## Solution Time for different percentiles of solved molecules - 700 0.0 106.0 57.0 69.0 90.0 94.0 18.0 78.0 46.0 109.0 37.0 0.05 224.6 192.7 208.9 194.6 57.4 172.9 99.8 185.1 75.4 196.8 600 Percentile 0.1 242.1 233.7 226.7 230.9 216.9 82.6 208.8 121.5 219.4 110.4 500 0.25 254.0 253.8 247.0 249.8 242.0 108.8 235.5 157.0 237.8 167.5 Solved Molecules 400 0.5 273.0 277.0 272.5 256.0 170.5 256.5 215.0 252.0 230.5 267.5 - 300 0.75 286.2 301.0 287.0 288.8 274.8 236.2 277.0 285.0 274.5 285.5 0.9 299.1 352.0 313.0 327.4 304.1 353.3 305.1 363.5 303.7 371.4 - 200 0.95 311.9 396.1 398.3 432.1 352.6 420.2 334.9 398.9 350.3 471.5 - 100 1.0 555.0 600.0 646.0 576.0 487.0 526.0 414.0 494.0 518.0 719.0 10 10 constant-0 0.01 0.3 **Tanimoto** Emb fnps Emb gnn **Retro**\* Tanimoto \* 0.1 **Tanimoto** \* Tanimoto \* Emb fnps **Tanimoto** \* Algorithm