

TNBC human cell line Supplemental Figure 1. Prevalence of TNBC cell lines in literature.



Supplemental Figure 2. Correlation between tumorigenicity and metastasis in high and low metastatic potential cell lines. Correlation between high tumorigenic cell lines A) tumor volume and the number of lung metastasis B) tumor volume and size of lung metastasis C) size of lung metastasis and tumor volume. Correlation between intermediate and low tumorigenic cell lines D) tumor volume and the number of lung metastasis E) tumor volume and size of lung metastasis F) size of lung metastasis and tumor volume. Correlation between high metastatic potential cell line's G) tumor volume and the number of liver metastasis H) tumor volume and size of liver metastasis I) size of liver metastasis and tumor volume and size of liver metastasis J) tumor volume and size of liver metastasis A) tumor volume and size of liver metastasis J) tumor volume and size of liver metastasis J) tumor volume and size of liver metastasis A) tumor volume A) the number of liver metastasis A) tumor volume A) the number of liver me



Supplemental Figure 3. Characterization and clustering of cell line morphology Quantification of cell shape parameters for each cell line 231 (n=679 cells), BT549 (n=799 cells), Hs578T (n=538 cells), and SUM159 (n=892 cells) (A) Perimeter (****P<0.0001) (B) Form Factor (****P<0.0001), (C) Compactness (****P<0.0001). Principal component analysis of the cell morphology metrics for each cell line (D) loadings scores of each cell morphology metric projected onto PC1 and PC2. (E) PC scores of each cell line projected onto PC1 and PC2 (E)Significance was determined

using a one-way ANOVA with Dunnett's multiple comparisons test compared to 231 controls. Each data point represents a single cell.



Supplemental Figure 4. Characterization and clustering of cell lines 2D and 3D single cell motility Principal component analysis of the single cell motility metrics for each cell line (A) PC scores of each cell line projected onto PC1 and PC2 (B) loadings scores of each cell morphology metric projected onto PC1 and PC2.



Pearson Correlation

Supplemental Figure 5. Spearman correlation between *in vitro* metrics and *in vivo* behavior.