

Table 4S. Performance of prediction models using features from Table 3S. The accuracy in terms of MCC is based on 5-fold cross-validation of a linear model (LDA). Highlighted with bold face is the final feature space selected for MutaCYP.

Filter	Number of features in the model	MCC±SD
None	46	0.40±0.09
F-score \geq 0.1	37	0.48±0.09
F-score \geq 0.2	31	0.48±0.03
F-score \geq 0.3	22	0.47±0.10
F-score \geq 0.4	18	0.50±0.09
F-score \geq 0.5	11	0.46±0.06
F-score \geq 0.6	6	0.40±0.15
F-score \geq 0.4 and $r <$ 0.9	9	0.51±0.10
F-score \geq 0.4 and $r <$ 0.8	5	0.54±0.04
F-score \geq 0.4 and $r <$ 0.7	3	0.48±0.16