

## Computer Assisted Geometry Optimization for *in silico* Modeling

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**Table 1.** The name of the drug-like molecule, the PubChem compound identifier (CID) and active/not active status in the CNS (central nervous system)

Name	CID	CNSA	Name	CID	CNSA	Name	CID	CNSA
Adenosine	191	1	Amprenavir	2177	0	Isradipine	3784	0
Alfentanil	51263	1	Amrinone	3698	0	Ketotifen	3827	0
Alosetron	2099	1	Anastrozole	2187	0	Lamivudine	3877	0
Amiloride	16231	1	Anthralin	2202	0	Lansoprazole	3883	0
Aripiprazole	60795	1	Argatroban	92722	0	Latanoprost	5311221	0
Benzotropine	2344	1	Azathioprine	2265	0	Leflunomide	3899	0
Betaxolol	2369	1	Aztreonam	5362041	0	Letrozole	3902	0
Bisoprolol	2405	1	Baclofen	2284	0	Levamisole	26879	0
Brimonidine	2435	1	Balsalazide	5362070	0	Lindane	727	0
Bromocriptine	31101	1	Beclometasone	20469	0	Linezolid	3929	0
Butorphanol	2487	1	Benazepril	2311	0	Lisinopril	5362119	0
Chloralhydrate	2707	1	Bepidil	2351	0	Lodoxamide	44564	0
Chlordiazepoxide	2712	1	Brinzolamide	68844	0	Loracarbef	3956	0
Chlorpheniramine	2725	1	Budesonide	63006	0	Losartan	3961	0
Chlorzoxazone	2733	1	Bumetanide	2471	0	Lovastatin	53232	0
Citalopram	2771	1	Bupivacaine	2474	0	Mechlorethamine	4033	0
Clemastine	2781	1	Calcitriol	6398761	0	Medroxyprogesterone	10631	0
Clonazepam	2802	1	Candesartan	2541	0	Melphalan	4053	0
Clorzepate	2809	1	Capsaicine	2548	0	Mercaptopurine	667490	0
Clozapine	2818	1	Captopril	2550	0	Meropenem	64778	0
Cyclobenzaprine	2895	1	Cefaclor	2609	0	Mesalamine	4075	0
Cyproheptadine	2913	1	Cefadroxil	2610	0	Metaproterenol	4086	0
Dezocine	40841	1	Cefazolin	33255	0	Metformin	4091	0
Dipivefrin	3105	1	Cefdinir	6399011	0	Methimazole	1349907	0
Dolasetron	3148	1	Cefditoren	6437877	0	Methylergonovine	8226	0
Doxazosin	3157	1	Cefepime	2622	0	Metoclopramide	4168	0
Doxepin	667477	1	Cefixime	54362	0	Metolazone	4170	0
Dronabinol	2978	1	Cefmetazole	2626	0	Metyrosine	3125	0
Droperidol	3168	1	Cefonicid	43592	0	Mexiletine	4178	0
Emedastine	3219	1	Cefoperazone	135784	0	Miglitol	441314	0
Entacapone	5281081	1	Cefotaxime	2632	0	Milrinone	4197	0
Esmolol	59768	1	Cefoxitin	37194	0	Minoxidil	4201	0
Estazolam	3261	1	Cefpodoxime	6335986	0	Moexipril	91270	0
Fexofenadine	3348	1	Ceftazidime	157706	0	Moricizine	34633	0

CNSA=active(1) or inactive(0) in Central nervous system; CID=compound ID

Table 1. (continued)

Name	CID	CNSA	Name	CID	CNSA	Name	CID	CNSA
Fluoxetine	3386	1	Ceftibuten	5282242	0	Moxifloxacin	4259	0
Flurazepam	3393	1	Ceftizoxime	2655	0	MycophenolicAcid	446541	0
Fluvoxamine	5324346	1	Ceftriaxone	5479530	0	Nabumetone	4409	0
Formoterol	3410	1	Cefuroxime	2659	0	Naloxone	4425	0
Fosphenytoin	56339	1	Celecoxib	2662	0	Naphazoline	4436	0
Galantamine	3449	1	Cephalexin	27447	0	Naproxen	1302	0
Granisetron	3510	1	Chlorpropamide	2727	0	Nateglinide	4443	0
Hydrocodone	411697	1	Chlorthalidone	2732	0	Nedocromil	50294	0
Hydromorphone	3648	1	Cholecalciferol	6221	0	Nicardipine	4474	0
Isotretinoin	5538	1	Cholestyramine	3086319	0	Nifedipine	4485	0
Labetalol	3869	1	Ciclopirox	2749	0	Nimodipine	4497	0
Levobunolol	39468	1	Cidofovir	60613	0	Nisoldipine	4499	0
Levocabastine	54385	1	Cladribine	1546	0	Nitazoxanide	41684	0
Maprotiline	4011	1	Clindamycin	29029	0	Nitrofurantoin	4509	0
Meperidide	3034126	1	Clopidogrel	2806	0	Nitroglycerin	4510	0
Metaxalone	15459	1	Clotrimazole	2812	0	Nizatidine	4513	0
Methadone	4095	1	Colchicine	2833	0	Norgestrel	13109	0
Methocarbamol	4107	1	Cromolyn	2882	0	Ofloxacin	4583	0
Methoxamine	6082	1	Cyclopentolate	2905	0	Olopatadine	60865	0
Methyl dopa	4138	1	Cyclophosphamide	2907	0	Olsalazine	6816262	0
Molindone	23897	1	Cytarabine	596	0	Oseltamivir	65028	0
Nalbuphine	4419	1	Dantrolene	2952	0	Oxaprozin	4614	0
Naratriptan	4440	1	Dapsone	2955	0	Oxybutynin	4634	0
Nefazodone	4449	1	Delavirdinemesylate	5625	0	Pantoprazole	4679	0
Nortriptyline	4543	1	Dexamethasone	5743	0	Pemirolast	57697	0
Ondansetron	4595	1	Dexpanthenol	4678	0	Penbutolol	37464	0
Orphenadrine	4601	1	Diazoxide	3019	0	Penciclovir	4725	0
Oxcarbazepine	34312	1	Dibucaine	3025	0	Pentamidine	4735	0
Oxycodone	4635	1	Dicloxacillin	3041	0	Pentoxifylline	4740	0
Oxymorphone	4639	1	Digoxin	15478	0	Perindopril	107807	0
Paroxetine	4691	1	Diltiazem	3076	0	Pindolol	4828	0
Phenelzine	3675	1	Dinoprostone	9691	0	Pioglitazone	4829	0
Phenylephrine	6041	1	Disopyramide	3114	0	Pramoxine	4886	0
Pirbuterol	4845	1	Dofetilide	71329	0	Procainamide	4913	0
Pramipexole	4885	1	Dorzolamide	3154	0	Procarbazine	4915	0
Prazosin	4893	1	Econazole	33745	0	Propafenone	4932	0
Procyclidine	4919	1	Edrophoniumchloride	3202	0	Propylthiouracil	657298	0
Propoxyphene	10100	1	Ephedrine	5032	0	Pyridoxine	1054	0
Pseudoephedrine	7028	1	Eplerenone	443872	0	Quinapril	54892	0
Quazepam	4999	1	Epoprostenol	5280427	0	Quinidine	1065	0
Quetiapine	5002	1	Eprosartan	60879	0	Ramipril	5038	0
Rizatriptan	5078	1	Estramustine	18140	0	Rivastigmine	77991	0
Scopolamine	5184	1	Etidronicacid	3305	0	Rofecoxib	5090	0
Secobarbital	5193	1	Etodolac	3308	0	Rosiglitazone	77999	0
Sertraline	5203	1	Famciclovir	3324	0	Sildenafil	5212	0
Sibutramine	5210	1	Famotidine	3325	0	Simvastatin	54454	0
Sufentanil	41693	1	Fenoldopam	3341	0	Streptozocin	5299	0
Sumatriptan	5358	1	Fenopropfen	3342	0	Sulfacetamide	5320	0
Thiethylperazine	5440	1	Flavoxate	3354	0	Sulfasalazine	5353980	0
Thiothixene	5454	1	Flecainide	3356	0	Sulfipyrazone	5342	0
Tiagabine	5466	1	Floxuridine	3363	0	Sulindac	5352	0
Timolol	5478	1	Flunisolide	82153	0	Tamsulosin	129211	0
Tolazoline	5504	1	Fluoxymesterone	6446	0	Tazarotene	5381	0
Tramadol	5523	1	Flurbiprofen	3394	0	Terazosin	5401	0
Trazodone	5533	1	Flutamide	3397	0	Terbutaline	5403	0
Trimethobenzamide	5577	1	Fluvastatin	446155	0	Theophylline	2153	0
Venlafaxine	5656	1	Fosfomycin	3417	0	Thiamine	1130	0
Zaleplon	5719	1	Furosemide	3440	0	Ticlopidine	5472	0

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Table 1. (continued)

Name	CID	CNSA	Name	CID	CNSA	Name	CID	CNSA
Ziprasidone	60854	1	Ganciclovir	3454	0	Tocainide	38945	0
Zolpidem	5732	1	Gatifloxacin	5379	0	Tolazamide	5503	0
Zolmitriptan	5731	1	Gemcitabine	60750	0	Tolbutamide	5505	0
Acarbose	41774	0	Gemfibrozil	3463	0	Tolmetin	5509	0
Acetazolamide	1986	0	Glimepiride	3476	0	Torasemide	41781	0
Acetylcysteine	581	0	Glipizide	3478	0	Trandolapril	5484727	0
Acyclovir	2022	0	Glyburide	3488	0	Triamcinolone	31307	0
Adefovir	60172	0	Hydralazine	3637	0	Triamterene	5546	0
Allopurinol	2094	0	Ibutilide	60753	0	Valacyclovir	5647	0
Alprostadiol	214	0	Idarubicin	42890	0	Voriconazole	5231054	0
Altretamine	2123	0	Ifosfamide	3690	0	Warfarin	6691	0
Aminoglutethimide	2145	0	Imiquimod	57469	0	Zileuton	60490	0
Amlodipine	2162	0	Indapamide	3702	0	ZoledronicAcid	68740	0
Amoxicillin	2171	0	Isoetharine	3762	0			
Ampicillin	2174	0	Isosorbidedinitrate	170113	0			

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