

Model description	Threshold	Number of descriptors	accuracy 10-CV	precision 10-CV	recall 10-CV	accuracy test	precision test	recall test
Only Mordred descriptors	100 nM	1503	0.847	1	1	0.799	0.829	0.907
The combination of Fingerprints: Morgan, Topological, MACCS, and Avalon	100 nM	4775	0.844	1	1	0.872	0.888	0.957
Only Topological fps	100 nM	2058	0.847	1	1	0.866	0.881	0.957
Only MACCS fps	100 nM	177	0.815	1	1	0.779	0.874	0.836
Only Avalon fps	100 nM	522	0.859	1	1	0.819	0.887	0.879
The combination of Mordred descriptors and Morgan Fps	100 nM	3550	0.856	1	1	0.826	0.895	0.879
The combination of Mordred descriptors and Topological Fps	100 nM	3550	0.847	1	1	0.859	0.906	0.914
The combination of Mordred descriptors and MACCS Fps	100 nM	1669	0.854	1	1	0.826	0.875	0.905
The combination of Mordred descriptors and Avalon Fps	100 nM	2014	0.841	1	1	0.839	0.904	0.888
The combination of Mordred descriptors and Morgan Fps	100 nM	3550	0.847	1	1	0.846	0.904	0.897
Only Morgan fps	100 nM	2058	0.864	1	1	0.785	0.929	0.784