

# SIGMAP: an explainable artificial intelligence tool for SIGMA-1 receptor affinity Prediction

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## SUPPLEMENTARY MATERIAL

**Table S1.** Parameters optimized for each trained model based on the hyperparameter tuning performed on a 5-CV.

**Table S1**

| <b>Algorithm</b> | <b>Optimized parameters</b>     | <b>AtomPair</b> | <b>Morgan</b> | <b>Torsion</b> | <b>MACCS</b> | <b>CSFP</b> |
|------------------|---------------------------------|-----------------|---------------|----------------|--------------|-------------|
| <b>RF</b>        | split criterion                 | gini index      | gini index    | gini index     | gini index   | gini index  |
|                  | attribute sampling              | square root     | square root   | square root    | square root  | square root |
|                  | set of attributes for each tree | different       | different     | different      | different    | different   |
|                  | number of trees                 | 205             | 123           | 235            | 217          | 162         |
|                  | tree depth                      | 10              | 9             | 9              | 9            | 10          |
|                  | equal size sampling             | yes             | yes           | yes            | yes          | yes         |
| <b>KNN</b>       | number of neighbors to consider | 3               | 5             | 3              | 5            | 5           |
|                  | weight neighbors by distance    | yes             | yes           | no             | yes          | yes         |
| <b>GB</b>        | number of trees                 | 463             | 481           | 424            | 378          | 29          |
|                  | learning rate                   | 0.017           | 0.014         | 0.017          | 0.004        | 0.074       |
|                  | attribute sampling              | square root     | square root   | square root    | square root  | square root |
|                  | set of attributes for each tree | different       | different     | different      | different    | different   |
|                  | maximum tree depth              | 8               | 9             | 17             | 23           | 17          |
| <b>XGB</b>       | eta                             | 0.289           | 0.302         | 0.306          | 0.151        | 0.674       |
|                  | boosting rounds                 | 162             | 339           | 203            | 180          | 298         |
|                  | gamma                           | 0.621           | 0.481         | 0.334          | 0.315        | 2.405       |
|                  | lambda                          | 3.912           | 4.019         | 0.604          | 4.556        | 7.31        |
|                  | alpha                           | 0.411           | 0.409         | 9.061          | 0.411        | 1.258       |
|                  | maximum depth                   | 3               | 6             | 6              | 6            | 7           |
| <b>SVM</b>       | kernel                          | RBF             | RBF           | RBF            | RBF          | RBF         |
|                  | nu                              | 0.1             | 0.1           | 0.1            | 0.3          | 0.3         |
|                  | gamma                           | 0.02            | 0.02          | 0.02           | 0.32         | 0.07        |