Table S1. Biological properties of 37 APIs

API	B1	B2	B3	BB_{vivo}	CNS+/-	LactMed	LLL H	log U/D	M/P	PB	PhCharge
acetazolamid	-1.60	-1.29	0.52		1	1	2	-0.24	0.28	0.98	-1
amitriptyline	0.76	0.50	-0.45	0.89	1	1	2	-1.98	0.92	0.95	1
bupivacaine	0.16	0.03	1.25		1	1	2	-0.93	0.37	0.95	1
chloroquine	0.39	0.10	0.89		1	1	2	-3.27	2.65	0.55	2
citalopram	0.13	-0.03	-0.23		1	2	2	-2.37	1.03	0.80	1
clomipramine	0.79	0.44	-0.28		1	1	2	-2.26	1.13	0.98	1
colchicine	-0.93	-0.78	-1.99		1	2	4		0.95	0.39	0
diltiazem	-0.02	-0.40	-1.22		1	1	3	-1.74	0.99	0.75	1
doxepin	0.54	0.35	-0.18		1	1	5	-2.20	1.37	0.76	1
duloxetine	0.56	0.21	-0.65		1	1	3	-2.82	0.78	0.90	1
eletriptan	-0.19	-0.30	-0.84		1	1	3	-3.15	0.25	0.85	1
ethambutol	-0.86	-0.49	-0.52		0	1	2	-2.39	1.00	0.25	1
fluvoxamine	-0.14	-0.36	0.68		1	1	2	-2.19	1.33	0.79	1
gabapentin	-0.63	-0.47	-0.19		1	1	2	-0.29	1.00	0.03	0
gentamycin	-3.13	-2.65	-2.40		0	1	2	-2.57	0.36	0.15	5
hydrochlorotiazide	-1.62	-1.35	-2.29		0	1	2	-1.75	0.38	0.68	0
itraconazole	-0.66	-1.07	3.68		0	1	2	-0.73	1.14	1.00	0
ketorolac	-0.33	-0.40	0.23		1	1	2	-2.91	0.03	0.99	-1
levetiracetam	-0.93	-0.47	-1.02		1	1	3		1.00	0.10	0
lincomycin	-1.62	-1.47	-0.43		0		2	-1.58	0.15	0.70	1
mesalazine	-0.99	-0.79	-1.55		0	1	3	-5.30	2.69	0.43	-1
minoxidil	-1.00	-0.95	-0.18		1		3	-1.66	0.82	0.00	0
nitrendipine	-0.92	-1.22	-1.09		0	1	2	-4.41	0.30	0.99	0
ofloxacin	-0.66	-0.63	-1.97		0	1	2	-2.01	1.26	0.32	-1
oxcarbamazepine	-0.55	-0.47	-0.87		1		3	-6.53	0.50	0.40	0
pefloxacin	-0.52	-0.48	-1.44		0			-7.04	0.96	0.25	-1

pregabalin	-0.63	-0.47	-0.22		1	1	3	-0.57	0.55	0.00	0
primidone	-0.60	-0.38	-0.31		1	2	3	-5.06	0.72	0.70	0
propylthiouracil	-0.29	-0.11	-0.31		1	1	2	-0.43	0.17	0.82	0
quinine	-0.11	-0.18	-0.07		1	1	2	-2.08	0.23	0.70	1
rifampicin	-2.81	-2.98	-0.67		0	1	2	-2.24	0.40	0.89	1
rimantadine	0.26	0.13	0.43		1		3	-3.56	2.00	0.40	1
timolol	-0.85	-0.73	-0.06		0	1	2	-2.15	0.80	0.10	1
tinidazole	-1.35	-1.02	-0.65		1	1	3	-4.90	1.14	0.12	0
tramadol	0.01	0.02	-0.67		1	1	2	-2.41	2.30	0.20	1
trimethoprim	-1.33	-1.14	-1.90		1	1	2	-0.30	1.25	0.44	1
warfarin	-0.33	-0.47	-0.44		1	0	2	-2.70	0.00	0.99	-1

Table S2. Physicochemical properties of 37 APIs

API	a/b/n code[1]	DM	eH	eH-eL	eL[2]	HA	HD	log D	log P	MW[3]	pKa	PSA[4]	Sa[3]	V[3]
acetazolamid	0	0.89	-9.06	-9.13	0.69	5	2	-0.55	-0.26	2.22	7.44	11.50	4.69	2.9
amitriptyline	1	6.42	-9.9	-8.20	-17.01	1	0	3.15	4.41	2.77	9.18	0.32	3.61	1.56
bupivacaine	0	3.02	-9.03	-9.37	3.37	2	1	2.80	3.31	2.88	8.13	3.23	4.78	3.02
chloroquine	1	4.4	-8.6	-8.03	-5.71	3	1	1.87	4.41	3.20	10.47	2.82	5.94	3.11
citalopram	1	2.83	-7.98	-8.86	8.83	3	0	0.39	3.48	3.24	9.57	3.63	5.88	3.14
clomipramine	1	1.53	-8.49	-8.65	1.56	2	0	3.50	4.94	3.15	9.46	0.65	5.11	3.05
colchicine	0	5.95	-9.11	-8.52	-5.91	6	1	0.92	1.07	3.99		8.31	5.47	3.61
diltiazem	1	2.43	-8.71	-8.52	-1.86	4	0	2.10	4.73	4.15	8.94	5.91	6.17	3.96
doxepin	1	0.31	-9.11	-9.03	-0.81	2	0	2.08	3.84	2.79	9.40	1.25	4.69	2.81
duloxetine	1	0.96	-9.01	-8.63	-3.82	2	1	1.24	4.81	2.97	10.02	2.13	4.56	2.84
eletriptan	1	4.88	-8.5	-7.90	-5.96	3	1	0.36	2.98	3.83	10.35	5.32	4.69	3.57
ethambutol	1	1.11	-9.11	-11.45	23.39	4	4	-2.21	-0.29	2.04	9.59	6.45	4.95	2.18
fluvoxamine	1	3.9	-9.69	-8.87	-8.25	4	1	1.15	3.71	3.18	9.39	5.68	5.89	2.79
gabapentin	0	1.56	-9.35	-10.19	8.36	3	2	-1.31	1.08	1.71	7.50	6.33	2.38	1.7
gentamycin	1	4.31	-9.34	-11.20	18.62	12	8	-7.81	-2.04	4.78	9.77	19.97	4.71	4.25
hydrochlorotiazide	0	7.27	-9.64	-8.46	-11.83	5	3	-0.09	-0.02	2.98	8.95	11.84	3.85	2.01
itraconazole	0	6.11	-8.42	-7.65	-7.7	9	0	4.26	4.53	6.73	6.47	10.08	8.43	6.15
ketorolac	-1	2.14	-9.19	-8.83	-3.63	3	1	-0.95	2.68	2.55	4.29	5.93	3.87	2.39
levetiracetam	0	5.71	-9.8	-10.45	6.49	2	1	-0.67	-0.88	1.70		6.34	3.09	1.62
lincomycin	1	3.92	-8.5	-8.50	0.04	8	5	-0.48	0.72	4.07	8.78	12.60	6.35	3.89
mesalazine	-1	3.8	-8.18	-8.06	-1.23	4	3	-2.61	0.74	1.53	1.90	8.36	2.49	1.28
minoxidil	0	4.2	-8.07	-8.10	0.29	5	2	0.65	1.62	2.09	5.54	9.36	3.16	1.96
nitrendipine	0	6.92	-9.09	-8.00	-10.94	5	1	3.50	3.81	3.60	2.79	11.05	5.3	2.98
ofloxacin	-1	4.68	-8.72	-7.82	-8.97	7	1	-0.65	1.85	3.61	5.19	7.33	4.74	3.07
oxcarbamazepine	0	3.46	-9.31	-8.84	-4.73	2	1	1.25	1.66	2.52	13.73	6.34	3.02	2.26
pefloxacin	-1	9.41	-9.01	-7.97	-10.45	6	1	0.52	1.92	3.33	0.16	6.41	4.66	2.91
pregabalin	0	1.67	-9.53	-10.46	9.29	3	2	-1.38	1.09	1.59	7.77	6.33	3.54	1.65
primidone	0	2.84	-9.78	-9.77	-0.15	2	2	0.40	0.83	2.18	12.26	5.82	3.19	2.02

propylthiouracil	0	5.57	-9.2	-7.93	-12.71	1	2	1.18	1.15	1.70	7.63	4.11	3.32	1.51
quinine	1	1.73	-9.55	-9.54	-0.14	4	1	1.58	2.82	3.24	9.28	4.56	4.22	3.06
rifampicin	-1					14	6	-0.46	2.05	8.23	4.96	22.02		
rimantadine	1	1.22	-9.33	-12.28	29.54	1	1	0.08	3.31	1.79	10.76	2.60	2.43	1.91
timolol	1	3.06	-9.17	-8.05	-11.24	7	2	-1.39	1.28	3.16	9.35	7.97	4.95	2.88
tinidazole	0	2.34	-10.52	-9.24	-12.82	5	0	-0.27	-0.29	2.47	2.30	9.78	4.41	2
tramadol	1					3	1	0.36	2.32	2.63	9.61	3.27		
trimethoprim	0	2.09	-8.8	-8.68	-1.22	7	2	0.58	0.59	2.90	6.90	10.55	4.14	2.63
warfarin	-1	4.12	-7.38	-6.05	-13.35	3	1	-0.90	3.13	3.08	4.50	6.36	4.01	2.76

1 – code describing the acid-base properties: (-1) - acids; (0) - neutrals; (1) - bases

2 – multiplied by 10

3 – divided by 100

4 – divided by 10

Table S3. Chromatographic data and their derivatives obtained from NP TLC and RP TLC experiments

API	C_{NP}*	NP**	NP/C	NP/PSA	C_{RP}*	RP**	RP/C	RP/PSA	NP/B2	RP/B2	NP/PB	RP/PB	NP/logP	RP/logP
acetazolamid	0.94	0.94	1.00	0.817	0.97	0.96	0.99	0.834	-0.727	-0.742	0.959	0.980	-3.615	-3.692
amitriptyline	0.32	0.31	0.97	9.568	0.67	0.63	0.94	19.444	0.626	1.272	0.326	0.663	0.070	0.143
bupivacaine	0.67	0.67	1.00	2.072	0.74	0.75	1.01	2.319	22.666	25.372	0.705	0.789	0.202	0.227
chloroquine	0.17	0.17	1.00	0.604	0.40	0.30	0.75	1.065	1.763	3.111	0.309	0.545	0.039	0.068
citalopram	0.30	0.29	0.97	0.800	0.62	0.60	0.97	1.655	-8.745	-18.094	0.363	0.750	0.083	0.172
clomipramine	0.33	0.32	0.97	4.938	0.59	0.59	1.00	9.105	0.722	1.331	0.327	0.602	0.065	0.119
colchicine	0.79	0.77	0.97	0.927	0.91	0.91	1.00	1.095	-0.984	-1.163	1.974	2.333	0.720	0.850
diltiazem	0.49	0.49	1.00	0.829	0.76	0.72	0.95	1.219	-1.230	-1.808	0.653	0.960	0.104	0.152
doxepin	0.30	0.31	1.03	2.486	0.58	0.54	0.93	4.330	0.892	1.554	0.411	0.715	0.081	0.141
duloxetine	0.32	0.33	1.03	1.552	0.57	0.53	0.93	2.493	1.595	2.562	0.367	0.589	0.069	0.110
eletriptan	0.29	0.28	0.97	0.527	0.62	0.62	1.00	1.166	-0.922	-2.041	0.329	0.729	0.094	0.208
ethambutol	0.19	0.21	1.11	0.325	0.97	0.95	0.98	1.472	-0.433	-1.957	0.840	3.800	-0.724	-3.276
fluvoxamine	0.34	0.32	0.94	0.563	0.62	0.62	1.00	1.091	-0.883	-1.711	0.408	0.790	0.086	0.167
gabapentin	0.91	0.91	1.00	1.437	0.66	0.66	1.00	1.042	-1.952	-1.416	30.333	22.000	0.843	0.611
gentamycin	0.96	0.94	0.98	0.471	0.91	0.90	0.99	0.451	-0.355	-0.340	6.267	6.000	-0.461	-0.441
hydrochlorotiazide	0.96	0.96	1.00	0.811	0.97	0.96	0.99	0.811	-0.713	-0.713	1.414	1.414	-48.000	-48.000
itraconazole	0.96	0.97	1.01	0.962	0.86	0.84	0.98	0.833	-0.910	-0.788	0.972	0.842	0.214	0.185
ketorolac	0.92	0.91	0.99	1.535	0.96	0.96	1.00	1.619	-2.265	-2.389	0.919	0.970	0.340	0.358
levetiracetam	0.92	0.92	1.00	1.451	0.92	0.92	1.00	1.451	-1.968	-1.968	9.200	9.200	-1.045	-1.045
lincomycin	0.91	0.91	1.00	0.722	0.94	0.94	1.00	0.746	-0.620	-0.640	1.300	1.343	1.264	1.306
mesalazine	0.94	0.93	0.99	1.113	0.99	0.97	0.98	1.161	-1.178	-1.228	2.163	2.256	1.257	1.311
minoxidil	0.43	0.42	0.98	0.449	0.80	0.82	1.03	0.876	-0.442	-0.862			0.259	0.506
nitrendipine	0.97	0.97	1.00	0.878	0.86	0.86	1.00	0.779	-0.795	-0.705	0.980	0.869	0.255	0.226
ofloxacin	0.24	0.23	0.96	0.314	0.54	0.50	0.93	0.682	-0.367	-0.799	0.719	1.563	0.124	0.270
oxcarbamazepine	0.91	0.90	0.99	1.420	0.91	0.91	1.00	1.435	-1.926	-1.947	2.250	2.275	0.542	0.548
pefloxacin	0.30	0.29	0.97	0.452	0.76	0.70	0.92	1.092	-0.606	-1.463	1.160	2.800	0.151	0.365
pregabalin	0.76	0.76	1.00	1.200	0.41	0.41	1.00	0.648	-1.630	-0.880			0.697	0.376
primidone	0.90	0.93	1.03	1.598	0.93	0.97	1.04	1.667	-2.421	-2.525	1.329	1.386	1.120	1.169

propylthiouracil	0.94	0.94	1.00	2.285	0.93	0.93	1.00	2.261	-8.462	-8.372	1.146	1.134	0.817	0.809
quinine	0.30	0.29	0.97	0.636	0.66	0.64	0.97	1.404	-1.590	-3.508	0.414	0.914	0.103	0.227
rifampicin	0.73	0.77	1.05	0.350	0.95	0.94	0.99	0.427	-0.259	-0.316	0.865	1.056	0.376	0.459
rimantadine	0.92	0.92	1.00	3.536	0.95	0.95	1.00	3.651	7.040	7.270	2.300	2.375	0.278	0.287
timolol	0.34	0.32	0.94	0.401	0.97	0.97	1.00	1.216	-0.439	-1.331	3.200	9.700	0.250	0.758
tinidazole	0.89	0.88	0.99	0.900	0.94	0.93	0.99	0.951	-0.865	-0.914	7.333	7.750	-3.034	-3.207
tramadol	0.31	0.31	1.00	0.948	0.63	0.64	1.02	1.957	13.025	26.891	1.550	3.200	0.134	0.276
trimethoprim	0.57	0.59	1.04	0.559	0.84	0.83	0.99	0.787	-0.517	-0.727	1.341	1.886	1.000	1.407
warfarin	0.99	0.99	1.00	1.557	0.87	0.83	0.95	1.305	-2.104	-1.764	1.000	0.838	0.316	0.265

* Rf value from unimpregnated NP or RP plate (control)

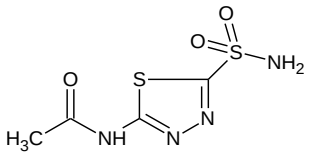
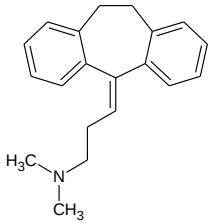
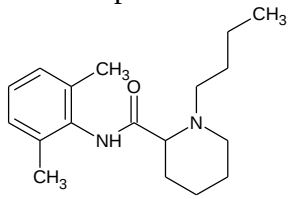
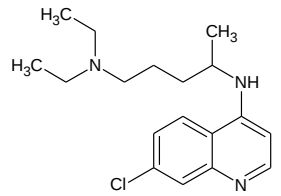
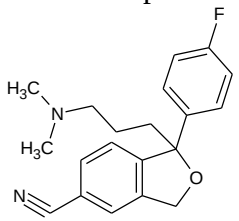
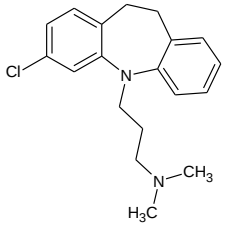
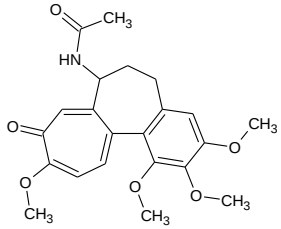
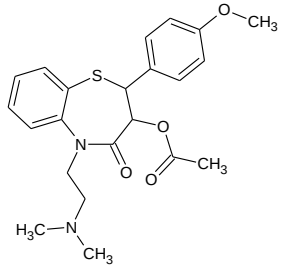
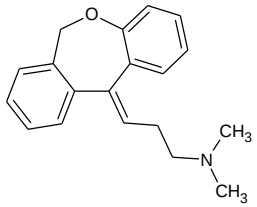
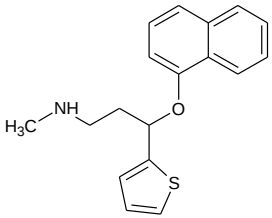
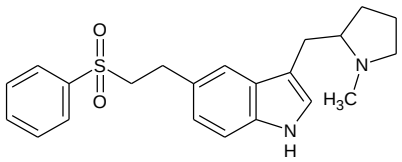
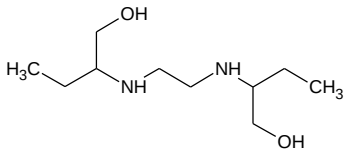
** Rf value from NP or RP plate impregnated with 2 mg/mL BSA solution

Table S4. Chromatographic data and their derivatives obtained from the $HPLC_{HSA}$ i $HPLC_{IAM}$ experiments

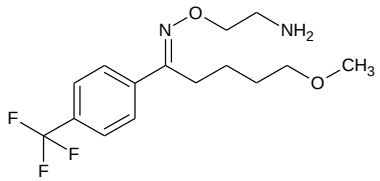
API	k_{HSA}	log k_{HSA}	log k_{HSA}/B2	log k_{HSA}/PB	log k_{HSA}/log P	k_{IAM}	log k_{IAM}
acetazolamid	0.74	-0.13	-0.575	0.760	-2.863	2.90	0.46
amitriptyline	5.87	0.77	11.854	6.178	1.331	1.56	0.19
bupivacaine	1.18	0.07	40.084	1.247	0.358	3.02	0.48
chloroquine	18.05	1.26	187.127	32.812	4.092	3.11	0.49
citalopram	2.67	0.43	-80.418	3.333	0.766	3.14	0.50
clomipramine	9.09	0.96	20.510	9.278	1.841	3.05	0.48
colchicine	0.28	-0.55	-0.362	0.726	0.265	3.61	0.56
diltiazem	1.74	0.24	-4.362	2.316	0.367	3.96	0.60
doxepin	4.25	0.63	12.220	5.624	1.106	2.81	0.45
duloxetine	8.16	0.91	39.435	9.063	1.696	2.84	0.45
eletriptan	3.78	0.58	-12.429	4.441	1.267	3.57	0.55
ethambutol	1.73	0.24	-3.557	6.906	-5.953	2.18	0.34
fluvoxamine	0.25	-0.60	-0.696	0.321	0.068	2.79	0.45
gabapentin	0.15	-0.84	-0.312	4.843	0.135	1.70	0.23
gentamycin	1.50	0.18	-0.568	10.028	-0.737	4.25	0.63
hydrochlorotiazide	0.61	-0.22	-0.452	0.897	-30.451	2.01	0.30
itraconazole	9.65	0.98	-9.055	9.668	2.130	6.15	0.79
ketorolac	9.65	0.98	-24.017	9.747	3.601	2.39	0.38
levetiracetam	0.07	-1.16	-0.149	0.696	-0.079	1.62	0.21
lincomycin	0.82	-0.08	-0.560	1.175	1.142	3.89	0.59
mesalazine	0.18	-0.73	-0.234	0.430	0.250	1.28	0.11
minoxidil	0.40	-0.40	-0.422		0.248	1.96	0.29
nitrendipine	3.55	0.55	-2.906	3.581	0.931	2.98	0.47
ofloxacin	6.62	0.82	-10.566	20.673	3.576	3.07	0.49
oxcarbamazepine	0.40	-0.40	-0.846	0.988	0.238	2.26	0.35
pefloxacin	12.43	1.09	-25.980	49.720	6.474	2.91	0.46
pregabalin	0.14	-0.87	-0.291		0.124	1.65	0.22
primidone	0.22	-0.66	-0.569	0.312	0.263	2.02	0.31

propylthiouracil	0.33	-0.48	-2.950	0.400	0.285	1.51	0.18
quinine	2.59	0.41	-14.194	3.699	0.918	3.06	0.49
rifampicin	0.03	-1.53	-0.010	0.034	0.015	8.37	0.92
rimantadine	0.16	-0.80	1.222	0.399	0.048	1.91	0.28
timolol	0.13	-0.88	-0.179	1.304	0.102	2.88	0.46
tinidazole	0.12	-0.92	-0.118	0.997	-0.413	2.00	0.30
tramadol	1.08	0.03	45.221	5.381	0.464	3.90	0.59
trimethoprim	0.85	-0.07	-0.749	1.943	1.449	2.63	0.42
warfarin	13.86	1.14	-29.454	14.001	4.428	2.76	0.44

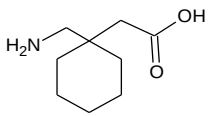
Table S5. Structures of 37 APIs

1. acetazolamid	2. amitriptyline	3. bupivacaine	4. chloroquine
			
5. citalopram	6. clomipramine	7. colchicine	8. diltiazem
			
9. doxepin	10. duloxetine	11. eletriptan	12. ethambutol
			

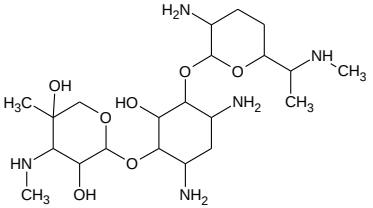
13. fluvoxamine



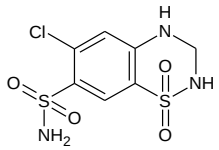
14. gabapentin



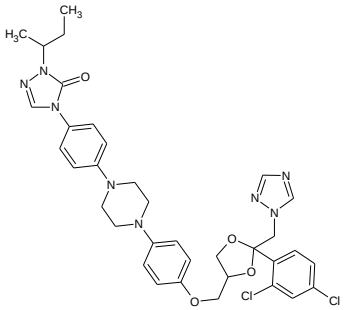
15. gentamicin



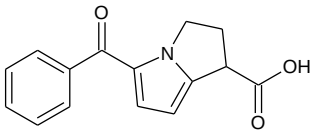
16. hydrochlorotiazide



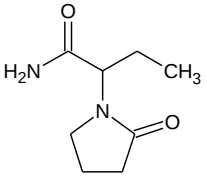
17. itraconazole



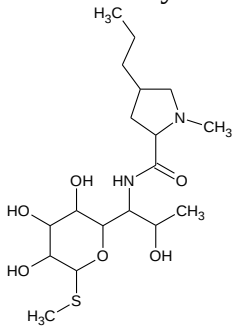
18. ketorolac



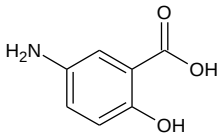
19. levetiracetam



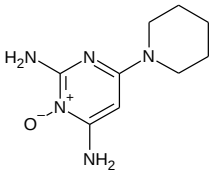
20. lincomycin



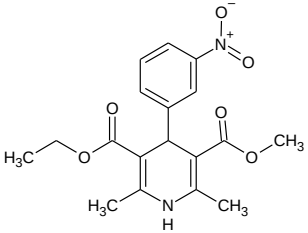
21. mesalazine



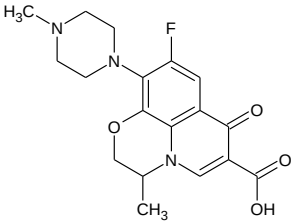
22. minoxidil



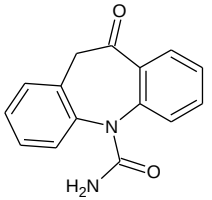
23. nitrendipine



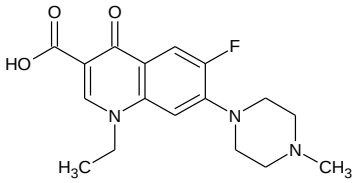
24. ofloxacin



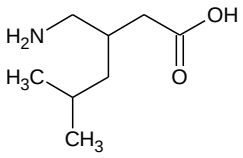
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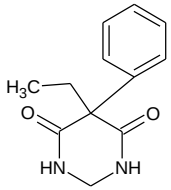
26. pefloxacin



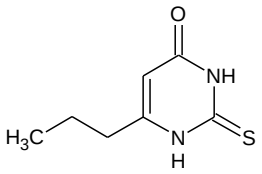
27. pregabalin



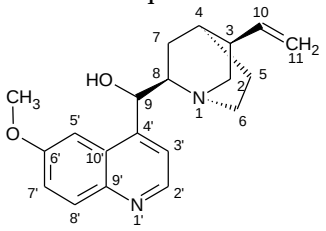
28. primidone



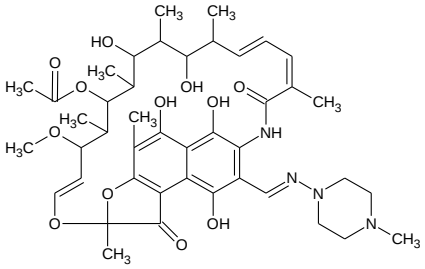
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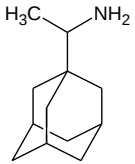
30. quinine



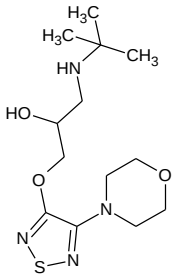
31. rifampicin



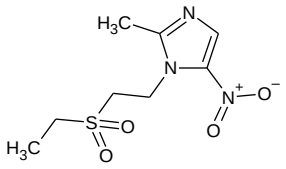
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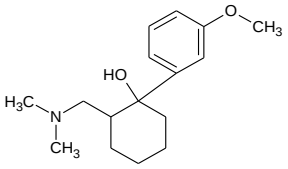
33. timolol



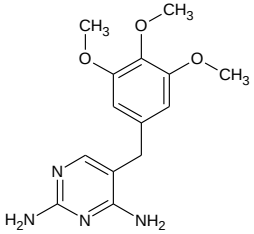
34. tinidazole



35. tramadol



36. trimethoprim



37. warfarin

