**Table S2.** Pockets predicted using DoGSiteScore for each SARS-CoV-2 Mpro PDB structure, corresponding size of clusters, values for chemical descriptors, and of score values (simple and druggability).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Pocket/Cluster** | **4MDS 1** | | | | | |
| **Size** | **volume** | **surface** | **hydrophobicity** | **simpleScore** | **drugScore** |
| **P\_1** | **13051** | **835,26** | **807,04** | **0,66** | **0,506** | **0,327** |
| P\_2 | 9517 | 609,09 | 707,20 | 0,69 | 0,462 | 0,233 |
| P\_3 | 4052 | 259,33 | 237,76 | 0,66 | 0,112 | 0,173 |
| P\_4 | 2818 | 180,35 | 157,44 | 0,81 | 0,446 | 0,217 |
| P\_5 | 2252 | 144,13 | 162,56 | 0,63 | 0,000 | 0,723 |
| P\_6 | 2179 | 139,46 | 183,04 | 0,65 | 0,006 | 0,220 |
|  | **5R83 2** | | | | | |
|  | **Size** | **volume** | **surface** | **hydrophobicity** | **simpleScore** | **drugScore** |
| P\_1 | 14005 | 896,32 | 994,24 | 0,71 | 0,671 | 0,524 |
| **P\_2** | **10134** | **648,58** | **568,32** | **0,67** | **0,438** | **0,431** |
| P\_3 | 4273 | 273,47 | 252,64 | 0,64 | 0,086 | 0,242 |
| P\_4 | 2827 | 180,93 | 114,88 | 0,52 | 0,000 | 0,056 |
| P\_5 | 2446 | 156,54 | 143,84 | 0,71 | 0,144 | 0,106 |
| P\_6 | 2342 | 149,89 | 164,00 | 0,69 | 0,098 | 0,430 |
|  | **6W63 3** | | | | | |
|  | **Size** | **volume** | **surface** | **hydrophobicity** | **simpleScore** | **drugScore** |
| P\_1 | 9397 | 601,41 | 695,68 | 0,70 | 0,481 | 0,271 |
| **P\_2** | **7083** | **453,31** | **394,08** | **0,68** | **0,340** | **0,563** |
| P\_3 | 4177 | 267,33 | 386,40 | 0,74 | 0,367 | 0,098 |
| P\_4 | 4152 | 265,73 | 233,44 | 0,63 | 0,050 | 0,260 |
| P\_5 | 2699 | 172,74 | 151,68 | 0,73 | 0,207 | 0,031 |
| **P\_6** | **2670** | **170,88** | **157,76** | **0,61** | **0,000** | **0,044** |

1 For PDB ID 4MDS the P\_1 was predicted as the active site, i.e. where the crystallographic ligand was originally bound into (see Fig. S1); 2 For PDB ID 5R83 the P\_2 was predicted as the active site. Note that P\_1 was predicted with higher scores due to inclusion/merge of additional subpockets, forming an improbably large pocket (see Fig. S2); 3 For PDB ID 6W63 the active site was split in two pockets i.e. pockets P\_2 and P\_6. Note that P\_1 was also predicted with higher scores due to inclusion/merge of additional subpockets, forming an improbably large pocket (see Fig. S3).