**Supplementary File 1**

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|  | Drug | Docking score | Clash score |
| 1 | Verapmil | 6.91 | 65 |
| 2 | Dopexamine | 6.76 | 68 |
| 3 | Lidoflazine | 6.52 | 70 |
| 4 | Doripenem | 6.42 | 58 |
| 5 | Bosentan | 5.80 | 102 |
| 6 | Montelukast | 5.61 | 138 |
| 7 | Saquinavir | 5.59 | 195 |
| 8 | Formoterol | 5.13 | 62 |
| 9 | Cloxacillin | 5.01 | 114 |
| 10 | Nicardipin | 4.98 | 89 |
| 11 | Perindoprin | 4.89 | 102 |
| 12 | Mupirocine | 4.67 | 118 |