**Table S3.** **AUC for the 4 DUD systems used for calculating the time performance.**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **Vina1** | **Glide SP1** | **rDock** | | | |
|  |  |  | **Grid-based SF** | | **Indexed SF** | |
|  |  |  | **VS2** | **Full1,3** | **VS2** | **Full1,3** |
| ADA | 0.39 | 0.67 | 0.68 | 0.64 | 0.57 | 0.62 |
| COMT | 0.51 | 0.69 | 0.67 | 0.62 | 0.65 | 0.64 |
| PARP | 0.68 | 0.9 | 0.88 | 0.86 | 0.87 | 0.86 |
| Trypsin | 0.74 | 0.49 | 0.63 | 0.62 | 0.66 | 0.76 |
| **Average** | **0.58** | **0.69** | **0.72** | **0.69** | **0.69** | **0.72** |

1 Default program parameters were used. 2 On HTVS mode, the average number of docking runs needed for these 4 systems is 10. 3 50 docking runs are used for default docking.