

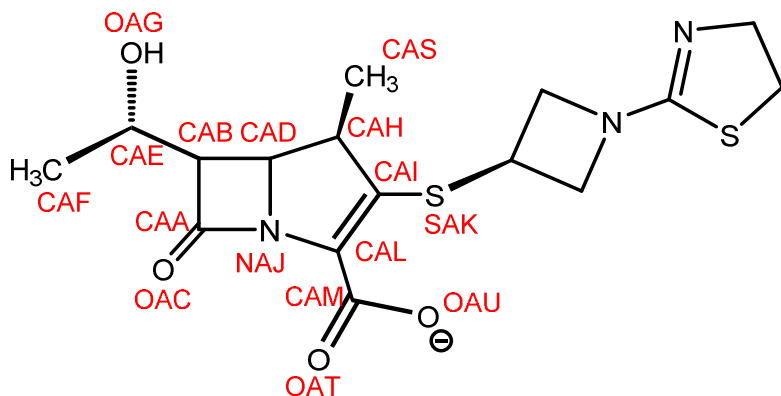
## Supplementary Material

for

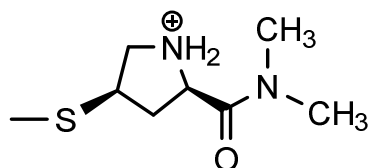
### Tebipenem, a New Carbapenem Antibiotic is a Slow Substrate that Inhibits the $\beta$ - Lactamase from *Mycobacterium tuberculosis*

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Numbering of tebipenem and meropenem common atoms used in Table S1

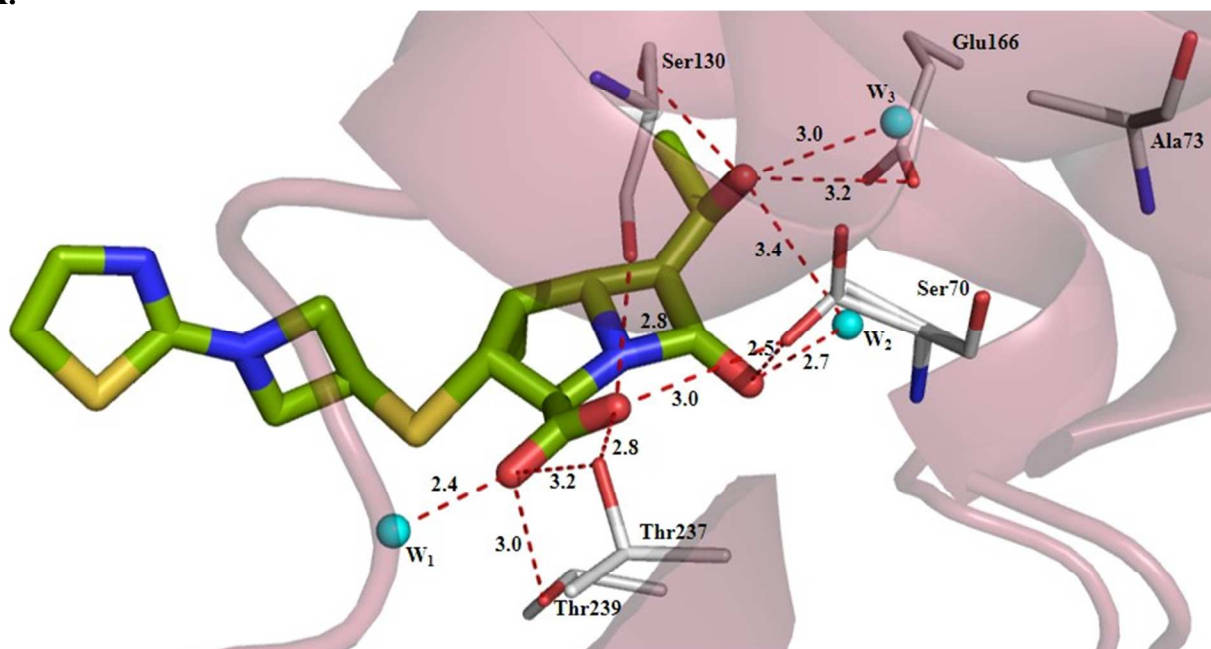


Side chain of meropenem

<b>Table S1: Interactions of Tebipenem and Meropenem covalent adducts with M. tuberculosis <math>\beta</math>-lactamase.</b>							
Tebipenem	Protein (BlaC)		Distance (Å)	Meropenem	Protein (BlaC)		Distance (Å)
	Residue	Atom Name			Residue	Atom Name	
CAE	Ser70	OG	3.1	CBE	HOH697	O	3.4
	Glu166	OE2	3.5	N	HOH697	O	3.4
	HOH572	O	3.4	CAS	Thr239	O	3.5
OAG	Ser70	OG	2.7		HOH639	O	3.4
	Glu166	OE2	2.7	CAM	Thr237	OG1	3.3
	Lys73	CE	3.4	OAT	Thr237	OG1	2.5
	Lys73	NZ	2.6		Ser130	OG	3.4
	Glu166	CD	3.2		Thr237	C	3.3
	HOH572	O	3.2		Thr237	O	3.4
CAB	Ser70	OG	2.6	OAU	HOH520	O	2.7
CAA	Ser70	OG	1.4		HOH520	OG1	3.5
	Ser70	CA	3.3		Thr237	OG1	3.2
	Ser70	CB	2.5	NAJ	Ser130	OG	2.7
	Ser70	N	3.3		Ser70	OG	3.0
	HOH572	O	2.9		Ser130	CB	3.3
OAC	Ser70	N	2.8	CAD	Ser70	OG	3.2
	Thr239	N	2.8	CAB	Ser70	OG	2.5
	Ser70	CA	3.3	CAE	Ser70	OG	2.9
	Ser70	CB	2.7		Glu166	OE1	3.4
	Ser70	OG	2.3		Glu166	OE2	3.4
	Thr239	O	2.9		HOH572	O	3.2
	HOH572	O	3.4	CAF	HOH514	O	3.3
CAD	Ser70	OG	3.1	OAG	Glu166	OE2	2.7
NAJ	Ser70	OG	2.8		Ser70	OG	2.8
	Ser130	OG	2.8		Lys73	CE	3.4
	Ser70	CB	3.4		Lys73	NZ	2.6
	Ser130	CB	3.4		Glu166	CD	3.2
CAL	Ser130	CB	3.3		Glu166	OE1	3.4
	Ser130	OG	3.2		HOH572	O	3.4
CAM	Thr237	OG1	3.4	CAA	Ser70	OG	1.4
	Thr239	OG1	3.4		Ser70	CA	3.2
OAT	Thr237	OG1	2.5		Ser70	CB	2.4
	Ser130	OG	3.3		Ser70	N	3.1
	Thr237	C	3.4		HOH572	O	2.9
	Thr237	CB	3.4	OAC	Ser70	N	2.7
OAU	HOH520	O	2.8		Thr239	N	2.9
	Thr239	OG1	2.9		Ser70	CA	3.2
C17	HOH863	O	3.4		Ser70	CB	2.7
C18	HOH863	O	3.1		Ser70	OG	2.3
C23	HOH706	O	3.4		Gly238	CA	3.3
N25	HOH687	O	2.9		Thr239	O	3.0
C17	HOH863	O	3.1		HOH572	O	3.4
C18	HOH863	O	3.1				
C20	HOH863	O	3.1				
N19	HOH863	O	3.1				

Figure S1:

A.



B.

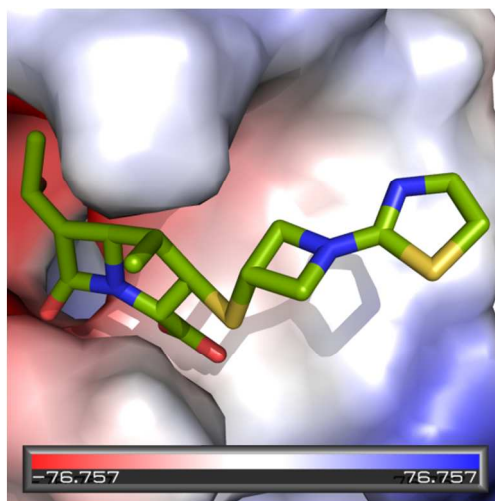
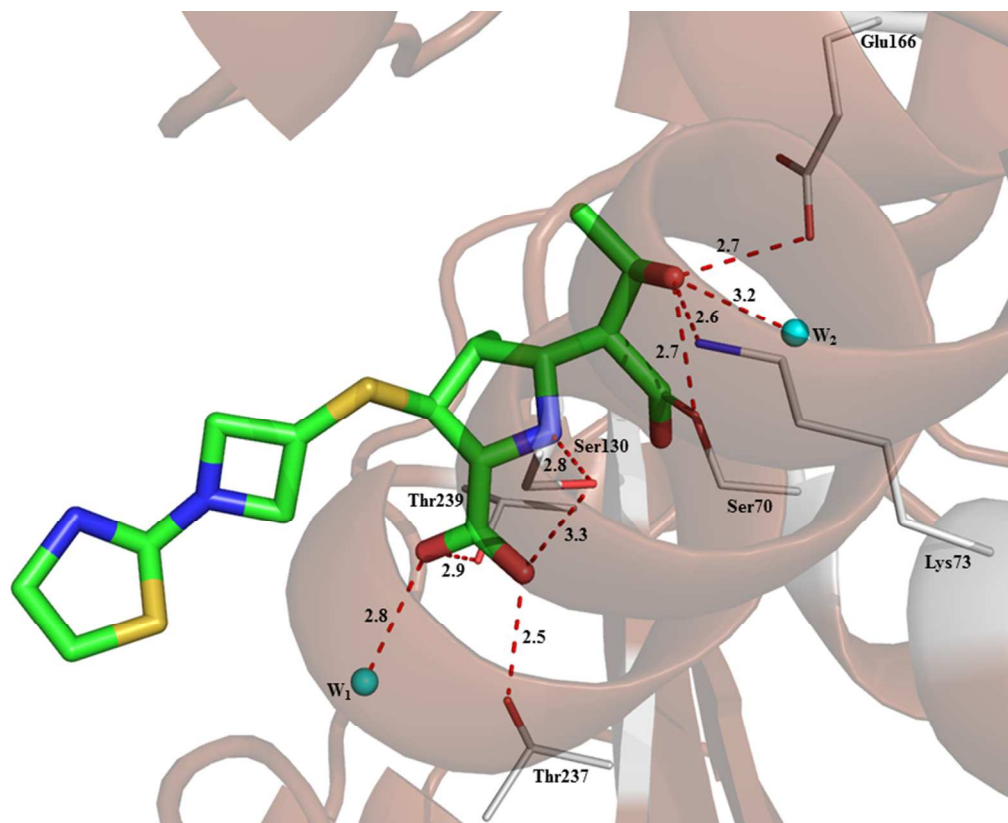


Figure S1: A. Active site molecular description of BlaC-Tebipenem Michaelis-Menten complex  
A. 3-D ribbon and ball-stick representation, B. Calculated electrostatic interaction map of BlaC-Tebipenem Michaelis-Menten complex.

Figure S2:

A.



B.

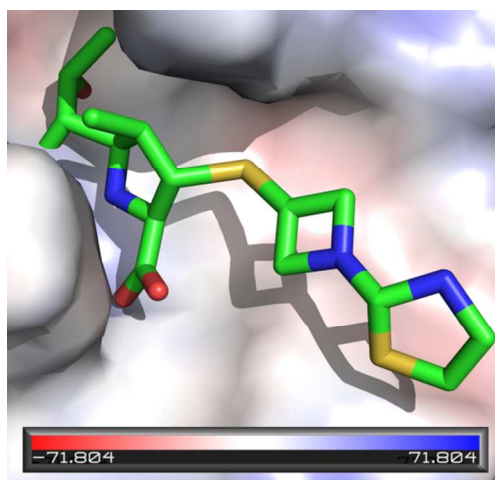


Figure S2: A. Active site molecular description of BlaC-Tebipenem covalent adduct: 3-D ribbon and ball-stick representation, B. Calculated electrostatic interaction map of BlaC-Tebipenem covalent adduct.