Supplementary Table. 2: Parameters used in PRISM and their default values

Name	Description	Default value
MAXRADIUS	size of the active site	10 Å
MAXDIST	distance over with PA is allowed between two atoms	5 Å
BALLRADIUS	radius of the ball which is between two atoms to ascertain spatial hindrance.	1 Å
ADJUSTRATIO	ratio in which the potential difference is distributed between the atoms involved in PA	3/4