Supplementary Material



Suppl. Figure 1. *In silico* selection of CD49f antagonists. Graphic representation of Z-scores obtained by docking of CD49f with 11,421 compounds using AutoDock Vina (A) and AutoDock (B) and their re-evaluation using DSX_089 in AutoDock Vina (C) and AutoDock (D). (E) Graphic representation of consensus Z-score values of CD49f docking. Red circles correspond to the selected candidates. Compounds are ranked by consensus Z-score, and the order is conserved in all graphs. (F) Selected compounds and their corresponding reported targets.



Suppl. Figure 2. CD49f (ITGA6) expression in triple negative breast cancer cell lines. Data from Heiser LM, et. al. (PNAS, 2012;109:2724. DOI: <u>10.1073/pnas.1018854108</u>) were analyzed using the UCSC Xena platform (Goldman M, et. al. bioRxiv 326470. DOI: <u>10.1101/326470</u>). Red arrow points to the cell line employed in this study.



Suppl. Figure 3. Representative pictures of the effect of evaluated drugs on mammosphere formation. Bar scale = $200 \ \mu m$.



Suppl. Figure 4. (A) Expression of CD49f in MCF-7 cells (pink histogram), assessed by FACS, versus its isotype control (gray histogram). (B) Representative pictures of the adhesion of MCF-7 to cell culture polystyrene (CCP), laminin (20 mg/ml), or bovine serum albumin (BSA; 20 mg/ml), and their corresponding quantification. Statistical significance was determined by Dunnett's test; P value < 0.05 (*), < 0.001 (****). (C) Effect of pranlukast (50 mM) on the adhesion of MCF-7 cells to laminin. Vehicle was DMSO (0.2%). Bar scale = 100 mm.



Suppl. Figure 5. (A) Evaluation of cell viability in MDA-MB-231 cells exposed to pranlukast for 24 h. Statistical significance was determined by Dunnett's test; P value < 0.05 (*). (B). Evaluation of apoptosis after 24 h of exposure to pranlukast. The annotated percentages correspond to the annexin V-positive population.