Analysis of surface binding sites (SBSs) in carbohydrate active enzymes with focus on glycoside hydrolase families 13 and 77: — a mini-review

Surface binding sites (SBSs) interact with carbohydrates outside of the enzyme active site. They are frequently situated on catalytic domains and are distinct from carbohydrate binding modules (CBMs). SBSs are found in a variety of enzymes and often seen in crystal structures. Notably about half of the > 45 enzymes (in 17 GH and two GT families) with an identified SBS are from GH13 and a few from GH77, both belonging to clan GH-H of carbohydrate active enzymes. The many enzymes of GH13 with SBSs provide an opportunity to analyse their distribution within this very large and diverse family. SBS containing enzymes in GH13 are spread among 15 subfamilies (two were not assigned a subfamily).

Comparison of these SBSs reveals a complex evolutionary history with evidence of conservation of key residues and/or structural location between some SBSs, while others are found at entirely distinct structural locations, suggesting convergent evolution. An array of investigations of the two SBSs in barley α-amylase demonstrated they play different functional roles in binding and degradation of polysaccharides. MalQ from Escherichia coli is an α-1,4-glucanotransferase of GH77, a family that is known to have at least one member that contains an SBS. Whereas MalQ is a single domain enzyme lacking CBMs, its plant orthologue DPE2 contains two N-terminal CBM20s. Surface plasmon resonance binding studies showed that MalQ and DPE2 have a similar affinity for β-cyclodextrin and that MalQ binds malto-oligosaccharides of >DP4 at a second site in competition with β-cyclodextrin yielding a stoichiometry >1. This suggests that MalQ may have an SBS, though its structural location remains unknown.

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