**ADME Prediction results of best hits**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Compund**  **(Pubchem CID)** | **MDCK Permeability** | **Pgp-inhibitor** | **PPB (plasma protein . binding)** | **BBB Penetration** | **Volume Distribution** | **CYP3A4 Inhibitor** | **CYP1A2 inhibitor** | **CL (clearance)** | **T1/2 (half life)** |
| **103646811** | **0.095** | **0.001** | **38.9%** | **0.76** | **0.69** | **0.05** | **0.01** | **6.97** | **0.62** |
| **75536** | **3-05** | **0.001** | **49.0%** | **0.98** | **0.58** | **0.09** | **0.02** | **4.02** | **0.52** |
| **7370** | **0.001** | **0.001** | **46.4%** | **0.16** | **0.59** | **0.08** | **0.47** | **0.78** | **0.30** |
| **139364956** | **0.006** | **0.001** | **32.4%** | **0.96** | **0.56** | **0.06** | **0.07** | **4.57** | **0.69** |
| **141764153** | **0.002** | **0.001** | **37.2%** | **0.81** | **1.45** | **0.05** | **0.08** | **6.1** | **0.62** |
| **152760603** | **3.2-05** | **0.009** | **19.4%** | **0.90** | **1.44** | **0.05** | **0.06** | **4.62** | **0.52** |
| **156030339** | **0.015** | **0.0** | **55.0%** | **0.90** | **0.63** | **0.08** | **0.02** | **4.39** | **0.61** |
| **156530860** | **0.001** | **0.0** | **45.2%** | **0.16** | **0.60** | **0.01** | **0.12** | **1.0** | **0.36** |
| **17976419** | **3.4-05** | **0.001** | **48.9%** | **0.81** | **0.56** | **0.01** | **0.41** | **2.14** | **0.49** |
| **45080568** | **5-05** | **0.001** | **51.6%** | **0.93** | **0.5** | **0.04** | **0.01** | **6.17** | **0.85** |
| **64514083** | **0.001** | **0.002** | **32.6%** | **0.98** | **0.69** | **0.07** | **0.01** | **5.45** | **0.56** |
| **65050329** | **0.001** | **0.0** | **55.0%** | **0.90** | **0.63** | **0.08** | **0.02** | **4.39** | **0.61** |
| **67028586** | **5-05** | **0.001** | **51.6%** | **0.93** | **0.5** | **0.04** | **0.01** | **6.1** | **0.85** |
| **103646815** | **0.005** | **0.001** | **33.8%** | **0.88** | **0.86** | **0.06** | **0.01** | **5.85** | **0.55** |
| **118156306** | **0.002** | **0.0** | **55.8%** | **0.03** | **0.98** | **0.01** | **0.05** | **7.9** | **0.8** |
| **136574701** | **7-06** | **0.001** | **32.3%** | **0.39** | **1.5** | **0.01** | **0.01** | **3.18** | **0.62** |
| **156787384** | **1.6-05** | **0.002** | **32.5%** | **0.47** | **0.81** | **0.06** | **0.01** | **3.45** | **0.55** |
| **46175386** | **0.002** | **0.0** | **51.4%** | **0.04** | **0.79** | **0.07** | **0.03** | **7.47** | **0.78** |
| **90142128** | **0.001** | **0.0** | **73.9%** | **0.06** | **1.48** | **0.01** | **0.05** | **2.62** | **0.78** |

**Ranges :**

**(** MDCK Permeability : < 2 \* 10-6 cm/s; Pgp inhibitor :0 = non inhibitor and 1 = inhibitor ;

PPB : < 90% ; BBB Penetration : 0 = BBB- and 1 = BBB+ ; Volume Distribution : 0.04-20L/kg;

CYP3A4 inhibitor : 0 = non inhibitor and 1 = inhibitor ; CYP1A2 inhibitor : 0 = non substrate

and 1 = substrate ; Clearance : Low = < 5 ml/min/kg , Moderate = 5-15 ml/min/kg , High = >

20 ml/min/kg ; t ½ : 0 = short half life and 1 = long half life **)**

**Toxicity prediction results of best hits**

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Compund**  **(Pubchem CID)** | **Hepatotoxicity** | | **Carcinogenicity** | | **Immunotxicity** | | **Mutagenicity** | | **Cytotoxicity** |
| **103646811** | **Inactive**  **0.22** | | **Inactive**  **0.48** | | **Inactive**  **0.01** | | **Inactive**  **0.34** | | **Inactive**  **0.36** |
| **75536** | **Inactive**  **0.16** | | **Inactive**  **0.44** | | **Inactive**  **0.01** | | **Inactive**  **0.17** | | **Inactive**  **0.23** |
| **7370** | **Inactive**  **0.16** | | **Inactive**  **0.46** | | **Inactive**  **0.01** | | **Inactive**  **0.17** | | **Inactive**  **0.23** |
| **139364956** | **Inactive**  **0.26** | | **Inactive**  **0.39** | | **Inactive**  **0.01** | | **Inactive**  **0.30** | | **Inactive**  **0.27** |
| **141764153** | **Inactive**  **0.27** | | **Inactive**  **0.41** | | **Inactive**  **0.01** | | **Inactive**  **0.33** | | **Inactive**  **0.34** |
| **152760603** | **Inactive**  **0.27** | | **Inactive**  **0.47** | | **Inactive**  **0.01** | | **Inactive**  **0.31** | | **Inactive**  **0.44** |
| **156030339** | **Inactive**  **0.26** | | **Inactive**  **0.47** | | **Inactive**  **0.01** | | **Inactive**  **0.29** | | **Inactive**  **0.25** |
| **156530860** | **Inactive**  **0.25** | | **Inactive**  **0.37** | | **Inactive**  **0.02** | | **Inactive**  **0.27** | | **Inactive**  **0.22** |
| **17976419** | **Inactive**  **0.25** | | **Inactive**  **0.48** | | **Inactive**  **0.01** | | **Inactive**  **0.30** | | **Inactive**  **0.29** |
| **45080568** | **Inactive**  **0.48** | | **Inactive**  **0.44** | **Inactive**  **0.05** | | **Inactive**  **0.32** | | **Inactive**  **0.39** | |
| **64514083** | **Inactive**  **0.26** | | **Inactive**  **0.48** | **Inactive**  **0.01** | | **Inactive**  **0.29** | | **Inactive**  **0.25** | |
| **65050329** | **Inactive**  **0.26** | | **Inactive**  **0.47** | **Inactive**  **0.01** | | **Inactive**  **0.29** | | **Inactive**  **0.25** | |
| **67028586** | **Inactive**  **0.48** | | **Inactive**  **0.44** | **Inactive**  **0.05** | | **Inactive**  **0.32** | | **Inactive**  **0.39** | |
| **103646815** | **Inactive**  **0.22** | | **Inactive**  **0.48** | **Inactive**  **0.01** | | **Inactive**  **0.34** | | **Inactive**  **0.36** | |
| **90142128** | **Inactive**  **0.24** | | **Inactive**  **0.45** | **Inactive**  **0.001** | | **Inactive**  **0.28** | | **Inactive**  **0.23** | |
| **118156306** | **Inactive**  **0.36** | | **Inactive**  **0.48** | **Inactive**  **0.01** | | **Inactive**  **0.50** | | **Inactive**  **0.29** | |
| **118910321** | **Inactive**  **0.22** | **Inactive**  **0.48** | | **Inactive**  **0.01** | | **Inactive**  **0.35** | | **Inactive**  **0.25** | |

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **46175386** | **Inactive**  **0.42** | **Inactive**  **0.48** | **Inactive**  **0.01** | **Inactive**  **0.43** | **Inactive**  **0.34** |

**(The Values in table denote the probability of the specific toxicity occurring on administration of the compound as a drug. Compounds getting the result inactive with a probability of less than 0.49 as considered as hits)**