Supplementary information for "Learning retrosynthetic planning through simulated experience"

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Additional results

Table SI provides additional data for comparing the performance of the huerstic and learned policies. Figure S1 shows the full cost distribution for the heuristic policy (π_{sd}) and the learned optimal policy (π_*). Figure S2 shows additional data on the effect of noise ε on the performance of the heuristic policy.

Table SI: Comparison of the performance of π_{sd} versus π_*. The values show the percent that one policy found a lower cost than the other, or whether the two policies found pathways with identical cost (e.g., a tie), for the molecules in the training and testing sets. All percents were computed using the size of the training (~100,000) or testing set (~25,000).

	Train (100,00)			**Test** (25,000)		
	π_{sd} (%)	π_* (%)	Tie (%)	π_{sd} (%)	π_* (%)	Tie (%)
$c_{\text{tot}} < P_1$	0.4	35.0	47.9	6.1	21.3	47.9
$P_1 \leq \text{tot} < P_2$	3.9	5.2	5.1	3.4	8.6	9.9
$c_{\text{tot}} \geq P_2$	<1	1.6	<1	<1	1.1	1.3
Bulk	4.4	41.8	53.8	9.9	31.0	59.1

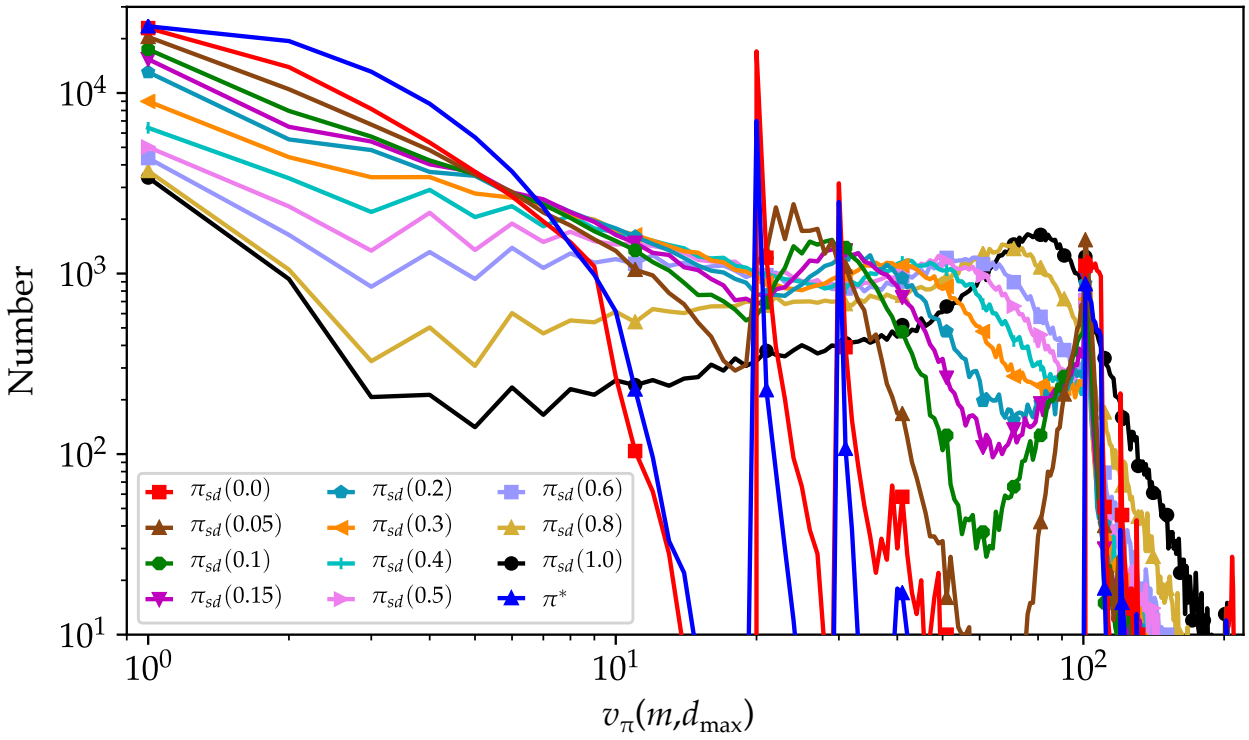

Figure S1: The distribution of expected costs $v_\pi(m, d_{\max})$ over the set of 100,000 target molecules is shown for the greedy optimal policy π_* and the symmetric disconnection policy π_{sd} for different values of noise ε.

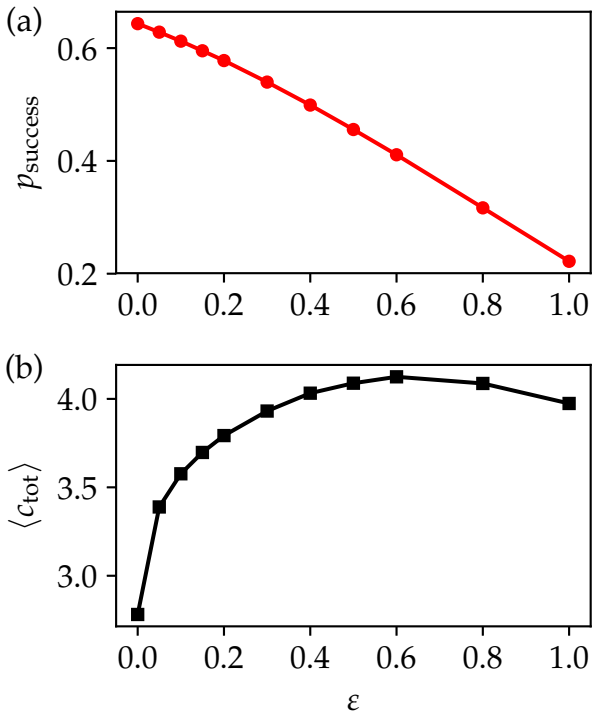

Figure S2: (a) The probability of successfully synthesizing the target molecule using the symmetric disconnection policy π_{sd} decreases with increasing noise ε. (b) For those successful syntheses, the average cost $\langle c_{\text{tot}} \rangle$ increases with increasing noise ε.