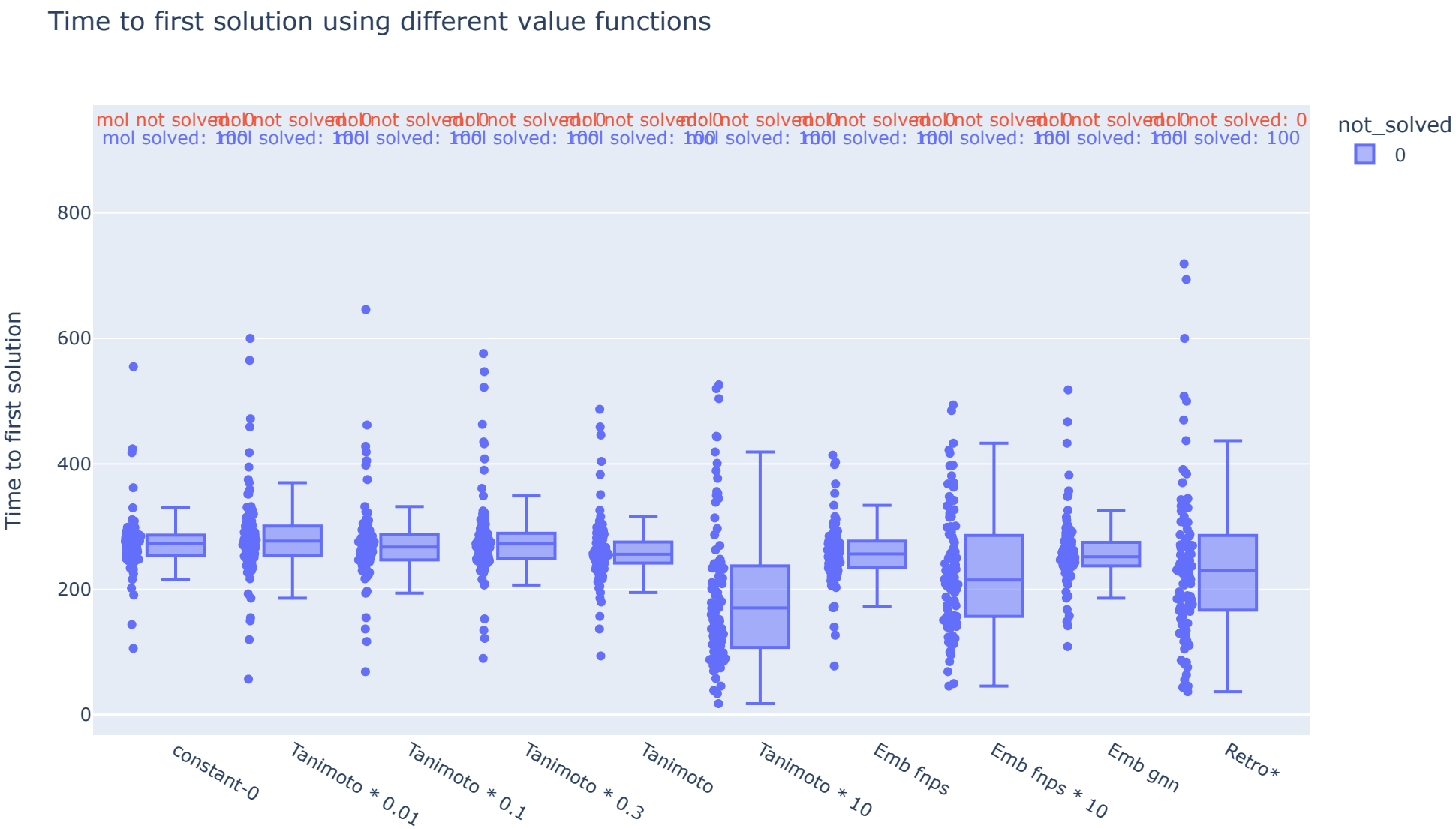
Time to first solution using different value functions
not_solved
0
Time to first solution
0
200
400
600
800
mol not solved: 0
mol solved: 100
constant-0
Tanimoto * 0.01
Tanimoto * 0.1
Tanimoto * 0.3
Tanimoto
Tanimoto * 10
Emb fnps
Emb fnps * 10
Emb gnn
Retro*