

The origin of heredity in protocells

Timothy West^{1,2}, Victor Sojo^{1,2,3}, Andrew Pomiankowski^{1,2} and Nick Lane^{1,2}

¹*Department of Genetics, Evolution and Environment, and* ²*Centre for Computation, Mathematics and Physics in the Life Sciences and Experimental Biology (CoMPLEX), University College London Gower Street, London WC1E 6BT*

³*Systems Biophysics, Faculty of Physics, Ludwig-Maximilian University of Munich. Amalienstr. 54. 80799 Munich, Germany.*

SI Table 1

Initial Values			
Symbol	Name	Value	Notes
$\bar{V}_{crys}^{cyto}(1)$	Initial mean crystal volume	$1 \times 10^{-15} \text{ cm}^3$	Cuboid nanocrystal of length ~500nm
$[crys]^{mem}(1)$	Initial concentration of crystal in membrane	$1 \times 10^{-9} \text{ mol dm}^{-3}$	Set very low
$[aa]^{cyto}(1)$	Initial concentration of amino acid in the cytosol	$1 \times 10^{-6} \text{ mol dm}^{-3}$	Set low
$[fa]^{cyto}(1)$	Initial concentration of fatty acid in the membrane	$1 \times 10^{-6} \text{ mol dm}^{-3}$	Set low
$SA^{cyto}(1)$	Initial cytoplasm surface area	$4.84 \times 10^{-6} \text{ cm}^2$	
$[crys]^{cyto}(1)$	Initial concentration of crystal in cytosol	$1 \times 10^{-6} \text{ mol dm}^{-3}$	Typical particulate FeS found in hydrothermal vent samples [1]
$V_{crys}^{cyto}(eq)$	Total crystal population volume (fixed)	$6 \times 10^{-10} \text{ cm}^3$	
Transport			
Symbol	Name	Value	Notes
p_{aa}^{cyto}	Permeability coefficient for amino acids from cytosol	$1 \times 10^{-9} \text{ cm s}^{-1}$	Set very low
p_{fa}^{cyto}	Permeability coefficient for fatty acids from cytosol	$1 \times 10^{-9} \text{ cm s}^{-1}$	Set very low
p_{crys}^{cyto}	Association constant for crystal permeation from cytosol	$1 \times 10^{-12} \text{ cm s}^{-1}$	Set very low
p_{crys}^{mem}	Association constant for crystal permeation from membrane	$1 \times 10^{-12} \text{ cm s}^{-1}$	Set very low
p_{crys}^{surf}	Permeability coefficient for FeS diffusion to crystal surface	$1 \times 10^{-12} \text{ cm s}^{-1}$	

Crystal Growth			
Symbol	Name	Value	Notes
k^{grow}	Rate constant for crystal growth	$1 \times 10^{-6} \text{ s}^{-1}$	
\bar{V}_{crys}^{min}	Minimum crystal size	$1 \times 10^{-16} \text{ cm}^3$	Minimum nanocrystal length ~50nm
K_{crys}	Saturation constant of FeS crystal nucleation	$1 \times 10^{-8} \text{ mol dm}^{-3}$	
Catalysis and Amino Acid Interactions			
Symbol	Name	Value	Notes
$[CO_2]_{in}$	Concentration of aqueous CO ₂ in cytosol	$1 \times 10^{-3} \text{ mol dm}^{-3}$	10x CO ₂ concentration at Lost City hydrothermal field [2]
K_{CO_2}	CO ₂ binding constant for iron-sulphur catalyst	$3 \times 10^{-4} \text{ mol dm}^{-3}$	~0.3mM affinity of CO ₂ for ferredoxins [3]
K_{aa}	Binding constant of amino acids for crystals	$1 \times 10^{-4.5} - 10^{-2} \text{ mol.dm}^{-3}$	(varied in simulations)
λ_{aa}	Fraction of organic yield that is amino acid	1/10	
λ_{fa}	Fraction of organic yield that is fatty acid	1/4	
R_{cat}	Areal turnover rate	$1 \times 10^{-11.8} - 10^{-9.3} \text{ mol cm}^{-2} \text{ s}^{-1}$	(varied in simulations)
Cell Geometry			
Symbol	Name	Value	Notes
r_{mem}	Thickness of fatty acid bilayer	$1 \times 10^{-6} \text{ cm}$	~10nm thick bilayer in yeast [4]
ϕ_{fa}	Headgroup area of fatty acid	$2 \times 10^{-15} \text{ cm}^2$	~0.2nm ² surface area of arachidic acid [5]
V_{cell}	Volume of protocell cytosol	$1 \times 10^{-9} \text{ cm}^3$	Cell of ~6000 μm ³
Concentrations			
Symbol	Name	Value	Notes
$[aa]_{sink}$	Concentration of amino acids in sink	$1 \times 10^{-6} \text{ mol dm}^{-3}$	~1uM concentrations in hydrothermal fluids and plume at Lost City [6]
$[fa]_{sink}$	Concentration of fatty acids in sink	$1 \times 10^{-6} \text{ mol dm}^{-3}$	
Constants			
Symbol	Name	Value	Notes
A_N	Avogadro's number	$6.023 \times 10^{23} \text{ mol}^{-1}$	

References for SI Table 1

1. Harmandas NG, Koutsoukos PG. 1996 The formation of iron(II) sulfides in aqueous solutions. *J Cryst. Growth* **167**, 719–724.
2. Fitzsimmons JN, Boyle EA, Jenkins WJ. 2014 Distal transport of dissolved hydrothermal iron in the deep South Pacific Ocean. *Proc. Natl. Acad. Sci. USA*. **111**, 16654–61.
3. Thauer RK, Käufer B, Fuchs G. 1975 The active species of “CO₂” utilized by reduced ferredoxin:CO₂ oxidoreductase from *Clostridium pasteurianum*. *Europ. J. Biochem.* **55**, 111–7.
4. Schneider R, Brügger B, Sandhoff R, Zellnig G, Leber A, Lampl M, et al. 1999. Electrospray ionization tandem mass spectrometry (ESI-MS/MS) analysis of the lipid molecular species composition of yeast subcellular membranes reveals acyl chain-based sorting/remodeling of distinct molecular species en route to the plasma membrane. *J. Cell Biol.* **146**, 741–54.
5. Johann R, Brezesinski G, Vollhardt D, Möhwald H. 2001 The effect of headgroup interactions on structure and morphology of arachidic acid monolayers. *J. Phys. Chem.* **105**, 2957–2965.
6. Fuchida S, Mizuno Y, Masuda H, Toki T, Makita H. 2014 Concentrations and distributions of amino acids in black and white smoker fluids at temperatures over 200°C. *Organic Geochemistry* **66**, 98–106.