

DRD2 - Sample limit

| | | | | | | | | | | | | | | | |
|-------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| LSTM-HC | 0.6 | 0.7 | 0.62 | 0.54 | 0.5 | 0.41 | 0.45 | 0.41 | 0.45 | 0.4 | 0.35 | 0.34 | 0.33 | 0.36 | 0.33 |
| AugmentedHC | 0.7 | 0.95 | 0.85 | 0.76 | 0.71 | 0.6 | 0.63 | 0.59 | 0.57 | 0.58 | 0.52 | 0.51 | 0.49 | 0.53 | 0.49 |
| Reinvent | 0.62 | 0.85 | 0.77 | 0.7 | 0.64 | 0.52 | 0.57 | 0.52 | 0.51 | 0.5 | 0.43 | 0.43 | 0.4 | 0.45 | 0.4 |
| BAR | 0.54 | 0.76 | 0.7 | 0.73 | 0.7 | 0.56 | 0.61 | 0.54 | 0.64 | 0.54 | 0.44 | 0.43 | 0.4 | 0.45 | 0.4 |
| VSMaxMin | 0.5 | 0.71 | 0.64 | 0.7 | 0.65 | 0.57 | 0.65 | 0.57 | 0.54 | 0.55 | 0.42 | 0.41 | 0.37 | 0.44 | 0.37 |
| AugMemory | 0.41 | 0.6 | 0.52 | 0.56 | 0.57 | 0.76 | 0.78 | 0.8 | 0.78 | 0.84 | 0.56 | 0.56 | 0.46 | 0.65 | 0.46 |
| GraphGA | 0.45 | 0.63 | 0.57 | 0.61 | 0.65 | 0.78 | 0.81 | 0.79 | 0.84 | 0.74 | 0.55 | 0.53 | 0.46 | 0.58 | 0.46 |
| VSRandom | 0.41 | 0.59 | 0.52 | 0.54 | 0.57 | 0.8 | 0.79 | 0.9 | 0.84 | 1.1 | 0.7 | 0.71 | 0.58 | 0.83 | 0.58 |
| LSTM-PPO | 0.45 | 0.57 | 0.51 | 0.64 | 0.54 | 0.78 | 0.84 | 0.84 | | 0.84 | 0.58 | 0.63 | 0.47 | 0.63 | 0.47 |
| Mimosa | 0.4 | 0.58 | 0.5 | 0.54 | 0.55 | 0.84 | 0.74 | 1.1 | 0.84 | 1.6 | 1.3 | 1.2 | 1 | 1.5 | 1 |
| SmilesGA | 0.35 | 0.52 | 0.43 | 0.44 | 0.42 | 0.56 | 0.55 | 0.7 | 0.58 | 1.3 | 0.73 | 1.1 | 0.47 | 1.3 | 0.47 |
| Stoned | 0.34 | 0.51 | 0.43 | 0.43 | 0.41 | 0.56 | 0.53 | 0.71 | 0.63 | 1.2 | 1.1 | 1.2 | 0.89 | 1.3 | 0.78 |
| Gflownet | 0.33 | 0.49 | 0.4 | 0.4 | 0.37 | 0.46 | 0.46 | 0.58 | 0.47 | 1 | 0.47 | 0.89 | 0 | 0.92 | 0 |
| GflownetDF | 0.36 | 0.53 | 0.45 | 0.45 | 0.44 | 0.65 | 0.58 | 0.83 | 0.63 | 1.5 | 1.3 | 1.3 | 0.92 | 1.3 | 0.86 |
| Mars | 0.33 | 0.49 | 0.4 | 0.4 | 0.37 | 0.46 | 0.46 | 0.58 | 0.47 | 1 | 0.47 | 0.78 | 0 | 0.86 | 0 |

DRD2 - Time limit

| | | | | | | | | | | | | | | | |
|-------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| LSTM-HC | 0.66 | 0.66 | 0.57 | 0.56 | 0.52 | 0.56 | 0.6 | 0.49 | 0.46 | 0.46 | 0.46 | 0.45 | 0.45 | 0.45 | 0.45 |
| AugmentedHC | 0.95 | 0.99 | 0.79 | 0.93 | 0.68 | 0.77 | 0.87 | 0.6 | 0.53 | 0.51 | 0.52 | 0.51 | 0.51 | 0.51 | 0.51 |
| Reinvent | 0.99 | 1 | 0.82 | 0.98 | 0.7 | 0.8 | 0.91 | 0.62 | 0.54 | 0.53 | 0.53 | 0.52 | 0.52 | 0.52 | 0.52 |
| BAR | 0.79 | 0.82 | 1.1 | 1.1 | 0.87 | 1.1 | 1.1 | 0.73 | 0.58 | 0.57 | 0.58 | 0.55 | 0.55 | 0.56 | 0.56 |
| VSMaxMin | 0.93 | 0.98 | 1.1 | | 0.87 | 1.1 | 1.1 | 0.76 | 0.67 | 0.66 | 0.67 | 0.65 | 0.65 | 0.66 | 0.66 |
| AugMemory | 0.68 | 0.7 | 0.87 | 0.87 | 0.91 | 1 | 0.94 | 0.72 | 0.52 | 0.49 | 0.5 | 0.46 | 0.46 | 0.48 | 0.48 |
| GraphGA | 0.77 | 0.8 | 1.1 | 1.1 | 1 | 1.2 | 1.1 | 0.83 | 0.65 | 0.63 | 0.65 | 0.61 | 0.61 | 0.62 | 0.62 |
| VSRandom | 0.87 | 0.91 | 1.1 | 1.1 | 0.94 | 1.1 | 1.1 | 0.78 | 0.67 | 0.65 | 0.66 | 0.64 | 0.64 | 0.65 | 0.65 |
| LSTM-PPO | 0.6 | 0.62 | 0.73 | 0.76 | 0.72 | 0.83 | 0.78 | 0.94 | 0.64 | 0.59 | 0.62 | 0.54 | 0.54 | 0.56 | 0.56 |
| Mimosa | 0.53 | 0.54 | 0.58 | 0.67 | 0.52 | 0.65 | 0.67 | 0.64 | 1.8 | 1.3 | 1.6 | 0.9 | 0.9 | 1.1 | 1.1 |
| SmilesGA | 0.51 | 0.53 | 0.57 | 0.66 | 0.49 | 0.63 | 0.65 | 0.59 | 1.3 | 1 | 1.4 | 0.54 | 0.54 | 0.66 | 0.66 |
| Stoned | 0.52 | 0.53 | 0.58 | 0.67 | 0.5 | 0.65 | 0.66 | 0.62 | 1.6 | 1.4 | 1.7 | 1 | 1 | 1.2 | 1.2 |
| Gflownet | 0.51 | 0.52 | 0.55 | 0.65 | 0.46 | 0.61 | 0.64 | 0.54 | 0.9 | 0.54 | 1 | 0 | 0 | 0.95 | 0.95 |
| GflownetDF | 0.51 | 0.52 | 0.55 | 0.65 | 0.46 | 0.61 | 0.64 | 0.54 | 0.9 | 0.54 | 1 | 0 | 0 | 0.55 | 0.55 |
| Mars | 0.51 | 0.52 | 0.56 | 0.66 | 0.48 | 0.62 | 0.65 | 0.56 | 1.1 | 0.66 | 1.2 | 0.95 | 0.55 | 0.93 | 0.93 |

GSK3β - Sample limit

| | | | | | | | | | | | | | | | |
|-------------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| LSTM-HC | 0.78 | 0.73 | 0.59 | 0.55 | 0.5 | 0.47 | 0.47 | 0.46 | 0.47 | 0.43 | 0.41 | 0.42 | 0.43 | 0.42 | 0.4 |
| AugmentedHC | 0.73 | 0.67 | 0.58 | 0.54 | 0.48 | 0.45 | 0.45 | 0.45 | 0.48 | 0.41 | 0.39 | 0.41 | 0.42 | 0.4 | 0.39 |
| Reinvent | 0.59 | 0.58 | 0.54 | 0.53 | 0.45 | 0.41 | 0.41 | 0.41 | 0.37 | 0.35 | 0.32 | 0.34 | 0.36 | 0.33 | 0.31 |
| BAR | 0.55 | 0.54 | 0.53 | 0.51 | 0.44 | 0.39 | 0.39 | 0.38 | 0.36 | 0.31 | 0.28 | 0.31 | 0.33 | 0.3 | 0.27 |
| VSMaxMin | 0.5 | 0.48 | 0.45 | 0.44 | 0.65 | 0.61 | 0.61 | 0.59 | 0.53 | 0.45 | 0.39 | 0.45 | 0.48 | 0.42 | 0.37 |
| AugMemory | 0.47 | 0.45 | 0.41 | 0.39 | 0.61 | 0.76 | 0.83 | 0.78 | 0.69 | 0.58 | 0.47 | 0.56 | 0.61 | 0.53 | 0.44 |
| GraphGA | 0.47 | 0.45 | 0.41 | 0.39 | 0.61 | 0.83 | 0.99 | 0.84 | 0.84 | 0.72 | 0.6 | 0.72 | 0.68 | 0.65 | 0.56 |
| VSRandom | 0.46 | 0.45 | 0.41 | 0.38 | 0.59 | 0.78 | 0.84 | 0.79 | 0.77 | 0.58 | 0.47 | 0.57 | 0.6 | 0.53 | 0.44 |
| LSTM-PPO | 0.47 | 0.48 | 0.37 | 0.36 | 0.53 | 0.69 | 0.84 | 0.77 | | 0.76 | 0.58 | 0.75 | 0.53 | 0.64 | 0.46 |
| Mimosa | 0.43 | 0.41 | 0.35 | 0.31 | 0.45 | 0.58 | 0.72 | 0.58 | 0.76 | 1.6 | 0.68 | 1.4 | 0.43 | 1.5 | 0.52 |
| SmilesGA | 0.41 | 0.39 | 0.32 | 0.28 | 0.39 | 0.47 | 0.6 | 0.47 | 0.58 | 0.68 | 0.24 | 0.59 | 0.3 | 0.56 | 0.17 |
| Stoned | 0.42 | 0.41 | 0.34 | 0.31 | 0.45 | 0.56 | 0.72 | 0.57 | 0.75 | 1.4 | 0.59 | 1.3 | 0.41 | 1.3 | 0.47 |
| Gflownet | 0.43 | 0.42 | 0.36 | 0.33 | 0.48 | 0.61 | 0.68 | 0.6 | 0.53 | 0.43 | 0.3 | 0.41 | 0.42 | 0.37 | 0.27 |
| GflownetDF | 0.42 | 0.4 | 0.33 | 0.3 | 0.42 | 0.53 | 0.65 | 0.53 | 0.64 | 1.5 | 0.56 | 1.3 | 0.37 | 1.8 | 0.43 |
| Mars | 0.4 | 0.39 | 0.31 | 0.27 | 0.37 | 0.44 | 0.56 | 0.44 | 0.46 | 0.52 | 0.17 | 0.47 | 0.27 | 0.43 | 0.11 |

GSK3β - Time limit

| | | | | | | | | | | | | | | | |
|-------------|------|------|------|------|------|------|------|------|------|------|------|-------|------|------|------|
| LSTM-HC | 0.87 | 0.73 | 0.76 | 0.64 | 0.59 | 0.66 | 0.59 | 0.52 | 0.48 | 0.47 | 0.47 | 0.47 | 0.48 | 0.47 | 0.47 |
| AugmentedHC | 0.83 | 0.69 | 0.73 | 0.62 | 0.55 | 0.62 | 0.56 | 0.49 | 0.45 | 0.44 | 0.44 | 0.44 | 0.45 | 0.44 | 0.44 |
| Reinvent | 0.69 | 1 | 0.96 | 0.86 | 0.76 | 0.9 | 0.78 | 0.64 | 0.54 | 0.53 | 0.53 | 0.52 | 0.54 | 0.53 | 0.53 |
| BAR | 0.73 | 0.96 | 1 | 0.8 | 0.71 | 0.83 | 0.72 | 0.61 | 0.53 | 0.52 | 0.52 | 0.51 | 0.53 | 0.51 | 0.51 |
| VSMaxMin | 0.62 | 0.86 | 0.8 | | 1 | 1.2 | 1.1 | 0.87 | 0.73 | 0.72 | 0.71 | 0.72 | 0.75 | 0.71 | 0.71 |
| AugMemory | 0.55 | 0.76 | 0.71 | 1 | 0.83 | 1 | 0.87 | 0.62 | 0.46 | 0.44 | 0.44 | 0.42 | 0.46 | 0.43 | 0.43 |
| GraphGA | 0.62 | 0.9 | 0.83 | 1.2 | 1 | 1.2 | 1 | 0.8 | 0.64 | 0.63 | 0.63 | 0.61 | 0.65 | 0.62 | 0.62 |
| VSRandom | 0.56 | 0.78 | 0.72 | 1.1 | 0.87 | 1 | 1.1 | 0.87 | 0.66 | 0.64 | 0.64 | 0.62 | 0.67 | 0.63 | 0.63 |
| LSTM-PPO | 0.49 | 0.64 | 0.61 | 0.87 | 0.62 | 0.8 | 0.87 | 0.78 | 0.55 | 0.5 | 0.51 | 0.47 | 0.55 | 0.49 | 0.49 |
| Mimosa | 0.45 | 0.54 | 0.53 | 0.73 | 0.46 | 0.64 | 0.66 | 0.55 | 1.5 | 1.3 | 1.3 | 0.52 | 0.52 | 1.1 | 1.1 |
| SmilesGA | 0.44 | 0.53 | 0.52 | 0.72 | 0.44 | 0.63 | 0.64 | 0.5 | 1.3 | 1.5 | 1.6 | 0.44 | 0.36 | 1.2 | 1.2 |
| Stoned | 0.44 | 0.53 | 0.52 | 0.71 | 0.44 | 0.63 | 0.64 | 0.51 | 1.3 | 1.6 | 1.6 | 0.48 | 0.36 | 1.3 | 1.3 |
| Gflownet | 0.44 | 0.52 | 0.51 | 0.72 | 0.42 | 0.61 | 0.62 | 0.47 | 0.52 | 0.44 | 0.48 | 0.049 | 0.25 | 0.27 | 0.27 |
| GflownetDF | 0.45 | 0.54 | 0.53 | 0.75 | 0.46 | 0.65 | 0.67 | 0.55 | 0.52 | 0.36 | 0.36 | 0.25 | 0.4 | 0.3 | 0.3 |
| Mars | 0.44 | 0.53 | 0.51 | 0.71 | 0.43 | 0.62 | 0.63 | 0.49 | 1.1 | 1.2 | 1.3 | 0.27 | 0.3 | 0.88 | 0.88 |

JNK3 - Sample limit

| | | | | | | | | | | | | | | | |
|-------------|------|------|-------|------|------|------|------|------|------|------|------|------|------|------|-------|
| LSTM-HC | 0.7 | 0.67 | 0.43 | 0.53 | 0.39 | 0.42 | 0.4 | 0.4 | 0.42 | 0.41 | 0.38 | 0.38 | 0.37 | 0.39 | 0.37 |
| AugmentedHC | 0.67 | 0.86 | 0.53 | 0.76 | 0.51 | 0.58 | 0.52 | 0.53 | 0.53 | 0.54 | 0.5 | 0.49 | 0.48 | 0.51 | 0.48 |
| Reinvent | 0.43 | 0.53 | 0.17 | 0.4 | 0.14 | 0.19 | 0.16 | 0.16 | 0.15 | 0.16 | 0.12 | 0.12 | 0.1 | 0.14 | 0.099 |
| BAR | 0.53 | 0.76 | 0.4 | 0.86 | 0.53 | 0.62 | 0.56 | 0.57 | 0.48 | 0.57 | 0.51 | 0.5 | 0.47 | 0.53 | 0.47 |
| VSMaxMin | 0.39 | 0.51 | 0.14 | 0.53 | 0.18 | 0.36 | 0.25 | 0.26 | 0.18 | 0.29 | 0.17 | 0.14 | 0.11 | 0.21 | 0.1 |
| AugMemory | 0.42 | 0.58 | 0.19 | 0.62 | 0.36 | 0.55 | 0.57 | 0.55 | 0.53 | 0.69 | 0.47 | 0.38 | 0.34 | 0.54 | 0.34 |
| GraphGA | 0.4 | 0.52 | 0.16 | 0.56 | 0.25 | 0.57 | 0.76 | 0.81 | 0.64 | 0.85 | 0.6 | 0.55 | 0.43 | 0.64 | 0.41 |
| VSRandom | 0.4 | 0.53 | 0.16 | 0.57 | 0.26 | 0.55 | 0.81 | 0.78 | 0.65 | 0.99 | 0.67 | 0.57 | 0.47 | 0.74 | 0.46 |
| LSTM-PPO | 0.42 | 0.53 | 0.15 | 0.48 | 0.18 | 0.53 | 0.64 | 0.65 | | 1 | 0.59 | 0.7 | 0.37 | 0.81 | 0.33 |
| Mimosa | 0.41 | 0.54 | 0.16 | 0.57 | 0.29 | 0.69 | 0.85 | 0.99 | 1 | 1.3 | 0.99 | 1 | 0.87 | 1.5 | 0.85 |
| SmilesGA | 0.38 | 0.5 | 0.12 | 0.51 | 0.17 | 0.47 | 0.6 | 0.67 | 0.59 | 0.99 | 0.62 | 0.63 | 0.49 | 1 | 0.47 |
| Stoned | 0.38 | 0.49 | 0.12 | 0.5 | 0.14 | 0.38 | 0.55 | 0.57 | 0.7 | 1 | 0.63 | 0.6 | 0.55 | 1.1 | 0.47 |
| Gflownet | 0.37 | 0.48 | 0.1 | 0.47 | 0.11 | 0.34 | 0.43 | 0.47 | 0.37 | 0.87 | 0.49 | 0.55 | 1 | 1 | |
| GflownetDF | 0.39 | 0.51 | 0.14 | 0.53 | 0.21 | 0.54 | 0.64 | 0.74 | 0.81 | 1.5 | 1 | 1.1 | 1 | 1.5 | 1 |
| Mars | 0.37 | 0.48 | 0.099 | 0.47 | 0.1 | 0.34 | 0.41 | 0.46 | 0.33 | 0.85 | 0.47 | 0.47 | | 1 | |

JNK3 - Time limit

| | | | | | | | | | | | | | | |
|-------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| -0.91 | 0.77 | 0.72 | 0.67 | 0.54 | 0.61 | 0.62 | 0.6 | 0.51 | 0.49 | 0.49 | 0.49 | 0.48 | 0.48 | 0.49 |
| -0.77 | 0.79 | 0.82 | 0.75 | 0.59 | 0.65 | 0.67 | 0.63 | 0.5 | 0.46 | 0.46 | 0.46 | 0.45 | 0.45 | 0.45 |
| -0.72 | 0.82 | 0.89 | 0.83 | 0.7 | 0.71 | 0.73 | 0.69 | 0.52 | 0.47 | 0.47 | 0.48 | 0.46 | 0.46 | 0.47 |
| -0.67 | 0.75 | 0.83 | 0.9 | 0.81 | 0.79 | 0.84 | 0.77 | 0.55 | 0.49 | 0.49 | 0.5 | 0.47 | 0.47 | 0.48 |
| -0.54 | 0.59 | 0.7 | 0.81 | | 0.87 | 1.1 | 1.1 | 0.71 | 0.65 | 0.63 | 0.64 | 0.61 | 0.61 | 0.62 |
| -0.61 | 0.65 | 0.71 | 0.79 | 0.87 | 0.78 | 0.9 | 0.81 | 0.52 | 0.44 | 0.44 | 0.45 | 0.42 | 0.42 | 0.43 |
| -0.62 | 0.67 | 0.73 | 0.84 | 1.1 | 0.9 | 1.1 | 1.1 | 0.76 | 0.64 | 0.64 | 0.65 | 0.62 | 0.62 | 0.63 |
| -0.6 | 0.63 | 0.69 | 0.77 | 1.1 | 0.81 | 1.1 | 1 | 0.73 | 0.61 | 0.61 | 0.63 | 0.59 | 0.59 | 0.6 |
| -0.51 | 0.5 | 0.52 | 0.55 | 0.71 | 0.52 | 0.76 | 0.73 | 0.99 | 0.7 | 0.69 | 0.74 | 0.59 | 0.59 | 0.66 |
| -0.49 | 0.46 | 0.47 | 0.49 | 0.65 | 0.44 | 0.64 | 0.61 | 0.7 | 1.4 | 1.2 | 1.6 | 0.9 | 0.9 | 1.2 |
| -0.49 | 0.46 | 0.47 | 0.49 | 0.63 | 0.44 | 0.64 | 0.61 | 0.69 | 1.2 | 0.74 | 1.1 | 0.5 | 0.5 | 0.91 |
| -0.49 | 0.46 | 0.48 | 0.5 | 0.64 | 0.45 | 0.65 | 0.63 | 0.74 | 1.6 | 1.1 | 1.5 | 1 | 1 | 1.4 |
| -0.48 | 0.45 | 0.46 | 0.47 | 0.61 | 0.42 | 0.62 | 0.59 | 0.59 | 0.9 | 0.5 | 1 | 0 | 0 | 0.75 |
| -0.48 | 0.45 | 0.46 | 0.47 | 0.61 | 0.42 | 0.62 | 0.59 | 0.59 | 0.9 | 0.5 | 1 | 0 | | 0.75 |
| -0.49 | 0.45 | 0.47 | 0.48 | 0.62 | 0.43 | 0.63 | 0.6 | 0.66 | 1.2 | 0.91 | 1.4 | 0.75 | 0.75 | 0.89 |