Nowak-Chen Model – July 27, 2015

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1 Parameters of the model

Model was presented in the papers [1–3]

- We assume that there are enough of activated monomers in the system, so that their concentrations are constant. This way we don't have to track them in the simulations.
- Polymers can therefore spontaneously grow with the rate α. Without loss of generality we can put this parameter equal 1; all other rates with be relative to the growth rate in this case.
- Activated monomers decay into regular ones with the rate $a \gg 1$. This imitates input of food into the system. It is safe to assume that decay of activated monomers happens much faster than spontaneous growth of polymers. Therefore we explore values of $a \propto 10^2, 10^3\alpha$
- Dilution parameter d mimics cell division and loss of the matter because of that. From 2.1 we see that total mass of the system is $M \propto \frac{a}{\alpha}$, $d \approx \alpha$ or $d \gg \alpha$ and $M \propto \frac{a}{\alpha}\frac{d}{2\alpha}$, $d \ll \alpha$. Therefore we explore valued of d from $\propto 0.01\alpha$ to $\propto 1\alpha$.
- Hydrolysis has constant rate d_h per bond; it varies from $\propto 0.01$ to $\propto 1$.

  For instance, the uncatalyzed hydrolysis of glycylglycine under neutral conditions at 25 1C proceeds with a rate constant of $6.310^{-11}M^{-1}s^{-1}$ (i.e. an half life of 350 y), whereas values of $9.310^{-11}s^{-1}$ have been reported for glycylvaline at 37 C under neutral conditions[4], and $1.310^{-10}s^{-1}$ for benzoylglycylphenylalanine (t1/2 = 128 y)[5].

  kinetics are depending on the position of the residues within the peptide chain [6]

- Folding and unfolding reactions happen very quickly with the rates $k_{unf} \gg 1$ and $k_{unf} \cdot \exp(E_{native}/kT)$ correspondingly.
- Catalysis rate is proportional to the exponent of hydrophobic energy E_h and number of contacting hydrophobes n_c: $\alpha \cdot \exp(E_h \cdot n_c/kT)$
- Some experiments also include aggregation reactions for the long hydrophobic chains.

2 Kinetics

We enumerate all the polymers, so that x_i is population of i^{th} monomer, and $x_{i'}$ is a population of its precursor.

Equations are:

$$\text{One mers:} \quad \dot{x_i} = a - 2\alpha x_i - dx_i \tag{1}$$

$$\text{2+ mers:} \quad \dot{x_i} = \alpha x_{i'} - (2\alpha + d)x_i \tag{2}$$

2.1 Steady State Kinetics

Steady state: $\dot{x_i} = 0$

$$\text{One mers:} \quad 0 = a - 2\alpha x_i - dx_i \tag{3}$$

$$\text{2+ mers:} \quad 0 = \alpha x_{i'} - (2\alpha + d)x_i \tag{4}$$

So we have:

$$\text{One mers:} \quad x_i = \frac{a}{2\alpha + d} \tag{5}$$

$$\text{2+ mers:} \quad x_i = \frac{\alpha}{2\alpha + d} x_{i'} \tag{6}$$

Therefore for every sequence of length l we get:

$$\boxed{x_l = \frac{a}{\alpha}\left(\frac{\alpha}{2\alpha + d}\right)^l} \tag{7}$$

Population of all the sequence of length l is therefore:

$$p_l = \frac{a}{\alpha}\left(\frac{\alpha}{2\alpha + d}\right)^l 2^l = \frac{a}{\alpha}\left(\frac{2\alpha}{2\alpha + d}\right)^l = \frac{a}{\alpha}\left(\frac{1}{1 + d/2\alpha}\right)^l \tag{8}$$

If we denote $x \equiv \frac{d}{2\alpha}$, population of all the sequences of length l will be:

$$\boxed{p_l = \frac{a}{\alpha}\left(\frac{1}{1 + x}\right)^l} \tag{9}$$

Total mass of all the sequences is:

$$M = \sum_{l=0}^{\infty} l p_l \tag{10}$$

$$M = \sum_{l=0}^{\infty} \frac{a}{\alpha} l \left(\frac{1}{1+x}\right)^l \tag{11}$$

According to [7] the sum will be

$$M = \frac{a}{\alpha} \frac{\frac{1}{1+x}}{\left(1-\frac{1}{1+x}\right)^2} = \frac{a}{\alpha}\left(\frac{1+x}{x}\right) \tag{12}$$

Therefore total mass is:

$$M = \frac{a}{\alpha}\left(1+\frac{1}{x}\right) \tag{13}$$

Remember that $x = d/2\alpha$. It means that values of d $d \approx \alpha$ or $d \gg \alpha$ produce total masses

$$M \propto \frac{a}{\alpha}, \qquad d \approx \alpha \quad \text{or} \quad d \gg \alpha \tag{14}$$

while very small values of $d:\ d \ll \alpha$ produce total masses

$$M \propto \frac{a}{\alpha}\frac{d}{2\alpha}, \qquad d \ll \alpha \tag{15}$$

References

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