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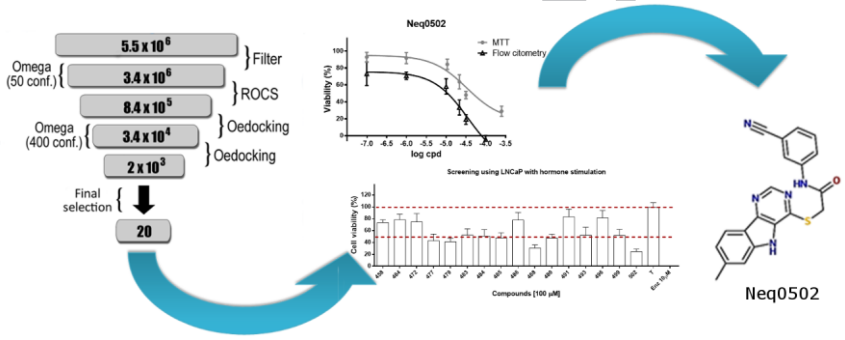
Graphical abstract



Abstract

Prostate cancer is one of the most prevalent types of cancer in male population. It is a hormone driven disease, especially in its initial phase. Hence, androgen deprivation therapy (ADT) is the major chemotherapeutic effort and novel AR inhibitors with improved pharmacological profiles are needed. In this report, a novel bioactive compound was selected and investigated using *in silico* and cell-based assays. Neq0502 compound was selective for the testosterone stimulated AR-dependent prostate cancer cell (LNCaP, GI_{50} = 22.4 µM) when compared with unstimulated LNCaP or AR-insensitive (DU145 and PC-3) cell lines. Cell cycle arrest study provided the same profile for Neq0502 and the reference drug enzalutamide. Moreover, this compound is not cytotoxic for fibroblast Balb/C 3T3 clone A31 cells up to 250