**Supplementary Table 1. 3D drug molecules from Protein Data Bank with their respective ID**

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| **Drug** | **PDB ID** |
| Chlorpromazine | 5NUJ |
| Fluvoxamine | 4MMA |
| Sertraline  | 3GWU |
| Amiloride  | 4NTX |
| Vinblastine | 5BMV |
| Iitraconazole  | 6UOX |
| Imipramine  | 2Q72 |
| Metronidazole  | 1W3R |
| Ivermectin  | 5VDI |
| Doxycycline  | 5OM3 |
| Minocycline  | 4A99 |
| Quinoline  | 5L6K |
| Quinine  | 4UIL |
| Chloroquine  | 1CET |
| Amodiaquine  | 4FGZ |
| Primaquine  | 4FGJ |
| Dexamethasone  | 3GN8 |
| Nicotine  | 2YK1 |
| Nitaoxanide  | 3V35 |
| Calcifediol  | 5IEN |
| Cholecalciferol  | 5IEP |
| Calcitriol  | 2ZBZ |
| Thymoquinone  | 4HCO |
| Quercetin  | 1H1I |
| Chlorpromazine  | 5NUJ |

**Supplementary Table 2.** The binding affinity and the inhibition constant value of 32 compounds

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| **S.No** | **Drug** | **Binding affinity (kcal/mol)** | **Inhibition constant (μM)** |
| 1 | Chlorpromazine | -5.99 | 40.48 |
| 2 | Fluvoxamine | -3.48 | 2.8 |
| 3 | Sertraline | -6.46 | 18.48 |
| 4 | Amiloride | -5.34 | 122.59 |
| 5 | Vinblastine | -6.41 | 19.97 |
| 6 | Itraconazole | -6.48 | 17.82 |
| 7 | Imipramine | -6.23 | 27.21 |
| 8 | Metronidazole | -6.91 | 8.6 |
| 9 | Doxycycline | -8.88 | 312.23 |
| 10 | Quinoline | -5.76 | 59.7 |
| 11 | Quinine | -6.94 | 8.14 |
| 12 | Chloroquine | -4.09 | 1.01 |
| 13 | Amodiaquine | -6.35 | 22.12 |
| 14 | Primaquine | -5.16 | 163.77 |
| 15 | Nicotine | -4.07 | 1.4 |
| 16 | Cholecalciferol | -7.3 | 4.46 |
| 17 | Enoxaparin | 0.37 | --- |
| 18 | 24-25-Dihydroxycholecalciferol | -7.56 | 2.88 |
| 19 | Terfanadine | -6.0 | 39.86 |
| 20 | Penduline | -5.95 | 43.35 |
| 21 | Nystatin | -5.82 | 54.48 |
| 22 | Niclosamide | -6.64 | 13.67 |
| 23 | Neomycin | -1.44 | 87.28 |
| 24 | Flubendazole | -6.78 | 10.78 |
| 25 | Fenbendazone | -6.38 | 21.21 |
| 26 | Cepharanthine | -8.68 | 436.66 |
| 27 | Hydroxychloroquine | -4.03 | 1.11 |
| 28 | Aspirin | -6.69 | 12.43 |
| 29 | Promethazine | -5.63 | 75.08 |
| 30 | Nystatin | -5.82 | 54.48 |
| 31 | Methylene blue | -5.64 | 73.26 |
| 32 | Andrographolide | -7.13 | 5.94 |

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