Electronic Supplementary Material (ESI) for Lab on a Chip

Electronic Supplementary Information

In silico evolution of guiding track designs for molecular shuttles powered by kinesin motors

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This electronic supplementary information contains:

(1) A description of the evolutionary strategy algorithms employed in this research, and
(2) Supplementary Figures showing the variability of results from the evolutionary runs.

(1) Description of the evolutionary strategy algorithms employed in this research:

Selection:

In order to pick up parent chromosomes from the population in the current generation, we employed the tournament selection (Fig. S1).

Two chromosomes were randomly picked up from the current generation, regardless of their performances. Then, the performances of the two chromosomes were compared. The chromosome having the better performance between the two was selected as one of two parent chromosomes. Due to this comparison, the expected value of the performance of the parent chromosome was higher than that among all the chromosomes in the current generation.

The other parent chromosome was selected in the same way. The two parent chromosomes were subjected to crossover (described below and in Fig. S2) to generate offspring chromosomes. We allowed a chromosome to be selected multiple times.

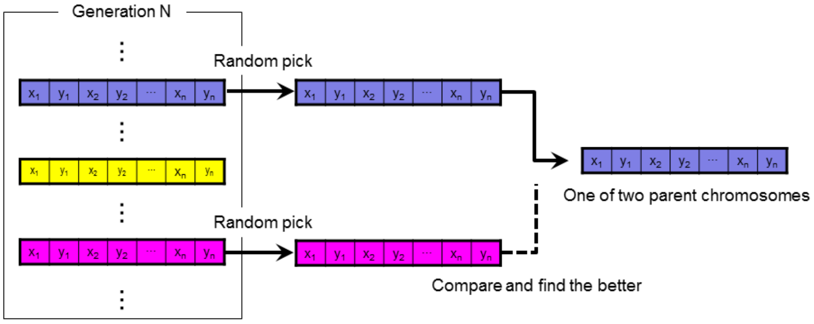

Fig. S1 Schematic of tournament selection.

Crossover:

Two offspring chromosomes were generated from two parent chromosomes through the two-point crossover. Two crossover points were randomly generated along the parent chromosomes. The parts of the two chromosomes between the two crossover points were swapped between the two chromosomes.

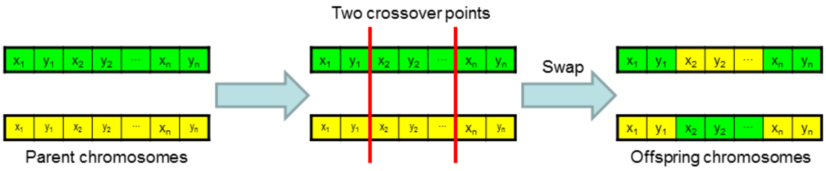

Fig. S2 Schematic of two-point crossover.

Mutation:

Anchor points may be subjected to mutation. Exceptions are anchor points located at the ends of inlet/outlet channels. If a mutation occurred at an anchor point, the anchor point was displaced at random around the original position. The distance and direction of the displacement occurred with a probability expressed as:

$$p(x,y) = \frac{1}{\sqrt{2\pi\sigma^2}} exp\left(-\frac{(x-x_0)^2-(y-y_0)^2}{2\sigma^2}\right), \qquad \text{(S1)}$$

where x and y are the x- and y-coordinates after the mutation, respectively; x_0 and y_0 are the x- and y-coordinates before the mutation, respectively; σ was set to be 2.5μm.

Constraint:

Each offspring chromosome generated was check whether some of spline curves connecting the anchor points, which described guiding track boundaries, crossed each other. If they did, the chromosome was discarded. Also, we put two constraints on the guiding tracks: The narrowest part in a module structure must be wider than 2 μm to facilitate fabrication by photolithography; the radius of curvature of the sharpest part of a module structure must be larger than the breaking radius of curvature for microtubules of 600 nm, which limits the sharpest curvature in a guiding track design. If the guiding track structure did not satisfy the constraints, it was discarded.

The selection, the crossover and mutation were repeated until the prescribed numbers of the offspring were generated.

Implementation:

The computations were performed with Windows computers. The programming language used was Fortran 90, compiled with the Fujitsu compiler.

(2) Supplementary Figures showing the variability of results from the evolutionary runs:

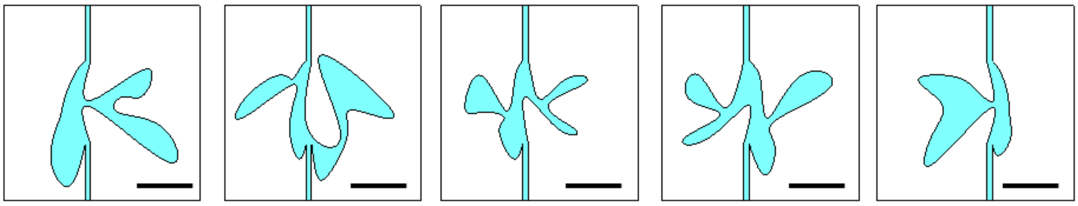

Fig. S3 The five structures of the rectifiers with PEG-coated SiO_2 barriers which showed the highest performance obtained through five independent evolution runs. The evolutions proceeded for 250 generations. The regions colored with light blue show those accessible to molecular shuttles. Scale bar = 20 μm.

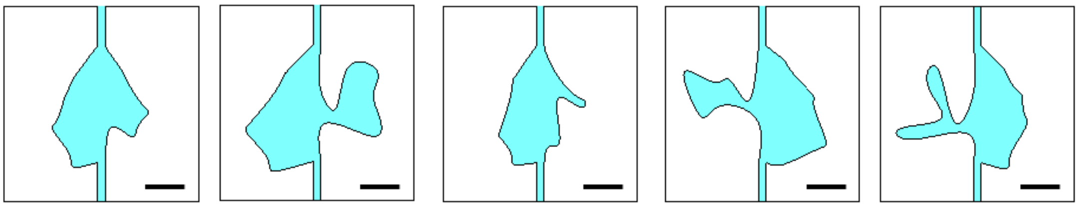

Fig. S4 The five structures of the rectifiers with PEO-coated SU8 barriers which showed the highest performance obtained through five independent evolution runs. The evolutions proceeded for 250 generations. The regions colored with light blue show those accessible to molecular shuttles. Scale bar, 10 μm.

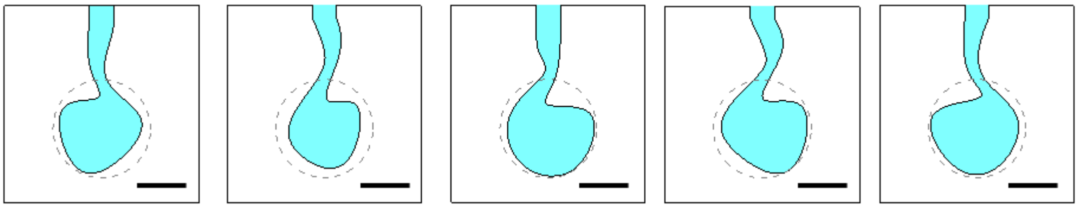

Fig. S5 The five structures of Concentrators which showed the highest performance obtained through five independent evolution runs. The evolutions proceeded for 50 generations. The regions colored with light blue show those accessible to molecular shuttles. Scale bar, 10 μm.

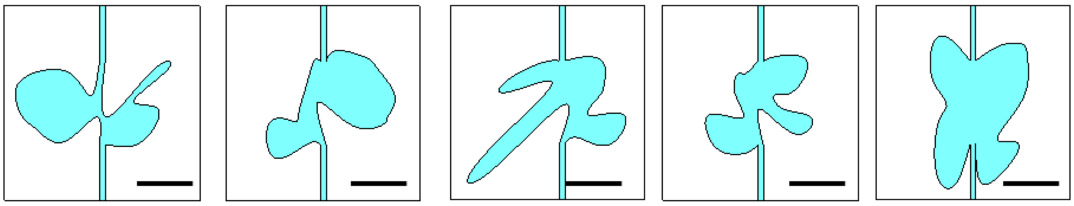

Fig. S6 The five structures of the pulse splitters with PEG-coated SiO_2 barriers which showed the highest performance obtained through five independent evolution runs. The evolutions proceeded for 500 generations. The regions colored with light blue show those accessible to molecular shuttles. Scale bar, 20 μm.