

Supplementary Table S1: Binding Scores of all inhibitors

Drug	Affinity (kcal/mol)
Dutasteride	-9.7
Cepharantine	-9.6
Zafirlukast	-9.5
Carbenoxolone	-9.2
Telmisartan	-9.2
Atovaquone	-9.1
Doxorubicin	-8.9
Pirarubicin	-8.9
Profenamine	-8.7
Ritanserlin	-8.7
Solasodine	-8.7
Tomatidine	-8.7
Astemizole	-8.6
Daunorubicin	-8.6
Diosmin	-8.6
Droperidol	-8.4
Montelukast	-8.3
Flunarizine	-8.2
SB-222200	-8.2
Sertindole	-8.1
Trifluoperidol	-8.1
Domperidone	-8
Fusidic-acid	-8
Conessine	-7.9
Dexamethasone	-7.9
Donepezil	-7.9
Enoxolone	-7.9
Lercanidipine	-7.9
Raloxifene	-7.9
Spiperone	-7.9
Bromocriptine	-7.8
Calcipotriol	-7.8
Cinnarizine	-7.8
Fipexide	-7.8
Phenserine	-7.8
Pirenperone	-7.8

Progesterone	-7.8
Clofazimine	-7.7
Desloratadine	-7.7
Flavoxate	-7.7
Flupenthixol	-7.7
Idarubicin	-7.7
Stanozolol	-7.7
Sulindac	-7.7
Cypermethrin	-7.6
Fluspirilene	-7.6
Hydrocortisone	-7.6
Loperamide	-7.6
Mifepristone	-7.6
Moexipril	-7.6
Nelfinavir	-7.6
Penfluridool	-7.6
Pranlukast	-7.6
Acrivastine	-7.5
Cyproheptadine	-7.5
Fexofenadine	-7.5
Barnidipine	-7.4
Clebopride	-7.4
Emetine	-7.4
Haloperidol	-7.4
Loratadine	-7.4
Terfenadine	-7.4
Bromperidol	-7.3
Cisapride	-7.3
Cyclofenil	-7.3
Fulvestrant	-7.3
Indomethacin	-7.3
Quetiapine	-7.3
Cilnidipine	-7.2
Encainide	-7.2
Noscapine	-7.2
Pimethixene	-7.2
Pimozide	-7.2
Pipamperone	-7.2

Tofisopam	-7.2
Yohimbine	-7.2
Zolantidine	-7.2
Azaperone	-7.1
Butenafine	-7.1
Flecainide	-7.1
Flufenamic-acid	-7.1
Flupirtine	-7.1
ketotifen	-7.1
Opipramol	-7.1
Allylestrenol	-7
AY-9944	-7
Butorphanol	-7
Carbamazepine	-7
Clozapine	-7
Fluphenazine	-7
Mianserin	-7
Retinol	-7
Apomorphin	-6.9
Chlorotrianisene	-6.9
Phenothrin	-6.9
Tamoxifen	-6.9
Tirofiban	-6.9
Trifluoperazine	-6.9
Chlorprothixene	-6.8
Diazepam	-6.8
Fenspiride	-6.8
Hydroxyzin	-6.8
Mirtazapine	-6.8
Oxyphencyclimine	-6.8
Phenytoin	-6.8
Repaglinide	-6.8
Tibolone	-6.8
Vinpocetine	-6.8
Warfarin	-6.8
Amorolfine	-6.7
Bepridil	-6.7
Dibenzosuberane	-6.7

Epinastine	-6.7
Fenofibrate	-6.7
Hydroquinine	-6.7
Mebhydroline	-6.7
Quinine	-6.7
Sulpiride	-6.7
Cyclobenzaprine	-6.6
Diphenylpyralin	-6.6
FG7142	-6.6
Mesoridazine	-6.6
Perphenazine	-6.6
Thioridazin	-6.6
Thioridazine	-6.6
Tiagabine	-6.6
Alaproclate	-6.5
Amitriptyline	-6.5
Benztropine	-6.5
Biperidene	-6.5
Biperiden	-6.5
Clomiphene	-6.5
Desogestrel	-6.5
Hydroxyzine	-6.5
Lynestrenol	-6.5
Maprotiline	-6.5
Meclofenamic_acid	-6.5
Mibefradil	-6.5
Paroxentine	-6.5
Rolipram	-6.5
Vincamine	-6.5
Cloricromen	-6.4
Colchicine	-6.4
Fluoxetine	-6.4
Leukomethylene_blue	-6.4
Mepacrine	-6.4
Naproxen	-6.4
Papaverine	-6.4
Pridinol	-6.4
Sertraline	-6.4

Triprolidine	-6.4
Aprindine	-6.3
Atropine	-6.3
Betaxolol	-6.3
Diltiazeml	-6.3
Doxepin	-6.3
Ibuprofen	-6.3
Mebeverine	-6.3
Nortriptyline	-6.3
Trihexyphenidyl	-6.3
Amiodarone	-6.2
Antazoline	-6.2
Benzbromarone	-6.2
Citalopram	-6.2
Clemastine	-6.2
Isoxsuprine	-6.2
Lamotrigine	-6.2
Pergolide	-6.2
Perhexiline	-6.2
Phentolamine	-6.2
Procyclidine	-6.2
Carvedilol	-6.1
Disopyramide	-6.1
Lofepramine	-6.1
Norfluoxetine	-6.1
Propafenone	-6.1
Protriptyline	-6.1
Uridine	-6.1
Ambroxol	-6
Dextromethorphan	-6
Fendiline	-6
Harmine	-6
Naphazoline	-6
Tacrine	-6
Tramadol	-6
Triflupromazine	-6
Trimipramine	-6
Venlafaxine	-6

Amlodipine	-5.9
Cibenzoline	-5.9
Cyclazocine	-5.9
Imipramine	-5.9
Reboxentine	-5.9
Sparteine	-5.9
Bromhexine	-5.8
Clomipramine	-5.8
Diphenhydramine	-5.8
Mitotane	-5.8
Orphenadrine	-5.8
Oxolamine	-5.8
Quinacrine	-5.8
Xylometazoline	-5.8
Benfluorex	-5.7
Brompheniramine	-5.7
Carbetapentane	-5.7
Chloroquine	-5.7
Chlorpheniramine	-5.7
Cloperastine	-5.7
Cyclopentolate	-5.7
Drofenine	-5.7
Fluvoxamine	-5.7
Oxybutynine	-5.7
Oxymetazoline	-5.7
Promazin	-5.7
Promazine	-5.7
Desipramine	-5.6
Ethopropazine	-5.6
Promethazin	-5.6
Promethazine	-5.6
Pyrilamine	-5.6
Tripelennamine	-5.6
Chloropyramine	-5.5
Chlorpromazine	-5.5
Dicyclomine	-5.5
Etomidate	-5.5
Fenfluramine	-5.5

Proparacaine	-5.5
Ropinirole	-5.5
Alprenolol	-5.4
Bromopride	-5.4
Chlorquinaldol	-5.4
Dienestrol	-5.4
Gabapentin	-5.3
Propranolol	-5.3
Tetracaine	-5.3
Lidocaine	-5.2
Moxisylyte	-5.2
Oxeladin	-5.2
Paraxanthine	-5.2
Camylofin	-5.1
Clonidine	-5.1
Metoclopramide	-5.1
Suloctidil	-5.1
Clenbuterol	-5
Gentisic_acid	-5
Alverine	-4.9
Bupropion	-4.9
D_Mannitol	-4.9
Methapyrilene	-4.8
Phenylmethysulfonyl_flouride	-4.8
Tulobuterol	-4.8
Memantine	-4.7
Rimantadine	-4.6
L_Leucine_methyl_ester	-4.4
Mecamylamine	-4.3
Amantadine	-4.1
Putrescine	-3.2