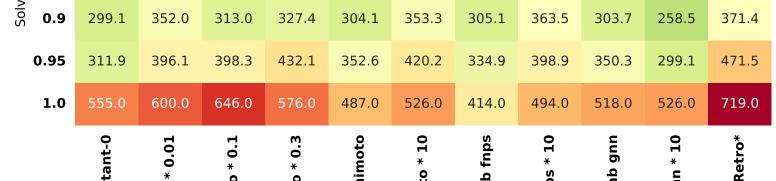
Solution Time for different percentiles of solved molecules - 700 0.0 106.0 90.0 94.0 18.0 78.0 46.0 109.0 28.0 57.0 69.0 37.0 0.05 224.6 192.7 196.8 208.9 194.6 57.4 172.9 99.8 185.1 65.8 75.4 600 82.6 121.5 110.4 Percentile 0.1 242.1 233.7 226.7 230.9 216.9 208.8 219.4 77.9 - 500 0.25 254.0 253.8 247.0 249.8 242.0 108.8 235.5 157.0 237.8 112.2 167.5 Solved Molecules - 400 0.5 273.0 277.0 267.5 272.5 256.0 170.5 256.5 215.0 252.0 151.5 230.5 - 300 0.75 286.2 301.0 287.0 288.8 274.8 236.2 277.0 285.0 274.5 210.0 285.5 0.9 299.1 352.0 313.0 327.4 304.1 353.3 305.1 363.5 303.7 258.5 371.4 - 200

- 100

* uub

Emb

Emb



10 10 constant-0 0.01 0.1 0.3 **Tanimoto** Emb fnps **Tanimoto** * × **Tanimoto** * **Tanimoto** * **Emb fnps Tanimoto** * Algorithm