FIGURE 2. Operation of the molecular computer.

From the following article:

An autonomous molecular computer for logical control of gene expression
(/nature/journal/v429/n6990/full/nature02551.html)

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doi: 10.1038/nature02551
The complete sequences for all molecules shown are given in the Supplementary Methods. a, Part of the computation path for the diagnostic molecule for prostate cancer with all molecular indicators present, ending in drug release. The initial diagnostic molecule consists of a diagnosis moiety (grey) that encodes the left-hand side of the diagnostic rule (Fig. 1b) and a drug-administration moiety (light purple) incorporating an inactive drug loop (dark purple). At each computation step, the prevailing transition is shown, except for the processing of the symbol $PIM1^\uparrow$, for which details of the stochastic choice, accomplished by a regulated pair of competing transition molecules, are shown (dashed box, see c). b, Regulation of the two transitions for $PIM1^\uparrow$ by sub-sequences (tags) of overexpressed $PIM1$. 
mRNA, resulting in a relatively high level of the Yes $\rightarrow PIM1^{\uparrow}$Yes transition molecules and low level of the Yes $\rightarrow PIM1^{\uparrow}$No molecules. Each transition molecule contains regulation (green, orange) and computation (blue, grey) fragments. The 'inactivation tag' of PIM1 mRNA (light orange) displaces the 5' $\rightarrow$ 3' strand of the transition molecule Yes $\rightarrow PIM1^{\uparrow}$No and destroys its computation fragment. The 'activation tag' of PIM1 mRNA (light green) activates the transition molecule Yes $\rightarrow PIM1^{\uparrow}$Yes. Initially, a protecting oligonucleotide (green) partially hybridizes to the 3' $\rightarrow$ 5' strand of the transition molecule and blocks the correct annealing of its 5' $\rightarrow$ 3' strand. The 'activation tag' displaces the protecting strand, allowing such annealing and rendering an active Yes $\rightarrow PIM1^{\uparrow}$Yes transition. Ideally, one PIM1 mRNA molecule inactivates one Yes $\rightarrow PIM1^{\uparrow}$No and activates one Yes $\rightarrow PIM1^{\uparrow}$Yes transition molecule. c, Stochastic processing of the symbol PIM1 $\uparrow$ by a regulated pair of competing transition molecules. The probability of a Yes $\rightarrow$ Yes transition is high, resulting in a high level of diagnostic molecules in the state Yes and a low level in state No. d, Combining computation results for both types of diagnostic molecules, both with high Yes and low No final states, results in high release of drug and low release of drug suppressor, and hence in the administration of the drug.