**PROJECT DATA**

| **DISEASE CONDITION** | **CYSTIC FIBROSIS** | **SICKLE CELL ANEMIA** |
| --- | --- | --- |
| **DISEASE IDENTIFIER** | **ORPHA:586 / OMIM: 219700** | **ORPHA:232 / OMIM: 603903** |
| **GENE ASSOCIATIONS** | **delF508 gene→ CFTR** | **HBB gene -> SS** |
| **EXISTING DRUGS** | **Ivacaftor** | **Voxelotor** |
| **SMILES STRING OF EXISTING DRUGS** | **Ivacaftor** | **Voxelotor** |
| **MOLECULAR FINGERPRINTS** | **Using Google CoLab** | **Using Google CoLab** |
| **MOLECULAR GRAPHS** | **Using Google CoLab** | **Using Google CoLab** |
| **FASTA SEQUENCES** | **Using Google CoLab** | **Using Google CoLab** |
| **SEQUENCE EMBEDDINGS** | **Using Google CoLab** | **Using Google CoLab** |
| **POCKET FEATURES** | **Using Google CoLab** | **Using Google CoLab** |
| **REFERENCES** | **Zoete, V., Daina, A., Bovigny, C., & Michielin, O. SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening., J. Chem. Inf. Model., 2016, 56(8), 1399-1404.** | **Zoete, V., Daina, A., Bovigny, C., & Michielin, O. SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening., J. Chem. Inf. Model., 2016, 56(8), 1399-1404.** |
| **ML FILE INPUT** | **JSON, CSV** | **JSON, CSV** |
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