# QSAR model for CYP450 2C9 substrate (v2.0)

ProtoADME by ProtoQSAR

## ProtoADME

ProtoADME is a computational (*in silico*) tool focused on the prediction of endpoints related with the ADME (Absortion, Distribution, Metabolism and Excretion) of chemical substances.

## Endpoint

**Toxicokinetic: CYP450 2C9 substrate.**

The microsomal cytochrome P450 (CYP) family 4 monooxygenases are the major fatty acid omega-hydroxylases. These enzymes remove excess free fatty acids to prevent lipotoxicity, catabolize leukotrienes and prostanoids, and also produce bioactive metabolites from arachidonic acid omega-hydroxylation. In addition to endogenous substrates, recent evidence indicates that CYP4 monooxygenases can also metabolize xenobiotics, including therapeutic drugs. If a compound is a CYP substrate means that the compound will be subjected to metabolic clearance.

## Metrics

### Training set

| Experimental values | QSAR predictions | |
|---|---|---|
| | **Non-substrate** | **Substrate** |
| **Non-substrate** | 288 | 27 |
| **Substrate** | 16 | 305 |

### Validation set

| Experimental values | QSAR predictions | |
|---|---|---|
| | **Non-substrate** | **Substrate** |
| **Non-substrate** | 27 | 8 |
| **Substrate** | 7 | 46 |

| Parameters | Training | Validation |
|---|---|---|
| Accuracy | 0.93 | 0.83 |
| Sensitivity / recall | 0.95 | 0.87 |
| Specificity | 0.91 | 0.77 |
| Precision | 0.92 | 0.85 |
| Negative predictive value | 0.95 | 0.79 |
| F-score | 0.93 | 0.86 |
| Matthews Correlation Coefficient | 0.87 | 0.64 |
| Critical Success Index | 0.88 | 0.75 |
| Area under the ROC | 0.93 | 0.82 |

ProtoADME is part of ProtoPRED

ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, using proprietary (Q)SAR models.

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