The structure of a novel glucuronoyl esterase from *Myceliophthora thermophila* gives new insights into its role as a potential biocatalyst

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Supplementary Material

Table S1. Secondary structure assignment by *PROMOTIF* (Hutchinson & Thornton, 1996)

Promotif	*St*GE2	S213A mutant	S213A complex	Cip2_GE
Beta-sheet	1	1	1	1
Alpha/beta units	4	4	4	4
Beta hairpins	2	2	2	2
Psi loop	1	1	1	1
Beta buldges	2	2	2	3
Strands	10	10	10	10
Helices	18	18	19	18
Helix-helix interactions	17	17	17	21
Beta turn	31	30	27	22
Gamma-turns	5	5	7	4
Disulphides	3	3	3	3

Table S2*a*. Hydrogen bond interactions of the catalytic Ser213 in *St*GE2 structure

Ser213 / atom	Atom	Distance (Å)	Angle (°)
N	Gln235 O	3.0	167.4
O	Gly216 N	2.9	127.7
	Lys217 N	3.1	160.0
OG	His346 NE2	2.7	173.7
	Arg214 N	3.2	120.1
	Wat567 O	2.7	-
	...Arg214 NH2	3.1	166.3
	...Arg214 N	3.1	160.5
	...Wat577 O	2.8	-

Table S2*b*. Hydrogen bond interactions of the catalytic Glu236 in *St*GE2 structure

Glu236 / atom	Atom		Distance (Å)	Angle (°)
OE1	His346 ND1		2.8	146.8
	Asn306 ND2		3.0	156.6
OE2	Cys347 N		2.8	147.4
	Wat560 O		2.8	-
O	Gln235 O		3.3	105.0
	Wat568 O		3.0	-
	...Lys217 NZ		3.1	-
	...Ser237 O		3.0	100.9
	…Wat578 O		3.0	-
		...Lys217 NZ	2.8	-
		...Gln259 OE1	2.8	141.6
		...Wat740 O		-
N	Phe304 O		2.8	161.4

Table S2*c*. Hydrogen bond interactions of the catalytic His346 in *St*GE2 structure

His346 / atom	Atom	Distance (Å)	Angle (^{o})
ND1	Glu236 OE1	2.8	123.8
NE2	Ser213 OG	2.7	96.0
N	Wat700 O	2.8	-
O	Wat867 O	2.8	-
	...Wat775 O	3.0	-
	...Asn345 ND2	3.3	138.5

Table S3*a*. Hydrogen bond interactions of the mutated catalytic Ser213 to Ala in the mutant structure

Ala213 / atom	Atom	Distance (Å)	Angle (^{o})
N	Gln235 O	3.0	169.7
O	Gly216 N	2.9	120.1
	Lys217 N	3.0	156.2

Table S3*b*. Hydrogen bond interactions of the catalytic Glu236 in the mutant structure

Glu236 / atom	Atom		Distance (Å)	Angle (°)
OE1	His346 ND1		2.6	157.9
	Asn306 ND2		3.3	145.7
OE2	Cys347 N		2.8	154.3
	Wat539 O		2.8	-
	…Gln235 NE2		2.9	173.1
	…Wat514 O		2.9	-
		…Glu305	2.9	112.0
		…Gln353	2.7	122.9
		…Wat539	2.9	-
N	Phe304 O		2.7	165.8
O	Gln235 O		3.3	103.9
	Wat906 O		3.0	147.1
	...Lys217 NZ		3.1	-
	...Ser237 O		3.0	96.4

Table S3*c*. Hydrogen bond interactions of the catalytic His346 in the mutant structure

His346 / atom	Atom	Distance (Å)	Angle (^{o})
ND1	Glu236 OE1	2.6	129.1
NE2	Wat557	2.9	-
	…Wat511	2.8	-
	...Arg214 N		
	…Arg214 NH2		
	…Wat654		
N	Wat707 O	2.8	-

Table S4*a*. Hydrogen bond interactions of the mutated catalytic Ser213 to Ala in the mutant complex structure

Ala213 / atom	Atom	Distance (Å)	Angle (^{o})
N	Gln235 O	3.0	166.6
O	Lys217 N	3.0	144.0

Table S4*b*. Hydrogen bond interactions of Glu236 in the mutant complex structure

Glu236 / atom	Atom		Distance (Å)	Angle (°)
OE1	His346 ND1		2.6	147.9
	Asn306 ND2		3.3	154.0
OE2	Cys347 N		2.9	152.6
	Asn306 ND2		3.3	143.4
	Wat567 O		2.8	-
	…Gln235 NE2		2.9	156.2
	…Wat596 O		2.9	-
		…Glu305	2.9	119.0
		…Gln353	2.7	124.6
N	Phe304 O		2.7	164.4

Table S4*c*. Hydrogen bond interactions of the catalytic His346 in the mutant complex structure

His346 / atom	Atom	Distance (Å)	Angle (^{o})
ND1	Glu236 OE1	2.6	138.2

Table S5*a*. Hydrogen bonds interactions of EDO408 at the catalytic pocket of the mutant structure

EDO408 Atom	Protein atom	Distance (Å)	Angle (°)
O1	Lys 217A NZ	2.8	-
	Gln 259A OE1	2.6	131.9
O2	Gln 259A NE2	3.3	128.7
	Glu 267A OE2	2.8	110.6
	Trp 310A NE1	2.8	159.6

Table S5*b*. Hydrogen bonds interactions of EDO406 at the vicinity of the catalytic pocket of the mutant structure

EDO408 Atom	Protein atom	Distance (Å)	Angle (°)
O2	Wat 557A O	3.2	-

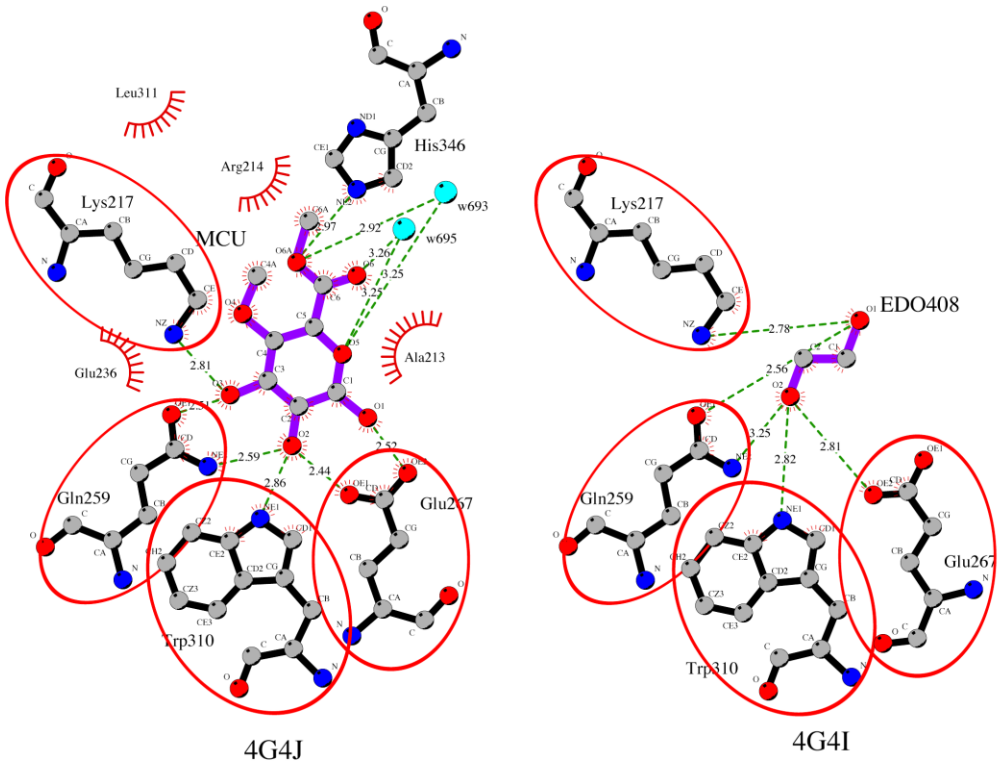

Figure S1

LIGPLOT diagram of the methyl 4-*O*-methyl-*β*-D-glucopyranuronate (MCU, left) and EDO408 (right) interacting with residues lying in the vicinity. The substrate analogue and EDO408 bonds are shown in purple while bonds of the residues lining the site in black. Hydrogen bonds are black dashed lines with indicated distances (in Å). Residues forming Van der Waals interactions with MCU are represented by red semicircles with radiating spokes.