| Cutoff | ncP52 inhibitors from ChEMBL | ncRandoms | cP52 inhibitors of X-ray | cRandoms | Initial candidate SSIs |
|--------|-------------------------------|-----------|-------------------------|----------|-----------------------|
| > -1   | 31                            | 37        | 7104                    | 6        | 5450                  | 11,714 |
| > -0.9 | 30                            | 8         | 345                     | 6        | 0                     | 313    | 947    |
| > -0.8 | 30                            | 8         | 334                     | 6        | 0                     | 313    | 946    |
| > -0.7 | 29                            | 8         | 328                     | 6        | 0                     | 313    | 943    |
| > -0.6 | 29                            | 8         | 297                     | 6        | 0                     | 312    | 915    |
| > -0.5 | 29                            | 8         | 283                     | 6        | 0                     | 299    | 861    |
| > -0.4 | 29                            | 8         | 258                     | 6        | 0                     | 280    | 783    |
| > -0.3 | 28                            | 8         | 225                     | 6        | 0                     | 260    | 619    |
| > -0.2 | 28                            | 8         | 206                     | 6        | 0                     | 239    | 474    |
| > -0.1 | 27                            | 7         | 174                     | 6        | 0                     | 200    | 352    |
| > 0    | 26                            | 6         | 153                     | 6        | 0                     | 162    | 228    |
| > 0.1  | 25                            | 4         | 143                     | 6        | 0                     | 131    | 136    |
| > 0.2  | 23                            | 4         | 124                     | 5        | 0                     | 103    | 95     |
| > 0.3  | 23                            | 4         | 113                     | 5        | 0                     | 80     | 84     |
| > 0.4  | 16                            | 3         | 70                      | 5        | 0                     | 69     | 65     |
| > 0.5  | 16                            | 3         | 60                      | 4        | 0                     | 51     | 52     |
| > 0.6  | 14                            | 3         | 45                      | 3        | 0                     | 37     | 38     |
| > 0.7  | 11                            | 3         | 43                      | 3        | 0                     | 21     | 28     |
| > 0.8  | 10                            | 3         | 33                      | 3        | 0                     | 14     | 17     |
| > 0.85 | 10                            | 1         | 33                      | 3        | 0                     | 14     | 13     |
| > 0.9 |  10 |  0 |  33 |  2 |  0 |  7 |  11 |