HP World Model – December 22, 2015

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1 Parameters of the model

Model is based on [1–3]. In addition to the parameters introduced in Nowak-Chen Model (edit) we also have:

- Hydrolysis has constant rate d_h per bond. Half-life time of hydrolysis bonds in neutral conditions and temperatures around room temperature are on the order of hundreds of years.

  •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]

  In our simulation it has constant rate constant d_h per bond; it varies from $\propto 0.01$ to $\propto 1$.

- Folding and unfolding reactions happen very quickly with the unfolding rate constants of $k_{unf} \gg \alpha$ and folding rate constant of $k_{unf} \cdot \exp(E_{native}/kT)$.

  E_h in our experiments is around $1 - 2$kT[]. k_{unf} we keep $\propto 10^2$, which gives us range of unfolding rates from a reaction per hours and days and range of folding rates from a reaction per hours to fractions of a second.

- Catalysis rate is proportional to the exponent of hydrophobic energy E_h and number of contacting hydrophobes n_c: $\alpha \cdot \exp(E_h \cdot n_c/kT)$. Number of hydrophobic contacts for the short HP-sequences is about $3 - 6$. With the hydrophobic energies of $1 - 2$kT this gives us catalysis rates around hours and days for one reaction. For the calculations

of the folding rate constants derived from theories of K.Dill see Folding kinetics and dynamics (edit)

- Some experiments also include aggregation reactions for the long hydrophobic chains.

Rate constant name	Symbol	Normalized simulation value	Simulation value (deduced) per $1M$	Value from literature, per $1M$
Polymerization	α	1	$\propto 1\,month^{-1}$	??
Hydrolysis	d_h	$\propto 10^{-1}$–10^{-4}	$\propto 1\,month^{-1} - -10^{-3}year^{-1}$	$\propto 10^{-3}year^{-1}$ [4–6]
Dilution	d	$\propto 10^{-2} - 1$	$\propto 0.1year^{-1} - -10^{-3}year^{-1}$	— Is used to keep model from overflowing
Monomer import	a	$\propto 10^2 - 10^3$	$\propto 1 - 10^2 day^{-1}$	??
Number of rotational freedoms	z	$1.5 - 2.5$	$1.5 - 2.5$	??
Hydrophobic energy per kT	e_h	$1 - 2$	$1 - 2$	$0 - 3.3$ [8]

Tab. 1: !

References

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