

Supporting Information

On the Role of Catabolic Enzymes in Biosynthetic Models of Glycogen Molecular Weight Distributions

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THEORETICAL CLDS

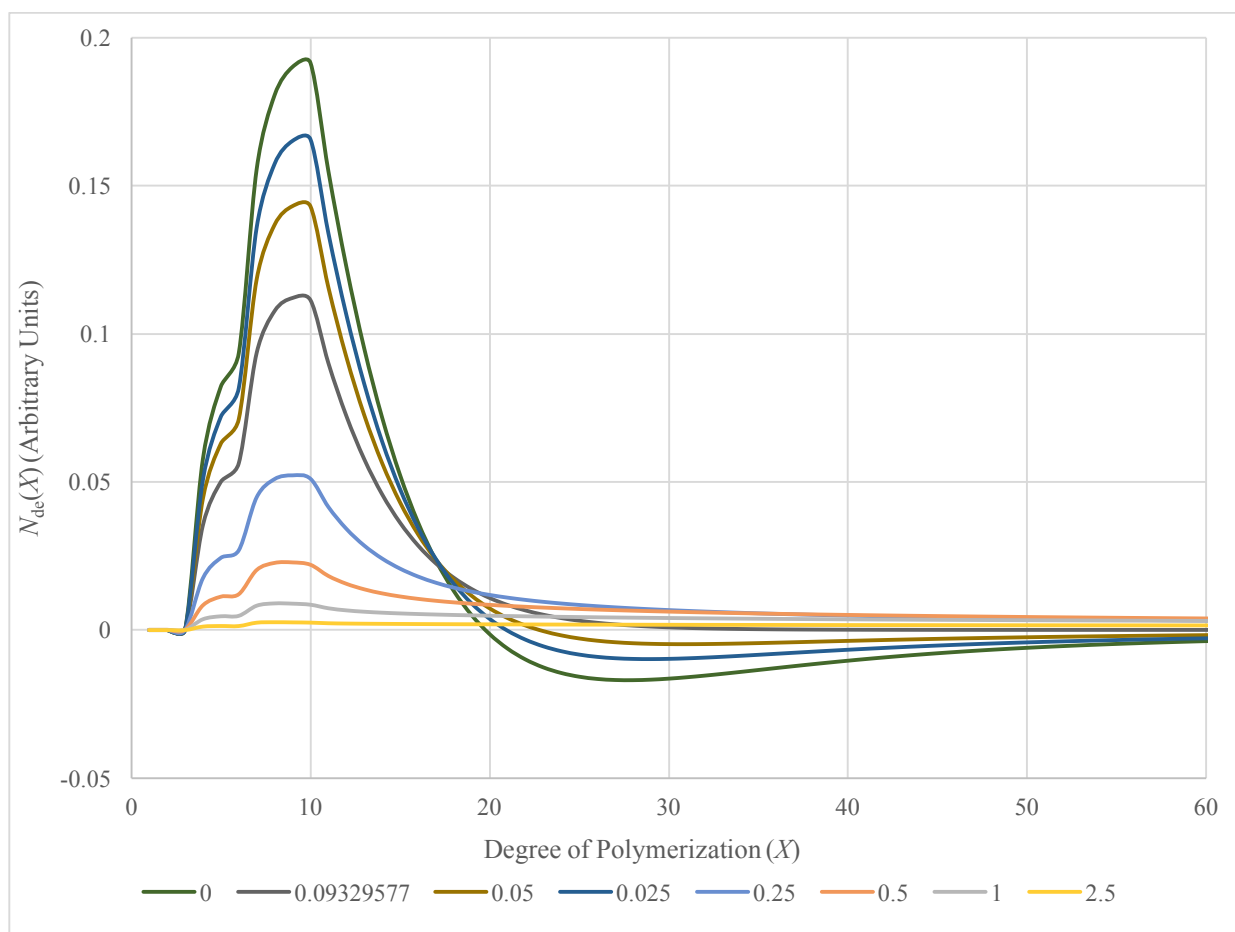


Figure S1. A plot of the data in Figure 1 of the main text that has not been normalized so that all series have the same maximum and showing a larger range of DP.

MATRICES

In order for matrix equations of the form shown in Equation 1 of the main text to be solved, they must first be truncated. This is effected by removing the first $(X_0 + X_{\min} - 1)$ rows and columns of the coefficient matrix as well as the first $(X_0 + X_{\min} - 1)$ components of the right hand and solution vectors (Equation S1). The highest DP considered in this illustrative matrix is set arbitrarily.

$$\begin{bmatrix} -N(13) & 0 & 0 & 0 & 0 & 0 & N(19)/7 & N(20)/4 \\ 0 & -N(14) & 0 & 0 & 0 & 0 & 0 & N(20)/8 \\ 0 & 0 & -N(15) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -N(16) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -N(17) & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -N(18) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -N(19) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -N(20) \end{bmatrix} \times \begin{bmatrix} \beta(13) \\ \beta(14) \\ \beta(15) \\ \beta(16) \\ \beta(17) \\ \beta(18) \\ \beta(19) \\ \beta(20) \end{bmatrix} = \begin{bmatrix} -N(12) + N(13) \\ -N(13) + N(14) \\ -N(14) + N(15) \\ -N(15) + N(16) \\ -N(16) + N(17) \\ -N(17) + N(18) \\ -N(18) + N(19) \\ -N(19) + N(20) \end{bmatrix}$$

(S1)

[illegible][illegible]

S4

MODEL CALCULATIONS

Significant oscillatory behavior is observed in the calculated values of $\beta(X)$ shown in Figures 3-5 of the main text. To illustrate that this is an artifactual result of experimental noise in the CLDs used to perform the calculations and not due to instability in the solving method, model CLDs were generated according to the equation¹ $N_{\text{de}}(X) = X e^{-AX}$ (Figure S2), a continuous function free from the small uncertainty inherently present in experimental discrete values of $N_{\text{de}}(X)$. Values of $\beta(X)$ calculated from these CLDs were found to exhibit smooth change with no oscillatory behavior (Figure S3).

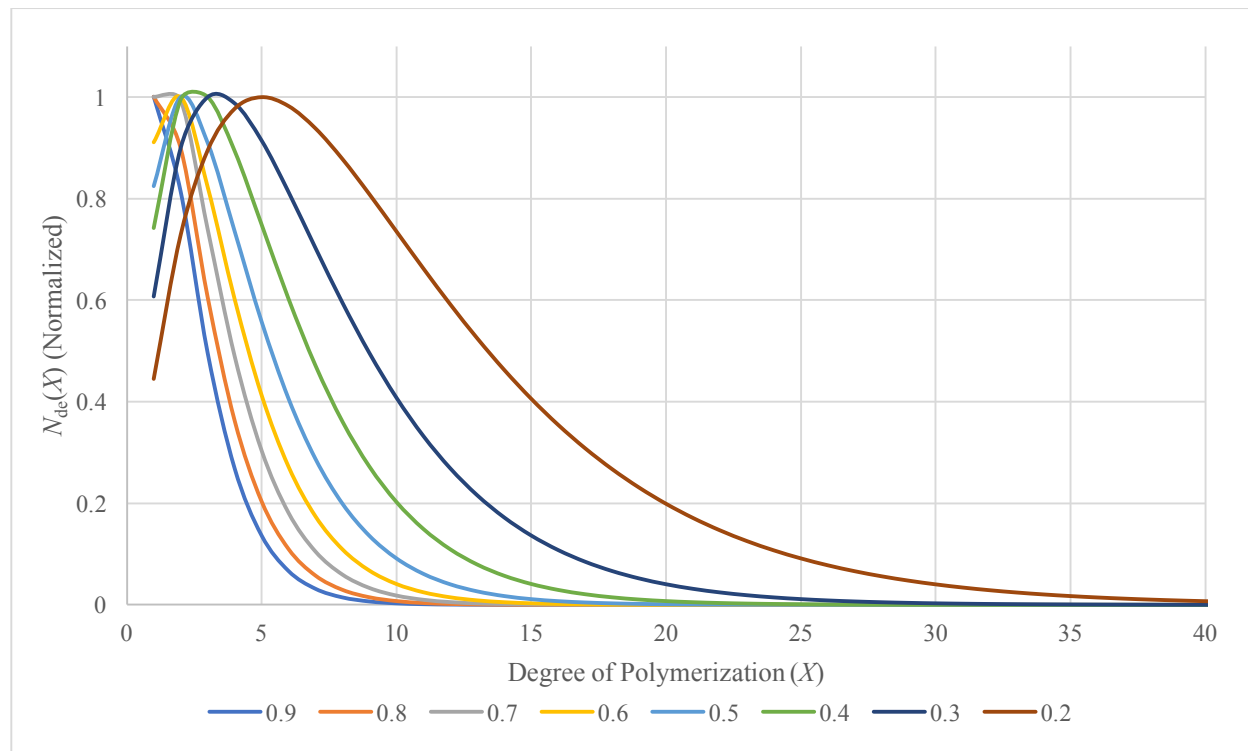


Figure S2. Model CLDs generated using the equation $N_{\text{de}}(X) = X e^{-AX}$ to test for oscillatory behavior in calculated values of $\beta(X)$. Values of A used for each series are listed in the legend. All series have been normalized to have the same maximum.

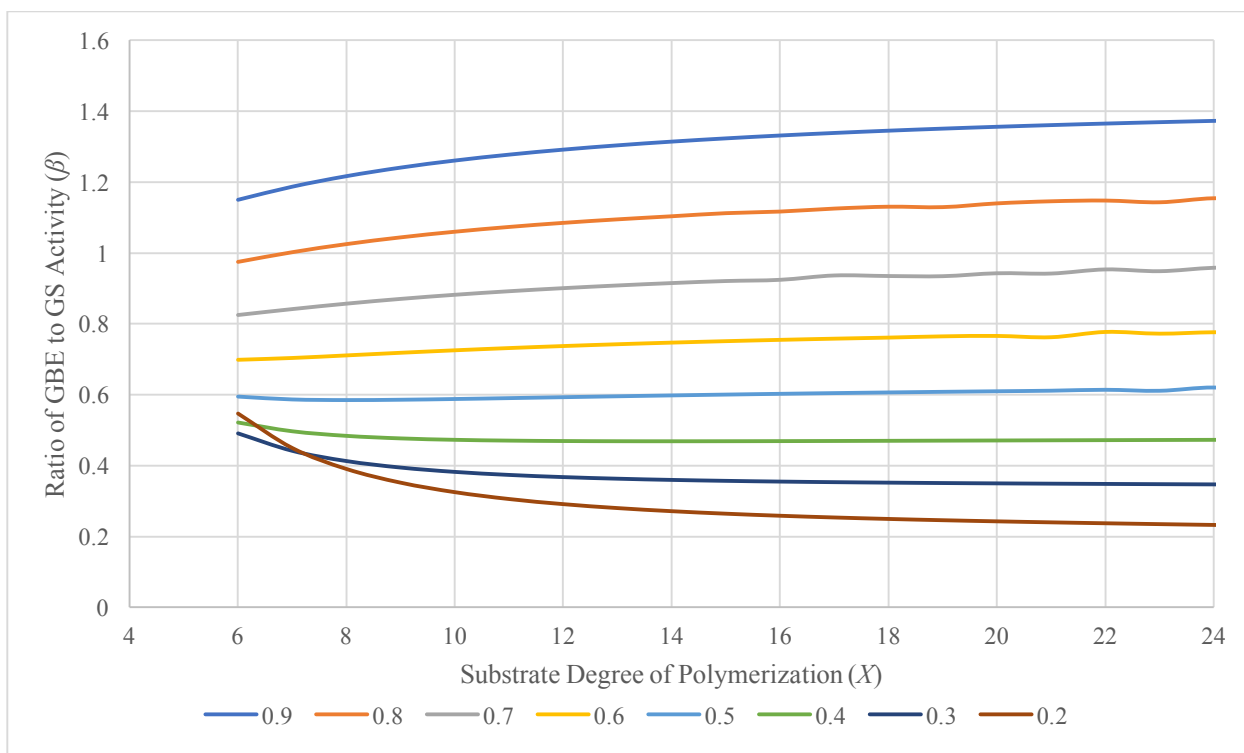


Figure S3. Values of $\beta(X)$ calculated from the CLDs in Figure S2. All series were calculated using the parameters $X_0 = 3$, $X_{\min} = 3$, $\delta = 0$, $\epsilon = 0$, and a maximum DP of 40 considered. Unlike in the analysis of experimental CLDs in the main text, analysis of these model CLDs yielded no oscillations in the values of $\beta(X)$ calculated.

EFFECTS OF VARIATION OF PARAMETERS ON CALCULATED VALUES OF BETA

As the computing time needed to find analytical solutions to the systems described by this model increases exponentially with the size of the truncated matrix (Equation S1) used, it is useful to determine the point of diminishing returns on the precision of calculated values versus the size of the matrix used. This was done by varying the maximum DP (X_{\max}) considered in the system while keeping other parameters constant, and locating the threshold value of X_{\max} after which negligible change was observed in calculated values of $\beta(X)$ (Figure S4).

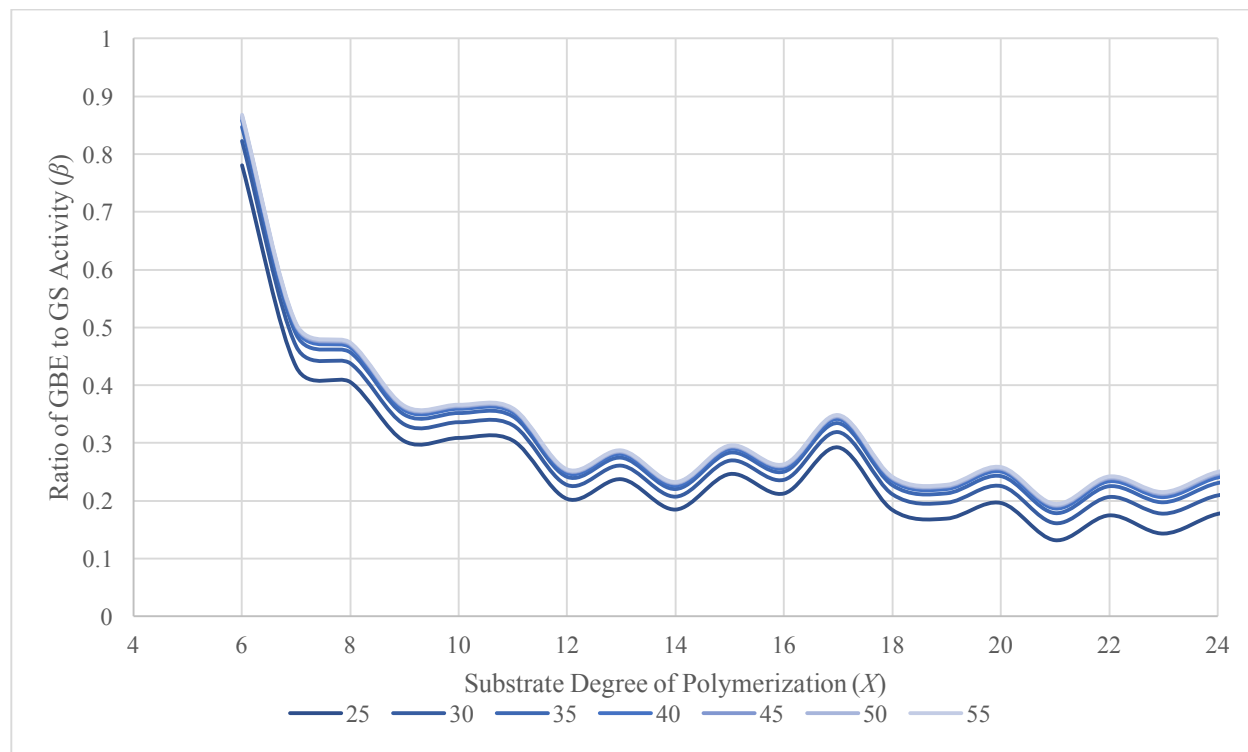


Figure S4. Effect of changing the size of the matrix used (and thus, the highest DP considered in the CLD) when calculating values of $\beta(X)$. All series were calculated using the Mouse 2-A (4AM) series from Figure 2 of the main text and the parameters $X_0 = 3$, $X_{\min} = 3$, $\delta = 0$, and $\varepsilon = 0$. The maximum DP considered for each calculation (X_{\max}) is listed in the legend. Changes in calculated values of $\beta(X)$ were found to be negligible as the maximum DP considered increased past 40 (and thus, as the size of the truncated matrix, which is equal to $X_{\max} - (X_0 + X_{\min} - 1)$, increased past 35).

Interestingly, the sum of $X_0 + X_{\min}$ (Figure S5) as well as the individual values of $X_0 + X_{\min}$ (Figure S6) had minimal impact on values of $\beta(X)$ calculated for valid DP ($X \geq X_0 + X_{\min}$) in each system. Conversely, while the sum of $\delta + \varepsilon$ qualitatively affected calculated values of $\beta(X)$ (Figure S7), variations in the individual values of δ and ε comprising a given sum had no effect (Figure S8).

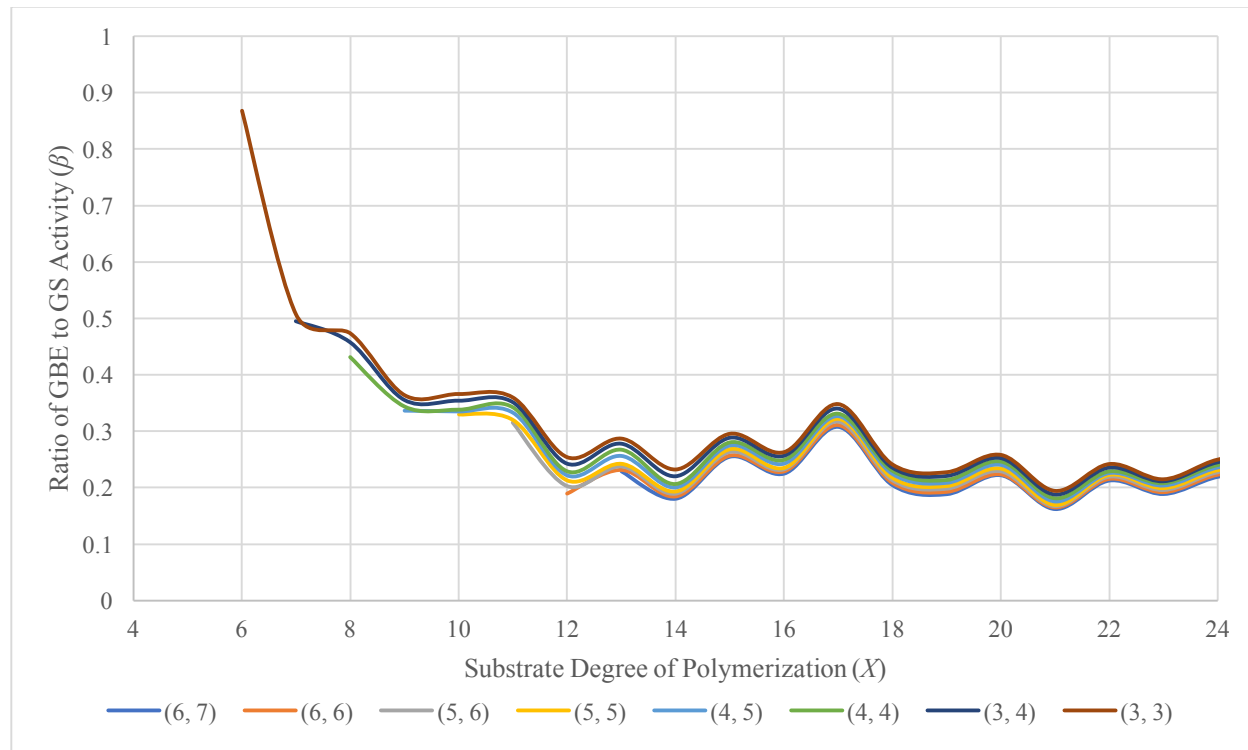


Figure S5. Effect of changing values of X_0 and X_{\min} (listed in the legend as (X_0, X_{\min})) on $\beta(X)$. Changes in the sum of $X_0 + X_{\min}$ had minimal impact on the calculated substrate preference of GBE. All series were calculated using the Mouse 2-A (4AM) series from Figure 2 of the main text and the parameters $\delta = 0$ and $\varepsilon = 0$, with a maximum DP of 55 considered.

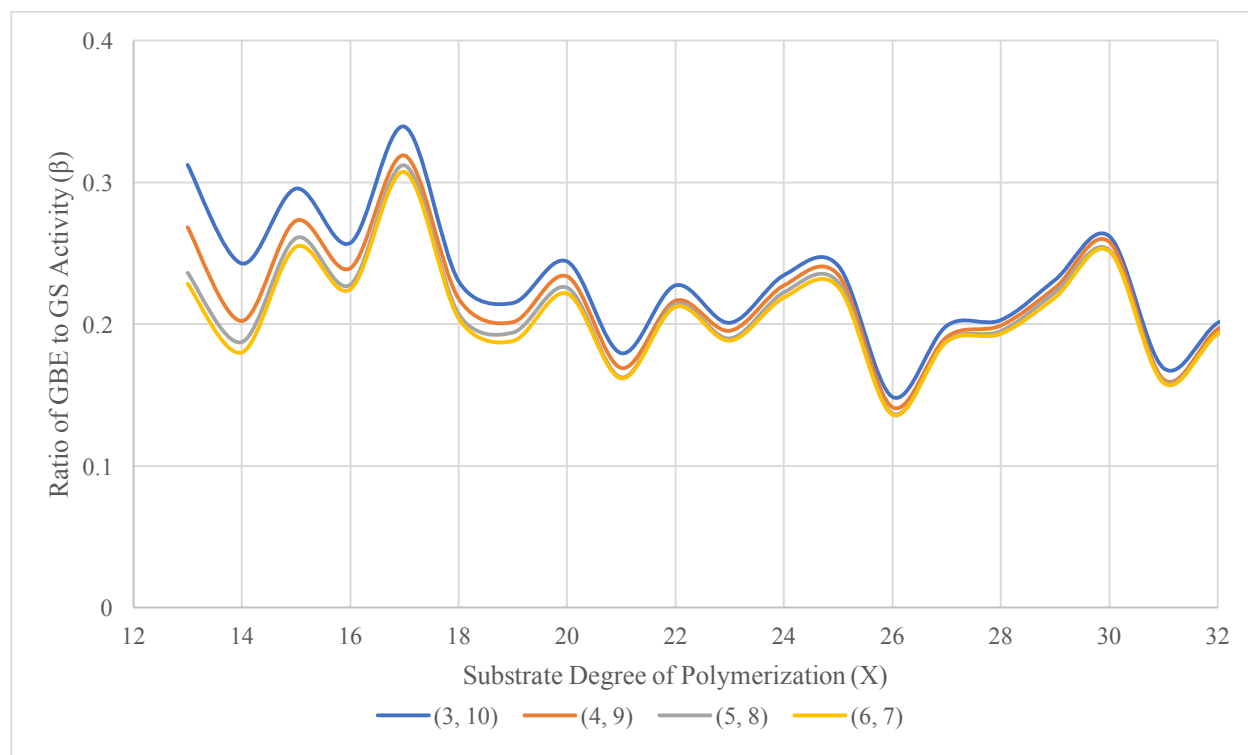


Figure S6. Effect of changing values of X_0 and X_{\min} (listed in the legend as (X_0, X_{\min})) on $\beta(X)$ while keeping the sum of $X_0 + X_{\min}$ constant. Changes in the individual values of X_0 and X_{\min} had minimal impact on the calculated substrate preference of GBE. All series were calculated using the Mouse 2-A (4AM) series from Figure 2 of the main text and the parameters $\delta = 0$ and $\varepsilon = 0$, with a maximum DP of 55 considered.

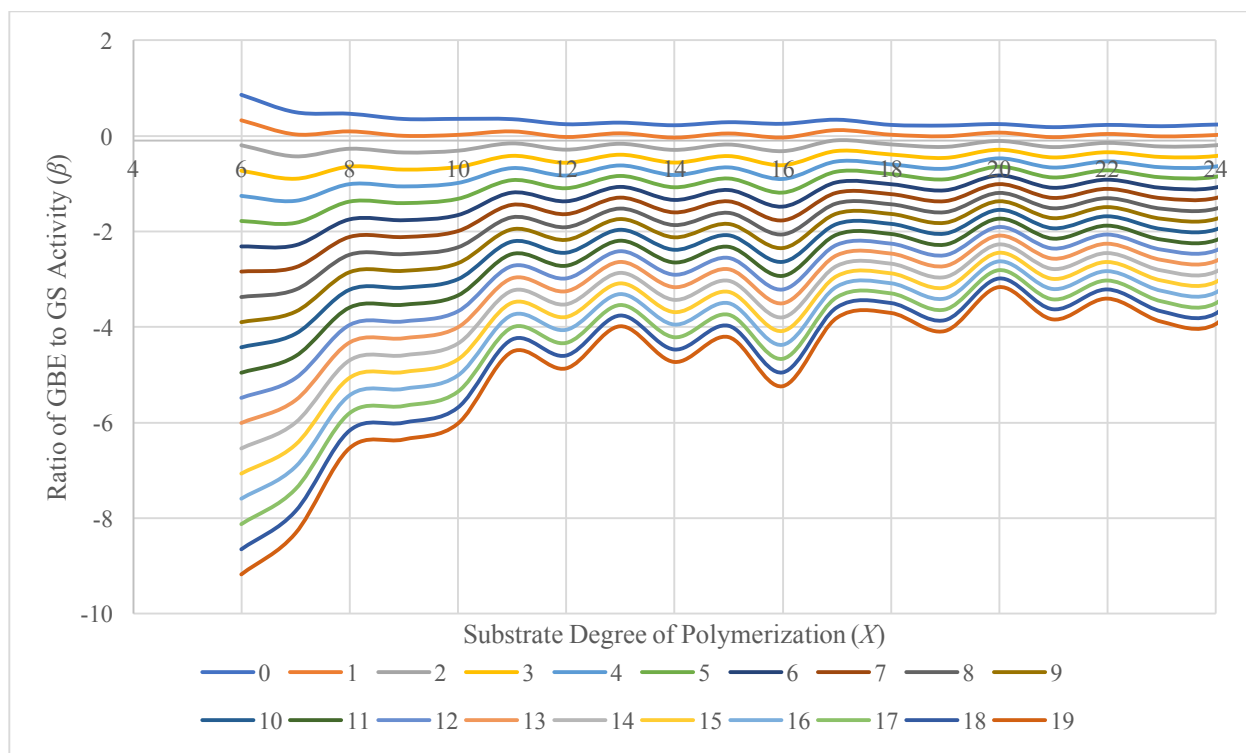


Figure S7. Effect of changing values of the sum of $\delta + \epsilon$ (listed in the legend) on $\beta(X)$. Sufficiently large sums of $\delta + \epsilon$ caused the values of $\beta(X)$ to decay at low DP, in contrast to the increase in values seen without these representations of degradative enzymes (Figure 4 of the main text). All series were calculated using the Mouse 2-A (4AM) series from Figure 2 of the main text and the parameters $X_0 = 3$ and $X_{\min} = 3$, with a maximum DP of 40 considered.

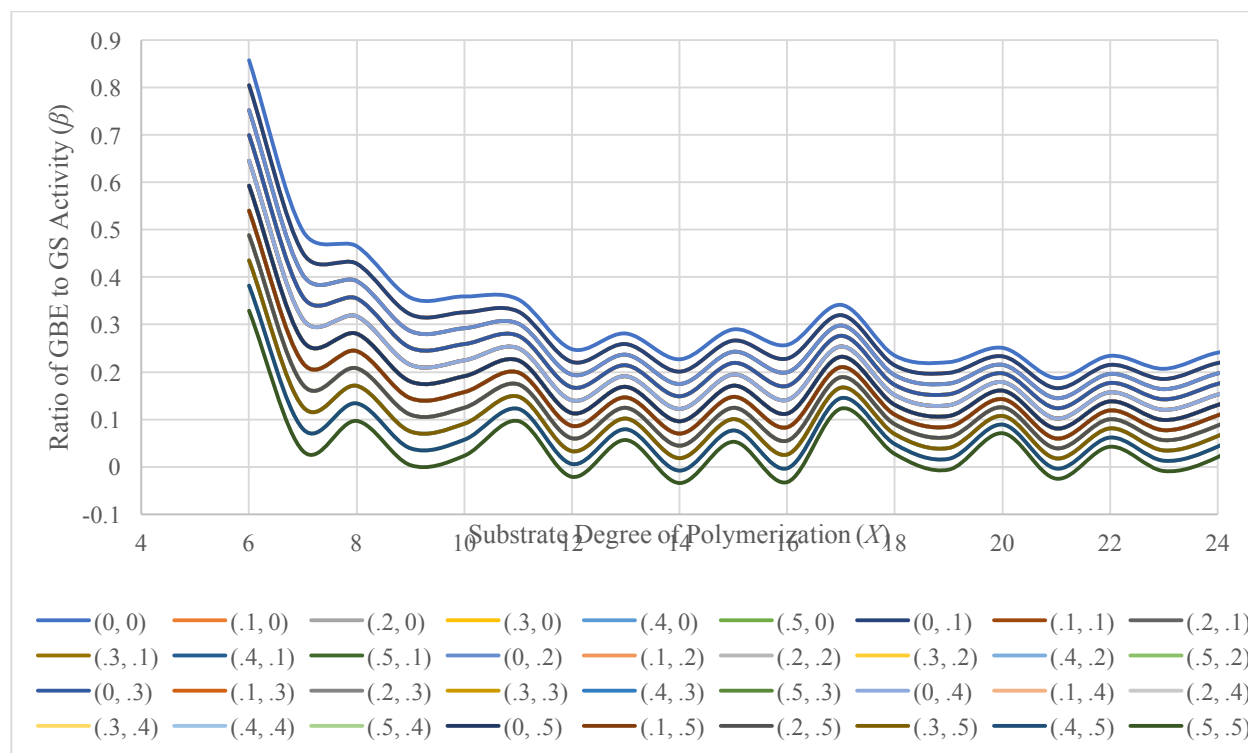


Figure S8. Effect of changing values of δ and ε (listed in the legend as (δ, ε)) on $\beta(X)$. While the sum of $\delta + \varepsilon$ had an effect on the values of $\beta(X)$ calculated, the individual values of δ and ε had no effect. As a result, only 10 series (representing the 10 different possible sums of $\delta + \varepsilon$) are visible in the plot, despite 36 series being plotted. All series were calculated using the Mouse 2-A (4AM) series from Figure 2 of the main text and the parameters $X_0 = 3$ and $X_{\min} = 3$, with a maximum DP of 40 considered.

REFERENCES

1. Gray-Weale, A.; Gilbert, R. G., General description of the structure of branched polymers. *J. Polym. Sci., Part A: Polym. Chem.* **2009**, 47 (15), 3914–3930.