Predicting Diagnostic Potential of Cathepsin in Epithelial Ovarian Cancer: A Design Validated by Computational, Biophysical and Electrochemical Data	
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Publication Year	2021
Grant Number	
DOI link	10.3390/biom12010053

Abstract: Background: Epithelial ovarian cancer remains one of the leading variants of gynecological cancer with a high mortality rate. Feasibility and technical competence for screening and detection of epithelial ovarian cancer remain a major obstacle and the development of point of care diagnostics (POCD) may offer a simple solution for monitoring its progression. Cathepsins have been implicated as biomarkers for cancer progression and metastasis; being a protease, it has an inherent tendency to interact with Cystatin C, a cysteine protease inhibitor. This interaction was assessed for designing a POCD module. Methods: A combinatorial approach encompassing computational, biophysical and electron-transfer kinetics has been used to assess this protease-inhibitor interaction. Results: Calculations predicted two cathepsin candidates, Cathepsin K and Cathepsin L based on their binding energies and structural alignment and both predictions were confirmed experimentally. Differential pulse voltammetry was used to verify the potency of Cathepsin K and Cathepsin L interaction with Cystatin C and assess the selectivity and sensitivity of their electrochemical interactions. Electrochemical measurements indicated selectivity for both the ligands, but with increasing concentrations, there was a marked difference in the sensitivity of the detection. Conclusions: This work validated the utility of dry-lab integration in the wet-lab technique to generate leads for the design of electrochemical diagnostics for epithelial ovarian cancer.