

## INHIBITION DYNAMICS OF VIABILITY OF MELANOMA CELLS

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Melanoma cells express chemokine receptor 4 (CXCR-4). When bound to chemokine ligand 12 (CXCL12) it activates signalling pathways such as mitogen-activated protein kinase (MAPK) and phosphatidylinositol 3-kinase (PI3K) that promote tumour cell proliferation, migration and adhesion. An inhibiting agent is a molecule which docks on the receptor CXCR-4, but does not activate the mentioned signalling pathway. The inhibiting agents tested within the framework of this research are CTCE9908, L-kynurenine Quinolinic acid, Kynurenic acid. The basic dynamics of the inhibition process can be represented via of mass-action reaction kinetics. The reaction network is easily restated as a system of ODEs and analyzed as such. The system has a unique globally asymptotically stable equilibrium.

Establishing inhibitory concentrations of a drug required to obtain 50 percent of the desired efficacy is a widely employed benchmark to determine the appropriateness. Numerical estimates of the IC50 estimates rely on computational software that perform a regression, which is subject to the choice of the curve used and often very sensitive to the parameters used in the curve. This motivates the use of the underlying dynamics before the regression while calculating the IC50 values. This needs the extra effort in terms of computation, but finds motivation in cutting the cost during assay performances by having fewer experiments, and thus also to simultaneously shorten the time frame to obtain the assay results. To fit the parameters of the inhibition and cell viability model would require large amount of data, which is time consuming and costly to obtain. We adopt data-driven methods on the available assay data itself to obtain a cell viability versus concentration graph and thus the IC50 values. In the he data-driven approach, we employ the information from the dynamics of the cell viability of the known concentrations for forecasting the cell-viability of the unknown concentrations at any time-instant.

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