**Supplementary Table 5: Number of the drugs used in each step of the machine learning process.** In parenthesis, the number of drugs when using “Targets” feature.

|  |  |  |  |
| --- | --- | --- | --- |
| **Type of drug** | **Number of drugs** | | |
| **Complete dataset** | **Training** | **Testing** |
| DILIrank drugs | 175 (172) | 72 | 30 |
| DILI-Concern drugs | 124 (121) | 36 | 15 |
| Most-DILI-Concern drugs | 37 (36) | 11 | 4 |
| Less-DILI-Concern drugs | 87 (85) | 25 | 11 |
| No-DILI-Concern drugs | 51 (51) | 36 | 15 |
| Independent hold-out test dataset drugs | 55 (53) |  |  |