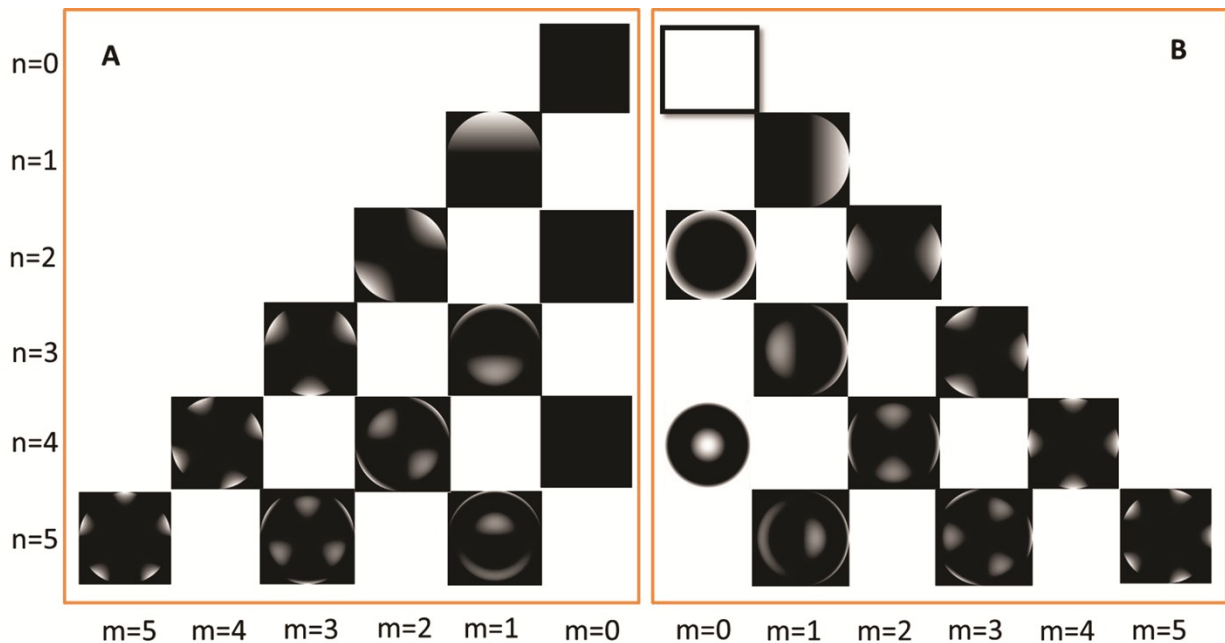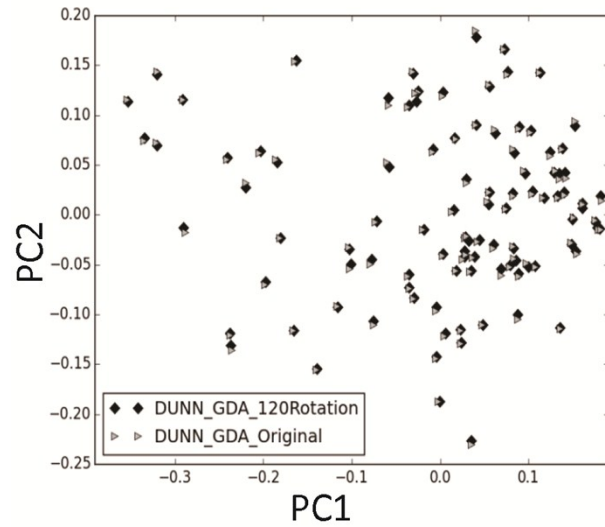## Supplementary Information


Supplementary Figure 1: Zernike polynomials representation. In this figure, Zernike polynomials are plotted from n=0 to n=5. A) Imaginary part of Zernike polynomials. B) Real part of Zernike polynomials. Zernike polynomials with even order and zero repetition are symmetrical under rotation.

Supplementary Figure 2: Rotation invariant Zernike moments. Zernike moments of DUNN cell line on GDA substrate and its Zernike moments of 120 degrees rotated images in principal component space shows that they are almost equal. This confirms that, Zernike moments used in this study are rotation invariant.
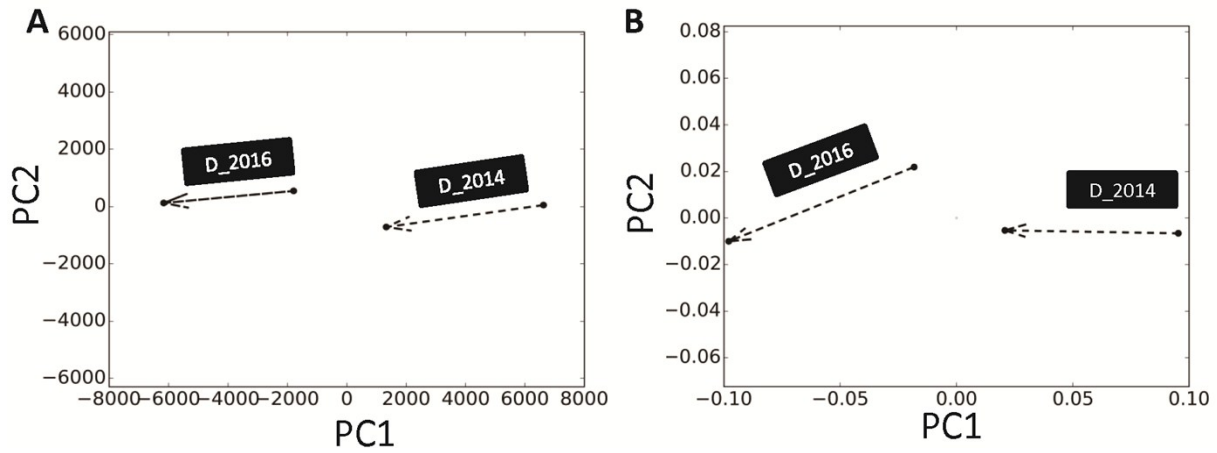
Supplementary Figure 3: Reproducibility of shape changes. Data from two separate experimental batches year in principal component space (A) Geometric parameters: PC1 and PC2 changes are similar for experiments done in 2014 and 2016 (B) Zernike moments: PC1 changes is very similar for the experiments done in 2014 and 2016.
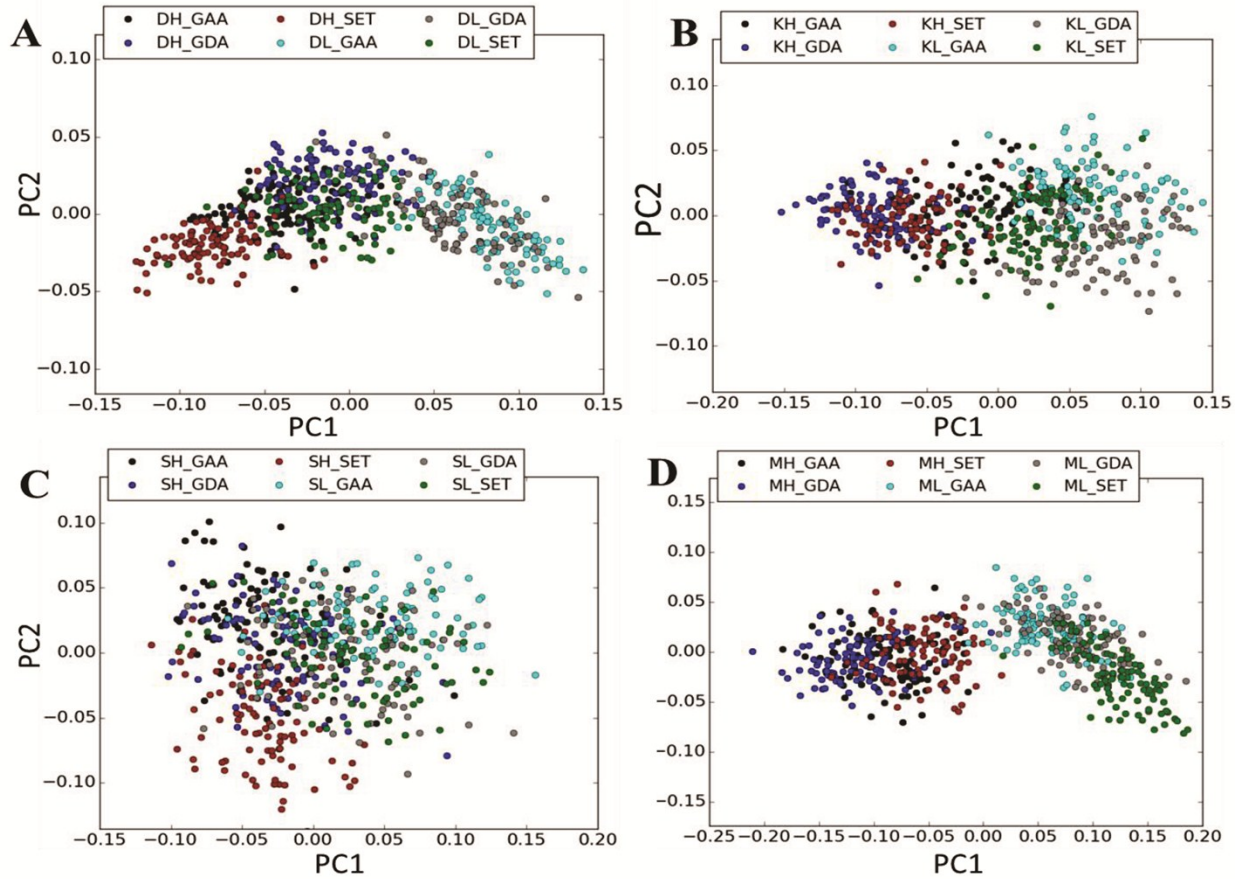
Supplementary Figure 4: Clustering of each paired line on different substrates in principal component space. A) D paired cell lines, B) K paired cell lines, C) S paired cell lines, D) M paired cell lines.

S. No.	Original Cell Line Name	Metastatic Classification	Nomenclature in this paper
1.	DUNN	Low	DL
2.	DLM8	High	DH
3.	K12	Low	KL
4.	K7M2	High	KH
5.	SAOS2	Low	SL
6.	SAOS-LM7	High	SH
7.	MG63	Low	ML
8.	MG63.2	High	MH

Table S1. The cell lines and the abbreviations used to describe them in this paper. The abbreviation is based on the first letter of each pair of cell lines, with the second letter denoting whether it is classified as having low or high metastatic potential. Cell lines 1-4 are murine while cell lines 5-8 are human.

Training and Test cell lines	Validation cell lines	Substrate	Accuracy
DL versus DH	KL versus KH	All	0.69
DL versus DH	KL versus KH	GAA	0.52
DL versus DH	KL versus KH	GDA	0.85
DL versus DH	KL versus KH	SET	0.785
DL versus DH	SL versus SH	All	0.68
DL versus DH	SL versus SH	GAA	0.81
DL versus DH	SL versus SH	GDA	0.625
DL versus DH	SL versus SH	SET	0.69
KL versus KH	DL versus DH	All	0.67
KL versus KH	DL versus DH	GAA	0.565
KL versus KH	DL versus DH	GDA	0.525
KL versus KH	DL versus DH	SET	0.615
KL versus KH	SL versus SH	All	0.63
KL versus KH	SL versus SH	GAA	0.52
KL versus KH	SL versus SH	GDA	0.66
KL versus KH	SL versus SH	SET	0.405
SL versus SH	DL versus DH	All	0.725
SL versus SH	DL versus DH	GAA	0.635
SL versus SH	DL versus DH	GDA	0.665
SL versus SH	DL versus DH	SET	0.81
SL versus SH	KL versus KH	All	0.83
SL versus SH	KL versus KH	GAA	0.57
SL versus SH	KL versus KH	GDA	0.895
SL versus SH	KL versus KH	SET	0.64
SL and DL versus SH and DH	KL versus KH	All	0.725
SL and DL versus SH and DH	KL versus KH	GAA	0.58
SL and DL versus SH and DH	KL versus KH	GDA	0.945
SL and DL versus SH and DH	KL versus KH	SET	0.495
SL and KL versus KL and KH	DL versus DH	All	0.675
SL and KL versus KL and KH	DL versus DH	GAA	0.925
SL and KL versus KL and KH	DL versus DH	GDA	0.54
SL and KL versus KL and KH	DL versus DH	SET	0.205
KL and DL versus KH and DH	SL versus SH	All	0.66
KL and DL versus KH and DH	SL versus SH	GAA	0.775
KL and DL versus KH and DH	SL versus SH	GDA	0.59
KL and DL versus KH and DH	SL versus SH	SET	0.66

Table S2. Prediction accuracy of the neural network when it is trained on one set of cell lines and another set of cell lines are used for validation. The best performing cases are highlighted here and reported in Table 4 of the main text.

PC1		PC2	
Attributes	Weights	Attributes	Weights
4_0	0.401406	10_2	0.110873
6_0	0.382081	12_2	0.109819
2_0	0.309363	14_2	0.099882
8_0	0.278669	8_2	0.097855
10_2	0.160788	18_4	0.08918
12_2	0.155303	15_1	0.088992
8_2	0.138404	16_2	0.088989
10_0	0.131511	16_4	0.086615
14_2	0.126728	17_1	0.085775
0_0	0.116983	20_4	0.085324
6_2	0.09455	13_1	0.082725
16_4	0.09018	18_2	0.08064
16_2	0.08985	19_1	0.080287
18_4	0.086394	22_4	0.079989
14_4	0.086118	20_2	0.078865

Table S3. Sorted weights for PCA. For each principal component Zernike moments are sorted based on their weights. First column is sorted Zernike moments for PC1 and third column is sorted Zernike moments for PC2. It can be seen that in PC1 early even orders with m=0 and for PC2 later even orders with m=2 have the largest weights.