Supporting Information

Possible Roles of Amphiphilic Molecules in the Origin of Biological Homochirality

Nozomu Suzuki [1,2,*] and Yutaka Itabashi [3,4,*]

[1] Department of Chemistry, College of Science, Rikkyo University, Toshima-ku, Tokyo 171-8501, Japan
[2] Department of Molecular Design and Engineering, Graduate School of Engineering, Nagoya University, Chikusa-ku, Nagoya 464-8603, Japan
[3] Faculty of Fisheries Sciences, Hokkaido University, Hakodate 041-8611, Japan
[4] Japan Association for Inspection and Investigation of Foods Including Fats and Oils, 3-27-8, Nihonbashi-Hamacho, Chuo-ku, Tokyo 103-0007, Japan
* Correspondence: nsuzuki@chembio.nagoya-u.ac.jp (N.S.); yutaka@fish.hokudai.ac.jp (Y.I.)

Index

1. Dynamic Equations

1.1. General Relationship Among Parameters

In addition to eq S1, S2, and S3, some useful equations to derive dynamic equations are described in this section. These equations describe relationships among parameters x_L, x_D, k_L, k_D, g, η, and θ.

$$\frac{d\eta}{dt} = \left(-2x_L\frac{dx_D}{dt} + 2x_D\frac{dx_L}{dt}\right)/(x_L + x_D)^2 \tag{S1}$$

$$k_L = \frac{1+g}{1-g}k_D \tag{S2}$$

$$\frac{k_D}{1-g} = \frac{1}{2}(k_L + k_D) \tag{S3}$$

$$x_L x_D = \frac{(x_L + x_D)^2 - (x_L - x_D)^2}{4} = -\frac{1}{4}\theta^2(\eta^2 - 1) \tag{S4}$$

$$x_L{}^2 + x_D{}^2 = (x_L - x_D)^2 + 2x_L x_D = \frac{1}{2}\theta^2(\eta^2 + 1) \tag{S5}$$

$$x_L{}^3 + x_D{}^3 = (x_L + x_D)(x_L{}^2 - x_L x_D + x_D{}^2) = \frac{1}{4}\theta^3(3\eta^2 + 1) \tag{S6}$$

$$x_L{}^3 - x_D{}^3 = (x_L - x_D)(x_L{}^2 + x_L x_D + x_D{}^2) = \frac{1}{4}\eta\theta^3(\eta^2 + 3) \tag{S7}$$

1.2. Reaction Formula and Differential Equations

1.2.1. Block I: Synthesis

$$\mathrm{A} \xrightarrow{k_L} \mathrm{L} \tag{S8}$$

$$A \xrightarrow{k_D} \mathrm{D} \tag{S9}$$

$$\frac{dx_L}{dt} = k_L x_A \tag{S10}$$

$$\frac{dx_D}{dt} = k_D x_A \tag{S11}$$

1.2.2. Block II: Racemization

$$\mathrm{L} \xrightarrow{k_L} \mathrm{D} \tag{S12}$$

$$\mathrm{D} \xrightarrow{k_D} \mathrm{L} \tag{S13}$$

$$\frac{dx_L}{dt} = -k_L x_L + k_D x_D \tag{S14}$$

$$\frac{dx_D}{dt} = -k_D x_D + k_L x_L \tag{S15}$$

1.2.3. Block III: Accidental Autocatalysis

$$\mathrm{A} + \mathrm{L} \xrightarrow{k_L} \mathrm{L} + \mathrm{D} \tag{S16}$$

$$\mathrm{A} + \mathrm{D} \xrightarrow{k_D} \mathrm{L} + \mathrm{D} \tag{S17}$$

$$\frac{dx_L}{dt} = k_D x_A x_D \tag{S18}$$

$$\frac{dx_D}{dt} = k_L x_A x_L \tag{S19}$$

1.2.4. Block IV: Binary Racemization

$$2\mathrm{L} \xrightarrow{k_L} \mathrm{L} + \mathrm{D} \tag{S20}$$

$$2D \xrightarrow{k_D} L + D \tag{S21}$$

$$\frac{dx_L}{dt} = k_D {x_D}^2 - k_L {x_L}^2 \tag{S22}$$

$$\frac{dx_D}{dt} = k_L {x_L}^2 - k_D {x_D}^2 \tag{S23}$$

1.2.5. Block V: Binary Racemization

$$2L \xrightarrow{k_L} A + B \tag{S24}$$

$$2D \xrightarrow{k_D} A + B \tag{S25}$$

$$\frac{dx_L}{dt} = -2k_L {x_L}^2 \tag{S26}$$

$$\frac{dx_D}{dt} = -2k_D {x_D}^2 \tag{S27}$$

1.2.6. Block VI: Accidental Superautocatalysis

$$A + 2L \xrightarrow{k_L} 2L + D \tag{S28}$$

$$A + 2D \xrightarrow{k_D} L + 2D \tag{S29}$$

$$\frac{dx_L}{dt} = k_D x_A {x_D}^2 \tag{S30}$$

$$\frac{dx_D}{dt} = k_L x_A {x_L}^2 \tag{S31}$$

1.2.7. Block VII: Destruction

$$L \xrightarrow{k_L} A \tag{S32}$$

$$D \xrightarrow{k_D} A \tag{S33}$$

$$\frac{dx_L}{dt} = -k_L x_L \tag{S34}$$

$$\frac{dx_D}{dt} = -k_D x_D \tag{S35}$$

1.2.8. Block VIII: Autocatalysis

$$A + L \xrightarrow{k_L} 2L \tag{S36}$$

$$A + D \xrightarrow{k_D} 2D \tag{S37}$$

$$\frac{dx_L}{dt} = k_L x_A x_L \tag{S38}$$

$$\frac{dx_D}{dt} = k_D x_A x_D \tag{S39}$$

1.2.9. Block IX: Cross-inversion

$$L + D \xrightarrow{k_L} 2L \tag{S40}$$

$$L + D \xrightarrow{k_D} 2D \tag{S41}$$

$$\frac{dx_{\mathrm{L}}}{dt} = k_{\mathrm{L}}x_{\mathrm{D}}x_{\mathrm{L}} - k_{\mathrm{D}}x_{\mathrm{L}}x_{\mathrm{D}} \tag{S42}$$

$$\frac{dx_{\mathrm{D}}}{dt} = k_{\mathrm{D}}x_{\mathrm{L}}x_{\mathrm{D}} - k_{\mathrm{L}}x_{\mathrm{D}}x_{\mathrm{L}} \tag{S43}$$

1.2.10. Block X: Annihilation

$$\mathrm{L} + \mathrm{D} \xrightarrow{k} \mathrm{A} + \mathrm{B} \tag{S44}$$

$$\frac{dx_{\mathrm{L}}}{dt} = -kx_{\mathrm{L}}x_{\mathrm{D}} \tag{S45}$$

$$\frac{dx_{\mathrm{D}}}{dt} = -kx_{\mathrm{L}}x_{\mathrm{D}} \tag{S46}$$

1.2.11. Block XI: Superautocatalysis

$$\mathrm{A} + 2\mathrm{L} \xrightarrow{k_{\mathrm{L}}} 3\mathrm{L} \tag{S47}$$

$$\mathrm{A} + 2\mathrm{D} \xrightarrow{k_{\mathrm{D}}} 3\mathrm{D} \tag{S48}$$

$$\frac{dx_{\mathrm{L}}}{dt} = k_{\mathrm{L}}x_{\mathrm{A}}{x_{\mathrm{L}}}^2 \tag{S49}$$

$$\frac{dx_{\mathrm{D}}}{dt} = k_{\mathrm{D}}x_{\mathrm{A}}{x_{\mathrm{D}}}^2 \tag{S50}$$

1.3. An Example of Deriving Dynamic Equations (Block VI)

As an example, derivation ($d\eta/dt$) of Block VI is described in this section. First, dx_{L}/dt and dx_{D}/dt in eq S1 are substituted by equations S30 and S31.

$$\frac{d\eta}{dt} = (-2x_{\mathrm{L}}k_{\mathrm{L}}x_{\mathrm{A}}{x_{\mathrm{L}}}^2 + 2x_{\mathrm{D}}k_{\mathrm{D}}x_{\mathrm{A}}{x_{\mathrm{D}}}^2)/(x_{\mathrm{L}} + x_{\mathrm{D}})^2 = -2x_{\mathrm{A}}(k_{\mathrm{L}}{x_{\mathrm{L}}}^3 - k_{\mathrm{D}}{x_{\mathrm{D}}}^3)/\theta^2 \tag{S51}$$

By substituting k_{L} using eq S2, following equation can be obtained.

$$\frac{d\eta}{dt} = -2x_{\mathrm{A}}(\frac{1+g}{1-g}k_{\mathrm{D}}{x_{\mathrm{L}}}^3 - k_{\mathrm{D}}{x_{\mathrm{D}}}^3)/\theta = -2x_{\mathrm{A}}\frac{k_{\mathrm{D}}}{1-g}((1+g){x_{\mathrm{L}}}^3 - (1-g){x_{\mathrm{D}}}^3)/\theta^2 \tag{S52}$$

By substituting $k_{\mathrm{D}}/(1\text{-}g)$ using eq S3, following equation can be obtained.

$$\frac{d\eta}{dt} = -2x_{\mathrm{A}} \times \frac{1}{2}(k_{\mathrm{L}} + k_D)({x_{\mathrm{L}}}^3 - {x_{\mathrm{D}}}^3 + g({x_{\mathrm{L}}}^3 + {x_{\mathrm{D}}}^3))/\theta^2 \tag{S53}$$

Using cubic equations S6 and S7, the dynamic equations becomes as follows.

$$\begin{aligned}\frac{d\eta}{dt} &= -x_{\mathrm{A}}(k_{\mathrm{L}} + k_D)(\frac{1}{4}\eta\theta^3(\eta^2+3) + g(\frac{1}{4}\theta^3(3\eta^2+1)))/\theta^2 \\ &= -\frac{1}{4}(k_L + k_D)x_A\theta(g + 3\eta + 3g\eta^2 + \eta^3)\end{aligned} \tag{S54}$$