Solution Time for different percentiles of solved molecules 106.0 18.0 6.0 78.0 46.0 3.0 28.0 0.0 94.0 109.0 3.0 37.0 2000 - 1750 65.8 0.05 224.6 194.6 57.4 7.0 172.9 99.8 8.0 185.1 7.0 75.4 - 1500 - 1250 8.0 9.0 Percentile 0.1 242.1 216.9 82.6 208.8 121.5 12.9 219.4 77.9 110.4 - 1000 14.0 0.25 254.0 242.0 108.8 16.8 235.5 157.0 36.8 237.8 112.2 167.5 - 750 - 500 Solved Molecules 0.5 273.0 256.0 170.5 37.5 256.5 215.0 89.5 252.0 151.5 28.0 230.5 - 250 0.75 286.2 274.8 236.2 88.0 277.0 285.0 221.8 274.5 210.0 65.0 285.5 0.9 353.3 299.1 304.1 260.8 305.1 363.5 377.8 303.7 258.5 150.0 371.4 0.95 311.9 352.6 420.2 498.8 334.9 398.9 642.4 350.3 299.1 327.6 471.5 1.0 526.0 2258.4 414.0 1882.0 518.0 526.0 2258.4 555.0 487.0 494.0 719.0 0 10 10 100 100 **GNN** 10 100 constant-0 **Tanimoto** FNP-NN Tanimoto * **Tanimoto**

Retro* PT * NNS **FNP-NN*** * NNS FNP-NN Algorithm