**Supplementary Materials**

**Article Title -** A Dynamic Quantitative Systems Pharmacology Model of Inflammatory Bowel Disease: Part 1 – Model Framework

**Authors:** Katharine V. Rogers, Steve W. Martin, Indranil Bhattacharya, Ravi Shankar Prasad Singh, Satyaprakash Nayak

**List of Supplementary Materials Included:**

**Table 1**: Model\_Information.xls – contains information about the model. Within this excel file, the description of each spreadsheet is as follows:

**Sheet 1**: Model\_Species.xls – contains species name, description, location, and units

**Sheet 2**: Model\_Species\_Values.xls – contains species, description, location, unit in model, disease, converted units, min value, best value, max value, key type, reference, and assumptions

**Sheet 3**: Model\_Reaction.xls – contains reaction name, reaction, and reaction rate

**Sheet 4**: Model\_Parameters.xls – contains parameter name, description, units, and approximate range

**Sheet 5**: Parameters\_Weighted.xlsx – contains list of parameters changed and description

**Sheet 6:** Simulated PK Params.xlsx – contains the PK parameters of the drugs simulated in the model with references.

**Supplementary Figure 1**: Selection of baseline CD population was done using the virtual population generation method by Allen *et al., (*[*https://doi.org/10.1002/psp4.12063*](https://doi.org/10.1002/psp4.12063)*).* To implement this method, first bounds were defined for the input parameters (rate constant values) and model outputs (cytokine, cell, and biomarker levels). If the bounds were not known, we used physiological considerations to constrain them. Using these values, a set containing a large number of `plausible patients` was generated which contained input parameter values failing in the ranges set in the step before. A virtual population from this plausible patient set was selected based on the criteria of matching an empirical distribution of interest, by calculating a probability of inclusion of a plausible patient into the virtual population. Comparison of the plausible population (N = 40,000) with (a-b) multivariate distribution of CRP and FCP from two studies (covariance was assumed similar to all internal data) and (c)2D projection of the 95% confidence surface of the estimated probability density function. Comparison of the virtual population subset (N = 357) with (d-e) multivariate distribution of CRP and FCP from two studies (covariance was assumed similar to all internal data) and (f)2D projection of the 95% confidence surface of the estimated probability density function. G. Histogram of the plausible population (PP) selection probability, where red is the virtual population (Vpop) selected.

**ModelCode.zip –** Contains the MATLAB code for the underlying model (a .xml file) and helper files to simulate the model, find steady state, parameters to vary/weigh and an example of running the model. The baseline virtual population parameters are also provided as a csv file.