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| **Table S1. Performance comparison in terms of the Accuracy, AUC, and AUPR metrics for two distinct negative sample selection methods and three different feature selection methods.** | | | | | | | | | | | | | | |
| Target groups and  Performance  metrics  negative selection and feature selection method | | Nuclear receptor | | | GPCR | | | Ion channel | | | | Enzyme | | |
| ACC | AUC | AUPR | ACC | AUC | AUPR | ACC | AUC | AUPR | ACC | | AUC | AUPR |
| BRNS | SSFSM-DTI | 0.96 | 0.99 | 0.99 | 0.92 | 0.99 | 0.53 | 0.93 | 0.98 | 0.98 | 0.69 | | 0.71 | 0.81 |
| SUPL\_FS | 0.95 | 0.98 | 0.99 | 0.91 | 0.99 | 0.53 | 0.90 | 0.97 | 0.98 | 0.65 | | 0.66 | 0.79 |
| INFO\_GAIN\_FS | 0.92 | 0.96 | 0.98 | 0.84 | 0.88 | 0.55 | 0.92 | 0.94 | 0.96 | 0.64 | | 0.65 | 0.77 |
| Random | SSFSM-DTI | 0.31 | 0.64 | 0.75 | 0.53 | 0.74 | 0.62 | 0.51 | 0.73 | 0.56 | 0.55 | | 0.55 | 0.48 |
| SUPL\_FS | 0.43 | 0.79 | 0.83 | 0.52 | 0.75 | 0.65 | 0.50 | 0.58 | 0.77 | 0.63 | | 0.68 | 0.65 |
| INFO\_GAIN\_FS | 0.34 | 0.63 | 0.69 | 0.54 | 0.59 | 0.74 | 0.44 | 0.64 | 0.75 | 0.54 | | 0.51 | 0.45 |