**Table S4.** The MMP-12 non-inhibitors in the testing set.

|  |  |  |
| --- | --- | --- |
| Index | Name | Structure |
| 1 | 10571165-1a |  |
| 2 | 10514279-12f |  |
| 3 | 10514279-5i |  |
| 4 | 10514279-5n |  |
| 5 | 10514279-4e |  |
| 6 | 10514279-5h |  |
| 7 | 10571165-12b |  |
| 8 | 10571165-18 |  |
| 9 | 10514279-6 |  |
| 10 | 10514279-4k |  |
| 11 | 110685 |  |
| 12 | 10903 |  |
| 13 | 10571165-12a |  |
| 14 | 10571165-1c |  |
| 15 | 10514279-8 |  |
| 16 | 108056 |  |
| 17 | 108956 |  |
| 18 | 109817 |  |
| 19 | 105495 |  |
| 20 | 103462 |  |
| 21 | 104683 |  |
| 22 | 109008 |  |
| 23 | 104169 |  |
| 24 | 102256 |  |
| 25 | 10514279-15b |  |
| 26 | 106354 |  |
| 27 | 10589 |  |
| 28 | 105979 |  |
| 29 | 10514279-4h |  |
| 30 | 107553 |  |
| 31 | 110311 |  |
| 32 | 105651 |  |
| 33 | 110434 |  |
| 34 | 107130 |  |
| 35 | 10514279-14d |  |
| 36 | 107475 |  |
| 37 | 100293 |  |
| 38 | 105951 |  |
| 39 | 10590 |  |
| 40 | 104452 |  |
| 41 | 109162 |  |
| 42 | 105303 |  |
| 43 | 109858 |  |
| 44 | 1036 |  |
| 45 | 108066 |  |
| 46 | 109706 |  |
| 47 | 109178 |  |