HP World Model – August 10, 2015

EG

Home (edit)
Research: Calculations (edit)

Contents

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

[1] Martin A Nowak and Hisashi Ohtsuki. Prevolutionary dynamics and the origin of evolution. *Proceedings of the National Academy of Sciences*, 105(39):14924–14927, September 2008.

[2] Hisashi Ohtsuki and Martin A Nowak. Prelife catalysts and replicators. *Proceedings. Biological sciences / The Royal Society*, 276(1674):3783–90, November 2009.

[3] Irene A Chen and Martin A Nowak. From Prelife to Life: How Chemical Kinetics Become Evolutionary Dynamics. *Accounts of chemical research*, 45(12), February 2012.

[4] Robert M. Smith and David E. Hansen. The pH-Rate Profile for the Hydrolysis of a Peptide Bond. *Journal of the American Chemical Society*, 120(35):8910–8913, September 1998.

[5] Rebecca A R Bryant and David E Hansen. Direct Measurement of the Uncatalyzed Rate of Hydrolysis of a Peptide Bond. *Journal of the American Chemical Society*, 118(23):5498–5499, January 1996.

[6] Grégoire Danger, Raphaël Plasson, and Robert Pascal. Pathways for the formation and evolution of peptides in prebiotic environments. *Chemical Society reviews*, 41(16):5416–29, August 2012.

[7]

[8] William C. Wimley and Stephen H. White. Experimentally determined hydrophobicity scale for proteins at membrane interfaces. *Nature Structural Biology*, 3(10):842–848, October 1996.