

Table S2.- Results obtained for log P from MLR analysis.

Compound	logPexp ^a	logPcalc ^b	logPcalc(cv) ^c
Acyclovir	-1.56	-1.87	-1.90
Althiazine	1.17	1.36	1.38
Amiodarone	7.57	6.18	5.80
Amodiaquine	3.99	3.89	3.88
Artemether	3.53	2.29	2.24
Artemisinin	2.9	2.27	2.24
Aspirin	1.19	0.06	-0.02
Azatadine	3.59	3.47	3.46
Azytromycin	4.02	3.35	3.04
Baclofene	-0.96	1.84	1.97
Benzoquinone	3.43	3.14	3.07
Bitertanol	4.16	4.55	4.61
Chloramphenicol	1.14	0.50	0.46
Chlorfenac	3.2	3.50	3.56
Ciprofloxacin	0.28	-0.26	-0.32
Clemizole	4.4	4.67	4.69
Clindamycin	2.16	2.19	2.19
Clofazimine	7.66	7.55	7.48
Codeine	1.19	2.42	2.46
Cortenil	3.08	2.82	2.80
Chloroquine	4.63	3.66	3.59
Dacarbazine	-0.24	0.10	0.12
Dapsone	0.97	1.58	1.62
Deptropine	5.27	4.63	4.57
Didanosine	-1.24	-0.12	-0.04
Dopamine	-0.98	-0.97	-0.97
Doxycycline	-0.02	-0.52	-0.60
Enprofyl	0.33	0.21	0.20
Ganciclovir	-1.66	-2.01	-2.05
Hydrocortisone	1.61	1.19	1.16
Ibuprofen	3.97	2.90	2.84
Indomethacin	4.27	2.82	2.77
Ketoconazole	4.35	5.30	5.42
Metronidazole	-0.02	-1.96	-2.34
Morphine	0.89	1.98	2.01
Nalorphine	1.86	2.31	2.33
Naphthoquinone	1.71	2.57	2.60
Norfloxacin	-1.03	-0.52	-0.46
Paracetamol	0.46	1.43	1.56
Pipemidic acid	-2.15	0.04	0.27
Proguanil	2.53	3.25	3.33
Pyrimethamine	2.69	2.46	2.45
Quinidine	3.44	3.23	3.22
Quinine	3.44	3.23	3.22
Sotalol	0.24	2.16	2.34
Sulfadoxine	0.7	0.99	1.01

Testosterone	3.32	2.92	2.90
Tinidazole	-0.35	-0.14	-0.11
Triclosan	4.76	4.36	4.32
Trifluridine	-0.46	-1.27	-3.39
trovafloxacin	0.31	-0.09	-0.14
Vincristine	2.82	3.48	3.64
Verapamil	3.79	3.02	2.99
Vidarabine	-1.11	-1.40	-1.46
Vinblastine	3.7	3.55	3.52
Zalcitabine	-1.3	-0.43	-0.37
Zidovudine	0.05	-0.16	-0.16

^a from database ChemIDplus (National Library of Medicine, US) ^b from the mathematical model. ^c from cross-validation analysis

Table S3.- Compounds selected by mathematical models FD1 and FD2 as potentially active against liver stage of *P. yoelii* from Merck Index

Compounds	Therapeutic Category ^a	DF1 ^b (class)	DF2 ^c (class)
Azelastine	Antihistaminic	5.59(A)	1.80(HA)
Bidisomide	Antiarrhythmic	5.19(A)	4.98(HA)
Butenafine	Antifungal	9.14(A)	5.89(HA)
Butoconazol	Antifungal	0.89(A)	3.42(HA)
Cinnarizine	Antihistaminic	10.46(A)	-15.06(NC)
Cloconazole	Antifungal	3.12(A)	-4.10(A)
Cyclamic acid	Non nutritive sweetener	4.89(A)	-3.40(A)
Cyclandelate	Vasodilator agent	6.84(A)	-4.98(A)
Denopamine	Beta adrenergic agonist	5.25(A)	-4.05(A)
Dichlorophen	Algicid / bactericide / fungicide	2.61(A)	7.05(HA)
Digitalin	Cardiotonic	10.61(A)	-40.55(NC)
Dimemorfan	Antitussive	7.46(A)	0.25(A)
Dobutamine	Cardiotonic	5.75(A)	1.52(HA)
Domiphen bromide	Topical anti-infective	1.98(A)	2.08(HA)
Doxenitoin	Anticonvulsant	5.37(A)	-0.72(A)
Doxycycline	Antibiotic	2.84(A)	-5.93(A)
Epitiostanol	Antineoplastic / Antioestrogenic agent	3.90(A)	-17.17(NC)
Fantofarone	Calcium channel antagonist	6.35(A)	2.82(HA)
Fenticonazole	Antifungal	4.74(A)	-5.07(A)
Fenvalerate	Insecticide	10.37(A)	-0.66(A)
Flumethrin	Insecticide	9.86(A)	2.13(HA)
Flunarizine	Calcium channel blocker	9.77(A)	-10.68(A)
Fluspirilene	Calcium channel blocker (Tranquilizer)	7.60(A)	-5.73(A)
Gallopamil	Calcium channel antagonist	9.69(A)	17.46(NC)
Isoxicam	Nonsteroid	5.15(A)	-1.17(A)
Lercanidipine	Antihypertensive / calcium channel blocker	10.97(A)	-0.20(A)
Levocabastine	Antihistaminic	8.79(A)	3.66(HA)

Lidoflazine	Coronary vasodilator	8.83(A)	0.85(A)
Mitotane	Antineoplastic	0.49(A)	1.12(HA)
Mofezolac	Analgesic	4.33(A)	-0.95(A)
Naftifin	Antifungal	10.43(A)	-4.03(A)
Naphthacen	Antifungal / antibiotic	9.18(A)	-0.45(A)
Naproxen	Analgesic	3.68(A)	-0.78(A)
Nifenazone	Analgesic	2.03(A)	-6.75(A)
Nifurprazine	Antifungal/topical	2.68(A)	-16.36(NC)
Oleandomycin	Macrolide	6.36(A)	-25.40(NC)
Omoconazole	Antifungal	3.13(A)	3.78(HA)
Oxyclozanide	Antihelminthic (flukicide)	0.37(NC)	12.97(HC)
Paroxypropione	Pituitary gonadotropic hormone inhibitor	2.90(A)	3.46(HA)
Patchouli alcohol	Tricyclic sesquiterpene alcohol	2.43(A)	-5.11(A)
Penamecillin	Antirheumatic	5.42(A)	-5.08(A)
Phenesterine	Antineoplastic	6.79(A)	-12.81(A)
Piperocaine	Local anesthetic	1.04(A)	-6.32(A)
Prednimustine	Antineoplastic	7.42(A)	0.91(A)
Saperconazole	Antifungal	8.50(A)	-9.00(A)
Siccanin	Antifungal	5.53(A)	1.80(HA)
Talastine	Antihistaminic	6.10(A)	1.01(HA)
Thymyl n-isoamyl carbamide	Antihelminthic	4.32(A)	10.03(HA)
Zorubicin	Antineoplastic	4.41(A)	-0.73(A)

^a From Merck Index.

^b From discriminant function DF1.

^c From discriminant function DF2.