

Make Predictions

- Please choose a model and enter a decimal number for each of the 6 chemical descriptors
- Helpful definitions are available for each descriptor. To access them click the question mark icon

Please choose a model to make predictions

Random Forest Classifier

Molecular Weight (MW) ?

12.00 - +

Topological Polar Surface Area (TPSA) ?

10.00 - +

XLogP3-AA (XLogP) ?

3.00 - +

Hydrogen Bond Donor Count (NHD) ?

4.00 - +

Hydrogen Bond Acceptor Count (NHA) ?

6.00 - +

Rotatable Bond Count (NRB) ?

12.00 - +

Predict

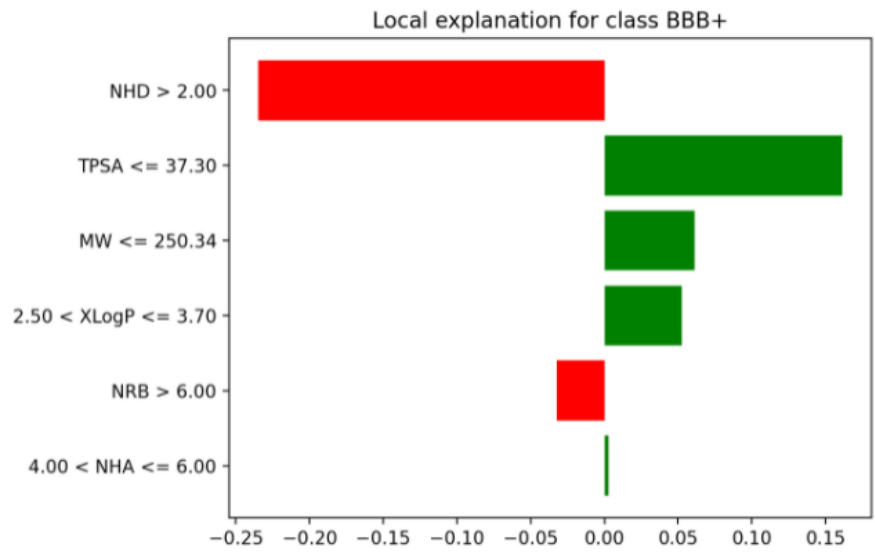
Result

Probability that it cannot enter the brain: **0.32370**

Probability that it can enter the brain: **0.67630**

The model has predicted that the compound/drug with the specific chemical properties you have specified **Can cross the BBB**

Prediction Explanation



Model Weights

	feature	weight	std
0	TPSA	0.3228	0.1082
1	MW	0.1870	0.0393
2	XLogP	0.1503	0.0281
3	NHD	0.1360	0.0911
4	NHA	0.1145	0.0688
5	NRB	0.0894	0.0148