Leak reaction case study - tutorials/leak_casestudy/case1.py

In this code, we study a system where the top strand of an eight-basepair duplex is invaded by a strand that carries an extra toehold, like so:


```
          Starting Multistrand 3.0    (c) 2008-2016 Caltech
Running first step mode simulations for GTCGATGC (with Boltzmann sampling)...
Computing 500010 trials,  using 14 threads  .. Done.  58.51437 seconds
('Was success:', 381)
('Was failure:', 499629)
Running first step mode simulations for TCGAGTGA (with Boltzmann sampling)...
Computing 500010 trials,  using 14 threads  .. Done.  77.83514 seconds
('Was success:', 620)
('Was failure:', 499390)
```

It is obvious that this reaction is not really supposed to occur. But it could. We compare the case where the ends are given by CG vs. AT pairs. The simulation matches our intuition: for CG ends, fewer side reactions occur (381 vs. 620 trajectories). From this, we can estimate rate constants for these reactions.

We use the first step mode to directly trigger a bimolecular step at the start of the simulation. In this simulation, two complexes are combined for the starting state: the complex that consists of the duplex, and the complex that consists of the single strand. By using complex.boltzmann_count = trials and complex.boltzmann_sample = True we sample over the Boltzmann distribution of secondary structures, which then serve as the initial state. So some simulations may start in the completely hybridized state (8 basepairs), while others may start with one of the basepairs at the end dissociated (7 basepairs). The secondary structure of the invading strand is also sampled according to this distribution. The stopping states are defined as either having completed the leak reaction (success) or having the invading strand fall off again (failed).