect. Docking studies has shown that ligand 15 (Linoleic acid ethylester), ligand27 (Ergosta-5,7,9(11),22-tetraen-3ol, (3. beta.,22E)-), ligand 28 (Stigmasta-5,22-dien-3-ol, acetate, (3. beta., 22Z)-), ligand 30 (Ergosta-5, 7, 22-Trien-3-OI,(3.Beta.,22E)-) and ligand 32 (Gamma.-Sitosterol) exhibited better binding affinities with EGFR, PR and NF-kB proteins. This suggest that ethanolic extract may have downregulated these signaling cascades to act as an anticancer agent. From this study it can be ascertained that Oyster mushrooms are not only beneficial to our taste buds but at the same time they provide us with necessary elements, variety of phytochemicals compounds and has protective function e.g., antioxidant, antibacterial and

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