Contribution ID: **37** Type: **Poster (Chemistry SIG)**

Computational studies, Synthesis and antiproliferative activities of coumarin-tagged 1,3,4-oxadiazole conjugates against MDA-MB-231 and MCF-7 human breast cancer cells

Abstract
Using a ligand-based pharmacophore screening workflow, two well-defined molecular drug targets were identified; these are epidermal growth factor receptor (EGFR) and estrogen receptor-α (ERα). These proteins have been imperative chemotherapeutic targets in current treatment regimens of breast cancer. Molecular docking studies were performed on the most active compounds for each scaffold in their respective drug targets to highlight important binding interactions of the drug candidates with potential targets. The binding profile Ospemifene, an ER inhibitor comprising of a significant contribution from hydrophobic interactions Leu41, Ala45, Trp78, Leu82 and Leu220 (bond distance = 3.93, 3.23, 3.70, 3.64 and 3.53 Å, respectively); and a hydrogen bond between the hydrogen bond donor Asp46 and ligand (bond distance = 1.91 Å, bond angle = 133.13). It is evident from the ospemifene-ERα complex that the active site of ERα is composed of a significant hydrophobic pocket, thus the selective binding of the potential anti-breast cancer agents will rely largely on contributions from hydrophobic interactions. The 3D structures of tested compounds were further optimized using the force field, MMFF94s in the Avogadro package (V 1.2.0). AutoDock Tools (V 1.5.6) was used to establish the grid box parameters.

Presenter Biography

Primary authors: Mr DHAWAN, Sanjeev (University of KwaZulu natal, westville campus); Dr SINGH, Parvesh (UKZN); Prof. JONNALAGADDAS, Sreekantha (UKZN)

Presenter: Mr DHAWAN, Sanjeev (University of KwaZulu natal, westville campus)

Session Classification: Chemistry and Material Science SIG Seminar

Track Classification: Chemistry and Material Science SIG Seminar