

# Computational analysis of the interactions of OppA from *Yersinia pseudotuberculosis* and its ligands.

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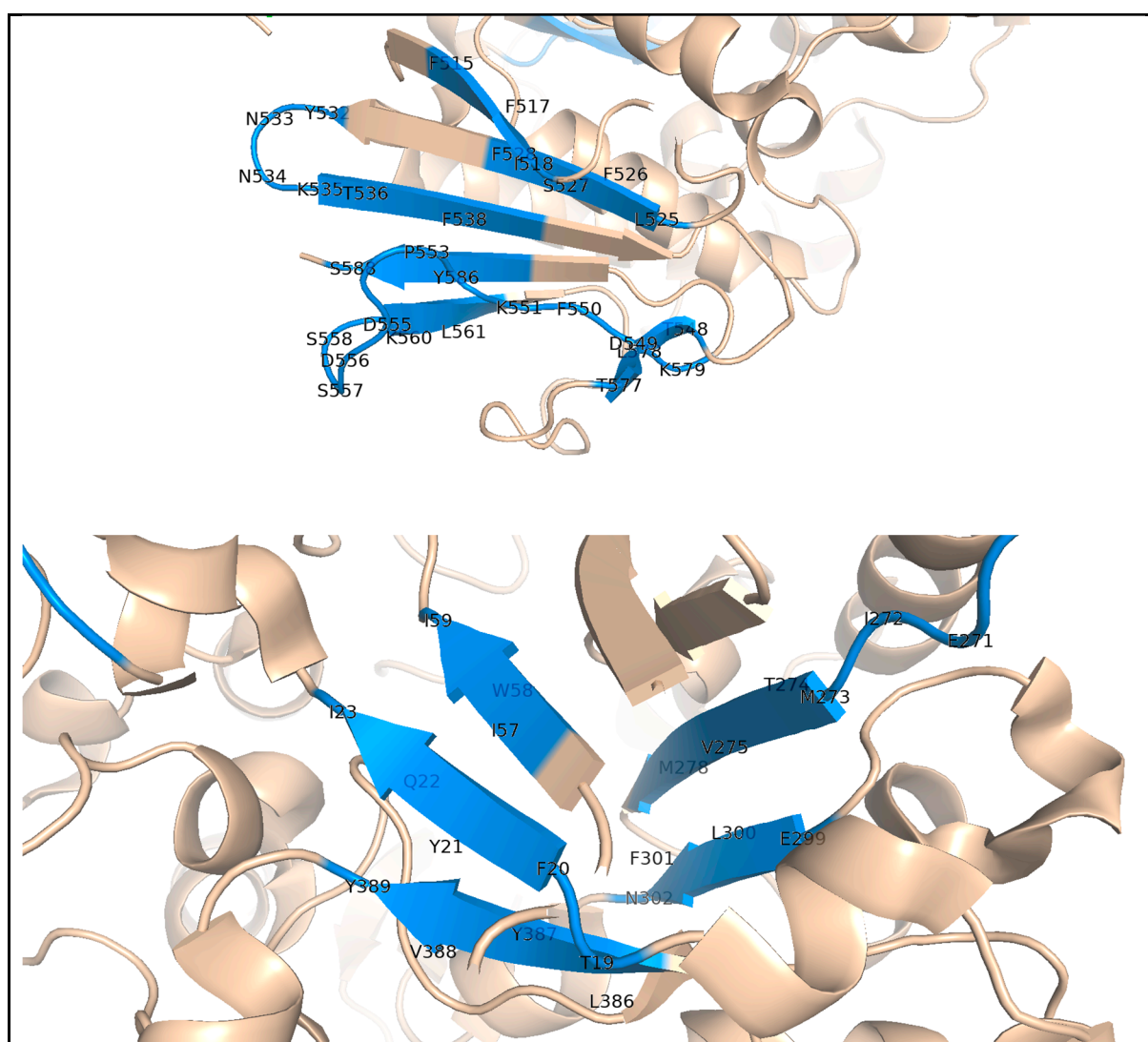
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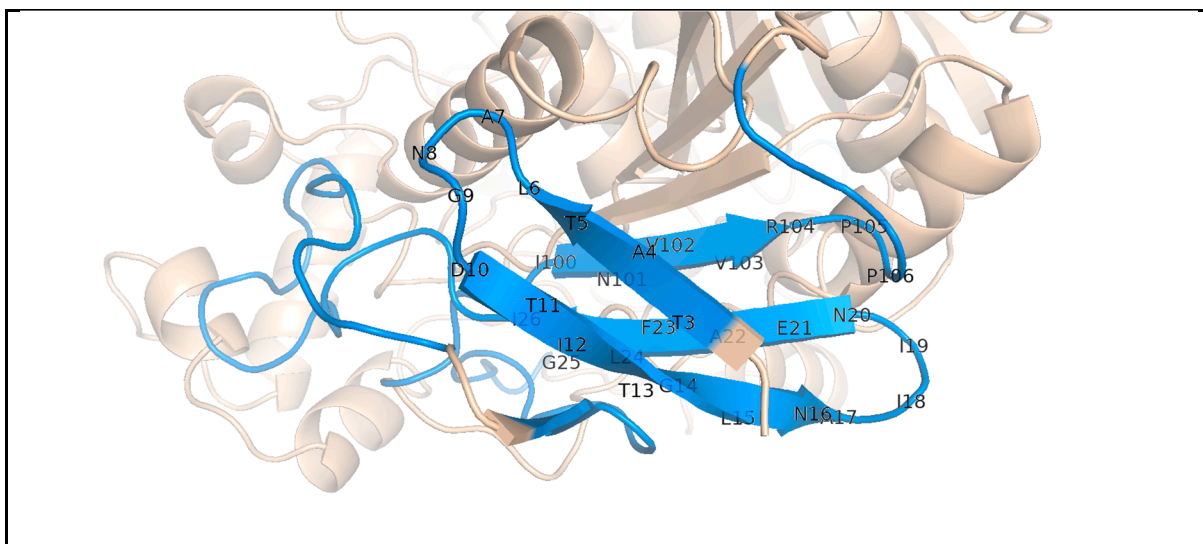
## Supplementary material

Figure S1

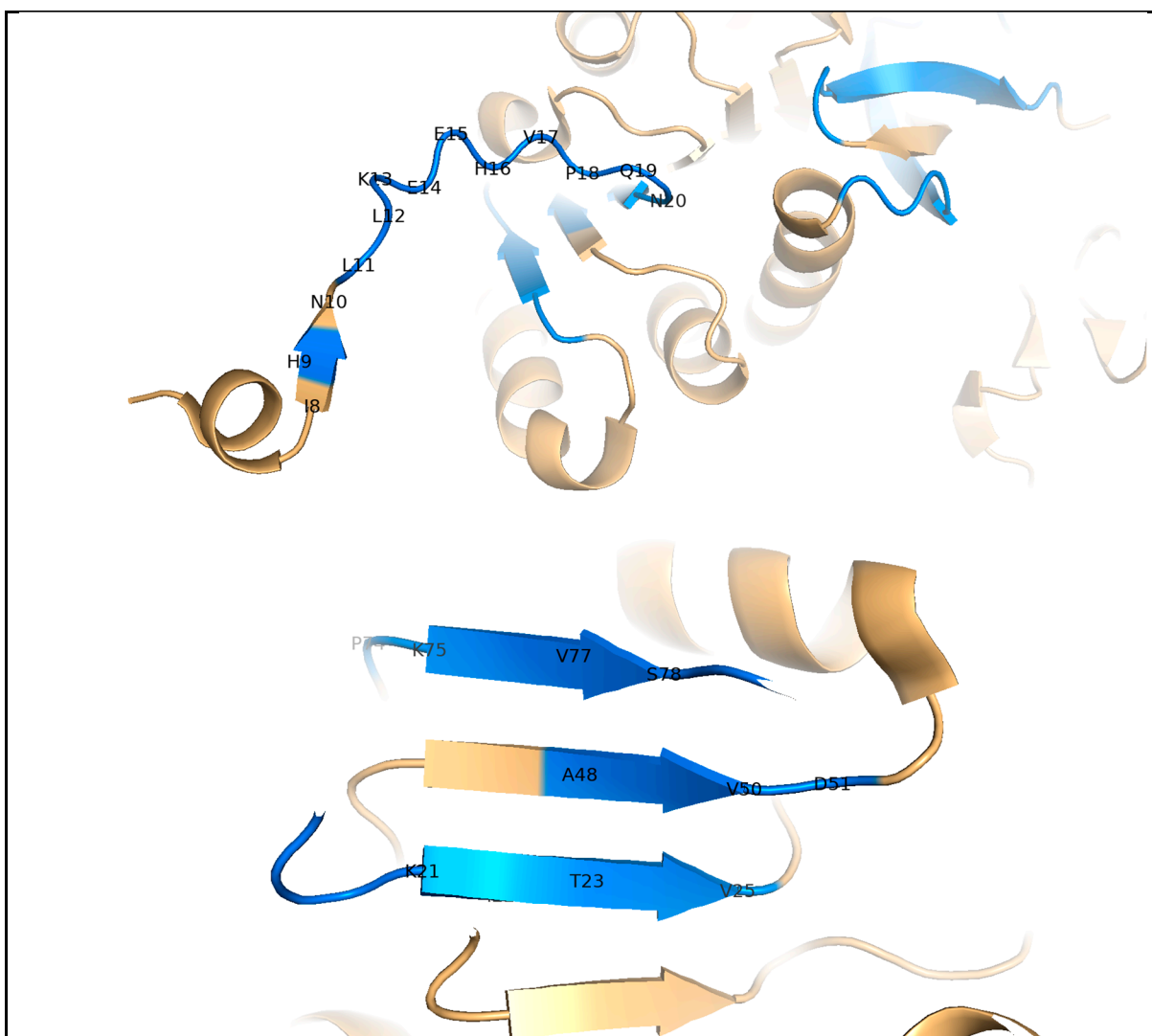
OppA interaction zones with four different enzymes (Mal12, LDH, *EcoRI* and THG)

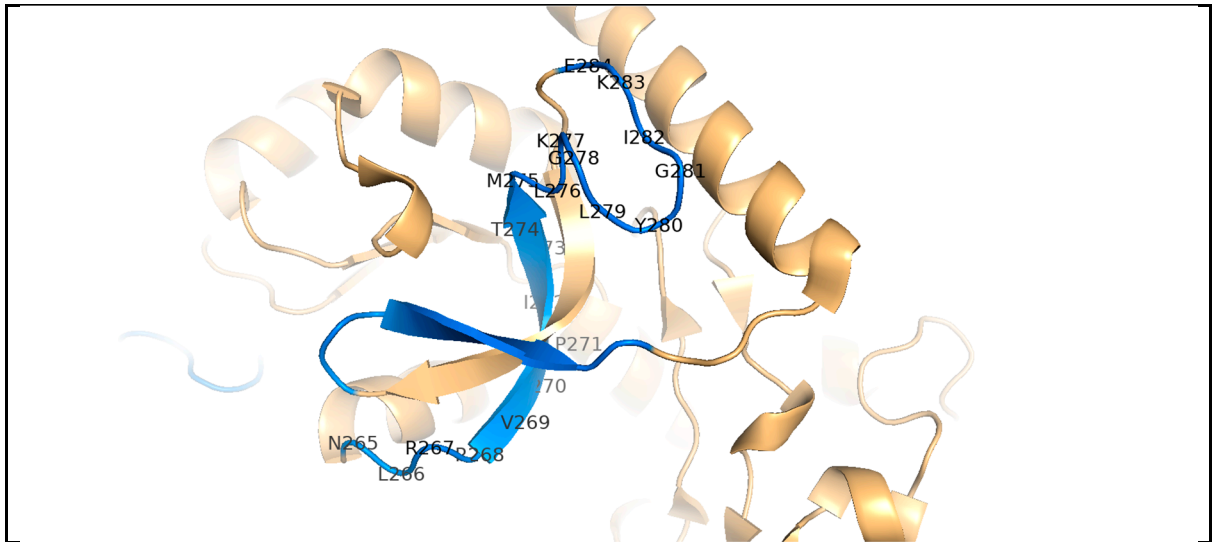
### MAL12 enzyme



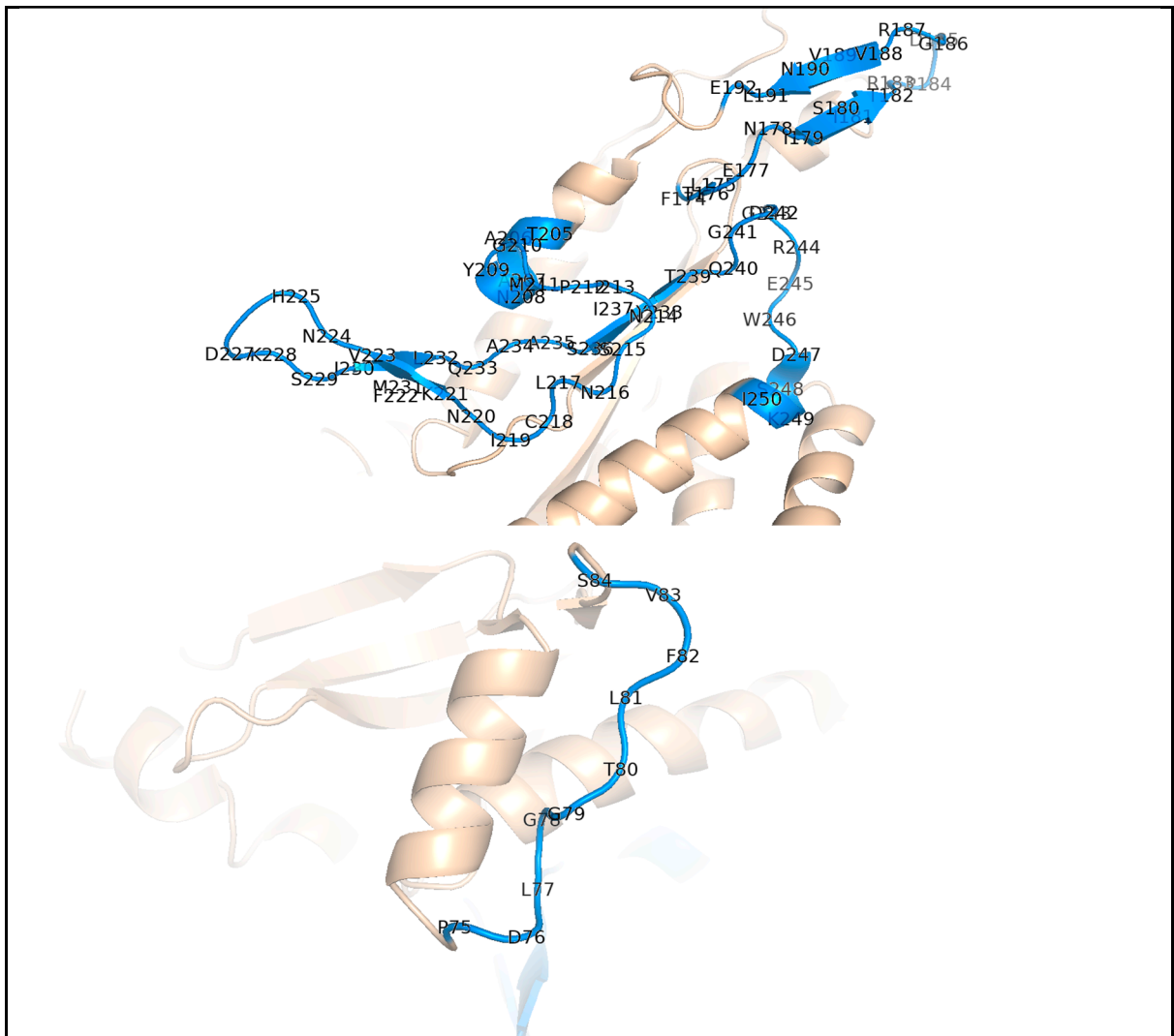


LDH-A enzyme





*EcoRI* enzyme



## THG enzyme

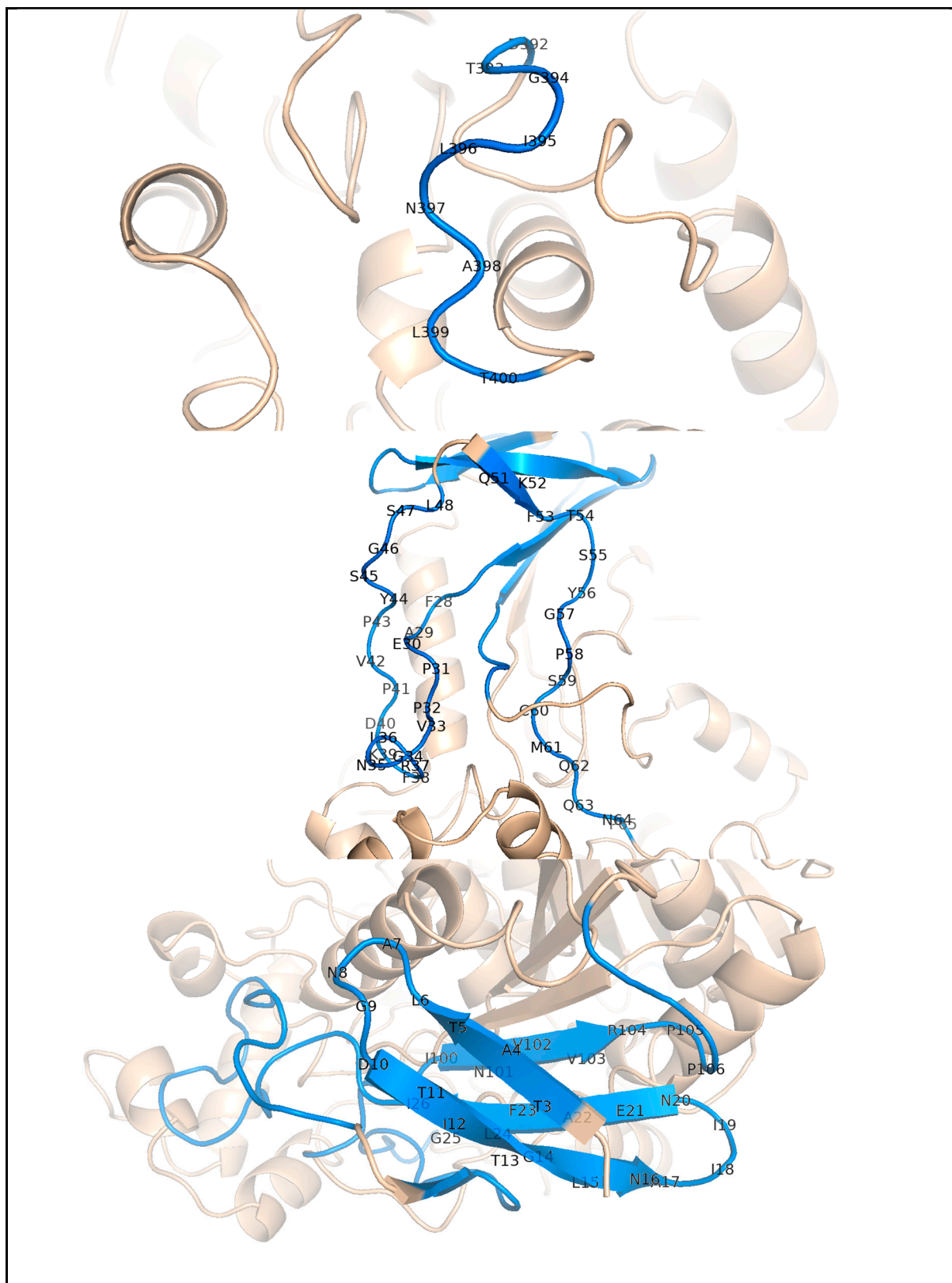


Table S1

## HYDROGEN-BOND NETWORK AA

Enzyme	OppA
Mal12_4.5	
PHE, LYS, LEU, GLU, PHE, GLY	TYR_485, TYR_245, ARG_413, VAL_34, CYS_417, GLN_32, GLY_33, SER_37, ALA_418, TYR_269, ASN_246
MAL12_5.5:	
THR, VAL, GLY, GLU, MET GLN	TYR_109, CYS_417, ALA_415, GLY_20, ASN_366, ARG_413, TYR_245, GLU_32, ASP_419
LDH_1.2	
GLY, SER, ASP, VAL, VAL	ASP_419, TYR_109, CYS_417, ARG_404, ARG_413, HIS_371, SER_37, ALA_418
LDH_4.4	
LYS, ILE, VAL	TYR_109, GLU_32, VAL_34, ALA_415, HIS_371, ARG_413, CYS_417, ALA_418, ASP_419
EcoRI_3.1	
ARG, VAL, LEU, GLY, ARG	TYR_109, CYS_417, ARG_413, HIS_371, GLU_396, GLU_229, THR_367, SER_227, ALA_418, ASP_419
EcoRI_5.1	
ASP, ASP, LEU, THR, PHE	TYR_269, ARG_41, ASN_506, HIS_161, SER_37, CYS_417, GLU_32, VAL_34, ARG_413, TYR_245, ASN_247, HIS_371, ASN_366, ARG_413
THG_2.1	
GLY, LEU, ALA, ASP, PHE	HIS_161, CYS_417, ARG_404, ALA_415, ARG_413, THR_367, ASN_366, SER_21, TYR_245, ASN_246, VAL_34, TYR_269
THG_3.1	
PHE, LYS LEU, GLU, PHE	GLU_32, ARG_404, ASN_366, HIS_371, TYR_245, ALA_415, VAL_34

Table S2

AA THAT HAS OPPA'S HYDROPHOBIC INTERACTIONS WITH Mal12, LDH, *EcoRI* and THG.

Enzime	OppA
Mal12_4.5	
PHE, LYS, LEU, GLU, PHE, GLY	SER_487, HIS_371, ASN_247, ALA_415, ASN_38, PRO_35, LEU_504, ASP_505, ARG_41, ASN_506, HIS_161, ILE_31, TYR_109, TRP_416, LEU_401, TRP_397, ARG_404
MAL12_5.5:	
THR, VAL, GLY, GLU, MET GLN	TRP_416, ASN_436, GLY_33, ARG_404, TRP_397, SER_227, SER_21, GLU_229, THR_367, SER_368, PRO_35, HIS_371, TYR_269, ASN_247, ASN_246, VAL_34, TYR_485, CYS_271
LDH_1.2	
GLY, ILE, SER, ASP, VAL, VAL	PRO_162, LEU_504, HIS_161, TRP_416, GLY_33, GLU_32, ALA_415, SER_368, TYR_485, GLU_229, TRP_397, GLY_20, SER_21, PRO_35, ASN_247, ASN_366, ASN_246, VAL_34, ARG_41, ASN_506, ASP_505, TYR_269
LDH_4.4	
LYS, ILE, THR, VAL, VAL	TRP_416, ASN_506, ARG_404, LEU_401, ASN_247, TYR_485, PRO_335, SER_21, GLU_229, TYR_245, GLY_20, ASN_366, TRP_397, SER_37, HIS_161, GLY_33
<i>EcoRI</i> _3.1	
ARG, VAL, LEU, GLY, ARG	PRO_162, HIS_161, TRP_416, ALA_415, TYR_269, SER_21, PRO_35, GLY_20, ASN_366, SER_368, ASN_246, ASN_247, TYR_245, TRP_397, TYR_485, VAL_34, GLY_33, SER_37, ASN_506, GLU_32
<i>EcoRI</i> _5.1	
ASP, ASP, LEU, THR, PHE	ASP_419, TYR_109, TRP_416, GLY_33, ALA_418, ARG_404, ALA_415, TRP_397, THR_367, SER_227, GLY_20, SER_21, PRO_35, ASP_505, LEU_504
THG_2.1	
GLY, LEU, LYS, ALA, ASP, PHE	ASP_419, SER_37, TRP_416, GLU_32, TYR_109, LEU_401, SER_227, GLY_20, HIS_371, SER_368, PRO_35, GLU_229, TRP_397, ASN_247, ASN_506, GLY_33, ALA_418, LEU_504
THG_3.1	
PHE, LYS LEU, GLU, PHE, GLY	ASP_419, TYR_109, ARG_413, MET_429, GLY_33, TRP_416, LEU_401, ALA_414, TRP_397, THR_367, SER_21, GLU_396, SER_227, SER_368, GLY_20, ILE_226, GLU_229, ASP_232, ASN_18, ASN_247,

	ASN_246, PRO_35, TYR_269, TYR_485, CLY_417, SER_37, HIS_161
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Table S2

Hydrogen bond distance values and average (in Å) between OppA and Mal12, LDH, *EcoRI*, THG.

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	Average
<b>Mal 12_4.5</b>	2.3 Ala 418	3.0 Asp 419	3.0 Asp 419	3.1 Cys 417	2.9 Cys 417	3.0 Gly 33	2.6 Ser 37	2.9 Cys 417	2.8 Glu 32	2.3 Val 34	3.2 Arg 413	3.0 Tyr 245	2.8 Tyr 485	3.0 Asn 246	2.5 Tyr 269		2.8
<b>Mal 12_5.5</b>	3.1 Asp 419	2.8 Tyr 109	3.0 Cys 417	3.1 Cys 417	2.7 Glu 32	2.6 Ala 415	2.5 Tyr 245	3.3 Arg 413	2.5 Arg 413	2.8 Arg 413	2.9 Asn 366	2.9 Gly 20					2.8
<b>LDH_1.2</b>	3.1 Asp 419	3.1 Ala 418	2.7 Ser 37	3.2 Asp 419	3.1 Tyr 109	2.8 Cys 417	2.2 Arg 404	2.7 Arg 413	2.9 His 371	3.0 Tyr 245	3.9 His 371						3.0
<b>LDH_4.4</b>	3.1 Ala 418	3.2 Trp 416	2.9 Cys 417	2.8 Cys 418	2.8 Asp 419	2.8 Tyr 109	2.6 Glu 32	3.2 Val 34	2.6 Ala 415	3.0 Arg 413	2.3 Arg 413	2.8 His 371					2.8
<b>EcoRI_3.1</b>	3.0 Thr 367	2.8 Glu 229	3.0 Thr 367	2.8 Ser 227	2.9 His 371	2.5 Arg 413	3.0 Arg 413	3.3 Arg 413	3.1 Cys 417	2.9 Cys 417	3.1 Tyr 109	3.0 Ala 418	3.0 Ala 418				2.9
<b>EcoRI_5.1</b>	2.8 Tyr 269	3.1 Arg 41	3.3 Asn 506	2.7 His 161	2.8 Ser 37	2.7 Ser 37	2.7 Cys 417	3.1 Glu 32	3.7 Val 34	3 Arg 413	2.7 Tyr 245	2.4 Asn 247	2.8 His 371	2.5 Asn 366	2.7 Arg 413	3	2.9
<b>THG_2.1</b>	2.8 Thr 367	2.2 Asn 366	2.9 Ser 21	2.8 Tyr 245	3 Asn 246	3.2 Tyr 269	3.1 Arg 413	2.1 Arg 413	3.0 Val 34	3.0 Arg 404	3.0 Arg 404	3.0 Ala 415	3.1 Cys 417	3.2 His 161			2.9
<b>THG_3.1</b>	2.0 Val 34	2.8 Glu 32	2.8 Glu 32	2.7 Arg 404	3.2 Ala 415	3.2 Tyr 245	3.0 Asn 366	3.7 His 371	2.2 Asn 366								2.8