

SUPPLEMENTARY DATA

Supplementary Table S1. Comparison of Factors Affecting the binding of N-sulfotransferase inhibitory peptides to other sulfotransferases

Sulfotransferase	PDB code	Number of residues	Total volume (Å³)	Pocket volume (Å³)	Solvent accessibility for catalytic site LYS residues	Relative solvent accessibility for PAPS*	NMQALSMPVT theoretical Ki
NDST	1NS T	282	27373	712	K614: 4.05; K833: 33.83	0.07	0.82 μM
3OST	1T8T	268	52874	697	K162: 3.24; K366: 100.12	0.03	infinite
2OST	3F5F	656	62187	689	K1083: 7.71; K1293: 85.34	0.04	infinite

*Relative solvent accessibility is the ratio of solvent-accessible surface area for the ligand bound to the protein against that for an isolated ligand, calculated by NACCESS.