

Supplementary data

Table S1. Known drugs containing aryl amine, amide and nitro moieties.

Name of Drug	DFT		
	Drug group	Mulliken	NBO
Aromatic amines and amides			
Abacavir	secondary	0.084	-0.269
Acebutalol	amide	0.085	-0.333
Acetaminophen	amide	0.061	-0.292
Acetazolamide	amide	0.125	-0.302
Aciclovir	primary	-0.291	-0.427
Adefovir Dipivoxil	primary	-0.229	-0.351
Adenine	primary	-0.165	-0.311
Adenosine	primary	-0.243	-0.353
Adenosine monophosphate	primary	-0.212	-0.332
Adenosine triphosphate	primary	-0.253	-0.366
Albendazole	amide	-0.398	-0.421
Alfuzosin	primary	-0.314	-0.483
Almitrine	secondary	-0.020	-0.211
Amiloride	primary	-0.274	-0.449
Aminoglutethimide	primary	-0.248	-0.354
Aminohippurate	primary	-0.257	-0.383
Aminosalicylic Acid	primary	-0.303	-0.343
Amisulpride	primary	-0.267	-0.427
Amlexanox	primary	-0.199	-0.279
Amodiaquine	secondary	0.077	-0.311
Amprenavir	primary	-0.336	-0.396
Amrinone	primary	-0.311	-0.385
Amsacrine	secondary	-0.040	-0.593
Anileridine	primary	-0.320	-0.420
Antrafenine	secondary	0.065	-0.321
Apraclonidine	secondary	0.085	-0.334
Arformoterol	amide	-0.094	-0.348
Atorvastatin	amide	0.216	-0.387

Azacitidine	primary	-0.197	-0.287
Bentiromide	amide	0.270	-0.288
Benzocaine	primary	-0.220	-0.322
Benzonatate	secondary	0.142	-0.207
Bicalutamide	amide	0.316	-0.248
Bleomycin	primary	-0.357	-0.470
Bosentan	secondary	-0.091	-0.545
Brimonidine	secondary	-0.007	-0.326
Bromfenac	primary	-0.319	-0.364
Bumetanide	secondary	0.204	-0.211
Bupivacaine	amide	0.235	-0.375
Capecitabine	amide	-0.036	-0.276
cefdinir	primary	-0.328	-0.395
Cefditoren	primary	-0.302	-0.494
Cefepime	primary	-0.295	-0.489
Cefixime	primary	-0.295	-0.464
Cefmenoxime	primary	-0.336	-0.559
Cefotaxime	primary	-0.282	-0.456
Cefpodoxime	primary	-0.284	-0.474
Ceftazidime	primary	-0.259	-0.491
Ceftizoxime	primary	-0.277	-0.467
Ceftriaxone	primary	-0.324	-0.540
Chlorhexidine	secondary	-0.103	-0.540
Chloriprocaine	primary	-0.282	-0.394
Chloroquine	secondary	0.303	-0.293
Cidofovir	primary	-0.231	-0.321
Cladribine	primary	-0.109	-0.354
Clenbuterol	primary	-0.093	-0.404
Clofarabine	primary	-0.243	-0.357
Clofazimine	secondary	0.222	-0.307
Clonidine	secondary	0.153	-0.311
Conivaptan	amide	0.179	-0.348
Cytarabine	primary	-0.169	-0.278
Dactinomycin	primary	-0.170	-0.506
Dapsone	primary	-0.270	-0.390
Darunavir	primary	-0.259	-0.377
Dasatinib	secondary	-0.154	-0.348
Decitabine	primary	-0.135	-0.220
Delavirdine	secondary	0.168	-0.338
Diclofenac	secondary	0.340	-0.282
Dofetilide	secondary	-0.047	-0.568
Doxazosin	primary	-0.436	-0.557
Dutasteride	amide	0.288	-0.683

Emtricitabine	primary	-0.178	-0.295
Entecavir	primary	-0.285	-0.429
Erlotinib	secondary	-0.080	-0.351
Ertapenem	amide	0.063	-0.405
Famciclovir	primary	-0.251	-0.356
Flucytosine	primary	-0.264	-0.418
Fludarabine	primary	-0.124	-0.349
Flutamide	amide	0.190	-0.218
Folic acid	secondary	-0.239	-0.395
Formoterol	amide	-0.072	-0.344
Fosamprenavir	primary	-0.262	-0.389
Furosemide	secondary	0.212	-0.229
Ganciclovir	primary	-0.356	-0.477
Gefitinib	secondary	-0.054	-0.365
Gemcitabine	primary	-0.187	-0.266
Glycodiazine	secondary	0.002	-0.464
Hydralazine	secondary	0.094	-0.030
Hydroxychloroquine	secondary	0.302	-0.297
Ibutilide	secondary	-0.041	-0.552
Imatinib	secondary	-0.084	-0.327
Imiquimod	primary	-0.249	-0.352
Lamivudine	primary	-0.142	-0.245
Lamotrigine	primary	-0.302	-0.479
Lapatinib	secondary	-0.080	No data
Leflunomide	amide	0.117	-0.273
Lenalidomide	primary	-0.278	-0.354
Leucovorin	secondary	-0.375	-0.571
Levobupivacaine	amide	-0.220	-0.337
Levosimendan	secondary	0.091	-0.073
Lucanthone	secondary	0.268	-0.442
Lumiracoxib	secondary	0.224	-0.282
Mebendazole	amide	-0.346	-0.376
Meclofenamic acid	secondary	0.505	-0.228
Mefenamic acid	secondary	0.262	-0.234
Mepivacaine	amide	0.252	-0.362
Mesalazine	primary	-0.255	-0.366
Methotrexate	primary	-0.369	-0.467
Metoclopramide	primary	-0.223	-0.439
Minaprine	secondary	0.010	-0.466
MInoxidil	primary	-0.504	-0.648
Mitomycin	primary	-0.279	-0.452
Mitoxantrone	secondary	0.290	-0.263
Moricizine	amide	-0.143	-0.332

Nelarabine	primary	-0.266	-0.382
Niflumic Acid	secondary	-0.182	-0.342
Nltazoxanide	amide	0.169	-0.352
Olsalazine	secondary	0.092	-0.034
Oxybuprocaine	primary	-0.337	-0.405
Pemetrexed	primary	-0.245	-0.413
Pencilovir	primary	-0.284	-0.419
Phenazopyridine	primary	-0.341	-0.491
piroxicam	amide	0.212	-0.446
Pramipexole	primary	-0.280	-0.465
Pranlukast	amide	0.077	-0.334
Prazosin	primary	-0.465	-0.572
Primaquine	secondary	0.330	-0.201
Procainamide	primary	-0.282	-0.407
Procaine	primary	-0.303	-0.426
Proflavine	primary	-0.280	-0.402
Proparacaine	primary	-0.352	-0.394
Pyrimethamine	primary	-0.371	-0.511
Quinacrine	secondary	0.298	-0.751
Rifabutin	amide	0.040	-0.366
Rifaximin	amide	-0.245	-0.521
Riluzole	primary	-0.226	-0.416
Ropivacaine	amide	0.221	-0.373
S-Adenosylmethionine	primary	-0.217	-0.314
Saprisartan	secondary	-0.080	-0.615
Silver Sulfadiazine	primary	-0.159	-0.250
Sorafenib	amide	-0.076	-0.423
Sotalol	secondary	-0.034	-0.522
Sparfloxacin	primary	-0.385	-0.376
Sulfacetamide	primary	-0.213	-0.318
sulfacytine	secondary	-0.269	-0.384
Sulfadiazine	secondary	-0.231	-0.342
Sulfadoxine	secondary	0.030	-0.572
Sulfamerazine	secondary	-0.235	-0.347
Sulfamethazine	secondary	-0.242	-0.353
Sulfamethizole	secondary	-0.058	-0.538
Sulfamethoxazole	secondary	-0.120	-0.516
Sulfanilamide	primary	-0.219	-0.322
Sulfapyridine	secondary	-0.055	-0.543
Sulfasalazine	secondary	0.434	0.005
Sulfisoxazole	secondary	-0.030	-0.571
Tacrine	primary	-0.319	-0.422
Tamibarotene	primary	0.140	-0.295

Tenofovir	primary	-0.243	-0.357
Tenoxicam	secondary	0.104	-0.397
Terazosin	primary	-0.441	-0.560
Tetrahydrobiopterin	primary	-0.396	-0.581
Tetrahydrofolic acid	primary	0.001	-0.373
Thiamine	primary	-0.125	-0.243
Thioguanine	primary	-0.299	-0.434
Tigecycline	amide	0.005	-0.420
Tipranavir	secondary	0.278	-0.479
Tocainide	amide	0.296	-0.329
Torasemide	secondary	0.284	-0.204
Triamterene	primary	-0.356	-0.497
Trimethoprim	primary	-0.475	-0.605
Tremexate	primary	-0.471	-0.577
Valaciclovir	primary	-0.231	-0.393
Valganciclovir	primary	-0.345	-0.455
Vidarabine	primary	-0.240	-0.348
Vorinostat	amide	0.159	-0.273
Zafirluast	amide	-0.043	-0.321
Zalcitabine	primary	-0.153	-0.260

Nitro aromatic (NO₂)

Acenocoumarol		-0.296	-0.418
Azathioprine		-0.353	-0.460
Chloramphenicol		-0.254	-0.370
Clonazepam		-0.276	-0.406
Dantrolene		-0.324	-0.589
Entacapone		-0.286	-0.359
Flutamide		-0.277	-0.393
Furazolidone		-0.347	-0.477
Lercanidipine		-0.280	-0.392
Metronidazole		-0.340	-0.460
Nicardipine		-0.269	-0.382
Nifedipine		-0.235	-0.420
Nilutamide		-0.270	-0.377
Nimodipine		-0.385	-0.546
Nisoldipine		-0.287	-0.461
Nitazoxanide		-0.284	-0.458
Nitisinone		-0.284	-0.311
Nitrazepam		-0.279	-0.407
Nitrendipine		-0.255	-0.366
Nitrofurantoin		-0.346	-0.481

Nitrofurazone	-0.344	-0.481
Nitroxoline	-0.314	-0.436
Oxamniquine	-0.304	-0.445
Tinidazole	-0.380	-0.480

Table S2. Ames positive primary aromatic amines compounds.

Ames positive	DFT	
	Mulliken	NBO
1-Amino-2, 4-dibromoanthraquinone	-0.324	-0.374
9,10-Anthracenedione, 1-amino-2-methyl-	-0.189	-0.316
Benzenamine, 2,4,6-trimethyl-	-0.274	-0.396
Aniline-o-sulfonic acid	-0.226	-0.269
2-amino-4-chloro-5-methylbenzenesulfonic acid	-0.187	-0.322
2-Naphthalenamine	-0.203	-0.292
4-Aminobiphenyl	-0.282	-0.398
Benzenamine, 3,4-dimethyl-	-0.241	-0.350
Benzenamine, 4-chloro-2-methyl-	-0.235	-0.379
Benzenamine, 2,5-dimethyl-	-0.231	-0.367
2-amino-4-methylphenol	-0.382	-0.444
5-Chloro-2-hydroxyaniline	-0.284	-0.364
2-Aminothiazole	-0.123	-0.316
1,4-Benzenediamine, N,N-dimethyl-	-0.319	-0.433
N-(3-aminophenyl)acetamide	-0.057	-0.307
Benzenamine, 4-methoxy-2-methyl-	-0.300	-0.407
2-Aminoanthraquinone	-0.239	-0.328
Acetamide, N-(4-aminophenyl)-	0.061	-0.322
Fluoren-2-amine	-0.303	-0.423
4-Ethoxyaniline	-0.297	-0.398
2,4-Difluoroaniline	-0.276	-0.335
p-Fluoroaniline	-0.241	-0.334
Benzenamine, 2,6-diethyl-	-0.303	-0.386
2-Quinolinamine	-0.278	-0.352
Phenol, 3-amino-	-0.240	-0.322
2-Anthracenamine	-0.308	-0.430
O-toluidine, hydrochloride	-0.249	-0.338
Adenine, 9-methyl-	-0.210	-0.237
Benzeneacetic acid, 4-amino-	-0.241	-0.334
4-Aminostyrene	-0.281	-0.381
1,2,3,4-tetrahydroacridin-9-amine	-0.289	-0.421
3-Aminophenanthrene	-0.296	-0.413
2-phenylaniline	-0.246	-0.390
[1,1'-Biphenyl]-3-amine	-0.261	-0.347

3-Fluoranthenamine	-0.292	-0.438
Phenol, 2-amino-5-methyl-	-0.289	-0.376
2-acetamido-6-aminobenzoic acid	-0.321	-0.615
6-methyl-1H-benzimidazol-2-amine	-0.312	-0.470
3-Aminofluorene	-0.280	-0.368
Benzenamine, 4-(2-phenylethyl)-	-0.265	-0.382
1-methylimidazo[4,5-b][1,7]naphthyridin-2-amine	-0.433	-0.453
4-Chloroaniline	-0.258	-0.357
4-methoxyaniline	-0.286	-0.389
3-methyl-1,2-thiazol-5-amine hydrochloride	-0.209	-0.371
1,2-benzothiazol-5-amine	-0.267	-0.378
2-amino-3H-benzimidazole-5-carbonitrile	-0.299	-0.448
1,2-benzothiazol-7-amine	-0.247	-0.398
3-chloro-1,2-benzothiazol-5-amine	-0.264	-0.375
3-chloro-1,2-benzothiazol-7-amine	-0.256	-0.405
3-methoxy-1,2-benzothiazol-6-amine	-0.258	-0.359