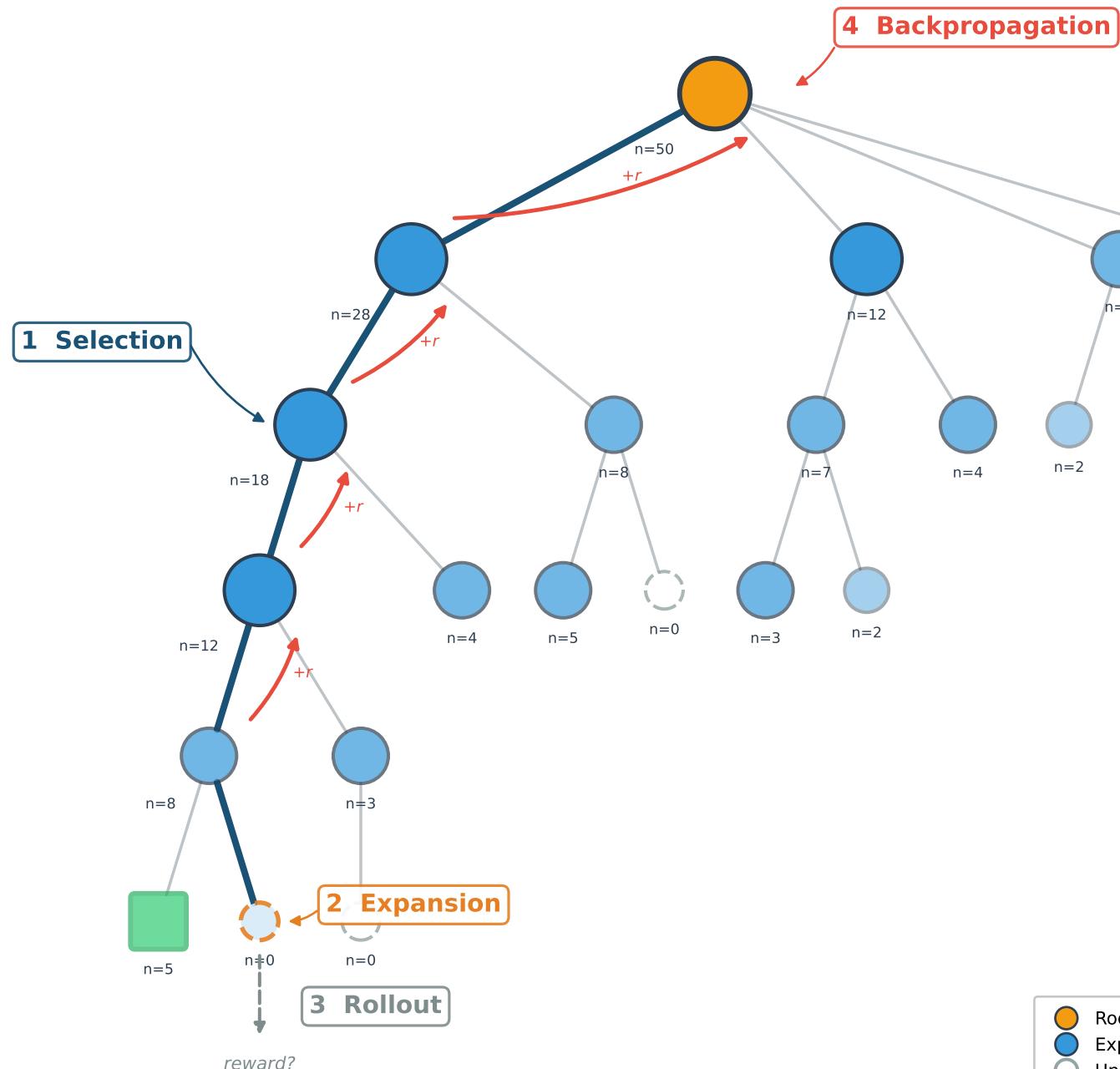


# Monte Carlo Tree Search for Retrosynthesis

Asymmetric exploration guided by UCB1 selection policy



- Root (target molecule)
- Explored node (darker = more visits)
- Unexpanded node
- Building block (terminal)
- Newly expanded node
- Selection path (UCB1)
- Backpropagation (+reward)

## Breadth-First Search

uniform exploration

