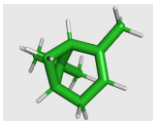
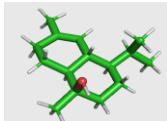
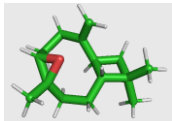
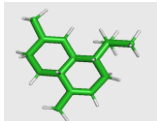
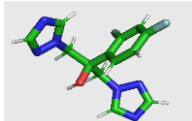


## Supplementary data

**Table S1.** Forward and reverse primers used for qRT-PCR

Genes	Forward primer	Reverse primer
<b>CYP51</b>	GACAACGTCATGGAGGAGATG	CCACCTGGACTGGCTTTAAT
<b>ODC</b>	GCACGCGCTTCTCATGAACGTATT	CGAAGAGGATGCAGTTGAAGCTGT
<b>SPS</b>	ACTTCTACACGAATGTGCTCCGCA	CATTGCGTACTTGACCGTGGCAAA
<b>TryS</b>	TGTCATGAGCGAATGACCAACCGAT	GCTTGCCATTCAACAAACGTCAGGT
<b>TR</b>	AATGAGGACGGCTCGAATCACGTT	ATGGCGTAGATGTTGTCCACCGAT
<b>CTP</b>	CCAACGGCAGCTTCAAGAAGATCA	TGAAGTCGAGCGGGTAGAAGAAGA
<b>MTP</b>	AAGCTAAACACGCAGGTTGTTGCG	TCGATCAGCACACCATAGTCACGA

**Table S2.** Characteristics and structures of  $\alpha$ -Pinene, t-Cadinol, Caryophyllene oxide,  $\alpha$ -Cadinene and Fluconazole obtained from Pub Chem

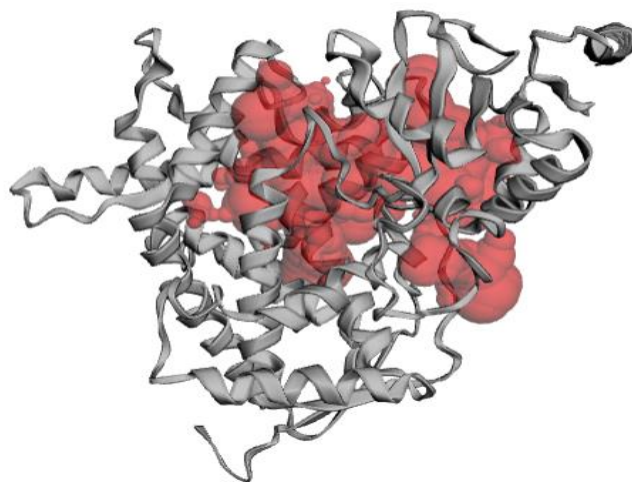
Sample Name	$\alpha$ -Pinene	t-Cadinol	Caryophyllene oxide	$\alpha$ -Cadinene	Fluconazole
molecular formula	$C_{10}H_{16}$	$C_{15}H_{26}O$	$C_{15}H_{24}O$	$C_{15}H_{24}$	$C_{13}H_{12}F_2N_6O$
Canonical SMILES <sup>a</sup>	<chem>CC1=CCC2C1C2(C)C</chem>	<chem>CC1=CC2C(CC(C2CC1)(C)O)C(C)C</chem>	<chem>CC1(CC2C1CC3(C(O3)CCC2=C)C)C</chem>	<chem>CC1=CC2C(C1)C(=CCC2C(C)C)C</chem>	<chem>C1=CC(=C(C=C1F)C(CN2C=NC=N2)(CN3C=NC=N3)O</chem>
3D Structure <sup>b</sup>					

a: PubChem

b :USCF Chimera 1.17.

**Table S3.** Selected Grid parameters for target enzymes

Protein	Species	PDB ID	Resolution (Å)	Grid Box Center Coordinates			Grid Box Size
				x	y	z	
<b>Sterol 14-alpha demethylase (CYP51)</b>	<i>Leishmania infantum</i>	3L4D	2.75	32.676	-25.214	-3.329	40 x 40 x 40



**Figure S1.** The active sites of sterol 14-alpha demethylase (CYP51) from *Leishmania*

The active amino acid sites of sterol 14-alpha demethylase (CYP51) was predicted using the CASTp server. The CASTp server predicted the binding site amino acids of sterol 14-alpha demethylase (CYP51) from *Leishmania*. Beside, this enzyme had a pocket ID of an area (SA) Å<sup>2</sup> of 2295.980 and a volume of (SA) Å<sup>3</sup> of 1427.802.: ILE.45 , ILE.46 , PHE.48, GLY.49, LYS.50, PRO.52, LEU.53, PHE.55, MET.56, LEU.57, PHE.67, MET.69, ILE.71, CYS.72, ASN.74, ILE.76, VAL.78, PHE.89, ASN.93, SER.97, PRO.98, ARG.99, GLU.100, VAL.101, TYR.102, PHE.104, MET.105, VAL.106, PHE.109, VAL.113, ALA.114, TYR.115, TYR.119, MET.122, ARG.123, GLN.125, LEU.126, ASN.127, LEU.129, GLU.132, LEU.133, LYS.137, PHE.138, ASP.168, SER.171, ALA.172, ILE.174, ILE.175, ALA.178, CYS.181, LEU.182, ALA.197, GLN.198, LEU.200, ALA.201, GLU.204, SER.205, ILE.208, PRO.209, VAL.212, PHE.213, PRO.215, LEU.260, MET.283, ALA.286, ALA.287, MET.288, PHE.289, ALA.290, GLY.291, GLN.292, HIS.293, THR.294, SER.295, THR.296, THR.298, TRP.301, SER.302, HIS.305, GLU.342, ALA.345, ARG.346, GLU.347, SER.348, ILE.349, ARG.350, ARG.351, ASP.352, PRO.353, PRO.354, LEU.355, VAL.356, MET.357, LEU.358, MET.359, ARG.360, LYS.361, ILE.378, ALA.380, PRO.383, LEU.384, LEU.385, HIS.387, GLN.388, PHE.393, PRO.396, ARG.397, GLU.398, ASN.400, MET.405, GLY.414, PHE.415, GLY.416, VAL.419, HIS.420, LYS.421, CYS.422, ILE.423, GLY.424, GLU.425, PHE.427, GLY.428, LEU.429, GLN.431, VAL.432, LYS.433,

LEU.451, GLU.453, PRO.454, TYR.456, HIS.457, THR.458, MET.459, VAL.460, VAL.462 of  
chain-A.