Solution Time for different percentiles of solved molecules - 700 0.0 106.0 94.0 37.0 0.05 224.6 194.6 75.4 - 600 0.1 242.1 216.9 110.4 - 500 Solved Molecules Percentile 0.25 254.0 242.0 167.5 - 400

0.5 273.0 256.0 230.5 0.75 286.2 274.8 285.5 - 300 0.9 299.1 371.4 304.1 - 200 0.95 311.9 352.6 471.5 - 100 1.0 555.0 719.0 487.0 constant-0 **Tanimoto** Retro* Algorithm