**Baseline model:**
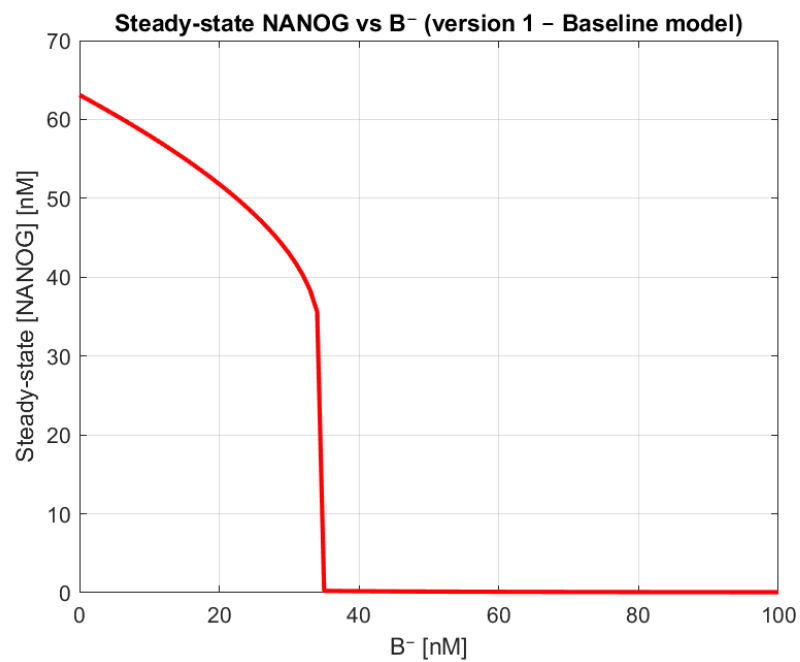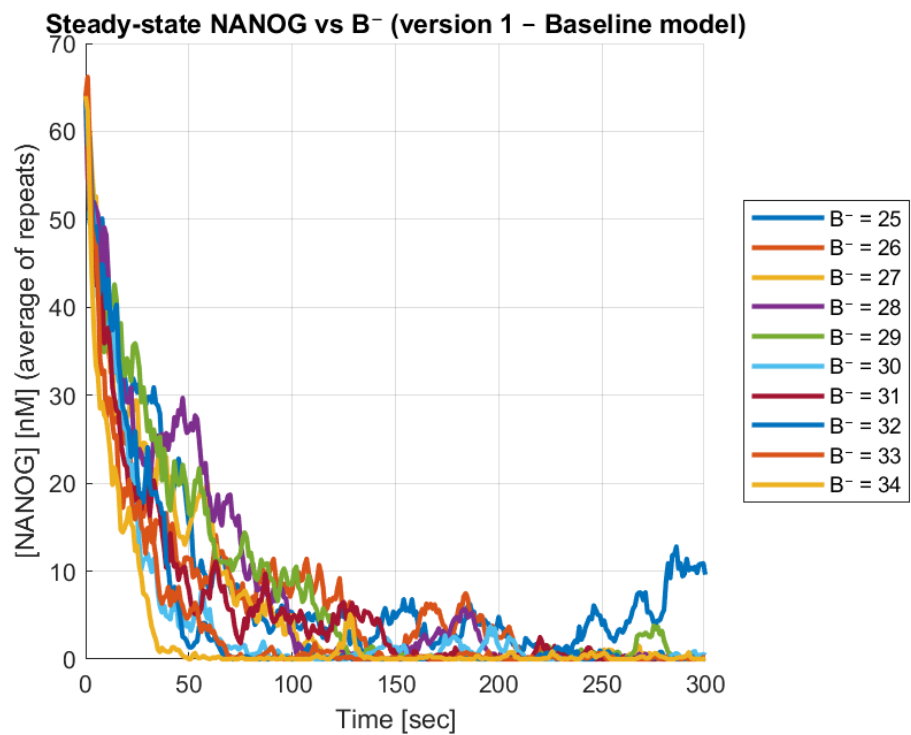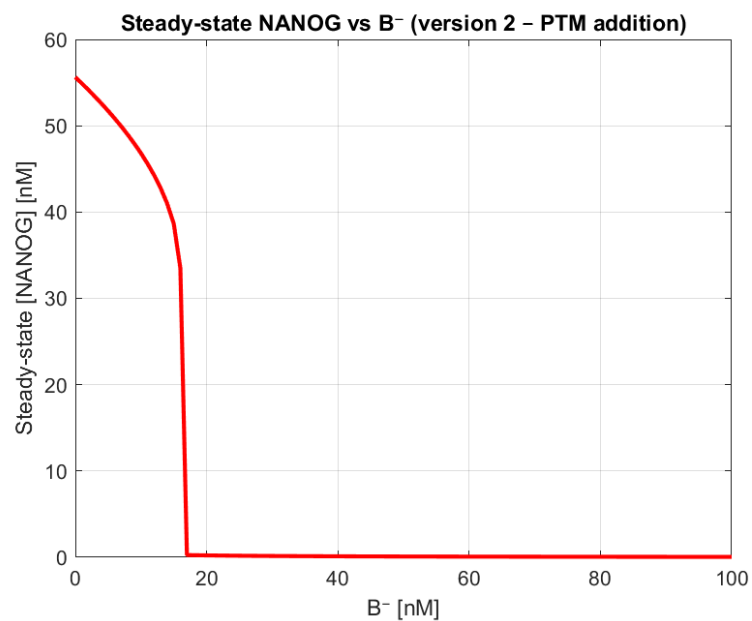
- Deterministic solution (threshold = ~36):



- Stochastic solution (convergence radius = ~10 ):

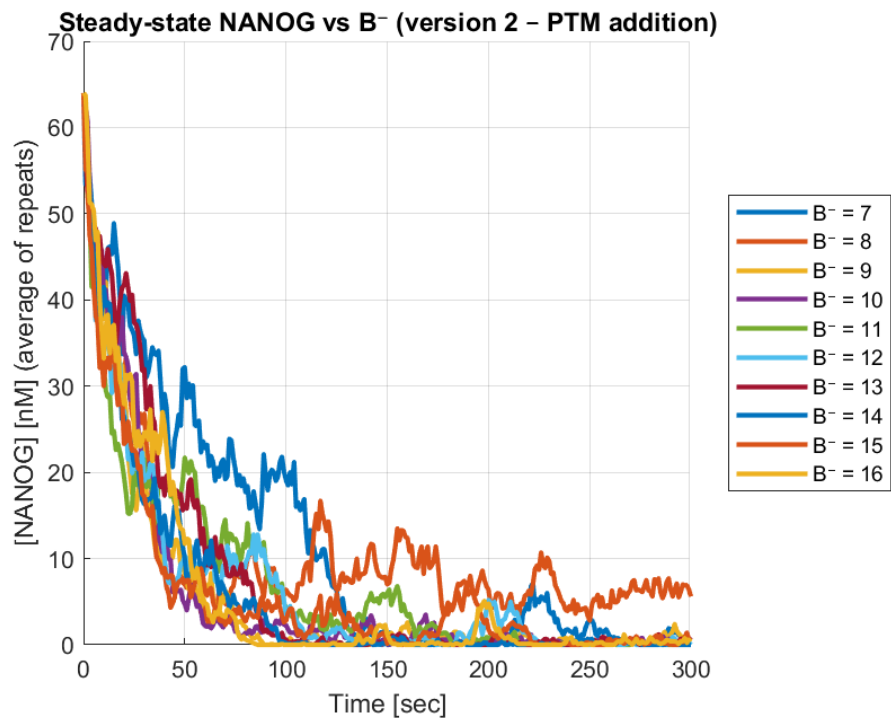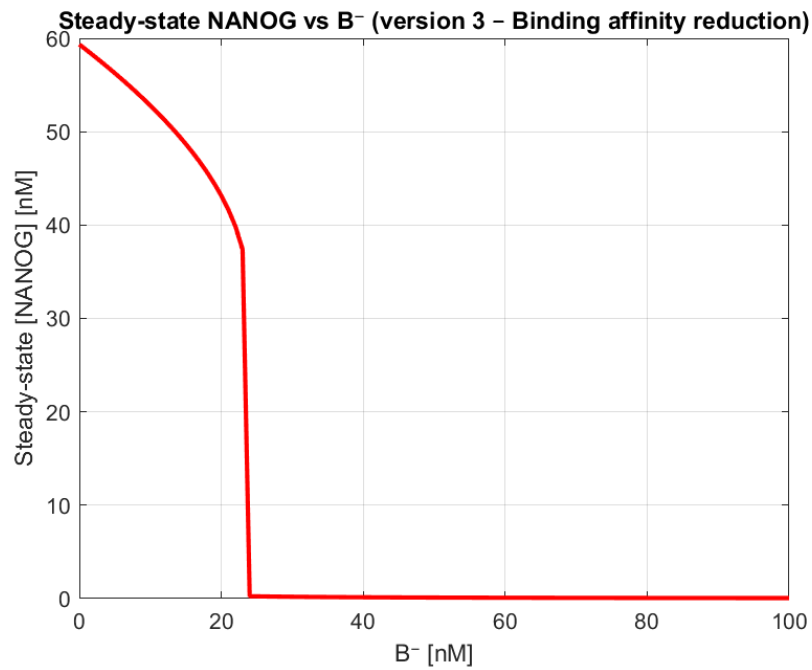**PMT addition model:**

- Deterministic solution (threshold = ~17):



- Stochastic solution ( convergence radius = ~8):

**Weaker binding affinity model:**

- Deterministic solution (threshold = ~ 24):



- Stochastic solution (convergence radius = ~ 6):