

TABLE I  
Grid box size and position for both enzymes models

	Centre position			Box size		
	x	y	z	x	y	z
IIWO	-5.077	-47.902	8.882	28	26	30
PfATP	-4.857	-24.528	7.832	26	32	28

TABLE II  
Flexible amino acids of the active sites from the mammalian and parasite enzymes

IIWO			PfATP6		
Residue	Symbol	Position	Residue	Symbol	Position
Leucine	LEU	253	Isoleucine	ILE	251
Glutamate	GLU	255	Leucine	LEU	253
Phenylalanine	PHE	256	Phenylalanine	PHE	254
Glutamine	GLN	259	Glutamine	GLN	257
Leucine	LEU	260	Leucine	LEU	258
Valine	VAL	263	Isoleucine	ILE	261
Isoleucine	ILE	761	Isoleucine	ILE	748
Isoleucine	ILE	765	Isoleucine	ILE	752
Aspartate	ASN	768	Aspartate	ASN	755
Valine	VAL	769	Isoleucine	ILE	756
Valine	VAL	772	Valine	VAL	759
Valine	VAL	773	Phenylalanine	PHE	763
Phenylalanine	PHE	776	Leucine	LEU	815
Leucine	LEU	828	Isoleucine	ILE	816
Isoleucine	ILE	829	Leucine	LEU	821
Phenylalanine	PHE	834	Tyrosine	TYR	824
Tyrosine	TYR	837	Isoleucine	ILE	825
Methionine	MET	838	-	-	-

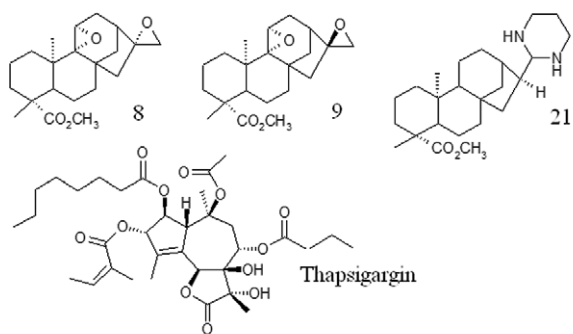


Fig. 1: chemical structure of *ent*-kaurane diterpenes 8, 9, 21 and the natural inhibitor thapsigargin.

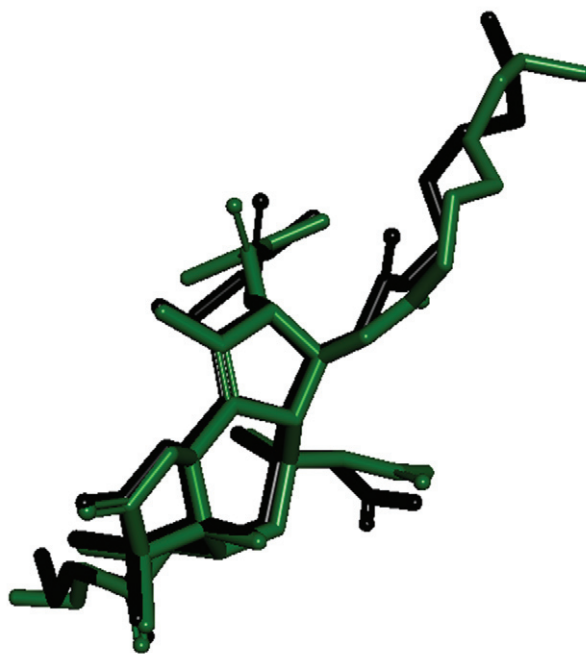


Fig. 2: redocking results. In green colour is the crystallographic PDB structure and in black is the docked one.