BIOINFORMATION

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Supplementary material:

Table 1: Function regions of CYP4V2 predicted using ConSurf server with high amino acid conservation score (9 - conserved, 1 - variable).

Residue	Conservation score	Buried (B)/Exposed (E)	Residual variety
W130	9	B	W,G
L131	9	B	M,I,L
G132	9	E	S,A,N,R,K,G
L133	5	E	A,F,S,T,N,K,E,Q,C,D,R,I,L
G134	9	B	S,C,G
L135	9	E	M,P,I,L
L136	8	B	F,M,I,L,V
T137	8	E	T,N,R,I,L,V
S138	9	E	F,A,S,T,N,C,D,G,L
L150	8	B	A,F,M,I,L
T151	9	E	A,W,T,D,N,I,G
P152	9	E	S,Q,M,P
T153	8	E	S,A,T,C
F154	9	B	F,L
H155	9	B	H,N,P
F156	9	B	H,S,F,L,Y
R320	9	E	Q,C,I,K,R,L
E321	9	E	A,Q,N,D,K,E
E322	9	E	Q,EV
V323	9	B	I,V
D324	9	E	H,N,D,E
T325	9	B	T,I,LF
F326	9	B	F,I,V
M327	9	B	T,M,I,L,V
F328	9	B	F,I,L
E329	8	E	A,R,G,E
G330	9	B	A,G,BV
H331	9	E	H,Q,N
D332	9	E	D,E
T333	9	E	S,T
F398	5	B	F,T,Y,V,H,Q,M,I,L
I506	8	B	T,I,L,V
L507	8	B	T,N,V,H,M,I,R,L
R508	8	E	S,M,T,I,K,R,L

Table 2: Ligand properties

Ligand	Molar weight	LogP	H acceptor	H donor	pKa	pKb	psa	logD	logK	Total charge
Caprylic acid	143.204	2.44	2	1	5.19	0	37.30	0.63	1.417	0.001
Lauric acid	200.318	3.21	2	2	11.88	4.03	40.46	3.21	-5.2	0.002
Myristic acid	227.363	4.82	2	1	4.95	0	37.30	2.78	-8.031	0.001
Palmitic acid	255.416	5.61	2	1	4.95	0	37.30	3.57	-13.55	0.001

Table 3: Docking analysis of CYP4V2 with selected ligands

Ligand	Free Energy of Binding (kcal/mol)	Inhibition Constant, Ki (uM)	vdW + Hbond + desolv Energy (kcal/mol)	Electrostatic Energy (kcal/mol)	Total Intermolec. Energy (kcal/mol)	Interact. Surface
Caprylic acid	-4.30	707.14	-5.85	-0.05	-5.89	353.002
Lauric acid	-5.99	40.85	-7.64	-0.05	-7.69	427.342
Myristic acid	-5.72	64.20	-8.70	0.07	-8.63	480.982
Palmitic acid	-6.14	31.58	-9.60	-0.03	-9.63	534.563

Table 4: Details of intermolecular interactions in the binding site of CYP4V2 with ligands

Ligand complex	Hydrophobic*	Polar	Cation	Other
Caprylic acid	C2-LEU136 (3.25), C1-LEU136 (3.13), C7-PHE328 (3.62), C6-PHE398 (3.76)	O2 -SER394 (3.38)	-	C1-GLU329(3.51), C3-GLU329(3.58), C3-THR333(3.63) C5-THR333(3.38) C7-THR333(3.33) C8-SER394(3.89) O1-SER394 (3.61) O2-SER394(3.48) O2-PHE398(3.43)
Lauric acid	C10-LEU136 (3.87) C11-ILE230 (3.51) C11-PHE231(3.87) C5-PHE328(3.68) C7-PHE328(3.84) C9-PHE328(3.48) C11-PHE328(3.77) C6-PHE398(3.59) C8-PHE398(3.82) C7-ILE506(3.69) C9-ILE506(3.89) C11-ILE506(3.50)	-	H1-PHE328(3.35)	O1-LEU136(3.52) C9-SER227(3.36) C11-SER227(3.78) H1-GLU329(3.67) O2-GLU329(3.53) H2-GLU329(3.53) C7-ASP332(3.86) C9-ASP332(3.10) O2-THR333(3.31) H2-THR333(3.36) C4-SER394(3.76)
Myristic Acid	C6-LEU136(3.53) C13-ILE230(3.84) C10-PHE328 C12-PHE329(3.71) C14-PHE328(3.62) C2-PHE398(3.78) C1-PHW398(3.65) C3-PHE398(3.69) C9-PHE398(3.51) C11-LEU505(3.40) C13-LEU505(3.71) C7-ILE506(3.76) C14-ILE506(3.90)	O2-ASP332(3.14)	-	O1-PHE328(3.42) C14-ASP332(3.90) C8-THR333(3.64) C10-THR333(3.87) O2-THR333(3.71) C3-SER394(3.32) C5-SER394(3.26) O2-ILE506(3.80) O1-ILE506(3.77)
Palmitic acid	C2-LEU136 (3.11) C1-LEU136 (3.61) C4-LEU136 (3.64) C12-ILE230 (3.80) C15-PRO393 (3.37) C5-PHE398 (3.45) C2-PHE398 (3.20) C4-PHE398 (3.76) C6-PHE398 (3.30) C8-PHE398 (3.88) C10-PHE398 (3.14) C12-LEU505(3.14) C14-LEU505(3.17)	-	-	C11-THR333(3.33) C13-THR333(3.84) C15-THR(3.63) C7-SER394(3.36) C9-SER394(3.32) C13-SER394(3.32) C15-SER394(3.58) O2-PHE398(3.84)

*C(X) –R(X) (D):
C(X) - atom name, R(X) - residue name, number within 4 Angstrom from the given ligand atom, (D) - lowest inter atomic distance between the given ligand atom and the residue. For example: C2-LEU136 (3.11), here C2 is C(X), LEU136 is R(X) and 3.11 is (D)