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SUPPL. MATERIAL

In silico antimalarial bioprospecting of neem (*Azadirachta indica*) quinine-derivative alkaloids

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Table 1. Autodock Vina's search space for three selected receptors.

Receptor (lr)4-6	Binding Site Residue	Chain	Coordinate X	Coordinate Y	Coordinate Z	Dimension X	Dimension Y	Dimension Z
PNP (PDB ID: 5ZNC)	His7, Arg45, Cys92, Gly93, Ser157, Tyr160, Glu182, Met183, Asp206, Trp212, Asp218	A	64.7963	63.3105	14.0424	All set to 25 Å		
DHODH (PDB ID: 6GJG)	Gly181, Cys184, His185, Phe188, Phe227, Ile263, Arg265, Val532, Met536	A	11.7281	-7.9624	-6.7855			
EMP1 (PDB ID: 6S8U)	Asn973, Asn974, Glu1098, Glu1099, Gln1103, Gly1114 (*)	A	-17.0929	-54.4949	-7.2024			

Note: For PNP and DHODH, the binding sites referred to the active sites of the proteins. As for EMP1, residues marked with (*) referred to the binding sites where the protein EMP1 binds to intercellular adhesion molecule 1 (ICAM1) polypeptide molecule.

Table 2. List of enzymes targeted by the control and studied compounds.

Compounds and their respective targets						
IZP	**Quinine**	**A**	**B**	**C**	**D**	**E**
11-β-hydroxysteroid dehydrogenase 1	Mitogen-activated protein kinase kinase kinase 12	Aldehyde dehydrogenase 1A1	Steryl-sulfatase	**6-phosphofructo-2-kinase/fructose-2,6-bisphosphatase 3**	**11-β-hydroxysteroid dehydrogenase 1 (by homology)**	PH domain leucine-rich repeat-containing protein phosphatase 2

Acyl-CoA desaturase	**Nitric oxide synthase, inducible**	Aldo-keto reductase family 1 member B10	**Acyl-CoA desaturase (by homology)**	**6-phosphofructo-2-kinase/fructose-2,6-bisphosphatase 3**	Quinone reductase 2
Arachidonate 15-lipoxygenase	Phenylethanolamine N-methyltransferase	Aldehyde reductase	α-1,6-mannosyl-glycoprotein 2-beta-N-acetylglucosaminyltransferase	Acetyl-CoA carboxylase 1	
Elongation of very long chain fatty acids protein 6	**PI3-kinase p110-α subunit**	Anandamide amidohydrolase	Acyl coenzyme A:cholesterol acyltransferase 1	Aldose reductase	
Estradiol 17-β-dehydrogenase 2	S-methyl-5-thioadenosine phosphorylase	Leukocyte common antigen	Adenosine kinase	Autotaxin	
Glutaminyl-peptide cyclotransferase	Telomerase reverse transcriptase	Macrophage migration inhibitory factor	Arachidonate 12-lipoxygenase	Geranylgeranyltransferase type I	
Indoleamine 2,3-dioxygenase		Myeloperoxidase	Arachidonate 15-lipoxygenase, type II	Group IID secretory phospholipase A2	
PI3-kinase p110-α subunit		Nicotinamide phosphoribosyltransferase	Carnitine O-palmitoyltransferase 1, liver isoform	Hexokinase type IV	
PI3-kinase p110-δ subunit		**Nitric oxide synthase, inducible (by homology)**	Deoxycytidine kinase	Liver glycogen phosphorylase	
PI3-kinase p110-γ subunit		Poly [ADP-ribose] polymerase-1	Diacylglycerol O-acyltransferase 2	Peptidyl-prolyl cis-trans isomerase NIMA-interacting 1	
Poly [ADP-ribose] polymerase-1		**Protein-glutamine γ-glutamyltransferase**	Estradiol 17-β-dehydrogenase 1	Prostaglandin E synthase	
Poly [ADP-ribose] polymerase 2		Steryl-sulfatase	Estradiol 17-β-dehydrogenase 2	Protein farnesyltransferase	

Tankyrase-2	Thymidine phosphorylase	Prostaglandin E synthase	Squalene synthase (by homology)
Tankyrase-1		Isocitrate dehydrogenase [NADP] cytoplasmic	
Thymidine phosphorylase		Peptidyl-prolyl cis-trans isomerase FKBP5	
		Phosphoglycerate kinase 1	
		Protein-glutamine γ-glutamyltransferase	
		Protein-glutamine gamma-glutamyltransferase K	

Note: Enzymes in bold letters are the shared enzymes that target the compounds.