

Supplementary material:

Table 1: List of energy for BglB-CBI, BglB-CTT and BglB-CTR complexes obtained from docking experimental

	<i>BglB-CBI</i>	<i>BglB-CTT</i>	<i>BglB-CTR</i>
Binding Energy, ΔG_b (kcal/mol)	-6.2	-5.68	-5.63
Ligand Efficiency	-0.27	-0.13	-0.17
Inhibition Constant, K_i (μm)	28.39	68.76	74.94
Intermol. Energy(kJ/mol)	-9.78	-12.84	-10.4
VDW Desolvation (kcal/mol)	-9.42	-11.48	-9.39
Electrostatical energy(kcal/mol)	-0.36	-1.35	-1.07
Total Internal(kJ/mol)	-3.83	-9.09	-5.66
Torsional Energy(kJ/mol)	3.58	7.16	4.77
Unbound Energy(kJ/mol)	-3.83	-9.09	-5.66
Hydrogen Bond Formed	10	7	7

Table 2: List of hydrogen bond length for BglB-CBI, BglB-CTT and BglB-CTR complexes

<i>Enzyme-Substrates Complex</i>	<i>H-Bonds No.</i>	<i>Ligand Atom</i>	<i>Receptor Atom</i>	<i>Length (Å)</i>
BglB-CBI	1	O5	GLU356 OE1	2.85
	2	O5	ASN166 OD1	2.88
	3	O6	GLU167 OE1	2.97
	4	O6	GLU167 OE2	2.81
	5	O4	GLN22 OE1	2.81
	6	O3	GLN22 NE2	2.91
	7	O10	GLU409 O	3.09
	8	O11	GLU409 OE2	2.68
	9	O10	HIS181 N	3.15
	10	O3	GLU409 OE2	2.85
BglB-CTT	1	O6	GLN22 NE2	3.08
	2	O6	TRP402 NE1	3.16
	3	O7	GLU409 OE2	2.68
	4	O9	HIS181 NE2	2.84
	5	O1	HIS181 NE2	3.3
	6	O14	GLU180 OE2	2.62
	7	O15	GLU180 OE1	3.05
BglB-CTR	1	O6	GLN22 NE2	3.08
	2	O6	TRP402 NE1	3.16
	3	O9	HIS181 NE2	2.84
	4	O7	GLU409 OE2	2.68
	5	O14	GLU180 OE2	2.62
	6	O1	HIS181 NE2	3.3
	7	O15	GLU180 OE1	3.05