The efficacy of cancer treatments have improved constantly in the last decade. However, therapeutic resistance and the lack of curative treatments in metastatic disease, suggest that conventional anticancer therapies do not affect the subpopulation cancer initiating cells (CICs), constitute a self-renewing stem cell-like population responsible for the progression, metastasis, resistance to treatment, and recurrence of several tumors. The aim of this work is the identification of adjuvant molecules that can be associated to an oncoantigen-driven vaccination. By microarray analysis and data mining we have identified a set of drugs targeting genes that are associated to breast cancer stem cells (CSC): Atorvastatin, Bumetanide, Radafaxine, ICA 17043, YSL. In vitro characterization of two of these drugs, Atorvastatin and YSL, showed their ability to impair mammosphere formation, which is a peculiarity of normal and cancer stem cells. A mathematical model to simulate the effect of the combination of adjuvant and vaccination was designed and parameters defined on the basis of ErbB2-driven vaccination and Atorvastatin activity on CSC. The model suggests that reduction and halting of tumor mass increment can be reached by combining the effect of ErbB2 vaccination and Atorvastatin as adjuvant.