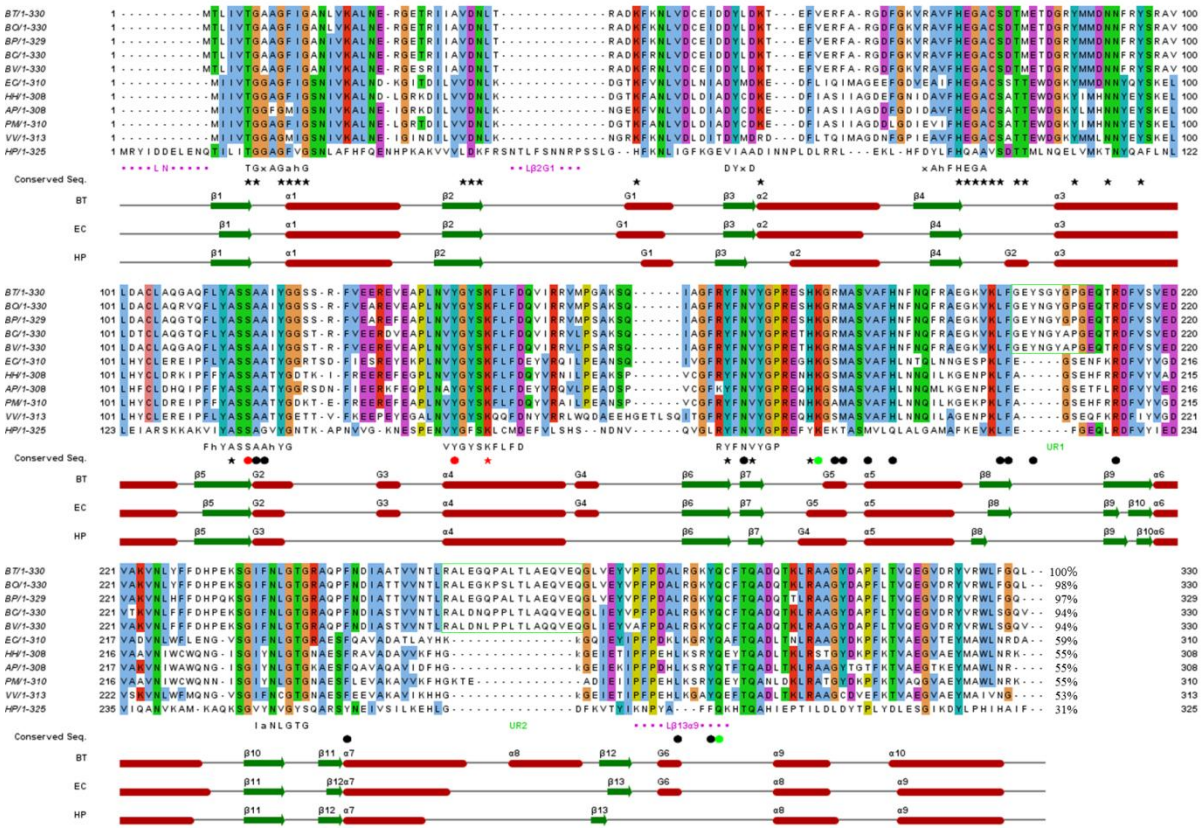
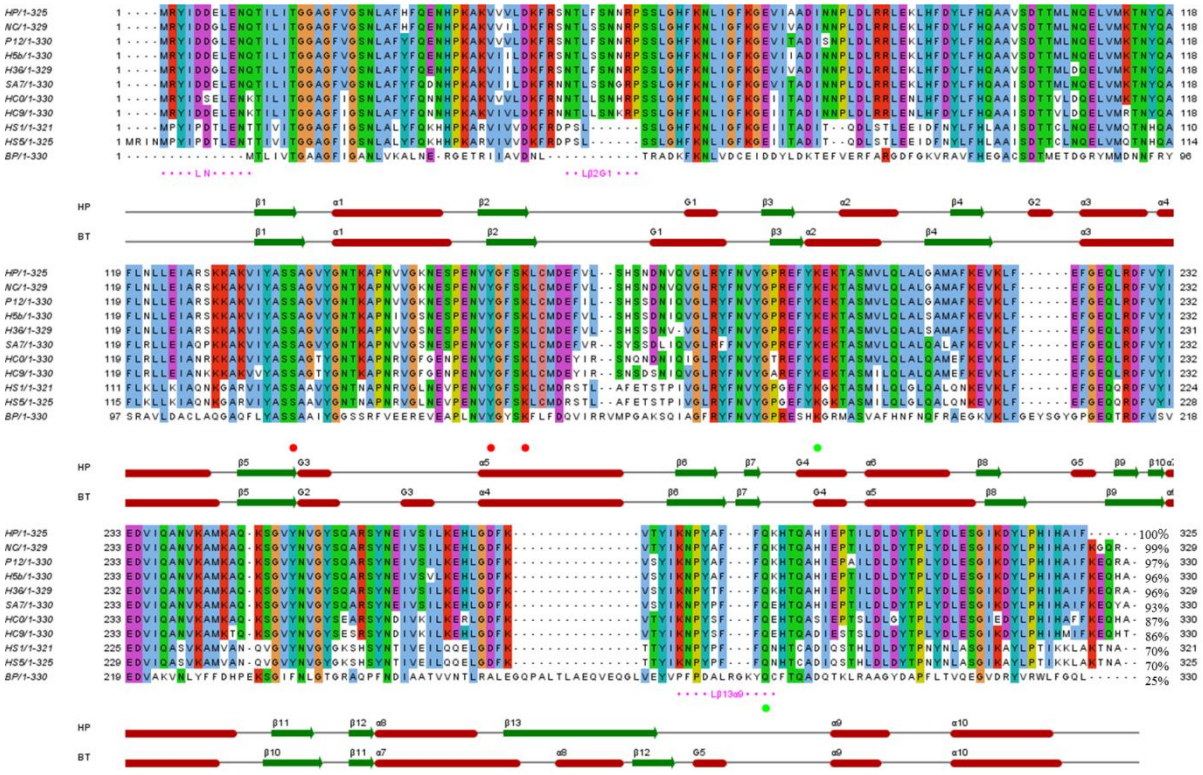
Supplementary Material

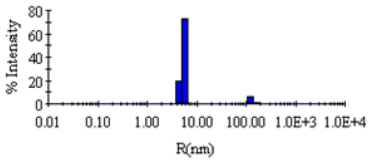


Supplementary Figure S1. Sequence comparison between *Bt*AGME and its homologues. Abbreviations are as follows: *B. thailandensis* (Bt), *B. oklahomensis* C6786 (BO), *B. pseudomallei* (BP), *B. cenocepacia* H111 (BC), *B. vietnamiensis* G4 (BV), *E. coli* str. K-12 substr. MG1655 (EC), *Haemophilus haemolyticus* M21639 (HH), *Actinobacillus pleuropneumoniae* serovar 10 str. D13039 (AP), *Pasteurella multocida* subsp. multocida str. Pm70 (PM), *Vibrio vulnificus* MO6-24/O (VV), *Helicobacter pylori* (HP). Secondary structural elements of *Bt*AGME and *Hp*AGME are represented below the sequence alignment rows (α, α-helix; β, β-strand; G, 3_{10}-helix). The filled stars represent residues comprising the $NADP^+$ binding cavity and the filled circles for residues comprising the substrate binding cavity. One red star and two red circles represent the catalytic triad (Ser116, Tyr139, Lys143) and the green circles for the residues, Lys177 and Gln293, forming hydrogen bonds with the real substrate, ADP-D,D-Hep, in the docking model. The two unique regions for *Burkholderia* species are boxed in green. Percent sequence identities (%) are listed compared with the sequence of *B. thailandensis*. The three flexible loops, LN, Lβ2G1 and Lβ13α9, of *Hp*AGME are represented by pink dots. The figure was drawn with the Jalview program (Waterhouse *et al*., 2009). The consensus amino acid is colored according to the Clustal X color scheme provided by this program.



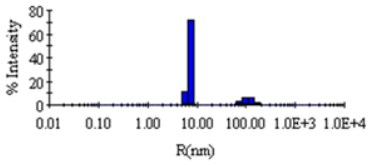
Supplementary Figure S2. Sequence comparison between *Bt*AGME and *Hp*AGME homologues. Abbreviations are as follow : *H. pylori G27* (HP), *H. pylori* NCTC 11637 (NC), *H. pylori* P12 (P12), *H. pylori* Hp H-5b (H5b), *H. pylori* Hp H-36 (H36), *H. pylori* SouthAfrica7 (SA), *H. cetorum* MIT 00-7128 (HC0), *H. cetorum* MIT 99-5656 (HC9), *H. suis* HS1 (HS1), *H. suis* HS5 (HS5), *B. thailandensis* (BT). Refer to supplement figure S1 for labels.

(a)



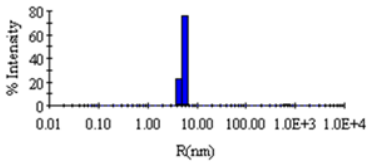
Item	R (nm)	%Pd	MW-R (kDa)	%Int	%Mass
Peak 1	5.6	10.6	187	92.1	100
Peak 2	135.5	12	327719	7.9	0
Peak 3	3659.2	0	7.32E+08	----	----

(b)



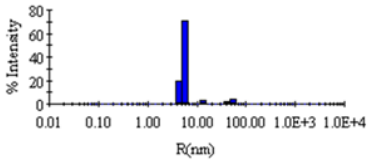
Item	R (nm)	%Pd	MW-R (kDa)	%Int	%Mass
Peak 1	0.3	0	0	----	----
Peak 2	7.5	8.7	376	83.1	100
Peak 3	112.6	25.9	212662	16.9	0

(c)



Item	R (nm)	%Pd	MW-R (kDa)	%Int	%Mass
Peak 1	5.5	10.8	186	98.6	100
Peak 2	682.2	0	14388600	1.4	0

(d)



Item	R (nm)	%Pd	MW-R (kDa)	%Int	%Mass
Peak 1	5.5	10.6	186	90.7	99.7
Peak 2	13.6	0	1503	3.6	0.2
Peak 3	50.2	12.8	32108	5.7	0

Supplementary Figure S3. Monodisperse peaks from DLS experiments. DLS experiments were performed with *Bt*AGME in the following conditions. (a) 0.5 mg/ml wild type in 0.1 M Tris-HCl, pH 7.5 (b) 0.25 mg/ml wild type in 0.1 M Sodium succinate, pH 4.5 (c) 0.5 mg/ml E210G mutant in 0.1 M Tris-HCl, pH 7.5 (d) 0.5 mg/ml E210G mutant in 0.1 M Sodium Citrate, pH 5.0. Since E210G mutant precipitated below pH 5.0, data could not be collected at pH 4.5.

Supplementary Table S1a. CScore analysis of the docking of *Bt*AGME with ADP-D,D-Hep using Surflex-Dock.

Model	Total_Score	Crash	Polar	D_SCORE	PMF_SCORE	G_SCORE	CHEMSCORE	CSCORE
1	10.36	-2.11	8.93	-191.35	-116.50	-265.00	-6.41	2
2	9.94	-1.92	6.32	-209.75	-131.18	-299.38	0.63	2
3	9.93	-2.14	6.91	-174.11	-133.52	-326.40	-2.45	4
4	9.82	-1.94	8.14	-197.47	-117.57	-267.58	-5.15	2
5	9.35	-3.80	7.46	-233.75	-132.19	-314.24	-5.78	5
6	9.15	-2.58	8.21	-206.70	-117.45	-279.16	-6.78	1
7	9.09	-4.94	9.96	-230.49	-114.34	-341.29	-7.66	3
8	9.05	-3.82	9.08	-226.43	-124.04	-361.57	-1.42	3
9	9.05	-3.16	5.18	-226.80	-106.34	-327.56	4.15	2
10	8.93	-3.10	7.95	-219.18	-139.79	-317.54	-6.34	4
11	8.91	-1.94	5.53	-201.60	-121.57	-315.41	-3.06	2
12	8.91	-2.89	5.74	-224.10	-120.07	-317.64	0.78	2
13	8.84	-2.40	7.43	-203.46	-110.44	-290.86	-1.56	0
14	8.81	-1.73	7.71	-189.94	-128.82	-251.39	-3.40	2
15	8.75	-2.20	7.69	-175.61	-130.52	-294.00	-5.54	2
16	8.63	-3.36	6.60	-223.84	-112.33	-336.56	0.32	2
17	8.39	-1.71	6.41	-194.14	-115.46	-271.76	3.10	0
18	8.22	-3.34	7.34	-228.31	-114.61	-324.76	-1.61	2
19	8.22	-3.62	4.78	-245.98	-113.20	-355.46	1.49	2
20	8.12	-1.83	6.21	-199.44	-109.03	-297.90	-3.72	1

Total_Score The total Surflex-Dock score expressed as -log(K_d). The total score includes the Crash score.
Crash The degree of inappropriate penetration by the ligand into the protein and of interpenetration (self-clash) between ligand atoms that are separated by rotatable bonds.
Polar Contribution of the polar interactions to the total score.
D_SCORE is using only the charge and van der Waals interactions between the protein and the ligand:
PMF_SCORE is based upon ligand-receptor atom-pair interaction potentials (Potential of Mean Force, PMF).
G_SCORE is using the hydrogen bonding, complex (ligand-protein), and internal (ligand-ligand) energies.
CHEMSCORE includes terms for hydrogen bonding, metal-ligand interaction, lipophilic contact, and rotational entropy, along with an intercept term.
CSCORE is the consensus score computed from the Surflex-Dock Total Score, ChemScore, G-Score, D-Score, and PMF-Score.

Supplementary Table S1b. CScore analysis of the docking of *Bt*AGME with ADP-D,D-Hep using Surflex-Dock GeomX.

Name	Total_Score	Crash	Polar	D_SCORE	PMF_SCORE	G_SCORE	CHEMSCORE	CSCORE
1	12.33	-2.68	10.41	-224.43	-1.61	-342.88	16.64	4
2	10.76	-2.60	8.50	-218.81	21.41	-329.42	17.64	3
3	10.17	-2.83	9.74	-199.41	-5.31	-281.12	17.76	3
4	10.17	-3.07	10.06	-198.79	0.83	-274.78	17.88	2
5	9.91	-2.28	8.86	-200.69	-15.41	-277.69	17.72	2
6	9.71	-2.69	7.60	-220.08	13.19	-321.11	17.52	3
7	9.55	-1.10	8.30	-185.71	-3.44	-249.04	15.37	1
8	9.50	-2.72	8.97	-214.85	-7.96	-271.36	16.54	2
9	9.27	-2.39	8.03	-215.39	5.88	-288.89	18.39	3
10	8.97	-3.17	8.78	-201.80	-8.25	-271.90	17.77	2
11	8.88	-3.01	7.57	-207.38	19.51	-294.22	16.04	2
12	8.83	-2.82	6.97	-211.27	0.50	-330.37	17.57	3
13	8.63	-1.95	7.57	-189.94	43.19	-261.41	18.64	0
14	8.46	-3.37	9.13	-210.99	-4.00	-262.46	11.20	3
15	8.45	-2.86	6.73	-223.43	-13.30	-344.38	17.07	3
16	8.14	-2.22	7.38	-214.27	-10.25	-279.80	16.78	2
17	7.98	-1.81	8.28	-193.27	-4.41	-262.85	18.43	1
18	7.84	-1.54	7.67	-183.92	-10.70	-247.19	14.15	2
19	7.81	-2.29	7.21	-213.68	-10.93	-285.41	17.33	3
20	7.58	-1.40	8.08	-173.46	1.75	-218.19	13.56	2

This CScore analysis was obtained from Surflex-Dock GeomX with the fifth conformer in the Supplementary Table S1a.

Supplementary Table S1c. CScore analysis of the docking of *Ec*AGME with ADP-D,D-Hep using Surflex-Dock.

Name	Total_Score	Crash	Polar	D_SCORE	PMF_SCORE	G_SCORE	CHEMSCORE	CSCORE
1	10.69	-2.89	7.99	-252.64	-135.25	-368.33	-2.07	4
2	9.38	-3.59	7.19	-250.74	-132.68	-340.65	-0.26	3
3	8.89	-4.72	8.37	-256.48	-106.61	-336.88	-3.80	3
4	8.57	-5.35	8.47	-246.12	-101.45	-343.52	-6.12	2
5	8.48	-3.44	5.65	-252.12	-132.62	-344.20	5.00	2
6	7.64	-3.79	6.53	-247.80	-113.55	-345.91	0.83	1
7	7.16	-4.86	5.95	-245.21	-129.99	-344.83	2.43	1
8	6.59	-6.58	8.02	-249.62	-114.18	-330.92	-1.90	1
9	6.42	-5.02	6.83	-260.77	-117.59	-343.38	1.79	1
10	6.37	-5.07	4.78	-257.60	-112.86	-383.84	1.17	2
11	6.34	-5.18	5.27	-263.13	-122.16	-362.64	-1.53	4
12	6.21	-5.91	5.28	-258.06	-119.62	-364.77	3.09	3
13	6.18	-4.94	4.70	-258.29	-121.48	-369.07	1.12	4
14	6.04	-5.48	6.27	-250.33	-103.84	-359.80	1.33	1
15	5.77	-4.98	5.38	-251.97	-112.06	-352.69	5.72	0
16	5.64	-6.52	5.33	-254.09	-114.42	-328.01	-3.68	2
17	5.43	-5.07	3.90	-259.17	-128.42	-385.46	7.92	3
18	5.29	-5.69	5.62	-256.15	-126.89	-387.93	8.41	3
19	5.06	-6.31	5.80	-254.77	-133.35	-343.57	6.64	2
20	4.95	-5.88	5.55	-245.02	-100.70	-344.97	0.10	1

Supplementary Table S1d. CScore analysis of the docking of *Ec*AGME with ADP-D,D-Hep using Surflex-Dock GeomX.

Name	Total_Score	Crash	Polar	D_SCORE	PMF_SCORE	G_SCORE	CHEMSCORE	CSCORE
1	14.44	-2.12	11.58	-230.90	-147.42	-319.42	-12.88	3
2	14.32	-2.47	11.18	-241.78	-131.05	-312.11	-11.58	3
3	14.31	-1.65	11.54	-238.55	-141.74	-309.84	-7.57	3
4	13.46	-1.64	8.06	-241.79	-123.97	-370.34	0.32	3
5	13.37	-1.67	9.29	-240.81	-135.35	-335.38	-6.86	4
6	13.31	-3.27	8.83	-237.77	-125.54	-336.56	-6.67	2
7	13.23	-3.54	9.87	-247.56	-111.12	-397.87	-5.48	2
8	13.22	-2.49	9.67	-234.84	-140.09	-306.45	-9.53	2
9	12.99	-2.08	12.25	-235.68	-154.29	-306.23	-15.70	2
10	12.98	-2.29	9.41	-228.28	-127.06	-311.51	-8.38	1
11	12.82	-2.37	10.95	-236.77	-130.50	-263.71	-10.07	1
12	12.73	-1.30	7.94	-244.70	-140.02	-348.24	-2.13	3
13	12.73	-1.97	9.73	-242.89	-143.16	-331.17	-7.15	3
14	12.60	-2.40	10.49	-238.96	-140.42	-320.10	-12.59	3
15	12.38	-1.86	10.31	-237.90	-133.07	-317.45	-4.62	1
16	12.38	-3.24	8.45	-246.96	-111.58	-360.66	-1.85	2
17	12.32	-3.98	10.16	-243.84	-116.14	-312.26	-6.94	1
18	12.30	-2.64	11.80	-235.09	-125.20	-314.12	-12.97	1
19	12.29	-2.85	9.85	-245.33	-148.24	-306.68	-7.45	2
20	12.16	-1.68	9.99	-243.69	-150.84	-293.06	-5.57	2

This CScore analysis was obtained from Surflex-Dock GeomX with the first conformer in the Supplementary Table S1c.