

How accurate are the P450 models?

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The accuracies of the models for each isoform when tested on independent test sets are shown below:

Results of the P450 Regioselectivity Models on independent test sets

Isoform	N *	Top-2**	Top-3**
CYP3A4	352	84.5%	90.5%
CYP2D6	221	91.1%	92.9%
CYP2C9	222	85.7%	93.9%
CYP1A2	238	87.7%	89.5%
CYP2C8	114	81.5%	92.6%
CYP2C19	213	85.7%	89.8%
CYP2E1	134	90%	93.3%

* N = number of compounds in independent test set.

** Observed metabolites in the top 2/3 predicted sites