

Supporting Table S2. PyRosetta computed absolute energies and computed binding energies (kcal/mol)

SUBSTRATES	UNPRODUCTIVE		PRODUCTIVE	
	Absolute	Binding	Absolute	Binding
Testosterone	-43	-7	-47	-11
Finasteride	-41	-6	-63	-27
$\beta$ -sitosterol AutoDock	-30	-6	-51	-15
Stigmasterol AutoDock	-44	-7	-49	-12
Campesterol AutoDock	-41	-4	-50	-13
Daucosterol AutoDock	-58	-22	-44	-7
$\beta$ -sitosterol Manual	-38	-2	-64	-28
Stigmasterol Manual	-36	0.1	-66	-29
Campesterol Manual	-36	0.5	-45	-8
Daucosterol Manual	-71	-34	-67	-30
Oleic acid	-47	-12	-69	-34
Lauric acid	-39	-3	Not binding	Not Binding
Myristic acid	-43	-8	-55	-20
Palmitic acid	-44	-12	-45	-13
Linoleic acid	-43	-7	-64	-28