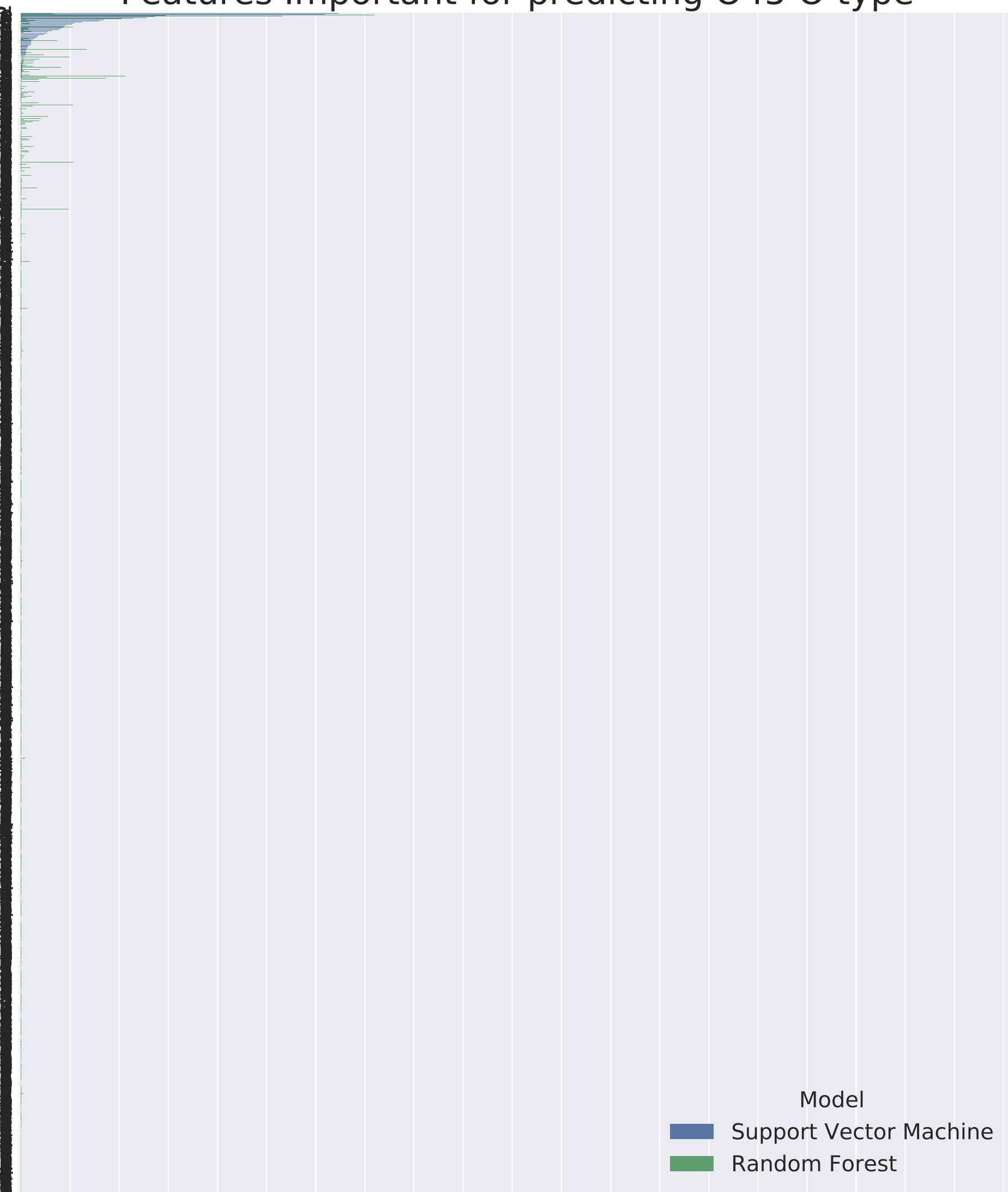


Features Important for predicting O45 O type

Sample Distribution

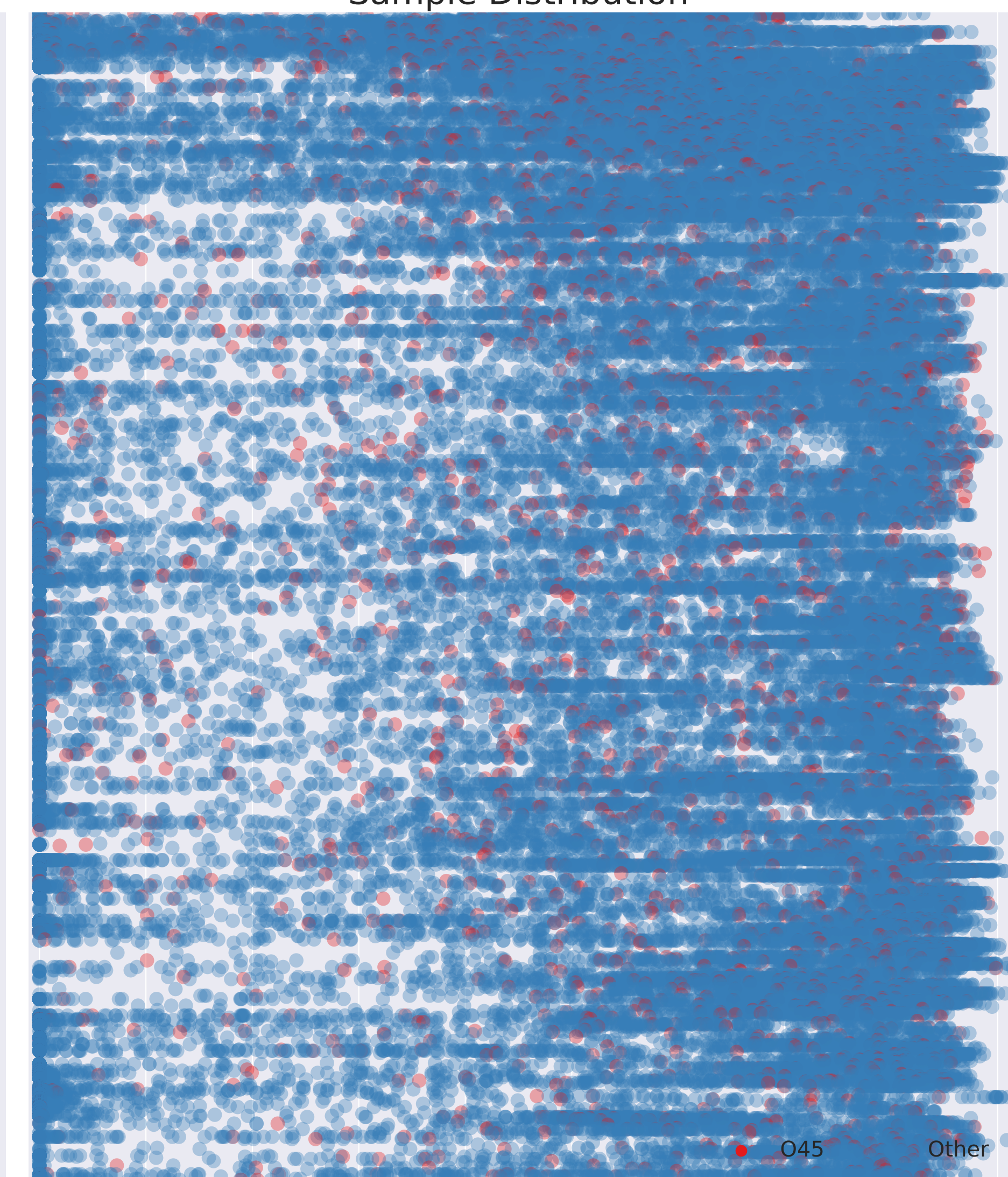
Feature

100mM Sodium Chloride
50mM Sodium Chloride
5-Bromo-4-chloro-3-iodo-2-pyridinecarboxamide
Thymidine
100mM Sodium Chloride
200mM Sodium Chloride
5-Bromo-4-chloro-3-iodo-2-pyridinecarboxamide
5-Bromo-4-chloro-3-iodo-2-pyridinecarboxamide
5-Bromo-4-chloro-3-iodo-2-pyridinecarboxamide
Dimethyl Sulphoxide
2-Amino-6-methyl-4-pyridinecarboxamide
5-Methyl-2-pyridinecarboxamide
5-Bromo-4-chloro-3-iodo-2-pyridinecarboxamide
Uridine-5-phosphate
2,4-Diamino-6,7,5-Dioxypyrimidine
3-Amino-2-pyridinecarboxamide
Guanidine
Potassium
N-Acetylglucosamine
D-Glucose
Methylsulfonyl
Adenosine-3-phosphate
Octylmethyl
1-Chloro-2,4-Diamino-6,7,5-Dioxypyrimidine
2-Deoxy-2-pyridinecarboxamide
D-Glucose
Thymidine
Methyltriethylammonium
D,L-Cysteine
D,L-Cysteine
Thalium
20mM Sodium Chloride
D,L-Cysteine
3,4-Dimethyl-2-pyridinecarboxamide
Semicarbazide
Dodecyltrimethylammonium
Hexyltrimethylammonium
p-Glutamic Acid
p-Hydroxybenzoic Acid
4-Hydroxy-1-naphthol
[5]4-Amino-1-naphthol
8-Nicotinamide
5-Bromo-4-chloro-3-iodo-2-pyridinecarboxamide
5-Bromo-4-chloro-3-iodo-2-pyridinecarboxamide
5-Chloro-7-iodo-2-pyridinecarboxamide
1-Chloro-2,4-Diamino-6,7,5-Dioxypyrimidine
4-Hydroxy-1-naphthol
Dodecyltrimethylammonium
5-Bromo-4-chloro-3-iodo-2-pyridinecarboxamide
3-O-β-D-Galactopyranoside
5-Bromo-4-chloro-3-iodo-2-pyridinecarboxamide
Adenosine-3-phosphate
Manganese
5-Bromo-4-chloro-3-iodo-2-pyridinecarboxamide
L-Proline
100mM Sodium Chloride
5-Chloro-7-iodo-2-pyridinecarboxamide
3,4-Dimethyl-2-pyridinecarboxamide
L-Glutamic Acid
Methyltriethylammonium
a-Phenylisopropylamine



0.0 0.05 0.1 0.15 0.2 0.25 0.3 0.35 0.4 0.45 0.5 0.55 0.6 0.65 0.7 0.75 0.8 0.85 0.9 0.95 1.0
Score

Model
Support Vector Machine
Random Forest



0 100 200 300 400 500 600 700 800 900
Omnilog Are Under the Curve
O45
Other