|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | CID | Antineoplastic | Anti-Diabetic | Antiviral |
| Pa | Pi | Pa | Pi | Pa | Pi |
| 1 | 5481882 | 0,835 | 0,008 | 0,547 | 0,017 | 0,290 | 0,040 |
| 2 | 21310440 | 0,835 | 0,008 | 0,547 | 0,017 | 0,290 | 0,040 |
| 3 | 14749097 | 0,835 | 0,008 | 0,547 | 0,017 | 0,290 | 0,040 |
| 4 | 44258911 | 0,835 | 0,008 | 0,547 | 0,017 | 0,290 | 0,040 |
| 5 | 5316673 | 0,855 | 0,006 | 0,543 | 0,018 | 0,251 | 0,059 |
| 6 | 15558501 | 0,855 | 0,006 | 0,543 | 0,018 | 0,251 | 0,059 |
| 7 | 22838616 | 0,855 | 0,006 | 0,543 | 0,018 | 0,251 | 0,059 |
| 8 | 5835713 | 0,855 | 0,006 | 0,543 | 0,018 | 0,251 | 0,059 |
| 9 | 14749098 | 0,925 | 0,003 | 0,547 | 0,017 | 0,290 | 0,040 |

**Table 1.** Biological pass prediction spectrum computation of Chlorogenic acid derivatives

Table 2: Data of Lipinski rule, Pharmacokinetics, and Drug likeness

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Ligand No | CID | Molecular weight | Hydrogen bond acceptor | Hydrogen bond donor | Molar Refractivity | **Consensus** **Log Po/w** | Lipinski rule |
| Result | violation |
| L01 | 5481882 | **418.35 g/mol** | 10 | 6 | 102.17 | 0.35 | yes | 1 violation |
| L02 | 21310440 | **418.35 g/mol** | 10 | 6 | 102.17 | 0.38 | yes | 1violation |
| L03 | 14749097 | **418.35 g/mol** | 10 | 6 | 102.17 | 0.24 | yes | 1 violation  |
| L04 | 44258911 | **418.35 g/mol** | 10 | 6 | 102.17 | 0.32 | yes | 1 violation |
| L05 | 5316673 | **432.38 g/mol** | 10 | 6 | 106.97 | 0.67 | yes | 1 violation |
| L06 | 15558501 | **432.38 g/mol** | 10 | 6 | 106.97 | 0.57 | yes | 1 violation  |
| L07 | 22838616 | **432.38 g/mol** | 10 | 6 | 106.97 | 0.61 | yes | 1 violation |
| L08 | 5835713 | **432.38 g/mol** | 10 | 6 | 106.97 | 0.60 | yes | 1 violation |
| L09 | 14749098 | **418.35 g/mol** | 10 | 6 | 102.17 | 0.28 | yes | 1 violation |

**Table 3:** Molecular docking score

|  |  |  |
| --- | --- | --- |
| Drug Molecules No | Human CYP3A4 bound to metformin (PDB ID 5G5J) | Human dipeptidyl peptidase-IV (PDB ID: 4A5S) |
|  | Binding Affinity(kcal/mol) | Binding Affinity(kcal/mol) |
| 5481882 | -9.6 | -8.3 |
| 21310440 | -9.7 | -7.8 |
| 14749097 | -9.6 | -9.1 |
| 44258911 | -9.6 | -8.4 |
| 5316673 | -9.7 | -8.5 |
| 15558501 | -9.8 | -8.6 |
| 22838616 | -10.0 | -8.5 |
| 5835713 | -9.3 | -9.1 |
| 14749098 | -9.9 | -8.3 |

**Table 4: Chemical structure with molecular docking score**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| SLNO | Drug Molecules No | Chemical structure | Human CYP3A4 bound to metformin (PDB ID 5G5J) | Human dipeptidyl peptidase-IV (PDB ID: 4A5S) |
| Binding Affinity(kcal/mol) | Binding Affinity(kcal/mol) |
| 1 | 5481882 |  | **-9.6** | **-8.3** |
| 2 | 21310440 |  | **-9.7** | **-7.8** |
| 3 | 14749097 |  | **-9.6** | **-9.1** |
| 4 | 44258911 |  | **-9.6** | **-8.4** |
| 5 | 5316673 |  | **-9.7** | **-8.5** |
| 6 | 15558501 |  | **-9.8** | **-8.6** |
| 7 | 22838616 |  | **-10.0** | **-8.5** |
| 8 | 5835713 |  | **-9.3** | **-9.1** |
| 9 | 14749098 |  | **-9.9** | **-8.3** |
| 10 | Standard (Metformin) |  | **-4.9** | **-5.3** |

Table 5: **Computational ADMET Data Prediction**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | CID | **Absorption** | **Distribution** | **Metabolism** | **Excretion** | **Toxicity** |
| SI No | Water solubilityLog S | Human Intestinal Absorption (%) | VDss (log L/kg) | BBBPermeability | CYP450 1A2Inhibitor | CYP450 2C9Substrate | Total Clearance (ml/min/kg) | Renal OCT2substrate | Max. tolerated dose(Log mg/kg/day) | Skin Sensitization | Hepatotoxicity |
| 01 | 5481882 | **-2.967** | **59.181** | **1.135** | **-1.243** | No | No | **0.431** | No | **0.543** | No | No |
| 02 | 21310440 | **-2.967** | **59.181** | **1.135** | **-1.243** | No | No | **0.431** | NO | **0.543** | No | No |
| 03 | 14749097 | **-2.967** | **59.181** | **1.135** | **-1.243** | No | No | **0.431** | No | **0.543** | No | No |
| 04 | 44258911 | **-2.967** | **59.181** | **1.135** | **-1.243** | No | No | **0.431** | No | **0.543** | No | No |
| 05 | 5316673 | **-2.969** | **60.006** | **1.15** | **-1.265** | No | No | **0.431** | No | **0.544** | No |  No |
| 06 | 15558501 | **-2.892** | **82.505** | **0.011** | **0.142** | Yes | No | **-35.249** | No | **0.438** | No | No |
| 07 | 22838616 | **-2.969** | **60.006** | **1.15** | **-1.265** | No | NO | **0.431** | No | **0.544** | No | No |
| 08 | 5835713 | **-2.892** | **82.505** | **0.011** | **0.142** | Yes | No | **-35.249** | No | **0.438** | No | No |
| 09 | 14749098 | **-2.967** | **59.181** | **1.135** | **-1.243** | No | No | **0.431** | No | **0.543** | No | No |

Table:6 **Quantitative structure-activity relationship (QSAR) and PlogIC50**

|  |
| --- |
| Data of QSAR |
| **Ligand** | **CID** | **Chiv5** | **bcutm1** | **(MRVSA9)**  | **(MRVSA6)**  | **(PEOEVSA5)**  | **GATSv4** | **J** | **Diametert** | **PIC50** |
| 01 | 5481882 | 2.151 | 4.119 | 10.969 | 46.622 | 0.0 | 0.957 | 1.551 | 12.0 | 4.88 |
| 02 | 21310440 | 2.151 | 4.119 | 10.969 | 46.622 | 0.0 | 0.957 | 1.551 | 12.0 | 4.88 |
| 03 | 14749097 | 2.151 | 4.119 | 10.969 | 46.622 | 0.0 | 0.957 | 1.551 | 12.0 | 4.88 |
| 04 | 44258911 | 2.151 | 4.119 | 10.969 | 46.622 | 0.0 | 0.957 | 1.551 | 12.0 | 4.88 |
| 05 | 5316673 | 2.292 | 4.119 | 10.969 | 46.622 | 0.0 | 1.003 | 1.567 | 12.0 | 4.89 |
| 06 | 15558501 | 2.292 | 4.119 | 10.969 | 46.622 | 0.0 | 1.003 | 1.567 | 12.0 | 4.89 |
| 07 | 22838616 | 2.292 | 4.119 | 10.969 | 46.622 | 0.0 | 1.003 | 1.567 | 12.0 | 4.89 |
| 08 | 5835713 | 2.292 | 4.119 | 10.969 | 46.622 | 0.0 | 1.003 | 1.567 | 12.0 | 4.89 |
| 09 | 14749098 | 2.151 | 4.119 | 10.969 | 46.622 | 0.0 | 0.957 | 1.551 | 12.0 | 4.88 |