

Table 1. OATP1B1 models: Description of the used settings

| <b>Model Name</b>   | <b>Descriptors</b>   | <b>weka.classifier</b>  | <b>Cost matrix</b>                                   |
|---------------------|--|---|--|
| <b>B1_6MOE_RF</b>   | 6 MOE descriptors:<br>a_acc, a_don, logP (o/w),<br>mr, TPSA and weight   | trees.RandomForest<br>(numTrees: 10, default)   | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 8.0, 0.0]" |
| <b>B1_6MOE_SMO</b>  | 6 MOE descriptors:<br>a_acc, a_don, logP (o/w),<br>mr, TPSA and weight   | functions.SMO.Puk.kernel<br>(buildLogisticModels:True,<br>the rest settings at default) | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 8.0, 0.0]" |
| <b>B1_6PaD_RF</b>   | 6 PaDEL descriptors:<br>CrippenLogP, CrippenMR,<br>nHBAcc_Lipinski,<br>nHBDOn_Lipinski,<br>TopoPSA, MW   | trees.RandomForest<br>(numTrees: 10, default)   | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 8.0, 0.0]" |
| <b>B1_6PaD_SMO</b>  | 6 PaDEL descriptors:<br>CrippenLogP, CrippenMR,<br>nHBAcc_Lipinski,<br>nHBDOn_Lipinski,<br>TopoPSA, MW   | functions.SMO.Puk.kernel<br>(buildLogisticModels:True,<br>the rest settings at default) | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 8.0, 0.0]" |
| <b>B1_11PaD_RF</b>  | 11 PaDEL descriptors:<br>CrippenLogP, CrippenMR,<br>nHBAcc_Lipinski,<br>nHBDOn_Lipinski,<br>TopoPSA, MW, nRotB,<br>topoRadius,<br>topoDiameter,<br>topoShape,<br>globalTopoChargeIndex | trees.RandomForest<br>(numTrees: 10, default)   | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 8.0, 0.0]" |
| <b>B1_11PaD_SMO</b> | 11 PaDEL descriptors:<br>CrippenLogP, CrippenMR,<br>nHBAcc_Lipinski,<br>nHBDOn_Lipinski,<br>TopoPSA, MW, nRotB,<br>topoRadius,<br>topoDiameter,<br>topoShape,<br>globalTopoChargeIndex | functions.SMO.Puk.kernel<br>(buildLogisticModels:True,<br>the rest settings at default) | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 8.0, 0.0]" |

Table 2. OATP1B3 models: Description of the used settings

| <b>Model Name</b>   | <b>Descriptors</b>   | <b>weka.classifier</b>  | <b>Cost matrix</b>                                    |
|---------------------|--|---|---|
| <b>B3_6MOE_RF</b>   | 6 MOE descriptors:<br>a_acc, a_don, logP (o/w),<br>mr, TPSA and weight   | trees.RandomForest<br>(numTrees: 10, default)   | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 13.0, 0.0]" |
| <b>B3_6MOE_SMO</b>  | 6 MOE descriptors:<br>a_acc, a_don, logP (o/w),<br>mr, TPSA and weight   | functions.SMO.Puk.kernel<br>(buildLogisticModels:True,<br>the rest settings at default) | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 13.0, 0.0]" |
| <b>B3_6PaD_RF</b>   | 6 PaDEL descriptors:<br>CrippenLogP, CrippenMR,<br>nHBAcc_Lipinski,<br>nHBDon_Lipinski,<br>TopoPSA, MW   | trees.RandomForest<br>(numTrees: 10, default)   | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 13.0, 0.0]" |
| <b>B3_6PaD_SMO</b>  | 6 PaDEL descriptors:<br>CrippenLogP, CrippenMR,<br>nHBAcc_Lipinski,<br>nHBDon_Lipinski,<br>TopoPSA, MW   | functions.SMO.Puk.kernel<br>(buildLogisticModels:True,<br>the rest settings at default) | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 13.0, 0.0]" |
| <b>B3_11PaD_RF</b>  | 11 PaDEL descriptors:<br>CrippenLogP, CrippenMR,<br>nHBAcc_Lipinski,<br>nHBDon_Lipinski,<br>TopoPSA, MW, nRotB,<br>topoRadius,<br>topoDiameter,<br>topoShape,<br>globalTopoChargeIndex | trees.RandomForest<br>(numTrees: 10, default)   | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 13.0, 0.0]" |
| <b>B3_11PaD_SMO</b> | 11 PaDEL descriptors:<br>CrippenLogP, CrippenMR,<br>nHBAcc_Lipinski,<br>nHBDon_Lipinski,<br>TopoPSA, MW, nRotB,<br>topoRadius,<br>topoDiameter,<br>topoShape,<br>globalTopoChargeIndex | functions.SMO.Puk.kernel<br>(buildLogisticModels:True,<br>the rest settings at default) | meta.MetaCost -cost-matrix<br>"[0.0, 1.0; 8.0, 0.0]"  |