**Table S3.** The MMP-12 inhibitors in the testing set.

|  |  |  |
| --- | --- | --- |
| Index | Name | Structure |
| 1 | 104-1 |  |
| 2 | 104-26S |  |
| 3 | 27-1j |  |
| 4 | 105-1205 |  |
| 5 | 170-ADAM10 |  |
| 6 | 103-19S |  |
| 7 | 104-8 |  |
| 8 | 104-10aR |  |
| 9 | 104-19S |  |
| 10 | 104-23S |  |
| 11 | 103-16S |  |
| 12 | 104-9aR |  |
| 13 | 104-5aR |  |
| 14 | 104-28S |  |
| 15 | 103-28S |  |
| 16 | 104-6aR |  |
| 17 | 104-4aR |  |
| 18 | 104-14S |  |
| 19 | 104-22S |  |
| 20 | 102-19 |  |
| 21 | 104-30S |  |
| 22 | 112-1a |  |
| 23 | 104-13S |  |
| 24 | 101-15 |  |
| 25 | 102-18 |  |
| 26 | 103-21S |  |
| 27 | 104-3aR |  |
| 28 | 104-24aR |  |
| 29 | 104-20S |  |
| 30 | 117-10i |  |
| 31 | 122-10nR |  |
| 32 | 115-6501 |  |
| 33 | 100-4c |  |
| 34 | 96-3 |  |
| 35 | 117-10e |  |
| 36 | 96-8 |  |
| 37 | 103-14S |  |
| 38 | 101-7a |  |
| 39 | 27-1e |  |
| 40 | 102-16 |  |
| 41 | 102-7 |  |
| 42 | 115-5401 |  |
| 43 | 104-16S |  |
| 44 | 115-2801 |  |
| 45 | 112-1c |  |
| 46 | 96-7 |  |
| 47 | 101-6e |  |
| 48 | 101-7d |  |
| 49 | 3-PF |  |
| 50 | 117-10a |  |
| 51 | 100-4j |  |
| 52 | 102-8 |  |