

TABLE S1

Five rankings of pharmaceuticals in the PEIAR database. Rankings differ in the combination of data categories used to create them (Table 3). Uncertainty values indicate the amount of missing data; larger values indicate larger data gaps.

Name	Class-Subclass	Aquatic Env		ECOSAR		All Data		All-ECOSAR		Most Data	
		Rank	Uncertainty value	Rank	Rank	Uncertainty Value	Rank	Uncertainty Value	Rank	Uncertainty value	
Erythromycin Base	Al-abio	1	0.430493274	61	5	0.528746466	6	0.798876404	154	0.671304348	
Oxytetracycline (anhydrous)	Al-abio	2	0.562780269	276	10	0.724787936	4	0.806741573	235	0.883478261	
Sulfamethoxazole	Al-abio	3	0.488789238	64	2	0.424128181	3	0.797752809	25	0.795096322	
Fluoxetine Hydrochloride	CNS-psy	4	0.365470852	13	8	0.315739868	11	0.77752809	1	0.77408056	
Nitroglycerin	CRD-ah/di	5	0.5	93	13	0.560791706	14	0.830337079	60	0.781085814	
Clofibrate	CRD-alip	6	0.524663677	26	12	0.605089538	13	0.759550562	172	0.744347826	
Ibuprofen	CNS-ana	7	0.428251121	47	1	0.318567389	2	0.737078652	22	0.65323993	
Acetaminophen	CNS-ana	8	0.459641256	91	3	0.356267672	1	0.735955056	6	0.753064799	
Estradiol	HOR-sex	9	0.452914798	12	18	0.461828464	27	0.791011236	42	0.711033275	
Diclofenac Sodium	CNS-ana	10	0.428251121	124	23	0.57869934	17	0.770786517	102	0.929947461	
Caffeine	RESP	11	0.562780269	107	11	0.586239397	9	0.747191011	77	0.907180385	
Carvedilol	CRD-ah/di	12	0.493273543	44	20	0.496701225	24	0.784269663	88	0.893169877	
Metronidazole	Al-oth	13	0.614349776	111	27	0.627709708	25	0.841573034	54	0.758318739	
Trimethoprim	Al-abio	14	0.578475336	72	6	0.440150801	8	0.742696629	34	0.747810858	
Tetracycline Hydrochloride	Al-abio	15	0.68161435	146	15	0.681432611	12	0.782022472	241	0.822608696	
Propranolol Hydrochloride	CRD-ah/di	16	0.717488789	116	29	0.652214892	26	0.835955056	166	0.636521739	
Gemfibrozil	CRD-alip	17	0.470852018	20	14	0.474081056	21	0.77752809	83	0.882661996	
Naproxen	CNS-ana	18	0.560538117	73	7	0.422243167	7	0.912359551	58	0.887915937	
Diazepam	CNS-psy	19	0.522421525	46	4	0.374175306	5	0.739325843	40	0.702276708	
Paroxetine	CNS-ana	20	0.535874439	78	33	0.481621112	31	0.814606742	68	0.88441331	
Clarithromycin	Al-abio	21	0.531390135	39	28	0.528746466	32	0.801123596	92	0.903677758	
Amitriptyline Hydrochloride	CNS-psy	22	0.641255605	74	21	0.512723845	19	0.984269663	87	0.891418564	
Carbamazepine	CNS-oth	23	0.547085202	68	9	0.518378888	10	0.841573034	136	1	
Risperidone	CNS-psy	24	0.569506726	34	38	0.535344015	46	0.947191011	79	0.866900175	
Nitrofurazone	Al-abio	25	0.643497758	38	60	0.715362865	81	0.980898876	107	0.956217163	
Chloramphenicol	Al-abio	26	0.578475336	19	26	0.597549482	33	0.808988764	50	0.742556918	
Codeine Phosphate (anhydrous)	CNS-ana	27	0.659192825	132	56	0.603204524	44	0.84494382	14	0.633975482	
Phenobarbital	CNS-oth	28	0.616591928	147	48	0.676720075	36	0.817977528	144	0.756521739	
Fosinopril sodium	CRD-ah/di	29	0.360986547	233	102	0.638077286	74	0.95505618	103	0.936952715	

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Fenofibrate	CRD-alip	30	0.51793722	6	37	0.484448633	56	0.883146067	49	0.740805604	
Furosemide	CNS-oth	31	0.641255605	104	17	0.471253534	15	0.791011236	86	0.88966725	
Sulfamethazine	Al-abio	32	0.621076233	56	64	0.717247879	78	0.973033708	108	0.957968476	
Atenolol	CRD-ah/di	33	0.623318386	117	22	0.471253534	16	0.9	12	0.630472855	
Dicyclomine Hydrochloride	GAS	34	0.405829596	16	58	0.53063148	87	0.996629213	8	0.61821366	
Cimetidine	GAS	35	0.600896861	103	46	0.650329877	38	0.824719101	90	0.896672504	
Lisinopril Dihydrate	CRD-ah/di	36	0.401345291	255	45	0.459000943	29	0.797752809	21	0.665499124	
Streptomycin	Al-abio	37	0.674887892	164	98	0.820923657	73	0.970786517	134	1	
Simvastatin	CRD-alip	38	0.540358744	7	35	0.412818096	51	0.937078652	19	0.647985989	
Verapamil Hydrochloride	CRD-ah/di	39	0.52690583	121	24	0.486333648	18	0.92247191	105	0.949211909	
Nicotinic Acid/Niacin	NUT	40	0.576233184	135	88	0.673892554	70	0.948314607	65	0.798598949	
Budesonide	HOR-oth	41	0.674887892	76	67	0.622997172	71	0.949438202	127	1	
Ethinyl Estradiol	HOR-sex	42	0.567264574	10	19	0.362865221	28	0.898876404	10	0.625218914	
Chlortetracycline	Al-abio	43	0.692825112	95	44	0.722902922	39	0.833707865	150	0.526956522	
Ciprofloxacin	Al-abio	44	0.618834081	144	30	0.564561734	20	0.774157303	45	0.840630473	
Promethazine Hydrochloride	RESP	45	0.470852018	45	54	0.463713478	65	0.935955056	2	0.691768827	
Norethindrone	HOR-sex	46	0.609865471	42	63	0.571159284	82	0.982022472	69	0.915936953	
Sertraline Hydrochloride	CNS-psy	47	0.448430493	75	55	0.43732328	61	0.929213483	9	0.619964974	
Nefazodone Hydrochloride	CNS-psy	48	0.558295964	269	138	0.762488219	102	1	269	0.900869565	
Atorvastatin Calcium	CRD-alip	49	0.587443946	174	77	0.567389255	55	0.91011236	153	0.532173913	
Diltiazem	CRD-ah/di	50	0.569506726	218	70	0.57869934	48	0.859550562	89	0.894921191	
Nystatin	Al-oth	51	0.48206278	83	92	0.58529689	96	1	73	0.824868651	
Doxazosin Mesylate	CRD-ah/di	52	0.511210762	36	74	0.538171536	92	1	16	0.670753065	
Zolpidem Tartrate	CNS-oth	53	0.529147982	313	87	0.558906692	60	0.925842697	38	0.697022767	
Norfloxacin	Al-abio	54	0.659192825	151	122	0.786993402	95	1	116	0.987740806	
Paroxetine Hydrochloride	CNS-psy	55	0.531390135	79	39	0.448633365	37	0.897752809	11	0.625218914	
Sulfadiazine	Al-abio	56	0.834080717	89	118	0.820923657	129	0.662582469	163	0.737391304	
Amphetamine (Alpha-Meythylphenethylamine)	CNS-oth	57	0.565022422	60	36	0.477851084	40	0.834831461	7	0.614711033	
Levofloxacin	Al-abio	58	0.874439462	252	120	0.763430726	88	0.995505618	200	0.660869565	
Albuterol Sulfate (salbutamol)	RESP	59	0.621076233	66	32	0.434495759	30	0.8	3	0.611208406	
Tramadol Hydrochloride	CNS-ana	60	0.708520179	306	113	0.67200754	85	0.992134831	185	0.620869565	
Venlafaxine Hydrochloride	CNS-psy	61	0.596412556	82	59	0.518378888	62	0.93258427	4	0.704028021	
Omeprazole	GAS	62	0.632286996	32	40	0.509896324	50	0.905617978	33	0.684763573	
Clonidine Hydrochloride	CRD-ah/di	63	0.576233184	71	42	0.500471254	42	0.840449438	17	0.642732049	
Terazosin Hydrochloride Dihydrate	CRD-ah/di	64	0.587443946	303	149	0.716305372	111	0.699340245	106	0.954465849	

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Azithromycin	Al-abio	65	0.589686099	35	16	0.374175306	23	0.788764045	20	0.798598949	
Prednisone	HOR-oth	66	0.650224215	98	84	0.561734213	83	0.984269663	35	0.6882662	
Enalapril Maleate	CRD-ah/di	67	0.594170404	222	97	0.618284637	69	0.94494382	51	0.751313485	
Tolterodine tartrate	Al-abio	68	0.587443946	304	146	0.705937795	110	0.815268615	111	0.968476357	
Roxithromycin	Al-abio	69	0.679372197	54	82	0.728557964	94	1	202	0.796521739	
Lomefloxacin	Al-abio	70	0.670403587	139	141	0.818096136	131	0.657869934	143	0.67826087	
Hydrocodone	CRD-oth	71	0.587443946	67	65	0.470311027	75	0.96741573	5	0.61295972	
Acetylsalicylic acid	CNS-ana	72	0.697309417	125	43	0.625824694	35	0.813483146	71	0.861646235	
Ampicillin	Al-abio	73	0.614349776	112	143	0.763430726	147	0.767200754	130	1	
Phenazopyridine Hydrochloride	CNS-ana	74	0.591928251	87	128	0.670122526	143	0.763430726	98	0.91943958	
Methylphenidate Hydrochloride	CNS-oth	75	0.639013453	122	112	0.630537229	98	1	23	0.65849387	
Niacin	CRD-alip	76	0.639013453	136	140	0.712535344	135	0.61734213	66	0.900175131	
Digoxin	CRD-oth	77	0.69955157	99	25	0.492931197	22	0.782022472	64	0.821366025	
Naproxen Sodium	CNS-ana	78	0.67264574	268	131	0.657869934	93	1	186	0.622608696	
Minocycline Hydrochloride	Al-abio	79	0.656950673	261	167	0.743638077	137	0.737983035	93	0.905429072	
Butalbital	CNS-psy	80	0.627802691	140	169	0.754005655	155	0.739868049	147	0.532173913	
Cephalexin	Al-abio	81	0.67264574	133	73	0.568331762	59	0.923595506	37	0.712784588	
Isosorbide Mononitrate	CRD-ah/di	82	0.670403587	143	66	0.613572102	54	0.882022472	36	0.690017513	
Warfarin Sodium Salt	MISC	83	0.899103139	120	89	0.671065033	79	0.974157303	118	0.99474606	
Losartan Potassium	CRD-ah/di	84	0.64573991	30	75	0.51460886	97	1	47	0.726795096	
Sulfafurazole	Al-abio	85	0.760089686	51	93	0.718190386	113	0.67200754	99	0.921190893	
Fentanyl Transdermal System	CNS-ana	86	0.616591928	25	81	0.581526861	105	1	41	0.709281961	
Captopril	CRD-ah/di	87	0.66367713	106	79	0.65598492	72	0.952808989	56	0.840630473	
Lansoprazole	GAS	88	0.903587444	250	76	0.691800189	53	0.879775281	168	0.580869565	
Enoxacin	Al-abio	89	0.688340807	149	188	0.838831291	178	0.725730443	146	0.75826087	
Methocarbamol	CNS-oth	90	0.670403587	130	165	0.747408106	160	0.757775683	110	0.961471103	
Glyburide	HOR-oth	91	0.607623318	8	71	0.481621112	99	1	24	0.663747811	
Cefaclor	Al-abio	92	0.677130045	131	172	0.773798303	170	0.771913289	119	0.992994746	
Carisoprodol	CNS-oth	93	0.643497758	59	95	0.573986805	114	0.589066918	32	0.751313485	
Sulfathiazole	Al-abio	94	0.742152466	57	134	0.774740811	180	0.845428841	124	1	
Amoxicillin	Al-abio	95	0.670403587	101	52	0.501413761	52	0.870786517	13	0.735551664	
Felodipine	CRD-ah/di	96	0.621076233	9	107	0.62393968	165	0.747408106	78	0.851138354	
Tobramycin	Al-abio	97	0.710762332	166	187	0.807728558	164	0.647502356	101	0.936952715	
Vancomycin	Al-abio	98	0.701793722	153	151	0.796418473	128	0.670122526	121	1	
Bacitracin	Al-abio	99	0.919282511	177	168	0.898209237	138	0.762488219	274	0.911304348	
Kanamycin A	Al-abio	100	0.713004484	248	204	0.867106503	194	0.8133836	140	0.669565217	

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			value								Value
Diltiazem Hydrochloride	CRD-ah/di	101	0.719730942	40	51	0.529688973	64	0.943820225	59	0.772329247	
Nabumetone	CNS-ana	102	0.634529148	29	109	0.625824694	156	0.6399623	67	0.812609457	
Amlodipine Besylate	CRD-ah/di	103	0.639013453	49	41	0.440150801	43	0.902247191	18	0.679509632	
Ceftriaxone	AI-abio	104	0.724215247	196	196	0.843543827	182	0.800188501	128	1	
Probucol	CRD-alip	105	0.607623318	1	126	0.674835061	199	0.844486334	148	0.740869565	
Irbesartan	CRD-ah/di	106	0.609865471	245	159	0.672950047	122	0.786993402	215	0.699130435	
Mirtazapine d	CNS-psy	107	0.612107623	262	178	0.725730443	146	0.705937795	240	0.794782609	
Lovastatin	CRD-alip	108	0.625560538	11	78	0.538171536	108	0.688972667	48	0.732049037	
Ceftriaxone sodium	AI-abio	109	0.726457399	197	199	0.844486334	186	0.779453346	129	1	
Ofloxacin	AI-abio	110	0.894618834	272	96	0.7332705	68	0.942696629	189	0.732173913	
Bupropion Hydrochloride	CNS-psy	111	0.728699552	181	139	0.675777568	103	1	28	0.749562172	
Temazepam	CNS-psy	112	0.66367713	70	68	0.576814326	76	0.969662921	53	0.847635727	
Itraconazole	AI-oth	113	0.621076233	246	198	0.795475966	184	0.719132893	271	0.906086957	
Indomethacin	CNS-ana	114	0.746636771	41	31	0.57869934	34	0.894382022	120	0.99474606	
Clotrimazole	AI-oth	115	0.621076233	2	49	0.53063148	77	0.97752809	84	0.894921191	
Clonazepam	CNS-oth	116	0.661434978	53	47	0.499528746	58	0.914606742	26	0.672504378	
Famotidine	GAS	117	0.769058296	127	160	0.757775683	154	0.686145146	112	0.971978984	
Loratadine	RESP	118	0.625560538	3	57	0.547596607	90	1	80	0.900175131	
Amikacin	AI-abio	119	0.730941704	169	180	0.845428841	151	0.796418473	142	0.667826087	
Meclizine Hydrochloride (monohydrate)	RESP	120	0.623318386	256	179	0.724787936	148	0.673892554	238	0.784347826	
Desogestrel	HOR-sex	121	0.627802691	85	145	0.684260132	168	0.898209237	181	0.613913043	
Bisoprolol Fumarate	CRD-ah/di	122	0.905829596	77	132	0.75871819	152	0.750235627	152	0.627826087	
Hydrocortisone	HOR-oth	123	0.683856502	97	150	0.711592837	167	0.743638077	109	0.95971979	
Ferrous Fumarate	NUT	124	0.69955157	113	127	0.634307257	118	0.820923657	46	0.77408056	
Valacyclovir	AI-oth	125	0.739910314	310	175	0.75871819	145	0.684260132	70	0.816112084	
Folic Acid	NUT	126	0.923766816	161	158	0.798303487	130	0.638077286	193	0.673043478	
Lorazepam	CNS-psy	127	0.67264574	58	91	0.542884072	106	0.566446748	27	0.674255692	
Carbenicillin	AI-abio	128	0.692825112	134	182	0.800188501	183	0.811498586	178	0.608695652	
Meloxicam	CNS-ana	129	0.656950673	90	136	0.672950047	159	0.672950047	138	0.754782609	
Norgestimate	HOR-sex	130	0.639013453	5	83	0.511781338	123	0.639019793	44	0.718038529	
Fluvastatin Sodium	CRD-alip	131	0.641255605	123	171	0.727615457	174	0.754005655	223	0.775652174	
Extended Phenytoin Sodium	CNS-oth	132	0.67264574	154	62	0.629594722	47	0.849438202	162	0.659130435	
Cyclobenzaprine Hydrochloride	CNS-oth	133	0.643497758	69	106	0.566446748	120	0.763430726	91	0.900175131	
Spironolactone	CRD-oth	134	0.674887892	43	53	0.543826579	66	0.939325843	55	0.828371278	
Donepezil Hydrochloride	CNS-oth	135	0.751121076	219	185	0.786050895	162	0.812441093	95	0.908931699	

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Methylprednisolone	HOR-oth	136	0.695067265	88	100	0.618284637	100	1	63	0.793345009	
Ketoconazole	AI-oth	137	0.65470852	17	80	0.590009425	109	0.625824694	104	0.940455342	
Gatifloxacin	AI-abio	138	0.755605381	234	194	0.8133836	176	0.737983035	115	0.985989492	
Propoxyphene Napsylate	CNS-ana	139	0.659192825	157	135	0.61734213	107	0.62393968	156	0.55826087	
Levothyroxine Sodium	HOR-oth	140	0.661434978	253	69	0.549481621	45	0.892134831	149	0.704347826	
Levonorgestrel	HOR-sex	141	0.67264574	27	105	0.589066918	149	0.716305372	62	0.786339755	
Norgestrel	HOR-sex	142	0.674887892	28	117	0.654099906	172	0.773798303	117	0.989492119	
Dexamethasone	HOR-oth	143	0.704035874	94	116	0.705937795	121	0.745523091	139	0.556521739	
Atomoxetine HCl	CNS-oth	144	0.764573991	173	186	0.779453346	163	0.664467484	97	0.912434326	
Nifedipine	CRD-oth	145	0.69955157	31	125	0.654099906	179	0.724787936	76	0.84938704	
Sulfonamide	AI-abio	146	0.751121076	86	147	0.767200754	171	0.727615457	96	0.910683012	
Nalidixic acid	AI-abio	147	0.715246637	119	133	0.772855796	124	0.650329877	197	0.68173913	
Felodipine	CRD-ah/di	148	0.68161435	229	205	0.807728558	196	0.843543827	264	0.890434783	
Zolpidem	CNS-psy	149	0.683856502	24	85	0.496701225	112	0.630537229	31	0.690017513	
Griseofulvin (microsize)	AI-oth	150	0.721973094	81	155	0.739868049	188	0.838831291	165	0.714782609	
Gabapentin	CNS-oth	151	0.773542601	158	154	0.686145146	126	0.674835061	52	0.753064799	
Quinapril Hydrochloride	CRD-ah/di	152	0.688340807	126	94	0.613572102	84	0.991011236	159	0.603478261	
Pravastatin Sodium	CRD-alip	153	0.764573991	114	124	0.650329877	116	0.705937795	39	0.707530648	
Benazepril Hydrochloride	CRD-ah/di	154	0.695067265	178	163	0.664467484	132	0.75871819	184	0.617391304	
Glipizide	HOR-oth	155	0.721973094	37	99	0.56267672	139	0.675777568	30	0.677758319	
Medroxyprogesterone Acetate	HOR-sex	156	0.697309417	14	101	0.57869934	158	0.798303487	61	0.782837128	
Betamethasone Dipropionate	HOR-oth	157	0.706278027	22	123	0.639019793	185	0.786050895	94	0.912434326	
Penicillin V Potassium	AI-abio	158	0.773542601	165	176	0.737983035	150	0.711592837	208	0.692173913	
Methotrexate	AN	159	0.791479821	138	86	0.729500471	67	0.941573034	114	0.985989492	
Cefuroxime Axetil	AI-abio	160	0.744394619	96	174	0.754005655	198	0.795475966	135	1	
Quinine sulfate	AI-oth	161	0.704035874	286	152	0.750235627	115	0.571159284	250	0.819130435	
Tamoxifen Citrate	HOR-oth	162	0.834080717	23	111	0.699340245	166	0.673892554	43	0.716287215	
Methyltestosterone	HOR-sex	163	0.706278027	18	90	0.653157399	136	0.672950047	141	0.747826087	
Ramipril	CRD-ah/di	164	0.706278027	65	114	0.589066918	142	0.690857681	85	0.88441331	
Alprazolam	CNS-psy	165	0.728699552	21	34	0.428840716	41	0.891011236	15	0.635726795	
Ceftiofur	AI-abio	166	0.968609865	194	234	0.986804901	227	0.811498586	298	0.994782609	
Triamcinolone Acetonide	CNS-ana	167	0.735426009	308	166	0.673892554	134	0.774740811	137	0.627826087	
Topiramate	CNS-oth	168	0.795964126	305	121	0.745523091	89	1	113	0.975481611	
Amlodipine Besylate	CRD-ah/di	169	0.721973094	171	156	0.6399623	117	0.654099906	157	0.551304348	
Hydrochlorothiazide	CRD-ah/di	170	0.874439462	145	61	0.610744581	49	0.862921348	125	1	
Fexofenadine Hydrochloride	RESP	171	0.733183857	84	115	0.571159284	127	0.634307257	74	0.831873905	

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Allopurinol	CNS-ana	172	0.793721973	110	72	0.622997172	63	0.933707865	57	0.765323993	
Triamterene	CRD-oth	173	0.766816143	63	50	0.505183789	57	0.892134831	29	0.69352014	
Acyclovir	AI-oth	174	0.807174888	142	170	0.771913289	157	0.730442978	122	1	
Citalopram hydrobromide	CNS-psy	175	0.744394619	206	184	0.719132893	161	0.7332705	207	0.68	
Metoclopramide Hydrochloride	GAS	176	0.746636771	33	130	0.638077286	187	0.807728558	100	0.926444834	
Metaxalone	CNS-oth	177	0.746636771	52	144	0.673892554	195	0.725730443	132	1	
Trazodone Hydrochloride	CNS-ana	178	0.748878924	307	129	0.662582469	91	1	192	0.63826087	
Benzonatate	RESP	179	0.753363229	115	189	0.760603205	202	0.79736098	211	0.749565217	
Doxepin Hydrochloride	CNS-psy	180	0.760089686	15	142	0.690857681	212	0.770028275	123	1	
Cephalothin	AI-abio	181	0.807174888	199	240	0.915174364	236	0.8133836	246	0.913043478	
Hydroxyzine Hydrochloride	RESP	182	0.764573991	62	148	0.673892554	191	0.783223374	131	1	
Alendronate Sodium	MISC	183	0.908071749	167	173	0.737983035	144	0.673892554	169	0.587826087	
Hydrocodone Bitartrate	CNS-ana	184	0.771300448	239	164	0.647502356	133	0.772855796	151	0.526956522	
Cefoxitin	AI-abio	185	0.816143498	192	245	0.911404336	242	0.832233742	243	0.897391304	
Hyoscyamine Sulfate	GAS	186	0.789237668	240	218	0.830348728	211	0.766258247	253	0.864347826	
Hyoscyamine Sulfate	GAS	187	0.789237668	241	219	0.831291235	214	0.776625825	255	0.907826087	
Oxybutynin Chloride	GAS	188	0.791479821	55	153	0.683317625	200	0.753063148	126	1	
Salmeterol Xinafoate	RESP	189	0.937219731	298	230	0.916116871	224	0.8133836	265	0.892173913	
Brimonidine tartrate	CRD-ah/di	190	0.852017937	180	223	0.867106503	218	0.830348728	183	0.615652174	
Dextroamphetamine Salts	CNS-oth	191	0.802690583	216	110	0.815268615	80	0.975280899	297	0.993043478	
Nortriptyline Hydrochloride	CNS-psy	192	0.804932735	92	103	0.701225259	104	1	179	0.747826087	
Cefprozil	AI-abio	193	0.838565022	108	197	0.798303487	222	0.78793591	209	0.753043478	
Nitrofurantoin	AI-abio	194	0.849775785	48	108	0.688972667	141	0.818096136	81	0.910683012	
Gemifloxacin mesylate	AI-abio	195	0.869955157	235	248	0.914231857	245	0.911404336	222	0.72	
Fluconazole	AI-oth	196	0.831838565	230	200	0.753063148	189	0.760603205	203	0.674782609	
Divalproex Sodium	CNS-oth	197	0.83632287	155	161	0.7332705	140	0.712535344	206	0.695652174	
Amoxicillin Trihydrate	AI-abio	198	0.838565022	102	202	0.79736098	234	0.986804901	205	0.751304348	
Estradiol	HOR-sex	199	0.937219731	227	206	0.815268615	197	0.798303487	195	0.650434783	
Lamotrigine	CNS-oth	200	0.887892377	249	162	0.812441093	125	0.654099906	190	0.633043478	
Pseudoephedrine Sulfate	RESP	201	0.843049327	284	256	0.909519321	253	0.866163996	283	0.949565217	
Loracarbef	AI-abio	202	0.865470852	129	226	0.868991517	249	0.852968897	248	0.817391304	
Pantoprazole Sodium Sesquihydrate	GAS	203	0.84529148	279	193	0.725730443	175	0.75871819	180	0.693913043	
Metformin Hydrochloride	HOR-oth	204	0.943946188	148	104	0.658812441	86	0.993258427	133	1	
Cefotaxime	AI-abio	205	0.856502242	100	216	0.853911404	258	0.873704053	233	0.84173913	
Cefditoren pivoxil	AI-abio	206	0.903587444	189	254	0.918001885	251	0.861451461	230	0.845217391	

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Codeine Phosphate	CNS-ana	207	0.865470852	210	195	0.725730443	177	0.703110273	175	0.59826087	
Tamsulosin hydrochloride	MISC	208	0.867713004	301	209	0.788878417	203	0.751178134	219	0.834782609	
Cetirizine Hydrochloride/ Cetirizine dihydrochloride	RESP	209	0.923766816	201	192	0.731385485	173	0.737983035	160	0.563478261	
Ranitidine Hydrochloride	GAS	210	0.887892377	293	203	0.751178134	193	0.725730443	187	0.627826087	
Rosuvastatin	CRD-alip	211	0.899103139	297	228	0.824693685	223	0.867106503	229	0.754782609	
Cefixime	Al-abio	212	0.901345291	109	231	0.866163996	263	0.899151744	232	0.829565217	
Propoxyphene Napsylate	CNS-ana	213	0.912556054	283	201	0.737983035	190	0.7332705	170	0.584347826	
Doxycycline Hyclate	Al-abio	214	0.917040359	220	224	0.8133836	219	0.831291235	221	0.71826087	
Sumatriptan Succinate	CNS-ana	215	0.975336323	300	238	0.867106503	233	0.934967012	236	0.773913043	
Clindamycin Hydrochloride	Al-abio	216	0.919282511	162	221	0.808671065	220	0.784165881	216	0.709565217	
Ranitidine	GAS	217	0.979820628	292	191	0.783223374	169	0.754005655	191	0.636521739	
Latamoxef	Al-abio	218	0.941704036	105	252	0.91328935	281	0.950989632	245	0.813913043	
Ipratropium Bromide	RESP	219	0.950672646	150	229	0.824693685	239	0.824693685	214	0.714782609	
Fosfomycin	Al-abio	220	0.964125561	232	278	0.952874647	272	0.959472196	281	0.937391304	
Oxytetracycline (dihydrate)	Al-abio	221	0.97309417	277	288	0.981149859	285	0.960414703	291	0.975652174	
Pseudoephedrine HCl	RESP	222	0.979820628	159	227	0.811498586	231	0.866163996	198	0.667826087	
Apramycin	Al-abio	223	0.993273543	168	294	0.994344958	295	0.992459943	295	0.989565217	
Neomycin	Al-abio	224	0.997757848	170	261	0.946277097	259	0.882186616	280	0.930434783	
Pantoprazole sodium	GAS	225	1	278	137	0.737983035	101	1	182	0.706086957	
Esomeprazole Magnesium	GAS	226	1	225	157	0.730442978	119	0.691800189	167	0.579130435	
Desloratadine	RESP	227	1	215	183	0.811498586	153	0.683317625	225	0.733913043	
Oxycodone Hydrochloride	CNS-ana	228	1	128	190	0.7332705	181	0.695570217	145	0.699130435	
Meclizine Hydrochloride (anhydrous)	RESP	229	1	4	119	0.691800189	192	0.731385485	72	0.817863398	
Fluticasone Propionate	CNS-ana	230	1	231	208	0.752120641	201	0.737983035	155	0.542608696	
Metoprolol Succinate	CRD-ah/di	231	1	259	210	0.757775683	204	0.867106503	158	0.553043478	
Conjugated Estrogens	HOR-sex	232	1	213	211	0.766258247	205	0.807728558	161	0.568695652	
Gentamycin	Al-abio	233	1	152	207	0.883129123	206	0.815268615	252	0.833043478	
Valsartan	CRD-ah/di	234	1	311	212	0.770028275	207	0.883129123	164	0.575652174	
Escitalopram oxalate	CNS-psy	235	1	224	214	0.776625825	208	0.752120641	171	0.587826087	
Montelukast sodium	RESP	236	1	265	215	0.778510839	209	0.788878417	173	0.591304348	
Celecoxib	CNS-ana	237	1	198	217	0.779453346	210	0.757775683	174	0.593043478	
Metoprolol Tartrate	CRD-ah/di	238	1	80	181	0.695570217	213	0.918944392	82	0.92469352	
Amphotericin B	Al-oth	239	1	163	213	0.918944392	215	0.778510839	278	0.926956522	
Clavulanate Potassium	Al-abio	240	1	207	220	0.784165881	216	0.853911404	176	0.768695652	

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Clopidogrel bisulfate	CRD-oth	241	1	208	222	0.78793591	217	0.779453346	177	0.60173913	
Raloxifene Hydrochloride	HOR-oth	242	1	290	225	0.798303487	221	0.808671065	188	0.627826087	
Niacin /Lovastatin SR		243	1	271	232	0.807728558	225	0.798303487	194	0.645217391	
Ertapenem	Al-abio	244	1	223	233	0.934967012	226	0.868991517	284	0.954782609	
Sildenafil citrate	MISC	245	1	299	235	0.810556079	228	0.824693685	196	0.796521739	
Rofecoxib	CNS-ana	246	1	295	236	0.8133836	229	0.824693685	199	0.655652174	
Destrothyroxine sodium	CRD-alip	247	1	50	177	0.703110273	230	0.916116871	75	0.863397548	
Rosiglitazone maleate	HOR-oth	248	1	296	237	0.819038643	232	0.807728558	201	0.666086957	
Insulin	HOR-oth	249	1	243	239	0.824693685	235	0.810556079	204	0.676521739	
Pioglitazone hydrochloride	HOR-oth	250	1	281	241	0.830348728	237	0.819038643	210	0.686956522	
Risedronate sodium	MISC	251	1	294	242	0.832233742	238	0.867106503	212	0.690434783	
Mometasone Furoate	CNS-ana	252	1	263	243	0.833176249	240	0.915174364	213	0.692173913	
Ezetimibe	CRD-alip	253	1	228	244	0.839773798	241	0.830348728	217	0.704347826	
Rabeprazole sodium	GAS	254	1	288	246	0.843543827	243	0.833176249	218	0.711304348	
Drospirenone	HOR-sex	255	1	221	247	0.847313855	244	0.839773798	220	0.713043478	
Quetiapine fumerate	CNS-psy	256	1	285	249	0.852968897	246	0.843543827	224	0.728695652	
Raloxifene Hydrochloride	HOR-oth	257	1	291	250	0.860508954	247	0.847313855	226	0.742608696	
Latanoprost	HOR-oth	258	1	251	251	0.861451461	248	0.914231857	227	0.744347826	
Ipratropium Bromide	RESP	259	1	244	253	0.866163996	250	0.860508954	228	0.753043478	
Olanzapine	CNS-psy	260	1	273	255	0.869934025	252	0.91328935	231	0.76	
Azactam lyoph	Al-abio	261	1	175	257	0.955702168	254	0.918001885	288	0.96173913	
Metoclopramide Hydrochloride (anhydrous)	GAS	262	1	258	258	0.873704053	255	0.869934025	234	0.766956522	
Cefdinir	Al-abio	263	1	188	259	0.882186616	256	0.909519321	237	0.782608696	
Moxifloxacin	Al-abio	264	1	266	260	0.885014138	257	0.955702168	239	0.787826087	
Buspirone Hydrochloride	CNS-psy	265	1	182	262	0.891611687	260	0.885014138	242	0.8	
Pimecrolimus	MISC	266	1	280	263	0.899151744	261	0.946277097	244	0.911304348	
Olopatadine hydrochloride	MISC	267	1	275	264	0.901036758	262	0.891611687	247	0.885217391	
Olmesartan medoxomil	CRD-ah/di	268	1	274	265	0.901979265	264	0.901036758	249	0.862608696	
Esterified Estrogens	HOR-sex	269	1	226	266	0.909519321	265	0.901979265	251	0.826086957	
Chlorpheniramine	RESP	270	1	202	268	0.928369463	266	0.909519321	256	0.852173913	
Calcitonin-salmon	HOR-oth	271	1	184	270	0.935909519	267	0.950047125	260	0.925217391	
Calcitonin	HOR-oth	272	1	183	274	0.937794533	268	0.928369463	262	0.895652174	
Mupirocin	Al-abio	273	1	267	275	0.940622055	269	0.946277097	263	0.885217391	
Polymyxin	Al-abio	274	1	282	276	0.943449576	270	0.935909519	266	0.893913043	
Gentamicin	Al-abio	275	1	236	277	0.944392083	271	0.951932139	267	0.895652174	

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Cefadroxil	Al-abio	276	1	186	279	0.946277097	273	0.943449576	268	0.897391304	
Cholestyramine	CRD-alip	277	1	204	280	0.949104618	274	0.937794533	270	0.904347826	
Colesevelam	CRD-alip	278	1	211	281	0.950989632	275	0.940622055	272	0.913043478	
telithromycin	Al-abio	279	1	302	282	0.951932139	276	0.943449576	273	0.909565217	
Folate	NUT	280	1	160	273	0.943449576	277	0.944392083	261	0.883478261	
Cefpodoxime Proxetil	Al-abio	281	1	193	283	0.956644675	278	0.952874647	275	0.913043478	
Colestipol hydrochloride	CRD-alip	282	1	212	284	0.957587182	279	0.946277097	276	0.92	
linezolid	Al-abio	283	1	254	285	0.960414703	280	0.949104618	277	0.92173913	
Vancomycin	Al-abio	284	1	312	286	0.962299717	282	0.951932139	279	0.937391304	
Cefazolin sodium	Al-abio	285	1	187	287	0.972667295	283	0.956644675	282	0.940869565	
Ceftazidime	Al-abio	286	1	141	269	0.946277097	284	0.957587182	257	0.867826087	
Cefepime	Al-abio	287	1	190	289	0.97737983	286	0.962299717	285	0.956521739	
daptomycin	Al-abio	288	1	214	290	0.978322337	287	0.972667295	286	0.95826087	
Imipenem	Al-abio	289	1	242	291	0.979264844	288	0.981149859	287	0.96	
Cefotetan disodium	Al-abio	290	1	137	271	0.951932139	289	0.97737983	258	0.900869565	
Meropenem	Al-abio	291	1	257	292	0.984919887	290	0.978322337	289	0.968695652	
Kanamycin	Al-abio	292	1	247	293	0.986804901	291	0.979264844	290	0.972173913	
Quinupristin	Al-abio	293	1	287	295	0.992459943	292	0.984919887	292	0.986086957	
Ceftizoxime sodium	Al-abio	294	1	195	296	0.993402451	293	0.986804901	293	0.986086957	
Trovofloxacin mesylate	Al-abio	295	1	309	297	0.994344958	294	0.994344958	294	0.987826087	
Cerivastatin sodium	CRD-alip	296	1	200	298	0.996229972	296	0.993402451	296	0.994782609	
Furosemide	CNS-oth	297	1	118	267	0.950047125	297	0.994344958	254	0.850434783	
Oxycodone Hydrochloride	CNS-ana	298	1	156	272	0.959472196	298	0.996229972	259	0.911304348	
Amphotericin B	Al-oth	299	1	172	299	1	299	1	299	1	
Azithromycin Dihydrate	Al-abio	300	1	176	300	1	300	1	300	1	
Bisoprolol Fumarate	CRD-ah/di	301	1	179	301	1	301	1	301	1	
Cefaclor (monohydrate)	Al-abio	302	1	185	302	1	302	1	302	1	
Cefepime	Al-abio	303	1	191	303	1	303	1	303	1	
Chlorpheniramine	RESP	304	1	203	304	1	304	1	304	1	
Ciprofloxacin Hydrochloride	Al-abio	305	1	205	305	1	305	1	305	1	
Clopidogrel bisulfate	CRD-oth	306	1	209	306	1	306	1	306	1	
DEXTROTHTYROXINE SODIUM	CRD-alip	307	1	217	307	1	307	1	307	1	
Glimepiride	HOR-oth	308	1	237	308	1	308	1	308	1	
Grepafloxacin Hydrochloride	Al-abio	309	1	238	309	1	309	1	309	1	
Metoprolol Tartrate	CRD-ah/di	310	1	260	310	1	310	1	310	1	
Mometasone furoate monohydrate	CNS-ana	311	1	264	311	1	311	1	311	1	

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Neomycin A (neamine)	Al-abio	312	1	270	312	1	312	1	312	1
Rabeprazole sodium	GAS	313	1	289	313	1	313	1	313	1