**Table S2.** The MMP-12 non-inhibitors in the training set.

|  |  |  |
| --- | --- | --- |
| Index | Name | Structure |
| 1 | 10514279-5l |  |
| 2 | 10514279-12a |  |
| 3 | 10514279-5b |  |
| 4 | 10514279-5k |  |
| 5 | 10514279-4d |  |
| 6 | 10514279-5c |  |
| 7 | 10514279-5g |  |
| 8 | 10514279-5a |  |
| 9 | 10514279-4j |  |
| 10 | 10514279-11 |  |
| 11 | 10514279-4b |  |
| 12 | 110269 |  |
| 13 | 109529 |  |
| 14 | 103276 |  |
| 15 | 104992 |  |
| 16 | 109060 |  |
| 17 | 10514279-12e |  |
| 18 | 10547 |  |
| 19 | 10571165-12c |  |
| 20 | 10514279-5e |  |
| 21 | 104806 |  |
| 22 | 10514279-12c |  |
| 23 | 104705 |  |
| 24 | 103130 |  |
| 25 | 102897 |  |
| 26 | 100877 |  |
| 27 | 102653 |  |
| 28 | 10514279-7 |  |
| 29 | 109263 |  |
| 30 | 104814 |  |
| 31 | 10514279-12d |  |
| 32 | 102317 |  |
| 33 | 106009 |  |
| 34 | 100645 |  |
| 35 | 106466 |  |
| 36 | 10514279-14b |  |
| 37 | 100400 |  |
| 38 | 106010 |  |
| 39 | 10514279-4g |  |
| 40 | 10571165-1b |  |
| 41 | 107112 |  |
| 42 | 107400 |  |
| 43 | 105755 |  |
| 44 | 104491 |  |
| 45 | 110318 |  |
| 46 | 10514279-4c |  |
| 47 | 10556 |  |
| 48 | 106786 |  |
| 49 | 106575 |  |
| 50 | 10571165-3 |  |
| 51 | 109388 |  |
| 52 | 10514279-15c |  |
| 53 | 106412 |  |
| 54 | 10532 |  |
| 55 | 1011 |  |
| 56 | 108193 |  |
| 57 | 109338 |  |
| 58 | 10514279-10 |  |
| 59 | 107536 |  |
| 60 | 105211 |  |
| 61 | 102982 |  |
| 62 | 10514279-9 |  |
| 63 | 100350 |  |
| 64 | 110540 |  |
| 65 | 103196 |  |
| 66 | 100090 |  |
| 67 | 10837 |  |
| 68 | 10417 |  |
| 69 | 10088 |  |
| 70 | 103522 |  |
| 71 | 102612 |  |
| 72 | 1080 |  |
| 73 | 10514279-4i |  |
| 74 | 10514279-4a |  |
| 75 | 107367 |  |
| 76 | 102065 |  |
| 77 | 105888 |  |
| 78 | 110255 |  |
| 79 | 100501 |  |
| 80 | 10514279-14a |  |
| 81 | 10514279-4f |  |
| 82 | 100790 |  |
| 83 | 101063 |  |
| 84 | 101140 |  |
| 85 | 102496 |  |
| 86 | 103249 |  |
| 87 | 105911 |  |
| 88 | 106528 |  |
| 89 | 106794 |  |
| 90 | 107434 |  |
| 91 | 10772 |  |
| 92 | 108248 |  |
| 93 | 109216 |  |
| 94 | 109515 |  |