

Spontaneous Emergence of Information in Simple Biological Systems

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Short Communication

Information, no doubt plays an important role in the processes leading to the appearance of life on Earth. Hence, in this perspective, it is important to understand how a system, or a simple biological system, can generate such information. Let us consider, for instance, a simple process where a primitive catalyst, E, randomly binds two substrates, A and B, before releasing the products. The aim of the present paper is to raise the question to know whether such system can generate information.

Simple Enzyme System and its Information

Let us consider the simple process involving an enzyme E that randomly binds two substrates A and B before releasing the corresponding product(s). In such a system one can define the probabilities of occurrence of events A and B as

$$p(A) = \frac{K_1[A](1 + K_2[B]) + u_{EA}}{1 + K_1[A] + K_3[B] + K_1K_2[A][B] + u_{EA} + u_{EB} + u_E} \quad (1)$$

And

$$p(B) = \frac{K_3[B](1 + K_4[A]) + u_{EB}}{1 + K_1[A] + K_3[B] + K_1K_2[A][B] + u_{EA} + u_{EB} + u_E} \quad (2)$$

In these expressions, K_1, K_2, \dots are the apparent equilibrium constants of A and B to the various states of the protein. However, as the real system is not in equilibrium it has to be "corrected" by the so-called u functions defined as [1]

$$\begin{aligned} u_E &= \frac{k(k_{-1} + k_2[B])(k_{-3} + k_4[A])}{k_{-3}k_{-4}(k_{-1} + k_2[B]) + k_{-1}k_{-2}(k_{-3} + k_4[A])} \\ u_{EA} &= \frac{k_1[A]}{k_{-1} + k_2[B]} u_E \\ u_{EB} &= \frac{k_3[B]}{k_{-3} + k_4[A]} u_E \\ u_{EB}^* &= u_{EB} / k_3[B] \end{aligned} \quad (3)$$

Thus the biochemical network possesses nodes, i.e. the free enzyme E and the two enzyme-substrate complexes EA and EB. The u 's thus represent local reaction circuits that maintain an approximate steady state of the system. u_E is a reaction flow leading to the E node and both u_{EA} and u_{EB} are flows leading to nodes EA and EB. Hence the u 's are intrinsic flows that confer some dynamics to the system.

The information consumed, or generated, in such a system is defined as

$$I(A : B) = \log \frac{p(A|B)}{p(A)} \quad (4)$$

or as

$$I(A : B) = I(A) - I(A|B) \quad (5)$$

which implies that

$$I(A) = -\log p(A) \quad (6)$$

And

$$I(A|B) = -\log p(A|B) \quad (7)$$

Information is generated by the system if [2,3]

$$p(A|B) > p(A) \quad (8)$$

Looking back at expressions (1) and (2) allows to write

$$p(A|B) = \frac{[EAB]}{[EB] + [EAB]} = \frac{K_4[A]}{1 + K_4[A] + (u_{EB} / K_3[B])} \quad (9)$$

and it follows that

$$\frac{p(A|B)}{p(A)} = \frac{K_4[A]}{1 + K_4[A] + (u_{EB} / K_3[B])} \frac{1 + K_1[A] + K_3[B] + K_1K_2[A][B] + u_{EA} + u_{EB} + u_E}{K_1[A](1 + K_3[B]) + u_{EA}} \quad (10)$$

The numerator, N, and the denominator, D, of this expression can be rewritten as

$$N = K_4[A] + K_1K_4[A]^2 + K_3K_4[A][B] + K_1K_2K_4[A]^2[B] + K_4[A]u_E + K_4[A]u_{EA} + K_4[A]u_{EB} \quad (11)$$

$$D = K_1[A] + K_1K_2[A][B] + u_{EA} + K_1K_4[A]^2 + K_1K_2K_4[A]^2[B] + K_4[A]u_{EA} + K_1[A]u_{EB}^* + K_1K_2[A][B]u_{EB}^* + u_{EA}$$

and the difference $D-N$ can be expressed as

$$D-N = K_1[A] - K_4[A] + K_1K_2[A][B]u_{EB}^* - K_4[A]u_E + K_1[A]u_{EB}^* - K_4[A]u_{EB} + u_{EB}^*u_{EA} + u_{EA} \quad (12)$$

Moreover one has

$$K_1K_2[A][B]u_{EB}^* - K_4[A]u_E = \frac{K_1K_2[A][B] - K_4[A](k_{-3} + k_4[A])}{k_{-3} + k_4[A]} u_E \quad (13)$$

Similarly one has

$$K_1[A]u_{EB}^* - K_4[A]u_{EB} = \frac{(K_1[A] - K_4[A])k_3[B]}{k_{-3} + k_4[A]} u_E \quad (14)$$

Hence it appears that the differences above can be positive or negative whereas $u_{EB}^*u_{EA}$ and u_{EA} are of necessity positive, namely

$$K_1[A] - K_4[A]; K_1K_2[A][B]u_{EB}^* - K_4[A]u_E; K_1[A]u_{EB}^* - K_4[A]u_{EB}; u_{EB}^*u_{EA}; u_{EA} \quad (15)$$

It follows from these simple mathematical developments that the system considered can generate, or alternatively consume, information.

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Expressions (13) and (14) show that if $K_4 > K_1$ then the system generates information.

General Considerations and Conclusions

It can be noticed that, within a simple biochemical system such as an enzyme catalysed reaction, the interaction between several elements of this system can produce, or dissipate, information. We have seen previously that two situations have particularly interesting implications, namely:

Situation 1: $D(u)-N(u)>0$

Situation 2: $D(u)-N(u)<0$

The first situation (a) implies that

$$k_3[B] > k_3 + k_4[A] \quad (a)$$

$$K_2[B] < 1$$

And the second situation (b) means that

$$k_{-3} + k_4[A] > k_3[B] \quad (b)$$

$$K_2[B] > 1$$

Condition (a) means that EA and EB accumulate in the system and condition (b) means that E and EAB accumulate. The latter condition is indeed in favor of a chemical transformation of A and B into the corresponding products P and Q . In a way, one can consider that the system “choose” between these two possibilities. This choice is a consequence of the topology of the system. It also appears that the local reaction circuits u play a major role in the emergence, or the lack of emergence, of information in the system.

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