**Table S2.** Description of the training and validation sets in the term of P450 inhibition.

|  |  |  |  |
| --- | --- | --- | --- |
| dataset | P450 non-inhibitor (n) | non-extensive P450 inhibitor (n) | multi-P450 inhibitor (n) |
| training set | 1681 | 2188 | 1563 |
| validation set | 841 | 1095 | 780 |