Electronic Supplementary Information (ESI)

Modeling Continuum of Epithelial Mesenchymal Transition Plasticity

Mousumi Mandal[1] , Biswajoy Ghosh[1,*], Anji Anura[1] , Pabitra Mitra[2] , Tanmaya Pathak[3] , and Jyotirmoy Chatterjee[1]

[1] Indian Institute of Technology Kharagpur, School of Medical Science and Technology, Kharagpur, 721302, India [2] Indian Institute of Technology Kharagpur, Dept. of Computer Science and Engineering, Kharagpur, 721302, India [3] Indian Institute of Technology Kharagpur, Dept. of Chemistry, Kharagpur, 721302, India

*Email: biswajoyghosh@smst.iitkgp.ernet.in

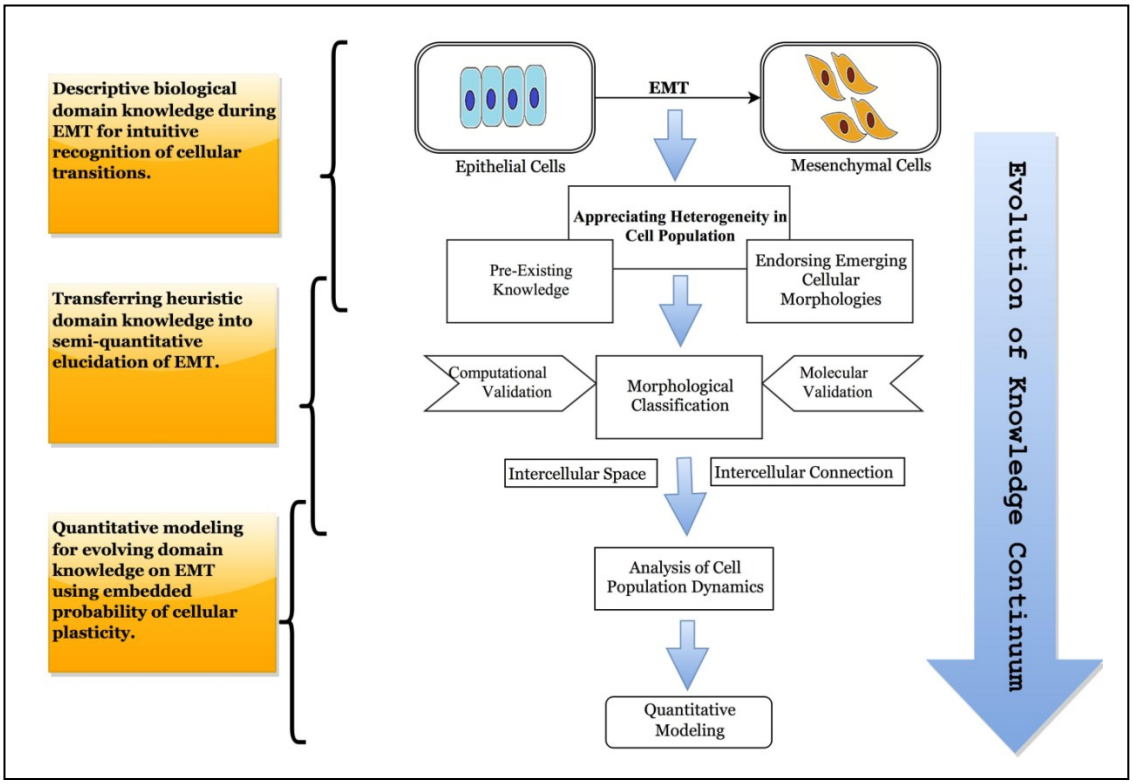

Fig. S1. Schematic diagram illustrating a multi-step appreciation of EMT – an evolutionary biological phenomenon with critical but ambiguous manifestations in development, healing and carcinogenesis – by minimizing loss of relevant information in understanding inherent dynamism. Suitable heuristics may be considered for semi-quantitative model formulation exploring understanding patterns of the process.

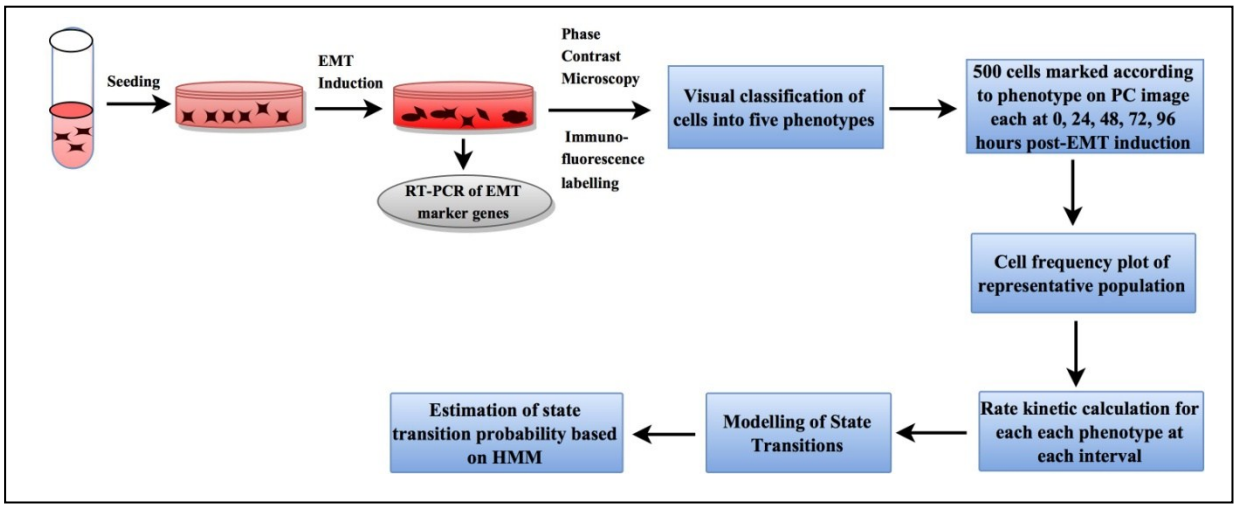

Fig. S2: A schematic diagram describing the journey from *in vitro* cell culture towards achievement of computational modeling.

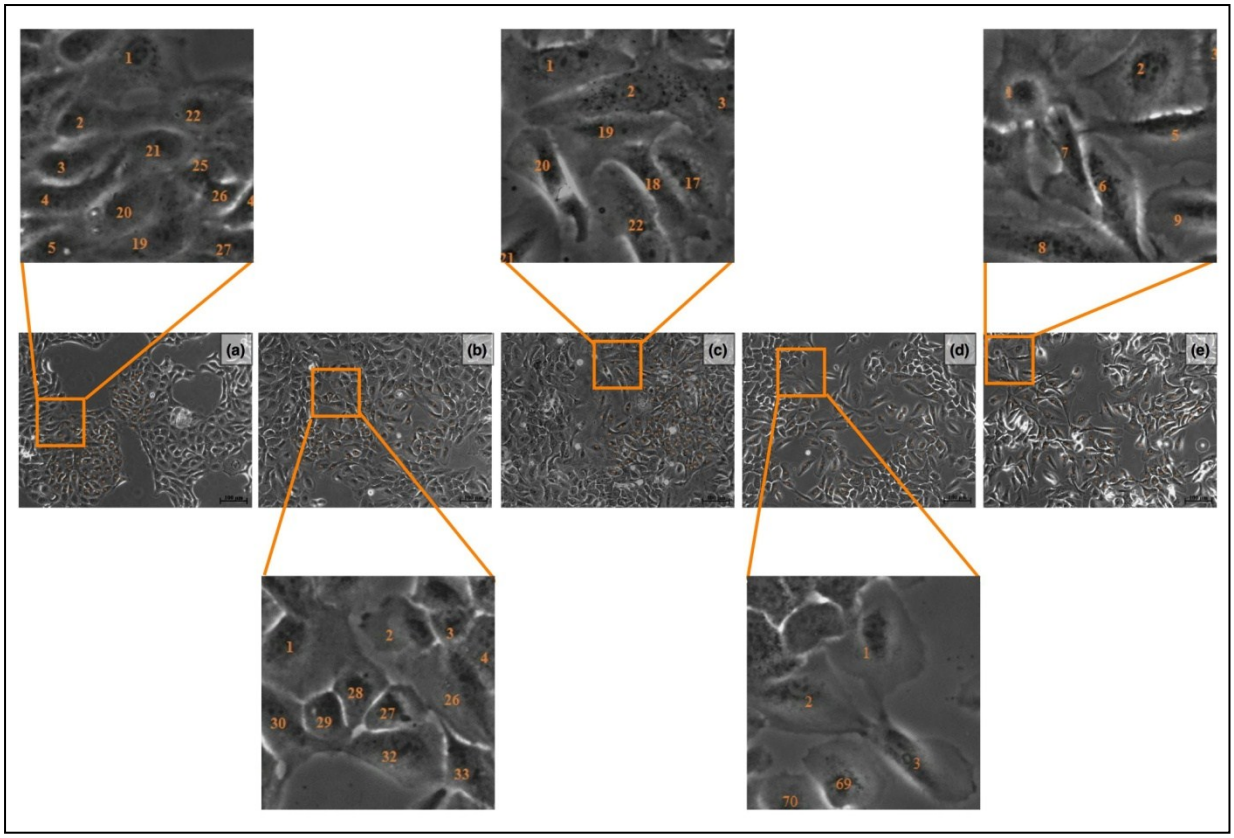

Fig. S3. The image displays annotation method of cells from phase contrast microscopy images for sampling of representative cell population in a single set of experiment. The frames are shown for 0, 24, 48, 72, and 96 hrs in (a), (b), (c), (d), and (e) respectively.

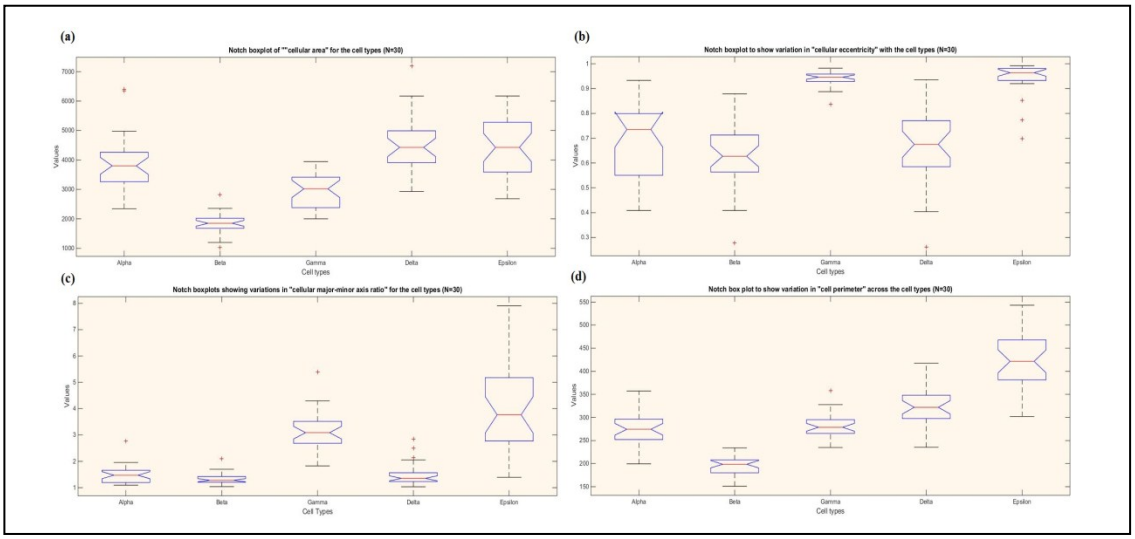

Fig. S4. Notch box-plots showing the spread of morphometric features in the cell phenotypes. A set of 30 randomly selected cells from each type was used to determine the (a) area, (b) eccentricity, (c) major-minor axis ratio, and (d) perimeter.

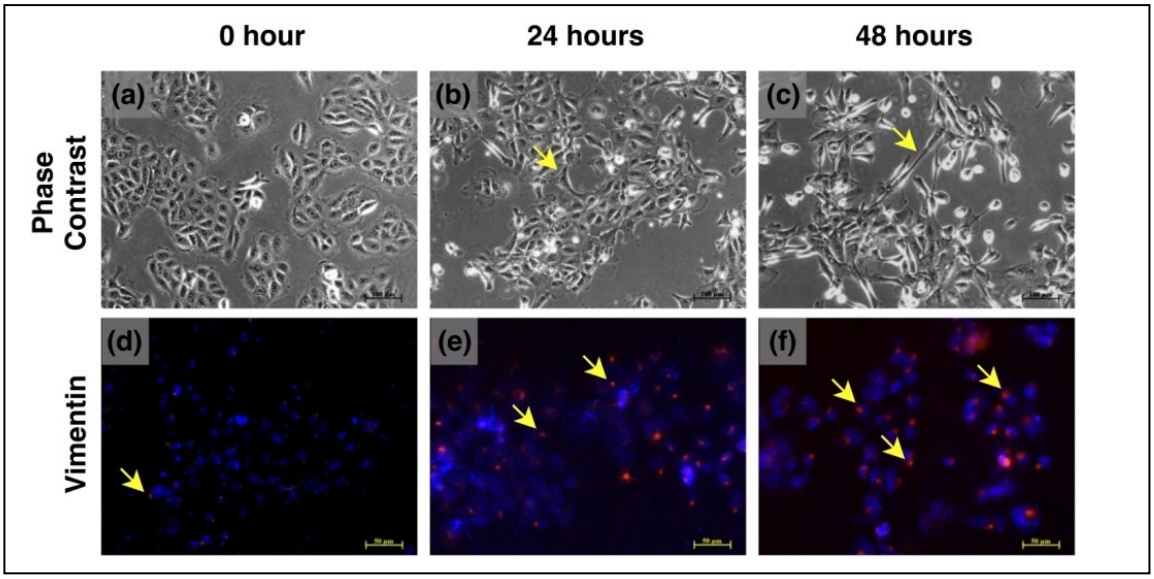

Fig. S5. Figure illustrating morphological changes, population heterogeneity, and relevant molecular expression during EMT (induced in AW13516 population) at different time points. (a-c) Phase Contrast micrographs (Objective 10 X). The arrows indicate occurrence of elongated mesenchymal-like cells (b, c). (d-f) Immunofluorescence micrographs showing progressive molecular expression of Vimentin (red) at 20 X objective magnification. The arrows indicate vimentin expression (d-f). (*DAPI was used for nuclear staining (blue)*)

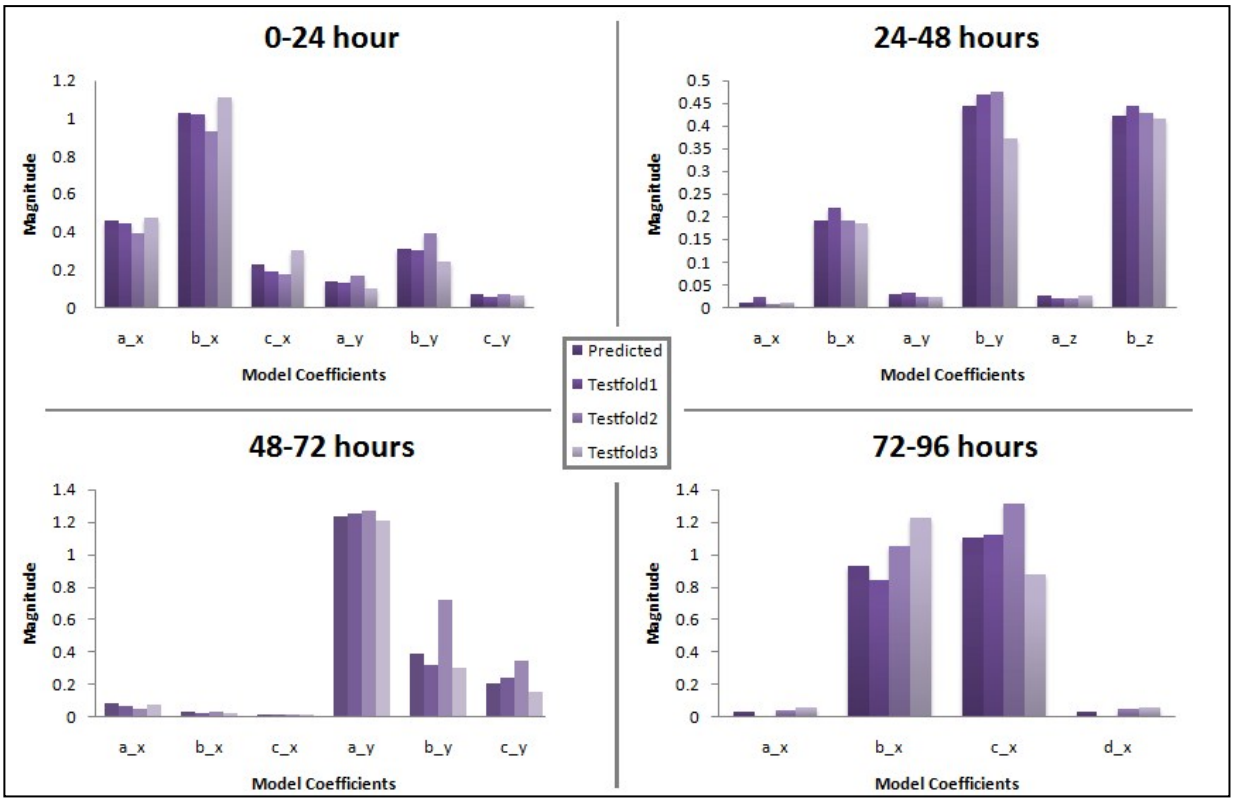

Fig. S6. The plot illustrates the prediction and 3-fold cross validation result of the EMT plasticity model coefficients. Here a, b, c ... represent the contributory cells and x, y, z ... represent the forming cells. The coefficients p_q signifies the coefficient of 'p' phenotype in forming the 'q' phenotype.

Table S1: Primer sequences and cycling conditions maintained for Real Time Polymerase Chain Reaction.

Gene	Primer	Sequence (5' to 3')	Annealing Temp (°C)
18S rRNA	For	GTAACCCGTTGAACCCCATT	51.8
	Rev	CCATCCAATCGGTAGTAGCG	53.8
N-Cadherin	For	CAACTTGCCAGAAAACTCCAGG	54.84
	Rev	GCTTCCTGTAGGTGGCAATC	54.36
Vimentin	For	CGAGAACTTTGCCGTTGAAGC	51.8
	Rev	ATGAAACCGGGCTATCTGCTC	53.8
Fibronectin	For	GAGCTATTCCCTGCACCTGA	53.83
	Rev	CGTGCAAGGCAACCACACT	53.25

***Cycling Conditions**: 95 °C for 10 min (1 cycle), 95 °C for 15 s, 55 °C for 10 s, 72 °C for 15 s (40 cycles).*