

T/P	Side Effects (SE)		Indications (I)		SE + I	
	Training	Validation	Training	Validation	Training	Validation
A.	.863±.030	.739±.023	.725±.033	.661±.016	.905±.026	.760±.021
AUC	.841±.038	.709±.031	.640±.095	.585±.077	.894±.031	.739±.029
F <sub>1</sub> <sup>&amp;</sup>	.861±.031	.737±.024	.675±.063	.606±.046	.905±.026	.760±.021
F <sub>1(+)</sub> <sup>^</sup>	.895±.026	.802±.020	.800±.044	.754±.053	.926±.022	.814±.018
F <sub>1(-)</sub> <sup>#</sup>	.796±.052	.615±.048	.421±.230	.320±.216	.863±.040	.658±.040

Each data field shows average ± std of 1000 random splits of drugs known permeability

<sup>&</sup>: macro weighted F<sub>1</sub> from total samples;

<sup>^</sup>: positive samples;

<sup>#</sup>: negative samples.