

Supplementary Materials

Supplementary Figures

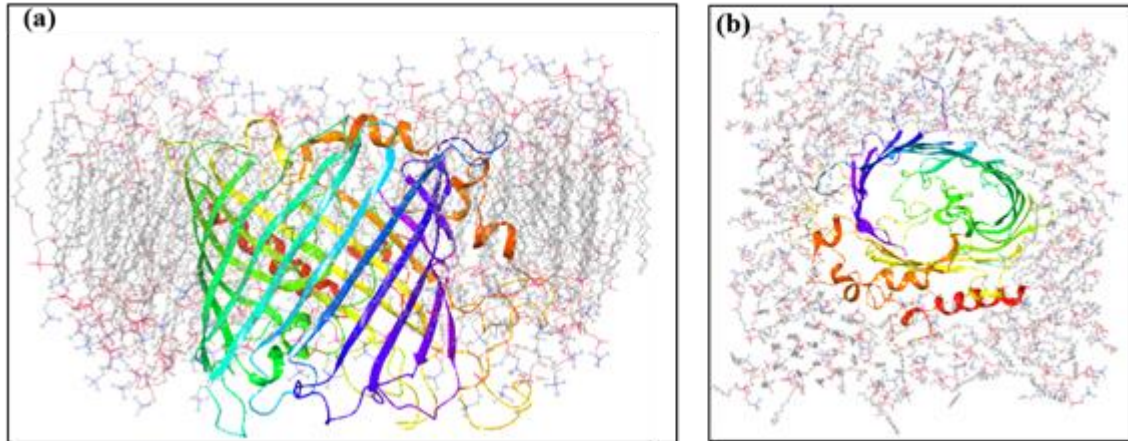


Fig S1. (a) Snapshot of membrane system of Porin embedded in bilayer lipid of DMPC, and the structure over view and it is seen in cylindrical shape; (b) view of Porin from extracellular side of pore channel.

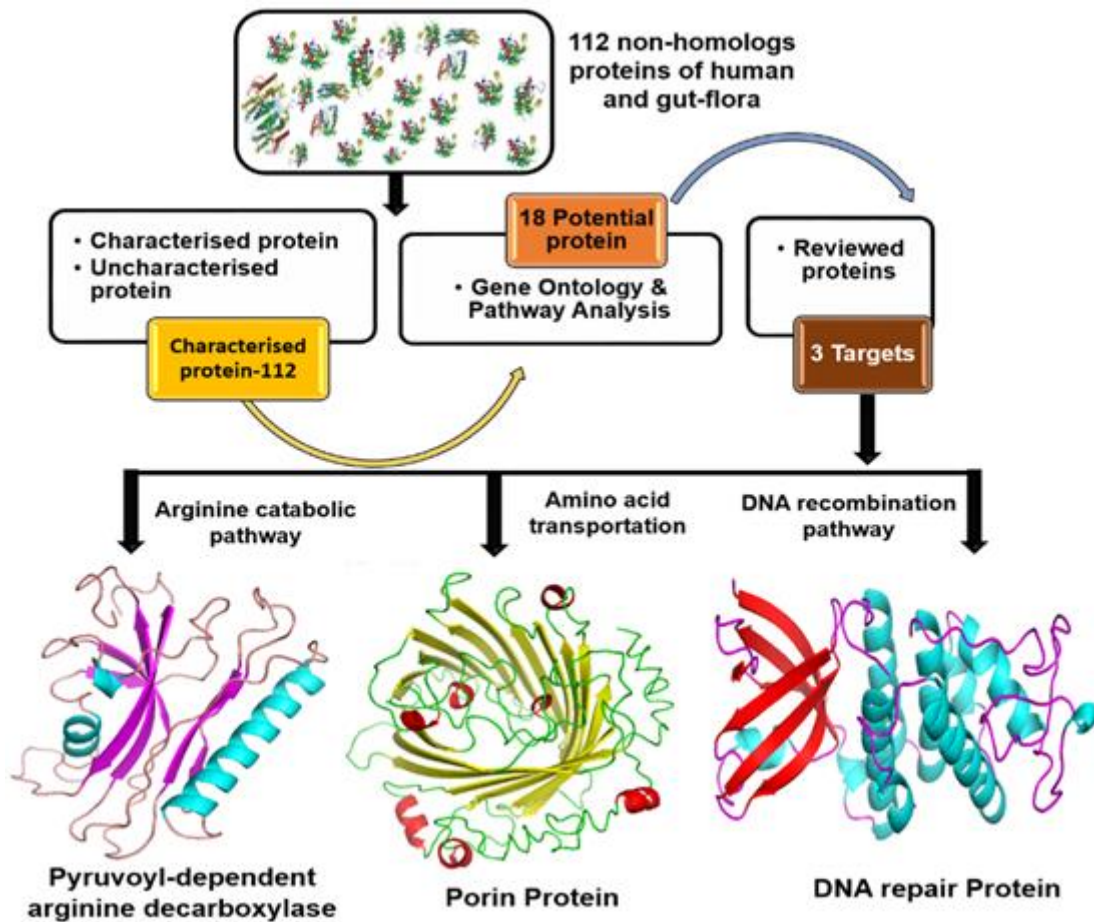


Fig S2. Identification of three potential targets through stringent filtration process

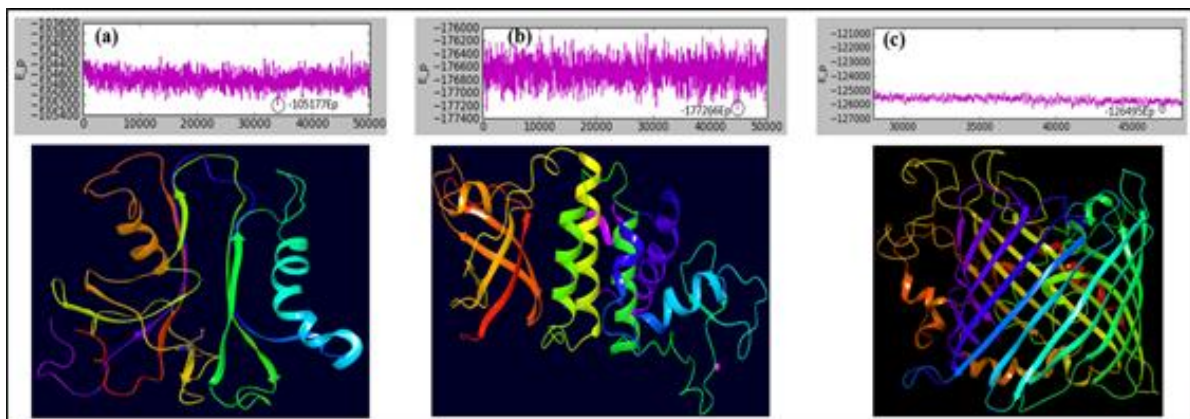


Fig S3: Potential energy trajectory showing lowest potential energy dip; (a) Potential energy plot showing the lowest potential structure of PvlArgDC; (b) Potential energy plot showing the lowest potential structure of RecO; (c) Potential energy plot showing the lowest potential structure Porin

Supplementary Tables

Table S1. Physicochemical descriptors for ADME based on QikProp for top hits from virtual screening of NCI and Maybridge data sets

| Potential targets | Ligand | MolWt | Volume | SASA | Dipole | HB donor | HB Acceptor | Qlog BB | PSA | Metab | Human Oral absorption | Rule of Five | Rule of three |
|-------------------|--------------|---------|----------|---------|--------|----------|-------------|---------|---------|-------|-----------------------|--------------|---------------|
| PvlArgDC | NSC_13086 | 263.422 | 1024.242 | 568.408 | 1.577 | 1 | 2.75 | 0.514 | 19.948 | 4 | 3 | 0 | 0 |
| | NSC_525651 | 272.475 | 679.243 | 423.018 | 1.936 | 2.25 | 5.25 | -0.845 | 119.765 | 0 | 3 | 0 | 0 |
| RecO | MFCD00276409 | 462.52 | 1466.83 | 850.713 | 11.872 | 2.25 | 7.75 | -3.595 | 185.528 | 4 | 1 | 0 | 2 |
| | NSC_159881 | 407.314 | 1201.324 | 699.781 | 4.121 | 2 | 5.2 | -0.86 | 73.582 | 3 | 1 | 0 | 1 |
| Porin | MFCD05662003 | 354.459 | 1008.804 | 586.767 | 11.225 | 4 | 7 | -2.037 | 128.706 | 7 | 2 | 0 | 2 |
| | MFCD01567048 | 437.931 | 1150.277 | 615.13 | 5.005 | 0 | 5.25 | 0.139 | 47.453 | 4 | 3 | 0 | 0 |