**Table 1: Amino acids codes used by Uniprot for FASTA Sequence of Protein CDK5R1 indicating the part-by-part building of 3D structure.**

|  |
| --- |
| Ab initio Modeling |
| MGTVLSLSPSYRKATLFEDGAATVGHYTAVQNSKNAKDKNLKRHSIISVLPWKRIVAVSAKKKNSKKVQPNSSYQNNITHLNNENLKKSLSCANLSTFAQPPPAQPPAPPASQLSGSQTGGSSSVKKAPHPAVTSAGTPKRVIVQA |
| Homology Modeling |
| STSELLRCLGEFLCRRCYRLKHLSPTDPVLWLRSVDRSLLLQGWQDQGFITPANVVFLYMLCRDVISSEVGSDHELQAVLLTCLYLSYSYMGNEISYPLKPFLVESCKEAFWDRCLSVINLMSSKMLQINADPHYFTQVFSDLKNES |
| Ab initio Modeling |
| GQEDKKRLLLGLDR |

**Table 2: Structure metrics information of CDK5R1 generated by homology modeling in SWISS MODEL**

|  |  |
| --- | --- |
| **Sequence Identity** | **100** |
| **Method** | **X Ray** |
| **Sequence Similarity** | **0.61** |
| **Coverage** | **0.60** |
| **Range** | **Amino acid 147-293** |

**Table 3: Model information generated by ab initio method from I-TASSER.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Model no.** | **Favored Region (F)** | **Allowed Region (A)** | **Outlier** | **F+A (%)** |
| Model1 | 52.1 | 28.5 | 19.4 | 80.6 |
| Model2 | 58.3 | 27.8 | 13.9 | 86.1 |
| Model3 | 37.5 | 31.9 | 30.6 | 69.4 |
| Model4 | 72.2 | 18.8 | 9 | 91 |
| Model5 | 56.9 | 24.3 | 18.8 | 81.2 |

**Table 4: Selected Pockets generated by CASTp along with three dimensional coordinates**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Sl. No. | Pocket ID | MS Volume | Openings | X | Y | Z |
| 1 | 19 | 23.5 | 1 | 85.661 | 103.504 | 75.785 |
| 2 | 11 | 23.8 | 1 | 107.556 | 72.157 | 72.960 |
| 3 | 12 | 27.6 | 1 | 82.279 | 34.399 | 84.043 |
| 4 | 10 | 35.2 | 1 | 71.184 | 101.835 | 77.681 |
| 5 | 9 | 44.0 | 1 | 113.004 | 41.495 | 54.763 |
| 6 | 6 | 55.1 | 1 | 82.835 | 44.349 | 93.795 |
| 7 | 5 | 86.8 | 1 | 101.551 | 60.283 | 54.743 |
| 8 | 8 | 102.2 | 1 | 78.885 | 92.611 | 74.852 |
| 9 | 7 | 118.2 | 1 | 112.637 | 53.718 | 64.741 |

**Table 5: Draggability information of the selected molecules by RPBS Mobyle web server**

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Ligand | MW | logP | tPSA | Flexibility | Lipinski Violation | Solubility  (mg/l) | Solubility Forecast Index | Oral Bioavailability |
| 2 | 447.59 | 3.34 | 70.23 | 0.22 | 0 | 5562.36 | Good | Good |
| 4 | 309.33 | 4.05 | 25.84 | 0.37 | 0 | 5286.07 | Good | Good |
| 10 | 451.56 | 3.09 | 80.07 | 0.24 | 0 | 6819.5 | Good | Good |
| 11 | 375.47 | 1.21 | 91.07 | 0.23 | 0 | 27514.02 | Good | Good |
| 47 | 416.51 | 0.91 | 98.77 | 0.34 | 0 | 37510.97 | Good | Good |
| 52 | 251.33 | 3.06 | 56.32 | 0.16 | 0 | 8088.12 | Good | Good |
| 53 | 408.54 | 3.76 | 64.61 | 0.35 | 0 | 5269.59 | Good | Good |
| 54 | 337.37 | 2.69 | 77.24 | 0.25 | 0 | 10022.87 | Reduced Solubility | Good |

**Table 6: Binding affinity of the selected Lead Compounds**

|  |  |
| --- | --- |
| Compound | Binding affinity (Kcal/mol) |
| Compound 2 | -83.07 |
| Compound 4 | -83.89 |
| Compound 10 | -85.35 |
| Compound 11 | -95.84 |
| Compound 47 | -96.72 |
| Compound 52 | -88.80 |
| Compound 53 | -87.48 |
| Compound 54 | -91.65 |